



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 9, 2024 – 12:28 pm GMT

PDB ID : 5DM7  
Title : Crystal structure of the 50S ribosomal subunit from *Deinococcus radiodurans* in complex with hygromycin A  
Authors : Kaminishi, T.; Schedlbauer, A.; Ochoa-Lizarralde, B.; Connell, S.R.; Fucini, P.  
Deposited on : 2015-09-08  
Resolution : 3.00 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

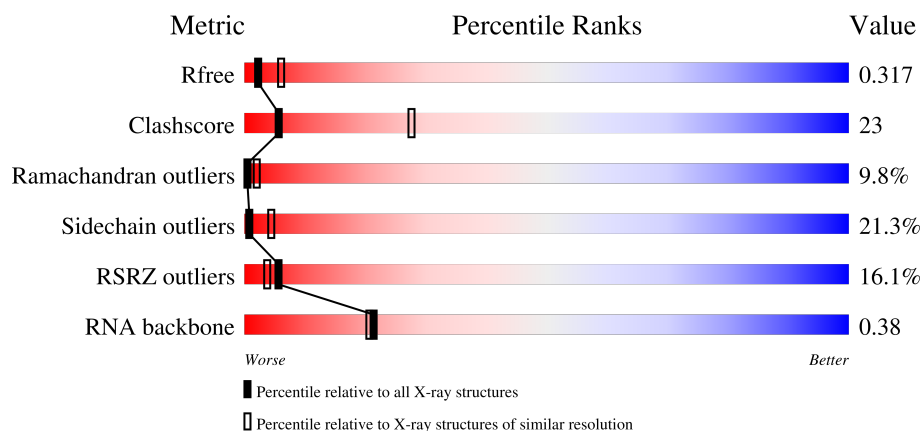
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	2511 (3.00-3.00)
Clashscore	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)
RSRZ outliers	164620	2523 (3.00-3.00)
RNA backbone	3690	1019 (3.20-2.80)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	0	224	
2	A	274	
3	B	205	

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	C	197	
5	D	177	
6	E	171	
7	F	144	
8	G	142	
9	H	134	
10	I	141	
11	J	136	
12	K	113	
13	L	104	
14	M	109	
15	N	117	
16	O	94	
17	P	127	
18	Q	93	
19	R	110	
20	S	175	
21	T	84	
22	U	72	
23	V	66	
24	W	55	
25	Z	57	
26	1	54	
27	2	47	
28	3	65	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	X	2881	
30	Y	122	

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
31	MG	X	6001	-	-	-	X
31	MG	X	6003	-	-	-	X
31	MG	X	6006	-	-	-	X
31	MG	X	6010	-	-	-	X
31	MG	X	6013	-	-	-	X
31	MG	X	6018	-	-	-	X
31	MG	X	6022	-	-	-	X
31	MG	X	6025	-	-	-	X
31	MG	X	6027	-	-	-	X
31	MG	X	6031	-	-	-	X
31	MG	X	6033	-	-	-	X
31	MG	X	6042	-	-	-	X
31	MG	X	6045	-	-	-	X
31	MG	X	6046	-	-	-	X
31	MG	X	6048	-	-	-	X
31	MG	X	6049	-	-	-	X
31	MG	X	6051	-	-	-	X
31	MG	X	6052	-	-	-	X
31	MG	X	6053	-	-	-	X
31	MG	X	6057	-	-	-	X
31	MG	X	6060	-	-	-	X
31	MG	X	6062	-	-	-	X
31	MG	X	6072	-	-	-	X
31	MG	X	6074	-	-	-	X
31	MG	X	6076	-	-	-	X
31	MG	X	6085	-	-	-	X
31	MG	X	6087	-	-	-	X
31	MG	X	6089	-	-	-	X
31	MG	X	6091	-	-	-	X
31	MG	X	6092	-	-	-	X
31	MG	X	6099	-	-	-	X
31	MG	X	6100	-	-	-	X
31	MG	X	6101	-	-	-	X

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	MG	X	6105	-	-	-	X
31	MG	X	6111	-	-	-	X
31	MG	X	6114	-	-	-	X
31	MG	X	6116	-	-	-	X
31	MG	X	6117	-	-	-	X
31	MG	X	6123	-	-	-	X
31	MG	X	6124	-	-	-	X
31	MG	X	6125	-	-	-	X
31	MG	X	6127	-	-	-	X
31	MG	X	6129	-	-	-	X
31	MG	X	6132	-	-	-	X
31	MG	X	6133	-	-	-	X
31	MG	X	6135	-	-	-	X
31	MG	X	6141	-	-	-	X
31	MG	X	6142	-	-	-	X
31	MG	X	6147	-	-	-	X
31	MG	X	6149	-	-	-	X
31	MG	X	6150	-	-	-	X
31	MG	X	6153	-	-	-	X
31	MG	X	6154	-	-	-	X
31	MG	X	6155	-	-	-	X
31	MG	X	6157	-	-	-	X
31	MG	X	6159	-	-	-	X
31	MG	X	6160	-	-	-	X
31	MG	X	6162	-	-	-	X
31	MG	X	6167	-	-	-	X
31	MG	X	6168	-	-	-	X
31	MG	X	6169	-	-	-	X
31	MG	X	6170	-	-	-	X
31	MG	X	6175	-	-	-	X
31	MG	X	6177	-	-	-	X
31	MG	Y	201	-	-	-	X
31	MG	Y	203	-	-	-	X
31	MG	Y	204	-	-	-	X

## 2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 89361 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 protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	224	Total	C	N	O	S	0	0	0
			1651	1031	302	313	5			

- Molecule 2 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	274	Total	C	N	O	S	0	0	0
			2107	1313	423	368	3			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	LYS	ARG	conflict	UNP Q9RXJ9
A	25	ALA	THR	conflict	UNP Q9RXJ9
A	270	LEU	ILE	conflict	UNP Q9RXJ9

- Molecule 3 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	205	Total	C	N	O	S	0	0	0
			1540	965	295	272	8			

- Molecule 4 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	197	Total	C	N	O	S	0	0	0
			1507	935	287	283	2			

- Molecule 5 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	177	Total	C	N	O	S	0	0	0
			1401	892	247	255	7			

- Molecule 6 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	E	171	Total	C	N	O	S	0	0	0
			1287	812	237	237	1			

- Molecule 7 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	F	144	Total	C	N	O	S	0	0	0
			1048	663	183	197	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	2	ARG	LYS	conflict	UNP Q9RSS7
F	3	ARG	LYS	conflict	UNP Q9RSS7

- Molecule 8 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	G	142	Total	C	N	O	S	0	0	0
			1115	704	209	199	3			

- Molecule 9 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	134	Total	C	N	O	S	0	0	0
			997	614	198	180	5			

- Molecule 10 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	I	141	Total	C	N	O	0	0	0
			1068	655	216	197			

- Molecule 11 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	136	Total	C	N	O	S	0	0	0
			1091	696	202	186	7			

- Molecule 12 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	113	Total	C	N	O	S	0	0	0
			879	541	178	158	2			

- Molecule 13 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	L	104	Total	C	N	O	0	0	0
			778	476	159	143			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	26	LYS	ARG	conflict	UNP Q9RSL2

- Molecule 14 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	M	109	Total	C	N	O	0	0	0
			867	540	171	156			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	?	-	LEU	deletion	UNP Q9RWB4
M	?	-	ARG	deletion	UNP Q9RWB4
M	?	-	GLU	deletion	UNP Q9RWB4
M	?	-	LEU	deletion	UNP Q9RWB4

- Molecule 15 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	N	117	Total	C	N	O	S	0	0	0
			978	608	210	159	1			

- Molecule 16 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
16	O	94	Total	C	N	O	0	0	0
			742	465	139	138			

- Molecule 17 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	P	127	Total	C	N	O	S	0	0	0
			1014	639	199	174	2			

- Molecule 18 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Q	93	Total	C	N	O	S	0	0	0
			727	458	136	131	2			

- Molecule 19 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	R	110	Total	C	N	O	S	0	0	0
			826	513	160	152	1			

- Molecule 20 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	S	175	Total	C	N	O	S	0	0	0
			1346	849	236	255	6			

- Molecule 21 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	T	84	Total	C	N	O	S	0	0	0
			626	393	122	110	1			

- Molecule 22 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	U	72	Total	C	N	O	0	0	0
			553	341	116	96			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	67	ILE	LEU	conflict	UNP Q9RRG8

- Molecule 23 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	V	66	Total	C	N	O	S	0	0	0
			534	327	107	97	3			

- Molecule 24 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	W	55	Total	C	N	O	S	0	0	0
			424	264	82	76	2			

- Molecule 25 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Z	57	Total	C	N	O	S	0	0	0
			453	278	93	77	5			

- Molecule 26 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	1	54	Total	C	N	O	S	0	0	0
			404	256	73	74	1			

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	0	ALA	-	insertion	UNP Q9RSS4
1	1	ALA	-	insertion	UNP Q9RSS4
1	3	GLY	LYS	conflict	UNP Q9RSS4
1	4	ALA	ASP	conflict	UNP Q9RSS4
1	5	ALA	GLY	conflict	UNP Q9RSS4
1	45	ALA	LYS	conflict	UNP Q9RSS4
1	46	HIS	LYS	conflict	UNP Q9RSS4
1	47	VAL	HIS	conflict	UNP Q9RSS4
1	49	PHE	VAL	conflict	UNP Q9RSS4
1	50	ALA	PHE	conflict	UNP Q9RSS4
1	51	ALA	-	insertion	UNP Q9RSS4
1	52	ALA	-	insertion	UNP Q9RSS4
1	53	ALA	-	insertion	UNP Q9RSS4

- Molecule 27 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	2	47	Total	C	N	O	S	0	0	0
			393	235	92	64	2			

- Molecule 28 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	3	65	Total	C	N	O	S	0	0	0
			509	320	104	80	5			

- Molecule 29 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	X	2780	Total	C	N	O	P	0	0	0
			59673	26617	11011	19265	2780			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	1526	U	UNK	conflict	GB 11612676

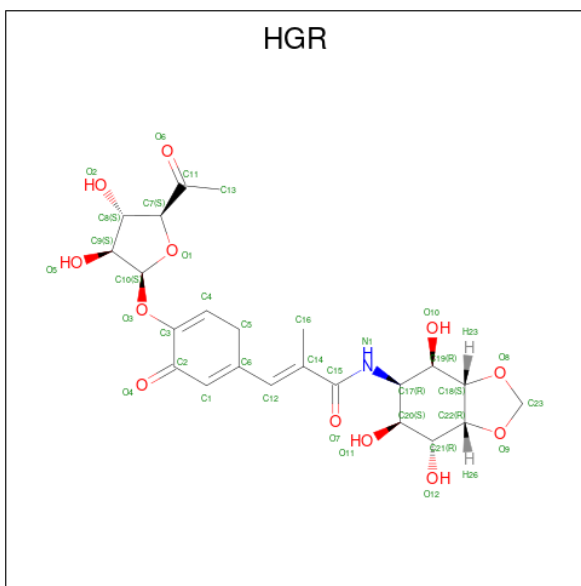
- Molecule 30 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	Y	122	Total	C	N	O	P	0	0	0
			2601	1161	476	842	122			

- Molecule 31 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
31	A	1	Total	Mg	0	0
			1	1		
31	H	1	Total	Mg	0	0
			1	1		
31	M	1	Total	Mg	0	0
			1	1		
31	N	1	Total	Mg	0	0
			1	1		
31	X	177	Total	Mg	0	0
			177	177		
31	Y	5	Total	Mg	0	0
			5	5		

- Molecule 32 is Hygromycin A (three-letter code: HGR) (formula:  $C_{23}H_{29}NO_{12}$ ).

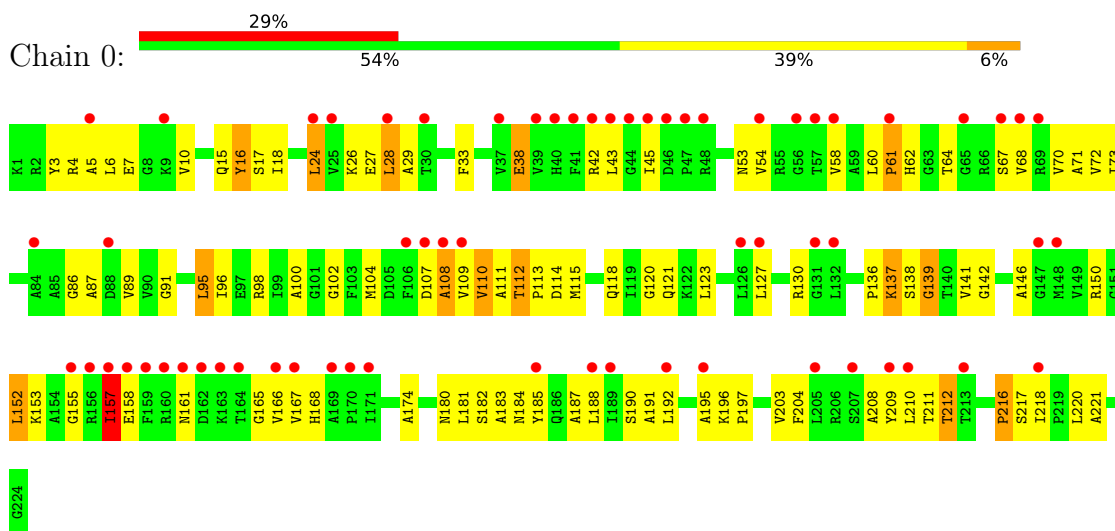


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	X	1	Total	C	N	O	0	0
			36	23	1	12		

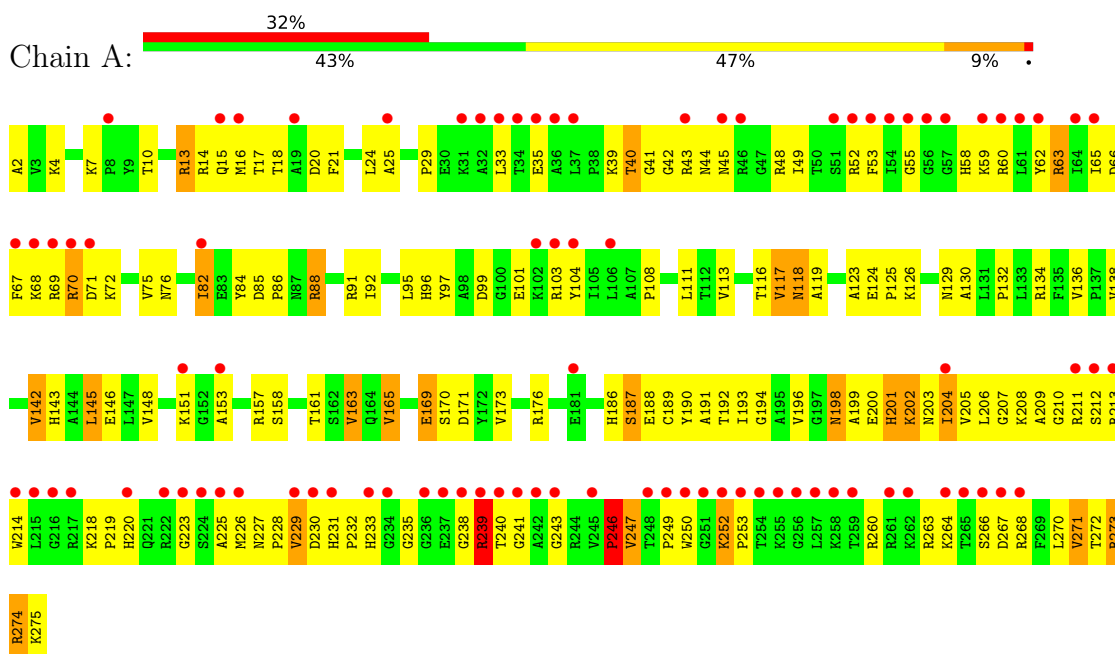
### 3 Residue-property plots [i](#)

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

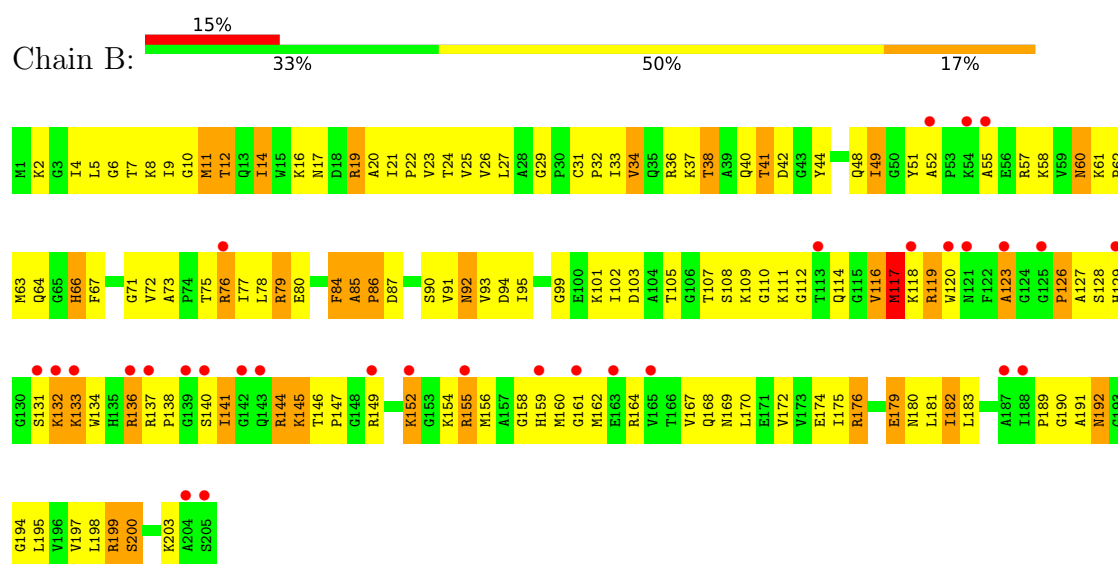
#### • Molecule 1: 50S ribosomal protein L1



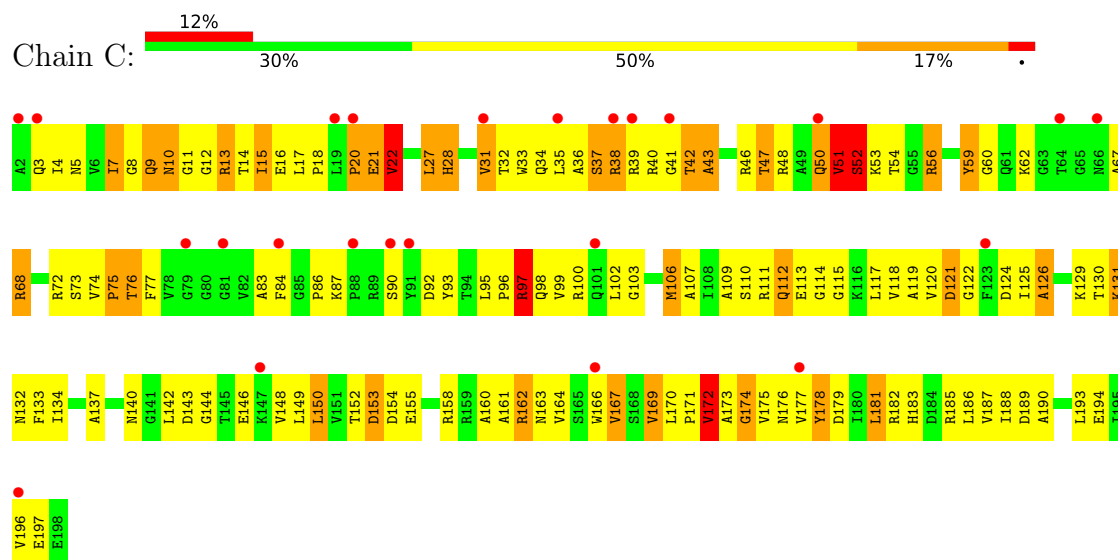
#### • Molecule 2: 50S ribosomal protein L2



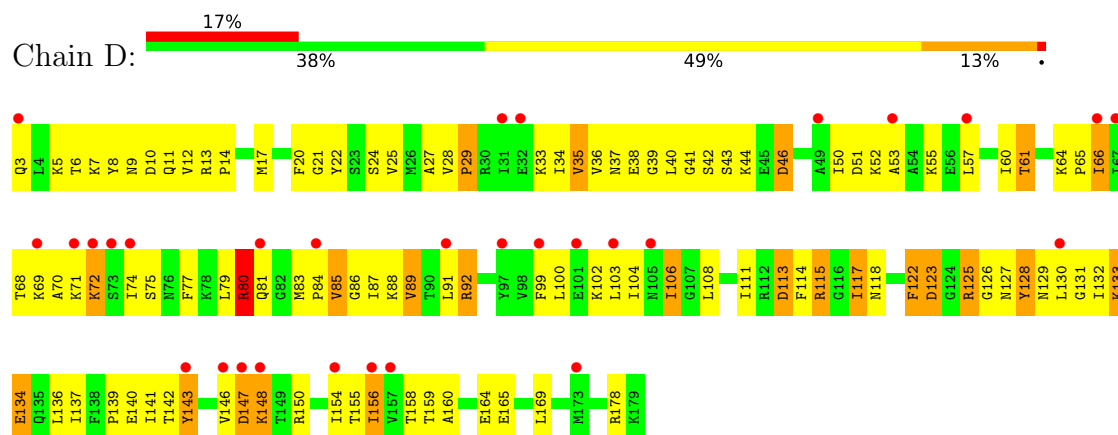
#### • Molecule 3: 50S ribosomal protein L3



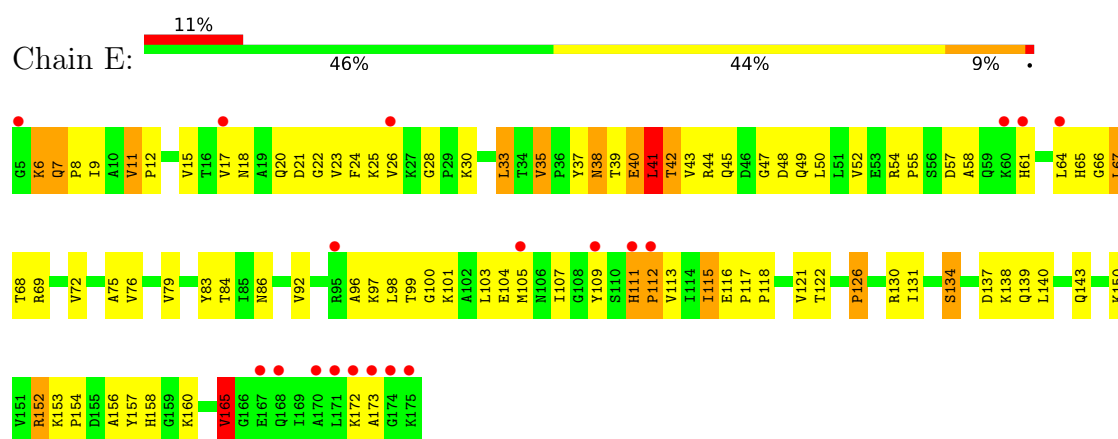
• Molecule 4: 50S ribosomal protein L4



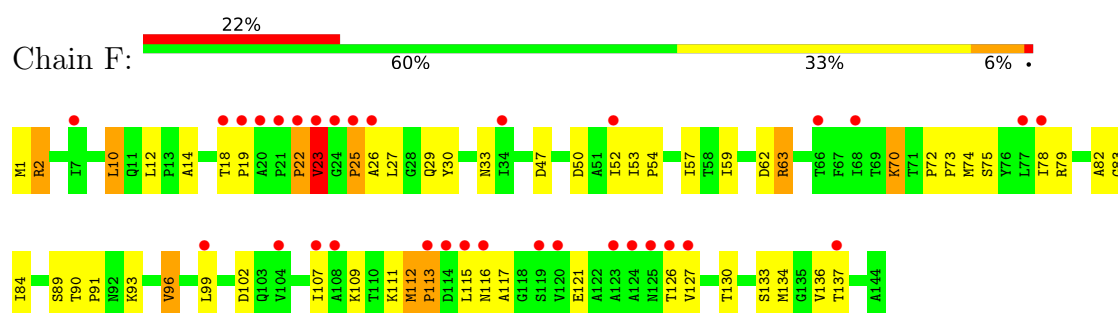
• Molecule 5: 50S ribosomal protein L5



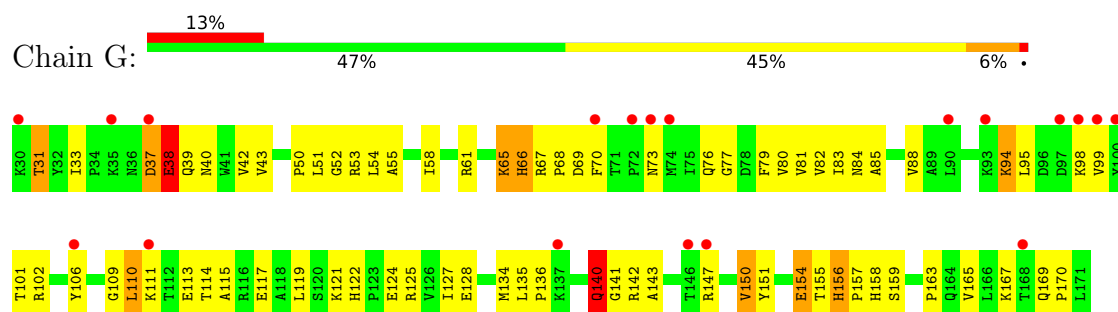
• Molecule 6: 50S ribosomal protein L6



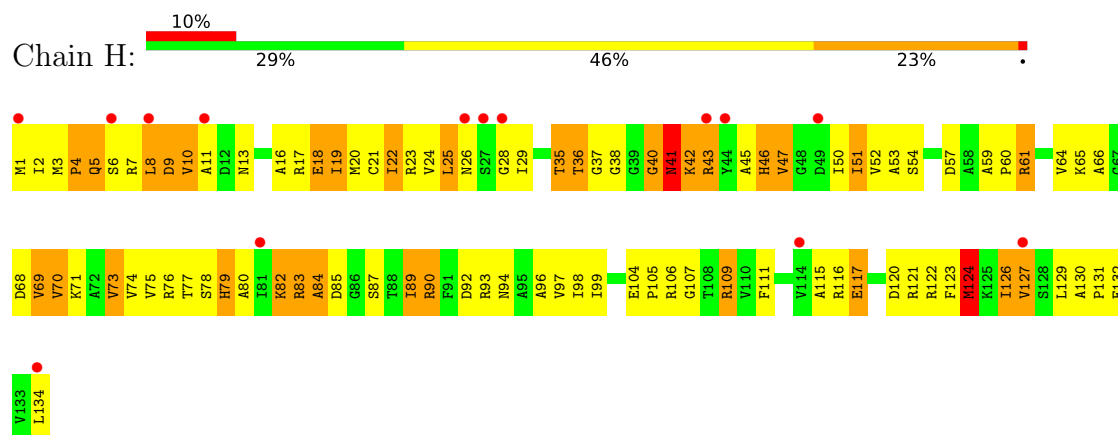
- Molecule 7: 50S ribosomal protein L11



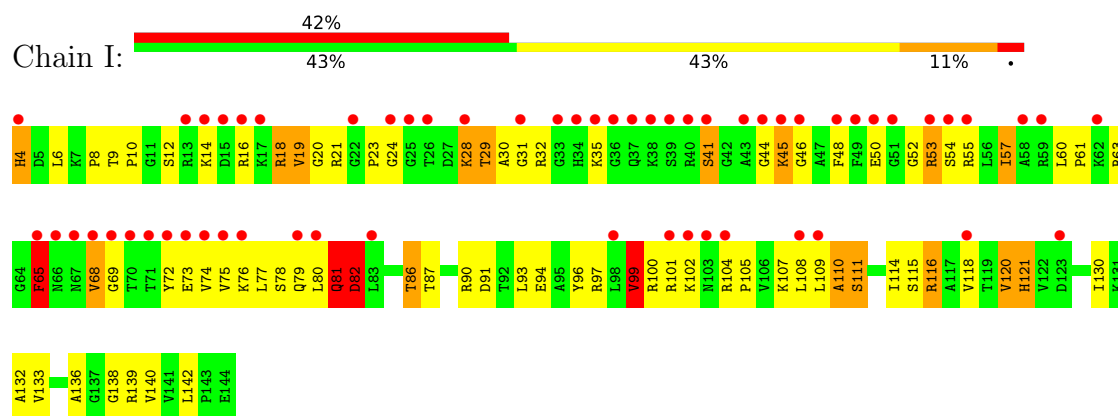
- Molecule 8: 50S ribosomal protein L13



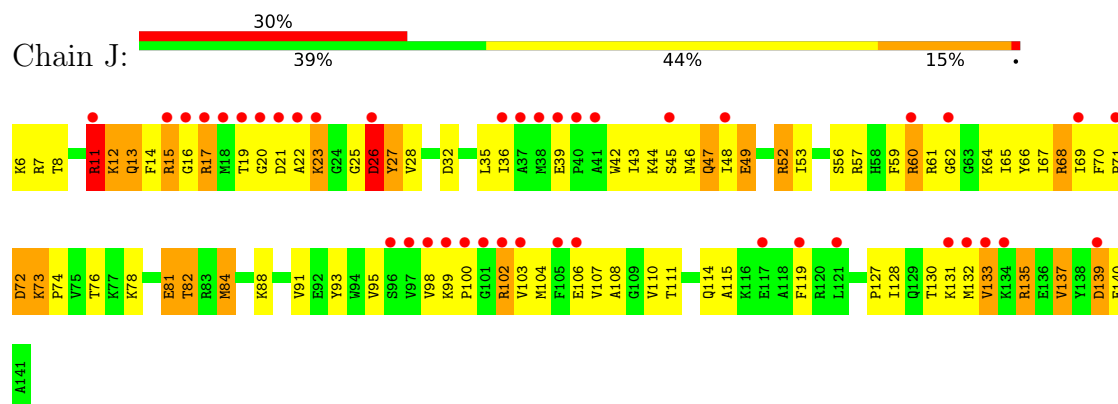
- Molecule 9: 50S ribosomal protein L14



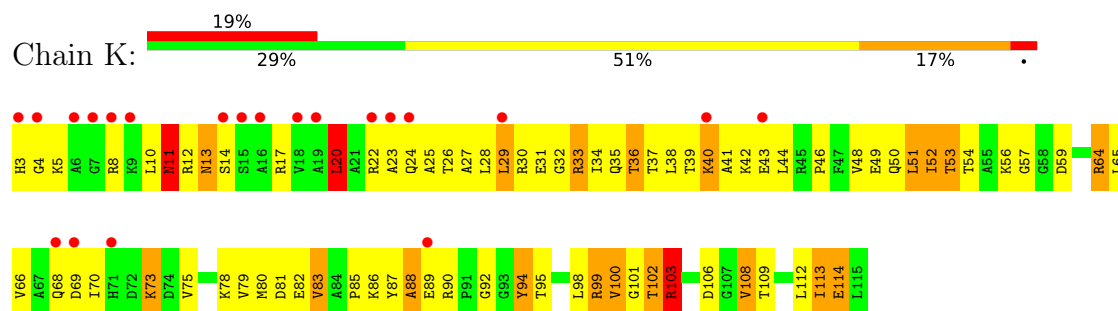
- Molecule 10: 50S ribosomal protein L15



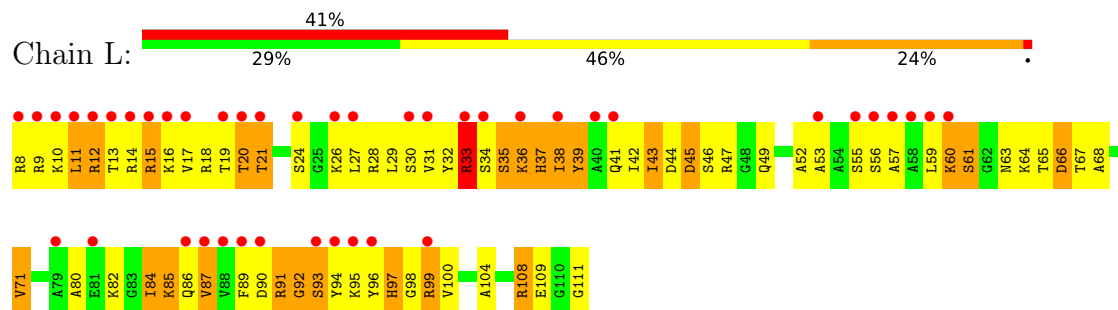
- Molecule 11: 50S ribosomal protein L16



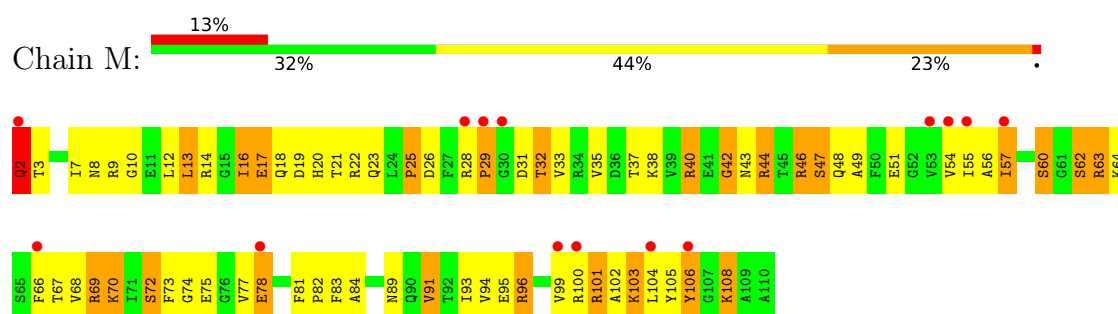
- Molecule 12: 50S ribosomal protein L17



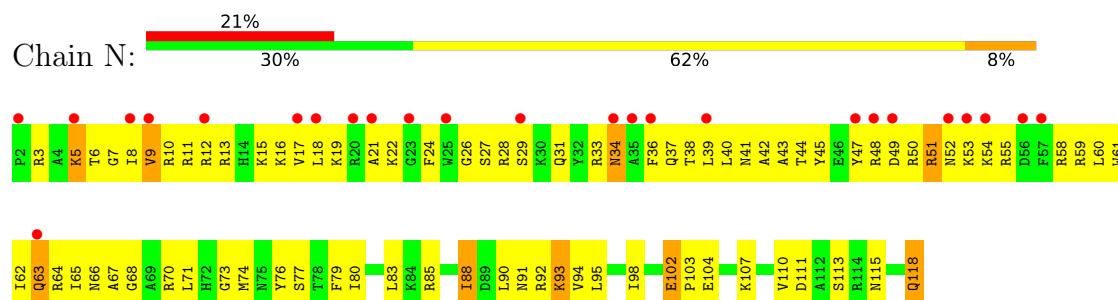
- Molecule 13: 50S ribosomal protein L18



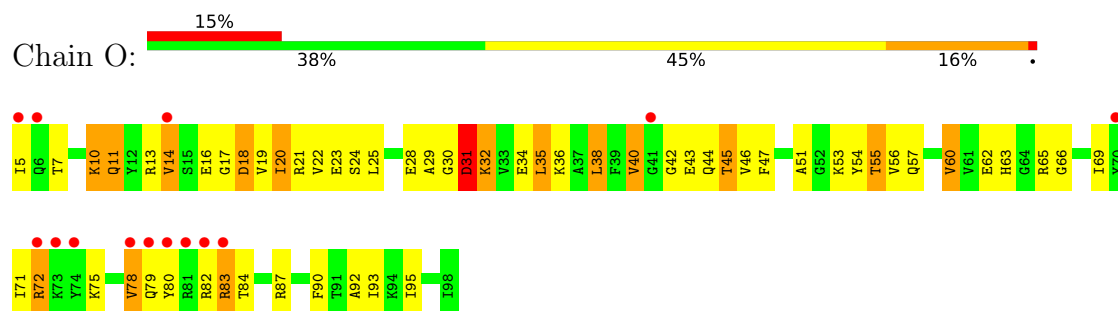
- Molecule 14: 50S ribosomal protein L19



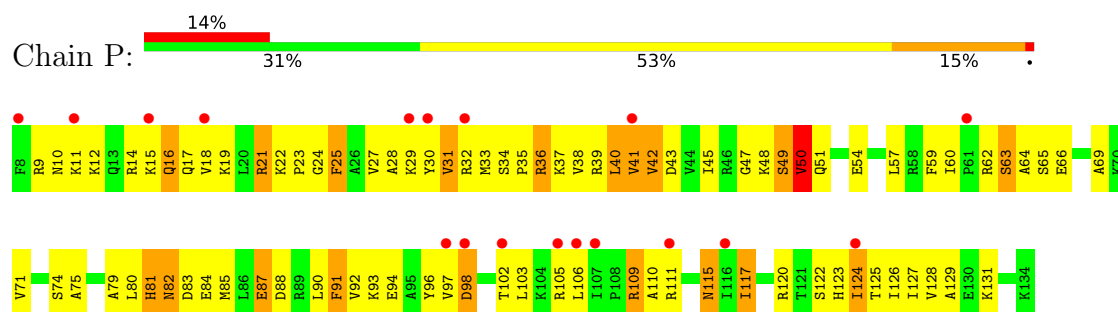
• Molecule 15: 50S ribosomal protein L20



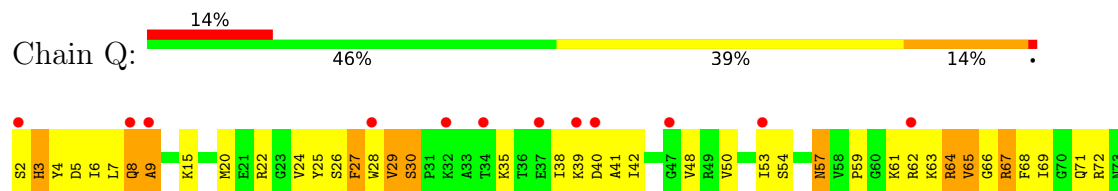
• Molecule 16: 50S ribosomal protein L21

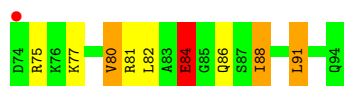


• Molecule 17: 50S ribosomal protein L22

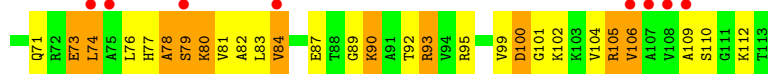
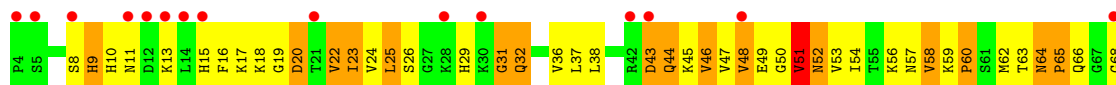


• Molecule 18: 50S ribosomal protein L23

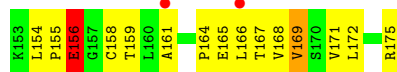
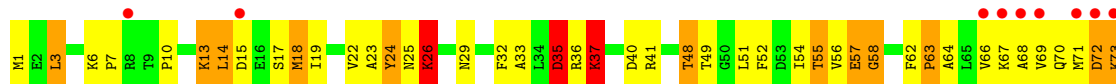




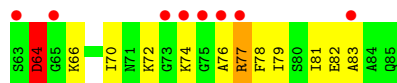
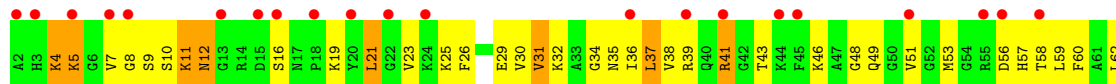
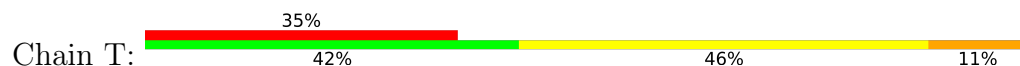
• Molecule 19: 50S ribosomal protein L24



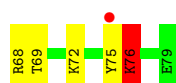
• Molecule 20: 50S ribosomal protein L25



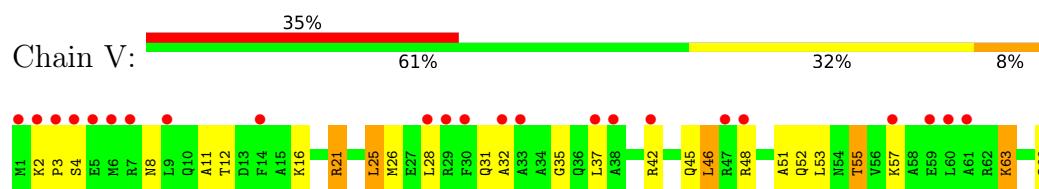
• Molecule 21: 50S ribosomal protein L27



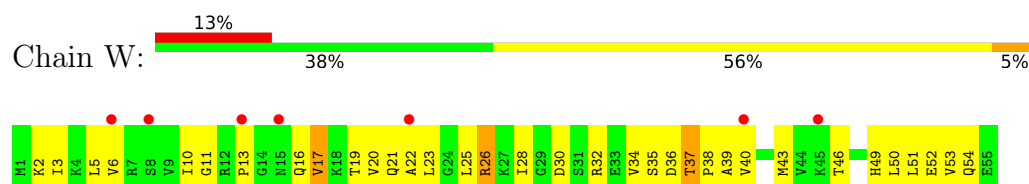
• Molecule 22: 50S ribosomal protein L28



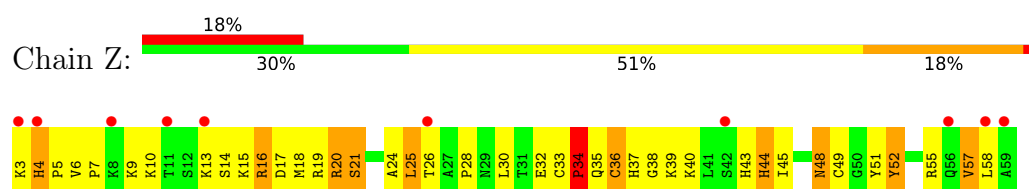
- Molecule 23: 50S ribosomal protein L29



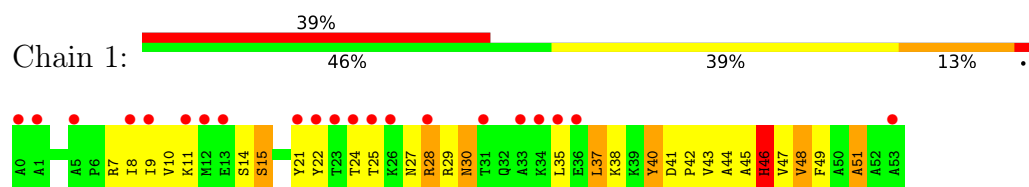
- Molecule 24: 50S ribosomal protein L30



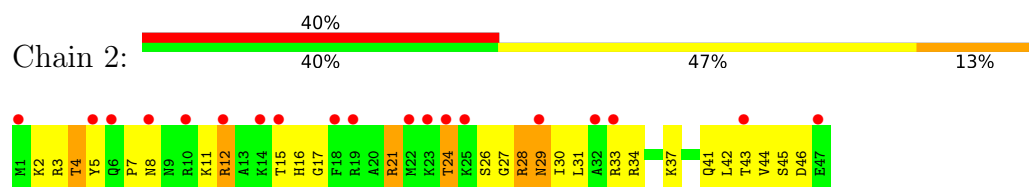
- Molecule 25: 50S ribosomal protein L32



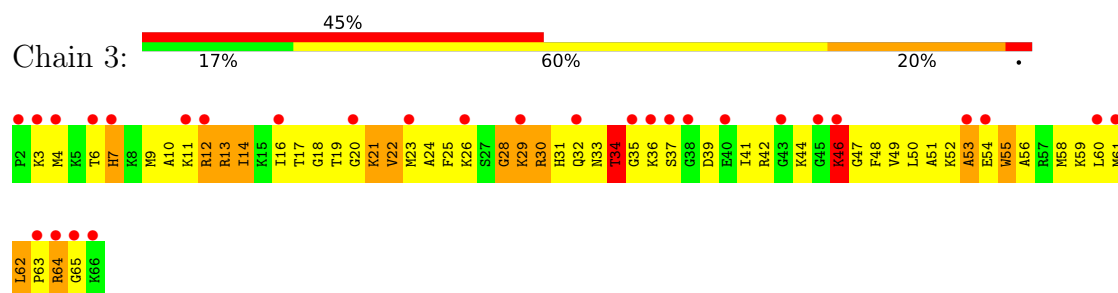
- Molecule 26: 50S ribosomal protein L33



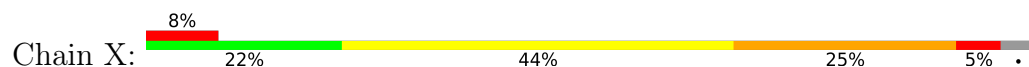
- Molecule 27: 50S ribosomal protein L34



- Molecule 28: 50S ribosomal protein L35



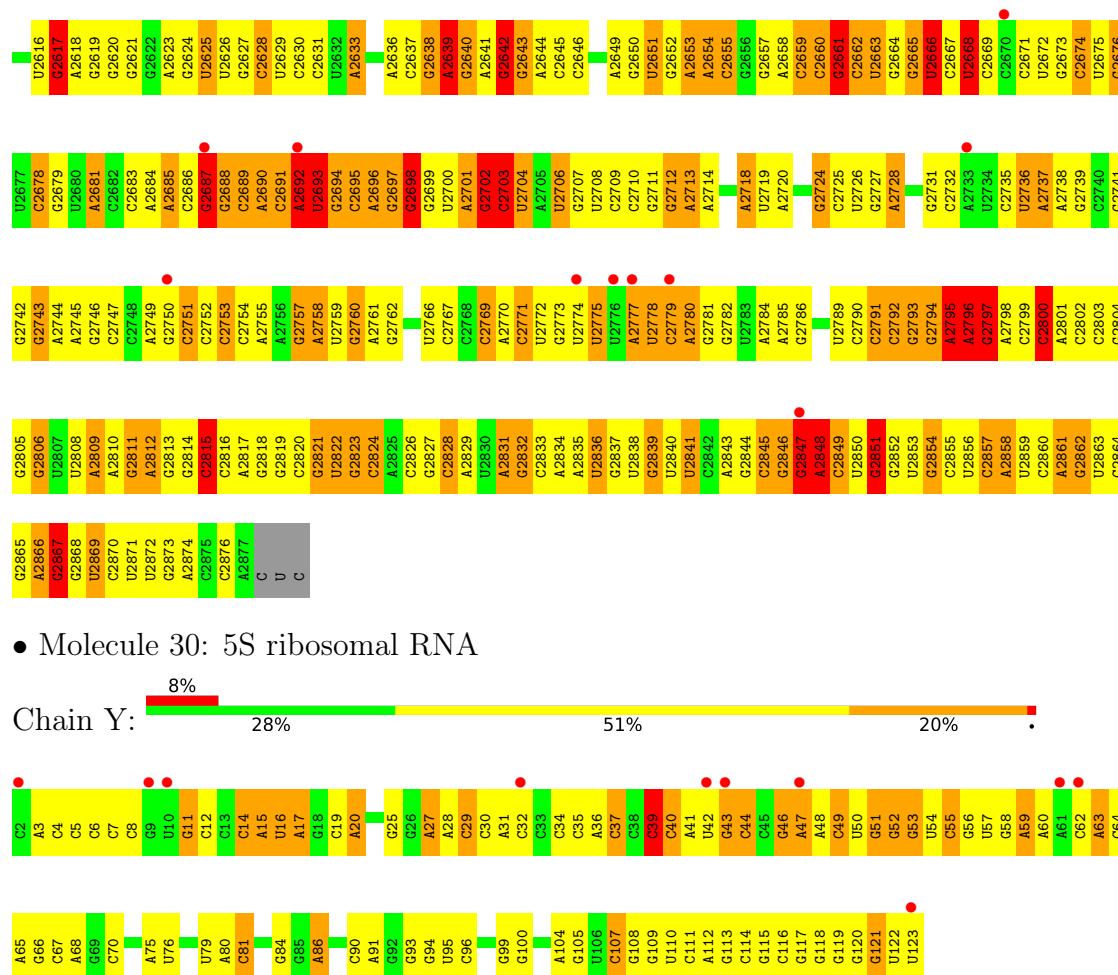
- Molecule 29: 23S ribosomal RNA











## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	169.82Å 411.54Å 695.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.02 – 3.00 57.02 – 3.00	Depositor EDS
% Data completeness (in resolution range)	91.9 (57.02-3.00) 76.2 (57.02-3.00)	Depositor EDS
$R_{merge}$	0.21	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.27 (at 3.01Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.284 , 0.326 0.272 , 0.317	Depositor DCC
$R_{free}$ test set	22814 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	67.3	Xtriage
Anisotropy	0.451	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.20 , 38.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	89361	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	142.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	O	0.25	0/1674	0.46	0/2257
2	A	0.40	0/2149	0.62	0/2890
3	B	0.66	0/1568	0.92	2/2105 (0.1%)
4	C	0.50	0/1530	0.75	0/2070
5	D	0.36	0/1420	0.59	0/1903
6	E	0.39	0/1309	0.61	0/1771
7	F	0.30	0/1067	0.55	0/1446
8	G	0.47	0/1139	0.74	0/1539
9	H	0.72	0/1007	1.02	1/1352 (0.1%)
10	I	0.49	0/1082	0.78	0/1448
11	J	0.60	0/1114	0.83	1/1486 (0.1%)
12	K	0.81	0/887	1.11	4/1188 (0.3%)
13	L	0.54	0/784	0.79	1/1045 (0.1%)
14	M	0.76	0/880	1.02	3/1179 (0.3%)
15	N	0.65	0/994	0.77	0/1323
16	O	0.54	0/751	0.75	0/1000
17	P	0.75	0/1027	0.93	0/1373
18	Q	0.46	0/738	0.63	0/988
19	R	0.58	0/836	0.87	0/1121
20	S	0.40	0/1371	0.68	0/1862
21	T	0.52	0/634	0.70	0/838
22	U	0.52	0/557	0.88	1/741 (0.1%)
23	V	0.40	0/538	0.58	0/714
24	W	0.51	0/426	0.74	0/568
25	Z	0.67	0/465	0.99	1/622 (0.2%)
26	1	0.47	0/411	0.68	0/554
27	2	0.47	0/397	0.70	0/521
28	3	0.56	0/516	0.75	0/673
29	X	0.79	28/66826 (0.0%)	1.38	1078/104247 (1.0%)
30	Y	0.61	0/2907	1.12	10/4529 (0.2%)
All	All	0.73	28/97004 (0.0%)	1.25	1102/145353 (0.8%)

