



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 04:05 PM GMT

PDB ID : 3V2F  
Title : Crystal structure of YfiA bound to the 70S ribosome. This PDB entry contains coordinates for the 50S subunit of the 2nd ribosome in the ASU  
Authors : Polikanov, Y.S.; Blaha, G.M.; Steitz, T.A.  
Deposited on : 2011-12-12  
Resolution : 2.70 Å(reported)

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

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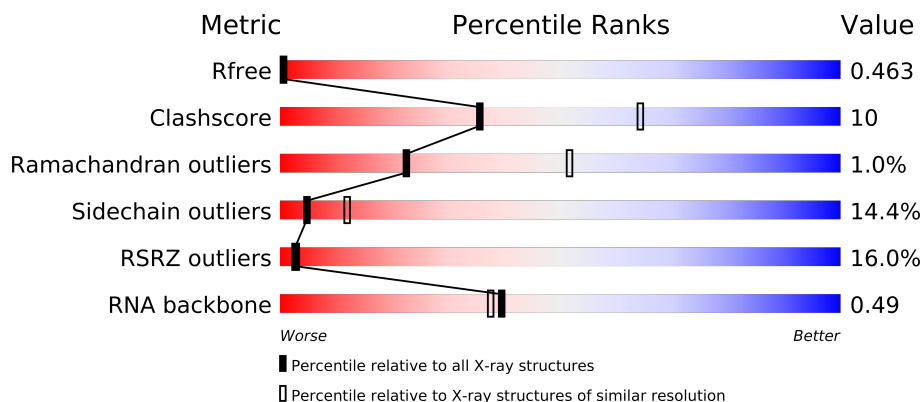
The following versions of software and data (see [references](#)) were used in the production of this report:

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

# 1 Overall quality at a glance

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.












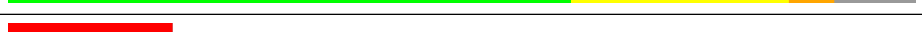

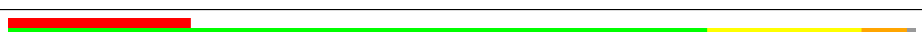
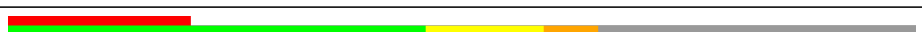

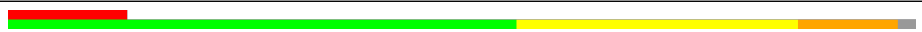




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)
RNA backbone	1838	1042 (3.20-2.20)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	2915	
2	B	122	
3	D	276	
4	E	206	
5	F	210	
6	G	182	
7	H	180	
8	I	148	
9	N	140	
10	O	122	
11	P	150	
12	Q	141	

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Mol	Chain	Length	Quality of chain
13	R	118	
14	S	112	
15	T	146	
16	U	118	
17	V	101	
18	W	113	
19	X	96	
20	Y	110	
21	Z	206	
22	0	85	
23	1	98	
24	2	72	
25	3	60	
26	4	71	
27	5	60	
28	6	54	
29	7	49	
30	8	65	
31	9	37	

## 2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 91815 atoms, of which 0 are hydrogen and 0 are deuterium.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2798	Total	C	N	O	P	0	0	0
			60264	26820	11274	19374	2796			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

- Molecule 3 is a protein called 50S Ribosomal Protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			

- Molecule 4 is a protein called 50S Ribosomal Protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	204	Total	C	N	O	S	0	0	0
			1555	982	297	270	6			

- Molecule 5 is a protein called 50S Ribosomal Protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	203	Total	C	N	O	S	0	0	1
			1572	1003	298	269	2			

- Molecule 6 is a protein called 50S Ribosomal Protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	181	Total	C	N	O	S	0	0	0
			1368	879	242	244	3			

- Molecule 7 is a protein called 50S Ribosomal Protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	174	Total	C	N	O	S	0	0	0
			1317	837	243	236	1			

- Molecule 8 is a protein called 50S Ribosomal Protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	146	Total	C	N	O	S	0	0	0
			1043	672	180	190	1			

- Molecule 9 is a protein called 50S Ribosomal Protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	N	140	Total	C	N	O	S	0	0	0
			1112	717	207	184	4			

- Molecule 10 is a protein called 50S Ribosomal Protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	O	122	Total	C	N	O	S	0	0	0
			923	583	168	168	4			

- Molecule 11 is a protein called 50S Ribosomal Protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	P	149	Total	C	N	O	S	0	0	0
			1131	703	229	196	3			

- Molecule 12 is a protein called 50S Ribosomal Protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	Q	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 13 is a protein called 50S Ribosomal Protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	R	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 14 is a protein called 50S Ribosomal Protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	S	110	Total	C	N	O			
			873	550	174	149	0	0	0

- Molecule 15 is a protein called 50S Ribosomal Protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	T	130	Total	C	N	O	S			
			1058	663	212	182	1	0	0	0

- Molecule 16 is a protein called 50S Ribosomal Protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	U	116	Total	C	N	O	S			
			959	608	201	149	1	0	0	0

- Molecule 17 is a protein called 50S Ribosomal Protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	V	101	Total	C	N	O	S			
			775	498	141	135	1	0	0	0

- Molecule 18 is a protein called 50S Ribosomal Protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	W	111	Total	C	N	O	S			
			877	552	171	152	2	0	0	0

- Molecule 19 is a protein called 50S Ribosomal Protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	X	95	Total	C	N	O	S			
			732	477	130	124	1	0	0	0

- Molecule 20 is a protein called 50S Ribosomal Protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	Y	107	Total	C	N	O	S			
			781	502	145	128	6	0	0	0

- Molecule 21 is a protein called 50S Ribosomal Protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	Z	203	Total	C	N	O	S	0	0	0
			1528	973	268	284	3			

- Molecule 22 is a protein called 50S Ribosomal Protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	0	77	Total	C	N	O	S	0	0	0
			607	376	126	104	1			

- Molecule 23 is a protein called 50S Ribosomal Protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	1	97	Total	C	N	O	S	0	0	0
			745	469	144	131	1			

- Molecule 24 is a protein called 50S Ribosomal Protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	2	71	Total	C	N	O	S	0	0	0
			584	361	118	103	2			

- Molecule 25 is a protein called 50S Ribosomal Protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	3	59	Total	C	N	O	0	0	0
			463	295	87	81			

- Molecule 26 is a protein called 50S Ribosomal Protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	4	46	Total	C	N	O	S	0	0	0
			349	223	57	64	5			

- Molecule 27 is a protein called 50S Ribosomal Protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	5	59	Total	C	N	O	S	0	0	0
			451	283	89	74	5			

- Molecule 28 is a protein called 50S Ribosomal Protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	6	53	Total	C	N	O	S	0	0	0
			437	272	84	77	4			

- Molecule 29 is a protein called 50S Ribosomal Protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	7	48	Total	C	N	O	S	0	0	0
			402	248	97	55	2			

- Molecule 30 is a protein called 50S Ribosomal Protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	8	64	Total	C	N	O	S	0	0	0
			509	326	99	82	2			

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	9	36	Total	C	N	O	S	0	0	0
			297	182	66	46	3			

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	P	4	Total	Mg	0	0
			4	4		
32	0	1	Total	Mg	0	0
			1	1		
32	Q	4	Total	Mg	0	0
			4	4		
32	D	4	Total	Mg	0	0
			4	4		
32	E	3	Total	Mg	0	0
			3	3		
32	B	10	Total	Mg	0	0
			10	10		
32	1	1	Total	Mg	0	0
			1	1		
32	W	1	Total	Mg	0	0
			1	1		
32	A	637	Total	Mg	0	0
			637	637		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	T	2	Total 2	Mg 2	0	0
32	5	2	Total 2	Mg 2	0	0
32	8	1	Total 1	Mg 1	0	0
32	O	1	Total 1	Mg 1	0	0
32	R	2	Total 2	Mg 2	0	0
32	9	1	Total 1	Mg 1	0	0
32	F	5	Total 5	Mg 5	0	0

- Molecule 33 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	9	1	Total 1	Zn 1	0	0
33	Y	1	Total 1	Zn 1	0	0
33	4	1	Total 1	Zn 1	0	0
33	6	1	Total 1	Zn 1	0	0
33	5	1	Total 1	Zn 1	0	0

- Molecule 34 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	A	1493	Total 1493	O 1493	0	0
34	B	32	Total 32	O 32	0	0
34	D	15	Total 15	O 15	0	0
34	E	9	Total 9	O 9	0	0
34	F	10	Total 10	O 10	0	0

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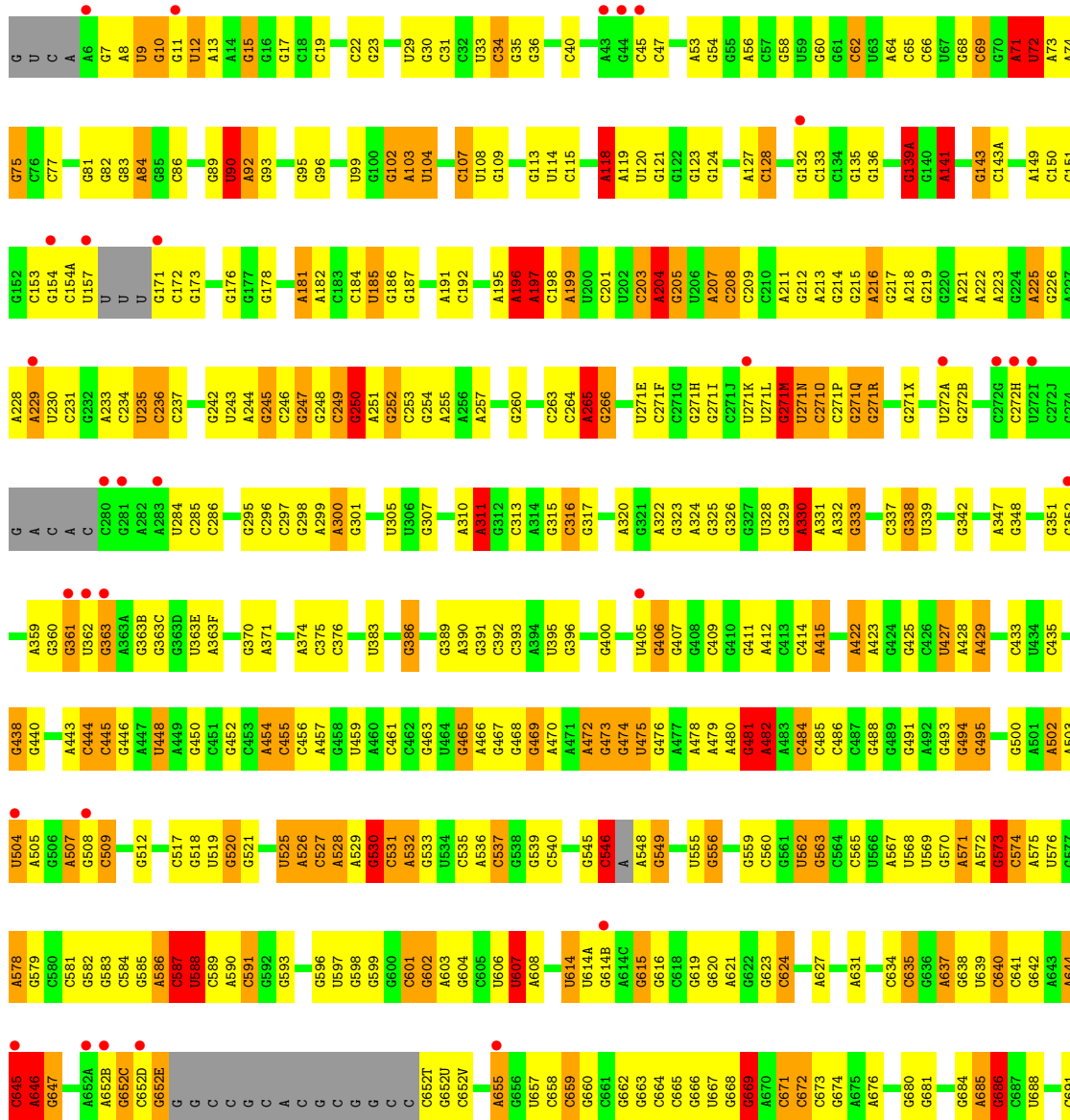
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	N	2	Total	O	0	0
			2	2		
34	O	5	Total	O	0	0
			5	5		
34	P	12	Total	O	0	0
			12	12		
34	Q	2	Total	O	0	0
			2	2		
34	R	5	Total	O	0	0
			5	5		
34	T	4	Total	O	0	0
			4	4		
34	U	1	Total	O	0	0
			1	1		
34	V	1	Total	O	0	0
			1	1		
34	W	4	Total	O	0	0
			4	4		
34	X	3	Total	O	0	0
			3	3		
34	Y	2	Total	O	0	0
			2	2		
34	0	1	Total	O	0	0
			1	1		
34	1	3	Total	O	0	0
			3	3		
34	2	1	Total	O	0	0
			1	1		
34	3	1	Total	O	0	0
			1	1		
34	5	3	Total	O	0	0
			3	3		
34	6	3	Total	O	0	0
			3	3		
34	7	1	Total	O	0	0
			1	1		
34	8	6	Total	O	0	0
			6	6		
34	9	1	Total	O	0	0
			1	1		

### 3 Residue-property plots

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.

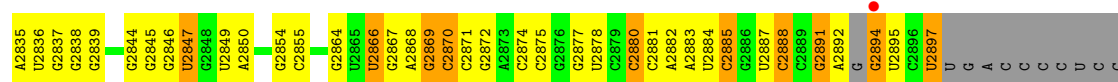
- Molecule 1: 23S Ribosomal RNA

Chain A: 



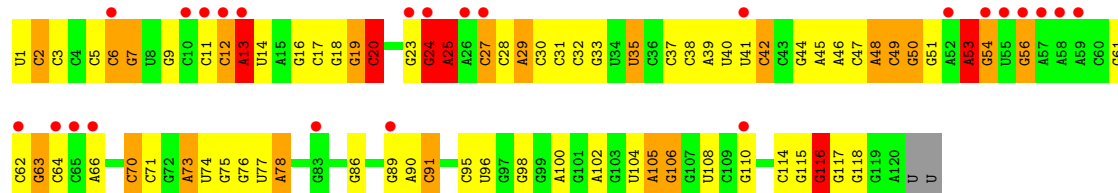






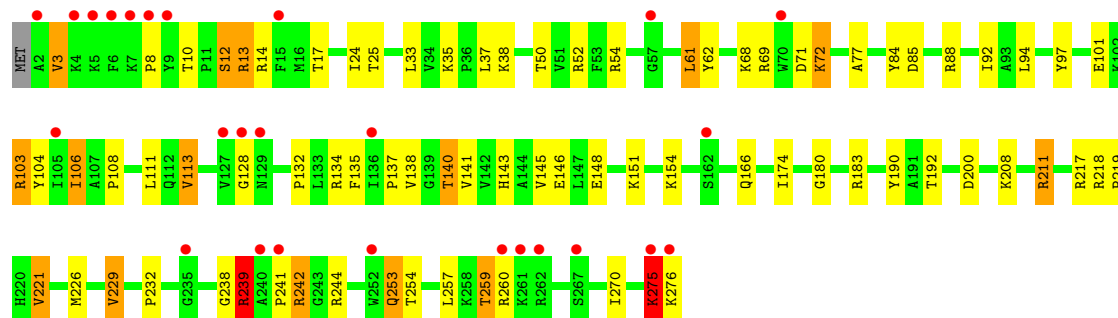
• Molecule 2: 5S Ribosomal RNA

Chain B:



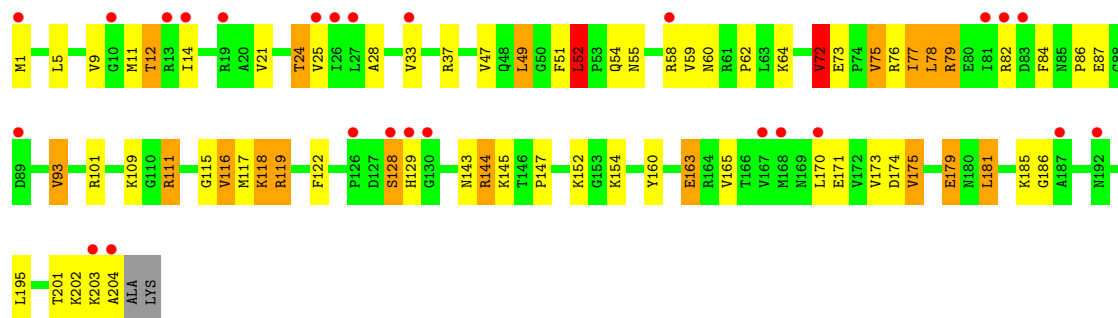
• Molecule 3: 50S Ribosomal Protein L2

Chain D:



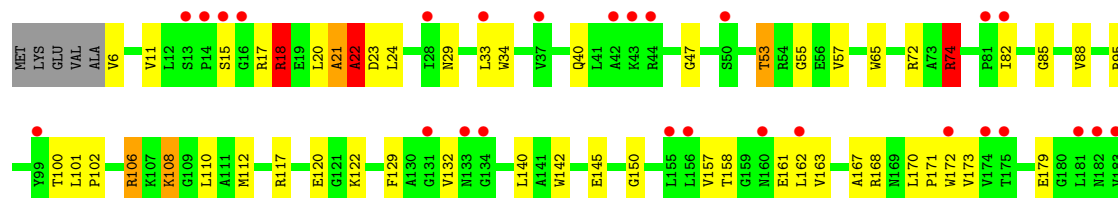
• Molecule 4: 50S Ribosomal Protein L3

Chain E:



• Molecule 5: 50S Ribosomal Protein L4

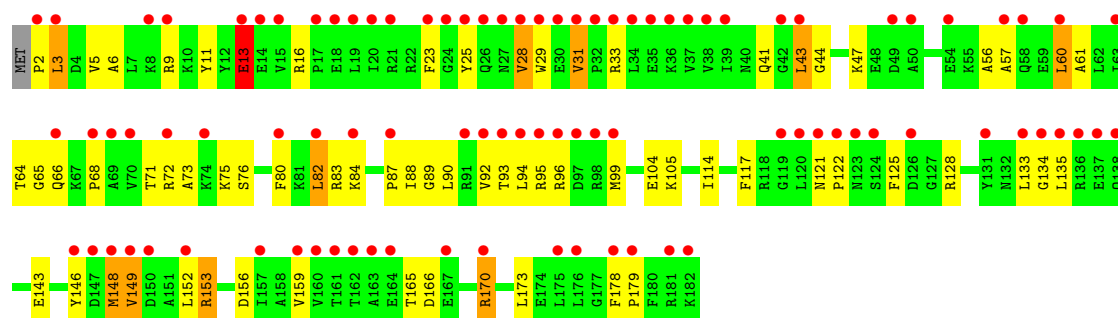
Chain F:





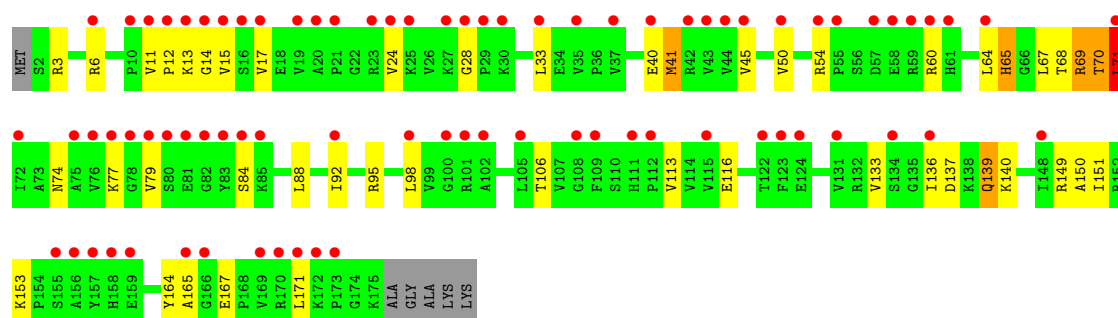
• Molecule 6: 50S Ribosomal Protein L5

Chain G:



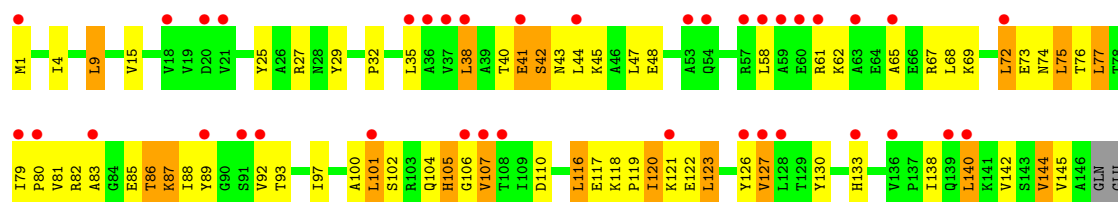
• Molecule 7: 50S Ribosomal Protein L6

Chain H:



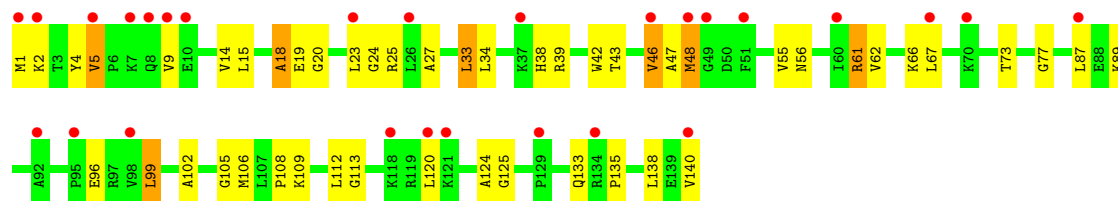
• Molecule 8: 50S Ribosomal Protein L9

Chain I:



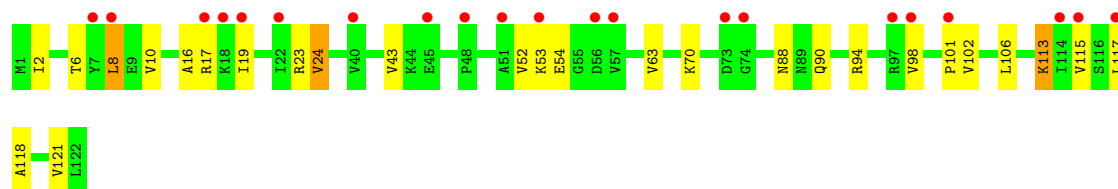
• Molecule 9: 50S Ribosomal Protein L13

Chain N:



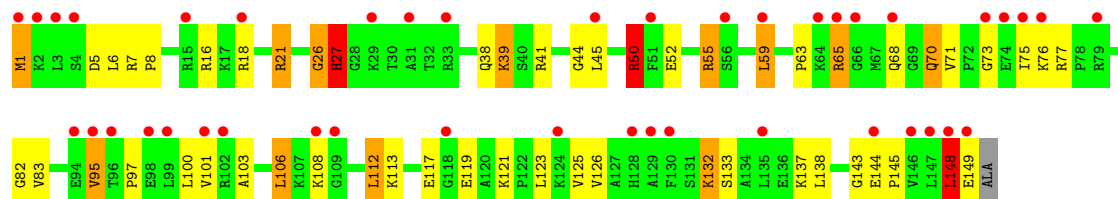
• Molecule 10: 50S Ribosomal Protein L14

Chain O:



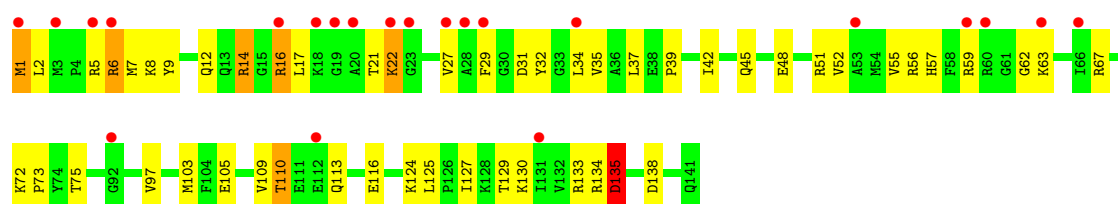
- Molecule 11: 50S Ribosomal Protein L15

Chain P:



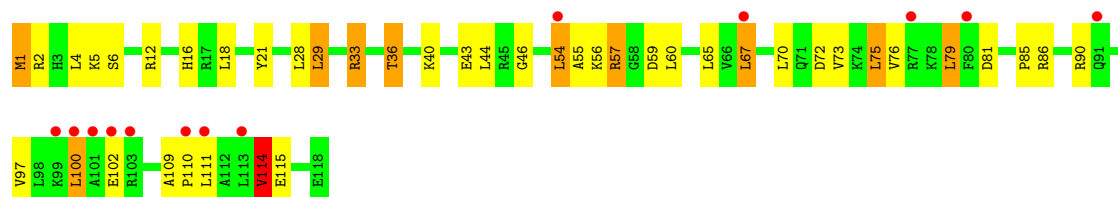
- Molecule 12: 50S Ribosomal Protein L16

Chain Q:



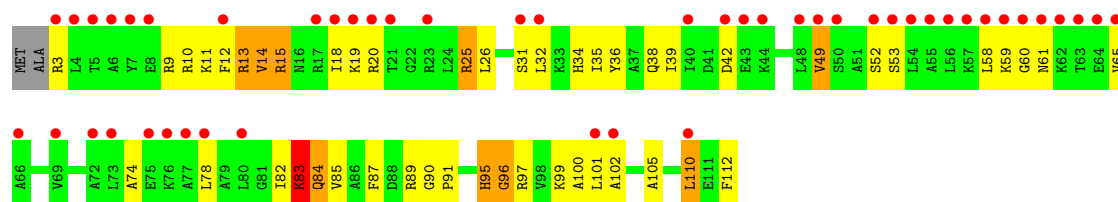
- Molecule 13: 50S Ribosomal Protein L17

Chain R:



- Molecule 14: 50S Ribosomal Protein L18

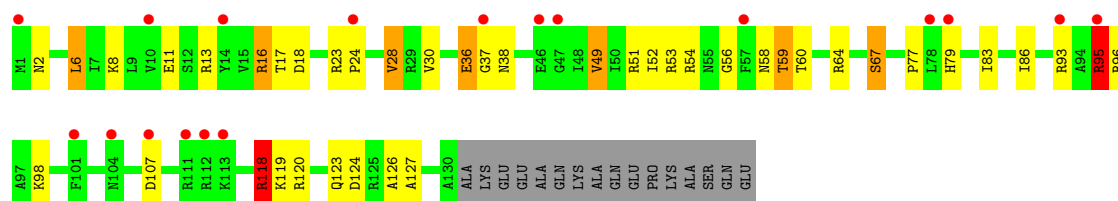
Chain S:



- Molecule 15: 50S Ribosomal Protein L19

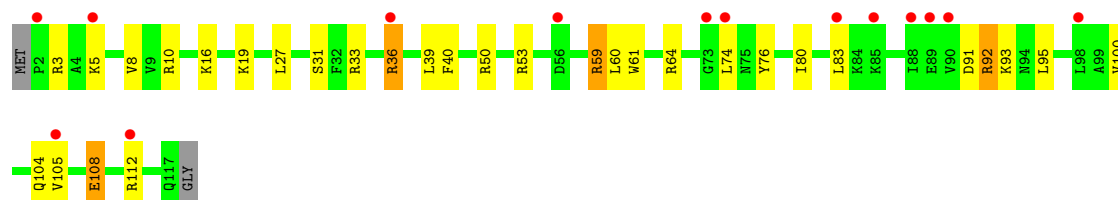
Chain T:





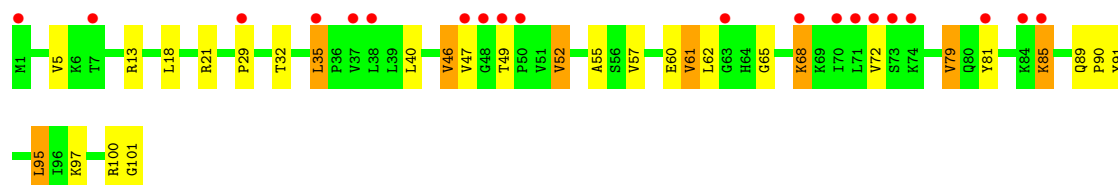
• Molecule 16: 50S Ribosomal Protein L20

Chain U:



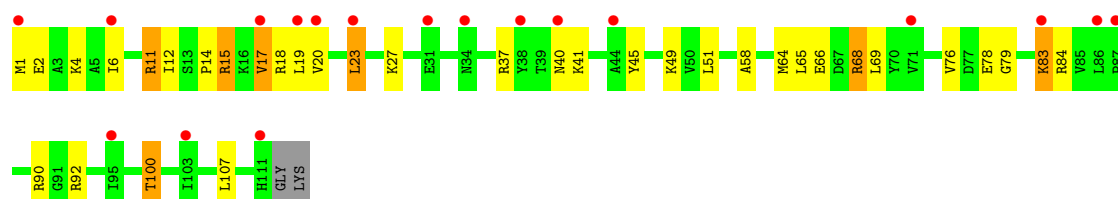
• Molecule 17: 50S Ribosomal Protein L21

Chain V:



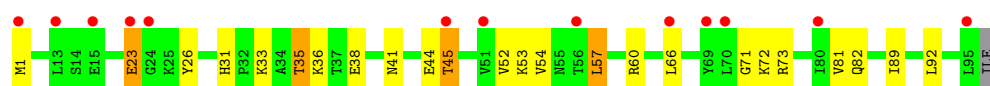
• Molecule 18: 50S Ribosomal Protein L22

Chain W:



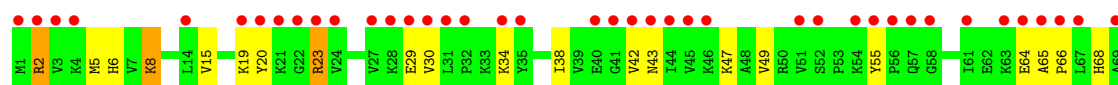
• Molecule 19: 50S Ribosomal Protein L23

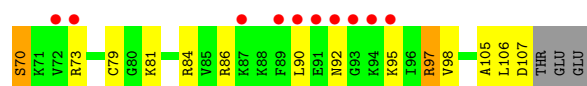
Chain X:



• Molecule 20: 50S Ribosomal Protein L24

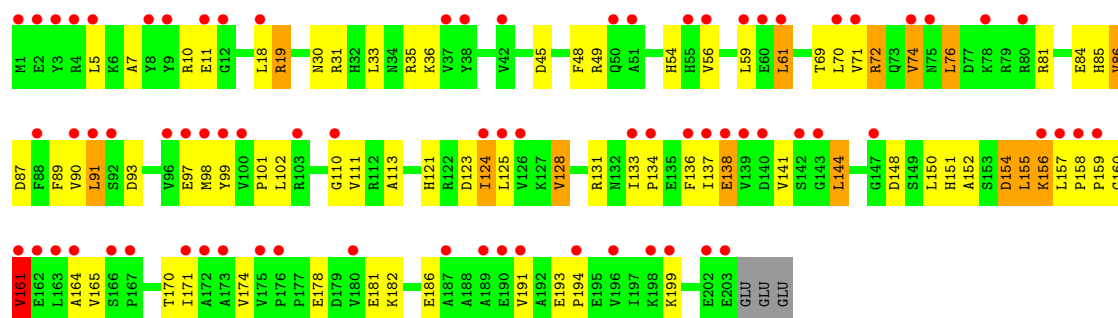
Chain Y:





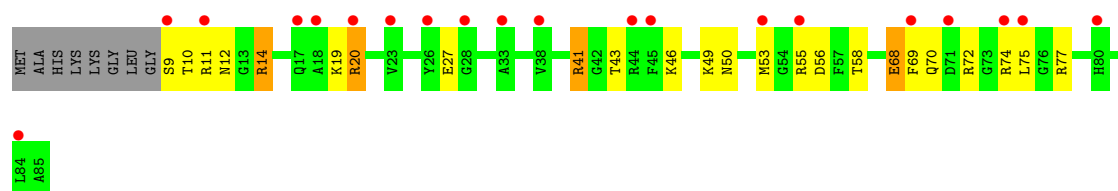
• Molecule 21: 50S Ribosomal Protein L25

Chain Z:



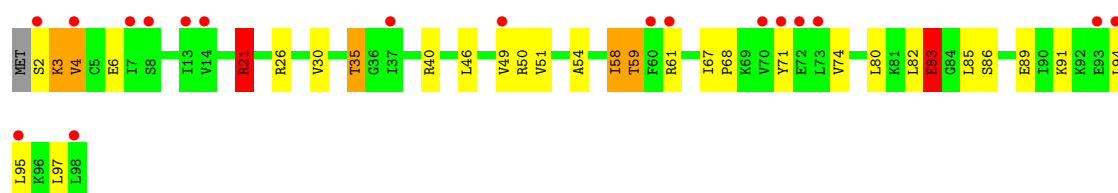
• Molecule 22: 50S Ribosomal Protein L27

Chain 0:



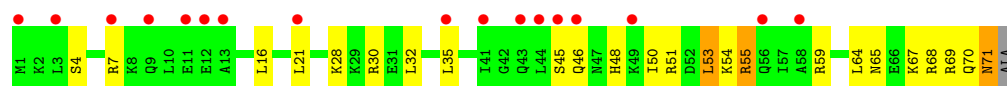
• Molecule 23: 50S Ribosomal Protein L28

Chain 1:



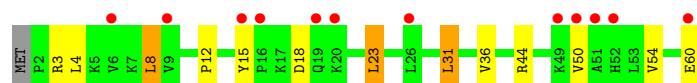
• Molecule 24: 50S Ribosomal Protein L29

Chain 2:



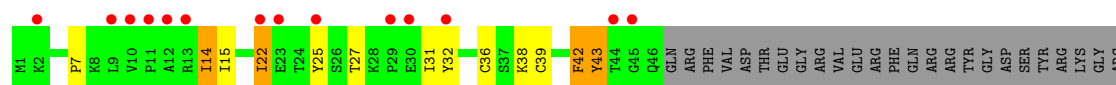
• Molecule 25: 50S Ribosomal Protein L30

Chain 3:



• Molecule 26: 50S Ribosomal Protein L31

Chain 4: 



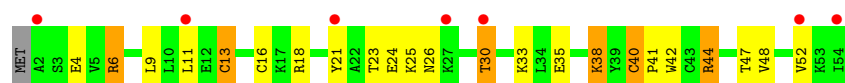
- Molecule 27: 50S Ribosomal Protein L32

Chain 5: 



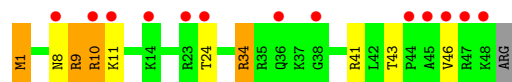
- Molecule 28: 50S Ribosomal Protein L33

Chain 6: 



- Molecule 29: 50S Ribosomal Protein L34

Chain 7: 



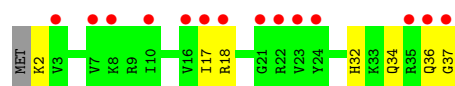
- Molecule 30: 50S Ribosomal Protein L35

Chain 8: 



- Molecule 31: 50S ribosomal protein L36

Chain 9: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	209.63Å 449.30Å 620.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.71 – 2.70 49.71 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.4 (49.71-2.70) 98.4 (49.71-2.70)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.20 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, $R_{free}$	0.217 , 0.254 0.460 , 0.463	Depositor DCC
$R_{free}$ test set	78243 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	55.6	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 38.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 1557851 reflections	Xtriage
$F_o, F_c$ correlation	0.60	EDS
Total number of atoms	91815	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.42% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

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	1.17	125/67486 (0.2%)	1.62	1697/105338 (1.6%)
2	B	1.27	9/2878 (0.3%)	1.51	51/4490 (1.1%)
3	D	0.79	0/2186	0.96	2/2944 (0.1%)
4	E	0.79	1/1588 (0.1%)	0.96	1/2145 (0.0%)
5	F	0.71	0/1607	0.91	4/2178 (0.2%)
6	G	0.69	0/1393	0.80	0/1892
7	H	0.63	0/1343	0.75	0/1820
8	I	0.64	0/1058	0.90	1/1449 (0.1%)
9	N	0.71	0/1139	0.89	1/1538 (0.1%)
10	O	0.77	0/933	0.91	1/1257 (0.1%)
11	P	0.72	0/1148	0.97	5/1529 (0.3%)
12	Q	0.76	0/1143	0.90	2/1527 (0.1%)
13	R	0.71	0/982	0.92	1/1312 (0.1%)
14	S	0.78	0/883	0.89	1/1176 (0.1%)
15	T	0.73	0/1072	0.97	4/1437 (0.3%)
16	U	0.78	0/977	0.83	0/1301
17	V	0.77	0/786	0.89	0/1053
18	W	0.85	0/887	0.91	1/1192 (0.1%)
19	X	0.78	0/746	0.88	1/1005 (0.1%)
20	Y	0.73	0/794	1.03	3/1067 (0.3%)
21	Z	0.71	0/1561	0.84	3/2131 (0.1%)
22	0	0.76	0/615	0.90	0/820
23	1	0.76	0/752	0.92	2/1003 (0.2%)
24	2	0.73	0/586	0.78	0/779
25	3	0.74	0/468	0.75	0/628
26	4	0.73	0/358	0.80	0/487
27	5	0.85	1/465 (0.2%)	0.99	1/630 (0.2%)
28	6	0.81	0/444	0.86	0/595
29	7	0.81	0/410	0.99	1/543 (0.2%)
30	8	0.82	0/516	1.06	5/679 (0.7%)
31	9	0.77	0/300	1.02	0/395
All	All	1.07	136/97504 (0.1%)	1.47	1788/146340 (1.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
3	D	0	1
4	E	0	1
5	F	0	2
6	G	0	1
7	H	0	1
9	N	0	1
11	P	0	2
14	S	0	1
15	T	0	1
19	X	0	1
21	Z	0	1
23	1	0	1
26	4	0	1
27	5	0	1
30	8	0	1
All	All	0	18

All (136) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2123	G	P-OP2	-12.16	1.28	1.49
1	A	1142(A)	A	N9-C4	-12.11	1.30	1.37
1	A	2287	A	N9-C4	-11.93	1.30	1.37
1	A	528	A	N9-C4	-11.85	1.30	1.37
1	A	1021	A	N9-C4	-11.75	1.30	1.37
1	A	2335	A	C6-N6	-11.70	1.24	1.33
1	A	945	A	N9-C4	-9.87	1.31	1.37
1	A	1821	A	C5-C4	-9.47	1.32	1.38
1	A	546	C	P-OP2	-9.35	1.33	1.49
1	A	2296	U	C4-C5	8.68	1.51	1.43
1	A	1026	U	P-OP1	-8.67	1.34	1.49
1	A	1762	A	P-OP1	-8.31	1.34	1.49
1	A	330	A	N9-C4	-8.21	1.32	1.37
1	A	272(A)	U	C1'-N1	7.97	1.60	1.48
1	A	530	G	N9-C8	7.95	1.43	1.37
1	A	1698	A	N9-C4	-7.92	1.33	1.37
1	A	945	A	C5-C6	-7.83	1.34	1.41
1	A	2143	C	P-OP1	-7.82	1.35	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2143	C	P-OP2	-7.77	1.35	1.49
2	B	27	C	P-OP2	-7.64	1.35	1.49
1	A	1026	U	P-OP2	-7.62	1.35	1.49
2	B	27	C	P-OP1	-7.62	1.35	1.49
1	A	786	C	N1-C6	7.48	1.41	1.37
1	A	2638	G	N7-C5	-7.46	1.34	1.39
1	A	530	G	C8-N7	7.45	1.35	1.30
1	A	2322	A	N7-C5	7.36	1.43	1.39
27	5	49	CYS	CB-SG	-7.21	1.70	1.82
1	A	2322	A	N9-C4	7.13	1.42	1.37
1	A	546	C	P-OP1	-7.04	1.36	1.49
1	A	530	G	C2-N3	-6.99	1.27	1.32
1	A	1762	A	P-OP2	-6.88	1.37	1.49
1	A	2296	U	N1-C2	6.86	1.44	1.38
1	A	2003	G	C6-N1	-6.79	1.34	1.39
1	A	1698	A	N9-C8	6.68	1.43	1.37
1	A	12	U	N1-C2	6.67	1.44	1.38
1	A	2050	C	N3-C4	6.66	1.38	1.33
1	A	2322	A	C6-N1	6.63	1.40	1.35
1	A	757	U	C4-O4	-6.61	1.18	1.23
2	B	53	A	N9-C4	6.61	1.41	1.37
1	A	71	A	N9-C4	6.61	1.41	1.37
1	A	2322	A	C5-C6	6.58	1.47	1.41
1	A	2774	C	N1-C6	6.50	1.41	1.37
1	A	2707	G	C2-N3	6.50	1.38	1.32
1	A	2689	U	C3'-O3'	6.46	1.51	1.42
1	A	945	A	N1-C2	6.44	1.40	1.34
1	A	1021	A	N3-C4	-6.31	1.31	1.34
1	A	528	A	N9-C8	6.30	1.42	1.37
1	A	1799	G	N9-C4	6.26	1.43	1.38
1	A	472	A	N7-C5	-6.25	1.35	1.39
1	A	945	A	N7-C5	-6.22	1.35	1.39
1	A	1698	A	N3-C4	-6.20	1.31	1.34
1	A	2609	U	C2-N3	-6.08	1.33	1.37
1	A	2335	A	C5-C4	-6.05	1.34	1.38
1	A	2454	G	C8-N7	6.05	1.34	1.30
1	A	2207	G	N7-C5	-6.01	1.35	1.39
1	A	777	A	N3-C4	-6.01	1.31	1.34
1	A	1142(A)	A	N3-C4	-6.01	1.31	1.34
1	A	90	U	C2-N3	5.99	1.42	1.37
1	A	741	G	N1-C2	-5.97	1.32	1.37
1	A	1783	A	N3-C4	-5.96	1.31	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2286	A	C5-C4	5.94	1.43	1.38
1	A	2322	A	C8-N7	5.93	1.35	1.31
1	A	528	A	C2-N3	-5.93	1.28	1.33
2	B	76	G	N7-C5	5.91	1.42	1.39
1	A	772	C	C4-C5	-5.88	1.38	1.43
1	A	1958	C	N1-C6	-5.86	1.33	1.37
1	A	2286	A	N7-C5	-5.86	1.35	1.39
1	A	1815	A	N3-C4	-5.83	1.31	1.34
1	A	1654	A	C6-N1	-5.83	1.31	1.35
1	A	2602	A	N9-C4	5.82	1.41	1.37
4	E	163	GLU	CG-CD	5.82	1.60	1.51
1	A	2249	U	C2-N3	-5.80	1.33	1.37
1	A	1204	A	N9-C4	-5.77	1.34	1.37
1	A	2829	C	N3-C4	5.75	1.38	1.33
1	A	563	G	N7-C5	5.72	1.42	1.39
1	A	1762	A	C5'-C4'	-5.69	1.44	1.51
1	A	2599	G	C6-N1	-5.68	1.35	1.39
2	B	49	C	N1-C6	5.66	1.40	1.37
1	A	2579	C	N1-C6	-5.66	1.33	1.37
1	A	2515	C	N3-C4	-5.64	1.29	1.33
2	B	48	A	N7-C5	5.64	1.42	1.39
1	A	2029	G	C8-N7	5.63	1.34	1.30
1	A	910	A	C6-N1	-5.62	1.31	1.35
1	A	118	A	N9-C4	-5.60	1.34	1.37
1	A	249	C	N1-C6	-5.57	1.33	1.37
1	A	733	G	N7-C5	-5.54	1.35	1.39
1	A	1788	C	N3-C4	-5.53	1.30	1.33
1	A	2346	A	N7-C5	-5.52	1.35	1.39
1	A	1992	G	N1-C2	-5.52	1.33	1.37
1	A	774	A	C6-N1	-5.52	1.31	1.35
1	A	2069	G	N7-C5	-5.51	1.35	1.39
1	A	2287	A	C5-C6	-5.50	1.36	1.41
1	A	139(A)	G	N9-C4	5.48	1.42	1.38
1	A	726	G	C8-N7	5.46	1.34	1.30
1	A	1392	A	N3-C4	5.45	1.38	1.34
1	A	2598	A	C5-C4	-5.45	1.34	1.38
1	A	2607	G	C6-O6	-5.43	1.19	1.24
1	A	2572	A	C5-C4	-5.43	1.34	1.38
1	A	2607	G	C5-C6	-5.36	1.36	1.42
1	A	2882	A	N7-C5	-5.35	1.36	1.39
1	A	948	G	C8-N7	5.33	1.34	1.30
2	B	13	A	N9-C4	-5.33	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1698	A	C5-C4	5.33	1.42	1.38
1	A	1300	U	C3'-O3'	5.32	1.49	1.42
1	A	2690	C	N1-C6	-5.30	1.33	1.37
2	B	25	A	N3-C4	5.26	1.38	1.34
1	A	803	U	C2-O2	-5.25	1.17	1.22
1	A	2894	G	C5-C4	5.25	1.42	1.38
1	A	1558	A	N3-C4	-5.24	1.31	1.34
1	A	798	G	C8-N7	5.24	1.34	1.30
1	A	254	G	N3-C4	-5.23	1.31	1.35
1	A	2434	A	N9-C4	5.22	1.41	1.37
1	A	1359	A	N7-C5	5.22	1.42	1.39
1	A	706	A	N7-C5	-5.21	1.36	1.39
1	A	300	A	N3-C4	5.20	1.38	1.34
1	A	2331	G	C8-N7	5.20	1.34	1.30
1	A	2332	U	C4-C5	5.18	1.48	1.43
1	A	1321	A	N7-C5	-5.17	1.36	1.39
2	B	114	C	C4-C5	5.13	1.47	1.43
1	A	2335	A	N3-C4	5.13	1.38	1.34
1	A	1641	A	N3-C4	-5.13	1.31	1.34
1	A	1788	C	N1-C6	-5.12	1.34	1.37
1	A	685	A	C6-N1	-5.12	1.31	1.35
1	A	728	G	N9-C4	5.12	1.42	1.38
1	A	2593	U	C4-O4	-5.12	1.19	1.23
1	A	1997	G	N1-C2	-5.10	1.33	1.37
1	A	777	A	N7-C5	-5.10	1.36	1.39
1	A	2034	U	C2-N3	5.09	1.41	1.37
1	A	1298	C	P-OP2	-5.07	1.40	1.49
1	A	526	A	N9-C4	5.06	1.40	1.37
1	A	2437	U	N3-C4	-5.05	1.33	1.38
1	A	1657	C	N3-C4	-5.05	1.30	1.33
1	A	254	G	N9-C4	-5.04	1.33	1.38
1	A	567	A	N9-C4	-5.04	1.34	1.37
1	A	1776	G	C2-N3	5.04	1.36	1.32
1	A	933	A	C5-C4	5.02	1.42	1.38

