Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 03:57 PM 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.; Jogl, G.
Deposited on	:	2012-02-16
Resolution	:	3.97 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

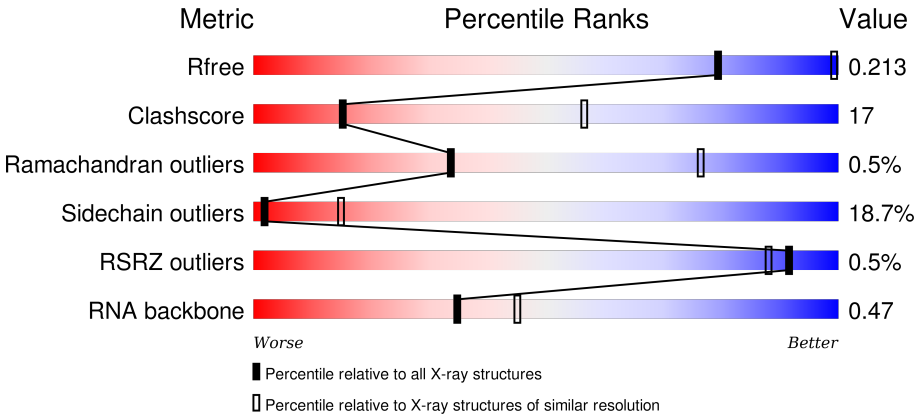
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.97 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}	91344	1011 (4.38-3.54)
Clashscore	102246	1025 (4.32-3.60)
Ramachandran outliers	100387	1008 (4.34-3.58)
Sidechain outliers	100360	1027 (4.36-3.56)
RSRZ outliers	91569	1015 (4.38-3.54)
RNA backbone	2183	1079 (5.04-2.80)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1522	23% 41% 27% 8%
2	B	256	48% 38% 6% 8%
3	C	239	40% 38% 9% 13%
4	D	209	56% 37% 7%

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Mol	Chain	Length	Quality of chain
5	E	162	54% 31% 8% 7%
6	F	101	50% 40% 10%
7	G	156	63% 31%
8	H	138	53% 38% 9%
9	I	128	3% 48% 41% 9%
10	J	105	2% 37% 46% 10% 6%
11	K	129	2% 59% 26% 8% 8%
12	L	135	% 47% 39% 7% 7%
13	M	126	% 40% 44% 9% 6%
14	N	61	39% 46% 11%
15	O	89	2% 47% 43% 8%
16	P	88	43% 44% 8% 5%
17	Q	105	44% 38% 13% 5%
18	R	88	2% 50% 30% 17%
19	S	93	40% 38% 8% 13%
20	T	106	49% 39% 5% 7%
21	U	27	52% 33% 7% 7%
22	V	3	33% 33% 33%
23	W	15	20% 60% 13% 7%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	PAR	A	1608	-	-	-	X
24	PAR	A	1610	-	-	-	X
24	PAR	A	1611	-	-	-	X
24	PAR	A	1612	-	-	-	X
24	PAR	A	1613	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	PAR	A	1614	-	-	-	X
24	PAR	A	1615	-	-	-	X
24	PAR	A	1616	-	-	-	X
24	PAR	A	1617	-	-	-	X
24	PAR	A	1618	-	-	-	X
25	MG	A	1619	-	-	-	X
25	MG	A	1651	-	-	-	X
25	MG	A	1694	-	-	-	X
25	MG	A	1740	-	-	-	X
25	MG	A	1794	-	-	-	X
25	MG	A	1803	-	-	-	X
25	MG	A	1818	-	-	-	X
25	MG	A	1823	-	-	-	X
25	MG	A	1832	-	-	-	X
25	MG	A	1853	-	-	-	X
25	MG	A	1862	-	-	-	X
25	MG	A	1867	-	-	-	X
25	MG	A	1883	-	-	-	X
25	MG	A	1888	-	-	-	X
25	MG	A	1890	-	-	-	X
25	MG	A	1912	-	-	-	X
25	MG	A	1914	-	-	-	X
25	MG	A	1918	-	-	-	X
25	MG	A	1934	-	-	-	X
25	MG	A	1935	-	-	-	X
25	MG	N	102	-	-	-	X
26	ZN	D	301	-	-	-	X

2 Entry composition

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	1512	32504	14477	6011	10505	1511	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	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			

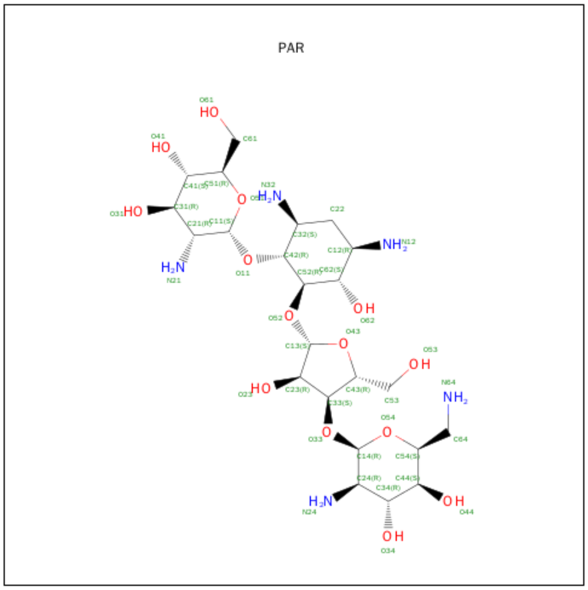
- Molecule 22 is a RNA chain called 5'-R(*UP*UP*U)-3'.

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: $C_{23}H_{45}N_5O_{14}$).



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

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

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

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

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

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

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

- Molecule 27 is water.

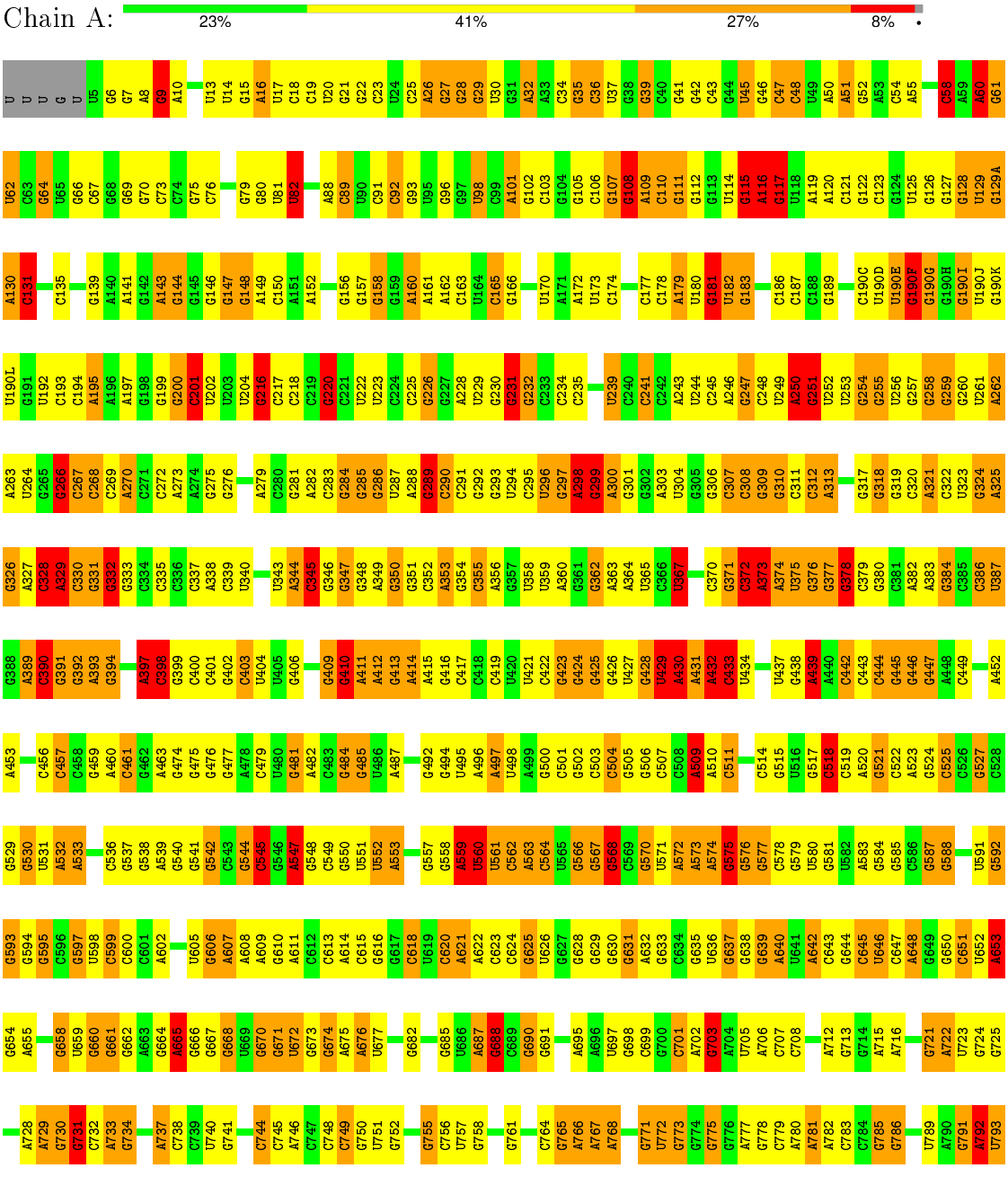
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	480	Total O 480 480	0	0
27	C	1	Total O 1 1	0	0
27	D	2	Total O 2 2	0	0
27	E	5	Total O 5 5	0	0
27	K	1	Total O 1 1	0	0
27	L	2	Total O 2 2	0	0
27	N	2	Total O 2 2	0	0
27	O	4	Total O 4 4	0	0
27	V	1	Total O 1 1	0	0

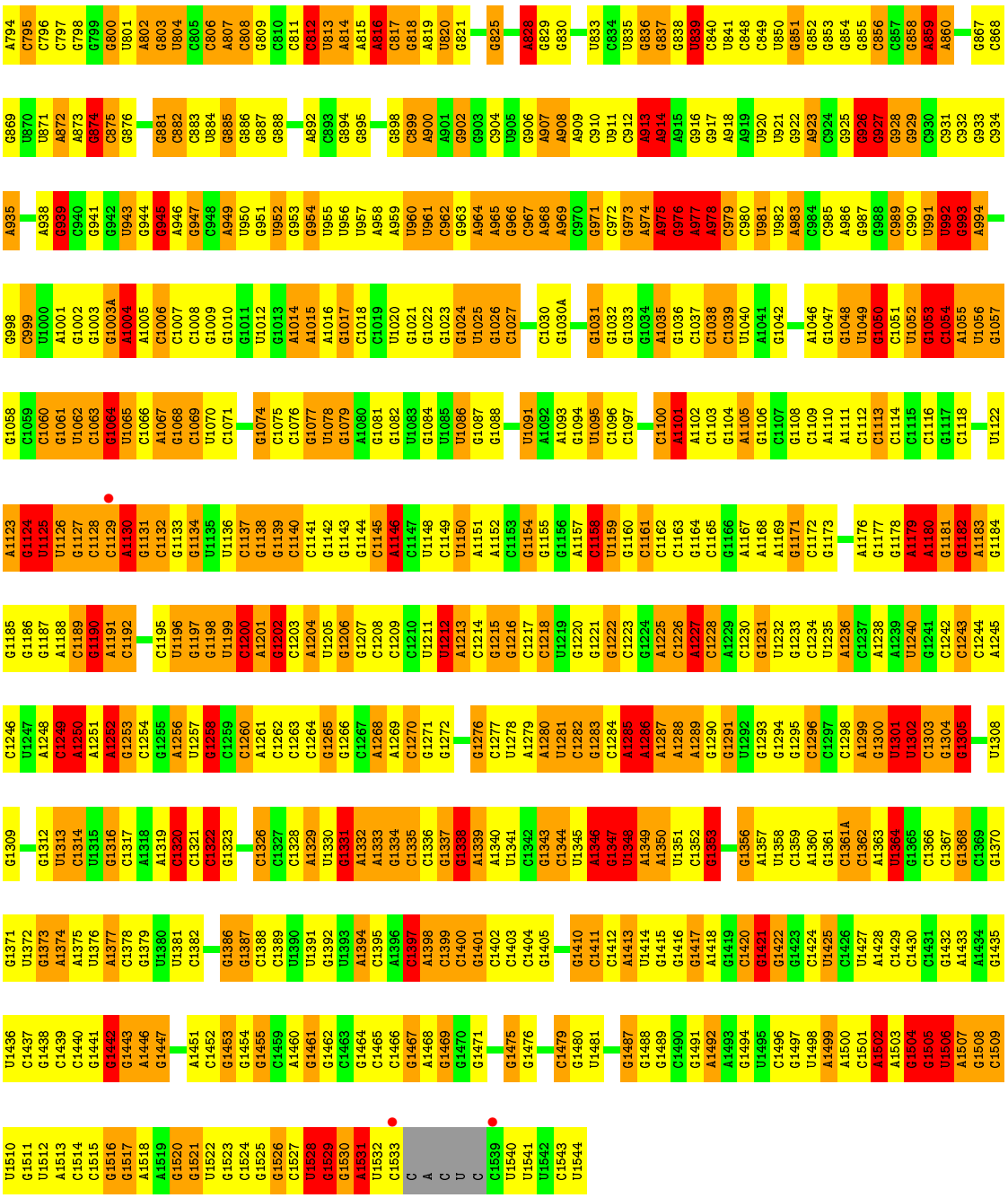
3 Residue-property plots (i)

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

- Molecule 1: 16S rRNA

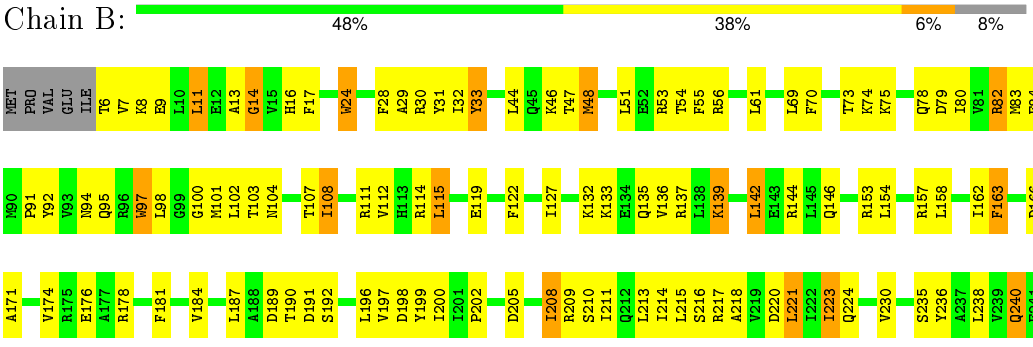
Chain A:





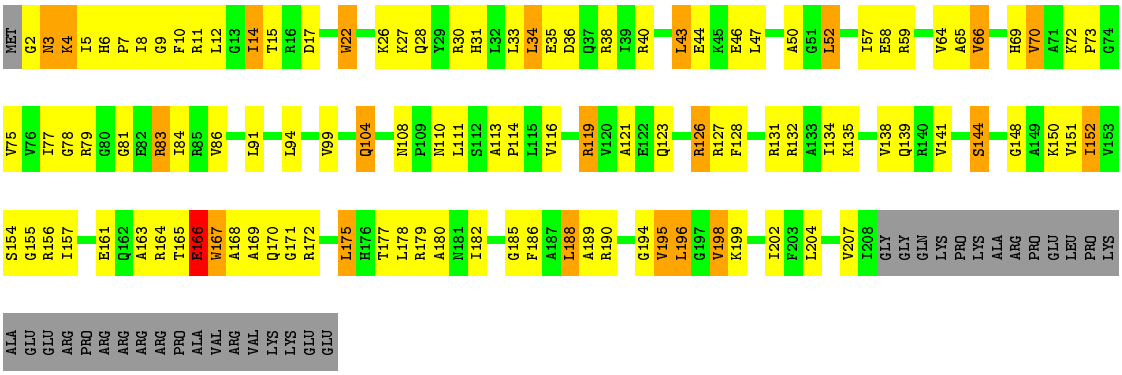
• Molecule 2: 30S ribosomal protein S2

Chain B:



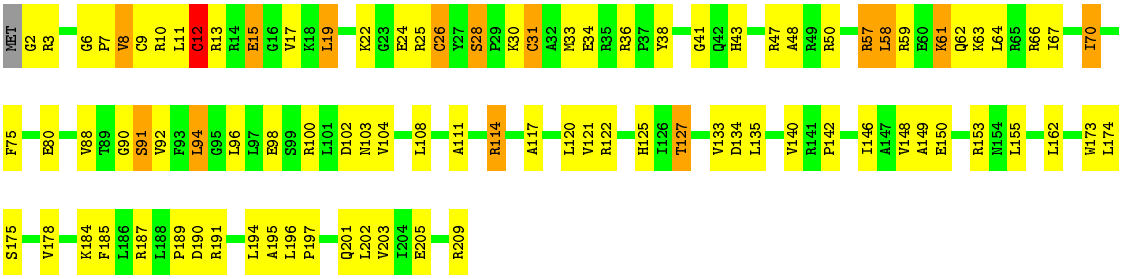
- Molecule 3: 30S ribosomal protein S3

Chain C:



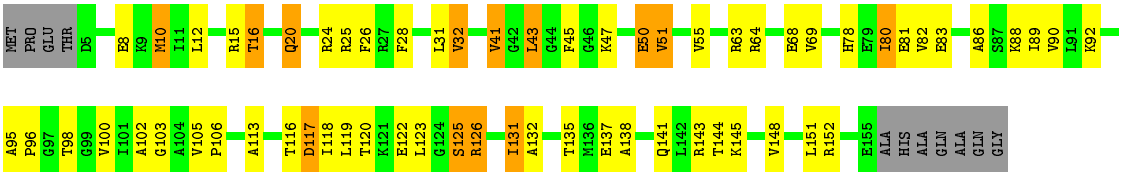
- Molecule 4: 30S ribosomal protein S4

Chain D:



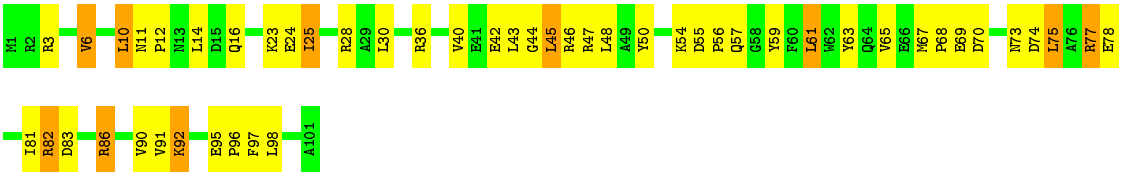
- Molecule 5: 30S ribosomal protein S5

Chain E:



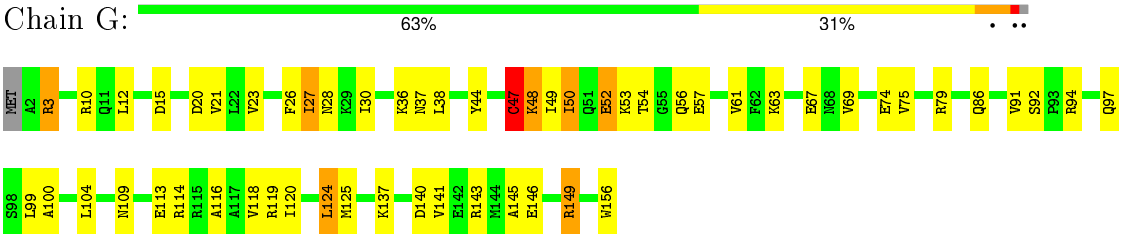
- Molecule 6: 30S ribosomal protein S6

Chain F:



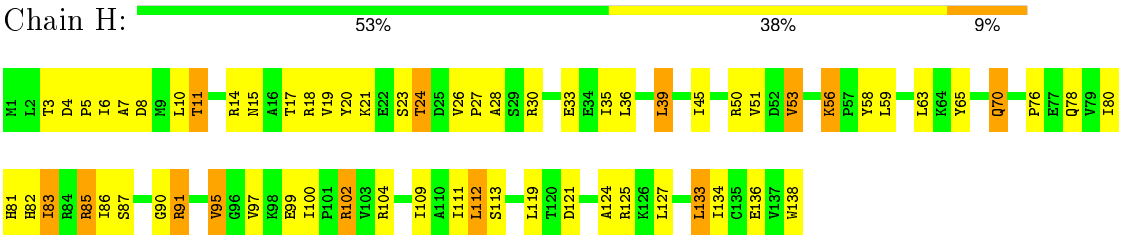
• Molecule 7: 30S ribosomal protein S7

Chain G:



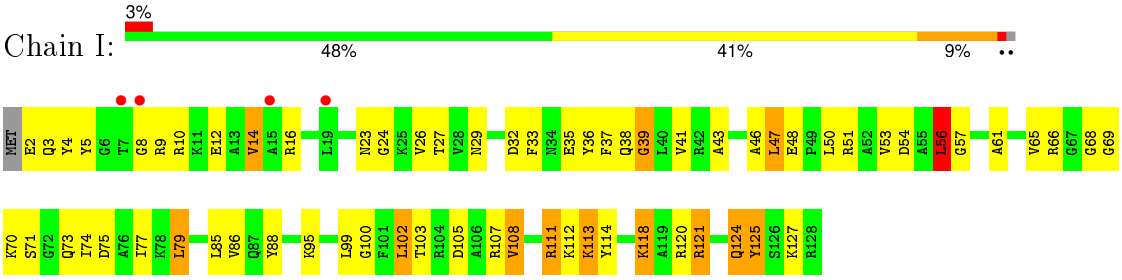
• Molecule 8: 30S ribosomal protein S8

Chain H:



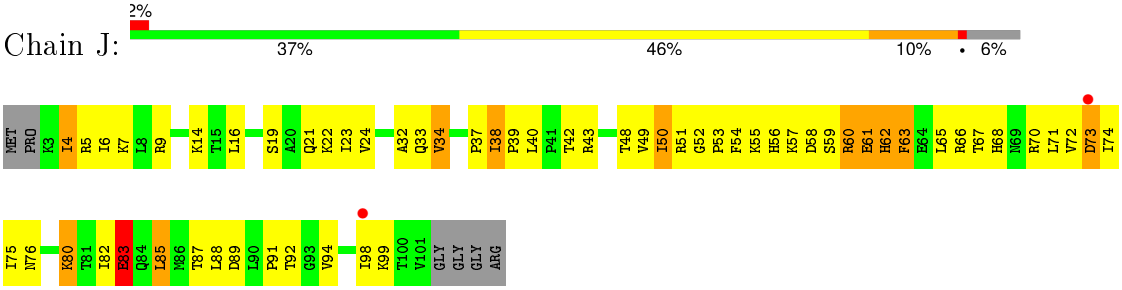
• Molecule 9: 30S ribosomal protein S9

Chain I:



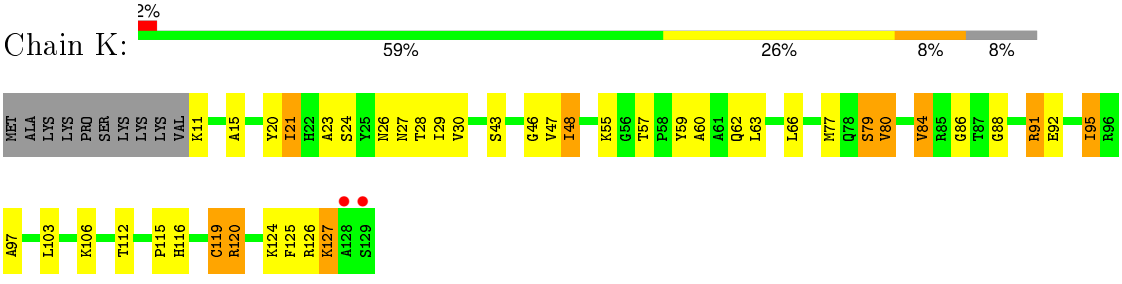
• Molecule 10: 30S ribosomal protein S10

Chain J:



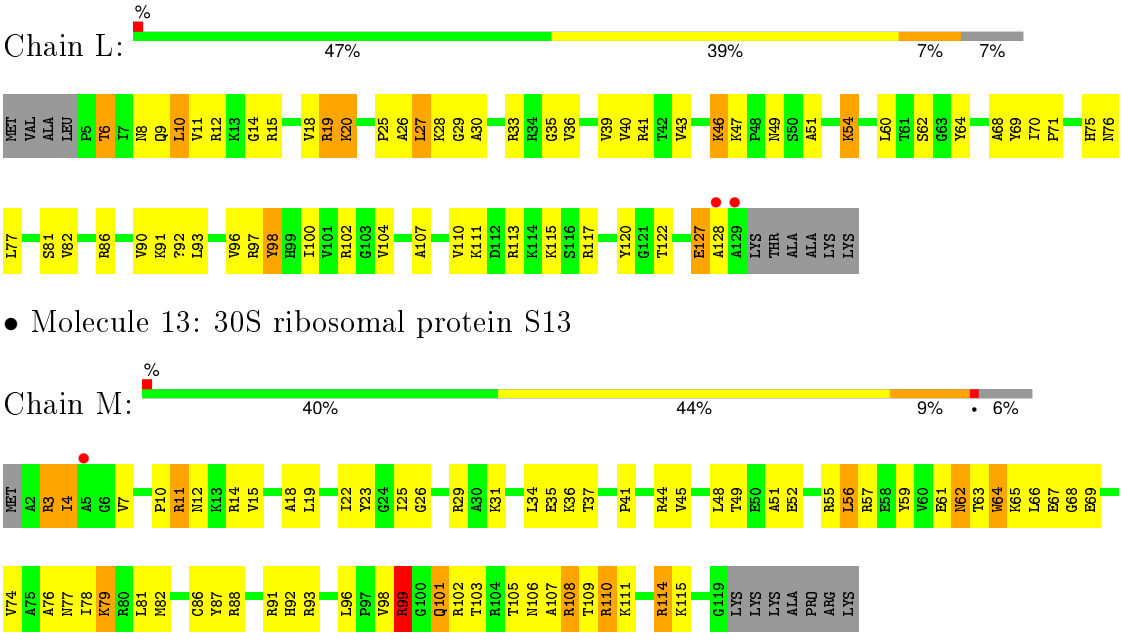
• Molecule 11: 30S ribosomal protein S11

Chain K:



• Molecule 12: 30S ribosomal protein S12

Chain L:

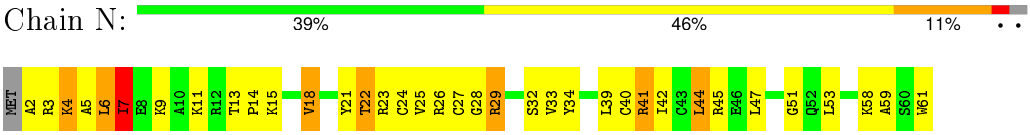


• Molecule 13: 30S ribosomal protein S13

Chain M:

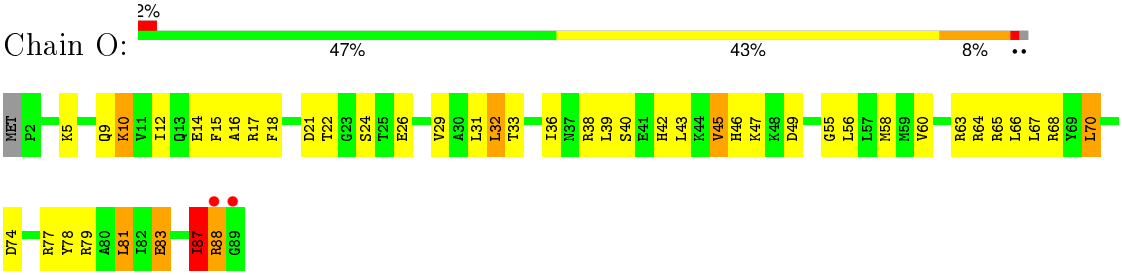
• Molecule 14: 30S ribosomal protein S14

Chain N:



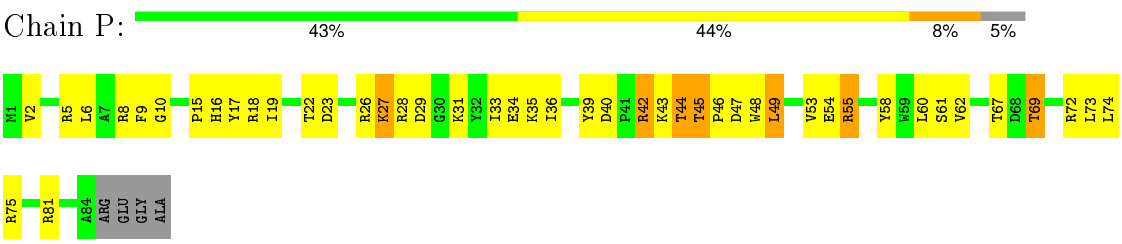
• Molecule 15: 30S ribosomal protein S15

