



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:26 PM GMT

PDB ID : 4LF5  
Title : Crystal Structure of 30S ribosomal subunit from *Thermus thermophilus*  
Authors : Demirci, H.; Belardinelli, R.; Carr, J.; Murphy IV, F.; Jögl, G.; Dahlberg, A.E.; Gregory, S.T.  
Deposited on : 2013-06-26  
Resolution : 3.75 Å(reported)

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

---

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

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

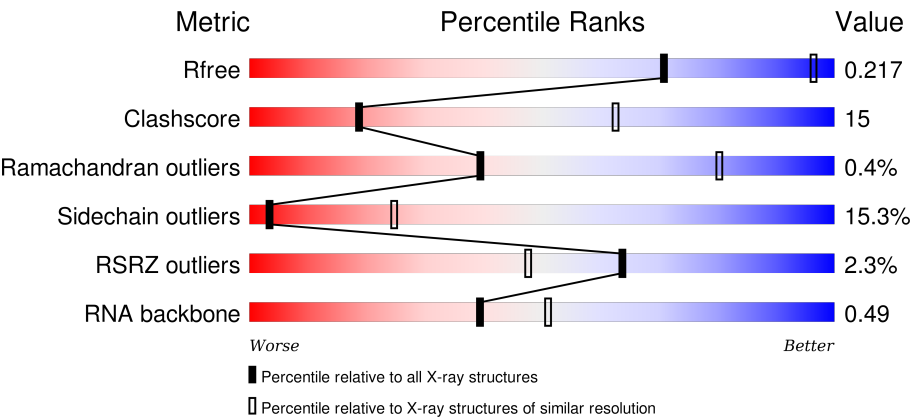
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.75 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R <sub>free</sub>	91344	1268 (4.02-3.50)
Clashscore	102246	1407 (4.02-3.50)
Ramachandran outliers	100387	1346 (4.02-3.50)
Sidechain outliers	100360	1342 (4.02-3.50)
RSRZ outliers	91569	1276 (4.02-3.50)
RNA backbone	2183	1069 (4.70-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	1522	<div><div>2%</div><div><div></div><div>37%</div><div>44%</div><div>16%</div><div>••</div></div></div>
2	B	256	<div><div>%</div><div><div></div><div>51%</div><div>32%</div><div>9%</div><div>8%</div></div></div>
3	C	239	<div><div>5%</div><div><div></div><div>42%</div><div>38%</div><div>7%</div><div>13%</div></div></div>
4	D	209	<div><div></div><div><div></div><div>51%</div><div>40%</div><div>9%</div></div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	162	
6	F	101	
7	G	156	
8	H	138	
9	I	128	
10	J	105	
11	K	129	
12	L	135	
13	M	126	
14	N	61	
15	O	89	
16	P	88	
17	Q	105	
18	R	88	
19	S	93	
20	T	106	
21	U	27	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	MG	A	1603	-	-	-	X
22	MG	A	1604	-	-	-	X
22	MG	A	1608	-	-	-	X
22	MG	A	1614	-	-	-	X
22	MG	A	1617	-	-	-	X
22	MG	A	1622	-	-	-	X
22	MG	A	1634	-	-	-	X
22	MG	A	1635	-	-	-	X

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	MG	A	1641	-	-	-	X
22	MG	A	1642	-	-	-	X
22	MG	A	1647	-	-	-	X
22	MG	A	1654	-	-	-	X
22	MG	A	1659	-	-	-	X
22	MG	A	1668	-	-	-	X
22	MG	A	1669	-	-	-	X
22	MG	A	1670	-	-	-	X
22	MG	A	1671	-	-	-	X
22	MG	A	1672	-	-	-	X
22	MG	A	1678	-	-	-	X
22	MG	A	1679	-	-	-	X
22	MG	A	1681	-	-	-	X
22	MG	A	1683	-	-	-	X
22	MG	A	1707	-	-	-	X
22	MG	A	1709	-	-	-	X
22	MG	B	301	-	-	-	X
22	MG	D	302	-	-	-	X
22	MG	M	201	-	-	-	X
23	K	A	1699	-	-	-	X

## 2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 51823 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1513	Total	C	N	O	P	0	0	0
			32522	14483	6016	10511	1512			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1533	C	A	CONFLICT	GB M26923.1
A	1534	A	C	CONFLICT	GB M26923.1

- Molecule 2 is a protein called ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	236	Total	C	N	O	S	0	0	1
			1874	1195	336	338	5			

- Molecule 3 is a protein called ribosomal protein S3.

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

- Molecule 4 is a protein called ribosomal protein S4.

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

- Molecule 5 is a protein called ribosomal protein S5.

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

- Molecule 6 is a protein called ribosomal protein S6.

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

- Molecule 7 is a protein called ribosomal protein S7.

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

- Molecule 8 is a protein called ribosomal protein S8.

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

- Molecule 9 is a protein called ribosomal protein S9.

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

- Molecule 10 is a protein called ribosomal protein S10.

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

- Molecule 11 is a protein called ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 12 is a protein called ribosomal protein S12.

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

- Molecule 13 is a protein called ribosomal protein S13.

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

- Molecule 14 is a protein called ribosomal protein S14.

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

- Molecule 15 is a protein called ribosomal protein S15.

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

- Molecule 16 is a protein called ribosomal protein S16.

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

- Molecule 17 is a protein called ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 18 is a protein called ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	73	Total	C	N	O	0	0	0
			598	381	118	99			

- Molecule 19 is a protein called ribosomal protein S19.

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

- Molecule 20 is a protein called ribosomal protein S20.

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

- Molecule 21 is a protein called ribosomal protein THX.

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

- Molecule 22 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

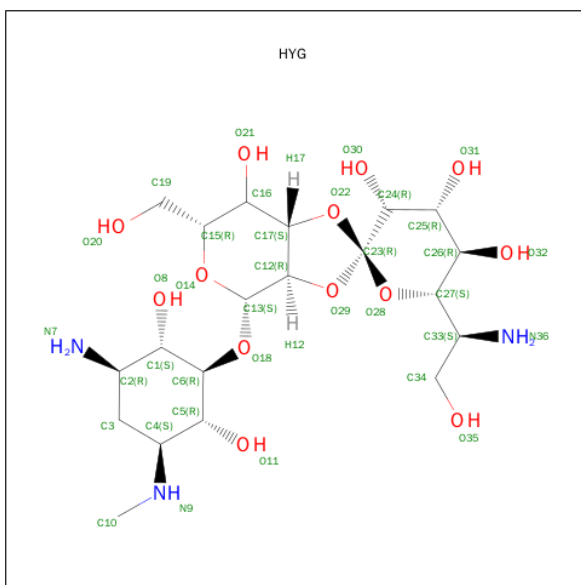
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	D	2	Total	Mg	0	0
			2	2		
22	K	1	Total	Mg	0	0
			1	1		
22	E	1	Total	Mg	0	0
			1	1		
22	H	2	Total	Mg	0	0
			2	2		
22	B	1	Total	Mg	0	0
			1	1		
22	A	108	Total	Mg	0	0
			108	108		
22	L	1	Total	Mg	0	0
			1	1		
22	S	1	Total	Mg	0	0
			1	1		
22	M	1	Total	Mg	0	0
			1	1		

- Molecule 23 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	A	8	Total	K	0	0
			8	8		

- Molecule 24 is HYGROMYCIN B (three-letter code: HYG) (formula: C<sub>20</sub>H<sub>37</sub>N<sub>3</sub>O<sub>13</sub>).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	0
			36	20	3	13		

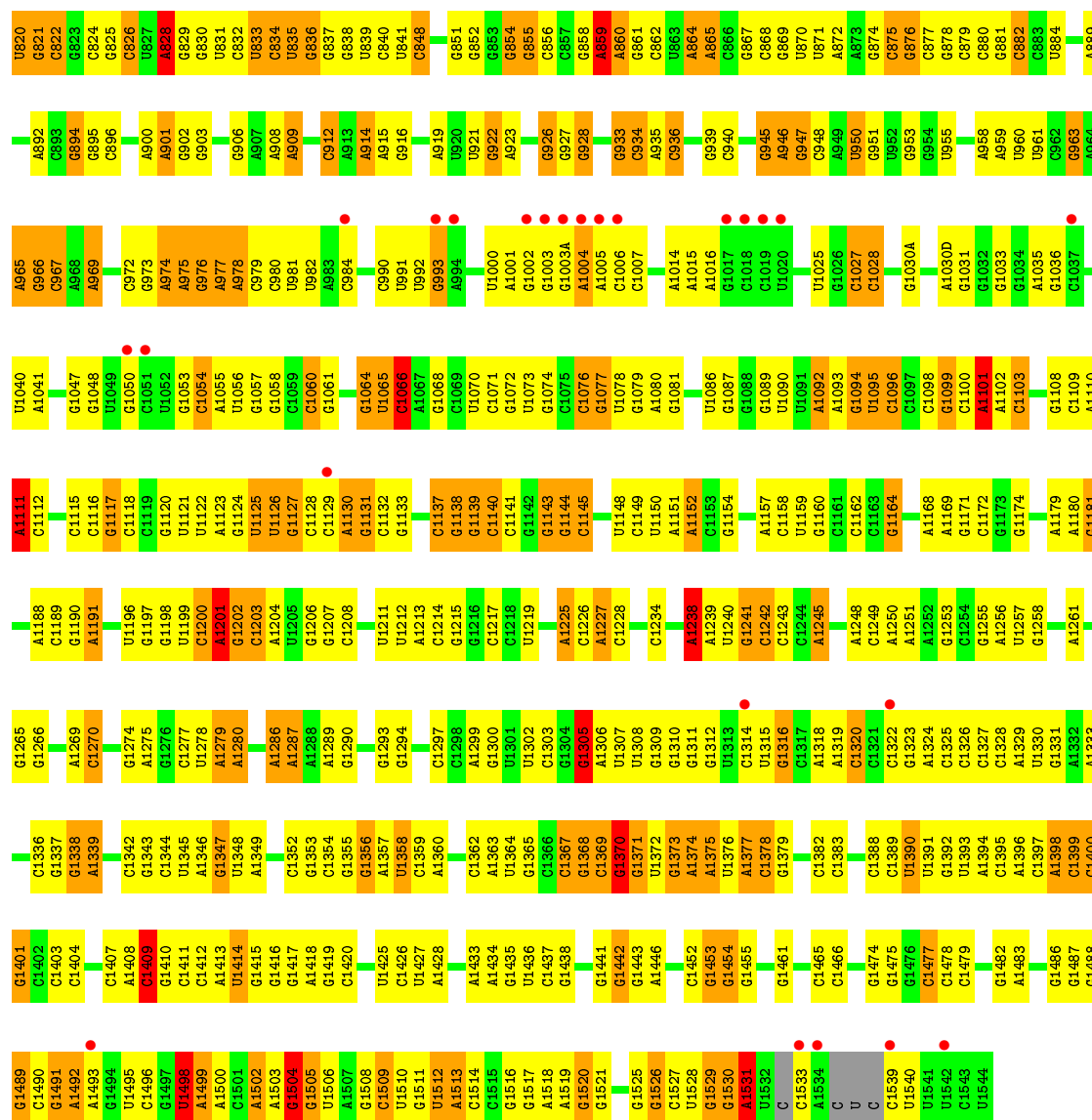
- Molecule 25 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

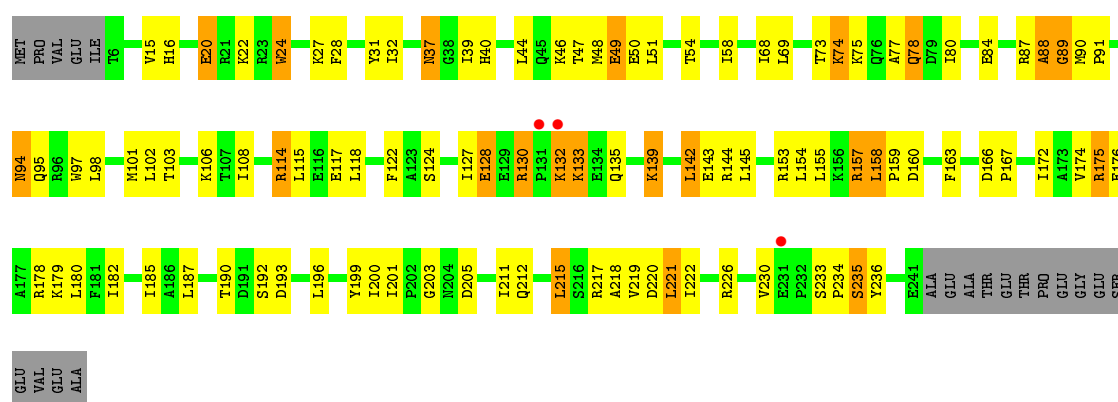
- Molecule 26 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	A	11	Total	O	0	0
			11	11		
26	E	6	Total	O	0	0
			6	6		
26	Q	1	Total	O	0	0
			1	1		

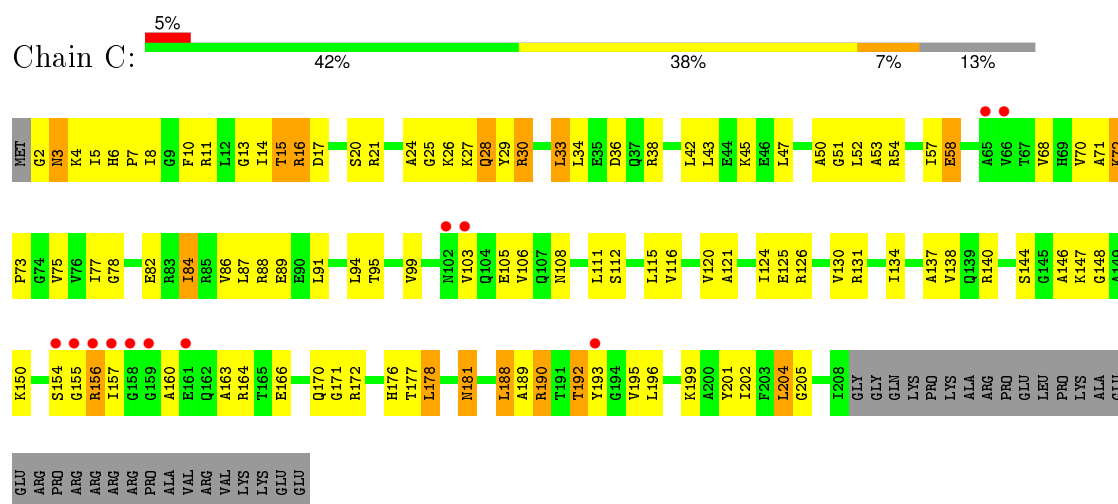




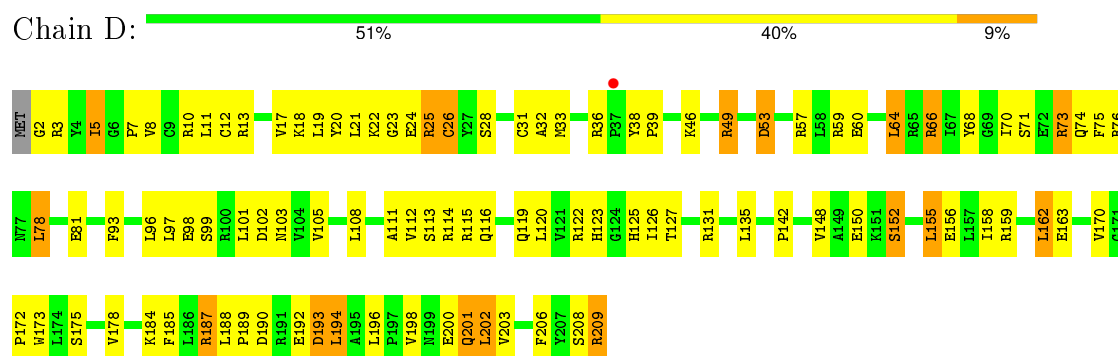
- Molecule 2: ribosomal protein S2



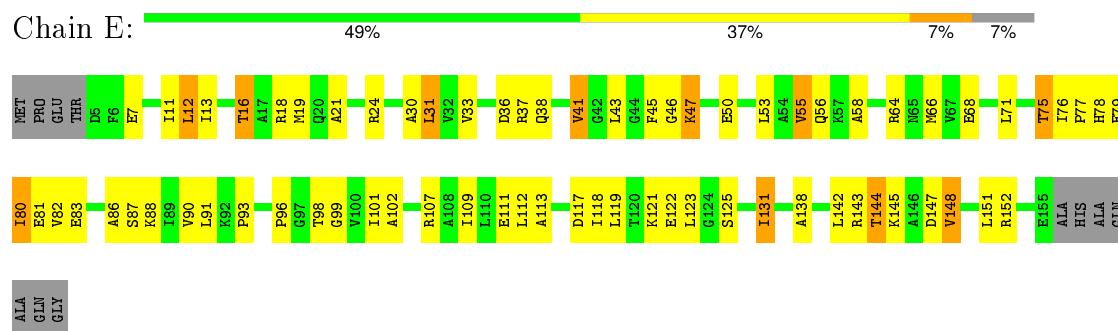
- Molecule 3: ribosomal protein S3



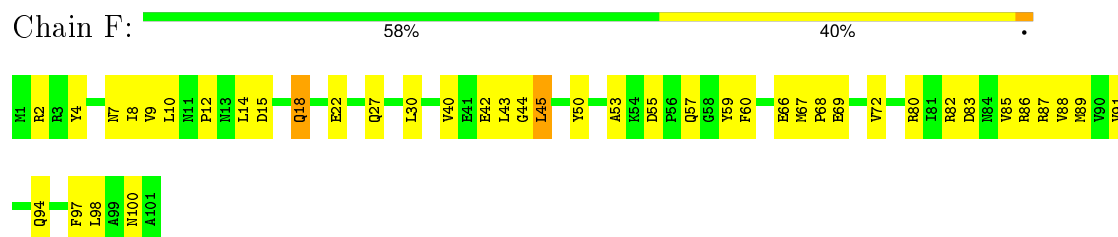
- Molecule 4: ribosomal protein S4



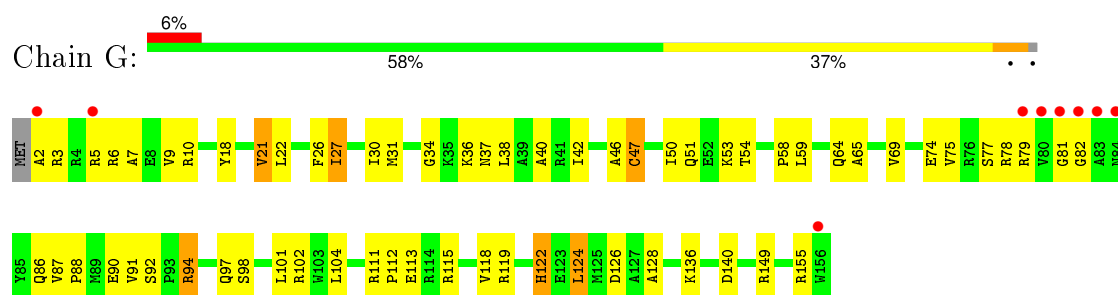
- Molecule 5: ribosomal protein S5



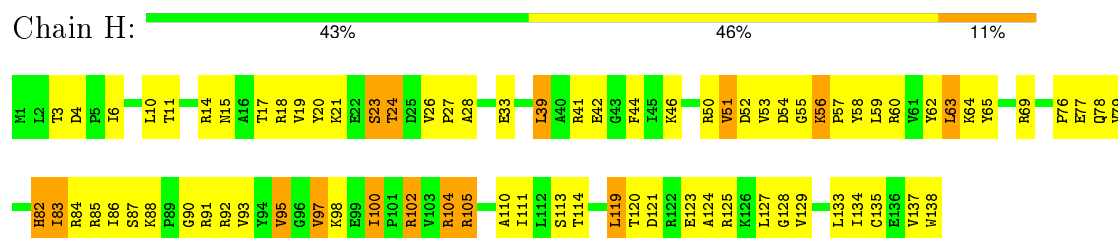
- Molecule 6: ribosomal protein S6



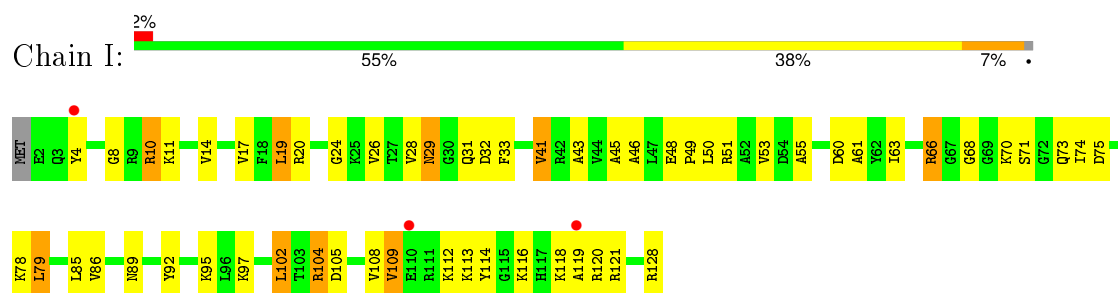
- Molecule 7: ribosomal protein S7



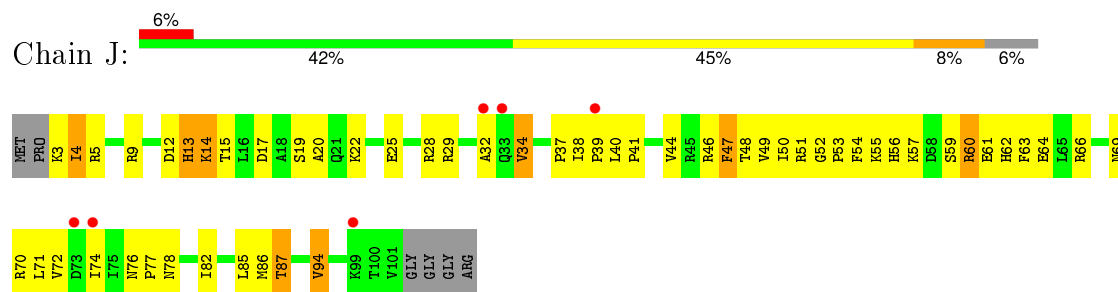
- Molecule 8: ribosomal protein S8



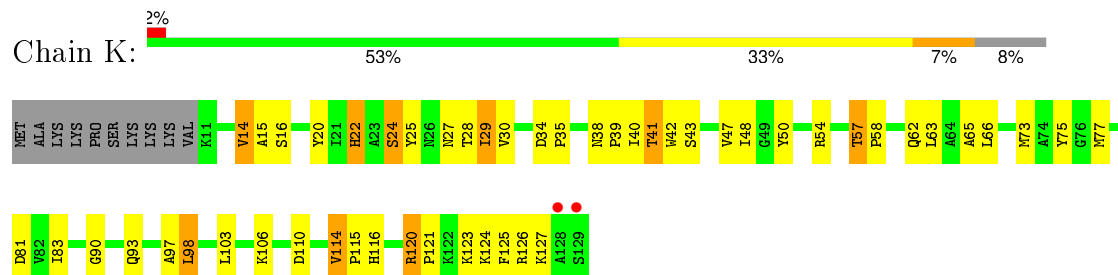
- Molecule 9: ribosomal protein S9



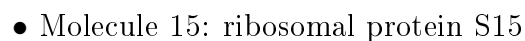
- Molecule 10: ribosomal protein S10

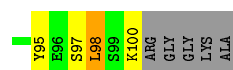


- Molecule 11: ribosomal protein S11

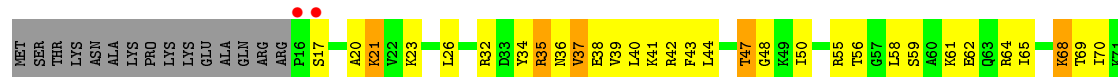


- Molecule 12: ribosomal protein S12

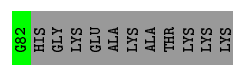




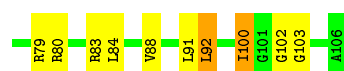
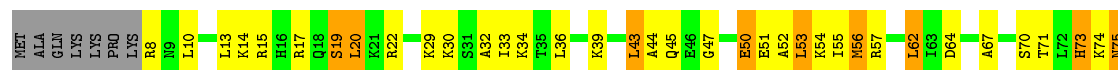
- Molecule 18: ribosomal protein S18



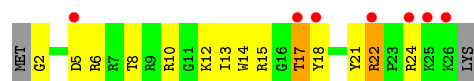
- Molecule 19: ribosomal protein S19



- Molecule 20: ribosomal protein S20



- Molecule 21: ribosomal protein THX



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	401.83Å 401.83Å 174.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.59 – 3.75 34.59 – 3.75	Depositor EDS
% Data completeness (in resolution range)	97.7 (34.59-3.75) 97.5 (34.59-3.75)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.88 (at 3.76Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1119)	Depositor
R, $R_{free}$	0.163 , 0.218 0.169 , 0.217	Depositor DCC
$R_{free}$ test set	7022 reflections (5.23%)	DCC
Wilson B-factor (Å <sup>2</sup> )	137.9	Xtriage
Anisotropy	0.350	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 110.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 141557 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	51823	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	147.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.87% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.89	41/36113 (0.1%)	1.47	568/56360 (1.0%)
2	B	0.57	0/1909	0.73	1/2579 (0.0%)
3	C	0.41	0/1637	0.60	0/2207
4	D	0.56	1/1733 (0.1%)	0.70	1/2318 (0.0%)
5	E	0.72	0/1163	0.86	2/1566 (0.1%)
6	F	0.46	0/856	0.65	0/1154
7	G	0.47	0/1276	0.62	0/1709
8	H	0.82	1/1136 (0.1%)	0.89	0/1527
9	I	0.45	0/1029	0.67	0/1379
10	J	0.43	0/806	0.72	0/1084
11	K	0.56	0/900	0.76	0/1213
12	L	0.58	0/978	0.84	0/1308
13	M	0.48	0/947	0.65	0/1270
14	N	0.50	0/501	0.63	0/664
15	O	0.61	0/745	0.77	1/992 (0.1%)
16	P	0.61	0/717	0.77	0/965
17	Q	0.71	0/836	0.90	1/1117 (0.1%)
18	R	0.56	0/604	0.73	0/801
19	S	0.40	0/662	0.66	0/892
20	T	0.55	0/765	0.78	0/1007
21	U	0.43	0/213	0.63	0/279
All	All	0.79	43/55526 (0.1%)	1.29	574/82391 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2
3	C	0	1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	#Chirality outliers	#Planarity outliers
8	H	0	1
10	J	0	2
18	R	0	1
All	All	0	7