All (1788) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2335	A	C5-C6-N1	22.57	128.98	117.70
1	A	2296	U	N3-C4-O4	-22.36	103.75	119.40
1	A	2296	U	C2-N3-C4	-21.07	114.36	127.00
1	A	1021	A	C2-N3-C4	-19.52	100.84	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2296	U	C5-C6-N1	-19.05	113.17	122.70
1	A	528	A	C2-N3-C4	-18.67	101.27	110.60
1	A	945	A	N1-C6-N6	18.34	129.61	118.60
1	A	1142(A)	A	C2-N3-C4	-18.04	101.58	110.60
1	A	945	A	C2-N3-C4	-16.76	102.22	110.60
1	A	2287	A	C2-N3-C4	-16.41	102.40	110.60
1	A	528	A	N3-C4-C5	16.30	138.21	126.80
1	A	2296	U	C2-N1-C1'	-15.96	98.54	117.70
1	A	528	A	N3-C4-N9	-15.63	114.90	127.40
1	A	2322	A	C6-N1-C2	-15.30	109.42	118.60
1	A	2296	U	C5-C4-O4	14.60	134.66	125.90
1	A	2322	A	C5-C6-N1	14.56	124.98	117.70
1	A	945	A	C5-N7-C8	-14.41	96.69	103.90
2	B	115	G	C8-N9-C4	14.16	112.06	106.40
1	A	2286	A	N7-C8-N9	13.62	120.61	113.80
1	A	2296	U	N1-C2-N3	13.57	123.04	114.90
1	A	1698	A	C2-N3-C4	-13.41	103.90	110.60
1	A	1698	A	C5-N7-C8	-13.37	97.21	103.90
20	Y	2	ARG	NE-CZ-NH1	-12.81	113.89	120.30
1	A	2287	A	N3-C4-C5	12.81	135.76	126.80
1	A	1142(A)	A	N3-C4-N9	-12.62	117.31	127.40
1	A	2286	A	C8-N9-C4	-12.57	100.77	105.80
1	A	1142(A)	A	N3-C4-C5	12.55	135.58	126.80
1	A	945	A	C4-C5-N7	12.53	116.96	110.70
1	A	945	A	C6-C5-N7	-12.49	123.56	132.30
1	A	2286	A	C6-C5-N7	-12.45	123.59	132.30
1	A	2286	A	C2-N3-C4	-12.39	104.41	110.60
1	A	2322	A	N1-C6-N6	-12.34	111.19	118.60
1	A	847	U	C5-C6-N1	-12.12	116.64	122.70
1	A	141	A	N7-C8-N9	11.88	119.74	113.80
1	A	2286	A	N1-C6-N6	11.69	125.61	118.60
1	A	2296	U	N3-C4-C5	11.63	121.58	114.60
1	A	933	A	C5-N7-C8	-11.59	98.11	103.90
1	A	2335	A	C5-C6-N6	-11.58	114.43	123.70
1	A	1372	U	C5-C4-O4	-11.56	118.96	125.90
1	A	2312	U	N3-C2-O2	-11.56	114.11	122.20
1	A	1021	A	N3-C4-C5	11.54	134.88	126.80
1	A	2286	A	C5-C6-N1	-11.54	111.93	117.70
1	A	2335	A	C6-N1-C2	-11.47	111.72	118.60
1	A	2286	A	C5-N7-C8	-11.44	98.18	103.90
1	A	1698	A	N7-C8-N9	11.38	119.49	113.80
1	A	141	A	C5-N7-C8	-11.33	98.23	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2296	U	C6-N1-C1'	11.30	137.02	121.20
1	A	330	A	C2-N3-C4	-11.25	104.97	110.60
1	A	847	U	C2-N1-C1'	-11.21	104.24	117.70
1	A	1698	A	C8-N9-C4	-11.10	101.36	105.80
1	A	1654	A	N1-C6-N6	-11.01	111.99	118.60
1	A	1021	A	N3-C4-N9	-10.98	118.62	127.40
1	A	2287	A	C5-N7-C8	-10.98	98.41	103.90
1	A	528	A	C5-N7-C8	-10.98	98.41	103.90
1	A	1558	A	C2-N3-C4	-10.78	105.21	110.60
1	A	2296	U	N3-C2-O2	-10.75	114.67	122.20
1	A	2286	A	C4-C5-C6	10.72	122.36	117.00
1	A	1021	A	N1-C2-N3	10.69	134.65	129.30
1	A	1021	A	C5-N7-C8	-10.60	98.60	103.90
1	A	933	A	N7-C8-N9	10.50	119.05	113.80
2	B	115	G	N7-C8-N9	-10.30	107.95	113.10
1	A	945	A	C5-C6-N6	-10.29	115.47	123.70
1	A	2312	U	C6-N1-C2	-10.27	114.84	121.00
1	A	1379	A	N1-C6-N6	10.19	124.72	118.60
1	A	528	A	C5-C6-N1	-10.12	112.64	117.70
1	A	1204	A	C5-N7-C8	-10.11	98.84	103.90
1	A	1558	A	N1-C2-N3	10.09	134.35	129.30
1	A	803	U	N3-C4-O4	-10.04	112.37	119.40
1	A	1653	G	C8-N9-C4	-10.04	102.38	106.40
1	A	1142(A)	A	C5-N7-C8	-9.99	98.91	103.90
20	Y	2	ARG	NE-CZ-NH2	9.87	125.24	120.30
1	A	1955	U	C5-C6-N1	-9.84	117.78	122.70
1	A	330	A	C5-N7-C8	-9.82	98.99	103.90
1	A	729	G	C8-N9-C4	-9.80	102.48	106.40
1	A	527	C	C4-C5-C6	9.79	122.30	117.40
1	A	2287	A	N3-C4-N9	-9.71	119.63	127.40
1	A	2318	G	C5-N7-C8	9.69	109.14	104.30
1	A	2206	G	C8-N9-C4	9.67	110.27	106.40
1	A	2226	C	C6-N1-C2	9.64	124.16	120.30
1	A	2517	C	N1-C2-O2	-9.64	113.12	118.90
1	A	2322	A	C2-N3-C4	9.62	115.41	110.60
1	A	2818	G	C8-N9-C4	9.61	110.25	106.40
1	A	945	A	N1-C2-N3	9.59	134.10	129.30
1	A	219	G	C5-C6-N1	-9.56	106.72	111.50
1	A	587	C	N3-C2-O2	-9.50	115.25	121.90
1	A	2286	A	N1-C2-N3	9.49	134.05	129.30
1	A	530	G	N3-C4-N9	-9.47	120.32	126.00
1	A	2712	U	C5-C4-O4	-9.44	120.23	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2698	U	C5-C6-N1	-9.38	118.01	122.70
1	A	530	G	C8-N9-C4	-9.35	102.66	106.40
1	A	945	A	N7-C8-N9	9.32	118.46	113.80
1	A	1021	A	C5-C6-N1	-9.31	113.04	117.70
1	A	1296	G	C5-C6-O6	9.31	134.18	128.60
1	A	2713	A	N1-C6-N6	-9.30	113.02	118.60
1	A	2866	U	C5-C6-N1	-9.29	118.06	122.70
1	A	528	A	C6-N1-C2	9.27	124.16	118.60
1	A	1675	C	C6-N1-C2	9.27	124.01	120.30
1	A	1304	C	C6-N1-C2	9.22	123.99	120.30
1	A	527	C	C5-C6-N1	-9.21	116.39	121.00
1	A	2324	C	N3-C4-C5	9.19	125.58	121.90
1	A	1142(A)	A	C5-C6-N1	-9.15	113.12	117.70
1	A	1488	G	C8-N9-C4	-9.13	102.75	106.40
1	A	1758	G	N1-C6-O6	9.11	125.36	119.90
1	A	2070	G	N1-C2-N2	-9.09	108.02	116.20
1	A	465	G	C8-N9-C4	-9.06	102.78	106.40
1	A	2335	A	C4-C5-C6	-9.06	112.47	117.00
1	A	1956	U	N1-C2-O2	-9.04	116.47	122.80
1	A	2137	C	N3-C2-O2	-9.02	115.58	121.90
1	A	114	U	N3-C4-O4	9.00	125.70	119.40
1	A	1698	A	N3-C4-N9	-8.99	120.21	127.40
1	A	195	A	C5-N7-C8	8.97	108.39	103.90
1	A	2705	A	C8-N9-C4	8.92	109.37	105.80
1	A	1776	G	N3-C4-N9	8.91	131.34	126.00
1	A	1698	A	C5-C6-N1	-8.90	113.25	117.70
1	A	1990	C	N1-C2-N3	8.88	125.41	119.20
1	A	2347	C	N3-C2-O2	-8.84	115.72	121.90
1	A	1204	A	C4-C5-N7	8.83	115.12	110.70
1	A	113	G	N3-C4-N9	-8.82	120.70	126.00
1	A	2137	C	C6-N1-C2	-8.81	116.77	120.30
1	A	527	C	N1-C2-N3	8.81	125.37	119.20
1	A	195	A	N7-C8-N9	-8.80	109.40	113.80
1	A	133	C	C6-N1-C2	8.78	123.81	120.30
1	A	584	C	C6-N1-C2	8.77	123.81	120.30
1	A	2585	U	C2-N1-C1'	8.76	128.22	117.70
1	A	1978	A	N9-C4-C5	8.76	109.30	105.80
1	A	2070	G	N3-C2-N2	8.75	126.02	119.90
1	A	141	A	C8-N9-C4	-8.74	102.30	105.80
1	A	645	C	N1-C2-O2	8.72	124.13	118.90
1	A	961	C	N1-C2-O2	-8.70	113.68	118.90
1	A	2373	G	C2-N3-C4	-8.69	107.55	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	495	G	C4-C5-N7	-8.68	107.33	110.80
1	A	2312	U	N1-C2-O2	8.67	128.87	122.80
1	A	1638	C	C6-N1-C2	8.66	123.77	120.30
1	A	2617	C	C6-N1-C2	8.66	123.76	120.30
1	A	776	G	C8-N9-C4	-8.65	102.94	106.40
1	A	1978	A	N1-C6-N6	-8.64	113.41	118.60
1	A	624	C	N1-C2-O2	-8.64	113.72	118.90
1	A	1963	U	C2-N1-C1'	8.61	128.03	117.70
1	A	1372	U	N3-C4-O4	8.61	125.42	119.40
1	A	560	C	C6-N1-C2	8.60	123.74	120.30
2	B	104	U	C5-C6-N1	-8.59	118.41	122.70
1	A	2036	C	N1-C2-O2	-8.58	113.75	118.90
1	A	495	G	C5-N7-C8	8.58	108.59	104.30
1	A	2312	U	C2-N1-C1'	8.58	127.99	117.70
1	A	141	A	C4-C5-N7	8.57	114.98	110.70
1	A	2605	U	C5-C4-O4	8.56	131.04	125.90
1	A	527	C	N3-C2-O2	-8.53	115.93	121.90
1	A	468	G	C8-N9-C4	8.53	109.81	106.40
1	A	115	C	C6-N1-C2	8.52	123.71	120.30
1	A	823	G	C5-C6-O6	8.50	133.70	128.60
1	A	1698	A	N3-C4-C5	8.49	132.74	126.80
1	A	570	G	N1-C6-O6	-8.47	114.81	119.90
1	A	71	A	C2-N3-C4	8.47	114.83	110.60
1	A	2605	U	N3-C4-O4	-8.47	113.47	119.40
1	A	2253	G	N1-C6-O6	8.46	124.98	119.90
1	A	1302	A	N7-C8-N9	-8.46	109.57	113.80
1	A	271(M)	G	N3-C4-N9	8.45	131.07	126.00
2	B	117	G	N1-C6-O6	8.39	124.93	119.90
1	A	2287	A	C4-C5-N7	8.38	114.89	110.70
1	A	2084	C	C6-N1-C2	8.37	123.65	120.30
1	A	1787	A	C8-N9-C4	8.36	109.14	105.80
1	A	1558	A	C8-N9-C4	-8.36	102.46	105.80
1	A	1266	G	C5-C6-O6	-8.34	123.60	128.60
1	A	2287	A	N1-C6-N6	8.33	123.60	118.60
1	A	2322	A	N9-C4-C5	8.32	109.13	105.80
1	A	1204	A	C2-N3-C4	-8.32	106.44	110.60
1	A	1990	C	N3-C2-O2	-8.32	116.08	121.90
1	A	2226	C	C5-C6-N1	-8.32	116.84	121.00
1	A	1698	A	C4-C5-N7	8.31	114.86	110.70
1	A	2260	C	N1-C2-O2	-8.30	113.92	118.90
1	A	1296	G	N1-C6-O6	-8.26	114.94	119.90
1	A	2439	A	C2-N3-C4	-8.24	106.48	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2420	C	C6-N1-C2	8.23	123.59	120.30
1	A	2105	C	C6-N1-C2	-8.22	117.01	120.30
1	A	608	A	C8-N9-C4	-8.21	102.52	105.80
1	A	271(M)	G	C4-N9-C1'	8.20	137.16	126.50
1	A	2579	C	C6-N1-C2	8.19	123.58	120.30
1	A	528	A	C4-C5-C6	-8.17	112.92	117.00
1	A	933	A	C4-C5-N7	8.16	114.78	110.70
1	A	1317	A	N1-C6-N6	-8.16	113.70	118.60
1	A	529	A	C5-N7-C8	-8.16	99.82	103.90
1	A	1654	A	C5-C6-N6	8.15	130.22	123.70
1	A	1957	C	N3-C4-N4	-8.15	112.30	118.00
1	A	1678	G	C8-N9-C4	-8.14	103.14	106.40
1	A	823	G	N1-C6-O6	-8.13	115.02	119.90
1	A	113	G	N3-C4-C5	8.12	132.66	128.60
1	A	40	C	N1-C2-O2	-8.10	114.04	118.90
1	A	1681	G	C8-N9-C4	8.10	109.64	106.40
1	A	208	C	N3-C2-O2	8.10	127.57	121.90
1	A	502	A	N1-C6-N6	-8.10	113.74	118.60
1	A	2103	C	C2-N3-C4	8.08	123.94	119.90
1	A	1204	A	C6-C5-N7	-8.06	126.66	132.30
5	F	74	ARG	NE-CZ-NH1	8.06	124.33	120.30
1	A	1302	A	C8-N9-C4	8.06	109.02	105.80
1	A	1258	C	C6-N1-C2	8.04	123.52	120.30
1	A	2347	C	N1-C2-O2	8.04	123.72	118.90
1	A	729	G	N7-C8-N9	8.04	117.12	113.10
1	A	1635	G	N1-C6-O6	8.03	124.72	119.90
1	A	2059	A	N1-C6-N6	8.01	123.41	118.60
1	A	528	A	C8-N9-C1'	7.99	142.09	127.70
1	A	1359	A	N1-C2-N3	-7.99	125.31	129.30
1	A	776	G	N9-C4-C5	7.97	108.59	105.40
1	A	856	C	C6-N1-C2	-7.96	117.12	120.30
1	A	740	U	C5-C4-O4	7.95	130.67	125.90
1	A	2380	C	N1-C2-O2	-7.95	114.13	118.90
2	B	102	A	C8-N9-C4	7.95	108.98	105.80
1	A	943	U	N3-C2-O2	-7.94	116.64	122.20
1	A	1254	A	C8-N9-C4	-7.94	102.62	105.80
1	A	1657	C	C5-C6-N1	-7.93	117.03	121.00
1	A	1288	U	N3-C2-O2	-7.93	116.65	122.20
1	A	1776	G	C5-C6-O6	-7.92	123.85	128.60
1	A	205	G	C8-N9-C4	7.92	109.57	106.40
1	A	1248	G	N3-C2-N2	7.91	125.43	119.90
1	A	2744	G	C2-N3-C4	-7.90	107.95	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	204	A	C5-C6-N1	7.89	121.65	117.70
1	A	2028	U	C5-C6-N1	-7.88	118.76	122.70
1	A	1256	G	C8-N9-C4	7.88	109.55	106.40
1	A	2304	G	C6-C5-N7	7.87	135.12	130.40
1	A	2079	U	N1-C2-N3	7.86	119.61	114.90
1	A	2585	U	C6-N1-C1'	-7.85	110.21	121.20
1	A	1226	A	C8-N9-C4	7.83	108.93	105.80
1	A	1681	G	N9-C4-C5	-7.83	102.27	105.40
1	A	1776	G	N9-C4-C5	-7.83	102.27	105.40
1	A	2137	C	N1-C2-O2	7.81	123.58	118.90
1	A	2644	G	C2-N3-C4	-7.80	108.00	111.90
1	A	1638	C	C2-N3-C4	-7.79	116.00	119.90
1	A	1757	U	C2-N3-C4	-7.79	122.33	127.00
1	A	1957	C	C5-C4-N4	7.79	125.65	120.20
1	A	570	G	C5-C6-N1	7.78	115.39	111.50
1	A	1757	U	C5-C6-N1	-7.77	118.82	122.70
1	A	2625	G	C8-N9-C4	7.77	109.51	106.40
1	A	527	C	C5-C4-N4	7.76	125.64	120.20
1	A	847	U	C6-N1-C1'	7.76	132.06	121.20
1	A	2318	G	C4-C5-N7	-7.75	107.70	110.80
1	A	1488	G	N7-C8-N9	7.75	116.98	113.10
1	A	2143	C	C5-C6-N1	7.75	124.88	121.00
1	A	2154	G	C5-C6-O6	7.75	133.25	128.60
1	A	2609	U	C5-C6-N1	-7.75	118.83	122.70
1	A	915	C	C6-N1-C2	-7.75	117.20	120.30
1	A	2624	G	N7-C8-N9	-7.74	109.23	113.10
1	A	2253	G	C5-C6-O6	-7.74	123.95	128.60
1	A	139(A)	G	N3-C4-N9	7.74	130.64	126.00
1	A	560	C	N3-C4-C5	7.73	124.99	121.90
1	A	945	A	N3-C4-C5	7.71	132.20	126.80
1	A	546	C	C2-N1-C1'	7.70	127.27	118.80
1	A	12	U	N3-C2-O2	-7.70	116.81	122.20
1	A	798	G	C5-C6-O6	7.70	133.22	128.60
1	A	2304	G	C2-N3-C4	7.69	115.75	111.90
1	A	587	C	N1-C2-O2	7.67	123.50	118.90
1	A	847	U	C5-C4-O4	7.66	130.50	125.90
1	A	139(A)	G	N3-C4-C5	-7.66	124.77	128.60
1	A	2304	G	C5-C6-N1	7.66	115.33	111.50
1	A	912	C	C6-N1-C2	-7.66	117.24	120.30
1	A	2791	C	C2-N1-C1'	7.66	127.22	118.80
1	A	2626	C	C6-N1-C2	7.64	123.36	120.30
1	A	1785	A	N9-C4-C5	7.64	108.86	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	265	A	N7-C8-N9	7.63	117.61	113.80
1	A	646	A	C8-N9-C4	-7.62	102.75	105.80
1	A	2502	G	C5-C6-N1	7.62	115.31	111.50
1	A	2032	G	C5-N7-C8	7.62	108.11	104.30
1	A	1948	G	N9-C4-C5	7.61	108.44	105.40
1	A	1775	U	N1-C2-O2	-7.61	117.48	122.80
1	A	2611	U	N1-C2-N3	7.61	119.46	114.90
1	A	2287	A	C5-C6-N1	-7.60	113.90	117.70
1	A	2312	U	C5-C6-N1	7.60	126.50	122.70
1	A	2697	G	C8-N9-C4	7.59	109.44	106.40
1	A	2206	G	N3-C4-C5	7.59	132.39	128.60
1	A	1778	U	C5-C4-O4	-7.58	121.35	125.90
1	A	2437	U	C5-C4-O4	7.58	130.45	125.90
1	A	1653	G	N3-C4-C5	-7.57	124.81	128.60
1	A	1821	A	N7-C8-N9	-7.57	110.02	113.80
1	A	265	A	C2-N3-C4	-7.56	106.82	110.60
1	A	728	G	C5-C6-O6	7.56	133.13	128.60
1	A	802	A	N1-C6-N6	-7.55	114.07	118.60
1	A	1791	A	C2-N3-C4	7.55	114.37	110.60
1	A	2322	A	C6-C5-N7	7.54	137.58	132.30
1	A	271(M)	G	N3-C4-C5	-7.54	124.83	128.60
1	A	728	G	C5-N7-C8	7.53	108.06	104.30
1	A	141	A	C6-C5-N7	-7.53	127.03	132.30
1	A	330	A	N3-C4-C5	7.52	132.06	126.80
1	A	2385	C	N3-C2-O2	7.52	127.16	121.90
1	A	2137	C	N3-C4-C5	-7.51	118.89	121.90
2	B	49	C	C5-C6-N1	7.51	124.75	121.00
1	A	2579	C	C5-C6-N1	-7.50	117.25	121.00
1	A	1653	G	N9-C4-C5	7.50	108.40	105.40
1	A	691	C	C4-C5-C6	7.49	121.14	117.40
1	A	2303	G	N9-C4-C5	7.48	108.39	105.40
1	A	2611	U	N1-C2-O2	-7.48	117.56	122.80
1	A	803	U	N3-C2-O2	-7.48	116.97	122.20
1	A	1779	U	C6-N1-C2	7.47	125.48	121.00
1	A	2335	A	N9-C4-C5	-7.47	102.81	105.80
1	A	2516	G	N1-C2-N2	-7.46	109.48	116.20
1	A	2206	G	C4-N9-C1'	-7.46	116.80	126.50
1	A	407	G	C8-N9-C4	7.46	109.38	106.40
1	A	1828	G	N1-C6-O6	7.45	124.37	119.90
1	A	1029	A	N1-C6-N6	7.45	123.07	118.60
5	F	22	ALA	CB-CA-C	-7.44	98.94	110.10
1	A	2375	G	N9-C4-C5	-7.44	102.42	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2304	G	C4-C5-N7	-7.44	107.83	110.80
1	A	2017	U	C4-C5-C6	7.43	124.16	119.70
1	A	1204	A	N7-C8-N9	7.42	117.51	113.80
1	A	2253	G	C4-C5-N7	7.42	113.77	110.80
1	A	1948	G	N3-C2-N2	-7.42	114.71	119.90
1	A	768	G	C8-N9-C4	-7.41	103.44	106.40
1	A	2729	G	N9-C4-C5	-7.41	102.44	105.40
1	A	2057	A	N1-C2-N3	7.41	133.00	129.30
1	A	236	C	C6-N1-C2	7.40	123.26	120.30
1	A	568	U	C2-N3-C4	-7.39	122.57	127.00
1	A	2463	C	C5-C4-N4	-7.38	115.03	120.20
1	A	265	A	C5-N7-C8	-7.38	100.21	103.90
1	A	2324	C	C2-N3-C4	-7.38	116.21	119.90
2	B	115	G	N9-C4-C5	-7.38	102.45	105.40
1	A	588	U	C5-C6-N1	7.37	126.39	122.70
1	A	390	A	C8-N9-C4	7.37	108.75	105.80
1	A	2003	G	N1-C6-O6	-7.36	115.48	119.90
1	A	1204	A	N1-C6-N6	7.36	123.02	118.60
1	A	1790	C	C2-N3-C4	7.36	123.58	119.90
1	A	933	A	C8-N9-C4	-7.35	102.86	105.80
1	A	530	G	C5-N7-C8	-7.35	100.62	104.30
1	A	1612	C	C2-N3-C4	-7.35	116.22	119.90
1	A	1675	C	N3-C2-O2	7.35	127.04	121.90
1	A	271(M)	G	C6-C5-N7	-7.34	126.00	130.40
1	A	1826	G	N1-C6-O6	-7.33	115.50	119.90
1	A	614	U	C5-C4-O4	7.33	130.30	125.90
1	A	2287	A	C6-N1-C2	7.33	123.00	118.60
1	A	2022	U	C5-C4-O4	-7.32	121.51	125.90
1	A	114	U	C5-C4-O4	-7.32	121.51	125.90
1	A	1294	U	N1-C2-N3	7.31	119.29	114.90
1	A	1155	A	N1-C2-N3	-7.31	125.65	129.30
1	A	2028	U	C6-N1-C2	7.30	125.38	121.00
1	A	1126	A	N1-C6-N6	7.30	122.98	118.60
1	A	518	G	N1-C6-O6	-7.29	115.53	119.90
1	A	1676	A	C2-N3-C4	7.29	114.25	110.60
1	A	776	G	N1-C6-O6	-7.29	115.53	119.90
1	A	2646	C	C6-N1-C2	7.28	123.21	120.30
1	A	2464	C	C6-N1-C1'	-7.28	112.07	120.80
1	A	1351	C	N1-C2-O2	-7.28	114.53	118.90
1	A	1834	U	N3-C2-O2	-7.27	117.11	122.20
1	A	2622	C	N3-C4-C5	7.26	124.81	121.90
1	A	2260	C	C2-N3-C4	-7.24	116.28	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2543	G	C8-N9-C4	7.22	109.29	106.40
1	A	2689	U	C2-N3-C4	-7.22	122.67	127.00
1	A	1638	C	C5-C6-N1	-7.22	117.39	121.00
1	A	2240	C	N3-C4-C5	7.22	124.79	121.90
1	A	2615	U	N3-C4-O4	-7.22	114.35	119.40
1	A	481	G	C8-N9-C4	-7.21	103.52	106.40
1	A	139(A)	G	C2-N3-C4	7.21	115.50	111.90
1	A	2218	U	N1-C2-O2	7.21	127.85	122.80
1	A	2063	C	C2-N3-C4	-7.19	116.31	119.90
1	A	1807	G	C8-N9-C4	7.18	109.27	106.40
1	A	1799	G	N3-C4-C5	-7.17	125.02	128.60
1	A	2161	C	C5-C4-N4	7.16	125.22	120.20
1	A	2249	U	N3-C4-C5	7.16	118.90	114.60
1	A	2003	G	C5-C6-O6	7.15	132.89	128.60
1	A	2625	G	N7-C8-N9	-7.15	109.53	113.10
1	A	2454	G	N1-C6-O6	-7.15	115.61	119.90
1	A	1490	A	N1-C6-N6	-7.15	114.31	118.60
19	X	57	LEU	CA-CB-CG	7.14	131.71	115.30
1	A	2042	A	C8-N9-C4	7.13	108.65	105.80
5	F	22	ALA	N-CA-C	7.13	130.25	111.00
1	A	2191	G	N1-C6-O6	7.12	124.17	119.90
1	A	1363	C	N3-C4-C5	7.11	124.74	121.90
1	A	2607	G	C5-C6-N1	7.11	115.05	111.50
1	A	271(M)	G	C8-N9-C1'	-7.10	117.77	127.00
1	A	1698	A	N1-C6-N6	7.10	122.86	118.60
1	A	1997	G	N3-C4-C5	-7.09	125.05	128.60
1	A	2322	A	C4-C5-N7	-7.09	107.15	110.70
1	A	1142(A)	A	N1-C2-N3	7.09	132.85	129.30
1	A	2074	U	N1-C2-N3	7.09	119.15	114.90
1	A	1359	A	C2-N3-C4	7.08	114.14	110.60
1	A	2894	G	C6-C5-N7	-7.08	126.15	130.40
1	A	961	C	N3-C2-O2	7.08	126.86	121.90
23	1	21	ARG	NE-CZ-NH1	7.07	123.84	120.30
1	A	1785	A	C8-N9-C4	-7.07	102.97	105.80
1	A	1524	G	C6-C5-N7	7.07	134.64	130.40
1	A	659	C	C6-N1-C2	7.07	123.13	120.30
1	A	2500	U	N3-C4-O4	-7.06	114.45	119.40
1	A	1830	C	C5-C4-N4	-7.06	115.26	120.20
1	A	465	G	N7-C8-N9	7.05	116.62	113.10
1	A	1813	G	C8-N9-C4	7.05	109.22	106.40
1	A	330	A	C4-C5-N7	7.04	114.22	110.70
1	A	798	G	C4-C5-N7	-7.04	107.98	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1652	A	N1-C6-N6	7.04	122.82	118.60
1	A	2818	G	N7-C8-N9	-7.03	109.58	113.10
1	A	933	A	C2-N3-C4	-7.03	107.09	110.60
1	A	645	C	C2-N1-C1'	7.02	126.53	118.80
1	A	525	U	N3-C2-O2	7.02	127.11	122.20
1	A	2729	G	N1-C6-O6	7.01	124.11	119.90
1	A	2784	C	C2-N3-C4	-7.01	116.39	119.90
1	A	1779	U	C5-C6-N1	-7.00	119.20	122.70
1	A	1611	C	C6-N1-C2	-7.00	117.50	120.30
1	A	2375	G	C5-C6-O6	-7.00	124.40	128.60
1	A	2030	A	N1-C6-N6	6.98	122.79	118.60
1	A	427	U	N3-C2-O2	-6.98	117.31	122.20
1	A	791	C	C2-N3-C4	-6.98	116.41	119.90
1	A	1571	A	C6-N1-C2	-6.98	114.41	118.60
1	A	2084	C	C5-C6-N1	-6.98	117.51	121.00
1	A	141	A	N1-C6-N6	6.98	122.78	118.60
1	A	1625	C	N3-C4-N4	-6.97	113.12	118.00
1	A	528	A	C4-C5-N7	6.97	114.19	110.70
1	A	587	C	C6-N1-C2	-6.97	117.51	120.30
1	A	1493	C	C2-N1-C1'	6.97	126.47	118.80
1	A	2373	G	C5-C6-N1	-6.97	108.01	111.50
1	A	766	C	C5-C6-N1	-6.97	117.52	121.00
1	A	2699	C	C6-N1-C2	6.96	123.08	120.30
1	A	758	C	C6-N1-C2	-6.96	117.52	120.30
1	A	2074	U	C6-N1-C2	-6.96	116.83	121.00
1	A	568	U	C5-C4-O4	-6.94	121.73	125.90
1	A	2062	A	C2-N3-C4	-6.94	107.13	110.60
1	A	2279	G	C8-N9-C4	6.94	109.17	106.40
1	A	1313	U	C6-N1-C2	-6.94	116.84	121.00
1	A	1475	G	N3-C2-N2	-6.94	115.05	119.90
1	A	2296	U	O4'-C1'-N1	6.94	113.75	108.20
1	A	1123	C	C6-N1-C2	6.93	123.07	120.30
1	A	2026	C	C6-N1-C2	6.93	123.07	120.30
1	A	803	U	N3-C4-C5	6.92	118.75	114.60
1	A	2838	G	C8-N9-C4	6.92	109.17	106.40
1	A	1757	U	N3-C4-C5	6.91	118.75	114.60
9	N	46	VAL	N-CA-C	6.91	129.66	111.00
1	A	530	G	C4-C5-C6	-6.91	114.65	118.80
1	A	804	A	N1-C2-N3	6.91	132.76	129.30
1	A	1029	A	C5-C6-N6	-6.91	118.17	123.70
1	A	2789	C	C6-N1-C2	6.91	123.06	120.30
2	B	71	C	C6-N1-C2	6.91	123.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	311	A	C8-N9-C4	6.91	108.56	105.80
1	A	1012	U	C5-C6-N1	-6.91	119.25	122.70
1	A	1935	G	C5-C6-O6	-6.90	124.46	128.60
1	A	2689	U	N1-C2-N3	6.89	119.04	114.90
1	A	2698	U	C2-N3-C4	-6.89	122.86	127.00
1	A	203	C	N1-C2-O2	-6.88	114.77	118.90
1	A	2137	C	C2-N1-C1'	6.88	126.37	118.80
1	A	2226	C	C2-N3-C4	-6.88	116.46	119.90
1	A	528	A	C4-N9-C1'	-6.88	113.92	126.30
1	A	472	A	C8-N9-C4	-6.88	103.05	105.80
1	A	781	A	C2-N3-C4	6.86	114.03	110.60
1	A	508	G	N1-C6-O6	6.86	124.02	119.90
1	A	1787	A	N9-C4-C5	-6.85	103.06	105.80
1	A	2375	G	C4-C5-N7	6.84	113.54	110.80
1	A	2238	G	N3-C4-N9	6.84	130.10	126.00
1	A	2422	A	N1-C2-N3	6.84	132.72	129.30
30	8	13	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	A	2503	A	N1-C2-N3	-6.84	125.88	129.30
1	A	1997	G	N1-C6-O6	-6.84	115.80	119.90
1	A	1948	G	C8-N9-C4	-6.83	103.67	106.40
1	A	1383	C	N1-C2-O2	-6.83	114.80	118.90
1	A	1826	G	C4-C5-N7	-6.83	108.07	110.80
1	A	2303	G	C4-C5-N7	-6.83	108.07	110.80
1	A	121	G	C5-C6-N1	6.82	114.91	111.50
1	A	1379	A	C5-C6-N6	-6.82	118.25	123.70
1	A	448	U	C5-C6-N1	-6.81	119.29	122.70
1	A	1331	A	C5-N7-C8	6.81	107.31	103.90
1	A	2385	C	N1-C2-O2	-6.81	114.81	118.90
1	A	729	G	C4-N9-C1'	6.81	135.35	126.50
1	A	1753	G	N3-C2-N2	6.81	124.67	119.90
1	A	1331	A	N7-C8-N9	-6.81	110.40	113.80
1	A	2286	A	C4-N9-C1'	6.80	138.55	126.30
1	A	2332	U	C5-C6-N1	-6.80	119.30	122.70
1	A	2375	G	C5-N7-C8	-6.80	100.90	104.30
1	A	213	A	C8-N9-C4	6.80	108.52	105.80
1	A	2028	U	N3-C4-C5	6.80	118.68	114.60
1	A	1524	G	N1-C6-O6	-6.79	115.82	119.90
1	A	1826	G	N9-C4-C5	6.79	108.11	105.40
1	A	1997	G	C5-N7-C8	6.79	107.69	104.30
1	A	2729	G	C8-N9-C4	6.78	109.11	106.40
1	A	141	A	C2-N3-C4	-6.78	107.21	110.60
1	A	1448	G	N1-C6-O6	6.78	123.97	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2866	U	C4-C5-C6	6.77	123.76	119.70
1	A	139(A)	G	C4-N9-C1'	6.77	135.30	126.50
1	A	205	G	N7-C8-N9	-6.77	109.71	113.10
1	A	570	G	N3-C2-N2	6.77	124.64	119.90
1	A	92	A	C8-N9-C4	-6.77	103.09	105.80
1	A	1640	C	C5-C6-N1	6.76	124.38	121.00
1	A	1757	U	C6-N1-C2	6.76	125.06	121.00
1	A	1939	U	N3-C4-C5	6.76	118.66	114.60
1	A	2335	A	C8-N9-C4	6.76	108.50	105.80
1	A	2260	C	N1-C2-N3	6.76	123.93	119.20
1	A	1977	A	C8-N9-C4	6.76	108.50	105.80
1	A	574	C	N3-C4-C5	-6.75	119.20	121.90
1	A	645	C	C6-N1-C2	-6.75	117.60	120.30
1	A	1776	G	C6-C5-N7	-6.75	126.35	130.40
1	A	1963	U	N1-C2-O2	6.75	127.52	122.80
1	A	791	C	C4-C5-C6	6.74	120.77	117.40
1	A	2063	C	C5-C4-N4	-6.74	115.48	120.20
1	A	192	C	N1-C2-O2	-6.74	114.86	118.90
1	A	2032	G	N7-C8-N9	-6.74	109.73	113.10
1	A	199	A	N9-C4-C5	6.74	108.49	105.80
1	A	1997	G	C4-C5-N7	-6.74	108.11	110.80
1	A	1140	C	C6-N1-C2	-6.73	117.61	120.30
1	A	2687	U	N3-C2-O2	6.73	126.91	122.20
1	A	1998	G	N1-C6-O6	-6.73	115.86	119.90
1	A	2029	G	N9-C4-C5	6.72	108.09	105.40
1	A	448	U	C2-N3-C4	-6.72	122.97	127.00
18	W	92	ARG	NE-CZ-NH1	-6.72	116.94	120.30
1	A	1612	C	C5-C6-N1	-6.72	117.64	121.00
1	A	504	U	C5-C4-O4	6.71	129.93	125.90
1	A	2070	G	N1-C6-O6	-6.71	115.87	119.90
1	A	933	A	N1-C6-N6	6.71	122.62	118.60
1	A	1248	G	N9-C4-C5	-6.71	102.72	105.40
1	A	2330	G	C5-C6-N1	-6.70	108.15	111.50
1	A	2286	A	C4-C5-N7	6.70	114.05	110.70
1	A	2608	G	C6-N1-C2	-6.70	121.08	125.10
1	A	2318	G	N7-C8-N9	-6.70	109.75	113.10
1	A	2408	U	N3-C2-O2	-6.69	117.52	122.20
1	A	785	G	C5-C6-N1	6.69	114.84	111.50
1	A	2330	G	N1-C6-O6	6.69	123.91	119.90
1	A	2448	A	C5-C6-N6	-6.68	118.35	123.70
1	A	1668	A	N1-C6-N6	-6.67	114.60	118.60
1	A	2543	G	N7-C8-N9	-6.66	109.77	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2467	C	N3-C4-C5	-6.66	119.24	121.90
1	A	2306	C	C5-C6-N1	6.65	124.33	121.00
1	A	777	A	C8-N9-C4	-6.65	103.14	105.80
1	A	740	U	N3-C4-O4	-6.65	114.75	119.40
1	A	796	C	N1-C2-O2	6.65	122.89	118.90
1	A	2805	G	N3-C4-C5	-6.65	125.28	128.60
1	A	271(X)	G	C4-C5-N7	-6.64	108.14	110.80
1	A	199	A	C5-N7-C8	6.64	107.22	103.90
1	A	759	G	C2-N3-C4	6.64	115.22	111.90
1	A	2888	C	C6-N1-C2	-6.64	117.64	120.30
1	A	2103	C	N1-C2-O2	6.63	122.88	118.90
1	A	2506	U	N3-C4-O4	-6.63	114.76	119.40
1	A	529	A	C4-C5-N7	6.63	114.01	110.70
1	A	2253	G	C6-C5-N7	-6.62	126.42	130.40
1	A	1609	A	C8-N9-C4	6.62	108.45	105.80
1	A	1758	G	C5-C6-O6	-6.62	124.63	128.60
1	A	1948	G	N3-C4-N9	-6.62	122.03	126.00
1	A	1379	A	N9-C4-C5	-6.62	103.15	105.80
2	B	63	G	C8-N9-C4	6.61	109.05	106.40
1	A	2699	C	C2-N1-C1'	-6.61	111.53	118.80
2	B	105	A	C8-N9-C4	6.61	108.44	105.80
1	A	390	A	N7-C8-N9	-6.61	110.50	113.80
1	A	2345	G	N3-C2-N2	6.60	124.52	119.90
1	A	2453	A	C5-N7-C8	6.60	107.20	103.90
1	A	1022	G	N3-C2-N2	-6.60	115.28	119.90
1	A	2894	G	N7-C8-N9	6.60	116.40	113.10
1	A	948	G	N9-C4-C5	6.60	108.04	105.40
1	A	2379	G	C5-C6-O6	-6.59	124.64	128.60
1	A	2506	U	C5-C4-O4	6.59	129.85	125.90
2	B	114	C	C5-C6-N1	-6.59	117.70	121.00
1	A	781	A	C6-N1-C2	-6.59	114.65	118.60
1	A	2236	C	C5-C6-N1	-6.59	117.71	121.00
1	A	2042	A	C2-N3-C4	-6.59	107.31	110.60
1	A	1558	A	C5-C6-N1	-6.58	114.41	117.70
1	A	133	C	C5-C6-N1	-6.57	117.71	121.00
1	A	2441	C	C2-N3-C4	-6.57	116.61	119.90
1	A	2689	U	N3-C2-O2	-6.57	117.60	122.20
1	A	834	C	N3-C4-C5	6.56	124.53	121.90
1	A	2078	C	N1-C2-O2	-6.56	114.96	118.90
2	B	115	G	C2-N3-C4	-6.56	108.62	111.90
1	A	82	G	N3-C4-N9	6.56	129.93	126.00
1	A	56	A	N1-C6-N6	-6.55	114.67	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	231	C	C6-N1-C2	-6.55	117.68	120.30
1	A	915	C	N3-C2-O2	-6.55	117.32	121.90
1	A	1289	C	C2-N3-C4	-6.55	116.63	119.90
1	A	1997	G	C2-N3-C4	6.55	115.17	111.90
1	A	2003	G	N1-C2-N3	6.55	127.83	123.90
11	P	50	ARG	NE-CZ-NH1	-6.55	117.03	120.30
1	A	1978	A	C8-N9-C4	-6.54	103.18	105.80
1	A	803	U	C2-N3-C4	-6.54	123.08	127.00
1	A	2489	G	C8-N9-C4	6.54	109.02	106.40
1	A	1777	U	N1-C2-N3	6.54	118.82	114.90
1	A	1609	A	N7-C8-N9	-6.54	110.53	113.80
1	A	1882	C	N1-C2-O2	6.53	122.82	118.90
1	A	197	A	N1-C2-N3	-6.53	126.03	129.30
2	B	6	C	C6-N1-C2	6.53	122.91	120.30
1	A	1289	C	C5-C6-N1	-6.52	117.74	121.00
1	A	2517	C	N3-C2-O2	6.52	126.46	121.90
3	D	218	ARG	NE-CZ-NH2	-6.52	117.04	120.30
1	A	2335	A	C4-C5-N7	6.51	113.96	110.70
1	A	1248	G	C4-C5-N7	6.51	113.40	110.80
1	A	1124	C	C5-C4-N4	-6.51	115.64	120.20
1	A	113	G	C4-N9-C1'	-6.50	118.05	126.50
1	A	2441	C	C4-C5-C6	6.50	120.65	117.40
1	A	673	C	C6-N1-C2	6.49	122.90	120.30
1	A	1187	G	N1-C6-O6	-6.49	116.00	119.90
1	A	427	U	N1-C2-O2	6.49	127.34	122.80
1	A	2237	G	C8-N9-C4	6.49	109.00	106.40
1	A	635	C	C6-N1-C2	-6.48	117.71	120.30
1	A	1141	U	C2-N3-C4	-6.48	123.11	127.00
1	A	923	C	C6-N1-C2	-6.48	117.71	120.30
1	A	530	G	N3-C4-C5	6.48	131.84	128.60
1	A	1977	A	N7-C8-N9	-6.48	110.56	113.80
1	A	756	C	N1-C2-O2	-6.47	115.02	118.90
1	A	693	C	C5-C6-N1	-6.47	117.77	121.00
1	A	1126	A	N9-C4-C5	-6.47	103.21	105.80
1	A	2207	G	N1-C6-O6	6.47	123.78	119.90
1	A	1904	G	C5-C6-N1	6.46	114.73	111.50
1	A	2161	C	N3-C4-N4	-6.46	113.48	118.00
1	A	199	A	C4-C5-N7	-6.46	107.47	110.70
1	A	2829	C	N1-C2-O2	-6.45	115.03	118.90
1	A	833	U	N3-C4-O4	6.45	123.92	119.40
1	A	2483	C	C6-N1-C2	-6.45	117.72	120.30
1	A	688	U	N1-C2-N3	6.44	118.77	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	34	C	N3-C4-C5	-6.44	119.32	121.90
1	A	1631	C	N1-C2-O2	-6.44	115.04	118.90
1	A	348	G	N7-C8-N9	-6.44	109.88	113.10
10	O	8	LEU	CA-CB-CG	6.43	130.10	115.30
1	A	1021	A	N7-C8-N9	6.43	117.02	113.80
1	A	2191	G	C4-C5-N7	6.43	113.37	110.80
1	A	2464	C	C5-C4-N4	-6.43	115.70	120.20
1	A	495	G	N7-C8-N9	-6.42	109.89	113.10
1	A	2335	A	C2-N3-C4	6.42	113.81	110.60
1	A	1679	U	C4-C5-C6	6.41	123.55	119.70
1	A	1252	G	N7-C8-N9	-6.41	109.89	113.10
1	A	2612	C	C6-N1-C2	6.41	122.86	120.30
11	P	148	LEU	CA-CB-CG	6.41	130.05	115.30
1	A	809	G	C5-N7-C8	6.41	107.50	104.30
1	A	2284	C	C6-N1-C2	6.41	122.86	120.30
1	A	652(T)	C	N1-C2-O2	6.40	122.74	118.90
1	A	114	U	C2-N1-C1'	6.40	125.38	117.70
1	A	646	A	N7-C8-N9	6.39	117.00	113.80
1	A	728	G	C4-C5-N7	-6.39	108.24	110.80
1	A	1670	C	N3-C4-C5	-6.39	119.34	121.90
1	A	1721	G	C4-C5-N7	6.39	113.36	110.80
30	8	34	TRP	O-C-N	-6.39	112.47	122.70
1	A	1037	G	N1-C6-O6	6.39	123.73	119.90
1	A	1695	G	N7-C8-N9	6.39	116.30	113.10
1	A	1992	G	C8-N9-C4	-6.39	103.84	106.40
1	A	2870	C	N1-C2-O2	-6.39	115.07	118.90
1	A	1796	U	N1-C2-O2	6.39	127.27	122.80
1	A	1835	G	N3-C4-N9	6.38	129.83	126.00
1	A	361	G	N1-C6-O6	6.38	123.73	119.90
1	A	812	C	C6-N1-C2	-6.38	117.75	120.30
1	A	1774	C	N3-C4-C5	-6.38	119.35	121.90
1	A	1990	C	C6-N1-C2	-6.38	117.75	120.30
1	A	107	C	N3-C4-C5	6.38	124.45	121.90
1	A	330	A	N1-C6-N6	6.38	122.43	118.60
1	A	1683	C	N3-C2-O2	6.38	126.36	121.90
1	A	2791	C	N1-C2-O2	6.37	122.72	118.90
1	A	2087	G	N1-C6-O6	6.37	123.72	119.90
1	A	1345	C	C4-C5-C6	6.37	120.58	117.40
1	A	121	G	C5-C6-O6	-6.37	124.78	128.60
2	B	91	C	C5-C4-N4	-6.36	115.75	120.20
1	A	757	U	C2-N3-C4	-6.36	123.19	127.00
1	A	750	A	N9-C4-C5	-6.36	103.26	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	883	G	C5-C6-O6	-6.35	124.79	128.60
1	A	2454	G	N3-C2-N2	6.35	124.34	119.90
1	A	2645	G	N3-C4-N9	-6.35	122.19	126.00
1	A	115	C	N3-C2-O2	6.34	126.34	121.90
1	A	2284	C	C5-C6-N1	-6.34	117.83	121.00
1	A	936	C	N1-C2-O2	-6.34	115.10	118.90
1	A	720	C	C6-N1-C2	6.34	122.83	120.30
1	A	1984	G	C8-N9-C4	-6.34	103.87	106.40
1	A	1399	C	C2-N3-C4	-6.33	116.73	119.90
1	A	1882	C	C2-N1-C1'	6.33	125.77	118.80
1	A	2864	G	C5-C6-O6	6.33	132.40	128.60
2	B	13	A	C8-N9-C4	6.33	108.33	105.80
1	A	530	G	C8-N9-C1'	6.33	135.23	127.00
1	A	562	U	N3-C2-O2	-6.33	117.77	122.20
1	A	1776	G	N3-C2-N2	6.32	124.33	119.90
1	A	2486	G	N1-C6-O6	6.32	123.69	119.90
1	A	2453	A	C2-N3-C4	6.32	113.76	110.60
1	A	317	G	N1-C6-O6	6.32	123.69	119.90
1	A	739	G	C2-N3-C4	6.31	115.06	111.90
1	A	2154	G	C6-N1-C2	6.31	128.89	125.10
1	A	1647	G	C5-C6-O6	-6.31	124.81	128.60
1	A	1778	U	N3-C4-O4	6.31	123.82	119.40
1	A	1822	G	N9-C4-C5	6.31	107.92	105.40
1	A	229	A	C8-N9-C4	-6.31	103.28	105.80
1	A	1807	G	N7-C8-N9	-6.31	109.95	113.10
1	A	537	C	N3-C4-C5	6.30	124.42	121.90
1	A	2371	G	N9-C4-C5	-6.30	102.88	105.40
1	A	826	U	N1-C2-O2	-6.30	118.39	122.80
1	A	752	A	N7-C8-N9	6.30	116.95	113.80
1	A	1558	A	N7-C8-N9	6.30	116.95	113.80
1	A	1239	G	C5-C6-O6	-6.29	124.82	128.60
1	A	1302	A	C5-N7-C8	6.29	107.05	103.90
1	A	2280	G	C5-C6-O6	-6.29	124.82	128.60
1	A	2283	C	N1-C2-O2	-6.29	115.13	118.90
1	A	525	U	N1-C2-O2	-6.28	118.40	122.80
1	A	981	A	N1-C2-N3	-6.28	126.16	129.30
1	A	1475	G	N3-C4-N9	-6.28	122.23	126.00
1	A	2705	A	N9-C4-C5	-6.28	103.29	105.80
1	A	964	C	N3-C4-C5	-6.28	119.39	121.90
1	A	444	C	C2-N3-C4	-6.28	116.76	119.90
1	A	2463	C	N3-C4-N4	6.28	122.39	118.00
1	A	738	G	N1-C6-O6	-6.27	116.14	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1635	G	C5-C6-O6	-6.26	124.84	128.60
2	B	117	G	C5-C6-O6	-6.26	124.84	128.60
1	A	1958	C	N1-C2-O2	-6.26	115.14	118.90
1	A	1973	G	N1-C6-O6	-6.26	116.15	119.90
1	A	2567	G	C6-N1-C2	-6.25	121.35	125.10
1	A	546	C	C5-C6-N1	6.25	124.13	121.00
1	A	1625	C	N3-C2-O2	-6.25	117.53	121.90
1	A	2335	A	N3-C4-N9	6.25	132.40	127.40
1	A	2866	U	C5-C4-O4	6.25	129.65	125.90
1	A	425	G	N3-C2-N2	6.25	124.27	119.90
1	A	520	G	C5-C6-O6	6.25	132.35	128.60
1	A	2029	G	C8-N9-C4	-6.25	103.90	106.40
1	A	1317	A	N9-C4-C5	6.24	108.30	105.80
1	A	2007	C	N1-C2-O2	-6.24	115.16	118.90
1	A	2013	A	N1-C2-N3	6.24	132.42	129.30
1	A	2063	C	N3-C4-C5	6.24	124.40	121.90
2	B	91	C	C6-N1-C2	6.24	122.80	120.30
15	T	95	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	A	2304	G	N1-C6-O6	-6.23	116.16	119.90
1	A	243	U	N3-C2-O2	-6.22	117.84	122.20
1	A	113	G	N1-C2-N2	6.22	121.80	116.20
1	A	692	C	C6-N1-C2	6.22	122.79	120.30
1	A	2017	U	C5-C6-N1	-6.22	119.59	122.70
1	A	2296	U	C4-C5-C6	6.22	123.43	119.70
1	A	139(A)	G	C5-C6-O6	-6.21	124.87	128.60
1	A	1343	G	N1-C6-O6	-6.21	116.17	119.90
1	A	1284	A	N1-C6-N6	6.21	122.33	118.60
1	A	1901	A	C6-N1-C2	-6.21	114.88	118.60
1	A	2817	G	C6-N1-C2	-6.21	121.38	125.10
1	A	2866	U	N1-C2-N3	6.21	118.62	114.90
1	A	527	C	C2-N3-C4	-6.20	116.80	119.90
1	A	1992	G	P-O3'-C3'	6.20	127.14	119.70
1	A	1040	C	N3-C4-C5	6.20	124.38	121.90
1	A	2694	G	C8-N9-C4	6.20	108.88	106.40
1	A	2364	C	C5-C6-N1	-6.20	117.90	121.00
1	A	2040	C	C6-N1-C2	6.20	122.78	120.30
1	A	596	G	N1-C6-O6	-6.19	116.18	119.90
1	A	1204	A	N1-C2-N3	6.19	132.40	129.30
1	A	1247	A	C2-N3-C4	-6.19	107.50	110.60
1	A	2791	C	C6-N1-C2	-6.19	117.82	120.30
1	A	529	A	N1-C6-N6	6.19	122.31	118.60
1	A	571	A	C8-N9-C4	6.19	108.28	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	G	N3-C2-N2	-6.19	115.57	119.90
1	A	1665	A	N7-C8-N9	-6.19	110.71	113.80
1	A	2828	C	N3-C4-C5	6.19	124.38	121.90
1	A	448	U	N1-C2-N3	6.18	118.61	114.90
1	A	530	G	N7-C8-N9	6.18	116.19	113.10
1	A	645	C	N3-C2-O2	-6.18	117.58	121.90
1	A	1854	A	N1-C6-N6	-6.18	114.89	118.60
1	A	2127	G	C6-N1-C2	6.17	128.80	125.10
1	A	1276	A	C8-N9-C4	6.17	108.27	105.80
1	A	1640	C	C6-N1-C2	-6.17	117.83	120.30
1	A	2303	G	N3-C2-N2	-6.17	115.58	119.90
1	A	607	U	C5-C6-N1	-6.17	119.61	122.70
1	A	1226	A	N7-C8-N9	-6.17	110.72	113.80
1	A	1318	C	N1-C2-O2	-6.17	115.20	118.90
1	A	2028	U	N3-C4-O4	-6.17	115.08	119.40
1	A	2611	U	C6-N1-C2	-6.17	117.30	121.00
1	A	1340	U	C5-C6-N1	-6.16	119.62	122.70
1	A	265	A	C8-N9-C4	-6.16	103.34	105.80
1	A	1359	A	C8-N9-C4	6.16	108.26	105.80
1	A	2304	G	C8-N9-C1'	6.16	135.01	127.00
1	A	686	G	C8-N9-C4	6.16	108.86	106.40
1	A	526	A	N1-C6-N6	-6.15	114.91	118.60
1	A	781	A	C5-N7-C8	6.15	106.98	103.90
14	S	96	GLY	N-CA-C	-6.15	97.72	113.10
1	A	803	U	C5-C6-N1	-6.15	119.62	122.70
1	A	347	A	C8-N9-C4	6.15	108.26	105.80
1	A	587	C	C5-C4-N4	6.15	124.50	120.20
1	A	223	A	C8-N9-C4	-6.15	103.34	105.80
1	A	1541	G	C8-N9-C4	-6.14	103.94	106.40
1	A	494	G	C2-N3-C4	-6.14	108.83	111.90
1	A	429	A	N1-C6-N6	-6.13	114.92	118.60
1	A	1681	G	N3-C4-C5	6.13	131.67	128.60
1	A	2260	C	C4-C5-C6	6.13	120.47	117.40
1	A	532	A	C5-C6-N1	-6.13	114.63	117.70
1	A	2304	G	C6-N1-C2	-6.13	121.42	125.10
1	A	1192	G	C8-N9-C4	6.13	108.85	106.40
1	A	1945	G	C8-N9-C4	6.13	108.85	106.40
1	A	933	A	C6-C5-N7	-6.13	128.01	132.30
1	A	776	G	C5-C6-O6	6.13	132.28	128.60
1	A	823	G	C4-C5-N7	-6.12	108.35	110.80
1	A	1010	A	N1-C2-N3	-6.12	126.24	129.30
1	A	1339	G	C8-N9-C4	6.12	108.85	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1022	G	N9-C4-C5	6.12	107.85	105.40
1	A	2567	G	C4-C5-N7	-6.12	108.35	110.80
1	A	2526	G	C5-C6-N1	-6.11	108.44	111.50
1	A	2697	G	N7-C8-N9	-6.11	110.04	113.10
1	A	236	C	N1-C2-O2	-6.11	115.23	118.90
1	A	825	C	C6-N1-C2	6.11	122.74	120.30
1	A	535	C	C2-N1-C1'	-6.11	112.08	118.80
1	A	2044	C	C2-N3-C4	-6.11	116.85	119.90
1	A	1002	G	N3-C2-N2	6.10	124.17	119.90
1	A	192	C	C5-C6-N1	-6.10	117.95	121.00
1	A	530	G	N9-C4-C5	6.10	107.84	105.40
1	A	680	G	C8-N9-C4	6.10	108.84	106.40
1	A	2027	G	C4-C5-N7	-6.09	108.36	110.80
1	A	2237	G	N9-C4-C5	-6.09	102.96	105.40
1	A	92	A	N7-C8-N9	6.09	116.85	113.80
1	A	250	G	C5-C6-N1	6.09	114.55	111.50
1	A	982	C	N3-C4-N4	6.09	122.26	118.00
1	A	2604	U	C5-C6-N1	-6.09	119.65	122.70
1	A	1311	G	N1-C6-O6	-6.09	116.25	119.90
1	A	2033	A	C4-C5-N7	-6.09	107.66	110.70
1	A	1541	G	C5-C6-O6	6.09	132.25	128.60
1	A	1800	C	N3-C2-O2	-6.09	117.64	121.90
1	A	1995	U	N3-C2-O2	-6.09	117.94	122.20
1	A	568	U	N1-C2-O2	-6.08	118.54	122.80
1	A	2207	G	C6-C5-N7	-6.08	126.75	130.40
1	A	124	G	C5-C6-O6	-6.08	124.95	128.60
1	A	207	A	C2-N3-C4	-6.08	107.56	110.60
1	A	574	C	C2-N3-C4	6.08	122.94	119.90
1	A	1975	G	N1-C6-O6	-6.08	116.25	119.90
1	A	2709	G	N3-C2-N2	6.08	124.16	119.90
1	A	2877	G	C8-N9-C4	6.08	108.83	106.40
1	A	1675	C	C5-C6-N1	-6.08	117.96	121.00
1	A	1963	U	C6-N1-C1'	-6.08	112.69	121.20
1	A	217	G	C8-N9-C4	6.08	108.83	106.40
1	A	271(H)	G	N3-C4-N9	6.08	129.65	126.00
1	A	693	C	C2-N3-C4	-6.07	116.86	119.90
1	A	1243	G	N9-C4-C5	6.07	107.83	105.40
1	A	737	C	C4-C5-C6	6.07	120.43	117.40
1	A	1620	G	N9-C4-C5	6.07	107.83	105.40
1	A	2869	G	C8-N9-C4	-6.07	103.97	106.40
1	A	2059	A	N9-C4-C5	-6.06	103.38	105.80
1	A	1313	U	C2-N1-C1'	6.06	124.97	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	945	A	C8-N9-C4	-6.06	103.38	105.80
1	A	2191	G	C6-C5-N7	-6.06	126.77	130.40
1	A	772	C	N3-C2-O2	6.06	126.14	121.90
1	A	1126	A	C5-C6-N6	-6.06	118.86	123.70
1	A	935	C	C6-N1-C2	6.05	122.72	120.30
1	A	1005	C	N3-C2-O2	-6.05	117.66	121.90
1	A	1698	A	C6-C5-N7	-6.05	128.06	132.30
1	A	1828	G	N9-C4-C5	-6.05	102.98	105.40
1	A	2441	C	C5-C6-N1	-6.05	117.97	121.00
1	A	139(A)	G	C5-C6-N1	6.05	114.53	111.50
1	A	208	C	N1-C2-O2	-6.05	115.27	118.90
1	A	817	C	N1-C2-O2	6.05	122.53	118.90
1	A	2622	C	C4-C5-C6	-6.04	114.38	117.40
1	A	1377	G	N1-C2-N2	-6.04	110.76	116.20
1	A	2453	A	N7-C8-N9	-6.04	110.78	113.80
1	A	149	A	N1-C6-N6	6.04	122.22	118.60
15	T	127	ALA	N-CA-C	-6.04	94.70	111.00
1	A	2436	G	N1-C6-O6	-6.04	116.28	119.90
1	A	1313	U	N1-C2-N3	6.03	118.52	114.90
1	A	2065	C	C5-C4-N4	6.03	124.42	120.20
1	A	195	A	C8-N9-C4	6.03	108.21	105.80
1	A	944	G	N7-C8-N9	6.03	116.11	113.10
1	A	2515	C	C2-N3-C4	-6.03	116.89	119.90
1	A	2087	G	C8-N9-C4	6.02	108.81	106.40
1	A	2624	G	C5-N7-C8	6.02	107.31	104.30
1	A	1755	A	C2-N3-C4	-6.01	107.59	110.60
1	A	139(A)	G	C8-N9-C4	-6.01	104.00	106.40
1	A	2260	C	C5-C6-N1	-6.01	118.00	121.00
1	A	1828	G	C5-C6-O6	-6.00	125.00	128.60
1	A	1602	U	N1-C2-O2	-6.00	118.60	122.80
1	A	893	C	C2-N1-C1'	6.00	125.39	118.80
1	A	2467	C	C6-N1-C2	-6.00	117.90	120.30
1	A	2502	G	C5-C6-O6	-5.99	125.00	128.60
1	A	1260	G	N7-C8-N9	-5.99	110.11	113.10
1	A	348	G	C5-N7-C8	5.99	107.29	104.30
1	A	214	G	C5-C6-N1	5.99	114.49	111.50
1	A	219	G	C6-N1-C2	5.98	128.69	125.10
1	A	2875	C	C2-N3-C4	-5.98	116.91	119.90
1	A	438	G	N1-C6-O6	5.98	123.49	119.90
1	A	737	C	C5-C6-N1	-5.98	118.01	121.00
1	A	1697	G	N1-C6-O6	5.98	123.49	119.90
1	A	2505	G	N1-C6-O6	-5.98	116.31	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1021	A	C4-C5-N7	5.97	113.69	110.70
1	A	271(H)	G	C8-N9-C1'	-5.97	119.24	127.00
1	A	1651	G	C2-N3-C4	5.97	114.89	111.90
1	A	1990	C	C5-C4-N4	5.97	124.38	120.20
1	A	2023	G	C8-N9-C4	-5.97	104.01	106.40
1	A	2827	C	C6-N1-C2	5.97	122.69	120.30
1	A	723	G	C8-N9-C4	-5.97	104.01	106.40
1	A	1684	C	N1-C2-O2	-5.97	115.32	118.90
1	A	2373	G	N1-C2-N3	5.97	127.48	123.90
1	A	484	C	C2-N3-C4	-5.97	116.92	119.90
1	A	665	C	N3-C2-O2	-5.96	117.72	121.90
1	A	532	A	C2-N3-C4	-5.96	107.62	110.60
1	A	2192	G	C4-C5-N7	5.96	113.18	110.80
1	A	2059	A	C8-N9-C4	5.96	108.18	105.80
1	A	738	G	N3-C4-C5	-5.95	125.62	128.60
1	A	481	G	N7-C8-N9	5.95	116.07	113.10
11	P	27	HIS	CB-CA-C	-5.94	98.51	110.40
1	A	2707	G	C6-N1-C2	-5.94	121.53	125.10
1	A	2049	G	C5-C6-O6	5.93	132.16	128.60
1	A	2356	C	N1-C2-O2	-5.93	115.34	118.90
1	A	1650	G	N9-C4-C5	5.93	107.77	105.40
1	A	1775	U	N3-C2-O2	5.93	126.35	122.20
1	A	2322	A	N3-C4-C5	-5.93	122.65	126.80
13	R	114	VAL	CB-CA-C	-5.93	100.13	111.40
1	A	1530	C	C5-C4-N4	-5.93	116.05	120.20
1	A	2420	C	C5-C6-N1	-5.92	118.04	121.00
1	A	2007	C	N1-C2-N3	5.92	123.35	119.20
1	A	2627	G	C8-N9-C4	5.92	108.77	106.40
1	A	313	C	N3-C4-C5	-5.92	119.53	121.90
1	A	2617	C	N3-C4-C5	5.91	124.27	121.90
1	A	1654	A	C5-N7-C8	5.91	106.86	103.90
1	A	2821	A	C5-N7-C8	-5.91	100.94	103.90
2	B	20	C	C6-N1-C1'	-5.91	113.71	120.80
1	A	1826	G	C5-C6-O6	5.90	132.14	128.60
1	A	809	G	N7-C8-N9	-5.90	110.15	113.10
1	A	1900	A	C6-N1-C2	-5.90	115.06	118.60
1	A	1956	U	C2-N3-C4	-5.90	123.46	127.00
1	A	2030	A	C5-C6-N6	-5.90	118.98	123.70
1	A	2585	U	N1-C2-O2	5.90	126.93	122.80
1	A	601	C	C5-C6-N1	-5.90	118.05	121.00
1	A	745	G	N3-C2-N2	-5.90	115.77	119.90
1	A	266	G	C8-N9-C4	5.89	108.76	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	530	G	N3-C2-N2	-5.89	115.78	119.90
1	A	607	U	N3-C4-O4	-5.89	115.28	119.40
1	A	249	C	C6-N1-C2	5.88	122.65	120.30
1	A	444	C	N3-C4-C5	5.88	124.25	121.90
1	A	1721	G	N3-C4-N9	5.88	129.53	126.00
1	A	2503	A	C8-N9-C4	5.88	108.15	105.80