Chain O:



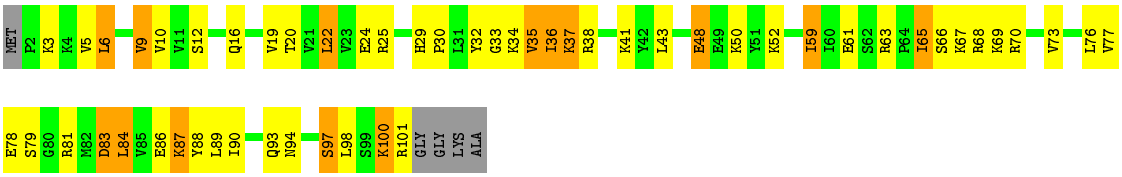
• Molecule 16: 30S ribosomal protein S16

Chain P:



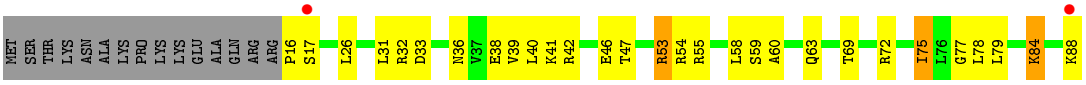
• Molecule 17: 30S ribosomal protein S17

Chain Q:



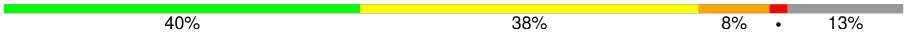
- Molecule 18: 30S ribosomal protein S18

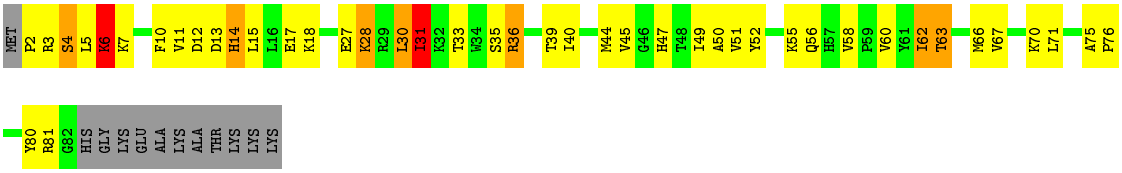
Chain R:



- Molecule 19: 30S ribosomal protein S19

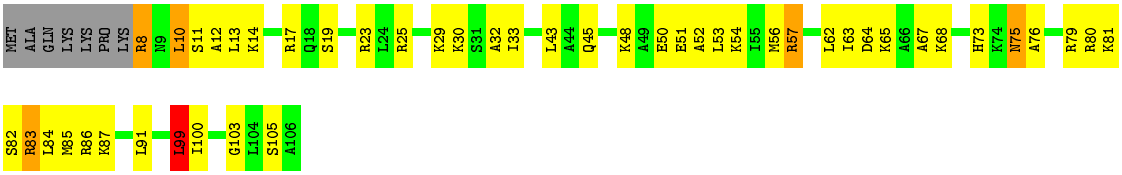
Chain S:





- Molecule 20: 30S ribosomal protein S20

Chain T:

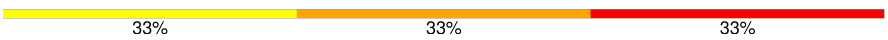


- Molecule 21: 30S ribosomal protein THX

Chain U:

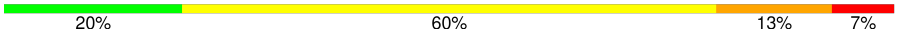
- Molecule 22: 5'-R(*UP*UP*U)-3'

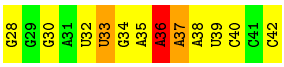
Chain V:



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

Chain W:




G28
G29
G30
A31
U32
U33
G34
A35
A36
A37
A38
U39
C40
C41
C42

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	2.94 (at 4.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_978)	Depositor
R, R_{free}	0.153 , 0.212 0.159 , 0.213	Depositor DCC
R_{free} test set	6190 reflections (5.28%)	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 , 94.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32504	0	16432	801	0
2	B	1896	0	1936	77	0
3	C	1613	0	1677	81	0
4	D	1703	0	1763	78	0
5	E	1147	0	1207	41	0
6	F	843	0	857	32	0
7	G	1257	0	1296	41	0
8	H	1116	0	1177	58	0
9	I	1010	0	1037	49	0
10	J	793	0	835	57	0
11	K	885	0	904	30	0
12	L	973	0	1058	39	0
13	M	937	0	995	46	0
14	N	492	0	529	35	0
15	O	734	0	771	34	0
16	P	701	0	720	39	0
17	Q	834	0	906	43	0
18	R	598	0	670	25	0
19	S	648	0	673	30	0
20	T	763	0	861	28	0
21	U	209	0	221	10	0
22	V	57	0	32	3	0
23	W	319	0	164	9	0
24	A	756	0	810	61	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
25	N	1	0	0	0	0
25	O	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	7	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	37531	1549	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (1549) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:15:ALA:HA	11:K:77:MET:HA	1.47	0.97
1:A:1053:G:HO2'	1:A:1199:U:H5	0.97	0.92
1:A:737:A:H1'	6:F:73:ASN:HD21	1.34	0.91
19:S:33:THR:HG22	19:S:35:SER:H	1.38	0.88
1:A:975:A:H4'	1:A:976:G:H5"	1.57	0.87
1:A:983:A:O2'	1:A:1050:G:OP2	1.91	0.86
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
20:T:57:ARG:HH21	20:T:100:ILE:HG23	1.43	0.83
1:A:1271:G:OP1	24:A:1616:PAR:N32	2.11	0.83
10:J:19:SER:HB3	10:J:91:PRO:HG3	1.61	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
1:A:664:G:H22	1:A:741:G:H1	1.25	0.81
3:C:58:GLU:HB3	10:J:92:THR:HG21	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:150:LYS:HG3	3:C:169:ALA:HB2	1.63	0.80
1:A:966:M2G:HM13	1:A:967:5MC:H1'	1.60	0.80
24:A:1605:PAR:O53	24:A:1605:PAR:N21	2.14	0.80
3:C:11:ARG:HD3	3:C:180:ALA:HB3	1.63	0.79
24:A:1608:PAR:H531	24:A:1608:PAR:HN22	1.48	0.79
5:E:83:GLU:HG3	5:E:88:LYS:HE3	1.65	0.79
3:C:180:ALA:HB1	3:C:182:ILE:HG13	1.65	0.78
1:A:108:G:H5"	1:A:109:A:H5"	1.65	0.78
1:A:376:G:H5"	16:P:5:ARG:HD2	1.65	0.78
1:A:946:A:H2'	1:A:947:G:H8	1.47	0.78
17:Q:66:SER:HB3	17:Q:69:LYS:HG3	1.64	0.78
1:A:1212:U:O2'	1:A:1213:A:O5'	2.02	0.78
1:A:353:A:H5'	1:A:353:A:H8	1.47	0.78
16:P:18:ARG:HD3	16:P:35:LYS:HD2	1.66	0.77
1:A:424:G:N7	24:A:1611:PAR:N21	2.30	0.77
7:G:75:VAL:HG21	7:G:86:GLN:HB3	1.64	0.77
1:A:946:A:H2'	1:A:947:G:C8	2.19	0.77
9:I:43:ALA:HA	9:I:74:ILE:HD13	1.66	0.77
10:J:4:ILE:HD12	10:J:74:ILE:HG13	1.64	0.77
1:A:447:G:H2'	1:A:485:G:H22	1.49	0.77
1:A:1367:C:H5'	10:J:60:ARG:NH1	2.00	0.77
15:O:39:LEU:HD12	15:O:56:LEU:HD13	1.68	0.76
1:A:734:G:H21	18:R:75:ILE:HD11	1.49	0.76
1:A:258:G:H2'	1:A:259:G:H8	1.51	0.76
19:S:55:LYS:HG2	19:S:56:GLN:HG2	1.66	0.75
14:N:27:CYS:SG	14:N:29:ARG:HB2	2.25	0.75
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
5:E:82:VAL:HG21	5:E:138:ALA:HA	1.68	0.74
4:D:57:ARG:HH11	4:D:57:ARG:HG3	1.52	0.74
1:A:1328:C:H2'	1:A:1329:A:H8	1.52	0.74
1:A:442:C:H42	1:A:492:G:H1	1.35	0.74
1:A:951:G:OP2	13:M:102:ARG:NH2	2.21	0.74
1:A:825:G:H21	8:H:11:THR:HG21	1.53	0.74
2:B:97:TRP:HZ2	2:B:102:LEU:HD13	1.52	0.74
10:J:49:VAL:O	10:J:61:GLU:N	2.20	0.73
1:A:1127:G:H21	1:A:1146:A:H62	1.36	0.73
1:A:192:U:H1'	20:T:103:GLY:HA2	1.69	0.73
10:J:48:THR:HA	10:J:62:HIS:HB3	1.71	0.73
1:A:927:G:O2'	1:A:1503:A:N7	2.21	0.73
1:A:51:A:OP2	24:A:1604:PAR:H24	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1399:C:H4'	1:A:1400:5MC:H5"	1.70	0.72
1:A:1387:G:O2'	27:A:2274:HOH:O	2.07	0.72
1:A:47:C:OP1	24:A:1604:PAR:N32	2.23	0.72
16:P:15:PRO:HD2	16:P:42:ARG:HD3	1.70	0.72
8:H:85:ARG:NH1	8:H:87:SER:O	2.21	0.72
5:E:10:MET:HA	5:E:32:VAL:HG22	1.72	0.72
1:A:382:A:H2'	1:A:383:A:C8	2.23	0.72
1:A:1003(A):G:H2'	1:A:1004:A:H4'	1.71	0.72
1:A:235:C:H5'	17:Q:70:ARG:HG2	1.72	0.72
12:L:47:LYS:NZ	22:V:3:U:OP1	2.23	0.72
11:K:24:SER:HB3	11:K:26:ASN:H	1.55	0.72
1:A:1281:U:H5'	1:A:1282:C:H5	1.54	0.71
1:A:737:A:H1'	6:F:73:ASN:ND2	2.05	0.71
7:G:137:LYS:O	7:G:141:VAL:HG23	1.90	0.71
12:L:77:LEU:HD21	12:L:107:ALA:HB2	1.71	0.71
10:J:50:ILE:HA	10:J:60:ARG:HA	1.72	0.71
9:I:53:VAL:HG21	9:I:85:LEU:HD21	1.72	0.71
1:A:1031:G:H2'	1:A:1032:G:H8	1.55	0.71
1:A:1366:C:H2'	1:A:1367:C:C6	2.26	0.71
13:M:49:THR:HG22	13:M:51:ALA:H	1.55	0.71
8:H:82:HIS:HD1	8:H:138:TRP:HE1	1.38	0.71
8:H:17:THR:O	8:H:78:GLN:NE2	2.24	0.71
9:I:51:ARG:HA	9:I:56:LEU:HD22	1.72	0.70
10:J:24:VAL:HG13	10:J:34:VAL:HG11	1.72	0.70
4:D:140:VAL:HG11	4:D:146:ILE:HD11	1.72	0.70
1:A:433:C:H5"	1:A:433:C:H6	1.56	0.70
1:A:795:C:H5"	1:A:796:C:OP2	1.91	0.70
18:R:38:GLU:HA	18:R:41:LYS:HE2	1.72	0.70
1:A:329:A:O2'	1:A:332:G:N7	2.25	0.70
4:D:13:ARG:HD2	4:D:38:TYR:O	1.91	0.70
1:A:642:A:N3	8:H:113:SER:OG	2.25	0.70
1:A:250:A:H4'	1:A:251:G:O5'	1.92	0.70
1:A:355:C:H5'	1:A:389:A:OP2	1.90	0.70
1:A:1326:C:OP1	21:U:12:LYS:NZ	2.23	0.70
1:A:114:U:H2'	1:A:115:G:C8	2.27	0.70
20:T:64:ASP:OD2	20:T:81:LYS:NZ	2.22	0.70
24:A:1613:PAR:O23	24:A:1613:PAR:N21	2.25	0.70
4:D:61:LYS:HB2	4:D:203:VAL:HG13	1.73	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
1:A:1291:G:H4'	9:I:39:GLY:HA3	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:1616:PAR:N24	24:A:1616:PAR:O53	2.26	0.69
23:W:36:A:H2'	23:W:37:A:H8	1.55	0.69
3:C:78:GLY:HA3	3:C:83:ARG:HB3	1.74	0.69
1:A:1284:C:H3'	1:A:1285:A:H8	1.57	0.69
24:A:1602:PAR:N24	24:A:1602:PAR:O44	2.24	0.69
1:A:1338:G:H2'	1:A:1339:A:C8	2.28	0.69
1:A:1504:G:OP1	1:A:1507:A:H4'	1.92	0.69
8:H:35:ILE:O	8:H:39:LEU:HD22	1.93	0.69
15:O:10:LYS:HE2	15:O:14:GLU:HB2	1.75	0.69
3:C:131:ARG:HA	3:C:134:ILE:HD12	1.75	0.69
18:R:17:SER:HB3	18:R:54:ARG:HH11	1.58	0.69
1:A:1360:A:H2'	1:A:1361:G:O4'	1.93	0.69
13:M:11:ARG:HG3	13:M:12:ASN:HB2	1.75	0.68
1:A:1328:C:H2'	1:A:1329:A:C8	2.28	0.68
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:156:ARG:H	3:C:163:ALA:HA	1.58	0.68
10:J:34:VAL:HA	10:J:74:ILE:HG22	1.75	0.68
3:C:164:ARG:NH1	3:C:166:GLU:OE1	2.26	0.68
1:A:1401:G:C2	1:A:1402:4OC:H1'	2.28	0.68
7:G:44:TYR:HA	7:G:47:CYS:HB2	1.75	0.68
24:A:1612:PAR:N21	24:A:1612:PAR:H42	2.09	0.68
7:G:20:ASP:OD2	7:G:63:LYS:NZ	2.25	0.68
1:A:414:A:OP2	24:A:1611:PAR:N12	2.27	0.67
11:K:57:THR:HG22	11:K:59:TYR:H	1.59	0.67
1:A:1023:G:O6	1:A:1024:G:N2	2.24	0.67
5:E:144:THR:O	5:E:148:VAL:HG23	1.94	0.67
12:L:49:ASN:ND2	12:L:92:0TD:SB	2.67	0.67
1:A:1356:G:H2'	1:A:1357:A:C8	2.28	0.67
1:A:37:U:O2'	1:A:500:G:H4'	1.95	0.67
1:A:928:G:O2'	1:A:1533:C:OP1	2.11	0.67
1:A:1154:G:H2'	1:A:1155:G:H8	1.59	0.67
3:C:126:ARG:HG2	3:C:128:PHE:HD1	1.60	0.67
1:A:1124:G:HO2'	1:A:1145:C:N4	1.92	0.67
1:A:972:C:OP1	10:J:57:LYS:NZ	2.22	0.67
1:A:372:C:H4'	1:A:373:A:O5'	1.94	0.67
1:A:1528:U:O2'	1:A:1529:G:OP2	2.12	0.67
20:T:33:ILE:HD13	20:T:63:ILE:HG12	1.77	0.67
10:J:6:ILE:HD13	10:J:72:VAL:HB	1.77	0.66
1:A:1305:G:H5"	21:U:4:GLY:HA3	1.75	0.66
1:A:1008:C:N3	1:A:1022:G:N2	2.42	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:74:GLU:HG2	7:G:91:VAL:HG22	1.77	0.66
18:R:36:ASN:O	18:R:40:LEU:HD12	1.95	0.66
12:L:62:SER:HB3	12:L:64:TYR:HD1	1.61	0.66
1:A:1454:G:H2'	1:A:1455:G:H8	1.60	0.66
1:A:1263:C:H42	1:A:1272:G:H1	1.43	0.66
1:A:475:G:H2'	1:A:476:G:H8	1.59	0.66
2:B:197:VAL:HB	2:B:200:ILE:HG12	1.78	0.66
10:J:54:PHE:HD2	10:J:55:LYS:HG2	1.61	0.66
14:N:6:LEU:HD12	14:N:23:ARG:HH21	1.60	0.65
16:P:26:ARG:HD2	16:P:31:LYS:O	1.96	0.65
6:F:28:ARG:HB2	6:F:28:ARG:HH11	1.61	0.65
1:A:1062:U:H2'	1:A:1063:C:C6	2.31	0.65
10:J:61:GLU:OE2	14:N:58:LYS:NZ	2.29	0.65
23:W:36:A:H2'	23:W:37:A:C8	2.32	0.65
7:G:15:ASP:HB3	7:G:20:ASP:H	1.60	0.65
1:A:560:U:H5'	1:A:566:G:N2	2.12	0.65
1:A:975:A:H5"	1:A:975:A:H8	1.62	0.65
17:Q:67:LYS:HA	17:Q:70:ARG:HH12	1.62	0.65
1:A:382:A:H2'	1:A:383:A:H8	1.59	0.65
1:A:1350:A:OP2	9:I:118:LYS:HE3	1.95	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
3:C:156:ARG:HH21	3:C:161:GLU:HA	1.62	0.65
24:A:1610:PAR:O44	24:A:1610:PAR:N24	2.30	0.64
6:F:10:LEU:HD12	6:F:59:TYR:HB3	1.78	0.64
1:A:1443:G:H4'	1:A:1446:A:C5'	2.27	0.64
1:A:1488:G:H2'	1:A:1489:G:H8	1.62	0.64
1:A:192:U:C1'	20:T:103:GLY:HA2	2.27	0.64
16:P:69:THR:HG22	16:P:72:ARG:HD3	1.79	0.64
1:A:1343:G:H2'	1:A:1344:C:C6	2.32	0.64
1:A:1182:G:O2'	1:A:1183:A:OP2	2.13	0.64
1:A:204:U:H5'	1:A:216:G:OP1	1.97	0.64
1:A:1060:C:C5	3:C:2:GLY:HA2	2.33	0.64
11:K:24:SER:HB2	11:K:27:ASN:H	1.62	0.64
8:H:86:ILE:HG21	8:H:133:LEU:HD13	1.79	0.64
5:E:81:GLU:HG2	5:E:90:VAL:HG22	1.79	0.64
6:F:25:ILE:HD13	6:F:82:ARG:HD2	1.78	0.64
1:A:665:A:H2'	1:A:732:C:O2	1.96	0.64
11:K:57:THR:HB	11:K:60:ALA:H	1.63	0.64
1:A:749:C:H2'	1:A:750:G:H8	1.62	0.64
17:Q:29:HIS:HB2	17:Q:36:ILE:CD1	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:135:LYS:HE3	5:E:50:GLU:HG2	1.80	0.64
6:F:91:VAL:HG13	18:R:72:ARG:NH2	2.12	0.64
1:A:976:G:H5'	1:A:1358:U:O2'	1.97	0.64
7:G:23:VAL:O	7:G:27:ILE:HG12	1.98	0.64
3:C:116:VAL:HG21	3:C:202:ILE:HD11	1.79	0.64
19:S:27:GLU:HG2	19:S:28:LYS:H	1.63	0.64
4:D:111:ALA:HB2	4:D:120:LEU:HD12	1.79	0.64
1:A:1498:UR3:O2'	1:A:1499:A:OP2	2.14	0.63
1:A:1031:G:H2'	1:A:1032:G:C8	2.33	0.63
24:A:1603:PAR:H532	24:A:1603:PAR:HN61	1.63	0.63
1:A:217:C:O2'	1:A:461:C:N4	2.30	0.63
1:A:731:G:OP1	1:A:766:A:H1'	1.99	0.63
7:G:26:PHE:CE2	7:G:30:ILE:HD11	2.34	0.63
1:A:1149:C:H2'	1:A:1150:U:H6	1.64	0.63
24:A:1616:PAR:N64	24:A:1616:PAR:O44	2.30	0.62
10:J:49:VAL:HG23	14:N:41:ARG:HD2	1.81	0.62
2:B:75:LYS:HA	2:B:78:GLN:HB2	1.81	0.62
1:A:390:C:H2'	1:A:391:G:C8	2.33	0.62
9:I:46:ALA:HB2	9:I:74:ILE:HG23	1.82	0.62
1:A:447:G:H2'	1:A:485:G:N2	2.12	0.62
19:S:31:ILE:HG22	19:S:50:ALA:H	1.64	0.62
1:A:1308:U:OP2	13:M:99:ARG:HG3	1.98	0.62
8:H:7:ALA:HA	8:H:85:ARG:HG3	1.81	0.62
3:C:148:GLY:HA3	3:C:172:ARG:O	1.99	0.62
1:A:445:G:H2'	1:A:446:G:H8	1.64	0.62
1:A:1060:C:C4	3:C:2:GLY:HA2	2.35	0.62
1:A:1392:G:H21	1:A:1502:A:H8	1.45	0.62
2:B:220:ASP:O	2:B:224:GLN:HB3	1.99	0.62
9:I:4:TYR:CE2	9:I:88:TYR:HD1	2.17	0.62
1:A:353:A:H5'	1:A:353:A:C8	2.31	0.62
15:O:55:GLY:HA2	15:O:58:MET:HE2	1.82	0.62
1:A:1505:G:O2'	1:A:1506:U:OP2	2.12	0.62
1:A:1368:G:H5"	9:I:112:LYS:HD3	1.82	0.62
5:E:98:THR:HB	5:E:117:ASP:HB3	1.81	0.61
1:A:559:A:OP1	5:E:126:ARG:NH2	2.33	0.61
1:A:981:U:H5'	14:N:21:TYR:CE1	2.35	0.61
1:A:1296:C:H4'	1:A:1302:U:C5	2.34	0.61
20:T:45:GLN:HA	20:T:91:LEU:HD22	1.81	0.61
8:H:5:PRO:HB2	8:H:6:ILE:HD12	1.82	0.61
1:A:428:G:H4'	1:A:429:U:O5'	2.00	0.61
19:S:31:ILE:HG21	19:S:49:ILE:HG23	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:978:A:H1'	1:A:1322:C:O2	2.00	0.61
1:A:721:G:H4'	1:A:722:A:O4'	2.01	0.61
1:A:273:A:H1'	17:Q:16:GLN:HE21	1.66	0.61
9:I:24:GLY:HA3	9:I:57:GLY:HA2	1.82	0.61
10:J:82:ILE:HA	10:J:85:LEU:HB2	1.81	0.61
1:A:592:G:H2'	1:A:593:G:H8	1.65	0.61
1:A:1288:A:H2'	1:A:1289:A:O4'	1.99	0.61
1:A:1190:G:HO2'	1:A:1191:A:P	2.23	0.61
13:M:34:LEU:HD12	13:M:41:PRO:HA	1.83	0.61
1:A:1343:G:H2'	1:A:1344:C:H6	1.65	0.61
1:A:665:A:H3'	1:A:725:G:N2	2.15	0.61
1:A:344:A:H5'	1:A:345:C:C5	2.36	0.61
1:A:598:U:H2'	1:A:599:C:C6	2.36	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
4:D:8:VAL:O	4:D:11:LEU:N	2.25	0.61
9:I:70:LYS:O	9:I:74:ILE:HG13	2.00	0.61
18:R:33:ASP:O	18:R:40:LEU:HD11	2.01	0.61
4:D:31:CYS:C	4:D:33:MET:H	2.04	0.60
2:B:80:ILE:HD11	2:B:208:ILE:HG22	1.82	0.60
1:A:109:A:C6	1:A:326:G:C6	2.89	0.60
9:I:29:ASN:ND2	9:I:65:VAL:O	2.26	0.60
1:A:595:G:H22	1:A:643:C:N4	1.99	0.60
1:A:110:C:H2'	1:A:111:G:O4'	2.01	0.60
1:A:433:C:H5"	1:A:433:C:C6	2.36	0.60
1:A:1256:A:H5'	1:A:1258:G:H1'	1.83	0.60
1:A:81:U:H2'	1:A:82:U:H5"	1.83	0.60
1:A:103:C:OP1	20:T:17:ARG:NH1	2.33	0.60
2:B:7:VAL:N	2:B:9:GLU:HG3	2.17	0.60
3:C:155:GLY:HA2	3:C:164:ARG:H	1.66	0.60
4:D:100:ARG:HB3	4:D:102:ASP:OD1	2.01	0.60
1:A:179:A:H2'	1:A:180:U:C6	2.37	0.60
12:L:6:THR:OG1	12:L:9:GLN:HG3	2.02	0.60
1:A:1127:G:N2	1:A:1145:C:N3	2.50	0.60
2:B:84:GLU:OE1	2:B:216:SER:HA	2.02	0.60
1:A:1101:A:H4'	1:A:1102:A:O5'	2.02	0.60
1:A:226:G:N7	24:A:1617:PAR:O31	2.34	0.60
8:H:10:LEU:HD22	8:H:83:ILE:HD11	1.83	0.59
11:K:43:SER:HA	11:K:47:VAL:HG21	1.83	0.59
1:A:1256:A:N6	1:A:1278:U:O4'	2.28	0.59
12:L:90:VAL:HB	12:L:93:LEU:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1488:G:H2'	1:A:1489:G:C8	2.37	0.59
2:B:133:LYS:O	2:B:137:ARG:HG3	2.01	0.59
3:C:11:ARG:HH22	3:C:175:LEU:HD23	1.68	0.59
8:H:6:ILE:O	8:H:10:LEU:HG	2.01	0.59
13:M:66:LEU:O	13:M:69:GLU:HB2	2.02	0.59
10:J:39:PRO:HA	10:J:70:ARG:HD3	1.85	0.59
1:A:438:G:O2'	1:A:495:U:O4	2.20	0.59
1:A:362:G:N2	1:A:365:U:OP2	2.36	0.59
1:A:1086:U:H6	1:A:1086:U:O5'	1.85	0.59
5:E:148:VAL:O	5:E:152:ARG:HG3	2.02	0.59
24:A:1618:PAR:HN21	24:A:1618:PAR:H322	1.51	0.59
1:A:1316:G:H4'	14:N:18:VAL:HG11	1.83	0.59
1:A:985:C:C2	1:A:1221:G:N2	2.71	0.59
1:A:1285:A:H4'	1:A:1286:A:O5'	2.03	0.59
18:R:17:SER:OG	18:R:55:ARG:HG2	2.03	0.59
1:A:1454:G:H2'	1:A:1455:G:C8	2.38	0.59
21:U:10:ARG:HD3	21:U:13:ILE:HD11	1.85	0.59
1:A:1065:U:H5"	1:A:1190:G:N2	2.17	0.59
20:T:10:LEU:HG	20:T:12:ALA:H	1.68	0.59
1:A:1112:C:H1'	3:C:179:ARG:HD3	1.83	0.59
3:C:6:HIS:HD2	3:C:8:ILE:H	1.49	0.59
1:A:1212:U:HO2'	1:A:1213:A:P	2.26	0.58
14:N:24:CYS:HB3	14:N:28:GLY:H	1.68	0.58
1:A:595:G:H22	1:A:643:C:H42	1.51	0.58
4:D:15:GLU:HG2	4:D:63:LYS:HG3	1.85	0.58
5:E:43:LEU:HD11	5:E:132:ALA:HB1	1.85	0.58
7:G:20:ASP:HB3	7:G:23:VAL:HG23	1.84	0.58
4:D:173:TRP:O	4:D:174:LEU:HD23	2.03	0.58
1:A:1402:4OC:HM22	1:A:1403:C:H5'	1.85	0.58
4:D:47:ARG:HE	4:D:48:ALA:H	1.51	0.58
4:D:148:VAL:HG12	4:D:149:ALA:H	1.68	0.58
23:W:28:G:H2'	23:W:28:G:N3	2.18	0.58
1:A:370:C:C2'	1:A:371:G:H5'	2.33	0.58
15:O:79:ARG:NH1	15:O:83:GLU:HB2	2.18	0.58
11:K:79:SER:HB2	11:K:106:LYS:HD3	1.85	0.58
4:D:13:ARG:HD3	4:D:36:ARG:O	2.04	0.58
1:A:1159:U:O4'	1:A:1182:G:N2	2.36	0.58
1:A:91:C:H2'	1:A:92:C:H6	1.68	0.58
1:A:551:U:H2'	1:A:552:U:C6	2.37	0.58
13:M:81:LEU:HD22	13:M:88:ARG:HB2	1.86	0.58
4:D:7:PRO:HB2	4:D:10:ARG:HD2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:929:G:H1	1:A:1388:C:H42	1.50	0.58
1:A:376:G:H2'	1:A:377:G:H8	1.67	0.58
1:A:558:G:C8	1:A:559:A:H2'	2.38	0.58
1:A:1026:G:H3'	1:A:1027:C:H5"	1.85	0.58
15:O:56:LEU:O	15:O:60:VAL:HG23	2.03	0.58
9:I:48:GLU:HG2	9:I:51:ARG:HH21	1.69	0.58
7:G:15:ASP:HB2	7:G:20:ASP:O	2.03	0.58
16:P:45:THR:HB	16:P:47:ASP:H	1.69	0.58
4:D:100:ARG:O	4:D:104:VAL:HG23	2.04	0.58
15:O:26:GLU:OE1	15:O:77:ARG:HB3	2.04	0.58
1:A:975:A:C5'	1:A:975:A:H8	2.17	0.57
12:L:25:PRO:C	12:L:27:LEU:H	2.07	0.57
9:I:24:GLY:CA	9:I:57:GLY:HA2	2.33	0.57
4:D:117:ALA:O	4:D:121:VAL:HG23	2.04	0.57
1:A:677:U:H3	1:A:713:G:H22	1.52	0.57
7:G:54:THR:HG22	7:G:56:GLN:H	1.68	0.57
12:L:54:LYS:HG2	12:L:75:HIS:CD2	2.39	0.57
16:P:19:ILE:HG22	16:P:36:ILE:HG13	1.86	0.57
1:A:474:G:H2'	1:A:475:G:H8	1.67	0.57
8:H:33:GLU:HB2	8:H:59:LEU:HD21	1.85	0.57
1:A:1517:G:H2'	1:A:1518:MA6:H8	1.87	0.57
17:Q:59:ILE:HD12	17:Q:73:VAL:HA	1.86	0.57
18:R:53:ARG:HG2	18:R:63:GLN:HG2	1.86	0.57
19:S:33:THR:HG22	19:S:35:SER:N	2.15	0.57
1:A:1049:U:H4'	1:A:1050:G:C5'	2.34	0.57
1:A:994:A:N7	1:A:1216:G:H4'	2.19	0.57
1:A:1179:A:O2'	1:A:1180:A:OP1	2.22	0.57
1:A:427:U:H3'	1:A:428:G:H2'	1.86	0.57
1:A:1349:A:OP1	9:I:120:ARG:HB2	2.04	0.57
18:R:53:ARG:HH11	18:R:53:ARG:HG3	1.70	0.57
1:A:998:G:N2	1:A:999:C:N3	2.53	0.57
20:T:82:SER:O	20:T:86:ARG:HG3	2.05	0.57
1:A:376:G:H2'	1:A:377:G:C8	2.40	0.57
3:C:155:GLY:HA2	3:C:164:ARG:O	2.05	0.57
7:G:23:VAL:HG12	7:G:27:ILE:HD11	1.87	0.57
1:A:765:G:H5"	1:A:766:A:OP1	2.04	0.57
11:K:21:ILE:HG23	11:K:30:VAL:HG22	1.86	0.57
1:A:1125:U:O2'	1:A:1281:U:O2	2.22	0.57
1:A:291:C:O2'	1:A:292:G:H5'	2.04	0.57
5:E:95:ALA:HB1	5:E:96:PRO:HD2	1.87	0.57
1:A:432:A:H2'	1:A:433:C:O4'	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559:A:H4'	1:A:560:U:O5'	2.03	0.57
1:A:372:C:C4	1:A:387:U:H5	2.23	0.56
4:D:28:SER:O	4:D:30:LYS:N	2.38	0.56
7:G:50:ILE:HD13	7:G:125:MET:HG3	1.86	0.56
5:E:51:VAL:O	5:E:55:VAL:HG23	2.04	0.56
1:A:318:G:N2	1:A:335:C:O2	2.36	0.56
1:A:1048:G:H5"	14:N:3:ARG:HG3	1.86	0.56
24:A:1605:PAR:O44	24:A:1605:PAR:N64	2.36	0.56
17:Q:10:VAL:HG13	17:Q:19:VAL:HB	1.86	0.56
1:A:429:U:H1'	1:A:430:A:H5"	1.87	0.56
20:T:81:LYS:O	20:T:85:MET:HG3	2.04	0.56
6:F:28:ARG:NH1	6:F:28:ARG:HB2	2.19	0.56
6:F:44:GLY:HA2	6:F:59:TYR:CE2	2.40	0.56
17:Q:29:HIS:HB2	17:Q:36:ILE:HD11	1.87	0.56
1:A:800:G:H8	1:A:800:G:O5'	1.89	0.56
1:A:443:C:H2'	1:A:444:C:H6	1.69	0.56
1:A:872:A:C8	1:A:874:G:C8	2.93	0.56
1:A:413:G:N2	1:A:428:G:H1'	2.20	0.56
11:K:59:TYR:HE2	11:K:63:LEU:HD11	1.70	0.56
1:A:1331:G:H4'	1:A:1332:A:H5'	1.88	0.56
1:A:757:U:H2'	1:A:758:G:O4'	2.04	0.56
11:K:48:ILE:HD13	11:K:48:ILE:H	1.70	0.56
1:A:355:C:OP1	24:A:1604:PAR:N21	2.39	0.56
1:A:143:A:H2	1:A:220:G:H22	1.53	0.56
1:A:807:A:H2'	1:A:808:C:C6	2.41	0.56
1:A:1136:U:H5"	1:A:1137:C:OP2	2.05	0.56
10:J:61:GLU:HG2	10:J:63:PHE:CE2	2.41	0.56
2:B:213:LEU:O	2:B:217:ARG:HG2	2.06	0.56
11:K:23:ALA:HB1	11:K:88:GLY:HA3	1.88	0.56
1:A:372:C:N3	1:A:387:U:H5	2.04	0.56
15:O:70:LEU:HD21	15:O:77:ARG:HB2	1.88	0.56
10:J:49:VAL:HG23	14:N:41:ARG:HB2	1.87	0.56
1:A:1502:A:H2	1:A:1505:G:H1	1.51	0.56
1:A:502:G:OP1	12:L:117:ARG:N	2.38	0.56
1:A:749:C:H2'	1:A:750:G:C8	2.41	0.56
9:I:111:ARG:HD2	14:N:61:TRP:OXT	2.05	0.56
9:I:8:GLY:HA2	9:I:79:LEU:HD13	1.88	0.56
1:A:954:G:H21	1:A:1227:A:H62	1.53	0.56
3:C:43:LEU:O	3:C:47:LEU:HB2	2.06	0.56
17:Q:24:GLU:OE1	17:Q:37:LYS:HD2	2.05	0.56
1:A:1063:C:H2'	1:A:1064:G:C8	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:G:H2'	1:A:259:G:C8	2.39	0.55
4:D:150:GLU:HA	4:D:153:ARG:CZ	2.35	0.55
20:T:65:LYS:O	20:T:68:LYS:HB2	2.06	0.55
1:A:272:C:H2'	1:A:273:A:H8	1.71	0.55
1:A:1510:U:H2'	1:A:1511:G:C8	2.41	0.55
16:P:58:TYR:O	16:P:62:VAL:HG22	2.05	0.55
1:A:532:A:N6	1:A:1206:G:O2'	2.39	0.55
2:B:47:THR:HA	2:B:202:PRO:HG2	1.87	0.55
13:M:49:THR:HB	13:M:52:GLU:H	1.71	0.55
7:G:149:ARG:HB3	11:K:59:TYR:CE1	2.42	0.55
12:L:11:VAL:HG22	17:Q:29:HIS:CD2	2.41	0.55
1:A:1261:A:N6	1:A:1262:C:O2	2.38	0.55
5:E:69:VAL:HG21	5:E:113:ALA:HB1	1.87	0.55
20:T:63:ILE:HD13	20:T:80:ARG:HB2	1.87	0.55
3:C:72:LYS:HE3	3:C:75:VAL:HG21	1.88	0.55
13:M:25:ILE:HG23	13:M:29:ARG:HB2	1.88	0.55
1:A:1124:G:O2'	1:A:1145:C:N4	2.40	0.55
2:B:79:ASP:O	2:B:82:ARG:HG3	2.06	0.55
1:A:254:G:OP1	17:Q:67:LYS:O	2.25	0.55
1:A:1497:G:C2'	1:A:1498:UR3:H5'	2.37	0.55
13:M:11:ARG:HG3	13:M:12:ASN:N	2.22	0.55
17:Q:3:LYS:HB3	17:Q:61:GLU:HB3	1.89	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
13:M:34:LEU:CD1	13:M:41:PRO:HA	2.37	0.55
7:G:50:ILE:HD11	7:G:124:LEU:HB3	1.89	0.55
19:S:11:VAL:HG22	19:S:39:THR:HB	1.89	0.55
1:A:437:U:H5"	4:D:155:LEU:HD22	1.88	0.55
4:D:22:LYS:HB2	4:D:26:CYS:SG	2.46	0.55
1:A:1420:C:H2'	1:A:1421:G:C8	2.42	0.55
1:A:600:C:OP1	8:H:97:VAL:HG12	2.07	0.55
2:B:13:ALA:HB1	2:B:209:ARG:HB3	1.89	0.55
18:R:40:LEU:HB3	18:R:79:LEU:HD11	1.89	0.55
9:I:105:ASP:OD1	9:I:107:ARG:HG3	2.06	0.55
1:A:756:C:N4	27:A:2114:HOH:O	2.39	0.55
12:L:36:VAL:HG22	12:L:82:VAL:HA	1.88	0.55
20:T:76:ALA:HA	20:T:79:ARG:NH1	2.21	0.55
1:A:1314:C:C5	19:S:6:LYS:HE2	2.42	0.55
12:L:70:ILE:HD13	12:L:77:LEU:HD12	1.89	0.54
1:A:580:U:H2'	1:A:581:G:O4'	2.08	0.54
18:R:32:ARG:HA	18:R:69:THR:HG21	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:180:ALA:HB1	3:C:182:ILE:CG1	2.36	0.54
1:A:1060:C:C5'	10:J:51:ARG:HB3	2.38	0.54
1:A:986:A:C2	1:A:1220:G:C2	2.95	0.54
1:A:443:C:H2'	1:A:444:C:C6	2.42	0.54
1:A:1420:C:H2'	1:A:1421:G:H8	1.72	0.54
20:T:79:ARG:O	20:T:83:ARG:HG3	2.07	0.54
1:A:64:G:C2	1:A:67:C:N4	2.75	0.54
8:H:20:TYR:CE1	8:H:76:PRO:HG2	2.41	0.54
1:A:1435:G:H2'	1:A:1436:U:C6	2.43	0.54
6:F:30:LEU:HD23	6:F:75:LEU:HD11	1.89	0.54
1:A:772:U:OP1	24:A:1615:PAR:H222	2.08	0.54
1:A:397:A:H5'	1:A:398:C:OP1	2.07	0.54
11:K:91:ARG:HD3	11:K:92:GLU:OE1	2.07	0.54
1:A:1347:G:O2'	1:A:1348:U:P	2.65	0.54
2:B:223:ILE:HD12	2:B:224:GLN:H	1.72	0.54
1:A:1054:C:P	1:A:1197:G:OP2	2.65	0.54
3:C:121:ALA:HB2	3:C:198:VAL:HG21	1.88	0.54
1:A:660:G:OP2	15:O:5:LYS:HE2	2.08	0.54
1:A:976:G:OP1	14:N:32:SER:N	2.33	0.54
1:A:475:G:H2'	1:A:476:G:C8	2.42	0.54
1:A:977:A:C2'	1:A:978:A:H5'	2.38	0.54
1:A:855:G:C5	1:A:856:C:C5	2.96	0.54
8:H:36:LEU:HD12	8:H:59:LEU:HD22	1.90	0.54
1:A:1521:G:H2'	1:A:1522:U:C6	2.43	0.54
1:A:775:G:N2	1:A:804:U:O4	2.41	0.54
1:A:263:A:O2'	1:A:264:U:H5'	2.07	0.54
1:A:960:U:H4'	1:A:961:U:C5'	2.38	0.54
1:A:1154:G:H2'	1:A:1155:G:C8	2.41	0.54
8:H:20:TYR:HA	8:H:65:TYR:CZ	2.43	0.54
1:A:160:A:H2'	1:A:161:A:O4'	2.08	0.54
5:E:86:ALA:HB1	5:E:125:SER:HB3	1.90	0.54
4:D:25:ARG:HE	4:D:30:LYS:HB2	1.73	0.54
1:A:1123:A:H4'	10:J:37:PRO:HD2	1.88	0.54
3:C:33:LEU:HD21	14:N:53:LEU:HD22	1.89	0.54
8:H:6:ILE:N	8:H:6:ILE:HD12	2.23	0.54
13:M:15:VAL:HB	13:M:34:LEU:HD11	1.90	0.54
3:C:50:ALA:HB2	3:C:75:VAL:HB	1.88	0.54
17:Q:87:LYS:HA	17:Q:90:ILE:HD12	1.90	0.54
1:A:390:C:H2'	1:A:391:G:H8	1.73	0.53
1:A:232:G:H1'	1:A:262:A:N1	2.23	0.53
1:A:1428:A:H2'	1:A:1429:C:C6	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:53:LEU:O	20:T:57:ARG:HD2	2.08	0.53
1:A:1006:C:H42	1:A:1024:G:N2	2.06	0.53
3:C:123:GLN:O	3:C:128:PHE:HB2	2.08	0.53
1:A:456:C:H2'	1:A:457:C:C6	2.43	0.53
1:A:413:G:N2	1:A:429:U:OP2	2.23	0.53
1:A:1152:A:OP1	10:J:68:HIS:ND1	2.41	0.53
3:C:14:ILE:HG23	3:C:15:THR:HG23	1.91	0.53
1:A:1497:G:H2'	1:A:1498:UR3:H5'	1.90	0.53
1:A:978:A:O2'	1:A:1322:C:N3	2.36	0.53
7:G:120:ILE:O	7:G:124:LEU:HB2	2.08	0.53
9:I:111:ARG:HD3	9:I:113:LYS:HD2	1.90	0.53
8:H:95:VAL:HG12	8:H:99:GLU:HB2	1.89	0.53
1:A:778:G:H8	1:A:778:G:O5'	1.92	0.53
2:B:181:PHE:CD2	8:H:70:GLN:HB2	2.43	0.53
4:D:24:GLU:HG2	4:D:25:ARG:N	2.23	0.53
1:A:958:A:N3	1:A:985:C:O2'	2.35	0.53
15:O:17:ARG:HD3	15:O:77:ARG:NH1	2.23	0.53
1:A:1300:G:HO2'	1:A:1301:U:P	2.32	0.53
5:E:83:GLU:HG2	5:E:88:LYS:HB2	1.91	0.53
1:A:687:A:H4'	1:A:688:G:O5'	2.09	0.53
3:C:134:ILE:HG22	3:C:168:ALA:HB3	1.89	0.53
1:A:1527:C:O2'	1:A:1528:U:H5'	2.09	0.53
1:A:21:G:H2'	1:A:22:G:C8	2.43	0.53
1:A:836:G:C6	1:A:851:G:C6	2.96	0.53
17:Q:94:ASN:O	17:Q:97:SER:HB3	2.09	0.53
1:A:410:G:N1	1:A:429:U:O2	2.42	0.53
1:A:201:C:H42	1:A:216:G:H1	1.57	0.53
1:A:1240:U:OP2	7:G:116:ALA:N	2.34	0.53
2:B:16:HIS:HB3	2:B:44:LEU:HD11	1.91	0.53
1:A:1347:G:O2'	1:A:1348:U:O5'	2.27	0.53