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
3	B	0	1
9	H	0	1
10	I	0	1
13	L	0	1
14	M	0	2
19	R	0	1
All	All	0	7

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	X	774	A	N3-C4	7.61	1.39	1.34
29	X	774	A	C5-C4	7.18	1.43	1.38
29	X	1682	A	N7-C5	-6.86	1.35	1.39
29	X	1975	G	N7-C5	6.29	1.43	1.39
29	X	2823	G	N9-C8	-6.08	1.33	1.37
29	X	2409	A	N9-C4	5.99	1.41	1.37
29	X	1750	A	N3-C4	-5.93	1.31	1.34
29	X	1686	A	N3-C4	-5.84	1.31	1.34
29	X	1680	U	N1-C2	5.74	1.43	1.38
29	X	2611	A	N9-C4	-5.67	1.34	1.37
29	X	1680	U	C2-N3	5.62	1.41	1.37
29	X	2618	A	N9-C4	5.59	1.41	1.37
29	X	2795	A	N9-C4	5.46	1.41	1.37
29	X	513	A	N3-C4	-5.40	1.31	1.34
29	X	2488	G	C6-N1	-5.35	1.35	1.39
29	X	1681	A	C5-C6	-5.34	1.36	1.41
29	X	1680	U	C2-O2	5.33	1.27	1.22
29	X	1278	A	N7-C5	-5.29	1.36	1.39
29	X	2398	U	C2-N3	5.25	1.41	1.37
29	X	540	G	C5-C4	5.22	1.42	1.38
29	X	2548	G	C6-O6	5.20	1.28	1.24
29	X	2489	C	C4-C5	-5.19	1.38	1.43
29	X	774	A	C6-N1	5.08	1.39	1.35
29	X	1692	C	N1-C6	-5.07	1.34	1.37
29	X	527	C	N1-C2	5.06	1.45	1.40
29	X	1678	G	N7-C5	5.05	1.42	1.39
29	X	1975	G	N9-C4	-5.03	1.33	1.38
29	X	2797	G	N1-C2	-5.02	1.33	1.37

All (1102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	1678	G	C8-N9-C4	14.96	112.38	106.40
29	X	1292	A	C8-N9-C4	14.80	111.72	105.80
29	X	774	A	N1-C6-N6	13.97	126.98	118.60
29	X	1679	U	C5-C6-N1	-13.00	116.20	122.70
29	X	1678	G	N7-C8-N9	-12.95	106.62	113.10
29	X	1724	C	C6-N1-C2	12.83	125.43	120.30
29	X	1681	A	N1-C6-N6	12.46	126.08	118.60
29	X	2704	U	N1-C2-O2	-12.39	114.12	122.80
29	X	497	C	N1-C2-O2	-11.87	111.78	118.90
29	X	2548	G	C5-C6-N1	-11.76	105.62	111.50
29	X	1679	U	C2-N3-C4	-11.74	119.95	127.00
29	X	1647	U	N3-C4-C5	-11.63	107.62	114.60
29	X	527	C	C6-N1-C2	-11.22	115.81	120.30
29	X	774	A	C5-N7-C8	-10.93	98.43	103.90
29	X	1992	G	C8-N9-C4	10.93	110.77	106.40
29	X	2019	C	C6-N1-C2	-10.90	115.94	120.30
29	X	522	G	N1-C6-O6	10.89	126.43	119.90
29	X	2550	C	C6-N1-C2	-10.87	115.95	120.30
29	X	1973	C	C6-N1-C2	-10.77	115.99	120.30
29	X	774	A	N7-C8-N9	10.66	119.13	113.80
29	X	2857	C	C6-N1-C2	-10.49	116.11	120.30
29	X	774	A	C4-C5-N7	10.39	115.90	110.70
29	X	1702	C	C6-N1-C2	10.38	124.45	120.30
29	X	661	C	C6-N1-C2	-9.98	116.31	120.30
29	X	1647	U	C6-N1-C2	-9.93	115.05	121.00
29	X	563	U	C6-N1-C2	9.90	126.94	121.00
29	X	1670	G	C8-N9-C4	9.90	110.36	106.40
29	X	2845	C	C6-N1-C2	-9.87	116.35	120.30
29	X	1681	A	C5-C6-N6	-9.84	115.83	123.70
29	X	2624	G	C8-N9-C4	-9.75	102.50	106.40
29	X	957	G	N1-C6-O6	-9.67	114.10	119.90
29	X	1289	A	C8-N9-C4	9.50	109.60	105.80
29	X	2815	C	C6-N1-C2	9.50	124.10	120.30
29	X	2854	G	C4-C5-N7	9.42	114.57	110.80
29	X	1336	G	C5-C6-O6	-9.36	122.98	128.60
29	X	1681	A	N9-C4-C5	-9.34	102.06	105.80
29	X	2523	G	C8-N9-C4	-9.33	102.67	106.40
29	X	1999	U	C2-N1-C1'	9.31	128.87	117.70
29	X	2523	G	C6-C5-N7	-9.28	124.83	130.40
29	X	1678	G	C5-N7-C8	9.26	108.93	104.30
29	X	2541	U	N3-C2-O2	-9.21	115.75	122.20
29	X	2867	G	N3-C4-C5	9.19	133.19	128.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	1682	A	C8-N9-C4	-9.14	102.14	105.80
29	X	2655	C	C6-N1-C2	9.13	123.95	120.30
29	X	955	G	C6-C5-N7	-9.12	124.92	130.40
29	X	2049	C	C6-N1-C2	-9.09	116.66	120.30
29	X	2369	U	C5-C6-N1	9.08	127.24	122.70
29	X	1313	U	C2-N1-C1'	-9.01	106.89	117.70
29	X	1681	A	C6-C5-N7	-9.01	126.00	132.30
29	X	1775	A	C8-N9-C4	9.00	109.40	105.80
29	X	2478	C	C6-N1-C2	-8.98	116.71	120.30
29	X	2594	U	N1-C2-N3	-8.97	109.52	114.90
29	X	2822	U	N3-C4-O4	8.97	125.68	119.40
29	X	1756	C	C6-N1-C2	8.94	123.87	120.30
29	X	2662	C	C6-N1-C2	-8.93	116.73	120.30
29	X	774	A	C6-C5-N7	-8.93	126.05	132.30
29	X	1163	C	C6-N1-C2	-8.90	116.74	120.30
29	X	2554	C	C6-N1-C2	-8.90	116.74	120.30
29	X	2038	C	C6-N1-C2	-8.86	116.76	120.30
29	X	2590	U	C2-N1-C1'	8.82	128.28	117.70
29	X	1933	G	C8-N9-C4	-8.81	102.87	106.40
29	X	1715	A	N1-C6-N6	8.78	123.87	118.60
29	X	1335	A	C8-N9-C4	8.74	109.30	105.80
29	X	497	C	N3-C2-O2	8.73	128.01	121.90
29	X	1992	G	N7-C8-N9	-8.73	108.74	113.10
29	X	579	G	C8-N9-C4	-8.71	102.92	106.40
29	X	1244	U	C5-C6-N1	8.67	127.04	122.70
29	X	2695	C	C6-N1-C2	-8.66	116.83	120.30
29	X	2522	G	N3-C4-C5	-8.65	124.27	128.60
29	X	2576	G	N1-C6-O6	8.65	125.09	119.90
29	X	1339	U	N3-C4-O4	8.64	125.45	119.40
29	X	2523	G	N7-C8-N9	8.61	117.41	113.10
29	X	1155	G	C8-N9-C4	8.57	109.83	106.40
29	X	1336	G	C4-C5-N7	8.56	114.22	110.80
29	X	1292	A	N7-C8-N9	-8.53	109.53	113.80
29	X	2433	G	N1-C6-O6	-8.53	114.78	119.90
29	X	1725	C	C6-N1-C2	-8.53	116.89	120.30
29	X	563	U	C5-C6-N1	-8.53	118.44	122.70
29	X	754	G	C4-C5-N7	8.51	114.20	110.80
29	X	1678	G	C4-C5-N7	-8.51	107.40	110.80
29	X	2596	C	C6-N1-C2	8.51	123.70	120.30
29	X	2495	G	N3-C4-C5	-8.49	124.35	128.60
29	X	1975	G	N3-C4-N9	-8.49	120.91	126.00
29	X	2523	G	N3-C4-C5	-8.49	124.36	128.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	1681	A	C4-C5-N7	8.47	114.94	110.70
29	X	1973	C	C5-C6-N1	8.45	125.22	121.00
29	X	527	C	N3-C2-O2	-8.43	116.00	121.90
29	X	1679	U	N1-C2-N3	8.43	119.96	114.90
29	X	1678	G	C6-C5-N7	8.41	135.44	130.40
29	X	1339	U	C5-C6-N1	8.40	126.90	122.70
29	X	206	U	N1-C2-O2	8.39	128.68	122.80
29	X	1634	A	N1-C6-N6	-8.39	113.56	118.60
29	X	1340	C	C6-N1-C2	-8.36	116.96	120.30
29	X	1704	G	C4-C5-N7	8.35	114.14	110.80
29	X	496	C	C6-N1-C2	8.34	123.63	120.30
29	X	2033	C	N3-C2-O2	-8.31	116.08	121.90
29	X	2240	C	C6-N1-C2	-8.28	116.99	120.30
30	Y	32	C	C6-N1-C2	-8.23	117.01	120.30
29	X	1244	U	C6-N1-C2	-8.20	116.08	121.00
30	Y	81	C	C6-N1-C2	-8.16	117.04	120.30
29	X	16	G	C8-N9-C4	8.15	109.66	106.40
29	X	1751	A	C8-N9-C4	8.11	109.05	105.80
29	X	2718	A	C8-N9-C4	8.11	109.05	105.80
29	X	540	G	C5-C6-N1	-8.11	107.45	111.50
29	X	1339	U	C5-C4-O4	-8.11	121.04	125.90
29	X	2038	C	C5-C6-N1	8.09	125.04	121.00
29	X	1679	U	N3-C4-O4	-8.07	113.75	119.40
29	X	2867	G	N3-C4-N9	-8.06	121.16	126.00
29	X	1312	G	N1-C6-O6	8.03	124.72	119.90
29	X	1683	G	N1-C6-O6	-8.01	115.09	119.90
29	X	1749	G	C8-N9-C4	-7.99	103.20	106.40
29	X	955	G	N7-C8-N9	7.99	117.09	113.10
14	M	3	THR	N-CA-C	-7.94	89.56	111.00
29	X	1636	G	N1-C6-O6	7.94	124.66	119.90
29	X	1333	G	C8-N9-C4	-7.93	103.23	106.40
29	X	1961	A	C8-N9-C4	-7.88	102.65	105.80
29	X	1975	G	N1-C6-O6	-7.84	115.19	119.90
29	X	1313	U	C5-C6-N1	-7.83	118.78	122.70
29	X	1001	A	C8-N9-C4	-7.83	102.67	105.80
29	X	1652	G	C4-C5-N7	7.83	113.93	110.80
29	X	2747	C	C6-N1-C2	7.81	123.42	120.30
29	X	1238	A	N1-C6-N6	-7.80	113.92	118.60
29	X	1696	C	N3-C4-C5	-7.79	118.78	121.90
29	X	1775	A	N9-C4-C5	-7.79	102.69	105.80
29	X	472	C	C6-N1-C2	-7.78	117.19	120.30
29	X	1305	C	C6-N1-C2	7.77	123.41	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	2624	G	N7-C8-N9	7.77	116.98	113.10
29	X	2862	G	N3-C4-C5	-7.77	124.72	128.60
29	X	806	A	C8-N9-C4	7.77	108.91	105.80
29	X	522	G	C6-C5-N7	-7.76	125.74	130.40
29	X	2661	G	C5-C6-O6	-7.75	123.95	128.60
29	X	2698	G	N1-C6-O6	7.74	124.54	119.90
29	X	1704	G	C5-C6-O6	-7.74	123.96	128.60
29	X	1974	U	C6-N1-C2	-7.71	116.37	121.00
9	H	25	LEU	CA-CB-CG	7.70	133.00	115.30
29	X	206	U	C2-N1-C1'	7.70	126.94	117.70
29	X	522	G	C4-C5-N7	7.70	113.88	110.80
29	X	2433	G	C5-C6-O6	7.69	133.21	128.60
29	X	175	C	C2-N1-C1'	7.68	127.25	118.80
29	X	1677	C	N3-C2-O2	-7.66	116.54	121.90
29	X	574	C	C5-C6-N1	7.66	124.83	121.00
29	X	2009	U	C5-C6-N1	7.65	126.52	122.70
12	K	103	ARG	NE-CZ-NH2	-7.62	116.49	120.30
29	X	2704	U	N1-C2-N3	7.62	119.47	114.90
29	X	2369	U	C6-N1-C2	-7.61	116.43	121.00
29	X	2693	U	N3-C2-O2	-7.61	116.87	122.20
29	X	2797	G	N3-C4-N9	7.59	130.55	126.00
29	X	990	A	N1-C6-N6	-7.59	114.05	118.60
29	X	1770	U	C5-C6-N1	-7.58	118.91	122.70
29	X	2495	G	C2-N3-C4	7.55	115.68	111.90
29	X	2854	G	C6-C5-N7	-7.55	125.87	130.40
29	X	955	G	C4-C5-N7	7.54	113.82	110.80
29	X	1480	G	N1-C6-O6	7.54	124.42	119.90
29	X	660	G	N3-C4-N9	-7.54	121.48	126.00
29	X	2839	G	N1-C6-O6	-7.53	115.38	119.90
29	X	2854	G	C5-N7-C8	-7.51	100.54	104.30
29	X	1292	A	N9-C4-C5	-7.51	102.80	105.80
29	X	2799	C	C6-N1-C2	-7.50	117.30	120.30
29	X	1269	G	N1-C6-O6	7.50	124.40	119.90
29	X	1715	A	C5-C6-N6	-7.50	117.70	123.70
29	X	1721	G	C4-N9-C1'	-7.48	116.78	126.50
30	Y	39	C	C2-N1-C1'	7.48	127.03	118.80
29	X	1269	G	C5-C6-O6	-7.47	124.12	128.60
29	X	2623	A	C8-N9-C4	7.44	108.77	105.80
29	X	2815	C	C5-C6-N1	-7.43	117.28	121.00
29	X	774	A	N9-C4-C5	-7.43	102.83	105.80
29	X	1277	G	N1-C6-O6	-7.42	115.44	119.90
29	X	1663	C	C5-C6-N1	7.42	124.71	121.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	2845	C	C5-C6-N1	7.42	124.71	121.00
29	X	527	C	N1-C2-O2	7.39	123.33	118.90
29	X	2522	G	C8-N9-C4	-7.39	103.44	106.40
29	X	501	G	C5-C6-O6	7.37	133.02	128.60
29	X	1963	G	C8-N9-C4	-7.37	103.45	106.40
29	X	1977	C	N3-C4-C5	7.35	124.84	121.90
29	X	1760	G	N7-C8-N9	7.35	116.77	113.10
29	X	2700	U	N3-C2-O2	-7.34	117.06	122.20
29	X	2668	U	C6-N1-C2	7.34	125.41	121.00
29	X	2854	G	C5-C6-O6	-7.34	124.20	128.60
29	X	1776	A	C8-N9-C4	-7.33	102.87	105.80
29	X	2659	C	N3-C4-C5	-7.33	118.97	121.90
29	X	1269	G	C4-C5-N7	7.32	113.73	110.80
29	X	955	G	N1-C6-O6	7.31	124.29	119.90
29	X	1933	G	C2-N3-C4	7.31	115.55	111.90
29	X	1345	G	C4-N9-C1'	7.30	136.00	126.50
29	X	2835	A	N1-C6-N6	7.30	122.98	118.60
29	X	1009	C	C5-C6-N1	-7.30	117.35	121.00
29	X	2523	G	N3-C4-N9	7.27	130.36	126.00
29	X	20	C	C6-N1-C2	-7.26	117.40	120.30
29	X	527	C	C2-N1-C1'	7.24	126.76	118.80
29	X	1714	A	N1-C6-N6	7.24	122.94	118.60
29	X	656	U	N3-C2-O2	-7.22	117.14	122.20
29	X	1270	C	N3-C4-C5	-7.22	119.01	121.90
29	X	2671	C	N3-C4-N4	7.22	123.06	118.00
29	X	206	U	N3-C2-O2	-7.21	117.15	122.20
29	X	661	C	C5-C6-N1	7.21	124.60	121.00
29	X	943	U	C2-N1-C1'	7.20	126.34	117.70
29	X	1336	G	N9-C4-C5	-7.20	102.52	105.40
29	X	538	A	N1-C6-N6	-7.18	114.29	118.60
29	X	1652	G	C5-C6-O6	-7.18	124.29	128.60
29	X	2019	C	C5-C6-N1	7.17	124.58	121.00
29	X	2542	U	N3-C2-O2	-7.15	117.19	122.20
29	X	672	C	C6-N1-C2	7.13	123.15	120.30
29	X	1313	U	C5-C4-O4	7.13	130.18	125.90
29	X	1336	G	N1-C6-O6	7.13	124.18	119.90
29	X	1684	G	N9-C4-C5	7.13	108.25	105.40
29	X	1219	C	N1-C2-O2	7.12	123.17	118.90
29	X	2478	C	C5-C6-N1	7.11	124.56	121.00
29	X	1665	C	C5-C6-N1	-7.09	117.45	121.00
29	X	1341	G	C5-C6-N1	7.09	115.05	111.50
29	X	2688	G	C8-N9-C4	7.07	109.23	106.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	1704	G	N1-C6-O6	7.07	124.14	119.90
29	X	2857	C	N3-C4-C5	-7.07	119.07	121.90
29	X	2523	G	C4-N9-C1'	7.07	135.68	126.50
29	X	1016	C	C2-N1-C1'	7.05	126.56	118.80
29	X	700	C	C6-N1-C2	-7.04	117.48	120.30
29	X	1167	A	C8-N9-C4	7.04	108.62	105.80
29	X	1278	A	C4-C5-C6	7.03	120.52	117.00
29	X	1989	C	C5-C6-N1	7.03	124.52	121.00
29	X	1974	U	N3-C2-O2	-7.03	117.28	122.20
29	X	2314	A	C8-N9-C4	-7.02	102.99	105.80
29	X	754	G	C6-C5-N7	-7.02	126.19	130.40
29	X	2273	C	C6-N1-C2	-7.01	117.49	120.30
29	X	1167	A	N9-C4-C5	-7.01	103.00	105.80
29	X	2749	A	N1-C6-N6	7.00	122.80	118.60
29	X	2662	C	C5-C6-N1	6.99	124.50	121.00
29	X	2535	C	C6-N1-C2	6.99	123.10	120.30
29	X	2398	U	N3-C4-C5	-6.99	110.41	114.60
29	X	1269	G	N9-C4-C5	-6.98	102.61	105.40
29	X	2433	G	C4-C5-N7	-6.98	108.01	110.80
29	X	1770	U	C4-C5-C6	6.97	123.88	119.70
29	X	1647	U	C4-C5-C6	6.96	123.88	119.70
29	X	1647	U	N1-C2-N3	6.95	119.07	114.90
29	X	2854	G	N9-C4-C5	-6.95	102.62	105.40
29	X	2500	C	C6-N1-C2	-6.94	117.52	120.30
29	X	2597	G	N3-C4-N9	6.93	130.16	126.00
29	X	1270	C	C6-N1-C2	-6.92	117.53	120.30
29	X	1636	G	C8-N9-C4	6.92	109.17	106.40
29	X	1474	A	C8-N9-C4	-6.92	103.03	105.80
29	X	466	A	N1-C6-N6	-6.92	114.45	118.60
29	X	989	G	C8-N9-C4	6.92	109.17	106.40
29	X	1704	G	C6-C5-N7	-6.90	126.26	130.40
29	X	2862	G	N3-C4-N9	6.90	130.14	126.00
29	X	2555	G	C8-N9-C4	6.90	109.16	106.40
29	X	985	G	C8-N9-C4	-6.89	103.64	106.40
29	X	2867	G	C2-N3-C4	-6.89	108.45	111.90
29	X	1033	G	N3-C4-C5	-6.89	125.16	128.60
29	X	943	U	N1-C2-O2	6.88	127.61	122.80
29	X	1941	C	C6-N1-C2	6.88	123.05	120.30
29	X	1984	A	N3-C4-C5	6.86	131.60	126.80
29	X	773	G	N3-C4-N9	6.86	130.11	126.00
29	X	22	C	C2-N1-C1'	6.85	126.33	118.80
29	X	1312	G	C5-C6-O6	-6.85	124.49	128.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	Y	39	C	C6-N1-C1'	-6.85	112.58	120.80
29	X	700	C	C5-C6-N1	6.83	124.41	121.00
29	X	591	G	C8-N9-C4	6.82	109.13	106.40
29	X	2422	C	C6-N1-C2	-6.81	117.58	120.30
29	X	2028	C	C5-C4-N4	-6.81	115.44	120.20
29	X	501	G	N1-C6-O6	-6.80	115.82	119.90
29	X	2702	G	N3-C4-C5	-6.79	125.21	128.60
29	X	1343	C	N3-C4-N4	6.78	122.75	118.00
29	X	1974	U	C5-C4-O4	6.78	129.97	125.90
29	X	2592	U	N1-C2-O2	-6.78	118.05	122.80
29	X	774	A	C5-C6-N6	-6.78	118.28	123.70
29	X	2023	C	C6-N1-C2	6.77	123.01	120.30
29	X	2037	A	C8-N9-C4	-6.76	103.09	105.80
29	X	615	C	N3-C2-O2	-6.76	117.17	121.90
29	X	1343	C	C5-C4-N4	-6.76	115.47	120.20
29	X	2800	C	N1-C2-O2	6.75	122.95	118.90
29	X	1016	C	C5-C6-N1	6.74	124.37	121.00
29	X	1652	G	N9-C4-C5	-6.74	102.70	105.40
29	X	522	G	N9-C4-C5	-6.74	102.70	105.40
29	X	1305	C	C5-C6-N1	-6.74	117.63	121.00
29	X	2624	G	C4-N9-C1'	6.74	135.26	126.50
29	X	2465	G	C8-N9-C4	-6.73	103.71	106.40
29	X	1975	G	C6-C5-N7	6.72	134.43	130.40
29	X	1696	C	C6-N1-C2	-6.72	117.61	120.30
29	X	2421	C	C6-N1-C2	-6.72	117.61	120.30
29	X	2552	C	C6-N1-C2	-6.72	117.61	120.30
29	X	1347	C	C6-N1-C2	-6.71	117.61	120.30
29	X	1279	G	N3-C2-N2	6.71	124.60	119.90
29	X	1950	C	C6-N1-C2	-6.71	117.62	120.30
29	X	2704	U	C5-C6-N1	-6.70	119.35	122.70
29	X	2572	U	C6-N1-C2	-6.69	116.99	121.00
29	X	2573	C	C6-N1-C2	-6.69	117.62	120.30
29	X	2662	C	N3-C4-C5	-6.68	119.23	121.90
29	X	2523	G	C4-C5-C6	6.68	122.81	118.80
29	X	2851	G	C8-N9-C4	6.68	109.07	106.40
29	X	519	C	N3-C4-C5	-6.67	119.23	121.90
29	X	522	G	C5-N7-C8	-6.66	100.97	104.30
29	X	968	C	C5-C6-N1	6.66	124.33	121.00
29	X	2586	G	C6-C5-N7	-6.66	126.40	130.40
29	X	2597	G	C8-N9-C1'	-6.66	118.34	127.00
29	X	1326	U	N3-C2-O2	-6.66	117.54	122.20
29	X	2548	G	C4-C5-C6	6.64	122.79	118.80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	1634	A	C5-C6-N6	6.64	129.01	123.70
29	X	576	A	N1-C6-N6	-6.64	114.62	118.60
29	X	1039	A	C8-N9-C4	-6.64	103.14	105.80
29	X	1995	G	N3-C4-N9	6.64	129.98	126.00
25	Z	16	ARG	NE-CZ-NH2	-6.63	116.98	120.30
29	X	1474	A	N1-C6-N6	-6.63	114.62	118.60
29	X	1686	A	C8-N9-C4	-6.63	103.15	105.80
29	X	787	A	N1-C6-N6	6.63	122.58	118.60
29	X	2524	G	C5-C6-N1	6.62	114.81	111.50
29	X	2870	C	C6-N1-C2	-6.62	117.65	120.30
29	X	22	C	N3-C2-O2	-6.61	117.27	121.90
29	X	225	G	N1-C6-O6	6.61	123.87	119.90
29	X	1770	U	N3-C2-O2	-6.61	117.57	122.20
29	X	689	A	N7-C8-N9	6.61	117.10	113.80
29	X	983	G	C8-N9-C4	-6.61	103.76	106.40
29	X	2822	U	C5-C4-O4	-6.60	121.94	125.90
29	X	957	G	N3-C4-C5	-6.59	125.30	128.60
29	X	1289	A	N7-C8-N9	-6.59	110.50	113.80
29	X	1975	G	C4-C5-C6	-6.59	114.84	118.80
29	X	1683	G	C5-C6-O6	6.58	132.55	128.60
29	X	2854	G	N1-C6-O6	6.58	123.85	119.90
29	X	2398	U	C6-N1-C2	-6.58	117.05	121.00
29	X	430	C	C6-N1-C2	-6.58	117.67	120.30
29	X	2687	G	C8-N9-C4	6.57	109.03	106.40
29	X	2598	C	C6-N1-C2	-6.57	117.67	120.30
29	X	955	G	C5-N7-C8	-6.57	101.02	104.30
29	X	2479	U	C5-C6-N1	6.57	125.98	122.70
29	X	526	C	N3-C2-O2	-6.56	117.31	121.90
29	X	2554	C	N3-C4-N4	6.56	122.59	118.00
29	X	2576	G	C6-C5-N7	-6.56	126.47	130.40
29	X	1744	G	N3-C4-C5	-6.56	125.32	128.60
29	X	2821	G	C8-N9-C4	6.55	109.02	106.40
29	X	1016	C	C6-N1-C2	-6.55	117.68	120.30
29	X	1207	G	N1-C6-O6	6.55	123.83	119.90
29	X	2757	G	N9-C4-C5	-6.55	102.78	105.40
29	X	1212	U	C5-C6-N1	-6.54	119.43	122.70
29	X	124	A	C8-N9-C4	-6.54	103.19	105.80
29	X	1636	G	N9-C4-C5	-6.53	102.79	105.40
29	X	2867	G	C4-N9-C1'	-6.53	118.02	126.50
29	X	2698	G	C5-C6-O6	-6.53	124.69	128.60
14	M	42	GLY	N-CA-C	-6.52	96.79	113.10
29	X	2060	A	C8-N9-C4	-6.51	103.19	105.80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	2659	C	C6-N1-C2	-6.51	117.70	120.30
29	X	2697	G	C8-N9-C4	-6.51	103.80	106.40
29	X	497	C	N3-C4-N4	6.50	122.55	118.00
29	X	1760	G	C8-N9-C4	-6.50	103.80	106.40
29	X	1652	G	N1-C6-O6	6.50	123.80	119.90
29	X	2548	G	N1-C6-O6	6.50	123.80	119.90
29	X	2039	G	C8-N9-C4	-6.50	103.80	106.40
29	X	557	U	N3-C2-O2	-6.50	117.65	122.20
29	X	2488	G	C5-C6-N1	6.50	114.75	111.50
29	X	2279	G	N1-C6-O6	6.49	123.80	119.90
29	X	1142	G	N9-C4-C5	-6.48	102.81	105.40
29	X	1721	G	N3-C4-C5	6.48	131.84	128.60
29	X	2704	U	C2-N1-C1'	-6.48	109.92	117.70
29	X	2828	C	C6-N1-C2	-6.48	117.71	120.30
29	X	576	A	N9-C4-C5	6.48	108.39	105.80
29	X	493	A	C8-N9-C4	6.47	108.39	105.80
29	X	1661	C	N3-C2-O2	-6.47	117.37	121.90
29	X	2481	G	N3-C4-C5	-6.46	125.37	128.60
29	X	2696	A	C8-N9-C4	-6.46	103.21	105.80
29	X	2712	G	N1-C2-N2	-6.46	110.38	116.20
29	X	225	G	C4-C5-N7	6.46	113.38	110.80
14	M	35	VAL	CB-CA-C	-6.46	99.13	111.40
29	X	991	A	C8-N9-C4	-6.46	103.22	105.80
29	X	2666	U	N1-C2-O2	-6.45	118.28	122.80
29	X	1656	U	C6-N1-C2	6.44	124.86	121.00
29	X	1647	U	C5-C4-O4	6.43	129.76	125.90
29	X	646	C	C6-N1-C2	-6.42	117.73	120.30
29	X	2419	C	N1-C2-O2	-6.41	115.05	118.90
29	X	2383	C	C6-N1-C2	-6.41	117.74	120.30
29	X	1667	A	C8-N9-C4	6.40	108.36	105.80
29	X	2703	C	N1-C2-O2	-6.40	115.06	118.90
29	X	2538	C	C5-C6-N1	6.39	124.20	121.00
3	B	179	GLU	N-CA-C	-6.39	93.75	111.00
29	X	522	G	C2-N3-C4	-6.38	108.71	111.90
29	X	1333	G	N1-C6-O6	-6.38	116.07	119.90
29	X	1964	A	C8-N9-C4	-6.37	103.25	105.80
29	X	2587	G	C8-N9-C4	-6.37	103.85	106.40
29	X	2240	C	C5-C6-N1	6.37	124.18	121.00
29	X	660	G	N3-C4-C5	6.37	131.78	128.60
29	X	1313	U	C6-N1-C1'	6.37	130.11	121.20
29	X	2617	G	N1-C6-O6	-6.36	116.08	119.90
29	X	968	C	N1-C2-O2	6.35	122.71	118.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	338	G	C8-N9-C4	-6.35	103.86	106.40
29	X	2044	G	N3-C4-C5	-6.33	125.44	128.60
29	X	175	C	C6-N1-C1'	-6.33	113.21	120.80
29	X	2479	U	C6-N1-C2	-6.33	117.20	121.00
29	X	2007	G	C8-N9-C4	6.32	108.93	106.40
29	X	2538	C	C6-N1-C2	-6.31	117.78	120.30
29	X	2757	G	C5-C6-O6	-6.31	124.81	128.60
29	X	2563	U	C2-N1-C1'	6.30	125.26	117.70
29	X	2841	U	N3-C2-O2	-6.30	117.79	122.20
29	X	854	G	C8-N9-C4	-6.30	103.88	106.40
29	X	540	G	C4-C5-N7	-6.30	108.28	110.80
29	X	773	G	N3-C4-C5	-6.29	125.45	128.60
29	X	1457	A	C8-N9-C4	6.29	108.32	105.80
29	X	2554	C	C5-C6-N1	6.28	124.14	121.00
29	X	2623	A	N7-C8-N9	-6.28	110.66	113.80
29	X	1002	C	C6-N1-C2	-6.27	117.79	120.30
29	X	1281	A	C8-N9-C4	6.27	108.31	105.80
29	X	1713	G	N9-C4-C5	6.26	107.91	105.40
29	X	2273	C	C5-C6-N1	6.26	124.13	121.00
29	X	2847	G	N3-C2-N2	-6.26	115.52	119.90
29	X	750	C	C6-N1-C2	-6.26	117.80	120.30
29	X	2867	G	C8-N9-C1'	6.26	135.14	127.00
12	K	103	ARG	NE-CZ-NH1	6.26	123.43	120.30
29	X	2695	C	C5-C6-N1	6.26	124.13	121.00
29	X	2606	G	N1-C6-O6	6.26	123.65	119.90
29	X	774	A	C6-N1-C2	6.25	122.35	118.60
29	X	587	A	N1-C6-N6	-6.25	114.85	118.60
29	X	2797	G	C8-N9-C1'	-6.24	118.89	127.00
29	X	2300	G	C8-N9-C4	-6.24	103.90	106.40
29	X	972	C	C6-N1-C2	-6.24	117.81	120.30
29	X	1999	U	C6-N1-C1'	-6.24	112.47	121.20
29	X	993	C	N1-C2-O2	6.23	122.64	118.90
29	X	1271	C	N3-C2-O2	-6.22	117.54	121.90
29	X	774	A	C2-N3-C4	-6.22	107.49	110.60
29	X	508	G	N1-C6-O6	6.22	123.63	119.90
29	X	2048	C	C6-N1-C2	-6.22	117.81	120.30
29	X	2693	U	N1-C2-N3	6.22	118.63	114.90
29	X	2845	C	N3-C4-N4	6.22	122.35	118.00
29	X	1289	A	N9-C4-C5	-6.21	103.31	105.80
29	X	1465	G	C8-N9-C4	-6.21	103.92	106.40
29	X	1672	A	N1-C6-N6	6.21	122.32	118.60
29	X	2639	A	C2-N3-C4	6.20	113.70	110.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	1981	A	N1-C6-N6	6.20	122.32	118.60
29	X	2637	C	C6-N1-C2	6.20	122.78	120.30
29	X	1142	G	N1-C6-O6	6.20	123.62	119.90
29	X	1339	U	C2-N1-C1'	6.19	125.13	117.70
29	X	2199	C	N1-C2-O2	6.19	122.61	118.90
29	X	219	G	C4-N9-C1'	-6.19	118.45	126.50
29	X	2597	G	C4-N9-C1'	6.19	134.55	126.50
29	X	993	C	N3-C2-O2	-6.18	117.57	121.90
29	X	2858	A	C8-N9-C4	-6.18	103.33	105.80
29	X	334	G	N1-C6-O6	6.18	123.61	119.90
29	X	540	G	C4-N9-C1'	6.18	134.53	126.50
29	X	2797	G	N9-C4-C5	-6.17	102.93	105.40
29	X	2690	A	N1-C2-N3	6.16	132.38	129.30
29	X	2822	U	C5-C6-N1	6.16	125.78	122.70
29	X	880	C	N1-C2-O2	6.15	122.59	118.90
29	X	2590	U	N3-C2-O2	-6.13	117.91	122.20
29	X	579	G	N7-C8-N9	6.13	116.16	113.10
29	X	576	A	C4-C5-N7	-6.13	107.64	110.70
29	X	1208	A	C8-N9-C4	-6.12	103.35	105.80
29	X	1308	C	C2-N1-C1'	6.12	125.53	118.80
29	X	615	C	N1-C2-O2	6.12	122.57	118.90
29	X	2671	C	C6-N1-C2	-6.11	117.86	120.30
29	X	1315	A	C4-C5-N7	-6.11	107.65	110.70
29	X	107	G	C4-N9-C1'	6.11	134.44	126.50
29	X	2383	C	C2-N1-C1'	6.10	125.51	118.80
29	X	2233	C	C6-N1-C2	6.10	122.74	120.30
29	X	528	G	N3-C2-N2	-6.10	115.63	119.90
29	X	713	G	N1-C6-O6	6.10	123.56	119.90
29	X	2628	C	N3-C2-O2	-6.10	117.63	121.90
29	X	774	A	C5-C6-N1	-6.09	114.65	117.70
29	X	2371	A	C8-N9-C4	-6.09	103.36	105.80
29	X	1256	C	C6-N1-C2	6.09	122.73	120.30
29	X	1990	U	N3-C4-C5	-6.09	110.95	114.60
29	X	2662	C	C2-N3-C4	6.09	122.94	119.90
29	X	931	G	N3-C4-N9	6.08	129.65	126.00
29	X	2841	U	N1-C2-O2	6.08	127.05	122.80
29	X	2009	U	C6-N1-C2	-6.08	117.35	121.00
29	X	1744	G	N3-C4-N9	6.08	129.65	126.00
29	X	2240	C	N1-C2-O2	6.08	122.55	118.90
29	X	931	G	N9-C4-C5	-6.07	102.97	105.40
29	X	2015	G	C5-N7-C8	-6.07	101.26	104.30
29	X	2592	U	N3-C2-O2	6.07	126.45	122.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	1984	A	C4-C5-C6	-6.07	113.97	117.00
29	X	2594	U	N3-C4-O4	6.07	123.65	119.40
29	X	1990	U	N3-C4-O4	6.06	123.64	119.40
29	X	20	C	C5-C6-N1	6.06	124.03	121.00
29	X	2561	G	N1-C6-O6	-6.06	116.27	119.90
29	X	688	A	C8-N9-C4	-6.05	103.38	105.80
29	X	1668	G	C4-C5-N7	6.05	113.22	110.80
29	X	2655	C	N3-C4-C5	6.05	124.32	121.90
29	X	319	G	C4-C5-N7	6.05	113.22	110.80
29	X	673	G	C8-N9-C4	6.04	108.82	106.40
29	X	2382	C	C6-N1-C2	-6.04	117.88	120.30
29	X	1775	A	N1-C6-N6	6.03	122.22	118.60
29	X	2828	C	C5-C6-N1	6.03	124.02	121.00
29	X	968	C	C2-N1-C1'	6.03	125.43	118.80
29	X	574	C	C6-N1-C2	-6.03	117.89	120.30
29	X	1736	C	C6-N1-C2	-6.03	117.89	120.30
29	X	2617	G	N3-C2-N2	6.02	124.12	119.90
29	X	2696	A	N1-C6-N6	-6.02	114.99	118.60
29	X	1407	G	C5-C6-O6	-6.01	124.99	128.60
29	X	1724	C	C5-C6-N1	-6.01	117.99	121.00
29	X	2690	A	C2-N3-C4	-6.01	107.59	110.60
29	X	754	G	N9-C4-C5	-6.01	103.00	105.40
29	X	2704	U	N3-C2-O2	6.01	126.41	122.20
29	X	1231	A	N7-C8-N9	6.00	116.80	113.80
29	X	1982	C	N3-C2-O2	-6.00	117.70	121.90
29	X	2524	G	N3-C4-C5	-6.00	125.60	128.60
29	X	1706	A	N1-C6-N6	6.00	122.20	118.60
29	X	2044	G	C4-C5-N7	-6.00	108.40	110.80
29	X	672	C	N3-C4-C5	5.99	124.30	121.90
29	X	2569	A	C8-N9-C4	5.99	108.20	105.80
29	X	1950	C	C5-C6-N1	5.99	123.99	121.00
29	X	1684	G	C4-C5-N7	-5.99	108.41	110.80
29	X	2546	G	N3-C4-C5	-5.98	125.61	128.60
29	X	652	C	C6-N1-C2	5.98	122.69	120.30
29	X	2704	U	C2-N3-C4	-5.97	123.42	127.00
29	X	522	G	C5-C6-O6	-5.97	125.02	128.60
29	X	2522	G	C5-C6-O6	5.97	132.18	128.60
29	X	968	C	C4-C5-C6	-5.97	114.42	117.40
29	X	1684	G	C5-C6-O6	5.97	132.18	128.60
29	X	673	G	C4-N9-C1'	-5.96	118.75	126.50
29	X	1337	G	C5-C6-N1	5.96	114.48	111.50
29	X	1679	U	N3-C4-C5	5.96	118.18	114.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	2412	A	N1-C6-N6	-5.96	115.02	118.60
29	X	1681	A	C8-N9-C1'	-5.95	116.99	127.70
29	X	2408	G	N3-C4-C5	-5.95	125.63	128.60
29	X	2561	G	C5-C6-N1	5.95	114.47	111.50
29	X	1681	A	C4-N9-C1'	5.94	136.99	126.30
29	X	1983	G	N1-C2-N3	5.94	127.46	123.90
29	X	1950	C	C2-N1-C1'	5.94	125.33	118.80
29	X	2590	U	N1-C2-O2	5.94	126.95	122.80
29	X	2666	U	C2-N1-C1'	-5.93	110.58	117.70
29	X	1995	G	C5-C6-N1	5.93	114.47	111.50
29	X	1339	U	C6-N1-C2	-5.93	117.44	121.00
29	X	2239	C	C6-N1-C2	-5.92	117.93	120.30
29	X	2492	G	N1-C6-O6	-5.92	116.35	119.90
29	X	1323	G	N1-C6-O6	5.91	123.45	119.90
29	X	931	G	N3-C2-N2	5.91	124.04	119.90
29	X	2724	G	C8-N9-C4	-5.91	104.04	106.40
29	X	1763	G	C8-N9-C4	5.90	108.76	106.40
29	X	1721	G	C8-N9-C1'	5.90	134.67	127.00
29	X	522	G	C5-C6-N1	-5.90	108.55	111.50
29	X	1747	G	N3-C4-N9	5.90	129.54	126.00
29	X	2550	C	C5-C6-N1	5.90	123.95	121.00
29	X	2696	A	C2-N3-C4	5.89	113.55	110.60
29	X	1980	A	N1-C2-N3	5.89	132.25	129.30
29	X	2191	A	N1-C6-N6	-5.89	115.07	118.60
29	X	1989	C	N3-C2-O2	5.89	126.02	121.90
29	X	689	A	C5-N7-C8	-5.89	100.96	103.90
29	X	1221	C	C6-N1-C2	-5.89	117.94	120.30
29	X	2831	A	C8-N9-C4	-5.88	103.45	105.80
29	X	2598	C	N1-C2-O2	5.88	122.43	118.90
29	X	1744	G	N3-C2-N2	5.88	124.02	119.90
29	X	1999	U	C5-C6-N1	5.88	125.64	122.70
29	X	927	C	C6-N1-C2	-5.87	117.95	120.30
29	X	1627	C	C6-N1-C2	-5.87	117.95	120.30
29	X	566	U	C5-C6-N1	5.87	125.64	122.70
29	X	1683	G	N9-C4-C5	5.87	107.75	105.40
29	X	1219	C	C5-C6-N1	5.87	123.93	121.00
29	X	1333	G	C4-N9-C1'	5.87	134.13	126.50
29	X	526	C	N1-C2-O2	5.86	122.42	118.90
29	X	919	U	C5-C6-N1	-5.86	119.77	122.70
29	X	1219	C	C6-N1-C2	-5.86	117.96	120.30
29	X	2484	G	C8-N9-C4	-5.86	104.06	106.40
29	X	1269	G	C6-C5-N7	-5.85	126.89	130.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	1474	A	C5-C6-N6	5.85	128.38	123.70
29	X	458	G	C4-C5-N7	5.84	113.14	110.80
29	X	1636	G	N3-C4-C5	5.84	131.52	128.60
29	X	863	C	C6-N1-C2	-5.84	117.96	120.30
29	X	1470	G	N1-C6-O6	-5.84	116.39	119.90
29	X	968	C	N1-C2-N3	-5.84	115.11	119.20
29	X	1008	G	N9-C4-C5	-5.84	103.06	105.40
29	X	1258	G	C8-N9-C4	-5.84	104.06	106.40
29	X	2273	C	C2-N1-C1'	5.84	125.22	118.80
29	X	2028	C	N3-C4-N4	5.83	122.08	118.00
30	Y	84	G	C8-N9-C4	5.83	108.73	106.40
29	X	2605	C	N3-C2-O2	-5.83	117.82	121.90
29	X	2797	G	C4-N9-C1'	5.83	134.08	126.50
29	X	1778	U	N3-C2-O2	-5.83	118.12	122.20
29	X	1661	C	C2-N1-C1'	5.83	125.21	118.80
29	X	2671	C	N3-C4-C5	-5.83	119.57	121.90
29	X	1132	C	C6-N1-C2	-5.82	117.97	120.30
29	X	2846	G	C8-N9-C1'	-5.82	119.43	127.00
29	X	1672	A	C5-C6-N6	-5.82	119.04	123.70
29	X	2698	G	C6-C5-N7	-5.82	126.91	130.40
29	X	1631	C	N1-C2-O2	-5.82	115.41	118.90
29	X	920	G	C8-N9-C4	5.82	108.73	106.40
29	X	2858	A	N9-C4-C5	5.81	108.12	105.80
29	X	2516	U	C6-N1-C2	5.81	124.49	121.00
29	X	1662	G	N1-C6-O6	-5.80	116.42	119.90
29	X	1940	C	C6-N1-C1'	-5.80	113.84	120.80
29	X	1315	A	C5-C6-N6	5.80	128.34	123.70
29	X	2797	G	C4-C5-N7	5.80	113.12	110.80
29	X	2757	G	C8-N9-C4	5.79	108.72	106.40
29	X	2465	G	N7-C8-N9	5.79	116.00	113.10
29	X	1678	G	C4-N9-C1'	-5.78	118.98	126.50
29	X	2823	G	C4-C5-N7	-5.78	108.49	110.80
29	X	2489	C	C5-C4-N4	-5.78	116.15	120.20
29	X	923	A	N1-C6-N6	5.78	122.07	118.60
29	X	2199	C	N3-C2-O2	-5.78	117.86	121.90
29	X	2568	A	C8-N9-C4	5.78	108.11	105.80
29	X	1134	C	C6-N1-C2	-5.77	117.99	120.30
29	X	2033	C	C6-N1-C2	-5.77	117.99	120.30
29	X	2437	G	C6-C5-N7	-5.76	126.94	130.40
29	X	749	C	C6-N1-C2	-5.76	118.00	120.30
29	X	1308	C	C6-N1-C2	-5.76	118.00	120.30
29	X	1768	U	N1-C2-O2	5.76	126.83	122.80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	2420	C	C6-N1-C2	-5.76	118.00	120.30
29	X	2366	U	N1-C2-O2	-5.75	118.77	122.80
29	X	548	G	N1-C6-O6	5.75	123.35	119.90
29	X	1744	G	N1-C2-N2	-5.75	111.02	116.20
29	X	1405	A	C2-N3-C4	5.75	113.47	110.60
29	X	90	G	N3-C4-C5	-5.75	125.73	128.60
29	X	2553	G	C4-C5-N7	5.75	113.10	110.80
29	X	1294	G	C8-N9-C4	-5.75	104.10	106.40
29	X	773	G	C4-N9-C1'	5.74	133.97	126.50
29	X	2559	U	C2-N3-C4	5.74	130.45	127.00
29	X	2598	C	C5-C6-N1	5.74	123.87	121.00
29	X	1260	A	C8-N9-C4	5.74	108.10	105.80
29	X	2597	G	N3-C4-C5	-5.74	125.73	128.60
29	X	1301	U	N3-C4-C5	-5.74	111.16	114.60
29	X	2240	C	C2-N1-C1'	5.73	125.11	118.80
29	X	476	G	C4-C5-N7	-5.73	108.51	110.80
29	X	493	A	N7-C8-N9	-5.73	110.93	113.80
29	X	2594	U	N3-C2-O2	5.73	126.21	122.20
29	X	1281	A	N7-C8-N9	-5.73	110.93	113.80
29	X	1155	G	N7-C8-N9	-5.73	110.24	113.10
29	X	508	G	C5-C6-O6	-5.73	125.16	128.60
29	X	796	A	N7-C8-N9	5.73	116.66	113.80
29	X	2279	G	C6-C5-N7	-5.73	126.96	130.40
29	X	2846	G	N9-C4-C5	-5.73	103.11	105.40
29	X	1345	G	C8-N9-C1'	-5.73	119.56	127.00
29	X	1766	U	C5-C6-N1	-5.73	119.84	122.70
29	X	1692	C	C4-C5-C6	5.72	120.26	117.40
29	X	2491	C	N3-C4-C5	5.72	124.19	121.90
29	X	2492	G	C4-C5-N7	-5.72	108.51	110.80
29	X	2642	G	C8-N9-C4	5.72	108.69	106.40
29	X	1332	G	C6-C5-N7	-5.72	126.97	130.40
29	X	2654	A	C8-N9-C4	5.72	108.09	105.80
29	X	968	C	C2-N3-C4	5.71	122.76	119.90
29	X	2794	G	C6-N1-C2	-5.71	121.67	125.10
29	X	501	G	C4-C5-N7	-5.71	108.52	110.80
29	X	1292	A	C2-N3-C4	-5.71	107.74	110.60
29	X	789	G	C6-C5-N7	-5.71	126.97	130.40
29	X	2661	G	N1-C2-N2	5.71	121.34	116.20
29	X	2594	U	C2-N3-C4	5.70	130.42	127.00
29	X	545	C	C2-N1-C1'	-5.70	112.53	118.80
29	X	16	G	N7-C8-N9	-5.70	110.25	113.10
29	X	1332	G	C4-N9-C1'	5.70	133.91	126.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	2851	G	N3-C2-N2	5.69	123.89	119.90
29	X	237	G	N3-C4-C5	-5.69	125.75	128.60
29	X	596	C	C6-N1-C2	-5.69	118.02	120.30
29	X	1975	G	N3-C4-C5	5.68	131.44	128.60
29	X	2300	G	C2-N3-C4	5.68	114.74	111.90
29	X	1318	A	C8-N9-C4	5.68	108.07	105.80
29	X	2712	G	N9-C4-C5	-5.68	103.13	105.40
29	X	761	G	N3-C4-C5	5.68	131.44	128.60
29	X	1332	G	N3-C4-N9	5.67	129.40	126.00
29	X	1142	G	C8-N9-C4	5.67	108.67	106.40
29	X	1315	A	N1-C6-N6	-5.67	115.20	118.60
29	X	1326	U	C2-N1-C1'	5.67	124.50	117.70
29	X	2451	G	N3-C4-C5	-5.67	125.77	128.60
29	X	2590	U	C6-N1-C1'	-5.67	113.27	121.20
29	X	927	C	N1-C2-O2	5.67	122.30	118.90
12	K	29	LEU	CB-CG-CD1	-5.66	101.37	111.00
29	X	758	G	C8-N9-C4	5.66	108.67	106.40
29	X	1989	C	C2-N3-C4	5.66	122.73	119.90
29	X	1681	A	N3-C4-N9	5.66	131.93	127.40
29	X	1672	A	C6-C5-N7	-5.66	128.34	132.30
29	X	1550	C	C6-N1-C2	-5.66	118.04	120.30
29	X	2366	U	N3-C2-O2	5.66	126.16	122.20
29	X	516	G	C4-C5-N7	5.65	113.06	110.80
29	X	2831	A	N9-C4-C5	5.65	108.06	105.80
29	X	2368	G	N3-C4-C5	-5.65	125.78	128.60
29	X	1747	G	N3-C4-C5	-5.64	125.78	128.60
29	X	1685	A	C8-N9-C4	5.64	108.06	105.80
29	X	2857	C	C5-C4-N4	5.64	124.15	120.20
29	X	343	A	N9-C4-C5	5.64	108.06	105.80
29	X	968	C	C6-N1-C1'	-5.64	114.03	120.80
29	X	1207	G	C5-C6-O6	-5.64	125.22	128.60
29	X	2597	G	N1-C2-N2	-5.64	111.12	116.20
29	X	1465	G	N1-C2-N3	5.64	127.28	123.90
29	X	1312	G	C4-C5-N7	5.63	113.05	110.80
29	X	2002	A	C2-N3-C4	5.63	113.42	110.60
29	X	2419	C	C6-N1-C2	-5.63	118.05	120.30
29	X	2848	A	C8-N9-C4	-5.63	103.55	105.80
29	X	1403	U	C2-N1-C1'	5.63	124.46	117.70
29	X	2693	U	C4-C5-C6	5.62	123.08	119.70
29	X	319	G	C5-C6-O6	-5.62	125.23	128.60
30	Y	32	C	C5-C6-N1	5.62	123.81	121.00
29	X	700	C	N3-C4-C5	-5.61	119.66	121.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	1274	C	N1-C2-O2	5.61	122.27	118.90
29	X	1335	A	N7-C8-N9	-5.61	111.00	113.80
29	X	2618	A	C2-N3-C4	5.61	113.41	110.60
29	X	2806	G	C2-N3-C4	-5.61	109.09	111.90
29	X	2848	A	N1-C6-N6	-5.61	115.24	118.60
29	X	1197	U	N1-C2-O2	5.61	126.72	122.80
29	X	1997	A	C4-C5-C6	5.61	119.80	117.00
29	X	2666	U	C6-N1-C1'	5.60	129.04	121.20
29	X	1272	G	N1-C6-O6	-5.60	116.54	119.90
29	X	769	C	N1-C2-O2	-5.60	115.54	118.90
29	X	2812	A	C8-N9-C4	-5.60	103.56	105.80
29	X	943	U	N3-C2-O2	-5.59	118.28	122.20
29	X	2317	G	C8-N9-C4	-5.59	104.16	106.40
29	X	1645	U	N3-C2-O2	-5.59	118.29	122.20
29	X	1707	A	N1-C6-N6	5.59	121.95	118.60
29	X	1918	G	N1-C6-O6	-5.59	116.55	119.90
29	X	2495	G	N3-C4-N9	5.59	129.35	126.00
29	X	2839	G	C6-C5-N7	5.59	133.75	130.40
29	X	1775	A	C8-N9-C1'	-5.59	117.64	127.70
29	X	1966	C	C6-N1-C2	5.59	122.54	120.30
29	X	2572	U	C5-C6-N1	5.59	125.49	122.70
29	X	2668	U	C5-C6-N1	-5.58	119.91	122.70
29	X	2434	G	C8-N9-C1'	-5.58	119.74	127.00
29	X	2681	A	N1-C6-N6	5.58	121.95	118.60
29	X	1678	G	N1-C6-O6	-5.58	116.55	119.90
29	X	499	G	N3-C4-N9	5.58	129.35	126.00
29	X	1008	G	C8-N9-C4	5.58	108.63	106.40
29	X	1272	G	C5-C6-O6	5.58	131.94	128.60
29	X	2033	C	N1-C2-O2	5.58	122.25	118.90
29	X	2665	G	N3-C4-N9	-5.58	122.65	126.00
29	X	2598	C	C2-N1-C1'	5.57	124.93	118.80
29	X	1288	A	C5-C6-N6	-5.57	119.24	123.70
29	X	1298	G	C6-C5-N7	-5.57	127.06	130.40
29	X	2311	U	C2-N1-C1'	5.56	124.38	117.70
29	X	563	U	N3-C4-C5	5.56	117.94	114.60
29	X	661	C	C2-N1-C1'	5.56	124.92	118.80
29	X	1298	G	N9-C4-C5	-5.56	103.18	105.40
29	X	1345	G	N7-C8-N9	5.56	115.88	113.10
29	X	1344	C	N3-C4-C5	5.55	124.12	121.90
29	X	1656	U	N1-C2-N3	-5.55	111.57	114.90
29	X	2757	G	N1-C6-O6	5.55	123.23	119.90
29	X	2366	U	C2-N1-C1'	-5.55	111.04	117.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	1670	G	N9-C4-C5	-5.55	103.18	105.40
29	X	2233	C	C5-C6-N1	-5.55	118.23	121.00
29	X	2794	G	N3-C4-C5	-5.55	125.83	128.60
29	X	343	A	C4-C5-N7	-5.55	107.93	110.70
29	X	1232	U	C6-N1-C2	-5.54	117.67	121.00
29	X	1405	A	C8-N9-C4	-5.54	103.58	105.80
29	X	1681	A	C5-N7-C8	-5.54	101.13	103.90
29	X	1683	G	C8-N9-C1'	5.54	134.20	127.00
29	X	2610	G	N3-C4-N9	-5.54	122.68	126.00
29	X	2618	A	N3-C4-C5	-5.54	122.92	126.80
29	X	1965	U	C2-N1-C1'	5.54	124.35	117.70
29	X	1333	G	N3-C4-C5	-5.54	125.83	128.60
29	X	1947	G	N1-C6-O6	-5.54	116.58	119.90
29	X	1973	C	C2-N1-C1'	5.53	124.89	118.80
29	X	2041	A	N1-C6-N6	5.53	121.92	118.60
29	X	2546	G	N3-C4-N9	5.53	129.32	126.00
29	X	528	G	N1-C2-N2	5.53	121.17	116.20
29	X	567	G	C4-C5-N7	-5.53	108.59	110.80
29	X	1776	A	N9-C4-C5	5.53	108.01	105.80
29	X	2311	U	N3-C2-O2	-5.53	118.33	122.20
29	X	1918	G	C8-N9-C4	-5.52	104.19	106.40
29	X	1332	G	C5-C6-O6	-5.51	125.29	128.60
29	X	792	U	C5-C6-N1	-5.51	119.94	122.70
29	X	1658	A	C8-N9-C4	-5.51	103.59	105.80
29	X	12	U	C6-N1-C2	-5.51	117.69	121.00
29	X	919	U	C2-N1-C1'	-5.51	111.09	117.70
29	X	505	G	C2-N3-C4	-5.51	109.15	111.90
29	X	1461	C	C6-N1-C2	-5.51	118.10	120.30
29	X	236	C	C6-N1-C2	-5.50	118.10	120.30
29	X	789	G	C4-N9-C1'	5.50	133.65	126.50
29	X	583	C	C6-N1-C2	-5.50	118.10	120.30
29	X	1704	G	C5-N7-C8	-5.50	101.55	104.30
29	X	1296	G	C8-N9-C4	-5.49	104.20	106.40
29	X	2582	G	C8-N9-C1'	-5.49	119.86	127.00
29	X	2824	C	C5-C6-N1	-5.49	118.25	121.00
29	X	778	G	C6-C5-N7	-5.49	127.11	130.40
29	X	2712	G	N3-C2-N2	5.49	123.74	119.90
29	X	1670	G	N7-C8-N9	-5.49	110.36	113.10
29	X	2437	G	C5-C6-O6	-5.48	125.31	128.60
3	B	119	ARG	NE-CZ-NH2	-5.48	117.56	120.30
29	X	319	G	N1-C6-O6	5.48	123.19	119.90
29	X	1691	G	C5-C6-N1	5.48	114.24	111.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	2637	C	N3-C4-C5	5.48	124.09	121.90
29	X	2357	A	N1-C6-N6	5.47	121.89	118.60
29	X	107	G	C8-N9-C1'	-5.47	119.89	127.00
29	X	824	U	N1-C2-N3	5.47	118.18	114.90
29	X	1213	U	C5-C6-N1	5.47	125.43	122.70
29	X	2669	C	N1-C2-O2	5.47	122.18	118.90
29	X	1694	A	C5-N7-C8	-5.46	101.17	103.90
29	X	2699	G	C5-C6-O6	5.46	131.88	128.60
29	X	1714	A	N9-C4-C5	-5.46	103.61	105.80
29	X	2227	C	C6-N1-C1'	-5.46	114.25	120.80
29	X	1747	G	C2-N3-C4	5.46	114.63	111.90
29	X	2547	C	C5-C6-N1	5.46	123.73	121.00
29	X	585	U	N3-C4-O4	5.45	123.22	119.40
29	X	63	A	N1-C6-N6	5.45	121.87	118.60
29	X	1709	U	N3-C2-O2	-5.45	118.39	122.20
29	X	751	G	N3-C4-C5	-5.45	125.88	128.60
29	X	548	G	C6-C5-N7	-5.45	127.13	130.40
29	X	2481	G	N1-C2-N2	-5.45	111.30	116.20
29	X	9	U	N3-C2-O2	-5.44	118.39	122.20
29	X	996	C	C6-N1-C2	5.44	122.48	120.30
29	X	2696	A	N9-C4-C5	5.44	107.98	105.80
29	X	568	G	N1-C6-O6	-5.44	116.64	119.90
29	X	470	U	N3-C2-O2	-5.44	118.39	122.20
29	X	1449	C	C6-N1-C2	-5.43	118.13	120.30
29	X	1975	G	N9-C4-C5	5.43	107.57	105.40
29	X	2048	C	C5-C6-N1	5.43	123.72	121.00
30	Y	79	U	C5-C6-N1	-5.43	119.98	122.70
29	X	2412	A	C8-N9-C4	-5.43	103.63	105.80
29	X	2560	G	C8-N9-C4	-5.43	104.23	106.40
29	X	1991	C	C5-C6-N1	-5.43	118.29	121.00
29	X	793	G	C2-N3-C4	-5.42	109.19	111.90
29	X	1250	A	N1-C6-N6	5.42	121.85	118.60
29	X	1230	C	C6-N1-C2	-5.42	118.13	120.30
29	X	2470	U	C2-N1-C1'	5.42	124.21	117.70
29	X	1321	A	N1-C6-N6	-5.42	115.35	118.60
29	X	1960	A	C8-N9-C4	5.42	107.97	105.80
29	X	2704	U	C6-N1-C1'	5.42	128.78	121.20
29	X	2487	G	C5-C6-N1	5.42	114.21	111.50
29	X	528	G	N3-C4-N9	-5.41	122.75	126.00
29	X	993	C	C4-C5-C6	5.41	120.11	117.40
29	X	1933	G	N9-C4-C5	5.41	107.56	105.40
29	X	2851	G	N9-C4-C5	-5.41	103.23	105.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	1929	U	C5-C6-N1	-5.41	120.00	122.70
29	X	1946	U	C5-C6-N1	5.41	125.40	122.70
29	X	2698	G	C4-C5-C6	5.41	122.04	118.80
12	K	108	VAL	CB-CA-C	-5.41	101.13	111.40
29	X	931	G	N1-C2-N2	-5.41	111.34	116.20
29	X	1717	A	N1-C6-N6	-5.40	115.36	118.60
29	X	2638	G	N1-C6-O6	5.40	123.14	119.90
29	X	774	A	C8-N9-C4	-5.40	103.64	105.80
29	X	1689	U	C6-N1-C2	5.40	124.24	121.00
29	X	2496	C	N3-C4-C5	5.40	124.06	121.90
29	X	2796	A	N1-C6-N6	-5.40	115.36	118.60
29	X	760	U	N1-C2-N3	5.40	118.14	114.90
29	X	2543	A	C5-C6-N6	-5.40	119.38	123.70
29	X	2583	U	C5-C6-N1	-5.40	120.00	122.70
29	X	2553	G	N3-C4-C5	5.39	131.30	128.60
29	X	2753	C	C6-N1-C2	-5.39	118.14	120.30
29	X	1469	U	N1-C2-O2	-5.39	119.03	122.80
29	X	2227	C	C2-N1-C1'	5.39	124.73	118.80
29	X	507	A	N1-C6-N6	-5.39	115.37	118.60
29	X	2599	U	C5-C6-N1	5.39	125.39	122.70
29	X	504	G	C4-C5-N7	5.38	112.95	110.80
29	X	1712	G	N3-C4-N9	5.38	129.23	126.00
29	X	2437	G	N1-C6-O6	5.38	123.13	119.90
29	X	1624	A	C4-C5-C6	5.38	119.69	117.00
29	X	1480	G	C6-C5-N7	-5.38	127.17	130.40
29	X	1636	G	C2-N3-C4	-5.38	109.21	111.90
29	X	2500	C	N3-C2-O2	-5.38	118.14	121.90
29	X	2314	A	N9-C4-C5	5.37	107.95	105.80
29	X	789	G	C8-N9-C1'	-5.37	120.02	127.00
29	X	2407	G	C8-N9-C4	-5.37	104.25	106.40
29	X	2408	G	N3-C4-N9	5.37	129.22	126.00
29	X	940	G	N1-C6-O6	-5.37	116.68	119.90
29	X	1933	G	N3-C4-C5	-5.37	125.92	128.60
29	X	1995	G	N3-C4-C5	-5.37	125.92	128.60
29	X	2669	C	N3-C2-O2	-5.36	118.14	121.90
29	X	2698	G	N3-C4-C5	-5.36	125.92	128.60
29	X	1986	G	C4-C5-N7	-5.36	108.66	110.80
29	X	2483	U	C5-C6-N1	5.36	125.38	122.70
29	X	2689	C	C2-N1-C1'	-5.36	112.91	118.80
29	X	1984	A	C6-N1-C2	5.35	121.81	118.60
29	X	1243	G	C5-C6-O6	-5.35	125.39	128.60
29	X	30	G	C8-N9-C4	-5.35	104.26	106.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	1775	A	N7-C8-N9	-5.35	111.13	113.80
29	X	2014	A	C8-N9-C4	-5.35	103.66	105.80
29	X	2307	A	C2-N3-C4	-5.35	107.93	110.60
29	X	845	U	C5-C6-N1	5.34	125.37	122.70
29	X	1704	G	N9-C4-C5	-5.34	103.26	105.40
29	X	2661	G	N1-C6-O6	5.34	123.11	119.90
29	X	1976	U	N3-C2-O2	-5.34	118.46	122.20
29	X	741	G	C8-N9-C4	5.34	108.53	106.40
22	U	17	SER	C-N-CA	5.33	135.03	121.70
29	X	1704	G	N3-C4-N9	5.33	129.20	126.00
29	X	1305	C	N1-C2-O2	-5.33	115.70	118.90
29	X	2687	G	N3-C4-C5	5.33	131.26	128.60
29	X	2843	A	C8-N9-C4	5.33	107.93	105.80
29	X	33	C	N1-C2-O2	5.32	122.09	118.90
29	X	2598	C	N3-C2-O2	-5.32	118.18	121.90
29	X	567	G	N3-C4-N9	-5.32	122.81	126.00
29	X	576	A	C5-C6-N6	5.32	127.95	123.70
29	X	1346	C	C6-N1-C2	-5.32	118.17	120.30
29	X	488	A	C8-N9-C4	-5.32	103.67	105.80
29	X	786	U	N3-C2-O2	-5.31	118.48	122.20
29	X	1300	A	C8-N9-C4	-5.31	103.67	105.80
29	X	2315	A	N1-C6-N6	-5.31	115.41	118.60
29	X	12	U	N3-C2-O2	-5.31	118.48	122.20
29	X	2679	G	C8-N9-C4	5.31	108.52	106.40
29	X	749	C	C2-N1-C1'	5.31	124.64	118.80
29	X	2699	G	C6-N1-C2	5.31	128.28	125.10
29	X	557	U	C6-N1-C2	-5.30	117.82	121.00
29	X	749	C	C5-C6-N1	5.30	123.65	121.00
29	X	2692	A	C4-C5-C6	-5.30	114.35	117.00
29	X	1668	G	C5-N7-C8	-5.30	101.65	104.30
29	X	2700	U	N1-C2-O2	5.30	126.51	122.80
29	X	1333	G	C5-C6-O6	5.30	131.78	128.60
29	X	1756	C	N3-C2-O2	5.30	125.61	121.90
29	X	2697	G	N7-C8-N9	5.30	115.75	113.10
29	X	2015	G	C4-C5-N7	5.29	112.92	110.80
29	X	2594	U	C5-C6-N1	5.29	125.35	122.70
29	X	1751	A	N7-C8-N9	-5.29	111.16	113.80
29	X	957	G	C5-C6-O6	5.29	131.77	128.60
29	X	2561	G	C4-C5-C6	-5.29	115.63	118.80
29	X	829	C	N3-C4-C5	5.29	124.01	121.90
29	X	2055	G	N3-C2-N2	5.28	123.60	119.90
29	X	1308	C	N3-C4-N4	5.28	121.70	118.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	2853	U	C5-C6-N1	-5.28	120.06	122.70
29	X	536	A	C6-N1-C2	-5.27	115.44	118.60
29	X	755	C	C6-N1-C2	5.27	122.41	120.30
29	X	1295	U	C6-N1-C2	-5.27	117.84	121.00
29	X	2665	G	C4-N9-C1'	-5.27	119.65	126.50
29	X	956	A	C2-N3-C4	5.27	113.23	110.60
29	X	664	C	N1-C2-O2	5.26	122.06	118.90
29	X	2498	U	N3-C4-C5	-5.26	111.44	114.60
29	X	689	A	N1-C6-N6	5.26	121.76	118.60
29	X	2702	G	N3-C4-N9	5.26	129.16	126.00
29	X	350	U	C5-C6-N1	5.26	125.33	122.70
29	X	13	A	C4-C5-C6	5.26	119.63	117.00
29	X	2049	C	N3-C2-O2	-5.26	118.22	121.90
29	X	2554	C	C5-C4-N4	-5.26	116.52	120.20
29	X	957	G	C5-C6-N1	5.25	114.13	111.50
29	X	2239	C	N3-C2-O2	-5.25	118.22	121.90
29	X	2251	U	C6-N1-C2	5.25	124.15	121.00
29	X	778	G	N1-C6-O6	5.25	123.05	119.90
29	X	2398	U	N3-C4-O4	5.25	123.07	119.40
29	X	1686	A	N7-C8-N9	5.24	116.42	113.80
29	X	2051	U	N3-C2-O2	-5.24	118.53	122.20
29	X	2383	C	N3-C2-O2	-5.24	118.23	121.90
29	X	2441	U	N3-C2-O2	-5.24	118.53	122.20
29	X	2561	G	C2-N3-C4	5.24	114.52	111.90
29	X	579	G	N9-C4-C5	5.24	107.50	105.40
29	X	2297	G	C4-C5-N7	-5.24	108.70	110.80
29	X	21	A	C8-N9-C4	-5.24	103.70	105.80
29	X	2795	A	C8-N9-C4	-5.24	103.70	105.80
29	X	1250	A	C6-C5-N7	-5.24	128.63	132.30
29	X	2660	C	C4-C5-C6	5.24	120.02	117.40
29	X	2015	G	C8-N9-C1'	5.24	133.81	127.00
29	X	2524	G	C2-N3-C4	5.23	114.52	111.90
29	X	2845	C	N3-C4-C5	-5.23	119.81	121.90
29	X	700	C	C2-N3-C4	5.23	122.51	119.90
29	X	1715	A	C4-C5-N7	5.23	113.31	110.70
29	X	2569	A	N7-C8-N9	-5.23	111.19	113.80
29	X	2578	G	N3-C4-N9	5.23	129.14	126.00
29	X	1693	A	N9-C4-C5	-5.23	103.71	105.80
29	X	1993	G	N1-C6-O6	5.23	123.03	119.90
29	X	2482	A	N1-C2-N3	5.23	131.91	129.30
29	X	1683	G	C6-C5-N7	5.22	133.53	130.40
29	X	1766	U	C6-N1-C2	5.22	124.14	121.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	2543	A	N1-C6-N6	5.22	121.73	118.60
29	X	2620	G	N1-C6-O6	5.22	123.03	119.90
29	X	2001	G	C8-N9-C4	-5.22	104.31	106.40
29	X	2402	U	C6-N1-C2	-5.22	117.87	121.00
29	X	1981	A	C8-N9-C4	5.22	107.89	105.80
29	X	2695	C	N3-C2-O2	-5.21	118.25	121.90
29	X	2843	A	N7-C8-N9	-5.21	111.19	113.80
29	X	1663	C	N3-C4-N4	5.21	121.65	118.00
29	X	1939	U	C6-N1-C2	-5.21	117.87	121.00
29	X	1666	G	C8-N9-C4	5.21	108.48	106.40
29	X	1690	U	C5-C6-N1	5.21	125.31	122.70
29	X	955	G	C8-N9-C4	-5.21	104.32	106.40
29	X	2483	U	N1-C2-O2	5.21	126.45	122.80
30	Y	34	C	C6-N1-C2	-5.21	118.22	120.30
29	X	12	U	C2-N1-C1'	5.21	123.95	117.70
29	X	746	G	N3-C4-C5	-5.20	126.00	128.60
29	X	22	C	C6-N1-C1'	-5.20	114.56	120.80
29	X	2000	U	N1-C2-O2	-5.20	119.16	122.80
29	X	1721	G	N3-C4-N9	-5.20	122.88	126.00
29	X	679	C	N3-C2-O2	-5.20	118.26	121.90
29	X	754	G	C5-N7-C8	-5.20	101.70	104.30
29	X	989	G	C4-N9-C1'	-5.20	119.74	126.50
29	X	1245	G	N7-C8-N9	5.20	115.70	113.10
29	X	1629	G	N1-C6-O6	-5.20	116.78	119.90
29	X	2300	G	N3-C4-C5	-5.20	126.00	128.60
29	X	2712	G	C8-N9-C1'	-5.20	120.25	127.00
29	X	796	A	C8-N9-C4	-5.19	103.72	105.80
29	X	2009	U	N3-C4-O4	5.19	123.03	119.40
29	X	2053	G	C4-N9-C1'	-5.19	119.75	126.50
29	X	1465	G	N3-C4-C5	-5.19	126.01	128.60
29	X	2611	A	C2-N3-C4	-5.19	108.01	110.60
29	X	1974	U	N3-C4-C5	-5.19	111.49	114.60
29	X	469	G	N1-C6-O6	-5.18	116.79	119.90
29	X	2606	G	C6-C5-N7	-5.18	127.29	130.40
29	X	2676	G	C4-C5-C6	5.18	121.91	118.80
29	X	2792	C	C5-C6-N1	-5.18	118.41	121.00
29	X	1255	A	N1-C6-N6	-5.18	115.49	118.60
29	X	1674	C	C5-C6-N1	-5.18	118.41	121.00
29	X	219	G	C8-N9-C1'	5.17	133.73	127.00
29	X	1317	G	C8-N9-C1'	5.17	133.73	127.00
29	X	2437	G	N3-C4-N9	5.17	129.10	126.00
29	X	544	U	N1-C2-O2	5.17	126.42	122.80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	1142	G	C5-C6-O6	-5.17	125.50	128.60
29	X	224	G	N3-C4-N9	5.17	129.10	126.00
29	X	1970	G	N3-C4-C5	-5.17	126.02	128.60
29	X	2215	C	C6-N1-C2	5.17	122.37	120.30
29	X	2821	G	N7-C8-N9	-5.17	110.52	113.10
29	X	1704	G	N7-C8-N9	5.16	115.68	113.10
29	X	567	G	C6-C5-N7	5.16	133.50	130.40
29	X	2542	U	C5-C4-O4	5.16	129.00	125.90
29	X	1753	A	N7-C8-N9	5.16	116.38	113.80
29	X	595	A	C4-C5-C6	-5.16	114.42	117.00
29	X	1975	G	C8-N9-C1'	5.16	133.70	127.00
29	X	2524	G	N1-C6-O6	-5.16	116.81	119.90
29	X	1035	G	N3-C4-C5	-5.15	126.02	128.60
29	X	1323	G	C6-C5-N7	-5.15	127.31	130.40
29	X	945	G	C8-N9-C4	-5.15	104.34	106.40
29	X	1291	G	C8-N9-C4	5.15	108.46	106.40
29	X	1315	A	N9-C4-C5	5.15	107.86	105.80
29	X	1476	G	C8-N9-C4	-5.15	104.34	106.40
29	X	2870	C	N3-C2-O2	-5.15	118.30	121.90
29	X	943	U	C6-N1-C1'	-5.15	113.99	121.20
29	X	968	C	C5-C4-N4	-5.15	116.60	120.20
29	X	2806	G	N1-C2-N2	-5.15	111.57	116.20
29	X	2835	A	N9-C4-C5	-5.15	103.74	105.80
29	X	1714	A	C5-C6-N6	-5.14	119.58	123.70
29	X	2854	G	N7-C8-N9	5.14	115.67	113.10
29	X	2327	U	C5-C6-N1	5.14	125.27	122.70
29	X	2461	G	C4-N9-C1'	5.14	133.19	126.50
29	X	472	C	C5-C6-N1	5.14	123.57	121.00
29	X	1279	G	N1-C2-N2	-5.14	111.57	116.20
29	X	1632	A	N1-C6-N6	5.14	121.69	118.60
29	X	1679	U	C4-C5-C6	5.14	122.78	119.70
29	X	1238	A	C6-C5-N7	5.14	135.90	132.30
29	X	1931	G	N1-C6-O6	5.14	122.98	119.90
29	X	854	G	N7-C8-N9	5.13	115.67	113.10
29	X	2869	U	C6-N1-C2	-5.13	117.92	121.00
29	X	483	A	C2-N3-C4	-5.13	108.03	110.60
29	X	1862	C	C6-N1-C2	-5.13	118.25	120.30
29	X	526	C	C6-N1-C2	-5.13	118.25	120.30
29	X	545	C	C6-N1-C1'	5.13	126.96	120.80
29	X	1690	U	C5-C4-O4	-5.13	122.82	125.90
29	X	1984	A	C2-N3-C4	-5.13	108.03	110.60
29	X	2422	C	N3-C2-O2	-5.13	118.31	121.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	J	42	TRP	N-CA-C	-5.13	97.15	111.00
29	X	1984	A	N3-C4-N9	-5.13	123.30	127.40
29	X	2541	U	N1-C2-O2	5.13	126.39	122.80
29	X	2559	U	C5-C6-N1	5.13	125.26	122.70
29	X	8	A	C6-N1-C2	-5.13	115.52	118.60
29	X	1940	C	C2-N1-C1'	5.13	124.44	118.80
29	X	1989	C	C4-C5-C6	-5.13	114.84	117.40
30	Y	93	G	N1-C6-O6	5.13	122.98	119.90
29	X	990	A	N7-C8-N9	-5.12	111.24	113.80
29	X	1663	C	N1-C2-O2	5.12	121.97	118.90
29	X	2442	C	C6-N1-C2	-5.12	118.25	120.30
29	X	2492	G	C5-C6-O6	5.12	131.67	128.60
29	X	1661	C	C6-N1-C2	-5.12	118.25	120.30
29	X	2227	C	N1-C2-O2	5.12	121.97	118.90
29	X	2559	U	C2-N1-C1'	5.12	123.85	117.70
29	X	2489	C	N3-C4-N4	5.12	121.58	118.00
29	X	541	C	C5-C6-N1	-5.12	118.44	121.00
29	X	934	G	C8-N9-C4	-5.12	104.35	106.40
29	X	931	G	C8-N9-C1'	-5.12	120.35	127.00
29	X	1013	G	N3-C4-N9	5.11	129.07	126.00
29	X	1308	C	C5-C6-N1	5.11	123.56	121.00
29	X	1779	C	C6-N1-C2	5.11	122.34	120.30
29	X	2660	C	C5-C6-N1	-5.11	118.44	121.00
29	X	39	C	C6-N1-C2	-5.11	118.26	120.30
29	X	1663	C	C6-N1-C2	-5.11	118.26	120.30
29	X	1971	C	N3-C4-C5	5.11	123.94	121.90
29	X	1344	C	C6-N1-C2	5.10	122.34	120.30
29	X	534	U	N1-C2-O2	-5.10	119.23	122.80
29	X	689	A	C8-N9-C4	-5.10	103.76	105.80
29	X	1298	G	N3-C4-N9	5.10	129.06	126.00
29	X	2017	U	C5-C6-N1	5.10	125.25	122.70
29	X	2800	C	C5-C6-N1	5.10	123.55	121.00
29	X	1332	G	C4-C5-N7	5.10	112.84	110.80
29	X	2494	C	C6-N1-C2	5.10	122.34	120.30
29	X	1939	U	N3-C2-O2	-5.10	118.63	122.20
29	X	2007	G	N7-C8-N9	-5.09	110.55	113.10
29	X	2559	U	N1-C2-N3	-5.09	111.85	114.90
29	X	852	U	C6-N1-C2	5.09	124.05	121.00
29	X	974	U	N3-C4-O4	5.09	122.96	119.40
29	X	1138	A	C8-N9-C4	-5.09	103.76	105.80
29	X	660	G	N3-C2-N2	-5.09	116.34	119.90
29	X	2599	U	C6-N1-C2	-5.09	117.95	121.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	540	G	N3-C2-N2	-5.08	116.34	119.90
29	X	2510	A	N1-C6-N6	5.08	121.65	118.60
29	X	597	U	C6-N1-C2	5.08	124.05	121.00
29	X	1016	C	N3-C4-N4	5.07	121.55	118.00
13	L	92	GLY	N-CA-C	-5.07	100.42	113.10
29	X	1750	A	C4-C5-C6	5.07	119.53	117.00
29	X	2398	U	C5-C6-N1	5.07	125.23	122.70
29	X	812	G	C8-N9-C4	-5.06	104.38	106.40
30	Y	107	C	C6-N1-C2	-5.06	118.28	120.30
29	X	1292	A	N3-C4-C5	5.06	130.34	126.80
29	X	1332	G	C8-N9-C1'	-5.06	120.42	127.00
29	X	2718	A	N7-C8-N9	-5.06	111.27	113.80
29	X	1301	U	C2-N3-C4	5.06	130.03	127.00
29	X	496	C	N1-C2-N3	-5.05	115.66	119.20
29	X	1238	A	C5-C6-N6	5.05	127.74	123.70
29	X	2542	U	N1-C2-N3	5.05	117.93	114.90
29	X	1663	C	C2-N3-C4	5.05	122.42	119.90
29	X	1652	G	C6-C5-N7	-5.05	127.37	130.40
29	X	2576	G	C5-C6-N1	-5.05	108.98	111.50
29	X	1723	U	N3-C2-O2	-5.04	118.67	122.20
29	X	1750	A	C8-N9-C4	-5.04	103.78	105.80
29	X	2563	U	N3-C2-O2	-5.04	118.67	122.20
29	X	2685	A	N1-C6-N6	-5.04	115.58	118.60
29	X	559	C	C5-C6-N1	5.03	123.52	121.00
29	X	174	A	C2-N3-C4	5.03	113.12	110.60
29	X	1231	A	C8-N9-C4	-5.03	103.79	105.80
29	X	1748	U	N3-C2-O2	5.03	125.72	122.20
29	X	2425	G	C4-N9-C1'	5.03	133.04	126.50
29	X	2553	G	N3-C4-N9	-5.03	122.98	126.00
29	X	632	A	N1-C6-N6	-5.03	115.58	118.60
29	X	1692	C	N1-C2-O2	-5.03	115.88	118.90
29	X	1253	C	N3-C2-O2	-5.03	118.38	121.90
29	X	1975	G	C4-N9-C1'	-5.03	119.96	126.50
29	X	413	G	N3-C4-C5	-5.02	126.09	128.60
29	X	2522	G	N1-C6-O6	-5.02	116.89	119.90
29	X	476	G	C5-C6-O6	5.02	131.61	128.60
29	X	2605	C	N1-C2-O2	5.02	121.91	118.90
29	X	2704	U	C4-C5-C6	5.02	122.71	119.70
29	X	90	G	N3-C4-N9	5.01	129.01	126.00
29	X	1250	A	C4-C5-C6	5.01	119.51	117.00
29	X	1657	A	C8-N9-C4	5.01	107.81	105.80
29	X	2483	U	C2-N1-C1'	5.01	123.72	117.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	1333	G	N1-C2-N2	-5.01	111.69	116.20
29	X	1715	A	C6-C5-N7	-5.01	128.79	132.30
29	X	1138	A	N7-C8-N9	5.01	116.30	113.80
29	X	2586	G	N3-C4-N9	5.01	129.00	126.00
29	X	2597	G	C4-C5-C6	5.01	121.81	118.80
29	X	223	C	C6-N1-C2	-5.01	118.30	120.30
29	X	540	G	C8-N9-C4	-5.01	104.40	106.40
29	X	829	C	C5-C6-N1	-5.01	118.50	121.00
29	X	334	G	C5-C6-O6	-5.00	125.60	128.60
29	X	762	A	C4-C5-N7	5.00	113.20	110.70