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	868	C	N3-C4	-7.21	1.28	1.33
1	A	1502	A	N9-C4	-7.07	1.33	1.37
1	A	882	C	N3-C4	-7.01	1.29	1.33
1	A	569	C	N3-C4	-6.87	1.29	1.33
1	A	828	A	N9-C4	-6.76	1.33	1.37
1	A	1502	A	C5-C6	-6.71	1.35	1.41
1	A	300	A	N3-C4	-6.65	1.30	1.34
1	A	901	A	N9-C4	-6.50	1.33	1.37
1	A	817	C	N1-C6	-6.42	1.33	1.37
1	A	1227	A	N9-C4	-6.39	1.34	1.37
4	D	12	CYS	CB-SG	6.33	1.93	1.82
1	A	1502	A	N7-C5	-6.19	1.35	1.39
1	A	1513	A	N9-C4	-6.03	1.34	1.37
1	A	130	A	N9-C4	-5.94	1.34	1.37
1	A	864	A	N3-C4	-5.89	1.31	1.34
1	A	822	C	N1-C6	-5.87	1.33	1.37
1	A	300	A	N9-C4	-5.86	1.34	1.37
1	A	1502	A	N3-C4	-5.82	1.31	1.34
1	A	1077	G	N9-C8	-5.68	1.33	1.37
1	A	1377	A	N9-C4	-5.67	1.34	1.37
1	A	1509	C	N3-C4	-5.64	1.30	1.33
1	A	919	A	N9-C4	-5.51	1.34	1.37
1	A	766	A	N9-C4	-5.47	1.34	1.37
1	A	109	A	N9-C4	-5.47	1.34	1.37
1	A	824	C	N1-C6	-5.46	1.33	1.37
1	A	864	A	C6-N1	-5.46	1.31	1.35
8	H	135	CYS	CB-SG	-5.44	1.73	1.81
1	A	865	A	C5-C4	-5.42	1.34	1.38
1	A	1500	A	N3-C4	-5.41	1.31	1.34
1	A	1525	G	C6-N1	-5.37	1.35	1.39
1	A	1504	G	N7-C5	-5.37	1.36	1.39
1	A	1377	A	N3-C4	-5.34	1.31	1.34
1	A	1513	A	N3-C4	-5.33	1.31	1.34
1	A	915	A	N9-C4	-5.27	1.34	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	568	G	C6-N1	-5.20	1.35	1.39
1	A	1066	C	N1-C6	-5.17	1.34	1.37
1	A	807	A	N9-C4	-5.12	1.34	1.37
1	A	584	G	N7-C5	-5.12	1.36	1.39
1	A	722	A	C5-C6	-5.07	1.36	1.41
1	A	298	A	N3-C4	-5.07	1.31	1.34
1	A	124	G	C6-N1	-5.03	1.36	1.39
1	A	876	G	C5-C4	-5.01	1.34	1.38
1	A	574	A	C5-C4	-5.00	1.35	1.38

All (574) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	573	A	C8-N9-C4	-11.59	101.16	105.80
1	A	1502	A	N1-C6-N6	11.23	125.34	118.60
1	A	266	G	N1-C6-O6	11.03	126.52	119.90
1	A	117	G	N1-C6-O6	10.91	126.45	119.90
1	A	691	G	N1-C6-O6	10.59	126.25	119.90
1	A	266	G	C6-C5-N7	-10.58	124.05	130.40
1	A	572	A	N1-C6-N6	-10.51	112.30	118.60
1	A	232	G	N9-C4-C5	-10.28	101.29	105.40
1	A	572	A	C5-C6-N1	10.22	122.81	117.70
1	A	232	G	N1-C6-O6	10.22	126.03	119.90
1	A	815	A	C8-N9-C4	9.89	109.76	105.80
1	A	1502	A	C6-C5-N7	-9.64	125.55	132.30
1	A	266	G	C2-N3-C4	-9.49	107.15	111.90
1	A	122	G	N1-C6-O6	9.49	125.59	119.90
1	A	117	G	C6-C5-N7	-9.29	124.83	130.40
1	A	1502	A	C5-N7-C8	-9.21	99.29	103.90
1	A	1054	C	C2-N1-C1'	9.21	128.93	118.80
1	A	922	G	N1-C6-O6	9.05	125.33	119.90
1	A	1370	G	C8-N9-C4	-8.92	102.83	106.40
1	A	864	A	C5-C6-N6	8.88	130.81	123.70
1	A	577	G	C8-N9-C4	8.77	109.91	106.40
1	A	864	A	N1-C6-N6	-8.76	113.35	118.60
1	A	579	G	N1-C6-O6	8.72	125.14	119.90
1	A	729	A	N1-C6-N6	8.70	123.82	118.60
1	A	1395	C	O5'-P-OP2	-8.59	97.97	105.70
1	A	295	C	C6-N1-C2	8.56	123.72	120.30
1	A	317	G	N1-C6-O6	8.53	125.02	119.90
1	A	1502	A	C4-C5-N7	8.50	114.95	110.70
1	A	310	G	C5-C6-O6	-8.50	123.50	128.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	377	G	N1-C6-O6	8.50	125.00	119.90
1	A	1074	G	C5-C6-N1	-8.40	107.30	111.50
1	A	328	C	N1-C2-O2	8.34	123.91	118.90
1	A	1369	C	C6-N1-C2	-8.33	116.97	120.30
1	A	331	G	N1-C6-O6	8.22	124.83	119.90
1	A	285	G	N1-C6-O6	8.18	124.81	119.90
1	A	299	G	C5-C6-N1	-8.18	107.41	111.50
1	A	691	G	C6-C5-N7	-8.13	125.52	130.40
1	A	232	G	C8-N9-C4	8.12	109.65	106.40
1	A	1054	C	N1-C2-O2	8.10	123.76	118.90
1	A	16	A	C8-N9-C4	8.03	109.01	105.80
1	A	299	G	C5-C6-O6	7.96	133.38	128.60
1	A	584	G	C5-C6-O6	-7.95	123.83	128.60
1	A	292	G	N1-C6-O6	7.94	124.67	119.90
1	A	872	A	N9-C4-C5	-7.91	102.64	105.80
1	A	7	G	C5-C6-O6	-7.90	123.86	128.60
1	A	576	G	N1-C2-N3	7.90	128.64	123.90
1	A	875	C	C5-C6-N1	-7.88	117.06	121.00
1	A	572	A	N9-C4-C5	7.86	108.94	105.80
1	A	724	G	C4-C5-N7	7.84	113.94	110.80
1	A	875	C	C2-N3-C4	-7.83	115.99	119.90
1	A	583	A	N1-C6-N6	7.83	123.30	118.60
1	A	835	U	N3-C2-O2	-7.80	116.74	122.20
1	A	360	A	N1-C6-N6	7.79	123.28	118.60
1	A	133	U	C5-C4-O4	7.76	130.56	125.90
1	A	128	G	N1-C6-O6	7.73	124.54	119.90
1	A	1504	G	P-O3'-C3'	7.69	128.93	119.70
1	A	676	A	C8-N9-C4	7.62	108.85	105.80
1	A	569	C	C5-C6-N1	-7.61	117.20	121.00
1	A	229	U	N1-C2-N3	7.56	119.44	114.90
1	A	1502	A	C2-N3-C4	-7.56	106.82	110.60
1	A	283	C	C6-N1-C2	-7.55	117.28	120.30
1	A	722	A	C2-N3-C4	-7.46	106.87	110.60
1	A	864	A	N9-C4-C5	7.44	108.78	105.80
1	A	1455	G	N1-C6-O6	7.44	124.36	119.90
1	A	1128	C	C6-N1-C2	-7.43	117.33	120.30
1	A	569	C	N3-C4-N4	-7.42	112.81	118.00
1	A	821	G	O5'-P-OP1	-7.42	99.03	105.70
1	A	922	G	C4-N9-C1'	7.42	136.14	126.50
1	A	232	G	C6-C5-N7	-7.40	125.96	130.40
1	A	584	G	N1-C6-O6	7.39	124.34	119.90
1	A	1374	A	O5'-P-OP2	-7.38	99.06	105.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	724	G	C5-C6-O6	-7.37	124.18	128.60
1	A	691	G	C5-C6-O6	-7.37	124.18	128.60
1	A	1373	G	N3-C4-C5	-7.37	124.92	128.60
1	A	154	C	N3-C4-C5	7.35	124.84	121.90
1	A	1528	U	C6-N1-C2	7.33	125.40	121.00
1	A	266	G	C4-C5-N7	7.32	113.73	110.80
1	A	154	C	C6-N1-C2	7.32	123.23	120.30
1	A	852	G	N1-C6-O6	7.31	124.29	119.90
1	A	126	G	C5-C6-N1	-7.31	107.84	111.50
1	A	618	C	C6-N1-C2	7.29	123.22	120.30
1	A	232	G	N3-C4-N9	7.26	130.36	126.00
1	A	573	A	N9-C4-C5	7.26	108.70	105.80
1	A	812	C	P-O3'-C3'	7.25	128.40	119.70
1	A	872	A	N1-C6-N6	7.23	122.94	118.60
1	A	289	G	N1-C6-O6	7.17	124.20	119.90
1	A	1414	U	N3-C2-O2	-7.17	117.18	122.20
1	A	600	C	C5-C6-N1	-7.14	117.43	121.00
1	A	892	A	C2-N3-C4	-7.11	107.05	110.60
1	A	331	G	C5-C6-O6	-7.09	124.34	128.60
1	A	572	A	C6-N1-C2	-7.09	114.35	118.60
1	A	362	G	C5-C6-N1	-7.09	107.96	111.50
1	A	128	G	C5-C6-O6	-7.06	124.36	128.60
1	A	1373	G	N3-C4-N9	7.05	130.23	126.00
1	A	576	G	C8-N9-C1'	-7.04	117.84	127.00
1	A	1054	C	C6-N1-C1'	-7.04	112.35	120.80
1	A	659	U	C5-C6-N1	-7.03	119.18	122.70
1	A	948	C	C6-N1-C2	7.02	123.11	120.30
1	A	389	A	N1-C2-N3	7.01	132.81	129.30
1	A	1074	G	N1-C6-O6	7.01	124.10	119.90
1	A	945	G	C5-C6-O6	-6.99	124.41	128.60
1	A	870	U	N1-C2-O2	6.97	127.68	122.80
1	A	878	G	N1-C6-O6	6.96	124.08	119.90
1	A	1348	U	O5'-P-OP2	-6.96	99.44	105.70
1	A	855	G	C8-N9-C4	6.94	109.18	106.40
1	A	1504	G	OP2-P-O3'	6.94	120.47	105.20
1	A	980	C	N1-C2-O2	6.94	123.06	118.90
1	A	882	C	N3-C2-O2	-6.93	117.05	121.90
1	A	328	C	N3-C2-O2	-6.93	117.05	121.90
1	A	567	G	N9-C4-C5	6.93	108.17	105.40
1	A	128	G	C4-C5-N7	6.92	113.57	110.80
1	A	774	G	C5-C6-O6	-6.92	124.45	128.60
1	A	329	A	C2-N3-C4	-6.91	107.14	110.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	880	C	N3-C4-N4	6.91	122.83	118.00
1	A	117	G	C2-N3-C4	-6.91	108.45	111.90
1	A	454	C	N1-C2-O2	6.90	123.04	118.90
1	A	117	G	C5-C6-O6	-6.90	124.46	128.60
1	A	1403	C	C6-N1-C2	6.89	123.06	120.30
1	A	232	G	C8-N9-C1'	-6.89	118.05	127.00
1	A	1461	G	C8-N9-C4	6.88	109.15	106.40
1	A	107	G	C4-C5-N7	6.87	113.55	110.80
1	A	820	U	O5'-P-OP2	-6.87	99.52	105.70
1	A	922	G	C8-N9-C1'	-6.86	118.09	127.00
1	A	912	C	C5-C4-N4	-6.86	115.40	120.20
1	A	285	G	C8-N9-C4	6.85	109.14	106.40
1	A	21	G	C8-N9-C1'	-6.81	118.14	127.00
1	A	16	A	N7-C8-N9	-6.79	110.41	113.80
1	A	569	C	C2-N3-C4	-6.79	116.51	119.90
1	A	300	A	C2-N3-C4	-6.78	107.21	110.60
1	A	317	G	C5-C6-O6	-6.76	124.54	128.60
1	A	27	G	C4-C5-N7	6.74	113.50	110.80
1	A	569	C	N3-C4-C5	6.74	124.60	121.90
1	A	366	C	N1-C2-O2	6.73	122.94	118.90
1	A	945	G	C5-C6-N1	6.73	114.86	111.50
1	A	872	A	C2-N3-C4	-6.73	107.24	110.60
1	A	122	G	C5-C6-O6	-6.71	124.57	128.60
1	A	326	G	C4-C5-N7	-6.70	108.12	110.80
1	A	567	G	C4-C5-N7	-6.70	108.12	110.80
1	A	190(A)	C	C6-N1-C2	-6.70	117.62	120.30
1	A	1054	C	C5-C6-N1	6.70	124.35	121.00
1	A	331	G	C4-C5-N7	6.70	113.48	110.80
1	A	21	G	N3-C4-N9	6.69	130.02	126.00
1	A	295	C	C5-C6-N1	-6.68	117.66	121.00
1	A	1111	A	N1-C6-N6	-6.68	114.59	118.60
1	A	1079	G	C8-N9-C4	-6.68	103.73	106.40
1	A	579	G	C6-C5-N7	-6.67	126.40	130.40
1	A	317	G	C4-C5-N7	6.66	113.47	110.80
1	A	824	C	C5-C6-N1	-6.65	117.67	121.00
1	A	317	G	N9-C4-C5	-6.65	102.74	105.40
1	A	201	C	C2-N1-C1'	6.64	126.11	118.80
1	A	266	G	C5-C6-N1	-6.64	108.18	111.50
1	A	328	C	C2-N1-C1'	6.64	126.11	118.80
1	A	689	C	C6-N1-C2	-6.64	117.64	120.30
1	A	722	A	C4-C5-N7	6.64	114.02	110.70
1	A	229	U	N1-C2-O2	-6.63	118.16	122.80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	283	C	C5-C6-N1	6.62	124.31	121.00
1	A	201	C	C6-N1-C2	-6.62	117.65	120.30
1	A	292	G	C6-C5-N7	-6.61	126.43	130.40
1	A	573	A	N7-C8-N9	6.58	117.09	113.80
1	A	778	G	C5-C6-N1	-6.58	108.21	111.50
1	A	328	C	N3-C4-C5	6.56	124.52	121.90
1	A	266	G	C5-N7-C8	-6.54	101.03	104.30
1	A	600	C	C2-N3-C4	-6.54	116.63	119.90
1	A	721	G	C6-C5-N7	-6.54	126.48	130.40
1	A	266	G	O5'-P-OP2	-6.53	99.82	105.70
1	A	21	G	O5'-P-OP2	-6.53	99.83	105.70
1	A	824	C	C6-N1-C2	6.52	122.91	120.30
1	A	27	G	C5-C6-O6	-6.51	124.69	128.60
1	A	818	G	N1-C6-O6	6.50	123.80	119.90
1	A	1370	G	C4-N9-C1'	6.48	134.93	126.50
1	A	922	G	C6-C5-N7	-6.48	126.51	130.40
1	A	377	G	C5-C6-O6	-6.47	124.72	128.60
1	A	722	A	N1-C6-N6	6.47	122.48	118.60
1	A	354	G	C8-N9-C4	-6.46	103.81	106.40
1	A	586	C	C5-C6-N1	-6.46	117.77	121.00
1	A	307	C	N1-C2-O2	6.45	122.77	118.90
1	A	15	G	N1-C6-O6	6.44	123.77	119.90
1	A	9	G	N1-C6-O6	6.44	123.76	119.90
1	A	774	G	N1-C6-O6	6.44	123.76	119.90
1	A	1377	A	N1-C6-N6	-6.43	114.74	118.60
1	A	121	C	C6-N1-C2	6.42	122.87	120.30
1	A	596	C	C6-N1-C2	6.41	122.86	120.30
1	A	577	G	N1-C6-O6	6.41	123.75	119.90
1	A	815	A	N7-C8-N9	-6.41	110.59	113.80
1	A	115	G	P-O3'-C3'	6.41	127.39	119.70
1	A	1099	G	N3-C4-N9	-6.41	122.16	126.00
1	A	300	A	N1-C2-N3	6.39	132.50	129.30
1	A	292	G	C5-C6-O6	-6.39	124.77	128.60
1	A	1128	C	C5-C6-N1	6.39	124.19	121.00
1	A	561	U	C6-N1-C2	6.38	124.83	121.00
1	A	281	G	C4-C5-N7	6.38	113.35	110.80
1	A	703	G	C4-C5-N7	-6.37	108.25	110.80
1	A	687	A	P-O3'-C3'	6.37	127.35	119.70
1	A	1531	A	N7-C8-N9	6.36	116.98	113.80
1	A	1238	A	C8-N9-C4	-6.36	103.26	105.80
1	A	825	G	C5-C6-O6	-6.34	124.80	128.60
1	A	303	A	C2-N3-C4	-6.34	107.43	110.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1370	G	N7-C8-N9	6.34	116.27	113.10
1	A	122	G	C4-C5-N7	6.33	113.33	110.80
1	A	855	G	N7-C8-N9	-6.33	109.94	113.10
1	A	572	A	C2-N3-C4	6.32	113.76	110.60
1	A	258	G	C5-C6-N1	-6.31	108.34	111.50
1	A	1370	G	C4-C5-C6	6.29	122.58	118.80
1	A	9	G	O5'-P-OP2	-6.28	100.05	105.70
1	A	15	G	C5-C6-N1	-6.28	108.36	111.50
1	A	201	C	C5-C6-N1	6.28	124.14	121.00
1	A	818	G	C5-C6-O6	-6.28	124.83	128.60
1	A	587	G	O5'-P-OP2	-6.27	100.06	105.70
1	A	1502	A	N7-C8-N9	6.25	116.92	113.80
1	A	130	A	N1-C6-N6	6.24	122.34	118.60
1	A	703	G	C5-C6-O6	6.21	132.33	128.60
1	A	774	G	C6-C5-N7	-6.21	126.67	130.40
1	A	807	A	C2-N3-C4	-6.21	107.50	110.60
1	A	1509	C	N3-C4-N4	-6.21	113.66	118.00
1	A	770	C	N3-C4-C5	6.19	124.38	121.90
1	A	238	G	C5-C6-N1	-6.19	108.41	111.50
1	A	580	U	N3-C4-C5	-6.17	110.90	114.60
1	A	1414	U	N1-C2-O2	6.17	127.12	122.80
1	A	654	G	C2-N3-C4	-6.16	108.82	111.90
1	A	856	C	N3-C4-C5	-6.15	119.44	121.90
1	A	21	G	N3-C2-N2	6.14	124.20	119.90
1	A	428	G	P-O3'-C3'	6.13	127.06	119.70
1	A	1509	C	C5-C6-N1	-6.13	117.94	121.00
1	A	310	G	N1-C6-O6	6.12	123.58	119.90
1	A	815	A	N9-C4-C5	-6.12	103.35	105.80
1	A	266	G	N1-C2-N3	6.12	127.57	123.90
1	A	757	U	C5-C6-N1	-6.12	119.64	122.70
1	A	59	A	C5-C6-N1	6.11	120.76	117.70
1	A	128	G	C6-C5-N7	-6.11	126.73	130.40
1	A	721	G	C8-N9-C1'	-6.11	119.06	127.00
1	A	615	C	C6-N1-C2	-6.09	117.86	120.30
1	A	608	A	C2-N3-C4	-6.09	107.55	110.60
1	A	7	G	N1-C6-O6	6.08	123.55	119.90
1	A	872	A	C8-N9-C4	6.08	108.23	105.80
1	A	805	C	C6-N1-C2	6.07	122.73	120.30
1	A	570	G	N3-C4-C5	-6.06	125.57	128.60
1	A	721	G	C4-N9-C1'	6.06	134.38	126.50
1	A	864	A	C4-C5-N7	-6.04	107.68	110.70
1	A	576	G	C4-N9-C1'	6.03	134.34	126.50