1	A	2582	G	N3-C2-N2	5.88	124.02	119.90
1	A	645	C	C5-C6-N1	5.88	123.94	121.00
1	A	2036	C	N3-C4-C5	5.88	124.25	121.90
1	A	82	G	N9-C4-C5	-5.88	103.05	105.40
1	A	961	C	C2-N3-C4	-5.88	116.96	119.90
1	A	2036	C	C5-C4-N4	-5.88	116.09	120.20
1	A	468	G	N7-C8-N9	-5.88	110.16	113.10
1	A	1776	G	N1-C2-N2	-5.88	110.91	116.20
1	A	2712	U	N3-C4-C5	5.87	118.12	114.60
1	A	265	A	C5-C6-N1	-5.87	114.77	117.70
1	A	1678	G	N1-C2-N3	5.87	127.42	123.90
2	B	117	G	N3-C4-C5	5.87	131.53	128.60
1	A	214	G	C5-C6-O6	-5.87	125.08	128.60
1	A	1126	A	C8-N9-C4	5.87	108.15	105.80
1	A	1238	G	C8-N9-C4	5.87	108.75	106.40
1	A	2332	U	N3-C2-O2	-5.87	118.09	122.20
1	A	1288	U	N1-C2-O2	5.86	126.90	122.80
1	A	1596	A	C8-N9-C4	5.86	108.15	105.80
1	A	2279	G	N9-C4-C5	-5.86	103.06	105.40
1	A	2014	A	N1-C6-N6	5.86	122.11	118.60
1	A	2444	G	C4-C5-N7	-5.86	108.46	110.80
1	A	333	G	N7-C8-N9	5.85	116.03	113.10
1	A	1997	G	N7-C8-N9	-5.85	110.17	113.10
1	A	923	C	C5-C6-N1	5.85	123.92	121.00
1	A	966	G	C5-C6-O6	5.85	132.11	128.60
1	A	676	A	N1-C6-N6	5.85	122.11	118.60
1	A	433	C	C6-N1-C2	-5.84	117.96	120.30
1	A	1441	G	C8-N9-C4	5.84	108.74	106.40
1	A	2773	C	N3-C4-C5	5.84	124.24	121.90
1	A	546	C	C6-N1-C2	-5.84	117.97	120.30
1	A	495	G	C5-C6-O6	5.84	132.10	128.60
1	A	2619	C	C5-C6-N1	-5.84	118.08	121.00
1	A	948	G	N3-C2-N2	-5.83	115.81	119.90
1	A	2296	U	C1'-O4'-C4'	-5.83	105.23	109.90
1	A	2328	A	N9-C4-C5	5.83	108.13	105.80
1	A	1303	G	N3-C2-N2	5.83	123.98	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	86	G	C8-N9-C4	5.83	108.73	106.40
1	A	847	U	C4-C5-C6	5.83	123.20	119.70
1	A	1674	G	C4-N9-C1'	5.83	134.08	126.50
1	A	1683	C	N1-C2-O2	-5.83	115.40	118.90
1	A	1760	A	N1-C6-N6	-5.83	115.10	118.60
1	A	1493	C	C6-N1-C1'	-5.83	113.80	120.80
1	A	454	A	N1-C6-N6	5.83	122.10	118.60
1	A	1038	C	N1-C2-O2	5.83	122.39	118.90
1	A	1782	C	N3-C4-C5	5.83	124.23	121.90
1	A	750	A	N1-C6-N6	5.82	122.09	118.60
1	A	1453	U	N1-C2-O2	-5.82	118.73	122.80
1	A	1799	G	C8-N9-C4	-5.82	104.07	106.40
1	A	1697	G	N3-C2-N2	-5.82	115.83	119.90
2	B	104	U	C6-N1-C2	5.82	124.49	121.00
1	A	608	A	N7-C8-N9	5.81	116.70	113.80
1	A	1343	G	C5-C6-O6	5.81	132.09	128.60
1	A	752	A	C8-N9-C4	-5.81	103.48	105.80
1	A	1780	A	C5-C6-N1	-5.81	114.80	117.70
1	A	1653	G	C6-N1-C2	-5.80	121.62	125.10
1	A	260	G	C4-C5-N7	-5.80	108.48	110.80
1	A	2495	G	C5-C6-N1	-5.80	108.60	111.50
1	A	2543	G	C5-N7-C8	5.80	107.20	104.30
1	A	2891	G	C5-C6-O6	-5.80	125.12	128.60
1	A	784	A	C8-N9-C4	5.80	108.12	105.80
1	A	1249	U	C4-C5-C6	5.80	123.18	119.70
1	A	425	G	C8-N9-C4	5.79	108.72	106.40
1	A	1821	A	C5-C6-N6	-5.79	119.06	123.70
2	B	49	C	C6-N1-C2	-5.79	117.98	120.30
1	A	2399	G	N1-C6-O6	-5.79	116.42	119.90
1	A	1828	G	C8-N9-C4	5.79	108.72	106.40
1	A	2134	A	N1-C6-N6	-5.79	115.13	118.60
1	A	2304	G	C4-N9-C1'	-5.79	118.97	126.50
1	A	62	C	C5-C6-N1	-5.79	118.11	121.00
1	A	272(H)	C	N3-C4-C5	5.79	124.22	121.90
1	A	1258	C	C5-C6-N1	-5.79	118.11	121.00
1	A	1953	A	N9-C4-C5	-5.79	103.48	105.80
1	A	395	U	N1-C2-O2	5.79	126.85	122.80
1	A	1984	G	N7-C8-N9	5.79	115.99	113.10
2	B	29	A	N1-C6-N6	5.78	122.07	118.60
1	A	2828	C	N3-C4-N4	-5.78	113.95	118.00
1	A	1841	U	N3-C4-O4	5.78	123.44	119.40
1	A	2231	C	C6-N1-C2	5.78	122.61	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	78	A	C5-C6-N6	-5.78	119.08	123.70
1	A	948	G	C8-N9-C4	-5.78	104.09	106.40
1	A	1901	A	N9-C4-C5	5.78	108.11	105.80
1	A	2600	A	N1-C6-N6	-5.78	115.13	118.60
1	A	912	C	C5-C6-N1	5.77	123.89	121.00
1	A	2053	G	C8-N9-C4	5.77	108.71	106.40
1	A	2784	C	C5-C6-N1	-5.77	118.11	121.00
2	B	118	G	N3-C4-C5	5.77	131.49	128.60
1	A	961	C	C6-N1-C2	5.77	122.61	120.30
1	A	2304	G	N9-C4-C5	5.77	107.71	105.40
3	D	239	ARG	N-CA-C	-5.77	95.43	111.00
1	A	2386	C	C5-C6-N1	-5.77	118.12	121.00
1	A	406	G	C4-C5-N7	5.76	113.11	110.80
1	A	2080	G	N1-C2-N3	5.76	127.36	123.90
1	A	2487	G	N1-C6-O6	5.76	123.36	119.90
1	A	348	G	C8-N9-C4	5.76	108.70	106.40
1	A	886	C	C5-C6-N1	5.76	123.88	121.00
1	A	1453	U	C2-N3-C4	-5.76	123.54	127.00
1	A	2124	G	C6-N1-C2	5.76	128.56	125.10
1	A	2050	C	C5-C4-N4	-5.76	116.17	120.20
1	A	107	C	C2-N3-C4	-5.76	117.02	119.90
1	A	680	G	N7-C8-N9	-5.76	110.22	113.10
1	A	2897	U	C5-C6-N1	5.76	125.58	122.70
1	A	791	C	C5-C6-N1	-5.75	118.12	121.00
1	A	2363	C	C2-N1-C1'	-5.75	112.47	118.80
1	A	1653	G	N7-C8-N9	5.75	115.97	113.10
1	A	191	A	N7-C8-N9	-5.75	110.92	113.80
1	A	2068	U	N1-C2-N3	5.75	118.35	114.90
1	A	1558	A	N3-C4-N9	-5.75	122.80	127.40
1	A	1939	U	N3-C4-O4	-5.74	115.38	119.40
21	Z	151	HIS	N-CA-C	5.74	126.51	111.00
1	A	640	C	C5-C6-N1	5.74	123.87	121.00
1	A	1901	A	C8-N9-C4	-5.74	103.50	105.80
1	A	893	C	C6-N1-C1'	-5.74	113.91	120.80
1	A	1204	A	N9-C4-C5	-5.74	103.50	105.80
2	B	56	G	N1-C6-O6	-5.74	116.46	119.90
1	A	1305	C	N1-C2-O2	5.74	122.34	118.90
1	A	1886	C	N3-C4-C5	5.74	124.19	121.90
1	A	454	A	C5-C6-N6	-5.74	119.11	123.70
1	A	2379	G	N1-C6-O6	5.74	123.34	119.90
1	A	444	C	N1-C2-O2	-5.73	115.46	118.90
1	A	71	A	N3-C4-C5	-5.73	122.79	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1022	G	N3-C4-N9	-5.73	122.56	126.00
1	A	1490	A	C8-N9-C4	5.73	108.09	105.80
1	A	961	C	N3-C4-C5	5.73	124.19	121.90
1	A	456	C	C6-N1-C2	5.72	122.59	120.30
1	A	1541	G	C4-C5-N7	-5.72	108.51	110.80
1	A	2743	C	C5-C6-N1	-5.72	118.14	121.00
1	A	1681	G	C4-C5-N7	5.72	113.09	110.80
1	A	1684	C	N3-C2-O2	5.72	125.90	121.90
1	A	2193	G	N1-C6-O6	5.72	123.33	119.90
1	A	811	U	C5-C4-O4	5.72	129.33	125.90
1	A	1750	G	C8-N9-C4	-5.72	104.11	106.40
1	A	2584	U	C5-C4-O4	-5.72	122.47	125.90
1	A	676	A	C5-N7-C8	-5.71	101.04	103.90
1	A	1650	G	N3-C4-N9	-5.71	122.57	126.00
1	A	2716	U	N3-C2-O2	-5.71	118.20	122.20
1	A	33	U	C2-N3-C4	-5.71	123.57	127.00
1	A	759	G	C4-C5-N7	-5.71	108.52	110.80
1	A	1478	G	N3-C4-C5	-5.71	125.75	128.60
1	A	1975	G	C5-C6-O6	5.71	132.03	128.60
1	A	1657	C	C4-C5-C6	5.71	120.25	117.40
1	A	133	C	C2-N3-C4	-5.71	117.05	119.90
1	A	1170	G	C8-N9-C4	-5.70	104.12	106.40
1	A	2036	C	C2-N3-C4	-5.70	117.05	119.90
2	B	56	G	C5-C6-O6	5.70	132.02	128.60
1	A	1721	G	N9-C4-C5	-5.70	103.12	105.40
2	B	78	A	N1-C6-N6	5.70	122.02	118.60
1	A	764	A	C2-N3-C4	5.70	113.45	110.60
1	A	2743	C	C6-N1-C2	5.70	122.58	120.30
1	A	796	C	N3-C2-O2	-5.70	117.91	121.90
1	A	1478	G	N3-C4-N9	5.70	129.42	126.00
1	A	684	G	C8-N9-C4	-5.69	104.12	106.40
2	B	20	C	C2-N1-C1'	5.69	125.06	118.80
1	A	192	C	C4-C5-C6	5.69	120.25	117.40
1	A	747	U	C6-N1-C2	5.69	124.41	121.00
1	A	2320	A	C2-N3-C4	5.69	113.44	110.60
1	A	652(T)	C	C2-N3-C4	5.69	122.74	119.90
1	A	1248	G	N1-C2-N2	-5.69	111.08	116.20
1	A	272(H)	C	C6-N1-C2	5.68	122.57	120.30
1	A	686	G	N1-C2-N3	5.68	127.31	123.90
1	A	2598	A	C2-N3-C4	5.68	113.44	110.60
1	A	1304	C	C5-C6-N1	-5.68	118.16	121.00
1	A	2296	U	C6-N1-C2	5.68	124.41	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1394	U	N3-C2-O2	-5.68	118.22	122.20
1	A	2474	C	N3-C4-C5	5.68	124.17	121.90
1	A	579	G	N1-C6-O6	5.68	123.31	119.90
1	A	2304	G	C5-N7-C8	5.68	107.14	104.30
1	A	841	A	N9-C4-C5	5.68	108.07	105.80
1	A	2228	G	N1-C6-O6	-5.68	116.49	119.90
1	A	2773	C	C2-N3-C4	-5.68	117.06	119.90
1	A	1901	A	N1-C6-N6	-5.68	115.19	118.60
1	A	235	U	C5-C4-O4	-5.67	122.50	125.90
1	A	507	A	C8-N9-C4	5.67	108.07	105.80
1	A	706	A	C5-N7-C8	-5.67	101.06	103.90
1	A	2345	G	N1-C2-N2	-5.67	111.09	116.20
1	A	2817	G	N3-C4-C5	-5.67	125.76	128.60
1	A	90	U	C5-C6-N1	5.67	125.54	122.70
1	A	187	G	N7-C8-N9	-5.67	110.26	113.10
1	A	461	C	N1-C2-O2	-5.67	115.50	118.90
1	A	1776	G	C4-C5-N7	5.67	113.07	110.80
1	A	1799	G	N9-C4-C5	5.67	107.67	105.40
1	A	966	G	N1-C6-O6	-5.67	116.50	119.90
1	A	2395	C	N3-C4-C5	5.67	124.17	121.90
1	A	1698	A	N1-C2-N3	5.67	132.13	129.30
1	A	663	G	C4-C5-N7	-5.67	108.53	110.80
1	A	1266	G	C5-C6-N1	5.67	114.33	111.50
1	A	1638	C	N3-C4-C5	5.67	124.17	121.90
1	A	53	A	N1-C2-N3	5.66	132.13	129.30
1	A	2253	G	C2-N3-C4	-5.66	109.07	111.90
1	A	2322	A	N1-C2-N3	5.66	132.13	129.30
1	A	1676	A	C5-C6-N1	5.66	120.53	117.70
1	A	68	G	C5-N7-C8	5.66	107.13	104.30
1	A	1211	U	C6-N1-C2	5.66	124.40	121.00
1	A	2864	G	N1-C6-O6	-5.66	116.50	119.90
1	A	217	G	N9-C4-C5	-5.66	103.14	105.40
1	A	2114	A	C8-N9-C4	-5.66	103.54	105.80
1	A	503	A	N1-C6-N6	-5.66	115.21	118.60
1	A	1453	U	C5-C6-N1	-5.66	119.87	122.70
1	A	1793	C	N3-C2-O2	-5.66	117.94	121.90
1	A	1803	A	N9-C4-C5	5.65	108.06	105.80
1	A	2319	G	C8-N9-C4	-5.65	104.14	106.40
1	A	2236	C	C2-N3-C4	-5.65	117.07	119.90
1	A	2607	G	C5-C6-O6	-5.65	125.21	128.60
1	A	1834	U	C5-C6-N1	-5.65	119.88	122.70
1	A	1612	C	C4-C5-C6	5.65	120.22	117.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1799	G	C2-N3-C4	5.65	114.72	111.90
1	A	2346	A	N1-C2-N3	5.65	132.12	129.30
1	A	474	G	P-O3'-C3'	5.64	126.47	119.70
1	A	2042	A	C5-C6-N1	-5.64	114.88	117.70
2	B	70	C	N1-C2-O2	5.64	122.28	118.90
1	A	2817	G	C8-N9-C4	-5.64	104.14	106.40
1	A	2838	G	N7-C8-N9	-5.64	110.28	113.10
1	A	1767	C	C6-N1-C2	5.64	122.55	120.30
1	A	752	A	C5-N7-C8	-5.63	101.08	103.90
1	A	559	G	C2-N3-C4	-5.63	109.08	111.90
1	A	1952	A	N7-C8-N9	-5.63	110.98	113.80
1	A	176	G	C8-N9-C4	-5.63	104.15	106.40
1	A	2237	G	N3-C2-N2	5.63	123.84	119.90
1	A	1239	G	N1-C6-O6	5.63	123.28	119.90
1	A	1624	G	C8-N9-C4	5.63	108.65	106.40
1	A	2543	G	N3-C2-N2	5.62	123.84	119.90
1	A	755	C	N1-C2-O2	5.62	122.27	118.90
1	A	686	G	N7-C8-N9	-5.62	110.29	113.10
1	A	2300	G	C8-N9-C4	-5.62	104.15	106.40
5	F	20	LEU	N-CA-C	5.62	126.17	111.00
1	A	781	A	N7-C8-N9	-5.62	110.99	113.80
1	A	68	G	C5-C6-O6	5.62	131.97	128.60
1	A	1721	G	C5-C6-N1	5.62	114.31	111.50
1	A	1950	G	C4-C5-N7	-5.62	108.55	110.80
1	A	260	G	C5-C6-O6	5.61	131.97	128.60
1	A	847	U	N3-C4-O4	-5.61	115.47	119.40
1	A	2334	G	N7-C8-N9	-5.61	110.29	113.10
1	A	1678	G	N3-C4-C5	-5.61	125.80	128.60
1	A	1816	G	C4-N9-C1'	-5.61	119.21	126.50
1	A	2017	U	N1-C2-N3	5.61	118.27	114.90
1	A	2375	G	N1-C6-O6	5.61	123.27	119.90
1	A	305	U	N3-C4-O4	5.61	123.33	119.40
1	A	1756	G	N7-C8-N9	-5.61	110.30	113.10
1	A	371	A	C2-N3-C4	-5.61	107.80	110.60
1	A	734	A	C2-N3-C4	-5.61	107.80	110.60
1	A	2149	G	N1-C2-N2	5.61	121.25	116.20
1	A	2416	C	C5-C4-N4	5.61	124.12	120.20
1	A	2259	G	C2-N3-C4	-5.61	109.10	111.90
1	A	531	C	C2-N3-C4	-5.60	117.10	119.90
1	A	1575	C	N3-C4-C5	5.60	124.14	121.90
1	A	2050	C	N1-C2-O2	-5.60	115.54	118.90
1	A	2247	A	C8-N9-C4	5.60	108.04	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1304	C	N3-C4-C5	5.60	124.14	121.90
1	A	1967	C	N3-C4-C5	5.60	124.14	121.90
27	5	58	LEU	CA-CB-CG	5.60	128.18	115.30
1	A	1721	G	N3-C2-N2	5.60	123.82	119.90
1	A	1816	G	N3-C4-N9	-5.60	122.64	126.00
1	A	1019	U	N1-C2-N3	5.60	118.26	114.90
1	A	1541	G	N9-C4-C5	5.59	107.64	105.40
1	A	2332	U	N3-C4-O4	-5.59	115.49	119.40
1	A	2710	C	C5-C6-N1	-5.59	118.20	121.00
1	A	2791	C	C5-C6-N1	5.59	123.80	121.00
1	A	847	U	N1-C2-N3	5.59	118.25	114.90
1	A	1945	G	N7-C8-N9	-5.59	110.31	113.10
1	A	2733	A	C8-N9-C4	-5.59	103.56	105.80
1	A	2517	C	C5-C4-N4	-5.58	116.29	120.20
1	A	2069	G	N9-C4-C5	5.58	107.63	105.40
1	A	1625	C	C5-C4-N4	5.58	124.11	120.20
1	A	2509	G	N1-C6-O6	5.58	123.25	119.90
1	A	71	A	C5-C6-N1	5.58	120.49	117.70
1	A	1124	C	C6-N1-C1'	-5.58	114.11	120.80
1	A	2828	C	C5-C6-N1	-5.57	118.21	121.00
1	A	2249	U	N3-C4-O4	-5.57	115.50	119.40
1	A	1260	G	C5-N7-C8	5.57	107.09	104.30
1	A	2248	C	N3-C4-C5	5.57	124.13	121.90
1	A	530	G	N1-C6-O6	-5.57	116.56	119.90
1	A	672	C	N3-C4-C5	5.57	124.13	121.90
1	A	1261	C	C2-N1-C1'	-5.57	112.68	118.80
1	A	2744	G	N1-C2-N3	5.57	127.24	123.90
1	A	1339	G	C5-C6-O6	-5.57	125.26	128.60
1	A	787	U	C6-N1-C2	-5.56	117.66	121.00
1	A	208	C	C6-N1-C2	5.56	122.53	120.30
1	A	236	C	N3-C4-C5	5.56	124.12	121.90
1	A	945	A	C5-C6-N1	-5.56	114.92	117.70
1	A	555	U	C6-N1-C2	5.56	124.33	121.00
1	A	1465	G	C8-N9-C4	-5.56	104.18	106.40
1	A	1530	C	C5-C6-N1	5.56	123.78	121.00
1	A	1956	U	N3-C2-O2	5.56	126.09	122.20
1	A	252	G	N9-C4-C5	5.55	107.62	105.40
1	A	1963	U	N3-C2-O2	-5.55	118.31	122.20
1	A	400	G	C8-N9-C4	5.55	108.62	106.40
1	A	2698	U	C6-N1-C2	5.55	124.33	121.00
1	A	236	C	N3-C2-O2	5.55	125.78	121.90
1	A	1140	C	N3-C4-C5	-5.55	119.68	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1676	A	N1-C2-N3	-5.54	126.53	129.30
1	A	2062	A	C5-C6-N1	-5.54	114.93	117.70
20	Y	2	ARG	CD-NE-CZ	5.54	131.36	123.60
1	A	706	A	N7-C8-N9	5.54	116.57	113.80
1	A	1448	G	C5-C6-O6	-5.54	125.28	128.60
1	A	187	G	C8-N9-C4	5.54	108.61	106.40
1	A	644	A	C8-N9-C4	-5.54	103.59	105.80
1	A	1990	C	C4-C5-C6	5.54	120.17	117.40
1	A	2325	G	C8-N9-C4	-5.54	104.19	106.40
1	A	1838	C	C4-C5-C6	5.53	120.17	117.40
30	8	57	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	A	2473	U	N1-C2-O2	5.53	126.67	122.80
1	A	2866	U	N3-C2-O2	-5.53	118.33	122.20
1	A	2465	C	C5-C6-N1	5.53	123.77	121.00
1	A	143(A)	C	C6-N1-C2	5.53	122.51	120.30
1	A	1803	A	C8-N9-C4	-5.53	103.59	105.80
1	A	2808	U	C6-N1-C2	5.53	124.32	121.00
1	A	827	U	N3-C2-O2	5.53	126.07	122.20
1	A	1950	G	N9-C4-C5	5.52	107.61	105.40
1	A	1955	U	C4-C5-C6	5.52	123.01	119.70
1	A	2502	G	C6-N1-C2	-5.52	121.79	125.10
1	A	1338	G	C5-C6-O6	5.52	131.91	128.60
1	A	2519	U	C5-C6-N1	-5.52	119.94	122.70
2	B	118	G	C4-N9-C1'	-5.52	119.32	126.50
1	A	2441	C	N3-C2-O2	-5.52	118.04	121.90
1	A	1958	C	C6-N1-C2	5.52	122.51	120.30
1	A	2238	G	N9-C4-C5	-5.52	103.19	105.40
1	A	1493	C	N1-C2-O2	5.52	122.21	118.90
1	A	599	G	C2-N3-C4	-5.51	109.14	111.90
1	A	978	G	C8-N9-C4	5.51	108.61	106.40
2	B	78	A	C8-N9-C4	-5.51	103.59	105.80
1	A	266	G	N9-C4-C5	-5.51	103.20	105.40
2	B	114	C	C2-N3-C4	-5.51	117.14	119.90
1	A	191	A	C8-N9-C4	5.51	108.00	105.80
1	A	527	C	N3-C4-N4	-5.50	114.15	118.00
1	A	1948	G	N1-C2-N2	5.50	121.16	116.20
1	A	1939	U	C4-C5-C6	-5.50	116.40	119.70
1	A	2448	A	C5-C6-N1	5.50	120.45	117.70
1	A	2027	G	N1-C6-O6	-5.50	116.60	119.90
2	B	117	G	C4-C5-N7	5.50	113.00	110.80
1	A	1834	U	C2-N3-C4	-5.50	123.70	127.00
1	A	2894	G	C4-N9-C1'	5.50	133.65	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2409	G	C5-C6-O6	-5.50	125.30	128.60
1	A	2526	G	C6-N1-C2	5.50	128.40	125.10
1	A	2570	G	N1-C6-O6	5.50	123.20	119.90
1	A	1192	G	N7-C8-N9	-5.50	110.35	113.10
1	A	1223	G	C5-C6-O6	5.49	131.90	128.60
1	A	1559	G	N9-C4-C5	-5.49	103.20	105.40
1	A	2182	G	C6-C5-N7	5.49	133.70	130.40
1	A	1835	G	N3-C2-N2	5.49	123.74	119.90
1	A	977	G	N1-C6-O6	-5.49	116.61	119.90
1	A	1377	G	N1-C6-O6	-5.49	116.61	119.90
1	A	2062	A	C5-N7-C8	-5.49	101.16	103.90
1	A	71	A	C5-C6-N6	-5.48	119.31	123.70
1	A	444	C	C2-N1-C1'	-5.48	112.77	118.80
1	A	1926	U	C5-C6-N1	-5.48	119.96	122.70
2	B	76	G	C8-N9-C4	5.48	108.59	106.40
1	A	2540	C	N1-C2-O2	-5.48	115.61	118.90
1	A	1019	U	N3-C2-O2	-5.48	118.37	122.20
1	A	1957	C	N3-C2-O2	-5.47	118.07	121.90
1	A	2207	G	C4-N9-C1'	5.47	133.62	126.50
1	A	1295	C	N3-C2-O2	-5.47	118.07	121.90
1	A	1379	A	C8-N9-C4	5.47	107.99	105.80
1	A	2053	G	C5-C6-N1	5.47	114.24	111.50
1	A	330	A	N1-C2-N3	5.47	132.04	129.30
1	A	1342	A	C5-C6-N6	-5.47	119.32	123.70
1	A	521	G	N9-C4-C5	5.47	107.59	105.40
1	A	781	A	C5-C6-N1	5.47	120.44	117.70
1	A	975	C	C5-C4-N4	5.47	124.03	120.20
1	A	1399	C	N3-C4-C5	5.47	124.09	121.90
1	A	1835	G	C6-C5-N7	-5.47	127.12	130.40
1	A	2500	U	C4-C5-C6	-5.47	116.42	119.70
2	B	78	A	C5-N7-C8	-5.46	101.17	103.90
1	A	1025	G	C8-N9-C4	-5.46	104.22	106.40
1	A	1559	G	C4-C5-N7	5.46	112.98	110.80
1	A	371	A	N1-C6-N6	5.46	121.88	118.60
1	A	1303	G	N1-C2-N2	-5.46	111.28	116.20
1	A	2029	G	N1-C2-N2	5.46	121.11	116.20
1	A	139(A)	G	N7-C8-N9	5.46	115.83	113.10
1	A	2514	U	N3-C2-O2	5.46	126.02	122.20
1	A	528	A	N7-C8-N9	5.45	116.53	113.80
1	A	2885	C	N3-C4-C5	-5.45	119.72	121.90
1	A	2894	G	N1-C2-N2	-5.45	111.29	116.20
1	A	1017	G	C8-N9-C4	-5.45	104.22	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	A	N3-C4-N9	5.45	131.76	127.40
1	A	135	G	C5-C6-O6	-5.45	125.33	128.60
1	A	1187	G	C5-C6-O6	5.45	131.87	128.60
1	A	2791	C	C2-N3-C4	5.45	122.62	119.90
2	B	116	G	C2-N3-C4	-5.45	109.17	111.90
1	A	2303	G	C6-C5-N7	5.45	133.67	130.40
1	A	1331	A	C8-N9-C4	5.44	107.98	105.80
23	1	21	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	A	2458	G	N3-C2-N2	-5.44	116.09	119.90
1	A	779	U	C5-C4-O4	-5.44	122.64	125.90
1	A	1678	G	N9-C4-C5	5.44	107.58	105.40
1	A	486	C	C6-N1-C2	5.44	122.47	120.30
1	A	602	G	C5-C6-O6	-5.44	125.34	128.60
1	A	1347	G	C8-N9-C4	-5.44	104.23	106.40
1	A	2352	A	C8-N9-C4	5.44	107.97	105.80
1	A	2206	G	N7-C8-N9	-5.43	110.38	113.10
1	A	1258	C	N3-C4-C5	5.43	124.07	121.90
1	A	2003	G	N1-C2-N2	-5.43	111.31	116.20
1	A	1188	U	N3-C4-O4	-5.43	115.60	119.40
1	A	1675	C	C2-N1-C1'	-5.43	112.83	118.80
2	B	24	G	N9-C4-C5	-5.43	103.23	105.40
1	A	245	G	C5-C6-O6	-5.43	125.34	128.60
1	A	1795	C	C5-C4-N4	-5.43	116.40	120.20
1	A	216	A	C2-N3-C4	-5.43	107.89	110.60
1	A	1527	G	N3-C4-N9	-5.43	122.74	126.00
1	A	1617	C	C5-C6-N1	-5.43	118.29	121.00
1	A	457	A	N1-C2-N3	-5.42	126.59	129.30
1	A	1780	A	C5-C6-N6	5.42	128.04	123.70
1	A	2207	G	C4-C5-C6	5.42	122.05	118.80
1	A	2487	G	N3-C4-C5	5.42	131.31	128.60
1	A	2878	U	C6-N1-C2	-5.42	117.75	121.00
1	A	1318	C	N3-C4-C5	-5.42	119.73	121.90
1	A	2572	A	N7-C8-N9	-5.42	111.09	113.80
1	A	512	G	N1-C6-O6	-5.42	116.65	119.90
1	A	2519	U	C6-N1-C2	5.41	124.25	121.00
1	A	1992	G	N3-C4-C5	-5.41	125.89	128.60
1	A	104	U	C5-C6-N1	-5.41	120.00	122.70
1	A	124	G	C8-N9-C4	5.41	108.56	106.40
1	A	593	G	N3-C4-N9	-5.41	122.75	126.00
1	A	2825	C	C6-N1-C2	5.41	122.46	120.30
1	A	205	G	N1-C2-N3	-5.41	120.66	123.90
11	P	50	ARG	NE-CZ-NH2	5.41	123.00	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1259	G	C5-C6-O6	5.40	131.84	128.60
1	A	777	A	N9-C4-C5	5.40	107.96	105.80
1	A	1137	G	N3-C2-N2	-5.40	116.12	119.90
1	A	2449	U	C5-C6-N1	-5.40	120.00	122.70
1	A	962	G	N7-C8-N9	-5.40	110.40	113.10
1	A	701	G	C5-C6-O6	5.40	131.84	128.60
1	A	2161	C	C2-N3-C4	5.40	122.60	119.90
1	A	512	G	O4'-C1'-N9	5.39	112.52	108.20
1	A	1695	G	C8-N9-C4	-5.39	104.24	106.40
1	A	546	C	N1-C2-O2	5.39	122.14	118.90
1	A	596	G	C5-C6-O6	5.39	131.84	128.60
1	A	864	G	C2-N3-C4	5.39	114.60	111.90
1	A	1164	G	C5-C6-O6	5.39	131.84	128.60
1	A	2506	U	C2-N1-C1'	-5.39	111.23	117.70
1	A	338	G	N3-C2-N2	5.39	123.67	119.90
1	A	2045	C	C5-C6-N1	-5.39	118.31	121.00
1	A	2628	C	C5-C4-N4	-5.39	116.43	120.20
1	A	2618	G	C4-C5-N7	-5.38	108.65	110.80
1	A	1492	G	C8-N9-C4	5.38	108.55	106.40
1	A	1978	A	C5-C6-N6	5.38	128.01	123.70
1	A	2362	G	C8-N9-C4	5.38	108.55	106.40
1	A	2585	U	N1-C2-N3	-5.38	111.67	114.90
1	A	33	U	N1-C2-N3	5.38	118.12	114.90
1	A	2688	U	C5-C4-O4	-5.38	122.67	125.90
1	A	2632	A	N1-C2-N3	-5.38	126.61	129.30
1	A	2881	C	N1-C2-O2	-5.38	115.67	118.90
1	A	1034	G	C5-C6-O6	-5.37	125.38	128.60
1	A	1142(A)	A	N1-C6-N6	5.37	121.82	118.60
1	A	1558	A	P-O3'-C3'	5.37	126.14	119.70
1	A	2014	A	C5-C6-N1	-5.37	115.02	117.70
1	A	113	G	C6-C5-N7	5.37	133.62	130.40
1	A	845	G	C5-C6-O6	-5.37	125.38	128.60
1	A	1558	A	N9-C4-C5	5.37	107.95	105.80
1	A	1816	G	C6-C5-N7	5.37	133.62	130.40
1	A	2631	G	C8-N9-C4	-5.37	104.25	106.40
1	A	1163	G	C8-N9-C4	5.36	108.55	106.40
1	A	1204	A	C4-N9-C1'	5.36	135.95	126.30
1	A	1799	G	C4-C5-N7	-5.36	108.66	110.80
1	A	1859	A	N1-C6-N6	5.36	121.82	118.60
1	A	2296	U	C3'-C2'-C1'	-5.36	97.21	101.50
1	A	2230	G	N1-C6-O6	5.36	123.12	119.90
1	A	271(H)	G	C6-C5-N7	-5.36	127.19	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1377	G	C5-C6-O6	5.36	131.81	128.60
1	A	2364	C	C6-N1-C2	5.36	122.44	120.30
1	A	2517	C	N3-C4-N4	5.36	121.75	118.00
1	A	223	A	N9-C4-C5	5.36	107.94	105.80
1	A	330	A	N3-C4-N9	-5.36	123.11	127.40
1	A	1300	U	P-O3'-C3'	5.36	126.13	119.70
1	A	2409	G	C6-C5-N7	-5.36	127.19	130.40
1	A	2489	G	N7-C8-N9	-5.36	110.42	113.10
1	A	671	C	C2-N1-C1'	-5.35	112.91	118.80
1	A	673	C	C5-C6-N1	-5.35	118.32	121.00
1	A	1261	C	N1-C2-O2	-5.35	115.69	118.90
1	A	2306	C	C2-N3-C4	5.35	122.58	119.90
1	A	2721	A	C5-C6-N1	-5.35	115.02	117.70
1	A	19	C	C2-N3-C4	-5.35	117.23	119.90
1	A	2241	A	C5-N7-C8	5.35	106.57	103.90
1	A	841	A	C8-N9-C4	-5.35	103.66	105.80
1	A	395	U	N3-C2-O2	-5.34	118.46	122.20
1	A	1998	G	C5-C6-O6	5.34	131.81	128.60
1	A	2261	C	N1-C2-O2	-5.34	115.69	118.90
1	A	2322	A	C5-N7-C8	5.34	106.57	103.90
1	A	1246	A	C2-N3-C4	-5.34	107.93	110.60
1	A	1359	A	N1-C6-N6	5.34	121.81	118.60
1	A	2729	G	C2-N3-C4	-5.34	109.23	111.90
2	B	115	G	N3-C4-C5	5.34	131.27	128.60
1	A	128	C	C4-C5-C6	5.34	120.07	117.40
1	A	1265	A	C8-N9-C4	5.34	107.94	105.80
1	A	2105	C	C5-C6-N1	5.34	123.67	121.00
15	T	118	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	1323	U	C5-C4-O4	-5.34	122.70	125.90
1	A	836	G	C5-C6-O6	-5.33	125.40	128.60
1	A	1745	C	C6-N1-C2	5.33	122.43	120.30
1	A	1571	A	C5-C6-N1	5.33	120.37	117.70
1	A	212	G	C8-N9-C4	-5.33	104.27	106.40
1	A	1294	U	N1-C2-O2	-5.33	119.07	122.80
1	A	1764	G	N7-C8-N9	-5.33	110.44	113.10
1	A	2093	G	N7-C8-N9	-5.33	110.44	113.10
2	B	14	U	N3-C2-O2	-5.33	118.47	122.20
1	A	390	A	C5-N7-C8	5.33	106.56	103.90
1	A	2357	U	N1-C2-O2	-5.33	119.07	122.80
1	A	2847	U	C5-C6-N1	-5.33	120.04	122.70
1	A	952	G	C8-N9-C4	-5.32	104.27	106.40
1	A	1117	G	C5-C6-O6	-5.32	125.41	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1527	G	N3-C4-C5	5.32	131.26	128.60
1	A	1641	A	N1-C2-N3	5.32	131.96	129.30
1	A	1990	C	C2-N3-C4	-5.32	117.24	119.90
1	A	2247	A	C5-N7-C8	5.32	106.56	103.90
1	A	204	A	C6-N1-C2	-5.32	115.41	118.60
1	A	60	G	C4-C5-N7	5.32	112.93	110.80
1	A	2713	A	C2-N3-C4	5.32	113.26	110.60
11	P	103	ALA	N-CA-C	-5.32	96.64	111.00
1	A	2524	G	C8-N9-C4	-5.32	104.27	106.40
1	A	708	C	C5-C6-N1	5.31	123.66	121.00
1	A	981	A	C4-C5-C6	-5.31	114.34	117.00
1	A	1217	C	N1-C2-O2	-5.31	115.71	118.90
1	A	123	G	C8-N9-C4	5.31	108.52	106.40
1	A	474	G	N1-C6-O6	-5.31	116.72	119.90
1	A	1284	A	C5-N7-C8	-5.31	101.25	103.90
1	A	2048	G	C6-C5-N7	-5.31	127.22	130.40
1	A	1628	G	C5-C6-O6	-5.30	125.42	128.60
30	8	57	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	A	211	A	C8-N9-C4	5.30	107.92	105.80
1	A	823	G	C5-N7-C8	5.30	106.95	104.30
1	A	1623	G	N1-C6-O6	-5.30	116.72	119.90
1	A	1830	C	N3-C4-N4	5.30	121.71	118.00
1	A	2844	G	N1-C6-O6	5.30	123.08	119.90
1	A	1296	G	C4-C5-N7	-5.30	108.68	110.80
1	A	507	A	N1-C2-N3	-5.30	126.65	129.30
1	A	2389	G	N9-C4-C5	5.30	107.52	105.40
1	A	2769	C	C5-C6-N1	-5.30	118.35	121.00
1	A	2789	C	N3-C2-O2	5.30	125.61	121.90
1	A	124	G	N9-C4-C5	-5.29	103.28	105.40
1	A	1659	U	N1-C2-O2	-5.29	119.09	122.80
1	A	1899	G	N3-C4-N9	5.29	129.18	126.00
1	A	1453	U	C4-C5-C6	5.29	122.88	119.70
1	A	910	A	N1-C6-N6	-5.29	115.43	118.60
1	A	409	C	C6-N1-C2	5.29	122.42	120.30
1	A	1820	U	C6-N1-C2	5.29	124.17	121.00
1	A	2638	G	C6-C5-N7	-5.29	127.23	130.40
1	A	803	U	N1-C2-N3	5.29	118.07	114.90
1	A	560	C	C2-N3-C4	-5.28	117.26	119.90
1	A	1975	G	C8-N9-C4	-5.28	104.29	106.40
1	A	2138	C	C2-N3-C4	5.28	122.54	119.90
1	A	2755	C	C5-C6-N1	5.28	123.64	121.00
1	A	2757	A	N7-C8-N9	5.28	116.44	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1217	C	C4-C5-C6	5.28	120.04	117.40
1	A	1685	C	C5-C4-N4	-5.28	116.50	120.20
1	A	1968	G	C5-C6-O6	-5.28	125.43	128.60
1	A	271(H)	G	C4-N9-C1'	5.28	133.36	126.50
1	A	1248	G	N3-C4-N9	5.28	129.17	126.00
1	A	887	A	C2-N3-C4	5.28	113.24	110.60
1	A	473	G	N3-C2-N2	-5.28	116.20	119.90
1	A	12	U	N1-C2-O2	5.28	126.49	122.80
1	A	196	A	C4-C5-N7	5.28	113.34	110.70
1	A	425	G	N9-C4-C5	-5.28	103.29	105.40
1	A	693	C	N3-C4-N4	-5.28	114.31	118.00
1	A	1787	A	N1-C6-N6	5.28	121.77	118.60
1	A	2327	A	C5-C6-N1	5.28	120.34	117.70
1	A	246	C	N3-C2-O2	5.27	125.59	121.90
1	A	943	U	N1-C2-O2	5.27	126.49	122.80
1	A	1566	A	C5-C6-N6	-5.27	119.48	123.70
1	A	2049	G	C2-N3-C4	-5.27	109.26	111.90
1	A	2644	G	N1-C2-N3	5.27	127.06	123.90
1	A	535	C	C6-N1-C1'	5.27	127.12	120.80
1	A	2515	C	N3-C4-C5	5.27	124.01	121.90
1	A	1294	U	C2-N3-C4	-5.27	123.84	127.00
1	A	2363	C	N3-C4-N4	-5.27	114.31	118.00
1	A	570	G	N1-C2-N2	-5.27	111.46	116.20
1	A	1611	C	C2-N1-C1'	5.27	124.59	118.80
1	A	700	G	N1-C6-O6	-5.26	116.74	119.90
1	A	1321	A	C4-C5-C6	5.26	119.63	117.00
1	A	2006	C	N3-C4-N4	5.26	121.69	118.00
1	A	2346	A	C4-C5-C6	5.26	119.63	117.00
1	A	2704	C	C6-N1-C2	-5.26	118.19	120.30
1	A	2041	U	N1-C2-O2	-5.26	119.12	122.80
2	B	74	U	N1-C2-N3	5.26	118.06	114.90
1	A	571	A	N9-C4-C5	-5.26	103.70	105.80
1	A	791	C	N1-C2-O2	-5.26	115.74	118.90
1	A	2185	C	C5-C4-N4	5.26	123.88	120.20
1	A	699	A	N7-C8-N9	-5.26	111.17	113.80
29	7	34	ARG	NE-CZ-NH2	5.26	122.93	120.30
1	A	454	A	C2-N3-C4	5.25	113.23	110.60
1	A	812	C	N3-C4-N4	5.25	121.68	118.00
1	A	2364	C	C2-N3-C4	-5.25	117.27	119.90
1	A	207	A	C8-N9-C4	5.25	107.90	105.80
1	A	1124	C	N3-C4-C5	5.25	124.00	121.90
1	A	1265	A	N7-C8-N9	-5.25	111.17	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1367	A	N1-C2-N3	5.25	131.93	129.30
1	A	23	G	N1-C6-O6	-5.25	116.75	119.90
1	A	2599	G	N1-C6-O6	-5.25	116.75	119.90
1	A	2700	C	C6-N1-C2	5.25	122.40	120.30
1	A	2024	G	C2-N3-C4	-5.25	109.28	111.90
1	A	1802	A	N7-C8-N9	-5.25	111.18	113.80
1	A	576	U	C5-C4-O4	5.24	129.05	125.90
1	A	1524	G	C5-C6-O6	5.24	131.75	128.60
1	A	2069	G	N3-C2-N2	-5.24	116.23	119.90
1	A	599	G	N1-C2-N2	-5.24	111.48	116.20
2	B	14	U	N1-C2-O2	5.24	126.47	122.80
1	A	71	A	P-O3'-C3'	5.24	125.99	119.70
1	A	2324	C	C6-N1-C1'	-5.24	114.51	120.80
1	A	1204	A	O4'-C1'-N9	5.24	112.39	108.20
1	A	1657	C	N3-C2-O2	-5.24	118.23	121.90
1	A	2593	U	N3-C2-O2	-5.24	118.54	122.20
1	A	2712	U	C2-N3-C4	-5.24	123.86	127.00
1	A	482	A	C8-N9-C4	5.23	107.89	105.80
1	A	1940	U	N3-C4-O4	5.23	123.06	119.40
1	A	2420	C	C5-C4-N4	-5.23	116.54	120.20
2	B	76	G	N3-C4-C5	5.23	131.22	128.60
1	A	1619	G	C2-N3-C4	5.23	114.51	111.90
1	A	2357	U	C5-C6-N1	-5.23	120.09	122.70
1	A	2438	U	C5-C4-O4	-5.23	122.76	125.90
1	A	2061	G	N7-C8-N9	-5.22	110.49	113.10
1	A	2495	G	N1-C6-O6	5.22	123.03	119.90
1	A	2743	C	C2-N1-C1'	-5.22	113.05	118.80
1	A	1240	U	C5-C4-O4	-5.22	122.77	125.90
1	A	1653	G	N1-C2-N3	5.22	127.03	123.90
1	A	2699	C	N3-C2-O2	5.22	125.55	121.90
1	A	205	G	N3-C2-N2	5.22	123.55	119.90
2	B	104	U	C2-N1-C1'	-5.22	111.44	117.70
1	A	1524	G	C4-C5-N7	-5.22	108.71	110.80
1	A	143	G	N3-C4-N9	-5.22	122.87	126.00
1	A	1323	U	C6-N1-C2	5.22	124.13	121.00
1	A	2713	A	C5-C6-N6	5.22	127.87	123.70
1	A	391	G	C5-N7-C8	5.21	106.91	104.30
1	A	697	C	C2-N3-C4	5.21	122.51	119.90
1	A	153	C	N1-C2-O2	5.21	122.03	118.90
1	A	2505	G	C5-C6-O6	5.21	131.73	128.60
1	A	491	G	C8-N9-C4	-5.21	104.32	106.40
1	A	732	C	C4-C5-C6	5.21	120.00	117.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1040	C	C2-N3-C4	-5.21	117.30	119.90
1	A	1816	G	C8-N9-C1'	5.21	133.77	127.00
1	A	2631	G	N3-C4-C5	-5.21	126.00	128.60
1	A	1573	G	C8-N9-C4	5.21	108.48	106.40
1	A	2894	G	C4-C5-C6	5.21	121.92	118.80
1	A	1890	A	C8-N9-C4	5.21	107.88	105.80
1	A	72	U	C5-C4-O4	-5.20	122.78	125.90
1	A	2362	G	N1-C6-O6	-5.20	116.78	119.90
1	A	2516	G	N3-C2-N2	5.20	123.54	119.90
1	A	2612	C	C2-N3-C4	-5.20	117.30	119.90
1	A	785	G	N1-C6-O6	-5.20	116.78	119.90
1	A	1787	A	N1-C2-N3	-5.20	126.70	129.30
1	A	585	G	C6-N1-C2	-5.20	121.98	125.10
1	A	945	A	N3-C4-N9	-5.19	123.25	127.40
1	A	196	A	N1-C6-N6	5.19	121.72	118.60
1	A	757	U	N1-C2-O2	-5.19	119.17	122.80
1	A	2505	G	N9-C4-C5	5.19	107.48	105.40
1	A	1834	U	N1-C2-N3	5.19	118.01	114.90
1	A	115	C	N1-C2-O2	-5.19	115.79	118.90
1	A	1644	C	N1-C2-O2	5.19	122.01	118.90
1	A	2885	C	C2-N3-C4	5.19	122.49	119.90
1	A	845	G	C6-C5-N7	-5.19	127.29	130.40
1	A	2066	C	N3-C2-O2	-5.18	118.27	121.90
1	A	2303	G	C8-N9-C1'	5.18	133.74	127.00
1	A	1904	G	N3-C4-C5	-5.18	126.01	128.60
1	A	755	C	N3-C2-O2	-5.18	118.28	121.90
1	A	1653	G	P-O3'-C3'	5.18	125.91	119.70
1	A	1964	G	N3-C2-N2	5.18	123.53	119.90
1	A	389	G	C5-C6-O6	-5.18	125.49	128.60
1	A	1530	C	N3-C4-N4	5.18	121.62	118.00
1	A	2352	A	C2-N3-C4	-5.18	108.01	110.60
1	A	686	G	N1-C2-N2	-5.17	111.54	116.20
1	A	1038	C	N3-C4-C5	5.17	123.97	121.90
1	A	1361	G	N1-C6-O6	-5.17	116.80	119.90
1	A	2087	G	C5-C6-N1	-5.17	108.91	111.50
1	A	2399	G	C5-C6-O6	5.17	131.71	128.60
1	A	2505	G	C8-N9-C4	-5.17	104.33	106.40
1	A	68	G	N7-C8-N9	-5.17	110.51	113.10
1	A	1311	G	C8-N9-C4	-5.17	104.33	106.40
1	A	1490	A	C6-C5-N7	5.17	135.92	132.30
1	A	2604	U	N3-C2-O2	-5.17	118.58	122.20
2	B	77	U	N3-C2-O2	5.17	125.82	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	393	C	N1-C2-O2	-5.17	115.80	118.90
1	A	409	C	N3-C4-C5	5.17	123.97	121.90
1	A	1979	C	N3-C4-C5	5.17	123.97	121.90
1	A	2042	A	N3-C4-C5	5.17	130.42	126.80
1	A	2207	G	C8-N9-C1'	-5.17	120.28	127.00
1	A	2228	G	C5-C6-O6	5.17	131.70	128.60
1	A	1271	G	N1-C2-N3	5.17	127.00	123.90
1	A	1358	G	C8-N9-C4	5.17	108.47	106.40
1	A	247	G	C4-C5-N7	-5.17	108.73	110.80
1	A	518	G	C8-N9-C4	-5.17	104.33	106.40
1	A	944	G	N3-C4-C5	-5.16	126.02	128.60
1	A	1117	G	N1-C6-O6	5.16	123.00	119.90
1	A	1404	C	N3-C2-O2	-5.16	118.29	121.90
8	I	120	ILE	CB-CA-C	-5.16	101.28	111.60
1	A	254	G	N3-C4-C5	5.16	131.18	128.60
1	A	1271	G	C2-N3-C4	-5.16	109.32	111.90
1	A	337	C	N3-C4-C5	5.16	123.96	121.90
1	A	1212	G	C5-C6-O6	-5.16	125.50	128.60
1	A	2182	G	N3-C4-N9	-5.16	122.91	126.00
1	A	2408	U	N1-C2-O2	5.16	126.41	122.80
1	A	192	C	C2-N1-C1'	-5.16	113.13	118.80
1	A	981	A	C5-C6-N1	5.16	120.28	117.70
1	A	1540	U	C6-N1-C2	-5.16	117.91	121.00
1	A	58	G	C5-C6-O6	5.16	131.69	128.60
1	A	201	C	N1-C2-O2	-5.16	115.81	118.90
1	A	1675	C	N1-C2-O2	-5.16	115.81	118.90
1	A	2294	C	N3-C4-C5	5.15	123.96	121.90
1	A	135	G	C4-N9-C1'	-5.15	119.80	126.50
1	A	601	C	C2-N3-C4	-5.15	117.33	119.90
1	A	1899	G	C4-C5-N7	5.15	112.86	110.80
1	A	1290	C	C2-N3-C4	-5.15	117.33	119.90
1	A	1821	A	C5-C6-N1	5.15	120.27	117.70
1	A	1998	G	C4-C5-N7	-5.15	108.74	110.80
1	A	934	G	C5-N7-C8	5.15	106.87	104.30
1	A	58	G	C8-N9-C4	-5.14	104.34	106.40
1	A	666	G	C2-N3-C4	-5.14	109.33	111.90
1	A	1401	G	N3-C4-C5	5.14	131.17	128.60
21	Z	86	VAL	CB-CA-C	-5.14	101.62	111.40
1	A	22	C	C6-N1-C2	5.14	122.36	120.30
1	A	351	G	C5-C6-O6	-5.14	125.51	128.60
1	A	389	G	C6-N1-C2	-5.14	122.02	125.10
1	A	972	G	C5-C6-O6	5.14	131.69	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1260	G	C5-C6-O6	5.14	131.69	128.60
1	A	1756	G	C5-N7-C8	5.14	106.87	104.30
1	A	2249	U	N1-C2-O2	5.14	126.40	122.80
1	A	2365	G	C5-C6-N1	5.14	114.07	111.50
1	A	2821	A	N1-C6-N6	5.14	121.68	118.60
1	A	265	A	N1-C6-N6	5.14	121.68	118.60
1	A	762	U	C2-N1-C1'	5.14	123.86	117.70
1	A	1164	G	N1-C2-N3	5.14	126.98	123.90
1	A	624	C	N3-C2-O2	5.14	125.50	121.90
1	A	817	C	N3-C2-O2	-5.14	118.30	121.90
1	A	1819	A	N9-C4-C5	5.14	107.86	105.80
2	B	89	G	N1-C6-O6	5.14	122.98	119.90
1	A	2462	U	C5-C6-N1	-5.13	120.13	122.70
1	A	2464	C	N3-C2-O2	5.13	125.49	121.90
1	A	54	G	C4-C5-N7	-5.13	108.75	110.80
1	A	635	C	N3-C4-C5	-5.13	119.85	121.90
1	A	2462	U	N3-C2-O2	5.13	125.79	122.20
1	A	113	G	C8-N9-C1'	5.13	133.67	127.00
1	A	1475	G	N1-C2-N2	5.13	120.82	116.20
1	A	655	A	C8-N9-C4	-5.13	103.75	105.80
1	A	2871	C	N1-C2-O2	-5.13	115.82	118.90
1	A	139(A)	G	C8-N9-C1'	-5.13	120.33	127.00
1	A	2104	G	C4-N9-C1'	5.13	133.16	126.50
1	A	2363	C	C6-N1-C2	5.13	122.35	120.30
1	A	488	G	C2-N3-C4	-5.12	109.34	111.90
1	A	249	C	C5-C6-N1	-5.12	118.44	121.00
1	A	569	U	N1-C2-O2	-5.12	119.21	122.80
1	A	1654	A	C6-C5-N7	5.12	135.89	132.30
1	A	1831	G	C2-N3-C4	-5.12	109.34	111.90
1	A	2089	U	N3-C2-O2	-5.12	118.61	122.20
1	A	2516	G	N1-C2-N3	5.12	126.97	123.90
1	A	576	U	N3-C2-O2	-5.12	118.61	122.20
1	A	932	G	C2-N3-C4	-5.12	109.34	111.90
1	A	1792	G	N3-C2-N2	5.12	123.49	119.90
12	Q	14	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	A	2334	G	C8-N9-C4	5.12	108.45	106.40
1	A	33	U	C5-C6-N1	-5.12	120.14	122.70
1	A	467	G	C8-N9-C4	5.12	108.45	106.40
1	A	614	U	N3-C2-O2	-5.12	118.62	122.20
1	A	2430	A	C2-N3-C4	5.12	113.16	110.60
1	A	1943	U	N1-C2-N3	5.11	117.97	114.90
1	A	2669	G	C8-N9-C4	5.11	108.44	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1007	C	N1-C2-O2	-5.11	115.83	118.90
1	A	1897	G	C5-C6-O6	-5.11	125.53	128.60
1	A	2226	C	N3-C4-C5	5.11	123.94	121.90
1	A	2779	U	N3-C4-C5	5.11	117.67	114.60
1	A	1996	C	C5-C4-N4	-5.11	116.62	120.20
1	A	961	C	C5-C4-N4	-5.11	116.62	120.20
1	A	2611	U	N3-C4-O4	5.11	122.98	119.40
1	A	135	G	N1-C6-O6	5.11	122.96	119.90
1	A	469	G	C6-N1-C2	-5.11	122.04	125.10
1	A	2000	G	C5-C6-O6	-5.10	125.54	128.60
1	A	2675	A	C6-N1-C2	-5.10	115.54	118.60
1	A	1563	G	N1-C2-N2	-5.10	111.61	116.20
1	A	1899	G	C6-C5-N7	-5.10	127.34	130.40
1	A	2675	A	N1-C2-N3	5.10	131.85	129.30
1	A	407	G	N7-C8-N9	-5.10	110.55	113.10
1	A	708	C	N3-C4-C5	5.10	123.94	121.90
1	A	1438	U	C5-C4-O4	-5.10	122.84	125.90
1	A	1681	G	N1-C6-O6	5.10	122.96	119.90
30	8	35	GLN	N-CA-C	5.10	124.77	111.00
1	A	1654	A	C4-C5-N7	-5.10	108.15	110.70
1	A	2357	U	C2-N3-C4	-5.10	123.94	127.00
1	A	2582	G	N1-C2-N3	-5.10	120.84	123.90
1	A	1204	A	C3'-C2'-C1'	-5.10	97.42	101.50
1	A	832	G	N9-C4-C5	5.09	107.44	105.40
1	A	1541	G	N3-C4-C5	-5.09	126.05	128.60
1	A	1620	G	C5-C6-N1	-5.09	108.95	111.50
1	A	1800	C	C4-C5-C6	5.09	119.95	117.40
1	A	565	C	C5-C4-N4	5.09	123.77	120.20
1	A	757	U	C5-C6-N1	-5.09	120.15	122.70
1	A	1959	G	C8-N9-C4	-5.09	104.36	106.40
1	A	2105	C	C2-N3-C4	5.09	122.44	119.90
1	A	2500	U	N3-C4-C5	5.09	117.65	114.60
1	A	2757	A	N1-C6-N6	5.09	121.65	118.60
2	B	20	C	C5-C4-N4	-5.09	116.64	120.20
1	A	121	G	C6-N1-C2	-5.09	122.05	125.10
1	A	114	U	C6-N1-C1'	-5.09	114.08	121.20
1	A	445	C	N1-C2-O2	-5.09	115.85	118.90
1	A	798	G	N1-C6-O6	-5.09	116.85	119.90
1	A	1028	A	N9-C4-C5	5.09	107.83	105.80
1	A	591	C	C2-N1-C1'	-5.08	113.21	118.80
1	A	1835	G	N1-C2-N2	-5.08	111.62	116.20
1	A	185	U	C5-C6-N1	-5.08	120.16	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	751	A	C8-N9-C4	5.08	107.83	105.80
1	A	1904	G	N3-C4-N9	5.08	129.05	126.00
4	E	78	LEU	CA-CB-CG	5.08	126.99	115.30
1	A	136	G	N1-C6-O6	5.08	122.95	119.90
1	A	2191	G	C5-C6-O6	-5.08	125.55	128.60
1	A	2199	A	C4-N9-C1'	5.08	135.45	126.30
1	A	463	G	C5-C6-O6	5.08	131.65	128.60
1	A	2015	A	N9-C4-C5	5.08	107.83	105.80
1	A	2066	C	C4-C5-C6	5.08	119.94	117.40
1	A	482	A	N9-C4-C5	-5.07	103.77	105.80
1	A	546	C	C6-N1-C1'	-5.07	114.71	120.80
1	A	2248	C	C2-N3-C4	-5.07	117.36	119.90
1	A	893	C	C5-C4-N4	-5.07	116.65	120.20
1	A	2036	C	N3-C2-O2	5.07	125.45	121.90
1	A	2142	C	C6-N1-C1'	5.07	126.89	120.80
2	B	64	C	N3-C2-O2	-5.07	118.35	121.90
1	A	934	G	C4-C5-N7	-5.07	108.77	110.80
1	A	271(M)	G	N7-C8-N9	5.07	115.63	113.10
1	A	573	G	C6-C5-N7	-5.07	127.36	130.40
1	A	2027	G	C6-N1-C2	-5.07	122.06	125.10
12	Q	135	ASP	CB-CA-C	-5.07	100.27	110.40
1	A	2466	C	N3-C2-O2	-5.07	118.35	121.90
1	A	109	G	N1-C6-O6	-5.06	116.86	119.90
1	A	469	G	C5-C6-O6	-5.06	125.56	128.60
1	A	783	A	C2-N3-C4	5.06	113.13	110.60
1	A	2869	G	N7-C8-N9	5.06	115.63	113.10
1	A	2249	U	C6-N1-C2	5.06	124.04	121.00
1	A	742	G	C2-N3-C4	-5.06	109.37	111.90
1	A	1518	U	C5-C4-O4	5.06	128.94	125.90
1	A	1942	C	C6-N1-C2	5.06	122.32	120.30
1	A	2234	G	N3-C2-N2	5.06	123.44	119.90
1	A	1960	A	C8-N9-C4	5.06	107.82	105.80
1	A	671	C	N1-C2-O2	-5.05	115.87	118.90
1	A	915	C	N1-C2-O2	5.05	121.93	118.90
1	A	1820	U	N3-C4-O4	-5.05	115.86	119.40
1	A	1189	A	N1-C6-N6	5.05	121.63	118.60
1	A	2063	C	C6-N1-C2	5.05	122.32	120.30
2	B	12	C	C2-N1-C1'	5.05	124.36	118.80
1	A	585	G	N1-C2-N3	5.05	126.93	123.90
1	A	980	A	C2-N3-C4	-5.05	108.07	110.60
1	A	2474	C	C6-N1-C2	5.05	122.32	120.30
1	A	47	C	C2-N3-C4	-5.05	117.38	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	236	C	C2-N3-C4	-5.05	117.38	119.90
1	A	681	G	C5-C6-O6	5.05	131.63	128.60
1	A	706	A	C8-N9-C4	-5.05	103.78	105.80
1	A	1943	U	C2-N3-C4	-5.05	123.97	127.00
1	A	2326	C	N3-C4-C5	-5.05	119.88	121.90
1	A	2371	G	C8-N9-C4	5.05	108.42	106.40
1	A	2772	C	C6-N1-C2	5.05	122.32	120.30
15	T	53	ARG	CB-CA-C	-5.04	100.31	110.40
1	A	114	U	C5-C6-N1	5.04	125.22	122.70
1	A	316	C	C5-C4-N4	-5.04	116.67	120.20
1	A	1897	G	C8-N9-C4	5.04	108.42	106.40
2	B	63	G	N9-C4-C5	-5.04	103.38	105.40
1	A	40	C	N3-C2-O2	5.04	125.43	121.90
1	A	214	G	C4-N9-C1'	-5.04	119.95	126.50
1	A	474	G	N3-C2-N2	5.04	123.43	119.90
1	A	728	G	N1-C6-O6	-5.04	116.88	119.90
1	A	1531	C	C5-C6-N1	5.04	123.52	121.00
1	A	2733	A	N7-C8-N9	5.04	116.32	113.80
1	A	1385	G	C2-N3-C4	-5.04	109.38	111.90
1	A	1900	A	C5-C6-N1	5.04	120.22	117.70
1	A	1217	C	C5-C6-N1	-5.04	118.48	121.00
1	A	2029	G	N3-C2-N2	-5.04	116.37	119.90
1	A	2318	G	C5-C6-O6	5.04	131.62	128.60
1	A	1231	G	N1-C6-O6	5.04	122.92	119.90
2	B	35	U	C5-C6-N1	-5.04	120.18	122.70
1	A	472	A	C6-N1-C2	-5.03	115.58	118.60
1	A	1745	C	N3-C2-O2	5.03	125.42	121.90
1	A	732	C	N3-C4-C5	-5.03	119.89	121.90
1	A	1819	A	C8-N9-C4	-5.03	103.79	105.80
1	A	669	G	C8-N9-C4	5.03	108.41	106.40
21	Z	74	VAL	CB-CA-C	-5.03	101.84	111.40
1	A	537	C	C2-N3-C4	-5.03	117.39	119.90
1	A	1142(A)	A	N7-C8-N9	5.03	116.31	113.80
1	A	1925	C	N1-C2-O2	-5.03	115.89	118.90
1	A	1933	G	C4-C5-N7	-5.03	108.79	110.80
1	A	1721	G	C5-C6-O6	-5.02	125.59	128.60
1	A	56	A	C5-C6-N6	5.02	127.72	123.70
1	A	798	G	C6-C5-N7	5.02	133.41	130.40
1	A	809	G	C4-C5-N7	-5.02	108.79	110.80
1	A	1555	G	N3-C2-N2	-5.02	116.39	119.90
1	A	2182	G	C8-N9-C1'	5.02	133.53	127.00
1	A	1266	G	C8-N9-C4	5.02	108.41	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2710	C	C2-N3-C4	-5.02	117.39	119.90
1	A	686	G	C6-N1-C2	-5.01	122.09	125.10
1	A	2131	G	C8-N9-C4	-5.01	104.39	106.40
1	A	465	G	N3-C4-C5	-5.01	126.09	128.60
1	A	578	A	N9-C4-C5	5.01	107.81	105.80
1	A	1243	G	N1-C6-O6	-5.01	116.89	119.90
1	A	1306	C	N1-C2-O2	5.01	121.91	118.90
1	A	833	U	N3-C4-C5	-5.01	111.59	114.60
1	A	1441	G	N7-C8-N9	-5.01	110.59	113.10
1	A	2821	A	C4-C5-N7	5.01	113.20	110.70
1	A	132	G	N3-C4-N9	-5.01	123.00	126.00
1	A	2778	A	N9-C4-C5	5.01	107.80	105.80
1	A	922	U	C5-C4-O4	-5.01	122.90	125.90
1	A	1249	U	C5-C6-N1	-5.01	120.20	122.70
1	A	1665	A	C5-N7-C8	5.01	106.40	103.90
1	A	153	C	C2-N1-C1'	5.00	124.30	118.80
1	A	271(X)	G	N9-C4-C5	5.00	107.40	105.40
1	A	1707	G	C8-N9-C4	5.00	108.40	106.40
1	A	1607	C	C5-C4-N4	-5.00	116.70	120.20
1	A	2045	C	C2-N3-C4	-5.00	117.40	119.90