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	85	ALA	Peptide
9	H	36	THR	Peptide
10	I	52	GLY	Peptide
13	L	87	VAL	Peptide
14	M	108	LYS	Peptide
14	M	2	GLN	Peptide
19	R	105	ARG	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	0	1651	0	1693	51	0
2	A	2107	0	2190	133	0
3	B	1540	0	1600	117	0
4	C	1507	0	1525	115	0
5	D	1401	0	1481	81	0
6	E	1287	0	1336	53	0
7	F	1048	0	1088	35	0
8	G	1115	0	1144	50	0
9	H	997	0	1046	81	0
10	I	1068	0	1103	68	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	J	1091	0	1125	66	0
12	K	879	0	930	79	0
13	L	778	0	820	57	0
14	M	867	0	890	64	0
15	N	978	0	1020	95	0
16	O	742	0	756	37	0
17	P	1014	0	1096	80	0
18	Q	727	0	753	31	0
19	R	826	0	881	65	0
20	S	1346	0	1372	71	0
21	T	626	0	655	38	0
22	U	553	0	604	50	0
23	V	534	0	558	13	0
24	W	424	0	470	24	0
25	Z	453	0	455	49	0
26	1	404	0	416	25	0
27	2	393	0	420	24	0
28	3	509	0	565	56	0
29	X	59673	0	30060	1967	0
30	Y	2601	0	1327	91	0
31	A	1	0	0	0	0
31	H	1	0	0	0	0
31	M	1	0	0	0	0
31	N	1	0	0	0	0
31	X	177	0	0	1	0
31	Y	5	0	0	0	0
32	X	36	0	29	2	0
All	All	89361	0	59408	3326	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 23.

All (3326) 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)
3:B:14:ILE:HB	14:M:20:HIS:HD2	1.16	1.11
12:K:79:VAL:HA	12:K:83:VAL:HG13	1.35	1.06
29:X:1225:G:H1'	29:X:1250:A:H61	1.21	1.03
29:X:517:A:H5''	29:X:518:A:H5'	1.37	1.02
29:X:2690:A:OP1	29:X:2692:A:OP2	1.78	0.99
29:X:2550:C:H5''	29:X:2551:A:H5'	1.42	0.98

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:U:21:ARG:HH12	29:X:400:U:H5'	1.28	0.98
15:N:48:ARG:HD2	29:X:1167:A:H61	1.27	0.97
24:W:43:MET:HE1	29:X:940:G:H21	1.30	0.97
29:X:320:A:N3	29:X:340:G:O2'	1.96	0.97
10:I:21:ARG:NH2	29:X:596:C:OP2	1.99	0.96
29:X:2796:A:H2'	29:X:2797:G:H8	1.30	0.96
29:X:623:G:O2'	29:X:626:A:N6	1.99	0.95
29:X:1230:C:H2'	29:X:1231:A:H8	1.31	0.94
3:B:14:ILE:HB	14:M:20:HIS:CD2	2.03	0.93
28:3:29:LYS:NZ	29:X:2398:U:OP2	2.01	0.93
25:Z:19:ARG:NH2	29:X:1277:G:OP1	2.02	0.92
14:M:25:PRO:HB3	14:M:93:ILE:HD11	1.53	0.91
29:X:2796:A:H2'	29:X:2797:G:C8	2.05	0.91
14:M:82:PRO:O	14:M:84:ALA:N	2.04	0.90
29:X:646:C:O2'	29:X:650:U:OP1	1.90	0.90
11:J:19:THR:HG22	11:J:20:GLY:H	1.37	0.89
12:K:36:THR:OG1	29:X:1291:G:OP1	1.91	0.89
17:P:31:VAL:HG11	17:P:124:ILE:HD11	1.54	0.89
8:G:140:GLN:HG3	29:X:567:G:H5'	1.55	0.88
29:X:2083:G:H1	29:X:2172:U:H3	1.21	0.88
14:M:42:GLY:O	14:M:44:ARG:N	2.08	0.87
28:3:34:THR:OG1	29:X:2399:C:OP1	1.92	0.86
3:B:75:THR:HG22	3:B:77:ILE:H	1.38	0.86
10:I:21:ARG:HA	29:X:824:U:H2'	1.55	0.86
6:E:22:GLY:HA3	6:E:39:THR:HG22	1.56	0.86
14:M:29:PRO:HD3	14:M:57:ILE:HD11	1.57	0.86
29:X:320:A:N6	29:X:1223:G:O2'	2.08	0.86
29:X:578:U:O2'	29:X:994:A:N1	2.08	0.86
12:K:53:THR:OG1	29:X:2815:C:OP1	1.92	0.85
24:W:25:LEU:HD22	24:W:30:ASP:HB3	1.57	0.85
17:P:49:SER:O	17:P:51:GLN:N	2.08	0.85
29:X:834:A:H1'	29:X:955:G:H5'	1.58	0.85
29:X:1230:C:H2'	29:X:1231:A:C8	2.12	0.84
29:X:1919:A:H2	29:X:1926:U:H3	1.24	0.84
13:L:18:ARG:NH2	29:X:2271:C:OP2	2.10	0.84
29:X:469:G:N2	29:X:481:A:OP2	2.08	0.84
29:X:1989:C:O2'	29:X:2798:A:N3	2.11	0.84
29:X:2821:G:H2'	29:X:2822:U:C6	2.12	0.83
12:K:11:ASN:HD22	12:K:11:ASN:H	1.25	0.83
29:X:841:G:H2'	29:X:842:A:C8	2.13	0.83
29:X:1202:U:H2'	29:X:1203:A:H8	1.44	0.83

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:U:17:SER:HB2	22:U:18:VAL:HB	1.60	0.83
27:2:43:THR:HG22	27:2:45:SER:H	1.41	0.83
29:X:2352:A:H2'	29:X:2353:G:C8	2.14	0.82
27:2:46:ASP:OD1	29:X:125:A:N6	2.13	0.82
29:X:1983:G:N2	29:X:2668:U:O4	2.10	0.82
29:X:2522:G:H2'	29:X:2523:G:C8	2.14	0.82
20:S:141:MET:HG2	20:S:145:ASP:HB2	1.62	0.81
29:X:693:A:H2'	29:X:694:G:H8	1.45	0.81
29:X:1060:C:H42	29:X:2731:G:H1	1.26	0.81
3:B:111:LYS:NZ	29:X:2704:U:OP1	2.13	0.81
15:N:37:GLN:HA	15:N:40:LEU:HD12	1.60	0.81
12:K:13:ASN:O	12:K:17:ARG:NH2	2.14	0.81
29:X:1244:U:H2'	29:X:1245:G:H8	1.45	0.81
29:X:1909:U:OP2	29:X:1912:G:N1	2.13	0.80
29:X:2668:U:O2	29:X:2693:U:H5''	1.82	0.80
29:X:1681:A:N6	29:X:1975:G:O6	2.14	0.80
29:X:2543:A:OP1	29:X:2627:G:O2'	1.97	0.80
3:B:189:PRO:HA	29:X:2659:C:H5'	1.61	0.80
15:N:49:ASP:HA	15:N:52:ASN:HB2	1.61	0.80
28:3:64:ARG:NH2	29:X:219:G:OP1	2.15	0.80
29:X:1336:G:H2'	29:X:1337:G:H5'	1.63	0.79
29:X:652:C:H42	29:X:657:A:H61	1.28	0.79
29:X:1674:C:H2'	29:X:1675:C:C6	2.17	0.79
29:X:698:A:OP1	29:X:699:G:N2	2.15	0.79
29:X:2309:G:N2	29:X:2365:U:O2	2.16	0.79
29:X:1573:G:H3'	29:X:1574:A:H5''	1.61	0.79
29:X:79:G:H2'	29:X:80:A:H8	1.48	0.79
22:U:48:LYS:HG2	22:U:49:LYS:H	1.48	0.79
17:P:109:ARG:NH1	29:X:760:U:O2'	2.15	0.79
29:X:833:A:N3	29:X:954:U:O2'	2.15	0.79
29:X:2118:A:N6	29:X:2140:G:O6	2.15	0.79
11:J:26:ASP:OD1	11:J:26:ASP:N	2.14	0.78
2:A:60:ARG:HD3	2:A:86:PRO:HB2	1.65	0.78
29:X:312:G:HO2'	29:X:313:U:H6	1.31	0.78
12:K:103:ARG:HH21	12:K:108:VAL:HB	1.48	0.78
2:A:16:MET:HG3	2:A:207:GLY:HA3	1.65	0.78
29:X:546:A:H2'	29:X:547:U:H6	1.49	0.78
29:X:2303:C:H5''	29:X:2304:G:H5''	1.66	0.78
26:I:45:ALA:HB1	29:X:2350:G:H4'	1.66	0.78
14:M:69:ARG:HD2	14:M:78:GLU:HG2	1.64	0.78
16:O:46:VAL:HG13	16:O:51:ALA:HB2	1.66	0.78

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:32:ARG:NH1	17:P:120:ARG:O	2.16	0.78
29:X:1164:C:H2'	29:X:1165:G:C8	2.18	0.78
5:D:75:SER:H	5:D:79:LEU:HD22	1.49	0.77
4:C:150:LEU:HA	4:C:187:VAL:HB	1.64	0.77
17:P:15:LYS:NZ	29:X:512:A:O2'	2.12	0.77
17:P:28:ALA:HB2	17:P:71:VAL:HG21	1.66	0.77
9:H:64:VAL:HG22	9:H:106:ARG:HH21	1.48	0.77
10:I:28:LYS:HB3	10:I:29:THR:HG23	1.67	0.77
2:A:157:ARG:NH1	29:X:1810:U:OP2	2.18	0.77
29:X:226:C:H4'	29:X:227:G:H5''	1.66	0.77
29:X:2283:G:H22	29:X:2291:U:H3	1.32	0.77
29:X:2772:U:H2'	29:X:2773:G:H8	1.48	0.77
14:M:60:SER:HA	14:M:64:LYS:HB2	1.64	0.77
20:S:67:LYS:HD2	20:S:84:TYR:HB2	1.66	0.77
22:U:32:ARG:H	22:U:32:ARG:NE	1.81	0.77
17:P:117:ILE:HD11	29:X:1995:G:H4'	1.66	0.77
29:X:7:G:H2'	29:X:8:A:H8	1.50	0.77
29:X:1097:A:O2'	29:X:1098:G:N7	2.17	0.77
8:G:88:VAL:HG21	8:G:127:ILE:HD11	1.67	0.77
29:X:2494:C:H42	29:X:2548:G:H1	1.30	0.77
3:B:6:GLY:HA3	3:B:27:LEU:O	1.85	0.77
2:A:69:ARG:HH12	2:A:192:THR:HG22	1.50	0.77
29:X:2418:A:H4'	29:X:2419:C:C5'	2.16	0.76
15:N:102:GLU:OE1	16:O:13:ARG:NH2	2.18	0.76
30:Y:40:C:O2	30:Y:50:U:O2'	2.01	0.76
29:X:1770:U:H5	29:X:1775:A:N7	1.83	0.76
29:X:1674:C:H2'	29:X:1675:C:H6	1.49	0.76
17:P:81:HIS:O	17:P:83:ASP:N	2.18	0.76
27:2:12:ARG:NH1	29:X:476:G:OP1	2.19	0.76
25:Z:15:LYS:O	25:Z:18:MET:N	2.18	0.76
29:X:1058:G:O2'	29:X:1120:C:N4	2.19	0.76
3:B:78:LEU:O	3:B:79:ARG:NE	2.17	0.76
10:I:28:LYS:O	10:I:30:ALA:N	2.19	0.76
6:E:107:ILE:O	6:E:152:ARG:NH1	2.19	0.76
29:X:693:A:H2'	29:X:694:G:C8	2.20	0.76
29:X:857:U:H3'	29:X:858:G:C8	2.21	0.76
11:J:32:ASP:H	11:J:108:ALA:HB2	1.51	0.76
20:S:25:ASN:HA	20:S:85:MET:HB2	1.68	0.76
24:W:40:VAL:HA	24:W:43:MET:HE3	1.67	0.75
5:D:111:ILE:HG12	5:D:137:ILE:HD12	1.65	0.75
19:R:37:LEU:HD11	19:R:49:GLU:HG3	1.68	0.75