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	285	G	C2-N3-C4	-6.03	108.89	111.90
1	A	589	C	C5-C6-N1	-6.02	117.99	121.00
1	A	722	A	C5-N7-C8	-6.00	100.90	103.90
1	A	122	G	C6-C5-N7	-5.99	126.81	130.40
1	A	832	C	C2-N3-C4	-5.99	116.91	119.90
1	A	1371	G	O5'-P-OP1	-5.99	100.31	105.70
1	A	647	C	C6-N1-C2	5.98	122.69	120.30
1	A	733	A	C2-N3-C4	-5.98	107.61	110.60
1	A	1388	C	C6-N1-C2	5.98	122.69	120.30
1	A	274	A	C8-N9-C4	5.97	108.19	105.80
1	A	328	C	P-O3'-C3'	5.96	126.86	119.70
1	A	21	G	OP2-P-O3'	5.96	118.32	105.20
1	A	724	G	C5-N7-C8	-5.96	101.32	104.30
1	A	1367	C	C6-N1-C2	-5.96	117.92	120.30
1	A	1527	C	N3-C4-C5	5.96	124.28	121.90
1	A	1103	C	C6-N1-C2	5.95	122.68	120.30
1	A	238	G	N7-C8-N9	5.95	116.08	113.10
1	A	21	G	O5'-P-OP1	5.95	117.84	110.70
1	A	597	G	O5'-P-OP1	-5.94	100.35	105.70
1	A	1455	G	C4-C5-N7	5.94	113.18	110.80
1	A	882	C	C4-C5-C6	5.93	120.37	117.40
1	A	126	G	N1-C6-O6	5.93	123.46	119.90
1	A	238	G	C8-N9-C4	-5.93	104.03	106.40
1	A	1227	A	C5-N7-C8	-5.93	100.94	103.90
1	A	17	U	N3-C4-O4	5.93	123.55	119.40
1	A	342	C	C6-N1-C2	-5.92	117.93	120.30
1	A	820	U	N1-C2-O2	-5.92	118.65	122.80
1	A	1370	G	C5-C6-N1	-5.91	108.54	111.50
1	A	362	G	N1-C6-O6	5.91	123.44	119.90
1	A	24	U	C5-C6-N1	-5.90	119.75	122.70
1	A	416	G	N1-C6-O6	5.90	123.44	119.90
1	A	232	G	C5-C6-N1	-5.89	108.56	111.50
1	A	755	G	N1-C6-O6	5.89	123.43	119.90
4	D	12	CYS	CA-CB-SG	5.89	124.59	114.00
1	A	892	A	N1-C2-N3	5.88	132.24	129.30
1	A	1181	G	C4-N9-C1'	-5.88	118.86	126.50
1	A	28	G	N1-C6-O6	5.87	123.42	119.90
1	A	90	U	C5-C6-N1	5.87	125.64	122.70
1	A	1531	A	N1-C6-N6	5.87	122.12	118.60
1	A	1370	G	C6-C5-N7	-5.87	126.88	130.40
1	A	583	A	C5-C6-N6	-5.87	119.01	123.70
1	A	360	A	C5-C6-N6	-5.85	119.02	123.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1504	G	N3-C4-C5	-5.85	125.68	128.60
1	A	1074	G	C6-C5-N7	-5.84	126.89	130.40
1	A	285	G	N9-C4-C5	-5.84	103.06	105.40
1	A	1090	U	N3-C4-C5	-5.83	111.10	114.60
1	A	900	A	C8-N9-C4	-5.83	103.47	105.80
1	A	1099	G	N9-C4-C5	5.83	107.73	105.40
1	A	623	C	C6-N1-C2	5.82	122.63	120.30
1	A	1203	C	C6-N1-C2	-5.82	117.97	120.30
1	A	1528	U	N1-C2-N3	-5.82	111.41	114.90
1	A	600	C	C4-C5-C6	5.82	120.31	117.40
1	A	577	G	N3-C4-C5	5.81	131.51	128.60
1	A	836	G	N1-C6-O6	5.81	123.39	119.90
1	A	628	G	N3-C4-C5	-5.81	125.70	128.60
1	A	1103	C	C5-C6-N1	-5.80	118.10	121.00
1	A	1529	G	C4-N9-C1'	5.80	134.04	126.50
1	A	834	C	N3-C4-C5	5.80	124.22	121.90
1	A	1299	A	C8-N9-C4	-5.80	103.48	105.80
1	A	1479	C	C6-N1-C2	-5.79	117.98	120.30
1	A	729	A	N9-C4-C5	-5.78	103.49	105.80
5	E	12	LEU	CA-CB-CG	5.78	128.59	115.30
1	A	566	G	N3-C4-N9	-5.77	122.54	126.00
1	A	878	G	C6-C5-N7	-5.75	126.95	130.40
1	A	299	G	C4-C5-N7	-5.75	108.50	110.80
1	A	32	A	N1-C2-N3	5.75	132.17	129.30
1	A	867	G	N1-C6-O6	5.74	123.35	119.90
1	A	48	C	O5'-P-OP1	-5.72	100.55	105.70
1	A	120	A	N1-C2-N3	5.72	132.16	129.30
1	A	1388	C	N3-C2-O2	5.72	125.91	121.90
1	A	21	G	N9-C4-C5	-5.72	103.11	105.40
1	A	804	U	N3-C2-O2	-5.72	118.20	122.20
1	A	117	G	C4-C5-N7	5.71	113.08	110.80
1	A	812	C	N3-C2-O2	-5.71	117.90	121.90
1	A	1239	A	C8-N9-C4	5.71	108.08	105.80
1	A	731	G	N1-C6-O6	5.71	123.32	119.90
1	A	576	G	N1-C2-N2	-5.70	111.07	116.20
1	A	1087	G	N1-C6-O6	5.70	123.32	119.90
1	A	266	G	C4-C5-C6	5.70	122.22	118.80
1	A	859	A	N1-C6-N6	5.69	122.02	118.60
1	A	32	A	C6-N1-C2	-5.69	115.19	118.60
1	A	880	C	C5-C4-N4	-5.69	116.22	120.20
1	A	729	A	C5-C6-N6	-5.68	119.15	123.70
1	A	916	G	C6-N1-C2	-5.68	121.69	125.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	679	C	C6-N1-C2	5.68	122.57	120.30
1	A	833	U	N3-C4-C5	-5.68	111.19	114.60
1	A	573	A	C4-C5-C6	5.67	119.84	117.00
1	A	692	U	N3-C4-C5	-5.67	111.20	114.60
1	A	1203	C	C5-C6-N1	5.67	123.84	121.00
1	A	1346	A	N1-C6-N6	-5.67	115.20	118.60
1	A	724	G	N1-C6-O6	5.67	123.30	119.90
1	A	1375	A	N1-C6-N6	-5.67	115.20	118.60
1	A	877	C	C5-C6-N1	-5.66	118.17	121.00
1	A	584	G	C4-C5-N7	5.66	113.06	110.80
1	A	922	G	C5-C6-N1	-5.65	108.68	111.50
1	A	934	C	C2-N1-C1'	-5.65	112.59	118.80
1	A	946	A	C8-N9-C4	-5.64	103.54	105.80
1	A	642	A	N1-C6-N6	-5.64	115.22	118.60
1	A	1526	G	C5-C6-O6	-5.63	125.22	128.60
1	A	129(A)	G	C4-N9-C1'	5.63	133.82	126.50
1	A	856	C	C4-C5-C6	5.61	120.21	117.40
1	A	825	G	C8-N9-C4	5.61	108.64	106.40
1	A	1455	G	C5-C6-O6	-5.61	125.23	128.60
1	A	676	A	N7-C8-N9	-5.60	111.00	113.80
1	A	921	U	N3-C4-O4	5.60	123.32	119.40
1	A	878	G	C5-C6-O6	-5.60	125.24	128.60
1	A	1530	G	C8-N9-C4	5.59	108.64	106.40
1	A	229	U	C6-N1-C2	-5.59	117.65	121.00
1	A	774	G	C4-C5-N7	5.58	113.03	110.80
1	A	805	C	N3-C4-C5	5.57	124.13	121.90
1	A	577	G	N7-C8-N9	-5.57	110.32	113.10
1	A	328	C	N3-C4-N4	-5.56	114.11	118.00
1	A	416	G	C6-C5-N7	-5.55	127.07	130.40
1	A	879	C	C5-C4-N4	-5.54	116.32	120.20
1	A	1452	C	C6-N1-C2	5.54	122.52	120.30
1	A	1504	G	C4-N9-C1'	5.54	133.70	126.50
1	A	1529	G	C8-N9-C4	-5.54	104.19	106.40
1	A	126	G	N3-C2-N2	-5.53	116.03	119.90
2	B	80	ILE	N-CA-C	-5.52	96.09	111.00
1	A	80	G	N3-C4-N9	5.52	129.31	126.00
1	A	257	G	N1-C6-O6	5.51	123.21	119.90
1	A	308	C	N1-C2-O2	5.51	122.21	118.90
1	A	1101	A	O5'-P-OP2	-5.51	100.74	105.70
1	A	131	C	C5-C6-N1	-5.51	118.24	121.00
1	A	190(D)	U	C5-C6-N1	-5.51	119.95	122.70
1	A	484	G	P-O3'-C3'	5.50	126.30	119.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	266	G	C5-C6-O6	-5.50	125.30	128.60
1	A	283	C	N3-C4-C5	-5.49	119.70	121.90
1	A	289	G	C5-C6-O6	-5.49	125.31	128.60
1	A	906	G	N1-C6-O6	5.49	123.19	119.90
1	A	945	G	C4-C5-N7	5.49	113.00	110.80
1	A	117	G	C4-C5-C6	5.48	122.09	118.80
1	A	394	G	C4-C5-N7	-5.48	108.61	110.80
1	A	589	C	C2-N3-C4	-5.47	117.16	119.90
1	A	867	G	C5-C6-O6	-5.47	125.31	128.60
1	A	74	C	C6-N1-C2	-5.47	118.11	120.30
1	A	1074	G	C4-C5-C6	5.47	122.08	118.80
1	A	107	G	N1-C6-O6	5.47	123.18	119.90
1	A	948	C	C5-C6-N1	-5.47	118.27	121.00
1	A	1181	G	C8-N9-C1'	5.47	134.11	127.00
1	A	366	C	C2-N1-C1'	5.46	124.81	118.80
1	A	655	A	C8-N9-C4	5.46	107.98	105.80
1	A	117	G	C5-N7-C8	-5.46	101.57	104.30
1	A	575	G	N3-C4-C5	5.45	131.33	128.60
1	A	1378	C	N1-C2-O2	-5.45	115.63	118.90
1	A	914	A	C8-N9-C4	5.44	107.98	105.80
1	A	127	G	C5-C6-O6	-5.44	125.33	128.60
1	A	254	G	O5'-P-OP1	-5.43	100.81	105.70
1	A	780	A	N1-C6-N6	-5.42	115.35	118.60
1	A	1390	U	C4-C5-C6	5.42	122.95	119.70
1	A	874	G	C6-N1-C2	-5.42	121.85	125.10
1	A	326	G	N3-C4-C5	-5.42	125.89	128.60
1	A	654	G	N3-C4-C5	5.41	131.31	128.60
1	A	38	G	C8-N9-C4	5.41	108.56	106.40
1	A	1452	C	N1-C2-N3	-5.41	115.41	119.20
1	A	129(A)	G	N3-C4-N9	5.40	129.24	126.00
1	A	559	A	P-O3'-C3'	5.40	126.18	119.70
1	A	566	G	N9-C4-C5	5.40	107.56	105.40
1	A	724	G	N9-C4-C5	-5.40	103.24	105.40
1	A	786	G	C5-C6-O6	-5.39	125.36	128.60
1	A	915	A	C2-N3-C4	-5.39	107.91	110.60
1	A	310	G	N9-C4-C5	-5.39	103.25	105.40
1	A	317	G	C2-N3-C4	-5.38	109.21	111.90
1	A	331	G	C6-C5-N7	-5.38	127.17	130.40
1	A	706	A	N1-C6-N6	5.38	121.83	118.60
1	A	125	U	C5-C6-N1	-5.38	120.01	122.70
1	A	1365	G	C8-N9-C4	-5.38	104.25	106.40
1	A	1502	A	C5-C6-N6	-5.38	119.40	123.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1356	G	N1-C6-O6	-5.37	116.68	119.90
1	A	258	G	N1-C6-O6	5.37	123.12	119.90
1	A	247	G	O5'-P-OP2	-5.36	100.88	105.70
1	A	1375	A	C5-N7-C8	5.36	106.58	103.90
1	A	1079	G	N9-C4-C5	5.36	107.54	105.40
1	A	1512	U	N3-C4-C5	-5.35	111.39	114.60
1	A	331	G	N9-C4-C5	-5.35	103.26	105.40
1	A	597	G	N3-C4-C5	-5.35	125.93	128.60
1	A	874	G	N3-C4-N9	5.35	129.21	126.00
1	A	21	G	N1-C2-N2	-5.34	111.39	116.20
1	A	307	C	C2-N1-C1'	5.34	124.68	118.80
1	A	607	A	N1-C6-N6	5.34	121.81	118.60
1	A	317	G	C6-C5-N7	-5.34	127.20	130.40
1	A	874	G	C8-N9-C4	5.34	108.54	106.40
1	A	761	G	N1-C6-O6	5.33	123.10	119.90
1	A	309	G	C5-C6-O6	-5.33	125.40	128.60
1	A	566	G	C8-N9-C4	-5.33	104.27	106.40
1	A	1279	A	N7-C8-N9	5.33	116.47	113.80
1	A	73	C	C6-N1-C2	-5.33	118.17	120.30
1	A	120	A	C2-N3-C4	-5.33	107.94	110.60
1	A	53	A	N1-C2-N3	5.33	131.96	129.30
1	A	565	U	C6-N1-C2	5.32	124.19	121.00
1	A	232	G	C5-C6-O6	-5.32	125.41	128.60
1	A	306	G	C8-N9-C4	5.31	108.53	106.40
1	A	824	C	C2-N3-C4	-5.31	117.24	119.90
1	A	867	G	C4-C5-N7	5.31	112.92	110.80
1	A	257	G	C6-C5-N7	-5.31	127.21	130.40
1	A	815	A	N1-C6-N6	5.31	121.79	118.60
1	A	128	G	C5-N7-C8	-5.31	101.65	104.30
1	A	609	A	C2-N3-C4	-5.30	107.95	110.60
1	A	1530	G	N3-C4-C5	5.30	131.25	128.60
1	A	872	A	C4-C5-N7	5.30	113.35	110.70
1	A	644	G	C5-C6-N1	5.29	114.15	111.50
1	A	21	G	C4-N9-C1'	5.29	133.38	126.50
1	A	820	U	C5-C6-N1	-5.29	120.06	122.70
1	A	1197	G	N3-C4-N9	5.29	129.18	126.00
1	A	1201	A	P-O3'-C3'	5.29	126.05	119.70
1	A	109	A	C5-N7-C8	-5.29	101.26	103.90
1	A	599	C	C6-N1-C2	5.29	122.41	120.30
1	A	729	A	C4-C5-N7	5.28	113.34	110.70
1	A	190(G)	G	N1-C6-O6	5.28	123.07	119.90
1	A	552	U	N1-C2-N3	5.28	118.07	114.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1531	A	C5-N7-C8	-5.28	101.26	103.90
1	A	691	G	N9-C4-C5	-5.28	103.29	105.40
1	A	541	G	N1-C6-O6	5.28	123.07	119.90
1	A	553	A	C5-C6-N1	5.27	120.34	117.70
1	A	380	G	C5-C6-N1	-5.27	108.86	111.50
1	A	723	U	C5-C6-N1	5.27	125.34	122.70
1	A	836	G	C5-C6-N1	-5.27	108.86	111.50
1	A	1227	A	C4-C5-N7	5.27	113.33	110.70
1	A	933	G	C6-C5-N7	-5.27	127.24	130.40
1	A	394	G	C5-C6-O6	5.26	131.76	128.60
1	A	832	C	C5-C6-N1	-5.26	118.37	121.00
1	A	691	G	C4-C5-N7	5.26	112.90	110.80
1	A	835	U	O4'-C1'-N1	5.26	112.41	108.20
1	A	936	C	OP2-P-O3'	5.26	116.76	105.20
1	A	1401	G	C8-N9-C4	5.26	108.50	106.40
1	A	1504	G	O4'-C1'-N9	-5.26	104.00	108.20
1	A	963	G	C8-N9-C4	-5.25	104.30	106.40
1	A	238	G	N1-C6-O6	5.25	123.05	119.90
1	A	559	A	C6-N1-C2	-5.25	115.45	118.60
1	A	19	C	N1-C2-O2	-5.25	115.75	118.90
1	A	1390	U	C6-N1-C2	-5.25	117.85	121.00
1	A	73	C	C5-C6-N1	5.24	123.62	121.00
1	A	190(G)	G	C6-C5-N7	-5.24	127.26	130.40
1	A	909	A	C6-N1-C2	-5.23	115.46	118.60
1	A	865	A	C5-C6-N1	5.23	120.32	117.70
1	A	965	A	C8-N9-C4	5.23	107.89	105.80
1	A	366	C	N3-C2-O2	-5.23	118.24	121.90
1	A	326	G	C5-C6-O6	5.23	131.74	128.60
1	A	599	C	C5-C6-N1	-5.22	118.39	121.00
1	A	1390	U	N3-C4-C5	-5.22	111.47	114.60
1	A	125	U	C4-C5-C6	5.22	122.83	119.70
1	A	1339	A	N7-C8-N9	-5.22	111.19	113.80
1	A	360	A	C6-C5-N7	-5.22	128.65	132.30
1	A	530	G	C8-N9-C4	-5.22	104.31	106.40
1	A	1238	A	N9-C4-C5	5.22	107.89	105.80
1	A	1305	G	C8-N9-C4	-5.21	104.31	106.40
1	A	854	G	C6-C5-N7	-5.21	127.27	130.40
1	A	692	U	N3-C4-O4	5.21	123.05	119.40
1	A	579	G	C5-C6-O6	-5.21	125.47	128.60
1	A	329	A	N1-C6-N6	5.21	121.72	118.60
1	A	867	G	C6-C5-N7	-5.21	127.28	130.40
1	A	81	U	C6-N1-C2	-5.21	117.88	121.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	138	G	C8-N9-C4	5.20	108.48	106.40
1	A	292	G	N3-C4-N9	5.20	129.12	126.00
1	A	785	G	N1-C6-O6	5.20	123.02	119.90
1	A	928	G	N1-C6-O6	5.20	123.02	119.90
1	A	78	G	N1-C6-O6	5.20	123.02	119.90
1	A	878	G	C2-N3-C4	-5.19	109.30	111.90
1	A	1100	C	OP2-P-O3'	5.19	116.63	105.20
1	A	1504	G	N3-C4-N9	5.19	129.12	126.00
1	A	779	C	C5-C6-N1	-5.19	118.41	121.00
1	A	874	G	C5-C6-O6	-5.19	125.49	128.60
1	A	1498	UR3	P-O3'-C3'	5.19	125.92	119.70
1	A	266	G	N7-C8-N9	5.18	115.69	113.10
1	A	722	A	C6-C5-N7	-5.18	128.67	132.30
1	A	993	G	C4-N9-C1'	5.17	133.22	126.50
1	A	107	G	C6-C5-N7	-5.17	127.30	130.40
1	A	232	G	C4-C5-N7	5.17	112.87	110.80
1	A	281	G	N3-C4-C5	5.16	131.18	128.60
1	A	837	G	C8-N9-C4	5.16	108.46	106.40
1	A	1369	C	N3-C2-O2	-5.15	118.29	121.90
1	A	18	C	C5-C6-N1	-5.15	118.42	121.00
1	A	21	G	C8-N9-C4	5.15	108.46	106.40
1	A	894	G	C4-C5-N7	5.15	112.86	110.80
1	A	238	G	C6-C5-N7	-5.15	127.31	130.40
1	A	281	G	C5-C6-O6	-5.14	125.51	128.60
1	A	1076	C	OP2-P-O3'	5.14	116.50	105.20
1	A	266	G	C4-N9-C1'	5.13	133.17	126.50
1	A	572	A	C8-N9-C4	-5.13	103.75	105.80
1	A	860	A	C2-N3-C4	-5.12	108.04	110.60
1	A	1502	A	N9-C4-C5	-5.12	103.75	105.80
1	A	1227	A	N1-C6-N6	5.12	121.67	118.60
1	A	281	G	C5-N7-C8	-5.11	101.74	104.30
1	A	912	C	N3-C4-N4	5.11	121.58	118.00
1	A	285	G	C6-C5-N7	-5.11	127.33	130.40
1	A	117	G	N7-C8-N9	5.11	115.66	113.10
1	A	906	G	C4-C5-N7	5.11	112.84	110.80
1	A	1409	C	C6-N1-C2	-5.11	118.26	120.30
1	A	914	A	OP2-P-O3'	5.09	116.41	105.20
1	A	1492	A	C2-N3-C4	5.09	113.15	110.60
1	A	947	G	N1-C6-O6	5.09	122.95	119.90
1	A	794	A	N1-C6-N6	-5.09	115.55	118.60
1	A	589	C	C6-N1-C2	5.09	122.33	120.30
1	A	721	G	C4-C5-C6	5.08	121.85	118.80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1318	A	C8-N9-C4	5.08	107.83	105.80
1	A	1373	G	C4-N9-C1'	5.08	133.11	126.50
1	A	133	U	N3-C2-O2	-5.08	118.64	122.20
1	A	828	A	C2-N3-C4	-5.08	108.06	110.60
1	A	922	G	O5'-P-OP2	-5.07	101.14	105.70
1	A	1508	G	OP2-P-O3'	5.07	116.36	105.20
1	A	575	G	N3-C4-N9	-5.07	122.96	126.00
1	A	1504	G	C6-C5-N7	-5.07	127.36	130.40
1	A	27	G	C6-C5-N7	-5.06	127.36	130.40
1	A	779	C	C2-N3-C4	-5.06	117.37	119.90
17	Q	31	LEU	CA-CB-CG	-5.06	103.67	115.30
1	A	825	G	N7-C8-N9	-5.06	110.57	113.10
1	A	1111	A	C5-C6-N6	5.06	127.75	123.70
1	A	477	G	N1-C6-O6	5.05	122.93	119.90
1	A	249	U	C5-C4-O4	5.05	128.93	125.90
1	A	1333	A	C8-N9-C4	-5.05	103.78	105.80
1	A	17	U	N1-C2-O2	-5.05	119.27	122.80
1	A	20	U	C5-C6-N1	-5.05	120.18	122.70
1	A	377	G	C6-C5-N7	-5.05	127.37	130.40
1	A	658	G	C8-N9-C1'	-5.05	120.44	127.00
1	A	1512	U	N1-C2-N3	5.05	117.93	114.90
1	A	326	G	C5-N7-C8	5.04	106.82	104.30
1	A	862	C	N3-C4-C5	5.04	123.92	121.90
1	A	292	G	N9-C4-C5	-5.04	103.39	105.40
1	A	690	G	C5-C6-O6	5.04	131.62	128.60
1	A	600	C	N1-C2-N3	5.03	122.72	119.20
1	A	586	C	C6-N1-C2	5.03	122.31	120.30
1	A	293	G	N1-C6-O6	5.03	122.92	119.90
1	A	307	C	C5-C6-N1	5.02	123.51	121.00
1	A	328	C	C6-N1-C1'	-5.02	114.77	120.80
1	A	757	U	C4-C5-C6	5.02	122.71	119.70
15	O	67	LEU	CA-CB-CG	-5.02	103.75	115.30
1	A	832	C	N3-C4-C5	5.02	123.91	121.90
1	A	570	G	C6-N1-C2	-5.02	122.09	125.10
1	A	229	U	C4-C5-C6	5.02	122.71	119.70
1	A	59	A	C2-N3-C4	5.01	113.11	110.60
5	E	41	VAL	CB-CA-C	-5.01	101.88	111.40
1	A	26	A	C2-N3-C4	-5.01	108.09	110.60
1	A	181	G	P-O3'-C3'	5.01	125.71	119.70
1	A	666	G	C2-N3-C4	-5.01	109.40	111.90
1	A	690	G	C4-C5-N7	-5.00	108.80	110.80

There are no chirality outliers.



All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	130	ARG	Peptide
2	B	88	ALA	Peptide
3	C	166	GLU	Peptide
8	H	90	GLY	Peptide
10	J	12	ASP	Peptide
10	J	87	THR	Peptide
18	R	20	ALA	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32522	0	16437	648	0
2	B	1874	0	1887	74	0
3	C	1613	0	1677	78	0
4	D	1703	0	1763	81	0
5	E	1147	0	1207	49	0
6	F	843	0	857	34	0
7	G	1257	0	1296	48	0
8	H	1116	0	1177	51	0
9	I	1010	0	1037	41	0
10	J	793	0	835	43	0
11	K	885	0	904	34	0
12	L	973	0	1058	33	0
13	M	937	0	995	43	0
14	N	492	0	529	44	0
15	O	734	0	771	30	0
16	P	701	0	720	16	0
17	Q	823	0	891	36	0
18	R	598	0	670	30	0
19	S	648	0	673	24	0
20	T	763	0	861	34	0
21	U	209	0	221	20	0
22	A	108	0	0	0	0
22	B	1	0	0	0	0
22	D	2	0	0	0	0
22	E	1	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	H	2	0	0	0	0
22	K	1	0	0	0	0
22	L	1	0	0	0	0
22	M	1	0	0	0	0
22	S	1	0	0	0	0
23	A	8	0	0	0	0
24	A	36	0	37	4	0
25	D	1	0	0	0	0
25	N	1	0	0	0	0
26	A	11	0	0	0	0
26	E	6	0	0	0	0
26	Q	1	0	0	0	0
All	All	51823	0	36503	1335	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (1335) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:G:H5''	12:L:114:LYS:HB2	1.55	0.88
1:A:959:A:HO2'	1:A:984:C:HO2'	1.18	0.88
16:P:57:ARG:NH1	16:P:79:VAL:O	2.07	0.86
1:A:279:A:OP2	17:Q:95:TYR:OH	1.93	0.85
5:E:11:ILE:HB	5:E:31:LEU:HB3	1.57	0.85
2:B:75:LYS:HA	2:B:78:GLN:HB2	1.59	0.84
10:J:48:THR:HG1	10:J:62:HIS:HD1	0.85	0.84
1:A:144:G:H1	1:A:178:C:H42	1.26	0.84
13:M:86:CYS:SG	13:M:87:TYR:N	2.51	0.84
8:H:51:VAL:HG11	8:H:60:ARG:HG3	1.61	0.83
1:A:1133:G:H1	1:A:1141:C:H42	1.27	0.83
1:A:664:G:H22	1:A:741:G:H1	1.26	0.83
20:T:30:LYS:HE3	20:T:80:ARG:HH12	1.42	0.82
18:R:17:SER:HB3	18:R:55:ARG:HG2	1.62	0.81
10:J:48:THR:OG1	10:J:62:HIS:ND1	2.03	0.81
1:A:235:C:H5'	17:Q:70:ARG:HG2	1.62	0.81
5:E:80:ILE:HD11	5:E:138:ALA:HB1	1.62	0.81
19:S:7:LYS:NZ	19:S:7:LYS:O	2.13	0.80
1:A:1376:U:OP1	7:G:98:SER:OG	1.99	0.80
1:A:792:A:H4'	1:A:793:U:H5'	1.64	0.79
1:A:974:A:OP2	14:N:41:ARG:NH1	2.14	0.79

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:6:ARG:HH21	21:U:15:ARG:HH21	1.29	0.79
6:F:2:ARG:HE	6:F:69:GLU:HG2	1.46	0.79
2:B:103:THR:N	2:B:176:GLU:OE1	2.16	0.78
1:A:692:U:OP1	11:K:124:LYS:NZ	2.15	0.78
1:A:1028:C:N3	1:A:1033:G:N2	2.31	0.77
1:A:1060:C:OP1	14:N:45:ARG:NH2	2.16	0.77
13:M:4:ILE:HD12	13:M:56:LEU:HD12	1.64	0.77
1:A:1368:G:H5'	9:I:112:LYS:HB3	1.66	0.77
1:A:103:C:OP1	20:T:17:ARG:NH1	2.15	0.77
1:A:1028:C:H42	1:A:1033:G:H1	1.33	0.77
7:G:79:ARG:HG3	7:G:81:GLY:H	1.51	0.76
19:S:33:THR:HG22	19:S:35:SER:H	1.49	0.76
11:K:40:ILE:HG22	11:K:41:THR:HG22	1.69	0.75
2:B:78:GLN:O	2:B:94:ASN:ND2	2.17	0.75
2:B:158:LEU:H	2:B:158:LEU:HD12	1.52	0.75
9:I:97:LYS:HA	9:I:102:LEU:HD11	1.68	0.75
1:A:1356:G:H2'	1:A:1357:A:C8	2.22	0.75
13:M:81:LEU:HD23	13:M:84:ILE:HD11	1.68	0.75
13:M:16:ASP:OD1	13:M:16:ASP:N	2.19	0.75
1:A:427:U:OP1	4:D:13:ARG:NH2	2.18	0.75
1:A:413:G:N2	1:A:429:U:OP2	2.17	0.75
20:T:30:LYS:HE2	20:T:34:LYS:HE2	1.68	0.74
1:A:1219:U:OP1	14:N:19:ARG:NH2	2.15	0.74
20:T:53:LEU:HD12	20:T:102:GLY:HA3	1.70	0.74
10:J:17:ASP:HA	10:J:20:ALA:HB3	1.70	0.74
1:A:1086:U:H3	1:A:1099:G:H22	1.35	0.74
2:B:102:LEU:HB2	2:B:176:GLU:HG2	1.69	0.74
13:M:5:ALA:HB3	13:M:22:ILE:HD11	1.69	0.74
9:I:112:LYS:NZ	9:I:116:LYS:O	2.21	0.73
1:A:1496:C:N4	24:A:1717:HYG:O11	2.22	0.73
16:P:21:VAL:HG12	16:P:33:ILE:HD12	1.70	0.73
1:A:955:U:H1'	1:A:1227:A:H61	1.52	0.73
2:B:77:ALA:HB2	2:B:211:ILE:HD13	1.70	0.73
18:R:32:ARG:HA	18:R:69:THR:HG21	1.70	0.73
9:I:50:LEU:HB3	9:I:55:ALA:HB2	1.68	0.73
16:P:68:ASP:OD1	16:P:68:ASP:N	2.18	0.73
1:A:290:C:H42	1:A:310:G:H1	1.36	0.72
16:P:4:ILE:HG12	16:P:21:VAL:HG22	1.71	0.72
1:A:258:G:H2'	1:A:259:G:H8	1.55	0.71
8:H:46:LYS:HG3	8:H:64:LYS:HB3	1.70	0.71
4:D:64:LEU:HD23	4:D:198:VAL:HG21	1.71	0.71