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
23	1	83	GLU	Peptide
26	4	42	PHE	Peptide
27	5	53	ALA	Peptide
30	8	34	TRP	Mainchain
1	A	271(Q)	G	Sidechain
3	D	275	LYS	Peptide
4	E	72	VAL	Peptide
5	F	21	ALA	Mainchain
5	F	85	GLY	Peptide
6	G	13	GLU	Peptide
7	H	70	THR	Peptide
9	N	124	ALA	Peptide
11	P	26	GLY	Peptide
11	P	44	GLY	Peptide
14	S	83	LYS	Peptide
15	T	126	ALA	Peptide
19	X	23	GLU	Mainchain

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Mol	Chain	Res	Type	Group
21	Z	159	PRO	Peptide

## 5.2 Close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	60264	0	30391	904	0
2	B	2573	0	1306	51	0
3	D	2136	0	2218	61	0
4	E	1555	0	1607	46	0
5	F	1572	0	1613	43	0
6	G	1368	0	1324	49	0
7	H	1317	0	1376	24	0
8	I	1043	0	1054	51	0
9	N	1112	0	1180	28	0
10	O	923	0	981	15	0
11	P	1131	0	1201	45	0
12	Q	1122	0	1179	30	0
13	R	968	0	1033	30	0
14	S	873	0	927	49	0
15	T	1058	0	1098	28	0
16	U	959	0	1019	23	0
17	V	775	0	841	16	0
18	W	877	0	932	18	0
19	X	732	0	777	16	0
20	Y	781	0	829	22	0
21	Z	1528	0	1476	59	0
22	0	607	0	622	18	0
23	1	745	0	804	22	0
24	2	584	0	623	16	0
25	3	463	0	507	8	0
26	4	349	0	336	12	0
27	5	451	0	461	11	0
28	6	437	0	440	16	0
29	7	402	0	434	5	0
30	8	509	0	565	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	9	297	0	316	6	0
32	0	1	0	0	0	0
32	1	1	0	0	0	0
32	5	2	0	0	0	0
32	8	1	0	0	0	0
32	9	1	0	0	0	0
32	A	637	0	0	0	0
32	B	10	0	0	0	0
32	D	4	0	0	0	0
32	E	3	0	0	0	0
32	F	5	0	0	0	0
32	O	1	0	0	0	0
32	P	4	0	0	0	0
32	Q	4	0	0	0	0
32	R	2	0	0	0	0
32	T	2	0	0	0	0
32	W	1	0	0	0	0
33	4	1	0	0	0	0
33	5	1	0	0	0	0
33	6	1	0	0	0	0
33	9	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	1	0	0	0	0
34	1	3	0	0	0	0
34	2	1	0	0	0	0
34	3	1	0	0	1	0
34	5	3	0	0	0	0
34	6	3	0	0	0	0
34	7	1	0	0	0	0
34	8	6	0	0	0	0
34	9	1	0	0	0	0
34	A	1493	0	0	107	0
34	B	32	0	0	6	0
34	D	15	0	0	2	0
34	E	9	0	0	0	0
34	F	10	0	0	0	0
34	N	2	0	0	0	0
34	O	5	0	0	0	0
34	P	12	0	0	0	0
34	Q	2	0	0	1	0
34	R	5	0	0	0	0
34	T	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	U	1	0	0	0	0
34	V	1	0	0	0	0
34	W	4	0	0	0	0
34	X	3	0	0	0	0
34	Y	2	0	0	0	0
All	All	91815	0	59470	1548	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

All (1548) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2296:U:O4	1:A:2335:A:N6	1.59	1.33
1:A:2322:A:H61	1:A:2335:A:N6	1.49	1.08
1:A:885:C:N4	1:A:890:A:N6	2.02	1.08
1:A:1783:A:OP1	34:A:3845:HOH:O	1.74	1.04
1:A:885:C:H42	1:A:890:A:N6	1.54	1.02
1:A:571:A:H5'	1:A:2030:A:H62	1.24	1.00
1:A:1204:A:H2	1:A:1241:A:H62	1.08	0.99
1:A:1359:A:H61	1:A:1372:U:H3	1.13	0.97
22:0:11:ARG:O	22:0:14:ARG:NH2	2.00	0.95
1:A:2136:C:N4	1:A:2155:G:H1	1.66	0.94
1:A:1689:A:H62	1:A:1698:A:H2	1.17	0.93
19:X:31:HIS:HD2	19:X:33:LYS:H	1.15	0.92
23:1:21:ARG:HH11	23:1:21:ARG:HG2	1.36	0.90
1:A:2287:A:H62	1:A:2344:U:H3	1.17	0.89
1:A:2100:G:H1	1:A:2189:U:H3	1.14	0.89
1:A:1332:G:OP1	34:A:3795:HOH:O	1.91	0.88
1:A:1530:C:O2'	1:A:1531:C:O5'	1.91	0.87
14:S:82:ILE:HA	14:S:83:LYS:HB2	1.58	0.86
21:Z:160:GLY:HA2	21:Z:161:VAL:HB	1.57	0.86
1:A:2304:G:H1	1:A:2312:U:H3	1.21	0.86
15:T:54:ARG:HA	15:T:59:THR:HB	1.58	0.86
1:A:2624:G:N7	34:A:5142:HOH:O	2.08	0.85
4:E:47:VAL:HG21	4:E:86:PRO:HD2	1.56	0.85
1:A:2206:G:H5'	1:A:2207:G:N7	1.90	0.85
1:A:1017:G:N7	34:A:5104:HOH:O	2.09	0.85
1:A:1798:U:H5'	3:D:259:THR:HG22	1.58	0.85
8:I:110:ASP:N	8:I:130:TYR:OH	2.10	0.84
1:A:2499:C:OP2	34:A:3839:HOH:O	1.97	0.83
1:A:2283:C:OP2	34:A:4878:HOH:O	1.97	0.83
1:A:1784:A:OP2	34:A:3845:HOH:O	1.96	0.82