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1225:G:H1'	29:X:1250:A:N6	1.98	0.75
29:X:1104:G:H21	29:X:1109:A:H62	1.33	0.75
21:T:25:LYS:HB2	21:T:37:LEU:HA	1.67	0.75
29:X:2629:U:H2'	29:X:2630:C:H6	1.52	0.75
16:O:14:VAL:HG11	16:O:95:ILE:HG13	1.69	0.74
17:P:15:LYS:HB3	29:X:512:A:H4'	1.67	0.74
9:H:22:ILE:HD11	29:X:1935:A:C6	2.22	0.74
5:D:14:PRO:HA	5:D:17:MET:HB2	1.68	0.74
29:X:43:A:H61	29:X:447:U:H3	1.36	0.74
15:N:12:ARG:NH1	29:X:1229:C:OP2	2.21	0.74
19:R:15:HIS:CD2	19:R:16:PHE:HD2	2.06	0.74
29:X:867:G:H1	29:X:935:C:H42	1.32	0.74
14:M:93:ILE:HD12	14:M:93:ILE:H	1.52	0.74
29:X:455:A:H2	29:X:1258:G:N3	1.85	0.74
29:X:1437:A:H2'	29:X:1438:G:H8	1.52	0.74
30:Y:4:C:N4	30:Y:121:G:O6	2.18	0.74
29:X:2543:A:H5'	29:X:2627:G:H4'	1.69	0.74
29:X:2789:U:H3	29:X:2861:A:H61	1.36	0.74
29:X:2672:U:H2'	29:X:2673:G:H8	1.52	0.74
5:D:131:GLY:HA2	5:D:154:ILE:H	1.52	0.73
13:L:39:TYR:OH	30:Y:118:G:N3	2.21	0.73
29:X:205:A:H2'	29:X:206:U:H5'	1.68	0.73
29:X:2639:A:N3	29:X:2639:A:H5''	2.02	0.73
5:D:38:GLU:HB3	5:D:87:ILE:HB	1.70	0.73
17:P:109:ARG:NH2	29:X:1996:A:N3	2.37	0.73
29:X:517:A:C5'	29:X:518:A:H5'	2.18	0.73
7:F:73:PRO:O	7:F:75:SER:N	2.20	0.73
29:X:333:A:H5'	29:X:351:A:H1'	1.70	0.73
29:X:2417:U:O2'	29:X:2419:C:OP1	2.06	0.73
29:X:2811:G:H2'	29:X:2812:A:C8	2.23	0.73
5:D:92:ARG:NH2	30:Y:47:A:OP1	2.21	0.73
8:G:151:TYR:OH	8:G:158:HIS:NE2	2.21	0.73
12:K:81:ASP:O	12:K:85:PRO:HG3	1.88	0.73
5:D:60:ILE:HG22	5:D:140:GLU:HB2	1.70	0.73
10:I:130:ILE:HG12	10:I:140:VAL:HG21	1.70	0.73
29:X:692:C:H2'	29:X:693:A:H8	1.54	0.73
29:X:2550:C:H5''	29:X:2551:A:C5'	2.18	0.73
17:P:62:ARG:HH11	25:Z:25:LEU:HD11	1.53	0.73
19:R:16:PHE:CE2	19:R:81:VAL:HG11	2.23	0.73
19:R:93:ARG:NH2	29:X:312:G:OP2	2.19	0.73
29:X:1279:G:O2'	29:X:1995:G:O6	2.06	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1479:G:H2'	29:X:1480:G:C8	2.24	0.72
29:X:1726:C:O2'	29:X:2834:A:N3	2.21	0.72
2:A:201:HIS:O	2:A:203:ASN:N	2.21	0.72
29:X:402:A:N7	29:X:2392:G:O2'	2.22	0.72
29:X:2270:U:O2'	29:X:2353:G:N3	2.21	0.72
29:X:421:G:H2'	29:X:422:C:H6	1.54	0.72
29:X:2611:A:H61	29:X:2766:U:H3	1.36	0.72
2:A:108:PRO:HB3	2:A:143:HIS:HE1	1.53	0.72
23:V:51:ALA:O	23:V:55:THR:OG1	2.08	0.72
9:H:21:CYS:SG	9:H:22:ILE:N	2.62	0.72
13:L:89:PHE:O	13:L:91:ARG:NH2	2.22	0.72
29:X:834:A:H5'	29:X:835:U:H6	1.53	0.72
9:H:22:ILE:HG22	9:H:52:VAL:HG12	1.70	0.72
15:N:48:ARG:NH2	29:X:987:G:OP1	2.22	0.72
29:X:488:A:H2'	29:X:489:A:C8	2.25	0.72
29:X:2014:A:C6	29:X:2477:C:H1'	2.25	0.72
2:A:17:THR:OG1	2:A:205:VAL:N	2.22	0.72
3:B:84:PHE:CD2	3:B:86:PRO:HD3	2.25	0.72
2:A:239:ARG:HG3	29:X:2569:A:H5''	1.72	0.72
28:3:52:LYS:O	28:3:54:GLU:N	2.23	0.72
29:X:1164:C:H2'	29:X:1165:G:H8	1.53	0.72
12:K:87:TYR:CD1	12:K:90:ARG:HD2	2.25	0.72
24:W:5:LEU:HB2	24:W:25:LEU:HD13	1.71	0.72
29:X:46:C:H2'	29:X:47:G:H8	1.52	0.72
29:X:2336:G:N2	29:X:2339:A:OP2	2.22	0.72
2:A:39:LYS:NZ	2:A:58:HIS:H	1.88	0.71
9:H:47:VAL:HG23	9:H:77:THR:HG23	1.72	0.71
10:I:63:ARG:NH1	29:X:2396:C:OP1	2.22	0.71
20:S:54:ILE:HB	20:S:62:PHE:HB2	1.70	0.71
29:X:1437:A:H2'	29:X:1438:G:C8	2.25	0.71
29:X:2522:G:H2'	29:X:2523:G:H8	1.54	0.71
15:N:26:GLY:O	15:N:28:ARG:N	2.23	0.71
20:S:148:THR:HB	20:S:165:GLU:HA	1.71	0.71
12:K:3:HIS:O	12:K:5:LYS:N	2.21	0.71
15:N:111:ASP:O	15:N:115:ASN:ND2	2.22	0.71
19:R:77:HIS:HD2	29:X:339:U:H4'	1.55	0.71
29:X:1333:G:C2	29:X:1342:U:H5''	2.26	0.71
29:X:2761:A:H5''	29:X:2762:G:H5'	1.72	0.71
19:R:22:VAL:HG11	19:R:81:VAL:HG22	1.70	0.71
23:V:2:LYS:NZ	29:X:76:C:OP1	2.17	0.71
7:F:75:SER:O	7:F:79:ARG:NH1	2.23	0.71