19:S:50:ALA:HA	19:S:58:VAL:O	2.07	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:O5'	1:A:1190:G:H8	1.91	0.53
1:A:427:U:OP2	4:D:36:ARG:NH2	2.36	0.53
1:A:60:A:H4'	1:A:61:G:O5'	2.09	0.53
8:H:24:THR:HG22	8:H:63:LEU:HD21	1.90	0.53
7:G:109:ASN:OD1	7:G:119:ARG:NH2	2.35	0.53
1:A:1366:C:H2'	1:A:1367:C:H6	1.69	0.52
1:A:636:U:O4	24:A:1610:PAR:H54	2.09	0.52
1:A:1202:G:C2	14:N:42:ILE:HG21	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:A:P	24:A:1611:PAR:N12	2.82	0.52
10:J:61:GLU:OE1	14:N:45:ARG:HD2	2.09	0.52
10:J:80:LYS:O	10:J:83:GLU:HB2	2.08	0.52
1:A:1128:C:O2'	1:A:1130:A:C8	2.61	0.52
12:L:20:LYS:H	12:L:20:LYS:HD2	1.74	0.52
1:A:1346:A:N1	1:A:1374:A:H5"	2.24	0.52
1:A:474:G:H5"	16:P:81:ARG:NH2	2.24	0.52
3:C:5:ILE:HD12	3:C:6:HIS:O	2.09	0.52
14:N:14:PRO:O	14:N:15:LYS:HB3	2.09	0.52
1:A:1331:G:O2'	1:A:1332:A:P	2.68	0.52
3:C:6:HIS:CD2	3:C:8:ILE:H	2.27	0.52
2:B:100:GLY:O	2:B:104:ASN:N	2.41	0.52
1:A:1163:C:H2'	1:A:1164:G:C8	2.45	0.52
5:E:103:GLY:H	5:E:106:PRO:HG2	1.74	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
2:B:103:THR:HG23	2:B:176:GLU:OE1	2.10	0.52
1:A:1206:G:C6	1:A:1207:2MG:C5	2.98	0.52
16:P:22:THR:OG1	16:P:23:ASP:N	2.43	0.52
16:P:15:PRO:HD2	16:P:42:ARG:CD	2.38	0.52
1:A:1097:C:O2'	1:A:1168:A:N3	2.38	0.52
1:A:1015:A:H2'	1:A:1016:A:C8	2.45	0.52
5:E:80:ILE:HD12	5:E:138:ALA:HB1	1.92	0.52
9:I:48:GLU:HG2	9:I:51:ARG:NH2	2.25	0.52
6:F:97:PHE:HB3	18:R:32:ARG:HG3	1.91	0.52
3:C:121:ALA:HB1	3:C:189:ALA:HB2	1.92	0.52
6:F:95:GLU:HG2	6:F:96:PRO:HD2	1.92	0.52
1:A:519:C:H2'	1:A:520:A:C8	2.44	0.52
1:A:190(E):U:O2	17:Q:63:ARG:NH2	2.43	0.52
6:F:70:ASP:N	6:F:70:ASP:OD1	2.42	0.52
1:A:6:G:O2'	1:A:7:G:H5"	2.10	0.52
2:B:53:ARG:HA	2:B:56:ARG:NH1	2.25	0.52
1:A:665:A:H3'	1:A:725:G:H21	1.75	0.52
1:A:229:U:H5"	16:P:33:ILE:HD13	1.92	0.52
8:H:80:ILE:H	8:H:80:ILE:HD12	1.75	0.52
1:A:1260:C:O5'	1:A:1284:C:H4'	2.10	0.51
1:A:594:G:H2'	1:A:595:G:H5'	1.91	0.51
7:G:37:ASN:OD1	9:I:41:VAL:HG23	2.10	0.51
3:C:110:ASN:O	3:C:141:VAL:HG22	2.10	0.51
12:L:69:TYR:HE2	12:L:71:PRO:HA	1.75	0.51
6:F:12:PRO:HD2	6:F:86:ARG:NH1	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:238:LEU:C	2:B:240:GLN:H	2.12	0.51
1:A:1312:G:H2'	1:A:1313:U:H6	1.75	0.51
1:A:1413:A:C2	1:A:1488:G:C2	2.98	0.51
19:S:31:ILE:HG22	19:S:49:ILE:HA	1.92	0.51
1:A:858:G:O2'	1:A:859:A:H5'	2.10	0.51
1:A:520:A:OP2	12:L:51:ALA:HB1	2.10	0.51
1:A:1190:G:O2'	1:A:1191:A:P	2.67	0.51
1:A:254:G:H5"	17:Q:69:LYS:HD2	1.91	0.51
2:B:97:TRP:CZ2	2:B:102:LEU:HD13	2.39	0.51
1:A:1003(A):G:N2	1:A:1038:C:O2	2.43	0.51
7:G:15:ASP:HB3	7:G:20:ASP:N	2.26	0.51
1:A:390:C:O3'	16:P:28:ARG:NH2	2.44	0.51
2:B:187:LEU:HD12	2:B:214:ILE:HG21	1.92	0.51
14:N:34:TYR:N	14:N:39:LEU:O	2.41	0.51
1:A:1250:A:H4'	9:I:68:GLY:N	2.25	0.51
24:A:1610:PAR:H33	24:A:1610:PAR:N24	2.23	0.51
15:O:16:ALA:HB1	15:O:21:ASP:HB3	1.92	0.51
1:A:371:G:O2'	1:A:372:C:H5'	2.11	0.51
24:A:1610:PAR:O34	24:A:1610:PAR:O54	2.27	0.51
1:A:1242:C:H2'	1:A:1243:C:H6	1.76	0.51
2:B:91:PRO:HB3	2:B:154:LEU:HB2	1.92	0.51
1:A:539:A:H2'	1:A:540:G:C8	2.46	0.51
1:A:839:U:O2	1:A:839:U:H2'	2.09	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
2:B:122:PHE:CE2	2:B:139:LYS:HG2	2.45	0.51
1:A:9:G:OP1	5:E:122:GLU:HG3	2.11	0.51
1:A:974:A:OP2	14:N:29:ARG:NH1	2.38	0.51
1:A:1281:U:H5'	1:A:1282:C:C5	2.39	0.51
3:C:6:HIS:HD2	3:C:8:ILE:N	2.09	0.51
1:A:229:U:H2'	1:A:230:G:H8	1.76	0.51
7:G:140:ASP:OD2	7:G:143:ARG:NH2	2.44	0.51
2:B:55:PHE:CE2	2:B:218:ALA:HA	2.44	0.51
3:C:108:ASN:HD21	3:C:144:SER:HB2	1.76	0.51
7:G:52:GLU:HG2	7:G:53:LYS:HZ2	1.76	0.51
1:A:806:C:H4'	24:A:1613:PAR:H13	1.93	0.51
5:E:144:THR:HG22	5:E:145:LYS:N	2.26	0.51
1:A:665:A:H1'	1:A:733:A:O4'	2.11	0.51
6:F:91:VAL:HG12	6:F:92:LYS:O	2.11	0.51
1:A:552:U:H2'	1:A:553:A:C8	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:892:A:C2	1:A:907:A:C4	2.99	0.51
17:Q:100:LYS:HG2	17:Q:101:ARG:NH2	2.26	0.51
9:I:33:PHE:CE2	9:I:47:LEU:HD11	2.46	0.51
1:A:651:C:O2'	1:A:652:U:H5'	2.10	0.51
11:K:62:GLN:HG3	11:K:97:ALA:HB2	1.93	0.51
12:L:40:VAL:HG21	12:L:77:LEU:O	2.12	0.50
1:A:803:G:H2'	1:A:804:U:O4'	2.11	0.50
1:A:1234:C:O2'	1:A:1235:U:H5'	2.11	0.50
1:A:811:C:H4'	1:A:900:A:N6	2.25	0.50
12:L:86:ARG:O	12:L:98:TYR:HB3	2.11	0.50
1:A:370:C:O2'	1:A:371:G:H5'	2.11	0.50
9:I:50:LEU:HB3	9:I:56:LEU:H	1.75	0.50
2:B:55:PHE:HE2	2:B:218:ALA:HA	1.76	0.50
1:A:1010:G:N2	1:A:1020:U:H1'	2.25	0.50
1:A:106:C:O2'	1:A:379:C:OP1	2.29	0.50
1:A:1213:A:C6	1:A:1215:G:C4	2.99	0.50
1:A:547:A:OP2	4:D:2:GLY:HA3	2.12	0.50
5:E:137:GLU:O	5:E:141:GLN:HG3	2.12	0.50
1:A:1208:C:H2'	1:A:1209:C:H6	1.75	0.50
3:C:52:LEU:HA	3:C:70:VAL:HG13	1.93	0.50
1:A:22:G:H2'	1:A:23:C:C6	2.47	0.50
3:C:38:ARG:HD3	3:C:94:LEU:HD11	1.92	0.50
10:J:62:HIS:O	14:N:59:ALA:HB3	2.12	0.50
2:B:189:ASP:HB2	2:B:205:ASP:OD2	2.12	0.50
3:C:156:ARG:N	3:C:163:ALA:HA	2.25	0.50
1:A:1314:C:OP2	19:S:6:LYS:HD3	2.12	0.50
2:B:211:ILE:O	2:B:215:LEU:HB2	2.11	0.50
2:B:29:ALA:HA	2:B:32:ILE:HD12	1.94	0.50
1:A:838:G:N2	1:A:849:C:C2	2.80	0.50
1:A:428:G:H8	1:A:428:G:OP1	1.94	0.50
3:C:6:HIS:NE2	3:C:8:ILE:HB	2.26	0.50
2:B:174:VAL:O	2:B:178:ARG:HG2	2.12	0.50
1:A:932:C:C5	7:G:3:ARG:HD3	2.47	0.50
15:O:45:VAL:HB	15:O:46:HIS:HD2	1.77	0.50
1:A:377:G:N2	1:A:387:U:O2	2.44	0.50
1:A:1403:C:O2'	1:A:1404:5MC:H5'	2.12	0.50
1:A:1339:A:H2'	1:A:1340:A:O4'	2.12	0.50
1:A:456:C:H2'	1:A:457:C:H6	1.75	0.50
1:A:1179:A:H2'	1:A:1180:A:O4'	2.12	0.50
2:B:132:LYS:O	2:B:136:VAL:HG23	2.12	0.50
19:S:14:HIS:O	19:S:17:GLU:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1475:G:H2'	1:A:1476:G:H8	1.77	0.50
1:A:377:G:OP1	16:P:5:ARG:NH1	2.43	0.50
8:H:82:HIS:HE1	8:H:136:GLU:OE2	1.94	0.50
1:A:431:A:C2'	1:A:432:A:H5'	2.42	0.50
4:D:6:GLY:O	4:D:8:VAL:HG12	2.11	0.50
8:H:36:LEU:HA	8:H:39:LEU:HD23	1.94	0.50
1:A:1252:A:H2'	1:A:1253:G:O4'	2.11	0.50
1:A:1375:A:P	7:G:28:ASN:HD22	2.35	0.50
6:F:6:VAL:HG13	6:F:90:VAL:HG22	1.93	0.50
16:P:9:PHE:CD1	16:P:18:ARG:HG3	2.47	0.50
10:J:51:ARG:HB2	10:J:59:SER:HB2	1.94	0.50
1:A:345:C:O2	1:A:346:G:N2	2.44	0.50
1:A:1206:G:O4'	3:C:194:GLY:HA2	2.11	0.50
1:A:830:G:N2	1:A:856:C:O2	2.39	0.50
16:P:49:LEU:HD13	16:P:73:LEU:HD22	1.94	0.50
1:A:35:G:C6	1:A:36:C:N4	2.80	0.50
20:T:56:MET:HG3	20:T:84:LEU:HD22	1.94	0.50
19:S:31:ILE:CG2	19:S:49:ILE:HA	2.42	0.49
9:I:121:ARG:HH11	9:I:121:ARG:HG2	1.77	0.49
13:M:78:ILE:HD13	13:M:92:HIS:CE1	2.47	0.49
4:D:57:ARG:NH1	4:D:57:ARG:HG3	2.26	0.49
24:A:1603:PAR:C53	24:A:1603:PAR:HN61	2.24	0.49
1:A:1256:A:H5'	1:A:1258:G:C1'	2.43	0.49
1:A:658:G:H2'	1:A:659:U:C6	2.47	0.49
1:A:814:A:H2'	1:A:816:A:H5"	1.94	0.49
1:A:1192:C:O2	5:E:25:ARG:NH2	2.32	0.49
11:K:27:ASN:OD1	11:K:28:THR:N	2.45	0.49
1:A:1014:A:H4'	19:S:14:HIS:CD2	2.47	0.49
13:M:19:LEU:O	13:M:22:ILE:HG12	2.11	0.49
1:A:1283:G:H2'	1:A:1284:C:H6	1.76	0.49
2:B:48:MET:HA	2:B:51:LEU:HD12	1.95	0.49
13:M:63:THR:HG23	13:M:64:TRP:H	1.78	0.49
1:A:673:G:H2'	1:A:674:G:C8	2.46	0.49
1:A:1038:C:H2'	1:A:1039:C:H6	1.76	0.49
3:C:83:ARG:HA	3:C:86:VAL:HG23	1.94	0.49
1:A:1056:U:H5'	3:C:163:ALA:HB2	1.93	0.49
15:O:74:ASP:OD2	15:O:77:ARG:HG3	2.12	0.49
1:A:267:C:O2'	1:A:268:C:H5'	2.12	0.49
7:G:48:LYS:HG3	7:G:49:ILE:N	2.26	0.49
1:A:1002:G:H2'	1:A:1003:G:C8	2.47	0.49
10:J:32:ALA:HB3	10:J:75:ILE:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
15:O:39:LEU:HD12	15:O:56:LEU:HB2	1.94	0.49
1:A:1060:C:O2'	10:J:56:HIS:ND1	2.43	0.49
1:A:1104:G:OP1	2:B:111:ARG:HD2	2.13	0.49
17:Q:5:VAL:C	17:Q:6:LEU:HD23	2.33	0.49
1:A:141:A:H1'	1:A:182:U:O2	2.13	0.49
21:U:5:ASP:HB3	21:U:8:THR:OG1	2.12	0.49
3:C:188:LEU:HD22	3:C:195:VAL:HG22	1.93	0.49
1:A:325:A:H2'	1:A:326:G:O4'	2.13	0.49
24:A:1602:PAR:N24	24:A:1602:PAR:H33	2.27	0.49
1:A:1511:G:H2'	1:A:1512:U:O4'	2.13	0.49
1:A:343:U:O2'	1:A:346:G:O6	2.27	0.49
13:M:36:LYS:HD3	13:M:59:TYR:OH	2.13	0.49
8:H:23:SER:HA	8:H:63:LEU:HD22	1.94	0.49
2:B:53:ARG:HA	2:B:56:ARG:HH12	1.77	0.49
12:L:76:ASN:O	12:L:76:ASN:CG	2.51	0.49
1:A:1004:A:H5'	27:A:2449:HOH:O	2.11	0.49
1:A:1052:U:H2'	1:A:1055:A:OP1	2.13	0.49
1:A:533:A:C6	1:A:536:C:C2	3.01	0.49
9:I:71:SER:O	9:I:74:ILE:HB	2.12	0.49
1:A:268:C:H2'	1:A:269:C:H6	1.77	0.49
1:A:767:A:H2'	1:A:768:A:O4'	2.12	0.49
1:A:1048:G:O3'	1:A:1049:U:H3'	2.13	0.49
1:A:1347:G:O6	9:I:10:ARG:NH2	2.45	0.49
16:P:28:ARG:HG3	16:P:29:ASP:OD2	2.12	0.49
1:A:1220:G:H2'	1:A:1221:G:C8	2.48	0.49
4:D:121:VAL:O	4:D:134:ASP:HA	2.12	0.49
8:H:100:ILE:HG22	8:H:125:ARG:HH12	1.78	0.49
1:A:637:G:H2'	1:A:638:G:H8	1.76	0.49
1:A:922:G:C6	1:A:923:A:C6	3.01	0.49
19:S:45:VAL:HA	19:S:62:ILE:HD13	1.95	0.49
3:C:154:SER:O	3:C:196:LEU:HD11	2.12	0.48
1:A:975:A:H5"	1:A:975:A:C8	2.46	0.48
1:A:1347:G:H3'	9:I:108:VAL:O	2.13	0.48
1:A:1443:G:H4'	1:A:1446:A:O5'	2.12	0.48
13:M:81:LEU:O	13:M:86:CYS:HB3	2.13	0.48
1:A:1279:A:H5"	1:A:1280:A:OP1	2.13	0.48
9:I:5:TYR:CE1	9:I:16:ARG:HG2	2.48	0.48
1:A:1061:G:C6	1:A:1062:U:N3	2.80	0.48
1:A:518:C:H2'	1:A:530:G:N3	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1137:C:H4'	1:A:1138:G:C2	2.47	0.48
1:A:1163:C:H2'	1:A:1164:G:H8	1.78	0.48
13:M:23:TYR:HB2	13:M:67:GLU:OE2	2.13	0.48
1:A:670:G:OP2	24:A:1613:PAR:N24	2.45	0.48
1:A:932:C:H5	7:G:3:ARG:NH1	2.11	0.48
1:A:511:C:O3'	4:D:43:HIS:NE2	2.45	0.48
1:A:1264:C:H2'	1:A:1265:G:H8	1.78	0.48
10:J:6:ILE:CD1	10:J:72:VAL:HB	2.43	0.48
10:J:54:PHE:CD2	10:J:55:LYS:HG2	2.45	0.48
4:D:120:LEU:HD23	4:D:125:HIS:CD2	2.48	0.48
1:A:1288:A:C6	1:A:1289:A:C5	3.02	0.48
1:A:247:G:OP2	17:Q:100:LYS:HB2	2.12	0.48
15:O:29:VAL:HG11	15:O:67:LEU:HD21	1.95	0.48
1:A:708:C:H6	1:A:708:C:O5'	1.96	0.48
20:T:29:LYS:O	20:T:32:ALA:HB3	2.13	0.48
1:A:574:A:N3	1:A:883:C:H1'	2.29	0.48
12:L:117:ARG:O	12:L:120:TYR:N	2.47	0.48
1:A:1054:C:N3	23:W:34:G:O4'	2.46	0.48
1:A:1128:C:N3	1:A:1144:G:N2	2.61	0.48
1:A:811:C:H4'	1:A:900:A:H62	1.78	0.48
4:D:58:LEU:HD22	4:D:62:GLN:HG2	1.96	0.48
3:C:138:VAL:HG23	3:C:151:VAL:HG23	1.95	0.48
19:S:44:MET:O	19:S:47:HIS:HB2	2.12	0.48
1:A:956:U:C2	1:A:1225:A:C2	3.01	0.48
17:Q:9:VAL:HG21	17:Q:84:LEU:HD12	1.95	0.48
13:M:57:ARG:HG3	13:M:61:GLU:HG3	1.95	0.48
15:O:32:LEU:HD22	15:O:32:LEU:HA	1.73	0.48
1:A:1158:C:O2	1:A:1181:G:N2	2.34	0.48
1:A:929:G:H1	1:A:1388:C:N4	2.11	0.48
18:R:53:ARG:NH1	18:R:60:ALA:HA	2.29	0.48
23:W:37:A:H2'	23:W:38:A:O4'	2.14	0.48
8:H:28:ALA:HA	8:H:59:LEU:CD1	2.44	0.48
1:A:989:C:H42	1:A:1216:G:H1	1.62	0.48
1:A:1054:C:HO2'	1:A:1055:A:P	2.37	0.48
1:A:1427:U:H2'	1:A:1428:A:C8	2.48	0.48
10:J:42:THR:HG23	10:J:67:THR:O	2.14	0.48
6:F:45:LEU:HD12	6:F:47:ARG:HH22	1.79	0.48
1:A:1126:U:C2	1:A:1127:G:C8	3.02	0.48
1:A:1401:G:N2	1:A:1402:4OC:H1'	2.28	0.48
1:A:1492:A:OP1	12:L:47:LYS:HA	2.12	0.48
1:A:1168:A:C6	1:A:1169:A:C6	3.01	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1410:G:H2'	1:A:1411:C:C6	2.49	0.48
1:A:157:G:C2	1:A:158:G:C8	3.02	0.48
15:O:87:ILE:O	15:O:88:ARG:HB2	2.13	0.48
1:A:340:U:C2	1:A:350:G:N2	2.82	0.48
20:T:43:LEU:HD13	20:T:51:GLU:HB3	1.96	0.48
14:N:2:ALA:HB1	14:N:7:ILE:HD11	1.94	0.48
1:A:1061:G:H2'	1:A:1062:U:O4'	2.13	0.48
1:A:966:M2G:HM13	1:A:967:5MC:C1'	2.37	0.48
1:A:592:G:N2	1:A:648:A:C4	2.81	0.48
2:B:70:PHE:O	2:B:92:TYR:HA	2.13	0.48
4:D:12:CYS:HA	4:D:19:LEU:CD2	2.44	0.48
13:M:74:VAL:O	13:M:77:ASN:HB2	2.14	0.48
1:A:925:G:H1	1:A:1391:U:H3	1.62	0.48
24:A:1613:PAR:H322	24:A:1613:PAR:H11	1.78	0.48
9:I:118:LYS:O	9:I:120:ARG:N	2.43	0.48
1:A:1007:C:H2'	1:A:1008:C:C6	2.49	0.48
12:L:27:LEU:HD13	12:L:64:TYR:HE1	1.78	0.48
1:A:1412:C:H2'	1:A:1413:A:C8	2.49	0.48
1:A:1287:A:C6	1:A:1288:A:C6	3.01	0.48
1:A:1351:U:O2'	1:A:1352:C:H5'	2.14	0.48
19:S:10:PHE:O	19:S:39:THR:OG1	2.19	0.48
1:A:1300:G:C6	1:A:1335:C:C5	3.01	0.48
1:A:1376:U:H2'	1:A:1377:A:C8	2.49	0.48
1:A:269:C:H2'	1:A:270:A:C8	2.49	0.48
19:S:63:THR:HG23	19:S:66:MET:SD	2.54	0.48
17:Q:66:SER:O	17:Q:70:ARG:NH1	2.46	0.47
11:K:24:SER:CB	11:K:26:ASN:H	2.26	0.47
1:A:410:G:OP2	4:D:25:ARG:HD2	2.14	0.47
2:B:73:THR:HG23	2:B:95:GLN:O	2.14	0.47
9:I:26:VAL:HG13	9:I:61:ALA:HB3	1.95	0.47
2:B:70:PHE:CE2	2:B:163:PHE:HD1	2.32	0.47
1:A:149:A:H2'	1:A:150:C:C6	2.49	0.47
1:A:16:A:C2'	1:A:17:U:H5'	2.44	0.47
1:A:285:G:O2'	1:A:286:G:H5'	2.14	0.47
1:A:1095:U:H5"	1:A:1109:C:O2	2.12	0.47
1:A:825:G:N2	8:H:11:THR:HG21	2.26	0.47
1:A:1158:C:H5"	1:A:1159:U:OP2	2.15	0.47
1:A:179:A:H2'	1:A:180:U:H6	1.76	0.47
1:A:707:C:H5"	11:K:20:TYR:CD2	2.49	0.47
4:D:175:SER:HB3	4:D:184:LYS:HB2	1.95	0.47
1:A:1074:G:C6	1:A:1075:C:C4	3.03	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:102:ARG:H	8:H:102:ARG:HD2	1.79	0.47
1:A:668:G:N2	1:A:738:C:O2	2.44	0.47
1:A:662:G:O6	24:A:1605:PAR:H62	2.14	0.47
1:A:740:U:H4'	15:O:42:HIS:CD2	2.48	0.47
10:J:51:ARG:HG2	14:N:45:ARG:NH1	2.28	0.47
1:A:426:G:H2'	1:A:427:U:C6	2.50	0.47
10:J:6:ILE:HB	10:J:72:VAL:CG2	2.44	0.47
1:A:665:A:N3	1:A:732:C:H2'	2.29	0.47
1:A:103:C:OP2	20:T:14:LYS:HD2	2.13	0.47
1:A:803:G:OP1	24:A:1615:PAR:O41	2.31	0.47
1:A:1071:C:H42	1:A:1104:G:H1	1.63	0.47
1:A:177:C:H2'	1:A:178:C:H6	1.79	0.47
1:A:728:A:H2'	1:A:729:A:O4'	2.14	0.47
1:A:1442:G:C5	1:A:1446:A:N6	2.83	0.47
1:A:1288:A:N3	1:A:1352:C:O2'	2.36	0.47
13:M:86:CYS:SG	13:M:87:TYR:N	2.88	0.47
1:A:1300:G:O2'	1:A:1301:U:P	2.71	0.47
13:M:79:LYS:HA	13:M:82:MET:HE2	1.96	0.47
8:H:119:LEU:HD12	8:H:124:ALA:HB2	1.96	0.47
10:J:5:ARG:HA	10:J:73:ASP:OD1	2.14	0.47
1:A:1391:U:H2'	1:A:1392:G:C8	2.49	0.47
1:A:1466:C:H2'	1:A:1467:G:O4'	2.15	0.47
1:A:558:G:H8	1:A:559:A:H2'	1.79	0.47
13:M:99:ARG:NH2	19:S:2:PRO:HG2	2.28	0.47
1:A:1122:U:O4	1:A:1123:A:N6	2.48	0.47
1:A:1002:G:C6	1:A:1003:G:C6	3.03	0.47
1:A:148:G:H2'	1:A:149:A:H8	1.79	0.47
1:A:620:C:C2	4:D:135:LEU:HD22	2.50	0.47
1:A:1191:A:H5"	3:C:4:LYS:HE2	1.95	0.47
1:A:1392:G:N2	1:A:1502:A:H8	2.11	0.47
1:A:1056:U:C5'	3:C:163:ALA:HB2	2.45	0.47
2:B:75:LYS:CA	2:B:78:GLN:HB2	2.43	0.47
7:G:54:THR:HG22	7:G:56:GLN:HB3	1.97	0.47
1:A:955:U:H1'	1:A:1227:A:H61	1.79	0.47
1:A:781:A:C8	1:A:802:A:C2	3.02	0.47
1:A:992:U:H4'	1:A:993:G:O5'	2.14	0.47
21:U:17:THR:O	21:U:22:ARG:NH1	2.44	0.47
13:M:4:ILE:HD11	13:M:56:LEU:HB3	1.97	0.47
11:K:120:ARG:HB3	11:K:120:ARG:HH11	1.79	0.47
1:A:1057:G:H5"	3:C:154:SER:HB2	1.97	0.47
24:A:1608:PAR:H531	24:A:1608:PAR:N21	2.24	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:19:SER:HA	10:J:22:LYS:HE3	1.97	0.47
1:A:974:A:H8	1:A:974:A:OP1	1.98	0.47
20:T:33:ILE:HD11	20:T:63:ILE:HA	1.97	0.47
14:N:24:CYS:HB3	14:N:28:GLY:N	2.29	0.47
1:A:1157:A:H4'	1:A:1158:C:O5'	2.15	0.47
1:A:1118:C:H1'	1:A:1179:A:C4	2.50	0.47
1:A:961:U:H2'	1:A:962:C:H5'	1.95	0.47
4:D:91:SER:HB3	4:D:191:ARG:HB2	1.96	0.47
1:A:506:G:C6	1:A:507:C:C4	3.03	0.47
15:O:12:ILE:HG12	15:O:31:LEU:HD11	1.97	0.47
1:A:738:C:H5"	6:F:69:GLU:HB3	1.97	0.47
10:J:91:PRO:HB2	10:J:94:VAL:HB	1.97	0.47
4:D:25:ARG:HA	4:D:28:SER:HB3	1.97	0.47
1:A:29:G:O2'	1:A:295:C:H4'	2.15	0.47
1:A:393:A:O2'	1:A:394:G:H5'	2.14	0.47
6:F:78:GLU:HA	6:F:81:ILE:HG12	1.97	0.47
9:I:32:ASP:HB3	9:I:35:GLU:HB2	1.97	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:1316:G:N2	1:A:1319:A:OP2	2.41	0.47
2:B:235:SER:O	2:B:238:LEU:HB2	2.13	0.47
1:A:1091:U:O2	1:A:1093:A:C8	2.67	0.47
2:B:54:THR:HG23	2:B:199:TYR:HB3	1.96	0.47
16:P:8:ARG:O	16:P:9:PHE:HD2	1.98	0.47
1:A:501:C:H2'	1:A:502:G:H8	1.80	0.47
1:A:1441:G:O2'	1:A:1460:A:N6	2.46	0.47
1:A:346:G:H2'	1:A:347:G:O4'	2.15	0.47
1:A:956:U:H2'	1:A:957:U:O4'	2.14	0.47
1:A:737:A:H2'	1:A:738:C:C6	2.50	0.46
1:A:1501:C:N4	1:A:1504:G:C2	2.83	0.46
1:A:432:A:C8	1:A:433:C:C6	3.03	0.46
4:D:25:ARG:O	4:D:25:ARG:HG2	2.15	0.46
6:F:10:LEU:CD1	6:F:59:TYR:HB3	2.42	0.46
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:943:U:H1'	9:I:124:GLN:HE22	1.80	0.46
13:M:45:VAL:HG13	13:M:48:LEU:HD12	1.96	0.46
6:F:50:TYR:CE1	18:R:77:GLY:HA2	2.51	0.46
1:A:310:G:OP2	16:P:27:LYS:HE2	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:745:C:H2'	1:A:746:A:C8	2.50	0.46
1:A:1015:A:C6	1:A:1016:A:C6	3.03	0.46
1:A:1009:G:N2	1:A:1020:U:O2	2.32	0.46
3:C:114:PRO:HA	3:C:185:GLY:HA3	1.97	0.46
1:A:101:A:O2'	1:A:102:G:H5'	2.16	0.46
1:A:585:G:H4'	12:L:8:ASN:OD1	2.16	0.46
1:A:668:G:O4'	15:O:49:ASP:HB2	2.16	0.46
1:A:1249:C:H2'	9:I:68:GLY:O	2.15	0.46
8:H:17:THR:HB	8:H:78:GLN:HE22	1.80	0.46
19:S:30:LEU:HB3	19:S:31:ILE:H	1.54	0.46
1:A:1103:C:H5"	2:B:98:LEU:HD13	1.96	0.46
1:A:1417:G:H8	1:A:1417:G:O5'	1.99	0.46
1:A:625:G:H4'	16:P:16:HIS:CD2	2.50	0.46
1:A:1309:G:C6	1:A:1329:A:C2	3.04	0.46
1:A:620:C:N1	4:D:135:LEU:HD13	2.30	0.46
1:A:297:G:N2	1:A:300:A:OP2	2.48	0.46
1:A:1298:C:H4'	1:A:1299:A:O4'	2.16	0.46
1:A:881:G:H2'	1:A:882:C:O4'	2.15	0.46
20:T:75:ASN:OD1	20:T:75:ASN:N	2.49	0.46
1:A:965:A:C2	1:A:969:A:C2	3.04	0.46
1:A:716:A:N7	24:A:1613:PAR:O41	2.47	0.46
1:A:1413:A:H2'	1:A:1414:U:O4'	2.16	0.46
13:M:106:ASN:HB3	13:M:107:ALA:H	1.50	0.46
1:A:1357:A:H61	1:A:1363:A:H2	1.63	0.46
1:A:1386:G:O2'	1:A:1387:G:H5'	2.15	0.46
1:A:266:G:H5"	1:A:267:C:C5	2.51	0.46
1:A:1226:C:H4'	19:S:80:TYR:CZ	2.50	0.46
1:A:222:U:H2'	1:A:223:U:C6	2.51	0.46
1:A:1053:G:N7	1:A:1200:C:H5"	2.30	0.46
1:A:1358:U:H5"	1:A:1359:C:OP2	2.16	0.46
1:A:234:C:H2'	1:A:235:C:C6	2.50	0.46
5:E:78:HIS:ND1	8:H:104:ARG:HD2	2.30	0.46
1:A:1503:A:H5'	1:A:1531:A:H1'	1.98	0.46
17:Q:36:ILE:HG12	17:Q:36:ILE:H	1.49	0.46
1:A:730:G:C5	1:A:731:G:H1'	2.51	0.46
1:A:583:A:N6	1:A:758:G:O2'	2.49	0.46
1:A:1069:C:O2'	1:A:1192:C:H1'	2.16	0.46
20:T:43:LEU:HB2	20:T:52:ALA:HB2	1.98	0.46
1:A:1230:C:H2'	1:A:1231:G:H8	1.79	0.46
17:Q:20:THR:HA	17:Q:43:LEU:HD23	1.98	0.46
1:A:1468:A:H2'	1:A:1469:G:O4'	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1149:C:H2'	1:A:1150:U:C6	2.46	0.46
9:I:53:VAL:CG2	9:I:85:LEU:HD21	2.43	0.46
1:A:646:U:H2'	1:A:647:C:C6	2.51	0.46
4:D:148:VAL:HG12	4:D:149:ALA:N	2.31	0.46
4:D:17:VAL:O	4:D:19:LEU:HD23	2.16	0.46
4:D:191:ARG:O	4:D:191:ARG:HD2	2.16	0.46
1:A:1081:G:P	5:E:16:THR:HG1	2.39	0.46
1:A:875:C:H1'	8:H:15:ASN:HD21	1.81	0.46
3:C:31:HIS:O	3:C:34:LEU:HD23	2.16	0.46
11:K:124:LYS:HE3	11:K:125:PHE:CE2	2.50	0.46
1:A:509:A:H3'	1:A:509:A:C8	2.51	0.46
1:A:1022:G:H2'	1:A:1023:G:C8	2.51	0.46
1:A:922:G:H4'	5:E:20:GLN:HA	1.97	0.46
11:K:80:VAL:HG11	11:K:103:LEU:HD13	1.97	0.46
10:J:14:LYS:HB3	10:J:14:LYS:HE2	1.67	0.46
1:A:426:G:H2'	1:A:427:U:H6	1.81	0.46
24:A:1603:PAR:H11	24:A:1603:PAR:O52	2.16	0.46
13:M:99:ARG:NH1	19:S:2:PRO:HG2	2.31	0.46
4:D:47:ARG:NE	4:D:48:ALA:H	2.12	0.46
1:A:1051:C:H2'	1:A:1052:U:C6	2.51	0.46
1:A:1055:A:C6	1:A:1206:G:C5	3.04	0.46
1:A:744:C:H2'	1:A:745:C:C6	2.51	0.46
21:U:5:ASP:O	21:U:11:GLY:HA3	2.15	0.46
13:M:67:GLU:HB3	13:M:68:GLY:H	1.51	0.46
4:D:12:CYS:HA	4:D:19:LEU:HD21	1.98	0.46
1:A:792:A:H4'	1:A:793:U:O5'	2.16	0.46
2:B:115:LEU:HD11	2:B:146:GLN:HG3	1.97	0.46
8:H:104:ARG:NE	8:H:138:TRP:CZ2	2.84	0.45
1:A:51:A:H4'	1:A:52:G:C5'	2.47	0.45
11:K:63:LEU:HD23	11:K:63:LEU:HA	1.62	0.45
1:A:1263:C:N4	1:A:1272:G:H1	2.11	0.45
1:A:1442:G:O6	1:A:1461:G:N2	2.50	0.45
1:A:598:U:H2'	1:A:599:C:H6	1.80	0.45
7:G:140:ASP:HA	7:G:143:ARG:NH2	2.31	0.45
15:O:33:THR:HG23	15:O:63:ARG:HH12	1.81	0.45
13:M:37:THR:HG22	13:M:55:ARG:NH1	2.31	0.45
1:A:1113:C:O2'	1:A:1114:C:H5'	2.16	0.45
1:A:1057:G:C5	1:A:1204:A:C2	3.04	0.45
15:O:39:LEU:O	15:O:43:LEU:HG	2.16	0.45
1:A:1127:G:H1	1:A:1145:C:H42	1.62	0.45
9:I:9:ARG:HG3	9:I:14:VAL:HG13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:15:PRO:CD	16:P:42:ARG:HD3	2.44	0.45
18:R:38:GLU:O	18:R:42:ARG:HG2	2.17	0.45
1:A:200:G:H2'	1:A:201:C:O4'	2.16	0.45
3:C:116:VAL:O	3:C:119:ARG:HB3	2.17	0.45
13:M:64:TRP:HE3	13:M:66:LEU:HD21	1.81	0.45
4:D:98:GLU:HG2	4:D:189:PRO:HG3	1.98	0.45
12:L:69:TYR:CE2	12:L:71:PRO:HA	2.51	0.45
1:A:241:C:H42	1:A:285:G:H1	1.65	0.45
1:A:786:G:C2	1:A:797:C:C2	3.04	0.45
2:B:101:MET:HA	2:B:108:ILE:HG21	1.98	0.45
9:I:125:TYR:HE1	9:I:127:LYS:HB2	1.81	0.45
1:A:820:U:H4'	1:A:821:G:OP2	2.16	0.45
4:D:127:THR:OG1	4:D:127:THR:O	2.29	0.45
1:A:131:C:OP1	1:A:190(F):G:N2	2.46	0.45
1:A:231:G:N7	24:A:1612:PAR:H612	2.31	0.45
1:A:778:G:H1'	11:K:119:CYS:HB3	1.98	0.45
17:Q:83:ASP:O	17:Q:86:GLU:HB2	2.16	0.45
4:D:9:CYS:HA	4:D:12:CYS:HB2	1.98	0.45
1:A:781:A:H2	1:A:1514:C:O4'	1.99	0.45
1:A:1226:C:H2'	13:M:103:THR:OG1	2.16	0.45
2:B:83:MET:HA	2:B:86:GLU:HB2	1.97	0.45
7:G:54:THR:C	7:G:56:GLN:H	2.20	0.45
7:G:52:GLU:HG2	7:G:53:LYS:NZ	2.32	0.45
1:A:791:G:H2'	1:A:792:A:H5'	1.98	0.45
6:F:23:LYS:HD2	6:F:42:GLU:OE1	2.16	0.45
4:D:92:VAL:O	4:D:96:LEU:HD13	2.16	0.45
1:A:1305:G:H22	1:A:1331:G:H2'	1.81	0.45
1:A:1001:A:H2'	1:A:1002:G:C8	2.52	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
2:B:184:VAL:N	2:B:198:ASP:OD2	2.36	0.45
1:A:1330:U:O4	1:A:1331:G:N1	2.50	0.45
1:A:391:G:C6	1:A:392:G:C5	3.04	0.45
19:S:58:VAL:HG21	19:S:75:ALA:HB2	1.98	0.45
18:R:53:ARG:HG3	18:R:53:ARG:NH1	2.32	0.45
1:A:1216:G:H5"	14:N:5:ALA:HB2	1.98	0.45
1:A:1161:C:H2'	1:A:1162:C:H6	1.82	0.45
1:A:899:C:H2'	1:A:900:A:O4'	2.17	0.45
16:P:73:LEU:HA	16:P:73:LEU:HD23	1.73	0.45
3:C:34:LEU:HB2	14:N:25:VAL:HG21	1.98	0.45
1:A:567:G:H2'	1:A:568:G:O4'	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:108:LEU:HA	4:D:108:LEU:HD23	1.79	0.45
24:A:1613:PAR:H23	24:A:1613:PAR:H52	1.65	0.45
1:A:27:G:N2	1:A:557:G:H1'	2.32	0.45
24:A:1610:PAR:N21	24:A:1610:PAR:O43	2.50	0.45
9:I:24:GLY:O	9:I:26:VAL:HG23	2.17	0.45
1:A:375:U:H4'	16:P:17:TYR:CE2	2.51	0.45
1:A:358:U:H2'	1:A:359:U:C6	2.52	0.45
20:T:50:GLU:HB2	20:T:99:LEU:HD22	1.99	0.45
1:A:740:U:O3'	15:O:39:LEU:HD23	2.17	0.45
5:E:80:ILE:HA	8:H:104:ARG:NH2	2.31	0.45
1:A:1148:U:C5	1:A:1149:C:C4	3.04	0.45
1:A:1148:U:H2'	1:A:1149:C:O4'	2.16	0.45
1:A:1283:G:H2'	1:A:1284:C:C6	2.51	0.45
1:A:474:G:H5"	16:P:81:ARG:CZ	2.47	0.45
1:A:129(A):G:C2	1:A:190(E):U:H5"	2.52	0.45
1:A:148:G:H2'	1:A:149:A:C8	2.52	0.45
1:A:1254:C:H41	10:J:43:ARG:HH21	1.64	0.45
1:A:165:C:C2	1:A:166:G:C8	3.05	0.45
5:E:8:GLU:OE1	5:E:63:ARG:NH2	2.49	0.45
2:B:28:PHE:CD2	2:B:190:THR:HA	2.52	0.45
2:B:30:ARG:HG3	2:B:31:TYR:CD2	2.52	0.45
1:A:527:7MG:H5"	1:A:527:7MG:H81	1.98	0.45
4:D:57:ARG:HD3	4:D:202:LEU:HD22	1.98	0.45
1:A:1189:C:P	10:J:51:ARG:HH22	2.40	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
6:F:95:GLU:CG	6:F:96:PRO:HD2	2.47	0.45
3:C:188:LEU:HD21	3:C:195:VAL:HG13	1.98	0.45
1:A:1172:C:H2'	1:A:1173:G:H8	1.81	0.45
1:A:1049:U:H4'	1:A:1050:G:O5'	2.16	0.45
10:J:4:ILE:O	10:J:73:ASP:HA	2.17	0.45