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:21:LYS:O	8:H:65:TYR:OH	2.09	0.71
1:A:946:A:H2'	1:A:947:G:C8	2.26	0.71
1:A:359:U:H2'	1:A:360:A:C8	2.24	0.71
13:M:34:LEU:HA	13:M:37:THR:HG22	1.72	0.71
11:K:15:ALA:HA	11:K:77:MET:HA	1.71	0.71
1:A:285:G:H2'	1:A:286:G:H8	1.56	0.71
20:T:56:MET:HG3	20:T:88:VAL:HG21	1.74	0.70
15:O:70:LEU:HD13	15:O:78:TYR:HA	1.71	0.70
1:A:1133:G:N2	1:A:1141:C:N3	2.35	0.70
5:E:98:THR:HB	5:E:117:ASP:HB3	1.72	0.70
1:A:299:G:H2'	1:A:300:A:C8	2.27	0.70
11:K:66:LEU:HG	11:K:97:ALA:HB1	1.74	0.70
10:J:50:ILE:HD11	10:J:57:LYS:HD2	1.74	0.69
1:A:1358:U:H5''	14:N:35:ARG:HD3	1.75	0.69
8:H:20:TYR:CE1	8:H:76:PRO:HD2	2.28	0.69
6:F:100:ASN:ND2	18:R:23:LYS:O	2.25	0.68
13:M:27:LYS:HE3	21:U:21:TYR:HE2	1.58	0.68
1:A:1266:G:N2	1:A:1269:A:OP2	2.26	0.68
5:E:83:GLU:HG2	5:E:88:LYS:HG3	1.75	0.68
13:M:57:ARG:HG2	13:M:61:GLU:HG3	1.76	0.68
12:L:10:LEU:HD23	17:Q:32:TYR:CZ	2.29	0.68
1:A:129:U:O3'	1:A:129(A):G:H3'	1.93	0.68
1:A:21:G:H2'	1:A:22:G:C8	2.29	0.68
1:A:1047:G:H5''	14:N:4:LYS:HG3	1.76	0.68
1:A:677:U:H3	1:A:713:G:H22	1.42	0.67
1:A:89:C:H2'	1:A:90:U:C6	2.29	0.67
1:A:407:G:OP1	4:D:115:ARG:NH2	2.26	0.67
9:I:48:GLU:OE2	9:I:51:ARG:NH2	2.23	0.67
3:C:155:GLY:HA2	3:C:164:ARG:H	1.60	0.67
1:A:9:G:OP2	5:E:121:LYS:NZ	2.16	0.67
1:A:1415:G:C2	1:A:1486:G:C6	2.82	0.67
2:B:212:GLN:HE21	2:B:235:SER:HB2	1.60	0.67
1:A:1189:C:H5''	3:C:5:ILE:HG12	1.77	0.67
12:L:113:ARG:NH1	12:L:116:SER:H	1.93	0.66
1:A:1058:G:OP1	3:C:199:LYS:NZ	2.28	0.66
15:O:45:VAL:HB	15:O:46:HIS:CD2	2.30	0.66
8:H:41:ARG:NH1	8:H:123:GLU:OE2	2.28	0.66
10:J:4:ILE:HG21	10:J:77:PRO:HG3	1.75	0.66
1:A:76:C:H42	1:A:93:G:H1	1.42	0.66
18:R:38:GLU:HA	18:R:41:LYS:HE2	1.78	0.66
6:F:10:LEU:HB2	6:F:59:TYR:HB3	1.77	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539:A:H2'	1:A:540:G:C8	2.31	0.66
1:A:316:G:OP2	1:A:351:G:O2'	2.14	0.66
2:B:20:GLU:HA	2:B:39:ILE:HG13	1.79	0.65
1:A:191:G:O2'	20:T:102:GLY:O	2.12	0.65
1:A:633:G:H2'	1:A:634:C:H6	1.62	0.65
7:G:79:ARG:HD2	7:G:82:GLY:H	1.61	0.65
1:A:1286:A:H2'	1:A:1287:A:H4'	1.77	0.65
1:A:101:A:H2'	1:A:102:G:H8	1.60	0.65
8:H:10:LEU:HD22	8:H:83:ILE:HD11	1.79	0.65
1:A:838:G:H1	1:A:848:C:H42	1.44	0.65
4:D:152:SER:HB3	4:D:155:LEU:HD12	1.78	0.65
10:J:13:HIS:HB3	10:J:14:LYS:HD3	1.77	0.65
13:M:54:VAL:HG22	13:M:57:ARG:HH12	1.61	0.65
1:A:1329:A:H5'	13:M:29:ARG:HD2	1.79	0.65
3:C:130:VAL:O	3:C:134:ILE:HG13	1.96	0.65
4:D:49:ARG:HD2	4:D:49:ARG:H	1.62	0.65
1:A:263:A:OP2	20:T:79:ARG:NH1	2.30	0.65
1:A:1401:G:O6	1:A:1504:G:N2	2.31	0.64
1:A:527:7MG:O2'	1:A:535:A:N1	2.30	0.64
1:A:1126:U:H2'	1:A:1127:G:H8	1.63	0.64
13:M:37:THR:HG23	13:M:39:ILE:H	1.62	0.64
1:A:1148:U:H2'	1:A:1149:C:O4'	1.98	0.64
17:Q:62:SER:OG	17:Q:72:ARG:HG3	1.97	0.64
1:A:946:A:H2'	1:A:947:G:H8	1.60	0.64
1:A:633:G:H2'	1:A:634:C:C6	2.33	0.64
3:C:78:GLY:HA3	3:C:82:GLU:HB3	1.78	0.64
1:A:811:C:O2'	1:A:901:A:N1	2.28	0.64
18:R:86:VAL:HG12	18:R:87:ARG:HG3	1.80	0.64
14:N:16:PHE:HB2	14:N:19:ARG:HB2	1.79	0.64
1:A:835:U:H3	1:A:851:G:H1	1.44	0.64
1:A:875:C:O2'	8:H:14:ARG:NH1	2.31	0.64
3:C:156:ARG:H	3:C:163:ALA:HA	1.62	0.64
9:I:46:ALA:HB2	9:I:74:ILE:HG23	1.80	0.64
8:H:113:SER:HB2	8:H:134:ILE:HD11	1.80	0.64
1:A:266:G:H5'	1:A:268:C:H41	1.61	0.63
1:A:1309:G:OP2	13:M:99:ARG:NH2	2.31	0.63
11:K:43:SER:HA	11:K:47:VAL:HG21	1.78	0.63
13:M:4:ILE:HG22	13:M:5:ALA:H	1.64	0.63
16:P:3:LYS:HG3	16:P:24:ALA:HB2	1.79	0.63
13:M:12:ASN:H	13:M:45:VAL:HB	1.63	0.63
10:J:82:ILE:HA	10:J:85:LEU:HB2	1.79	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:85:LEU:HB3	15:O:87:ILE:HG23	1.81	0.63
1:A:1435:G:H2'	1:A:1436:U:C6	2.34	0.63
4:D:111:ALA:HB2	4:D:120:LEU:HD12	1.80	0.63
1:A:512:U:OP1	4:D:46:LYS:NZ	2.30	0.63
20:T:50:GLU:HA	20:T:100:ILE:HB	1.81	0.62
18:R:37:VAL:O	18:R:40:LEU:N	2.30	0.62
1:A:109:A:H2'	1:A:326:G:N2	2.14	0.62
1:A:951:G:OP2	13:M:102:ARG:NH2	2.32	0.62
8:H:23:SER:HB2	8:H:62:TYR:CD1	2.34	0.62
1:A:76:C:N4	1:A:93:G:H1	1.97	0.62
4:D:111:ALA:HB1	4:D:116:GLN:HG2	1.82	0.62
1:A:192:U:O4'	20:T:103:GLY:HA2	1.99	0.62
1:A:1411:C:H42	1:A:1490:C:N4	1.97	0.62
4:D:150:GLU:CD	4:D:150:GLU:H	2.02	0.62
1:A:544:G:OP1	4:D:59:ARG:NH2	2.32	0.62
1:A:1149:C:O2'	1:A:1280:A:N1	2.33	0.62
11:K:30:VAL:HG21	11:K:65:ALA:HA	1.82	0.62
3:C:202:ILE:HG22	3:C:204:LEU:HD23	1.81	0.62
13:M:62:ASN:OD1	13:M:62:ASN:N	2.32	0.62
1:A:579:G:H5'	1:A:728:A:H1'	1.82	0.61
1:A:1347:G:N2	1:A:1373:G:H2'	2.15	0.61
3:C:116:VAL:HG21	3:C:202:ILE:HD11	1.80	0.61
1:A:1164:G:H1	1:A:1172:C:H42	1.47	0.61
7:G:90:GLU:HG2	7:G:91:VAL:H	1.65	0.61
1:A:976:G:OP2	1:A:1358:U:O2'	2.17	0.61
9:I:118:LYS:O	9:I:120:ARG:N	2.30	0.61
1:A:1316:G:N1	1:A:1319:A:OP2	2.30	0.61
1:A:1412:C:N3	1:A:1489:G:N2	2.49	0.61
6:F:14:LEU:HD13	6:F:18:GLN:HB2	1.83	0.61
15:O:45:VAL:HG12	15:O:46:HIS:H	1.66	0.61
18:R:43:PHE:HD2	18:R:56:THR:HG22	1.64	0.61
1:A:1278:U:H5''	1:A:1279:A:C8	2.36	0.61
13:M:19:LEU:O	13:M:22:ILE:HG22	2.00	0.60
15:O:39:LEU:HD12	15:O:56:LEU:HB2	1.82	0.60
1:A:1133:G:H1	1:A:1141:C:N4	1.99	0.60
1:A:1404:5MC:H1'	1:A:1499:A:C2	2.35	0.60
9:I:8:GLY:HA2	9:I:79:LEU:HD12	1.82	0.60
1:A:419:C:H42	1:A:424:G:H1	1.47	0.60
1:A:278:G:OP2	17:Q:41:LYS:NZ	2.33	0.60
1:A:1425:U:H2'	1:A:1426:C:H6	1.66	0.60
4:D:78:LEU:HD11	4:D:96:LEU:HB3	1.84	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:24:VAL:HG13	12:L:98:TYR:CE2	2.37	0.60
1:A:501:C:H2'	1:A:502:G:C8	2.36	0.60
21:U:6:ARG:HE	21:U:15:ARG:NH2	1.99	0.60
1:A:1162:C:H42	1:A:1174:G:H1	1.50	0.60
21:U:6:ARG:HH21	21:U:15:ARG:NH2	1.98	0.60
1:A:1053:G:HO2'	1:A:1199:U:H5	1.50	0.60
12:L:24:VAL:HG13	12:L:98:TYR:HE2	1.66	0.60
10:J:61:GLU:OE1	14:N:45:ARG:NH1	2.35	0.60
1:A:1373:G:H5''	7:G:36:LYS:HE2	1.83	0.60
14:N:33:VAL:HA	14:N:40:CYS:HA	1.83	0.60
3:C:42:LEU:HA	3:C:45:LYS:HE3	1.83	0.59
1:A:1190:G:O2'	3:C:3:ASN:HB3	2.02	0.59
9:I:19:LEU:HG	9:I:61:ALA:HB2	1.84	0.59
1:A:1240:U:OP1	7:G:119:ARG:NH2	2.35	0.59
4:D:53:ASP:OD1	4:D:53:ASP:N	2.34	0.59
1:A:1397:C:O2'	1:A:1398:A:OP1	2.18	0.59
10:J:63:PHE:HE1	14:N:45:ARG:HA	1.66	0.59
20:T:33:ILE:HD12	20:T:62:LEU:HD13	1.83	0.59
4:D:187:ARG:NH2	4:D:193:ASP:OD1	2.36	0.59
1:A:1425:U:H2'	1:A:1426:C:C6	2.37	0.59
9:I:10:ARG:HD3	9:I:105:ASP:HB3	1.84	0.59
1:A:1056:U:H5'	3:C:163:ALA:HB2	1.84	0.59
1:A:1487:G:H2'	1:A:1488:G:C8	2.37	0.59
2:B:91:PRO:HG3	2:B:154:LEU:HB2	1.84	0.59
8:H:124:ALA:O	8:H:128:GLY:N	2.33	0.59
14:N:27:CYS:HB3	14:N:43:CYS:SG	2.41	0.59
1:A:1510:U:H2'	1:A:1511:G:C8	2.38	0.59
2:B:84:GLU:OE2	2:B:235:SER:OG	2.21	0.59
1:A:1191:A:OP1	3:C:4:LYS:NZ	2.36	0.59
1:A:438:G:N1	1:A:496:A:OP2	2.32	0.59
1:A:277:C:H5'	17:Q:68:ARG:HH12	1.68	0.59
10:J:14:LYS:HE3	10:J:15:THR:HG23	1.85	0.58
1:A:1238:A:H5'	1:A:1336:C:H41	1.68	0.58
1:A:384:G:H2'	1:A:385:C:C6	2.38	0.58
7:G:136:LYS:NZ	7:G:140:ASP:OD2	2.36	0.58
1:A:130:A:O2'	1:A:131:C:H5''	2.03	0.58
1:A:1399:C:H4'	1:A:1400:5MC:H5''	1.85	0.58
20:T:10:LEU:O	20:T:13:LEU:HB2	2.03	0.58
1:A:518:C:H4'	1:A:519:C:H5''	1.85	0.58
9:I:75:ASP:HA	9:I:78:LYS:HG3	1.84	0.58
1:A:232:G:H1'	1:A:262:A:N1	2.19	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:8:GLU:CD	13:M:22:ILE:HA	2.24	0.58
1:A:1441:G:H4'	1:A:1442:G:C2	2.39	0.58
7:G:51:GLN:C	7:G:53:LYS:H	2.07	0.58
2:B:97:TRP:HZ2	2:B:102:LEU:HD13	1.69	0.58
13:M:8:GLU:OE1	13:M:23:TYR:N	2.32	0.58
1:A:284:G:H2'	1:A:285:G:H8	1.69	0.58
1:A:1057:G:H5''	3:C:154:SER:HB2	1.85	0.58
12:L:53:ARG:NH1	12:L:92:OTD:OD2	2.25	0.58
1:A:580:U:H2'	1:A:581:G:O4'	2.04	0.58
1:A:457:C:H2'	1:A:458:C:H6	1.69	0.58
1:A:1498:UR3:O2'	1:A:1499:A:OP2	2.20	0.58
1:A:17:U:H2'	1:A:18:C:C6	2.39	0.58
12:L:90:VAL:HG21	12:L:93:LEU:HD12	1.85	0.58
3:C:106:VAL:HG11	3:C:112:SER:HB3	1.86	0.57
1:A:784:C:H2'	1:A:785:G:O4'	2.04	0.57
1:A:963:G:O2'	1:A:1199:U:H5''	2.05	0.57
1:A:79:G:C6	1:A:80:G:N7	2.72	0.57
1:A:836:G:C6	1:A:851:G:C6	2.92	0.57
1:A:1241:G:H2'	1:A:1242:C:H6	1.69	0.57
2:B:211:ILE:O	2:B:215:LEU:HB2	2.03	0.57
8:H:86:ILE:HG22	8:H:87:SER:N	2.20	0.57
1:A:1316:G:H4'	14:N:18:VAL:HG11	1.86	0.57
1:A:1188:A:O3'	14:N:58:LYS:NZ	2.33	0.57
1:A:1137:C:H4'	1:A:1138:G:C2	2.39	0.57
14:N:16:PHE:HD1	14:N:19:ARG:HD2	1.68	0.57
3:C:150:LYS:HB3	3:C:201:TYR:HB2	1.86	0.57
11:K:114:VAL:HG23	11:K:115:PRO:HD2	1.86	0.57
12:L:54:LYS:HB3	12:L:70:ILE:HD12	1.87	0.57
1:A:95:U:H2'	1:A:96:G:C8	2.39	0.57
1:A:614:A:H2'	1:A:615:C:C6	2.40	0.57
1:A:731:G:OP1	1:A:766:A:H1'	2.05	0.57
21:U:5:ASP:O	21:U:8:THR:OG1	2.23	0.57
9:I:53:VAL:HG21	9:I:85:LEU:HD11	1.86	0.57
1:A:1200:C:O2	1:A:1204:A:N6	2.38	0.57
1:A:392:G:H2'	1:A:393:A:H8	1.70	0.57
1:A:144:G:H1	1:A:178:C:N4	1.99	0.57
7:G:18:TYR:HB3	7:G:59:LEU:HD22	1.86	0.57
15:O:45:VAL:HB	15:O:46:HIS:HD2	1.71	0.56
1:A:1425:U:H3	1:A:1475:G:H1	1.51	0.56
1:A:790:A:H2'	1:A:791:G:C8	2.40	0.56
3:C:43:LEU:HD21	3:C:91:LEU:HD11	1.86	0.56