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:10:LEU:O	12:K:12:ARG:N	2.24	0.71
29:X:789:G:N1	29:X:2055:G:OP1	2.17	0.71
30:Y:25:G:H1	30:Y:62:C:H42	1.37	0.71
22:U:31:GLY:HA2	22:U:32:ARG:HH11	1.56	0.70
29:X:1030:U:H3	29:X:1153:A:N6	1.89	0.70
29:X:1505:U:H1'	29:X:1506:C:H2'	1.73	0.70
29:X:2665:G:C2	29:X:2704:U:O2	2.44	0.70
4:C:148:VAL:HG13	4:C:185:ARG:HB3	1.73	0.70
29:X:542:A:OP1	29:X:570:G:N2	2.24	0.70
29:X:1212:U:H2'	29:X:1213:U:C6	2.26	0.70
29:X:1997:A:H2'	29:X:1998:A:C8	2.26	0.70
28:3:13:ARG:NH2	29:X:227:G:OP2	2.24	0.70
29:X:713:G:H22	29:X:745:C:H5	1.38	0.70
29:X:870:C:N4	29:X:871:U:O4	2.25	0.70
29:X:2013:A:H4'	29:X:2014:A:C8	2.26	0.70
15:N:37:GLN:HG3	29:X:1265:G:H1	1.55	0.70
24:W:35:SER:O	24:W:37:THR:N	2.22	0.70
29:X:2418:A:H4'	29:X:2419:C:H5''	1.74	0.70
3:B:176:ARG:HH21	14:M:16:ILE:HA	1.54	0.70
12:K:90:ARG:NH1	29:X:2855:C:O2'	2.25	0.70
25:Z:33:CYS:O	25:Z:35:GLN:N	2.23	0.70
29:X:1662:G:H5''	29:X:1663:C:H5'	1.71	0.70
29:X:1939:U:H1'	29:X:2531:U:OP1	1.90	0.70
20:S:74:ARG:HH22	30:Y:94:G:H5''	1.54	0.70
29:X:1053:G:H1	29:X:1124:U:H3	1.38	0.70
29:X:2387:U:H2'	29:X:2388:G:C8	2.27	0.70
8:G:169:GLN:HG2	8:G:170:PRO:HD2	1.73	0.70
13:L:44:ASP:O	13:L:46:SER:N	2.24	0.70
19:R:100:ASP:HB3	19:R:101:GLY:HA3	1.74	0.70
29:X:2123:G:N2	29:X:2134:U:O2	2.25	0.70
5:D:39:GLY:HA2	5:D:86:GLY:HA2	1.74	0.69
29:X:1267:A:H5''	29:X:1268:U:H5''	1.72	0.69
29:X:2378:G:H1	29:X:2396:C:H42	1.40	0.69
3:B:110:GLY:HA2	3:B:161:GLY:HA3	1.74	0.69
30:Y:64:C:H2'	30:Y:65:A:C8	2.27	0.69
1:0:42:ARG:HH22	1:0:209:TYR:HB2	1.56	0.69
29:X:172:A:H5''	29:X:173:A:OP2	1.92	0.69
29:X:1937:G:O2'	29:X:1939:U:O4	2.10	0.69
2:A:274:ARG:NH2	29:X:1788:C:OP2	2.24	0.69
4:C:111:ARG:HH11	4:C:181:LEU:HA	1.56	0.69
5:D:50:ILE:HG22	5:D:87:ILE:HD11	1.74	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:104:LEU:HA	14:M:106:TYR:CE2	2.27	0.69
29:X:2187:A:H2	29:X:2198:U:H3	1.38	0.69
29:X:2775:U:O2'	29:X:2778:U:OP2	2.08	0.69
2:A:198:ASN:O	2:A:200:GLU:N	2.26	0.69
10:I:86:THR:OG1	10:I:116:ARG:NH1	2.26	0.69
29:X:57:G:N2	29:X:68:C:O2	2.24	0.69
29:X:2845:C:N4	29:X:2846:G:O6	2.25	0.69
30:Y:27:A:OP2	30:Y:27:A:H8	1.75	0.69
6:E:143:GLN:HG3	29:X:2725:C:H1'	1.74	0.69
10:I:60:LEU:O	28:3:13:ARG:NH1	2.26	0.69
11:J:22:ALA:HB2	11:J:99:LYS:HB2	1.74	0.69
11:J:65:ILE:HA	11:J:107:VAL:HG12	1.74	0.69
11:J:15:ARG:HG2	11:J:74:PRO:HD2	1.75	0.69
22:U:31:GLY:HA2	22:U:32:ARG:NH1	2.08	0.69
29:X:711:C:O2'	29:X:747:A:N6	2.25	0.69
12:K:3:HIS:N	29:X:2795:A:H4'	2.08	0.69
21:T:34:GLY:HA3	29:X:2332:G:H1'	1.75	0.69
29:X:877:G:H1	29:X:924:C:H42	1.39	0.69
10:I:75:VAL:HG22	10:I:99:VAL:HG11	1.75	0.68
29:X:1185:C:H2'	29:X:1186:G:H2'	1.74	0.68
2:A:243:GLY:HA3	29:X:2576:G:H5'	1.74	0.68
4:C:72:ARG:HE	4:C:77:PHE:HE2	1.41	0.68
12:K:29:LEU:HD13	12:K:79:VAL:HB	1.75	0.68
13:L:33:ARG:HE	13:L:38:ILE:HG21	1.57	0.68
17:P:50:VAL:HB	17:P:91:PHE:HA	1.75	0.68
29:X:796:A:H4'	29:X:2567:G:H4'	1.75	0.68
30:Y:5:C:N3	30:Y:120:G:N2	2.37	0.68
8:G:109:GLY:O	8:G:111:LYS:N	2.26	0.68
9:H:23:ARG:HG3	9:H:24:VAL:H	1.57	0.68
9:H:69:VAL:HG12	9:H:70:VAL:H	1.58	0.68
15:N:54:LYS:NZ	29:X:1006:C:OP2	2.27	0.68
29:X:1043:A:H2	29:X:1133:G:H22	1.39	0.68
1:O:208:ALA:HB3	1:O:220:LEU:HB2	1.75	0.68
29:X:511:A:O2'	29:X:512:A:OP1	2.09	0.68
29:X:1255:A:H2'	29:X:1256:C:H6	1.59	0.68
29:X:2032:G:N2	29:X:2598:C:O2	2.24	0.68
9:H:134:LEU:HA	14:M:48:GLN:HE22	1.59	0.68
26:1:15:SER:OG	26:1:48:VAL:O	2.12	0.68
2:A:161:THR:H	2:A:196:VAL:HB	1.59	0.68
3:B:132:LYS:NZ	29:X:2590:U:OP1	2.27	0.68
4:C:47:THR:H	4:C:50:GLN:HG3	1.58	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:76:TYR:HE2	29:X:1163:C:HO2'	1.41	0.68
29:X:33:C:N4	29:X:458:G:O2'	2.27	0.68
29:X:1116:U:H2'	29:X:1117:G:C8	2.29	0.68
15:N:92:ARG:NH2	29:X:1009:C:OP2	2.26	0.67
29:X:796:A:OP1	29:X:1778:U:O2'	2.12	0.67
29:X:1556:A:H2'	29:X:1557:G:H8	1.58	0.67
29:X:1850:G:O4'	29:X:1867:A:N6	2.26	0.67
29:X:2690:A:OP1	29:X:2692:A:P	2.52	0.67
29:X:79:G:H2'	29:X:80:A:C8	2.28	0.67
29:X:654:A:O2'	29:X:655:A:OP1	2.12	0.67
29:X:2485:U:O2	32:X:6178:HGR:H23	1.93	0.67
8:G:142:ARG:NH2	29:X:539:A:OP2	2.24	0.67
24:W:43:MET:HE1	29:X:940:G:N2	2.05	0.67
29:X:198:A:N1	29:X:242:A:O2'	2.26	0.67
29:X:677:G:O2'	29:X:952:A:OP2	2.12	0.67
29:X:580:A:H4'	29:X:581:A:OP1	1.95	0.67
29:X:2440:C:H2'	29:X:2441:U:H6	1.58	0.67
2:A:173:VAL:HG23	2:A:187:SER:HB3	1.76	0.67
4:C:62:LYS:NZ	29:X:2043:A:H3'	2.10	0.67
29:X:1005:U:O2'	29:X:1007:A:OP1	2.10	0.67
29:X:2043:A:H1'	29:X:2481:G:C1'	2.24	0.67
4:C:129:LYS:HB3	4:C:132:ASN:ND2	2.10	0.67
29:X:1401:G:H1	29:X:1412:C:H42	1.40	0.67
29:X:1407:G:O6	29:X:1408:A:N6	2.28	0.67
29:X:2225:G:H2'	29:X:2226:A:H8	1.58	0.67
29:X:219:G:N2	29:X:231:G:H2'	2.10	0.67
29:X:1507:A:H2'	29:X:1508:G:C8	2.30	0.67
29:X:2816:C:C2	29:X:2852:G:N2	2.63	0.67
4:C:112:GLN:HA	4:C:117:LEU:HG	1.76	0.67
1:O:104:MET:SD	1:O:130:ARG:NH1	2.68	0.67
20:S:1:MET:HG3	20:S:52:PHE:HD2	1.60	0.67
16:O:35:LEU:HD23	16:O:36:LYS:H	1.60	0.67
29:X:168:A:H2'	29:X:169:C:C6	2.30	0.67
2:A:55:GLY:HA3	2:A:218:LYS:HG3	1.77	0.66
4:C:4:ILE:HG22	4:C:13:ARG:HH12	1.60	0.66
9:H:25:LEU:HD22	9:H:52:VAL:HG23	1.77	0.66
28:3:58:MET:HA	28:3:61:MET:HG3	1.76	0.66
29:X:1686:A:OP2	31:X:6021:MG:MG	1.38	0.66
29:X:546:A:H2'	29:X:547:U:C6	2.28	0.66
29:X:1301:U:O2'	29:X:1664:G:N2	2.29	0.66
29:X:1679:U:O2	29:X:2666:U:H5''	1.94	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:3:LEU:HG	20:S:32:PHE:CD1	2.30	0.66
29:X:403:A:H4'	29:X:404:A:H5'	1.76	0.66
29:X:1195:U:H2'	29:X:1196:G:C8	2.30	0.66
29:X:2873:G:H2'	29:X:2874:A:C8	2.29	0.66
10:I:68:VAL:HG13	10:I:69:GLY:H	1.60	0.66
12:K:31:GLU:O	12:K:33:ARG:N	2.25	0.66
15:N:24:PHE:HB2	15:N:29:SER:HB3	1.76	0.66
21:T:46:LYS:HE2	21:T:77:ARG:H	1.60	0.66
27:2:8:ASN:HB3	27:2:11:LYS:HB3	1.77	0.66
29:X:474:G:N2	29:X:477:A:OP2	2.28	0.66
29:X:1454:U:H2'	29:X:1455:C:H6	1.61	0.66
29:X:2241:U:H2'	29:X:2242:C:H6	1.61	0.66
29:X:2791:C:C2	29:X:2806:G:N2	2.63	0.66
30:Y:64:C:H2'	30:Y:65:A:H8	1.60	0.66
2:A:274:ARG:HH22	29:X:1788:C:P	2.18	0.66
29:X:2826:C:H2'	29:X:2827:G:O4'	1.95	0.66
11:J:68:ARG:O	11:J:102:ARG:NH2	2.29	0.66
29:X:1030:U:H3	29:X:1153:A:H62	1.44	0.66
1:0:127:LEU:HD23	1:0:130:ARG:HG3	1.76	0.66
7:F:96:VAL:HB	7:F:136:VAL:HG12	1.75	0.66
9:H:40:GLY:HA3	29:X:2545:A:H61	1.61	0.66
24:W:39:ALA:O	29:X:864:C:O2'	2.14	0.66
29:X:1697:U:O2'	29:X:1754:G:N7	2.25	0.66
29:X:2226:A:H2'	29:X:2227:C:H6	1.61	0.66
3:B:119:ARG:HG2	3:B:120:TRP:CD1	2.31	0.66
16:O:22:VAL:HG12	16:O:23:GLU:H	1.60	0.66
29:X:1223:G:H4'	29:X:1224:A:H5''	1.78	0.66
29:X:1624:A:H1'	29:X:1626:A:OP2	1.96	0.66
26:1:14:SER:HB2	26:1:47:VAL:HG11	1.77	0.66
29:X:1454:U:H2'	29:X:1455:C:C6	2.30	0.66
29:X:2450:A:N6	29:X:2455:A:O2'	2.29	0.66
29:X:2690:A:P	29:X:2692:A:OP2	2.54	0.66
12:K:46:PRO:O	12:K:50:GLN:HG3	1.96	0.65
15:N:13:ARG:NH1	29:X:1264:C:H5''	2.11	0.65
1:0:212:THR:O	29:X:2106:G:N2	2.28	0.65
4:C:9:GLN:O	4:C:10:ASN:ND2	2.16	0.65
7:F:12:LEU:HD22	7:F:18:THR:HG21	1.78	0.65
26:1:7:ARG:NH2	29:X:2265:A:OP2	2.28	0.65
29:X:1753:A:H8	29:X:1753:A:O5'	1.78	0.65
29:X:1856:U:OP1	29:X:2389:G:O2'	2.12	0.65
10:I:90:ARG:HB2	10:I:93:LEU:HB2	1.76	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:66:ASN:HA	15:N:76:TYR:HB2	1.77	0.65
29:X:335:A:N6	29:X:349:G:O2'	2.28	0.65
29:X:573:C:H2'	29:X:574:C:H6	1.59	0.65
29:X:1482:U:O4'	29:X:1562:G:N2	2.30	0.65
5:D:37:ASN:OD1	29:X:2291:U:O2'	2.13	0.65
6:E:28:GLY:HA3	6:E:79:VAL:HB	1.78	0.65
14:M:40:ARG:HB3	14:M:40:ARG:HH11	1.59	0.65
17:P:90:LEU:HD11	17:P:128:VAL:HB	1.76	0.65
7:F:112:MET:HG3	7:F:113:PRO:HD3	1.77	0.65
12:K:20:LEU:O	12:K:22:ARG:N	2.29	0.65
29:X:1467:U:O2	29:X:1468:A:N6	2.30	0.65
29:X:421:G:H1	29:X:432:C:H42	1.44	0.65
29:X:1359:G:O6	29:X:1616:C:N4	2.27	0.65
5:D:36:VAL:HB	5:D:89:VAL:HG23	1.79	0.65
12:K:108:VAL:HG12	12:K:109:THR:O	1.96	0.65
2:A:238:GLY:O	2:A:240:THR:OG1	2.13	0.65
6:E:45:GLN:NE2	6:E:47:GLY:O	2.30	0.65
26:1:29:ARG:O	26:1:30:ASN:ND2	2.30	0.65
29:X:992:A:N1	29:X:2010:G:O2'	2.25	0.65
29:X:2191:A:H5''	29:X:2192:U:H5	1.61	0.65
1:0:152:LEU:HD23	1:0:157:ILE:HD12	1.79	0.65
2:A:206:LEU:HB2	29:X:1782:A:O3'	1.97	0.65
12:K:11:ASN:HD22	12:K:11:ASN:N	1.92	0.65
29:X:1255:A:H2'	29:X:1256:C:C6	2.32	0.65
4:C:164:VAL:HB	4:C:167:VAL:HG22	1.79	0.65
11:J:81:GLU:HB3	21:T:4:LYS:HE2	1.80	0.65
12:K:87:TYR:HD1	12:K:90:ARG:HD2	1.62	0.65
29:X:510:G:H22	29:X:513:A:H5'	1.61	0.65
29:X:1140:A:O2'	29:X:2494:C:O2	2.14	0.65
2:A:225:ALA:HB1	29:X:795:A:O2'	1.98	0.64
7:F:115:LEU:O	7:F:117:ALA:N	2.24	0.64
29:X:2410:U:O2	29:X:2412:A:H8	1.79	0.64
11:J:23:LYS:O	20:S:73:LYS:NZ	2.29	0.64
13:L:16:LYS:NZ	13:L:90:ASP:OD1	2.29	0.64
18:Q:66:GLY:O	18:Q:68:PHE:N	2.29	0.64
19:R:58:VAL:HA	29:X:494:A:H5'	1.79	0.64
2:A:223:GLY:HA2	2:A:226:MET:HG3	1.77	0.64
29:X:876:A:H2'	29:X:877:G:C8	2.33	0.64
8:G:124:GLU:HB3	8:G:150:VAL:HB	1.80	0.64
11:J:52:ARG:HG3	11:J:67:ILE:HD11	1.79	0.64
12:K:73:LYS:H	12:K:73:LYS:CE	2.10	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:33:ARG:HG2	13:L:99:ARG:HG3	1.79	0.64
29:X:104:C:H2'	29:X:105:G:H8	1.62	0.64
23:V:2:LYS:HE2	23:V:52:GLN:NE2	2.12	0.64
29:X:746:G:N7	29:X:774:A:C6	2.66	0.64
29:X:1981:A:HO2'	29:X:2704:U:HO2'	1.40	0.64
30:Y:16:U:H1'	30:Y:109:G:H21	1.62	0.64
29:X:2691:C:O2'	29:X:2692:A:O5'	2.13	0.64
29:X:7:G:H2'	29:X:8:A:C8	2.33	0.64
29:X:10:A:H2'	29:X:11:G:H8	1.63	0.64
29:X:531:G:H2'	29:X:532:A:H8	1.61	0.64
29:X:540:G:N2	29:X:2006:G:OP1	2.27	0.64
29:X:1838:G:H2'	29:X:1839:A:C8	2.33	0.64
29:X:2099:G:OP2	29:X:2149:G:O2'	2.14	0.64
18:Q:29:VAL:HG12	18:Q:30:SER:H	1.63	0.64
29:X:794:A:H2	29:X:1767:G:N3	1.96	0.64
29:X:2299:A:N6	29:X:2312:A:O2'	2.30	0.64
22:U:28:GLY:O	22:U:30:VAL:N	2.30	0.64
26:1:38:LYS:HG2	26:1:48:VAL:HG22	1.80	0.64
29:X:14:A:C6	29:X:536:A:C2	2.86	0.64
29:X:2775:U:H4'	29:X:2777:A:H3'	1.79	0.64
3:B:51:TYR:N	3:B:75:THR:HG21	2.13	0.64
3:B:149:ARG:O	29:X:2035:G:H1'	1.98	0.64
6:E:137:ASP:OD1	6:E:138:LYS:N	2.30	0.64
13:L:90:ASP:OD2	13:L:91:ARG:N	2.31	0.64
15:N:6:THR:HG21	15:N:10:ARG:HB2	1.80	0.64
29:X:88:G:H5''	29:X:89:A:H5''	1.79	0.64
29:X:1237:G:O2'	29:X:1238:A:H5'	1.97	0.64
29:X:2617:G:O2'	29:X:2755:A:N1	2.31	0.64
29:X:1090:C:N4	29:X:1099:A:OP1	2.28	0.63
29:X:1116:U:H2'	29:X:1117:G:H8	1.60	0.63
29:X:1366:A:H2'	29:X:1367:A:C8	2.32	0.63
1:O:10:VAL:HG21	1:O:216:PRO:HG2	1.80	0.63
10:I:18:ARG:NH2	29:X:1263:G:N7	2.47	0.63
11:J:82:THR:HG23	21:T:4:LYS:HG3	1.81	0.63
29:X:2040:A:H2'	29:X:2041:A:C8	2.33	0.63
29:X:104:C:H2'	29:X:105:G:C8	2.33	0.63
2:A:134:ARG:HB3	2:A:187:SER:HB2	1.79	0.63
4:C:173:ALA:O	4:C:175:VAL:N	2.32	0.63
29:X:1393:G:O2'	29:X:1585:A:N6	2.31	0.63
29:X:2278:A:H61	29:X:2296:U:H3	1.45	0.63
10:I:90:ARG:O	10:I:121:HIS:ND1	2.32	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:2:5:TYR:HE1	29:X:699:G:C8	2.17	0.63
29:X:942:U:H2'	29:X:943:U:H6	1.63	0.63
29:X:1329:U:H2'	29:X:1330:G:H8	1.63	0.63
29:X:1429:A:C6	29:X:1600:U:H4'	2.34	0.63
4:C:126:ALA:HB3	4:C:132:ASN:ND2	2.14	0.63
28:3:22:VAL:HG13	28:3:55:TRP:CD1	2.33	0.63
29:X:5:A:H2'	29:X:6:A:C8	2.33	0.63
29:X:2043:A:H1'	29:X:2481:G:O4'	1.97	0.63
29:X:2736:U:H4'	29:X:2737:A:OP1	1.99	0.63
10:I:16:ARG:HH22	29:X:598:U:P	2.22	0.63
12:K:11:ASN:H	12:K:11:ASN:ND2	1.95	0.63
20:S:68:ALA:HB3	20:S:82:ASP:HB2	1.80	0.63
5:D:34:ILE:HG22	5:D:91:LEU:HB2	1.79	0.63
15:N:50:ARG:HA	15:N:53:LYS:HE2	1.81	0.63
21:T:56:ASP:HB2	21:T:58:THR:OG1	1.99	0.63
29:X:89:A:H4'	29:X:90:G:O5'	1.97	0.63
29:X:1507:A:H2'	29:X:1508:G:H8	1.62	0.63
2:A:71:ASP:HB3	2:A:103:ARG:HH12	1.64	0.62
9:H:76:ARG:O	9:H:94:ASN:HA	1.98	0.62
17:P:93:LYS:HD3	17:P:94:GLU:HG3	1.81	0.62
19:R:23:ILE:HA	19:R:32:GLN:O	1.98	0.62
29:X:1705:U:O4'	29:X:1718:A:N6	2.32	0.62
7:F:90:THR:HB	29:X:1087:C:H1'	1.80	0.62
3:B:102:ILE:N	3:B:170:LEU:O	2.31	0.62
13:L:37:HIS:HE1	13:L:39:TYR:CD1	2.18	0.62
29:X:652:C:N4	29:X:657:A:H61	1.95	0.62
29:X:858:G:O2'	29:X:859:U:OP2	2.17	0.62
29:X:2191:A:OP1	29:X:2193:C:N4	2.32	0.62
29:X:2674:C:H2'	29:X:2675:U:C6	2.33	0.62
2:A:123:ALA:HB1	2:A:129:ASN:HD22	1.64	0.62
6:E:17:VAL:HG22	6:E:26:VAL:HG13	1.81	0.62
15:N:3:ARG:HB3	29:X:1261:G:C5	2.34	0.62
29:X:2102:A:O4'	29:X:2155:U:O2'	2.17	0.62
29:X:2240:C:O2	29:X:2258:G:N2	2.19	0.62
29:X:2369:U:H3'	29:X:2369:U:H6	1.64	0.62
10:I:94:GLU:N	10:I:97:ARG:HH11	1.97	0.62
28:3:25:PHE:HA	28:3:47:GLY:HA2	1.80	0.62
29:X:1703:C:H2'	29:X:1704:G:O4'	1.99	0.62
3:B:27:LEU:HD23	3:B:29:GLY:H	1.64	0.62
26:1:46:HIS:HD2	29:X:2350:G:O2'	1.83	0.62
29:X:334:G:OP1	29:X:349:G:N2	2.32	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:2640:G:H2'	29:X:2641:A:C8	2.35	0.62
7:F:62:ASP:OD1	7:F:63:ARG:NH1	2.32	0.62
22:U:23:LYS:HD2	22:U:35:THR:HG21	1.81	0.62
29:X:421:G:H2'	29:X:422:C:C6	2.34	0.62
29:X:1454:U:H3	29:X:1567:A:H61	1.47	0.62
29:X:1654:A:H4'	29:X:2690:A:O2'	2.00	0.62
3:B:132:LYS:O	3:B:134:TRP:N	2.33	0.62
9:H:124:MET:O	9:H:127:VAL:HG12	1.99	0.62
14:M:104:LEU:HA	14:M:106:TYR:HE2	1.64	0.62
25:Z:14:SER:O	25:Z:18:MET:HG3	2.00	0.62
29:X:160:C:O2'	29:X:445:A:N3	2.31	0.62
29:X:427:C:H2'	29:X:428:A:C8	2.34	0.62
29:X:494:A:H3'	29:X:495:C:H6	1.65	0.62
29:X:2285:U:H5'	29:X:2286:G:C8	2.35	0.62
19:R:84:VAL:HG22	19:R:89:GLY:HA2	1.80	0.62
28:3:17:THR:OG1	28:3:18:GLY:N	2.33	0.62
29:X:1642:G:H5''	29:X:1643:A:OP1	2.00	0.62
29:X:2033:C:N4	29:X:2034:A:N1	2.48	0.62
30:Y:68:A:N6	30:Y:111:C:OP2	2.33	0.62
13:L:27:LEU:HD13	13:L:84:ILE:HG23	1.82	0.61
29:X:170:U:N3	29:X:180:C:O2	2.32	0.61
29:X:1192:A:H2'	29:X:1193:G:H8	1.63	0.61
2:A:63:ARG:HH21	2:A:86:PRO:HD3	1.65	0.61
4:C:149:LEU:HD21	4:C:170:LEU:HD12	1.82	0.61
29:X:555:U:C2	29:X:1243:G:C2	2.88	0.61
29:X:571:U:HO2'	29:X:581:A:H8	1.47	0.61
29:X:753:U:H2'	29:X:754:G:C8	2.34	0.61
29:X:1790:G:N2	29:X:1811:A:OP2	2.31	0.61
29:X:2186:G:H2'	29:X:2187:A:C8	2.36	0.61
9:H:2:ILE:N	9:H:45:ALA:O	2.27	0.61
29:X:1030:U:O2	29:X:1155:G:N2	2.33	0.61
29:X:1066:G:H1	29:X:1115:C:H42	1.48	0.61
11:J:43:ILE:O	11:J:95:VAL:HA	2.00	0.61
19:R:51:VAL:HG13	19:R:73:GLU:HB3	1.81	0.61
19:R:93:ARG:NH2	29:X:311:A:O5'	2.33	0.61
29:X:510:G:N2	29:X:513:A:H5'	2.16	0.61
29:X:1077:U:O2'	29:X:1079:G:N7	2.28	0.61
9:H:51:ILE:HD11	9:H:53:ALA:HB2	1.81	0.61
29:X:98:U:O2	29:X:100:G:N1	2.33	0.61
29:X:759:C:OP1	29:X:761:G:H4'	2.01	0.61
29:X:1511:A:N1	29:X:1512:A:N6	2.48	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:67:ALA:HA	29:X:1268:U:C5	2.35	0.61
9:H:41:ASN:HB2	29:X:2654:A:H5'	1.83	0.61
17:P:94:GLU:HB2	17:P:127:ILE:HB	1.83	0.61
29:X:1608:U:H2'	29:X:1609:G:C8	2.36	0.61
3:B:12:THR:OG1	14:M:17:GLU:OE1	2.18	0.61
17:P:111:ARG:HG2	29:X:764:A:O4'	2.01	0.61
29:X:220:U:H2'	29:X:221:A:H8	1.65	0.61
2:A:142:VAL:HG23	2:A:193:ILE:HA	1.82	0.61
3:B:55:ALA:H	3:B:58:LYS:NZ	1.97	0.61
8:G:67:ARG:O	8:G:70:PHE:HB2	2.01	0.61
16:O:55:THR:OG1	16:O:56:VAL:N	2.33	0.61
17:P:98:ASP:OD1	29:X:23:G:N2	2.29	0.61
18:Q:2:SER:OG	18:Q:3:HIS:N	2.32	0.61
29:X:1770:U:H6	29:X:1775:A:H62	1.49	0.61
19:R:25:LEU:HD11	19:R:82:ALA:HB2	1.83	0.61
16:O:40:VAL:HG12	16:O:42:GLY:H	1.66	0.61
19:R:68:GLY:N	29:X:494:A:O2'	2.33	0.61
29:X:90:G:H5''	29:X:91:A:OP2	2.01	0.61
29:X:926:C:H42	30:Y:104:A:H5'	1.66	0.61
29:X:2672:U:H2'	29:X:2673:G:C8	2.35	0.61
13:L:104:ALA:O	13:L:108:ARG:N	2.31	0.60
15:N:18:LEU:HA	15:N:21:ALA:HB3	1.83	0.60
22:U:20:ARG:NE	29:X:393:U:OP1	2.34	0.60
29:X:653:G:H21	29:X:656:U:H3	1.49	0.60
29:X:761:G:C8	29:X:763:A:C8	2.89	0.60
29:X:836:G:H2'	29:X:837:U:C6	2.36	0.60
29:X:2201:G:H2'	29:X:2202:G:H8	1.66	0.60
2:A:210:GLY:HA2	29:X:777:A:H5'	1.82	0.60
3:B:26:VAL:HG12	3:B:182:ILE:HB	1.82	0.60
9:H:16:ALA:CB	9:H:98:ILE:HD11	2.31	0.60
29:X:174:A:N6	29:X:2409:A:O2'	2.33	0.60
29:X:588:G:O2'	29:X:2002:A:OP1	2.14	0.60
29:X:761:G:C8	29:X:763:A:N7	2.69	0.60
29:X:1863:U:H2'	29:X:1864:G:C8	2.34	0.60
1:O:123:LEU:HB3	1:O:127:LEU:HB2	1.84	0.60
3:B:189:PRO:HA	29:X:2659:C:C5'	2.31	0.60
4:C:40:ARG:NH2	29:X:39:C:O2	2.32	0.60
4:C:133:PHE:HB2	4:C:160:ALA:HB1	1.82	0.60
12:K:46:PRO:HB3	29:X:2814:G:H5'	1.82	0.60
29:X:1690:U:O2'	29:X:1691:G:OP1	2.18	0.60
9:H:8:LEU:HD23	9:H:8:LEU:H	1.64	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:106:ASP:N	29:X:1300:A:N7	2.49	0.60
19:R:83:LEU:O	19:R:92:THR:OG1	2.20	0.60
20:S:127:PRO:HA	20:S:130:ILE:HD11	1.82	0.60
22:U:51:ILE:HG23	22:U:59:THR:HA	1.83	0.60
29:X:531:G:H2'	29:X:532:A:C8	2.35	0.60
29:X:957:G:H2'	29:X:958:G:H8	1.66	0.60
29:X:2208:U:H2'	29:X:2209:G:H8	1.66	0.60
29:X:2038:C:H2'	29:X:2483:U:H4'	1.82	0.60
29:X:2246:A:H61	29:X:2251:U:H3	1.48	0.60
30:Y:6:C:H2'	30:Y:7:C:C6	2.36	0.60
5:D:72:LYS:HG3	5:D:81:GLN:HG3	1.83	0.60
11:J:36:ILE:HG12	11:J:103:VAL:HG13	1.83	0.60
12:K:11:ASN:OD1	29:X:1669:A:N6	2.35	0.60
20:S:167:THR:OG1	29:X:888:G:H4'	2.01	0.60
29:X:490:A:N3	29:X:492:G:H5''	2.17	0.60
29:X:505:G:H8	29:X:505:G:O5'	1.84	0.60
29:X:1982:C:OP1	29:X:2703:C:O2'	2.19	0.60
29:X:2639:A:H3'	29:X:2640:G:C8	2.37	0.60
29:X:330:C:H2'	29:X:331:U:H6	1.67	0.60
29:X:691:C:H2'	29:X:692:C:H6	1.65	0.60
30:Y:17:A:OP1	30:Y:110:U:O2'	2.13	0.60
5:D:34:ILE:HG13	5:D:156:ILE:HG23	1.83	0.60
9:H:40:GLY:CA	29:X:2545:A:H61	2.14	0.60
13:L:19:THR:O	13:L:21:THR:N	2.34	0.60
17:P:24:GLY:O	17:P:127:ILE:HA	2.01	0.60
4:C:62:LYS:HZ2	29:X:2043:A:H5'	1.67	0.60
4:C:142:LEU:HB3	4:C:166:TRP:HH2	1.66	0.60
5:D:35:VAL:HG11	29:X:2293:G:H5'	1.83	0.60
6:E:137:ASP:OD1	6:E:139:GLN:N	2.35	0.60
29:X:2579:A:H2'	29:X:2580:C:C6	2.37	0.60
9:H:38:GLY:O	29:X:2627:G:H1'	2.01	0.60
16:O:32:LYS:HZ3	16:O:57:GLN:HB3	1.66	0.60
17:P:63:SER:HB2	29:X:1993:G:H5''	1.83	0.60
20:S:91:PRO:HG3	20:S:126:GLY:H	1.66	0.60
20:S:154:LEU:HD22	20:S:158:CYS:HB2	1.83	0.60
29:X:633:G:C2	29:X:634:G:C8	2.90	0.60
29:X:1479:G:H2'	29:X:1480:G:H8	1.66	0.60
29:X:1681:A:N3	29:X:2706:U:C2	2.69	0.60
29:X:1992:G:O2'	29:X:1993:G:H5'	2.02	0.60
29:X:2277:A:C2	29:X:2278:A:H1'	2.36	0.60
6:E:83:TYR:CE1	6:E:138:LYS:HB2	2.37	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:87:VAL:HG21	13:L:108:ARG:HH12	1.67	0.59
22:U:51:ILE:O	22:U:52:ARG:NH2	2.33	0.59
29:X:70:A:H4'	29:X:71:A:H5''	1.84	0.59
29:X:389:G:H1	29:X:411:C:H42	1.50	0.59
29:X:825:C:H2'	29:X:826:U:H6	1.67	0.59
29:X:1556:A:H2'	29:X:1557:G:C8	2.35	0.59
2:A:208:LYS:HB2	29:X:742:G:C5	2.37	0.59
20:S:105:GLN:O	20:S:109:GLN:NE2	2.35	0.59
25:Z:19:ARG:HA	29:X:2029:G:H5'	1.84	0.59
28:3:33:ASN:O	28:3:35:GLY:N	2.35	0.59
6:E:17:VAL:HG13	6:E:26:VAL:HG22	1.82	0.59
11:J:39:GLU:HB2	11:J:128:ILE:HG22	1.83	0.59
29:X:1701:C:C2	29:X:1722:G:N2	2.69	0.59
5:D:113:ASP:HB3	5:D:115:ARG:HH12	1.65	0.59
7:F:89:SER:HA	29:X:1075:C:H4'	1.84	0.59
12:K:20:LEU:O	12:K:23:ALA:N	2.36	0.59
21:T:23:VAL:HB	21:T:38:VAL:HG22	1.83	0.59
29:X:451:A:H2'	29:X:452:G:C8	2.37	0.59
29:X:663:G:H2'	29:X:664:C:H4'	1.84	0.59
29:X:1117:G:H2'	29:X:1118:G:H8	1.66	0.59
29:X:2013:A:H4'	29:X:2014:A:H8	1.66	0.59
2:A:33:LEU:HD13	2:A:104:TYR:HD2	1.66	0.59
2:A:273:ARG:HB2	2:A:275:LYS:HE2	1.85	0.59
7:F:54:PRO:HG2	7:F:70:LYS:HB2	1.83	0.59
11:J:72:ASP:OD2	11:J:72:ASP:N	2.35	0.59
12:K:37:THR:HB	12:K:40:LYS:HG3	1.85	0.59
19:R:77:HIS:O	19:R:79:SER:N	2.35	0.59
29:X:388:G:OP1	29:X:406:G:OP1	2.20	0.59
29:X:1504:G:N2	29:X:1517:C:O2	2.35	0.59
1:0:113:PRO:HG3	1:0:142:GLY:HA2	1.84	0.59
4:C:131:LYS:HA	4:C:134:ILE:HD12	1.85	0.59
9:H:75:VAL:HG22	9:H:96:ALA:HA	1.84	0.59
11:J:47:GLN:OE1	11:J:127:PRO:HD3	2.01	0.59
14:M:16:ILE:O	14:M:18:GLN:N	2.32	0.59
29:X:118:U:H4'	29:X:119:G:H5''	1.83	0.59
29:X:129:A:H61	29:X:142:U:H3	1.50	0.59
29:X:1909:U:H5''	29:X:1911:A:OP2	2.02	0.59
29:X:2791:C:O2	29:X:2858:A:O2'	2.19	0.59
2:A:70:ARG:NH1	2:A:146:GLU:OE2	2.35	0.59
3:B:9:ILE:HD11	3:B:27:LEU:HB2	1.83	0.59
5:D:37:ASN:ND2	29:X:2291:U:O2	2.35	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:R:19:GLY:H	19:R:36:VAL:HB	1.68	0.59
29:X:575:U:O2'	29:X:822:G:OP2	2.20	0.59
29:X:1053:G:N2	29:X:1124:U:O2	2.29	0.59
29:X:2821:G:H2'	29:X:2822:U:H6	1.64	0.59
1:0:174:ALA:HA	1:0:181:LEU:HD21	1.83	0.59
2:A:263:ARG:NH1	29:X:2206:C:OP1	2.35	0.59
29:X:627:A:H2'	29:X:628:A:C8	2.38	0.59
29:X:2180:U:H2'	29:X:2203:G:H1	1.67	0.59
1:0:138:SER:OG	1:0:139:GLY:N	2.34	0.59
15:N:33:ARG:HB3	29:X:1265:G:C2	2.38	0.59
29:X:511:A:HO2'	29:X:512:A:P	2.26	0.59
29:X:712:A:H2'	29:X:713:G:O4'	2.03	0.59
29:X:847:C:HO2'	29:X:2337:A:HO2'	1.51	0.59
29:X:1827:G:H1'	29:X:1914:U:C2	2.38	0.59
29:X:2088:U:H3	29:X:2167:A:H61	1.50	0.59
29:X:2559:U:H5''	29:X:2560:G:OP2	2.03	0.59
29:X:2792:C:C2	29:X:2805:G:N2	2.71	0.59
13:L:38:ILE:HD12	13:L:39:TYR:H	1.67	0.59
18:Q:35:LYS:HD2	18:Q:53:ILE:HD13	1.85	0.59
25:Z:38:GLY:O	25:Z:39:LYS:HG2	2.01	0.59
26:1:35:LEU:HB3	26:1:51:ALA:HB2	1.83	0.59
30:Y:25:G:H1	30:Y:62:C:N4	2.01	0.59
1:0:15:GLN:HB3	1:0:221:ALA:HB2	1.85	0.58
1:0:136:PRO:HA	1:0:141:VAL:HG11	1.84	0.58
19:R:77:HIS:CD2	29:X:339:U:H4'	2.37	0.58
29:X:82:G:N2	29:X:100:G:H1'	2.18	0.58
29:X:641:G:N2	29:X:644:A:OP2	2.34	0.58
29:X:1465:G:N2	29:X:1466:C:C2	2.71	0.58
3:B:4:ILE:HG12	3:B:5:LEU:H	1.67	0.58
4:C:84:PHE:CE1	29:X:596:C:H5'	2.38	0.58
12:K:92:GLY:HA2	12:K:94:TYR:CE2	2.38	0.58
19:R:26:SER:HB2	29:X:321:A:H5'	1.85	0.58
29:X:455:A:C2	29:X:1258:G:N3	2.68	0.58
29:X:1326:U:H4'	29:X:1345:G:H4'	1.85	0.58
29:X:1679:U:H2'	29:X:1680:U:O4'	2.02	0.58
29:X:2516:U:H2'	29:X:2517:C:C6	2.37	0.58
8:G:140:GLN:HG3	29:X:567:G:C5'	2.30	0.58
9:H:115:ALA:O	9:H:117:GLU:N	2.36	0.58
20:S:103:ARG:HH22	20:S:107:GLU:HB3	1.67	0.58
23:V:32:ALA:HA	23:V:37:LEU:HB2	1.84	0.58
29:X:548:G:H1	29:X:564:U:H3	1.50	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:970:A:N3	29:X:2436:U:O2'	2.33	0.58
29:X:1100:G:H5'	29:X:1101:U:OP2	2.04	0.58
4:C:125:ILE:HD12	4:C:133:PHE:HA	1.85	0.58
8:G:31:THR:OG1	29:X:1006:C:N3	2.37	0.58
18:Q:88:ILE:HD11	18:Q:91:LEU:HB2	1.85	0.58
23:V:42:ARG:NH1	23:V:45:GLN:OE1	2.36	0.58
29:X:243:G:H1	29:X:439:C:H42	1.50	0.58
29:X:930:A:H4'	30:Y:100:G:N3	2.18	0.58
29:X:958:G:H2'	29:X:959:C:C6	2.38	0.58
10:I:77:LEU:O	10:I:79:GLN:N	2.37	0.58
12:K:3:HIS:O	12:K:3:HIS:CD2	2.56	0.58
14:M:102:ALA:O	14:M:103:LYS:NZ	2.26	0.58
15:N:19:LYS:NZ	29:X:1233:A:OP1	2.36	0.58
15:N:31:GLN:NE2	29:X:589:C:H4'	2.18	0.58
15:N:91:ASN:HD22	15:N:93:LYS:HB3	1.69	0.58
29:X:1117:G:H2'	29:X:1118:G:C8	2.38	0.58
29:X:1655:C:H5''	29:X:2689:C:H1'	1.85	0.58
29:X:1815:G:H2'	29:X:1816:G:H8	1.68	0.58
29:X:2226:A:H2'	29:X:2227:C:C6	2.37	0.58
5:D:128:TYR:HB3	5:D:156:ILE:HD12	1.84	0.58
6:E:150:LYS:NZ	29:X:2741:G:H21	2.00	0.58
11:J:16:GLY:O	11:J:73:LYS:NZ	2.36	0.58
13:L:32:TYR:O	13:L:34:SER:N	2.36	0.58
19:R:8:SER:OG	19:R:9:HIS:N	2.36	0.58
26:1:42:PRO:HG3	29:X:2327:U:O2'	2.03	0.58
29:X:622:U:H2'	29:X:623:G:C8	2.38	0.58
29:X:2418:A:H4'	29:X:2419:C:H5'	1.84	0.58
29:X:2633:A:N1	29:X:2644:A:H5''	2.17	0.58
13:L:43:ILE:HG22	13:L:45:ASP:H	1.69	0.58
14:M:70:LYS:NZ	14:M:72:SER:OG	2.37	0.58
15:N:83:LEU:HD22	15:N:88:ILE:HD12	1.85	0.58
28:3:64:ARG:HH21	29:X:219:G:P	2.26	0.58
29:X:2565:C:H2'	29:X:2566:A:C8	2.39	0.58
10:I:72:TYR:HD1	10:I:107:LYS:HZ2	1.52	0.58
13:L:49:GLN:HG2	30:Y:116:C:H4'	1.86	0.58
17:P:41:VAL:HG11	17:P:65:SER:HA	1.84	0.58
29:X:1035:G:C6	29:X:1036:G:C6	2.92	0.58
29:X:1040:A:C8	29:X:1041:G:C8	2.92	0.58
29:X:1124:U:H2'	29:X:1125:G:C8	2.39	0.58
29:X:1298:G:C6	29:X:1342:U:C6	2.92	0.58
29:X:1621:C:O2	29:X:1626:A:O2'	2.20	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1921:A:O2'	29:X:1922:U:H5'	2.03	0.58
29:X:2625:U:O5'	29:X:2625:U:H6	1.87	0.58
10:I:75:VAL:HG12	10:I:108:LEU:HD13	1.85	0.58
14:M:31:ASP:OD1	14:M:96:ARG:HA	2.04	0.58
22:U:48:LYS:HE3	29:X:2074:U:H1'	1.85	0.58
29:X:1033:G:N2	29:X:1034:U:O4	2.28	0.58
1:O:182:SER:HA	1:O:185:TYR:HB3	1.86	0.58
14:M:106:TYR:CE1	29:X:1745:C:H5'	2.39	0.58
15:N:3:ARG:HB3	29:X:1261:G:C4	2.39	0.58
21:T:53:MET:HG2	21:T:57:HIS:HA	1.86	0.58
29:X:834:A:H5'	29:X:835:U:C6	2.38	0.58
4:C:86:PRO:HD3	29:X:1261:G:C8	2.38	0.57
9:H:90:ARG:NH2	14:M:78:GLU:OE1	2.37	0.57
9:H:97:VAL:HG11	9:H:126:ILE:HD13	1.86	0.57
14:M:46:ARG:HG2	14:M:47:SER:H	1.68	0.57
15:N:58:ARG:O	15:N:62:ILE:HG13	2.04	0.57
19:R:13:LYS:NZ	29:X:349:G:OP1	2.30	0.57
20:S:123:VAL:HG23	20:S:161:ALA:HB2	1.84	0.57
24:W:2:LYS:HB3	24:W:54:GLN:HB2	1.87	0.57
29:X:333:A:H5'	29:X:351:A:C1'	2.33	0.57
29:X:501:G:H2'	29:X:502:A:O4'	2.04	0.57
29:X:2531:U:H2'	29:X:2533:U:OP2	2.04	0.57
30:Y:58:G:H4'	30:Y:59:A:H5''	1.84	0.57
2:A:62:TYR:HE1	29:X:1808:C:H3'	1.69	0.57
5:D:66:ILE:HD11	30:Y:43:G:H2'	1.85	0.57
6:E:66:GLY:HA3	29:X:2728:A:H4'	1.86	0.57
15:N:59:ARG:HH22	29:X:1019:U:H4'	1.69	0.57
16:O:71:ILE:HB	16:O:84:THR:OG1	2.04	0.57
25:Z:3:LYS:HD2	29:X:2556:A:H4'	1.84	0.57
29:X:484:G:H2'	29:X:485:G:H8	1.69	0.57
29:X:622:U:H2'	29:X:623:G:H8	1.68	0.57
29:X:836:G:N2	29:X:847:C:O2	2.37	0.57
29:X:936:A:H2'	29:X:937:C:C6	2.40	0.57
29:X:1281:A:H2'	29:X:1282:A:C8	2.40	0.57
29:X:1608:U:H2'	29:X:1609:G:H8	1.68	0.57
29:X:2198:U:H3'	29:X:2199:C:H4'	1.85	0.57
29:X:2424:G:H2'	29:X:2425:G:H8	1.69	0.57
1:O:187:ALA:HA	1:O:190:SER:HB3	1.86	0.57
9:H:25:LEU:CD2	9:H:52:VAL:HG23	2.34	0.57
11:J:11:ARG:NH2	11:J:72:ASP:HB2	2.19	0.57
13:L:35:SER:OG	13:L:36:LYS:N	2.37	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:R:58:VAL:HG13	19:R:60:PRO:HD2	1.85	0.57
29:X:548:G:C2	29:X:549:G:C8	2.91	0.57
29:X:992:A:H5''	29:X:993:C:OP2	2.04	0.57
29:X:1067:G:H1'	29:X:1114:A:H61	1.69	0.57
29:X:1072:U:N3	29:X:1080:A:OP1	2.38	0.57
29:X:1336:G:C2'	29:X:1337:G:H5'	2.32	0.57
29:X:2391:A:C8	29:X:2392:G:C8	2.91	0.57
2:A:210:GLY:HA3	29:X:777:A:OP1	2.04	0.57
8:G:33:ILE:HG21	29:X:548:G:H5'	1.84	0.57
11:J:27:TYR:HB3	11:J:137:VAL:HB	1.85	0.57
19:R:106:VAL:O	19:R:112:LYS:HB2	2.04	0.57
29:X:668:A:H4'	29:X:669:G:H5'	1.85	0.57
29:X:2197:U:H2'	29:X:2198:U:C6	2.38	0.57
16:O:34:GLU:HG3	16:O:57:GLN:HA	1.86	0.57
17:P:31:VAL:HG12	17:P:122:SER:O	2.05	0.57
17:P:59:PHE:HD1	25:Z:30:LEU:HD11	1.70	0.57
29:X:691:C:H2'	29:X:692:C:C6	2.39	0.57
2:A:108:PRO:HB3	2:A:143:HIS:CE1	2.36	0.57
13:L:37:HIS:CE1	13:L:39:TYR:HD1	2.23	0.57
29:X:1464:A:H61	29:X:1477:C:H42	1.50	0.57
30:Y:39:C:H5''	30:Y:40:C:C5	2.39	0.57
3:B:92:ASN:OD1	3:B:92:ASN:N	2.37	0.57
4:C:8:GLY:H	4:C:121:ASP:HB3	1.70	0.57
15:N:6:THR:O	15:N:8:ILE:N	2.35	0.57
16:O:32:LYS:NZ	16:O:57:GLN:HB3	2.20	0.57
20:S:63:PRO:HB2	20:S:86:VAL:HG22	1.87	0.57
29:X:308:C:H2'	29:X:309:G:C8	2.40	0.57
29:X:485:G:C6	29:X:520:C:N4	2.73	0.57
29:X:497:C:O2	29:X:505:G:N2	2.38	0.57
2:A:142:VAL:HA	2:A:194:GLY:H	1.69	0.57
5:D:5:LYS:HA	5:D:8:TYR:CD2	2.40	0.57
5:D:126:GLY:O	5:D:160:ALA:HB3	2.04	0.57
8:G:84:ASN:ND2	8:G:154:GLU:OE1	2.34	0.57
17:P:80:LEU:HD11	17:P:87:GLU:HB2	1.87	0.57
27:2:12:ARG:HD2	27:2:44:VAL:HG11	1.87	0.57
29:X:1787:U:H2'	29:X:1788:C:H6	1.70	0.57
29:X:1981:A:H4'	29:X:2704:U:O2'	2.03	0.57
2:A:211:ARG:HD2	2:A:214:TRP:CZ3	2.40	0.57
2:A:260:ARG:NH2	2:A:267:ASP:OD1	2.24	0.57
12:K:24:GLN:HB3	12:K:44:LEU:HD22	1.87	0.57
15:N:24:PHE:CE1	29:X:543:G:H5'	2.40	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:958:G:H2'	29:X:959:C:H6	1.70	0.57
29:X:1071:U:H4'	29:X:1072:U:H5'	1.86	0.57
29:X:1192:A:H2'	29:X:1193:G:C8	2.40	0.57
29:X:2124:C:N4	29:X:2125:C:N3	2.53	0.57
29:X:2354:G:N2	29:X:2357:A:OP2	2.34	0.57
29:X:2691:C:H2'	29:X:2694:G:H5''	1.85	0.57
1:0:53:ASN:ND2	1:0:161:ASN:OD1	2.37	0.57
15:N:50:ARG:O	15:N:53:LYS:HG2	2.04	0.57
17:P:31:VAL:HG11	17:P:124:ILE:CD1	2.33	0.57
29:X:533:C:H5''	29:X:550:C:O2'	2.05	0.57
28:3:24:ALA:O	28:3:48:PHE:N	2.33	0.56
29:X:654:A:H2'	29:X:655:A:C8	2.39	0.56
29:X:1458:A:H5''	29:X:1459:U:OP2	2.05	0.56
29:X:1529:C:H2'	29:X:1530:U:C6	2.40	0.56
29:X:1982:C:H2'	29:X:1983:G:O4'	2.05	0.56
4:C:189:ASP:OD1	4:C:190:ALA:N	2.37	0.56
24:W:13:PRO:HG2	24:W:16:GLN:HB2	1.87	0.56
28:3:28:GLY:HA3	28:3:32:GLN:OE1	2.06	0.56
29:X:602:C:H42	29:X:678:G:H1	1.52	0.56
29:X:874:A:H2'	29:X:875:G:O4'	2.05	0.56
29:X:1845:A:H2'	29:X:1846:A:C8	2.40	0.56
29:X:1935:A:C6	29:X:1936:A:N1	2.73	0.56
29:X:2048:C:H5''	29:X:2231:G:H1'	1.86	0.56
1:0:73:ILE:HG12	1:0:95:LEU:HB3	1.86	0.56
3:B:141:ILE:HD12	29:X:2035:G:C8	2.40	0.56
3:B:144:ARG:HD3	29:X:2551:A:C8	2.41	0.56
3:B:152:LYS:HB3	8:G:106:TYR:CE1	2.41	0.56
14:M:100:ARG:NH2	29:X:1744:G:OP1	2.34	0.56
19:R:43:ASP:OD2	19:R:43:ASP:N	2.38	0.56
22:U:20:ARG:HB3	22:U:43:ARG:NH2	2.20	0.56
28:3:3:LYS:HA	29:X:602:C:H1'	1.88	0.56
29:X:340:G:H4'	29:X:341:A:OP2	2.06	0.56
29:X:837:U:H2'	29:X:838:A:C8	2.39	0.56
29:X:1002:C:H5'	29:X:1200:G:OP2	2.05	0.56
29:X:1793:A:H2'	29:X:1794:A:C8	2.40	0.56
29:X:2197:U:H2'	29:X:2198:U:C5	2.40	0.56
29:X:2251:U:H5''	29:X:2252:A:OP1	2.05	0.56
30:Y:16:U:O2'	30:Y:17:A:OP2	2.21	0.56
5:D:69:LYS:NZ	30:Y:43:G:H1	2.04	0.56
8:G:95:LEU:HA	8:G:115:ALA:HB3	1.88	0.56
11:J:12:LYS:O	11:J:13:GLN:HB2	2.05	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:69:ARG:NH2	14:M:108:LYS:HA	2.20	0.56
15:N:37:GLN:HG3	29:X:1265:G:N1	2.20	0.56
17:P:27:VAL:HG22	17:P:125:THR:OG1	2.05	0.56
17:P:36:ARG:NH1	25:Z:20:ARG:HH21	2.04	0.56
4:C:97:ARG:NH2	29:X:630:G:N7	2.53	0.56
29:X:16:G:H2'	29:X:17:G:H8	1.71	0.56
29:X:52:A:H5''	29:X:53:G:OP2	2.05	0.56
29:X:224:G:H4'	29:X:399:G:C4	2.41	0.56
29:X:858:G:H8	29:X:858:G:OP2	1.87	0.56
29:X:1863:U:H2'	29:X:1864:G:H8	1.70	0.56
29:X:2605:C:H2'	29:X:2606:G:H8	1.70	0.56
29:X:2662:C:C2'	29:X:2663:U:H5'	2.35	0.56
2:A:48:ARG:HH21	29:X:791:G:H5'	1.70	0.56
3:B:7:THR:HG23	3:B:194:GLY:O	2.06	0.56
3:B:109:LYS:HG2	3:B:191:ALA:HB2	1.87	0.56
8:G:51:LEU:HD12	8:G:88:VAL:HG11	1.87	0.56
28:3:56:ALA:HA	28:3:59:LYS:HG3	1.88	0.56
29:X:1329:U:H2'	29:X:1330:G:C8	2.40	0.56
29:X:1909:U:P	29:X:1912:G:H1	2.26	0.56
29:X:1956:G:H2'	29:X:1957:C:C6	2.41	0.56
29:X:1989:C:O5'	29:X:1989:C:H6	1.88	0.56
2:A:142:VAL:HG23	2:A:193:ILE:HD13	1.86	0.56
3:B:2:LYS:HA	3:B:84:PHE:HE1	1.70	0.56
3:B:107:THR:O	3:B:190:GLY:HA3	2.05	0.56
29:X:840:U:H4'	29:X:841:G:C8	2.41	0.56
29:X:2129:U:H2'	29:X:2130:G:H8	1.70	0.56
29:X:2308:A:H2'	29:X:2309:G:C8	2.40	0.56
4:C:158:ARG:O	4:C:161:ALA:N	2.39	0.56
8:G:136:PRO:O	8:G:141:GLY:HA3	2.06	0.56
13:L:11:LEU:HD21	29:X:2273:C:OP1	2.06	0.56
29:X:1016:C:H1'	29:X:1023:U:N3	2.20	0.56
29:X:1428:G:HO2'	29:X:1429:A:H8	1.53	0.56
4:C:188:ILE:HB	4:C:189:ASP:O	2.05	0.56
12:K:73:LYS:H	12:K:73:LYS:HE2	1.71	0.56
20:S:3:LEU:HB2	20:S:33:ALA:O	2.06	0.56
26:1:9:ILE:HA	26:1:25:THR:HG22	1.87	0.56
29:X:10:A:H2'	29:X:11:G:C8	2.40	0.56
29:X:628:A:H2'	29:X:629:C:C6	2.40	0.56
29:X:692:C:H2'	29:X:693:A:C8	2.37	0.56
29:X:1383:C:H3'	29:X:1384:G:H8	1.71	0.56
29:X:1736:C:H2'	29:X:1737:G:C8	2.41	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:52:ARG:HG2	2:A:53:PHE:CD2	2.41	0.56
15:N:94:VAL:O	15:N:98:ILE:HG12	2.06	0.56
21:T:9:SER:HB3	29:X:2235:G:O2'	2.05	0.56
25:Z:7:PRO:HA	29:X:2594:U:C2	2.42	0.56
29:X:415:A:H61	29:X:435:A:H61	1.54	0.56
29:X:806:A:OP2	29:X:2054:A:O2'	2.24	0.56
29:X:861:G:H22	29:X:943:U:H1'	1.69	0.56
29:X:861:G:N3	29:X:944:A:H1'	2.21	0.56
29:X:995:A:P	29:X:996:C:H41	2.28	0.56
29:X:1426:U:H3	29:X:1605:A:H61	1.54	0.56
29:X:1656:U:OP1	29:X:2688:G:N2	2.39	0.56
29:X:1707:A:H3'	29:X:1708:C:H6	1.71	0.56
29:X:1856:U:H3	29:X:1861:G:H1	1.52	0.56
29:X:2225:G:H2'	29:X:2226:A:C8	2.40	0.56
29:X:2387:U:H2'	29:X:2388:G:H8	1.70	0.56
4:C:146:GLU:O	4:C:166:TRP:HE3	1.90	0.55
13:L:37:HIS:HD2	30:Y:29:C:O3'	1.89	0.55
17:P:60:ILE:HD11	25:Z:28:PRO:HD3	1.88	0.55
22:U:30:VAL:O	22:U:32:ARG:NH1	2.39	0.55
29:X:1342:U:O5'	29:X:1343:C:H5	1.87	0.55
29:X:1690:U:H6	29:X:1690:U:H3'	1.72	0.55
29:X:2434:G:H2'	29:X:2435:C:C6	2.41	0.55
29:X:2516:U:H2'	29:X:2517:C:H6	1.70	0.55
5:D:13:ARG:HB2	5:D:14:PRO:HD3	1.88	0.55
5:D:85:VAL:HG23	29:X:2291:U:H5'	1.88	0.55
9:H:2:ILE:HD12	9:H:6:SER:OG	2.06	0.55
16:O:66:GLY:O	16:O:87:ARG:HD2	2.06	0.55
20:S:69:VAL:HG22	20:S:81:VAL:HG22	1.88	0.55
29:X:1244:U:H2'	29:X:1245:G:C8	2.36	0.55
29:X:2198:U:C2	29:X:2199:C:H1'	2.41	0.55
2:A:142:VAL:HG21	2:A:191:ALA:HB1	1.89	0.55
15:N:61:TRP:O	15:N:65:ILE:HG13	2.05	0.55
16:O:28:GLU:O	16:O:30:GLY:N	2.39	0.55
20:S:151:ASP:OD2	20:S:151:ASP:N	2.37	0.55
22:U:22:GLY:C	22:U:39:LYS:HZ3	2.08	0.55
29:X:165:G:O2'	29:X:1378:A:N6	2.39	0.55
29:X:568:G:H2'	29:X:569:C:O4'	2.07	0.55
29:X:652:C:N3	29:X:658:G:N2	2.54	0.55
29:X:787:A:O2'	29:X:788:G:O4'	2.24	0.55
29:X:810:U:H2'	29:X:811:G:O4'	2.06	0.55
2:A:246:PRO:HG2	29:X:1884:A:O2'	2.07	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:23:GLU:O	16:O:25:LEU:N	2.38	0.55
19:R:58:VAL:HA	29:X:494:A:H4'	1.87	0.55
22:U:54:ASN:O	22:U:56:GLN:N	2.39	0.55
29:X:1975:G:N2	29:X:1979:C:O2'	2.37	0.55
29:X:2031:A:H2'	29:X:2032:G:H5''	1.89	0.55
29:X:2234:G:H2'	29:X:2235:G:O4'	2.07	0.55
29:X:2586:G:H2'	29:X:2587:G:O4'	2.05	0.55
1:O:68:VAL:HG22	1:O:153:LYS:HA	1.89	0.55
2:A:43:ARG:HA	2:A:48:ARG:O	2.06	0.55
2:A:208:LYS:HB2	29:X:742:G:C6	2.41	0.55
8:G:94:LYS:O	8:G:98:LYS:N	2.31	0.55
8:G:125:ARG:NH1	29:X:2619:G:OP1	2.36	0.55
15:N:13:ARG:O	15:N:16:LYS:HB2	2.06	0.55
21:T:46:LYS:HZ3	21:T:76:ALA:HA	1.71	0.55
28:3:52:LYS:O	28:3:55:TRP:N	2.39	0.55
29:X:877:G:H1	29:X:924:C:N4	2.03	0.55
29:X:1283:C:H5''	29:X:1284:G:H5'	1.88	0.55
29:X:1325:U:H4'	29:X:1326:U:O5'	2.05	0.55
29:X:1819:U:H2'	29:X:1820:G:O4'	2.06	0.55
29:X:2443:C:H42	29:X:2465:G:H1	1.52	0.55
28:3:33:ASN:HB3	29:X:2398:U:H5''	1.89	0.55
29:X:495:C:H2'	29:X:496:C:C6	2.42	0.55
29:X:1550:C:H2'	29:X:1553:G:H1	1.71	0.55
29:X:2328:G:O6	29:X:2361:G:N2	2.30	0.55
5:D:99:PHE:HA	5:D:102:LYS:HD2	1.88	0.55
19:R:23:ILE:HG13	19:R:31:GLY:HA2	1.88	0.55
29:X:774:A:H8	29:X:774:A:O5'	1.90	0.55
29:X:1710:U:H3	29:X:1821:A:H61	1.55	0.55
29:X:1922:U:OP1	29:X:2583:U:O2'	2.25	0.55
29:X:2546:G:H2'	29:X:2547:C:C6	2.42	0.55
30:Y:41:A:O2'	30:Y:48:A:N1	2.35	0.55
1:O:123:LEU:HD13	1:O:127:LEU:HD12	1.87	0.55
5:D:92:ARG:NH2	30:Y:46:G:H3'	2.22	0.55
8:G:61:ARG:HD3	8:G:66:HIS:CE1	2.42	0.55
29:X:2277:A:H2'	29:X:2278:A:O4'	2.07	0.55
29:X:2604:G:H2'	29:X:2605:C:O4'	2.07	0.55
10:I:65:PHE:HA	28:3:12:ARG:HD2	1.89	0.55
11:J:66:TYR:HE2	29:X:886:A:HO2'	1.55	0.55
11:J:78:LYS:NZ	11:J:84:MET:HG3	2.22	0.55
14:M:63:ARG:HD3	29:X:2661:G:H4'	1.88	0.55
21:T:21:LEU:HD11	21:T:41:ARG:NE	2.21	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:T:64:ASP:OD1	21:T:64:ASP:N	2.40	0.55
25:Z:17:ASP:HB3	29:X:16:G:OP1	2.07	0.55
27:2:12:ARG:CD	27:2:44:VAL:HG11	2.36	0.55
29:X:518:A:H5''	29:X:518:A:H8	1.71	0.55
29:X:974:U:H2'	29:X:975:C:C6	2.42	0.55
29:X:1108:U:H3'	29:X:1109:A:C8	2.41	0.55
29:X:1221:C:C2	29:X:1222:G:C8	2.95	0.55
29:X:1484:G:H2'	29:X:1485:U:C6	2.42	0.55
29:X:2053:G:H2'	29:X:2054:A:C8	2.41	0.55
1:O:38:GLU:HB2	1:O:211:THR:HB	1.88	0.55
3:B:84:PHE:HD2	3:B:86:PRO:HD3	1.71	0.55
13:L:64:LYS:HZ3	30:Y:53:G:H5''	1.72	0.55
20:S:168:VAL:HG12	20:S:169:VAL:H	1.71	0.55
24:W:17:VAL:O	24:W:20:VAL:N	2.40	0.55
25:Z:3:LYS:HB2	29:X:2590:U:O2	2.07	0.55
29:X:68:C:H2'	29:X:69:G:C8	2.41	0.55
29:X:713:G:O5'	29:X:713:G:H8	1.90	0.55
29:X:751:G:H2'	29:X:752:G:C8	2.41	0.55
29:X:2145:A:H4'	29:X:2155:U:H5''	1.89	0.55
3:B:22:PRO:HB3	29:X:2661:G:C2	2.42	0.54
3:B:134:TRP:CD1	3:B:137:ARG:HB2	2.42	0.54
9:H:4:PRO:O	9:H:5:GLN:HB2	2.07	0.54
13:L:19:THR:HG21	13:L:28:ARG:HD3	1.88	0.54
15:N:10:ARG:HG3	15:N:13:ARG:HH22	1.72	0.54
29:X:562:G:H2'	29:X:563:U:O4'	2.07	0.54
29:X:618:A:H2'	29:X:619:A:C8	2.43	0.54
29:X:825:C:HO2'	29:X:1239:A:HO2'	1.55	0.54
30:Y:7:C:H2'	30:Y:8:C:H6	1.72	0.54
3:B:116:VAL:HG11	3:B:138:PRO:HB3	1.89	0.54
5:D:24:SER:OG	30:Y:57:U:O3'	2.15	0.54
5:D:65:PRO:HA	5:D:89:VAL:HG13	1.89	0.54
10:I:90:ARG:HD2	10:I:93:LEU:HG	1.88	0.54
18:Q:84:GLU:OE2	18:Q:86:GLN:NE2	2.40	0.54
20:S:26:LYS:HE3	30:Y:107:C:H4'	1.89	0.54
21:T:12:ASN:OD1	21:T:12:ASN:N	2.40	0.54
26:1:37:LEU:HG	29:X:2323:U:O2'	2.06	0.54
27:2:37:LYS:HG2	29:X:469:G:C8	2.41	0.54
29:X:165:G:H2'	29:X:166:G:O4'	2.08	0.54
29:X:313:U:H2'	29:X:314:G:H8	1.72	0.54
29:X:1773:C:O4'	29:X:2588:U:C2	2.60	0.54
13:L:85:LYS:HD2	13:L:86:GLN:HG2	1.89	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:82:PRO:C	14:M:84:ALA:H	2.09	0.54
29:X:867:G:H1	29:X:935:C:N4	2.02	0.54
29:X:1298:G:C6	29:X:1342:U:C5	2.95	0.54
29:X:1987:G:C5	29:X:1988:A:C8	2.96	0.54
29:X:2482:A:H4'	29:X:2483:U:OP1	2.06	0.54
29:X:2605:C:H2'	29:X:2606:G:C8	2.43	0.54
4:C:117:LEU:HD22	4:C:188:ILE:HD11	1.88	0.54
24:W:19:THR:HG23	24:W:43:MET:HG2	1.88	0.54
29:X:1818:G:H2'	29:X:1819:U:H6	1.71	0.54
29:X:2030:U:H2'	29:X:2031:A:C8	2.42	0.54
29:X:2495:G:N2	29:X:2548:G:H1'	2.23	0.54
29:X:2574:G:N2	29:X:2577:A:OP2	2.39	0.54
29:X:2779:C:H2'	29:X:2780:A:H8	1.72	0.54
30:Y:86:A:C2	30:Y:96:C:N3	2.76	0.54
2:A:145:LEU:HD22	2:A:163:VAL:HG11	1.90	0.54
3:B:57:ARG:NH2	29:X:2809:A:H5'	2.21	0.54
3:B:108:SER:OG	3:B:162:MET:N	2.41	0.54
5:D:117:ILE:HG21	5:D:130:LEU:HD21	1.89	0.54
6:E:96:ALA:HA	6:E:104:GLU:O	2.08	0.54
14:M:106:TYR:CD2	14:M:106:TYR:N	2.75	0.54
18:Q:2:SER:O	18:Q:4:TYR:N	2.34	0.54
29:X:510:G:H2'	29:X:511:A:H3'	1.88	0.54
29:X:573:C:H2'	29:X:574:C:C6	2.41	0.54
29:X:659:G:H2'	29:X:660:G:C8	2.41	0.54
29:X:1296:G:N2	29:X:1299:A:H5'	2.23	0.54
29:X:1974:U:H2'	29:X:1975:G:H5'	1.89	0.54
1:O:112:THR:HB	1:O:115:MET:HB2	1.89	0.54
2:A:39:LYS:HZ1	2:A:58:HIS:H	1.54	0.54
8:G:31:THR:HG21	15:N:61:TRP:HE1	1.71	0.54
14:M:40:ARG:HB3	14:M:40:ARG:NH1	2.21	0.54
16:O:18:ASP:N	16:O:18:ASP:OD1	2.39	0.54
16:O:78:VAL:HG23	16:O:80:TYR:H	1.73	0.54
27:2:34:ARG:HD3	29:X:478:G:OP2	2.07	0.54
29:X:854:G:H1'	29:X:949:G:H22	1.71	0.54
29:X:932:G:H2'	29:X:933:G:C8	2.42	0.54
29:X:1030:U:OP1	29:X:1046:U:O2'	2.21	0.54
29:X:1385:C:H2'	29:X:1386:A:O4'	2.08	0.54
29:X:2285:U:H5	29:X:2290:A:C6	2.26	0.54
29:X:2660:C:C4	29:X:2704:U:C5	2.95	0.54
3:B:164:ARG:O	29:X:2753:C:H5''	2.08	0.54
3:B:175:ILE:HG12	3:B:182:ILE:HD11	1.90	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:80:ALA:HB2	13:L:111:GLY:O	2.08	0.54
20:S:49:THR:HG21	20:S:96:VAL:HG13	1.89	0.54
29:X:588:G:H1	29:X:1274:C:H42	1.55	0.54
29:X:706:A:H2'	29:X:707:U:O4'	2.08	0.54
29:X:994:A:N7	29:X:995:A:C6	2.76	0.54
29:X:1353:A:H3'	29:X:1354:A:C8	2.42	0.54
29:X:2557:G:H2'	29:X:2558:C:C6	2.43	0.54
5:D:64:LYS:HD3	30:Y:44:C:H4'	1.90	0.54
10:I:61:PRO:HG2	28:3:25:PHE:HB2	1.89	0.54
17:P:45:ILE:HD11	17:P:57:LEU:HG	1.90	0.54
29:X:597:U:H2'	29:X:598:U:C6	2.42	0.54
29:X:1818:G:H2'	29:X:1819:U:C6	2.43	0.54
2:A:260:ARG:HH22	2:A:266:SER:HB2	1.72	0.54
29:X:521:U:O4	29:X:522:G:N2	2.41	0.54
29:X:2594:U:H2'	29:X:2595:C:H6	1.73	0.54
8:G:106:TYR:CD2	29:X:2621:G:H5'	2.42	0.54
14:M:8:ASN:HA	29:X:2851:G:OP1	2.08	0.54
23:V:21:ARG:HG3	23:V:46:LEU:HD23	1.89	0.54
29:X:24:G:H2'	29:X:25:U:C6	2.43	0.54
29:X:1542:G:H2'	29:X:1543:G:C8	2.43	0.54
29:X:2433:G:H2'	29:X:2434:G:H8	1.73	0.54
29:X:2819:G:H2'	29:X:2820:C:H6	1.73	0.54
5:D:74:ILE:HA	5:D:79:LEU:HB2	1.90	0.53
6:E:41:LEU:HG	6:E:54:ARG:HA	1.90	0.53
11:J:78:LYS:HZ2	11:J:84:MET:HG3	1.73	0.53
18:Q:64:ARG:HB2	18:Q:69:ILE:HD13	1.90	0.53
18:Q:65:VAL:HG23	29:X:63:A:H1'	1.88	0.53
25:Z:45:ILE:HD13	25:Z:57:VAL:HG22	1.90	0.53
29:X:525:A:H2'	29:X:526:C:H5'	1.90	0.53
29:X:555:U:H5'	29:X:556:A:C2	2.43	0.53
29:X:1324:G:OP2	29:X:1324:G:N2	2.29	0.53
29:X:1329:U:H5'	29:X:1405:A:H1'	1.89	0.53
3:B:105:THR:HB	3:B:197:VAL:HG13	1.90	0.53
17:P:11:LYS:HG3	17:P:14:ARG:NH2	2.22	0.53
20:S:52:PHE:N	20:S:64:ALA:O	2.32	0.53
26:1:22:TYR:OH	29:X:2326:C:O2'	2.20	0.53
28:3:56:ALA:O	28:3:60:LEU:HG	2.08	0.53
29:X:957:G:H2'	29:X:958:G:C8	2.43	0.53