1:A:542:G:H5'	4:D:41:GLY:HA3	1.98	0.45
8:H:36:LEU:HA	8:H:36:LEU:HD23	1.79	0.45
1:A:1347:G:N2	1:A:1374:A:OP2	2.33	0.45
1:A:500:G:H2'	1:A:501:C:C6	2.52	0.45
14:N:23:ARG:NH1	14:N:28:GLY:O	2.50	0.45
1:A:390:C:H6	1:A:390:C:O5'	1.99	0.45
14:N:9:LYS:HE3	14:N:21:TYR:O	2.17	0.45
4:D:63:LYS:O	4:D:67:ILE:HD12	2.17	0.45
3:C:50:ALA:O	3:C:70:VAL:HG12	2.15	0.45
1:A:701:C:H5"	1:A:703:G:O4'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:952:U:O2'	1:A:953:G:H5'	2.17	0.45
13:M:108:ARG:NH2	13:M:114:ARG:HA	2.32	0.45
1:A:373:A:H1'	1:A:481:G:N3	2.32	0.44
12:L:27:LEU:O	12:L:29:GLY:N	2.50	0.44
21:U:10:ARG:O	21:U:13:ILE:HG13	2.17	0.44
17:Q:59:ILE:HA	17:Q:59:ILE:HD12	1.55	0.44
4:D:150:GLU:HA	4:D:153:ARG:NH2	2.32	0.44
3:C:186:PHE:HD1	3:C:198:VAL:O	2.00	0.44
1:A:1251:A:H2'	1:A:1252:A:O4'	2.17	0.44
1:A:628:G:H2'	1:A:629:G:H8	1.82	0.44
5:E:118:ILE:HG12	5:E:119:LEU:N	2.32	0.44
1:A:496:A:C2	1:A:497:A:C4	3.05	0.44
4:D:94:LEU:HD23	4:D:94:LEU:HA	1.75	0.44
18:R:55:ARG:HB3	18:R:55:ARG:HH11	1.82	0.44
1:A:1321:C:C5	1:A:1322:C:C2	3.04	0.44
4:D:173:TRP:CD2	4:D:189:PRO:HB3	2.52	0.44
4:D:98:GLU:OE2	4:D:103:ASN:ND2	2.44	0.44
17:Q:100:LYS:HG2	17:Q:101:ARG:HH21	1.80	0.44
1:A:1375:A:C2	1:A:1376:U:C2	3.05	0.44
16:P:39:TYR:CD2	16:P:73:LEU:HD11	2.52	0.44
1:A:1333:A:H2'	1:A:1334:G:O4'	2.18	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:1276:G:H8	1:A:1276:G:O5'	2.00	0.44
16:P:9:PHE:HE1	16:P:18:ARG:CZ	2.30	0.44
1:A:1030(A):G:N2	1:A:1031:G:O6	2.50	0.44
2:B:154:LEU:HA	2:B:154:LEU:HD23	1.73	0.44
1:A:312:C:H2'	1:A:313:A:C8	2.53	0.44
1:A:624:C:H2'	1:A:625:G:C8	2.52	0.44
2:B:97:TRP:HZ3	2:B:176:GLU:OE2	2.01	0.44
1:A:1127:G:N2	1:A:1145:C:C2	2.86	0.44
1:A:1402:4OC:HM41	1:A:1498:UR3:H3U3	1.99	0.44
1:A:518:C:H2'	1:A:530:G:C2	2.52	0.44
4:D:36:ARG:HB3	4:D:38:TYR:CE2	2.52	0.44
1:A:1284:C:H3'	1:A:1285:A:C8	2.45	0.44
1:A:949:A:H1'	1:A:1364:U:N3	2.32	0.44
1:A:284:G:H2'	1:A:285:G:H8	1.82	0.44
1:A:945:G:C2	1:A:1337:G:C2	3.06	0.44
10:J:60:ARG:H	10:J:60:ARG:HG2	1.40	0.44
15:O:26:GLU:HA	15:O:81:LEU:HD13	1.99	0.44
1:A:1242:C:H2'	1:A:1243:C:C6	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:76:LEU:HD12	17:Q:77:VAL:N	2.33	0.44
5:E:102:ALA:HA	5:E:120:THR:OG1	2.18	0.44
1:A:1357:A:C5	1:A:1358:U:C4	3.06	0.44
1:A:1371:G:O3'	9:I:69:GLY:HA3	2.17	0.44
5:E:135:THR:O	5:E:138:ALA:HB3	2.18	0.44
8:H:104:ARG:HG3	8:H:138:TRP:CD2	2.53	0.44
1:A:1503:A:OP1	1:A:1531:A:O2'	2.33	0.44
7:G:56:GLN:HG2	7:G:57:GLU:H	1.81	0.44
5:E:15:ARG:HD3	5:E:28:PHE:HE2	1.83	0.44
1:A:1054:C:H42	23:W:34:G:C1'	2.30	0.44
1:A:1425:U:H3	1:A:1475:G:H1	1.65	0.44
1:A:243:A:H4'	1:A:244:U:O5'	2.18	0.44
6:F:56:PRO:HG2	6:F:57:GLN:HG3	1.98	0.44
1:A:671:G:H2'	1:A:672:U:O4'	2.17	0.44
1:A:976:G:N7	1:A:1358:U:C2	2.86	0.44
1:A:625:G:H4'	16:P:16:HIS:CG	2.53	0.44
5:E:78:HIS:HE2	5:E:143:ARG:H	1.65	0.44
1:A:413:G:H21	1:A:428:G:H1'	1.83	0.44
10:J:66:ARG:HD3	10:J:68:HIS:CE1	2.53	0.44
6:F:68:PRO:HB2	6:F:70:ASP:OD1	2.18	0.44
7:G:53:LYS:HD3	7:G:53:LYS:HA	1.78	0.44
1:A:116:A:OP1	27:A:2017:HOH:O	2.21	0.44
1:A:1046:A:H3'	1:A:1047:G:H8	1.83	0.44
16:P:10:GLY:H	16:P:16:HIS:H	1.65	0.44
8:H:82:HIS:ND1	8:H:138:TRP:CD1	2.83	0.44
1:A:1039:C:H2'	1:A:1040:U:C6	2.53	0.44
1:A:530:G:O2'	23:W:35:A:H4'	2.17	0.44
20:T:64:ASP:O	20:T:67:ALA:HB3	2.17	0.44
1:A:1236:A:O2'	1:A:1304:G:H4'	2.18	0.44
1:A:1256:A:C2	1:A:1277:C:N4	2.86	0.44
3:C:6:HIS:CD2	3:C:9:GLY:H	2.35	0.44
1:A:751:U:H4'	15:O:24:SER:HA	1.99	0.44
2:B:55:PHE:HD2	2:B:221:LEU:HD12	1.81	0.44
1:A:1103:C:H2'	1:A:1104:G:O4'	2.18	0.44
12:L:10:LEU:HD23	12:L:14:GLY:HA2	2.00	0.44
10:J:87:THR:O	10:J:88:LEU:HD23	2.17	0.44
1:A:1440:C:C2	1:A:1462:G:C2	3.06	0.44
17:Q:68:ARG:NH1	17:Q:68:ARG:HB3	2.32	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
8:H:6:ILE:HG21	8:H:85:ARG:HH21	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1509:C:H2'	1:A:1510:U:O4'	2.17	0.44
21:U:10:ARG:HA	21:U:13:ILE:HD11	2.00	0.44
15:O:26:GLU:HA	15:O:81:LEU:CD1	2.48	0.44
1:A:1009:G:H1'	1:A:1021:G:H22	1.83	0.44
1:A:358:U:O2'	1:A:359:U:H5'	2.18	0.44
1:A:1132:C:H42	1:A:1142:G:H1	1.66	0.44
3:C:35:GLU:OE2	3:C:59:ARG:NH2	2.29	0.44
12:L:111:LYS:HA	12:L:111:LYS:NZ	2.33	0.44
16:P:40:ASP:OD1	16:P:44:THR:HG23	2.17	0.44
1:A:1049:U:H4'	1:A:1050:G:H5'	2.00	0.43
1:A:372:C:H1'	1:A:373:A:OP2	2.18	0.43
1:A:321:A:H62	1:A:328:C:H1'	1.83	0.43
7:G:149:ARG:HB3	11:K:59:TYR:HE1	1.83	0.43
5:E:15:ARG:HD2	5:E:26:PHE:CD2	2.53	0.43
1:A:129:U:O3'	1:A:129(A):G:H3'	2.17	0.43
1:A:439:A:C4	1:A:497:A:C2	3.06	0.43
8:H:91:ARG:NH1	17:Q:33:GLY:HA3	2.32	0.43
19:S:51:VAL:HG21	19:S:71:LEU:HB3	1.99	0.43
1:A:1507:A:C2	1:A:1508:G:C4	3.05	0.43
10:J:57:LYS:HG2	10:J:58:ASP:OD1	2.18	0.43
1:A:558:G:H3'	1:A:559:A:H3'	1.99	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:1516:G:H2'	1:A:1518:MA6:OP2	2.18	0.43
7:G:50:ILE:CD1	7:G:125:MET:HG3	2.48	0.43
1:A:1361(A):C:H2'	1:A:1362:C:H5"	2.00	0.43
6:F:74:ASP:O	6:F:77:ARG:HB3	2.19	0.43
1:A:1329:A:H62	21:U:7:ARG:HH21	1.65	0.43
2:B:97:TRP:CZ3	2:B:176:GLU:OE2	2.71	0.43
1:A:926:G:H3'	1:A:1505:G:H21	1.84	0.43
8:H:85:ARG:HD3	8:H:87:SER:O	2.17	0.43
24:A:1602:PAR:H51	24:A:1602:PAR:H322	1.82	0.43
10:J:6:ILE:HG23	10:J:98:ILE:HG12	1.99	0.43
2:B:48:MET:O	2:B:51:LEU:HB2	2.19	0.43
1:A:1055:A:C8	1:A:1206:G:C2	3.06	0.43
1:A:1421:G:C6	1:A:1480:G:N1	2.86	0.43
1:A:157:G:H2'	1:A:158:G:H8	1.83	0.43
23:W:39:U:H2'	23:W:40:C:C6	2.54	0.43
1:A:885:G:O2'	1:A:914:A:N1	2.43	0.43
6:F:61:LEU:HB2	6:F:63:TYR:CE2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:938:A:N6	1:A:939:G:C6	2.86	0.43
1:A:88:A:H2'	1:A:89:C:O4'	2.18	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
3:C:43:LEU:HD22	3:C:43:LEU:HA	1.66	0.43
1:A:266:G:H8	1:A:266:G:H2'	1.58	0.43
3:C:81:GLY:O	3:C:84:ILE:HG22	2.18	0.43
4:D:114:ARG:HG3	4:D:114:ARG:HH11	1.83	0.43
1:A:975:A:C5'	1:A:975:A:C8	3.01	0.43
1:A:1399:C:C2	1:A:1401:G:C5	3.07	0.43
1:A:382:A:C2	1:A:383:A:C4	3.06	0.43
5:E:144:THR:HG22	5:E:145:LYS:H	1.84	0.43
1:A:1526:G:O2'	1:A:1527:C:H5'	2.19	0.43
1:A:218:C:O5'	1:A:218:C:H6	2.01	0.43
1:A:345:C:OP2	1:A:345:C:H6	2.02	0.43
2:B:7:VAL:H	2:B:9:GLU:HG3	1.84	0.43
4:D:173:TRP:HB2	4:D:187:ARG:O	2.18	0.43
1:A:1376:U:H2'	1:A:1377:A:H8	1.83	0.43
1:A:575:G:C5	1:A:881:G:C2	3.06	0.43
1:A:690:G:C6	1:A:691:G:C6	3.07	0.43
3:C:77:ILE:O	3:C:81:GLY:HA2	2.19	0.43
11:K:126:ARG:HB3	11:K:127:LYS:H	1.56	0.43
1:A:190(C):C:C5	1:A:190(D):U:C5	3.07	0.43
10:J:49:VAL:HG13	10:J:61:GLU:HB3	2.01	0.43
12:L:110:VAL:HG23	12:L:120:TYR:HB3	2.01	0.43
1:A:1331:G:O2'	1:A:1332:A:O5'	2.37	0.43
1:A:476:G:C2	1:A:477:G:C4	3.07	0.43
1:A:581:G:H4'	15:O:64:ARG:HH22	1.83	0.43
2:B:112:VAL:HG21	2:B:153:ARG:HA	2.00	0.43
5:E:82:VAL:HG21	5:E:138:ALA:CA	2.41	0.43
1:A:329:A:H4'	1:A:330:C:OP2	2.18	0.43
1:A:1116:C:O2'	9:I:108:VAL:HG21	2.18	0.43
1:A:216:G:O2'	1:A:217:C:O5'	2.36	0.43
1:A:892:A:O2'	1:A:1415:G:H4'	2.19	0.43
1:A:35:G:H2'	1:A:36:C:C6	2.54	0.43
12:L:35:GLY:HA3	12:L:60:LEU:HD13	1.99	0.43
1:A:200:G:N2	1:A:218:C:C2	2.87	0.43
15:O:58:MET:HE2	15:O:58:MET:HB2	1.76	0.43
1:A:1070:U:O2'	1:A:1071:C:H5'	2.18	0.43
8:H:121:ASP:HB2	8:H:125:ARG:NH2	2.34	0.43
1:A:620:C:H2'	1:A:621:A:O4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1134:G:N2	1:A:1140:C:O2	2.49	0.43
1:A:309:G:H1'	1:A:608:A:C2	2.54	0.43
1:A:812:C:O2'	1:A:813:U:OP2	2.24	0.43
8:H:111:ILE:O	8:H:134:ILE:HB	2.18	0.43
16:P:60:LEU:HD23	16:P:60:LEU:HA	1.67	0.43
1:A:255:G:H2'	1:A:256:U:C6	2.53	0.43
1:A:255:G:C2	1:A:272:C:C2	3.07	0.43
17:Q:69:LYS:HB3	17:Q:69:LYS:HE2	1.69	0.43
1:A:1404:5MC:O4'	1:A:1499:A:C2	2.71	0.43
18:R:17:SER:O	18:R:17:SER:OG	2.32	0.43
1:A:1475:G:H2'	1:A:1476:G:C8	2.53	0.43
9:I:121:ARG:NH1	9:I:121:ARG:HG2	2.34	0.43
1:A:768:A:H5'	1:A:1524:C:H1'	2.01	0.43
3:C:73:PRO:O	3:C:77:ILE:HG12	2.18	0.43
12:L:19:ARG:HG3	12:L:19:ARG:H	1.57	0.43
17:Q:65:ILE:H	17:Q:65:ILE:HD12	1.84	0.43
1:A:1018:C:H6	1:A:1018:C:O5'	2.01	0.43
10:J:63:PHE:HA	14:N:59:ALA:H	1.84	0.43
1:A:409:G:H1	1:A:433:C:H42	1.65	0.43
24:A:1601:PAR:H11	24:A:1601:PAR:O52	2.19	0.43
4:D:70:ILE:HD11	4:D:100:ARG:CZ	2.49	0.43
4:D:15:GLU:OE2	4:D:59:ARG:NE	2.49	0.43
1:A:800:G:H2'	1:A:801:U:C6	2.54	0.43
15:O:21:ASP:OD2	15:O:24:SER:HB3	2.19	0.43
2:B:135:GLN:O	2:B:139:LYS:HB2	2.19	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
1:A:75:G:C6	1:A:96:G:C6	3.07	0.43
1:A:399:G:H2'	1:A:400:C:C6	2.53	0.43
17:Q:22:LEU:HA	17:Q:22:LEU:HD12	1.56	0.43
5:E:123:LEU:HD23	5:E:123:LEU:HA	1.67	0.43
3:C:11:ARG:CD	3:C:180:ALA:HB3	2.43	0.42
15:O:36:ILE:HD13	15:O:60:VAL:HG22	2.00	0.42
1:A:1038:C:H2'	1:A:1039:C:C6	2.53	0.42
15:O:70:LEU:HD22	15:O:78:TYR:N	2.33	0.42
1:A:771:G:N2	1:A:808:C:O2	2.44	0.42
2:B:181:PHE:HD2	8:H:70:GLN:HB2	1.83	0.42
2:B:238:LEU:C	2:B:240:GLN:N	2.72	0.42
13:M:91:ARG:HH22	13:M:103:THR:HG21	1.84	0.42
2:B:24:TRP:HB2	2:B:190:THR:HG22	2.01	0.42
17:Q:78:GLU:OE1	17:Q:81:ARG:HD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:965:A:H4'	1:A:966:M2G:OP2	2.19	0.42
1:A:1127:G:H4'	1:A:1148:U:O2	2.18	0.42
1:A:1526:G:C2'	1:A:1527:C:H5'	2.50	0.42
10:J:6:ILE:HB	10:J:72:VAL:HB	2.02	0.42
15:O:17:ARG:HD3	15:O:77:ARG:HH11	1.83	0.42
16:P:58:TYR:CD1	16:P:58:TYR:C	2.91	0.42
1:A:22:G:O2'	1:A:23:C:H5'	2.18	0.42
1:A:1230:C:H2'	1:A:1231:G:C8	2.54	0.42
1:A:337:C:H2'	1:A:338:A:C8	2.54	0.42
12:L:68:ALA:HB1	12:L:100:ILE:HG13	2.01	0.42
7:G:99:LEU:HA	7:G:99:LEU:HD23	1.87	0.42
9:I:100:GLY:O	9:I:102:LEU:HD12	2.18	0.42
5:E:89:ILE:HG21	5:E:135:THR:HA	2.01	0.42
1:A:1505:G:H3'	1:A:1505:G:C8	2.53	0.42
1:A:328:C:O2	1:A:328:C:H2'	2.19	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
19:S:75:ALA:HA	19:S:76:PRO:HD2	1.83	0.42
7:G:54:THR:HG22	7:G:56:GLN:CB	2.50	0.42
17:Q:90:ILE:O	17:Q:93:GLN:N	2.51	0.42
4:D:133:VAL:HG12	4:D:135:LEU:H	1.85	0.42
16:P:6:LEU:HD23	16:P:17:TYR:CB	2.49	0.42
3:C:69:HIS:CE1	3:C:104:GLN:HB3	2.55	0.42
1:A:1397:C:H4'	1:A:1398:A:OP2	2.17	0.42
13:M:65:LYS:HE3	13:M:65:LYS:HB2	1.84	0.42
1:A:982:U:H4'	1:A:983:A:O5'	2.19	0.42
16:P:9:PHE:N	16:P:16:HIS:O	2.51	0.42
1:A:1309:G:N2	1:A:1329:A:H1'	2.34	0.42
1:A:1030:C:H42	1:A:1031:G:H1	1.67	0.42
1:A:872:A:N3	1:A:872:A:H2'	2.35	0.42
1:A:147:G:C2	1:A:148:G:C8	3.08	0.42
1:A:252:U:C4	1:A:253:U:O4	2.72	0.42
4:D:88:VAL:HG12	4:D:90:GLY:H	1.84	0.42
1:A:913:A:OP1	12:L:91:LYS:HE3	2.19	0.42
2:B:167:PRO:O	2:B:171:ALA:HB2	2.18	0.42
16:P:74:LEU:HA	16:P:74:LEU:HD23	1.78	0.42
1:A:106:C:H2'	1:A:107:G:H8	1.84	0.42
1:A:424:G:H2'	1:A:425:G:H8	1.85	0.42
1:A:239:U:O4	24:A:1603:PAR:H642	2.20	0.42
1:A:344:A:H4'	1:A:345:C:OP2	2.20	0.42
2:B:82:ARG:HB3	2:B:94:ASN:HD21	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:688:G:H5'	11:K:46:GLY:C	2.40	0.42
1:A:707:C:H2'	1:A:708:C:C6	2.54	0.42
1:A:285:G:C2	1:A:286:G:C8	3.08	0.42
5:E:92:LYS:O	5:E:119:LEU:HB2	2.19	0.42
8:H:91:ARG:NH1	17:Q:32:TYR:O	2.52	0.42
10:J:7:LYS:HG3	10:J:71:LEU:HD21	2.01	0.42
1:A:1422:G:N2	1:A:1479:C:C2	2.87	0.42
9:I:36:TYR:HD2	9:I:37:PHE:CE2	2.36	0.42
1:A:403:C:O2'	1:A:404:U:H5'	2.19	0.42
9:I:69:GLY:O	9:I:73:GLN:HG3	2.19	0.42
1:A:254:G:H2'	1:A:255:G:H8	1.83	0.42
8:H:81:HIS:HB2	8:H:138:TRP:O	2.20	0.42
1:A:1399:C:C2	1:A:1502:A:N6	2.87	0.42
1:A:1460:A:H2'	1:A:1461:G:O4'	2.20	0.42
17:Q:100:LYS:HB3	17:Q:101:ARG:HE	1.84	0.42
6:F:23:LYS:HE2	6:F:23:LYS:HB3	1.78	0.42
6:F:61:LEU:HD12	6:F:63:TYR:HE2	1.83	0.42
1:A:1077:G:N2	1:A:1079:G:H3'	2.34	0.42
18:R:46:GLU:CD	18:R:46:GLU:H	2.23	0.42
1:A:1200:C:H1'	1:A:1204:A:H62	1.85	0.42
1:A:414:A:H2'	1:A:415:A:O4'	2.20	0.42
19:S:52:TYR:HA	19:S:56:GLN:O	2.20	0.42
4:D:57:ARG:CG	4:D:57:ARG:HH11	2.29	0.42
16:P:42:ARG:H	16:P:42:ARG:HG2	1.44	0.42
8:H:83:ILE:HG21	8:H:83:ILE:HD13	1.73	0.42
1:A:430:A:P	4:D:8:VAL:H	2.41	0.42
2:B:223:ILE:HD12	2:B:224:GLN:N	2.34	0.42
2:B:7:VAL:HG13	2:B:48:MET:SD	2.59	0.42
1:A:397:A:C6	1:A:548:G:N7	2.88	0.42
20:T:43:LEU:CD1	20:T:51:GLU:HB3	2.49	0.42
1:A:1035:A:H2'	1:A:1036:G:H8	1.83	0.42
1:A:653:A:OP1	8:H:56:LYS:HE2	2.19	0.42
3:C:58:GLU:HB3	10:J:92:THR:CG2	2.42	0.42
3:C:58:GLU:H	3:C:65:ALA:HB3	1.84	0.42
17:Q:66:SER:HB3	17:Q:69:LYS:CG	2.41	0.42
1:A:1402:4OC:O2	1:A:1500:A:N1	2.52	0.42
1:A:503:C:H6	1:A:503:C:O5'	2.03	0.42
1:A:593:G:H1	1:A:646:U:H3	1.68	0.42
3:C:6:HIS:HA	3:C:7:PRO:HD2	1.71	0.42
1:A:778:G:H2'	1:A:779:C:O4'	2.20	0.42
1:A:1300:G:O2'	1:A:1301:U:O5'	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1417:G:HO2'	1:A:1418:A:H8	1.64	0.42
14:N:40:CYS:O	14:N:44:LEU:HB3	2.19	0.42
14:N:26:ARG:NH1	14:N:47:LEU:HD21	2.34	0.42
12:L:127:GLU:HB2	12:L:128:ALA:H	1.63	0.42
1:A:190(L):U:O2	20:T:105:SER:HB2	2.20	0.42
8:H:27:PRO:HA	8:H:58:TYR:CD2	2.54	0.42
1:A:587:G:O2'	1:A:588:G:OP2	2.30	0.42
5:E:131:ILE:HD13	5:E:131:ILE:HA	1.78	0.42
12:L:49:ASN:ND2	12:L:92:0TD:OD2	2.48	0.42
12:L:60:LEU:HB3	12:L:62:SER:H	1.85	0.42
16:P:45:THR:HG22	16:P:46:PRO:HD2	2.01	0.42
1:A:1054:C:OP1	1:A:1197:G:OP2	2.37	0.42
1:A:1161:C:H2'	1:A:1162:C:C6	2.55	0.42
1:A:859:A:H2'	1:A:860:A:O4'	2.20	0.42
13:M:91:ARG:HD2	13:M:91:ARG:HA	1.75	0.42
1:A:691:G:O2'	1:A:797:C:H4'	2.19	0.42
10:J:49:VAL:CG2	14:N:41:ARG:HB2	2.50	0.42
1:A:192:U:C2	1:A:193:C:C6	3.08	0.42
1:A:410:G:OP1	4:D:30:LYS:NZ	2.53	0.42
1:A:989:C:O2'	1:A:1017:G:O2'	2.21	0.42
14:N:11:LYS:O	14:N:14:PRO:HD3	2.20	0.42
1:A:1375:A:N1	1:A:1376:U:C2	2.88	0.42
1:A:367:U:C6	1:A:394:G:N2	2.88	0.42
2:B:14:GLY:O	2:B:17:PHE:HB2	2.20	0.42
13:M:3:ARG:NH2	13:M:7:VAL:HG12	2.35	0.42
1:A:117:G:O5'	1:A:117:G:H8	2.03	0.42
1:A:431:A:O2'	1:A:432:A:H5'	2.20	0.41
1:A:1348:U:O3'	9:I:120:ARG:HG3	2.19	0.41
1:A:560:U:H4'	1:A:561:U:H5"	2.01	0.41
2:B:217:ARG:O	2:B:220:ASP:HB2	2.19	0.41
1:A:157:G:N3	1:A:158:G:C8	2.88	0.41
1:A:1334:G:O5'	1:A:1334:G:H8	2.03	0.41
1:A:837:G:N2	1:A:850:U:O2	2.53	0.41
10:J:52:GLY:HA2	10:J:53:PRO:HD3	1.68	0.41
2:B:119:GLU:HG3	2:B:142:LEU:HD21	2.02	0.41
1:A:1217:C:H2'	1:A:1218:C:O4'	2.20	0.41
1:A:122:G:C2	1:A:123:C:C2	3.08	0.41
1:A:306:G:O2'	1:A:307:C:H5'	2.20	0.41
1:A:1105:A:H2'	1:A:1106:G:C8	2.54	0.41
4:D:162:LEU:HA	4:D:162:LEU:HD23	1.74	0.41
1:A:1281:U:O2'	1:A:1282:C:OP1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1320:C:O2'	1:A:1321:C:H5'	2.19	0.41
3:C:43:LEU:HD13	3:C:47:LEU:HD22	2.01	0.41
3:C:14:ILE:CG2	3:C:15:THR:HG23	2.51	0.41
1:A:129(A):G:N3	1:A:190(E):U:H5"	2.34	0.41
1:A:1424:C:H2'	1:A:1425:U:O4'	2.20	0.41
1:A:268:C:O2'	1:A:269:C:H5'	2.20	0.41
15:O:33:THR:HG23	15:O:63:ARG:NH1	2.34	0.41
1:A:1176:A:H2'	1:A:1177:G:C8	2.54	0.41
1:A:538:G:OP2	12:L:115:LYS:HG3	2.20	0.41
11:K:55:LYS:HE3	11:K:55:LYS:HB2	1.82	0.41
1:A:828:A:H4'	1:A:828:A:OP1	2.20	0.41
1:A:442:C:H6	1:A:442:C:OP2	2.04	0.41
3:C:126:ARG:HG2	3:C:128:PHE:CD1	2.48	0.41
1:A:1453:G:N2	1:A:1454:G:C5	2.89	0.41
3:C:113:ALA:HA	3:C:116:VAL:HG23	2.01	0.41
1:A:955:U:H1'	1:A:1227:A:N6	2.34	0.41
17:Q:83:ASP:N	17:Q:83:ASP:OD1	2.53	0.41
8:H:102:ARG:N	8:H:102:ARG:CD	2.83	0.41
8:H:91:ARG:HH12	17:Q:33:GLY:HA3	1.86	0.41
8:H:53:VAL:HG23	8:H:58:TYR:CD1	2.56	0.41
4:D:196:LEU:HA	4:D:197:PRO:HD3	1.87	0.41
7:G:145:ALA:O	7:G:146:GLU:HB2	2.20	0.41
1:A:524:G:H2'	1:A:525:C:C6	2.56	0.41
3:C:111:LEU:HD23	3:C:111:LEU:HA	1.73	0.41
24:A:1609:PAR:H33	24:A:1609:PAR:H24	1.74	0.41
18:R:58:LEU:HD23	18:R:58:LEU:HA	1.73	0.41
3:C:178:LEU:HA	3:C:178:LEU:HD12	1.59	0.41
3:C:57:ILE:HG12	3:C:66:VAL:HG22	2.02	0.41
4:D:8:VAL:O	4:D:10:ARG:N	2.53	0.41
2:B:73:THR:O	2:B:75:LYS:N	2.54	0.41
13:M:56:LEU:HD23	13:M:56:LEU:HA	1.71	0.41
1:A:299:G:C6	1:A:300:A:C6	3.09	0.41
9:I:100:GLY:O	9:I:103:THR:HB	2.21	0.41
2:B:166:ASP:HB3	2:B:169:LYS:HB3	2.02	0.41
3:C:12:LEU:HD23	3:C:12:LEU:HA	1.80	0.41
1:A:1160:G:O6	1:A:1181:G:O6	2.38	0.41
15:O:17:ARG:HB2	15:O:18:PHE:CD2	2.54	0.41
2:B:30:ARG:H	2:B:30:ARG:HG2	1.71	0.41
1:A:1373:G:H5"	7:G:36:LYS:HB2	2.03	0.41
1:A:325:A:N6	1:A:326:G:C2	2.88	0.41
1:A:1148:U:O3'	9:I:14:VAL:HG11	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:6:ILE:CD1	8:H:6:ILE:N	2.84	0.41
1:A:321:A:C2	1:A:333:G:C2	3.08	0.41
1:A:504:C:C2	1:A:542:G:C2	3.09	0.41
24:A:1613:PAR:H11	24:A:1613:PAR:N32	2.35	0.41
8:H:28:ALA:HA	8:H:59:LEU:HD12	2.02	0.41
1:A:1447:G:C6	1:A:1460:A:C2	3.08	0.41
2:B:98:LEU:N	2:B:98:LEU:HD23	2.36	0.41
3:C:12:LEU:HD11	14:N:51:GLY:HA2	2.03	0.41
13:M:31:LYS:HG2	13:M:35:GLU:OE1	2.20	0.41
1:A:973:G:H3'	1:A:974:A:H5"	2.02	0.41
1:A:1127:G:C2	1:A:1145:C:N3	2.88	0.41
8:H:17:THR:HB	8:H:78:GLN:NE2	2.35	0.41
22:V:1:U:N3	23:W:37:A:C2	2.89	0.41
18:R:16:PRO:HB2	18:R:17:SER:H	1.66	0.41
1:A:1054:C:H3'	1:A:1054:C:O2	2.20	0.41
2:B:33:TYR:HD1	2:B:44:LEU:HD22	1.85	0.41
16:P:43:LYS:HA	16:P:48:TRP:HB3	2.03	0.41
1:A:190(I):G:C6	1:A:190(J):U:C4	3.09	0.41
11:K:86:GLY:H	11:K:112:THR:HG23	1.86	0.41
8:H:112:LEU:N	8:H:112:LEU:HD23	2.36	0.41
4:D:25:ARG:HH21	4:D:30:LYS:HB3	1.86	0.41
18:R:55:ARG:HB3	18:R:55:ARG:NH1	2.35	0.41
17:Q:29:HIS:HA	17:Q:30:PRO:HD3	1.88	0.41
1:A:46:G:O2'	1:A:365:U:H1'	2.19	0.41
13:M:25:ILE:HG22	13:M:26:GLY:O	2.21	0.41
2:B:210:SER:O	2:B:214:ILE:HG12	2.20	0.41
20:T:43:LEU:HD12	20:T:52:ALA:HA	2.03	0.41
1:A:338:A:C2	1:A:339:C:C2	3.08	0.41
1:A:983:A:H1'	1:A:1049:U:O2	2.21	0.41
4:D:202:LEU:HD23	4:D:202:LEU:HA	1.66	0.41
1:A:1124:G:H2'	1:A:1145:C:H5	1.86	0.41
1:A:530:G:O6	22:V:3:U:H1'	2.20	0.41
8:H:30:ARG:O	8:H:33:GLU:HB3	2.21	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
12:L:27:LEU:O	12:L:30:ALA:N	2.42	0.41
1:A:964:A:O2'	10:J:55:LYS:HD3	2.21	0.41
24:A:1603:PAR:H43	24:A:1603:PAR:O54	2.20	0.41
1:A:1320:C:N3	19:S:36:ARG:HG3	2.36	0.41
5:E:28:PHE:CE1	5:E:51:VAL:HG22	2.55	0.41
1:A:1128:C:H1'	1:A:1130:A:N7	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:83:ASP:OD1	17:Q:84:LEU:HD23	2.21	0.41
1:A:1410:G:N2	1:A:1491:G:C4	2.89	0.41
1:A:177:C:H2'	1:A:178:C:C6	2.55	0.41
17:Q:20:THR:HG22	17:Q:41:LYS:HG2	2.02	0.41
1:A:1139:G:H4'	1:A:1140:C:OP1	2.21	0.41
4:D:64:LEU:HD12	4:D:75:PHE:HZ	1.85	0.41
11:K:66:LEU:HD23	11:K:66:LEU:HA	1.84	0.41
1:A:58:C:H6	1:A:58:C:H3'	1.86	0.41
1:A:676:A:H1'	11:K:115:PRO:HB3	2.03	0.41
4:D:142:PRO:HA	4:D:185:PHE:HD2	1.85	0.41
24:A:1616:PAR:H32	24:A:1616:PAR:H11	1.87	0.41
1:A:409:G:N2	1:A:433:C:N3	2.53	0.41
15:O:14:GLU:HG3	15:O:15:PHE:CD1	2.56	0.41
1:A:1024:G:H5"	1:A:1025:U:OP2	2.21	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
2:B:74:LYS:O	2:B:75:LYS:HB2	2.20	0.41
1:A:98:U:O4	24:A:1618:PAR:H12	2.21	0.41
1:A:1055:A:N6	1:A:1206:G:C5	2.89	0.41
1:A:855:G:C4	1:A:856:C:C6	3.09	0.41
1:A:1522:U:O2'	1:A:1523:G:H5'	2.21	0.41
6:F:67:MET:HB2	6:F:68:PRO:HD2	2.03	0.41
1:A:181:G:H4'	1:A:182:U:H5'	2.02	0.41
1:A:1203:C:OP1	14:N:2:ALA:N	2.54	0.41
4:D:64:LEU:HD12	4:D:75:PHE:CZ	2.56	0.41
13:M:10:PRO:HB2	13:M:18:ALA:HB1	2.02	0.41
11:K:84:VAL:HG21	11:K:95:ILE:HD11	2.03	0.41
19:S:40:ILE:O	19:S:67:VAL:HG13	2.21	0.41
1:A:1228:C:OP2	13:M:111:LYS:HE3	2.21	0.41
3:C:22:TRP:NE1	3:C:36:ASP:OD1	2.50	0.41
18:R:84:LYS:H	18:R:84:LYS:HG3	1.57	0.41
20:T:8:ARG:HD2	20:T:8:ARG:N	2.36	0.41
1:A:107:G:C2	1:A:108:G:H1'	2.56	0.40
1:A:386:C:C2'	1:A:387:U:H5'	2.51	0.40
1:A:1060:C:HO2'	10:J:56:HIS:CE1	2.37	0.40
1:A:1502:A:H2	1:A:1505:G:N1	2.17	0.40
1:A:1501:C:C5	1:A:1504:G:C4	3.09	0.40
18:R:36:ASN:CG	18:R:39:VAL:HG12	2.41	0.40
1:A:1256:A:H2	1:A:1277:C:N4	2.19	0.40
1:A:949:A:OP1	13:M:101:GLN:HB3	2.21	0.40
1:A:606:G:H5"	1:A:607:A:H5'	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:G:C6	1:A:290:C:N4	2.89	0.40
3:C:170:GLN:HG2	3:C:171:GLY:N	2.36	0.40
1:A:1057:G:H2'	1:A:1058:G:O4'	2.21	0.40
3:C:177:THR:O	3:C:180:ALA:HB2	2.21	0.40
9:I:74:ILE:HA	9:I:77:ILE:HD12	2.04	0.40
13:M:99:ARG:CZ	19:S:2:PRO:HG2	2.51	0.40
14:N:21:TYR:HD2	14:N:22:THR:O	2.03	0.40
1:A:994:A:N3	1:A:994:A:H2'	2.36	0.40
1:A:961:U:C2'	1:A:962:C:H5'	2.50	0.40
2:B:163:PHE:CE1	2:B:215:LEU:HD23	2.56	0.40
10:J:32:ALA:HB2	10:J:76:ASN:HB2	2.02	0.40
8:H:102:ARG:H	8:H:102:ARG:CD	2.34	0.40
6:F:61:LEU:HD13	6:F:63:TYR:OH	2.21	0.40
1:A:45:U:OP1	1:A:307:C:O2'	2.36	0.40
1:A:290:C:O5'	1:A:290:C:H6	2.04	0.40
2:B:127:ILE:H	2:B:127:ILE:HG13	1.70	0.40
12:L:15:ARG:HA	12:L:15:ARG:HD3	1.89	0.40
1:A:1329:A:H62	21:U:7:ARG:NH2	2.18	0.40
10:J:48:THR:OG1	10:J:62:HIS:HB3	2.21	0.40
8:H:4:ASP:OD1	8:H:7:ALA:N	2.41	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:1442:G:N7	1:A:1446:A:N6	2.70	0.40
13:M:59:TYR:CE1	13:M:63:THR:HG21	2.56	0.40
2:B:82:ARG:HB3	2:B:94:ASN:ND2	2.36	0.40
1:A:597:G:C6	1:A:644:G:C6	3.10	0.40
1:A:1313:U:O4	19:S:4:SER:OG	2.26	0.40
2:B:8:LYS:HA	2:B:11:LEU:HD13	2.02	0.40
3:C:40:ARG:O	3:C:44:GLU:HG3	2.21	0.40
3:C:152:ILE:HG22	3:C:199:LYS:HB2	2.02	0.40
4:D:194:LEU:HA	4:D:194:LEU:HD13	1.90	0.40
5:E:83:GLU:HA	5:E:88:LYS:HA	2.02	0.40
1:A:415:A:OP1	24:A:1611:PAR:N64	2.55	0.40
1:A:1060:C:H5"	10:J:51:ARG:HB3	2.02	0.40
6:F:45:LEU:HD12	6:F:47:ARG:NH2	2.36	0.40
1:A:1203:C:O5'	1:A:1203:C:H6	2.03	0.40
1:A:17:U:H2'	1:A:18:C:C6	2.56	0.40
13:M:76:ALA:HA	13:M:79:LYS:HB3	2.03	0.40
6:F:48:LEU:HD22	18:R:77:GLY:HA3	2.03	0.40
2:B:162:ILE:HD11	2:B:184:VAL:HG22	2.04	0.40
10:J:38:ILE:CG2	10:J:71:LEU:HB2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:69:VAL:HG12	7:G:100:ALA:HA	2.04	0.40
13:M:96:LEU:C	13:M:110:ARG:HG2	2.41	0.40
1:A:1190:G:O6	24:A:1608:PAR:N64	2.54	0.40
1:A:328:C:H4'	1:A:329:A:C5'	2.51	0.40
24:A:1602:PAR:O34	24:A:1602:PAR:O54	2.35	0.40
1:A:1352:C:H2'	1:A:1353:G:C8	2.57	0.40
12:L:93:LEU:HD13	12:L:96:VAL:HG21	2.04	0.40
1:A:989:C:N4	1:A:1216:G:H1	2.20	0.40
1:A:1227:A:C8	1:A:1227:A:H3'	2.57	0.40
7:G:140:ASP:O	7:G:143:ARG:HB3	2.22	0.40
1:A:909:A:H2'	1:A:910:C:O4'	2.21	0.40
1:A:1133:G:N2	1:A:1141:C:O2	2.48	0.40
1:A:1269:A:H2'	1:A:1270:C:O4'	2.21	0.40
1:A:639:G:O2'	1:A:640:A:H5'	2.21	0.40
7:G:104:LEU:HA	7:G:104:LEU:HD23	1.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	34	76
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%)	24	69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
10	J	97/105 (92%)	80 (82%)	14 (14%)	3 (3%)	5 44
11	K	117/129 (91%)	105 (90%)	11 (9%)	1 (1%)	21 66
12	L	122/135 (90%)	111 (91%)	10 (8%)	1 (1%)	24 69
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%)	16 62
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%)	7 48
20	T	97/106 (92%)	82 (84%)	14 (14%)	1 (1%)	19 65
21	U	23/27 (85%)	22 (96%)	1 (4%)	0	100 100
All	All	2353/2541 (93%)	2145 (91%)	197 (8%)	11 (0%)	34 76