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:54:ASP:OD2	8:H:55:GLY:N	2.37	0.56
17:Q:21:VAL:HG21	17:Q:59:ILE:HG13	1.87	0.56
14:N:16:PHE:CD1	14:N:19:ARG:HD2	2.40	0.56
9:I:48:GLU:N	9:I:49:PRO:HD2	2.19	0.56
12:L:92:0TD:N	12:L:92:0TD:OD1	2.36	0.56
19:S:12:ASP:OD1	19:S:37:ARG:NH1	2.31	0.56
20:T:51:GLU:HA	20:T:54:LYS:HE2	1.87	0.56
1:A:673:G:H5''	6:F:87:ARG:NH1	2.21	0.56
1:A:1412:C:H2'	1:A:1413:A:C8	2.40	0.56
6:F:10:LEU:HD23	6:F:85:VAL:HA	1.87	0.56
1:A:204:U:H5''	1:A:216:G:OP1	2.05	0.56
1:A:782:A:H2'	1:A:783:C:O4'	2.06	0.56
12:L:25:PRO:C	12:L:27:LEU:H	2.07	0.56
1:A:184:G:H2'	1:A:185:A:H8	1.71	0.56
5:E:31:LEU:HD23	5:E:45:PHE:HD1	1.70	0.56
2:B:24:TRP:HB2	2:B:190:THR:HG22	1.88	0.56
5:E:145:LYS:O	5:E:148:VAL:HG23	2.06	0.56
6:F:80:ARG:NH2	6:F:88:VAL:O	2.39	0.56
3:C:156:ARG:NE	3:C:160:ALA:O	2.31	0.56
4:D:113:SER:OG	4:D:114:ARG:N	2.39	0.56
10:J:51:ARG:HD2	10:J:59:SER:HB2	1.87	0.56
12:L:27:LEU:O	12:L:29:GLY:N	2.37	0.56
1:A:1305:G:N2	1:A:1331:G:H1'	2.20	0.56
13:M:40:ASN:HD22	13:M:43:THR:HG23	1.70	0.56
1:A:1379:G:O6	7:G:2:ALA:N	2.39	0.56
10:J:38:ILE:HB	10:J:71:LEU:HB2	1.87	0.56
1:A:359:U:H2'	1:A:360:A:H8	1.67	0.56
19:S:28:LYS:HD3	19:S:29:ARG:H	1.71	0.56
5:E:102:ALA:O	5:E:107:ARG:NH1	2.38	0.56
1:A:1234:C:H1'	1:A:1364:U:O2	2.06	0.56
1:A:413:G:O2'	1:A:428:G:N2	2.37	0.56
11:K:65:ALA:HB1	11:K:98:LEU:HD23	1.87	0.56
9:I:89:ASN:HB3	9:I:92:TYR:CE1	2.41	0.56
1:A:1414:U:C2	1:A:1415:G:C8	2.94	0.56
1:A:1441:G:O2'	1:A:1442:G:N2	2.38	0.56
1:A:1250:A:H4'	9:I:68:GLY:N	2.21	0.56
1:A:344:A:H5'	1:A:345:C:C5	2.41	0.56
1:A:115:G:O2'	1:A:289:G:H5''	2.06	0.56
8:H:111:ILE:HG22	8:H:134:ILE:HD12	1.87	0.55
1:A:614:A:H2'	1:A:615:C:H6	1.71	0.55
4:D:192:GLU:N	4:D:192:GLU:OE2	2.39	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:78:HIS:ND1	8:H:104:ARG:HG3	2.22	0.55
1:A:1408:A:H2'	1:A:1409:C:O4'	2.06	0.55
1:A:1486:G:C6	1:A:1487:G:C6	2.94	0.55
3:C:21:ARG:HB2	3:C:58:GLU:HB3	1.87	0.55
21:U:12:LYS:O	21:U:22:ARG:NH1	2.39	0.55
9:I:26:VAL:HB	9:I:33:PHE:HB2	1.89	0.55
4:D:31:CYS:C	4:D:33:MET:H	2.09	0.55
1:A:328:C:O2	1:A:328:C:H2'	2.06	0.55
11:K:27:ASN:OD1	11:K:28:THR:N	2.39	0.55
8:H:83:ILE:HB	8:H:137:VAL:HG13	1.88	0.55
1:A:164:U:H2'	1:A:165:C:C6	2.41	0.55
14:N:11:LYS:HE3	14:N:14:PRO:HA	1.88	0.55
1:A:581:G:O3'	15:O:64:ARG:NH2	2.40	0.55
1:A:1198:G:H2'	1:A:1199:U:C6	2.42	0.55
1:A:97:G:H2'	1:A:98:U:O4'	2.06	0.55
1:A:908:A:C2	1:A:909:A:C4	2.94	0.55
4:D:7:PRO:HG2	4:D:10:ARG:HD2	1.89	0.55
1:A:278:G:C6	17:Q:95:TYR:HD2	2.25	0.55
1:A:1265:G:H1	1:A:1270:C:H42	1.55	0.55
4:D:173:TRP:HB2	4:D:187:ARG:O	2.07	0.55
7:G:51:GLN:O	7:G:53:LYS:N	2.40	0.55
1:A:1320:C:H5'	19:S:70:LYS:HD3	1.88	0.55
11:K:110:ASP:HB2	18:R:88:LYS:HD2	1.89	0.55
1:A:258:G:H2'	1:A:259:G:C8	2.40	0.55
7:G:88:PRO:O	7:G:155:ARG:NH1	2.40	0.55
11:K:123:LYS:HA	11:K:126:ARG:HG3	1.89	0.55
15:O:32:LEU:HD21	15:O:62:GLN:HB3	1.89	0.55
11:K:41:THR:OG1	11:K:42:TRP:N	2.40	0.55
10:J:34:VAL:HG11	10:J:74:ILE:HA	1.87	0.55
3:C:91:LEU:HB3	3:C:99:VAL:HG21	1.88	0.55
1:A:1150:U:O4	1:A:1151:A:N6	2.40	0.55
8:H:97:VAL:HG23	8:H:129:VAL:O	2.06	0.55
1:A:321:A:H2'	1:A:322:C:H6	1.72	0.55
2:B:118:LEU:HB3	2:B:142:LEU:HG	1.89	0.55
16:P:14:ASN:OD1	16:P:42:ARG:NH2	2.39	0.55
19:S:33:THR:HG22	19:S:35:SER:N	2.20	0.54
1:A:1207:2MG:HM23	1:A:1208:C:H1'	1.89	0.54
4:D:93:PHE:CE1	4:D:97:LEU:HD11	2.41	0.54
2:B:178:ARG:HD2	2:B:196:LEU:O	2.07	0.54
9:I:108:VAL:HG12	9:I:109:VAL:H	1.72	0.54
1:A:279:A:OP1	1:A:280:C:O2'	2.21	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:104:ARG:NH1	9:I:105:ASP:O	2.37	0.54
1:A:1338:G:H2'	1:A:1339:A:C8	2.43	0.54
1:A:858:G:O2'	1:A:859:A:H5''	2.07	0.54
1:A:664:G:OP1	18:R:64:ARG:HD2	2.07	0.54
8:H:65:TYR:HA	8:H:79:VAL:HG23	1.88	0.54
5:E:88:LYS:HD2	5:E:123:LEU:HD12	1.89	0.54
3:C:121:ALA:HA	3:C:124:ILE:HD12	1.89	0.54
9:I:10:ARG:HH21	9:I:11:LYS:HE3	1.72	0.54
10:J:40:LEU:HD12	10:J:69:ASN:HB2	1.89	0.54
1:A:243:A:C2	1:A:246:A:C8	2.96	0.54
3:C:137:ALA:HA	3:C:140:ARG:HE	1.72	0.54
1:A:644:G:C5	1:A:645:C:C5	2.95	0.54
1:A:665:A:N3	1:A:732:C:H2'	2.22	0.54
13:M:2:ALA:O	13:M:10:PRO:HD2	2.07	0.54
7:G:21:VAL:HG22	7:G:22:LEU:HD12	1.90	0.54
1:A:560:U:H5'	1:A:566:G:N2	2.21	0.54
8:H:119:LEU:HD12	8:H:124:ALA:HA	1.90	0.54
2:B:139:LYS:HE2	2:B:143:GLU:HG3	1.90	0.54
14:N:25:VAL:HG23	14:N:38:GLY:HA3	1.89	0.54
6:F:22:GLU:OE1	6:F:82:ARG:NH1	2.40	0.54
1:A:345:C:OP2	1:A:345:C:H6	1.89	0.54
5:E:144:THR:O	5:E:148:VAL:HG22	2.07	0.54
1:A:1207:2MG:H2'	1:A:1208:C:C6	2.43	0.54
1:A:1323:G:H2'	1:A:1324:A:C8	2.43	0.54
3:C:6:HIS:CE1	3:C:8:ILE:HB	2.43	0.54
3:C:121:ALA:HB1	3:C:189:ALA:HB2	1.90	0.53
1:A:1139:G:H21	1:A:1143:G:H21	1.55	0.53
4:D:152:SER:O	4:D:155:LEU:HB2	2.08	0.53
15:O:36:ILE:HG23	15:O:56:LEU:HD11	1.89	0.53
1:A:381:C:H2'	1:A:382:A:O4'	2.08	0.53
14:N:48:ALA:HA	14:N:53:LEU:HB2	1.89	0.53
1:A:401:C:H1'	1:A:622:A:H1'	1.91	0.53
1:A:438:G:H4'	4:D:123:HIS:CD2	2.43	0.53
1:A:542:G:OP1	4:D:10:ARG:NH2	2.38	0.53
6:F:67:MET:HB2	6:F:68:PRO:HD2	1.90	0.53
5:E:152:ARG:NE	8:H:44:PHE:HE1	2.07	0.53
3:C:84:ILE:HG23	3:C:88:ARG:HH21	1.74	0.53
1:A:1509:C:H42	1:A:1526:G:H1	1.57	0.53
1:A:56:U:H2'	1:A:57:G:C8	2.43	0.53
10:J:19:SER:HA	10:J:22:LYS:HE2	1.91	0.53
1:A:1109:C:H2'	1:A:1110:A:O4'	2.07	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1511:G:H2'	1:A:1512:U:O4'	2.08	0.53
3:C:52:LEU:HD12	3:C:70:VAL:HG12	1.90	0.53
4:D:32:ALA:O	4:D:36:ARG:N	2.29	0.53
1:A:421:U:H5'	1:A:422:C:H5	1.73	0.53
1:A:1427:U:H2'	1:A:1428:A:C8	2.43	0.53
1:A:646:U:H2'	1:A:647:C:C6	2.43	0.53
17:Q:87:LYS:HA	17:Q:90:ILE:HD12	1.89	0.53
12:L:19:ARG:H	12:L:19:ARG:HD2	1.72	0.53
1:A:74:C:H2'	1:A:75:G:O4'	2.08	0.53
8:H:23:SER:HB2	8:H:62:TYR:HD1	1.72	0.53
1:A:141:A:H1'	1:A:182:U:O2	2.09	0.53
20:T:29:LYS:O	20:T:32:ALA:HB3	2.09	0.53
1:A:539:A:H2'	1:A:540:G:H8	1.71	0.53
14:N:17:LYS:HE2	14:N:18:VAL:HG13	1.91	0.53
1:A:1124:G:N7	1:A:1145:C:O2'	2.40	0.53
12:L:93:LEU:O	12:L:96:VAL:HG23	2.08	0.53
2:B:88:ALA:O	2:B:90:MET:N	2.42	0.53
12:L:27:LEU:HG	12:L:28:LYS:H	1.74	0.53
17:Q:10:VAL:HG13	17:Q:19:VAL:HB	1.91	0.53
1:A:199:G:H1	1:A:218:C:H42	1.57	0.53
1:A:673:G:H2'	1:A:674:G:C8	2.43	0.52
2:B:87:ARG:HE	2:B:219:VAL:HG11	1.74	0.52
1:A:1342:C:H2'	1:A:1343:G:C8	2.44	0.52
20:T:44:ALA:O	20:T:47:GLY:N	2.34	0.52
7:G:65:ALA:HB2	7:G:128:ALA:HB2	1.92	0.52
14:N:29:ARG:HH12	14:N:41:ARG:HH12	1.56	0.52
13:M:19:LEU:HD21	13:M:56:LEU:HD11	1.91	0.52
1:A:103:C:OP2	20:T:14:LYS:HD2	2.10	0.52
1:A:149:A:H2'	1:A:150:C:H6	1.74	0.52
1:A:587:G:N2	1:A:754:C:OP2	2.39	0.52
4:D:162:LEU:HD12	4:D:178:VAL:HG13	1.90	0.52
3:C:111:LEU:HD22	3:C:146:ALA:HB2	1.90	0.52
21:U:17:THR:HG22	21:U:18:TYR:H	1.75	0.52
1:A:1101:A:H4'	1:A:1102:A:O5'	2.08	0.52
18:R:44:LEU:HD21	18:R:70:ILE:HD13	1.90	0.52
4:D:102:ASP:OD1	4:D:103:ASN:N	2.43	0.52
5:E:75:THR:OG1	5:E:76:ILE:N	2.43	0.52
1:A:1111:A:N1	3:C:177:THR:HG23	2.25	0.52
1:A:443:C:H42	1:A:491:G:H1	1.57	0.52
1:A:1065:U:O2'	1:A:1066:C:OP2	2.23	0.52
7:G:46:ALA:O	7:G:50:ILE:HG12	2.10	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:181:ASN:O	3:C:181:ASN:ND2	2.41	0.52
1:A:1000:U:H2'	1:A:1001:A:C8	2.45	0.52
1:A:79:G:N1	1:A:91:C:C4	2.78	0.52
1:A:1241:G:H2'	1:A:1242:C:C6	2.44	0.52
14:N:53:LEU:HD12	14:N:56:VAL:HG21	1.91	0.52
1:A:1255:G:OP1	3:C:26:LYS:NZ	2.33	0.52
6:F:7:ASN:HB2	6:F:89:MET:O	2.09	0.52
8:H:82:HIS:C	8:H:82:HIS:CD2	2.83	0.52
1:A:1140:C:H2'	1:A:1141:C:H6	1.75	0.52
1:A:131:C:O2'	1:A:132:C:O5'	2.26	0.52
20:T:39:LYS:HG2	20:T:55:ILE:HD13	1.91	0.52
6:F:12:PRO:HG3	6:F:57:GLN:HB2	1.92	0.52
1:A:1356:G:H2'	1:A:1357:A:H8	1.74	0.52
17:Q:31:LEU:HD23	17:Q:32:TYR:CE2	2.44	0.52
15:O:25:THR:O	15:O:29:VAL:HG23	2.10	0.52
1:A:912:C:H5''	12:L:46:LYS:HE3	1.92	0.52
1:A:881:G:H2'	1:A:882:C:O4'	2.10	0.52
16:P:4:ILE:HG13	16:P:64:ALA:HB1	1.92	0.52
16:P:57:ARG:HG2	16:P:57:ARG:HH11	1.74	0.51
1:A:979:C:N4	14:N:18:VAL:O	2.30	0.51
2:B:167:PRO:HG2	2:B:192:SER:CB	2.41	0.51
1:A:652:U:O4	1:A:752:G:O2'	2.27	0.51
4:D:60:GLU:HA	4:D:60:GLU:OE1	2.10	0.51
1:A:92:C:H2'	1:A:93:G:C8	2.45	0.51
3:C:77:ILE:HG12	3:C:103:VAL:HG21	1.91	0.51
1:A:940:C:OP1	7:G:102:ARG:HD3	2.10	0.51
3:C:130:VAL:HG21	3:C:157:ILE:HG23	1.92	0.51
1:A:392:G:H2'	1:A:393:A:C8	2.46	0.51
1:A:627:G:H2'	1:A:628:G:H8	1.75	0.51
11:K:121:PRO:HB2	11:K:125:PHE:HB2	1.92	0.51
2:B:32:ILE:HG21	2:B:40:HIS:HB3	1.92	0.51
1:A:234:C:H2'	1:A:235:C:C6	2.45	0.51
5:E:107:ARG:O	5:E:111:GLU:HB2	2.10	0.51
14:N:47:LEU:HB3	14:N:53:LEU:HD23	1.92	0.51
2:B:217:ARG:O	2:B:220:ASP:HB2	2.09	0.51
1:A:1157:A:H1'	1:A:1181:G:N2	2.25	0.51
1:A:74:C:C4	1:A:75:G:N7	2.78	0.51
17:Q:59:ILE:HG23	17:Q:71:PHE:HB3	1.93	0.51
21:U:10:ARG:HG2	21:U:13:ILE:HD12	1.92	0.51
1:A:552:U:H2'	1:A:553:A:C8	2.46	0.51
10:J:64:GLU:HB3	14:N:59:ALA:HB2	1.90	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:102:ARG:H	8:H:102:ARG:HD2	1.75	0.51
1:A:1495:U:OP1	24:A:1717:HYG:N36	2.43	0.51
1:A:1125:U:H3'	1:A:1126:U:C5	2.45	0.51
1:A:1035:A:H2'	1:A:1036:G:C8	2.45	0.51
1:A:1305:G:OP1	21:U:2:GLY:N	2.44	0.51
1:A:56:U:H2'	1:A:57:G:H8	1.75	0.51
1:A:833:U:H2'	1:A:834:C:H6	1.76	0.51
1:A:818:G:O2'	1:A:819:A:H5''	2.11	0.51
16:P:15:PRO:HG2	16:P:41:PRO:HG2	1.93	0.51
1:A:285:G:N3	1:A:286:G:C8	2.79	0.51
1:A:1488:G:H2'	1:A:1489:G:C8	2.46	0.51
3:C:134:ILE:O	3:C:138:VAL:HG23	2.11	0.51
2:B:91:PRO:HG2	2:B:155:LEU:CD2	2.40	0.51
3:C:105:GLU:HG2	3:C:106:VAL:H	1.75	0.51
1:A:1179:A:H2'	1:A:1180:A:O4'	2.10	0.51
1:A:1325:C:O3'	21:U:17:THR:HG21	2.10	0.51
1:A:447:G:H2'	1:A:485:G:N2	2.26	0.51
8:H:4:ASP:OD2	8:H:85:ARG:NH1	2.44	0.51
1:A:79:G:C2	1:A:80:G:C8	2.99	0.51
1:A:92:C:H2'	1:A:93:G:H8	1.75	0.51
6:F:82:ARG:HB2	6:F:85:VAL:HG23	1.92	0.51
12:L:46:LYS:HG2	12:L:47:LYS:H	1.75	0.51
1:A:216:G:O2'	1:A:217:C:O4'	2.28	0.51
5:E:71:LEU:HD11	5:E:113:ALA:O	2.10	0.51
13:M:101:GLN:OE1	13:M:101:GLN:N	2.44	0.51
17:Q:24:GLU:HA	17:Q:39:SER:HB3	1.93	0.51
3:C:50:ALA:O	3:C:72:LYS:N	2.44	0.50
1:A:953:G:H5'	1:A:965:A:H61	1.76	0.50
1:A:75:G:C6	1:A:76:C:C4	2.99	0.50
18:R:38:GLU:CD	18:R:38:GLU:H	2.15	0.50
1:A:184:G:H2'	1:A:185:A:C8	2.47	0.50
1:A:1201:A:H4'	1:A:1202:G:O5'	2.11	0.50
14:N:27:CYS:SG	14:N:29:ARG:HB2	2.51	0.50
1:A:1435:G:H2'	1:A:1436:U:H6	1.75	0.50
7:G:5:ARG:HG3	7:G:7:ALA:H	1.76	0.50
1:A:981:U:H5'	14:N:21:TYR:CE1	2.45	0.50
13:M:6:GLY:HA3	13:M:67:GLU:HG3	1.92	0.50
4:D:142:PRO:HA	4:D:185:PHE:HD2	1.77	0.50
8:H:56:LYS:N	8:H:56:LYS:HD2	2.26	0.50
2:B:98:LEU:HB2	2:B:101:MET:HG3	1.94	0.50
1:A:1000:U:H2'	1:A:1001:A:H8	1.76	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:G:H2'	1:A:62:U:O4'	2.11	0.50
8:H:64:LYS:HG3	8:H:79:VAL:HG21	1.94	0.50
1:A:380:G:N2	1:A:382:A:H3'	2.27	0.50
2:B:167:PRO:HG2	2:B:192:SER:HB3	1.93	0.50
1:A:975:A:H5'	1:A:975:A:H8	1.76	0.50
1:A:369:C:OP2	1:A:388:G:N2	2.44	0.50
4:D:159:ARG:NH2	4:D:163:GLU:OE2	2.44	0.50
8:H:63:LEU:H	8:H:63:LEU:HD22	1.75	0.50
14:N:29:ARG:HH12	14:N:41:ARG:NH1	2.10	0.50
21:U:14:TRP:CE3	21:U:15:ARG:HG3	2.46	0.50
2:B:97:TRP:CZ2	2:B:101:MET:HB2	2.46	0.50
1:A:1048:G:H2'	1:A:1050:G:H8	1.77	0.50
8:H:110:ALA:HB3	8:H:121:ASP:HB3	1.93	0.50
2:B:54:THR:O	2:B:58:ILE:HG12	2.12	0.50
3:C:27:LYS:O	3:C:30:ARG:NH1	2.44	0.50
8:H:17:THR:O	8:H:78:GLN:NE2	2.42	0.50
16:P:74:LEU:O	16:P:79:VAL:HG23	2.12	0.50
1:A:1370:G:C2	1:A:1371:G:N7	2.80	0.50
3:C:11:ARG:NH1	3:C:177:THR:O	2.45	0.50
21:U:10:ARG:O	21:U:13:ILE:HB	2.12	0.50
9:I:24:GLY:H	9:I:60:ASP:HB2	1.77	0.50
20:T:75:ASN:N	20:T:75:ASN:OD1	2.45	0.50
11:K:20:TYR:CE1	11:K:83:ILE:HD13	2.47	0.50
4:D:155:LEU:HD23	4:D:156:GLU:N	2.26	0.49
1:A:234:C:H2'	1:A:235:C:H6	1.76	0.49
1:A:99:C:H2'	1:A:101:A:C8	2.46	0.49
1:A:301:G:H2'	1:A:302:G:C8	2.48	0.49
12:L:31:PRO:HB2	12:L:32:PHE:CE2	2.48	0.49
4:D:194:LEU:H	4:D:194:LEU:HD22	1.77	0.49
1:A:192:U:C1'	20:T:103:GLY:HA2	2.42	0.49
1:A:1127:G:H5'	9:I:66:ARG:HH22	1.77	0.49
1:A:321:A:H2'	1:A:322:C:C6	2.47	0.49
1:A:41:G:H2'	1:A:42:G:C8	2.47	0.49
4:D:175:SER:O	4:D:184:LYS:N	2.41	0.49
1:A:1411:C:H42	1:A:1490:C:H42	1.60	0.49
1:A:1121:U:H2'	1:A:1122:U:C6	2.47	0.49
11:K:50:TYR:CD2	11:K:54:ARG:HB3	2.47	0.49
1:A:620:C:C2	4:D:135:LEU:HD22	2.47	0.49
2:B:16:HIS:HB3	2:B:44:LEU:HD11	1.94	0.49
1:A:538:G:H2'	1:A:539:A:H8	1.77	0.49
13:M:37:THR:HG21	13:M:56:LEU:HD23	1.95	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:5:ALA:HB2	13:M:61:GLU:HG2	1.93	0.49
1:A:284:G:H2'	1:A:285:G:C8	2.48	0.49
3:C:155:GLY:O	3:C:196:LEU:HD22	2.13	0.49
4:D:119:GLN:HG3	4:D:123:HIS:ND1	2.27	0.49
1:A:1131:G:H2'	1:A:1132:C:C6	2.48	0.49
9:I:102:LEU:HD12	9:I:102:LEU:H	1.76	0.49
1:A:130:A:H1'	1:A:263:A:O2'	2.12	0.49
1:A:1277:C:H2'	1:A:1279:A:H8	1.77	0.49
1:A:1064:G:H1'	1:A:1190:G:H21	1.78	0.49
4:D:22:LYS:HB2	4:D:26:CYS:SG	2.52	0.49
15:O:26:GLU:OE2	15:O:77:ARG:HD3	2.12	0.49
6:F:4:TYR:CZ	6:F:72:VAL:HG21	2.48	0.49
1:A:933:G:OP2	7:G:3:ARG:HB3	2.11	0.49
20:T:43:LEU:HB3	20:T:52:ALA:HB2	1.95	0.49
1:A:1127:G:H1	1:A:1145:C:H42	1.60	0.49
3:C:120:VAL:HG12	3:C:124:ILE:HD11	1.95	0.49
1:A:149:A:H2'	1:A:150:C:C6	2.48	0.49
1:A:551:U:H2'	1:A:552:U:C6	2.47	0.49
1:A:1503:A:H8	1:A:1531:A:HO2'	1.61	0.49
1:A:629:G:H2'	1:A:630:G:O4'	2.12	0.49
6:F:45:LEU:HD23	6:F:45:LEU:H	1.77	0.49
5:E:80:ILE:HA	8:H:104:ARG:NH2	2.28	0.49
1:A:76:C:H2'	1:A:77:G:C8	2.47	0.49
1:A:1391:U:H2'	1:A:1392:G:C8	2.48	0.49
1:A:35:G:O2'	12:L:118:SER:O	2.24	0.49
5:E:36:ASP:OD1	5:E:38:GLN:N	2.37	0.49
1:A:958:A:N6	19:S:77:THR:O	2.45	0.49
1:A:767:A:H2'	1:A:768:A:O4'	2.12	0.49
1:A:1152:A:H5''	10:J:13:HIS:CE1	2.48	0.49
3:C:73:PRO:HG3	3:C:105:GLU:HB2	1.95	0.49
7:G:2:ALA:HB2	7:G:7:ALA:HB2	1.95	0.49
19:S:18:LYS:O	19:S:22:LEU:HG	2.12	0.49
19:S:29:ARG:HB3	19:S:30:LEU:HG	1.95	0.49
1:A:152:A:N6	1:A:170:U:C2	2.81	0.49
16:P:67:THR:HG22	16:P:69:THR:H	1.78	0.49
1:A:279:A:C5	17:Q:98:LEU:HD12	2.47	0.49
1:A:1358:U:H5'	14:N:35:ARG:H	1.77	0.49
1:A:1377:A:HO2'	7:G:2:ALA:N	2.09	0.49
6:F:97:PHE:C	6:F:98:LEU:HD13	2.33	0.49
5:E:33:VAL:HG12	5:E:112:LEU:HD12	1.94	0.49
1:A:735:C:OP1	18:R:68:LYS:NZ	2.36	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:91:VAL:HG21	18:R:72:ARG:CZ	2.43	0.49
2:B:101:MET:HA	2:B:108:ILE:HG13	1.95	0.48
2:B:103:THR:HG23	2:B:176:GLU:HG3	1.94	0.48
4:D:196:LEU:O	4:D:198:VAL:N	2.44	0.48
7:G:47:CYS:HA	7:G:50:ILE:HG12	1.95	0.48
3:C:30:ARG:HD3	3:C:30:ARG:H	1.78	0.48
1:A:1477:C:H2'	1:A:1478:C:C6	2.48	0.48
1:A:292:G:H5''	1:A:293:G:OP2	2.12	0.48
2:B:114:ARG:O	2:B:117:GLU:HB2	2.13	0.48
1:A:432:A:H2'	1:A:433:C:O4'	2.13	0.48
8:H:104:ARG:CZ	8:H:138:TRP:CZ2	2.97	0.48
13:M:22:ILE:CG2	13:M:25:ILE:HB	2.43	0.48
1:A:1502:A:C2	1:A:1504:G:C2	3.01	0.48
18:R:44:LEU:HD13	18:R:48:GLY:O	2.13	0.48
1:A:1202:G:C2	14:N:42:ILE:HG21	2.48	0.48
1:A:1217:C:OP1	14:N:5:ALA:HB1	2.13	0.48
1:A:457:C:C2	1:A:458:C:C5	3.01	0.48
9:I:43:ALA:HA	9:I:74:ILE:HD13	1.95	0.48
3:C:13:GLY:HA3	14:N:57:ARG:CZ	2.43	0.48
7:G:111:ARG:HG2	7:G:112:PRO:HD2	1.95	0.48
4:D:17:VAL:HG22	4:D:18:LYS:H	1.78	0.48
1:A:96:G:H2'	1:A:97:G:H8	1.78	0.48
1:A:1250:A:H2'	1:A:1251:A:C8	2.48	0.48
1:A:860:A:H2'	1:A:861:G:O4'	2.12	0.48
1:A:630:G:H3'	1:A:631:G:H8	1.78	0.48
1:A:238:G:OP1	17:Q:25:ARG:NH2	2.45	0.48
1:A:809:G:C6	1:A:810:C:C5	3.02	0.48
4:D:73:ARG:HD3	4:D:73:ARG:HA	1.71	0.48
2:B:102:LEU:HD23	2:B:182:ILE:HD12	1.96	0.48
1:A:426:G:OP1	4:D:38:TYR:OH	2.27	0.48
1:A:1002:G:H2'	1:A:1003:G:C8	2.48	0.48
7:G:97:GLN:O	7:G:101:LEU:HD23	2.14	0.48
8:H:28:ALA:HB2	8:H:59:LEU:HG	1.94	0.48
7:G:79:ARG:HG3	7:G:81:GLY:N	2.25	0.48
5:E:7:GLU:CD	5:E:37:ARG:HE	2.17	0.48
1:A:547:A:OP2	4:D:2:GLY:N	2.46	0.48
2:B:31:TYR:HE1	2:B:200:ILE:HG21	1.79	0.48
14:N:6:LEU:HB3	14:N:23:ARG:NH2	2.28	0.48
3:C:195:VAL:C	3:C:196:LEU:HD23	2.34	0.48
1:A:1489:G:H2'	1:A:1490:C:C6	2.48	0.48
15:O:14:GLU:HG2	15:O:15:PHE:CD1	2.49	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:91:PRO:HG2	2:B:155:LEU:HD23	1.96	0.48
2:B:135:GLN:O	2:B:139:LYS:HB2	2.13	0.48
1:A:1488:G:C5	1:A:1489:G:N7	2.81	0.48
1:A:1391:U:H2'	1:A:1392:G:H8	1.79	0.48
1:A:1065:U:H5''	1:A:1190:G:N2	2.29	0.48
7:G:50:ILE:CG2	7:G:58:PRO:HA	2.43	0.48
1:A:584:G:OP2	17:Q:87:LYS:NZ	2.29	0.48
1:A:13:U:O2	1:A:914:A:H3'	2.13	0.48
3:C:188:LEU:HD21	3:C:195:VAL:HB	1.95	0.48
1:A:301:G:H2'	1:A:302:G:H8	1.77	0.48
1:A:1030(A):G:N2	1:A:1030(D):A:OP2	2.42	0.48
10:J:49:VAL:HG13	14:N:41:ARG:HB2	1.95	0.48
1:A:358:U:H2'	1:A:359:U:H6	1.79	0.48
1:A:457:C:H2'	1:A:458:C:C6	2.48	0.48
1:A:1274:G:H2'	1:A:1275:A:C8	2.49	0.48
19:S:15:LEU:O	19:S:19:VAL:HG12	2.14	0.48
10:J:40:LEU:HD22	10:J:41:PRO:HD2	1.96	0.48
6:F:2:ARG:NE	6:F:69:GLU:HG2	2.22	0.47
1:A:80:G:H22	1:A:88:A:N6	2.11	0.47
11:K:48:ILE:HD12	11:K:63:LEU:HB2	1.96	0.47
2:B:187:LEU:HD22	2:B:205:ASP:HB3	1.96	0.47
15:O:67:LEU:HA	15:O:67:LEU:HD23	1.73	0.47
1:A:838:G:H1	1:A:848:C:N4	2.09	0.47
4:D:120:LEU:HD22	4:D:125:HIS:HB2	1.96	0.47
2:B:124:SER:O	2:B:127:ILE:HG13	2.13	0.47
1:A:830:G:C6	1:A:831:U:C4	3.02	0.47
7:G:50:ILE:HG21	7:G:58:PRO:HA	1.96	0.47
12:L:48:PRO:HD2	12:L:92:0TD:H8	1.96	0.47
20:T:45:GLN:HA	20:T:91:LEU:HD12	1.95	0.47
1:A:24:U:H2'	1:A:25:C:C6	2.49	0.47
10:J:25:GLU:HA	10:J:28:ARG:HB2	1.96	0.47
1:A:1382:C:H2'	1:A:1383:C:H6	1.79	0.47
1:A:575:G:N2	1:A:576:G:N7	2.54	0.47
11:K:14:VAL:HG23	11:K:15:ALA:H	1.79	0.47
1:A:1409:C:H3'	1:A:1410:G:H8	1.79	0.47
1:A:92:C:C2	1:A:93:G:C8	3.03	0.47
11:K:29:ILE:HG12	11:K:30:VAL:N	2.27	0.47
4:D:78:LEU:O	4:D:81:GLU:HB3	2.14	0.47
1:A:990:C:H42	1:A:1215:G:H1	1.61	0.47
19:S:62:ILE:HD12	19:S:66:MET:HE2	1.95	0.47
1:A:375:U:H2'	1:A:376:G:H8	1.79	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:854:G:N1	1:A:855:G:N7	2.62	0.47
2:B:172:ILE:HD12	2:B:172:ILE:H	1.79	0.47
6:F:44:GLY:HA2	6:F:59:TYR:CE1	2.49	0.47
1:A:164:U:H2'	1:A:165:C:H6	1.80	0.47
1:A:1048:G:H2'	1:A:1050:G:C8	2.49	0.47
1:A:410:G:H21	1:A:432:A:H62	1.62	0.47
1:A:854:G:C6	1:A:855:G:N7	2.83	0.47
7:G:38:LEU:O	7:G:42:ILE:HG13	2.15	0.47
13:M:88:ARG:HH12	19:S:3:ARG:HD2	1.79	0.47
8:H:53:VAL:HB	8:H:58:TYR:CD1	2.50	0.47
10:J:54:PHE:CD2	10:J:55:LYS:HG2	2.50	0.47
7:G:74:GLU:HG2	7:G:91:VAL:HG22	1.96	0.47
1:A:1370:G:H5''	9:I:109:VAL:HG21	1.97	0.47
1:A:718:G:C8	11:K:116:HIS:HB3	2.50	0.47
1:A:1314:C:H2'	1:A:1315:U:C6	2.50	0.47
1:A:966:M2G:HM22	1:A:967:5MC:C2	2.49	0.47
1:A:267:C:OP1	17:Q:67:LYS:HE3	2.15	0.47
1:A:1326:C:OP2	21:U:6:ARG:NH2	2.40	0.47
10:J:51:ARG:HH21	10:J:61:GLU:HB2	1.80	0.47
1:A:259:G:OP2	20:T:83:ARG:NE	2.48	0.47
1:A:1400:5MC:H3'	1:A:1401:G:H5'	1.97	0.47
1:A:950:U:H2'	1:A:951:G:C8	2.49	0.47
1:A:1425:U:C2	1:A:1426:C:C5	3.03	0.47
1:A:385:C:H2'	1:A:386:C:H6	1.79	0.47
19:S:22:LEU:HD13	19:S:28:LYS:HD2	1.96	0.47
8:H:85:ARG:NH1	8:H:88:LYS:HA	2.30	0.47
1:A:975:A:N6	1:A:1367:C:O4'	2.48	0.47
2:B:54:THR:OG1	2:B:199:TYR:HB3	2.15	0.47
1:A:750:G:N3	15:O:23:GLY:HA3	2.30	0.47
1:A:1061:G:N7	3:C:2:GLY:HA2	2.30	0.47
1:A:636:U:H2'	1:A:637:G:C8	2.49	0.47
11:K:90:GLY:HA2	11:K:93:GLN:HB2	1.97	0.47
20:T:64:ASP:O	20:T:67:ALA:HB3	2.15	0.47
3:C:51:GLY:HA3	3:C:71:ALA:HB3	1.97	0.47
1:A:114:U:H2'	1:A:115:G:C8	2.50	0.47
1:A:244:U:H4'	1:A:245:C:H5''	1.97	0.47
1:A:745:C:H2'	1:A:746:A:C8	2.50	0.47
5:E:13:ILE:HG22	5:E:30:ALA:HA	1.95	0.47
1:A:1015:A:H2'	1:A:1016:A:C8	2.49	0.47
1:A:70:G:H2'	1:A:73:C:C6	2.50	0.47
9:I:32:ASP:OD1	9:I:33:PHE:N	2.48	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:555:C:H2'	1:A:556:C:C6	2.50	0.47
1:A:266:G:H5''	1:A:267:C:C5	2.50	0.47
1:A:1520:G:H2'	1:A:1521:G:H8	1.80	0.47
1:A:803:G:C6	1:A:804:U:N3	2.83	0.47
1:A:1465:C:H2'	1:A:1466:C:O4'	2.15	0.47
1:A:976:G:C8	1:A:1358:U:O2	2.68	0.46
1:A:283:C:C2	1:A:284:G:C8	3.02	0.46
1:A:1409:C:H3'	1:A:1410:G:C8	2.50	0.46
20:T:51:GLU:O	20:T:55:ILE:HG13	2.15	0.46
1:A:815:A:N6	1:A:1509:C:H1'	2.30	0.46
3:C:72:LYS:HB3	3:C:75:VAL:HG23	1.97	0.46
8:H:26:VAL:HG23	8:H:27:PRO:HD2	1.97	0.46
1:A:974:A:H8	1:A:974:A:OP1	1.98	0.46
1:A:424:G:H2'	1:A:425:G:H8	1.79	0.46
1:A:551:U:H2'	1:A:552:U:H6	1.80	0.46
1:A:977:A:H2'	1:A:978:A:H5'	1.98	0.46
4:D:23:GLY:HA3	4:D:112:VAL:HG12	1.96	0.46
10:J:47:PHE:HB3	14:N:34:TYR:CE2	2.50	0.46
3:C:170:GLN:HG2	3:C:171:GLY:H	1.80	0.46
19:S:36:ARG:NH2	19:S:75:ALA:O	2.48	0.46
5:E:99:GLY:N	5:E:117:ASP:OD1	2.39	0.46
1:A:1265:G:C6	1:A:1266:G:C6	3.04	0.46
15:O:85:LEU:HD23	15:O:85:LEU:HA	1.40	0.46
4:D:119:GLN:NE2	4:D:123:HIS:HE1	2.13	0.46
12:L:49:ASN:HB2	12:L:92:OTD:SB	2.54	0.46
1:A:854:G:C2	1:A:855:G:C8	3.04	0.46
10:J:52:GLY:HA2	10:J:53:PRO:HD3	1.82	0.46
1:A:617:G:N2	1:A:618:C:N3	2.63	0.46
1:A:1080:A:O3'	5:E:16:THR:OG1	2.33	0.46
1:A:689:C:H2'	1:A:690:G:O4'	2.15	0.46
3:C:190:ARG:HA	3:C:195:VAL:HG12	1.98	0.46
1:A:567:G:H2'	1:A:568:G:O4'	2.16	0.46
1:A:269:C:H2'	1:A:270:A:C8	2.50	0.46
15:O:45:VAL:HG12	15:O:46:HIS:N	2.30	0.46
9:I:89:ASN:HB3	9:I:92:TYR:CZ	2.50	0.46
1:A:1513:A:H2'	1:A:1514:C:C6	2.50	0.46
15:O:18:PHE:CZ	15:O:21:ASP:HB2	2.50	0.46
1:A:748:C:H4'	1:A:749:C:O5'	2.15	0.46
12:L:78:GLN:H	12:L:81:SER:HB2	1.81	0.46
1:A:7:G:H5'	1:A:298:A:H5'	1.97	0.46
1:A:1117:G:N2	1:A:1180:A:O2'	2.48	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:158:ILE:O	4:D:162:LEU:HB2	2.15	0.46
1:A:1130:A:OP1	1:A:1131:G:H8	1.98	0.46
3:C:108:ASN:HD21	3:C:144:SER:HB3	1.79	0.46
4:D:101:LEU:O	4:D:105:VAL:HG23	2.15	0.46
5:E:55:VAL:HG12	5:E:56:GLN:N	2.31	0.46
5:E:87:SER:HB3	5:E:131:ILE:HD13	1.97	0.46
1:A:1245:A:C2	1:A:1293:G:C2	3.04	0.46
1:A:110:C:H2'	1:A:111:G:O4'	2.16	0.46
2:B:157:ARG:HG2	2:B:158:LEU:N	2.31	0.46
4:D:78:LEU:HA	4:D:78:LEU:HD22	1.84	0.46
1:A:794:A:C6	1:A:795:C:C4	3.03	0.46
7:G:40:ALA:HB1	9:I:41:VAL:HG21	1.98	0.46
1:A:45:U:H2'	1:A:46:G:C8	2.50	0.46
3:C:24:ALA:HB3	3:C:29:TYR:CD1	2.51	0.46
24:A:1717:HYG:H13	24:A:1717:HYG:H341	1.98	0.46
1:A:7:G:H5'	1:A:298:A:O4'	2.16	0.46
1:A:1407:5MC:H2'	1:A:1408:A:O4'	2.16	0.46
7:G:90:GLU:HG2	7:G:91:VAL:N	2.31	0.46
1:A:385:C:H2'	1:A:386:C:C6	2.50	0.46
1:A:8:A:H5'	5:E:101:ILE:HG22	1.97	0.46
1:A:186:C:H2'	1:A:187:C:C6	2.51	0.46
7:G:75:VAL:HG21	7:G:86:GLN:HB3	1.97	0.46
12:L:77:LEU:HD21	12:L:107:ALA:HB2	1.97	0.46
13:M:117:VAL:HG12	13:M:118:ALA:H	1.80	0.46
1:A:538:G:H2'	1:A:539:A:C8	2.50	0.46
2:B:101:MET:C	2:B:102:LEU:HD12	2.36	0.46
1:A:259:G:H2'	1:A:260:G:C8	2.51	0.46
1:A:112:G:O2'	1:A:113:G:H5'	2.15	0.46
1:A:620:C:C1'	4:D:135:LEU:HD13	2.45	0.46
7:G:9:VAL:HG13	7:G:94:ARG:HH12	1.80	0.46
1:A:1158:C:H4'	2:B:133:LYS:HG2	1.98	0.46
1:A:1168:A:H2'	1:A:1169:A:C8	2.51	0.46
7:G:31:MET:SD	7:G:34:GLY:HA2	2.56	0.46
2:B:73:THR:HG23	2:B:95:GLN:O	2.16	0.46
1:A:290:C:N4	1:A:310:G:H1	2.07	0.46
4:D:64:LEU:HD12	4:D:75:PHE:CZ	2.50	0.46
1:A:421:U:H5'	1:A:422:C:C5	2.51	0.46
1:A:627:G:H2'	1:A:628:G:C8	2.51	0.46
1:A:833:U:H2'	1:A:834:C:C6	2.50	0.46
9:I:114:TYR:CB	10:J:60:ARG:HG2	2.46	0.46
12:L:44:THR:HA	12:L:45:PRO:HD3	1.77	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:G:OP1	17:Q:67:LYS:O	2.35	0.45
1:A:1316:G:H4'	14:N:18:VAL:CG1	2.45	0.45
10:J:14:LYS:H	10:J:14:LYS:HD3	1.81	0.45
1:A:1127:G:H1	1:A:1145:C:N4	2.13	0.45
1:A:1207:2MG:H2'	1:A:1208:C:H6	1.81	0.45
5:E:112:LEU:HA	5:E:112:LEU:HD23	1.75	0.45
4:D:172:PRO:HD2	4:D:173:TRP:CZ3	2.51	0.45
13:M:67:GLU:HB3	13:M:68:GLY:H	1.45	0.45
1:A:894:G:H2'	1:A:895:G:H8	1.81	0.45
1:A:753:A:OP1	15:O:69:TYR:OH	2.31	0.45
2:B:130:ARG:HA	2:B:130:ARG:HD3	1.78	0.45
1:A:300:A:H8	1:A:300:A:O5'	2.00	0.45
1:A:1249:C:O2'	9:I:73:GLN:NE2	2.49	0.45
1:A:894:G:H2'	1:A:895:G:C8	2.51	0.45