29:X:1359:G:H2'	29:X:1360:G:H8	1.73	0.53
29:X:2245:A:H4'	29:X:2246:A:C2	2.43	0.53
4:C:130:THR:HG21	29:X:331:U:H2'	1.90	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:35:LYS:HE2	29:X:820:U:P	2.48	0.53
19:R:48:VAL:HG13	19:R:50:GLY:H	1.72	0.53
20:S:55:THR:O	20:S:55:THR:OG1	2.23	0.53
22:U:21:ARG:HH21	22:U:23:LYS:HG2	1.72	0.53
25:Z:36:CYS:SG	25:Z:49:CYS:N	2.73	0.53
29:X:163:A:H2'	29:X:164:G:C8	2.43	0.53
29:X:175:C:O2'	29:X:176:A:H5'	2.08	0.53
9:H:132:GLU:HB2	14:M:73:PHE:CE1	2.44	0.53
12:K:34:ILE:O	12:K:112:LEU:HA	2.08	0.53
14:M:106:TYR:N	14:M:106:TYR:HD2	2.07	0.53
15:N:24:PHE:HB3	15:N:28:ARG:HB3	1.89	0.53
15:N:104:GLU:O	15:N:107:LYS:HB3	2.09	0.53
21:T:32:LYS:HB3	21:T:35:ASN:OD1	2.09	0.53
28:3:36:LYS:HB3	28:3:41:ILE:HG13	1.90	0.53
29:X:651:C:H2'	29:X:652:C:C6	2.44	0.53
29:X:1840:A:H2'	29:X:1841:G:O4'	2.09	0.53
29:X:2081:U:H3	29:X:2174:G:H1	1.55	0.53
29:X:2310:G:C6	29:X:2311:U:C5	2.97	0.53
29:X:2490:U:H2'	29:X:2491:C:O4'	2.09	0.53
3:B:11:MET:HG2	3:B:24:THR:OG1	2.09	0.53
3:B:176:ARG:NH2	14:M:16:ILE:HA	2.20	0.53
4:C:74:VAL:HG12	4:C:76:THR:H	1.74	0.53
8:G:110:LEU:HD22	29:X:1142:G:H4'	1.91	0.53
11:J:111:THR:HG22	11:J:114:GLN:HG3	1.91	0.53
20:S:103:ARG:NH2	20:S:107:GLU:HB3	2.22	0.53
29:X:548:G:N2	29:X:564:U:O2	2.33	0.53
29:X:645:G:H2'	29:X:646:C:C6	2.43	0.53
29:X:839:U:OP1	29:X:2408:G:OP1	2.26	0.53
29:X:1770:U:C2	29:X:1774:A:N7	2.77	0.53
29:X:2200:G:H2'	29:X:2201:G:C8	2.43	0.53
29:X:2451:G:H2'	29:X:2454:C:H42	1.74	0.53
29:X:2726:U:O2	29:X:2739:G:N2	2.41	0.53
4:C:33:TRP:HD1	4:C:93:TYR:CE1	2.27	0.53
4:C:67:ALA:HA	29:X:1268:U:C6	2.44	0.53
4:C:68:ARG:NH2	29:X:2043:A:N6	2.55	0.53
4:C:106:MET:O	4:C:110:SER:OG	2.15	0.53
12:K:27:ALA:O	12:K:30:ARG:N	2.42	0.53
12:K:83:VAL:HG23	12:K:87:TYR:CE2	2.43	0.53
15:N:54:LYS:NZ	29:X:1005:U:H3'	2.24	0.53
29:X:310:A:N3	29:X:330:C:O2'	2.40	0.53
29:X:493:A:OP2	29:X:517:A:N6	2.28	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1007:A:H2'	29:X:1008:G:H8	1.71	0.53
29:X:1020:A:N7	29:X:1021:A:C6	2.76	0.53
29:X:1430:G:O2'	29:X:1603:A:N3	2.41	0.53
29:X:1699:A:H61	29:X:1723:U:H3	1.57	0.53
29:X:2198:U:H3'	29:X:2199:C:C4'	2.38	0.53
29:X:2375:G:C2	29:X:2400:G:C2	2.96	0.53
29:X:2820:C:C2	29:X:2821:G:C8	2.97	0.53
3:B:37:LYS:NZ	3:B:80:GLU:OE2	2.38	0.53
3:B:147:PRO:HG2	3:B:149:ARG:HG2	1.90	0.53
13:L:63:ASN:HB3	13:L:66:ASP:HB2	1.91	0.53
22:U:20:ARG:HD2	22:U:43:ARG:NH1	2.23	0.53
25:Z:36:CYS:SG	25:Z:48:ASN:HB2	2.49	0.53
29:X:186:C:H2'	29:X:187:U:O4'	2.09	0.53
29:X:218:A:N1	29:X:232:A:H5''	2.23	0.53
29:X:513:A:C6	29:X:516:G:C6	2.97	0.53
29:X:1340:C:H2'	29:X:1341:G:C8	2.44	0.53
29:X:1662:G:H5''	29:X:1663:C:C5'	2.38	0.53
29:X:2084:G:H2'	29:X:2085:G:C8	2.43	0.53
8:G:50:PRO:HG3	29:X:1152:C:C5	2.44	0.53
8:G:122:HIS:ND1	8:G:122:HIS:O	2.39	0.53
9:H:35:THR:HG21	29:X:2628:C:O3'	2.09	0.53
13:L:64:LYS:NZ	30:Y:53:G:H5''	2.24	0.53
19:R:100:ASP:HB3	19:R:101:GLY:CA	2.38	0.53
29:X:571:U:O2'	29:X:581:A:H8	1.91	0.53
29:X:1069:G:H2'	29:X:1070:G:H8	1.73	0.53
29:X:1436:G:O3'	29:X:1508:G:O2'	2.27	0.53
29:X:1495:G:H2'	29:X:1496:G:C8	2.44	0.53
29:X:1991:C:H2'	29:X:1992:G:C8	2.44	0.53
29:X:2369:U:H3'	29:X:2369:U:C6	2.43	0.53
29:X:2769:C:H1'	29:X:2866:A:H2	1.73	0.53
29:X:2817:A:C2	29:X:2851:G:C2	2.96	0.53
2:A:229:VAL:HG11	29:X:797:A:C4	2.43	0.53
3:B:99:GLY:N	3:B:172:VAL:O	2.42	0.53
5:D:74:ILE:HG12	5:D:80:ARG:O	2.09	0.53
9:H:82:LYS:NZ	9:H:82:LYS:HB3	2.24	0.53
12:K:39:THR:O	12:K:42:LYS:N	2.42	0.53
15:N:91:ASN:HB3	15:N:94:VAL:HG23	1.91	0.53
17:P:97:VAL:HG22	17:P:124:ILE:HG23	1.89	0.53
19:R:44:GLN:HG2	19:R:77:HIS:HE1	1.72	0.53
22:U:32:ARG:H	22:U:32:ARG:HE	1.54	0.53
27:2:12:ARG:HD3	29:X:699:G:O6	2.09	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:500:G:H5''	29:X:501:G:OP2	2.09	0.53
29:X:937:C:H1'	29:X:939:C:H41	1.74	0.53
29:X:1692:C:C5	29:X:1693:A:N7	2.77	0.53
29:X:2750:G:H8	29:X:2750:G:O5'	1.92	0.53
1:O:157:ILE:HD13	1:O:157:ILE:H	1.73	0.53
3:B:145:LYS:HB2	29:X:2551:A:N7	2.24	0.53
4:C:34:GLN:HE21	29:X:627:A:P	2.31	0.53
7:F:115:LEU:HD22	7:F:126:THR:HG21	1.91	0.53
10:I:23:PRO:HD2	29:X:826:U:OP1	2.08	0.53
10:I:87:THR:OG1	10:I:97:ARG:NH2	2.41	0.53
11:J:84:MET:HE3	29:X:970:A:H62	1.73	0.53
13:L:35:SER:OG	30:Y:30:C:OP1	2.10	0.53
15:N:13:ARG:HH12	29:X:1264:C:P	2.30	0.53
19:R:58:VAL:HA	29:X:494:A:C5'	2.39	0.53
20:S:149:ALA:HB3	20:S:164:PRO:HA	1.91	0.53
29:X:307:C:C2'	29:X:308:C:H5'	2.38	0.53
29:X:359:G:H2'	29:X:360:A:C8	2.43	0.53
29:X:1104:G:N3	29:X:1110:G:N2	2.56	0.53
29:X:1924:C:N4	29:X:1948:C:OP2	2.42	0.53
29:X:2098:G:O2'	29:X:2154:A:N6	2.42	0.53
3:B:16:LYS:HB2	3:B:21:ILE:HD11	1.92	0.52
8:G:37:ASP:HB2	8:G:38:GLU:HG3	1.91	0.52
11:J:115:ALA:O	11:J:119:PHE:HB2	2.09	0.52
15:N:11:ARG:O	15:N:15:LYS:HG3	2.08	0.52
21:T:26:PHE:CE1	29:X:870:C:H1'	2.44	0.52
22:U:17:SER:CB	22:U:18:VAL:HB	2.36	0.52
29:X:220:U:H2'	29:X:221:A:C8	2.43	0.52
29:X:1728:A:H61	29:X:1738:U:H3	1.57	0.52
29:X:1794:A:N6	29:X:1806:G:O2'	2.42	0.52
29:X:2038:C:H2'	29:X:2483:U:C4'	2.40	0.52
29:X:2262:C:C5	29:X:2368:G:H2'	2.45	0.52
29:X:2606:G:H21	29:X:2761:A:H2	1.56	0.52
1:O:112:THR:HG22	1:O:113:PRO:HD2	1.91	0.52
6:E:103:LEU:HD21	6:E:131:ILE:HD13	1.91	0.52
9:H:2:ILE:O	9:H:45:ALA:N	2.43	0.52
10:I:77:LEU:C	10:I:79:GLN:H	2.12	0.52
15:N:6:THR:O	15:N:9:VAL:HG23	2.10	0.52
19:R:59:LYS:N	19:R:60:PRO:HD2	2.24	0.52
22:U:51:ILE:HA	22:U:59:THR:O	2.09	0.52
25:Z:10:LYS:HB2	29:X:2000:U:O2	2.09	0.52
29:X:218:A:H61	29:X:232:A:H3'	1.74	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:627:A:C6	29:X:628:A:C6	2.96	0.52
29:X:670:U:H2'	29:X:671:A:C8	2.44	0.52
29:X:2630:C:H2'	29:X:2631:C:C6	2.44	0.52
6:E:99:THR:O	6:E:101:LYS:N	2.40	0.52
9:H:16:ALA:HB2	9:H:98:ILE:HD11	1.91	0.52
21:T:39:ARG:HH21	29:X:2334:C:H1'	1.73	0.52
28:3:17:THR:HG21	28:3:21:LYS:HG3	1.90	0.52
29:X:16:G:O2'	29:X:17:G:H5'	2.10	0.52
29:X:2651:U:C2	29:X:2652:G:C8	2.98	0.52
9:H:38:GLY:HA2	29:X:2627:G:N3	2.24	0.52
9:H:54:SER:HA	9:H:69:VAL:HA	1.91	0.52
14:M:55:ILE:O	14:M:103:LYS:O	2.28	0.52
14:M:73:PHE:O	14:M:75:GLU:N	2.42	0.52
17:P:40:LEU:HA	17:P:43:ASP:OD2	2.08	0.52
22:U:22:GLY:O	22:U:39:LYS:HG3	2.09	0.52
29:X:24:G:H2'	29:X:25:U:H6	1.73	0.52
29:X:58:C:H1'	29:X:72:A:H2'	1.91	0.52
29:X:490:A:H4'	29:X:491:A:OP1	2.09	0.52
29:X:529:U:C2	29:X:530:G:C8	2.98	0.52
29:X:1030:U:N3	29:X:1031:C:H5	2.06	0.52
29:X:1672:A:H3'	29:X:1673:C:C6	2.44	0.52
29:X:1686:A:H5''	29:X:1687:C:OP2	2.09	0.52
29:X:2707:G:H2'	29:X:2708:U:H6	1.74	0.52
10:I:114:ILE:HG21	10:I:132:ALA:O	2.09	0.52
11:J:49:GLU:O	11:J:53:ILE:HG13	2.10	0.52
11:J:100:PRO:HG2	20:S:74:ARG:HH11	1.74	0.52
13:L:89:PHE:HZ	13:L:100:VAL:HG22	1.74	0.52
18:Q:15:LYS:NZ	29:X:1353:A:OP1	2.38	0.52
20:S:155:PRO:O	20:S:156:GLU:HB3	2.10	0.52
29:X:812:G:H3'	29:X:813:A:H2'	1.91	0.52
29:X:1282:A:O5'	29:X:1282:A:H8	1.92	0.52
29:X:1774:A:H5'	29:X:2587:G:H4'	1.90	0.52
29:X:2001:G:C6	29:X:2002:A:C6	2.97	0.52
30:Y:16:U:O2'	30:Y:17:A:P	2.67	0.52
10:I:93:LEU:HB3	10:I:97:ARG:NH1	2.24	0.52
29:X:483:A:H3'	29:X:484:G:H5'	1.91	0.52
29:X:1903:C:H5'	29:X:1904:G:OP2	2.09	0.52
29:X:2779:C:H2'	29:X:2780:A:C8	2.45	0.52
9:H:70:VAL:HG21	9:H:106:ARG:NH1	2.25	0.52
12:K:54:THR:HG22	12:K:66:VAL:HG23	1.90	0.52
13:L:15:ARG:HH21	29:X:2272:A:P	2.32	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:60:LYS:HG2	13:L:61:SER:H	1.74	0.52
26:1:21:TYR:OH	29:X:2397:A:N3	2.43	0.52
29:X:739:G:O2'	29:X:740:A:OP2	2.27	0.52
29:X:1238:A:O2'	29:X:1239:A:O4'	2.25	0.52
29:X:2198:U:C3'	29:X:2199:C:H4'	2.39	0.52
11:J:19:THR:HG22	11:J:20:GLY:N	2.16	0.52
13:L:65:THR:OG1	30:Y:52:G:OP1	2.25	0.52
23:V:31:GLN:O	23:V:35:GLY:N	2.43	0.52
25:Z:3:LYS:HA	29:X:2556:A:O2'	2.10	0.52
29:X:501:G:H2'	29:X:502:A:C8	2.44	0.52
29:X:1744:G:C2	29:X:1747:G:C2	2.98	0.52
29:X:2230:G:H5''	29:X:2231:G:OP2	2.09	0.52
29:X:2791:C:N3	29:X:2806:G:N2	2.57	0.52
30:Y:39:C:H5''	30:Y:40:C:C6	2.45	0.52
2:A:250:TRP:CE2	29:X:1796:A:H5''	2.45	0.52
4:C:84:PHE:HE1	29:X:596:C:H5'	1.75	0.52
7:F:133:SER:OG	29:X:1073:G:N3	2.43	0.52
10:I:20:GLY:HA3	10:I:21:ARG:NH1	2.24	0.52
11:J:59:PHE:CD2	11:J:110:VAL:HG11	2.44	0.52
25:Z:5:PRO:HG3	29:X:2593:A:C8	2.45	0.52
29:X:242:A:H1'	29:X:243:G:H1'	1.91	0.52
29:X:1234:C:H42	29:X:1241:G:H1	1.58	0.52
29:X:1323:G:H1'	29:X:1627:C:H5'	1.91	0.52
29:X:1462:C:O2'	29:X:1560:A:N3	2.32	0.52
29:X:1533:G:H2'	29:X:1534:A:C8	2.44	0.52
29:X:1578:U:H2'	29:X:1579:G:H8	1.75	0.52
29:X:1889:G:O2'	29:X:1890:G:H5''	2.09	0.52
2:A:238:GLY:O	2:A:240:THR:N	2.43	0.52
4:C:51:VAL:O	4:C:53:LYS:N	2.43	0.52
10:I:18:ARG:HH22	29:X:1262:U:H2'	1.74	0.52
22:U:27:ASP:O	22:U:32:ARG:HD3	2.10	0.52
29:X:13:A:O2'	29:X:15:G:N7	2.43	0.52
29:X:1065:A:H2'	29:X:1066:G:C8	2.45	0.52
29:X:1194:U:H2'	29:X:1195:U:C6	2.45	0.52
29:X:1905:G:H8	29:X:1905:G:OP2	1.92	0.52
29:X:1982:C:H4'	29:X:2703:C:O2	2.09	0.52
29:X:2551:A:H5''	29:X:2553:G:H4'	1.91	0.52
29:X:2579:A:H2'	29:X:2580:C:C5	2.44	0.52
29:X:2676:G:C2	29:X:2690:A:C2	2.98	0.52
30:Y:59:A:H5'	30:Y:60:A:OP2	2.09	0.52
2:A:48:ARG:NH2	29:X:791:G:H5'	2.25	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:18:PRO:HB2	4:C:106:MET:HG3	1.92	0.51
7:F:2:ARG:NH2	7:F:29:GLN:O	2.43	0.51
18:Q:28:TRP:CZ3	18:Q:77:LYS:HB2	2.45	0.51
19:R:46:VAL:N	19:R:76:LEU:O	2.44	0.51
29:X:1278:A:H5'	29:X:1280:U:H1'	1.91	0.51
29:X:1533:G:H2'	29:X:1534:A:H8	1.74	0.51
29:X:2120:C:N4	29:X:2137:G:O6	2.42	0.51
29:X:2308:A:N6	29:X:2365:U:O4	2.39	0.51
2:A:124:GLU:O	2:A:126:LYS:N	2.44	0.51
2:A:231:HIS:CG	2:A:232:PRO:HD2	2.45	0.51
7:F:107:ILE:HG21	7:F:127:VAL:HG11	1.92	0.51
8:G:81:VAL:HG11	8:G:156:HIS:CD2	2.45	0.51
13:L:37:HIS:CE1	13:L:39:TYR:CD1	2.96	0.51
15:N:3:ARG:HG2	29:X:457:C:H5''	1.92	0.51
15:N:90:LEU:HD13	15:N:95:LEU:HD21	1.92	0.51
29:X:826:U:H2'	29:X:827:C:C6	2.45	0.51
29:X:1548:U:H3	29:X:1555:A:H61	1.57	0.51
29:X:1673:C:C2	29:X:1674:C:C5	2.98	0.51
4:C:130:THR:HG23	29:X:332:C:H5''	1.92	0.51
29:X:915:C:H2'	29:X:916:U:C6	2.45	0.51
29:X:1354:A:H2'	29:X:1410:U:O2	2.10	0.51
29:X:1441:A:H4'	29:X:1442:C:O5'	2.09	0.51
29:X:2859:U:C5	29:X:2860:C:C2	2.98	0.51
1:O:61:PRO:HG2	1:O:184:ASN:HA	1.91	0.51
10:I:86:THR:HG1	10:I:116:ARG:HH11	1.57	0.51
17:P:12:LYS:NZ	29:X:319:G:N7	2.41	0.51
17:P:48:LYS:O	17:P:50:VAL:N	2.37	0.51
22:U:21:ARG:NH1	29:X:400:U:H5'	2.12	0.51
22:U:38:THR:HG22	29:X:2412:A:H2	1.75	0.51
29:X:389:G:H1	29:X:411:C:N4	2.08	0.51
29:X:1662:G:OP1	29:X:1663:C:H5'	2.10	0.51
29:X:2340:C:H2'	29:X:2341:G:O4'	2.11	0.51
2:A:14:ARG:HG3	2:A:15:GLN:H	1.76	0.51
2:A:85:ASP:HB2	2:A:92:ILE:HD13	1.93	0.51
14:M:10:GLY:O	14:M:13:LEU:HB2	2.11	0.51
19:R:95:ARG:HH22	19:R:109:ALA:HA	1.75	0.51
23:V:25:LEU:HA	23:V:28:LEU:HD12	1.92	0.51
27:2:7:PRO:HB2	29:X:1322:G:H4'	1.93	0.51
28:3:29:LYS:O	28:3:30:ARG:HD3	2.11	0.51
28:3:64:ARG:HD2	29:X:220:U:H5'	1.92	0.51
29:X:854:G:H1'	29:X:949:G:N2	2.26	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:929:A:H2	30:Y:81:C:O2	1.93	0.51
29:X:1334:A:H2'	29:X:1335:A:O4'	2.11	0.51
29:X:1681:A:O5'	29:X:1681:A:C8	2.63	0.51
29:X:1685:A:N6	29:X:1693:A:H61	2.09	0.51
29:X:2440:C:H2'	29:X:2441:U:C6	2.42	0.51
3:B:112:GLY:O	3:B:159:HIS:HA	2.10	0.51
3:B:134:TRP:HA	3:B:137:ARG:HD3	1.93	0.51
4:C:149:LEU:HD11	4:C:170:LEU:HG	1.92	0.51
4:C:174:GLY:HA3	29:X:626:A:C4	2.45	0.51
9:H:83:ARG:CZ	9:H:89:ILE:HD11	2.40	0.51
12:K:22:ARG:HD3	12:K:69:ASP:HA	1.93	0.51
20:S:56:VAL:O	20:S:58:GLY:N	2.39	0.51
21:T:16:SER:OG	29:X:2241:U:OP2	2.20	0.51
29:X:67:G:H2'	29:X:68:C:H6	1.76	0.51
29:X:556:A:H4'	29:X:558:G:H21	1.76	0.51
29:X:1680:U:H4'	29:X:2666:U:OP1	2.10	0.51
29:X:2144:C:O2'	29:X:2156:A:H1'	2.10	0.51
29:X:2494:C:O2	29:X:2549:G:C2	2.63	0.51
29:X:2528:G:C2	29:X:2529:G:N7	2.79	0.51
29:X:2607:C:H1'	29:X:2761:A:C2	2.46	0.51
29:X:2665:G:N2	29:X:2704:U:O2	2.43	0.51
1:O:71:ALA:HB3	1:O:109:VAL:HG22	1.93	0.51
3:B:144:ARG:HD3	29:X:2551:A:N7	2.25	0.51
3:B:174:GLU:HB3	3:B:183:LEU:HD12	1.93	0.51
14:M:106:TYR:HE1	29:X:1745:C:H5'	1.75	0.51
17:P:9:ARG:NH2	29:X:318:G:OP1	2.43	0.51
22:U:46:LEU:HB2	29:X:2209:G:H4'	1.92	0.51
29:X:227:G:C6	29:X:228:A:C6	2.98	0.51
29:X:942:U:H2'	29:X:943:U:C6	2.46	0.51
29:X:1578:U:H2'	29:X:1579:G:C8	2.46	0.51
29:X:2097:A:H61	29:X:2102:A:N6	2.09	0.51
29:X:2477:C:O2'	29:X:2478:C:H5'	2.11	0.51
29:X:2542:U:O2	29:X:2544:A:H8	1.93	0.51
29:X:2867:G:OP2	29:X:2867:G:H8	1.92	0.51
4:C:193:LEU:HA	4:C:196:VAL:HG22	1.93	0.51
11:J:28:VAL:HB	11:J:135:ARG:HA	1.93	0.51
13:L:39:TYR:OH	30:Y:118:G:H1'	2.10	0.51
15:N:74:MET:HE2	15:N:110:VAL:HG13	1.93	0.51
28:3:22:VAL:HG22	28:3:50:LEU:HD23	1.91	0.51
29:X:959:C:H2'	29:X:960:U:C6	2.45	0.51
29:X:1764:A:H2'	29:X:1765:C:H5'	1.92	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1851:A:H3'	29:X:1852:G:H8	1.75	0.51
30:Y:7:C:H2'	30:Y:8:C:C6	2.45	0.51
2:A:24:LEU:HD22	2:A:82:ILE:O	2.11	0.51
5:D:129:ASN:HA	5:D:155:THR:HA	1.93	0.51
7:F:12:LEU:HD21	7:F:23:VAL:HG22	1.93	0.51
14:M:2:GLN:N	29:X:2795:A:H61	2.09	0.51
15:N:31:GLN:HB3	29:X:590:C:OP1	2.11	0.51
19:R:44:GLN:HG2	19:R:77:HIS:CE1	2.46	0.51
29:X:914:C:H2'	29:X:915:C:C6	2.46	0.51
29:X:1478:U:H2'	29:X:1479:G:H8	1.75	0.51
29:X:1889:G:H1	29:X:1908:C:H5''	1.76	0.51
29:X:2629:U:H2'	29:X:2630:C:C6	2.40	0.51
5:D:27:ALA:HB2	30:Y:59:A:H1'	1.91	0.51
7:F:10:LEU:HD22	7:F:27:LEU:HD21	1.92	0.51
11:J:26:ASP:HA	11:J:103:VAL:HG23	1.93	0.51
12:K:8:ARG:HB2	12:K:43:GLU:OE1	2.11	0.51
20:S:17:SER:HA	20:S:36:ARG:HH22	1.75	0.51
23:V:63:LYS:HG2	23:V:66:GLN:NE2	2.25	0.51
29:X:1683:G:H1	29:X:1977:C:N4	2.08	0.51
29:X:2447:G:HO2'	29:X:2448:A:H8	1.57	0.51
29:X:2847:G:C2	29:X:2848:A:N6	2.79	0.51
5:D:115:ARG:HB2	5:D:178:ARG:HG3	1.93	0.50
5:D:117:ILE:HG22	5:D:118:ASN:H	1.76	0.50
7:F:90:THR:OG1	7:F:93:LYS:HB2	2.10	0.50
10:I:101:ARG:O	10:I:102:LYS:HB2	2.11	0.50
12:K:28:LEU:HD23	12:K:48:VAL:HG11	1.92	0.50
25:Z:7:PRO:HB3	29:X:2594:U:H1'	1.93	0.50
27:2:37:LYS:O	29:X:469:G:H2'	2.11	0.50
29:X:1211:G:C2	29:X:1212:U:C5	2.98	0.50
29:X:1231:A:N6	29:X:1245:G:O6	2.44	0.50
29:X:1281:A:OP1	29:X:1989:C:OP1	2.28	0.50
29:X:1707:A:H3'	29:X:1708:C:C6	2.46	0.50
29:X:1971:C:H2'	29:X:1972:G:O4'	2.11	0.50
29:X:2283:G:N2	29:X:2291:U:H3	2.05	0.50
29:X:2695:C:H2'	29:X:2696:A:H8	1.76	0.50
4:C:72:ARG:NE	4:C:77:PHE:HE2	2.07	0.50
19:R:18:LYS:HA	19:R:36:VAL:CG1	2.40	0.50
29:X:522:G:OP1	29:X:1247:U:O2'	2.27	0.50
29:X:640:C:H4'	29:X:660:G:H21	1.75	0.50
29:X:967:G:H2'	29:X:968:C:H2'	1.93	0.50
29:X:1039:A:N6	29:X:1137:A:OP1	2.35	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1468:A:N7	29:X:2681:A:N6	2.59	0.50
5:D:10:ASP:HA	5:D:13:ARG:HG3	1.94	0.50
7:F:54:PRO:HD3	7:F:73:PRO:HD3	1.94	0.50
11:J:88:LYS:HG3	29:X:966:A:H5''	1.92	0.50
12:K:52:ILE:HG21	12:K:94:TYR:CG	2.45	0.50
12:K:103:ARG:NH2	12:K:108:VAL:HB	2.24	0.50
15:N:48:ARG:CD	29:X:1167:A:H61	2.13	0.50
18:Q:2:SER:C	18:Q:4:TYR:H	2.15	0.50
29:X:503:G:H2'	29:X:504:G:O4'	2.11	0.50
29:X:653:G:H2'	29:X:654:A:H3'	1.93	0.50
29:X:1238:A:H2'	29:X:1239:A:C8	2.46	0.50
30:Y:16:U:HO2'	30:Y:17:A:P	2.34	0.50
30:Y:39:C:H5'	30:Y:40:C:OP2	2.11	0.50
4:C:179:ASP:O	4:C:182:ARG:HB3	2.11	0.50
6:E:45:GLN:HG2	6:E:47:GLY:H	1.77	0.50
8:G:52:GLY:O	8:G:55:ALA:HB3	2.12	0.50
12:K:103:ARG:CZ	12:K:106:ASP:OD2	2.59	0.50
20:S:37:LYS:O	20:S:41:ARG:HG2	2.12	0.50
21:T:41:ARG:HE	21:T:41:ARG:HA	1.77	0.50
29:X:125:A:H5''	29:X:126:C:O4'	2.11	0.50
29:X:213:C:H2'	29:X:214:C:H6	1.75	0.50
29:X:661:C:H2'	29:X:662:G:C8	2.46	0.50
29:X:866:U:H2'	29:X:867:G:C8	2.45	0.50
29:X:1856:U:H2'	29:X:1857:G:C8	2.46	0.50
29:X:1991:C:H2'	29:X:1992:G:H8	1.77	0.50
29:X:2425:G:H2'	29:X:2480:C:H5	1.76	0.50
29:X:2563:U:HO2'	29:X:2564:U:H5	1.58	0.50
29:X:2595:C:H2'	29:X:2596:C:H6	1.76	0.50
29:X:2659:C:C2	29:X:2660:C:C5	3.00	0.50
30:Y:36:A:N6	30:Y:46:G:O2'	2.44	0.50
1:O:150:ARG:HG2	1:O:153:LYS:HD2	1.92	0.50
3:B:8:LYS:HG2	3:B:192:ASN:HD22	1.76	0.50
6:E:150:LYS:HZ1	29:X:2741:G:H21	1.60	0.50
10:I:72:TYR:HE2	10:I:105:PRO:HB2	1.76	0.50
11:J:44:LYS:O	11:J:47:GLN:N	2.44	0.50
12:K:98:LEU:HD23	12:K:99:ARG:NH2	2.27	0.50
17:P:81:HIS:HD1	17:P:82:ASN:N	2.10	0.50
17:P:106:LEU:HA	17:P:115:ASN:O	2.11	0.50
19:R:20:ASP:O	19:R:36:VAL:HG23	2.11	0.50
29:X:46:C:H2'	29:X:47:G:C8	2.41	0.50
29:X:991:A:C4	29:X:1146:G:O4'	2.64	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:2630:C:H2'	29:X:2631:C:H6	1.76	0.50
29:X:2649:A:H2'	29:X:2650:G:O4'	2.11	0.50
2:A:40:THR:O	2:A:40:THR:OG1	2.26	0.50
4:C:46:ARG:HB3	4:C:50:GLN:HB2	1.94	0.50
6:E:6:LYS:HB3	6:E:6:LYS:HZ3	1.76	0.50
6:E:67:LEU:HD11	29:X:2738:A:C5	2.47	0.50
6:E:158:HIS:NE2	29:X:2638:G:OP1	2.45	0.50
8:G:157:PRO:HG2	8:G:158:HIS:CE1	2.47	0.50
10:I:57:ILE:HD12	28:3:61:MET:SD	2.52	0.50
17:P:39:ARG:NH2	29:X:527:C:O2'	2.44	0.50
29:X:98:U:H4'	29:X:100:G:C8	2.45	0.50
29:X:1142:G:H1'	29:X:1143:A:C8	2.47	0.50
29:X:1353:A:H3'	29:X:1354:A:H8	1.76	0.50
2:A:40:THR:O	2:A:42:GLY:N	2.44	0.50
2:A:208:LYS:HD2	29:X:742:G:C8	2.47	0.50
3:B:146:THR:HG23	29:X:1141:U:C5	2.47	0.50
9:H:1:MET:SD	9:H:79:HIS:NE2	2.84	0.50
9:H:43:ARG:HH21	29:X:1979:C:P	2.34	0.50
29:X:5:A:H2'	29:X:6:A:H8	1.73	0.50
29:X:513:A:OP1	29:X:514:G:N2	2.39	0.50
29:X:1066:G:O2'	29:X:1096:A:N1	2.33	0.50
29:X:2230:G:H3'	29:X:2231:G:H8	1.76	0.50
29:X:2407:G:H4'	29:X:2408:G:C4	2.47	0.50
2:A:202:LYS:HB2	29:X:1812:U:C2	2.46	0.50
2:A:219:PRO:HG3	29:X:794:A:C8	2.46	0.50
22:U:21:ARG:O	22:U:39:LYS:HD2	2.11	0.50
29:X:61:U:H3	29:X:91:A:H2	1.58	0.50
29:X:1742:G:C2	29:X:1743:C:N3	2.80	0.50
29:X:2291:U:H2'	29:X:2292:C:H6	1.77	0.50
30:Y:35:C:H2'	30:Y:36:A:C8	2.47	0.50
2:A:18:THR:HG21	29:X:1581:C:H5''	1.92	0.50
2:A:227:ASN:CG	29:X:797:A:H5''	2.31	0.50
3:B:11:MET:O	29:X:2661:G:H5'	2.12	0.50
13:L:67:THR:HG22	13:L:71:VAL:HG12	1.94	0.50
15:N:33:ARG:HB3	29:X:1265:G:N2	2.27	0.50
29:X:12:U:O2	29:X:12:U:H2'	2.12	0.50
29:X:79:G:N2	29:X:104:C:O2	2.45	0.50
29:X:525:A:C2'	29:X:526:C:H5'	2.42	0.50
29:X:746:G:O6	29:X:774:A:C8	2.65	0.50
10:I:16:ARG:NH2	29:X:598:U:OP2	2.44	0.49
10:I:50:GLU:HA	29:X:846:A:C4'	2.42	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:53:ILE:O	11:J:57:ARG:HG2	2.11	0.49
12:K:99:ARG:H	12:K:99:ARG:NE	2.10	0.49
17:P:39:ARG:O	17:P:42:VAL:HG12	2.11	0.49
18:Q:53:ILE:HG12	18:Q:54:SER:N	2.27	0.49
20:S:100:THR:HG21	20:S:113:VAL:HG11	1.93	0.49
22:U:9:GLY:H	22:U:14:VAL:HG22	1.77	0.49
25:Z:4:HIS:ND1	25:Z:4:HIS:O	2.45	0.49
29:X:668:A:H2'	29:X:668:A:OP2	2.12	0.49
29:X:1354:A:H5''	29:X:1410:U:O2	2.11	0.49
29:X:1815:G:H2'	29:X:1816:G:C8	2.46	0.49
29:X:2410:U:O2	29:X:2412:A:C8	2.63	0.49
29:X:2587:G:H8	29:X:2587:G:O5'	1.95	0.49
29:X:2642:G:H2'	29:X:2643:G:O4'	2.12	0.49
4:C:152:THR:HA	4:C:189:ASP:OD2	2.12	0.49
12:K:102:THR:O	12:K:103:ARG:HB2	2.12	0.49
19:R:99:VAL:HB	19:R:105:ARG:HD2	1.93	0.49
24:W:26:ARG:NH1	29:X:1197:U:H5''	2.28	0.49
28:3:36:LYS:HB2	28:3:37:SER:HA	1.94	0.49
29:X:224:G:OP2	29:X:226:C:N4	2.44	0.49
29:X:513:A:C6	29:X:515:A:C6	3.00	0.49
29:X:580:A:N3	29:X:582:G:C8	2.80	0.49
29:X:991:A:N6	29:X:992:A:N6	2.60	0.49
29:X:1017:C:H2'	29:X:1018:C:H6	1.76	0.49
29:X:1830:C:H4'	29:X:1831:G:C8	2.47	0.49
29:X:2180:U:H2'	29:X:2203:G:N1	2.27	0.49
4:C:72:ARG:NH1	29:X:1271:C:OP1	2.32	0.49
5:D:8:TYR:O	5:D:12:VAL:HG23	2.12	0.49
11:J:15:ARG:HG3	11:J:73:LYS:HG3	1.93	0.49
12:K:83:VAL:O	12:K:86:LYS:HB2	2.11	0.49
14:M:48:GLN:HG2	14:M:49:ALA:H	1.76	0.49
20:S:66:VAL:HG22	20:S:83:PHE:HE1	1.77	0.49
20:S:149:ALA:HA	20:S:152:ILE:HD13	1.94	0.49
22:U:23:LYS:HB3	22:U:37:ILE:HG22	1.95	0.49
28:3:33:ASN:O	28:3:36:LYS:HA	2.13	0.49
29:X:974:U:H2'	29:X:975:C:H6	1.77	0.49
29:X:1428:G:N2	29:X:1601:U:O4'	2.45	0.49
29:X:1451:C:O2'	29:X:1533:G:H4'	2.10	0.49
29:X:1542:G:H2'	29:X:1543:G:H8	1.76	0.49
29:X:1872:A:N1	29:X:2213:G:H1'	2.27	0.49
29:X:2273:C:H2'	29:X:2274:C:C6	2.47	0.49
1:O:58:VAL:HG13	1:O:191:ALA:HB3	1.94	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:9:ILE:HD11	3:B:27:LEU:CB	2.42	0.49
5:D:92:ARG:HD3	30:Y:47:A:H8	1.77	0.49
6:E:153:LYS:HG3	6:E:154:PRO:HD2	1.94	0.49
7:F:78:ILE:HD11	7:F:107:ILE:HD11	1.93	0.49
9:H:10:VAL:HG22	9:H:19:ILE:HG22	1.94	0.49
10:I:31:GLY:O	29:X:1204:G:H5''	2.12	0.49
10:I:100:ARG:C	10:I:101:ARG:HD2	2.33	0.49
22:U:50:ALA:HB3	22:U:62:LEU:HB3	1.93	0.49
26:1:38:LYS:HB2	29:X:2323:U:H2'	1.94	0.49
29:X:358:C:H2'	29:X:359:G:H5'	1.95	0.49
29:X:464:G:H2'	29:X:465:C:C6	2.48	0.49
29:X:583:C:C5	29:X:2016:A:H4'	2.47	0.49
29:X:1326:U:O3'	29:X:1345:G:H5'	2.13	0.49
29:X:1669:A:H2	29:X:1989:C:N3	2.10	0.49
29:X:1681:A:C2	29:X:2706:U:C2	3.00	0.49
29:X:2511:G:H2'	29:X:2512:A:O4'	2.12	0.49
29:X:2837:G:H2'	29:X:2838:U:H6	1.77	0.49
30:Y:63:A:H2'	30:Y:64:C:H6	1.77	0.49
2:A:4:LYS:NZ	29:X:1581:C:OP1	2.40	0.49
3:B:159:HIS:NE2	29:X:2797:G:OP1	2.45	0.49
4:C:176:ASN:OD1	4:C:179:ASP:N	2.41	0.49
7:F:73:PRO:HB3	29:X:1071:U:OP1	2.13	0.49
9:H:42:LYS:HA	29:X:2653:A:O3'	2.13	0.49
10:I:50:GLU:HA	29:X:846:A:H4'	1.94	0.49
14:M:55:ILE:HD11	14:M:67:THR:HG21	1.93	0.49
25:Z:16:ARG:HG3	29:X:1277:G:OP1	2.12	0.49
28:3:32:GLN:OE1	28:3:44:LYS:HE2	2.12	0.49
29:X:54:G:C2	29:X:114:C:C2	2.99	0.49
29:X:78:C:H2'	29:X:79:G:H8	1.77	0.49
29:X:206:U:O2	29:X:206:U:H2'	2.11	0.49
29:X:1174:G:C2	29:X:1175:A:N7	2.80	0.49
29:X:1313:U:O2	29:X:1642:G:N1	2.46	0.49
29:X:2661:G:O6	29:X:2708:U:H1'	2.13	0.49
29:X:2802:C:H2'	29:X:2803:C:H6	1.76	0.49
11:J:19:THR:CG2	11:J:20:GLY:H	2.16	0.49
13:L:37:HIS:CD2	30:Y:29:C:O3'	2.65	0.49
17:P:29:LYS:HB2	29:X:503:G:H4'	1.95	0.49
20:S:23:ALA:HA	20:S:83:PHE:HB2	1.94	0.49
25:Z:7:PRO:O	29:X:1999:U:O2'	2.25	0.49
29:X:356:A:H2'	29:X:357:A:N7	2.26	0.49
29:X:457:C:H2'	29:X:458:G:H5''	1.93	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:564:U:H2'	29:X:565:A:C8	2.48	0.49
29:X:712:A:H5'	29:X:712:A:H8	1.75	0.49
29:X:1660:G:C6	29:X:1661:C:C5	3.01	0.49
29:X:1913:G:N2	29:X:1914:U:O4	2.38	0.49
29:X:1919:A:C2	29:X:1928:G:C8	3.00	0.49
29:X:2140:G:H2'	29:X:2140:G:N3	2.27	0.49
4:C:95:LEU:HD12	4:C:96:PRO:CD	2.42	0.49
25:Z:49:CYS:SG	25:Z:51:TYR:HB2	2.53	0.49
29:X:661:C:H2'	29:X:662:G:H8	1.77	0.49
29:X:754:G:H2'	29:X:755:C:C6	2.47	0.49
29:X:858:G:C8	29:X:858:G:OP2	2.65	0.49
29:X:1299:A:C6	29:X:1302:C:C2	3.01	0.49
29:X:1673:C:H2'	29:X:1674:C:H6	1.78	0.49
29:X:2378:G:H1	29:X:2396:C:N4	2.08	0.49
29:X:2713:A:H2'	29:X:2714:A:H8	1.78	0.49
3:B:133:LYS:NZ	29:X:758:G:OP2	2.28	0.49
12:K:51:LEU:HD13	12:K:70:ILE:HD11	1.95	0.49
18:Q:7:LEU:HD11	18:Q:41:ALA:HB1	1.94	0.49
20:S:106:GLY:HA2	20:S:109:GLN:HE22	1.77	0.49
28:3:46:LYS:HB3	28:3:47:GLY:H	1.40	0.49
29:X:331:U:H4'	29:X:333:A:C8	2.48	0.49
29:X:1099:A:H2'	29:X:1099:A:N3	2.28	0.49
29:X:2097:A:H2'	29:X:2098:G:O4'	2.13	0.49
29:X:2794:G:C6	29:X:2796:A:C2	3.00	0.49
30:Y:30:C:H42	30:Y:58:G:H1	1.58	0.49
3:B:141:ILE:HD11	29:X:2034:A:O4'	2.12	0.49
4:C:33:TRP:HD1	4:C:93:TYR:CZ	2.31	0.49
10:I:72:TYR:HB3	10:I:107:LYS:HB2	1.94	0.49
19:R:17:LYS:HG3	29:X:83:A:H3'	1.95	0.49
26:1:8:ILE:HD12	26:1:28:ARG:NE	2.28	0.49
29:X:171:G:H2'	29:X:172:A:C8	2.48	0.49
29:X:219:G:O2'	29:X:231:G:O6	2.19	0.49
29:X:229:G:H2'	29:X:230:C:H6	1.78	0.49
29:X:635:C:O2	29:X:670:U:H4'	2.12	0.49
29:X:1129:A:H2'	29:X:1130:U:O4'	2.13	0.49
29:X:1174:G:C2	29:X:1175:A:C5	3.00	0.49
29:X:1379:A:H2'	29:X:1380:C:C6	2.47	0.49
29:X:1499:A:H2'	29:X:1500:U:C6	2.48	0.49
29:X:1505:U:O2	29:X:1506:C:O2'	2.21	0.49
29:X:1611:U:H2'	29:X:1612:U:C6	2.48	0.49
29:X:1669:A:C2	29:X:1989:C:N3	2.81	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:2034:A:H2	29:X:2035:G:O6	1.95	0.49
29:X:2431:C:H1'	32:X:6178:HGR:C1	2.43	0.49
29:X:2592:U:H6	29:X:2592:U:H5'	1.78	0.49
2:A:199:ALA:HA	29:X:1812:U:H3	1.77	0.49
8:G:58:ILE:HG12	8:G:80:VAL:HG11	1.94	0.49
9:H:64:VAL:HG13	9:H:68:ASP:OD2	2.13	0.49
15:N:22:LYS:NZ	29:X:1232:U:OP1	2.46	0.49
15:N:60:LEU:HD11	15:N:64:ARG:HE	1.78	0.49
22:U:14:VAL:HB	22:U:15:VAL:H	1.41	0.49
28:3:17:THR:HG21	28:3:21:LYS:CG	2.43	0.49
29:X:408:U:H2'	29:X:409:G:C8	2.48	0.49
29:X:820:U:H2'	29:X:821:A:H8	1.78	0.49
29:X:1982:C:H5''	29:X:2703:C:H1'	1.95	0.49
2:A:124:GLU:C	2:A:126:LYS:H	2.17	0.48
2:A:201:HIS:O	2:A:204:ILE:HG13	2.13	0.48
3:B:175:ILE:HG12	3:B:182:ILE:CD1	2.43	0.48
9:H:10:VAL:HA	9:H:96:ALA:O	2.12	0.48
9:H:21:CYS:SG	9:H:51:ILE:HG13	2.53	0.48
11:J:70:PHE:HA	11:J:71:PRO:HD2	1.63	0.48
25:Z:55:ARG:HH21	25:Z:58:LEU:HA	1.77	0.48
29:X:590:C:H2'	29:X:591:G:H8	1.78	0.48
29:X:742:G:H2'	29:X:1766:U:O2	2.13	0.48
29:X:746:G:C8	29:X:774:A:C6	3.00	0.48
29:X:987:G:C2	29:X:988:G:N7	2.80	0.48
29:X:1761:G:C5	29:X:1762:C:C5	3.01	0.48
29:X:1989:C:O5'	29:X:1989:C:C6	2.65	0.48
29:X:2047:C:O2	29:X:2429:A:N6	2.46	0.48
2:A:132:PRO:O	2:A:136:VAL:HG23	2.12	0.48
3:B:22:PRO:HB3	29:X:2661:G:N3	2.28	0.48
4:C:56:ARG:HB2	29:X:810:U:OP1	2.13	0.48
21:T:23:VAL:HG11	29:X:870:C:H4'	1.94	0.48
27:2:34:ARG:NH2	27:2:41:GLN:HG3	2.28	0.48
29:X:202:A:C4	29:X:203:G:H1'	2.48	0.48
29:X:625:A:OP2	29:X:625:A:H4'	2.13	0.48
29:X:689:A:H8	29:X:2052:G:H21	1.60	0.48
29:X:966:A:N6	29:X:967:G:C6	2.81	0.48
29:X:1426:U:H3'	29:X:1427:G:H5''	1.95	0.48
29:X:1491:C:N3	29:X:1533:G:N2	2.60	0.48
29:X:1503:G:H2'	29:X:1504:G:C8	2.48	0.48
29:X:1904:G:H2'	29:X:1905:G:O4'	2.13	0.48
29:X:1917:C:C2'	29:X:1918:G:H5'	2.43	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:2409:A:O2'	29:X:2410:U:O5'	2.25	0.48
2:A:2:ALA:N	2:A:20:ASP:OD1	2.46	0.48
6:E:54:ARG:NE	6:E:57:ASP:OD2	2.37	0.48
13:L:91:ARG:HB2	13:L:94:TYR:HD1	1.78	0.48
16:O:21:ARG:HD3	16:O:90:PHE:CE1	2.48	0.48
19:R:18:LYS:HB2	29:X:84:G:OP2	2.13	0.48
20:S:3:LEU:HD11	20:S:56:VAL:HG22	1.95	0.48
29:X:750:C:H4'	29:X:779:U:O3'	2.14	0.48
29:X:1108:U:H2'	29:X:1109:A:O4'	2.13	0.48
29:X:1919:A:H2	29:X:1926:U:N3	2.02	0.48
29:X:1920:A:N7	29:X:1923:U:H5	2.11	0.48
9:H:83:ARG:O	9:H:85:ASP:N	2.41	0.48
17:P:14:ARG:O	17:P:18:VAL:HG22	2.13	0.48
25:Z:10:LYS:HG3	29:X:1276:U:H1'	1.96	0.48
29:X:306:G:H2'	29:X:307:C:C6	2.49	0.48
29:X:731:A:H2'	29:X:732:G:H5'	1.94	0.48
29:X:870:C:C4	29:X:871:U:C4	3.02	0.48
29:X:956:A:C4	29:X:2427:A:C2	3.01	0.48
29:X:965:G:O2'	29:X:2253:A:N1	2.34	0.48
29:X:1174:G:C2	29:X:1175:A:C8	3.02	0.48
29:X:1337:G:N2	29:X:1344:C:C2	2.82	0.48
29:X:1469:U:H4'	29:X:1470:G:OP1	2.14	0.48
29:X:2425:G:H2'	29:X:2480:C:C5	2.47	0.48
29:X:2769:C:H1'	29:X:2866:A:C2	2.48	0.48
2:A:243:GLY:HA3	29:X:2576:G:C5'	2.42	0.48
3:B:57:ARG:HH21	29:X:2809:A:H5'	1.78	0.48
3:B:144:ARG:NH1	29:X:2551:A:C4	2.81	0.48
13:L:46:SER:OG	13:L:47:ARG:N	2.47	0.48
24:W:49:HIS:CD2	24:W:50:LEU:HG	2.49	0.48
27:2:11:LYS:HE2	29:X:699:G:H5''	1.96	0.48
29:X:82:G:H21	29:X:83:A:N6	2.11	0.48
29:X:149:A:OP2	29:X:149:A:H8	1.97	0.48
29:X:219:G:H22	29:X:231:G:H2'	1.78	0.48
29:X:647:G:O2'	29:X:649:G:O2'	2.26	0.48
29:X:772:G:H2'	29:X:773:G:H8	1.79	0.48
29:X:1882:G:O2'	29:X:1883:A:OP2	2.27	0.48
29:X:2279:G:H8	29:X:2279:G:O5'	1.95	0.48
29:X:2498:U:C5	29:X:2520:A:C6	3.02	0.48
29:X:2533:U:H2'	29:X:2534:U:C6	2.48	0.48
29:X:2708:U:H2'	29:X:2709:C:C6	2.48	0.48
29:X:2840:U:C4	29:X:2841:U:C4	3.01	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:16:TYR:CZ	1:O:24:LEU:HD22	2.49	0.48
2:A:211:ARG:NE	29:X:1582:A:OP1	2.40	0.48
11:J:46:ASN:OD1	11:J:46:ASN:N	2.34	0.48
15:N:10:ARG:HG3	15:N:13:ARG:NH2	2.28	0.48
15:N:51:ARG:HA	15:N:54:LYS:HD2	1.96	0.48
17:P:93:LYS:HB2	17:P:129:ALA:HB3	1.95	0.48
19:R:25:LEU:CD1	19:R:82:ALA:HB2	2.42	0.48
20:S:147:ILE:HG23	20:S:151:ASP:HB2	1.95	0.48
27:2:30:ILE:HD13	29:X:477:A:H4'	1.95	0.48
29:X:1370:U:H3'	29:X:1371:G:C8	2.48	0.48
29:X:1509:A:H8	29:X:1510:A:C8	2.32	0.48
29:X:2495:G:C6	29:X:2496:C:N4	2.81	0.48
30:Y:65:A:H2'	30:Y:66:G:H8	1.79	0.48
1:O:210:LEU:HB2	1:O:217:SER:HA	1.94	0.48
4:C:142:LEU:HB3	4:C:166:TRP:CH2	2.48	0.48
6:E:7:GLN:H	6:E:8:PRO:CD	2.27	0.48
10:I:55:ARG:NH1	29:X:228:A:OP1	2.35	0.48
12:K:11:ASN:N	12:K:11:ASN:ND2	2.59	0.48
29:X:218:A:H5'	29:X:220:U:O4'	2.12	0.48
29:X:713:G:H2'	29:X:714:G:O4'	2.13	0.48
29:X:1096:A:H1'	29:X:1116:U:H1'	1.95	0.48
29:X:1727:C:O2'	29:X:2833:C:N3	2.43	0.48
29:X:2047:C:H1'	29:X:2429:A:C6	2.49	0.48
29:X:2784:A:C2	29:X:2866:A:C4	3.02	0.48
1:O:10:VAL:HG22	1:O:218:ILE:HD11	1.96	0.48
2:A:52:ARG:CZ	2:A:53:PHE:HE2	2.26	0.48
4:C:137:ALA:HB1	4:C:142:LEU:HD12	1.95	0.48
5:D:52:LYS:HE2	5:D:146:VAL:HB	1.96	0.48
5:D:122:PHE:HE2	5:D:130:LEU:N	2.12	0.48
6:E:83:TYR:O	6:E:134:SER:OG	2.20	0.48
10:I:81:GLN:HB3	10:I:82:ASP:H	1.43	0.48
20:S:24:TYR:O	20:S:26:LYS:NZ	2.42	0.48
29:X:639:G:O2'	29:X:661:C:O2'	2.22	0.48
29:X:1054:C:H2'	29:X:1055:A:C8	2.49	0.48
29:X:1401:G:H1	29:X:1412:C:N4	2.08	0.48
29:X:2265:A:H4'	29:X:2266:A:O4'	2.14	0.48
3:B:44:TYR:CE1	29:X:2616:U:H5'	2.49	0.48
10:I:115:SER:O	10:I:136:ALA:HB1	2.14	0.48
20:S:26:LYS:HD2	30:Y:107:C:O2'	2.14	0.48
24:W:2:LYS:HD2	24:W:32:ARG:O	2.14	0.48
24:W:35:SER:O	24:W:37:THR:OG1	2.28	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:2:2:LYS:HG2	27:2:3:ARG:N	2.28	0.48
29:X:174:A:C5	29:X:175:C:C5	3.02	0.48
29:X:341:A:H2'	29:X:341:A:N3	2.29	0.48
29:X:691:C:C2	29:X:692:C:C5	3.01	0.48
29:X:1672:A:C8	29:X:1673:C:C5	3.01	0.48
29:X:1979:C:H4'	29:X:1980:A:OP1	2.14	0.48
29:X:2492:G:H2'	29:X:2493:U:C6	2.48	0.48
11:J:99:LYS:O	11:J:102:ARG:HB3	2.14	0.48
14:M:105:TYR:HD2	29:X:2698:G:H5'	1.79	0.48
21:T:46:LYS:HB3	21:T:78:PHE:CD2	2.49	0.48
24:W:26:ARG:HH12	29:X:1197:U:H5''	1.78	0.48
26:1:40:TYR:CG	26:1:41:ASP:N	2.82	0.48
29:X:187:U:H2'	29:X:188:G:C8	2.48	0.48
29:X:322:A:H3'	29:X:323:G:C8	2.49	0.48
29:X:772:G:H2'	29:X:773:G:C8	2.49	0.48
29:X:1378:A:H2'	29:X:1378:A:N3	2.29	0.48
29:X:1882:G:N7	29:X:1885:C:N4	2.46	0.48
29:X:2345:A:H2'	29:X:2346:G:O4'	2.14	0.48
29:X:2565:C:H2'	29:X:2566:A:H8	1.78	0.48
4:C:149:LEU:HB2	4:C:183:HIS:ND1	2.29	0.47
6:E:35:VAL:HB	6:E:37:TYR:CZ	2.49	0.47
9:H:109:ARG:HA	9:H:129:LEU:HD22	1.95	0.47
12:K:88:ALA:O	12:K:90:ARG:N	2.47	0.47
15:N:52:ASN:O	15:N:55:ARG:N	2.47	0.47
16:O:14:VAL:HG13	16:O:20:ILE:HD11	1.96	0.47
22:U:10:LYS:HD3	22:U:11:LYS:H	1.78	0.47
22:U:49:LYS:HB2	22:U:61:TRP:CZ3	2.47	0.47
26:1:11:LYS:HB2	26:1:22:TYR:O	2.14	0.47
29:X:181:A:H2	29:X:182:G:H21	1.61	0.47
29:X:303:C:N3	29:X:359:G:N2	2.44	0.47
29:X:797:A:O2'	29:X:798:G:H8	1.97	0.47
29:X:1658:A:N6	29:X:1659:G:C2	2.83	0.47
29:X:2432:A:H2'	29:X:2433:G:H8	1.79	0.47
29:X:2456:U:H4'	29:X:2458:U:O4	2.14	0.47
29:X:2495:G:C6	29:X:2548:G:C2	3.01	0.47
29:X:2702:G:C2'	29:X:2703:C:H5'	2.44	0.47
29:X:2707:G:C4	29:X:2708:U:C5	3.02	0.47
29:X:2728:A:C6	29:X:2737:A:N7	2.83	0.47
29:X:2796:A:C6	29:X:2797:G:C6	3.02	0.47
29:X:2813:G:C4	29:X:2814:G:C8	3.02	0.47
1:O:72:VAL:HG13	1:O:110:VAL:HB	1.96	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:119:ALA:HA	4:C:188:ILE:HB	1.95	0.47
9:H:37:GLY:O	29:X:2627:G:O2'	2.32	0.47
10:I:110:ALA:O	10:I:111:SER:OG	2.26	0.47
12:K:34:ILE:HG13	12:K:113:ILE:HG22	1.97	0.47
13:L:92:GLY:O	13:L:94:TYR:N	2.43	0.47
17:P:11:LYS:NZ	17:P:15:LYS:HE2	2.27	0.47
17:P:18:VAL:O	17:P:19:LYS:HB2	2.14	0.47
21:T:48:GLY:H	21:T:51:VAL:CG2	2.27	0.47
29:X:699:G:H2'	29:X:801:A:N1	2.29	0.47
29:X:1606:C:H2'	29:X:1607:A:H8	1.79	0.47
29:X:1606:C:H2'	29:X:1607:A:C8	2.48	0.47
29:X:1987:G:C4	29:X:1988:A:C8	3.02	0.47
29:X:2662:C:C6	29:X:2663:U:H5	2.32	0.47
2:A:44:ASN:HB2	29:X:1804:U:O2'	2.13	0.47
3:B:136:ARG:NH1	29:X:1673:C:OP1	2.46	0.47
5:D:70:ALA:HB3	5:D:81:GLN:O	2.14	0.47
9:H:8:LEU:HD23	9:H:8:LEU:N	2.28	0.47
9:H:26:ASN:HB3	9:H:38:GLY:H	1.78	0.47
15:N:34:ASN:O	15:N:38:THR:OG1	2.29	0.47
15:N:61:TRP:HZ2	29:X:1006:C:O2	1.96	0.47
17:P:30:TYR:CD1	17:P:123:HIS:HE1	2.32	0.47
25:Z:33:CYS:HB3	25:Z:40:LYS:HB3	1.95	0.47
29:X:617:U:H5''	29:X:630:G:O6	2.14	0.47
29:X:1337:G:C4	29:X:1341:G:O6	2.67	0.47
29:X:1724:C:H42	29:X:1742:G:H1	1.61	0.47
29:X:2367:A:N7	29:X:2368:G:C5	2.83	0.47
29:X:2675:U:H2'	29:X:2676:G:C8	2.49	0.47
3:B:169:ASN:ND2	29:X:2711:G:OP1	2.38	0.47
6:E:97:LYS:HB3	6:E:98:LEU:H	1.49	0.47
7:F:133:SER:HB2	29:X:1099:A:N6	2.29	0.47
12:K:30:ARG:HG2	12:K:31:GLU:OE1	2.14	0.47
12:K:106:ASP:HB3	29:X:1666:G:O2'	2.13	0.47
13:L:30:SER:HB3	13:L:41:GLN:HB2	1.96	0.47
15:N:13:ARG:CZ	29:X:1264:C:H5''	2.43	0.47
15:N:91:ASN:HB2	16:O:11:GLN:HB2	1.97	0.47
19:R:77:HIS:O	19:R:80:LYS:HG3	2.15	0.47
21:T:5:LYS:HA	21:T:5:LYS:HE3	1.96	0.47
22:U:19:ILE:HD12	22:U:20:ARG:N	2.29	0.47
25:Z:21:SER:O	25:Z:21:SER:OG	2.32	0.47
28:3:6:THR:HG23	28:3:62:LEU:HB3	1.96	0.47
29:X:536:A:N6	29:X:2605:C:H4'	2.29	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1309:G:H1	29:X:1661:C:H42	1.62	0.47
29:X:1391:A:O2'	29:X:1392:U:OP2	2.33	0.47
29:X:1452:U:H2'	29:X:1453:A:O4'	2.13	0.47
29:X:2335:U:H2'	29:X:2336:G:C8	2.50	0.47
29:X:2645:C:H3'	29:X:2646:C:C6	2.49	0.47
29:X:2757:G:H4'	29:X:2758:A:H5''	1.96	0.47
4:C:194:GLU:O	4:C:197:GLU:HB3	2.14	0.47
5:D:104:ILE:HA	5:D:108:LEU:HD12	1.97	0.47
10:I:9:THR:HB	10:I:12:SER:HB2	1.97	0.47
15:N:11:ARG:HH12	29:X:29:U:C4'	2.28	0.47
16:O:10:LYS:H	16:O:10:LYS:HD3	1.80	0.47
19:R:99:VAL:O	19:R:100:ASP:HB2	2.14	0.47
24:W:35:SER:HB3	29:X:941:U:OP1	2.13	0.47
25:Z:44:HIS:ND1	25:Z:44:HIS:N	2.63	0.47
29:X:553:C:H1'	29:X:556:A:H8	1.79	0.47
29:X:746:G:N7	29:X:774:A:C5	2.83	0.47
29:X:840:U:H4'	29:X:841:G:N7	2.29	0.47
29:X:1909:U:P	29:X:1912:G:H22	2.37	0.47
29:X:1998:A:C8	29:X:1999:U:C5	3.02	0.47
29:X:2158:C:H2'	29:X:2159:A:C8	2.49	0.47
29:X:2827:G:H2'	29:X:2828:C:O4'	2.15	0.47
30:Y:39:C:N4	30:Y:50:U:O2'	2.47	0.47
2:A:227:ASN:OD1	29:X:797:A:H5''	2.14	0.47
5:D:5:LYS:HE2	5:D:104:ILE:HD12	1.96	0.47
5:D:41:GLY:O	5:D:43:SER:N	2.47	0.47
9:H:10:VAL:HG23	9:H:17:ARG:O	2.14	0.47
11:J:14:PHE:CD1	11:J:88:LYS:HD3	2.50	0.47
17:P:81:HIS:ND1	17:P:82:ASN:OD1	2.48	0.47
20:S:94:VAL:HG12	20:S:96:VAL:HG22	1.97	0.47
22:U:20:ARG:HB2	22:U:43:ARG:HD2	1.96	0.47
29:X:717:G:N3	29:X:739:G:N1	2.63	0.47
29:X:1212:U:H2'	29:X:1213:U:H6	1.75	0.47
29:X:1463:A:H2'	29:X:1464:A:H8	1.79	0.47
29:X:2033:C:C4	29:X:2034:A:C6	3.03	0.47
29:X:2594:U:H2'	29:X:2595:C:C6	2.49	0.47
29:X:2658:A:H2'	29:X:2659:C:O4'	2.15	0.47
29:X:2659:C:N4	29:X:2660:C:H41	2.11	0.47
30:Y:19:C:H2'	30:Y:20:A:C8	2.49	0.47
1:O:60:LEU:HB2	1:O:155:GLY:HA2	1.97	0.47
2:A:233:HIS:HE2	2:A:247:VAL:HG12	1.79	0.47
3:B:61:LYS:N	3:B:62:PRO:HD2	2.29	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:11:VAL:HG12	6:E:15:VAL:HG11	1.95	0.47
8:G:33:ILE:CD1	29:X:547:U:H4'	2.45	0.47
8:G:85:ALA:HB1	8:G:127:ILE:HG13	1.96	0.47
9:H:13:ASN:ND2	9:H:109:ARG:HG2	2.30	0.47
11:J:61:ARG:HG2	20:S:175:ARG:H	1.79	0.47
12:K:3:HIS:O	12:K:3:HIS:CG	2.68	0.47
12:K:82:GLU:O	12:K:85:PRO:HG2	2.14	0.47
15:N:55:ARG:O	15:N:58:ARG:HB3	2.15	0.47
17:P:90:LEU:HA	17:P:129:ALA:O	2.14	0.47
19:R:16:PHE:CZ	19:R:46:VAL:HG21	2.50	0.47
21:T:37:LEU:HD12	21:T:59:LEU:O	2.14	0.47
29:X:176:A:N6	29:X:2413:A:C6	2.83	0.47
29:X:640:C:H5''	29:X:660:G:O2'	2.14	0.47
29:X:1987:G:N7	29:X:1988:A:N7	2.62	0.47
29:X:2044:G:N2	29:X:2046:C:C2	2.83	0.47
29:X:2145:A:H5''	29:X:2155:U:C6	2.49	0.47
29:X:2396:C:H2'	29:X:2397:A:O4'	2.14	0.47
29:X:2612:G:H2'	29:X:2613:A:O4'	2.15	0.47
29:X:2662:C:H2'	29:X:2663:U:H5'	1.95	0.47
29:X:2836:U:O2'	29:X:2837:G:H5'	2.14	0.47
29:X:2871:U:H2'	29:X:2872:U:C6	2.50	0.47
30:Y:5:C:H42	30:Y:120:G:H1	1.63	0.47
30:Y:80:A:H2'	30:Y:81:C:O4'	2.13	0.47
3:B:8:LYS:HG2	3:B:192:ASN:HA	1.96	0.47
4:C:153:ASP:HA	4:C:158:ARG:HH22	1.78	0.47
12:K:73:LYS:H	12:K:73:LYS:HE3	1.77	0.47
13:L:42:ILE:HB	13:L:52:ALA:HB3	1.97	0.47
23:V:4:SER:O	23:V:8:ASN:ND2	2.48	0.47
25:Z:18:MET:CE	29:X:2028:C:H5'	2.45	0.47
29:X:389:G:H2'	29:X:390:U:C6	2.50	0.47
29:X:459:A:H5''	29:X:461:A:C5	2.50	0.47
29:X:475:U:C4	29:X:801:A:C5	3.03	0.47
29:X:494:A:H3'	29:X:495:C:C6	2.46	0.47
29:X:981:C:N4	29:X:982:C:N4	2.63	0.47
29:X:1174:G:N3	29:X:1175:A:C8	2.83	0.47
29:X:2087:U:H2'	29:X:2088:U:C6	2.49	0.47
29:X:2474:G:C6	29:X:2475:C:N3	2.82	0.47
29:X:2542:U:C2	29:X:2544:A:OP2	2.67	0.47
29:X:2697:G:H2'	29:X:2698:G:C8	2.49	0.47
29:X:2711:G:H2'	29:X:2712:G:C8	2.50	0.47
1:O:150:ARG:HA	1:O:153:LYS:HB2	1.97	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:39:ARG:HD2	29:X:455:A:N7	2.30	0.47
5:D:22:TYR:HE1	5:D:28:VAL:HG13	1.80	0.47
5:D:57:LEU:HD23	5:D:60:ILE:HD11	1.97	0.47
12:K:8:ARG:HD2	12:K:10:LEU:HD21	1.97	0.47
13:L:37:HIS:HB3	30:Y:30:C:OP1	2.14	0.47
15:N:58:ARG:HH21	15:N:92:ARG:HH12	1.61	0.47
15:N:115:ASN:HA	15:N:118:GLN:OE1	2.15	0.47
17:P:98:ASP:OD2	17:P:98:ASP:N	2.47	0.47
20:S:146:HIS:HB3	20:S:167:THR:HG23	1.97	0.47
21:T:35:ASN:OD1	29:X:2332:G:O2'	2.25	0.47
29:X:116:A:OP2	29:X:117:A:H2'	2.15	0.47
29:X:202:A:C5	29:X:203:G:H1'	2.50	0.47
29:X:828:C:N4	29:X:1206:G:H1	2.13	0.47
29:X:1141:U:H6	29:X:1141:U:O5'	1.98	0.47
29:X:2519:C:O2	29:X:2720:A:H2	1.98	0.47
29:X:2663:U:C2	29:X:2664:G:C8	3.02	0.47
29:X:2796:A:C4	29:X:2797:G:N7	2.83	0.47
4:C:137:ALA:CB	4:C:142:LEU:HD12	2.44	0.47
12:K:24:GLN:HB3	12:K:44:LEU:HD13	1.96	0.47
17:P:47:GLY:H	17:P:92:VAL:HB	1.78	0.47
29:X:587:A:OP1	29:X:1268:U:O2'	2.15	0.47
29:X:649:G:N2	29:X:661:C:H1'	2.30	0.47
29:X:754:G:H2'	29:X:755:C:H6	1.80	0.47
29:X:2487:G:C6	29:X:2561:G:O6	2.68	0.47
29:X:2701:A:H1'	29:X:2848:A:O2'	2.15	0.47
29:X:2789:U:H2'	29:X:2790:C:C6	2.50	0.47
29:X:2820:C:H42	29:X:2846:G:H1	1.62	0.47
2:A:171:ASP:O	2:A:187:SER:OG	2.27	0.46
9:H:130:ALA:HA	9:H:131:PRO:HD3	1.81	0.46
22:U:68:ARG:NH1	29:X:413:G:O4'	2.39	0.46
29:X:218:A:H4'	29:X:219:G:OP1	2.14	0.46
29:X:790:A:C2	29:X:791:G:C4	3.03	0.46
29:X:1690:U:H3'	29:X:1690:U:C6	2.50	0.46
29:X:2411:A:H8	29:X:2411:A:O5'	1.98	0.46
2:A:163:VAL:HA	2:A:176:ARG:O	2.15	0.46
3:B:103:ASP:OD1	3:B:168:GLN:HA	2.14	0.46
4:C:47:THR:N	4:C:50:GLN:HG3	2.28	0.46
5:D:57:LEU:O	5:D:61:THR:HG23	2.15	0.46
8:G:115:ALA:O	8:G:119:LEU:HB2	2.15	0.46
9:H:59:ALA:O	9:H:61:ARG:N	2.48	0.46
10:I:72:TYR:CE2	10:I:105:PRO:HB2	2.50	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:20:HIS:O	14:M:62:SER:HB2	2.15	0.46
27:2:15:THR:HG22	27:2:16:HIS:CG	2.50	0.46
29:X:646:C:H2'	29:X:647:G:O4'	2.16	0.46
29:X:991:A:H62	29:X:992:A:N6	2.13	0.46
29:X:1340:C:H2'	29:X:1341:G:O4'	2.16	0.46
29:X:1687:C:C4	29:X:1688:U:C2	3.03	0.46
29:X:1794:A:H5''	29:X:1795:C:OP2	2.15	0.46
29:X:2040:A:H2'	29:X:2041:A:H8	1.76	0.46
29:X:2406:C:H5''	29:X:2407:G:OP1	2.15	0.46
6:E:157:TYR:CE2	29:X:2510:A:H4'	2.50	0.46
17:P:109:ARG:HD2	29:X:761:G:OP2	2.15	0.46
19:R:10:HIS:NE2	29:X:338:G:H1'	2.31	0.46
20:S:26:LYS:HE2	20:S:84:TYR:CE1	2.51	0.46
28:3:23:MET:HA	28:3:49:VAL:HA	1.97	0.46
29:X:402:A:H8	29:X:2392:G:H4'	1.79	0.46
29:X:1153:A:C5	29:X:1155:G:C5	3.03	0.46
29:X:1179:A:C2	29:X:1196:G:C2	3.04	0.46
29:X:1301:U:C2	29:X:1340:C:O2	2.68	0.46
29:X:1511:A:C6	29:X:1512:A:C6	3.03	0.46
29:X:1715:A:C8	29:X:1717:A:O4'	2.68	0.46
29:X:2505:G:N2	29:X:2517:C:H1'	2.31	0.46
29:X:2802:C:H2'	29:X:2803:C:C6	2.50	0.46
29:X:2859:U:H5	29:X:2860:C:C4	2.33	0.46
2:A:123:ALA:HB1	2:A:129:ASN:ND2	2.29	0.46
2:A:232:PRO:HB2	2:A:233:HIS:CD2	2.50	0.46
4:C:48:ARG:HD2	4:C:75:PRO:HD2	1.97	0.46
5:D:46:ASP:OD2	5:D:46:ASP:N	2.49	0.46
7:F:23:VAL:HA	7:F:26:ALA:HB3	1.98	0.46
8:G:117:GLU:O	8:G:121:LYS:HB2	2.16	0.46
13:L:15:ARG:HD3	13:L:15:ARG:HA	1.38	0.46
21:T:60:PHE:CE2	29:X:2344:G:H4'	2.51	0.46
25:Z:43:HIS:HA	25:Z:52:TYR:OH	2.15	0.46
28:3:33:ASN:C	28:3:35:GLY:H	2.18	0.46
29:X:223:C:C4	29:X:224:G:N7	2.84	0.46
29:X:471:A:C2	29:X:481:A:C4	3.03	0.46
29:X:518:A:H5''	29:X:518:A:C8	2.50	0.46
29:X:713:G:N2	29:X:745:C:H5	2.09	0.46
29:X:860:U:H5'	29:X:861:G:OP2	2.16	0.46