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:990:A:OP2	34:A:4573:HOH:O	1.96	0.82
1:A:1359:A:N6	1:A:1372:U:H3	1.77	0.82
1:A:1381:G:N7	34:A:3878:HOH:O	2.12	0.82
1:A:2070:G:OP2	34:A:4393:HOH:O	1.97	0.81
19:X:31:HIS:CD2	19:X:33:LYS:H	1.98	0.81
1:A:2322:A:N6	1:A:2335:A:N6	2.29	0.81
1:A:83:G:N2	1:A:103:A:OP2	2.13	0.81
1:A:1427:A:H4'	1:A:1428:C:O5'	1.79	0.81
1:A:2079:U:OP1	23:1:21:ARG:NH2	2.15	0.80
15:T:118:ARG:HG3	15:T:118:ARG:HH11	1.46	0.80
2:B:48:A:H4'	14:S:95:HIS:HD2	1.47	0.80
1:A:2036:C:H6	1:A:2036:C:H5'	1.46	0.80
1:A:2375:G:H8	34:A:5002:HOH:O	1.64	0.80
1:A:383:U:O4	34:A:5036:HOH:O	1.99	0.80
1:A:1506:C:H2'	1:A:1507:A:H5'	1.64	0.80
1:A:2123:G:H1	1:A:2175:C:H42	1.26	0.80
1:A:885:C:N4	1:A:890:A:H61	1.80	0.79
16:U:76:TYR:OH	16:U:92:ARG:NH1	2.15	0.79
1:A:2206:G:H3'	1:A:2207:G:C8	2.17	0.79
6:G:76:SER:HA	6:G:83:ARG:HA	1.64	0.79
1:A:1771:C:OP1	34:A:4359:HOH:O	1.99	0.79
15:T:95:ARG:HG2	15:T:95:ARG:HH11	1.48	0.79
1:A:326:G:N7	34:A:4238:HOH:O	2.14	0.79
2:B:20:C:N4	2:B:63:G:O6	2.16	0.79
6:G:11:TYR:CZ	6:G:16:ARG:HD3	2.17	0.78
6:G:56:ALA:HB2	6:G:153:ARG:HE	1.47	0.78
1:A:927:G:N7	34:A:4495:HOH:O	2.15	0.78
1:A:1403:C:H5''	1:A:1471:A:H1'	1.63	0.78
2:B:66:A:H61	2:B:108:U:H2'	1.48	0.78
1:A:2533:A:OP2	34:A:4657:HOH:O	2.00	0.77
1:A:1803:A:O2'	3:D:259:THR:HG21	1.84	0.77
1:A:11:G:N7	34:A:4486:HOH:O	2.18	0.77
1:A:1375:C:H3'	34:A:4021:HOH:O	1.86	0.76
3:D:148:GLU:HB2	3:D:151:LYS:HD2	1.67	0.76
1:A:827:U:OP1	34:A:4825:HOH:O	2.03	0.76
1:A:323:G:HO2'	1:A:1205:U:H3	1.32	0.76
12:Q:32:TYR:CE2	12:Q:133:ARG:HG3	2.20	0.76
1:A:587:C:OP2	11:P:21:ARG:NH2	2.19	0.76
1:A:1488:G:O6	34:A:4590:HOH:O	2.01	0.76
1:A:641:C:O2'	1:A:2350:C:OP1	2.02	0.75
1:A:1253:A:N7	34:A:4829:HOH:O	2.19	0.75
20:Y:23:ARG:HG2	20:Y:42:VAL:HG22	1.69	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:392:C:OP1	34:A:4221:HOH:O	2.03	0.75
2:B:41:U:OP1	34:B:318:HOH:O	2.04	0.75
1:A:527:C:H5	34:A:5057:HOH:O	1.70	0.75
1:A:2602:A:H4'	1:A:2603:G:OP1	1.86	0.75
2:B:6:C:H2'	2:B:7:G:H5''	1.68	0.75
9:N:56:ASN:H	9:N:125:GLY:HA3	1.51	0.75
1:A:1420:U:O2'	1:A:1421:G:OP1	2.03	0.74
1:A:495:G:N7	34:A:4790:HOH:O	2.20	0.74
1:A:1577:C:OP2	34:A:4580:HOH:O	2.05	0.74
1:A:2319:G:H22	14:S:3:ARG:HE	1.35	0.74
1:A:1364:G:OP2	23:1:3:LYS:HG2	1.86	0.74
23:1:82:LEU:HA	23:1:85:LEU:HD23	1.70	0.74
1:A:2820:A:OP2	13:R:2:ARG:NH2	2.20	0.73
4:E:111:ARG:HG3	4:E:160:TYR:CD1	2.23	0.73
1:A:1359:A:N1	1:A:1372:U:O4	2.22	0.73
1:A:938:G:OP2	30:8:52:LYS:NZ	2.20	0.73
1:A:773:U:OP1	34:A:4781:HOH:O	2.04	0.73
1:A:197:A:OP1	34:A:3883:HOH:O	2.05	0.73
15:T:16:ARG:NH2	15:T:83:ILE:O	2.22	0.73
23:1:21:ARG:NH1	23:1:21:ARG:HG2	2.03	0.73
1:A:2126:A:H4'	1:A:2127:G:O5'	1.89	0.72
24:2:70:GLN:NE2	24:2:71:ASN:OD1	2.22	0.72
30:8:34:TRP:O	30:8:36:LYS:N	2.22	0.72
1:A:2207:G:O2'	1:A:2208:A:OP1	2.07	0.72
2:B:30:C:H5''	34:B:326:HOH:O	1.87	0.72
8:I:69:LYS:HG2	8:I:138:ILE:HG12	1.71	0.72
1:A:2145:C:O2'	1:A:2147:G:N2	2.23	0.72
1:A:15:G:OP2	34:A:4609:HOH:O	2.08	0.72
1:A:1560:G:OP1	34:A:4678:HOH:O	2.07	0.72
14:S:14:VAL:O	14:S:18:ILE:HG12	1.90	0.72
1:A:1798:U:C5'	3:D:259:THR:HG22	2.19	0.72
1:A:1352:U:OP2	34:A:4020:HOH:O	2.07	0.72
11:P:59:LEU:HD11	30:8:10:ALA:HB2	1.71	0.71
14:S:34:HIS:ND1	14:S:53:SER:OG	2.23	0.71
1:A:621:A:OP2	11:P:108:LYS:NZ	2.22	0.71
1:A:2584:U:O4	34:A:3859:HOH:O	2.05	0.71
26:4:7:PRO:HB2	26:4:27:THR:HG21	1.71	0.71
1:A:1019:U:HO2'	1:A:1021:A:H2	1.36	0.71
27:5:16:ARG:HH11	27:5:16:ARG:HG2	1.54	0.71
1:A:956:G:OP2	12:Q:14:ARG:NH2	2.23	0.71
22:0:10:THR:HG22	22:0:12:ASN:H	1.55	0.71
1:A:1327:C:OP2	34:A:4831:HOH:O	2.07	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:71:A:OP2	1:A:71:A:H3'	1.90	0.71
8:I:72:LEU:HD12	8:I:138:ILE:HG21	1.73	0.71
17:V:40:LEU:HB2	17:V:46:VAL:HG13	1.71	0.71
6:G:72:ARG:HH12	6:G:87:PRO:HG3	1.56	0.71
1:A:2136:C:H42	1:A:2155:G:H1	1.39	0.71
6:G:44:GLY:HA2	6:G:88:ILE:HG22	1.73	0.71
3:D:8:PRO:HB3	3:D:14:ARG:HB2	1.72	0.71
1:A:2144:U:HO2'	1:A:2147:G:H1	1.37	0.70
1:A:62:C:OP1	34:A:4180:HOH:O	2.09	0.70
2:B:96:U:O4	34:B:330:HOH:O	2.07	0.70
1:A:948:G:OP1	34:A:3787:HOH:O	2.09	0.70
5:F:65:TRP:HH2	5:F:72:ARG:HH21	1.38	0.70
1:A:1507:A:O2'	1:A:1508:A:O5'	2.09	0.70
1:A:2789:C:O2'	1:A:2790:A:O2'	2.08	0.70
1:A:1376:C:OP2	34:A:4021:HOH:O	2.09	0.70
14:S:96:GLY:N	14:S:99:LYS:H	1.90	0.70
8:I:102:SER:HA	8:I:106:GLY:HA2	1.73	0.69
3:D:239:ARG:N	34:D:405:HOH:O	2.25	0.69
1:A:994:C:OP1	16:U:53:ARG:NH2	2.25	0.69
14:S:102:ALA:HB1	14:S:112:PHE:HZ	1.58	0.69
8:I:77:LEU:HD13	8:I:79:ILE:HD11	1.75	0.69
30:8:23:VAL:HG11	30:8:47:LYS:HD3	1.75	0.69
14:S:58:LEU:HB2	14:S:59:LYS:HB2	1.75	0.69
2:B:35:U:OP2	34:B:316:HOH:O	2.08	0.69
18:W:18:ARG:NH1	18:W:76:VAL:O	2.27	0.68
1:A:17:G:OP2	34:A:4488:HOH:O	2.11	0.68
18:W:14:PRO:HG2	18:W:78:GLU:HG2	1.74	0.68
8:I:93:THR:HG22	8:I:119:PRO:HB3	1.75	0.68
12:Q:127:ILE:O	34:Q:301:HOH:O	2.11	0.68
3:D:238:GLY:O	3:D:239:ARG:HB2	1.92	0.68
1:A:1495:A:H2'	1:A:1496:A:C8	2.28	0.68
1:A:1782:C:OP1	34:A:3840:HOH:O	2.10	0.68
1:A:607:U:OP1	5:F:102:PRO:HA	1.93	0.68
12:Q:51:ARG:NH2	21:Z:186:GLU:OE1	2.26	0.68
21:Z:160:GLY:HA2	21:Z:161:VAL:CB	2.23	0.68
23:1:54:ALA:HB1	23:1:83:GLU:HG3	1.76	0.68
1:A:2448:A:OP2	34:A:3839:HOH:O	2.11	0.68
7:H:3:ARG:HD3	7:H:54:ARG:HH12	1.59	0.68
11:P:38:GLN:HA	11:P:41:ARG:HG2	1.76	0.68
1:A:1023:U:OP2	34:A:4986:HOH:O	2.10	0.68
1:A:2162:G:O3'	1:A:2172:U:O2'	2.12	0.68
1:A:2541:A:OP2	34:A:4626:HOH:O	2.11	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1430:C:H2'	1:A:1431:U:C6	2.29	0.68
1:A:2431:U:OP2	34:A:4101:HOH:O	2.11	0.68
9:N:47:ALA:HB2	9:N:112:LEU:HD11	1.76	0.67
1:A:2332:U:O2'	1:A:2335:A:N3	2.22	0.67
8:I:27:ARG:HD2	23:1:71:TYR:CE1	2.29	0.67
1:A:2140:C:H2'	1:A:2141:G:H8	1.60	0.67
10:O:2:ILE:HD12	10:O:6:THR:HG21	1.77	0.67
11:P:39:LYS:HB2	11:P:45:LEU:HG	1.77	0.67
1:A:1452:A:OP2	34:A:4903:HOH:O	2.13	0.67
1:A:2577:A:O4'	27:5:3:LYS:HB2	1.94	0.67
2:B:66:A:N6	2:B:108:U:H2'	2.10	0.67
1:A:139(A):G:N2	19:X:44:GLU:OE1	2.28	0.67
1:A:588:U:H2'	1:A:589:C:C6	2.30	0.67
1:A:1980:G:O2'	1:A:1982:C:OP2	2.10	0.66
23:1:50:ARG:HG2	23:1:59:THR:HG22	1.78	0.66
1:A:1355:G:OP1	3:D:38:LYS:NZ	2.24	0.66
25:3:8:LEU:HD13	25:3:31:LEU:HD23	1.77	0.66
1:A:2589:A:OP1	34:A:3761:HOH:O	2.14	0.66
19:X:53:LYS:HB3	19:X:82:GLN:HB3	1.78	0.66
12:Q:135:ASP:OD2	21:Z:49:ARG:NH2	2.28	0.66
1:A:2127:G:O6	1:A:2161:C:N3	2.28	0.66
1:A:631:A:OP1	11:P:65:ARG:NH1	2.29	0.66
1:A:2123:G:H1	1:A:2175:C:N4	1.94	0.66
1:A:1310:G:OP2	29:7:9:ARG:NH1	2.26	0.66
5:F:53:THR:CG2	5:F:55:GLY:H	2.09	0.65
1:A:2296:U:OP2	14:S:9:ARG:NH2	2.28	0.65
18:W:4:LYS:HE2	18:W:6:ILE:HD11	1.78	0.65
1:A:1877:A:H5'	1:A:1878:G:OP2	1.96	0.65
1:A:2845:G:O2'	1:A:2846:G:H5'	1.95	0.65
1:A:2580:U:H5"	34:A:3936:HOH:O	1.96	0.65
19:X:35:THR:HG22	19:X:38:GLU:H	1.62	0.65
1:A:2327:A:H2'	1:A:2328:A:C8	2.32	0.65
14:S:102:ALA:HA	14:S:105:ALA:HB3	1.78	0.65
1:A:1542:A:OP2	34:A:3757:HOH:O	2.15	0.65
1:A:1689:A:N6	1:A:1698:A:H2	1.92	0.65
6:G:41:GLN:HB3	6:G:43:LEU:HD13	1.77	0.65
1:A:2683:C:O2	10:O:70:LYS:NZ	2.26	0.65
21:Z:158:PRO:O	21:Z:161:VAL:HG11	1.96	0.65
1:A:253:C:OP2	30:8:5:LYS:NZ	2.28	0.65
1:A:1642:G:N7	34:A:4432:HOH:O	2.30	0.65
13:R:55:ALA:HB2	13:R:79:LEU:HD13	1.78	0.65
1:A:1778:U:H2'	1:A:1784:A:N6	2.12	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2365:G:O6	30:8:39:LYS:HE3	1.97	0.65
1:A:2104:G:N2	1:A:2105:C:O2	2.30	0.65
1:A:2526:G:H21	31:9:2:LYS:HD2	1.62	0.65
7:H:33:LEU:HD21	7:H:136:ILE:HG13	1.77	0.64
14:S:15:ARG:O	14:S:19:LYS:HG2	1.97	0.64
1:A:668:G:H5'	1:A:669:G:OP2	1.96	0.64
1:A:2810:A:N6	1:A:2891:G:O2'	2.30	0.64
4:E:77:ILE:HD12	4:E:195:LEU:HD13	1.79	0.64
1:A:1250:G:N7	11:P:18:ARG:NH2	2.45	0.64
1:A:1420:U:HO2'	1:A:1421:G:P	2.21	0.64
1:A:2166:G:N2	1:A:2172:U:O4	2.31	0.64
4:E:179:GLU:HB3	4:E:181:LEU:HD22	1.79	0.64
1:A:2839:G:H5'	13:R:46:GLY:HA2	1.79	0.64
1:A:2128:C:H42	1:A:2160:G:H1	1.43	0.64
14:S:95:HIS:C	14:S:99:LYS:HB3	2.18	0.64
15:T:95:ARG:HG2	15:T:95:ARG:NH1	2.12	0.64
21:Z:158:PRO:HD2	21:Z:161:VAL:HG21	1.79	0.64
1:A:1352:U:P	34:A:4020:HOH:O	2.55	0.64
1:A:2127:G:N1	1:A:2161:C:O2	2.29	0.64
1:A:2353:G:N7	34:A:4862:HOH:O	2.30	0.64
1:A:2434:A:N7	34:A:4099:HOH:O	2.30	0.64
5:F:185:ASP:HA	5:F:188:ARG:HD3	1.79	0.63
1:A:1405:U:H2'	1:A:1406:U:C6	2.33	0.63
4:E:55:ASN:HB3	4:E:58:ARG:HG3	1.81	0.63
1:A:527:C:OP1	34:A:4807:HOH:O	2.15	0.63
1:A:2114:A:O2'	1:A:2167:U:O3'	2.15	0.63
9:N:24:GLY:HA2	9:N:27:ALA:HB3	1.80	0.63
1:A:1153:C:OP1	16:U:92:ARG:NH1	2.25	0.63
1:A:2318:G:O2'	1:A:2319:G:OP1	2.15	0.63
10:O:98:VAL:HG13	10:O:117:LEU:HB3	1.80	0.63
30:8:29:LYS:HG2	30:8:44:LYS:HB3	1.81	0.63
8:I:104:GLN:C	8:I:105:HIS:HD1	2.02	0.63
11:P:100:LEU:HD12	11:P:112:LEU:HD11	1.81	0.63
3:D:137:PRO:O	3:D:140:THR:HG23	1.99	0.63
1:A:271(E):U:H2'	1:A:271(F):C:C6	2.34	0.63
1:A:885:C:H5''	34:A:5034:HOH:O	1.99	0.63
1:A:2577:A:H5'	27:5:3:LYS:HD2	1.81	0.63
1:A:911:A:H2'	12:Q:9:TYR:OH	1.98	0.63
1:A:2134:A:H1'	1:A:2159:G:H1'	1.81	0.63
1:A:1038:C:H42	1:A:1117:G:H1	1.46	0.63
16:U:92:ARG:HA	16:U:95:LEU:HB2	1.81	0.62
4:E:54:GLN:HB2	4:E:76:ARG:HB3	1.80	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2349:G:H5'	1:A:2350:C:OP2	1.99	0.62
3:D:71:ASP:HB3	3:D:103:ARG:HH22	1.64	0.62
21:Z:124:ILE:HG13	21:Z:125:LEU:H	1.64	0.62
20:Y:90:LEU:HB3	20:Y:92:ASN:H	1.64	0.62
1:A:2243:U:H2'	1:A:2244:U:C6	2.34	0.62
1:A:1300:U:H4'	1:A:1301:A:H5'	1.82	0.62
1:A:271(M):G:O2'	1:A:271(N):U:O5'	2.15	0.62
1:A:370:G:OP2	34:A:4247:HOH:O	2.16	0.62
21:Z:54:HIS:ND1	21:Z:101:PRO:HG3	2.14	0.62
1:A:1379:A:H4'	1:A:1380:G:OP2	2.00	0.62
1:A:509:C:O3'	34:A:3884:HOH:O	2.16	0.62
1:A:330:A:H2	1:A:1210:A:H2'	1.63	0.62
1:A:2887:U:H2'	1:A:2888:C:C6	2.34	0.62
1:A:1531:C:H42	1:A:1538:G:H1	1.46	0.62
1:A:1448:G:H4'	1:A:1542:A:OP1	2.00	0.62
1:A:2285:C:OP2	28:6:6:ARG:NH1	2.33	0.62
1:A:2113:U:H2'	1:A:2114:A:O4'	2.00	0.62
24:2:51:ARG:HA	24:2:54:LYS:HB2	1.81	0.62
1:A:84:A:H5''	20:Y:8:LYS:HE3	1.82	0.62
1:A:2777:G:H5''	1:A:2778:A:H5'	1.82	0.62
1:A:1364:G:OP1	23:1:2:SER:HA	2.00	0.62
1:A:2646:C:OP2	1:A:2732:G:O2'	2.17	0.62
27:5:51:TYR:CE1	27:5:56:LYS:HG2	2.33	0.62
1:A:300:A:P	20:Y:86:ARG:HH22	2.23	0.61
5:F:197:ASP:OD2	5:F:197:ASP:N	2.32	0.61
20:Y:79:CYS:HB2	20:Y:81:LYS:H	1.64	0.61
1:A:1633:G:OP2	34:A:4045:HOH:O	2.16	0.61
1:A:833:U:O2	11:P:55:ARG:NH2	2.33	0.61
1:A:2198:A:H4'	1:A:2199:A:OP1	2.00	0.61
15:T:24:PRO:HD3	15:T:52:ILE:HD12	1.82	0.61
1:A:1429:G:H2'	1:A:1430:C:C6	2.34	0.61
1:A:300:A:OP2	20:Y:86:ARG:NH2	2.33	0.61
4:E:116:VAL:HG13	4:E:122:PHE:HB2	1.81	0.61
1:A:2894:G:H8	1:A:2894:G:O5'	1.83	0.61
26:4:42:PHE:HB3	26:4:43:TYR:HB2	1.82	0.61
1:A:764:A:H2	3:D:219:PRO:HG3	1.64	0.61
1:A:2686:G:H5'	34:A:4438:HOH:O	2.00	0.61
1:A:2208:A:H1'	1:A:2219:G:C4	2.36	0.61
3:D:71:ASP:OD2	3:D:103:ARG:NH2	2.33	0.61
1:A:2497:A:H5''	34:A:3890:HOH:O	2.00	0.61
4:E:152:LYS:HD2	9:N:77:GLY:HA3	1.82	0.61
2:B:106:G:H5'	21:Z:31:ARG:HG2	1.82	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1040:C:H2'	1:A:1041:C:O4'	2.00	0.61
1:A:1266:G:O5'	18:W:15:ARG:NH2	2.33	0.61
1:A:301:G:OP2	20:Y:84:ARG:NH2	2.34	0.61
8:I:41:GLU:HA	8:I:44:LEU:HB2	1.82	0.61
30:8:62:LEU:HB3	30:8:65:GLU:HG2	1.83	0.61
1:A:530:G:N3	1:A:530:G:O4'	2.33	0.61
1:A:945:A:C2	34:A:4005:HOH:O	2.50	0.60
1:A:2114:A:H1'	1:A:2168:G:H5'	1.83	0.60
1:A:2142:C:H2'	1:A:2143:C:C6	2.36	0.60
15:T:24:PRO:HA	15:T:49:VAL:HG22	1.82	0.60
4:E:24:THR:HG22	4:E:186:GLY:O	2.01	0.60
1:A:11:G:H2'	1:A:12:U:H5'	1.82	0.60
5:F:101:LEU:HD12	5:F:102:PRO:HD2	1.82	0.60
12:Q:37:LEU:HD21	12:Q:130:LYS:HE2	1.83	0.60
5:F:184:TYR:CD2	5:F:188:ARG:HD2	2.36	0.60
11:P:63:PRO:HG2	30:8:25:MET:HB2	1.84	0.60
3:D:275:LYS:HG3	3:D:276:LYS:HB2	1.83	0.60
1:A:2122:U:H2'	1:A:2123:G:H8	1.66	0.60
21:Z:152:ALA:HA	21:Z:155:LEU:HD13	1.83	0.60
21:Z:161:VAL:O	21:Z:161:VAL:HG13	2.01	0.60
14:S:11:LYS:O	14:S:15:ARG:HB2	2.01	0.60
21:Z:33:LEU:HD23	21:Z:90:VAL:HG21	1.84	0.60
9:N:15:LEU:HB2	9:N:135:PRO:HB2	1.83	0.60
11:P:126:VAL:HG12	11:P:148:LEU:HD22	1.83	0.60
2:B:2:C:H2'	2:B:3:C:C6	2.36	0.60
1:A:830:G:H5'	34:A:4007:HOH:O	2.01	0.60
1:A:997:G:OP1	16:U:92:ARG:HG2	2.01	0.60
1:A:2130:U:H1'	1:A:2158:A:N1	2.16	0.60
1:A:1796:U:H2'	1:A:1797:C:C6	2.37	0.60
1:A:2833:G:H3'	1:A:2834:G:H5''	1.84	0.60
1:A:760:G:OP2	34:A:4035:HOH:O	2.16	0.60
20:Y:38:ILE:HD11	20:Y:66:PRO:HG3	1.84	0.59
1:A:1778:U:OP2	34:A:4364:HOH:O	2.17	0.59
3:D:71:ASP:HB3	3:D:103:ARG:NH2	2.17	0.59
21:Z:69:THR:HG22	21:Z:90:VAL:HA	1.85	0.59
22:O:27:GLU:HG3	22:O:68:GLU:HA	1.84	0.59
1:A:1929:G:H4'	1:A:1930:G:OP1	2.01	0.59
1:A:1125:G:H5'	31:9:37:GLY:HA2	1.84	0.59
1:A:1019:U:O2'	1:A:1021:A:H2	1.84	0.59
25:3:23:LEU:HD13	25:3:50:VAL:HG11	1.84	0.59
1:A:1025:G:C4	1:A:1135:C:H1'	2.37	0.59
1:A:885:C:H3'	1:A:886:C:H5''	1.83	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:S:82:ILE:CA	14:S:83:LYS:HB2	2.31	0.59
1:A:2074:U:H2'	1:A:2075:U:C6	2.38	0.59
1:A:662:G:H5''	11:P:16:ARG:HG2	1.84	0.59
14:S:25:ARG:NH1	14:S:42:ASP:OD2	2.36	0.59
1:A:2168:G:H22	1:A:2171:A:H2'	1.67	0.59
1:A:95:G:O2'	24:2:46:GLN:HA	2.03	0.59
20:Y:68:HIS:ND1	20:Y:70:SER:HB3	2.17	0.59
1:A:1359:A:H5'	1:A:1359:A:N3	2.17	0.59
28:6:6:ARG:NH1	28:6:26:ASN:HB2	2.17	0.59
1:A:203:C:H3'	1:A:204:A:H5''	1.85	0.59
1:A:1991:U:H2'	1:A:1992:G:H5''	1.83	0.59
1:A:928:G:O6	34:A:5039:HOH:O	2.16	0.58
1:A:1019:U:H3	1:A:1142(A):A:H62	1.50	0.58
1:A:1774:C:OP1	34:A:3831:HOH:O	2.17	0.58
1:A:2506:U:OP1	4:E:144:ARG:NH2	2.36	0.58
23:1:6:GLU:HG3	23:1:61:ARG:O	2.03	0.58
4:E:47:VAL:HG12	4:E:49:LEU:HD13	1.85	0.58
1:A:1022:G:H22	1:A:1142(A):A:H2	1.47	0.58
1:A:686:G:H5''	29:7:11:LYS:HE2	1.84	0.58
1:A:1439:A:OP1	34:A:4335:HOH:O	2.17	0.58
1:A:250:G:OP2	30:8:13:ARG:NH2	2.36	0.58
1:A:251:A:C5	1:A:252:G:H1'	2.38	0.58
6:G:75:LYS:HA	6:G:84:LYS:HE2	1.86	0.58
1:A:1430:C:H2'	1:A:1431:U:H6	1.69	0.58
3:D:275:LYS:HG3	3:D:276:LYS:N	2.19	0.58
1:A:861:A:C2	1:A:917:A:C4	2.91	0.58
1:A:889:C:O2'	1:A:890:A:H8	1.87	0.58
1:A:2469:A:H4'	12:Q:56:ARG:HG2	1.85	0.58
14:S:34:HIS:O	14:S:97:ARG:NH2	2.37	0.58
4:E:203:LYS:CB	4:E:204:ALA:HA	2.33	0.58
1:A:1204:A:H61	1:A:1240:U:H2'	1.69	0.58
15:T:118:ARG:NH1	15:T:118:ARG:HG3	2.16	0.58
27:5:16:ARG:NH1	27:5:17:ASP:OD1	2.37	0.58
1:A:1021:A:H3'	1:A:1021:A:C8	2.39	0.57
1:A:963:U:OP2	34:A:3787:HOH:O	2.17	0.57
1:A:1494:A:O2'	1:A:1495:A:H5'	2.04	0.57
1:A:1029:A:O2'	34:A:4875:HOH:O	2.07	0.57
3:D:3:VAL:HG13	3:D:17:THR:HB	1.86	0.57
1:A:2136:C:N3	1:A:2155:G:N2	2.45	0.57
1:A:2136:C:N4	1:A:2155:G:N1	2.46	0.57
19:X:31:HIS:HD2	19:X:33:LYS:N	1.95	0.57
5:F:101:LEU:O	5:F:106:ARG:NH1	2.29	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2023:G:H5'	1:A:2617:C:H4'	1.87	0.57
1:A:639:U:H2'	1:A:640:C:C6	2.39	0.57
1:A:2463:C:O2'	1:A:2464:C:H5'	2.04	0.57
7:H:113:VAL:HG11	7:H:151:ILE:HD13	1.86	0.57
1:A:2439:A:H5'	1:A:2439:A:C8	2.39	0.57
1:A:2115:G:O2'	1:A:2166:G:N2	2.36	0.57
1:A:1330:C:OP1	34:A:4709:HOH:O	2.17	0.57
1:A:1434:A:H61	1:A:1558:A:H62	1.51	0.57
21:Z:138:GLU:H	21:Z:156:LYS:NZ	2.03	0.57
1:A:539:G:H2'	1:A:540:C:H6	1.69	0.57
1:A:297:C:OP1	20:Y:95:LYS:NZ	2.37	0.57
28:6:11:LEU:HB2	28:6:21:TYR:HB2	1.85	0.57
1:A:2519:U:OP2	34:A:4625:HOH:O	2.17	0.57
14:S:96:GLY:HA2	14:S:97:ARG:C	2.25	0.57
26:4:15:ILE:O	26:4:32:TYR:HA	2.04	0.57
4:E:9:VAL:HG13	4:E:25:VAL:O	2.04	0.57
1:A:1622:G:OP2	34:A:4056:HOH:O	2.18	0.57
1:A:926:A:N7	34:A:4491:HOH:O	2.33	0.57
1:A:2611:U:OP2	1:A:2611:U:H3'	2.05	0.57
16:U:105:VAL:O	16:U:108:GLU:HB2	2.04	0.57
1:A:2137:C:O2	1:A:2137:C:H2'	2.05	0.57
1:A:83:G:N2	1:A:102:G:H1'	2.20	0.57
13:R:72:ASP:O	13:R:76:VAL:HG23	2.04	0.57
2:B:39:A:O2'	2:B:46:A:N1	2.34	0.57
7:H:137:ASP:HB3	7:H:140:LYS:HB3	1.87	0.57
2:B:11:C:H3'	2:B:12:C:C6	2.40	0.57
1:A:945:A:H2	34:A:4005:HOH:O	1.86	0.57
30:8:32:LEU:O	30:8:36:LYS:HE3	2.05	0.57
8:I:123:LEU:HB2	8:I:144:VAL:O	2.05	0.57
1:A:2152:G:H2'	1:A:2153:G:C8	2.40	0.56
1:A:271(Q):G:O2'	1:A:271(R):G:H8	1.88	0.56
8:I:67:ARG:O	8:I:68:LEU:HD22	2.05	0.56
15:T:60:THR:HG22	15:T:77:PRO:HA	1.87	0.56
1:A:1494:A:H2'	1:A:1495:A:C8	2.39	0.56
6:G:179:PRO:HG3	26:4:43:TYR:OH	2.05	0.56
1:A:644:A:H4'	1:A:645:C:C5	2.41	0.56
21:Z:7:ALA:HB3	21:Z:61:LEU:HD12	1.85	0.56
28:6:16:CYS:HB2	28:6:18:ARG:NH1	2.20	0.56
1:A:2295:C:C2'	1:A:2296:U:H5'	2.34	0.56
21:Z:128:VAL:HG23	21:Z:161:VAL:H	1.70	0.56
1:A:330:A:H2	1:A:1210:A:HO2'	1.52	0.56
5:F:120:GLU:HB2	5:F:122:LYS:HG2	1.87	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1486:A:H2'	1:A:1487:G:H8	1.70	0.56
1:A:1406:U:H2'	1:A:1407:C:C6	2.41	0.56
1:A:271(Q):G:OP1	8:I:42:SER:HB2	2.05	0.56
2:B:78:A:C2	2:B:100:A:C4	2.93	0.56
12:Q:110:THR:HG23	12:Q:113:GLN:OE1	2.06	0.56
1:A:1187:G:H5''	17:V:81:TYR:CE2	2.40	0.56
1:A:69:C:N4	34:A:4185:HOH:O	2.39	0.56
1:A:2130:U:O2'	1:A:2133:G:O2'	2.22	0.56
1:A:2111:C:H42	1:A:2147:G:N2	2.04	0.56
21:Z:45:ASP:OD2	21:Z:49:ARG:NH1	2.39	0.56
1:A:539:G:H2'	1:A:540:C:C6	2.40	0.56
1:A:7:G:H2'	1:A:8:A:O4'	2.05	0.56
1:A:141:A:C8	1:A:1408:C:O2'	2.59	0.56
1:A:910:A:N1	1:A:2277:G:H1'	2.21	0.56
2:B:44:G:C2	2:B:48:A:C2	2.94	0.56
1:A:141:A:H8	1:A:1408:C:HO2'	1.52	0.56
1:A:2723:C:OP2	4:E:109:LYS:NZ	2.39	0.56
24:2:4:SER:HA	24:2:7:ARG:NH1	2.21	0.56
21:Z:154:ASP:OD1	21:Z:154:ASP:N	2.38	0.56
1:A:886:C:H2'	1:A:887:A:H5''	1.88	0.55
1:A:2012:G:OP1	18:W:11:ARG:NH2	2.38	0.55
1:A:652(C):G:N2	1:A:652(V):C:O2	2.32	0.55
5:F:53:THR:HG23	5:F:55:GLY:H	1.69	0.55
1:A:1903:G:OP1	3:D:241:PRO:HB2	2.06	0.55
1:A:873:G:N2	1:A:905:U:C2	2.74	0.55
3:D:242:ARG:N	3:D:242:ARG:HD3	2.20	0.55
1:A:2206:G:O2'	1:A:2207:G:OP1	2.21	0.55
1:A:2887:U:H2'	1:A:2888:C:H6	1.69	0.55
1:A:1540:U:C2'	1:A:1541:G:H5'	2.36	0.55
1:A:1540:U:O2'	1:A:1541:G:H5'	2.06	0.55
1:A:450:G:O6	34:A:4153:HOH:O	2.18	0.55
1:A:2572:A:N7	4:E:144:ARG:HD2	2.20	0.55
1:A:2784:C:H1'	4:E:37:ARG:HH12	1.71	0.55
1:A:2382:G:N7	34:A:4409:HOH:O	2.32	0.55
1:A:244:A:C2	1:A:255:A:C4	2.94	0.55
1:A:2357:U:OP1	22:O:20:ARG:HD3	2.06	0.55
1:A:2884:U:H1'	27:5:53:ALA:HB2	1.87	0.55
1:A:330:A:HO2'	1:A:331:A:H8	1.55	0.55
5:F:157:VAL:HB	5:F:194:MET:HG2	1.88	0.55
1:A:2537:U:H2'	1:A:2538:C:C6	2.41	0.55
1:A:77:C:OP1	24:2:59:ARG:HD3	2.06	0.55
1:A:1178:C:H2'	1:A:1179:C:H6	1.72	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:G:60:LEU:HB3	6:G:68:PRO:HG3	1.89	0.55
1:A:330:A:H2	1:A:1210:A:C2'	2.19	0.55
1:A:271(Q):G:O2'	1:A:271(R):G:C8	2.60	0.55
1:A:1247:A:OP1	5:F:95:ARG:NH2	2.40	0.55
1:A:2114:A:H3'	1:A:2115:G:C8	2.42	0.55
27:5:16:ARG:HG2	27:5:16:ARG:NH1	2.22	0.55
13:R:102:GLU:OE2	18:W:37:ARG:NH1	2.33	0.55
1:A:2584:U:H2'	1:A:2585:U:H2'	1.87	0.55
1:A:1963:U:H4'	1:A:1964:G:OP1	2.07	0.55
1:A:796:C:H2'	1:A:797:C:C6	2.41	0.55
5:F:17:ARG:O	5:F:18:ARG:HB2	2.07	0.55
1:A:1693:U:O2'	3:D:14:ARG:NH2	2.40	0.55
1:A:218:A:C2	1:A:235:U:H4'	2.42	0.55
1:A:2473:U:H2'	1:A:2473:U:O2	2.07	0.55
1:A:2304:G:H21	6:G:156:ASP:CG	2.10	0.54
20:Y:23:ARG:HB2	20:Y:23:ARG:NH1	2.22	0.54
9:N:56:ASN:HA	9:N:125:GLY:H	1.71	0.54
21:Z:128:VAL:HG23	21:Z:161:VAL:N	2.23	0.54
9:N:102:ALA:O	9:N:106:MET:HG3	2.07	0.54
5:F:21:ALA:O	5:F:22:ALA:HB2	2.06	0.54
2:B:90:A:N7	2:B:91:C:H1'	2.22	0.54
1:A:1290:C:H2'	1:A:1291:C:H6	1.72	0.54
2:B:49:C:OP1	14:S:97:ARG:N	2.39	0.54
1:A:528:A:N1	1:A:2042:A:H2'	2.22	0.54
1:A:2463:C:C2'	1:A:2464:C:H5'	2.36	0.54
1:A:1669:A:H5''	1:A:2550:G:OP1	2.07	0.54
14:S:96:GLY:H	14:S:99:LYS:H	1.54	0.54
1:A:2001:A:H2'	1:A:2002:G:C8	2.43	0.54
1:A:1914:C:H2'	1:A:1915:U:C6	2.42	0.54
1:A:2319:G:H22	14:S:3:ARG:NE	2.03	0.54
1:A:2126:A:H1'	1:A:2127:G:OP2	2.08	0.54
8:I:69:LYS:HB3	8:I:73:GLU:OE1	2.08	0.54
4:E:28:ALA:HB3	4:E:93:VAL:HG13	1.89	0.54
5:F:129:PHE:CD2	5:F:163:VAL:HG21	2.42	0.54
1:A:2867:G:OP2	15:T:119:LYS:NZ	2.41	0.54
12:Q:138:ASP:OD2	21:Z:81:ARG:NH1	2.40	0.54
1:A:1529:G:C6	1:A:1530:C:N4	2.76	0.54
1:A:323:G:O2'	1:A:1205:U:N3	2.34	0.54
1:A:2693:A:H2'	1:A:2694:G:H8	1.73	0.54
1:A:2125:G:N2	1:A:2172:U:H3'	2.23	0.54
1:A:1020:A:N1	1:A:1141:U:O2'	2.36	0.54
8:I:126:TYR:HB2	8:I:142:VAL:HG23	1.89	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1882:C:H5'	1:A:1883:G:OP2	2.07	0.54
1:A:1843:C:H5'	3:D:253:GLN:NE2	2.23	0.54
1:A:359:A:H2'	1:A:360:G:O4'	2.08	0.54
11:P:143:GLY:O	11:P:145:PRO:HD3	2.08	0.54
1:A:1688:U:H1'	1:A:1701:A:C6	2.42	0.53
1:A:12:U:H2'	1:A:12:U:O2	2.07	0.53
1:A:1488:G:H5''	1:A:1488:G:H8	1.73	0.53
1:A:1288:U:C2	1:A:1327:C:O2	2.61	0.53
1:A:2329:G:H21	22:0:41:ARG:HG3	1.72	0.53
1:A:2186:G:H2'	1:A:2186:G:N3	2.23	0.53
1:A:1817:G:OP1	3:D:88:ARG:NH2	2.40	0.53
12:Q:6:ARG:HB3	21:Z:194:PRO:HG2	1.90	0.53
2:B:2:C:H2'	2:B:3:C:H6	1.73	0.53
1:A:2080:G:OP1	23:1:35:THR:HG21	2.08	0.53
18:W:40:ASN:O	18:W:41:LYS:HG3	2.08	0.53
1:A:2648:C:H2'	1:A:2649:U:C6	2.44	0.53
1:A:139(A):G:H22	19:X:44:GLU:CD	2.11	0.53
1:A:1503:U:H2'	1:A:1504:C:C6	2.43	0.53
1:A:96:G:H4'	24:2:48:HIS:CD2	2.44	0.53
1:A:729:G:C6	3:D:208:LYS:HB2	2.43	0.53
1:A:127:A:H5''	1:A:128:C:C6	2.44	0.53
1:A:774:A:H2'	1:A:774:A:N3	2.23	0.53
1:A:2850:A:OP2	1:A:2866:U:H5	1.90	0.53
1:A:1530:C:HO2'	1:A:1531:C:P	2.30	0.53
1:A:1366:A:OP1	23:1:3:LYS:NZ	2.39	0.53
1:A:1429:G:O2'	1:A:1430:C:H5'	2.09	0.53
8:I:27:ARG:HD2	23:1:71:TYR:CZ	2.43	0.53
12:Q:109:VAL:HG13	12:Q:113:GLN:HB2	1.89	0.53
14:S:96:GLY:HA2	14:S:100:ALA:H	1.74	0.53
11:P:38:GLN:O	11:P:39:LYS:CB	2.57	0.53
1:A:993:G:OP1	16:U:50:ARG:NH2	2.40	0.53
1:A:642:G:H21	1:A:646:A:H2	1.57	0.53
1:A:2131:G:OP1	1:A:2132:U:H3'	2.08	0.53
1:A:1138:G:O2'	9:N:105:GLY:HA3	2.09	0.53
1:A:1800:C:OP2	3:D:183:ARG:NH2	2.32	0.53
1:A:1530:C:H1'	1:A:1531:C:OP1	2.09	0.53
20:Y:20:TYR:CD2	20:Y:42:VAL:HG13	2.43	0.53
1:A:1178:C:H2'	1:A:1179:C:C6	2.43	0.53
7:H:150:ALA:HA	7:H:153:LYS:HD2	1.90	0.53
1:A:762:U:OP1	34:A:3843:HOH:O	2.19	0.53
5:F:184:TYR:CE2	5:F:188:ARG:HD2	2.44	0.53
21:Z:124:ILE:HG13	21:Z:125:LEU:N	2.22	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1138:G:H2'	9:N:106:MET:HE2	1.90	0.53
1:A:1794:U:H2'	1:A:1795:C:C6	2.44	0.53
1:A:2328:A:H2'	1:A:2329:G:C8	2.43	0.53
1:A:2022:U:O2'	1:A:2617:C:H5'	2.09	0.53
3:D:108:PRO:HB3	3:D:143:HIS:CE1	2.44	0.53
14:S:96:GLY:N	14:S:99:LYS:HB3	2.23	0.52
1:A:1507:A:O2'	1:A:1508:A:H8	1.92	0.52
11:P:59:LEU:HD21	30:8:10:ALA:HA	1.91	0.52
1:A:2464:C:O2'	1:A:2465:C:H5''	2.07	0.52
1:A:1810:A:H2'	1:A:1811:G:O4'	2.09	0.52
1:A:1329:U:H5''	1:A:1330:C:H5	1.74	0.52
1:A:1403:C:C5'	1:A:1471:A:H1'	2.35	0.52
1:A:2171:A:H4'	1:A:2172:U:OP1	2.09	0.52
1:A:2183:C:H2'	1:A:2184:G:C8	2.45	0.52
18:W:66:GLU:HA	18:W:69:LEU:HD12	1.91	0.52
28:6:13:CYS:SG	28:6:47:THR:HG21	2.49	0.52
21:Z:10:ARG:HG3	21:Z:36:LYS:HB3	1.90	0.52
1:A:657:U:H2'	1:A:658:C:C6	2.44	0.52
1:A:2849:U:OP2	15:T:95:ARG:NH1	2.42	0.52
6:G:16:ARG:HG3	6:G:16:ARG:HH11	1.74	0.52
6:G:16:ARG:HE	6:G:31:VAL:HG21	1.74	0.52
1:A:2166:G:H2'	1:A:2167:U:O4'	2.10	0.52
13:R:21:TYR:OH	13:R:43:GLU:HG2	2.10	0.52
1:A:2361:A:N6	34:A:4402:HOH:O	2.14	0.52
25:3:4:LEU:O	25:3:36:VAL:HA	2.09	0.52
17:V:35:LEU:HB2	17:V:57:VAL:HG22	1.90	0.52
8:I:82:ARG:O	8:I:89:TYR:HD1	1.91	0.52
1:A:2880:C:O3'	13:R:90:ARG:NH1	2.43	0.52
10:O:16:ALA:HB2	10:O:52:VAL:HG21	1.91	0.52
1:A:784:A:C8	1:A:792:G:C5	2.97	0.52
1:A:952:G:OP1	12:Q:16:ARG:NH2	2.42	0.52
1:A:839:U:H2'	1:A:840:C:C6	2.44	0.52
6:G:61:ALA:O	6:G:65:GLY:N	2.39	0.52
1:A:527:C:H4'	1:A:528:A:O5'	2.10	0.52
21:Z:81:ARG:HH21	21:Z:81:ARG:HG2	1.75	0.52
1:A:1162:G:O2'	17:V:90:PRO:HG2	2.09	0.52
1:A:578:A:OP2	34:A:3912:HOH:O	2.19	0.52
1:A:2406:U:H2'	1:A:2406:U:OP2	2.10	0.52
1:A:2036:C:C6	1:A:2036:C:H5'	2.35	0.52
21:Z:137:ILE:HG23	21:Z:156:LYS:HD2	1.91	0.52
28:6:16:CYS:SG	28:6:18:ARG:HG2	2.49	0.52
8:I:62:LYS:HA	8:I:65:ALA:HB3	1.91	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:E:201:THR:OG1	4:E:202:LYS:N	2.41	0.52
30:8:34:TRP:CG	30:8:35:GLN:N	2.77	0.52
1:A:2839:G:C5'	13:R:46:GLY:HA2	2.39	0.52
20:Y:43:ASN:OD1	20:Y:65:ALA:HB3	2.10	0.52
24:2:71:ASN:N	24:2:71:ASN:OD1	2.42	0.52
1:A:330:A:H2	1:A:1210:A:O2'	1.93	0.52
1:A:821:A:H2'	1:A:946:G:H5''	1.92	0.52
1:A:2158:A:H4'	1:A:2159:G:H5'	1.91	0.52
26:4:14:ILE:HD12	26:4:22:ILE:HD12	1.92	0.52
1:A:2563:U:O2	1:A:2565:A:H8	1.92	0.52
21:Z:125:LEU:HG	21:Z:164:ALA:HB3	1.90	0.51
24:2:45:SER:O	24:2:46:GLN:HB2	2.10	0.51
26:4:14:ILE:O	26:4:22:ILE:HG13	2.10	0.51
1:A:1371:G:HO2'	1:A:1372:U:H5	1.58	0.51
1:A:1021:A:H3'	1:A:1021:A:H8	1.75	0.51
30:8:23:VAL:CG1	30:8:47:LYS:HD3	2.38	0.51
1:A:1485:G:O2'	1:A:1486:A:H5'	2.10	0.51
1:A:1805:U:O2	3:D:50:THR:HB	2.10	0.51
4:E:12:THR:HG22	15:T:58:ASN:OD1	2.10	0.51
8:I:38:LEU:HB3	8:I:40:THR:HG23	1.91	0.51
19:X:26:TYR:CE1	19:X:89:ILE:HG13	2.44	0.51
7:H:12:PRO:O	7:H:14:GLY:HA2	2.10	0.51
1:A:30:G:H2'	1:A:31:C:C6	2.45	0.51
21:Z:30:ASN:ND2	21:Z:90:VAL:HB	2.26	0.51
17:V:60:GLU:HB2	17:V:97:LYS:HE2	1.92	0.51
1:A:999:U:O2'	1:A:1000:A:H5'	2.11	0.51
2:B:29:A:H2'	2:B:30:C:C6	2.46	0.51
8:I:92:VAL:HG22	8:I:120:ILE:HB	1.91	0.51
2:B:11:C:OP2	2:B:12:C:N4	2.28	0.51
1:A:848:G:C4	1:A:933:A:H8	2.29	0.51
1:A:886:C:H4'	1:A:886:C:OP1	2.10	0.51
1:A:2125:G:H21	1:A:2126:A:N6	2.08	0.51
4:E:12:THR:HG21	15:T:11:GLU:OE2	2.11	0.51
1:A:2203:U:O2'	1:A:2205:C:H5'	2.11	0.51
9:N:56:ASN:H	9:N:125:GLY:CA	2.21	0.51
16:U:76:TYR:CZ	16:U:80:ILE:HG13	2.46	0.51
28:6:18:ARG:HG3	28:6:42:TRP:CD1	2.46	0.51
24:2:16:LEU:O	24:2:67:LYS:NZ	2.44	0.51
1:A:1721:G:N1	1:A:1739:U:OP2	2.44	0.51
1:A:1654:A:OP1	13:R:1:MET:HA	2.10	0.51
5:F:53:THR:HG22	5:F:55:GLY:H	1.75	0.51
21:Z:101:PRO:O	21:Z:102:LEU:HD12	2.11	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
28:6:40:CYS:SG	28:6:42:TRP:HB2	2.50	0.51
1:A:1290:C:H2'	1:A:1291:C:C6	2.46	0.51
12:Q:12:GLN:HG2	12:Q:73:PRO:HD2	1.93	0.51
2:B:42:C:O2	6:G:93:THR:N	2.40	0.51
1:A:2322:A:H2'	1:A:2323:G:O4'	2.11	0.51
1:A:2287:A:N6	1:A:2344:U:H3	1.97	0.51
1:A:2109:U:H2'	1:A:2110:G:C8	2.46	0.51
1:A:455:C:N3	1:A:472:A:H2'	2.25	0.51
2:B:53:A:H2'	2:B:54:G:O4'	2.11	0.51
1:A:1140:C:O3'	9:N:25:ARG:NH1	2.43	0.50
1:A:90:U:O2'	1:A:92:A:O4'	2.28	0.50
8:I:81:VAL:HG22	8:I:145:VAL:O	2.11	0.50
1:A:1166:C:H2'	1:A:1167:U:C6	2.46	0.50
12:Q:103:MET:CE	12:Q:125:LEU:HD13	2.41	0.50
1:A:660:G:N2	34:A:3720:HOH:O	2.43	0.50
14:S:102:ALA:HB1	14:S:112:PHE:CZ	2.43	0.50
5:F:184:TYR:O	5:F:188:ARG:HG3	2.11	0.50
4:E:11:MET:HG2	4:E:24:THR:HB	1.93	0.50
15:T:120:ARG:HA	15:T:123:GLN:HG2	1.92	0.50
16:U:112:ARG:NH2	17:V:47:VAL:HB	2.26	0.50
7:H:88:LEU:CD2	7:H:165:ALA:HA	2.40	0.50
1:A:71:A:H5''	1:A:73:A:C8	2.46	0.50
1:A:528:A:C2	1:A:2043:C:H4'	2.47	0.50
1:A:2130:U:O2'	1:A:2158:A:N6	2.43	0.50
21:Z:72:ARG:NH2	21:Z:97:GLU:O	2.43	0.50
8:I:4:ILE:HD11	8:I:44:LEU:HD12	1.92	0.50
1:A:2357:U:O2	34:A:4405:HOH:O	2.19	0.50
26:4:14:ILE:HG23	26:4:31:ILE:HB	1.92	0.50
1:A:2273:A:H2'	1:A:2274:A:C8	2.47	0.50
1:A:484:C:H2'	1:A:485:C:C6	2.47	0.50
11:P:26:GLY:O	11:P:27:HIS:CD2	2.64	0.50
8:I:116:LEU:HD22	8:I:118:LYS:O	2.10	0.50
1:A:2143:C:N3	1:A:2148:G:O6	2.45	0.50
2:B:73:A:C4	2:B:105:A:C2	3.00	0.50
1:A:1721:G:H2'	1:A:1740:G:O6	2.11	0.50
18:W:45:TYR:CZ	18:W:49:LYS:HE3	2.46	0.50
18:W:79:GLY:HA3	18:W:100:THR:HG22	1.93	0.50
9:N:42:TRP:HA	9:N:48:MET:SD	2.51	0.50
1:A:1824:G:OP1	3:D:52:ARG:NH1	2.42	0.50
1:A:234:C:H2'	1:A:235:U:H6	1.76	0.50
2:B:42:C:O2	6:G:92:VAL:HA	2.12	0.50
6:G:3:LEU:HD13	26:4:25:TYR:CE1	2.46	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:N:96:GLU:H	9:N:96:GLU:CD	2.15	0.50
1:A:1784:A:H4'	1:A:1785:A:O5'	2.12	0.50
1:A:2111:C:H42	1:A:2147:G:H22	1.59	0.50
1:A:90:U:O2'	1:A:92:A:C8	2.65	0.50
8:I:101:LEU:HD23	8:I:105:HIS:HB2	1.94	0.50
1:A:2386:C:H2'	1:A:2387:U:C6	2.47	0.50
2:B:24:G:H4'	2:B:25:A:C8	2.47	0.50
1:A:652(D):C:H2'	1:A:652(E):G:O4'	2.11	0.50
1:A:2316:C:H2'	1:A:2317:C:C6	2.46	0.50
1:A:2317:C:C4	1:A:2318:G:N7	2.80	0.50
1:A:1429:G:H2'	1:A:1430:C:H6	1.77	0.49
1:A:2128:C:N4	1:A:2160:G:H1	2.09	0.49
3:D:180:GLY:HA3	3:D:275:LYS:HD3	1.94	0.49
1:A:443:A:H1'	1:A:1201:C:O4'	2.12	0.49
26:4:36:CYS:SG	26:4:38:LYS:O	2.70	0.49
1:A:870:A:C2	1:A:908:C:C2	2.99	0.49
5:F:6:VAL:HG22	5:F:23:ASP:H	1.76	0.49
1:A:1932:A:H2'	1:A:1933:G:O4'	2.11	0.49
21:Z:144:LEU:HD12	21:Z:148:ASP:HB3	1.94	0.49
7:H:139:GLN:HG3	7:H:140:LYS:N	2.27	0.49
17:V:5:VAL:HG11	17:V:57:VAL:HG21	1.94	0.49
1:A:1545:A:H2'	1:A:1546:C:O4'	2.12	0.49
1:A:207:A:H2'	1:A:208:C:O4'	2.13	0.49
1:A:2820:A:OP1	13:R:4:LEU:HD23	2.12	0.49
4:E:111:ARG:HA	13:R:1:MET:SD	2.53	0.49
1:A:2125:G:H21	1:A:2126:A:H62	1.60	0.49
3:D:238:GLY:N	34:D:405:HOH:O	2.45	0.49
2:B:11:C:H3'	2:B:12:C:H6	1.77	0.49
17:V:52:VAL:HG22	17:V:55:ALA:HB3	1.94	0.49
15:T:30:VAL:HG22	15:T:86:ILE:HG12	1.93	0.49
9:N:20:GLY:HA2	9:N:61:ARG:HD3	1.95	0.49
1:A:674:G:H1'	5:F:74:ARG:HD3	1.93	0.49
1:A:2251:G:H5'	34:A:4109:HOH:O	2.11	0.49
1:A:2205:C:O2	1:A:2220:G:C2	2.65	0.49
6:G:125:PHE:HB3	6:G:166:ASP:OD2	2.13	0.49
1:A:781:A:H2	1:A:1776:G:N3	2.11	0.49
1:A:2690:C:OP2	1:A:2690:C:H6	1.94	0.49
1:A:586:A:N1	1:A:809:G:O2'	2.41	0.49
1:A:2320:A:N3	1:A:2320:A:H2'	2.28	0.49
1:A:1580:A:H8	1:A:1580:A:OP2	1.94	0.49
1:A:2286:A:H4'	1:A:2287:A:O4'	2.12	0.49
25:3:8:LEU:HD13	25:3:31:LEU:CD2	2.43	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1815:A:OP2	3:D:54:ARG:NH2	2.46	0.49
29:7:34:ARG:NH1	29:7:41:ARG:O	2.45	0.49
1:A:2304:G:O6	1:A:2312:U:O4	2.30	0.49
11:P:121:LYS:HD3	11:P:123:LEU:HD11	1.93	0.49
18:W:83:LYS:O	18:W:84:ARG:HD3	2.11	0.49
1:A:1803:A:H4'	3:D:259:THR:HG23	1.94	0.49
1:A:1287:A:H5''	1:A:1288:U:OP2	2.13	0.49
1:A:1268:A:C2	1:A:2013:A:C4	3.00	0.49
1:A:362:U:O2'	1:A:363:G:H5''	2.12	0.49
1:A:35:G:H2'	1:A:36:G:O4'	2.12	0.49
1:A:198:C:H2'	34:A:3752:HOH:O	2.13	0.49
9:N:33:LEU:HD12	9:N:38:HIS:CE1	2.47	0.49
1:A:2321:G:H5''	1:A:2322:A:OP2	2.13	0.49
2:B:49:C:H2'	2:B:50:G:C8	2.47	0.49
1:A:1143:A:OP1	9:N:25:ARG:NH2	2.45	0.49
13:R:56:LYS:NZ	13:R:90:ARG:O	2.45	0.49
10:O:19:ILE:HG22	10:O:43:VAL:HG22	1.93	0.49
1:A:1604:C:OP2	34:A:3797:HOH:O	2.20	0.49
34:A:4966:HOH:O	3:D:61:LEU:HD21	2.12	0.49
1:A:616:G:H5'	5:F:205:ARG:HD2	1.95	0.49
2:B:23:G:O6	34:B:321:HOH:O	2.19	0.49
1:A:375:C:H2'	1:A:376:C:C6	2.48	0.49
1:A:330:A:O2'	1:A:331:A:H8	1.96	0.49
1:A:234:C:H2'	1:A:235:U:C6	2.48	0.49
1:A:1816:G:H8	3:D:62:TYR:CZ	2.31	0.49
30:8:33:ASN:O	30:8:34:TRP:O	2.30	0.49
1:A:90:U:HO2'	1:A:92:A:H8	1.59	0.49
1:A:2133:G:C2	1:A:2157:G:H2'	2.47	0.49
1:A:1300:U:H4'	1:A:1301:A:C5'	2.43	0.49
1:A:484:C:H2'	1:A:485:C:H6	1.78	0.49
8:I:85:GLU:HG3	8:I:86:THR:H	1.78	0.49
1:A:2404:C:O3'	11:P:77:ARG:NH2	2.46	0.49
1:A:587:C:P	11:P:21:ARG:HH22	2.36	0.48
1:A:1607:C:H4'	1:A:1608:A:O5'	2.13	0.48
13:R:97:VAL:HG22	13:R:114:VAL:HG13	1.94	0.48
1:A:562:U:C4	1:A:2036:C:O4'	2.66	0.48
12:Q:5:ARG:O	21:Z:194:PRO:HD2	2.12	0.48
1:A:1889:A:H2'	1:A:1890:A:C8	2.48	0.48
1:A:1159:U:O2'	1:A:1160:G:H5'	2.12	0.48
4:E:59:VAL:O	4:E:64:LYS:HE3	2.13	0.48
10:O:23:ARG:HG3	10:O:24:VAL:N	2.27	0.48
1:A:2336:A:H61	22:O:43:THR:HG22	1.78	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:517:C:OP1	27:5:16:ARG:NH2	2.45	0.48
1:A:1268:A:H2'	1:A:1269:A:O4'	2.13	0.48
1:A:2576:G:H1'	34:A:3837:HOH:O	2.13	0.48
2:B:27:C:C4	2:B:28:C:C4	3.00	0.48
8:I:9:LEU:HD21	8:I:35:LEU:HD13	1.96	0.48
1:A:2173:A:H2'	1:A:2174:C:H5'	1.95	0.48
7:H:41:MET:HE3	7:H:54:ARG:HA	1.96	0.48
1:A:1165:U:H2'	1:A:1166:C:C6	2.48	0.48
15:T:28:VAL:HG13	15:T:86:ILE:HG23	1.96	0.48
5:F:29:ASN:H	5:F:112:MET:CE	2.27	0.48
9:N:4:TYR:CD2	16:U:100:VAL:HG11	2.49	0.48
1:A:1587:A:H2'	1:A:1588:C:C6	2.49	0.48
1:A:2364:C:H2'	1:A:2365:G:O4'	2.12	0.48
1:A:774:A:HO2'	1:A:775:G:H8	1.60	0.48
1:A:1581:G:H2'	1:A:1582:C:O4'	2.12	0.48
1:A:236:C:H2'	1:A:237:C:C6	2.48	0.48
1:A:996:A:H4'	16:U:91:ASP:OD1	2.14	0.48
1:A:2138:C:H2'	1:A:2139:C:C6	2.49	0.48
1:A:1113:U:H2'	1:A:1114:G:C8	2.48	0.48
1:A:2836:U:H2'	1:A:2837:G:C8	2.48	0.48
1:A:2101:G:H2'	1:A:2102:U:O4'	2.13	0.48
1:A:866:A:O2'	1:A:867:C:H5'	2.13	0.48
12:Q:42:ILE:HD13	12:Q:97:VAL:HG21	1.95	0.48
2:B:33:G:H5'	6:G:2:PRO:HD3	1.95	0.48
5:F:150:GLY:HA2	5:F:172:TRP:CD2	2.48	0.48
1:A:1218:C:H5''	1:A:1218:C:H6	1.79	0.48
1:A:2052:G:H4'	4:E:143:ASN:O	2.13	0.48
1:A:2377:A:H2'	1:A:2378:A:C8	2.48	0.48
1:A:446:G:OP1	16:U:3:ARG:NH1	2.47	0.48
1:A:2869:G:H2'	1:A:2870:C:O4'	2.13	0.48
15:T:51:ARG:HG3	15:T:98:LYS:HE3	1.94	0.48
10:O:101:PRO:HG3	15:T:67:SER:OG	2.12	0.48
6:G:43:LEU:HB2	6:G:89:GLY:HA2	1.94	0.48
16:U:76:TYR:HH	16:U:92:ARG:NH1	2.11	0.48
2:B:6:C:C2'	2:B:7:G:H5''	2.40	0.48
22:O:10:THR:HG22	22:O:12:ASN:N	2.27	0.48
8:I:77:LEU:CB	8:I:142:VAL:HG12	2.43	0.48
1:A:2104:G:N7	1:A:2186:G:N2	2.62	0.48
7:H:67:LEU:O	7:H:71:LEU:HB2	2.13	0.48
1:A:226:G:H21	1:A:228:A:H62	1.61	0.48
14:S:83:LYS:HB3	14:S:84:GLN:O	2.14	0.48
1:A:300:A:P	20:Y:86:ARG:NH2	2.86	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
28:6:21:TYR:CE2	28:6:38:LYS:HG2	2.49	0.48
1:A:847:U:H5	1:A:933:A:H62	1.59	0.48
13:R:12:ARG:HG2	13:R:16:HIS:ND1	2.29	0.48
1:A:664:C:H4'	1:A:941:A:OP1	2.14	0.48
1:A:2147:G:H2'	1:A:2148:G:O4'	2.14	0.47
21:Z:45:ASP:O	21:Z:49:ARG:HG3	2.13	0.47
1:A:2526:G:H5'	1:A:2742:C:O2'	2.14	0.47
1:A:478:A:N1	1:A:500:G:H4'	2.29	0.47
1:A:482:A:OP2	1:A:507:A:N6	2.46	0.47
2:B:45:A:O4'	6:G:95:ARG:NH1	2.47	0.47
1:A:11:G:C2'	1:A:12:U:H5'	2.43	0.47
1:A:1028:A:N6	1:A:1125:G:H2'	2.29	0.47
22:0:72:ARG:HB2	22:0:75:LEU:HB2	1.96	0.47
1:A:1376:C:OP2	34:A:4019:HOH:O	2.20	0.47
1:A:2315:G:C6	1:A:2316:C:C4	3.02	0.47
1:A:89:G:H3'	1:A:90:U:H5''	1.97	0.47
2:B:105:A:OP1	21:Z:72:ARG:NH1	2.46	0.47
21:Z:150:LEU:O	21:Z:171:ILE:HG13	2.14	0.47
7:H:28:GLY:HA3	7:H:79:VAL:HB	1.95	0.47
7:H:17:VAL:HG21	7:H:50:VAL:HG21	1.97	0.47
14:S:11:LYS:HG3	14:S:91:PRO:HD3	1.97	0.47
1:A:1588:C:H2'	1:A:1589:C:C6	2.50	0.47
10:O:88:ASN:HD21	10:O:90:GLN:HB2	1.79	0.47
3:D:69:ARG:NH2	3:D:128:GLY:O	2.40	0.47
2:B:116:G:OP2	2:B:116:G:H8	1.97	0.47
1:A:620:G:H5'	1:A:620:G:N3	2.29	0.47
1:A:1506:C:C2'	1:A:1507:A:H5'	2.40	0.47
1:A:2134:A:H62	1:A:2157:G:H5'	1.79	0.47
7:H:11:VAL:HG21	7:H:50:VAL:HG23	1.96	0.47
6:G:96:ARG:O	6:G:99:MET:HB3	2.14	0.47
1:A:720:C:H2'	1:A:721:C:C6	2.49	0.47
1:A:2031:A:C6	1:A:2498:C:H1'	2.49	0.47
1:A:2076:U:O5'	1:A:2076:U:H6	1.97	0.47
1:A:886:C:H5''	34:A:5034:HOH:O	2.14	0.47
8:I:40:THR:O	8:I:44:LEU:N	2.48	0.47
4:E:28:ALA:HB3	4:E:93:VAL:CG1	2.45	0.47
1:A:883:G:H1	1:A:893:C:H42	1.63	0.47
4:E:5:LEU:HD11	4:E:79:ARG:HB2	1.96	0.47
1:A:2317:C:C2	1:A:2318:G:N7	2.83	0.47
8:I:72:LEU:HA	8:I:75:LEU:HD13	1.96	0.47
1:A:1494:A:C6	1:A:1495:A:C6	3.03	0.47
4:E:75:VAL:HG13	4:E:77:ILE:H	1.79	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
21:Z:125:LEU:HB3	21:Z:165:VAL:HG12	1.97	0.47
25:3:36:VAL:HG23	34:3:101:HOH:O	2.15	0.47
10:O:43:VAL:HG12	10:O:54:GLU:HA	1.95	0.47
1:A:1588:C:H2'	1:A:1589:C:H6	1.79	0.47
1:A:1274:A:N3	1:A:1297:C:H1'	2.30	0.47
1:A:1278:A:OP1	13:R:36:THR:HG23	2.13	0.47
1:A:2885:C:O2'	27:5:34:PRO:HG3	2.15	0.47
1:A:747:U:O2	1:A:2014:A:H1'	2.14	0.47
1:A:892:G:O5'	1:A:892:G:H8	1.98	0.47
1:A:9:U:O2'	1:A:10:G:OP1	2.32	0.47
1:A:284:U:H2'	1:A:285:C:C6	2.50	0.47
1:A:2317:C:N3	1:A:2318:G:N7	2.63	0.47
3:D:68:LYS:O	3:D:69:ARG:HB2	2.15	0.47
1:A:1297:C:OP1	1:A:2710:C:H4'	2.15	0.47
1:A:704:G:O2'	1:A:726:G:N2	2.35	0.47
1:A:438:G:H2'	1:A:440:G:C8	2.50	0.47
1:A:263:C:H2'	1:A:264:C:O4'	2.14	0.47
1:A:2017:U:OP1	34:A:3913:HOH:O	2.20	0.47
1:A:1593:G:H2'	1:A:1594:G:C8	2.50	0.47
8:I:29:TYR:O	8:I:32:PRO:HD2	2.15	0.47
3:D:101:GLU:OE1	3:D:103:ARG:HD3	2.15	0.47
1:A:2648:C:H2'	1:A:2649:U:H6	1.79	0.47
1:A:647:G:O5'	1:A:647:G:H8	1.98	0.47
25:3:12:PRO:O	25:3:15:TYR:HB2	2.15	0.47
1:A:1417:C:H2'	1:A:1418:G:O4'	2.14	0.47
31:9:32:HIS:O	31:9:34:GLN:HG3	2.14	0.47
1:A:2136:C:C4	1:A:2137:C:H5	2.33	0.47
1:A:2349:G:H3'	1:A:2350:C:H5''	1.96	0.47
8:I:101:LEU:O	8:I:106:GLY:N	2.44	0.47
1:A:271(N):U:O2'	1:A:271(O):C:H5'	2.15	0.47
3:D:25:THR:HG21	3:D:113:VAL:HG11	1.96	0.47
30:8:4:MET:HE3	30:8:63:PRO:HG3	1.97	0.47
1:A:546:C:H6	1:A:548:A:OP1	1.98	0.47
1:A:740:U:H2'	1:A:741:G:C8	2.50	0.47
6:G:28:VAL:O	6:G:31:VAL:HG13	2.15	0.46
1:A:811:U:O2'	11:P:21:ARG:HG3	2.14	0.46
14:S:105:ALA:O	14:S:110:LEU:HB2	2.15	0.46
1:A:271(P):C:H4'	8:I:42:SER:O	2.15	0.46
1:A:141:A:H8	1:A:1408:C:O2'	1.95	0.46
7:H:13:LYS:HA	7:H:14:GLY:HA2	1.63	0.46
17:V:65:GLY:HA3	17:V:91:TYR:CZ	2.50	0.46
1:A:2554:U:H2'	1:A:2555:U:C6	2.49	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:857:C:OP2	22:O:77:ARG:NH2	2.48	0.46
8:I:79:ILE:HA	8:I:80:PRO:HD3	1.59	0.46
14:S:59:LYS:HE2	14:S:60:GLY:HA2	1.96	0.46
1:A:904:C:H2'	1:A:905:U:C6	2.50	0.46
1:A:623:G:H2'	1:A:624:C:C6	2.50	0.46
6:G:173:LEU:O	6:G:178:PHE:HB2	2.15	0.46
1:A:1939:U:OP1	1:A:2604:U:O2'	2.30	0.46
21:Z:110:GLY:HA3	21:Z:174:VAL:HG11	1.97	0.46
31:9:17:ILE:HA	31:9:17:ILE:HD12	1.78	0.46
17:V:49:THR:HG22	17:V:49:THR:O	2.16	0.46
10:O:98:VAL:HG22	10:O:118:ALA:HA	1.98	0.46
1:A:298:G:H5''	1:A:299:A:OP1	2.16	0.46
5:F:21:ALA:O	5:F:22:ALA:CB	2.63	0.46
1:A:2682:U:O2'	15:T:58:ASN:ND2	2.47	0.46
1:A:455:C:N3	1:A:473:G:H5'	2.30	0.46
3:D:24:ILE:HD13	3:D:84:TYR:HB2	1.97	0.46
1:A:65:C:H2'	1:A:66:C:H6	1.80	0.46
1:A:2115:G:H21	1:A:2171:A:N6	2.11	0.46
1:A:143:G:H4'	19:X:35:THR:HG21	1.97	0.46
1:A:271(P):C:OP1	8:I:45:LYS:HD2	2.15	0.46
1:A:1503:U:H2'	1:A:1504:C:H6	1.77	0.46
5:F:108:LYS:O	5:F:112:MET:HG3	2.15	0.46
1:A:2836:U:C4	1:A:2883:A:N6	2.83	0.46
30:8:61:LEU:C	30:8:63:PRO:HD3	2.35	0.46
1:A:1221(A):C:C2	1:A:1229:G:C2	3.04	0.46
1:A:1243:G:O2'	11:P:7:ARG:NH2	2.48	0.46
3:D:145:VAL:HG12	3:D:146:GLU:O	2.15	0.46
4:E:173:VAL:CG2	4:E:185:LYS:HB2	2.44	0.46
1:A:958:U:H5''	12:Q:14:ARG:HD3	1.97	0.46
1:A:171:G:H2'	1:A:172:C:C6	2.51	0.46
1:A:2469:A:H5''	1:A:2470:G:OP2	2.16	0.46
1:A:1486:A:H2'	1:A:1487:G:C8	2.48	0.46
1:A:848:G:H2'	1:A:849:A:C8	2.50	0.46
1:A:1278:A:OP1	13:R:36:THR:CG2	2.64	0.46
1:A:452:G:OP2	34:A:4152:HOH:O	2.20	0.46
19:X:72:LYS:HE3	19:X:73:ARG:O	2.14	0.46
6:G:41:GLN:HE22	6:G:153:ARG:HB3	1.79	0.46
14:S:101:LEU:O	14:S:102:ALA:HB3	2.15	0.46
13:R:67:LEU:HD13	13:R:76:VAL:HG21	1.98	0.46
1:A:1006:C:C2	1:A:1138:G:N2	2.84	0.46
1:A:848:G:N9	1:A:933:A:H8	2.14	0.46
1:A:1321:A:H2'	1:A:1322:A:O4'	2.16	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1149:G:H2'	1:A:1150:C:C6	2.50	0.46
1:A:2557:G:H2'	1:A:2558:C:C6	2.51	0.46
1:A:1021:A:H8	1:A:1022:G:H5''	1.79	0.46
8:I:77:LEU:HB3	8:I:142:VAL:HG12	1.98	0.46
1:A:2687:U:OP2	34:A:4438:HOH:O	2.20	0.46
1:A:1540:U:H2'	1:A:1541:G:O4'	2.15	0.46
1:A:856:C:HO2'	1:A:857:C:P	2.39	0.46
1:A:322:A:OP1	5:F:168:ARG:HD2	2.16	0.46
1:A:708:C:H5'	1:A:709:U:OP2	2.16	0.46
7:H:40:GLU:OE1	7:H:60:ARG:NH1	2.47	0.46
1:A:81:G:HO2'	1:A:295:G:HO2'	1.63	0.46
15:T:18:ASP:N	15:T:18:ASP:OD1	2.45	0.46
21:Z:121:HIS:HB3	21:Z:123:ASP:O	2.16	0.46
1:A:2295:C:O2'	1:A:2296:U:H5'	2.16	0.46
8:I:72:LEU:C	8:I:74:ASN:H	2.19	0.46
1:A:1352:U:P	34:A:4022:HOH:O	2.73	0.46
1:A:1495:A:H2'	1:A:1496:A:H8	1.81	0.46
1:A:2134:A:N3	1:A:2159:G:O2'	2.41	0.46
3:D:3:VAL:O	3:D:3:VAL:HG12	2.15	0.46
1:A:185:U:H2'	1:A:186:G:C8	2.51	0.46
1:A:2693:A:H2'	1:A:2694:G:C8	2.49	0.46
10:O:115:VAL:HG13	10:O:121:VAL:HG21	1.96	0.46
1:A:864:G:C6	1:A:865:C:N4	2.84	0.46
2:B:61:G:C2	2:B:62:C:C2	3.04	0.46
1:A:2430:A:N3	1:A:2430:A:H2'	2.30	0.46
1:A:2297:C:H1'	1:A:2322:A:C2	2.50	0.46
1:A:307:G:H21	1:A:330:A:H62	1.62	0.46
1:A:1914:C:H2'	1:A:1915:U:H6	1.79	0.46
3:D:12:SER:HB3	3:D:208:LYS:HB3	1.98	0.46
12:Q:27:VAL:O	12:Q:67:ARG:NH1	2.49	0.46
1:A:2581:G:H4'	1:A:2582:G:C8	2.51	0.46
1:A:1009:A:O4'	16:U:59:ARG:HG2	2.16	0.46
9:N:1:MET:O	9:N:2:LYS:HB2	2.16	0.46
1:A:1027:A:C6	1:A:1126:A:C4	3.04	0.46
1:A:2549:G:C8	1:A:2549:G:H5''	2.51	0.46
1:A:1315:C:OP2	34:A:3795:HOH:O	2.20	0.46
1:A:1488:G:H5''	1:A:1488:G:C8	2.51	0.46
21:Z:144:LEU:HD21	21:Z:150:LEU:HG	1.98	0.46
5:F:150:GLY:HA2	5:F:172:TRP:CE3	2.51	0.46
1:A:2555:U:H5''	1:A:2556:C:OP2	2.16	0.46
1:A:2661:G:H2'	1:A:2662:A:C8	2.51	0.46
4:E:128:SER:OG	4:E:129:HIS:N	2.49	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1378:A:OP1	29:7:10:ARG:NH2	2.49	0.46
6:G:43:LEU:HA	6:G:43:LEU:HD12	1.82	0.45
1:A:1003:G:N2	1:A:1153:C:C2	2.84	0.45
1:A:1327:C:P	34:A:4831:HOH:O	2.74	0.45
5:F:129:PHE:HB2	5:F:132:VAL:HG22	1.98	0.45
1:A:2110:G:OP1	1:A:2118:U:N3	2.47	0.45
1:A:2549:G:H8	1:A:2549:G:H5''	1.81	0.45
21:Z:19:ARG:NH1	21:Z:84:GLU:O	2.49	0.45
7:H:84:SER:HA	7:H:133:VAL:O	2.16	0.45
4:E:101:ARG:CZ	4:E:171:GLU:HB2	2.46	0.45
6:G:23:PHE:HB2	6:G:25:TYR:CZ	2.51	0.45
5:F:179:GLU:CD	5:F:179:GLU:H	2.19	0.45
1:A:2319:G:N1	14:S:3:ARG:HA	2.31	0.45
14:S:35:ILE:HD13	14:S:101:LEU:HD12	1.97	0.45
1:A:1166:C:H2'	1:A:1167:U:H6	1.81	0.45
1:A:855:G:H2'	1:A:856:C:C6	2.51	0.45
1:A:986:C:O2'	1:A:987:G:H5'	2.16	0.45
19:X:41:ASN:O	19:X:45:THR:HG23	2.16	0.45
8:I:97:ILE:O	8:I:100:ALA:HB3	2.16	0.45
8:I:140:LEU:HA	8:I:140:LEU:HD23	1.70	0.45
29:7:1:MET:HB2	29:7:1:MET:HE2	1.90	0.45
10:O:113:LYS:H	10:O:113:LYS:HG2	1.43	0.45
1:A:1647:G:H3'	1:A:1647:G:P	2.56	0.45
12:Q:134:ARG:O	12:Q:138:ASP:HB2	2.16	0.45
4:E:143:ASN:HB2	4:E:147:PRO:HD2	1.98	0.45
18:W:65:LEU:HD12	18:W:68:ARG:HE	1.79	0.45
1:A:634:C:H2'	1:A:635:C:C6	2.51	0.45
1:A:64:A:O3'	19:X:71:GLY:HA3	2.16	0.45
1:A:71:A:N7	19:X:31:HIS:HE1	2.14	0.45
1:A:2745:C:C4	1:A:2746:U:C4	3.04	0.45
2:B:37:C:C5	2:B:38:C:C4	3.05	0.45
1:A:2793:G:H2'	1:A:2794:C:O4'	2.17	0.45
1:A:2793:G:N2	1:A:2804:C:H1'	2.31	0.45
1:A:118:A:N3	1:A:178:G:H1'	2.31	0.45
1:A:2713:A:H2'	1:A:2713:A:N3	2.31	0.45
5:F:129:PHE:CE2	5:F:163:VAL:HG11	2.52	0.45
15:T:23:ARG:HG3	15:T:120:ARG:NH1	2.32	0.45
1:A:646:A:H2'	1:A:647:G:O4'	2.17	0.45
7:H:149:ARG:NH1	7:H:167:GLU:OE1	2.49	0.45
1:A:1455:G:P	34:A:4904:HOH:O	2.74	0.45
3:D:10:THR:OG1	3:D:13:ARG:HB2	2.16	0.45
21:Z:76:LEU:HD12	21:Z:76:LEU:HA	1.81	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1204:A:N6	1:A:1240:U:H2'	2.30	0.45
1:A:2312:U:H5'	6:G:88:ILE:HD11	1.99	0.45
1:A:2208:A:H1'	1:A:2219:G:C5	2.50	0.45
1:A:2327:A:H2'	1:A:2328:A:H8	1.81	0.45
1:A:475:U:C4	1:A:481:G:O6	2.69	0.45
15:T:2:ASN:O	15:T:6:LEU:HD22	2.17	0.45
1:A:1899:G:H2'	1:A:1899:G:N3	2.31	0.45
22:O:14:ARG:HH11	22:O:14:ARG:HB2	1.82	0.45
14:S:74:ALA:HA	14:S:110:LEU:HD22	1.99	0.45
1:A:2134:A:C2	1:A:2159:G:H4'	2.51	0.45
4:E:52:LEU:O	4:E:76:ARG:N	2.38	0.45
24:2:51:ARG:O	24:2:55:ARG:HD2	2.17	0.45
8:I:4:ILE:HD11	8:I:44:LEU:CD1	2.47	0.45
1:A:1721:G:H5'	1:A:1722:A:OP2	2.16	0.45
1:A:459:U:OP2	1:A:469:G:N1	2.39	0.45
9:N:108:PRO:O	9:N:113:GLY:HA3	2.16	0.45
21:Z:91:LEU:HA	21:Z:91:LEU:HD12	1.75	0.45
1:A:1239:G:H2'	1:A:1240:U:O4'	2.17	0.45
23:1:21:ARG:CG	23:1:21:ARG:HH11	2.18	0.45
6:G:43:LEU:HB3	6:G:44:GLY:H	1.54	0.45
1:A:1507:A:O2'	1:A:1508:A:C8	2.70	0.45
21:Z:141:VAL:O	21:Z:144:LEU:HB2	2.17	0.45
1:A:2336:A:H61	22:O:43:THR:CG2	2.30	0.45
8:I:127:VAL:HA	8:I:140:LEU:O	2.17	0.45
21:Z:5:LEU:O	21:Z:59:LEU:HA	2.17	0.45
1:A:1530:C:O2'	1:A:1531:C:P	2.75	0.45
8:I:120:ILE:HG21	8:I:126:TYR:CE1	2.52	0.45
1:A:919:G:N2	1:A:2269:A:OP2	2.48	0.45
1:A:2815:C:H5'	27:5:29:THR:HG21	1.99	0.45
1:A:2854:G:H2'	1:A:2855:C:C6	2.52	0.45
13:R:109:ALA:HA	13:R:110:PRO:HD2	1.83	0.45
1:A:1292:U:H2'	1:A:1293:C:C6	2.52	0.45
4:E:51:PHE:CD1	4:E:52:LEU:HD22	2.52	0.45
3:D:71:ASP:CB	3:D:103:ARG:HH22	2.29	0.45
1:A:2294:C:P	14:S:89:ARG:HH22	2.39	0.45
1:A:1124:C:H1'	31:9:36:GLN:NE2	2.32	0.45
1:A:13:A:N1	1:A:525:U:H2'	2.31	0.45
1:A:1270:C:H5''	1:A:1271:G:O5'	2.17	0.45
1:A:185:U:H4'	1:A:218:A:H4'	1.99	0.44
1:A:2391:G:O6	1:A:2425:A:H8	2.00	0.44
1:A:789:A:N1	34:A:4262:HOH:O	2.36	0.44
14:S:39:ILE:HD12	14:S:85:VAL:HG21	1.98	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1549:C:H2'	1:A:1550:C:C6	2.52	0.44
14:S:97:ARG:O	14:S:100:ALA:HB3	2.18	0.44
5:F:47:GLY:HA3	5:F:95:ARG:O	2.17	0.44
1:A:181:A:H1'	1:A:435:C:H5'	1.98	0.44
2:B:13:A:C2	2:B:16:G:H1'	2.51	0.44
1:A:887:A:H1'	1:A:889:C:OP2	2.16	0.44
1:A:526:A:H5''	1:A:527:C:OP1	2.17	0.44
14:S:101:LEU:HD23	14:S:102:ALA:H	1.82	0.44
1:A:1379:A:O5'	1:A:1379:A:H8	2.00	0.44
1:A:2778:A:O2'	1:A:2781:A:H5'	2.17	0.44
1:A:2564:A:C2	1:A:2647:U:H4'	2.52	0.44
27:5:11:THR:HG23	27:5:15:ARG:HB3	1.98	0.44
1:A:1185:C:H5''	1:A:1186:G:OP1	2.17	0.44
1:A:1783:A:H5'	1:A:2608:G:H4'	1.98	0.44
23:1:82:LEU:HA	23:1:85:LEU:CD2	2.42	0.44
1:A:242:G:C8	30:8:5:LYS:HG2	2.52	0.44
1:A:2134:A:N6	1:A:2157:G:H5'	2.32	0.44
1:A:330:A:O2'	1:A:331:A:C8	2.69	0.44
12:Q:16:ARG:O	12:Q:17:LEU:HD23	2.17	0.44
1:A:2534:A:H3'	1:A:2535:G:H5''	2.00	0.44
8:I:83:ALA:HB1	8:I:87:LYS:O	2.17	0.44
23:1:51:VAL:HG11	23:1:74:VAL:HG21	1.99	0.44
12:Q:57:HIS:NE2	12:Q:116:GLU:HB3	2.33	0.44
9:N:18:ALA:O	9:N:19:GLU:HB3	2.17	0.44
11:P:6:LEU:HD23	11:P:6:LEU:HA	1.87	0.44
1:A:2122:U:H2'	1:A:2123:G:C8	2.50	0.44
1:A:2172:U:H4'	1:A:2173:A:OP2	2.17	0.44
1:A:830:G:H4'	1:A:831:G:OP2	2.17	0.44
6:G:3:LEU:HG	6:G:3:LEU:H	1.67	0.44
1:A:864:G:N2	1:A:913:U:C2	2.85	0.44
1:A:769:G:O2'	1:A:770:G:H5'	2.17	0.44
1:A:2670:A:O2'	1:A:2671:A:H5'	2.17	0.44
13:R:70:LEU:HA	13:R:70:LEU:HD23	1.57	0.44
1:A:1745(A):C:H5'	1:A:1746:G:OP2	2.17	0.44
17:V:29:PRO:HA	17:V:61:VAL:HG22	2.00	0.44
6:G:66:GLN:HE21	6:G:66:GLN:HB3	1.67	0.44
10:O:63:VAL:HG12	10:O:106:LEU:HD11	1.98	0.44
20:Y:23:ARG:HH11	20:Y:23:ARG:HB2	1.82	0.44
1:A:1022:G:N7	9:N:66:LYS:HE2	2.33	0.44
9:N:24:GLY:HA2	9:N:27:ALA:CB	2.48	0.44
15:T:119:LYS:O	15:T:123:GLN:HG2	2.18	0.44
1:A:2009:G:OP1	18:W:41:LYS:HE2	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:720:C:H2'	1:A:721:C:H6	1.82	0.44
1:A:320:A:H4'	1:A:322:A:N7	2.33	0.44
11:P:1:MET:HE3	11:P:5:ASP:HB2	2.00	0.44
24:2:65:ASN:OD1	24:2:69:ARG:NH1	2.51	0.44
1:A:1866:C:H2'	1:A:1876:A:O4'	2.17	0.44
1:A:2483:C:N3	12:Q:124:LYS:NZ	2.62	0.44
3:D:134:ARG:HD3	3:D:135:PHE:CZ	2.51	0.44
1:A:1559:G:OP2	34:A:4884:HOH:O	2.20	0.44
1:A:493:G:H2'	1:A:494:G:O4'	2.18	0.44
21:Z:178:GLU:HA	21:Z:178:GLU:OE2	2.18	0.44
1:A:2137:C:C2	1:A:2154:G:N2	2.85	0.44
15:T:16:ARG:HB2	15:T:79:HIS:ND1	2.32	0.44
1:A:831:G:O2'	11:P:38:GLN:HG2	2.18	0.44
1:A:2198:A:O2'	1:A:2224:G:N2	2.50	0.44
21:Z:138:GLU:H	21:Z:156:LYS:HZ1	1.65	0.44
1:A:1005:C:H2'	1:A:1006:C:C6	2.52	0.44
1:A:2630:G:H2'	1:A:2631:G:O4'	2.18	0.44
1:A:1263:U:C4	1:A:1264:G:C6	3.05	0.44
22:0:56:ASP:CG	22:0:58:THR:HG1	2.21	0.44
24:2:21:LEU:HD23	24:2:21:LEU:HA	1.86	0.44
1:A:2374:C:H3'	34:A:5002:HOH:O	2.18	0.44
1:A:328:U:H4'	20:Y:68:HIS:CG	2.52	0.44
8:I:62:LYS:HG2	8:I:133:HIS:NE2	2.33	0.44
1:A:2267:A:H2'	34:A:4671:HOH:O	2.17	0.44
23:1:58:ILE:HD11	23:1:91:LYS:HG3	1.99	0.44
1:A:637:A:H8	11:P:117:GLU:HG3	1.82	0.44
6:G:6:ALA:HB3	6:G:104:GLU:OE1	2.17	0.44
6:G:64:THR:HB	6:G:94:LEU:HD21	2.00	0.44
1:A:29:U:H6	1:A:29:U:O5'	2.00	0.44
11:P:138:LEU:HA	11:P:138:LEU:HD12	1.85	0.44
2:B:32:C:C2	2:B:51:G:N2	2.86	0.44
1:A:2420:C:OP2	30:8:33:ASN:HB2	2.17	0.44
1:A:530:G:C5	1:A:2022:U:H5''	2.53	0.44
1:A:804:A:H5''	1:A:805:G:OP1	2.18	0.44
15:T:37:GLY:HA2	15:T:38:ASN:HA	1.55	0.44
14:S:61:ASN:O	14:S:65:VAL:HG23	2.18	0.44
1:A:783:A:H2'	1:A:783:A:N3	2.32	0.44
1:A:1482:G:C6	1:A:1507:A:C6	3.05	0.43
1:A:1021:A:H62	1:A:1141:U:H3	1.66	0.43
28:6:11:LEU:HD23	28:6:11:LEU:HA	1.74	0.43
13:R:67:LEU:HD13	13:R:67:LEU:HA	1.73	0.43
1:A:185:U:H2'	1:A:186:G:H8	1.83	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:481:G:C4	1:A:507:A:C2	3.06	0.43
1:A:1518:U:OP2	34:A:4330:HOH:O	2.21	0.43
28:6:25:LYS:HE3	28:6:30:THR:O	2.17	0.43
1:A:2064:C:H2'	1:A:2065:C:C6	2.53	0.43
12:Q:1:MET:HG2	12:Q:2:LEU:H	1.83	0.43
1:A:245:G:O5'	11:P:73:GLY:HA2	2.18	0.43
1:A:813:U:H2'	1:A:814:C:C6	2.53	0.43
1:A:465:G:C6	1:A:466:A:N6	2.86	0.43
1:A:2279:G:O6	22:0:14:ARG:HD2	2.18	0.43
1:A:325:G:O2'	1:A:326:G:H5'	2.18	0.43
1:A:927:G:H2'	1:A:928:G:O4'	2.18	0.43
1:A:11:G:H2'	1:A:12:U:C5'	2.48	0.43
1:A:2602:A:H1'	1:A:2603:G:H5''	1.99	0.43
1:A:2125:G:H22	1:A:2172:U:H5''	1.82	0.43
14:S:26:LEU:HD22	14:S:87:PHE:CE1	2.53	0.43
24:2:35:LEU:HD12	24:2:53:LEU:HD12	2.00	0.43
21:Z:93:ASP:HB2	21:Z:131:ARG:HH22	1.83	0.43
6:G:148:MET:O	6:G:149:VAL:HB	2.17	0.43
1:A:2298:A:H2'	1:A:2299:G:O4'	2.19	0.43
1:A:2300:G:C6	1:A:2301:C:C4	3.06	0.43
1:A:1840:G:C6	1:A:1841:U:C4	3.06	0.43
20:Y:98:VAL:HG12	20:Y:105:ALA:HA	1.99	0.43
1:A:2152:G:H2'	1:A:2153:G:H8	1.82	0.43
1:A:65:C:H2'	1:A:66:C:C6	2.53	0.43
1:A:2308:G:O2'	1:A:2310:A:N7	2.51	0.43
15:T:56:GLY:O	15:T:59:THR:HG23	2.18	0.43
2:B:48:A:H4'	14:S:95:HIS:CD2	2.39	0.43
1:A:2115:G:H21	1:A:2171:A:H61	1.66	0.43
1:A:184:C:H2'	1:A:185:U:C6	2.53	0.43
17:V:95:LEU:HD13	17:V:97:LYS:HD3	2.00	0.43
1:A:866:A:C6	1:A:914:C:C5	3.06	0.43
1:A:1598:C:H5'	19:X:36:LYS:HB2	2.00	0.43
12:Q:34:LEU:HD11	12:Q:129:THR:HB	2.00	0.43
21:Z:111:VAL:C	21:Z:113:ALA:H	2.22	0.43
1:A:2287:A:O2'	1:A:2288:A:H3'	2.19	0.43
1:A:1803:A:H4'	3:D:259:THR:CG2	2.48	0.43
1:A:2317:C:N4	1:A:2318:G:O6	2.51	0.43
1:A:1405:U:H2'	1:A:1406:U:H6	1.82	0.43
1:A:574:C:O2	4:E:145:LYS:NZ	2.51	0.43
1:A:2464:C:O2'	1:A:2465:C:P	2.76	0.43
1:A:1478:G:O2'	1:A:1558:A:N1	2.52	0.43
7:H:164:TYR:HB2	7:H:167:GLU:HB2	1.99	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:H:69:ARG:HG3	7:H:70:THR:N	2.34	0.43
1:A:829:A:N7	1:A:2248:C:H5'	2.34	0.43
1:A:2679:A:H4'	4:E:165:VAL:HG11	2.01	0.43
13:R:33:ARG:NH1	13:R:115:GLU:OE2	2.43	0.43
1:A:1652:A:C2'	1:A:1653:G:H5'	2.49	0.43
21:Z:35:ARG:HA	21:Z:35:ARG:HD2	1.71	0.43
1:A:1701:A:H5''	1:A:1702:G:OP2	2.18	0.43
8:I:72:LEU:HD23	8:I:107:VAL:HG11	2.01	0.43
7:H:54:ARG:HD3	7:H:65:HIS:ND1	2.34	0.43
8:I:25:TYR:HE2	8:I:29:TYR:CD2	2.37	0.43
11:P:70:GLN:O	11:P:73:GLY:N	2.42	0.43
1:A:2169:A:H2'	1:A:2170:A:C8	2.53	0.43
7:H:64:LEU:O	7:H:68:THR:OG1	2.32	0.43
1:A:1858:G:H1'	1:A:1884:A:N6	2.33	0.43
14:S:10:ARG:O	14:S:14:VAL:HG13	2.19	0.43
2:B:41:U:H5''	34:B:318:HOH:O	2.17	0.43
1:A:1638:C:H4'	1:A:2710:C:O2	2.19	0.43
16:U:59:ARG:CB	16:U:59:ARG:HH11	2.32	0.43
2:B:13:A:H2'	2:B:70:C:O2'	2.17	0.43
21:Z:134:PRO:HB2	21:Z:136:PHE:O	2.19	0.43
6:G:121:ASN:HA	6:G:122:PRO:HD3	1.80	0.43
1:A:1536:C:O2'	1:A:1537:G:P	2.77	0.43
1:A:918:A:H5''	2:B:98:G:O2'	2.19	0.43
1:A:2772:C:H2'	1:A:2773:C:C6	2.53	0.43
1:A:2591:C:H2'	1:A:2592:G:C8	2.54	0.43
18:W:12:ILE:HD13	18:W:17:VAL:HG13	2.00	0.43
1:A:247:G:H4'	1:A:386:G:C5	2.54	0.43
1:A:1224:C:O2'	17:V:85:LYS:HA	2.18	0.43
1:A:2295:C:H5	14:S:13:ARG:NH2	2.16	0.43
1:A:323:G:C8	5:F:171:PRO:HG3	2.53	0.43
1:A:2611:U:H3'	1:A:2611:U:P	2.58	0.43
1:A:271(Q):G:O2'	1:A:271(R):G:P	2.76	0.43
1:A:1581:G:H8	1:A:1581:G:H5''	1.84	0.43
1:A:2331:G:O2'	22:O:43:THR:HG22	2.19	0.43
4:E:14:ILE:HD11	4:E:173:VAL:HG11	2.00	0.43
3:D:92:ILE:HD12	3:D:104:TYR:CD2	2.54	0.43
1:A:1188:U:H4'	17:V:79:VAL:HG22	1.99	0.43
4:E:1:MET:O	4:E:84:PHE:HB2	2.18	0.43
1:A:751:A:H5'	18:W:90:ARG:HA	2.01	0.43
13:R:81:ASP:O	13:R:85:PRO:HG2	2.19	0.43
13:R:75:LEU:HD22	13:R:75:LEU:O	2.18	0.43
1:A:886:C:H6	34:A:5034:HOH:O	2.02	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2165:G:H2'	1:A:2166:G:C8	2.54	0.43
1:A:832:G:OP1	11:P:38:GLN:O	2.36	0.43
5:F:129:PHE:HB2	5:F:132:VAL:CG2	2.49	0.43
1:A:978:G:C2	1:A:986:C:C2	3.06	0.43
21:Z:85:HIS:HE1	21:Z:87:ASP:OD2	2.01	0.43
1:A:735:A:H3'	1:A:736:C:C6	2.54	0.43
1:A:2061:G:H5''	1:A:2503:A:C2	2.53	0.43
1:A:746:A:H2'	1:A:2612:C:H5''	2.00	0.43
1:A:315:G:H2'	1:A:316:C:C6	2.54	0.43
1:A:1700:A:H2'	1:A:1701:A:O5'	2.19	0.43
9:N:56:ASN:N	9:N:125:GLY:HA3	2.28	0.43
1:A:2103:C:O2	1:A:2187:G:C2	2.72	0.43
1:A:1539:G:H2'	1:A:1540:U:O4'	2.19	0.43
2:B:31:C:O2'	2:B:53:A:N6	2.52	0.43
1:A:208:C:H2'	1:A:209:C:C6	2.54	0.43
1:A:2689:U:H4'	1:A:2690:C:H5'	2.01	0.43
11:P:1:MET:CE	11:P:5:ASP:HB2	2.49	0.43
23:1:94:LEU:O	23:1:97:LEU:HB2	2.19	0.43
1:A:72:U:OP1	19:X:1:MET:N	2.52	0.43
6:G:16:ARG:HE	6:G:31:VAL:CG2	2.31	0.42
3:D:72:LYS:HG3	3:D:103:ARG:NH2	2.34	0.42
1:A:1794:U:H2'	1:A:1795:C:H6	1.83	0.42
15:T:51:ARG:HG3	15:T:98:LYS:CE	2.49	0.42
13:R:29:LEU:HD23	13:R:70:LEU:HD11	2.01	0.42
24:2:53:LEU:HA	24:2:53:LEU:HD23	1.90	0.42
21:Z:70:LEU:O	21:Z:89:PHE:N	2.43	0.42
1:A:667:U:O2	30:8:2:PRO:HD2	2.19	0.42
1:A:583:G:OP2	16:U:10:ARG:HD2	2.19	0.42
1:A:1482:G:O6	1:A:1507:A:N6	2.52	0.42
1:A:2171:A:H1'	1:A:2172:U:C6	2.54	0.42
1:A:92:A:H2'	1:A:93:G:O4'	2.19	0.42
14:S:102:ALA:HA	14:S:105:ALA:CB	2.48	0.42
7:H:3:ARG:HG2	7:H:6:ARG:HG2	2.00	0.42
11:P:38:GLN:O	11:P:39:LYS:HB3	2.20	0.42
8:I:44:LEU:HA	8:I:44:LEU:HD12	1.68	0.42
1:A:1999:C:H4'	1:A:2723:C:O2	2.20	0.42
1:A:873:G:N2	1:A:905:U:O2	2.52	0.42
6:G:68:PRO:HB2	6:G:90:LEU:HB3	2.01	0.42
1:A:2405:G:OP1	11:P:77:ARG:NH2	2.52	0.42
8:I:25:TYR:CE2	8:I:29:TYR:CD2	3.07	0.42
1:A:708:C:C6	1:A:708:C:H5''	2.54	0.42
1:A:947:G:N2	1:A:971:C:C2	2.87	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:Y:5:MET:HG2	20:Y:30:VAL:HG11	2.01	0.42
11:P:133:SER:O	11:P:137:LYS:HG3	2.19	0.42
1:A:602:G:O2'	1:A:655:A:N6	2.52	0.42
6:G:114:ILE:HB	6:G:117:PHE:HB2	2.02	0.42
13:R:59:ASP:N	13:R:59:ASP:OD2	2.50	0.42
1:A:1688:U:H5'	1:A:1689:A:OP1	2.19	0.42
1:A:2070:G:C2	1:A:2442:C:C2	3.07	0.42
2:B:33:G:C2	2:B:50:G:C2	3.08	0.42
20:Y:15:VAL:HG21	20:Y:42:VAL:HG11	2.01	0.42
1:A:2318:G:O2'	1:A:2319:G:H5''	2.19	0.42
13:R:2:ARG:NH1	13:R:5:LYS:O	2.45	0.42
1:A:2104:G:H2'	1:A:2104:G:N3	2.34	0.42
24:2:50:ILE:O	24:2:51:ARG:HB3	2.19	0.42
1:A:572:A:H5''	1:A:573:G:OP2	2.19	0.42
5:F:11:VAL:HB	5:F:18:ARG:HB3	2.01	0.42
9:N:48:MET:H	9:N:48:MET:HG3	1.75	0.42
1:A:478:A:N6	1:A:502:A:H62	2.16	0.42
1:A:525:U:H5'	1:A:556:G:OP1	2.19	0.42
1:A:615:G:OP1	5:F:40:GLN:NE2	2.52	0.42
3:D:77:ALA:HB2	3:D:97:TYR:CD2	2.54	0.42
21:Z:54:HIS:CG	21:Z:101:PRO:HG3	2.54	0.42
1:A:2833:G:O2'	1:A:2834:G:P	2.77	0.42
1:A:1289:C:H2'	1:A:1290:C:C6	2.54	0.42
10:O:102:VAL:HB	10:O:106:LEU:HD12	2.01	0.42
1:A:2005:A:OP1	34:A:3815:HOH:O	2.22	0.42
1:A:2492:U:H2'	1:A:2493:U:H6	1.84	0.42
1:A:1666:G:O2'	1:A:1667:G:H5'	2.20	0.42
6:G:82:LEU:HB3	6:G:83:ARG:H	1.63	0.42
1:A:1406:U:H2'	1:A:1407:C:H6	1.84	0.42
5:F:195:ASP:HB3	5:F:197:ASP:H	1.85	0.42
4:E:144:ARG:HB3	4:E:145:LYS:H	1.51	0.42
1:A:645:C:H2'	1:A:645:C:O2	2.18	0.42
1:A:2536:G:C6	1:A:2537:U:C4	3.07	0.42
1:A:479:A:N3	1:A:481:G:H5''	2.34	0.42
1:A:582:G:H2'	1:A:583:G:C8	2.54	0.42
30:8:54:GLU:O	30:8:58:ILE:HG13	2.19	0.42
2:B:17:C:H2'	2:B:18:G:O4'	2.19	0.42
1:A:581:C:OP1	16:U:33:ARG:HG3	2.20	0.42
1:A:2312:U:H5'	6:G:88:ILE:CD1	2.50	0.42
1:A:2206:G:H3'	1:A:2207:G:H8	1.78	0.42
6:G:11:TYR:OH	6:G:33:ARG:HG3	2.19	0.42
23:1:3:LYS:HB3	23:1:4:VAL:H	1.49	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2173:A:C3'	1:A:2174:C:H5'	2.49	0.42
30:8:39:LYS:HA	30:8:42:ARG:NH1	2.35	0.42
1:A:2547:U:O2	10:O:23:ARG:NH2	2.52	0.42
18:W:1:MET:HE2	18:W:2:GLU:H	1.83	0.42
1:A:590:A:H2'	1:A:591:C:O4'	2.19	0.42
1:A:2375:G:C8	34:A:5002:HOH:O	2.51	0.42
1:A:196:A:H62	11:P:38:GLN:NE2	2.18	0.42
1:A:2224:G:H4'	1:A:2226:C:C2	2.54	0.42
1:A:311:A:C6	1:A:328:U:C4	3.08	0.42
6:G:73:ALA:O	6:G:84:LYS:HA	2.20	0.42
1:A:438:G:H2'	1:A:440:G:H8	1.84	0.42
1:A:1271:G:N2	1:A:1617:C:O4'	2.53	0.42
12:Q:29:PHE:HB2	12:Q:105:GLU:OE2	2.19	0.42
1:A:1514:U:H2'	1:A:1515:G:H8	1.84	0.42
1:A:862:G:H2'	1:A:863:A:O4'	2.19	0.42
1:A:1651:G:OP1	13:R:40:LYS:HE3	2.19	0.42
1:A:2291:U:H2'	1:A:2292:C:C6	2.54	0.42
1:A:2093:G:C6	1:A:2225:A:C8	3.08	0.42
14:S:84:GLN:HG2	14:S:84:GLN:H	1.48	0.42
3:D:148:GLU:OE1	3:D:151:LYS:NZ	2.43	0.42
1:A:1253:A:C5	34:A:4829:HOH:O	2.68	0.42
1:A:2172:U:H1'	1:A:2173:A:OP1	2.20	0.42
1:A:75:G:H4'	24:2:55:ARG:NH1	2.34	0.42
1:A:297:C:H2'	1:A:298:G:O4'	2.19	0.42
8:I:62:LYS:HE2	8:I:133:HIS:NE2	2.35	0.42
1:A:1000:A:C6	1:A:1001:A:C6	3.08	0.42
1:A:1190:G:O2'	1:A:1191:G:H5'	2.20	0.42
16:U:36:ARG:HD2	16:U:40:PHE:CZ	2.55	0.42
1:A:1784:A:H4'	1:A:1785:A:C5'	2.50	0.42
1:A:2153:G:H2'	1:A:2154:G:C8	2.55	0.42
1:A:2849:U:H4'	1:A:2868:A:C2	2.55	0.42
1:A:2318:G:N3	1:A:2318:G:H2'	2.33	0.42
1:A:1038:C:N4	1:A:1117:G:H1	2.13	0.42
1:A:2687:U:H2'	1:A:2688:U:O4'	2.19	0.42
1:A:760:G:H2'	1:A:761:A:O4'	2.20	0.42
1:A:2519:U:C6	1:A:2542:A:N6	2.88	0.42
5:F:132:VAL:CG2	5:F:163:VAL:HG22	2.50	0.42
8:I:29:TYR:C	8:I:32:PRO:HD2	2.40	0.42
1:A:519:U:H2'	1:A:520:G:C8	2.55	0.42
5:F:34:TRP:CE2	11:P:8:PRO:HD3	2.55	0.42
11:P:95:VAL:HG22	11:P:125:VAL:HG12	2.02	0.42
1:A:1168:G:C2	1:A:1182:A:C2	3.08	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2153:G:H2'	1:A:2154:G:H8	1.84	0.42
14:S:83:LYS:HA	14:S:83:LYS:HE2	2.02	0.42
1:A:1507:A:HO2'	1:A:1508:A:P	2.40	0.42
4:E:115:GLY:O	4:E:119:ARG:HB2	2.20	0.42
3:D:17:THR:O	3:D:211:ARG:NH2	2.51	0.42
1:A:1179:C:O2'	1:A:1180:C:H5'	2.20	0.42
2:B:31:C:H4'	6:G:29:TRP:CH2	2.55	0.42
6:G:125:PHE:CZ	6:G:170:ARG:HA	2.55	0.42
1:A:945:A:C4	1:A:2448:A:C2	3.07	0.41
4:E:181:LEU:HA	4:E:181:LEU:HD12	1.80	0.41
1:A:2464:C:H1'	34:A:4973:HOH:O	2.20	0.41
1:A:1557:C:H5''	1:A:1558:A:OP2	2.20	0.41
1:A:2542:A:O4'	34:A:4624:HOH:O	2.21	0.41
1:A:2722:G:H2'	1:A:2723:C:C6	2.54	0.41
1:A:781:A:N1	1:A:1776:G:O2'	2.47	0.41
6:G:146:TYR:O	6:G:149:VAL:HG12	2.20	0.41
4:E:174:ASP:OD2	4:E:175:VAL:N	2.52	0.41
5:F:167:ALA:HB1	5:F:173:VAL:HG11	2.01	0.41
1:A:2096:U:H3	1:A:2193:G:H1	1.68	0.41
1:A:2740:A:C6	1:A:2764:A:C8	3.08	0.41
3:D:221:VAL:HG22	3:D:226:MET:HE2	2.01	0.41
3:D:232:PRO:HB3	3:D:244:ARG:CZ	2.50	0.41
3:D:166:GLN:HB2	3:D:174:ILE:HG22	2.02	0.41
6:G:11:TYR:O	6:G:16:ARG:HG2	2.20	0.41
1:A:2420:C:H6	1:A:2420:C:O5'	2.03	0.41
1:A:89:G:H3'	1:A:90:U:C5'	2.50	0.41
28:6:40:CYS:HA	28:6:41:PRO:HD3	1.70	0.41
1:A:30:G:H2'	1:A:31:C:H6	1.85	0.41
1:A:1997:G:O2'	1:A:1998:G:H5'	2.20	0.41
22:0:49:LYS:O	22:0:50:ASN:HB2	2.20	0.41
20:Y:97:ARG:HG2	20:Y:97:ARG:H	1.65	0.41
2:B:19:G:H8	2:B:19:G:OP2	2.03	0.41
11:P:126:VAL:HG11	11:P:148:LEU:HD13	2.01	0.41
1:A:361:G:O2'	1:A:362:U:H5'	2.21	0.41
1:A:363(B):G:C4	1:A:363(C):G:C8	3.09	0.41
1:A:742:G:H4'	1:A:1676:A:H5'	2.03	0.41
6:G:13:GLU:H	6:G:13:GLU:HG3	1.56	0.41
1:A:2078:C:C4	1:A:2079:U:C4	3.09	0.41
1:A:2540:C:H2'	1:A:2541:A:O4'	2.20	0.41
1:A:252:G:P	11:P:50:ARG:HH12	2.42	0.41
1:A:638:G:H2'	1:A:639:U:O4'	2.20	0.41
1:A:2660:A:H2'	1:A:2661:G:O4'	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:37:C:C5	2:B:38:C:C5	3.09	0.41
1:A:1614:A:H8	1:A:1614:A:P	2.43	0.41
13:R:100:LEU:HA	13:R:100:LEU:HD12	1.74	0.41
2:B:1:U:H2'	2:B:1:U:O2	2.21	0.41
1:A:2317:C:H2'	1:A:2318:G:H5'	2.03	0.41
1:A:2788:C:N4	1:A:2789:C:N4	2.68	0.41
1:A:2103:C:N3	1:A:2104:G:N7	2.68	0.41
1:A:1041:C:H5'	1:A:1042:G:OP2	2.21	0.41
1:A:530:G:N1	34:A:3952:HOH:O	2.36	0.41
21:Z:19:ARG:HE	21:Z:19:ARG:HB2	1.74	0.41
23:1:67:ILE:N	23:1:68:PRO:HD2	2.34	0.41
1:A:536:A:H2'	1:A:537:C:C6	2.56	0.41
4:E:117:MET:O	4:E:118:LYS:HB3	2.21	0.41
1:A:1825:A:O4'	3:D:254:THR:HG21	2.21	0.41
16:U:39:LEU:HD23	16:U:39:LEU:HA	1.89	0.41
2:B:29:A:OP2	14:S:32:LEU:HD12	2.20	0.41
1:A:1142(A):A:C4	1:A:1144:G:C8	3.08	0.41
1:A:2789:C:H5''	1:A:2790:A:OP2	2.21	0.41
1:A:2262:U:H4'	1:A:2328:A:C2	2.56	0.41
21:Z:99:TYR:HA	21:Z:124:ILE:O	2.20	0.41
22:0:27:GLU:HB2	22:0:69:PHE:HD1	1.85	0.41
1:A:686:G:N2	1:A:788:A:H61	2.18	0.41
1:A:476:G:H4'	1:A:502:A:N1	2.36	0.41
1:A:225:A:O2'	1:A:257:A:H4'	2.20	0.41
11:P:82:GLY:HA2	11:P:113:LYS:O	2.20	0.41
13:R:54:LEU:O	13:R:57:ARG:HB2	2.20	0.41
11:P:132:LYS:HE2	11:P:132:LYS:HB2	1.84	0.41
17:V:40:LEU:HD11	17:V:101:GLY:HA2	2.02	0.41
1:A:1452:A:O2'	1:A:1453:U:H2'	2.20	0.41
21:Z:98:MET:O	21:Z:125:LEU:HD12	2.20	0.41
1:A:2536:G:C5	1:A:2537:U:C5	3.09	0.41
1:A:30:G:OP2	16:U:5:LYS:HE2	2.20	0.41
6:G:105:LYS:NZ	26:4:25:TYR:O	2.53	0.41
7:H:71:LEU:HD12	7:H:71:LEU:HA	1.68	0.41
20:Y:97:ARG:HH11	20:Y:107:ASP:C	2.23	0.41
1:A:422:A:H2'	1:A:423:A:C8	2.55	0.41
1:A:338:G:H2'	1:A:339:U:H6	1.85	0.41
1:A:2094:G:C2	1:A:2196:C:C2	3.09	0.41
1:A:998:C:H3'	34:A:4566:HOH:O	2.19	0.41
1:A:2699:C:H2'	1:A:2700:C:O4'	2.21	0.41
1:A:671:C:H2'	1:A:672:C:C6	2.55	0.41
1:A:1170:G:H5''	1:A:1170:G:H8	1.85	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:86:C:H4'	1:A:104:U:H1'	2.01	0.41
1:A:2305:A:H5''	6:G:134:GLY:HA3	2.02	0.41
1:A:1531:C:N4	1:A:1538:G:H1	2.15	0.41
14:S:11:LYS:HD3	14:S:15:ARG:NH1	2.35	0.41
1:A:699:A:C2	1:A:1633:G:N3	2.89	0.41
21:Z:152:ALA:N	21:Z:171:ILE:HG12	2.35	0.41
11:P:126:VAL:CG1	11:P:148:LEU:HD13	2.51	0.41
26:4:15:ILE:HB	26:4:32:TYR:CD2	2.56	0.41
1:A:1180:C:H2'	1:A:1181:C:H6	1.86	0.41
3:D:183:ARG:HG3	3:D:270:ILE:HG12	2.03	0.41
12:Q:72:LYS:HA	12:Q:73:PRO:HD3	1.89	0.41
1:A:1324:G:C5	1:A:1328:G:O6	2.73	0.41
1:A:1790:C:H2'	1:A:1791:A:C5	2.56	0.41
11:P:101:VAL:HA	11:P:106:LEU:O	2.21	0.41
1:A:2600:A:O2'	1:A:2601:C:H5'	2.21	0.41
4:E:60:ASN:OD1	4:E:62:PRO:HD2	2.21	0.41
25:3:3:ARG:HD3	25:3:60:GLU:OE1	2.21	0.41
1:A:659:C:H4'	5:F:100:THR:O	2.21	0.41
1:A:2768:C:H2'	1:A:2769:C:O4'	2.19	0.41
28:6:23:THR:OG1	28:6:24:GLU:N	2.54	0.41
1:A:886:C:H1'	1:A:890:A:N6	2.36	0.41
1:A:1702:G:H2'	1:A:1703:G:O4'	2.20	0.41
15:T:56:GLY:O	15:T:59:THR:CG2	2.69	0.41
30:8:34:TRP:CE2	30:8:35:GLN:HB3	2.56	0.41
1:A:1021:A:C3'	1:A:1021:A:C8	3.03	0.41
14:S:87:PHE:CE1	14:S:102:ALA:HB2	2.56	0.41
23:1:49:VAL:O	23:1:59:THR:HA	2.20	0.41
4:E:116:VAL:HG13	4:E:122:PHE:CB	2.50	0.41
26:4:42:PHE:CB	26:4:43:TYR:HB2	2.49	0.41
1:A:573:G:O2'	1:A:574:C:H3'	2.20	0.41
1:A:2040:C:H2'	1:A:2041:U:O4'	2.20	0.41
1:A:2473:U:C2	1:A:2474:C:C6	3.09	0.41
8:I:88:ILE:HG22	8:I:89:TYR:N	2.36	0.41
8:I:85:GLU:CG	8:I:86:THR:H	2.34	0.41
22:0:70:GLN:HG2	22:0:72:ARG:HG2	2.03	0.41
1:A:708:C:H6	1:A:708:C:H5''	1.86	0.41
1:A:1031:G:H21	31:9:36:GLN:HE22	1.68	0.41
1:A:1549:C:H2'	1:A:1550:C:H6	1.86	0.41
28:6:9:LEU:HD21	28:6:25:LYS:HB3	2.03	0.41
1:A:2095:C:H2'	1:A:2096:U:O4'	2.21	0.41
16:U:61:TRP:CD2	16:U:93:LYS:HA	2.56	0.41
1:A:2721:A:O2'	1:A:2874:C:H5'	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:265:A:H1'	1:A:266:G:O4'	2.21	0.41
1:A:1314:C:H6	1:A:1314:C:H5'	1.86	0.41
1:A:2716:U:O2'	1:A:2717:G:H5'	2.21	0.41
9:N:5:VAL:H	16:U:64:ARG:HH22	1.68	0.41
3:D:33:LEU:HA	3:D:33:LEU:HD23	1.86	0.41
17:V:68:LYS:HB3	17:V:68:LYS:HE3	1.70	0.41
28:6:44:ARG:HH11	28:6:44:ARG:HB3	1.86	0.41
1:A:83:G:H22	1:A:102:G:H1'	1.84	0.41
1:A:2316:C:H2'	1:A:2317:C:H6	1.84	0.41
1:A:2147:G:H2'	1:A:2148:G:C4'	2.51	0.41
1:A:2158:A:H1'	1:A:2159:G:C8	2.55	0.41
6:G:57:ALA:HA	6:G:68:PRO:HG2	2.01	0.41
1:A:784:A:C5	3:D:229:VAL:HG21	2.56	0.41
1:A:2266:A:H4'	1:A:2267:A:C4	2.55	0.41
1:A:960:A:H5''	1:A:961:C:OP2	2.21	0.41
1:A:414:C:O2'	1:A:415:A:H5'	2.21	0.41
19:X:54:VAL:HG13	19:X:81:VAL:HG12	2.02	0.41
1:A:107:C:H2'	1:A:108:U:H6	1.86	0.41
30:8:30:ARG:HD3	30:8:30:ARG:HA	1.82	0.41
9:N:109:LYS:HD2	9:N:109:LYS:N	2.35	0.41
1:A:1488:G:H5'	1:A:1489:U:OP2	2.20	0.40
11:P:97:PRO:HD3	11:P:126:VAL:O	2.20	0.40
1:A:296:C:O2'	1:A:297:C:H5'	2.20	0.40
1:A:271(P):C:C2'	1:A:271(Q):G:H5'	2.51	0.40
1:A:1816:G:O6	3:D:35:LYS:NZ	2.42	0.40
1:A:601:C:OP1	5:F:108:LYS:HE3	2.20	0.40
1:A:445:C:O2'	1:A:446:G:H5'	2.21	0.40
1:A:2119:A:C6	1:A:2170:A:C5	3.09	0.40
1:A:614:U:H2'	1:A:614(A):U:O4'	2.21	0.40
9:N:14:VAL:HG13	9:N:138:LEU:HG	2.03	0.40
1:A:922:U:H2'	1:A:923:C:C6	2.56	0.40
1:A:2597:G:H2'	1:A:2598:A:C8	2.56	0.40
1:A:597:U:H2'	1:A:598:G:C8	2.56	0.40
1:A:2702:U:H4'	1:A:2703:C:OP1	2.22	0.40
1:A:1913:A:H3'	1:A:1913:A:OP2	2.20	0.40
1:A:2136:C:C5	1:A:2137:C:H5	2.39	0.40
4:E:119:ARG:HG2	4:E:160:TYR:HB2	2.02	0.40
1:A:2104:G:N2	1:A:2105:C:C2	2.89	0.40
1:A:729:G:C5	3:D:208:LYS:HB2	2.56	0.40
13:R:97:VAL:CG2	13:R:114:VAL:HG13	2.51	0.40
1:A:1589:C:H2'	1:A:1590:U:C6	2.57	0.40
22:0:72:ARG:CB	22:0:75:LEU:HB2	2.51	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
28:6:30:THR:OG1	28:6:30:THR:O	2.39	0.40
1:A:1786:A:H1'	1:A:1938:A:N6	2.36	0.40
12:Q:48:GLU:O	12:Q:52:VAL:HG23	2.21	0.40
1:A:819:A:C4	1:A:1189:A:C2	3.08	0.40
9:N:23:LEU:HD12	9:N:99:LEU:HD23	2.02	0.40
16:U:16:LYS:HB3	16:U:16:LYS:HE2	1.66	0.40
1:A:2238:G:N3	1:A:2238:G:H2'	2.36	0.40
1:A:1371:G:O6	34:A:4321:HOH:O	2.22	0.40
1:A:1022:G:C5	1:A:1140:C:C4	3.09	0.40
14:S:110:LEU:HD12	14:S:110:LEU:HA	2.01	0.40
25:3:8:LEU:HD23	25:3:8:LEU:HA	1.81	0.40
14:S:90:GLY:HA3	14:S:91:PRO:HD2	1.78	0.40
11:P:52:GLU:HB3	11:P:55:ARG:HD2	2.03	0.40
12:Q:39:PRO:HA	12:Q:97:VAL:O	2.22	0.40
1:A:150:C:H2'	1:A:151:C:C6	2.56	0.40
18:W:58:ALA:HB1	18:W:64:MET:HB2	2.01	0.40
1:A:1686:C:H2'	1:A:1687:G:O4'	2.21	0.40
21:Z:48:PHE:HE2	21:Z:71:VAL:HG11	1.87	0.40
1:A:1744:C:O2'	1:A:1745:C:H5'	2.22	0.40
1:A:836:G:C5	1:A:837:C:C4	3.09	0.40
1:A:2295:C:OP1	14:S:10:ARG:NH1	2.55	0.40
21:Z:182:LYS:HE3	21:Z:186:GLU:OE2	2.22	0.40
5:F:129:PHE:HD1	5:F:142:TRP:CE2	2.39	0.40
5:F:132:VAL:HG23	5:F:163:VAL:HG22	2.04	0.40
1:A:548:A:O2'	1:A:549:G:OP1	2.37	0.40
1:A:863:A:P	12:Q:22:LYS:HG3	2.61	0.40
11:P:68:GLN:HG3	30:8:12:LYS:HG2	2.03	0.40
3:D:132:PRO:HD3	3:D:190:TYR:CZ	2.57	0.40
1:A:374:A:H5'	34:A:4881:HOH:O	2.20	0.40
1:A:1385:G:H4'	1:A:1386:C:OP1	2.22	0.40
1:A:982:C:H6	1:A:982:C:O5'	2.04	0.40
18:W:20:VAL:O	18:W:23:LEU:HB2	2.20	0.40
1:A:2296:U:O2'	1:A:2297:C:OP2	2.26	0.40
20:Y:20:TYR:N	20:Y:20:TYR:CD1	2.89	0.40
2:B:95:C:H2'	2:B:96:U:C6	2.57	0.40
1:A:250:G:P	30:8:13:ARG:HH22	2.44	0.40
8:I:68:LEU:HA	8:I:68:LEU:HD13	1.49	0.40
1:A:795:C:H2'	1:A:796:C:C6	2.57	0.40
3:D:85:ASP:OD2	3:D:88:ARG:NH1	2.43	0.40
3:D:106:ILE:O	3:D:108:PRO:HD3	2.20	0.40
7:H:71:LEU:O	7:H:74:ASN:HB2	2.22	0.40
1:A:228:A:H2'	1:A:230:U:O4'	2.21	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2492:U:H2'	1:A:2493:U:C6	2.56	0.40
21:Z:56:VAL:HG23	21:Z:133:ILE:HD13	2.04	0.40
23:1:86:SER:O	23:1:89:GLU:HG2	2.22	0.40
1:A:2756:U:H1'	1:A:2757:A:H5''	2.03	0.40
4:E:72:VAL:HA	4:E:73:GLU:HB3	2.04	0.40
1:A:897:C:H6	1:A:897:C:O5'	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	273/276 (99%)	262 (96%)	8 (3%)	3 (1%)	21	49
4	E	202/206 (98%)	187 (93%)	12 (6%)	3 (2%)	15	38
5	F	201/210 (96%)	191 (95%)	8 (4%)	2 (1%)	22	51
6	G	179/182 (98%)	148 (83%)	29 (16%)	2 (1%)	21	49
7	H	172/180 (96%)	160 (93%)	9 (5%)	3 (2%)	14	33
8	I	144/148 (97%)	119 (83%)	22 (15%)	3 (2%)	11	27
9	N	138/140 (99%)	125 (91%)	11 (8%)	2 (1%)	16	41
10	O	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
11	P	147/150 (98%)	130 (88%)	15 (10%)	2 (1%)	16	41
12	Q	139/141 (99%)	131 (94%)	6 (4%)	2 (1%)	16	41
13	R	116/118 (98%)	115 (99%)	1 (1%)	0	100	100
14	S	108/112 (96%)	98 (91%)	9 (8%)	1 (1%)	25	55
15	T	128/146 (88%)	124 (97%)	3 (2%)	1 (1%)	27	58
16	U	114/118 (97%)	114 (100%)	0	0	100	100
17	V	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
18	W	109/113 (96%)	108 (99%)	1 (1%)	0	100	100
19	X	93/96 (97%)	88 (95%)	4 (4%)	1 (1%)	21	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	Y	105/110 (96%)	97 (92%)	8 (8%)	0	100	100
21	Z	201/206 (98%)	181 (90%)	15 (8%)	5 (2%)	9	21
22	0	75/85 (88%)	71 (95%)	4 (5%)	0	100	100
23	1	95/98 (97%)	92 (97%)	1 (1%)	2 (2%)	11	27
24	2	69/72 (96%)	65 (94%)	4 (6%)	0	100	100
25	3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
26	4	44/71 (62%)	34 (77%)	10 (23%)	0	100	100
27	5	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
28	6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
29	7	46/49 (94%)	44 (96%)	1 (2%)	1 (2%)	10	25
30	8	62/65 (95%)	59 (95%)	1 (2%)	2 (3%)	6	14
31	9	34/37 (92%)	34 (100%)	0	0	100	100
All	All	3378/3526 (96%)	3145 (93%)	198 (6%)	35 (1%)	22	51