All (11) Ramachandran outliers are listed below:

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	201/220 (91%)	176 (88%)	25 (12%)	6 32
3	C	160/188 (85%)	121 (76%)	39 (24%)	1 7
4	D	180/181 (99%)	159 (88%)	21 (12%)	7 35
5	E	115/123 (94%)	91 (79%)	24 (21%)	1 11
6	F	90/90 (100%)	66 (73%)	24 (27%)	0 5
7	G	126/127 (99%)	105 (83%)	21 (17%)	3 20
8	H	119/119 (100%)	94 (79%)	25 (21%)	1 11
9	I	98/99 (99%)	75 (76%)	23 (24%)	1 8
10	J	87/92 (95%)	69 (79%)	18 (21%)	1 11
11	K	90/99 (91%)	78 (87%)	12 (13%)	5 30
12	L	103/110 (94%)	86 (84%)	17 (16%)	3 21
13	M	94/101 (93%)	75 (80%)	19 (20%)	1 12
14	N	49/50 (98%)	39 (80%)	10 (20%)	1 12
15	O	79/80 (99%)	63 (80%)	16 (20%)	1 12
16	P	72/74 (97%)	60 (83%)	12 (17%)	3 20
17	Q	95/97 (98%)	75 (79%)	20 (21%)	1 11
18	R	64/77 (83%)	56 (88%)	8 (12%)	6 32
19	S	71/80 (89%)	53 (75%)	18 (25%)	1 7
20	T	76/82 (93%)	60 (79%)	16 (21%)	1 11
21	U	19/22 (86%)	16 (84%)	3 (16%)	3 23
All	All	1988/2111 (94%)	1617 (81%)	371 (19%)	2 15

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
21	U	17	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	40	HIS
3	C	6	HIS
3	C	69	HIS
3	C	108	ASN
6	F	73	ASN
6	F	94	GLN
9	I	73	GLN
17	Q	16	GLN
20	T	18	GLN
20	T	73	HIS

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
1	A	1505	G
1	A	1528	U

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

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	17,26,27	2.30	4 (23%)	21,38,41	2.75	4 (19%)
1	5MC	A	1400	1	13,22,23	1.18	1 (7%)	15,32,35	1.04	1 (6%)
1	4OC	A	1402	1	13,23,24	0.82	0	18,32,35	0.82	1 (5%)
1	5MC	A	1404	1	13,22,23	1.02	1 (7%)	15,32,35	0.72	0
1	5MC	A	1407	1	13,22,23	1.10	1 (7%)	15,32,35	1.28	3 (20%)
1	UR3	A	1498	1	12,22,23	0.85	0	16,32,35	1.28	1 (6%)
1	MA6	A	1518	1	16,26,27	0.86	1 (6%)	18,38,41	1.48	5 (27%)
1	MA6	A	1519	1	16,26,27	1.29	3 (18%)	18,38,41	1.35	3 (16%)
1	PSU	A	1540	1	13,21,22	1.27	2 (15%)	18,30,33	3.92	5 (27%)
1	PSU	A	1541	1	13,21,22	1.18	2 (15%)	18,30,33	3.73	7 (38%)
1	PSU	A	516	1	13,21,22	1.41	2 (15%)	18,30,33	4.69	4 (22%)
1	7MG	A	527	1,25	19,26,27	2.91	7 (36%)	24,39,42	1.71	6 (25%)
1	M2G	A	966	1	17,27,28	1.25	1 (5%)	22,40,43	2.46	4 (18%)
1	5MC	A	967	1	13,22,23	0.79	0	15,32,35	0.79	1 (6%)
12	0TD	L	92	12	4,9,10	0.99	0	4,11,13	3.34	3 (75%)

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

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	7MG	C8-N9	-7.94	1.33	1.45
1	A	527	7MG	CM7-N7	-3.68	1.39	1.46
1	A	527	7MG	C8-N7	-2.54	1.31	1.43
1	A	1407	5MC	C4-N3	-2.39	1.31	1.35
1	A	527	7MG	O6-C6	-2.36	1.19	1.24
1	A	1404	5MC	C6-C5	-2.24	1.34	1.40
1	A	1540	PSU	C5-C1'	2.03	1.54	1.52
1	A	1400	5MC	C6-N1	2.05	1.38	1.35
1	A	516	PSU	C5-C1'	2.10	1.54	1.52
1	A	1518	MA6	C10-N6	2.20	1.51	1.45
1	A	1541	PSU	C5-C1'	2.24	1.54	1.52
1	A	1519	MA6	C4-N3	2.29	1.39	1.35
1	A	527	7MG	C6-N1	2.29	1.37	1.33
1	A	1519	MA6	C2-N1	2.39	1.38	1.33
1	A	1207	2MG	C2-N2	2.75	1.37	1.34
1	A	1207	2MG	O6-C6	2.87	1.31	1.24
1	A	1207	2MG	C2-N1	2.96	1.45	1.34
1	A	1541	PSU	C4-N3	3.02	1.38	1.33
1	A	1540	PSU	C4-N3	3.22	1.39	1.33
1	A	1519	MA6	C6-N1	3.28	1.38	1.34
1	A	516	PSU	C4-N3	3.47	1.39	1.33
1	A	966	M2G	C6-N1	4.02	1.40	1.33
1	A	527	7MG	C4-N3	5.20	1.41	1.34
1	A	527	7MG	C2-N2	5.55	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1207	2MG	C6-N1	7.53	1.47	1.33

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	516	PSU	N1-C2-N3	-17.40	117.23	128.33
1	A	1540	PSU	N1-C2-N3	-13.66	119.62	128.33
1	A	1541	PSU	N1-C2-N3	-13.39	119.79	128.33
1	A	1207	2MG	C5-C6-N1	-10.69	108.97	123.59
1	A	966	M2G	C5-C6-N1	-9.64	110.41	123.59
1	A	1540	PSU	C5-C1'-C2'	-5.08	106.50	115.52
12	L	92	0TD	CSB-SB-CB	-5.00	92.10	101.54
1	A	527	7MG	C5-C4-N3	-4.98	121.96	126.82
1	A	1518	MA6	C1'-N9-C4	-3.30	121.96	126.94
1	A	966	M2G	N1-C2-N2	-3.30	113.44	117.16
1	A	966	M2G	CM1-N2-C2	-3.12	118.13	121.34
12	L	92	0TD	C-CA-N	-2.97	103.62	109.83
1	A	527	7MG	C4-N9-C1'	-2.93	119.65	126.70
12	L	92	0TD	CB-CA-N	-2.87	103.44	109.66
1	A	527	7MG	N1-C2-N3	-2.72	121.08	125.53
1	A	1518	MA6	N1-C6-N6	-2.50	114.33	117.05
1	A	1207	2MG	CM2-N2-C2	-2.40	120.36	123.07
1	A	1519	MA6	C2'-C1'-N9	-2.35	110.69	114.29
1	A	966	M2G	C2-N3-C4	-2.32	112.30	115.09
1	A	1519	MA6	C1'-N9-C4	-2.23	123.57	126.94
1	A	1518	MA6	C2'-C1'-N9	-2.23	110.89	114.29
1	A	1540	PSU	C3'-C2'-C1'	-2.21	99.22	101.79
1	A	1541	PSU	C5-C6-N1	-2.16	121.34	124.39
1	A	1402	4OC	CM4-N4-C4	-2.13	121.13	122.98
1	A	1407	5MC	N4-C4-N3	-2.13	113.86	116.95
1	A	1541	PSU	C5-C1'-C2'	-2.03	111.92	115.52
1	A	1541	PSU	C4-C5-C1'	2.03	124.93	121.23
1	A	967	5MC	CM5-C5-C6	2.05	122.75	118.62
1	A	1518	MA6	C2-N1-C6	2.13	115.97	111.43
1	A	1207	2MG	C6-C5-C4	2.16	123.48	120.90
1	A	527	7MG	N2-C2-N1	2.28	120.98	117.20
1	A	1400	5MC	CM5-C5-C6	2.29	123.22	118.62
1	A	1407	5MC	C5-C4-N3	2.29	125.10	121.27
1	A	1518	MA6	N3-C2-N1	2.40	130.73	128.89
1	A	527	7MG	C6-N1-C2	2.46	119.35	115.94
1	A	516	PSU	O4'-C1'-C2'	2.70	107.48	104.73
1	A	1540	PSU	C6-N1-C2	2.77	119.92	115.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1498	UR3	C6-C5-C4	2.77	122.46	117.28
1	A	1541	PSU	O4'-C1'-C2'	2.80	107.58	104.73
1	A	527	7MG	N3-C4-N9	2.89	131.09	126.75
1	A	516	PSU	C6-N1-C2	3.05	120.37	115.47
1	A	1519	MA6	C2-N1-C6	3.05	117.93	111.43
1	A	1407	5MC	CM5-C5-C6	3.33	125.33	118.62
1	A	1541	PSU	C6-N1-C2	3.50	121.10	115.47
1	A	1207	2MG	C6-N1-C2	4.85	122.36	115.31
1	A	1541	PSU	C4-N3-C2	5.64	120.12	115.25
1	A	1540	PSU	C4-N3-C2	6.45	120.82	115.25
1	A	516	PSU	C4-N3-C2	8.34	122.46	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1207	2MG	1	0
1	A	1400	5MC	1	0
1	A	1402	4OC	5	0
1	A	1404	5MC	2	0
1	A	1498	UR3	4	0
1	A	1518	MA6	2	0
1	A	527	7MG	1	0
1	A	966	M2G	3	0
1	A	967	5MC	2	0
12	L	92	0TD	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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	1.39	6 (13%)	59,67,67	1.57	11 (18%)
24	PAR	A	1602	-	45,45,45	1.60	7 (15%)	59,67,67	1.71	12 (20%)
24	PAR	A	1603	-	45,45,45	1.41	8 (17%)	59,67,67	1.68	12 (20%)
24	PAR	A	1604	-	45,45,45	1.30	7 (15%)	59,67,67	1.56	11 (18%)
24	PAR	A	1605	-	45,45,45	1.30	8 (17%)	59,67,67	1.48	9 (15%)
24	PAR	A	1606	-	45,45,45	1.44	7 (15%)	59,67,67	1.66	12 (20%)
24	PAR	A	1607	-	45,45,45	1.68	9 (20%)	59,67,67	1.65	11 (18%)
24	PAR	A	1608	25	45,45,45	1.27	6 (13%)	59,67,67	1.60	12 (20%)
24	PAR	A	1609	-	45,45,45	1.76	14 (31%)	59,67,67	1.68	11 (18%)
24	PAR	A	1610	-	45,45,45	1.73	14 (31%)	59,67,67	1.71	12 (20%)
24	PAR	A	1611	-	45,45,45	1.59	6 (13%)	59,67,67	1.62	11 (18%)
24	PAR	A	1612	-	45,45,45	1.54	7 (15%)	59,67,67	1.60	10 (16%)
24	PAR	A	1613	-	45,45,45	1.66	8 (17%)	59,67,67	1.60	9 (15%)
24	PAR	A	1614	-	45,45,45	1.69	12 (26%)	59,67,67	1.59	10 (16%)
24	PAR	A	1615	-	45,45,45	2.06	11 (24%)	59,67,67	1.67	12 (20%)
24	PAR	A	1616	-	45,45,45	1.98	11 (24%)	59,67,67	1.62	12 (20%)
24	PAR	A	1617	25	45,45,45	2.07	13 (28%)	59,67,67	1.63	10 (16%)
24	PAR	A	1618	-	45,45,45	2.25	17 (37%)	59,67,67	1.61	10 (16%)

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	0/4/4/4
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	0/4/4/4
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	1/4/4/4
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 (171) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1604	PAR	C62-C12	-2.06	1.49	1.53
24	A	1602	PAR	C44-C34	-2.04	1.47	1.52
24	A	1610	PAR	C13-C23	2.00	1.55	1.52
24	A	1615	PAR	C41-C51	2.02	1.57	1.53
24	A	1603	PAR	C41-C51	2.02	1.57	1.53
24	A	1618	PAR	O54-C14	2.03	1.47	1.41
24	A	1609	PAR	C11-C21	2.03	1.56	1.52
24	A	1610	PAR	C24-N24	2.03	1.50	1.47
24	A	1610	PAR	C62-C52	2.06	1.58	1.52
24	A	1618	PAR	O33-C33	2.08	1.49	1.43
24	A	1610	PAR	O33-C14	2.08	1.47	1.41
24	A	1614	PAR	O54-C14	2.09	1.47	1.41
24	A	1604	PAR	C13-C23	2.11	1.55	1.52
24	A	1609	PAR	C64-C54	2.11	1.57	1.52
24	A	1605	PAR	C13-C23	2.12	1.55	1.52
24	A	1603	PAR	C14-C24	2.12	1.56	1.52
24	A	1609	PAR	O52-C52	2.13	1.49	1.43
24	A	1601	PAR	C62-C52	2.13	1.58	1.52
24	A	1605	PAR	C31-C21	2.14	1.56	1.53
24	A	1614	PAR	C24-N24	2.14	1.50	1.47
24	A	1609	PAR	C24-N24	2.14	1.50	1.47
24	A	1617	PAR	O52-C13	2.14	1.47	1.41
24	A	1606	PAR	C33-C43	2.14	1.59	1.52
24	A	1608	PAR	C62-C52	2.14	1.58	1.52
24	A	1607	PAR	O52-C52	2.15	1.49	1.43
24	A	1614	PAR	C64-C54	2.15	1.57	1.52
24	A	1606	PAR	C62-C52	2.15	1.58	1.52
24	A	1607	PAR	O33-C14	2.16	1.47	1.41
24	A	1604	PAR	O43-C13	2.21	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1610	PAR	O11-C11	2.21	1.47	1.41
24	A	1615	PAR	O11-C11	2.22	1.47	1.41
24	A	1611	PAR	O33-C14	2.22	1.47	1.41
24	A	1618	PAR	C44-C34	2.23	1.58	1.52
24	A	1618	PAR	O11-C11	2.24	1.47	1.41
24	A	1604	PAR	C42-C32	2.25	1.58	1.53
24	A	1609	PAR	C31-C21	2.25	1.56	1.53
24	A	1604	PAR	C64-C54	2.25	1.57	1.52
24	A	1614	PAR	C33-C43	2.25	1.59	1.52
24	A	1608	PAR	C14-C24	2.29	1.57	1.52
24	A	1612	PAR	C34-C24	2.29	1.56	1.53
24	A	1603	PAR	C11-C21	2.30	1.57	1.52
24	A	1617	PAR	C44-C54	2.30	1.58	1.53
24	A	1613	PAR	O52-C13	2.30	1.47	1.41
24	A	1604	PAR	C33-C43	2.30	1.59	1.52
24	A	1608	PAR	C34-C24	2.31	1.56	1.53
24	A	1616	PAR	O33-C14	2.32	1.48	1.41
24	A	1617	PAR	C42-C32	2.33	1.58	1.53
24	A	1610	PAR	C52-C42	2.33	1.57	1.52
24	A	1605	PAR	C33-C43	2.35	1.59	1.52
24	A	1617	PAR	O33-C33	2.35	1.49	1.43
24	A	1614	PAR	C62-C52	2.37	1.59	1.52
24	A	1614	PAR	O33-C14	2.38	1.48	1.41
24	A	1618	PAR	C11-C21	2.39	1.57	1.52
24	A	1608	PAR	O43-C13	2.41	1.45	1.41
24	A	1602	PAR	O54-C14	2.41	1.48	1.41
24	A	1615	PAR	C62-C12	2.42	1.58	1.53
24	A	1618	PAR	C64-C54	2.42	1.58	1.52
24	A	1605	PAR	C34-C24	2.43	1.56	1.53
24	A	1617	PAR	O11-C11	2.43	1.48	1.41
24	A	1608	PAR	C11-C21	2.43	1.57	1.52
24	A	1603	PAR	O43-C13	2.44	1.46	1.41
24	A	1601	PAR	C33-C43	2.46	1.60	1.52
24	A	1611	PAR	C14-C24	2.47	1.57	1.52
24	A	1615	PAR	C23-C33	2.47	1.58	1.53
24	A	1614	PAR	O52-C52	2.48	1.50	1.43
24	A	1616	PAR	O52-C13	2.48	1.48	1.41
24	A	1605	PAR	O54-C14	2.49	1.48	1.41
24	A	1618	PAR	C42-C32	2.50	1.59	1.53
24	A	1612	PAR	C11-C21	2.52	1.57	1.52
24	A	1610	PAR	C64-C54	2.53	1.58	1.52
24	A	1616	PAR	C11-C21	2.53	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1605	PAR	O33-C14	2.54	1.48	1.41
24	A	1609	PAR	C62-C52	2.54	1.59	1.52
24	A	1612	PAR	C41-C51	2.57	1.58	1.53
24	A	1609	PAR	C41-C51	2.57	1.58	1.53
24	A	1602	PAR	O33-C14	2.57	1.48	1.41
24	A	1605	PAR	O43-C13	2.59	1.46	1.41
24	A	1613	PAR	O52-C52	2.60	1.50	1.43
24	A	1618	PAR	O52-C13	2.61	1.48	1.41
24	A	1609	PAR	C52-C42	2.61	1.57	1.52
24	A	1615	PAR	C64-C54	2.62	1.58	1.52
24	A	1603	PAR	C62-C52	2.62	1.59	1.52
24	A	1617	PAR	O43-C13	2.62	1.46	1.41
24	A	1615	PAR	C31-C21	2.62	1.56	1.53
24	A	1610	PAR	O54-C54	2.65	1.51	1.44
24	A	1606	PAR	C13-C23	2.68	1.56	1.52
24	A	1607	PAR	C13-C23	2.71	1.56	1.52
24	A	1616	PAR	C62-C52	2.72	1.60	1.52
24	A	1613	PAR	O33-C14	2.73	1.49	1.41
24	A	1609	PAR	O33-C14	2.75	1.49	1.41
24	A	1606	PAR	O52-C52	2.75	1.50	1.43
24	A	1602	PAR	C52-C42	2.76	1.58	1.52
24	A	1608	PAR	C62-C12	2.76	1.59	1.53
24	A	1611	PAR	C31-C21	2.79	1.57	1.53
24	A	1614	PAR	C13-C23	2.79	1.56	1.52
24	A	1610	PAR	O54-C14	2.80	1.49	1.41
24	A	1602	PAR	O43-C13	2.80	1.46	1.41
24	A	1616	PAR	O52-C52	2.82	1.50	1.43
24	A	1618	PAR	O52-C52	2.83	1.51	1.43
24	A	1610	PAR	C41-C51	2.84	1.59	1.53
24	A	1618	PAR	C62-C52	2.85	1.60	1.52
24	A	1601	PAR	C52-C42	2.86	1.58	1.52
24	A	1617	PAR	C62-C52	2.88	1.60	1.52
24	A	1605	PAR	C64-C54	2.90	1.59	1.52
24	A	1612	PAR	C52-C42	2.91	1.58	1.52
24	A	1607	PAR	C44-C54	2.91	1.59	1.53
24	A	1609	PAR	C44-C54	2.92	1.59	1.53
24	A	1613	PAR	C62-C52	2.93	1.60	1.52
24	A	1614	PAR	C31-C21	2.93	1.57	1.53
24	A	1617	PAR	C14-C24	2.94	1.58	1.52
24	A	1603	PAR	C33-C43	2.94	1.61	1.52
24	A	1607	PAR	C64-C54	2.94	1.59	1.52
24	A	1613	PAR	C52-C42	2.95	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1601	PAR	C11-C21	3.01	1.58	1.52
24	A	1613	PAR	C13-C23	3.01	1.56	1.52
24	A	1603	PAR	C13-C23	3.01	1.56	1.52
24	A	1611	PAR	C52-C42	3.06	1.58	1.52
24	A	1610	PAR	C31-C21	3.07	1.57	1.53
24	A	1607	PAR	C62-C12	3.09	1.60	1.53
24	A	1609	PAR	C13-C23	3.16	1.57	1.52
24	A	1618	PAR	C31-C21	3.18	1.57	1.53
24	A	1617	PAR	O52-C52	3.23	1.52	1.43
24	A	1617	PAR	O33-C14	3.25	1.50	1.41
24	A	1616	PAR	C31-C21	3.28	1.57	1.53
24	A	1601	PAR	C13-C23	3.33	1.57	1.52
24	A	1609	PAR	O43-C13	3.40	1.47	1.41
24	A	1618	PAR	C14-C24	3.42	1.59	1.52
24	A	1618	PAR	O33-C14	3.46	1.51	1.41
24	A	1613	PAR	C14-C24	3.47	1.59	1.52
24	A	1606	PAR	C52-C42	3.47	1.59	1.52
24	A	1612	PAR	C14-C24	3.50	1.59	1.52
24	A	1610	PAR	C11-C21	3.54	1.59	1.52
24	A	1616	PAR	O43-C13	3.57	1.47	1.41
24	A	1614	PAR	C52-C42	3.58	1.59	1.52
24	A	1612	PAR	O43-C13	3.60	1.48	1.41
24	A	1616	PAR	C14-C24	3.60	1.59	1.52
24	A	1601	PAR	C31-C21	3.62	1.58	1.53
24	A	1607	PAR	C62-C52	3.67	1.62	1.52
24	A	1610	PAR	C14-C24	3.67	1.59	1.52
24	A	1615	PAR	O52-C13	3.72	1.51	1.41
24	A	1607	PAR	O43-C13	3.75	1.48	1.41
24	A	1614	PAR	C14-C24	3.76	1.59	1.52
24	A	1616	PAR	C52-C42	3.83	1.60	1.52
24	A	1609	PAR	C34-C24	3.84	1.58	1.53
24	A	1606	PAR	O43-C13	3.86	1.48	1.41
24	A	1606	PAR	C34-C24	3.96	1.58	1.53
24	A	1614	PAR	C34-C24	4.00	1.58	1.53
24	A	1609	PAR	C14-C24	4.02	1.60	1.52
24	A	1615	PAR	C52-C42	4.07	1.61	1.52
24	A	1607	PAR	C52-C42	4.13	1.61	1.52
24	A	1612	PAR	C13-C23	4.16	1.58	1.52
24	A	1603	PAR	C52-C42	4.17	1.61	1.52
24	A	1602	PAR	C31-C21	4.21	1.58	1.53
24	A	1615	PAR	O52-C52	4.22	1.54	1.43
24	A	1618	PAR	O43-C13	4.25	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1616	PAR	C34-C24	4.29	1.59	1.53
24	A	1604	PAR	C52-C42	4.55	1.62	1.52
24	A	1611	PAR	O43-C13	4.60	1.49	1.41
24	A	1610	PAR	O43-C13	4.64	1.49	1.41
24	A	1615	PAR	O43-C13	4.73	1.50	1.41
24	A	1617	PAR	C34-C24	4.78	1.59	1.53
24	A	1611	PAR	C34-C24	5.01	1.59	1.53
24	A	1618	PAR	C52-C42	5.03	1.63	1.52
24	A	1617	PAR	C13-C23	5.30	1.59	1.52
24	A	1616	PAR	C13-C23	5.33	1.59	1.52
24	A	1613	PAR	C34-C24	5.33	1.60	1.53
24	A	1602	PAR	C14-C24	5.36	1.63	1.52
24	A	1618	PAR	C13-C23	5.75	1.60	1.52
24	A	1617	PAR	C52-C42	5.75	1.64	1.52
24	A	1618	PAR	C34-C24	6.04	1.61	1.53
24	A	1615	PAR	C13-C23	6.43	1.61	1.52