17:Q:63:ARG:HG2	17:Q:64:PRO:HD2	1.98	0.45
1:A:255:G:C2	1:A:272:C:C2	3.05	0.45
1:A:667:G:H4'	15:O:51:HIS:ND1	2.32	0.45
18:R:17:SER:HB3	18:R:55:ARG:CG	2.40	0.45
1:A:1354:C:H2'	1:A:1355:G:H8	1.81	0.45
1:A:358:U:H2'	1:A:359:U:C6	2.51	0.45
4:D:3:ARG:NH1	4:D:5:ILE:HD11	2.31	0.45
1:A:1399:C:O2	1:A:1401:G:C5	2.69	0.45
17:Q:58:GLU:O	17:Q:59:ILE:HD13	2.16	0.45
1:A:1363:A:H4'	1:A:1364:U:H2'	1.99	0.45
1:A:1151:A:H5'	10:J:40:LEU:O	2.17	0.45
2:B:218:ALA:O	2:B:222:ILE:HG13	2.15	0.45
19:S:50:ALA:HA	19:S:58:VAL:O	2.16	0.45
1:A:494:G:HO2'	1:A:495:U:H6	1.62	0.45
2:B:37:ASN:N	2:B:37:ASN:OD1	2.49	0.45
1:A:1357:A:H2'	1:A:1358:U:C6	2.52	0.45
1:A:969:A:H4'	10:J:55:LYS:HZ3	1.80	0.45
10:J:54:PHE:HD2	10:J:55:LYS:HG2	1.81	0.45
2:B:115:LEU:HD12	2:B:145:LEU:HB2	1.97	0.45
1:A:1112:C:N3	3:C:178:LEU:HB2	2.31	0.45
3:C:38:ARG:HB3	3:C:94:LEU:HD21	1.98	0.45
17:Q:22:LEU:HA	17:Q:22:LEU:HD12	1.60	0.45
2:B:128:GLU:CD	2:B:128:GLU:H	2.20	0.45
1:A:191:G:N2	20:T:103:GLY:O	2.38	0.45
1:A:6:G:H4'	1:A:298:A:H4'	1.97	0.45
18:R:47:THR:HG22	18:R:48:GLY:H	1.82	0.45
1:A:201:C:H42	1:A:216:G:H1	1.65	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1343:G:H2'	1:A:1344:C:C6	2.51	0.45
1:A:146:G:H2'	1:A:147:G:C8	2.52	0.45
1:A:1517:G:H2'	1:A:1518:A:O4'	2.17	0.45
1:A:1092:A:C6	1:A:1093:A:C6	3.05	0.45
1:A:737:A:H2'	1:A:738:C:C6	2.52	0.45
2:B:27:LYS:HD2	2:B:193:ASP:OD2	2.16	0.45
6:F:50:TYR:CE1	18:R:77:GLY:HA2	2.52	0.45
1:A:532:A:H2'	1:A:532:A:N3	2.32	0.45
1:A:1143:G:H2'	1:A:1144:G:C8	2.52	0.45
1:A:382:A:H2'	1:A:383:A:C8	2.52	0.45
1:A:491:G:C2	1:A:492:G:C8	3.05	0.45
4:D:25:ARG:HA	4:D:28:SER:HB2	1.98	0.45
12:L:10:LEU:HB3	17:Q:32:TYR:CD1	2.52	0.45
1:A:9:G:OP1	5:E:122:GLU:HG3	2.16	0.45
1:A:77:G:C6	1:A:93:G:N1	2.85	0.45
1:A:1056:U:O2'	1:A:1057:G:H5'	2.17	0.45
1:A:1130:A:H4'	9:I:20:ARG:NH2	2.31	0.45
1:A:375:U:H2'	1:A:376:G:C8	2.52	0.45
8:H:100:ILE:CG2	8:H:125:ARG:HH11	2.30	0.45
1:A:524:G:H2'	1:A:525:C:C6	2.52	0.45
12:L:69:TYR:HE2	12:L:71:PRO:HA	1.82	0.45
1:A:1328:C:OP1	21:U:21:TYR:OH	2.27	0.45
1:A:1392:G:H21	1:A:1502:A:H8	1.65	0.45
1:A:1372:U:OP1	9:I:71:SER:HB3	2.17	0.45
12:L:47:LYS:HB3	12:L:48:PRO:HD3	1.99	0.45
1:A:673:G:H5''	6:F:87:ARG:CZ	2.47	0.45
1:A:113:G:H2'	1:A:114:U:H6	1.82	0.45
4:D:36:ARG:HB3	4:D:38:TYR:CE2	2.52	0.45
1:A:42:G:H1	1:A:400:C:H42	1.63	0.45
10:J:47:PHE:HB3	14:N:34:TYR:HE2	1.82	0.45
2:B:233:SER:HA	2:B:234:PRO:HD3	1.75	0.45
1:A:663:A:H2'	1:A:664:G:O4'	2.17	0.45
1:A:1486:G:H2'	1:A:1487:G:O4'	2.17	0.45
1:A:1486:G:O6	1:A:1487:G:C6	2.70	0.45
2:B:115:LEU:HD12	2:B:145:LEU:CB	2.47	0.45
1:A:807:A:H2'	1:A:808:C:C6	2.52	0.45
1:A:1539:C:H2'	1:A:1540:PSU:C6	2.52	0.45
11:K:73:MET:HG3	11:K:103:LEU:HD21	1.99	0.45
1:A:1349:A:C2	1:A:1374:A:C4	3.05	0.45
1:A:1374:A:C4	1:A:1375:A:C8	3.05	0.45
1:A:778:G:H2'	1:A:779:C:O4'	2.17	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:599:C:C2	1:A:640:A:C2	3.04	0.45
16:P:60:LEU:HD23	16:P:60:LEU:HA	1.74	0.45
1:A:241:C:H42	1:A:285:G:H1	1.64	0.44
1:A:1382:C:H2'	1:A:1383:C:C6	2.52	0.44
19:S:41:VAL:HG23	19:S:44:MET:HG3	1.99	0.44
1:A:1226:C:H6	13:M:103:THR:HG1	1.63	0.44
11:K:22:HIS:ND1	11:K:22:HIS:O	2.49	0.44
8:H:98:LYS:HZ3	8:H:98:LYS:H	1.64	0.44
13:M:82:MET:HB3	13:M:93:ARG:NH1	2.32	0.44
4:D:120:LEU:HD23	4:D:120:LEU:HA	1.56	0.44
20:T:62:LEU:HD23	20:T:62:LEU:HA	1.74	0.44
8:H:87:SER:HB2	8:H:93:VAL:HB	1.99	0.44
1:A:828:A:H2'	1:A:829:G:O4'	2.18	0.44
1:A:96:G:H2'	1:A:97:G:C8	2.53	0.44
3:C:120:VAL:O	3:C:124:ILE:HG13	2.17	0.44
1:A:383:A:C5	1:A:384:G:H1'	2.52	0.44
21:U:5:ASP:HB3	21:U:8:THR:OG1	2.17	0.44
2:B:28:PHE:CD2	2:B:190:THR:HA	2.52	0.44
1:A:1115:C:O2'	1:A:1116:C:H5'	2.18	0.44
1:A:1352:C:H42	1:A:1370:G:H1	1.65	0.44
6:F:91:VAL:HG21	18:R:72:ARG:NH1	2.33	0.44
17:Q:43:LEU:HD23	17:Q:43:LEU:HA	1.68	0.44
1:A:253:U:H2'	1:A:254:G:C8	2.52	0.44
1:A:1309:G:N2	1:A:1329:A:H1'	2.32	0.44
1:A:854:G:H3'	1:A:871:U:O4	2.17	0.44
1:A:597:G:H2'	1:A:598:U:H5'	1.98	0.44
18:R:59:SER:H	18:R:62:GLU:HB2	1.82	0.44
1:A:409:G:H1	1:A:433:C:H42	1.65	0.44
10:J:60:ARG:N	10:J:60:ARG:HD2	2.32	0.44
1:A:923:A:OP1	5:E:21:ALA:HB2	2.17	0.44
11:K:34:ASP:HB2	11:K:35:PRO:HD2	1.99	0.44
1:A:701:C:O2	1:A:703:G:N1	2.50	0.44
15:O:3:ILE:HG13	15:O:3:ILE:H	1.53	0.44
20:T:92:LEU:HD23	20:T:92:LEU:HA	1.82	0.44
12:L:54:LYS:N	12:L:54:LYS:HD2	2.33	0.44
14:N:59:ALA:HB1	14:N:61:TRP:HZ3	1.83	0.44
3:C:147:LYS:HE2	3:C:205:GLY:H	1.81	0.44
3:C:16:ARG:HD2	3:C:16:ARG:HA	1.63	0.44
13:M:13:LYS:O	13:M:45:VAL:HG23	2.18	0.44
13:M:15:VAL:HG23	13:M:43:THR:O	2.17	0.44
11:K:54:ARG:O	11:K:57:THR:OG1	2.36	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1061:G:H1'	10:J:56:HIS:CE1	2.52	0.44
1:A:1014:A:H2'	1:A:1015:A:C8	2.53	0.44
5:E:131:ILE:HD13	5:E:131:ILE:HA	1.56	0.44
1:A:922:G:C2	1:A:1396:A:C6	3.05	0.44
1:A:1123:A:H4'	10:J:37:PRO:HD2	2.00	0.44
5:E:143:ARG:NH1	8:H:77:GLU:OE2	2.51	0.44
1:A:137:C:H42	1:A:226:G:H1	1.64	0.44
18:R:39:VAL:HG13	18:R:40:LEU:HD23	2.00	0.44
15:O:56:LEU:HD12	15:O:59:MET:HE3	2.00	0.44
1:A:1249:C:H2'	1:A:1250:A:H5'	2.00	0.44
3:C:6:HIS:HA	3:C:7:PRO:HD3	1.70	0.44
4:D:98:GLU:HG2	4:D:189:PRO:HG3	2.00	0.44
20:T:67:ALA:O	20:T:73:HIS:ND1	2.50	0.44
3:C:178:LEU:HD13	3:C:178:LEU:HA	1.82	0.44
1:A:1289:A:H2'	1:A:1290:G:H5'	2.00	0.44
16:P:38:TYR:O	16:P:49:LEU:HD12	2.18	0.44
9:I:112:LYS:HG2	9:I:113:LYS:N	2.32	0.44
24:A:1717:HYG:H103	24:A:1717:HYG:H32A	1.68	0.44
3:C:116:VAL:O	3:C:120:VAL:HG23	2.18	0.44
1:A:1251:A:N3	1:A:1369:C:O2'	2.37	0.44
17:Q:75:ARG:NH2	17:Q:77:VAL:HG13	2.33	0.44
9:I:28:VAL:HG12	9:I:29:ASN:OD1	2.17	0.44
1:A:758:G:H8	1:A:758:G:O5'	2.00	0.44
13:M:8:GLU:OE2	13:M:22:ILE:HA	2.18	0.43
1:A:98:U:H2'	1:A:99:C:C6	2.52	0.43
1:A:419:C:N4	1:A:424:G:H1	2.12	0.43
1:A:953:G:C5'	1:A:965:A:H61	2.30	0.43
19:S:36:ARG:HH21	19:S:75:ALA:HB3	1.83	0.43
12:L:77:LEU:HD23	12:L:77:LEU:HA	1.88	0.43
1:A:928:G:H5''	1:A:1533:C:H41	1.82	0.43
8:H:105:ARG:HA	8:H:105:ARG:HD2	1.81	0.43
1:A:285:G:C2	1:A:286:G:C8	3.07	0.43
1:A:1486:G:N1	1:A:1487:G:C2	2.86	0.43
6:F:18:GLN:O	6:F:22:GLU:HG2	2.18	0.43
1:A:393:A:C2	1:A:394:G:C8	3.07	0.43
1:A:394:G:H2'	1:A:395:C:C6	2.53	0.43
8:H:28:ALA:CB	8:H:59:LEU:HG	2.49	0.43
19:S:40:ILE:HD13	19:S:62:ILE:HD13	2.00	0.43
1:A:376:G:N3	1:A:389:A:C2	2.86	0.43
3:C:25:GLY:O	3:C:29:TYR:HB2	2.18	0.43
3:C:29:TYR:CE2	3:C:33:LEU:HD23	2.53	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:95:VAL:HG11	8:H:100:ILE:HA	1.99	0.43
1:A:716:A:C6	1:A:717:C:C4	3.06	0.43
1:A:1228:C:OP1	13:M:108:ARG:NH2	2.46	0.43
1:A:1139:G:H4'	1:A:1140:C:H5'	2.00	0.43
1:A:429:U:H1'	1:A:430:A:H5''	2.00	0.43
5:E:81:GLU:CD	5:E:88:LYS:HD3	2.38	0.43
1:A:1392:G:H2'	1:A:1393:U:H6	1.82	0.43
1:A:1372:U:H2'	1:A:1373:G:O4'	2.19	0.43
1:A:405:U:O4	4:D:2:GLY:HA2	2.18	0.43
11:K:16:SER:O	11:K:35:PRO:HD3	2.17	0.43
1:A:517:G:N1	1:A:533:A:OP2	2.49	0.43
5:E:80:ILE:HD13	5:E:91:LEU:HB2	2.00	0.43
15:O:15:PHE:CD2	15:O:30:ALA:HB2	2.53	0.43
1:A:1342:C:H2'	1:A:1343:G:H8	1.82	0.43
1:A:1001:A:H2'	1:A:1002:G:C8	2.54	0.43
1:A:630:G:H3'	1:A:631:G:C8	2.54	0.43
4:D:57:ARG:HG3	4:D:202:LEU:HD13	1.99	0.43
6:F:27:GLN:HA	6:F:30:LEU:HD12	2.01	0.43
4:D:71:SER:OG	4:D:74:GLN:HB2	2.18	0.43
1:A:821:G:H2'	1:A:822:C:H6	1.83	0.43
5:E:142:LEU:HA	5:E:142:LEU:HD23	1.69	0.43
1:A:1140:C:H2'	1:A:1141:C:C6	2.53	0.43
20:T:53:LEU:HB2	20:T:100:ILE:HG21	2.00	0.43
1:A:91:C:O2'	1:A:92:C:H5'	2.17	0.43
11:K:22:HIS:ND1	11:K:22:HIS:C	2.71	0.43
1:A:1453:G:H5'	1:A:1454:G:OP2	2.18	0.43
1:A:500:G:C5	1:A:546:G:N2	2.87	0.43
14:N:24:CYS:SG	14:N:39:LEU:HA	2.59	0.43
4:D:148:VAL:HG11	4:D:158:ILE:HG21	2.00	0.43
21:U:18:TYR:CE2	21:U:24:ARG:HB3	2.53	0.43
1:A:575:G:OP1	1:A:575:G:H4'	2.19	0.43
1:A:376:G:C4	1:A:389:A:C2	3.07	0.43
1:A:636:U:H2'	1:A:637:G:H8	1.83	0.43
1:A:1306:A:C2	1:A:1307:U:H1'	2.52	0.43
3:C:20:SER:HA	3:C:57:ILE:O	2.19	0.43
2:B:201:ILE:O	2:B:203:GLY:N	2.51	0.43
12:L:113:ARG:HD3	12:L:114:LYS:H	1.83	0.43
13:M:34:LEU:HD12	13:M:41:PRO:HA	2.01	0.43
2:B:158:LEU:H	2:B:158:LEU:CD1	2.18	0.43
1:A:297:G:N2	1:A:300:A:OP2	2.45	0.43
1:A:1415:G:C2	1:A:1416:G:C8	3.06	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:15:LEU:HA	19:S:18:LYS:HB2	1.99	0.43
1:A:665:A:H2'	1:A:732:C:O2	2.17	0.43
10:J:19:SER:OG	10:J:94:VAL:HG21	2.19	0.43
1:A:939:G:H2'	1:A:940:C:C6	2.54	0.43
3:C:50:ALA:HB2	3:C:75:VAL:HB	2.00	0.43
4:D:24:GLU:HG2	4:D:25:ARG:N	2.34	0.43
1:A:895:G:H2'	1:A:896:C:C6	2.54	0.43
5:E:46:GLY:H	5:E:58:ALA:HB2	1.84	0.43
1:A:1089:G:H1	1:A:1096:C:H42	1.67	0.43
1:A:812:C:OP1	1:A:903:G:H1'	2.18	0.43
1:A:1076:C:OP2	2:B:179:LYS:NZ	2.52	0.43
4:D:200:GLU:H	4:D:200:GLU:CD	2.22	0.43
10:J:51:ARG:NH2	10:J:61:GLU:HB2	2.34	0.43
20:T:100:ILE:HG13	20:T:102:GLY:N	2.34	0.43
4:D:64:LEU:HD12	4:D:75:PHE:HZ	1.83	0.43
5:E:118:ILE:HG12	5:E:119:LEU:N	2.33	0.43
1:A:1399:C:C2	1:A:1401:G:C5	3.07	0.43
1:A:1027:C:OP1	1:A:1027:C:H4'	2.19	0.43
7:G:26:PHE:CE2	7:G:124:LEU:HD21	2.54	0.43
1:A:44:G:H2'	1:A:45:U:O4'	2.18	0.43
19:S:80:TYR:CZ	19:S:81:ARG:HB2	2.53	0.43
1:A:864:A:H2'	1:A:865:A:C8	2.53	0.43
8:H:19:VAL:HG23	8:H:19:VAL:O	2.18	0.43
1:A:1412:C:N4	1:A:1489:G:H1	2.16	0.43
14:N:25:VAL:HB	14:N:39:LEU:HD23	1.99	0.43
4:D:98:GLU:O	4:D:103:ASN:ND2	2.52	0.43
17:Q:24:GLU:HG2	17:Q:39:SER:HB3	2.00	0.43
1:A:389:A:C5	1:A:390:C:H1'	2.54	0.43
2:B:89:GLY:H	2:B:226:ARG:HH22	1.67	0.43
1:A:1248:A:N3	9:I:70:LYS:NZ	2.67	0.43
1:A:1068:G:N7	1:A:1094:G:H2'	2.33	0.43
1:A:1482:G:HO2'	1:A:1483:A:H8	1.60	0.43
2:B:49:GLU:HG3	2:B:50:GLU:N	2.34	0.43
20:T:53:LEU:HG	20:T:100:ILE:HG21	2.00	0.43
6:F:100:ASN:ND2	18:R:23:LYS:HG2	2.34	0.43
1:A:1053:G:N2	1:A:1058:G:O6	2.52	0.43
1:A:75:G:C2	1:A:96:G:C2	3.07	0.43
8:H:23:SER:OG	8:H:24:THR:N	2.52	0.43
15:O:33:THR:HA	15:O:36:ILE:HD12	2.01	0.43
4:D:190:ASP:H	4:D:193:ASP:CG	2.22	0.43
1:A:1441:G:HO2'	1:A:1442:G:N2	2.16	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:G:H1	1:A:165:C:H42	1.66	0.43
8:H:56:LYS:HA	8:H:57:PRO:HD3	1.73	0.43
7:G:26:PHE:HE1	7:G:104:LEU:HB3	1.83	0.43
17:Q:27:PHE:CE2	17:Q:36:ILE:HG13	2.54	0.43
1:A:247:G:OP1	17:Q:100:LYS:HE3	2.18	0.43
1:A:600:C:H42	1:A:638:G:H1	1.67	0.43
12:L:20:LYS:NZ	12:L:20:LYS:H	2.17	0.43
18:R:32:ARG:HH21	18:R:65:ILE:HD11	1.84	0.42
1:A:1433:A:N6	1:A:1434:A:C6	2.87	0.42
1:A:1487:G:C2	1:A:1488:G:C4	3.07	0.42
1:A:109:A:C6	1:A:326:G:C6	3.07	0.42
1:A:204:U:H3'	1:A:204:U:OP2	2.18	0.42
1:A:1377:A:H2'	7:G:7:ALA:CB	2.49	0.42
1:A:1378:C:H2'	1:A:1379:G:O4'	2.18	0.42
1:A:8:A:C5	4:D:209:ARG:HB2	2.54	0.42
3:C:38:ARG:HD3	3:C:94:LEU:HD11	2.00	0.42
4:D:11:LEU:HD13	4:D:66:ARG:HG3	2.01	0.42
11:K:66:LEU:HD23	11:K:66:LEU:HA	1.73	0.42
1:A:1053:G:O2'	1:A:1199:U:H5	2.02	0.42
1:A:18:C:H2'	1:A:19:C:O4'	2.20	0.42
7:G:18:TYR:CG	7:G:59:LEU:HD13	2.54	0.42
6:F:12:PRO:HD2	6:F:86:ARG:NH1	2.34	0.42
1:A:113:G:H2'	1:A:114:U:C6	2.54	0.42
7:G:78:ARG:HB3	7:G:87:VAL:HG21	2.00	0.42
5:E:36:ASP:CG	5:E:38:GLN:H	2.21	0.42
4:D:24:GLU:H	4:D:112:VAL:CG1	2.32	0.42
1:A:1419:G:C6	1:A:1420:C:C4	3.07	0.42
1:A:1437:C:H2'	1:A:1438:G:C8	2.54	0.42
5:E:19:MET:SD	5:E:24:ARG:HG2	2.59	0.42
1:A:1225:A:H2'	1:A:1225:A:N3	2.34	0.42
3:C:53:ALA:HB2	3:C:115:LEU:HD11	2.01	0.42
1:A:1495:U:H2'	1:A:1496:C:O4'	2.19	0.42
9:I:8:GLY:HA3	9:I:79:LEU:HB3	2.01	0.42
1:A:936:C:H42	1:A:1379:G:H1	1.66	0.42
1:A:630:G:H5'	1:A:631:G:OP2	2.19	0.42
1:A:237:C:H2'	1:A:238:G:H8	1.84	0.42
10:J:55:LYS:HE3	10:J:55:LYS:HB2	1.63	0.42
1:A:1006:C:H2'	1:A:1007:C:C6	2.55	0.42
1:A:1389:C:H2'	1:A:1390:U:O4'	2.20	0.42
1:A:945:G:C2	1:A:1337:G:C2	3.07	0.42
1:A:1040:U:H2'	1:A:1041:A:H8	1.84	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:973:G:H3'	1:A:974:A:H5''	2.01	0.42
1:A:1486:G:O6	1:A:1487:G:N1	2.52	0.42
6:F:8:ILE:HG22	6:F:10:LEU:HG	2.00	0.42
15:O:29:VAL:O	15:O:33:THR:HB	2.19	0.42
1:A:1064:G:H1'	1:A:1190:G:N2	2.34	0.42
4:D:38:TYR:HA	4:D:39:PRO:HD3	1.91	0.42
1:A:1427:U:H2'	1:A:1428:A:H8	1.84	0.42
1:A:60:A:H4'	1:A:61:G:O5'	2.19	0.42
5:E:87:SER:HB3	5:E:131:ILE:CD1	2.49	0.42
1:A:795:C:H5''	1:A:796:C:OP2	2.19	0.42
9:I:114:TYR:HB2	10:J:60:ARG:HG2	2.01	0.42
18:R:34:TYR:HE1	18:R:35:ARG:HD3	1.84	0.42
3:C:86:VAL:O	3:C:89:GLU:HB3	2.19	0.42
17:Q:40:LYS:HG3	17:Q:41:LYS:N	2.32	0.42
1:A:1414:U:N3	1:A:1415:G:C8	2.88	0.42
1:A:1490:C:O2'	1:A:1491:G:H5'	2.20	0.42
3:C:131:ARG:HA	3:C:134:ILE:HD12	2.01	0.42
1:A:397:A:H5'	1:A:398:C:OP1	2.19	0.42
5:E:47:LYS:HB3	5:E:47:LYS:HE2	1.93	0.42
4:D:201:GLN:HE21	4:D:201:GLN:HB3	1.72	0.42
16:P:82:GLN:HE21	16:P:82:GLN:HB3	1.67	0.42
11:K:24:SER:OG	11:K:25:TYR:N	2.47	0.42
13:M:86:CYS:SG	19:S:73:GLU:HB3	2.60	0.42
2:B:98:LEU:HA	2:B:98:LEU:HD13	1.74	0.42
10:J:51:ARG:HB2	10:J:59:SER:HB2	2.01	0.42
6:F:22:GLU:OE2	6:F:82:ARG:HD3	2.19	0.42
1:A:230:G:H2'	1:A:231:G:O4'	2.19	0.42
1:A:598:U:H2'	1:A:599:C:C6	2.54	0.42
1:A:256:U:H2'	1:A:257:G:C8	2.54	0.42
1:A:278:G:C6	17:Q:95:TYR:CD2	3.05	0.42
8:H:19:VAL:HG22	8:H:21:LYS:HG3	2.02	0.42
13:M:27:LYS:HE3	21:U:21:TYR:CE2	2.45	0.42
1:A:1408:A:H3'	1:A:1409:C:H5''	2.01	0.42
4:D:155:LEU:HD23	4:D:156:GLU:H	1.84	0.42
1:A:383:A:C6	1:A:384:G:H1'	2.54	0.42
6:F:86:ARG:O	6:F:87:ARG:HG2	2.20	0.42
5:E:144:THR:HG23	5:E:147:ASP:OD2	2.20	0.42
1:A:448:A:OP2	1:A:485:G:N1	2.44	0.42
4:D:18:LYS:HE3	4:D:20:TYR:CE2	2.55	0.42
1:A:556:C:H2'	1:A:557:G:O4'	2.20	0.42
4:D:21:LEU:HD11	4:D:66:ARG:O	2.19	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:A:C6	1:A:339:C:C4	3.08	0.42
3:C:14:ILE:HG22	3:C:15:THR:HG23	2.01	0.42
20:T:15:ARG:HA	20:T:15:ARG:HD3	1.86	0.42
2:B:102:LEU:HB3	2:B:180:LEU:HD12	2.01	0.42
1:A:79:G:C2	1:A:91:C:C2	3.08	0.42
1:A:859:A:H2'	1:A:860:A:O4'	2.19	0.42
1:A:826:C:O2	8:H:15:ASN:ND2	2.53	0.42
1:A:500:G:C6	1:A:546:G:C2	3.07	0.42
3:C:148:GLY:HA3	3:C:172:ARG:O	2.20	0.42
2:B:174:VAL:HG12	2:B:175:ARG:N	2.34	0.42
2:B:221:LEU:HA	2:B:221:LEU:HD22	1.75	0.42
1:A:1434:A:H2'	1:A:1435:G:O4'	2.19	0.42
1:A:93:G:C6	1:A:95:U:C4	3.07	0.42
1:A:1116:C:H2'	1:A:1117:G:H5''	2.01	0.42
7:G:104:LEU:HA	7:G:104:LEU:HD23	1.66	0.42
2:B:74:LYS:HE3	2:B:166:ASP:HB2	2.02	0.42
3:C:47:LEU:HD11	3:C:87:LEU:HD13	2.02	0.42
15:O:43:LEU:HA	15:O:43:LEU:HD23	1.74	0.42
1:A:1308:U:OP2	13:M:99:ARG:HG3	2.20	0.42
4:D:125:HIS:O	4:D:126:ILE:HD13	2.19	0.42
4:D:8:VAL:O	4:D:10:ARG:N	2.53	0.42
7:G:87:VAL:HA	7:G:88:PRO:HD3	1.81	0.42
2:B:132:LYS:HA	2:B:135:GLN:HB2	2.01	0.42
1:A:140:A:H2'	1:A:141:A:O4'	2.20	0.42
20:T:43:LEU:HA	20:T:43:LEU:HD13	1.81	0.42
1:A:1095:U:OP1	1:A:1108:G:N2	2.51	0.42
2:B:48:MET:HA	2:B:51:LEU:HD12	2.02	0.42
1:A:266:G:H2'	1:A:266:G:H8	1.61	0.41
17:Q:67:LYS:HA	17:Q:70:ARG:HH12	1.85	0.41
1:A:1103:C:H5'	2:B:98:LEU:HD12	2.02	0.41
13:M:34:LEU:HD13	13:M:39:ILE:O	2.19	0.41
2:B:212:GLN:NE2	2:B:235:SER:HB2	2.32	0.41
1:A:1250:A:C6	1:A:1251:A:C6	3.08	0.41
1:A:1116:C:O2'	9:I:108:VAL:HG21	2.20	0.41
2:B:122:PHE:HE1	2:B:139:LYS:NZ	2.18	0.41
6:F:97:PHE:CZ	18:R:61:LYS:HE3	2.54	0.41
1:A:324:G:OP1	20:T:22:ARG:NH1	2.52	0.41
11:K:38:ASN:HA	11:K:39:PRO:HD3	1.76	0.41
11:K:81:ASP:OD2	11:K:106:LYS:HB2	2.18	0.41
1:A:570:G:H1'	1:A:820:U:C4	2.55	0.41
8:H:51:VAL:HG23	8:H:52:ASP:N	2.35	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1286:A:H2	21:U:22:ARG:HH22	1.66	0.41
1:A:1098:C:H2'	1:A:1099:G:O4'	2.20	0.41
12:L:10:LEU:HD23	17:Q:32:TYR:CE1	2.55	0.41
9:I:45:ALA:O	9:I:48:GLU:HB2	2.20	0.41
18:R:43:PHE:C	18:R:44:LEU:HD23	2.41	0.41
2:B:68:ILE:O	2:B:90:MET:HB3	2.20	0.41
5:E:76:ILE:HA	5:E:77:PRO:HD2	1.83	0.41
14:N:6:LEU:HD13	14:N:6:LEU:HA	1.75	0.41
3:C:10:PHE:CE1	3:C:178:LEU:HD11	2.55	0.41
1:A:145:G:H1	1:A:177:C:H42	1.67	0.41
1:A:926:G:C6	1:A:1505:G:C6	3.08	0.41
21:U:6:ARG:O	21:U:12:LYS:HE3	2.19	0.41
6:F:42:GLU:OE1	6:F:59:TYR:OH	2.31	0.41
1:A:1399:C:C2	1:A:1502:A:N6	2.88	0.41
1:A:836:G:H8	1:A:836:G:H5''	1.85	0.41
7:G:51:GLN:HG3	7:G:58:PRO:HG3	2.02	0.41
1:A:673:G:O3'	6:F:87:ARG:NH2	2.53	0.41
1:A:243:A:H4'	1:A:244:U:H5''	2.02	0.41
1:A:583:A:H2'	1:A:584:G:O4'	2.20	0.41
5:E:76:ILE:O	5:E:93:PRO:HB3	2.20	0.41
11:K:57:THR:HG22	11:K:58:PRO:HD2	2.01	0.41
1:A:958:A:C2	19:S:55:LYS:HB2	2.56	0.41
5:E:33:VAL:HG11	5:E:109:ILE:HA	2.02	0.41
1:A:966:M2G:N7	1:A:967:5MC:HM52	2.35	0.41
18:R:50:ILE:HG13	18:R:74:ARG:NH2	2.35	0.41
1:A:1077:G:N2	1:A:1081:G:C4	2.87	0.41
9:I:17:VAL:HG13	9:I:63:ILE:HG12	2.01	0.41
1:A:1101:A:N6	2:B:176:GLU:OE2	2.54	0.41
1:A:1358:U:H5''	14:N:35:ARG:CD	2.48	0.41
1:A:6:G:H2'	5:E:119:LEU:HD11	2.02	0.41
3:C:155:GLY:HA2	3:C:164:ARG:O	2.20	0.41
1:A:1203:C:H2'	1:A:1204:A:O4'	2.20	0.41
1:A:706:A:O2'	11:K:29:ILE:HD11	2.20	0.41
3:C:70:VAL:O	3:C:105:GLU:HA	2.20	0.41
1:A:1120:G:C2	1:A:1121:U:C2	3.08	0.41
1:A:237:C:H2'	1:A:238:G:C8	2.56	0.41
18:R:74:ARG:O	18:R:77:GLY:N	2.39	0.41
1:A:434:U:C4	1:A:435:C:N4	2.88	0.41
1:A:1070:U:H2'	1:A:1071:C:H6	1.85	0.41
1:A:179:A:H2'	1:A:180:U:C6	2.55	0.41
20:T:19:SER:OG	20:T:20:LEU:HD23	2.20	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:6:ARG:NH2	21:U:15:ARG:HH21	2.07	0.41
1:A:544:G:C6	1:A:545:C:C4	3.08	0.41
1:A:1190:G:OP1	3:C:4:LYS:HA	2.21	0.41
3:C:47:LEU:CD2	3:C:68:VAL:HG11	2.50	0.41
10:J:86:MET:HG3	10:J:87:THR:H	1.86	0.41
8:H:33:GLU:OE1	8:H:50:ARG:NE	2.53	0.41
15:O:57:LEU:HA	15:O:57:LEU:HD12	1.84	0.41
15:O:6:GLU:OE1	15:O:6:GLU:N	2.40	0.41
5:E:90:VAL:O	5:E:91:LEU:HD23	2.21	0.41
1:A:7:G:C5'	1:A:298:A:H5'	2.50	0.41
4:D:3:ARG:HH11	4:D:115:ARG:HE	1.67	0.41
1:A:613:C:H2'	1:A:614:A:H8	1.85	0.41
1:A:790:A:C6	1:A:791:G:C6	3.08	0.41
17:Q:44:ALA:HA	17:Q:71:PHE:O	2.20	0.41
5:E:36:ASP:OD2	5:E:38:GLN:HB2	2.20	0.41
7:G:9:VAL:HG12	7:G:10:ARG:O	2.20	0.41
1:A:945:G:H2'	1:A:945:G:N3	2.36	0.41
10:J:39:PRO:HA	10:J:70:ARG:NH1	2.36	0.41
1:A:455:C:H6	1:A:455:C:O5'	2.04	0.41
1:A:1326:C:H2'	1:A:1327:C:C6	2.55	0.41
14:N:15:LYS:HG2	14:N:16:PHE:CE1	2.55	0.41
4:D:64:LEU:HD22	4:D:64:LEU:HA	1.82	0.41
1:A:1057:G:H5"	3:C:154:SER:CB	2.51	0.41
13:M:13:LYS:HB2	13:M:18:ALA:HB2	2.01	0.41
18:R:56:THR:HB	18:R:58:LEU:HG	2.02	0.41
2:B:185:ILE:HA	2:B:199:TYR:O	2.21	0.41
1:A:617:G:H1	1:A:623:C:H42	1.69	0.41
1:A:1243:C:H42	1:A:1294:G:H1	1.68	0.41
1:A:1329:A:H2'	1:A:1330:U:O4'	2.21	0.41
1:A:115:G:H1'	1:A:116:A:N7	2.35	0.41
1:A:1118:C:H1'	1:A:1179:A:C4	2.56	0.41
14:N:53:LEU:HA	14:N:54:PRO:HD3	1.91	0.41
1:A:446:G:C6	1:A:447:G:C4	3.08	0.41
1:A:41:G:H2'	1:A:42:G:H8	1.85	0.41
2:B:222:ILE:O	2:B:226:ARG:HG3	2.21	0.41
4:D:57:ARG:HB3	4:D:206:PHE:HB2	2.03	0.41
4:D:70:ILE:HG22	4:D:71:SER:O	2.21	0.41
7:G:118:VAL:O	7:G:122:HIS:HB2	2.21	0.41
1:A:714:G:H2'	1:A:715:A:O4'	2.21	0.41
6:F:53:ALA:C	6:F:55:ASP:H	2.23	0.41
8:H:39:LEU:O	8:H:42:GLU:N	2.54	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:28:GLN:CD	3:C:28:GLN:H	2.24	0.41
16:P:74:LEU:HB3	16:P:79:VAL:CG2	2.51	0.41
17:Q:40:LYS:HG2	17:Q:42:TYR:CE1	2.56	0.41
1:A:1355:G:H2'	1:A:1356:G:H8	1.86	0.41
1:A:1410:G:N1	1:A:1411:C:C4	2.89	0.41
1:A:1486:G:C6	1:A:1487:G:N1	2.89	0.41
1:A:97:G:C2'	1:A:98:U:H5'	2.51	0.41
4:D:126:ILE:HD13	4:D:126:ILE:HA	1.85	0.41
18:R:36:ASN:O	18:R:40:LEU:HG	2.21	0.41
1:A:1378:C:C5	1:A:1379:G:C8	3.09	0.41
10:J:32:ALA:O	10:J:34:VAL:HG23	2.20	0.41
1:A:768:A:C5	1:A:769:G:C8	3.09	0.41
4:D:25:ARG:O	4:D:25:ARG:HG2	2.19	0.41
7:G:27:ILE:HD11	7:G:40:ALA:HA	2.01	0.41
1:A:1206:G:H4'	3:C:192:THR:O	2.21	0.41
15:O:55:GLY:HA2	15:O:58:MET:HE2	2.01	0.41
17:Q:84:LEU:H	17:Q:84:LEU:HD12	1.86	0.41
10:J:76:ASN:HB3	10:J:78:ASN:ND2	2.36	0.41
1:A:264:U:H2'	1:A:265:G:O4'	2.21	0.41
19:S:5:LEU:HG	19:S:9:VAL:HG22	2.03	0.41
1:A:314:C:O2'	1:A:315:A:H5'	2.20	0.41
1:A:695:A:H61	1:A:797:C:H1'	1.85	0.41
6:F:2:ARG:O	6:F:66:GLU:HA	2.21	0.41
2:B:158:LEU:HB3	2:B:159:PRO:HD2	2.03	0.41
1:A:1345:U:OP1	9:I:120:ARG:NH1	2.50	0.41
1:A:1370:G:O5'	1:A:1370:G:H8	2.04	0.41
1:A:859:A:OP2	1:A:869:G:N1	2.35	0.41
1:A:559:A:H4'	1:A:560:U:O5'	2.21	0.41
7:G:65:ALA:O	7:G:69:VAL:HG23	2.20	0.41
1:A:688:G:H2'	1:A:689:C:H6	1.85	0.41
1:A:142:G:O2'	1:A:196:A:N1	2.37	0.41
13:M:48:LEU:HD12	13:M:53:VAL:HG23	2.03	0.41
1:A:439:A:C4	1:A:497:A:C2	3.09	0.41
10:J:49:VAL:HG21	14:N:44:LEU:HD23	2.03	0.40
1:A:129(A):G:H1'	1:A:190(E):U:H2'	2.03	0.40
1:A:76:C:H2'	1:A:77:G:H8	1.84	0.40
8:H:6:ILE:O	8:H:10:LEU:HG	2.20	0.40
3:C:121:ALA:O	3:C:125:GLU:HG3	2.21	0.40
1:A:522:C:H41	12:L:53:ARG:HH22	1.69	0.40
1:A:981:U:H5'	14:N:21:TYR:CZ	2.56	0.40
1:A:376:G:H5''	16:P:5:ARG:HB2	2.02	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1518:A:H2'	1:A:1519:A:C8	2.56	0.40
1:A:707:C:H2'	1:A:708:C:C6	2.56	0.40
1:A:451:A:H8	1:A:451:A:O5'	2.05	0.40
5:E:118:ILE:C	5:E:119:LEU:HD23	2.42	0.40
1:A:1328:C:H2'	1:A:1329:A:O4'	2.21	0.40
1:A:1413:A:N1	1:A:1489:G:C2	2.89	0.40
11:K:98:LEU:HA	11:K:98:LEU:HD22	1.61	0.40
1:A:35:G:C6	1:A:36:C:C4	3.09	0.40
1:A:1003(A):G:H2'	1:A:1004:A:H4'	2.03	0.40
2:B:115:LEU:CD2	2:B:153:ARG:HH21	2.34	0.40
4:D:203:VAL:O	4:D:206:PHE:HB3	2.21	0.40
8:H:127:LEU:HD23	8:H:127:LEU:HA	1.84	0.40
18:R:26:LEU:HD12	18:R:26:LEU:HA	1.73	0.40
1:A:1435:G:O5'	1:A:1435:G:H8	2.03	0.40
1:A:285:G:C4	1:A:286:G:C8	3.09	0.40
1:A:1148:U:O3'	9:I:14:VAL:HG11	2.22	0.40
1:A:1516:G:N2	1:A:1520:G:C4	2.89	0.40
7:G:51:GLN:HA	7:G:54:THR:O	2.21	0.40
1:A:446:G:N2	1:A:489:C:C2	2.89	0.40
7:G:26:PHE:HA	7:G:101:LEU:HD12	2.02	0.40
19:S:40:ILE:HD13	19:S:62:ILE:CD1	2.52	0.40
1:A:923:A:H8	1:A:923:A:O5'	2.04	0.40
5:E:86:ALA:O	5:E:125:SER:N	2.51	0.40
11:K:120:ARG:HH11	11:K:120:ARG:HD3	1.73	0.40
1:A:1072:G:C5	1:A:1073:U:C4	3.10	0.40
1:A:258:G:N3	1:A:259:G:C8	2.90	0.40
5:E:98:THR:HG21	5:E:119:LEU:HD21	2.03	0.40
15:O:30:ALA:HA	15:O:85:LEU:HD11	2.03	0.40
1:A:34:C:H1'	12:L:32:PHE:CZ	2.57	0.40
2:B:31:TYR:CD2	2:B:31:TYR:N	2.89	0.40
7:G:27:ILE:HA	7:G:30:ILE:HD12	2.04	0.40
17:Q:26:GLN:O	17:Q:27:PHE:HB3	2.21	0.40
15:O:10:LYS:HA	15:O:10:LYS:HD2	1.85	0.40
1:A:268:C:H2'	1:A:269:C:H6	1.86	0.40
1:A:241:C:N4	1:A:285:G:H1	2.19	0.40
1:A:79:G:C6	1:A:91:C:N4	2.89	0.40
1:A:1499:A:H1'	1:A:1520:G:H5'	2.02	0.40
1:A:36:C:O2'	1:A:501:C:OP1	2.36	0.40
1:A:1117:G:N2	1:A:1180:A:H1'	2.37	0.40
4:D:68:TYR:OH	4:D:98:GLU:OE1	2.26	0.40
17:Q:9:VAL:O	17:Q:11:VAL:HG13	2.22	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:9:VAL:HG22	6:F:60:PHE:CE2	2.57	0.40
2:B:106:LYS:HA	2:B:106:LYS:HD3	1.81	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	234/256 (91%)	202 (86%)	31 (13%)	1 (0%)	39	80
3	C	205/239 (86%)	181 (88%)	24 (12%)	0	100	100
4	D	206/209 (99%)	188 (91%)	17 (8%)	1 (0%)	34	77
5	E	149/162 (92%)	145 (97%)	4 (3%)	0	100	100
6	F	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
7	G	153/156 (98%)	139 (91%)	14 (9%)	0	100	100
8	H	136/138 (99%)	132 (97%)	4 (3%)	0	100	100
9	I	125/128 (98%)	108 (86%)	15 (12%)	2 (2%)	12	58
10	J	97/105 (92%)	78 (80%)	17 (18%)	2 (2%)	9	53
11	K	117/129 (91%)	103 (88%)	14 (12%)	0	100	100
12	L	122/135 (90%)	108 (88%)	12 (10%)	2 (2%)	12	58
13	M	116/126 (92%)	106 (91%)	10 (9%)	0	100	100
14	N	58/61 (95%)	52 (90%)	6 (10%)	0	100	100
15	O	86/89 (97%)	78 (91%)	8 (9%)	0	100	100
16	P	82/88 (93%)	79 (96%)	3 (4%)	0	100	100
17	Q	97/105 (92%)	91 (94%)	6 (6%)	0	100	100
18	R	71/88 (81%)	60 (84%)	10 (14%)	1 (1%)	14	59
19	S	79/93 (85%)	65 (82%)	14 (18%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	T	97/106 (92%)	86 (89%)	11 (11%)	0	100	100
21	U	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
All	All	2352/2541 (93%)	2116 (90%)	227 (10%)	9 (0%)	39	80