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	G	82	LEU
11	P	27	HIS
21	Z	161	VAL
30	8	34	TRP
30	8	35	GLN
3	D	239	ARG
5	F	18	ARG
5	F	22	ALA
6	G	149	VAL
7	H	71	LEU
8	I	122	GLU
9	N	18	ALA
12	Q	135	ASP
21	Z	199	LYS
23	1	3	LYS
3	D	275	LYS
4	E	52	LEU
8	I	117	GLU
11	P	39	LYS
15	T	36	GLU
19	X	23	GLU

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Mol	Chain	Res	Type
21	Z	193	GLU
29	7	46	VAL
4	E	118	LYS
7	H	65	HIS
21	Z	191	VAL
23	1	83	GLU
3	D	3	VAL
12	Q	62	GLY
14	S	49	VAL
7	H	92	ILE
21	Z	157	LEU
4	E	72	VAL
8	I	107	VAL
9	N	5	VAL

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	215/218 (99%)	190 (88%)	25 (12%)	8	18
4	E	163/166 (98%)	139 (85%)	24 (15%)	4	11
5	F	157/166 (95%)	135 (86%)	22 (14%)	5	12
6	G	128/156 (82%)	107 (84%)	21 (16%)	3	9
7	H	141/148 (95%)	128 (91%)	13 (9%)	13	29
8	I	100/124 (81%)	75 (75%)	25 (25%)	1	2
9	N	117/119 (98%)	99 (85%)	18 (15%)	4	10
10	O	98/100 (98%)	91 (93%)	7 (7%)	21	46
11	P	114/116 (98%)	95 (83%)	19 (17%)	3	8
12	Q	111/111 (100%)	95 (86%)	16 (14%)	5	12
13	R	101/101 (100%)	81 (80%)	20 (20%)	2	5
14	S	86/88 (98%)	70 (81%)	16 (19%)	2	6
15	T	110/127 (87%)	93 (84%)	17 (16%)	4	10
16	U	93/94 (99%)	81 (87%)	12 (13%)	6	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	V	81/82 (99%)	65 (80%)	16 (20%)	2	5
18	W	89/92 (97%)	78 (88%)	11 (12%)	7	16
19	X	73/78 (94%)	66 (90%)	7 (10%)	12	27
20	Y	79/91 (87%)	64 (81%)	15 (19%)	2	6
21	Z	155/179 (87%)	136 (88%)	19 (12%)	7	17
22	0	61/67 (91%)	51 (84%)	10 (16%)	3	9
23	1	78/83 (94%)	66 (85%)	12 (15%)	4	10
24	2	63/67 (94%)	55 (87%)	8 (13%)	6	15
25	3	50/52 (96%)	44 (88%)	6 (12%)	7	17
26	4	39/63 (62%)	35 (90%)	4 (10%)	10	23
27	5	49/52 (94%)	44 (90%)	5 (10%)	11	24
28	6	48/52 (92%)	37 (77%)	11 (23%)	1	3
29	7	38/42 (90%)	32 (84%)	6 (16%)	4	10
30	8	52/55 (94%)	45 (86%)	7 (14%)	6	13
31	9	32/34 (94%)	31 (97%)	1 (3%)	52	83
All	All	2721/2923 (93%)	2328 (86%)	393 (14%)	5	12

All (393) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	12	SER
3	D	13	ARG
3	D	37	LEU
3	D	61	LEU
3	D	72	LYS
3	D	94	LEU
3	D	103	ARG
3	D	106	ILE
3	D	111	LEU
3	D	113	VAL
3	D	138	VAL
3	D	140	THR
3	D	141	VAL
3	D	154	LYS
3	D	192	THR
3	D	200	ASP
3	D	211	ARG

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Mol	Chain	Res	Type
3	D	217	ARG
3	D	221	VAL
3	D	229	VAL
3	D	242	ARG
3	D	253	GLN
3	D	257	LEU
3	D	259	THR
3	D	260	ARG
4	E	12	THR
4	E	21	VAL
4	E	24	THR
4	E	33	VAL
4	E	49	LEU
4	E	52	LEU
4	E	75	VAL
4	E	77	ILE
4	E	78	LEU
4	E	79	ARG
4	E	82	ARG
4	E	87	GLU
4	E	93	VAL
4	E	111	ARG
4	E	116	VAL
4	E	119	ARG
4	E	128	SER
4	E	144	ARG
4	E	154	LYS
4	E	163	GLU
4	E	170	LEU
4	E	175	VAL
4	E	179	GLU
4	E	181	LEU
5	F	15	SER
5	F	18	ARG
5	F	24	LEU
5	F	33	LEU
5	F	53	THR
5	F	57	VAL
5	F	74	ARG
5	F	82	ILE
5	F	88	VAL
5	F	106	ARG

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Mol	Chain	Res	Type
5	F	108	LYS
5	F	110	LEU
5	F	117	ARG
5	F	140	LEU
5	F	145	GLU
5	F	158	THR
5	F	161	GLU
5	F	162	LEU
5	F	170	LEU
5	F	192	LEU
5	F	197	ASP
5	F	201	VAL
6	G	3	LEU
6	G	5	VAL
6	G	9	ARG
6	G	13	GLU
6	G	28	VAL
6	G	31	VAL
6	G	43	LEU
6	G	47	LYS
6	G	60	LEU
6	G	71	THR
6	G	80	PHE
6	G	128	ARG
6	G	133	LEU
6	G	135	LEU
6	G	143	GLU
6	G	148	MET
6	G	152	LEU
6	G	153	ARG
6	G	159	VAL
6	G	165	THR
6	G	170	ARG
7	H	15	VAL
7	H	24	VAL
7	H	41	MET
7	H	45	VAL
7	H	69	ARG
7	H	71	LEU
7	H	77	LYS
7	H	95	ARG
7	H	98	LEU

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Mol	Chain	Res	Type
7	H	106	THR
7	H	116	GLU
7	H	139	GLN
7	H	171	LEU
8	I	1	MET
8	I	9	LEU
8	I	15	VAL
8	I	38	LEU
8	I	41	GLU
8	I	42	SER
8	I	43	ASN
8	I	47	LEU
8	I	48	GLU
8	I	58	LEU
8	I	61	ARG
8	I	72	LEU
8	I	75	LEU
8	I	76	THR
8	I	77	LEU
8	I	86	THR
8	I	87	LYS
8	I	101	LEU
8	I	105	HIS
8	I	116	LEU
8	I	121	LYS
8	I	123	LEU
8	I	127	VAL
8	I	140	LEU
8	I	144	VAL
9	N	9	VAL
9	N	33	LEU
9	N	34	LEU
9	N	39	ARG
9	N	43	THR
9	N	46	VAL
9	N	48	MET
9	N	55	VAL
9	N	61	ARG
9	N	62	VAL
9	N	67	LEU
9	N	73	THR
9	N	87	LEU

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Mol	Chain	Res	Type
9	N	89	LYS
9	N	99	LEU
9	N	120	LEU
9	N	133	GLN
9	N	140	VAL
10	O	8	LEU
10	O	10	VAL
10	O	17	ARG
10	O	24	VAL
10	O	53	LYS
10	O	94	ARG
10	O	113	LYS
11	P	1	MET
11	P	21	ARG
11	P	50	ARG
11	P	55	ARG
11	P	59	LEU
11	P	65	ARG
11	P	70	GLN
11	P	71	VAL
11	P	75	ILE
11	P	76	LYS
11	P	83	VAL
11	P	95	VAL
11	P	106	LEU
11	P	112	LEU
11	P	119	GLU
11	P	132	LYS
11	P	144	GLU
11	P	148	LEU
11	P	149	GLU
12	Q	1	MET
12	Q	6	ARG
12	Q	7	MET
12	Q	8	LYS
12	Q	16	ARG
12	Q	21	THR
12	Q	22	LYS
12	Q	31	ASP
12	Q	35	VAL
12	Q	45	GLN
12	Q	55	VAL