All (197) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	1602	PAR	C34-C24-N24	-4.09	103.27	110.86
24	A	1603	PAR	C34-C24-N24	-3.70	104.00	110.86
24	A	1610	PAR	C34-C24-N24	-3.69	104.01	110.86
24	A	1612	PAR	C34-C24-N24	-3.49	104.39	110.86
24	A	1605	PAR	C34-C24-N24	-3.38	104.60	110.86
24	A	1607	PAR	O34-C34-C44	-3.36	102.76	110.34
24	A	1606	PAR	C34-C24-N24	-3.36	104.62	110.86
24	A	1608	PAR	C34-C24-N24	-3.33	104.69	110.86
24	A	1601	PAR	C34-C24-N24	-3.33	104.69	110.86
24	A	1608	PAR	C14-O33-C33	-3.32	109.33	118.01
24	A	1609	PAR	C34-C24-N24	-3.32	104.70	110.86
24	A	1602	PAR	O34-C34-C44	-3.32	102.86	110.34
24	A	1613	PAR	O34-C34-C44	-3.31	102.88	110.34
24	A	1610	PAR	O34-C34-C44	-3.26	103.00	110.34
24	A	1607	PAR	C14-O33-C33	-3.22	109.60	118.01
24	A	1615	PAR	C34-C24-N24	-3.11	105.09	110.86
24	A	1611	PAR	C14-O33-C33	-3.10	109.91	118.01
24	A	1617	PAR	C34-C24-N24	-3.10	105.12	110.86
24	A	1618	PAR	C14-O33-C33	-3.06	110.00	118.01
24	A	1615	PAR	C14-O33-C33	-3.01	110.14	118.01
24	A	1614	PAR	O34-C34-C44	-2.99	103.59	110.34
24	A	1616	PAR	C34-C24-N24	-2.99	105.31	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	1611	PAR	C34-C24-N24	-2.96	105.38	110.86
24	A	1614	PAR	C34-C24-N24	-2.94	105.42	110.86
24	A	1612	PAR	C14-O33-C33	-2.91	110.40	118.01
24	A	1604	PAR	C34-C24-N24	-2.90	105.49	110.86
24	A	1615	PAR	O34-C34-C44	-2.89	103.83	110.34
24	A	1606	PAR	C14-O33-C33	-2.86	110.52	118.01
24	A	1607	PAR	C34-C24-N24	-2.86	105.55	110.86
24	A	1616	PAR	O34-C34-C44	-2.81	104.01	110.34
24	A	1603	PAR	O34-C34-C44	-2.81	104.02	110.34
24	A	1605	PAR	O34-C34-C44	-2.80	104.03	110.34
24	A	1617	PAR	O34-C34-C44	-2.79	104.05	110.34
24	A	1618	PAR	C34-C24-N24	-2.78	105.70	110.86
24	A	1601	PAR	O34-C34-C44	-2.77	104.10	110.34
24	A	1604	PAR	C13-O52-C52	-2.74	110.84	118.01
24	A	1603	PAR	C13-O52-C52	-2.73	110.88	118.01
24	A	1608	PAR	O34-C34-C44	-2.72	104.22	110.34
24	A	1616	PAR	C14-O33-C33	-2.67	111.04	118.01
24	A	1613	PAR	C34-C24-N24	-2.67	105.91	110.86
24	A	1604	PAR	C14-O33-C33	-2.66	111.05	118.01
24	A	1611	PAR	O34-C34-C44	-2.66	104.34	110.34
24	A	1604	PAR	O34-C34-C44	-2.65	104.37	110.34
24	A	1601	PAR	C13-O52-C52	-2.65	111.09	118.01
24	A	1618	PAR	O34-C34-C44	-2.64	104.40	110.34
24	A	1609	PAR	C14-O33-C33	-2.61	111.18	118.01
24	A	1606	PAR	O34-C34-C44	-2.61	104.45	110.34
24	A	1612	PAR	O34-C34-C44	-2.55	104.59	110.34
24	A	1610	PAR	O34-C34-C24	-2.50	106.09	110.31
24	A	1607	PAR	O34-C34-C24	-2.49	106.10	110.31
24	A	1609	PAR	O34-C34-C44	-2.49	104.73	110.34
24	A	1613	PAR	C14-O33-C33	-2.48	111.52	118.01
24	A	1617	PAR	C14-O33-C33	-2.46	111.57	118.01
24	A	1605	PAR	C14-O33-C33	-2.39	111.77	118.01
24	A	1605	PAR	C13-O52-C52	-2.37	111.82	118.01
24	A	1610	PAR	C14-O33-C33	-2.35	111.86	118.01
24	A	1601	PAR	C14-O33-C33	-2.34	111.88	118.01
24	A	1612	PAR	C13-O52-C52	-2.33	111.91	118.01
24	A	1608	PAR	C13-O52-C52	-2.30	112.00	118.01
24	A	1614	PAR	O43-C13-C23	-2.29	101.57	104.78
24	A	1614	PAR	C14-O33-C33	-2.28	112.04	118.01
24	A	1603	PAR	O34-C34-C24	-2.28	106.46	110.31
24	A	1601	PAR	O43-C13-C23	-2.28	101.58	104.78
24	A	1601	PAR	O33-C14-O54	-2.27	104.93	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	1601	PAR	O34-C34-C24	-2.26	106.50	110.31
24	A	1608	PAR	O33-C14-O54	-2.24	105.01	110.68
24	A	1607	PAR	C13-O52-C52	-2.24	112.15	118.01
24	A	1615	PAR	O34-C34-C24	-2.23	106.54	110.31
24	A	1616	PAR	C13-O52-C52	-2.21	112.23	118.01
24	A	1617	PAR	C13-O52-C52	-2.20	112.25	118.01
24	A	1612	PAR	O33-C14-O54	-2.19	105.14	110.68
24	A	1606	PAR	O33-C14-O54	-2.18	105.17	110.68
24	A	1603	PAR	C14-O33-C33	-2.16	112.36	118.01
24	A	1602	PAR	O34-C34-C24	-2.12	106.73	110.31
24	A	1604	PAR	O33-C14-O54	-2.12	105.32	110.68
24	A	1602	PAR	C14-O33-C33	-2.12	112.47	118.01
24	A	1608	PAR	O34-C34-C24	-2.07	106.81	110.31
24	A	1610	PAR	C13-O52-C52	-2.06	112.63	118.01
24	A	1611	PAR	O33-C14-O54	-2.04	105.53	110.68
24	A	1606	PAR	C13-O52-C52	-2.03	112.72	118.01
24	A	1612	PAR	O34-C34-C24	-2.02	106.90	110.31
24	A	1603	PAR	O33-C14-O54	-2.01	105.58	110.68
24	A	1602	PAR	C34-C44-C54	-2.01	106.70	110.20
24	A	1602	PAR	O33-C14-O54	-2.01	105.60	110.68
24	A	1613	PAR	O52-C52-C42	2.01	112.74	107.49
24	A	1616	PAR	O54-C54-C44	2.02	113.47	109.68
24	A	1617	PAR	O52-C52-C42	2.06	112.88	107.49
24	A	1610	PAR	O51-C51-C61	2.06	111.57	106.36
24	A	1618	PAR	O54-C54-C44	2.06	113.56	109.68
24	A	1613	PAR	O51-C51-C61	2.07	111.59	106.36
24	A	1606	PAR	O51-C51-C61	2.10	111.65	106.36
24	A	1616	PAR	C11-O51-C51	2.10	117.83	113.75
24	A	1617	PAR	O51-C51-C61	2.11	111.68	106.36
24	A	1606	PAR	O54-C54-C44	2.11	113.64	109.68
24	A	1605	PAR	O54-C54-C44	2.11	113.65	109.68
24	A	1611	PAR	O54-C54-C44	2.12	113.65	109.68
24	A	1618	PAR	C22-C12-C62	2.13	113.38	110.11
24	A	1614	PAR	O43-C43-C53	2.13	113.79	109.17
24	A	1607	PAR	O51-C51-C61	2.13	111.75	106.36
24	A	1611	PAR	C22-C32-C42	2.15	115.28	109.53
24	A	1611	PAR	O52-C13-C23	2.17	112.26	107.75
24	A	1607	PAR	O54-C54-C44	2.18	113.78	109.68
24	A	1615	PAR	O51-C51-C61	2.21	111.94	106.36
24	A	1609	PAR	O54-C54-C44	2.21	113.83	109.68
24	A	1618	PAR	O52-C52-C42	2.22	113.29	107.49
24	A	1611	PAR	O51-C51-C61	2.23	111.98	106.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	1605	PAR	O51-C51-C61	2.23	111.98	106.36
24	A	1608	PAR	O51-C51-C61	2.23	112.00	106.36
24	A	1608	PAR	C11-O51-C51	2.26	118.12	113.75
24	A	1610	PAR	O54-C54-C44	2.27	113.94	109.68
24	A	1616	PAR	O52-C52-C42	2.29	113.48	107.49
24	A	1612	PAR	O51-C51-C61	2.31	112.18	106.36
24	A	1614	PAR	O51-C51-C61	2.31	112.18	106.36
24	A	1616	PAR	O51-C51-C61	2.31	112.20	106.36
24	A	1616	PAR	C22-C12-C62	2.32	113.67	110.11
24	A	1604	PAR	O51-C51-C61	2.32	112.22	106.36
24	A	1615	PAR	O54-C54-C44	2.33	114.05	109.68
24	A	1602	PAR	C22-C12-C62	2.33	113.69	110.11
24	A	1601	PAR	O51-C51-C61	2.34	112.27	106.36
24	A	1615	PAR	O11-C42-C52	2.36	113.65	107.49
24	A	1610	PAR	C22-C12-C62	2.36	113.73	110.11
24	A	1610	PAR	C31-C41-C51	2.36	114.32	110.20
24	A	1603	PAR	C11-O51-C51	2.37	118.34	113.75
24	A	1609	PAR	O51-C51-C41	2.39	114.17	109.68
24	A	1614	PAR	C22-C12-C62	2.41	113.81	110.11
24	A	1603	PAR	O51-C51-C61	2.43	112.49	106.36
24	A	1613	PAR	C22-C12-C62	2.43	113.84	110.11
24	A	1606	PAR	C11-O51-C51	2.46	118.52	113.75
24	A	1602	PAR	O54-C54-C44	2.48	114.33	109.68
24	A	1604	PAR	C11-O51-C51	2.50	118.59	113.75
24	A	1606	PAR	C22-C12-C62	2.50	113.95	110.11
24	A	1602	PAR	O51-C51-C61	2.52	112.73	106.36
24	A	1602	PAR	O11-C11-O51	2.53	117.09	110.68
24	A	1609	PAR	O51-C51-C61	2.55	112.80	106.36
24	A	1618	PAR	O51-C51-C61	2.55	112.81	106.36
24	A	1601	PAR	O11-C11-O51	2.61	117.28	110.68
24	A	1602	PAR	O52-C13-C23	2.61	113.18	107.75
24	A	1605	PAR	O11-C11-O51	2.62	117.30	110.68
24	A	1604	PAR	C22-C32-C42	2.62	116.52	109.53
24	A	1607	PAR	C22-C12-C62	2.63	114.15	110.11
24	A	1610	PAR	O52-C13-C23	2.68	113.33	107.75
24	A	1617	PAR	O54-C54-C44	2.68	114.71	109.68
24	A	1609	PAR	O11-C11-O51	2.69	117.48	110.68
24	A	1615	PAR	O52-C52-C42	2.69	114.52	107.49
24	A	1603	PAR	C22-C12-C62	2.73	114.30	110.11
24	A	1613	PAR	O11-C11-O51	2.76	117.68	110.68
24	A	1611	PAR	C11-O51-C51	2.80	119.19	113.75
24	A	1609	PAR	C22-C12-C62	2.86	114.50	110.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	1607	PAR	O11-C11-O51	2.87	117.96	110.68
24	A	1605	PAR	O52-C13-C23	2.98	113.94	107.75
24	A	1616	PAR	O11-C11-O51	2.98	118.22	110.68
24	A	1609	PAR	O52-C13-C23	3.00	113.99	107.75
24	A	1608	PAR	O11-C11-O51	3.01	118.29	110.68
24	A	1610	PAR	O11-C11-O51	3.04	118.37	110.68
24	A	1615	PAR	C22-C12-C62	3.05	114.79	110.11
24	A	1608	PAR	O52-C13-C23	3.06	114.11	107.75
24	A	1618	PAR	O52-C13-C23	3.06	114.11	107.75
24	A	1611	PAR	O11-C11-O51	3.11	118.56	110.68
24	A	1612	PAR	O52-C13-C23	3.15	114.30	107.75
24	A	1607	PAR	O52-C13-C23	3.17	114.35	107.75
24	A	1604	PAR	O52-C13-C23	3.21	114.42	107.75
24	A	1604	PAR	O11-C11-O51	3.22	118.83	110.68
24	A	1603	PAR	O11-C11-O51	3.24	118.87	110.68
24	A	1614	PAR	O11-C11-O51	3.28	118.97	110.68
24	A	1614	PAR	O52-C13-C23	3.30	114.61	107.75
24	A	1606	PAR	O11-C11-O51	3.34	119.13	110.68
24	A	1608	PAR	C22-C12-C62	3.35	115.26	110.11
24	A	1606	PAR	O52-C13-C23	3.50	115.04	107.75
24	A	1609	PAR	C11-O51-C51	3.59	120.71	113.75
24	A	1617	PAR	O11-C11-O51	3.66	119.95	110.68
24	A	1616	PAR	O52-C13-C23	3.67	115.38	107.75
24	A	1617	PAR	O52-C13-C23	3.69	115.44	107.75
24	A	1618	PAR	O11-C11-O51	3.72	120.10	110.68
24	A	1615	PAR	O11-C11-O51	3.80	120.30	110.68
24	A	1612	PAR	O11-C11-O51	3.88	120.49	110.68
24	A	1613	PAR	O52-C13-C23	3.90	115.86	107.75
24	A	1615	PAR	O52-C13-C23	3.98	116.03	107.75
24	A	1601	PAR	O52-C13-C23	4.03	116.12	107.75
24	A	1603	PAR	O52-C13-C23	4.12	116.32	107.75
24	A	1601	PAR	O33-C14-C24	5.11	117.42	107.96
24	A	1603	PAR	O33-C14-C24	5.23	117.65	107.96
24	A	1604	PAR	O33-C14-C24	5.27	117.72	107.96
24	A	1605	PAR	O33-C14-C24	5.55	118.24	107.96
24	A	1615	PAR	O33-C14-C24	5.63	118.39	107.96
24	A	1614	PAR	O33-C14-C24	5.73	118.56	107.96
24	A	1608	PAR	O33-C14-C24	5.93	118.94	107.96
24	A	1606	PAR	O33-C14-C24	6.01	119.09	107.96
24	A	1617	PAR	O33-C14-C24	6.05	119.16	107.96
24	A	1613	PAR	O33-C14-C24	6.13	119.31	107.96
24	A	1611	PAR	O33-C14-C24	6.15	119.36	107.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	1616	PAR	O33-C14-C24	6.17	119.39	107.96
24	A	1612	PAR	O33-C14-C24	6.29	119.60	107.96
24	A	1618	PAR	O33-C14-C24	6.35	119.72	107.96
24	A	1607	PAR	O33-C14-C24	6.45	119.90	107.96
24	A	1609	PAR	O33-C14-C24	6.48	119.96	107.96
24	A	1610	PAR	O33-C14-C24	7.06	121.04	107.96
24	A	1602	PAR	O33-C14-C24	7.65	122.12	107.96

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	1618	PAR	C33-O33-C14-C24
24	A	1613	PAR	C42-O11-C11-C21
24	A	1615	PAR	C33-O33-C14-C24
24	A	1612	PAR	C42-O11-C11-C21
24	A	1602	PAR	C33-O33-C14-C24
24	A	1610	PAR	C33-O33-C14-C24
24	A	1613	PAR	C52-O52-C13-C23
24	A	1609	PAR	C33-O33-C14-C24

All (6) ring outliers are listed below:

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

17 monomers are involved in 61 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	1601	PAR	2	0
24	A	1602	PAR	4	0
24	A	1603	PAR	7	0
24	A	1604	PAR	3	0
24	A	1605	PAR	4	0
24	A	1606	PAR	1	0
24	A	1608	PAR	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	1609	PAR	1	0
24	A	1610	PAR	6	0
24	A	1611	PAR	5	0
24	A	1612	PAR	4	0
24	A	1613	PAR	7	0
24	A	1614	PAR	1	0
24	A	1615	PAR	3	0
24	A	1616	PAR	5	0
24	A	1617	PAR	1	0
24	A	1618	PAR	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	1498/1522 (98%)	-0.40	3 (0%) 95 94	49, 88, 175, 339	0
2	B	236/256 (92%)	-0.33	0 100 100	70, 114, 159, 187	0
3	C	207/239 (86%)	-0.34	0 100 100	80, 108, 146, 160	0
4	D	208/209 (99%)	-0.48	0 100 100	56, 92, 128, 166	0
5	E	151/162 (93%)	-0.41	0 100 100	47, 73, 107, 151	0
6	F	101/101 (100%)	-0.44	0 100 100	68, 108, 134, 160	0
7	G	155/156 (99%)	-0.55	0 100 100	66, 106, 162, 193	0
8	H	138/138 (100%)	-0.58	0 100 100	47, 74, 104, 132	0
9	I	127/128 (99%)	0.02	4 (3%) 52 40	69, 112, 142, 158	0
10	J	99/105 (94%)	-0.04	2 (2%) 68 57	75, 127, 185, 199	0
11	K	119/129 (92%)	-0.30	2 (1%) 73 62	54, 94, 132, 210	0
12	L	124/135 (91%)	-0.20	2 (1%) 74 63	55, 80, 124, 185	0
13	M	118/126 (93%)	0.03	1 (0%) 87 82	78, 108, 137, 149	0
14	N	60/61 (98%)	-0.48	0 100 100	75, 99, 139, 181	0
15	O	88/89 (98%)	-0.28	2 (2%) 64 52	56, 90, 123, 172	0
16	P	84/88 (95%)	-0.40	0 100 100	58, 77, 107, 151	0
17	Q	100/105 (95%)	-0.06	0 100 100	63, 81, 120, 155	0
18	R	73/88 (82%)	0.06	2 (2%) 58 46	68, 100, 153, 221	0
19	S	81/93 (87%)	-0.31	0 100 100	89, 124, 151, 179	0
20	T	99/106 (93%)	-0.16	0 100 100	65, 85, 130, 168	0
21	U	25/27 (92%)	0.09	0 100 100	87, 113, 132, 139	0
22	V	3/3 (100%)	0.40	0 100 100	99, 99, 103, 105	0
23	W	15/15 (100%)	0.64	0 100 100	127, 144, 218, 227	0
All	All	3909/4081 (95%)	-0.33	18 (0%) 91 88	47, 96, 156, 339	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
12	L	129	ALA	6.7
1	A	1539	C	4.3
11	K	128	ALA	3.3
15	O	89	GLY	3.2
1	A	1129	C	3.2
12	L	128	ALA	3.1
13	M	5	ALA	2.8
9	I	15	ALA	2.7
18	R	17	SER	2.6
9	I	7	THR	2.3
9	I	8	GLY	2.2
11	K	129	SER	2.2
1	A	1533	C	2.2
18	R	88	LYS	2.1
10	J	98	ILE	2.1
15	O	88	ARG	2.1
9	I	19	LEU	2.1
10	J	73	ASP	2.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	5MC	A	1407	21/22	0.98	0.13	-	61,67,72,74	0
1	MA6	A	1519	24/25	0.96	0.27	-	55,57,64,67	0
1	M2G	A	966	25/26	0.96	0.16	-	66,100,115,127	0
1	PSU	A	1541	20/21	0.85	0.54	-	228,249,272,273	0
1	7MG	A	527	24/25	0.96	0.19	-	63,69,82,84	0
1	PSU	A	516	20/21	0.95	0.23	-	83,94,105,108	0
1	PSU	A	1540	20/21	0.80	0.73	-	210,258,270,270	0
12	0TD	L	92	10/11	0.97	0.40	-	55,83,98,428	0
1	5MC	A	967	21/22	0.98	0.14	-	59,75,118,121	0
1	UR3	A	1498	21/22	0.98	0.20	-	63,71,81,88	0
1	2MG	A	1207	24/25	0.95	0.12	-	91,106,114,118	0
1	5MC	A	1400	21/22	0.97	0.18	-	44,73,95,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	MA6	A	1518	24/25	0.98	0.20	-	58,69,75,78	0
1	4OC	A	1402	22/23	0.96	0.20	-	57,63,67,91	0
1	5MC	A	1404	21/22	0.98	0.14	-	55,64,71,72	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
25	MG	N	102	1/1	0.84	0.57	26.02	82,82,82,82	0
25	MG	A	1914	1/1	0.90	0.75	19.16	44,44,44,44	0
25	MG	A	1867	1/1	0.92	0.57	17.64	29,29,29,29	0
24	PAR	A	1618	42/42	0.79	0.37	15.47	166,166,166,166	0
25	MG	A	1912	1/1	0.91	0.34	14.32	51,51,51,51	0
25	MG	A	1888	1/1	0.71	0.66	13.55	71,71,71,71	0
25	MG	A	1619	1/1	0.96	0.34	10.83	69,69,69,69	0
25	MG	A	1803	1/1	0.69	0.36	10.31	71,71,71,71	0
25	MG	A	1823	1/1	0.98	0.36	9.59	57,57,57,57	0
25	MG	A	1853	1/1	0.49	0.54	9.11	44,44,44,44	0
24	PAR	A	1614	42/42	0.84	0.29	8.11	174,174,174,174	0
25	MG	A	1832	1/1	0.56	0.41	7.12	77,77,77,77	0
25	MG	A	1890	1/1	0.88	0.53	7.06	59,59,59,59	0
25	MG	A	1818	1/1	0.86	0.21	6.45	36,36,36,36	0
24	PAR	A	1611	42/42	0.91	0.30	6.43	131,131,131,131	0
25	MG	A	1794	1/1	0.80	0.34	6.37	61,61,61,61	0
25	MG	A	1883	1/1	0.74	0.37	5.84	62,62,62,62	0
25	MG	A	1694	1/1	0.92	0.26	5.27	108,108,108,108	0
25	MG	A	1934	1/1	0.85	0.25	5.04	69,69,69,69	0
24	PAR	A	1615	42/42	0.81	0.32	5.03	149,149,149,149	0
24	PAR	A	1616	42/42	0.76	0.28	4.51	216,216,216,216	0
24	PAR	A	1608	42/42	0.89	0.25	4.14	81,81,81,81	42