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	L	28	LYS
9	I	119	ALA
10	J	34	VAL
9	I	31	GLN
10	J	72	VAL
18	R	21	LYS
2	B	89	GLY
4	D	5	ILE
12	L	30	ALA

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	194/220 (88%)	165 (85%)	29 (15%)	4	26
3	C	160/188 (85%)	136 (85%)	24 (15%)	3	26
4	D	180/181 (99%)	153 (85%)	27 (15%)	3	26
5	E	115/123 (94%)	93 (81%)	22 (19%)	2	13
6	F	90/90 (100%)	83 (92%)	7 (8%)	16	55
7	G	126/127 (99%)	111 (88%)	15 (12%)	6	35
8	H	119/119 (100%)	94 (79%)	25 (21%)	1	10
9	I	98/99 (99%)	84 (86%)	14 (14%)	4	28
10	J	87/92 (95%)	74 (85%)	13 (15%)	4	26
11	K	90/99 (91%)	78 (87%)	12 (13%)	5	31

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	L	103/110 (94%)	81 (79%)	22 (21%)	1	10
13	M	94/101 (93%)	77 (82%)	17 (18%)	2	16
14	N	49/50 (98%)	45 (92%)	4 (8%)	14	53
15	O	79/80 (99%)	69 (87%)	10 (13%)	5	32
16	P	72/74 (97%)	64 (89%)	8 (11%)	8	39
17	Q	94/97 (97%)	80 (85%)	14 (15%)	4	26
18	R	64/77 (83%)	56 (88%)	8 (12%)	6	33
19	S	71/80 (89%)	60 (84%)	11 (16%)	3	24
20	T	76/82 (93%)	58 (76%)	18 (24%)	1	7
21	U	19/22 (86%)	17 (90%)	2 (10%)	8	41
All	All	1980/2111 (94%)	1678 (85%)	302 (15%)	3	25

All (302) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	15	VAL
2	B	20	GLU
2	B	22	LYS
2	B	24	TRP
2	B	37	ASN
2	B	46	LYS
2	B	47	THR
2	B	49	GLU
2	B	69	LEU
2	B	74	LYS
2	B	78	GLN
2	B	94	ASN
2	B	114	ARG
2	B	128	GLU
2	B	132	LYS
2	B	133	LYS
2	B	139	LYS
2	B	142	LEU
2	B	144	ARG
2	B	157	ARG
2	B	158	LEU
2	B	160	ASP
2	B	163	PHE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	175	ARG
2	B	215	LEU
2	B	221	LEU
2	B	230	VAL
2	B	235	SER
2	B	236	TYR
3	C	3	ASN
3	C	15	THR
3	C	16	ARG
3	C	17	ASP
3	C	28	GLN
3	C	30	ARG
3	C	33	LEU
3	C	34	LEU
3	C	36	ASP
3	C	54	ARG
3	C	58	GLU
3	C	72	LYS
3	C	84	ILE
3	C	95	THR
3	C	126	ARG
3	C	156	ARG
3	C	176	HIS
3	C	178	LEU
3	C	181	ASN
3	C	188	LEU
3	C	190	ARG
3	C	192	THR
3	C	193	TYR
3	C	204	LEU
4	D	19	LEU
4	D	25	ARG
4	D	26	CYS
4	D	49	ARG
4	D	53	ASP
4	D	64	LEU
4	D	66	ARG
4	D	73	ARG
4	D	76	ARG
4	D	78	LEU
4	D	99	SER
4	D	108	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
4	D	122	ARG
4	D	127	THR
4	D	131	ARG
4	D	152	SER
4	D	155	LEU
4	D	162	LEU
4	D	170	VAL
4	D	187	ARG
4	D	188	LEU
4	D	193	ASP
4	D	194	LEU
4	D	201	GLN
4	D	202	LEU
4	D	208	SER
4	D	209	ARG
5	E	12	LEU
5	E	16	THR
5	E	18	ARG
5	E	31	LEU
5	E	41	VAL
5	E	43	LEU
5	E	47	LYS
5	E	50	GLU
5	E	53	LEU
5	E	55	VAL
5	E	64	ARG
5	E	66	MET
5	E	68	GLU
5	E	75	THR
5	E	79	GLU
5	E	80	ILE
5	E	82	VAL
5	E	96	PRO
5	E	131	ILE
5	E	144	THR
5	E	148	VAL
5	E	151	LEU
6	F	15	ASP
6	F	18	GLN
6	F	40	VAL
6	F	43	LEU
6	F	45	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
6	F	83	ASP
6	F	94	GLN
7	G	6	ARG
7	G	21	VAL
7	G	27	ILE
7	G	37	ASN
7	G	47	CYS
7	G	64	GLN
7	G	77	SER
7	G	92	SER
7	G	94	ARG
7	G	113	GLU
7	G	115	ARG
7	G	122	HIS
7	G	124	LEU
7	G	126	ASP
7	G	149	ARG
8	H	3	THR
8	H	11	THR
8	H	18	ARG
8	H	23	SER
8	H	24	THR
8	H	39	LEU
8	H	51	VAL
8	H	56	LYS
8	H	63	LEU
8	H	69	ARG
8	H	82	HIS
8	H	83	ILE
8	H	84	ARG
8	H	91	ARG
8	H	92	ARG
8	H	95	VAL
8	H	97	VAL
8	H	100	ILE
8	H	102	ARG
8	H	104	ARG
8	H	105	ARG
8	H	114	THR
8	H	119	LEU
8	H	120	THR
8	H	133	LEU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
9	I	4	TYR
9	I	10	ARG
9	I	19	LEU
9	I	29	ASN
9	I	41	VAL
9	I	66	ARG
9	I	79	LEU
9	I	86	VAL
9	I	95	LYS
9	I	102	LEU
9	I	104	ARG
9	I	109	VAL
9	I	121	ARG
9	I	128	ARG
10	J	3	LYS
10	J	4	ILE
10	J	5	ARG
10	J	9	ARG
10	J	13	HIS
10	J	14	LYS
10	J	29	ARG
10	J	44	VAL
10	J	46	ARG
10	J	47	PHE
10	J	60	ARG
10	J	66	ARG
10	J	94	VAL
11	K	14	VAL
11	K	22	HIS
11	K	24	SER
11	K	29	ILE
11	K	41	THR
11	K	57	THR
11	K	62	GLN
11	K	75	TYR
11	K	98	LEU
11	K	114	VAL
11	K	120	ARG
11	K	127	LYS
12	L	7	ILE
12	L	10	LEU
12	L	18	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
12	L	20	LYS
12	L	28	LYS
12	L	33	ARG
12	L	36	VAL
12	L	41	ARG
12	L	42	THR
12	L	43	VAL
12	L	66	VAL
12	L	67	THR
12	L	78	GLN
12	L	79	GLU
12	L	80	HIS
12	L	83	VAL
12	L	90	VAL
12	L	97	ARG
12	L	113	ARG
12	L	114	LYS
12	L	126	LYS
12	L	127	GLU
13	M	4	ILE
13	M	7	VAL
13	M	8	GLU
13	M	27	LYS
13	M	34	LEU
13	M	49	THR
13	M	53	VAL
13	M	56	LEU
13	M	60	VAL
13	M	62	ASN
13	M	63	THR
13	M	70	LEU
13	M	81	LEU
13	M	102	ARG
13	M	110	ARG
13	M	115	LYS
13	M	117	VAL
14	N	9	LYS
14	N	12	ARG
14	N	27	CYS
14	N	53	LEU
15	O	3	ILE
15	O	17	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
15	O	21	ASP
15	O	32	LEU
15	O	33	THR
15	O	38	ARG
15	O	70	LEU
15	O	71	GLN
15	O	73	GLU
15	O	83	GLU
16	P	2	VAL
16	P	53	VAL
16	P	61	SER
16	P	62	VAL
16	P	68	ASP
16	P	69	THR
16	P	82	GLN
16	P	83	GLU
17	Q	35	VAL
17	Q	37	LYS
17	Q	40	LYS
17	Q	41	LYS
17	Q	52	LYS
17	Q	59	ILE
17	Q	60	ILE
17	Q	77	VAL
17	Q	84	LEU
17	Q	86	GLU
17	Q	91	ARG
17	Q	92	ARG
17	Q	97	SER
17	Q	98	LEU
18	R	21	LYS
18	R	35	ARG
18	R	37	VAL
18	R	42	ARG
18	R	47	THR
18	R	68	LYS
18	R	81	PHE
18	R	84	LYS
19	S	6	LYS
19	S	7	LYS
19	S	15	LEU
19	S	18	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
19	S	27	GLU
19	S	29	ARG
19	S	30	LEU
19	S	43	GLU
19	S	65	ASN
19	S	70	LYS
19	S	81	ARG
20	T	8	ARG
20	T	19	SER
20	T	20	LEU
20	T	36	LEU
20	T	43	LEU
20	T	50	GLU
20	T	53	LEU
20	T	56	MET
20	T	57	ARG
20	T	62	LEU
20	T	70	SER
20	T	71	THR
20	T	73	HIS
20	T	74	LYS
20	T	75	ASN
20	T	84	LEU
20	T	92	LEU
20	T	100	ILE
21	U	17	THR
21	U	22	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	136	GLN
4	D	123	HIS
9	I	73	GLN
9	I	124	GLN
10	J	56	HIS
10	J	78	ASN
16	P	16	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1510/1522 (99%)	284 (18%)	25 (1%)

All (284) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	9	G
1	A	32	A
1	A	38	G
1	A	39	G
1	A	47	C
1	A	48	C
1	A	51	A
1	A	54	C
1	A	73	C
1	A	74	C
1	A	77	G
1	A	79	G
1	A	82	U
1	A	88	A
1	A	90	U
1	A	91	C
1	A	98	U
1	A	108	G
1	A	109	A
1	A	115	G
1	A	116	A
1	A	121	C
1	A	129(A)	G
1	A	130	A
1	A	131	C
1	A	132	C
1	A	163	C
1	A	169	C
1	A	178	C
1	A	182	U
1	A	188	C
1	A	195	A
1	A	197	A
1	A	201	C
1	A	202	U
1	A	203	U
1	A	204	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	216	G
1	A	220	G
1	A	231	G
1	A	247	G
1	A	251	G
1	A	266	G
1	A	267	C
1	A	289	G
1	A	292	G
1	A	293	G
1	A	301	G
1	A	319	G
1	A	321	A
1	A	328	C
1	A	329	A
1	A	335	C
1	A	344	A
1	A	345	C
1	A	346	G
1	A	352	C
1	A	353	A
1	A	354	G
1	A	367	U
1	A	372	C
1	A	373	A
1	A	382	A
1	A	384	G
1	A	392	G
1	A	396	G
1	A	397	A
1	A	398	C
1	A	406	G
1	A	411	A
1	A	412	A
1	A	413	G
1	A	419	C
1	A	421	U
1	A	424	G
1	A	429	U
1	A	430	A
1	A	433	C
1	A	439	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	442	C
1	A	452	A
1	A	460	A
1	A	485	G
1	A	497	A
1	A	498	U
1	A	508	C
1	A	511	C
1	A	513	C
1	A	518	C
1	A	519	C
1	A	527	7MG
1	A	528	C
1	A	530	G
1	A	531	U
1	A	532	A
1	A	533	A
1	A	547	A
1	A	548	G
1	A	559	A
1	A	560	U
1	A	563	A
1	A	564	C
1	A	568	G
1	A	572	A
1	A	573	A
1	A	575	G
1	A	576	G
1	A	577	G
1	A	579	G
1	A	588	G
1	A	596	C
1	A	624	C
1	A	630	G
1	A	631	G
1	A	632	A
1	A	653	A
1	A	665	A
1	A	687	A
1	A	688	G
1	A	701	C
1	A	702	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	703	G
1	A	717	C
1	A	721	G
1	A	723	U
1	A	724	G
1	A	731	G
1	A	734	G
1	A	749	C
1	A	755	G
1	A	760	G
1	A	773	G
1	A	774	G
1	A	777	A
1	A	781	A
1	A	785	G
1	A	787	A
1	A	792	A
1	A	793	U
1	A	794	A
1	A	813	U
1	A	816	A
1	A	817	C
1	A	818	G
1	A	819	A
1	A	826	C
1	A	828	A
1	A	839	U
1	A	840	C
1	A	841	U
1	A	848	C
1	A	859	A
1	A	876	G
1	A	884	U
1	A	889	A
1	A	902	G
1	A	926	G
1	A	927	G
1	A	934	C
1	A	935	A
1	A	950	U
1	A	960	U
1	A	961	U