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Mol	Chain	Res	Type
12	Q	59	ARG
12	Q	63	LYS
12	Q	75	THR
12	Q	110	THR
12	Q	135	ASP
13	R	1	MET
13	R	6	SER
13	R	18	LEU
13	R	28	LEU
13	R	29	LEU
13	R	33	ARG
13	R	36	THR
13	R	44	LEU
13	R	54	LEU
13	R	57	ARG
13	R	60	LEU
13	R	65	LEU
13	R	67	LEU
13	R	73	VAL
13	R	75	LEU
13	R	79	LEU
13	R	86	ARG
13	R	100	LEU
13	R	111	LEU
13	R	114	VAL
14	S	12	PHE
14	S	13	ARG
14	S	14	VAL
14	S	15	ARG
14	S	20	ARG
14	S	25	ARG
14	S	31	SER
14	S	36	TYR
14	S	38	GLN
14	S	49	VAL
14	S	52	SER
14	S	78	LEU
14	S	83	LYS
14	S	84	GLN
14	S	95	HIS
14	S	110	LEU
15	T	6	LEU

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Mol	Chain	Res	Type
15	T	8	LYS
15	T	13	ARG
15	T	16	ARG
15	T	17	THR
15	T	28	VAL
15	T	36	GLU
15	T	49	VAL
15	T	59	THR
15	T	64	ARG
15	T	67	SER
15	T	93	ARG
15	T	95	ARG
15	T	96	ARG
15	T	107	ASP
15	T	118	ARG
15	T	124	ASP
16	U	8	VAL
16	U	19	LYS
16	U	27	LEU
16	U	31	SER
16	U	36	ARG
16	U	59	ARG
16	U	60	LEU
16	U	74	LEU
16	U	83	LEU
16	U	92	ARG
16	U	104	GLN
16	U	108	GLU
17	V	13	ARG
17	V	18	LEU
17	V	21	ARG
17	V	32	THR
17	V	35	LEU
17	V	46	VAL
17	V	52	VAL
17	V	61	VAL
17	V	62	LEU
17	V	68	LYS
17	V	72	VAL
17	V	79	VAL
17	V	85	LYS
17	V	89	GLN

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Mol	Chain	Res	Type
17	V	95	LEU
17	V	100	ARG
18	W	11	ARG
18	W	15	ARG
18	W	17	VAL
18	W	19	LEU
18	W	23	LEU
18	W	27	LYS
18	W	51	LEU
18	W	68	ARG
18	W	83	LYS
18	W	100	THR
18	W	107	LEU
19	X	35	THR
19	X	45	THR
19	X	52	VAL
19	X	57	LEU
19	X	60	ARG
19	X	66	LEU
19	X	92	LEU
20	Y	2	ARG
20	Y	6	HIS
20	Y	8	LYS
20	Y	19	LYS
20	Y	23	ARG
20	Y	29	GLU
20	Y	34	LYS
20	Y	47	LYS
20	Y	49	VAL
20	Y	55	TYR
20	Y	64	GLU
20	Y	70	SER
20	Y	73	ARG
20	Y	97	ARG
20	Y	106	LEU
21	Z	11	GLU
21	Z	18	LEU
21	Z	19	ARG
21	Z	61	LEU
21	Z	72	ARG
21	Z	74	VAL
21	Z	76	LEU

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Mol	Chain	Res	Type
21	Z	86	VAL
21	Z	91	LEU
21	Z	124	ILE
21	Z	128	VAL
21	Z	138	GLU
21	Z	144	LEU
21	Z	154	ASP
21	Z	155	LEU
21	Z	156	LYS
21	Z	161	VAL
21	Z	170	THR
21	Z	181	GLU
22	0	9	SER
22	0	14	ARG
22	0	19	LYS
22	0	20	ARG
22	0	41	ARG
22	0	46	LYS
22	0	53	MET
22	0	55	ARG
22	0	68	GLU
22	0	74	ARG
23	1	4	VAL
23	1	21	ARG
23	1	26	ARG
23	1	30	VAL
23	1	35	THR
23	1	40	ARG
23	1	46	LEU
23	1	58	ILE
23	1	59	THR
23	1	80	LEU
23	1	83	GLU
23	1	95	LEU
24	2	28	LYS
24	2	30	ARG
24	2	32	LEU
24	2	53	LEU
24	2	55	ARG
24	2	64	LEU
24	2	68	ARG
24	2	71	ASN

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Mol	Chain	Res	Type
25	3	8	LEU
25	3	18	ASP
25	3	23	LEU
25	3	31	LEU
25	3	44	ARG
25	3	54	VAL
26	4	14	ILE
26	4	22	ILE
26	4	39	CYS
26	4	43	TYR
27	5	15	ARG
27	5	16	ARG
27	5	29	THR
27	5	40	LYS
27	5	55	ARG
28	6	4	GLU
28	6	6	ARG
28	6	13	CYS
28	6	30	THR
28	6	33	LYS
28	6	35	GLU
28	6	38	LYS
28	6	40	CYS
28	6	44	ARG
28	6	48	VAL
28	6	52	VAL
29	7	1	MET
29	7	8	ASN
29	7	9	ARG
29	7	10	ARG
29	7	24	THR
29	7	43	THR
30	8	14	VAL
30	8	26	LYS
30	8	29	LYS
30	8	31	HIS
30	8	32	LEU
30	8	34	TRP
30	8	41	ILE
31	9	18	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:



Mol	Chain	Res	Type
3	D	253	GLN
5	F	8	GLN
5	F	69	HIS
5	F	75	HIS
5	F	169	ASN
6	G	40	ASN
8	I	43	ASN
9	N	133	GLN
11	P	27	HIS
11	P	38	GLN
15	T	58	ASN
19	X	31	HIS
19	X	82	GLN
21	Z	34	ASN
31	9	36	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2788/2915 (95%)	485 (17%)	64 (2%)
2	B	119/122 (97%)	21 (17%)	0
All	All	2907/3037 (95%)	506 (17%)	64 (2%)

All (506) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	G
1	A	15	G
1	A	34	C
1	A	45	C
1	A	69	C
1	A	71	A
1	A	72	U
1	A	74	A
1	A	75	G
1	A	84	A
1	A	90	U
1	A	99	U
1	A	102	G
1	A	103	A
1	A	118	A
1	A	119	A

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Mol	Chain	Res	Type
1	A	120	U
1	A	139(A)	G
1	A	141	A
1	A	154	G
1	A	154(A)	C
1	A	157	U
1	A	173	G
1	A	181	A
1	A	182	A
1	A	196	A
1	A	197	A
1	A	204	A
1	A	205	G
1	A	215	G
1	A	216	A
1	A	221	A
1	A	222	A
1	A	225	A
1	A	229	A
1	A	233	A
1	A	248	G
1	A	250	G
1	A	265	A
1	A	271(I)	G
1	A	271(K)	U
1	A	271(L)	U
1	A	271(M)	G
1	A	271(N)	U
1	A	271(O)	C
1	A	271(R)	G
1	A	272(B)	G
1	A	286	C
1	A	311	A
1	A	324	A
1	A	329	G
1	A	330	A
1	A	332	A
1	A	333	G
1	A	342	G
1	A	352	G
1	A	363	G
1	A	363(F)	A

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Mol	Chain	Res	Type
1	A	386	G
1	A	396	G
1	A	405	U
1	A	406	G
1	A	411	G
1	A	412	A
1	A	415	A
1	A	422	A
1	A	427	U
1	A	428	A
1	A	429	A
1	A	444	C
1	A	448	U
1	A	454	A
1	A	455	C
1	A	470	A
1	A	475	U
1	A	480	A
1	A	481	G
1	A	482	A
1	A	504	U
1	A	505	A
1	A	509	C
1	A	530	G
1	A	531	C
1	A	532	A
1	A	533	G
1	A	545	G
1	A	546	C
1	A	549	G
1	A	556	G
1	A	563	G
1	A	573	G
1	A	575	A
1	A	586	A
1	A	587	C
1	A	588	U
1	A	603	A
1	A	604	G
1	A	606	U
1	A	607	U
1	A	614(B)	G

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Mol	Chain	Res	Type
1	A	615	G
1	A	619	G
1	A	627	A
1	A	637	A
1	A	645	C
1	A	646	A
1	A	647	G
1	A	652(B)	A
1	A	652(C)	G
1	A	652(E)	G
1	A	652(U)	G
1	A	669	G
1	A	686	G
1	A	707	G
1	A	708	C
1	A	730	C
1	A	752	A
1	A	753	C
1	A	764	A
1	A	765	G
1	A	775	G
1	A	776	G
1	A	782	A
1	A	784	A
1	A	785	G
1	A	790	C
1	A	792	G
1	A	805	G
1	A	812	C
1	A	819	A
1	A	827	U
1	A	828	U
1	A	830	G
1	A	857	C
1	A	859	G
1	A	866	A
1	A	880	G
1	A	884	C
1	A	885	C
1	A	886	C
1	A	888	C
1	A	889	C

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Mol	Chain	Res	Type
1	A	890	A
1	A	896	A
1	A	897	C
1	A	899	A
1	A	900	A
1	A	901	A
1	A	910	A
1	A	916	G
1	A	917	A
1	A	932	G
1	A	938	G
1	A	941	A
1	A	945	A
1	A	946	G
1	A	958	U
1	A	959	A
1	A	961	C
1	A	974	G
1	A	975	C
1	A	983	A
1	A	996	A
1	A	1005	C
1	A	1012	U
1	A	1013	C
1	A	1022	G
1	A	1026	U
1	A	1027	A
1	A	1033	U
1	A	1038	C
1	A	1039	G
1	A	1042	G
1	A	1043	C
1	A	1128	A
1	A	1129	A
1	A	1130	U
1	A	1135	C
1	A	1136	G
1	A	1139	G
1	A	1155	A
1	A	1170	G
1	A	1171	G
1	A	1210	A

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Mol	Chain	Res	Type
1	A	1211	U
1	A	1219	G
1	A	1220	A
1	A	1253	A
1	A	1256	G
1	A	1271	G
1	A	1272	A
1	A	1273	U
1	A	1287	A
1	A	1288	U
1	A	1300	U
1	A	1301	A
1	A	1303	G
1	A	1305	C
1	A	1308	A
1	A	1314	C
1	A	1321	A
1	A	1329	U
1	A	1345	C
1	A	1352	U
1	A	1359	A
1	A	1360	A
1	A	1365	A
1	A	1370	C
1	A	1373	A
1	A	1380	G
1	A	1384	A
1	A	1385	G
1	A	1386	C
1	A	1404	C
1	A	1416	G
1	A	1417	C
1	A	1419	A
1	A	1421	G
1	A	1427	A
1	A	1428	C
1	A	1436	G
1	A	1437	C
1	A	1445	A
1	A	1449	A
1	A	1450	G
1	A	1452	A

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Mol	Chain	Res	Type
1	A	1459	G
1	A	1467	C
1	A	1471	A
1	A	1472	A
1	A	1482	G
1	A	1488	G
1	A	1489	U
1	A	1493	C
1	A	1496	A
1	A	1497	U
1	A	1507	A
1	A	1508	A
1	A	1509	C
1	A	1509(A)	A
1	A	1525	G
1	A	1531	C
1	A	1533	G
1	A	1537	G
1	A	1541	G
1	A	1542	A
1	A	1543	C
1	A	1547	C
1	A	1558	A
1	A	1559	G
1	A	1566	A
1	A	1569	A
1	A	1578	U
1	A	1580	A
1	A	1581	G
1	A	1582	C
1	A	1584	C
1	A	1586	A
1	A	1588	C
1	A	1598	C
1	A	1608	A
1	A	1609	A
1	A	1610	A
1	A	1617	C
1	A	1631	C
1	A	1640	C
1	A	1647	G
1	A	1648	C

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Mol	Chain	Res	Type
1	A	1654	A
1	A	1674	G
1	A	1696	G
1	A	1700	A
1	A	1701	A
1	A	1703	G
1	A	1721	G
1	A	1722	A
1	A	1739	U
1	A	1740	G
1	A	1742	G
1	A	1746	G
1	A	1756	G
1	A	1762	A
1	A	1763	G
1	A	1764	G
1	A	1773	A
1	A	1780	A
1	A	1782	C
1	A	1791	A
1	A	1799	G
1	A	1800	C
1	A	1801	G
1	A	1816	G
1	A	1820	U
1	A	1829	A
1	A	1830	C
1	A	1835	G
1	A	1839	G
1	A	1847	A
1	A	1858	G
1	A	1861	G
1	A	1877	A
1	A	1878	G
1	A	1881	C
1	A	1882	C
1	A	1889	A
1	A	1900	A
1	A	1906	G
1	A	1913	A
1	A	1914	C
1	A	1929	G

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Mol	Chain	Res	Type
1	A	1930	G
1	A	1934	C
1	A	1936	A
1	A	1937	A
1	A	1938	A
1	A	1955	U
1	A	1963	U
1	A	1967	C
1	A	1969	A
1	A	1970	A
1	A	1971	A
1	A	1972	A
1	A	1982	C
1	A	1991	U
1	A	1992	G
1	A	1993	U
1	A	1997	G
1	A	2020	A
1	A	2023	G
1	A	2031	A
1	A	2033	A
1	A	2036	C
1	A	2043	C
1	A	2055	C
1	A	2056	G
1	A	2060	A
1	A	2061	G
1	A	2062	A
1	A	2069	G
1	A	2102	U
1	A	2103	C
1	A	2105	C
1	A	2107	C
1	A	2108	C
1	A	2113	U
1	A	2116	G
1	A	2117	A
1	A	2118	U
1	A	2120	G
1	A	2126	A
1	A	2127	G
1	A	2131	G

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Mol	Chain	Res	Type
1	A	2133	G
1	A	2134	A
1	A	2138	C
1	A	2142	C
1	A	2144	U
1	A	2145	C
1	A	2146	C
1	A	2147	G
1	A	2148	G
1	A	2154	G
1	A	2159	G
1	A	2160	G
1	A	2165	G
1	A	2166	G
1	A	2172	U
1	A	2173	A
1	A	2174	C
1	A	2185	C
1	A	2186	G
1	A	2187	G
1	A	2190	G
1	A	2191	G
1	A	2192	G
1	A	2193	G
1	A	2198	A
1	A	2199	A
1	A	2200	C
1	A	2206	G
1	A	2207	G
1	A	2208	A
1	A	2218	U
1	A	2219	G
1	A	2225	A
1	A	2239	G
1	A	2240	C
1	A	2267	A
1	A	2268	A
1	A	2275	C
1	A	2283	C
1	A	2287	A
1	A	2289	G
1	A	2296	U

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Mol	Chain	Res	Type
1	A	2297	C
1	A	2305	A
1	A	2311	A
1	A	2318	G
1	A	2319	G
1	A	2320	A
1	A	2321	G
1	A	2325	G
1	A	2327	A
1	A	2334	G
1	A	2336	A
1	A	2347	C
1	A	2350	C
1	A	2370	G
1	A	2383	G
1	A	2385	C
1	A	2393	A
1	A	2400	G
1	A	2406	U
1	A	2410	G
1	A	2414	G
1	A	2422	A
1	A	2423	U
1	A	2425	A
1	A	2429	G
1	A	2430	A
1	A	2431	U
1	A	2435	A
1	A	2439	A
1	A	2441	C
1	A	2448	A
1	A	2465	C
1	A	2469	A
1	A	2474	C
1	A	2476	A
1	A	2478	A
1	A	2498	C
1	A	2502	G
1	A	2505	G
1	A	2506	U
1	A	2518	A
1	A	2525	G

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Mol	Chain	Res	Type
1	A	2529	G
1	A	2535	G
1	A	2549	G
1	A	2554	U
1	A	2555	U
1	A	2566	A
1	A	2567	G
1	A	2573	C
1	A	2602	A
1	A	2603	G
1	A	2611	U
1	A	2612	C
1	A	2615	U
1	A	2629	A
1	A	2630	G
1	A	2663	G
1	A	2673	G
1	A	2675	A
1	A	2689	U
1	A	2690	C
1	A	2702	U
1	A	2703	C
1	A	2712(A)	A
1	A	2713	A
1	A	2714	G
1	A	2726	U
1	A	2733	A
1	A	2757	A
1	A	2758	A
1	A	2760	C
1	A	2765	A
1	A	2766	G
1	A	2778	A
1	A	2789	C
1	A	2790	A
1	A	2791	C
1	A	2802	G
1	A	2803	C
1	A	2808	U
1	A	2820	A
1	A	2821	A
1	A	2834	G

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Mol	Chain	Res	Type
1	A	2835	A
1	A	2847	U
1	A	2872	G
1	A	2880	C
1	A	2892	A
1	A	2895	U
1	A	2897	U
2	B	2	C
2	B	5	C
2	B	7	G
2	B	9	G
2	B	13	A
2	B	19	G
2	B	20	C
2	B	24	G
2	B	25	A
2	B	40	U
2	B	42	C
2	B	47	C
2	B	50	G
2	B	53	A
2	B	54	G
2	B	56	G
2	B	73	A
2	B	75	G
2	B	106	G
2	B	110	G
2	B	116	G

All (64) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	9	U
1	A	71	A
1	A	102	G
1	A	196	A
1	A	199	A
1	A	215	G
1	A	249	C
1	A	271(K)	U
1	A	271(M)	G
1	A	310	A

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Mol	Chain	Res	Type
1	A	363(E)	U
1	A	405	U
1	A	474	G
1	A	481	G
1	A	587	C
1	A	669	G
1	A	685	A
1	A	746	A
1	A	752	A
1	A	764	A
1	A	774	A
1	A	827	U
1	A	856	C
1	A	859	G
1	A	900	A
1	A	958	U
1	A	974	G
1	A	1026	U
1	A	1155	A
1	A	1210	A
1	A	1300	U
1	A	1301	A
1	A	1379	A
1	A	1420	U
1	A	1427	A
1	A	1507	A
1	A	1530	C
1	A	1558	A
1	A	1608	A
1	A	1617	C
1	A	1653	G
1	A	1799	G
1	A	1800	C
1	A	1819	A
1	A	1913	A
1	A	1992	G
1	A	2126	A
1	A	2171	A
1	A	2172	U
1	A	2207	G
1	A	2288	A
1	A	2318	G

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Mol	Chain	Res	Type
1	A	2406	U
1	A	2422	A
1	A	2430	A
1	A	2439	A
1	A	2602	A
1	A	2611	U
1	A	2689	U
1	A	2726	U
1	A	2756	U
1	A	2778	A
1	A	2789	C
1	A	2802	G

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 684 ligands modelled in this entry, 684 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	2798/2915 (95%)	0.55	182 (6%)	18 21	27, 46, 118, 170	0
2	B	120/122 (98%)	1.16	24 (20%)	2 2	50, 81, 97, 130	0
3	D	275/276 (99%)	0.69	26 (9%)	8 8	26, 43, 55, 84	0
4	E	204/206 (99%)	0.91	25 (12%)	5 5	27, 48, 69, 84	0
5	F	203/210 (96%)	0.88	31 (15%)	3 3	28, 58, 84, 115	0
6	G	181/182 (99%)	2.65	92 (50%)	0 0	78, 96, 116, 140	0
7	H	174/180 (96%)	2.23	79 (45%)	1 0	61, 78, 92, 101	0
8	I	146/148 (98%)	1.24	38 (26%)	1 1	49, 81, 99, 107	0
9	N	140/140 (100%)	1.09	27 (19%)	2 2	35, 52, 73, 86	0
10	O	122/122 (100%)	0.89	21 (17%)	2 2	37, 47, 65, 68	0
11	P	149/150 (99%)	1.54	42 (28%)	1 1	30, 60, 87, 99	0
12	Q	141/141 (100%)	1.05	22 (15%)	3 3	39, 55, 69, 79	0
13	R	118/118 (100%)	0.78	13 (11%)	6 6	33, 42, 55, 67	0
14	S	110/112 (98%)	2.26	48 (43%)	1 0	59, 74, 87, 93	0
15	T	130/146 (89%)	0.83	18 (13%)	4 4	41, 50, 73, 105	0
16	U	116/118 (98%)	0.77	14 (12%)	5 5	33, 45, 61, 70	0
17	V	101/101 (100%)	1.03	20 (19%)	2 2	32, 59, 76, 85	0
18	W	111/113 (98%)	0.85	18 (16%)	2 3	32, 40, 58, 85	0
19	X	95/96 (98%)	1.08	13 (13%)	4 4	39, 50, 68, 89	0
20	Y	107/110 (97%)	2.39	50 (46%)	1 0	53, 63, 82, 91	0
21	Z	203/206 (98%)	1.86	76 (37%)	1 1	57, 78, 100, 126	0
22	0	77/85 (90%)	1.38	20 (25%)	1 1	44, 52, 67, 101	0
23	1	97/98 (98%)	1.26	18 (18%)	2 2	33, 48, 78, 85	0
24	2	71/72 (98%)	1.28	17 (23%)	1 1	51, 65, 76, 94	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	3	59/60 (98%)	1.24	12 (20%) 1 2	39, 50, 76, 96	0
26	4	46/71 (64%)	1.54	14 (30%) 1 1	89, 107, 118, 124	0
27	5	59/60 (98%)	0.67	6 (10%) 7 7	27, 43, 61, 73	0
28	6	53/54 (98%)	0.82	7 (13%) 4 4	47, 52, 60, 70	0
29	7	48/49 (97%)	1.42	13 (27%) 1 1	28, 33, 54, 82	0
30	8	64/65 (98%)	1.25	14 (21%) 1 2	38, 44, 50, 60	0
31	9	36/37 (97%)	1.77	14 (38%) 1 1	45, 55, 66, 76	0
All	All	6354/6563 (96%)	0.97	1014 (15%) 3 3	26, 51, 101, 170	0

All (1014) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2164	C	14.3
1	A	1533	G	11.7
14	S	54	LEU	11.2
6	G	25	TYR	10.6
1	A	2136	C	10.2
31	9	37	GLY	10.2
7	H	171	LEU	10.0
4	E	204	ALA	9.9
11	P	1	MET	9.9
7	H	43	VAL	9.9
6	G	182	LYS	9.8
3	D	276	LYS	9.5
6	G	120	LEU	9.3
21	Z	202	GLU	9.2
6	G	39	ILE	8.9
12	Q	59	ARG	8.9
21	Z	3	TYR	8.6
7	H	12	PRO	8.5
1	A	2176	A	8.4
6	G	92	VAL	8.4
7	H	108	GLY	8.2
14	S	56	LEU	8.0
1	A	1113	U	8.0
20	Y	1	MET	7.9
20	Y	89	PHE	7.8
6	G	97	ASP	7.7
21	Z	190	GLU	7.6
21	Z	1	MET	7.5

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Mol	Chain	Res	Type	RSRZ
1	A	2124	G	7.3
3	D	127	VAL	7.3
13	R	101	ALA	7.2
1	A	614(B)	G	7.2
1	A	2116	G	7.1
6	G	19	LEU	7.0
13	R	100	LEU	7.0
14	S	8	GLU	7.0
6	G	21	ARG	7.0
23	1	2	SER	7.0
1	A	2159	G	6.9
20	Y	29	GLU	6.9
8	I	126	TYR	6.9
20	Y	55	TYR	6.9
20	Y	90	LEU	6.9
6	G	49	ASP	6.8
6	G	134	GLY	6.8
6	G	26	GLN	6.7
1	A	1041	C	6.7
6	G	35	GLU	6.7
6	G	17	PRO	6.7
25	3	50	VAL	6.7
20	Y	3	VAL	6.6
6	G	69	ALA	6.6
29	7	47	ARG	6.6
7	H	13	LYS	6.6
14	S	55	ALA	6.5
6	G	2	PRO	6.5
20	Y	28	LYS	6.5
6	G	96	ARG	6.5
27	5	25	LEU	6.4
26	4	32	TYR	6.4
21	Z	91	LEU	6.4
6	G	146	TYR	6.4
1	A	2790	A	6.4
8	I	57	ARG	6.4
7	H	76	VAL	6.4
6	G	82	LEU	6.3
20	Y	63	LYS	6.3
1	A	2172	U	6.3
1	A	2140	C	6.2
20	Y	94	LYS	6.2

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Mol	Chain	Res	Type	RSRZ
7	H	58	GLU	6.2
20	Y	93	GLY	6.2
7	H	109	PHE	6.2
20	Y	45	VAL	6.2
21	Z	194	PRO	6.2
6	G	157	ILE	6.2
1	A	2789	C	6.2
1	A	2169	A	6.1
8	I	58	LEU	6.1
1	A	2165	G	6.1
7	H	19	VAL	6.1
14	S	102	ALA	6.1
1	A	2191	G	6.0
6	G	27	ASN	6.0
1	A	2125	G	6.0
21	Z	162	GLU	6.0
6	G	33	ARG	6.0
27	5	58	LEU	5.9
16	U	89	GLU	5.9
1	A	2134	A	5.9
20	Y	66	PRO	5.9
12	Q	112	GLU	5.9
20	Y	41	GLY	5.9
6	G	30	GLU	5.9
1	A	281	G	5.9
1	A	2166	G	5.9
21	Z	164	ALA	5.8
11	P	4	SER	5.8
24	2	9	GLN	5.8
1	A	2174	C	5.8
17	V	48	GLY	5.8
29	7	46	VAL	5.7
26	4	30	GLU	5.7
11	P	45	LEU	5.7
19	X	13	LEU	5.7
6	G	138	GLN	5.7
11	P	3	LEU	5.7
20	Y	22	GLY	5.7
7	H	159	GLU	5.6
7	H	101	ARG	5.6
7	H	72	ILE	5.6
6	G	38	VAL	5.6

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Mol	Chain	Res	Type	RSRZ
28	6	54	ILE	5.6
1	A	2135	A	5.5
7	H	44	VAL	5.5
1	A	1532	C	5.5
15	T	112	ARG	5.5
1	A	2802	G	5.5
20	Y	91	GLU	5.5
11	P	98	GLU	5.5
5	F	188	ARG	5.5
19	X	66	LEU	5.5
22	O	74	ARG	5.5
14	S	58	LEU	5.5
6	G	24	GLY	5.5
1	A	1509	C	5.4
11	P	135	LEU	5.4
14	S	20	ARG	5.4
20	Y	73	ARG	5.4
1	A	2171	A	5.4
17	V	72	VAL	5.4
1	A	2309	A	5.3
19	X	56	THR	5.3
1	A	2177	C	5.3
30	8	23	VAL	5.3
14	S	3	ARG	5.3
5	F	208	GLY	5.3
21	Z	191	VAL	5.3
14	S	52	SER	5.3
6	G	136	ARG	5.3
6	G	147	ASP	5.2
1	A	2139	C	5.2
20	Y	42	VAL	5.2
14	S	57	LYS	5.2
25	3	19	GLN	5.2
6	G	20	ILE	5.2
1	A	2173	A	5.1
9	N	5	VAL	5.1
11	P	149	GLU	5.1
5	F	131	GLY	5.1
15	T	78	LEU	5.1
14	S	44	LYS	5.1
6	G	18	GLU	5.1
9	N	140	VAL	5.1

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Mol	Chain	Res	Type	RSRZ
20	Y	32	PRO	5.1
31	9	17	ILE	5.1
4	E	203	LYS	5.1
24	2	58	ALA	5.1
6	G	68	PRO	5.1
10	O	114	ILE	5.1
10	O	48	PRO	5.0
20	Y	23	ARG	5.0
22	0	84	LEU	5.0
7	H	105	LEU	5.0
20	Y	14	LEU	5.0
11	P	76	LYS	5.0
1	A	1913	A	5.0
14	S	80	LEU	5.0
11	P	109	GLY	5.0
17	V	1	MET	5.0
7	H	173	PRO	5.0
24	2	46	GLN	5.0
1	A	2103	C	4.9
7	H	60	ARG	4.9
20	Y	92	ASN	4.9
19	X	23	GLU	4.9
21	Z	9	TYR	4.9
26	4	11	PRO	4.9
1	A	2129	C	4.9
19	X	51	VAL	4.9
7	H	165	ALA	4.9
1	A	2160	G	4.9
6	G	84	LYS	4.9
11	P	146	VAL	4.9
7	H	30	LYS	4.9
24	2	13	ALA	4.9
8	I	92	VAL	4.8
14	S	59	LYS	4.8
17	V	73	SER	4.8
1	A	352	G	4.8
7	H	75	ALA	4.8
6	G	37	VAL	4.8
21	Z	126	VAL	4.8
14	S	65	VAL	4.8
21	Z	42	VAL	4.8
6	G	162	THR	4.8

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Mol	Chain	Res	Type	RSRZ
13	R	77	ARG	4.8
21	Z	70	LEU	4.8
14	S	5	THR	4.8
8	I	21	VAL	4.7
20	Y	24	VAL	4.7
21	Z	56	VAL	4.7
29	7	48	LYS	4.7
6	G	29	TRP	4.7
7	H	92	ILE	4.7
6	G	94	LEU	4.7
8	I	72	LEU	4.7
6	G	160	VAL	4.7
1	A	2155	G	4.7
22	0	71	ASP	4.7
29	7	23	ARG	4.7
21	Z	196	VAL	4.7
8	I	91	SER	4.7
1	A	1043	C	4.7
20	Y	4	LYS	4.6
7	H	81	GLU	4.6
1	A	900	A	4.6
6	G	34	LEU	4.6
13	R	111	LEU	4.6
9	N	1	MET	4.6
12	Q	18	LYS	4.6
14	S	40	ILE	4.6
20	Y	44	ILE	4.6
21	Z	175	VAL	4.6
3	D	275	LYS	4.6
14	S	12	PHE	4.6
6	G	121	ASN	4.6
17	V	38	LEU	4.6
12	Q	22	LYS	4.5
21	Z	203	GLU	4.5
1	A	1207	C	4.5
8	I	41	GLU	4.5
7	H	172	LYS	4.5
17	V	47	VAL	4.5
14	S	21	THR	4.5
1	A	2133	G	4.5
24	2	49	LYS	4.5
21	Z	80	ARG	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	2791	C	4.5
19	X	69	TYR	4.5
23	1	98	LEU	4.5
3	D	8	PRO	4.5
16	U	36	ARG	4.5
1	A	1116	C	4.4
21	Z	156	LYS	4.4
11	P	79	ARG	4.4
27	5	60	VAL	4.4
17	V	71	LEU	4.4
23	1	37	ILE	4.4
12	Q	92	GLY	4.4
14	S	50	SER	4.4
20	Y	87	LYS	4.4
9	N	9	VAL	4.4
6	G	98	ARG	4.3
12	Q	60	ARG	4.3
21	Z	100	VAL	4.3
24	2	1	MET	4.3
1	A	652(A)	A	4.3
21	Z	138	GLU	4.3
4	E	1	MET	4.3
6	G	163	ALA	4.3
21	Z	50	GLN	4.3
1	A	2158	A	4.3
26	4	23	GLU	4.3
1	A	1886	C	4.3
8	I	65	ALA	4.3
4	E	26	ILE	4.3
16	U	73	GLY	4.2
10	O	53	LYS	4.2
1	A	2101	G	4.2
11	P	94	GLU	4.2
12	Q	16	ARG	4.2
1	A	1463	C	4.2
1	A	2163	C	4.2
1	A	1530	C	4.2
7	H	82	GLY	4.2
6	G	149	VAL	4.2
7	H	29	PRO	4.2
11	P	15	ARG	4.2
1	A	2894	G	4.1

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Mol	Chain	Res	Type	RSRZ
9	N	118	LYS	4.1
8	I	61	ARG	4.1
14	S	31	SER	4.1
5	F	133	ASN	4.1
1	A	1919	A	4.1
1	A	272(H)	C	4.1
20	Y	57	GLN	4.1
6	G	32	PRO	4.1
5	F	184	TYR	4.1
30	8	50	LEU	4.1
24	2	7	ARG	4.1
6	G	161	THR	4.1
8	I	20	ASP	4.1
8	I	127	VAL	4.0
11	P	73	GLY	4.0
11	P	147	LEU	4.0
8	I	1	MET	4.0
6	G	36	LYS	4.0
11	P	2	LYS	4.0
20	Y	65	ALA	4.0
21	Z	75	ASN	4.0
1	A	2122	U	4.0
7	H	83	TYR	4.0
7	H	64	LEU	4.0
13	R	102	GLU	4.0
21	Z	136	PHE	4.0
12	Q	19	GLY	4.0
7	H	37	VAL	3.9
18	W	44	ALA	3.9
1	A	271(K)	U	3.9
10	O	8	LEU	3.9
21	Z	51	ALA	3.9
21	Z	71	VAL	3.9
21	Z	97	GLU	3.9
21	Z	99	TYR	3.9
1	A	2190	G	3.9
2	B	110	G	3.9
7	H	100	GLY	3.9
20	Y	2	ARG	3.9
21	Z	2	GLU	3.9
12	Q	1	MET	3.8
14	S	60	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	1907	G	3.8
1	A	2792	G	3.8
7	H	157	TYR	3.8
9	N	92	ALA	3.8
6	G	54	GLU	3.8
11	P	144	GLU	3.8
6	G	70	VAL	3.8
7	H	136	ILE	3.8
1	A	2104	G	3.8
1	A	2123	G	3.8
20	Y	56	PRO	3.8
10	O	57	VAL	3.8
1	A	2175	C	3.8
21	Z	124	ILE	3.8
6	G	164	GLU	3.8
1	A	2162	G	3.8
23	1	60	PHE	3.8
8	I	107	VAL	3.8
20	Y	72	VAL	3.8
14	S	73	LEU	3.8
22	0	75	LEU	3.8
1	A	229	A	3.8
1	A	2334	G	3.8
14	S	101	LEU	3.8
21	Z	134	PRO	3.7
9	N	48	MET	3.7
23	1	4	VAL	3.7
21	Z	55	HIS	3.7
3	D	252	TRP	3.7
1	A	171	G	3.7
1	A	2157	G	3.7
7	H	155	SER	3.7
29	7	38	GLY	3.7
27	5	59	GLU	3.7
7	H	123	PHE	3.7
10	O	97	ARG	3.7
25	3	49	LYS	3.7
9	N	8	GLN	3.7
21	Z	142	SER	3.7
16	U	88	ILE	3.7
14	S	76	LYS	3.7
3	D	57	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
7	H	50	VAL	3.7
18	W	17	VAL	3.7
21	Z	98	MET	3.7
11	P	68	GLN	3.7
7	H	131	VAL	3.7
7	H	77	LYS	3.6
25	3	60	GLU	3.7
6	G	123	ASN	3.6
21	Z	4	ARG	3.6
21	Z	147	GLY	3.6
19	X	45	THR	3.6
8	I	79	ILE	3.6
20	Y	58	GLY	3.6
1	A	2148	G	3.6
5	F	33	LEU	3.6
1	A	878	A	3.6
6	G	74	LYS	3.6
7	H	15	VAL	3.6
19	X	95	LEU	3.6
20	Y	67	LEU	3.6
1	A	2156	G	3.6
11	P	129	ALA	3.6
31	9	23	VAL	3.6
20	Y	34	LYS	3.6
4	E	128	SER	3.6
26	4	25	TYR	3.6
14	S	66	ALA	3.6
1	A	2146	C	3.6
12	Q	6	ARG	3.6
14	S	69	VAL	3.6
15	T	10	VAL	3.6
23	1	70	VAL	3.5
11	P	56	SER	3.5
7	H	71	LEU	3.5
4	E	81	ILE	3.5
14	S	19	LYS	3.5
6	G	15	VAL	3.5
14	S	17	ARG	3.5
11	P	96	THR	3.5
1	A	1910	G	3.5
9	N	10	GLU	3.5
14	S	7	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	2132	U	3.5
18	W	19	LEU	3.5
6	G	63	ILE	3.5
1	A	362	U	3.5
7	H	115	VAL	3.5
1	A	2187	G	3.5
6	G	93	THR	3.5
4	E	129	HIS	3.5
23	1	7	ILE	3.5
6	G	181	ARG	3.4
7	H	59	ARG	3.4
1	A	2112	G	3.4
3	D	7	LYS	3.4
26	4	29	PRO	3.4
6	G	3	LEU	3.4
10	O	7	TYR	3.4
21	Z	37	VAL	3.4
1	A	2442	C	3.4
22	0	11	ARG	3.4
1	A	2803	C	3.4
20	Y	40	GLU	3.4
21	Z	74	VAL	3.4
2	B	56	G	3.4
21	Z	137	ILE	3.4
1	A	652(B)	A	3.4
3	D	5	LYS	3.4
11	P	148	LEU	3.4
24	2	21	LEU	3.4
3	D	4	LYS	3.4
8	I	38	LEU	3.4
1	A	11	G	3.4
1	A	2141	G	3.4
31	9	22	ARG	3.4
2	B	62	C	3.4
8	I	121	LYS	3.4
25	3	9	VAL	3.4
18	W	95	ILE	3.4
15	T	57	PHE	3.3
1	A	2126	A	3.3
1	A	2750	A	3.3
30	8	29	LYS	3.3
24	2	41	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
10	O	17	ARG	3.3
8	I	60	GLU	3.3
24	2	45	SER	3.3
1	A	1641	A	3.3
1	A	2115	G	3.3
1	A	2168	G	3.3
2	B	23	G	3.3
21	Z	78	LYS	3.3
25	3	20	LYS	3.3
21	Z	133	ILE	3.3
16	U	112	ARG	3.3
1	A	2150	U	3.3
6	G	60	LEU	3.3
7	H	98	LEU	3.3
24	2	35	LEU	3.3
1	A	1146	C	3.3
6	G	28	VAL	3.3
9	N	98	VAL	3.3
29	7	8	ASN	3.3
20	Y	20	TYR	3.3
14	S	4	LEU	3.3
21	Z	140	ASP	3.3
1	A	2100	G	3.3
1	A	2111	C	3.3
6	G	72	ARG	3.3
7	H	27	LYS	3.3
7	H	78	GLY	3.3
8	I	35	LEU	3.3
8	I	44	LEU	3.3
10	O	19	ILE	3.3
10	O	18	LYS	3.3
11	P	64	LYS	3.3
14	S	43	GLU	3.3
20	Y	21	LYS	3.3
5	F	14	PRO	3.2
9	N	49	GLY	3.2
23	1	72	GLU	3.2
10	O	40	VAL	3.2
1	A	2117	A	3.2
6	G	13	GLU	3.2
21	Z	59	LEU	3.2
14	S	23	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
22	0	17	GLN	3.2
14	S	64	GLU	3.2
3	D	2	ALA	3.2
6	G	66	GLN	3.2
1	A	2138	C	3.2
2	B	52	A	3.2
3	D	128	GLY	3.2
11	P	74	GLU	3.2
15	T	93	ARG	3.2
21	Z	143	GLY	3.2
26	4	45	GLY	3.2
21	Z	176	PRO	3.2
1	A	283	A	3.2
29	7	45	ALA	3.2
21	Z	199	LYS	3.2
30	8	20	GLY	3.2
14	S	61	ASN	3.1
26	4	2	LYS	3.1
5	F	134	GLY	3.1
31	9	16	VAL	3.1
23	1	61	ARG	3.1
7	H	61	HIS	3.1
8	I	106	GLY	3.1
21	Z	96	VAL	3.1
30	8	2	PRO	3.1
9	N	60	ILE	3.1
21	Z	18	LEU	3.1
18	W	1	MET	3.1
21	Z	110	GLY	3.1
20	Y	64	GLU	3.1
17	V	81	TYR	3.1
8	I	37	VAL	3.1
21	Z	161	VAL	3.1
4	E	14	ILE	3.1
1	A	2170	A	3.1
6	G	87	PRO	3.1
7	H	10	PRO	3.1
7	H	45	VAL	3.1
12	Q	27	VAL	3.1
17	V	37	VAL	3.1
17	V	68	LYS	3.1
10	O	22	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
4	E	89	ASP	3.1
15	T	14	TYR	3.1
17	V	74	LYS	3.1
20	Y	43	ASN	3.1
3	D	105	ILE	3.1
7	H	57	ASP	3.1
6	G	23	PHE	3.0
9	N	121	LYS	3.0
1	A	645	C	3.0
4	E	27	LEU	3.0
28	6	52	VAL	3.0
31	9	36	GLN	3.0
4	E	168	MET	3.0
11	P	75	ILE	3.0
1	A	1739	U	3.0
16	U	2	PRO	3.0
15	T	37	GLY	3.0
20	Y	35	TYR	3.0
21	Z	5	LEU	3.0
21	Z	139	VAL	3.0
17	V	70	ILE	3.0
1	A	1963	U	3.0
1	A	2602	A	3.0
6	G	124	SER	3.0
23	1	73	LEU	3.0
7	H	80	SER	3.0
1	A	1536	C	3.0
1	A	2182	G	3.0
6	G	176	LEU	3.0
21	Z	11	GLU	3.0
21	Z	92	SER	3.0
21	Z	61	LEU	3.0
7	H	17	VAL	3.0
22	0	18	ALA	3.0
2	B	54	G	3.0
1	A	1543	C	3.0
1	A	1236	G	2.9
5	F	81	PRO	2.9
24	2	56	GLN	2.9
11	P	128	HIS	2.9
1	A	1885	A	2.9
6	G	99	MET	2.9

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Mol	Chain	Res	Type	RSRZ
27	5	28	PRO	2.9
8	I	108	THR	2.9
1	A	154	G	2.9
7	H	111	HIS	2.9
30	8	15	LYS	2.9
2	B	13	A	2.9
8	I	63	ALA	2.9
26	4	13	ARG	2.9
1	A	1450	G	2.9
2	B	83	G	2.9
7	H	122	THR	2.9
26	4	10	VAL	2.9
6	G	50	ALA	2.9
21	Z	158	PRO	2.9
23	1	95	LEU	2.9
1	A	132	G	2.9
1	A	2131	G	2.9
7	H	16	SER	2.9
14	S	62	LYS	2.9
12	Q	66	ILE	2.9
26	4	9	LEU	2.9
1	A	45	C	2.9
7	H	169	VAL	2.9
11	P	95	VAL	2.9
7	H	6	ARG	2.9
1	A	655	A	2.9
1	A	2119	A	2.9
2	B	12	C	2.9
1	A	272(I)	U	2.9
1	A	2296	U	2.9
6	G	95	ARG	2.8
7	H	24	VAL	2.8
3	D	15	PHE	2.8
7	H	148	ILE	2.8
9	N	23	LEU	2.8
15	T	47	GLY	2.8
7	H	134	SER	2.8
6	G	91	ARG	2.8
22	0	20	ARG	2.8
6	G	43	LEU	2.8
6	G	175	LEU	2.8
20	Y	31	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
12	Q	23	GLY	2.8
14	S	75	GLU	2.8
17	V	50	PRO	2.8
11	P	65	ARG	2.8
15	T	95	ARG	2.8
4	E	170	LEU	2.8
18	W	86	LEU	2.8
11	P	130	PHE	2.8
13	R	91	GLN	2.8
5	F	174	VAL	2.8
1	A	2314	C	2.8
2	B	27	C	2.8
4	E	82	ARG	2.8
19	X	1	MET	2.8
1	A	1026	U	2.8
24	2	11	GLU	2.8
11	P	51	PHE	2.8
20	Y	27	VAL	2.8
3	D	240	ALA	2.8
6	G	57	ALA	2.8
9	N	2	LYS	2.8
20	Y	54	LYS	2.8
6	G	131	TYR	2.8
21	Z	38	TYR	2.8
23	1	14	VAL	2.8
9	N	46	VAL	2.8
17	V	49	THR	2.8
31	9	3	VAL	2.8
16	U	83	LEU	2.7
10	O	45	GLU	2.7
30	8	40	GLU	2.7
18	W	103	ILE	2.7
14	S	42	ASP	2.7
22	0	26	TYR	2.7
7	H	166	GLY	2.7
1	A	1464	C	2.7
22	0	53	MET	2.7
1	A	1112	G	2.7
1	A	1461	G	2.7
7	H	25	LYS	2.7
8	I	101	LEU	2.7
9	N	26	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	504	U	2.7
21	Z	187	ALA	2.7
6	G	58	GLN	2.7
23	1	13	ILE	2.7
1	A	2121	G	2.7
4	E	83	ASP	2.7
7	H	42	ARG	2.7
8	I	83	ALA	2.7
15	T	111	ARG	2.7
23	1	93	GLU	2.7
1	A	896	A	2.7
1	A	1379	A	2.7
1	A	2801(A)	A	2.7
11	P	99	LEU	2.7
16	U	98	LEU	2.7
21	Z	12	GLY	2.7
21	Z	180	VAL	2.7
26	4	12	ALA	2.7
1	A	899	A	2.7
9	N	129	PRO	2.7
15	T	107	ASP	2.7
21	Z	173	ALA	2.7
1	A	1178	C	2.7
6	G	137	GLU	2.7
1	A	361	G	2.7
18	W	6	ILE	2.7
31	9	10	ILE	2.7
11	P	59	LEU	2.6
17	V	35	LEU	2.6
25	3	16	PRO	2.6
30	8	28	GLY	2.6
15	T	113	LYS	2.6
18	W	20	VAL	2.6
1	A	1559	G	2.6
6	G	122	PRO	2.6
5	F	16	GLY	2.6
1	A	1450(A)	C	2.6
7	H	23	ARG	2.6
1	A	2535	G	2.6
20	Y	61	ILE	2.6
2	B	55	U	2.6
7	H	79	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
31	9	7	VAL	2.6
7	H	20	ALA	2.6
1	A	889	C	2.6
5	F	99	TYR	2.6
22	0	80	HIS	2.6
1	A	405	U	2.6
1	A	1906	G	2.6
13	R	80	PHE	2.6
24	2	12	GLU	2.6
7	H	54	ARG	2.6
11	P	29	LYS	2.6
1	A	2109	U	2.6
5	F	183	VAL	2.6
14	S	6	ALA	2.6
19	X	70	LEU	2.6
24	2	44	LEU	2.6
15	T	104	ASN	2.6
1	A	363	G	2.6
1	A	1042	G	2.6
1	A	1115	G	2.6
1	A	1170	G	2.6
5	F	13	SER	2.6
8	I	89	TYR	2.6
1	A	1741	A	2.6
1	A	2114	A	2.6
17	V	84	LYS	2.6
1	A	652(D)	C	2.6
1	A	2188	C	2.6
4	E	167	VAL	2.6
5	F	187	VAL	2.6
18	W	71	VAL	2.6
11	P	118	GLY	2.6
9	N	51	PHE	2.6
17	V	29	PRO	2.6
18	W	38	TYR	2.6
6	G	148	MET	2.6
14	S	72	ALA	2.6
24	2	43	GLN	2.6
16	U	56	ASP	2.5
5	F	15	SER	2.5
7	H	55	PRO	2.5
7	H	112	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
14	S	53	SER	2.5
31	9	24	TYR	2.5
11	P	101	VAL	2.5
16	U	5	LYS	2.5
1	A	2804	C	2.5
5	F	43	LYS	2.5
26	4	44	THR	2.5
21	Z	189	ALA	2.5
21	Z	166	SER	2.5
7	H	21	PRO	2.5
18	W	83	LYS	2.5
1	A	6	A	2.5
1	A	2518	A	2.5
2	B	26	A	2.5
22	0	28	GLY	2.5
5	F	155	LEU	2.5
8	I	140	LEU	2.5
13	R	99	LYS	2.5
18	W	31	GLU	2.5
21	Z	159	PRO	2.5
8	I	18	VAL	2.5
14	S	78	LEU	2.5
1	A	44	G	2.5
1	A	2206	G	2.5
1	A	2319	G	2.5
2	B	24	G	2.5
6	G	31	VAL	2.5
21	Z	157	LEU	2.5
1	A	272(A)	U	2.5
1	A	1918	A	2.5
2	B	6	C	2.5
1	A	2833	G	2.5
3	D	136	ILE	2.5
8	I	136	VAL	2.5
22	0	23	VAL	2.5
8	I	80	PRO	2.5
4	E	10	GLY	2.5
6	G	167	GLU	2.5
7	H	14	GLY	2.5
7	H	124	GLU	2.5
29	7	24	THR	2.5
12	Q	20	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
23	1	49	VAL	2.5
1	A	1114	G	2.4
31	9	18	ARG	2.4
22	0	45	PHE	2.4
5	F	160	ASN	2.4
11	P	102	ARG	2.4
14	S	63	THR	2.4
4	E	25	VAL	2.4
11	P	108	LYS	2.4
14	S	48	LEU	2.4
16	U	90	VAL	2.4
23	1	94	LEU	2.4
1	A	2441	C	2.4
1	A	2805	G	2.4
6	G	150	ASP	2.4
3	D	162	SER	2.4
5	F	42	ALA	2.4
7	H	11	VAL	2.4
25	3	6	VAL	2.4
28	6	2	ALA	2.4
10	O	101	PRO	2.4
2	B	10	C	2.4
10	O	73	ASP	2.4
1	A	43	A	2.4
2	B	58	A	2.4
1	A	770	G	2.4
25	3	15	TYR	2.4
3	D	241	PRO	2.4
1	A	280	C	2.4
8	I	36	ALA	2.4
1	A	1331	A	2.4
3	D	261	LYS	2.4
13	R	103	ARG	2.4
25	3	52	HIS	2.4
6	G	80	PHE	2.4
21	Z	60	GLU	2.4
9	N	67	LEU	2.4
20	Y	19	LYS	2.4
23	1	8	SER	2.4
1	A	2161	C	2.4
30	8	25	MET	2.4
1	A	2310	A	2.4

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Mol	Chain	Res	Type	RSRZ
10	O	56	ASP	2.4
4	E	33	VAL	2.4
16	U	74	LEU	2.4
31	9	35	ARG	2.4
4	E	126	PRO	2.4
2	B	11	C	2.4
28	6	27	LYS	2.4
7	H	170	ARG	2.4
22	0	44	ARG	2.4
30	8	47	LYS	2.3
29	7	36	GLN	2.3
11	P	31	ALA	2.3
9	N	7	LYS	2.3
31	9	8	LYS	2.3
6	G	179	PRO	2.3
4	E	19	ARG	2.3
30	8	27	THR	2.3
7	H	102	ALA	2.3
12	Q	131	ILE	2.3
21	Z	171	ILE	2.3
1	A	272(G)	C	2.3
1	A	2464	C	2.3
18	W	34	ASN	2.3
23	1	71	TYR	2.3
19	X	15	GLU	2.3
5	F	156	LEU	2.3
6	G	42	GLY	2.3
13	R	54	LEU	2.3
30	8	24	ALA	2.3
1	A	2110	G	2.3
3	D	6	PHE	2.3
1	A	1909	C	2.3
29	7	11	LYS	2.3
6	G	14	GLU	2.3
30	8	19	SER	2.3
17	V	7	THR	2.3
10	O	98	VAL	2.3
16	U	105	VAL	2.3
17	V	85	LYS	2.3
4	E	192	ASN	2.3
22	0	69	PHE	2.3
7	H	28	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
13	R	67	LEU	2.3
13	R	113	LEU	2.3
12	Q	63	LYS	2.3
25	3	51	ALA	2.3
15	T	1	MET	2.3
25	3	26	LEU	2.3
1	A	859	G	2.3
1	A	1034	G	2.3
1	A	1921	G	2.3
4	E	187	ALA	2.3
20	Y	30	VAL	2.3
20	Y	69	ALA	2.3
1	A	1887	C	2.3
2	B	64	C	2.3
5	F	162	LEU	2.3
6	G	126	ASP	2.2
7	H	35	VAL	2.2
7	H	85	LYS	2.2
3	D	260	ARG	2.2
3	D	262	ARG	2.2
5	F	44	ARG	2.2
14	S	18	ILE	2.2
18	W	111	HIS	2.2
6	G	119	GLY	2.2
12	Q	5	ARG	2.2
5	F	172	TRP	2.2
8	I	139	GLN	2.2
2	B	65	C	2.2
1	A	1591	G	2.2
1	A	1929	G	2.2
5	F	37	VAL	2.2
3	D	129	ASN	2.2
31	9	21	GLY	2.2
7	H	40	GLU	2.2
1	A	2062	A	2.2
14	S	32	LEU	2.2
12	Q	28	ALA	2.2
14	S	49	VAL	2.2
15	T	79	HIS	2.2
1	A	2145	C	2.2
5	F	28	ILE	2.2
18	W	87	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
12	Q	29	PHE	2.2
21	Z	125	LEU	2.2
12	Q	3	MET	2.2
6	G	170	ARG	2.2
22	0	33	ALA	2.2
15	T	24	PRO	2.2
27	5	41	PRO	2.2
3	D	267	SER	2.2
9	N	70	LYS	2.2
1	A	2106	G	2.2
8	I	53	ALA	2.2
30	8	21	LYS	2.2
20	Y	52	SER	2.2
7	H	33	LEU	2.2
11	P	18	ARG	2.2
29	7	10	ARG	2.2
1	A	2465	C	2.2
1	A	2475	C	2.2
28	6	30	THR	2.2
10	O	74	GLY	2.2
20	Y	51	VAL	2.2
21	Z	172	ALA	2.2
22	0	55	ARG	2.2
8	I	128	LEU	2.2
22	0	9	SER	2.1
1	A	157	U	2.1
2	B	89	G	2.1
6	G	133	LEU	2.1
4	E	130	GLY	2.1
14	S	77	ALA	2.1
10	O	115	VAL	2.1
29	7	44	PRO	2.1
29	7	14	LYS	2.1
1	A	923	C	2.1
1	A	2275	C	2.1
5	F	181	LEU	2.1
8	I	133	HIS	2.1
9	N	95	PRO	2.1
22	0	38	VAL	2.1
26	4	22	ILE	2.1
15	T	101	PHE	2.1
2	B	41	U	2.1