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
25	MG	A	1918	1/1	0.87	0.25	3.95	39,39,39,39	0
24	PAR	A	1613	42/42	0.92	0.24	3.94	120,120,120,120	0
24	PAR	A	1610	42/42	0.88	0.38	3.69	144,144,144,144	0
24	PAR	A	1617	42/42	0.87	0.30	3.61	189,189,189,189	0
25	MG	A	1862	1/1	0.90	0.27	3.34	38,38,38,38	0
25	MG	A	1935	1/1	0.83	0.32	3.27	57,57,57,57	0
24	PAR	A	1612	42/42	0.90	0.22	2.99	131,131,131,131	0
25	MG	A	1651	1/1	0.96	0.20	2.60	48,48,48,48	0
25	MG	A	1740	1/1	0.98	0.17	2.58	113,113,113,113	0
26	ZN	D	301	1/1	0.98	0.30	2.03	141,141,141,141	0
24	PAR	A	1604	42/42	0.95	0.24	1.98	64,64,64,64	0
25	MG	A	1657	1/1	0.92	0.22	1.96	101,101,101,101	0
25	MG	A	1682	1/1	0.86	0.16	1.72	104,104,104,104	0
25	MG	S	101	1/1	0.97	0.28	1.72	22,22,22,22	0
24	PAR	A	1609	42/42	0.89	0.34	1.50	121,121,121,121	42
25	MG	A	1802	1/1	0.96	0.26	1.46	46,46,46,46	0
24	PAR	A	1606	42/42	0.93	0.21	1.39	113,113,113,113	0
25	MG	A	1915	1/1	0.96	0.22	1.37	59,59,59,59	0
25	MG	A	1635	1/1	0.88	0.26	1.18	45,45,45,45	0
25	MG	A	1649	1/1	0.91	0.19	0.93	47,47,47,47	0
24	PAR	A	1601	42/42	0.96	0.17	0.90	64,64,64,64	0
25	MG	A	1858	1/1	0.88	0.16	0.90	37,37,37,37	0
24	PAR	A	1605	42/42	0.90	0.23	0.89	94,94,94,94	42
25	MG	A	1760	1/1	0.94	0.18	0.87	44,44,44,44	0
25	MG	A	1764	1/1	0.96	0.22	0.82	65,65,65,65	0
25	MG	A	1754	1/1	0.90	0.22	0.77	67,67,67,67	0
24	PAR	A	1603	42/42	0.94	0.19	0.44	103,103,103,103	3
24	PAR	A	1607	42/42	0.92	0.23	0.33	99,99,99,99	42
25	MG	A	1673	1/1	0.94	0.17	0.21	73,73,73,73	0
25	MG	A	1879	1/1	0.96	0.17	0.02	56,56,56,56	0
25	MG	A	1678	1/1	0.97	0.20	-0.05	48,48,48,48	0
24	PAR	A	1602	42/42	0.95	0.16	-0.09	71,71,71,71	0
25	MG	A	1687	1/1	0.96	0.13	-0.11	53,53,53,53	0
25	MG	A	1759	1/1	0.82	0.16	-0.23	121,121,121,121	0
25	MG	A	1907	1/1	0.95	0.14	-0.31	53,53,53,53	0
26	ZN	N	101	1/1	0.99	0.14	-0.45	88,88,88,88	0
25	MG	A	1793	1/1	0.96	0.19	-0.55	22,22,22,22	0
25	MG	D	303	1/1	0.95	0.16	-0.87	73,73,73,73	0
25	MG	A	1844	1/1	0.85	0.17	-1.02	35,35,35,35	0
25	MG	A	1749	1/1	0.99	0.15	-1.04	72,72,72,72	0
25	MG	A	1666	1/1	0.97	0.13	-1.18	91,91,91,91	0
25	MG	A	1826	1/1	0.97	0.12	-1.25	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
25	MG	A	1661	1/1	0.95	0.10	-1.27	90,90,90,90	0
25	MG	A	1634	1/1	0.98	0.13	-1.48	42,42,42,42	0
25	MG	Q	201	1/1	0.93	0.15	-1.53	60,60,60,60	0
25	MG	A	1762	1/1	0.98	0.13	-1.60	63,63,63,63	0
25	MG	A	1910	1/1	0.96	0.10	-1.66	45,45,45,45	0
25	MG	A	1711	1/1	0.98	0.09	-1.70	64,64,64,64	0
25	MG	A	1942	1/1	0.92	0.08	-1.74	143,143,143,143	0
25	MG	A	1814	1/1	0.97	0.16	-1.85	26,26,26,26	0
25	MG	A	1646	1/1	0.96	0.12	-2.01	69,69,69,69	0
25	MG	A	1743	1/1	0.94	0.12	-2.05	71,71,71,71	0
25	MG	A	1938	1/1	0.97	0.05	-2.16	43,43,43,43	0
25	MG	A	1667	1/1	0.97	0.15	-2.35	56,56,56,56	0
25	MG	A	1774	1/1	0.89	0.08	-3.32	71,71,71,71	0
25	MG	A	1644	1/1	0.99	0.09	-3.32	40,40,40,40	0
25	MG	A	1775	1/1	0.99	0.07	-3.52	75,75,75,75	0
25	MG	A	1848	1/1	0.94	0.13	-3.74	42,42,42,42	0
25	MG	A	1658	1/1	0.98	0.08	-4.83	57,57,57,57	0
25	MG	A	1698	1/1	0.98	0.08	-5.37	56,56,56,56	0
25	MG	A	1751	1/1	0.93	0.08	-7.98	95,95,95,95	0
25	MG	A	1629	1/1	0.99	0.10	-8.18	60,60,60,60	0
25	MG	A	1874	1/1	0.98	0.37	-	13,13,13,13	0
25	MG	A	1648	1/1	0.99	0.13	-	64,64,64,64	0
25	MG	A	1880	1/1	0.81	0.28	-	60,60,60,60	0
25	MG	A	1729	1/1	0.99	0.04	-	73,73,73,73	0
25	MG	A	1840	1/1	0.87	0.34	-	22,22,22,22	0
25	MG	A	1654	1/1	0.98	0.09	-	75,75,75,75	0
25	MG	A	1913	1/1	0.89	0.37	-	49,49,49,49	0
25	MG	A	1919[A]	1/1	0.70	0.27	-	9,9,9,9	1
25	MG	A	1664	1/1	0.93	0.38	-	74,74,74,74	0
25	MG	A	1756	1/1	0.95	0.10	-	93,93,93,93	0
25	MG	A	1955	1/1	0.88	0.14	-	179,179,179,179	0
25	MG	A	1723	1/1	0.81	0.11	-	94,94,94,94	0
25	MG	A	1773	1/1	0.87	0.18	-	74,74,74,74	0
25	MG	A	1660	1/1	0.99	0.17	-	84,84,84,84	0
25	MG	A	1738	1/1	0.98	0.11	-	59,59,59,59	0
25	MG	A	1742	1/1	0.95	0.21	-	72,72,72,72	0
25	MG	A	1950	1/1	0.86	0.19	-	177,177,177,177	0
25	MG	A	1904	1/1	0.90	0.21	-	49,49,49,49	0
25	MG	A	1892	1/1	0.83	0.22	-	46,46,46,46	0
25	MG	A	1926	1/1	0.95	0.10	-	58,58,58,58	0
25	MG	A	1633	1/1	0.97	0.06	-	54,54,54,54	0
25	MG	A	1780	1/1	0.89	0.49	-	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
25	MG	A	1957	1/1	0.85	0.13	-	103,103,103,103	0
25	MG	A	1770	1/1	0.94	0.22	-	90,90,90,90	0
25	MG	A	1639	1/1	0.96	0.35	-	55,55,55,55	0
25	MG	A	1882[B]	1/1	0.74	0.60	-	0,0,0,0	1
25	MG	E	201	1/1	0.78	0.21	-	92,92,92,92	0
25	MG	A	1886	1/1	0.95	0.27	-	50,50,50,50	0
25	MG	A	1779	1/1	0.91	0.23	-	55,55,55,55	0
25	MG	A	1677	1/1	0.94	0.48	-	118,118,118,118	0
25	MG	A	1788	1/1	0.91	0.32	-	95,95,95,95	0
25	MG	A	1686	1/1	0.97	0.14	-	91,91,91,91	0
25	MG	A	1753	1/1	0.82	0.10	-	94,94,94,94	0
25	MG	E	203	1/1	0.89	0.10	-	80,80,80,80	0
25	MG	A	1632	1/1	0.99	0.10	-	65,65,65,65	0
25	MG	A	1638	1/1	0.91	0.26	-	56,56,56,56	0
25	MG	A	1778	1/1	0.86	0.39	-	59,59,59,59	0
25	MG	A	1836	1/1	0.42	0.30	-	75,75,75,75	0
25	MG	A	1768	1/1	0.86	0.16	-	103,103,103,103	0
25	MG	A	1732	1/1	0.95	0.09	-	84,84,84,84	0
25	MG	A	1791	1/1	0.89	0.26	-	30,30,30,30	0
25	MG	A	1931	1/1	0.76	0.69	-	58,58,58,58	0
25	MG	S	102	1/1	0.73	0.24	-	73,73,73,73	0
25	MG	A	1894	1/1	0.90	0.23	-	66,66,66,66	0
25	MG	A	1906	1/1	0.94	0.19	-	73,73,73,73	0
25	MG	A	1952	1/1	0.72	0.18	-	148,148,148,148	0
25	MG	A	1843	1/1	0.96	0.09	-	35,35,35,35	0
25	MG	A	1951	1/1	0.87	0.25	-	110,110,110,110	0
25	MG	A	1767	1/1	0.98	0.12	-	72,72,72,72	0
25	MG	A	1905	1/1	0.85	0.71	-	83,83,83,83	0
25	MG	A	1929	1/1	0.84	0.76	-	44,44,44,44	0
25	MG	A	1897[B]	1/1	0.86	0.53	-	0,0,0,0	1
25	MG	A	1721	1/1	0.76	0.83	-	43,43,43,43	0
25	MG	A	1769	1/1	0.85	0.16	-	114,114,114,114	0
25	MG	A	1835	1/1	0.77	0.24	-	71,71,71,71	0
25	MG	A	1709	1/1	0.95	0.08	-	94,94,94,94	0
25	MG	A	1670	1/1	0.76	0.19	-	64,64,64,64	0
25	MG	A	1869	1/1	0.52	0.88	-	59,59,59,59	0
25	MG	A	1898	1/1	0.86	0.31	-	61,61,61,61	0
25	MG	A	1676	1/1	0.91	0.27	-	75,75,75,75	0
25	MG	A	1817	1/1	0.88	0.63	-	54,54,54,54	0
25	MG	A	1855	1/1	0.91	0.16	-	24,24,24,24	0
25	MG	A	1893	1/1	0.75	0.55	-	53,53,53,53	0
25	MG	A	1700	1/1	0.84	0.38	-	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
25	MG	A	1662	1/1	0.74	0.43	-	77,77,77,77	0
25	MG	A	1838	1/1	0.97	0.56	-	50,50,50,50	0
25	MG	A	1882[A]	1/1	0.74	0.60	-	0,0,0,0	1
25	MG	A	1622	1/1	0.84	0.08	-	106,106,106,106	0
25	MG	A	1766	1/1	0.97	0.07	-	97,97,97,97	0
25	MG	A	1956	1/1	0.77	0.15	-	193,193,193,193	0
25	MG	A	1630	1/1	0.98	0.07	-	83,83,83,83	0
25	MG	A	1703	1/1	0.89	0.24	-	57,57,57,57	0
25	MG	A	1916	1/1	0.84	0.39	-	51,51,51,51	0
25	MG	A	1704	1/1	0.96	0.13	-	83,83,83,83	0
25	MG	A	1739	1/1	0.70	0.27	-	85,85,85,85	0
25	MG	A	1745	1/1	0.87	0.36	-	64,64,64,64	0
25	MG	A	1873	1/1	0.97	0.51	-	29,29,29,29	0
25	MG	P	103	1/1	0.87	0.20	-	44,44,44,44	0
25	MG	A	1798	1/1	0.71	0.17	-	70,70,70,70	0
25	MG	A	1801	1/1	0.70	0.84	-	57,57,57,57	0
25	MG	A	1679	1/1	0.93	0.18	-	47,47,47,47	0
25	MG	A	1800[A]	1/1	0.74	0.52	-	7,7,7,7	1
25	MG	A	1727	1/1	0.91	0.08	-	101,101,101,101	0
25	MG	A	1781	1/1	0.96	0.14	-	67,67,67,67	0
25	MG	A	1827	1/1	0.88	0.29	-	78,78,78,78	0
25	MG	A	1833	1/1	0.78	0.20	-	59,59,59,59	0
25	MG	A	1656	1/1	0.97	0.15	-	67,67,67,67	0
25	MG	A	1786	1/1	0.92	0.21	-	97,97,97,97	0
25	MG	A	1831	1/1	0.91	0.14	-	40,40,40,40	0
25	MG	A	1792	1/1	0.97	0.28	-	32,32,32,32	0
25	MG	A	1674	1/1	0.95	0.20	-	18,18,18,18	0
25	MG	A	1941	1/1	0.88	0.13	-	145,145,145,145	0
25	MG	A	1696	1/1	0.95	0.09	-	136,136,136,136	0
25	MG	A	1806	1/1	0.75	0.60	-	91,91,91,91	0
25	MG	A	1917	1/1	0.70	0.39	-	61,61,61,61	0
25	MG	A	1641	1/1	0.94	0.16	-	56,56,56,56	0
25	MG	A	1713	1/1	0.82	0.35	-	63,63,63,63	0
25	MG	A	1909	1/1	0.78	0.81	-	68,68,68,68	0
25	MG	H	201	1/1	0.95	0.55	-	53,53,53,53	0
25	MG	A	1695	1/1	0.96	0.17	-	94,94,94,94	0
25	MG	A	1799	1/1	0.96	0.34	-	59,59,59,59	0
25	MG	A	1868	1/1	0.69	0.41	-	68,68,68,68	0
25	MG	A	1652[A]	1/1	0.79	0.47	-	11,11,11,11	1
25	MG	A	1899	1/1	0.96	0.54	-	18,18,18,18	0
25	MG	A	1637	1/1	0.94	0.17	-	29,29,29,29	0
25	MG	A	1642	1/1	0.96	0.13	-	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
25	MG	A	1750	1/1	0.83	0.54	-	67,67,67,67	0
25	MG	A	1922	1/1	0.74	0.60	-	76,76,76,76	0
25	MG	A	1705	1/1	0.97	0.13	-	57,57,57,57	0
25	MG	A	1841	1/1	0.74	0.39	-	64,64,64,64	0
25	MG	A	1712	1/1	0.87	0.19	-	34,34,34,34	0
25	MG	A	1812	1/1	0.58	0.68	-	65,65,65,65	0
25	MG	A	1653[B]	1/1	0.87	0.60	-	11,11,11,11	1
25	MG	A	1821	1/1	0.87	0.29	-	33,33,33,33	0
25	MG	A	1924	1/1	0.86	0.39	-	54,54,54,54	0
25	MG	A	1684	1/1	0.99	0.09	-	25,25,25,25	0
25	MG	P	101	1/1	0.89	0.21	-	13,13,13,13	0
25	MG	A	1692	1/1	0.96	0.13	-	74,74,74,74	0
25	MG	A	1737	1/1	0.99	0.14	-	63,63,63,63	0
25	MG	A	1925	1/1	0.89	0.18	-	42,42,42,42	0
25	MG	E	202	1/1	0.75	0.37	-	45,45,45,45	0
25	MG	A	1860	1/1	0.97	0.24	-	55,55,55,55	0
25	MG	A	1881	1/1	0.74	0.37	-	63,63,63,63	0
25	MG	A	1693	1/1	0.83	0.26	-	96,96,96,96	0
25	MG	A	1797	1/1	0.54	0.55	-	47,47,47,47	0
25	MG	A	1620	1/1	0.94	0.07	-	70,70,70,70	0
25	MG	A	1825	1/1	0.82	0.34	-	59,59,59,59	0
25	MG	A	1627	1/1	0.97	0.10	-	30,30,30,30	0
25	MG	A	1744	1/1	0.98	0.30	-	62,62,62,62	0
25	MG	A	1901[A]	1/1	0.87	0.21	-	16,16,16,16	1
25	MG	A	1946	1/1	0.80	0.10	-	146,146,146,146	0
25	MG	V	101	1/1	0.59	0.56	-	75,75,75,75	0
25	MG	A	1640	1/1	0.94	0.12	-	59,59,59,59	0
25	MG	A	1854	1/1	0.97	0.14	-	40,40,40,40	0
25	MG	A	1631	1/1	0.99	0.09	-	75,75,75,75	0
25	MG	A	1834	1/1	0.92	0.16	-	57,57,57,57	0
25	MG	A	1675	1/1	0.74	0.38	-	74,74,74,74	0
25	MG	A	1872	1/1	0.93	0.25	-	30,30,30,30	0
25	MG	A	1933	1/1	0.95	0.11	-	82,82,82,82	0
25	MG	A	1947	1/1	0.86	0.09	-	133,133,133,133	0
25	MG	A	1708	1/1	0.99	0.07	-	55,55,55,55	0
25	MG	A	1685	1/1	0.99	0.08	-	57,57,57,57	0
25	MG	A	1936	1/1	0.88	0.30	-	68,68,68,68	0
25	MG	A	1896	1/1	0.76	0.40	-	57,57,57,57	0
25	MG	A	1908	1/1	0.89	0.54	-	66,66,66,66	0
25	MG	A	1655	1/1	0.96	0.10	-	78,78,78,78	0
25	MG	A	1747	1/1	0.93	0.21	-	108,108,108,108	0
25	MG	A	1805	1/1	0.92	0.41	-	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
25	MG	A	1746	1/1	0.84	0.39	-	146,146,146,146	0
25	MG	A	1804	1/1	0.95	0.17	-	62,62,62,62	0
25	MG	A	1626	1/1	0.95	0.06	-	100,100,100,100	0
25	MG	A	1715	1/1	0.89	0.32	-	82,82,82,82	0
25	MG	A	1659	1/1	0.94	0.25	-	87,87,87,87	0
25	MG	A	1911	1/1	0.89	0.16	-	49,49,49,49	0
25	MG	T	201	1/1	0.93	0.30	-	88,88,88,88	0
25	MG	A	1923	1/1	0.96	0.17	-	29,29,29,29	0
25	MG	A	1809	1/1	0.65	0.89	-	76,76,76,76	0
25	MG	A	1680	1/1	0.99	0.11	-	67,67,67,67	0
25	MG	A	1944	1/1	0.97	0.11	-	74,74,74,74	0
25	MG	A	1757	1/1	0.95	0.07	-	133,133,133,133	0
25	MG	A	1954	1/1	0.71	0.41	-	150,150,150,150	0
25	MG	A	1863	1/1	0.89	0.21	-	53,53,53,53	0
25	MG	A	1719	1/1	0.85	0.39	-	72,72,72,72	0
25	MG	A	1861	1/1	0.82	0.08	-	57,57,57,57	0
25	MG	A	1690	1/1	0.96	0.17	-	100,100,100,100	0
25	MG	A	1820	1/1	0.78	0.40	-	70,70,70,70	0
25	MG	A	1683	1/1	0.90	0.20	-	102,102,102,102	0
25	MG	A	1720	1/1	0.86	0.28	-	89,89,89,89	0
25	MG	A	1901[B]	1/1	0.87	0.21	-	16,16,16,16	1
25	MG	A	1672	1/1	0.95	0.17	-	56,56,56,56	0
25	MG	A	1714	1/1	0.81	0.24	-	66,66,66,66	0
25	MG	A	1717	1/1	0.86	0.12	-	110,110,110,110	0
25	MG	A	1864[B]	1/1	0.82	0.28	-	11,11,11,11	1
25	MG	A	1777	1/1	0.91	0.39	-	60,60,60,60	0
25	MG	A	1857	1/1	0.67	0.99	-	54,54,54,54	0
25	MG	A	1691	1/1	0.87	0.33	-	111,111,111,111	0
25	MG	A	1789	1/1	0.91	0.29	-	127,127,127,127	0
25	MG	A	1839	1/1	0.96	0.17	-	56,56,56,56	0
25	MG	A	1932	1/1	0.65	1.24	-	71,71,71,71	0
25	MG	A	1765	1/1	0.91	0.10	-	113,113,113,113	0
25	MG	A	1851	1/1	0.84	0.35	-	57,57,57,57	0
25	MG	A	1943	1/1	0.87	0.23	-	178,178,178,178	0
25	MG	A	1811	1/1	0.88	0.28	-	56,56,56,56	0
25	MG	A	1647	1/1	0.98	0.21	-	72,72,72,72	0
25	MG	A	1852	1/1	0.82	0.33	-	47,47,47,47	0
25	MG	A	1706	1/1	0.95	0.24	-	52,52,52,52	0
25	MG	A	1846	1/1	0.98	0.19	-	49,49,49,49	0
25	MG	A	1871	1/1	0.92	0.21	-	63,63,63,63	0
25	MG	A	1808	1/1	0.91	0.24	-	31,31,31,31	0
25	MG	A	1725	1/1	0.95	0.23	-	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
25	MG	A	1702	1/1	0.77	0.12	-	104,104,104,104	0
25	MG	A	1876	1/1	0.76	0.73	-	69,69,69,69	0
25	MG	A	1919[B]	1/1	0.70	0.27	-	9,9,9,9	1
25	MG	O	101	1/1	0.68	0.21	-	112,112,112,112	0
25	MG	A	1681	1/1	0.77	0.40	-	30,30,30,30	0
25	MG	A	1891	1/1	0.74	0.70	-	50,50,50,50	0
25	MG	A	1900	1/1	0.97	0.21	-	27,27,27,27	0
25	MG	A	1819	1/1	0.81	0.43	-	64,64,64,64	0
25	MG	A	1902	1/1	0.93	0.22	-	64,64,64,64	0
25	MG	A	1741	1/1	0.95	0.22	-	52,52,52,52	0
25	MG	A	1748	1/1	0.93	0.26	-	87,87,87,87	0
25	MG	A	1837	1/1	0.88	0.33	-	54,54,54,54	0
25	MG	A	1701	1/1	0.87	0.16	-	85,85,85,85	0
25	MG	A	1625	1/1	0.95	0.16	-	30,30,30,30	0
25	MG	A	1787	1/1	0.81	0.23	-	66,66,66,66	0
25	MG	A	1621	1/1	0.95	0.16	-	69,69,69,69	0
25	MG	A	1865	1/1	0.76	0.61	-	58,58,58,58	0
25	MG	A	1697	1/1	0.90	0.20	-	77,77,77,77	0
25	MG	A	1669	1/1	0.66	0.53	-	76,76,76,76	0
25	MG	A	1845	1/1	0.88	0.24	-	64,64,64,64	0
25	MG	A	1813	1/1	0.32	0.74	-	53,53,53,53	0
25	MG	A	1671	1/1	0.99	0.12	-	66,66,66,66	0
25	MG	A	1822	1/1	0.82	0.28	-	63,63,63,63	0
25	MG	A	1628	1/1	0.93	0.24	-	48,48,48,48	0
25	MG	A	1730	1/1	0.92	0.10	-	118,118,118,118	0
25	MG	A	1885	1/1	0.78	0.35	-	45,45,45,45	0
25	MG	A	1877	1/1	0.83	0.10	-	59,59,59,59	0
25	MG	E	204	1/1	0.77	0.20	-	70,70,70,70	0
25	MG	A	1795	1/1	0.94	0.22	-	57,57,57,57	0
25	MG	L	201	1/1	0.79	0.14	-	57,57,57,57	0
25	MG	A	1636	1/1	0.97	0.21	-	68,68,68,68	0
25	MG	A	1755	1/1	0.92	0.18	-	74,74,74,74	0
25	MG	A	1903	1/1	0.65	0.29	-	74,74,74,74	0
25	MG	A	1830	1/1	0.79	0.24	-	70,70,70,70	0
25	MG	A	1771	1/1	0.85	0.45	-	89,89,89,89	0
25	MG	A	1807	1/1	0.84	0.60	-	83,83,83,83	0
25	MG	A	1624	1/1	0.98	0.17	-	58,58,58,58	0
25	MG	A	1847	1/1	0.43	0.68	-	85,85,85,85	0
25	MG	A	1870	1/1	0.87	0.28	-	35,35,35,35	0
25	MG	A	1785	1/1	0.98	0.11	-	51,51,51,51	0
25	MG	A	1800[B]	1/1	0.74	0.52	-	7,7,7,7	1
25	MG	A	1716	1/1	0.95	0.23	-	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
25	MG	A	1940	1/1	0.79	0.50	-	82,82,82,82	0
25	MG	A	1688	1/1	0.93	0.15	-	60,60,60,60	0
25	MG	A	1920	1/1	0.95	0.54	-	50,50,50,50	0
25	MG	A	1726	1/1	0.87	0.10	-	93,93,93,93	0
25	MG	A	1949	1/1	0.81	0.28	-	228,228,228,228	0
25	MG	A	1782	1/1	0.99	0.10	-	68,68,68,68	0
25	MG	A	1699	1/1	0.85	0.20	-	79,79,79,79	0
25	MG	A	1689	1/1	0.97	0.11	-	75,75,75,75	0
25	MG	A	1731	1/1	0.93	0.10	-	121,121,121,121	0
25	MG	A	1772	1/1	0.58	0.66	-	61,61,61,61	0
25	MG	A	1824	1/1	0.87	0.35	-	64,64,64,64	0
25	MG	A	1668	1/1	0.95	0.48	-	66,66,66,66	0
25	MG	A	1815	1/1	0.79	0.44	-	45,45,45,45	0
25	MG	A	1945	1/1	0.94	0.16	-	156,156,156,156	0
25	MG	A	1816	1/1	0.76	0.79	-	53,53,53,53	0
25	MG	A	1790	1/1	0.87	0.15	-	162,162,162,162	0
25	MG	A	1850	1/1	0.89	0.22	-	71,71,71,71	0
25	MG	A	1884	1/1	0.90	0.37	-	55,55,55,55	0
25	MG	D	302	1/1	0.69	0.43	-	71,71,71,71	0
25	MG	A	1736	1/1	0.80	0.19	-	88,88,88,88	0
25	MG	A	1707	1/1	0.96	0.14	-	80,80,80,80	0
25	MG	A	1643	1/1	0.66	0.51	-	40,40,40,40	0
25	MG	A	1953	1/1	0.87	0.13	-	179,179,179,179	0
25	MG	A	1722	1/1	0.97	0.07	-	43,43,43,43	0
25	MG	A	1897[A]	1/1	0.86	0.53	-	0,0,0,0	1
25	MG	A	1783	1/1	0.74	0.76	-	41,41,41,41	0
25	MG	A	1829	1/1	0.98	0.16	-	37,37,37,37	0
25	MG	A	1927	1/1	0.86	0.18	-	62,62,62,62	0
25	MG	A	1733	1/1	0.83	0.30	-	61,61,61,61	0
25	MG	A	1663	1/1	0.98	0.08	-	36,36,36,36	0
25	MG	A	1939	1/1	0.45	0.27	-	57,57,57,57	0
25	MG	A	1735	1/1	0.92	0.34	-	67,67,67,67	0
25	MG	A	1796	1/1	0.60	0.84	-	58,58,58,58	0
25	MG	A	1728	1/1	0.91	0.11	-	103,103,103,103	0
25	MG	A	1864[A]	1/1	0.82	0.28	-	11,11,11,11	1
25	MG	A	1842	1/1	0.85	0.80	-	43,43,43,43	0
25	MG	A	1761	1/1	0.68	0.19	-	155,155,155,155	0
25	MG	A	1849	1/1	0.91	0.39	-	40,40,40,40	0
25	MG	A	1875	1/1	0.96	0.12	-	14,14,14,14	0
25	MG	A	1887	1/1	0.67	0.66	-	64,64,64,64	0
25	MG	A	1948	1/1	0.91	0.12	-	122,122,122,122	0
25	MG	A	1650	1/1	0.93	0.20	-	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
25	MG	A	1784	1/1	0.66	0.31	-	89,89,89,89	0
25	MG	A	1776	1/1	0.85	0.20	-	65,65,65,65	0
25	MG	A	1734	1/1	0.50	0.46	-	63,63,63,63	0
25	MG	A	1665	1/1	0.93	0.18	-	57,57,57,57	0
25	MG	A	1856	1/1	0.69	0.26	-	59,59,59,59	0
25	MG	A	1645	1/1	0.80	0.28	-	53,53,53,53	0
25	MG	A	1866	1/1	0.46	1.76	-	53,53,53,53	0
25	MG	A	1895	1/1	0.81	0.43	-	44,44,44,44	0
25	MG	A	1758	1/1	0.97	0.36	-	85,85,85,85	0
25	MG	A	1930	1/1	0.93	0.40	-	79,79,79,79	0
25	MG	A	1928	1/1	0.64	0.68	-	93,93,93,93	0
25	MG	A	1937	1/1	0.83	0.35	-	61,61,61,61	0
25	MG	A	1763	1/1	0.96	0.15	-	65,65,65,65	0
25	MG	A	1752	1/1	0.89	0.14	-	147,147,147,147	0
25	MG	A	1921	1/1	0.83	0.39	-	48,48,48,48	0
25	MG	A	1889	1/1	0.57	0.56	-	66,66,66,66	0
25	MG	A	1828	1/1	0.59	0.47	-	107,107,107,107	0
25	MG	A	1724	1/1	0.96	0.12	-	82,82,82,82	0
25	MG	A	1859	1/1	0.88	0.46	-	73,73,73,73	0
25	MG	A	1878	1/1	0.97	0.28	-	13,13,13,13	0
25	MG	P	102	1/1	0.84	0.25	-	51,51,51,51	0
25	MG	A	1710	1/1	0.82	0.35	-	82,82,82,82	0
25	MG	A	1810	1/1	0.44	0.77	-	71,71,71,71	0
25	MG	A	1623	1/1	0.61	0.48	-	64,64,64,64	0
25	MG	A	1718	1/1	0.76	0.96	-	80,80,80,80	0

6.5 Other polymers (i)

There are no such residues in this entry.