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	966	M2G
1	A	967	5MC
1	A	969	A
1	A	972	C
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	978	A
1	A	982	U
1	A	991	U
1	A	992	U
1	A	993	G
1	A	1004	A
1	A	1005	A
1	A	1025	U
1	A	1027	C
1	A	1028	C
1	A	1031	G
1	A	1054	C
1	A	1055	A
1	A	1060	C
1	A	1064	G
1	A	1065	U
1	A	1066	C
1	A	1078	U
1	A	1092	A
1	A	1094	G
1	A	1095	U
1	A	1096	C
1	A	1101	A
1	A	1111	A
1	A	1117	G
1	A	1125	U
1	A	1126	U
1	A	1127	G
1	A	1129	C
1	A	1130	A
1	A	1131	G
1	A	1137	C
1	A	1138	G
1	A	1139	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	1140	C
1	A	1143	G
1	A	1144	G
1	A	1145	C
1	A	1152	A
1	A	1154	G
1	A	1159	U
1	A	1160	G
1	A	1164	G
1	A	1171	G
1	A	1191	A
1	A	1196	U
1	A	1200	C
1	A	1201	A
1	A	1202	G
1	A	1211	U
1	A	1212	U
1	A	1213	A
1	A	1214	C
1	A	1225	A
1	A	1238	A
1	A	1241	G
1	A	1242	C
1	A	1245	A
1	A	1253	G
1	A	1257	U
1	A	1258	G
1	A	1261	A
1	A	1270	C
1	A	1280	A
1	A	1286	A
1	A	1287	A
1	A	1297	C
1	A	1300	G
1	A	1302	U
1	A	1303	C
1	A	1305	G
1	A	1310	G
1	A	1311	G
1	A	1312	G
1	A	1316	G
1	A	1320	C

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	1322	C
1	A	1338	G
1	A	1347	G
1	A	1353	G
1	A	1358	U
1	A	1359	C
1	A	1360	A
1	A	1362	C
1	A	1368	G
1	A	1370	G
1	A	1394	A
1	A	1398	A
1	A	1399	C
1	A	1400	5MC
1	A	1409	C
1	A	1418	A
1	A	1442	G
1	A	1443	G
1	A	1446	A
1	A	1453	G
1	A	1454	G
1	A	1474	G
1	A	1477	C
1	A	1489	G
1	A	1491	G
1	A	1492	A
1	A	1493	A
1	A	1498	UR3
1	A	1499	A
1	A	1504	G
1	A	1505	G
1	A	1506	U
1	A	1520	G
1	A	1529	G
1	A	1530	G
1	A	1531	A

All (25) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	115	G
1	A	129(A)	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	181	G
1	A	204	U
1	A	266	G
1	A	328	C
1	A	372	C
1	A	428	G
1	A	429	U
1	A	432	A
1	A	484	G
1	A	496	A
1	A	559	A
1	A	587	G
1	A	687	A
1	A	723	U
1	A	748	C
1	A	812	C
1	A	884	U
1	A	960	U
1	A	1065	U
1	A	1201	A
1	A	1256	A
1	A	1417	G
1	A	1504	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	2MG	A	1207	1	17,26,27	2.21	4 (23%)	21,38,41	2.21	3 (14%)
1	5MC	A	1400	1	13,22,23	1.27	1 (7%)	15,32,35	0.98	1 (6%)
1	4OC	A	1402	1	13,23,24	1.16	1 (7%)	18,32,35	0.60	0
1	5MC	A	1404	1	13,22,23	0.72	0	15,32,35	1.07	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	5MC	A	1407	1	13,22,23	1.52	2 (15%)	15,32,35	1.04	1 (6%)
1	UR3	A	1498	1	12,22,23	0.51	0	16,32,35	1.45	1 (6%)
1	PSU	A	1540	1	13,21,22	1.14	1 (7%)	18,30,33	3.65	6 (33%)
1	PSU	A	1541	1	13,21,22	1.07	1 (7%)	18,30,33	3.55	6 (33%)
1	PSU	A	516	1,22	13,21,22	0.94	1 (7%)	18,30,33	3.87	5 (27%)
1	7MG	A	527	1	19,26,27	2.72	5 (26%)	24,39,42	1.95	6 (25%)
1	M2G	A	966	1	17,27,28	1.99	4 (23%)	22,40,43	1.92	3 (13%)
1	5MC	A	967	1	13,22,23	0.90	0	15,32,35	0.87	1 (6%)
12	0TD	L	92	12	4,9,10	0.95	0	4,11,13	2.41	3 (75%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MG	A	1207	1	-	0/5/27/28	0/3/3/3
1	5MC	A	1400	1	-	0/3/25/26	0/2/2/2
1	4OC	A	1402	1	-	0/7/29/30	0/2/2/2
1	5MC	A	1404	1	-	0/3/25/26	0/2/2/2
1	5MC	A	1407	1	-	0/3/25/26	0/2/2/2
1	UR3	A	1498	1	-	0/3/25/26	0/2/2/2
1	PSU	A	1540	1	-	0/7/25/26	0/2/2/2
1	PSU	A	1541	1	-	0/7/25/26	0/2/2/2
1	PSU	A	516	1,22	-	0/7/25/26	0/2/2/2
1	7MG	A	527	1	-	0/7/37/38	0/3/3/3
1	M2G	A	966	1	-	0/7/29/30	0/3/3/3
1	5MC	A	967	1	-	0/3/25/26	0/2/2/2
12	0TD	L	92	12	-	0/2/12/14	0/0/0/0

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	7MG	C8-N9	-7.67	1.34	1.45
1	A	527	7MG	CM7-N7	-2.50	1.41	1.46
1	A	1207	2MG	C2-N1	2.16	1.42	1.34
1	A	1407	5MC	C6-N1	2.22	1.38	1.35
1	A	527	7MG	C6-N1	2.23	1.37	1.33
1	A	1207	2MG	C4-N3	2.38	1.39	1.35
1	A	1402	4OC	C5-C4	2.44	1.45	1.39

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	516	PSU	C4-N3	2.48	1.37	1.33
1	A	966	M2G	C2-N1	2.51	1.39	1.34
1	A	1541	PSU	C4-N3	2.87	1.38	1.33
1	A	1540	PSU	C4-N3	2.92	1.38	1.33
1	A	966	M2G	C4-N3	3.46	1.41	1.35
1	A	1400	5MC	C5-C4	3.54	1.46	1.41
1	A	1407	5MC	C5-C4	4.19	1.47	1.41
1	A	966	M2G	C2-N2	4.55	1.42	1.34
1	A	966	M2G	C6-N1	4.81	1.42	1.33
1	A	527	7MG	C2-N2	5.28	1.44	1.34
1	A	527	7MG	C4-N3	5.61	1.41	1.34
1	A	1207	2MG	C6-N1	5.70	1.43	1.33
1	A	1207	2MG	C2-N2	6.07	1.41	1.34

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	516	PSU	N1-C2-N3	-14.31	119.20	128.33
1	A	1540	PSU	N1-C2-N3	-13.09	119.98	128.33
1	A	1541	PSU	N1-C2-N3	-12.73	120.21	128.33
1	A	1207	2MG	C5-C6-N1	-7.92	112.76	123.59
1	A	966	M2G	C5-C6-N1	-7.68	113.09	123.59
1	A	527	7MG	C5-C4-N3	-6.46	120.53	126.82
12	L	92	0TD	CSB-SB-CB	-2.91	96.05	101.54
12	L	92	0TD	CB-CA-N	-2.90	103.37	109.66
1	A	1540	PSU	C5-C6-N1	-2.83	120.39	124.39
1	A	1541	PSU	C5-C1'-C2'	-2.83	110.49	115.52
1	A	1540	PSU	C5-C1'-C2'	-2.83	110.50	115.52
1	A	1407	5MC	N4-C4-N3	-2.78	112.91	116.95
1	A	1541	PSU	C5-C6-N1	-2.58	120.75	124.39
12	L	92	0TD	O-C-CA	-2.51	118.82	125.44
1	A	527	7MG	C4-N9-C1'	-2.39	120.94	126.70
1	A	527	7MG	N1-C2-N3	-2.36	121.67	125.53
1	A	516	PSU	C5-C6-N1	-2.35	121.08	124.39
1	A	1400	5MC	N4-C4-N3	-2.24	113.70	116.95
1	A	966	M2G	N1-C2-N2	-2.01	114.89	117.16
1	A	527	7MG	C2-N3-C4	2.03	120.44	114.53
1	A	967	5MC	CM5-C5-C6	2.14	122.92	118.62
1	A	1207	2MG	C4-C5-N7	2.17	111.47	109.48
1	A	1404	5MC	CM5-C5-C6	2.26	123.16	118.62
1	A	1541	PSU	O4'-C1'-C2'	2.72	107.50	104.73
1	A	516	PSU	O4'-C1'-C2'	2.87	107.66	104.73

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	527	7MG	C6-N1-C2	2.95	120.03	115.94
1	A	1541	PSU	C6-N1-C2	3.01	120.32	115.47
1	A	1540	PSU	O4'-C1'-C2'	3.03	107.82	104.73
1	A	516	PSU	C6-N1-C2	3.06	120.39	115.47
1	A	1540	PSU	C6-N1-C2	3.07	120.41	115.47
1	A	966	M2G	N3-C2-N2	3.14	120.71	117.16
1	A	1498	UR3	C6-C5-C4	3.40	123.63	117.28
1	A	527	7MG	N3-C4-N9	3.52	132.03	126.75
1	A	1207	2MG	C6-N1-C2	4.72	122.17	115.31
1	A	1540	PSU	C4-N3-C2	5.18	119.73	115.25
1	A	1541	PSU	C4-N3-C2	5.33	119.86	115.25
1	A	516	PSU	C4-N3-C2	6.13	120.55	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1207	2MG	3	0
1	A	1400	5MC	2	0
1	A	1404	5MC	1	0
1	A	1407	5MC	1	0
1	A	1498	UR3	1	0
1	A	1540	PSU	1	0
1	A	527	7MG	1	0
1	A	966	M2G	2	0
1	A	967	5MC	2	0
12	L	92	0TD	4	0

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 129 ligands modelled in this entry, 128 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	HYG	A	1717	-	35,39,39	1.81	6 (17%)	41,60,60	2.66	15 (36%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	HYG	A	1717	-	-	0/12/87/87	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1717	HYG	C26-C25	2.17	1.58	1.52
24	A	1717	HYG	C13-C12	2.60	1.59	1.52
24	A	1717	HYG	C16-C15	3.21	1.59	1.53
24	A	1717	HYG	C5-C4	3.21	1.59	1.52
24	A	1717	HYG	C34-C33	3.90	1.58	1.52
24	A	1717	HYG	C27-C33	6.14	1.60	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1717	HYG	C5-C6-C1	-3.56	106.19	110.89
24	A	1717	HYG	C16-C17-C12	-3.03	105.67	113.56
24	A	1717	HYG	O35-C34-C33	-2.38	106.52	111.53
24	A	1717	HYG	O32-C26-C27	-2.07	104.98	109.87
24	A	1717	HYG	C3-C2-C1	2.13	113.38	110.11
24	A	1717	HYG	O18-C6-C1	2.74	114.23	107.17
24	A	1717	HYG	C23-C24-C25	2.83	113.41	110.51
24	A	1717	HYG	C25-C26-C27	3.33	116.91	109.60
24	A	1717	HYG	C26-C25-C24	3.68	116.54	111.33
24	A	1717	HYG	O14-C15-C16	4.43	118.00	109.68
24	A	1717	HYG	C23-O28-C27	4.53	120.63	112.00
24	A	1717	HYG	C13-O14-C15	4.75	122.96	113.75
24	A	1717	HYG	O29-C12-C13	6.12	129.40	111.20

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1717	HYG	O28-C27-C26	6.61	117.19	108.56
24	A	1717	HYG	O18-C13-C12	6.81	123.08	109.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	1717	HYG	4	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	1501/1522 (98%)	-0.29	28 (1%) 70 54	69, 132, 256, 360	0
2	B	236/256 (92%)	-0.50	3 (1%) 79 65	77, 136, 231, 275	0
3	C	207/239 (86%)	-0.04	12 (5%) 26 16	94, 196, 235, 248	0
4	D	208/209 (99%)	-0.33	1 (0%) 91 85	87, 136, 186, 207	0
5	E	151/162 (93%)	-0.51	0 100 100	62, 100, 148, 192	0
6	F	101/101 (100%)	-0.56	0 100 100	114, 152, 178, 202	0
7	G	155/156 (99%)	-0.21	9 (5%) 26 16	125, 174, 240, 276	0
8	H	138/138 (100%)	-0.59	0 100 100	65, 91, 134, 149	0
9	I	127/128 (99%)	-0.12	3 (2%) 62 46	145, 190, 236, 264	0
10	J	99/105 (94%)	0.23	6 (6%) 25 15	81, 213, 309, 332	0
11	K	119/129 (92%)	-0.24	2 (1%) 73 58	88, 126, 169, 206	0
12	L	124/135 (91%)	-0.26	2 (1%) 74 59	64, 126, 162, 245	0
13	M	118/126 (93%)	-0.07	2 (1%) 73 58	133, 163, 190, 230	0
14	N	60/61 (98%)	0.39	7 (11%) 6 5	152, 187, 233, 271	0
15	O	88/89 (98%)	-0.36	0 100 100	85, 119, 169, 220	0
16	P	84/88 (95%)	-0.43	0 100 100	89, 128, 167, 247	0
17	Q	99/105 (94%)	-0.47	0 100 100	73, 110, 148, 169	0
18	R	73/88 (82%)	-0.44	2 (2%) 58 42	82, 126, 207, 231	0
19	S	81/93 (87%)	0.40	7 (8%) 13 9	96, 206, 253, 294	0
20	T	99/106 (93%)	-0.55	0 100 100	98, 133, 180, 200	0
21	U	25/27 (92%)	1.44	7 (28%) 1 1	81, 173, 190, 263	0
All	All	3893/4063 (95%)	-0.27	91 (2%) 64 47	62, 141, 236, 360	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	K	129	SER	11.7
11	K	128	ALA	11.5
3	C	193	TYR	6.5
14	N	12	ARG	6.3
1	A	1539	C	5.9
3	C	103	VAL	5.9
10	J	33	GLN	5.7
1	A	994	A	5.4
1	A	202	U	5.1
1	A	1129	C	5.0
14	N	13	THR	4.8
1	A	1003(A)	G	4.6
7	G	2	ALA	4.6
1	A	993	G	4.4
19	S	40	ILE	4.3
7	G	82	GLY	4.2
3	C	156	ARG	4.1
1	A	1018	C	4.0
3	C	155	GLY	4.0
1	A	1019	C	3.8
1	A	1005	A	3.5
19	S	38	SER	3.4
14	N	4	LYS	3.3
3	C	159	GLY	3.3
21	U	17	THR	3.3
1	A	1533	C	3.3
21	U	24	ARG	3.3
19	S	39	THR	3.3
7	G	5	ARG	3.3
21	U	25	LYS	3.3
21	U	18	TYR	3.2
9	I	119	ALA	3.2
19	S	28	LYS	3.2
3	C	157	ILE	3.1
13	M	7	VAL	3.0
14	N	3	ARG	2.9
10	J	32	ALA	2.9
21	U	22	ARG	2.9
9	I	4	TYR	2.9
1	A	1017	G	2.9
1	A	1037	C	2.8
2	B	132	LYS	2.8
3	C	66	VAL	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
7	G	81	GLY	2.8
7	G	83	ALA	2.7
21	U	5	ASP	2.7
19	S	69	HIS	2.7
4	D	37	PRO	2.7
1	A	1542	U	2.7
18	R	16	PRO	2.7
19	S	41	VAL	2.7
12	L	112	ASP	2.7
14	N	5	ALA	2.6
3	C	102	ASN	2.6
18	R	17	SER	2.6
13	M	118	ALA	2.6
3	C	65	ALA	2.6
14	N	2	ALA	2.5
10	J	39	PRO	2.5
1	A	1003	G	2.5
2	B	231	GLU	2.5
1	A	1006	C	2.5
7	G	84	ASN	2.5
7	G	156	TRP	2.4
10	J	74	ILE	2.4
1	A	1050	G	2.4
12	L	19	ARG	2.4
1	A	82	U	2.3
10	J	99	LYS	2.3
3	C	154	SER	2.3
1	A	1020	U	2.3
1	A	1322	C	2.3
21	U	26	LYS	2.3
1	A	1051	C	2.3
9	I	110	GLU	2.3
19	S	17	GLU	2.3
1	A	1493	A	2.2
14	N	6	LEU	2.2
1	A	1534	A	2.2
1	A	984	C	2.2
2	B	131	PRO	2.2
1	A	218	C	2.1
3	C	161	GLU	2.1
7	G	80	VAL	2.1
7	G	79	ARG	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
10	J	73	ASP	2.1
1	A	1314	C	2.1
1	A	532	A	2.0
1	A	1004	A	2.0
3	C	158	GLY	2.0
1	A	1002	G	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	5MC	A	1404	21/22	0.95	0.16	-	97,110,130,136	0
1	5MC	A	1407	21/22	0.95	0.22	-	142,156,190,190	0
1	4OC	A	1402	22/23	0.96	0.18	-	102,122,130,137	0
1	UR3	A	1498	21/22	0.95	0.23	-	115,129,138,150	0
1	7MG	A	527	24/25	0.93	0.18	-	97,110,123,130	0
1	PSU	A	516	20/21	0.92	0.12	-	137,146,155,158	0
1	M2G	A	966	25/26	0.96	0.14	-	130,149,169,172	0
1	5MC	A	1400	21/22	0.94	0.17	-	100,115,125,129	0
1	5MC	A	967	21/22	0.95	0.15	-	128,135,143,146	0
12	0TD	L	92	10/11	0.96	0.43	-	130,150,216,313	0
1	PSU	A	1540	20/21	0.70	0.95	-	325,348,352,353	0
1	PSU	A	1541	20/21	0.71	0.65	-	333,344,359,360	0
1	2MG	A	1207	24/25	0.90	0.19	-	200,220,224,230	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
22	MG	A	1672	1/1	0.93	0.50	58.50	37,37,37,37	0
22	MG	A	1608	1/1	0.86	0.94	45.76	70,70,70,70	0
22	MG	A	1635	1/1	0.78	1.10	29.28	74,74,74,74	0
22	MG	A	1679	1/1	0.97	0.47	26.21	78,78,78,78	0
22	MG	A	1670	1/1	0.80	1.22	25.91	91,91,91,91	0
22	MG	A	1668	1/1	0.94	1.14	25.41	77,77,77,77	0
22	MG	A	1707	1/1	0.97	0.63	22.15	76,76,76,76	0
22	MG	A	1603	1/1	0.92	0.44	16.63	64,64,64,64	0
22	MG	A	1622	1/1	0.98	0.46	11.76	55,55,55,55	0
22	MG	A	1681	1/1	0.96	0.56	10.78	76,76,76,76	0
22	MG	A	1614	1/1	0.93	0.58	9.43	46,46,46,46	0
22	MG	A	1654	1/1	0.95	0.47	8.13	84,84,84,84	0
22	MG	A	1669	1/1	0.94	0.41	7.05	59,59,59,59	0
22	MG	A	1634	1/1	0.79	0.37	6.72	83,83,83,83	0
22	MG	B	301	1/1	0.76	0.31	6.02	101,101,101,101	0
22	MG	A	1617	1/1	0.98	0.31	5.36	29,29,29,29	0
22	MG	A	1678	1/1	0.94	0.18	3.94	72,72,72,72	0
22	MG	A	1659	1/1	0.99	0.30	3.85	84,84,84,84	0
22	MG	D	302	1/1	0.92	0.33	3.72	112,112,112,112	0
22	MG	A	1671	1/1	0.91	0.47	3.70	94,94,94,94	0
23	K	A	1699	1/1	0.97	0.28	3.34	142,142,142,142	0
22	MG	M	201	1/1	0.98	0.42	3.29	113,113,113,113	0
22	MG	A	1642	1/1	0.99	0.24	3.12	103,103,103,103	0
22	MG	A	1647	1/1	0.92	0.22	2.61	50,50,50,50	0
22	MG	A	1683	1/1	0.99	0.24	2.43	76,76,76,76	0
22	MG	A	1604	1/1	0.98	0.27	2.32	98,98,98,98	0
22	MG	A	1709	1/1	0.17	0.29	2.01	130,130,130,130	0
22	MG	A	1641	1/1	0.54	0.53	1.94	80,80,80,80	0
22	MG	A	1684	1/1	0.96	0.39	1.90	141,141,141,141	0
22	MG	A	1667	1/1	0.93	0.26	1.25	73,73,73,73	0
25	ZN	D	301	1/1	0.99	0.37	0.89	119,119,119,119	0
22	MG	A	1673	1/1	0.99	0.20	0.81	48,48,48,48	0
24	HYG	A	1717	36/36	0.88	0.32	0.76	144,215,236,246	0
22	MG	A	1697	1/1	0.99	0.15	0.37	117,117,117,117	0
22	MG	A	1694	1/1	0.96	0.19	0.34	82,82,82,82	0
22	MG	L	201	1/1	0.96	0.21	-0.02	107,107,107,107	0
25	ZN	N	101	1/1	0.99	0.20	-0.14	199,199,199,199	0
22	MG	A	1698	1/1	0.98	0.23	-0.27	70,70,70,70	0
22	MG	A	1638	1/1	0.99	0.17	-0.55	55,55,55,55	0
22	MG	A	1689	1/1	0.99	0.12	-1.75	86,86,86,86	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
22	MG	A	1688	1/1	0.98	0.10	-2.66	62,62,62,62	0
22	MG	A	1693	1/1	0.90	0.07	-3.72	60,60,60,60	0
22	MG	A	1660	1/1	0.96	0.05	-8.01	64,64,64,64	0
22	MG	A	1632	1/1	0.96	0.55	-	86,86,86,86	0
22	MG	A	1616	1/1	0.99	0.13	-	101,101,101,101	0
22	MG	A	1644	1/1	0.91	0.13	-	109,109,109,109	0
22	MG	A	1690	1/1	0.94	0.22	-	84,84,84,84	0
22	MG	A	1657	1/1	0.96	0.12	-	127,127,127,127	0
22	MG	H	201	1/1	0.92	0.37	-	72,72,72,72	0
22	MG	A	1629	1/1	0.94	0.26	-	46,46,46,46	0
22	MG	A	1664	1/1	0.82	0.48	-	75,75,75,75	0
22	MG	A	1696	1/1	0.99	0.59	-	73,73,73,73	0
22	MG	A	1615	1/1	0.94	0.53	-	40,40,40,40	0
22	MG	A	1609	1/1	0.81	0.31	-	119,119,119,119	0
22	MG	A	1623	1/1	0.84	0.42	-	55,55,55,55	0
22	MG	A	1714	1/1	0.98	0.33	-	118,118,118,118	0
22	MG	A	1628	1/1	0.91	0.32	-	55,55,55,55	0
22	MG	A	1655	1/1	0.85	0.30	-	102,102,102,102	0
22	MG	A	1653	1/1	0.98	0.10	-	74,74,74,74	0
22	MG	A	1649	1/1	0.97	0.17	-	80,80,80,80	0
22	MG	A	1639	1/1	0.92	0.68	-	72,72,72,72	0
22	MG	A	1620	1/1	0.94	0.41	-	89,89,89,89	0
22	MG	A	1676	1/1	1.00	0.25	-	89,89,89,89	0
22	MG	A	1631	1/1	0.96	0.49	-	57,57,57,57	0
22	MG	A	1607	1/1	0.94	0.44	-	90,90,90,90	0
22	MG	A	1661	1/1	0.99	0.20	-	41,41,41,41	0
22	MG	A	1692	1/1	0.96	0.17	-	167,167,167,167	0
22	MG	A	1715	1/1	0.87	0.15	-	434,434,434,434	0
22	MG	A	1651	1/1	0.96	0.49	-	73,73,73,73	0
23	K	A	1702	1/1	0.92	0.23	-	161,161,161,161	0
22	MG	A	1630	1/1	0.61	0.48	-	56,56,56,56	0
23	K	A	1706	1/1	0.94	0.22	-	146,146,146,146	0
22	MG	A	1633	1/1	0.60	0.62	-	92,92,92,92	0
22	MG	A	1611	1/1	0.94	0.65	-	106,106,106,106	0
22	MG	A	1626	1/1	0.98	0.13	-	88,88,88,88	0
22	MG	A	1665	1/1	0.66	0.99	-	86,86,86,86	0
22	MG	A	1606	1/1	0.93	1.29	-	99,99,99,99	0
22	MG	A	1712	1/1	0.84	0.43	-	88,88,88,88	0
22	MG	A	1666	1/1	0.97	0.31	-	130,130,130,130	0
22	MG	A	1685	1/1	0.96	0.71	-	91,91,91,91	0
22	MG	A	1643	1/1	0.84	0.65	-	131,131,131,131	0
22	MG	A	1613	1/1	0.90	1.50	-	65,65,65,65	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
22	MG	A	1695	1/1	0.95	0.10	-	103,103,103,103	0
22	MG	A	1627	1/1	0.98	1.13	-	47,47,47,47	0
22	MG	A	1637	1/1	0.92	0.52	-	63,63,63,63	0
22	MG	A	1677	1/1	0.96	0.22	-	40,40,40,40	0
22	MG	A	1621	1/1	0.98	0.32	-	61,61,61,61	0
22	MG	D	303	1/1	0.85	0.16	-	88,88,88,88	0
22	MG	H	202	1/1	0.73	0.84	-	100,100,100,100	0
22	MG	A	1650	1/1	0.69	0.72	-	59,59,59,59	0
22	MG	A	1682	1/1	0.98	0.88	-	61,61,61,61	0
22	MG	A	1662	1/1	0.78	0.48	-	64,64,64,64	0
23	K	A	1701	1/1	0.99	0.36	-	100,100,100,100	0
22	MG	A	1674	1/1	0.98	0.59	-	49,49,49,49	0
22	MG	A	1602	1/1	0.82	0.88	-	54,54,54,54	0
22	MG	A	1636	1/1	0.78	0.86	-	54,54,54,54	0
22	MG	A	1648	1/1	0.92	0.55	-	81,81,81,81	0
22	MG	A	1686	1/1	0.96	0.21	-	102,102,102,102	0
23	K	A	1704	1/1	0.95	0.51	-	148,148,148,148	0
22	MG	A	1601	1/1	0.91	1.07	-	52,52,52,52	0
22	MG	A	1713	1/1	0.97	0.06	-	136,136,136,136	0
23	K	A	1705	1/1	0.96	0.60	-	157,157,157,157	0
22	MG	A	1624	1/1	0.98	0.07	-	71,71,71,71	0
22	MG	A	1711	1/1	0.88	0.34	-	122,122,122,122	0
22	MG	A	1612	1/1	0.96	0.30	-	66,66,66,66	0
23	K	A	1700	1/1	0.89	0.35	-	130,130,130,130	0
22	MG	A	1716	1/1	0.96	0.16	-	320,320,320,320	0
22	MG	A	1663	1/1	0.91	0.13	-	107,107,107,107	0
23	K	A	1703	1/1	0.96	0.46	-	166,166,166,166	0
22	MG	A	1610	1/1	0.88	1.12	-	62,62,62,62	0
22	MG	A	1625	1/1	0.94	0.47	-	65,65,65,65	0
22	MG	A	1710	1/1	0.86	0.30	-	71,71,71,71	0
22	MG	E	201	1/1	0.93	0.06	-	301,301,301,301	0
22	MG	A	1645	1/1	0.76	0.24	-	135,135,135,135	0
22	MG	A	1658	1/1	0.93	0.58	-	70,70,70,70	0
22	MG	A	1619	1/1	0.93	0.57	-	79,79,79,79	0
22	MG	A	1656	1/1	0.78	0.51	-	66,66,66,66	0
22	MG	A	1675	1/1	0.94	0.18	-	91,91,91,91	0
22	MG	A	1646	1/1	0.79	0.60	-	127,127,127,127	0
22	MG	K	201	1/1	0.87	0.28	-	59,59,59,59	0
22	MG	A	1680	1/1	0.97	0.41	-	88,88,88,88	0
22	MG	A	1605	1/1	0.96	0.34	-	67,67,67,67	0
22	MG	A	1640	1/1	0.72	0.39	-	88,88,88,88	0
22	MG	A	1687	1/1	0.99	0.29	-	89,89,89,89	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
22	MG	A	1652	1/1	0.83	1.10	-	71,71,71,71	0
22	MG	A	1618	1/1	0.91	0.51	-	40,40,40,40	0
22	MG	S	101	1/1	0.75	0.23	-	114,114,114,114	0
22	MG	A	1691	1/1	0.96	0.29	-	81,81,81,81	0
22	MG	A	1708	1/1	0.96	0.09	-	65,65,65,65	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.