29:X:1118:G:N1	29:X:1119:U:O2	2.47	0.46
29:X:1513:U:H6	29:X:1593:C:H5''	1.80	0.46
29:X:2151:G:N2	29:X:2154:A:O5'	2.46	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:2455:A:N3	29:X:2460:G:N1	2.54	0.46
2:A:201:HIS:C	2:A:203:ASN:H	2.19	0.46
14:M:2:GLN:HB3	29:X:2795:A:C2	2.51	0.46
14:M:32:THR:HG22	14:M:94:VAL:HB	1.98	0.46
15:N:44:THR:O	15:N:48:ARG:HG2	2.15	0.46
18:Q:63:LYS:HD2	18:Q:72:ARG:NH2	2.30	0.46
26:1:38:LYS:HD2	29:X:2323:U:OP1	2.15	0.46
29:X:143:A:H2'	29:X:144:U:C6	2.51	0.46
29:X:784:U:H2'	29:X:785:U:H6	1.81	0.46
29:X:828:C:H42	29:X:1206:G:H1	1.64	0.46
29:X:1235:C:H2'	29:X:1236:G:C8	2.51	0.46
29:X:1542:G:N2	29:X:1562:G:H1	2.14	0.46
29:X:1994:U:H2'	29:X:1995:G:C5'	2.45	0.46
29:X:2042:A:C5	29:X:2482:A:C2	3.03	0.46
8:G:38:GLU:OE2	8:G:67:ARG:NH2	2.48	0.46
17:P:74:SER:HA	29:X:498:C:H1'	1.98	0.46
19:R:76:LEU:HD23	19:R:76:LEU:HA	1.69	0.46
28:3:21:LYS:HE2	29:X:661:C:OP1	2.16	0.46
29:X:1:G:H2'	29:X:2:G:C8	2.51	0.46
29:X:169:C:H5''	29:X:170:U:OP2	2.15	0.46
29:X:1079:G:N2	29:X:1107:A:O5'	2.49	0.46
29:X:1655:C:O3'	29:X:2688:G:N2	2.48	0.46
29:X:1683:G:H1	29:X:1977:C:H42	1.62	0.46
30:Y:119:G:C6	30:Y:120:G:C5	3.04	0.46
3:B:2:LYS:NZ	3:B:95:ILE:HA	2.30	0.46
3:B:128:SER:OG	29:X:1693:A:H1'	2.15	0.46
4:C:62:LYS:HZ1	29:X:2043:A:H3'	1.81	0.46
9:H:42:LYS:NZ	29:X:2653:A:H5'	2.31	0.46
17:P:27:VAL:HB	29:X:504:G:H4'	1.98	0.46
28:3:7:HIS:O	28:3:10:ALA:N	2.43	0.46
29:X:515:A:H2'	29:X:516:G:H5'	1.97	0.46
29:X:590:C:H2'	29:X:591:G:C8	2.50	0.46
29:X:695:G:H2'	29:X:696:U:C6	2.51	0.46
29:X:1067:G:O2'	29:X:1098:G:O6	2.34	0.46
29:X:1103:C:H2'	29:X:1104:G:O4'	2.15	0.46
29:X:1222:G:O2'	29:X:1250:A:N1	2.42	0.46
29:X:1685:A:O4'	29:X:1686:A:C2	2.68	0.46
29:X:2237:C:O2'	29:X:2406:C:OP2	2.25	0.46
29:X:2441:U:H2'	29:X:2442:C:C6	2.50	0.46
4:C:149:LEU:HD22	4:C:179:ASP:HB3	1.98	0.46
5:D:3:GLN:O	5:D:6:THR:OG1	2.17	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:92:ASP:OD2	14:M:69:ARG:NH1	2.48	0.46
12:K:25:ALA:N	12:K:44:LEU:HD11	2.31	0.46
13:L:28:ARG:HH22	30:Y:11:G:H5'	1.81	0.46
17:P:34:SER:HB3	17:P:37:LYS:HG3	1.98	0.46
17:P:60:ILE:CD1	25:Z:28:PRO:HD3	2.46	0.46
19:R:62:MET:HA	19:R:63:THR:HA	1.70	0.46
24:W:16:GLN:O	24:W:20:VAL:HG23	2.15	0.46
29:X:78:C:H2'	29:X:79:G:C8	2.51	0.46
29:X:573:C:O2'	29:X:574:C:H5'	2.16	0.46
29:X:824:U:O2	29:X:1263:G:H3'	2.16	0.46
29:X:861:G:C4	29:X:862:A:C8	3.03	0.46
29:X:1067:G:H5''	29:X:1068:A:O4'	2.15	0.46
29:X:1495:G:N2	29:X:1529:C:O2	2.29	0.46
29:X:1511:A:H8	29:X:1594:U:HO2'	1.64	0.46
29:X:1733:U:H2'	29:X:1734:C:C5	2.50	0.46
29:X:1850:G:N3	29:X:1850:G:H2'	2.30	0.46
29:X:2415:G:H2'	29:X:2416:U:C6	2.51	0.46
29:X:2585:C:H2'	29:X:2586:G:H5'	1.98	0.46
5:D:60:ILE:HG13	5:D:61:THR:HG22	1.98	0.46
5:D:147:ASP:HB2	5:D:148:LYS:H	1.57	0.46
9:H:23:ARG:HG3	9:H:24:VAL:N	2.29	0.46
13:L:57:ALA:HB3	30:Y:119:G:H4'	1.97	0.46
20:S:126:GLY:HA3	20:S:128:ARG:NH2	2.31	0.46
29:X:1402:G:H2'	29:X:1403:U:C6	2.51	0.46
29:X:1464:A:C6	29:X:1465:G:C6	3.04	0.46
29:X:1698:C:O2'	29:X:1753:A:N3	2.37	0.46
29:X:1765:C:O5'	29:X:1765:C:H6	1.98	0.46
29:X:2447:G:O2'	29:X:2448:A:H8	1.99	0.46
29:X:2494:C:C2	29:X:2549:G:C2	3.04	0.46
29:X:2695:C:H2'	29:X:2696:A:C8	2.51	0.46
29:X:2767:C:HO2'	29:X:2785:A:HO2'	1.63	0.46
2:A:69:ARG:HD2	2:A:130:ALA:HB2	1.98	0.46
3:B:27:LEU:HD22	3:B:51:TYR:OH	2.15	0.46
5:D:70:ALA:O	5:D:72:LYS:N	2.43	0.46
6:E:117:PRO:HA	6:E:118:PRO:HD2	1.84	0.46
8:G:79:PHE:CE2	8:G:147:ARG:HD3	2.50	0.46
20:S:10:PRO:O	20:S:13:LYS:HG3	2.16	0.46
29:X:38:G:C2	29:X:454:G:C2	3.04	0.46
29:X:119:G:H1	29:X:128:C:H42	1.63	0.46
29:X:194:G:H2'	29:X:195:A:O4'	2.16	0.46
29:X:992:A:H2	29:X:2010:G:N3	2.13	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:998:C:O2'	29:X:1011:A:N3	2.37	0.46
29:X:1008:G:H1	29:X:1169:C:H42	1.64	0.46
29:X:1017:C:O2'	29:X:1018:C:H5'	2.16	0.46
29:X:1470:G:C2	29:X:1471:G:C8	3.04	0.46
29:X:1661:C:O2	29:X:1661:C:H2'	2.16	0.46
29:X:1669:A:N7	29:X:1670:G:C6	2.84	0.46
29:X:1769:U:H2'	29:X:1775:A:N6	2.31	0.46
29:X:2790:C:H2'	29:X:2791:C:C6	2.51	0.46
3:B:91:VAL:HG12	3:B:92:ASN:H	1.81	0.45
4:C:34:GLN:OE1	4:C:176:ASN:HB2	2.17	0.45
4:C:36:ALA:O	4:C:38:ARG:N	2.49	0.45
5:D:79:LEU:HD21	29:X:2289:A:H2	1.81	0.45
12:K:106:ASP:OD2	29:X:1300:A:C8	2.69	0.45
20:S:6:LYS:HA	20:S:32:PHE:HA	1.98	0.45
26:1:21:TYR:CE2	29:X:2378:G:H1'	2.51	0.45
28:3:62:LEU:HD13	28:3:65:GLY:HA2	1.97	0.45
29:X:165:G:H4'	29:X:1378:A:C5	2.51	0.45
29:X:1033:G:H22	29:X:1153:A:H2	1.63	0.45
29:X:1194:U:H2'	29:X:1195:U:H6	1.80	0.45
29:X:1510:A:H2'	29:X:1511:A:O4'	2.16	0.45
29:X:1685:A:H61	29:X:1693:A:H61	1.63	0.45
29:X:1813:A:H2'	29:X:1814:G:H8	1.81	0.45
3:B:38:THR:HG23	3:B:41:THR:OG1	2.16	0.45
3:B:60:ASN:HB2	3:B:63:MET:HB2	1.98	0.45
3:B:140:SER:HB2	29:X:2557:G:N7	2.31	0.45
4:C:53:LYS:HB2	4:C:73:SER:HB3	1.98	0.45
5:D:92:ARG:HD3	30:Y:47:A:C8	2.50	0.45
13:L:12:ARG:O	13:L:16:LYS:HB2	2.16	0.45
16:O:83:ARG:N	29:X:827:C:OP1	2.45	0.45
19:R:58:VAL:HG13	19:R:60:PRO:CD	2.46	0.45
22:U:8:THR:HA	22:U:13:LEU:HD12	1.98	0.45
27:2:4:THR:O	29:X:700:C:H5'	2.16	0.45
29:X:15:G:C5	29:X:16:G:N7	2.84	0.45
29:X:742:G:H2'	29:X:1766:U:H1'	1.98	0.45
29:X:1670:G:H8	29:X:1670:G:OP2	2.00	0.45
29:X:2227:C:H5''	29:X:2228:U:OP2	2.16	0.45
29:X:2727:G:O6	29:X:2735:C:H5''	2.15	0.45
29:X:2754:C:N4	29:X:2755:A:C5	2.84	0.45
30:Y:54:U:H4'	30:Y:54:U:OP1	2.16	0.45
2:A:39:LYS:NZ	2:A:58:HIS:O	2.34	0.45
5:D:74:ILE:HG23	5:D:80:ARG:HA	1.97	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:38:ASN:OD1	6:E:64:LEU:HD22	2.16	0.45
7:F:25:PRO:HB2	7:F:29:GLN:NE2	2.31	0.45
9:H:9:ASP:OD2	9:H:9:ASP:N	2.48	0.45
9:H:115:ALA:C	9:H:117:GLU:H	2.18	0.45
14:M:2:GLN:N	29:X:2795:A:N1	2.64	0.45
14:M:38:LYS:HZ2	14:M:89:ASN:HB2	1.82	0.45
18:Q:42:ILE:HD12	18:Q:80:VAL:HG21	1.99	0.45
18:Q:62:ARG:HA	18:Q:71:GLN:HA	1.98	0.45
18:Q:91:LEU:HD12	18:Q:91:LEU:HA	1.80	0.45
22:U:75:TYR:O	22:U:76:LYS:HB2	2.16	0.45
29:X:38:G:H2'	29:X:39:C:H6	1.81	0.45
29:X:314:G:H2'	29:X:315:G:C8	2.52	0.45
29:X:571:U:C2	29:X:581:A:C8	3.05	0.45
29:X:615:C:H1'	29:X:670:U:H1'	1.98	0.45
29:X:628:A:H8	29:X:628:A:O5'	1.99	0.45
29:X:1296:G:N2	29:X:1299:A:OP2	2.49	0.45
29:X:1302:C:O2'	29:X:1303:U:H5'	2.17	0.45
29:X:1336:G:O5'	29:X:1336:G:H8	1.99	0.45
29:X:2235:G:N2	29:X:2254:C:C4	2.85	0.45
29:X:2431:C:H2'	29:X:2432:A:C8	2.51	0.45
29:X:2468:G:C6	29:X:2469:G:C6	3.04	0.45
29:X:2555:G:OP1	29:X:2555:G:H3'	2.16	0.45
29:X:2686:C:C2'	29:X:2687:G:H5'	2.46	0.45
1:O:95:LEU:HD13	1:O:98:ARG:HB2	1.98	0.45
5:D:114:PHE:HE1	5:D:117:ILE:HG13	1.81	0.45
5:D:143:TYR:HA	5:D:146:VAL:HG22	1.98	0.45
8:G:69:ASP:HA	15:N:64:ARG:HH22	1.82	0.45
11:J:69:ILE:HG23	11:J:104:MET:HA	1.99	0.45
13:L:14:ARG:HG2	13:L:15:ARG:HH12	1.82	0.45
16:O:92:ALA:C	16:O:93:ILE:HD12	2.37	0.45
17:P:9:ARG:HG3	17:P:10:ASN:H	1.82	0.45
25:Z:36:CYS:HB3	25:Z:49:CYS:HB3	1.55	0.45
29:X:99:U:H5''	29:X:100:G:N7	2.32	0.45
29:X:158:A:H2	29:X:447:U:H4'	1.81	0.45
29:X:573:C:H2'	29:X:574:C:O4'	2.17	0.45
29:X:602:C:N4	29:X:678:G:H1	2.14	0.45
29:X:872:G:O2'	29:X:928:G:O6	2.30	0.45
29:X:1202:U:H2'	29:X:1203:A:C8	2.36	0.45
29:X:1888:C:OP1	29:X:1889:G:H5'	2.14	0.45
29:X:1918:G:H1'	29:X:1947:G:N2	2.31	0.45
29:X:1932:G:N2	29:X:1941:C:C2	2.85	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:2286:G:H3'	29:X:2287:G:H8	1.81	0.45
29:X:2792:C:C2	29:X:2805:G:C2	3.05	0.45
3:B:176:ARG:NE	14:M:16:ILE:HD13	2.31	0.45
4:C:162:ARG:HG3	4:C:169:VAL:HG21	1.98	0.45
5:D:164:GLU:HG3	5:D:165:GLU:HG2	1.98	0.45
6:E:40:GLU:H	6:E:40:GLU:HG3	1.55	0.45
12:K:64:ARG:O	12:K:68:GLN:HG3	2.17	0.45
18:Q:38:ILE:O	18:Q:42:ILE:HG13	2.16	0.45
28:3:58:MET:CA	28:3:61:MET:HG3	2.45	0.45
29:X:42:G:H2'	29:X:43:A:H8	1.81	0.45
29:X:534:U:H2'	29:X:535:U:C6	2.51	0.45
29:X:585:U:H4'	29:X:2481:G:N7	2.31	0.45
29:X:588:G:N2	29:X:1275:A:C4	2.85	0.45
29:X:591:G:C6	29:X:592:G:C6	3.04	0.45
29:X:650:U:H2'	29:X:651:C:C6	2.51	0.45
29:X:1069:G:H2'	29:X:1070:G:C8	2.52	0.45
29:X:1310:C:C2	29:X:1311:C:C5	3.05	0.45
29:X:2523:G:N3	29:X:2524:G:C8	2.85	0.45
1:O:7:GLU:HA	1:O:10:VAL:HB	1.98	0.45
2:A:186:HIS:O	2:A:189:CYS:N	2.47	0.45
3:B:20:ALA:HB2	9:H:85:ASP:O	2.16	0.45
3:B:61:LYS:O	3:B:64:GLN:HB2	2.16	0.45
4:C:148:VAL:HG12	4:C:187:VAL:HG23	1.99	0.45
11:J:32:ASP:OD2	11:J:135:ARG:NH2	2.40	0.45
12:K:11:ASN:ND2	29:X:1670:G:O6	2.49	0.45
17:P:97:VAL:HG22	17:P:124:ILE:HA	1.99	0.45
20:S:26:LYS:HD3	20:S:26:LYS:N	2.31	0.45
20:S:103:ARG:NH1	20:S:108:VAL:HG22	2.32	0.45
26:1:27:ASN:C	26:1:29:ARG:H	2.20	0.45
29:X:115:G:OP2	29:X:117:A:O2'	2.29	0.45
29:X:306:G:H2'	29:X:307:C:H6	1.82	0.45
29:X:476:G:H2'	29:X:477:A:C8	2.52	0.45
29:X:1269:G:N3	29:X:1269:G:H2'	2.32	0.45
29:X:1367:A:H2'	29:X:1368:G:O4'	2.16	0.45
29:X:1810:U:H4'	29:X:1813:A:H1'	1.99	0.45
29:X:2007:G:C2	29:X:2023:C:C2	3.05	0.45
29:X:2430:A:OP1	29:X:2476:A:N6	2.49	0.45
29:X:2523:G:C4	29:X:2524:G:C8	3.05	0.45
29:X:2529:G:C4	29:X:2530:C:C5	3.05	0.45
29:X:2837:G:H2'	29:X:2838:U:C6	2.51	0.45
6:E:97:LYS:H	6:E:104:GLU:HB2	1.80	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:64:VAL:HG22	9:H:106:ARG:NH2	2.25	0.45
11:J:11:ARG:HB3	11:J:12:LYS:H	1.41	0.45
20:S:112:LEU:HD12	20:S:113:VAL:H	1.82	0.45
21:T:46:LYS:NZ	21:T:76:ALA:HA	2.31	0.45
21:T:57:HIS:N	21:T:57:HIS:CD2	2.84	0.45
22:U:14:VAL:O	22:U:15:VAL:HG22	2.16	0.45
26:1:46:HIS:CE1	29:X:2351:G:HO2'	2.35	0.45
29:X:311:A:H1'	29:X:330:C:O4'	2.17	0.45
29:X:458:G:H5''	29:X:458:G:H8	1.82	0.45
29:X:2589:C:H4'	29:X:2590:U:H5'	1.99	0.45
29:X:2683:C:H2'	29:X:2684:A:O4'	2.17	0.45
29:X:2792:C:N3	29:X:2805:G:C2	2.84	0.45
1:0:43:LEU:HD12	1:0:167:VAL:HG11	1.99	0.45
3:B:9:ILE:HD12	3:B:9:ILE:N	2.32	0.45
14:M:33:VAL:HG11	14:M:91:VAL:HG12	1.98	0.45
21:T:36:ILE:HD11	29:X:2343:C:O2	2.16	0.45
29:X:491:A:H3'	29:X:492:G:H5''	1.97	0.45
29:X:697:G:C2	29:X:807:A:C2	3.05	0.45
29:X:769:C:C4	29:X:770:U:C4	3.05	0.45
29:X:1029:C:O3'	29:X:1131:G:N2	2.49	0.45
29:X:1298:G:N2	29:X:1341:G:H5'	2.32	0.45
29:X:1628:C:N3	29:X:1629:G:C8	2.85	0.45
29:X:1750:A:H2'	29:X:1751:A:H8	1.81	0.45
29:X:2264:C:H4'	29:X:2267:A:N7	2.32	0.45
29:X:2302:G:H1	29:X:2311:U:H5	1.65	0.45
29:X:2345:A:C6	29:X:2346:G:C4	3.05	0.45
29:X:2611:A:C2	29:X:2767:C:O2	2.70	0.45
29:X:2819:G:H2'	29:X:2820:C:C6	2.51	0.45
2:A:63:ARG:O	2:A:65:ILE:HG13	2.17	0.45
2:A:69:ARG:HH11	2:A:130:ALA:HB2	1.82	0.45
2:A:76:ASN:HB2	2:A:117:VAL:O	2.17	0.45
2:A:186:HIS:NE2	29:X:2201:G:H5'	2.32	0.45
2:A:218:LYS:HB3	2:A:218:LYS:HE3	1.49	0.45
4:C:3:GLN:O	4:C:12:GLY:HA3	2.17	0.45
4:C:14:THR:HB	4:C:15:ILE:H	1.58	0.45
4:C:172:VAL:HB	4:C:173:ALA:H	1.64	0.45
10:I:63:ARG:HD3	28:3:25:PHE:CE1	2.52	0.45
10:I:80:LEU:HD23	10:I:80:LEU:HA	1.75	0.45
11:J:22:ALA:HB2	11:J:99:LYS:CB	2.46	0.45
11:J:102:ARG:NH1	11:J:103:VAL:O	2.49	0.45
11:J:139:ASP:OD2	11:J:139:ASP:N	2.50	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:51:LEU:CD2	12:K:66:VAL:HG22	2.47	0.45
13:L:99:ARG:H	13:L:99:ARG:HG2	1.52	0.45
14:M:33:VAL:CG1	14:M:91:VAL:HG12	2.46	0.45
24:W:5:LEU:HB2	24:W:25:LEU:CD1	2.43	0.45
29:X:820:U:OP1	29:X:843:G:N2	2.50	0.45
29:X:831:G:N7	29:X:1201:G:C6	2.85	0.45
29:X:1309:G:H1	29:X:1661:C:N4	2.15	0.45
29:X:1478:U:C2	29:X:1479:G:C8	3.05	0.45
29:X:2217:G:H2'	29:X:2217:G:N3	2.32	0.45
29:X:2248:A:N3	29:X:2248:A:H2'	2.30	0.45
29:X:2494:C:N4	29:X:2548:G:H1	2.06	0.45
2:A:43:ARG:HH21	29:X:704:G:H4'	1.82	0.45
3:B:5:LEU:HD22	3:B:195:LEU:HD11	1.98	0.45
5:D:22:TYR:CE1	5:D:28:VAL:HG13	2.52	0.45
6:E:9:ILE:HD11	6:E:52:VAL:HG23	1.99	0.45
10:I:4:HIS:CD2	10:I:4:HIS:C	2.90	0.45
10:I:14:LYS:HD3	29:X:675:C:O2'	2.17	0.45
16:O:35:LEU:HD23	16:O:36:LYS:N	2.28	0.45
19:R:15:HIS:CD2	19:R:16:PHE:CD2	2.96	0.45
22:U:21:ARG:CG	22:U:22:GLY:H	2.30	0.45
29:X:1:G:H1	29:X:2876:C:H42	1.65	0.45
29:X:567:G:H2'	29:X:568:G:C8	2.52	0.45
29:X:1408:A:N1	29:X:1411:C:C2	2.85	0.45
29:X:1713:G:C6	29:X:1714:A:C5	3.05	0.45
29:X:1775:A:H4'	29:X:1776:A:OP1	2.15	0.45
29:X:2078:G:H2'	29:X:2079:A:C8	2.52	0.45
29:X:2691:C:HO2'	29:X:2692:A:P	2.36	0.45
30:Y:15:A:H4'	30:Y:17:A:H2'	1.99	0.45
2:A:232:PRO:HB2	2:A:233:HIS:HD2	1.82	0.44
4:C:62:LYS:HZ2	29:X:2043:A:H3'	1.82	0.44
4:C:118:VAL:O	4:C:120:VAL:HG23	2.17	0.44
4:C:133:PHE:CE1	4:C:161:ALA:HB2	2.51	0.44
6:E:126:PRO:HG2	6:E:130:ARG:HB2	1.99	0.44
8:G:140:GLN:O	8:G:143:ALA:N	2.50	0.44
10:I:118:VAL:O	10:I:138:GLY:HA3	2.17	0.44
14:M:81:PHE:HA	14:M:82:PRO:HD3	1.74	0.44
14:M:93:ILE:HD12	14:M:93:ILE:N	2.26	0.44
16:O:5:ILE:N	16:O:38:LEU:HD12	2.33	0.44
17:P:91:PHE:CZ	17:P:131:LYS:HG3	2.52	0.44
18:Q:7:LEU:HD21	18:Q:42:ILE:HG12	1.99	0.44
18:Q:8:GLN:O	18:Q:9:ALA:HB2	2.16	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Q:64:ARG:HH21	18:Q:69:ILE:HD11	1.82	0.44
28:3:17:THR:HG23	28:3:20:GLY:H	1.82	0.44
29:X:404:A:H1'	29:X:424:G:O4'	2.17	0.44
29:X:452:G:H2'	29:X:453:U:C6	2.51	0.44
29:X:498:C:N4	29:X:499:G:C6	2.85	0.44
29:X:944:A:OP2	29:X:944:A:H8	2.00	0.44
29:X:1236:G:C6	29:X:1240:G:C6	3.05	0.44
29:X:1611:U:H2'	29:X:1612:U:H6	1.82	0.44
29:X:2020:G:H2'	29:X:2021:G:C8	2.52	0.44
29:X:2048:C:H1'	29:X:2428:U:N3	2.32	0.44
29:X:2283:G:H2'	29:X:2283:G:N3	2.32	0.44
29:X:2831:A:H2'	29:X:2832:G:O4'	2.17	0.44
1:0:68:VAL:HG21	1:0:153:LYS:HG2	2.00	0.44
2:A:271:VAL:HG22	2:A:272:THR:HG23	1.98	0.44
3:B:119:ARG:HG2	3:B:120:TRP:NE1	2.33	0.44
4:C:95:LEU:O	4:C:100:ARG:NH1	2.45	0.44
10:I:19:VAL:O	10:I:21:ARG:NH1	2.51	0.44
12:K:27:ALA:O	12:K:31:GLU:N	2.49	0.44
15:N:40:LEU:O	15:N:43:ALA:HB3	2.18	0.44
18:Q:62:ARG:HG2	18:Q:71:GLN:HG3	1.98	0.44
20:S:36:ARG:HG2	20:S:40:ASP:OD2	2.17	0.44
24:W:49:HIS:HD2	24:W:50:LEU:HG	1.82	0.44
25:Z:13:LYS:HD3	29:X:527:C:OP2	2.17	0.44
29:X:420:C:H2'	29:X:421:G:H8	1.83	0.44
29:X:654:A:HO2'	29:X:655:A:P	2.40	0.44
29:X:1229:C:O5'	29:X:1229:C:H6	2.00	0.44
29:X:1348:C:H2'	29:X:1349:A:C8	2.52	0.44
29:X:1352:G:C6	29:X:1353:A:N6	2.85	0.44
29:X:1787:U:H2'	29:X:1788:C:C6	2.52	0.44
29:X:1882:G:N3	29:X:1882:G:H2'	2.32	0.44
29:X:2034:A:H2'	29:X:2557:G:OP1	2.17	0.44
30:Y:58:G:C4'	30:Y:59:A:H5''	2.47	0.44
2:A:233:HIS:NE2	2:A:247:VAL:HG12	2.33	0.44
4:C:17:LEU:HA	4:C:18:PRO:HD3	1.77	0.44
12:K:54:THR:CG2	12:K:66:VAL:HG23	2.47	0.44
17:P:22:LYS:HA	17:P:23:PRO:HD3	1.56	0.44
28:3:64:ARG:HH21	29:X:219:G:H5'	1.82	0.44
29:X:443:A:H5''	29:X:444:U:OP2	2.18	0.44
29:X:587:A:OP2	29:X:587:A:H8	2.00	0.44
29:X:742:G:H5'	29:X:743:A:H5''	2.00	0.44
29:X:828:C:H2'	29:X:829:C:H6	1.82	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1067:G:H2'	29:X:1113:C:H41	1.81	0.44
29:X:1142:G:C8	29:X:2008:C:H4'	2.52	0.44
29:X:1174:G:N2	29:X:1175:A:C4	2.85	0.44
29:X:1733:U:H3	29:X:1734:C:H41	1.64	0.44
29:X:1770:U:C5	29:X:1775:A:N7	2.73	0.44
29:X:1815:G:C4	29:X:1816:G:C8	3.06	0.44
29:X:1858:C:H2'	29:X:1859:A:O4'	2.16	0.44
29:X:2241:U:H2'	29:X:2242:C:C6	2.48	0.44
29:X:2375:G:N3	29:X:2400:G:N2	2.65	0.44
29:X:2662:C:H2'	29:X:2663:U:H6	1.82	0.44
30:Y:16:U:O2'	30:Y:110:U:H1'	2.18	0.44
2:A:225:ALA:HB1	29:X:795:A:HO2'	1.82	0.44
3:B:19:ARG:HH11	9:H:84:ALA:HB1	1.82	0.44
9:H:20:MET:HG2	9:H:21:CYS:N	2.29	0.44
14:M:106:TYR:HD1	29:X:1745:C:H4'	1.83	0.44
16:O:14:VAL:HG12	16:O:18:ASP:OD2	2.18	0.44
18:Q:9:ALA:O	18:Q:27:PHE:HB3	2.17	0.44
20:S:121:GLN:O	20:S:161:ALA:HB3	2.18	0.44
28:3:21:LYS:HB3	28:3:55:TRP:CH2	2.53	0.44
29:X:198:A:O2'	29:X:243:G:O6	2.35	0.44
29:X:526:C:H1'	29:X:1274:C:O2'	2.16	0.44
29:X:619:A:N6	29:X:630:G:O2'	2.51	0.44
29:X:1283:C:H5''	29:X:1284:G:C5'	2.47	0.44
29:X:1359:G:C6	29:X:1617:G:C6	3.05	0.44
29:X:1623:C:H4'	29:X:1624:A:O5'	2.17	0.44
29:X:2022:C:H2'	29:X:2023:C:C6	2.53	0.44
29:X:2067:U:H2'	29:X:2068:C:C6	2.53	0.44
29:X:2229:G:HO2'	29:X:2475:C:P	2.40	0.44
30:Y:30:C:H2'	30:Y:31:A:O4'	2.18	0.44
4:C:68:ARG:NH2	29:X:2043:A:H62	2.16	0.44
4:C:178:TYR:O	4:C:182:ARG:N	2.42	0.44
7:F:109:LYS:HD2	7:F:109:LYS:HA	1.60	0.44
7:F:130:THR:HG1	29:X:1071:U:H5	1.65	0.44
8:G:70:PHE:HA	8:G:76:GLN:OE1	2.18	0.44
8:G:128:GLU:HG3	8:G:150:VAL:HG21	1.99	0.44
9:H:1:MET:O	9:H:2:ILE:HD13	2.17	0.44
12:K:38:LEU:O	12:K:41:ALA:HB3	2.18	0.44
12:K:39:THR:O	12:K:41:ALA:N	2.51	0.44
15:N:47:TYR:CE2	15:N:51:ARG:CZ	3.00	0.44
20:S:66:VAL:HG22	20:S:83:PHE:CE1	2.53	0.44
20:S:91:PRO:HG2	20:S:124:ALA:HA	1.99	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:T:11:LYS:HE2	21:T:11:LYS:HB2	1.61	0.44
29:X:318:G:N1	29:X:321:A:OP2	2.47	0.44
29:X:757:U:H2'	29:X:758:G:O4'	2.17	0.44
29:X:875:G:O2'	30:Y:80:A:N3	2.38	0.44
29:X:1283:C:O5'	29:X:1283:C:H6	1.99	0.44
29:X:1629:G:C6	29:X:1633:C:C6	3.05	0.44
29:X:1724:C:N3	29:X:1747:G:C6	2.85	0.44
29:X:1951:G:O2'	29:X:1952:A:O4'	2.26	0.44
29:X:2011:U:H2'	29:X:2012:A:O4'	2.18	0.44
29:X:2427:A:OP1	29:X:2478:C:OP1	2.35	0.44
29:X:2741:G:C6	29:X:2742:G:N7	2.86	0.44
29:X:2817:A:H2'	29:X:2818:G:O4'	2.16	0.44
30:Y:16:U:O2'	30:Y:110:U:O2	2.34	0.44
30:Y:67:C:N4	30:Y:111:C:O2'	2.43	0.44
2:A:142:VAL:HG12	2:A:163:VAL:O	2.17	0.44
5:D:106:ILE:HB	5:D:139:PRO:HB3	2.00	0.44
14:M:60:SER:O	14:M:63:ARG:NH1	2.51	0.44
19:R:51:VAL:HG13	19:R:73:GLU:CB	2.48	0.44
29:X:7:G:C4	29:X:8:A:C8	3.06	0.44
29:X:42:G:H2'	29:X:43:A:C8	2.52	0.44
29:X:223:C:N4	29:X:224:G:O6	2.50	0.44
29:X:389:G:N2	29:X:412:U:H1'	2.32	0.44
29:X:1329:U:O2'	29:X:1330:G:H5'	2.17	0.44
29:X:1819:U:H5'	29:X:1954:A:O3'	2.17	0.44
29:X:1835:C:H2'	29:X:1836:C:C6	2.52	0.44
29:X:2038:C:O5'	29:X:2039:G:H5''	2.17	0.44
29:X:2039:G:N2	29:X:2040:A:C4	2.86	0.44
29:X:2233:C:C2'	29:X:2234:G:H5'	2.48	0.44
29:X:2290:A:N3	29:X:2290:A:H2'	2.33	0.44
29:X:2800:C:H5''	29:X:2801:A:OP2	2.17	0.44
6:E:7:GLN:H	6:E:8:PRO:HD3	1.82	0.44
6:E:111:HIS:HA	6:E:112:PRO:HD2	1.55	0.44
7:F:111:LYS:HD3	7:F:115:LEU:HG	1.99	0.44
11:J:25:GLY:HA3	29:X:919:U:OP1	2.18	0.44
15:N:68:GLY:HA2	15:N:71:LEU:HD12	2.00	0.44
16:O:31:ASP:HB2	16:O:60:VAL:HG21	2.00	0.44
16:O:53:LYS:HG3	16:O:54:TYR:CD1	2.53	0.44
17:P:33:MET:SD	17:P:64:ALA:HB2	2.58	0.44
17:P:75:ALA:HB1	17:P:128:VAL:HG22	1.99	0.44
20:S:18:MET:HA	20:S:35:ASP:HA	1.98	0.44
28:3:42:ARG:HD3	29:X:2328:G:OP2	2.16	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:349:G:H2'	29:X:350:U:C6	2.53	0.44
29:X:387:A:N6	29:X:413:G:O2'	2.51	0.44
29:X:488:A:H8	29:X:488:A:OP1	2.01	0.44
29:X:580:A:C8	29:X:2013:A:N6	2.86	0.44
29:X:1177:U:C2	29:X:1198:C:O2	2.71	0.44
29:X:1310:C:OP1	29:X:2689:C:H4'	2.17	0.44
29:X:1430:G:O2'	29:X:1603:A:H1'	2.18	0.44
29:X:1506:C:H4'	29:X:1507:A:OP1	2.17	0.44
29:X:2793:G:N2	29:X:2804:G:C4	2.86	0.44
1:0:96:ILE:HD11	1:0:118:GLN:HB3	2.00	0.44
1:0:96:ILE:HG23	1:0:123:LEU:HG	2.00	0.44
2:A:29:PRO:HG2	2:A:63:ARG:NH1	2.33	0.44
3:B:7:THR:O	3:B:9:ILE:HD12	2.17	0.44
3:B:55:ALA:H	3:B:58:LYS:HZ2	1.61	0.44
5:D:122:PHE:HB3	5:D:123:ASP:H	1.63	0.44
11:J:12:LYS:HG2	29:X:923:A:N6	2.33	0.44
13:L:9:ARG:O	13:L:11:LEU:N	2.51	0.44
13:L:91:ARG:CG	13:L:92:GLY:H	2.31	0.44
14:M:56:ALA:HB1	14:M:103:LYS:HE3	2.00	0.44
14:M:101:ARG:NH1	29:X:1745:C:OP1	2.47	0.44
20:S:91:PRO:HG3	20:S:126:GLY:N	2.32	0.44
28:3:3:LYS:HE3	29:X:219:G:OP2	2.17	0.44
28:3:11:LYS:HB3	28:3:11:LYS:HE2	1.68	0.44
29:X:213:C:H2'	29:X:214:C:C6	2.53	0.44
29:X:464:G:H2'	29:X:465:C:H6	1.83	0.44
29:X:471:A:C2	29:X:481:A:C5	3.06	0.44
29:X:534:U:P	29:X:549:G:H21	2.40	0.44
29:X:790:A:H2'	29:X:791:G:H8	1.83	0.44
29:X:1065:A:H2'	29:X:1066:G:H8	1.82	0.44
29:X:2309:G:H2'	29:X:2310:G:O4'	2.18	0.44
29:X:2571:G:C6	29:X:2572:U:N3	2.86	0.44
29:X:2578:G:C2	29:X:2579:A:C8	3.05	0.44
29:X:2857:C:N3	29:X:2858:A:C8	2.86	0.44
1:0:4:ARG:HG2	1:0:5:ALA:H	1.82	0.44
3:B:5:LEU:HD12	3:B:49:ILE:CD1	2.48	0.44
3:B:10:GLY:O	3:B:25:VAL:HG23	2.18	0.44
3:B:123:ALA:HB2	29:X:2491:C:OP1	2.17	0.44
3:B:199:ARG:H	3:B:199:ARG:HG3	1.65	0.44
4:C:5:ASN:N	4:C:5:ASN:OD1	2.51	0.44
10:I:41:SER:OG	29:X:684:C:H3'	2.18	0.44
15:N:91:ASN:ND2	15:N:93:LYS:HB3	2.33	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:65:C:H2'	29:X:66:U:O4'	2.18	0.44
29:X:199:A:O2'	29:X:200:A:O5'	2.29	0.44
29:X:228:A:C5	29:X:229:G:H1'	2.53	0.44
29:X:501:G:H2'	29:X:502:A:H8	1.82	0.44
29:X:1024:G:H2'	29:X:1025:A:C8	2.53	0.44
29:X:1174:G:H2'	29:X:1175:A:H8	1.82	0.44
29:X:1236:G:N2	29:X:1239:A:OP2	2.37	0.44
29:X:1254:G:C2	29:X:1255:A:C5	3.06	0.44
29:X:1642:G:H8	29:X:1642:G:O5'	2.01	0.44
29:X:2508:G:H5''	29:X:2509:A:H5''	2.00	0.44
29:X:2813:G:C5	29:X:2814:G:N7	2.86	0.44
3:B:60:ASN:HB3	3:B:62:PRO:HD2	2.00	0.43
4:C:154:ASP:OD1	4:C:154:ASP:N	2.50	0.43
5:D:92:ARG:CZ	30:Y:46:G:H5''	2.48	0.43
11:J:84:MET:HE2	29:X:967:G:H4'	2.00	0.43
11:J:111:THR:H	11:J:114:GLN:HG3	1.83	0.43
16:O:32:LYS:HB3	16:O:32:LYS:HE3	1.80	0.43
20:S:3:LEU:HD13	20:S:56:VAL:HA	2.00	0.43
25:Z:52:TYR:OH	29:X:2859:U:N3	2.50	0.43
28:3:17:THR:HG22	28:3:21:LYS:O	2.18	0.43
28:3:23:MET:HG2	28:3:49:VAL:HG22	1.99	0.43
29:X:567:G:H2'	29:X:568:G:H8	1.83	0.43
29:X:758:G:N2	29:X:766:A:C6	2.86	0.43
29:X:1474:A:H2'	29:X:1474:A:N3	2.32	0.43
29:X:1494:G:O2'	29:X:1574:A:N7	2.51	0.43
29:X:1600:U:H5''	29:X:1601:U:H5'	1.99	0.43
29:X:1734:C:H2'	29:X:1735:G:H5'	1.99	0.43
29:X:2433:G:C4	29:X:2434:G:C8	3.06	0.43
29:X:2684:A:O5'	29:X:2684:A:H8	2.01	0.43
1:0:110:VAL:HG12	1:0:111:ALA:H	1.83	0.43
1:0:196:LYS:HE2	1:0:204:PHE:CZ	2.53	0.43
3:B:48:GLN:HA	3:B:79:ARG:O	2.19	0.43
5:D:88:LYS:HD3	29:X:2292:C:H5''	1.99	0.43
9:H:7:ARG:HD3	9:H:18:GLU:OE2	2.17	0.43
13:L:33:ARG:NH2	13:L:38:ILE:HD13	2.32	0.43
17:P:36:ARG:NH1	25:Z:20:ARG:NH2	2.65	0.43
19:R:24:VAL:HA	19:R:80:LYS:O	2.18	0.43
20:S:19:ILE:HD11	20:S:36:ARG:HG3	2.00	0.43
29:X:312:G:N2	29:X:328:A:H1'	2.32	0.43
29:X:616:U:H4'	29:X:671:A:H4'	1.99	0.43
29:X:818:G:N2	29:X:842:A:OP1	2.51	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:825:C:H2'	29:X:826:U:C6	2.51	0.43
29:X:1146:G:N2	29:X:1147:G:C4	2.86	0.43
29:X:1436:G:O2'	29:X:1508:G:N3	2.51	0.43
29:X:1562:G:H3'	29:X:1563:U:H5'	2.01	0.43
29:X:2269:G:N2	29:X:2322:U:O2'	2.51	0.43
29:X:2273:C:H2'	29:X:2274:C:H6	1.82	0.43
29:X:2407:G:H5''	29:X:2408:G:O5'	2.17	0.43
29:X:2814:G:C2	29:X:2815:C:C2	3.06	0.43
2:A:76:ASN:HB3	2:A:118:ASN:CG	2.39	0.43
2:A:210:GLY:O	2:A:213:ARG:N	2.50	0.43
4:C:27:LEU:O	4:C:31:VAL:HG23	2.18	0.43
4:C:103:GLY:O	4:C:106:MET:N	2.51	0.43
5:D:129:ASN:HB3	5:D:155:THR:HG22	2.00	0.43
7:F:1:MET:HE2	7:F:2:ARG:HH11	1.83	0.43
15:N:51:ARG:O	15:N:54:LYS:HB2	2.18	0.43
16:O:78:VAL:O	16:O:79:GLN:HB2	2.18	0.43
18:Q:29:VAL:HG12	18:Q:30:SER:N	2.32	0.43
22:U:17:SER:OG	22:U:44:ALA:HA	2.18	0.43
24:W:37:THR:CB	29:X:940:G:H5'	2.48	0.43
29:X:18:U:O2'	29:X:563:U:OP1	2.33	0.43
29:X:851:C:C2	29:X:952:A:C6	3.07	0.43
29:X:1089:C:H1'	29:X:1099:A:H2	1.83	0.43
29:X:1424:U:H2'	29:X:1425:G:O4'	2.18	0.43
29:X:2097:A:H61	29:X:2102:A:H62	1.65	0.43
29:X:2212:U:H2'	29:X:2213:G:C8	2.53	0.43
29:X:2294:U:H2'	29:X:2295:C:C6	2.53	0.43
29:X:2349:G:C6	29:X:2350:G:C5	3.07	0.43
29:X:2511:G:C5	29:X:2512:A:N7	2.86	0.43
29:X:2678:C:O2	29:X:2688:G:N1	2.52	0.43
2:A:69:ARG:HH22	2:A:192:THR:HG21	1.84	0.43
3:B:129:HIS:CE1	29:X:1692:C:N3	2.86	0.43
4:C:28:HIS:CD2	10:I:8:PRO:HA	2.54	0.43
6:E:25:LYS:HG2	6:E:26:VAL:N	2.32	0.43
7:F:10:LEU:HD21	7:F:57:ILE:HG13	2.00	0.43
7:F:53:ILE:HG12	7:F:72:PRO:HB3	2.00	0.43
9:H:22:ILE:HD11	29:X:1935:A:N6	2.33	0.43
12:K:33:ARG:CB	12:K:114:GLU:HB2	2.49	0.43
15:N:67:ALA:O	15:N:71:LEU:HG	2.18	0.43
19:R:78:ALA:HA	19:R:81:VAL:HB	2.01	0.43
29:X:82:G:H1	29:X:100:G:HO2'	1.66	0.43
29:X:312:G:O2'	29:X:313:U:H6	1.95	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:350:U:H6	29:X:350:U:O5'	2.01	0.43
29:X:574:C:H4'	29:X:1266:G:C6	2.54	0.43
29:X:714:G:C2	29:X:745:C:C5	3.07	0.43
29:X:717:G:H1'	29:X:739:G:H22	1.84	0.43
29:X:1229:C:H2'	29:X:1230:C:C6	2.52	0.43
29:X:1310:C:H2'	29:X:1311:C:H6	1.84	0.43
29:X:2445:C:H42	29:X:2463:G:H1	1.66	0.43
29:X:2659:C:N3	29:X:2660:C:C5	2.86	0.43
2:A:62:TYR:CE1	29:X:1808:C:H3'	2.51	0.43
4:C:43:ALA:HB2	29:X:456:C:H4'	2.01	0.43
7:F:10:LEU:HD12	7:F:12:LEU:HG	2.00	0.43
10:I:73:GLU:HG3	10:I:105:PRO:O	2.19	0.43
15:N:28:ARG:HG2	15:N:38:THR:OG1	2.19	0.43
19:R:54:ILE:HD12	19:R:71:GLN:NE2	2.33	0.43
20:S:49:THR:HG22	20:S:94:VAL:HG13	2.00	0.43
20:S:72:ASP:O	20:S:76:ARG:N	2.49	0.43
25:Z:35:GLN:O	25:Z:37:HIS:N	2.52	0.43
29:X:502:A:H2'	29:X:503:G:O4'	2.19	0.43
29:X:1749:G:N3	29:X:1749:G:H5''	2.34	0.43
29:X:2499:C:C4	29:X:2546:G:C8	3.06	0.43
29:X:2666:U:O2'	29:X:2667:C:H5'	2.18	0.43
5:D:70:ALA:C	5:D:72:LYS:H	2.21	0.43
5:D:147:ASP:OD1	5:D:147:ASP:N	2.52	0.43
11:J:8:THR:HG22	11:J:70:PHE:CE2	2.53	0.43
17:P:36:ARG:CZ	25:Z:20:ARG:HH21	2.31	0.43
18:Q:15:LYS:HZ3	29:X:1354:A:H62	1.67	0.43
18:Q:57:ASN:OD1	18:Q:57:ASN:N	2.51	0.43
19:R:58:VAL:HA	29:X:494:A:C4'	2.48	0.43
21:T:56:ASP:CG	29:X:2343:C:H5'	2.39	0.43
23:V:11:ALA:HB1	23:V:57:LYS:HD2	2.01	0.43
29:X:26:G:O2'	29:X:27:G:H5'	2.18	0.43
29:X:436:A:N3	29:X:436:A:H2'	2.34	0.43
29:X:539:A:N7	29:X:2025:A:C2	2.87	0.43
29:X:676:G:C5	29:X:677:G:C8	3.07	0.43
29:X:777:A:O2'	29:X:778:G:H5'	2.19	0.43
29:X:783:G:N1	29:X:784:U:C2	2.87	0.43
29:X:1071:U:O4'	29:X:1073:G:H5'	2.18	0.43
29:X:1175:A:H2'	29:X:1176:U:C6	2.54	0.43
29:X:1419:G:H2'	29:X:1420:A:C8	2.53	0.43
29:X:1539:U:O5'	29:X:1539:U:H6	2.02	0.43
29:X:1678:G:C4	29:X:1983:G:N2	2.87	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1715:A:H8	29:X:1715:A:O5'	2.01	0.43
29:X:1865:C:H2'	29:X:1866:G:O4'	2.19	0.43
29:X:2269:G:N2	29:X:2322:U:H1'	2.34	0.43
29:X:2487:G:C2	29:X:2561:G:C6	3.07	0.43
29:X:2528:G:C2	29:X:2529:G:C8	3.05	0.43
30:Y:25:G:N2	30:Y:62:C:N3	2.52	0.43
30:Y:86:A:C2	30:Y:96:C:C2	3.07	0.43
4:C:59:TYR:HD1	4:C:60:GLY:N	2.15	0.43
4:C:114:GLY:N	4:C:115:GLY:HA2	2.33	0.43
7:F:22:PRO:HB2	7:F:23:VAL:H	1.61	0.43
10:I:73:GLU:OE2	10:I:104:ARG:HB2	2.19	0.43
19:R:38:LEU:O	19:R:46:VAL:HG23	2.19	0.43
29:X:717:G:N3	29:X:739:G:C2	2.87	0.43
29:X:998:C:O2	29:X:1011:A:H2	2.02	0.43
29:X:1110:G:H8	29:X:1110:G:O5'	2.01	0.43
29:X:1609:G:H2'	29:X:1610:A:O4'	2.18	0.43
29:X:1670:G:H5''	29:X:2797:G:N2	2.33	0.43
1:O:188:LEU:O	1:O:192:LEU:HB2	2.18	0.43
2:A:226:MET:HB3	2:A:230:ASP:HB2	2.01	0.43
3:B:44:TYR:CZ	29:X:2616:U:H5'	2.54	0.43
3:B:55:ALA:H	3:B:58:LYS:HZ1	1.64	0.43
9:H:11:ALA:O	9:H:111:PHE:N	2.46	0.43
11:J:52:ARG:O	11:J:56:SER:HB3	2.18	0.43
12:K:102:THR:HG22	12:K:103:ARG:H	1.83	0.43
15:N:63:GLN:H	15:N:63:GLN:HG2	1.56	0.43
21:T:72:LYS:HD3	30:Y:14:C:H5	1.84	0.43
25:Z:32:GLU:O	25:Z:34:PRO:HD3	2.18	0.43
29:X:330:C:C2	29:X:331:U:C6	3.06	0.43
29:X:444:U:O2'	29:X:445:A:H5'	2.19	0.43
29:X:547:U:H2'	29:X:548:G:C8	2.54	0.43
29:X:649:G:C5	29:X:650:U:C5	3.06	0.43
29:X:655:A:H8	29:X:655:A:O5'	2.01	0.43
29:X:817:A:H5''	29:X:818:G:OP1	2.19	0.43
29:X:1030:U:C4	29:X:1031:C:H5	2.36	0.43
29:X:1210:C:H1'	29:X:1239:A:C4	2.53	0.43
29:X:1339:U:C4'	29:X:1993:G:H21	2.32	0.43
29:X:1402:G:H2'	29:X:1403:U:H6	1.84	0.43
29:X:1527:G:H2'	29:X:1528:C:H6	1.83	0.43
29:X:1723:U:C6	29:X:1748:U:OP2	2.71	0.43
29:X:2021:G:C2	29:X:2022:C:C2	3.07	0.43
29:X:2238:G:C6	29:X:2261:G:O6	2.72	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:2655:C:O2	29:X:2712:G:N2	2.51	0.43
29:X:2662:C:C2	29:X:2663:U:C5	3.07	0.43
30:Y:63:A:H2'	30:Y:64:C:C6	2.53	0.43
2:A:71:ASP:CG	2:A:103:ARG:HH22	2.22	0.43
2:A:247:VAL:HA	2:A:253:PRO:HA	2.01	0.43
4:C:59:TYR:CD1	4:C:60:GLY:N	2.87	0.43
8:G:68:PRO:O	15:N:64:ARG:HG2	2.19	0.43
10:I:73:GLU:OE2	10:I:101:ARG:HB2	2.19	0.43
14:M:69:ARG:CZ	14:M:108:LYS:HG2	2.48	0.43
15:N:37:GLN:CG	29:X:1265:G:H1	2.27	0.43
17:P:9:ARG:HG3	17:P:10:ASN:N	2.33	0.43
20:S:168:VAL:HG12	20:S:169:VAL:N	2.34	0.43
22:U:38:THR:HG22	29:X:2412:A:C2	2.53	0.43
29:X:78:C:O2'	29:X:357:A:N3	2.43	0.43
29:X:167:A:H3'	29:X:168:A:H8	1.84	0.43
29:X:312:G:C4	29:X:313:U:C5	3.06	0.43
29:X:402:A:C8	29:X:2392:G:H4'	2.54	0.43
29:X:578:U:H1'	29:X:958:G:O4'	2.19	0.43
29:X:628:A:H2'	29:X:629:C:H6	1.80	0.43
29:X:1287:A:C2	29:X:1315:A:C2	3.07	0.43
29:X:1299:A:N6	29:X:1302:C:C2	2.87	0.43
29:X:1883:A:H5'	29:X:1953:A:H5'	2.00	0.43
29:X:2006:G:C2	29:X:2024:U:O2	2.72	0.43
29:X:2033:C:H5''	29:X:2034:A:OP2	2.19	0.43
29:X:2043:A:H1'	29:X:2481:G:H1'	1.99	0.43
29:X:2707:G:H2'	29:X:2708:U:C6	2.53	0.43
2:A:126:LYS:HB3	2:A:126:LYS:HE2	1.81	0.43
4:C:129:LYS:HB3	4:C:132:ASN:HD22	1.83	0.43
4:C:176:ASN:OD1	4:C:178:TYR:HB3	2.19	0.43
4:C:189:ASP:CG	4:C:190:ALA:H	2.19	0.43
9:H:85:ASP:CG	9:H:87:SER:H	2.22	0.43
12:K:8:ARG:NH1	29:X:1669:A:OP1	2.47	0.43
14:M:2:GLN:HB3	29:X:2795:A:N1	2.33	0.43
15:N:10:ARG:HG3	29:X:1264:C:OP1	2.18	0.43
15:N:31:GLN:HE22	29:X:589:C:H4'	1.83	0.43
15:N:107:LYS:O	15:N:110:VAL:HB	2.19	0.43
17:P:36:ARG:HA	17:P:39:ARG:HD2	2.01	0.43
22:U:8:THR:N	22:U:14:VAL:HG23	2.34	0.43
29:X:225:G:H2'	29:X:226:C:OP1	2.19	0.43
29:X:320:A:C6	29:X:341:A:C6	3.07	0.43
29:X:815:A:C5	29:X:816:U:C5	3.07	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:854:G:H22	29:X:948:C:N4	2.17	0.43
29:X:987:G:C2	29:X:988:G:C5	3.07	0.43
29:X:1021:A:N3	29:X:1164:C:H1'	2.34	0.43
29:X:1321:A:H61	29:X:1624:A:H61	1.66	0.43
29:X:1322:G:H1	29:X:1621:C:H42	1.67	0.43
29:X:2369:U:C6	29:X:2369:U:C3'	3.02	0.43
29:X:2429:A:OP1	29:X:2476:A:C8	2.71	0.43
29:X:2493:U:H2'	29:X:2494:C:C6	2.54	0.43
29:X:2604:G:C5	29:X:2605:C:C4	3.07	0.43
30:Y:42:U:H3'	30:Y:43:G:H5''	2.01	0.43
2:A:88:ARG:NH1	29:X:1809:G:OP1	2.51	0.42
3:B:34:VAL:HG21	3:B:67:PHE:HE1	1.83	0.42
3:B:52:ALA:O	3:B:76:ARG:N	2.48	0.42
6:E:45:GLN:HG3	6:E:49:GLN:O	2.18	0.42
9:H:43:ARG:NH2	29:X:1979:C:OP2	2.49	0.42
11:J:88:LYS:HG2	29:X:967:G:OP1	2.20	0.42
12:K:112:LEU:HD11	25:Z:57:VAL:HG13	2.01	0.42
25:Z:52:TYR:CZ	29:X:2859:U:N3	2.84	0.42
27:2:24:THR:O	27:2:28:ARG:HD3	2.19	0.42
28:3:4:MET:HE3	28:3:4:MET:HB2	1.91	0.42
29:X:351:A:H2'	29:X:352:G:H5'	2.01	0.42
29:X:469:G:N2	29:X:480:G:H2'	2.34	0.42
29:X:520:C:H2'	29:X:521:U:O4'	2.19	0.42
29:X:585:U:H4'	29:X:2481:G:C8	2.54	0.42
29:X:815:A:H5''	29:X:816:U:OP2	2.19	0.42
29:X:951:G:H2'	29:X:952:A:O4'	2.19	0.42
29:X:1028:G:C2	29:X:1157:G:C4	3.06	0.42
29:X:1104:G:N2	29:X:1109:A:H62	2.09	0.42
29:X:1287:A:C2	29:X:1315:A:H2	2.37	0.42
29:X:1672:A:H3'	29:X:1673:C:H6	1.84	0.42
29:X:1746:A:H8	29:X:1746:A:O5'	2.02	0.42
29:X:2214:G:H2'	29:X:2215:C:C6	2.54	0.42
29:X:2326:C:H2'	29:X:2327:U:C6	2.54	0.42
29:X:2512:A:H2'	29:X:2513:A:O4'	2.18	0.42
30:Y:55:C:H2'	30:Y:56:G:O4'	2.18	0.42
2:A:67:PHE:HB3	2:A:153:ALA:H	1.84	0.42
2:A:252:LYS:HA	2:A:253:PRO:HD3	1.90	0.42
3:B:23:VAL:HG11	3:B:183:LEU:HB3	2.00	0.42
3:B:33:ILE:HG12	3:B:36:ARG:HH21	1.84	0.42
4:C:22:VAL:HG22	4:C:106:MET:HG2	2.01	0.42
4:C:48:ARG:NH2	29:X:686:C:OP1	2.52	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:102:LEU:HD12	4:C:102:LEU:O	2.18	0.42
6:E:21:ASP:HB3	6:E:22:GLY:H	1.41	0.42
6:E:75:ALA:O	6:E:79:VAL:HG22	2.19	0.42
15:N:9:VAL:O	15:N:12:ARG:HB2	2.20	0.42
17:P:25:PHE:CD2	17:P:25:PHE:C	2.92	0.42
19:R:51:VAL:HG22	19:R:52:ASN:N	2.34	0.42
20:S:24:TYR:HB3	20:S:29:ASN:HB2	2.00	0.42
23:V:25:LEU:O	23:V:28:LEU:HB2	2.19	0.42
28:3:33:ASN:ND2	29:X:2398:U:O5'	2.50	0.42
29:X:1:G:H2'	29:X:2:G:H8	1.83	0.42
29:X:218:A:C6	29:X:232:A:H5''	2.54	0.42
29:X:351:A:N6	29:X:352:G:C2	2.86	0.42
29:X:1088:A:N1	29:X:1099:A:O2'	2.34	0.42
29:X:2432:A:H2'	29:X:2433:G:C8	2.54	0.42
29:X:2595:C:H2'	29:X:2596:C:C6	2.53	0.42
29:X:2660:C:C2	29:X:2704:U:O4	2.72	0.42
4:C:35:LEU:O	4:C:38:ARG:HG3	2.19	0.42
5:D:7:LYS:O	5:D:11:GLN:HG3	2.19	0.42
7:F:126:THR:HA	29:X:1091:C:O2'	2.19	0.42
13:L:8:ARG:HA	13:L:8:ARG:HD2	1.80	0.42
13:L:98:GLY:HA3	30:Y:51:G:OP1	2.19	0.42
15:N:59:ARG:O	15:N:63:GLN:HG2	2.19	0.42
16:O:71:ILE:HG13	29:X:1003:C:O2'	2.19	0.42
16:O:72:ARG:HA	16:O:82:ARG:O	2.19	0.42
17:P:38:VAL:O	17:P:41:VAL:HG23	2.18	0.42
19:R:64:ASN:HA	19:R:65:PRO:HD2	1.82	0.42
28:3:7:HIS:HD2	28:3:61:MET:CE	2.32	0.42
29:X:746:G:N7	29:X:774:A:N6	2.66	0.42
29:X:782:U:H2'	29:X:783:G:C8	2.54	0.42
29:X:828:C:N3	29:X:1207:G:C2	2.87	0.42
29:X:836:G:H2'	29:X:837:U:H6	1.80	0.42
29:X:919:U:HO2'	29:X:920:G:H8	1.68	0.42
29:X:1080:A:H4'	29:X:1081:A:H8	1.84	0.42
29:X:1091:C:H2'	29:X:1092:U:C6	2.54	0.42
29:X:1179:A:C2	29:X:1196:G:N1	2.87	0.42
29:X:1381:G:C2'	29:X:1799:A:H61	2.31	0.42
29:X:1674:C:C2	29:X:1675:C:C5	3.07	0.42
29:X:1942:G:H2'	29:X:1943:A:O4'	2.20	0.42
29:X:1950:C:N4	29:X:1951:G:C6	2.88	0.42
29:X:2057:U:C2	29:X:2415:G:C2	3.07	0.42
29:X:2450:A:C4	29:X:2451:G:C8	3.08	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:2543:A:C6	29:X:2544:A:N1	2.88	0.42
30:Y:36:A:H4'	30:Y:37:C:H5	1.84	0.42
2:A:72:LYS:O	2:A:75:VAL:HG12	2.19	0.42
4:C:20:PRO:C	4:C:21:GLU:HG2	2.39	0.42
4:C:42:THR:HG21	29:X:454:G:N3	2.33	0.42
11:J:60:ARG:O	11:J:62:GLY:HA2	2.19	0.42
11:J:100:PRO:C	11:J:102:ARG:H	2.22	0.42
13:L:65:THR:HG21	30:Y:52:G:OP2	2.19	0.42
16:O:75:LYS:HG3	16:O:80:TYR:HD1	1.84	0.42
19:R:58:VAL:C	19:R:60:PRO:HD2	2.39	0.42
25:Z:16:ARG:HD2	25:Z:20:ARG:HH12	1.85	0.42
29:X:587:A:H2'	29:X:588:G:H5''	1.99	0.42
29:X:718:A:H2'	29:X:719:A:C8	2.55	0.42
29:X:887:G:H1	29:X:915:C:H42	1.67	0.42
29:X:1667:A:H5''	29:X:1668:G:OP2	2.20	0.42
29:X:1720:G:C2	29:X:1721:G:C4	3.07	0.42
29:X:1977:C:O2	29:X:1977:C:H2'	2.19	0.42
29:X:2041:A:H8	29:X:2041:A:O5'	2.02	0.42
29:X:2255:G:C2	29:X:2256:G:C8	3.07	0.42
29:X:2691:C:O2	29:X:2692:A:H2'	2.19	0.42
8:G:61:ARG:HA	8:G:66:HIS:CE1	2.54	0.42
8:G:128:GLU:CD	29:X:2760:G:H1	2.23	0.42
10:I:94:GLU:HA	10:I:97:ARG:HE	1.84	0.42
17:P:16:GLN:NE2	29:X:511:A:O2'	2.52	0.42
17:P:30:TYR:H	17:P:123:HIS:CE1	2.37	0.42
19:R:90:LYS:C	19:R:92:THR:HG23	2.39	0.42
21:T:4:LYS:HA	21:T:4:LYS:HD3	1.42	0.42
29:X:192:G:H4'	29:X:193:A:H4'	2.01	0.42
29:X:303:C:H42	29:X:359:G:H1	1.66	0.42
29:X:681:A:C2	29:X:683:A:C6	3.07	0.42
29:X:752:G:H4'	29:X:753:U:OP1	2.20	0.42
29:X:813:A:O5'	29:X:813:A:H8	2.02	0.42
29:X:816:U:O2'	29:X:817:A:H5'	2.20	0.42
29:X:919:U:HO2'	29:X:920:G:C5'	2.32	0.42
29:X:953:G:O2'	29:X:1203:A:N3	2.44	0.42
29:X:1672:A:H3'	29:X:1673:C:C5	2.54	0.42
29:X:1699:A:H2'	29:X:1700:C:C6	2.55	0.42
29:X:1811:A:H1'	29:X:1813:A:C6	2.54	0.42
29:X:1830:C:H41	29:X:1882:G:P	2.42	0.42
29:X:2169:A:H2'	29:X:2170:C:C6	2.54	0.42
29:X:2223:U:H2'	29:X:2224:U:O4'	2.20	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:2536:G:O2'	29:X:2537:C:H5'	2.20	0.42
29:X:2543:A:C2	29:X:2626:U:H4'	2.54	0.42
29:X:2564:U:C6	29:X:2564:U:H5'	2.54	0.42
29:X:2720:A:C8	29:X:2743:G:N2	2.87	0.42
29:X:2844:G:C6	29:X:2845:C:N3	2.88	0.42
3:B:146:THR:HG23	29:X:1141:U:H5	1.84	0.42
11:J:78:LYS:HE3	11:J:78:LYS:HB2	1.64	0.42
15:N:64:ARG:O	15:N:67:ALA:HB3	2.19	0.42
17:P:62:ARG:NH1	25:Z:25:LEU:HD11	2.28	0.42
19:R:45:LYS:HA	19:R:76:LEU:O	2.19	0.42
29:X:74:G:OP1	29:X:74:G:H4'	2.20	0.42
29:X:740:A:OP1	29:X:1445:A:O2'	2.30	0.42
29:X:984:A:O4'	29:X:1202:U:C6	2.72	0.42
29:X:1713:G:H21	29:X:1961:A:H5'	1.85	0.42
29:X:1762:C:C2	29:X:1763:G:C8	3.08	0.42
29:X:2706:U:H3'	29:X:2707:G:H8	1.85	0.42
2:A:229:VAL:HG11	29:X:797:A:C5	2.54	0.42
3:B:19:ARG:HA	9:H:84:ALA:O	2.20	0.42
3:B:117:MET:O	3:B:119:ARG:N	2.53	0.42
3:B:203:LYS:NZ	29:X:2712:G:OP1	2.43	0.42
9:H:73:VAL:HG12	9:H:99:ILE:HD13	2.00	0.42
14:M:101:ARG:NH1	29:X:1745:C:P	2.92	0.42
15:N:39:LEU:HA	15:N:42:ALA:HB3	2.01	0.42
21:T:56:ASP:OD1	29:X:2343:C:H5'	2.19	0.42
22:U:72:LYS:HA	22:U:72:LYS:HD3	1.89	0.42
25:Z:6:VAL:O	29:X:2594:U:C4	2.71	0.42
27:2:16:HIS:HD2	29:X:699:G:O6	2.02	0.42
29:X:18:U:H6	29:X:18:U:O5'	2.03	0.42
29:X:389:G:H2'	29:X:390:U:H6	1.85	0.42
29:X:399:G:O2'	29:X:400:U:OP1	2.29	0.42
29:X:1298:G:C5	29:X:1342:U:C5	3.08	0.42
29:X:1374:G:O2'	29:X:1375:C:H5'	2.19	0.42
29:X:1541:G:C4	29:X:1542:G:C8	3.07	0.42
29:X:1554:G:H2'	29:X:1555:A:C8	2.54	0.42
29:X:1569:A:N6	29:X:1571:G:H1'	2.35	0.42
29:X:1750:A:C2	29:X:1751:A:C5	3.08	0.42
29:X:2001:G:C6	29:X:2002:A:C5	3.07	0.42
29:X:2849:C:H2'	29:X:2850:U:H6	1.84	0.42
30:Y:7:C:O2	30:Y:119:G:N2	2.52	0.42
3:B:41:THR:HB	3:B:42:ASP:OD1	2.20	0.42
4:C:95:LEU:HD12	4:C:96:PRO:HD2	2.00	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:86:ASN:HB2	6:E:165:VAL:HG22	2.02	0.42
11:J:6:LYS:HB3	11:J:7:ARG:H	1.67	0.42
15:N:91:ASN:O	15:N:95:LEU:HG	2.20	0.42
16:O:19:VAL:HG12	16:O:20:ILE:H	1.84	0.42
16:O:95:ILE:HD13	16:O:95:ILE:HA	1.83	0.42
17:P:28:ALA:O	17:P:123:HIS:HA	2.20	0.42
26:1:14:SER:HB3	26:1:49:PHE:CE1	2.54	0.42
27:2:28:ARG:O	27:2:31:LEU:HB2	2.19	0.42
29:X:13:A:N3	29:X:15:G:C6	2.88	0.42
29:X:14:A:N6	29:X:15:G:C2	2.88	0.42
29:X:511:A:C6	29:X:512:A:C2	3.08	0.42
29:X:728:G:H22	29:X:730:C:N4	2.18	0.42
29:X:763:A:C2	29:X:765:C:H4'	2.54	0.42
29:X:790:A:C2	29:X:791:G:C5	3.07	0.42
29:X:946:U:C2	29:X:947:C:C6	3.08	0.42
29:X:1040:A:H2	29:X:2444:C:O2	2.02	0.42
29:X:1135:C:C2	29:X:1136:G:C8	3.08	0.42
29:X:1345:G:N7	29:X:1626:A:C8	2.88	0.42
29:X:1643:A:H61	29:X:1656:U:H3	1.66	0.42
29:X:1693:A:C2	29:X:1976:U:H5'	2.55	0.42
29:X:1733:U:C5	29:X:1735:G:H1'	2.54	0.42
29:X:2019:C:O2'	29:X:2020:G:H5'	2.19	0.42
29:X:2425:G:N2	29:X:2480:C:N3	2.67	0.42
2:A:13:ARG:HA	2:A:13:ARG:HD3	1.44	0.42
2:A:108:PRO:HA	2:A:196:VAL:O	2.20	0.42
2:A:126:LYS:HB2	2:A:129:ASN:OD1	2.20	0.42
2:A:235:GLY:HA3	29:X:2577:A:H5''	2.01	0.42
4:C:106:MET:HB3	4:C:106:MET:HE2	1.86	0.42
4:C:186:LEU:HG	4:C:188:ILE:HA	2.02	0.42
5:D:34:ILE:HA	5:D:156:ILE:HG23	2.02	0.42
6:E:39:THR:OG1	6:E:40:GLU:N	2.53	0.42
8:G:69:ASP:HA	15:N:64:ARG:NH2	2.33	0.42
9:H:73:VAL:HG21	9:H:123:PHE:CE2	2.55	0.42
12:K:20:LEU:C	12:K:22:ARG:N	2.73	0.42
12:K:27:ALA:HA	12:K:30:ARG:HB3	2.02	0.42
12:K:100:VAL:HG12	12:K:101:GLY:N	2.34	0.42
14:M:56:ALA:CB	14:M:103:LYS:HE3	2.50	0.42
20:S:13:LYS:HB2	20:S:14:LEU:H	1.51	0.42
20:S:48:THR:O	20:S:48:THR:OG1	2.32	0.42
26:1:7:ARG:NH1	26:1:25:THR:O	2.53	0.42
29:X:139:A:H2'	29:X:140:G:C8	2.55	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:541:C:O2'	29:X:572:G:H5''	2.19	0.42
29:X:877:G:N2	29:X:925:U:O2	2.53	0.42
29:X:963:G:H5'	29:X:964:A:OP2	2.20	0.42
29:X:1681:A:O5'	29:X:1681:A:H8	2.01	0.42
29:X:1689:U:C2'	29:X:1690:U:H5'	2.50	0.42
29:X:1699:A:C2	29:X:1700:C:C2	3.08	0.42
29:X:1701:C:C2	29:X:1722:G:C2	3.08	0.42
29:X:2038:C:H6	29:X:2483:U:H5'	1.83	0.42
29:X:2201:G:C4	29:X:2202:G:C8	3.07	0.42
29:X:2310:G:N2	29:X:2364:C:C4	2.87	0.42
29:X:2494:C:H2'	29:X:2495:G:H8	1.85	0.42
29:X:2709:C:H2'	29:X:2710:C:C6	2.55	0.42
29:X:2829:A:C2	29:X:2839:G:C4	3.08	0.42
30:Y:90:C:H2'	30:Y:91:A:O4'	2.20	0.42
2:A:209:ALA:O	2:A:210:GLY:C	2.57	0.42
3:B:26:VAL:HG11	3:B:198:LEU:HD11	2.01	0.42
4:C:7:ILE:HD13	4:C:7:ILE:HA	1.74	0.42
4:C:107:ALA:HB2	4:C:177:VAL:HG13	2.02	0.42
12:K:44:LEU:O	12:K:44:LEU:HG	2.18	0.42
13:L:32:TYR:O	13:L:32:TYR:CG	2.72	0.42
14:M:82:PRO:C	14:M:84:ALA:N	2.71	0.42
15:N:13:ARG:NH2	29:X:1264:C:OP1	2.50	0.42
17:P:102:THR:HG22	17:P:120:ARG:HA	2.02	0.42
17:P:110:ALA:HB2	29:X:761:G:O5'	2.20	0.42
19:R:24:VAL:HB	19:R:29:HIS:O	2.19	0.42
21:T:66:LYS:HE2	21:T:66:LYS:HB3	1.72	0.42
25:Z:3:LYS:HG3	29:X:2591:C:OP2	2.20	0.42
29:X:167:A:C2	29:X:168:A:C4	3.07	0.42
29:X:215:G:H1'	29:X:619:A:H1'	2.01	0.42
29:X:457:C:C2'	29:X:458:G:H5''	2.50	0.42
29:X:961:G:C6	29:X:962:C:C4	3.08	0.42
29:X:1016:C:C2	29:X:1154:A:C5	3.08	0.42
29:X:1059:A:O5'	29:X:1059:A:H8	2.03	0.42
29:X:1314:A:H2	29:X:1642:G:N3	2.18	0.42
29:X:1704:G:H1'	29:X:1719:G:N2	2.34	0.42
29:X:2150:U:H2'	29:X:2151:G:C8	2.55	0.42
29:X:2461:G:H2'	29:X:2461:G:N3	2.34	0.42
29:X:2685:A:N1	29:X:2686:C:C2	2.87	0.42
30:Y:48:A:C5	30:Y:49:C:C4	3.07	0.42
2:A:151:LYS:HD3	29:X:2186:G:H4'	2.02	0.41
4:C:28:HIS:NE2	10:I:8:PRO:HB3	2.34	0.41