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Mol	Chain	Res	Type	RSRZ
3	D	235	GLY	2.1
19	X	24	GLY	2.1
4	E	58	ARG	2.1
7	H	84	SER	2.1
19	X	80	ILE	2.1
9	N	37	LYS	2.1
28	6	11	LEU	2.1
2	B	59	A	2.1
2	B	66	A	2.1
13	R	110	PRO	2.1
21	Z	90	VAL	2.1
16	U	85	LYS	2.1
21	Z	88	PHE	2.1
11	P	33	ARG	2.1
17	V	63	GLY	2.1
7	H	158	HIS	2.1
10	O	51	ALA	2.1
5	F	50	SER	2.1
1	A	1040	C	2.1
2	B	57	A	2.1
6	G	135	LEU	2.1
6	G	152	LEU	2.1
11	P	66	GLY	2.1
21	Z	163	LEU	2.1
7	H	156	ALA	2.1
1	A	1642	G	2.1
6	G	9	ARG	2.1
6	G	178	PHE	2.1
21	Z	103	ARG	2.1
28	6	21	TYR	2.1
14	S	110	LEU	2.1
18	W	23	LEU	2.1
1	A	2167	U	2.0
6	G	8	LYS	2.0
20	Y	46	LYS	2.0
15	T	46	GLU	2.0
9	N	87	LEU	2.0
10	O	117	LEU	2.0
11	P	124	LYS	2.0
24	2	3	LEU	2.0
1	A	1592	C	2.0
6	G	159	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
9	N	134	ARG	2.0
21	Z	167	PRO	2.0
1	A	901	A	2.0
5	F	82	ILE	2.0
3	D	9	TYR	2.0
20	Y	95	LYS	2.0
21	Z	8	TYR	2.0
21	Z	198	LYS	2.0
12	Q	34	LEU	2.0
18	W	40	ASN	2.0
8	I	54	GLN	2.0
8	I	59	ALA	2.0
3	D	70	TRP	2.0
1	A	508	G	2.0
5	F	182	ASN	2.0
9	N	120	LEU	2.0
4	E	13	ARG	2.0
1	A	2113	U	2.0
5	F	175	THR	2.0
12	Q	53	ALA	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
32	MG	A	3230	1/1	0.14	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3324	1/1	0.15	-	72,72,72,72	0
32	MG	A	3588	1/1	0.09	-	42,42,42,42	0
32	MG	A	3488	1/1	0.25	-	48,48,48,48	0
32	MG	Q	203	1/1	0.23	-	62,62,62,62	0
32	MG	A	3015	1/1	0.14	-	48,48,48,48	0
32	MG	A	3368	1/1	0.14	-	85,85,85,85	0
32	MG	A	3129	1/1	0.13	-	49,49,49,49	0
32	MG	A	3138	1/1	0.70	-	53,53,53,53	0
32	MG	A	3609	1/1	0.27	-	79,79,79,79	0
32	MG	A	3305	1/1	0.16	-	68,68,68,68	0
32	MG	A	3250	1/1	0.43	-	41,41,41,41	0
32	MG	A	3219	1/1	0.19	-	48,48,48,48	0
32	MG	A	3071	1/1	0.67	-	41,41,41,41	0
32	MG	A	3024	1/1	0.43	-	47,47,47,47	0
32	MG	A	3448	1/1	1.11	-	57,57,57,57	0
32	MG	A	3263	1/1	0.52	-	91,91,91,91	0
33	ZN	5	101	1/1	0.06	-	53,53,53,53	0
32	MG	A	3538	1/1	0.16	-	54,54,54,54	0
32	MG	A	3040	1/1	0.38	-	50,50,50,50	0
32	MG	A	3124	1/1	0.38	-	59,59,59,59	0
32	MG	A	3070	1/1	0.39	-	60,60,60,60	0
32	MG	A	3018	1/1	0.41	-	66,66,66,66	0
32	MG	A	3279	1/1	0.19	-	52,52,52,52	0
32	MG	A	3444	1/1	0.15	-	45,45,45,45	0
32	MG	A	3006	1/1	0.33	-	44,44,44,44	0
32	MG	A	3633	1/1	0.48	-	49,49,49,49	0
32	MG	A	3406	1/1	0.14	-	51,51,51,51	0
32	MG	A	3076	1/1	0.20	-	41,41,41,41	0
32	MG	A	3204	1/1	0.12	-	44,44,44,44	0
32	MG	A	3287	1/1	0.13	-	51,51,51,51	0
32	MG	A	3565	1/1	0.29	-	70,70,70,70	0
32	MG	A	3332	1/1	0.19	-	54,54,54,54	0
32	MG	A	3534	1/1	0.66	-	67,67,67,67	0
32	MG	D	303	1/1	0.19	-	39,39,39,39	0
32	MG	A	3445	1/1	0.34	-	68,68,68,68	0
32	MG	A	3507	1/1	0.22	-	73,73,73,73	0
32	MG	A	3007	1/1	0.23	-	27,27,27,27	0
32	MG	A	3052	1/1	0.24	-	46,46,46,46	0
32	MG	A	3245	1/1	0.16	-	41,41,41,41	0
32	MG	A	3531	1/1	0.17	-	58,58,58,58	0
32	MG	A	3128	1/1	0.38	-	38,38,38,38	0
32	MG	A	3316	1/1	0.16	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3431	1/1	0.11	-	67,67,67,67	0
32	MG	B	209	1/1	0.47	-	67,67,67,67	0
32	MG	A	3016	1/1	0.30	-	54,54,54,54	0
32	MG	A	3236	1/1	0.16	-	51,51,51,51	0
32	MG	A	3270	1/1	0.15	-	42,42,42,42	0
32	MG	A	3385	1/1	0.53	-	64,64,64,64	0
32	MG	A	3623	1/1	0.22	-	56,56,56,56	0
32	MG	A	3473	1/1	0.09	-	41,41,41,41	0
32	MG	A	3593	1/1	0.39	-	62,62,62,62	0
32	MG	A	3277	1/1	0.37	-	71,71,71,71	0
32	MG	A	3472	1/1	0.15	-	34,34,34,34	0
32	MG	A	3027	1/1	0.16	-	37,37,37,37	0
32	MG	A	3347	1/1	0.11	-	87,87,87,87	0
32	MG	A	3367	1/1	0.10	-	56,56,56,56	0
32	MG	A	3228	1/1	0.32	-	76,76,76,76	0
32	MG	A	3389	1/1	0.11	-	73,73,73,73	0
32	MG	A	3432	1/1	0.06	-	34,34,34,34	0
32	MG	A	3162	1/1	0.22	-	39,39,39,39	0
32	MG	A	3021	1/1	0.55	-	68,68,68,68	0
32	MG	A	3355	1/1	0.25	-	44,44,44,44	0
32	MG	A	3293	1/1	0.14	-	67,67,67,67	0
32	MG	A	3265	1/1	0.10	-	40,40,40,40	0
32	MG	A	3116	1/1	0.69	-	69,69,69,69	0
32	MG	A	3060	1/1	0.31	-	43,43,43,43	0
32	MG	A	3154	1/1	0.22	-	53,53,53,53	0
32	MG	A	3517	1/1	0.19	-	53,53,53,53	0
32	MG	A	3547	1/1	0.17	-	54,54,54,54	0
32	MG	T	201	1/1	0.15	-	52,52,52,52	0
32	MG	A	3599	1/1	0.13	-	33,33,33,33	0
32	MG	A	3557	1/1	0.49	-	70,70,70,70	0
32	MG	A	3152	1/1	0.08	-	32,32,32,32	0
32	MG	A	3172	1/1	0.09	-	34,34,34,34	0
32	MG	A	3413	1/1	0.05	-	66,66,66,66	0
32	MG	A	3426	1/1	0.13	-	24,24,24,24	0
32	MG	A	3159	1/1	0.10	-	42,42,42,42	0
32	MG	A	3545	1/1	0.20	-	64,64,64,64	0
32	MG	A	3278	1/1	0.47	-	66,66,66,66	0
32	MG	A	3446	1/1	0.28	-	58,58,58,58	0
32	MG	A	3457	1/1	0.32	-	58,58,58,58	0
32	MG	A	3584	1/1	0.15	-	36,36,36,36	0
32	MG	A	3286	1/1	0.24	-	52,52,52,52	0
32	MG	A	3115	1/1	0.17	-	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	9	102	1/1	0.34	-	51,51,51,51	0
32	MG	A	3416	1/1	0.17	-	59,59,59,59	0
32	MG	A	3176	1/1	0.17	-	32,32,32,32	0
32	MG	A	3298	1/1	0.09	-	33,33,33,33	0
33	ZN	Y	201	1/1	0.05	-	77,77,77,77	0
32	MG	A	3627	1/1	0.10	-	59,59,59,59	0
32	MG	A	3327	1/1	0.12	-	52,52,52,52	0
32	MG	A	3373	1/1	0.17	-	73,73,73,73	0
32	MG	A	3562	1/1	0.53	-	57,57,57,57	0
32	MG	A	3596	1/1	0.22	-	73,73,73,73	0
32	MG	A	3110	1/1	0.72	-	44,44,44,44	0
32	MG	A	3553	1/1	0.18	-	70,70,70,70	0
32	MG	A	3217	1/1	0.52	-	57,57,57,57	0
32	MG	A	3483	1/1	0.29	-	34,34,34,34	0
32	MG	A	3213	1/1	0.06	-	32,32,32,32	0
32	MG	A	3081	1/1	0.11	-	50,50,50,50	0
32	MG	A	3404	1/1	0.10	-	56,56,56,56	0
32	MG	A	3193	1/1	0.16	-	22,22,22,22	0
32	MG	A	3454	1/1	0.22	-	34,34,34,34	0
32	MG	A	3043	1/1	0.36	-	48,48,48,48	0
32	MG	A	3453	1/1	0.39	-	42,42,42,42	0
32	MG	A	3317	1/1	0.27	-	75,75,75,75	0
32	MG	A	3107	1/1	0.33	-	70,70,70,70	0
32	MG	A	3567	1/1	0.30	-	62,62,62,62	0
32	MG	A	3626	1/1	0.37	-	58,58,58,58	0
32	MG	A	3614	1/1	0.10	-	67,67,67,67	0
32	MG	A	3149	1/1	0.26	-	29,29,29,29	0
32	MG	A	3120	1/1	1.27	-	62,62,62,62	0
32	MG	A	3135	1/1	0.41	-	62,62,62,62	0
32	MG	A	3548	1/1	0.23	-	39,39,39,39	0
32	MG	A	3035	1/1	0.26	-	52,52,52,52	0
32	MG	A	3618	1/1	1.02	-	57,57,57,57	0
32	MG	A	3077	1/1	0.47	-	54,54,54,54	0
32	MG	A	3434	1/1	0.09	-	77,77,77,77	0
32	MG	A	3495	1/1	0.14	-	38,38,38,38	0
32	MG	A	3363	1/1	0.21	-	54,54,54,54	0
32	MG	A	3458	1/1	0.37	-	90,90,90,90	0
32	MG	A	3508	1/1	0.29	-	70,70,70,70	0
32	MG	A	3178	1/1	0.19	-	43,43,43,43	0
32	MG	A	3630	1/1	0.45	-	76,76,76,76	0
32	MG	A	3145	1/1	0.17	-	55,55,55,55	0
32	MG	A	3089	1/1	0.76	-	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3379	1/1	0.35	-	47,47,47,47	0
32	MG	F	304	1/1	0.44	-	41,41,41,41	0
32	MG	A	3034	1/1	0.41	-	62,62,62,62	0
32	MG	A	3285	1/1	0.16	-	69,69,69,69	0
32	MG	A	3420	1/1	0.21	-	44,44,44,44	0
32	MG	A	3256	1/1	0.16	-	40,40,40,40	0
32	MG	A	3549	1/1	0.26	-	51,51,51,51	0
32	MG	A	3057	1/1	0.36	-	43,43,43,43	0
32	MG	A	3179	1/1	0.15	-	29,29,29,29	0
32	MG	A	3209	1/1	0.30	-	47,47,47,47	0
32	MG	A	3276	1/1	0.19	-	60,60,60,60	0
32	MG	A	3097	1/1	0.26	-	52,52,52,52	0
32	MG	A	3216	1/1	0.25	-	54,54,54,54	0
32	MG	A	3051	1/1	0.26	-	28,28,28,28	0
32	MG	A	3535	1/1	0.42	-	76,76,76,76	0
32	MG	A	3026	1/1	0.17	-	62,62,62,62	0
32	MG	A	3393	1/1	0.18	-	59,59,59,59	0
32	MG	A	3569	1/1	0.35	-	63,63,63,63	0
32	MG	A	3309	1/1	0.64	-	47,47,47,47	0
32	MG	A	3221	1/1	0.13	-	37,37,37,37	0
32	MG	A	3467	1/1	0.21	-	66,66,66,66	0
32	MG	A	3231	1/1	0.43	-	45,45,45,45	0
32	MG	A	3042	1/1	0.42	-	55,55,55,55	0
32	MG	A	3353	1/1	0.17	-	39,39,39,39	0
32	MG	A	3022	1/1	0.91	-	64,64,64,64	0
32	MG	A	3439	1/1	0.25	-	65,65,65,65	0
32	MG	A	3281	1/1	0.17	-	64,64,64,64	0
32	MG	A	3121	1/1	0.87	-	58,58,58,58	0
32	MG	A	3331	1/1	0.10	-	28,28,28,28	0
32	MG	A	3094	1/1	0.60	-	65,65,65,65	0
32	MG	A	3189	1/1	0.14	-	43,43,43,43	0
32	MG	A	3577	1/1	0.36	-	45,45,45,45	0
32	MG	A	3102	1/1	0.41	-	48,48,48,48	0
32	MG	A	3153	1/1	0.21	-	47,47,47,47	0
32	MG	A	3249	1/1	0.40	-	38,38,38,38	0
32	MG	A	3275	1/1	0.24	-	76,76,76,76	0
32	MG	A	3098	1/1	1.27	-	54,54,54,54	0
32	MG	A	3126	1/1	0.18	-	24,24,24,24	0
32	MG	A	3452	1/1	0.14	-	49,49,49,49	0
32	MG	A	3345	1/1	0.21	-	57,57,57,57	0
32	MG	A	3267	1/1	0.14	-	54,54,54,54	0
32	MG	A	3311	1/1	0.13	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3528	1/1	0.19	-	65,65,65,65	0
32	MG	P	204	1/1	0.91	-	61,61,61,61	0
32	MG	A	3490	1/1	0.19	-	42,42,42,42	0
32	MG	B	201	1/1	0.47	-	67,67,67,67	0
32	MG	A	3620	1/1	0.11	-	41,41,41,41	0
32	MG	A	3500	1/1	0.14	-	85,85,85,85	0
32	MG	A	3505	1/1	0.23	-	57,57,57,57	0
32	MG	A	3240	1/1	0.20	-	47,47,47,47	0
32	MG	A	3506	1/1	0.16	-	90,90,90,90	0
32	MG	A	3570	1/1	0.44	-	53,53,53,53	0
32	MG	B	203	1/1	0.25	-	61,61,61,61	0
32	MG	A	3283	1/1	0.27	-	70,70,70,70	0
32	MG	A	3005	1/1	0.91	-	59,59,59,59	0
32	MG	A	3348	1/1	0.28	-	55,55,55,55	0
32	MG	A	3512	1/1	0.51	-	52,52,52,52	0
32	MG	A	3356	1/1	0.17	-	45,45,45,45	0
32	MG	A	3002	1/1	1.81	-	64,64,64,64	0
32	MG	A	3030	1/1	0.34	-	59,59,59,59	0
32	MG	A	3207	1/1	0.14	-	31,31,31,31	0
32	MG	A	3410	1/1	0.21	-	89,89,89,89	0
32	MG	A	3294	1/1	0.08	-	58,58,58,58	0
32	MG	A	3048	1/1	0.33	-	52,52,52,52	0
32	MG	A	3092	1/1	1.55	-	55,55,55,55	0
32	MG	A	3523	1/1	0.25	-	61,61,61,61	0
32	MG	A	3551	1/1	0.11	-	56,56,56,56	0
32	MG	A	3361	1/1	0.26	-	53,53,53,53	0
32	MG	A	3164	1/1	0.11	-	36,36,36,36	0
32	MG	A	3521	1/1	0.25	-	59,59,59,59	0
32	MG	A	3259	1/1	0.19	-	57,57,57,57	0
32	MG	A	3202	1/1	0.10	-	36,36,36,36	0
32	MG	F	301	1/1	0.30	-	51,51,51,51	0
32	MG	A	3301	1/1	0.24	-	51,51,51,51	0
32	MG	A	3337	1/1	0.79	-	67,67,67,67	0
32	MG	A	3496	1/1	0.44	-	40,40,40,40	0
32	MG	A	3478	1/1	0.18	-	66,66,66,66	0
32	MG	A	3559	1/1	0.15	-	57,57,57,57	0
32	MG	A	3598	1/1	0.32	-	45,45,45,45	0
32	MG	A	3438	1/1	0.17	-	57,57,57,57	0
32	MG	A	3257	1/1	0.13	-	35,35,35,35	0
32	MG	A	3566	1/1	0.13	-	57,57,57,57	0
32	MG	P	201	1/1	1.87	-	78,78,78,78	0
32	MG	A	3025	1/1	0.86	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	B	210	1/1	0.53	-	82,82,82,82	0
32	MG	D	302	1/1	0.17	-	53,53,53,53	0
32	MG	A	3134	1/1	0.16	-	59,59,59,59	0
32	MG	A	3480	1/1	0.13	-	51,51,51,51	0
32	MG	A	3440	1/1	0.18	-	63,63,63,63	0
32	MG	A	3492	1/1	0.18	-	33,33,33,33	0
32	MG	A	3418	1/1	0.09	-	51,51,51,51	0
32	MG	A	3011	1/1	0.36	-	60,60,60,60	0
32	MG	A	3471	1/1	0.67	-	73,73,73,73	0
32	MG	A	3268	1/1	0.07	-	36,36,36,36	0
32	MG	O	201	1/1	0.23	-	75,75,75,75	0
32	MG	A	3375	1/1	0.14	-	73,73,73,73	0
32	MG	A	3168	1/1	0.17	-	32,32,32,32	0
32	MG	A	3192	1/1	0.50	-	66,66,66,66	0
32	MG	A	3272	1/1	0.35	-	93,93,93,93	0
32	MG	A	3518	1/1	0.28	-	61,61,61,61	0
32	MG	A	3330	1/1	0.14	-	48,48,48,48	0
32	MG	A	3560	1/1	0.24	-	65,65,65,65	0
32	MG	A	3624	1/1	0.31	-	76,76,76,76	0
32	MG	A	3064	1/1	0.82	-	51,51,51,51	0
32	MG	A	3581	1/1	0.12	-	83,83,83,83	0
32	MG	T	202	1/1	0.17	-	62,62,62,62	0
32	MG	A	3195	1/1	0.10	-	37,37,37,37	0
32	MG	A	3442	1/1	0.19	-	51,51,51,51	0
32	MG	A	3308	1/1	0.14	-	45,45,45,45	0
32	MG	A	3539	1/1	0.35	-	48,48,48,48	0
32	MG	A	3165	1/1	0.23	-	56,56,56,56	0
32	MG	A	3101	1/1	0.48	-	48,48,48,48	0
32	MG	A	3069	1/1	0.23	-	39,39,39,39	0
32	MG	A	3387	1/1	0.31	-	73,73,73,73	0
32	MG	A	3489	1/1	0.12	-	60,60,60,60	0
32	MG	A	3072	1/1	0.23	-	46,46,46,46	0
32	MG	A	3191	1/1	0.11	-	37,37,37,37	0
32	MG	A	3238	1/1	0.34	-	46,46,46,46	0
32	MG	A	3499	1/1	0.21	-	56,56,56,56	0
32	MG	A	3099	1/1	0.33	-	56,56,56,56	0
32	MG	A	3088	1/1	0.23	-	45,45,45,45	0
32	MG	A	3422	1/1	0.15	-	37,37,37,37	0
32	MG	A	3218	1/1	0.08	-	32,32,32,32	0
32	MG	A	3611	1/1	0.14	-	49,49,49,49	0
32	MG	A	3020	1/1	0.16	-	37,37,37,37	0
32	MG	A	3463	1/1	0.11	-	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3056	1/1	0.35	-	38,38,38,38	0
32	MG	A	3460	1/1	0.12	-	76,76,76,76	0
32	MG	A	3359	1/1	0.16	-	36,36,36,36	0
32	MG	A	3397	1/1	0.13	-	53,53,53,53	0
32	MG	A	3117	1/1	0.61	-	75,75,75,75	0
32	MG	A	3220	1/1	0.07	-	27,27,27,27	0
32	MG	A	3300	1/1	0.12	-	31,31,31,31	0
32	MG	A	3211	1/1	0.21	-	32,32,32,32	0
32	MG	A	3533	1/1	0.31	-	53,53,53,53	0
32	MG	A	3631	1/1	0.23	-	54,54,54,54	0
32	MG	A	3421	1/1	0.34	-	71,71,71,71	0
32	MG	B	206	1/1	0.40	-	115,115,115,115	0
32	MG	A	3469	1/1	0.36	-	50,50,50,50	0
32	MG	A	3086	1/1	0.19	-	39,39,39,39	0
32	MG	A	3384	1/1	0.15	-	59,59,59,59	0
32	MG	A	3251	1/1	0.27	-	45,45,45,45	0
32	MG	A	3262	1/1	0.20	-	54,54,54,54	0
32	MG	A	3622	1/1	0.13	-	42,42,42,42	0
32	MG	A	3424	1/1	0.24	-	42,42,42,42	0
32	MG	A	3003	1/1	0.18	-	53,53,53,53	0
32	MG	A	3282	1/1	0.11	-	51,51,51,51	0
32	MG	A	3078	1/1	0.19	-	48,48,48,48	0
32	MG	A	3520	1/1	0.29	-	43,43,43,43	0
32	MG	A	3197	1/1	0.28	-	52,52,52,52	0
32	MG	A	3612	1/1	0.24	-	45,45,45,45	0
32	MG	A	3212	1/1	0.11	-	33,33,33,33	0
32	MG	A	3364	1/1	0.24	-	51,51,51,51	0
32	MG	A	3127	1/1	0.25	-	47,47,47,47	0
32	MG	A	3095	1/1	0.41	-	61,61,61,61	0
32	MG	A	3625	1/1	0.19	-	75,75,75,75	0
32	MG	A	3215	1/1	0.29	-	43,43,43,43	0
32	MG	A	3433	1/1	0.21	-	60,60,60,60	0
32	MG	A	3597	1/1	0.27	-	64,64,64,64	0
32	MG	A	3515	1/1	0.14	-	56,56,56,56	0
32	MG	A	3401	1/1	0.13	-	53,53,53,53	0
32	MG	A	3429	1/1	0.15	-	28,28,28,28	0
32	MG	A	3074	1/1	0.29	-	54,54,54,54	0
32	MG	A	3415	1/1	0.44	-	64,64,64,64	0
32	MG	A	3386	1/1	0.41	-	72,72,72,72	0
32	MG	A	3335	1/1	0.17	-	53,53,53,53	0
32	MG	A	3409	1/1	0.31	-	80,80,80,80	0
32	MG	A	3303	1/1	0.11	-	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3634	1/1	0.40	-	75,75,75,75	0
33	ZN	6	101	1/1	0.07	-	66,66,66,66	0
32	MG	Q	202	1/1	0.15	-	39,39,39,39	0
32	MG	A	3031	1/1	0.18	-	48,48,48,48	0
32	MG	A	3399	1/1	0.20	-	41,41,41,41	0
32	MG	A	3160	1/1	0.18	-	47,47,47,47	0
32	MG	A	3226	1/1	0.10	-	39,39,39,39	0
32	MG	A	3109	1/1	0.30	-	56,56,56,56	0
32	MG	A	3322	1/1	0.19	-	69,69,69,69	0
32	MG	A	3491	1/1	0.22	-	59,59,59,59	0
32	MG	A	3583	1/1	0.13	-	37,37,37,37	0
32	MG	A	3036	1/1	1.50	-	85,85,85,85	0
32	MG	A	3315	1/1	0.11	-	87,87,87,87	0
32	MG	A	3185	1/1	0.10	-	27,27,27,27	0
32	MG	A	3371	1/1	0.31	-	79,79,79,79	0
32	MG	A	3073	1/1	0.35	-	48,48,48,48	0
32	MG	A	3147	1/1	0.15	-	55,55,55,55	0
32	MG	A	3628	1/1	0.40	-	65,65,65,65	0
32	MG	A	3482	1/1	0.26	-	63,63,63,63	0
32	MG	A	3033	1/1	0.44	-	43,43,43,43	0
32	MG	A	3382	1/1	0.13	-	59,59,59,59	0
32	MG	A	3537	1/1	0.49	-	60,60,60,60	0
32	MG	A	3349	1/1	0.18	-	40,40,40,40	0
32	MG	A	3530	1/1	0.12	-	51,51,51,51	0
32	MG	A	3381	1/1	0.18	-	57,57,57,57	0
32	MG	A	3264	1/1	0.09	-	34,34,34,34	0
32	MG	A	3342	1/1	0.17	-	54,54,54,54	0
32	MG	A	3233	1/1	0.13	-	52,52,52,52	0
32	MG	A	3394	1/1	0.20	-	75,75,75,75	0
32	MG	A	3137	1/1	0.52	-	49,49,49,49	0
32	MG	A	3295	1/1	0.45	-	61,61,61,61	0
32	MG	A	3511	1/1	0.26	-	43,43,43,43	0
32	MG	A	3196	1/1	0.10	-	28,28,28,28	0
32	MG	A	3436	1/1	0.25	-	54,54,54,54	0
32	MG	A	3419	1/1	0.17	-	52,52,52,52	0
32	MG	A	3013	1/1	0.56	-	56,56,56,56	0
32	MG	P	202	1/1	0.17	-	53,53,53,53	0
32	MG	A	3059	1/1	0.17	-	45,45,45,45	0
32	MG	A	3214	1/1	0.07	-	30,30,30,30	0
32	MG	A	3585	1/1	0.15	-	142,142,142,142	0
32	MG	A	3103	1/1	0.47	-	51,51,51,51	0
32	MG	A	3229	1/1	0.26	-	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3019	1/1	0.14	-	32,32,32,32	0
32	MG	A	3163	1/1	0.25	-	64,64,64,64	0
32	MG	A	3494	1/1	0.23	-	34,34,34,34	0
32	MG	A	3543	1/1	0.39	-	67,67,67,67	0
32	MG	A	3354	1/1	0.17	-	67,67,67,67	0
32	MG	A	3338	1/1	0.08	-	53,53,53,53	0
32	MG	A	3380	1/1	0.22	-	55,55,55,55	0
32	MG	A	3582	1/1	0.23	-	35,35,35,35	0
32	MG	A	3180	1/1	0.14	-	50,50,50,50	0
32	MG	A	3119	1/1	0.16	-	47,47,47,47	0
32	MG	A	3194	1/1	0.39	-	33,33,33,33	0
32	MG	E	301	1/1	0.11	-	29,29,29,29	0
32	MG	A	3054	1/1	0.57	-	31,31,31,31	0
32	MG	A	3632	1/1	0.22	-	72,72,72,72	0
32	MG	A	3466	1/1	0.18	-	85,85,85,85	0
32	MG	A	3274	1/1	0.15	-	69,69,69,69	0
32	MG	A	3010	1/1	0.19	-	34,34,34,34	0
32	MG	A	3111	1/1	0.26	-	48,48,48,48	0
32	MG	F	302	1/1	0.44	-	63,63,63,63	0
32	MG	A	3412	1/1	0.16	-	78,78,78,78	0
32	MG	A	3561	1/1	0.62	-	65,65,65,65	0
32	MG	A	3087	1/1	0.33	-	50,50,50,50	0
32	MG	A	3468	1/1	0.31	-	56,56,56,56	0
32	MG	A	3456	1/1	0.15	-	59,59,59,59	0
32	MG	A	3510	1/1	0.58	-	44,44,44,44	0
32	MG	A	3554	1/1	0.35	-	63,63,63,63	0
32	MG	B	207	1/1	0.13	-	82,82,82,82	0
32	MG	A	3550	1/1	0.94	-	69,69,69,69	0
32	MG	A	3541	1/1	0.31	-	65,65,65,65	0
32	MG	A	3096	1/1	0.31	-	30,30,30,30	0
32	MG	A	3122	1/1	0.25	-	48,48,48,48	0
32	MG	A	3190	1/1	0.14	-	56,56,56,56	0
32	MG	A	3576	1/1	0.16	-	57,57,57,57	0
32	MG	A	3629	1/1	0.12	-	80,80,80,80	0
32	MG	A	3151	1/1	0.10	-	52,52,52,52	0
32	MG	A	3366	1/1	0.08	-	67,67,67,67	0
32	MG	A	3169	1/1	0.22	-	31,31,31,31	0
32	MG	A	3526	1/1	0.12	-	38,38,38,38	0
32	MG	A	3465	1/1	0.16	-	65,65,65,65	0
32	MG	A	3131	1/1	1.17	-	54,54,54,54	0
32	MG	A	3376	1/1	0.34	-	74,74,74,74	0
32	MG	A	3334	1/1	0.39	-	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3232	1/1	0.14	-	42,42,42,42	0
32	MG	A	3606	1/1	0.30	-	65,65,65,65	0
32	MG	D	301	1/1	0.11	-	32,32,32,32	0
32	MG	A	3289	1/1	0.13	-	47,47,47,47	0
32	MG	A	3171	1/1	0.18	-	30,30,30,30	0
32	MG	A	3400	1/1	0.26	-	56,56,56,56	0
32	MG	A	3312	1/1	0.16	-	34,34,34,34	0
32	MG	A	3066	1/1	0.21	-	38,38,38,38	0
32	MG	A	3009	1/1	0.19	-	45,45,45,45	0
32	MG	W	201	1/1	0.60	-	63,63,63,63	0
32	MG	A	3377	1/1	0.17	-	65,65,65,65	0
32	MG	5	103	1/1	0.12	-	61,61,61,61	0
32	MG	A	3339	1/1	0.16	-	72,72,72,72	0
32	MG	A	3388	1/1	0.29	-	82,82,82,82	0
32	MG	A	3310	1/1	0.20	-	31,31,31,31	0
32	MG	A	3032	1/1	0.14	-	34,34,34,34	0
32	MG	A	3063	1/1	0.15	-	74,74,74,74	0
32	MG	A	3555	1/1	0.32	-	87,87,87,87	0
32	MG	A	3343	1/1	0.14	-	56,56,56,56	0
32	MG	A	3605	1/1	0.77	-	82,82,82,82	0
32	MG	A	3136	1/1	1.34	-	45,45,45,45	0
32	MG	A	3504	1/1	0.19	-	66,66,66,66	0
32	MG	A	3199	1/1	0.14	-	34,34,34,34	0
32	MG	A	3208	1/1	0.07	-	45,45,45,45	0
32	MG	A	3108	1/1	0.41	-	57,57,57,57	0
32	MG	A	3146	1/1	1.36	-	52,52,52,52	0
32	MG	A	3477	1/1	0.31	-	64,64,64,64	0
32	MG	A	3028	1/1	0.75	-	63,63,63,63	0
32	MG	A	3141	1/1	0.19	-	48,48,48,48	0
32	MG	A	3029	1/1	0.17	-	46,46,46,46	0
32	MG	A	3187	1/1	0.29	-	51,51,51,51	0
32	MG	A	3575	1/1	0.13	-	36,36,36,36	0
32	MG	A	3435	1/1	0.22	-	77,77,77,77	0
32	MG	A	3321	1/1	0.20	-	61,61,61,61	0
32	MG	A	3459	1/1	0.15	-	32,32,32,32	0
32	MG	A	3613	1/1	0.65	-	92,92,92,92	0
32	MG	A	3340	1/1	0.43	-	60,60,60,60	0
32	MG	A	3290	1/1	0.31	-	64,64,64,64	0
32	MG	A	3573	1/1	0.12	-	77,77,77,77	0
32	MG	P	203	1/1	0.24	-	52,52,52,52	0
32	MG	A	3161	1/1	0.16	-	33,33,33,33	0
32	MG	A	3157	1/1	0.21	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3224	1/1	0.20	-	53,53,53,53	0
33	ZN	4	101	1/1	0.08	-	173,173,173,173	0
32	MG	A	3532	1/1	0.26	-	79,79,79,79	0
32	MG	A	3493	1/1	0.31	-	64,64,64,64	0
32	MG	A	3266	1/1	0.10	-	34,34,34,34	0
32	MG	A	3360	1/1	0.15	-	40,40,40,40	0
32	MG	A	3592	1/1	0.18	-	58,58,58,58	0
32	MG	A	3635	1/1	0.36	-	54,54,54,54	0
32	MG	A	3058	1/1	0.12	-	57,57,57,57	0
32	MG	A	3568	1/1	0.33	-	60,60,60,60	0
32	MG	A	3260	1/1	0.07	-	37,37,37,37	0
32	MG	A	3284	1/1	0.22	-	68,68,68,68	0
32	MG	A	3175	1/1	0.26	-	37,37,37,37	0
32	MG	A	3325	1/1	0.53	-	69,69,69,69	0
32	MG	A	3589	1/1	0.19	-	59,59,59,59	0
32	MG	A	3423	1/1	0.10	-	49,49,49,49	0
32	MG	A	3374	1/1	0.17	-	60,60,60,60	0
32	MG	A	3369	1/1	0.36	-	87,87,87,87	0
32	MG	A	3079	1/1	0.15	-	60,60,60,60	0
32	MG	A	3227	1/1	0.25	-	60,60,60,60	0
32	MG	A	3604	1/1	0.41	-	49,49,49,49	0
32	MG	E	302	1/1	0.37	-	37,37,37,37	0
32	MG	A	3320	1/1	0.33	-	74,74,74,74	0
32	MG	A	3280	1/1	0.18	-	85,85,85,85	0
32	MG	A	3001	1/1	0.28	-	34,34,34,34	0
32	MG	A	3519	1/1	0.19	-	74,74,74,74	0
32	MG	A	3484	1/1	0.13	-	33,33,33,33	0
32	MG	A	3556	1/1	0.13	-	55,55,55,55	0
32	MG	A	3411	1/1	0.55	-	75,75,75,75	0
32	MG	A	3441	1/1	0.13	-	59,59,59,59	0
32	MG	R	201	1/1	0.68	-	40,40,40,40	0
32	MG	A	3222	1/1	0.13	-	39,39,39,39	0
32	MG	A	3041	1/1	0.41	-	64,64,64,64	0
32	MG	A	3068	1/1	0.52	-	51,51,51,51	0
32	MG	A	3336	1/1	0.27	-	65,65,65,65	0
32	MG	A	3591	1/1	0.12	-	72,72,72,72	0
32	MG	A	3239	1/1	0.29	-	56,56,56,56	0
32	MG	A	3039	1/1	0.28	-	34,34,34,34	0
32	MG	A	3080	1/1	0.13	-	34,34,34,34	0
32	MG	A	3252	1/1	0.19	-	58,58,58,58	0
32	MG	A	3546	1/1	1.42	-	89,89,89,89	0
32	MG	A	3242	1/1	0.09	-	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3616	1/1	0.26	-	74,74,74,74	0
32	MG	A	3288	1/1	0.10	-	44,44,44,44	0
32	MG	A	3346	1/1	0.33	-	87,87,87,87	0
32	MG	A	3186	1/1	0.17	-	44,44,44,44	0
32	MG	A	3514	1/1	0.20	-	54,54,54,54	0
32	MG	A	3449	1/1	0.06	-	70,70,70,70	0
32	MG	A	3133	1/1	1.69	-	71,71,71,71	0
32	MG	B	202	1/1	0.31	-	67,67,67,67	0
32	MG	A	3200	1/1	0.11	-	29,29,29,29	0
32	MG	A	3527	1/1	0.54	-	36,36,36,36	0
32	MG	A	3055	1/1	0.11	-	53,53,53,53	0
32	MG	A	3273	1/1	0.17	-	51,51,51,51	0
32	MG	A	3198	1/1	0.15	-	29,29,29,29	0
32	MG	A	3243	1/1	0.16	-	32,32,32,32	0
32	MG	A	3173	1/1	0.19	-	24,24,24,24	0
32	MG	A	3563	1/1	0.43	-	61,61,61,61	0
32	MG	A	3579	1/1	0.22	-	39,39,39,39	0
32	MG	A	3140	1/1	1.69	-	70,70,70,70	0
32	MG	A	3067	1/1	0.54	-	67,67,67,67	0
32	MG	A	3574	1/1	0.13	-	98,98,98,98	0
32	MG	A	3481	1/1	0.23	-	69,69,69,69	0
32	MG	A	3113	1/1	0.20	-	36,36,36,36	0
32	MG	A	3391	1/1	0.14	-	43,43,43,43	0
32	MG	A	3090	1/1	0.54	-	41,41,41,41	0
32	MG	A	3084	1/1	0.36	-	54,54,54,54	0
32	MG	A	3306	1/1	0.31	-	79,79,79,79	0
32	MG	A	3235	1/1	0.10	-	40,40,40,40	0
32	MG	A	3188	1/1	0.21	-	36,36,36,36	0
32	MG	A	3082	1/1	0.65	-	45,45,45,45	0
32	MG	A	3234	1/1	0.54	-	58,58,58,58	0
32	MG	A	3104	1/1	0.34	-	54,54,54,54	0
32	MG	A	3479	1/1	0.09	-	57,57,57,57	0
32	MG	A	3304	1/1	0.64	-	66,66,66,66	0
32	MG	A	3177	1/1	0.16	-	42,42,42,42	0
32	MG	A	3253	1/1	0.12	-	39,39,39,39	0
32	MG	A	3603	1/1	0.18	-	72,72,72,72	0
32	MG	A	3403	1/1	0.14	-	62,62,62,62	0
32	MG	A	3486	1/1	0.35	-	65,65,65,65	0
32	MG	A	3170	1/1	0.13	-	28,28,28,28	0
32	MG	A	3617	1/1	0.86	-	93,93,93,93	0
32	MG	A	3261	1/1	0.53	-	55,55,55,55	0
32	MG	A	3571	1/1	0.12	-	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3143	1/1	0.23	-	54,54,54,54	0
32	MG	A	3254	1/1	0.14	-	51,51,51,51	0
32	MG	A	3083	1/1	0.22	-	60,60,60,60	0
32	MG	A	3437	1/1	0.31	-	54,54,54,54	0
32	MG	A	3155	1/1	0.14	-	34,34,34,34	0
32	MG	A	3299	1/1	0.14	-	29,29,29,29	0
32	MG	A	3012	1/1	0.49	-	73,73,73,73	0
32	MG	A	3017	1/1	0.47	-	46,46,46,46	0
32	MG	A	3558	1/1	1.32	-	76,76,76,76	0
32	MG	A	3037	1/1	0.77	-	57,57,57,57	0
32	MG	A	3552	1/1	0.22	-	64,64,64,64	0
32	MG	A	3049	1/1	0.28	-	73,73,73,73	0
32	MG	A	3425	1/1	0.16	-	55,55,55,55	0
32	MG	Q	204	1/1	0.27	-	67,67,67,67	0
32	MG	B	205	1/1	0.18	-	92,92,92,92	0
32	MG	A	3365	1/1	0.17	-	41,41,41,41	0
32	MG	A	3586	1/1	0.12	-	49,49,49,49	0
32	MG	A	3247	1/1	0.58	-	59,59,59,59	0
32	MG	A	3529	1/1	0.15	-	66,66,66,66	0
32	MG	F	305	1/1	0.39	-	74,74,74,74	0
32	MG	E	303	1/1	0.12	-	31,31,31,31	0
32	MG	A	3210	1/1	0.14	-	38,38,38,38	0
32	MG	A	3326	1/1	0.24	-	66,66,66,66	0
32	MG	A	3166	1/1	0.11	-	30,30,30,30	0
32	MG	A	3417	1/1	0.12	-	48,48,48,48	0
32	MG	A	3487	1/1	0.15	-	46,46,46,46	0
32	MG	A	3075	1/1	0.43	-	42,42,42,42	0
32	MG	A	3619	1/1	0.20	-	65,65,65,65	0
32	MG	A	3516	1/1	0.19	-	52,52,52,52	0
32	MG	A	3296	1/1	0.17	-	49,49,49,49	0
32	MG	A	3621	1/1	0.16	-	80,80,80,80	0
32	MG	A	3050	1/1	0.23	-	35,35,35,35	0
32	MG	A	3302	1/1	0.08	-	46,46,46,46	0
32	MG	A	3405	1/1	0.34	-	54,54,54,54	0
32	MG	A	3498	1/1	0.20	-	55,55,55,55	0
32	MG	A	3132	1/1	0.14	-	50,50,50,50	0
32	MG	A	3023	1/1	0.33	-	35,35,35,35	0
32	MG	A	3125	1/1	0.10	-	56,56,56,56	0
32	MG	A	3038	1/1	0.63	-	58,58,58,58	0
32	MG	A	3158	1/1	0.12	-	66,66,66,66	0
32	MG	A	3601	1/1	0.47	-	53,53,53,53	0
32	MG	A	3564	1/1	0.24	-	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3372	1/1	0.15	-	58,58,58,58	0
32	MG	A	3206	1/1	0.10	-	27,27,27,27	0
32	MG	A	3047	1/1	0.19	-	49,49,49,49	0
32	MG	A	3503	1/1	0.17	-	52,52,52,52	0
32	MG	A	3383	1/1	0.24	-	49,49,49,49	0
32	MG	A	3447	1/1	0.37	-	53,53,53,53	0
32	MG	A	3587	1/1	0.06	-	38,38,38,38	0
32	MG	A	3144	1/1	0.30	-	60,60,60,60	0
32	MG	A	3105	1/1	0.31	-	55,55,55,55	0
32	MG	A	3402	1/1	0.06	-	56,56,56,56	0
32	MG	A	3536	1/1	0.19	-	49,49,49,49	0
32	MG	A	3328	1/1	0.10	-	34,34,34,34	0
32	MG	A	3608	1/1	0.17	-	42,42,42,42	0
32	MG	A	3544	1/1	0.27	-	53,53,53,53	0
32	MG	A	3370	1/1	0.16	-	76,76,76,76	0
32	MG	A	3314	1/1	0.44	-	49,49,49,49	0
32	MG	A	3398	1/1	0.25	-	80,80,80,80	0
32	MG	A	3297	1/1	0.10	-	51,51,51,51	0
32	MG	Q	201	1/1	0.72	-	52,52,52,52	0
32	MG	A	3350	1/1	0.16	-	68,68,68,68	0
32	MG	A	3578	1/1	0.85	-	52,52,52,52	0
32	MG	F	303	1/1	0.26	-	56,56,56,56	0
32	MG	A	3637	1/1	0.68	-	63,63,63,63	0
32	MG	A	3475	1/1	0.21	-	95,95,95,95	0
32	MG	B	204	1/1	0.20	-	65,65,65,65	0
32	MG	A	3524	1/1	0.43	-	57,57,57,57	0
32	MG	A	3329	1/1	0.16	-	56,56,56,56	0
32	MG	A	3590	1/1	0.15	-	39,39,39,39	0
32	MG	A	3106	1/1	0.33	-	38,38,38,38	0
32	MG	A	3093	1/1	0.33	-	54,54,54,54	0
32	MG	A	3352	1/1	0.27	-	79,79,79,79	0
32	MG	A	3205	1/1	0.20	-	34,34,34,34	0
32	MG	A	3258	1/1	0.16	-	39,39,39,39	0
32	MG	A	3572	1/1	0.25	-	68,68,68,68	0
32	MG	A	3395	1/1	0.22	-	48,48,48,48	0
32	MG	A	3428	1/1	0.12	-	26,26,26,26	0
32	MG	A	3044	1/1	0.36	-	58,58,58,58	0
32	MG	A	3396	1/1	0.32	-	59,59,59,59	0
32	MG	A	3318	1/1	0.20	-	53,53,53,53	0
32	MG	1	101	1/1	0.16	-	59,59,59,59	0
32	MG	A	3184	1/1	0.23	-	47,47,47,47	0
32	MG	A	3461	1/1	0.29	-	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3091	1/1	0.64	-	54,54,54,54	0
32	MG	A	3225	1/1	0.05	-	41,41,41,41	0
32	MG	A	3112	1/1	0.40	-	56,56,56,56	0
32	MG	A	3313	1/1	0.09	-	31,31,31,31	0
32	MG	A	3061	1/1	0.15	-	47,47,47,47	0
32	MG	A	3540	1/1	0.43	-	46,46,46,46	0
32	MG	A	3085	1/1	0.24	-	52,52,52,52	0
32	MG	A	3139	1/1	0.41	-	60,60,60,60	0
32	MG	A	3014	1/1	0.20	-	64,64,64,64	0
32	MG	A	3476	1/1	0.49	-	63,63,63,63	0
32	MG	A	3123	1/1	0.82	-	69,69,69,69	0
32	MG	A	3392	1/1	0.26	-	52,52,52,52	0
32	MG	A	3150	1/1	0.15	-	31,31,31,31	0
32	MG	R	202	1/1	0.33	-	45,45,45,45	0
32	MG	5	102	1/1	0.52	-	44,44,44,44	0
32	MG	A	3602	1/1	0.11	-	44,44,44,44	0
32	MG	A	3615	1/1	0.46	-	63,63,63,63	0
32	MG	A	3008	1/1	0.28	-	48,48,48,48	0
32	MG	A	3451	1/1	0.14	-	45,45,45,45	0
32	MG	A	3174	1/1	0.30	-	31,31,31,31	0
32	MG	A	3455	1/1	0.24	-	45,45,45,45	0
32	MG	A	3004	1/1	0.78	-	42,42,42,42	0
32	MG	A	3130	1/1	0.18	-	25,25,25,25	0
32	MG	A	3497	1/1	0.22	-	39,39,39,39	0
32	MG	A	3513	1/1	0.29	-	92,92,92,92	0
32	MG	A	3255	1/1	0.11	-	57,57,57,57	0
32	MG	A	3341	1/1	1.03	-	40,40,40,40	0
32	MG	A	3580	1/1	0.14	-	46,46,46,46	0
32	MG	A	3357	1/1	0.20	-	59,59,59,59	0
32	MG	A	3307	1/1	0.56	-	70,70,70,70	0
32	MG	A	3362	1/1	0.23	-	51,51,51,51	0
32	MG	A	3333	1/1	0.12	-	45,45,45,45	0
32	MG	A	3181	1/1	0.15	-	45,45,45,45	0
32	MG	A	3522	1/1	0.12	-	73,73,73,73	0
32	MG	A	3595	1/1	0.33	-	60,60,60,60	0
32	MG	A	3323	1/1	0.26	-	86,86,86,86	0
32	MG	A	3100	1/1	0.35	-	60,60,60,60	0
32	MG	A	3474	1/1	0.43	-	60,60,60,60	0
32	MG	A	3358	1/1	0.26	-	69,69,69,69	0
32	MG	A	3203	1/1	0.10	-	32,32,32,32	0
32	MG	A	3407	1/1	0.14	-	54,54,54,54	0
32	MG	A	3248	1/1	0.14	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	3378	1/1	0.14	-	69,69,69,69	0
32	MG	A	3201	1/1	0.08	-	29,29,29,29	0
33	ZN	9	101	1/1	0.04	-	68,68,68,68	0
32	MG	A	3246	1/1	0.45	-	73,73,73,73	0
32	MG	D	304	1/1	0.38	-	56,56,56,56	0
32	MG	A	3292	1/1	0.32	-	85,85,85,85	0
32	MG	A	3114	1/1	0.35	-	33,33,33,33	0
32	MG	A	3610	1/1	0.26	-	57,57,57,57	0
32	MG	A	3237	1/1	0.12	-	44,44,44,44	0
32	MG	A	3414	1/1	0.21	-	53,53,53,53	0
32	MG	A	3607	1/1	0.47	-	74,74,74,74	0
32	MG	A	3182	1/1	0.14	-	36,36,36,36	0
32	MG	A	3241	1/1	0.09	-	36,36,36,36	0
32	MG	A	3443	1/1	0.19	-	73,73,73,73	0
32	MG	A	3450	1/1	0.14	-	60,60,60,60	0
32	MG	A	3525	1/1	0.19	-	42,42,42,42	0
32	MG	A	3509	1/1	0.22	-	46,46,46,46	0
32	MG	A	3271	1/1	0.25	-	69,69,69,69	0
32	MG	A	3427	1/1	0.31	-	36,36,36,36	0
32	MG	A	3244	1/1	0.35	-	37,37,37,37	0
32	MG	A	3470	1/1	0.10	-	41,41,41,41	0
32	MG	A	3065	1/1	0.12	-	58,58,58,58	0
32	MG	A	3148	1/1	0.24	-	46,46,46,46	0
32	MG	A	3053	1/1	0.39	-	25,25,25,25	0
32	MG	A	3062	1/1	0.13	-	36,36,36,36	0
32	MG	A	3156	1/1	0.19	-	33,33,33,33	0
32	MG	A	3430	1/1	0.12	-	27,27,27,27	0
32	MG	A	3485	1/1	0.21	-	44,44,44,44	0
32	MG	A	3462	1/1	0.36	-	67,67,67,67	0
32	MG	B	208	1/1	0.25	-	96,96,96,96	0
32	MG	A	3167	1/1	0.18	-	41,41,41,41	0
32	MG	A	3594	1/1	0.53	-	90,90,90,90	0
32	MG	A	3045	1/1	0.40	-	52,52,52,52	0
32	MG	A	3344	1/1	0.19	-	56,56,56,56	0
32	MG	A	3319	1/1	0.05	-	54,54,54,54	0
32	MG	A	3046	1/1	0.12	-	50,50,50,50	0
32	MG	A	3351	1/1	0.21	-	82,82,82,82	0
32	MG	A	3501	1/1	0.31	-	78,78,78,78	0
32	MG	A	3636	1/1	0.19	-	66,66,66,66	0
32	MG	A	3464	1/1	0.10	-	63,63,63,63	0
32	MG	A	3269	1/1	0.13	-	24,24,24,24	0
32	MG	A	3291	1/1	0.13	-	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	8	101	1/1	0.22	-	66,66,66,66	0
32	MG	A	3118	1/1	0.27	-	38,38,38,38	0
32	MG	0	101	1/1	1.15	-	78,78,78,78	0
32	MG	A	3542	1/1	0.20	-	54,54,54,54	0
32	MG	A	3183	1/1	0.13	-	33,33,33,33	0
32	MG	A	3390	1/1	0.16	-	62,62,62,62	0
32	MG	A	3142	1/1	0.25	-	62,62,62,62	0
32	MG	A	3408	1/1	0.26	-	53,53,53,53	0
32	MG	A	3600	1/1	0.09	-	32,32,32,32	0
32	MG	A	3502	1/1	0.53	-	59,59,59,59	0
32	MG	A	3223	1/1	0.12	-	60,60,60,60	0

## 6.5 Other polymers

There are no such residues in this entry.