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:153:ASP:HA	4:C:158:ARG:NH2	2.35	0.41
10:I:120:VAL:HG23	10:I:139:ARG:O	2.20	0.41
11:J:131:LYS:HD2	11:J:131:LYS:HA	1.93	0.41
21:T:31:VAL:HG22	21:T:35:ASN:HB2	2.01	0.41
22:U:27:ASP:CA	22:U:32:ARG:HH21	2.33	0.41
29:X:63:A:O2'	29:X:64:C:H5'	2.19	0.41
29:X:66:U:H2'	29:X:67:G:H8	1.85	0.41
29:X:71:A:O2'	29:X:74:G:N2	2.53	0.41
29:X:76:C:C2	29:X:108:G:C2	3.08	0.41
29:X:736:G:H2'	29:X:737:C:O4'	2.20	0.41
29:X:824:U:H1'	29:X:1264:C:O4'	2.20	0.41
29:X:830:C:O2	29:X:1205:G:N2	2.53	0.41
29:X:2269:G:H22	29:X:2322:U:H1'	1.85	0.41
29:X:2437:G:C8	29:X:2469:G:C6	3.08	0.41
29:X:2665:G:C6	29:X:2666:U:N3	2.88	0.41
29:X:2770:A:H4'	29:X:2771:C:O5'	2.20	0.41
30:Y:3:A:C6	30:Y:4:C:N4	2.88	0.41
3:B:179:GLU:O	3:B:181:LEU:N	2.53	0.41
5:D:125:ARG:HD2	29:X:2295:C:O4'	2.20	0.41
6:E:68:THR:O	6:E:72:VAL:HG23	2.21	0.41
8:G:39:GLN:HG3	8:G:79:PHE:CE1	2.55	0.41
15:N:33:ARG:HD3	29:X:1265:G:N3	2.35	0.41
15:N:74:MET:CE	15:N:79:PHE:HD1	2.33	0.41
17:P:41:VAL:HG13	17:P:60:ILE:HG21	2.03	0.41
20:S:112:LEU:O	20:S:171:VAL:HA	2.20	0.41
29:X:198:A:C8	29:X:243:G:C5	3.08	0.41
29:X:632:A:H2'	29:X:633:G:O4'	2.20	0.41
29:X:656:U:C5	29:X:657:A:C4	3.08	0.41
29:X:658:G:H2'	29:X:659:G:H8	1.85	0.41
29:X:753:U:O4'	29:X:1964:A:C4	2.73	0.41
29:X:786:U:H2'	29:X:787:A:H5'	2.02	0.41
29:X:787:A:O2'	29:X:790:A:H1'	2.21	0.41
29:X:1045:G:C6	29:X:1133:G:C2	3.08	0.41
29:X:1298:G:N1	29:X:1342:U:OP1	2.49	0.41
29:X:1302:C:H2'	29:X:1303:U:H6	1.84	0.41
29:X:1407:G:C6	29:X:1408:A:N6	2.89	0.41
29:X:1526:U:H4'	29:X:1527:G:OP1	2.20	0.41
29:X:1920:A:N7	29:X:1923:U:C5	2.88	0.41
29:X:1987:G:C6	29:X:1988:A:C4	3.08	0.41
29:X:2326:C:C5	29:X:2361:G:H1'	2.55	0.41
29:X:2639:A:H3'	29:X:2640:G:H8	1.81	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:231:HIS:ND1	2:A:249:PRO:HA	2.35	0.41
3:B:141:ILE:HD11	29:X:2034:A:C1'	2.50	0.41
4:C:17:LEU:HG	4:C:109:ALA:HB2	2.02	0.41
4:C:50:GLN:O	4:C:52:SER:N	2.53	0.41
5:D:36:VAL:HG22	5:D:154:ILE:HG13	2.01	0.41
5:D:60:ILE:HG21	5:D:141:ILE:HG12	2.02	0.41
6:E:30:LYS:HB2	6:E:79:VAL:O	2.21	0.41
22:U:67:ILE:HD13	22:U:67:ILE:HA	1.89	0.41
29:X:202:A:N6	29:X:203:G:N3	2.68	0.41
29:X:750:C:N3	29:X:751:G:C8	2.88	0.41
29:X:854:G:H8	29:X:854:G:O5'	2.03	0.41
29:X:1135:C:H2'	29:X:1136:G:H8	1.84	0.41
29:X:1147:G:N2	29:X:1148:G:H1'	2.35	0.41
29:X:1353:A:H4'	29:X:1407:G:H1'	2.02	0.41
29:X:1467:U:H4'	29:X:1468:A:C4	2.54	0.41
29:X:1665:C:C4	29:X:1666:G:N7	2.88	0.41
29:X:1710:U:H4'	29:X:1711:C:OP2	2.20	0.41
29:X:2010:G:C2	29:X:2020:G:C5	3.09	0.41
29:X:2044:G:N7	29:X:2480:C:H4'	2.34	0.41
29:X:2781:G:H2'	29:X:2782:G:C8	2.55	0.41
30:Y:58:G:H4'	30:Y:59:A:O4'	2.21	0.41
30:Y:117:G:H8	30:Y:117:G:O5'	2.03	0.41
2:A:95:LEU:HD23	2:A:95:LEU:HA	1.85	0.41
2:A:260:ARG:NH2	2:A:264:LYS:HD3	2.34	0.41
3:B:101:LYS:HA	3:B:170:LEU:O	2.20	0.41
4:C:77:PHE:CE1	29:X:1270:C:H4'	2.55	0.41
4:C:179:ASP:HA	4:C:182:ARG:HB3	2.02	0.41
5:D:100:LEU:O	5:D:103:LEU:HB3	2.20	0.41
6:E:115:ILE:HD12	6:E:115:ILE:HA	1.83	0.41
9:H:98:ILE:HG22	9:H:99:ILE:N	2.35	0.41
15:N:47:TYR:CZ	15:N:51:ARG:NH2	2.88	0.41
17:P:21:ARG:O	17:P:23:PRO:HD3	2.20	0.41
17:P:57:LEU:HD13	17:P:69:ALA:HA	2.03	0.41
18:Q:20:MET:HG3	18:Q:25:TYR:CE1	2.55	0.41
18:Q:22:ARG:HH12	18:Q:24:VAL:HG21	1.85	0.41
29:X:88:G:H5''	29:X:89:A:C5'	2.49	0.41
29:X:841:G:C2	29:X:842:A:N6	2.89	0.41
29:X:980:G:O5'	29:X:980:G:H8	2.03	0.41
29:X:982:C:H2'	29:X:983:G:O4'	2.21	0.41
29:X:1194:U:C4	29:X:1195:U:C4	3.08	0.41
29:X:1243:G:C2	29:X:1244:U:O2	2.73	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1261:G:H8	29:X:1261:G:O5'	2.04	0.41
29:X:1374:G:H2'	29:X:1375:C:H6	1.85	0.41
29:X:1440:G:C6	29:X:1441:A:C6	3.08	0.41
29:X:1802:A:H3'	29:X:1803:G:H8	1.85	0.41
29:X:1917:C:O2'	29:X:1918:G:H5'	2.19	0.41
29:X:2022:C:H2'	29:X:2023:C:H6	1.85	0.41
29:X:2177:U:H2'	29:X:2178:U:O4'	2.21	0.41
29:X:2311:U:H4'	29:X:2315:A:H62	1.85	0.41
29:X:2332:G:C6	29:X:2344:G:N2	2.88	0.41
29:X:2560:G:H22	29:X:2589:C:H2'	1.85	0.41
1:0:95:LEU:HD22	1:0:98:ARG:HD2	2.02	0.41
2:A:170:SER:HB3	2:A:171:ASP:H	1.67	0.41
2:A:209:ALA:O	2:A:212:SER:N	2.52	0.41
5:D:83:MET:HA	5:D:84:PRO:HD3	1.86	0.41
6:E:160:LYS:NZ	29:X:2636:A:O3'	2.52	0.41
9:H:22:ILE:HD12	9:H:22:ILE:HA	1.92	0.41
9:H:79:HIS:CG	9:H:80:ALA:H	2.38	0.41
10:I:14:LYS:O	29:X:675:C:H5'	2.20	0.41
10:I:32:ARG:HH22	29:X:684:C:P	2.43	0.41
18:Q:68:PHE:CD1	29:X:64:C:H1'	2.54	0.41
19:R:38:LEU:HB3	19:R:47:VAL:HG23	2.03	0.41
20:S:3:LEU:HG	20:S:32:PHE:HD1	1.84	0.41
23:V:48:ARG:HG2	23:V:52:GLN:HE21	1.85	0.41
27:2:21:ARG:O	27:2:27:GLY:HA3	2.21	0.41
28:3:29:LYS:HZ3	28:3:41:ILE:HG23	1.84	0.41
29:X:182:G:O2'	29:X:183:U:OP2	2.37	0.41
29:X:184:A:H2'	29:X:185:C:O4'	2.21	0.41
29:X:318:G:N2	29:X:321:A:C8	2.89	0.41
29:X:530:G:O2'	29:X:531:G:H5'	2.21	0.41
29:X:1109:A:H8	29:X:1109:A:O5'	2.02	0.41
29:X:1204:G:H2'	29:X:1205:G:C8	2.55	0.41
29:X:1581:C:O2'	29:X:1582:A:OP2	2.33	0.41
29:X:2325:A:H4'	29:X:2326:C:OP2	2.18	0.41
29:X:2359:U:H2'	29:X:2360:C:C6	2.56	0.41
29:X:2487:G:H2'	29:X:2488:G:O4'	2.21	0.41
1:0:28:LEU:HB3	1:0:216:PRO:HD3	2.02	0.41
2:A:119:ALA:HA	2:A:130:ALA:HB3	2.02	0.41
2:A:231:HIS:CE1	2:A:249:PRO:HA	2.55	0.41
3:B:33:ILE:HG12	3:B:36:ARG:HE	1.85	0.41
4:C:7:ILE:CG2	4:C:122:GLY:HA3	2.51	0.41
6:E:45:GLN:HA	6:E:50:LEU:HA	2.02	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:105:MET:HB2	6:E:113:VAL:O	2.20	0.41
8:G:51:LEU:HD11	8:G:127:ILE:HD13	2.02	0.41
11:J:19:THR:CG2	11:J:20:GLY:N	2.81	0.41
13:L:28:ARG:HH21	13:L:45:ASP:HB3	1.85	0.41
16:O:62:GLU:HG2	16:O:63:HIS:N	2.35	0.41
17:P:19:LYS:N	17:P:19:LYS:HD2	2.35	0.41
26:1:27:ASN:ND2	29:X:2264:C:OP1	2.53	0.41
29:X:36:G:N3	29:X:462:G:O2'	2.53	0.41
29:X:205:A:C2'	29:X:206:U:H5'	2.44	0.41
29:X:1066:G:H1	29:X:1115:C:N4	2.15	0.41
29:X:1513:U:C6	29:X:1593:C:H5''	2.56	0.41
29:X:1666:G:C6	29:X:1992:G:O6	2.74	0.41
29:X:1935:A:N6	29:X:1936:A:N1	2.68	0.41
29:X:1994:U:H2'	29:X:1995:G:H5'	2.01	0.41
29:X:2320:G:H2'	29:X:2321:C:O4'	2.20	0.41
29:X:2415:G:H2'	29:X:2416:U:H6	1.85	0.41
29:X:2604:G:H2'	29:X:2605:C:C6	2.55	0.41
29:X:2801:A:H2'	29:X:2801:A:N3	2.36	0.41
30:Y:104:A:C6	30:Y:105:G:C5	3.09	0.41
2:A:24:LEU:CD1	2:A:84:TYR:HB2	2.50	0.41
2:A:206:LEU:HD23	29:X:1783:G:OP1	2.21	0.41
5:D:38:GLU:HG2	5:D:53:ALA:HB1	2.03	0.41
5:D:125:ARG:H	5:D:125:ARG:HG2	1.50	0.41
8:G:33:ILE:HG12	29:X:547:U:O2'	2.21	0.41
8:G:134:MET:O	8:G:135:LEU:HG	2.20	0.41
9:H:1:MET:N	9:H:46:HIS:HB3	2.35	0.41
9:H:117:GLU:O	9:H:120:ASP:HB2	2.21	0.41
10:I:45:LYS:H	10:I:46:GLY:HA2	1.86	0.41
12:K:99:ARG:H	12:K:99:ARG:HE	1.69	0.41
19:R:44:GLN:HE21	19:R:44:GLN:HB2	1.70	0.41
21:T:41:ARG:NH1	29:X:2366:U:H1'	2.35	0.41
25:Z:55:ARG:NH2	25:Z:58:LEU:HA	2.36	0.41
29:X:315:G:C2	29:X:325:U:O2	2.74	0.41
29:X:399:G:HO2'	29:X:400:U:P	2.43	0.41
29:X:790:A:N3	29:X:791:G:C8	2.89	0.41
29:X:797:A:HO2'	29:X:798:G:H8	1.66	0.41
29:X:1340:C:C4	29:X:1341:G:C6	3.08	0.41
29:X:1495:G:H2'	29:X:1496:G:H8	1.84	0.41
29:X:1656:U:O2'	29:X:2678:C:H4'	2.20	0.41
29:X:1750:A:H2'	29:X:1751:A:C8	2.55	0.41
29:X:2151:G:N2	29:X:2153:A:H3'	2.35	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:2292:C:C2	29:X:2293:G:C8	3.09	0.41
29:X:2352:A:C6	29:X:2353:G:C6	3.09	0.41
29:X:2445:C:N3	29:X:2464:G:C2	2.89	0.41
29:X:2494:C:H2'	29:X:2495:G:C8	2.55	0.41
29:X:2728:A:C5	29:X:2737:A:N6	2.89	0.41
1:O:27:GLU:O	1:O:29:ALA:N	2.48	0.41
2:A:204:ILE:HG13	2:A:204:ILE:H	1.64	0.41
6:E:116:GLU:HA	6:E:117:PRO:HD2	1.96	0.41
7:F:2:ARG:NH2	7:F:30:TYR:HA	2.36	0.41
15:N:50:ARG:NH1	29:X:1004:A:OP1	2.42	0.41
15:N:74:MET:HE1	15:N:79:PHE:HD1	1.85	0.41
17:P:37:LYS:O	17:P:40:LEU:HB2	2.20	0.41
17:P:90:LEU:CD1	17:P:128:VAL:HB	2.47	0.41
19:R:51:VAL:HG21	19:R:74:LEU:O	2.20	0.41
20:S:62:PHE:HB3	20:S:85:MET:SD	2.60	0.41
20:S:172:LEU:HD23	20:S:172:LEU:HA	1.92	0.41
24:W:28:ILE:H	24:W:28:ILE:HG13	1.71	0.41
26:1:37:LEU:HD12	26:1:37:LEU:HA	1.80	0.41
28:3:52:LYS:HB3	28:3:53:ALA:H	1.68	0.41
29:X:23:G:C2	29:X:24:G:C8	3.09	0.41
29:X:140:G:H2'	29:X:141:G:C8	2.56	0.41
29:X:623:G:N1	29:X:627:A:C6	2.88	0.41
29:X:784:U:H2'	29:X:785:U:C6	2.55	0.41
29:X:1098:G:O6	29:X:1100:G:N2	2.54	0.41
29:X:1716:G:O6	29:X:1754:G:H1'	2.20	0.41
29:X:1787:U:O2'	29:X:1788:C:H5'	2.20	0.41
29:X:1885:C:C2	29:X:1886:G:H1'	2.56	0.41
29:X:2145:A:H5''	29:X:2155:U:H6	1.84	0.41
29:X:2165:A:H2'	29:X:2166:G:C8	2.55	0.41
29:X:2459:C:N4	29:X:2460:G:O6	2.54	0.41
29:X:2751:C:H2'	29:X:2752:C:C6	2.55	0.41
1:O:3:TYR:O	1:O:7:GLU:HB3	2.21	0.41
2:A:186:HIS:O	2:A:188:GLU:N	2.53	0.41
3:B:31:CYS:HA	3:B:32:PRO:HD3	1.75	0.41
3:B:126:PRO:O	3:B:128:SER:N	2.53	0.41
4:C:162:ARG:HH21	29:X:333:A:P	2.44	0.41
4:C:176:ASN:ND2	29:X:626:A:O2'	2.54	0.41
5:D:29:PRO:HB2	5:D:169:LEU:HD13	2.03	0.41
5:D:51:ASP:O	5:D:55:LYS:HG2	2.21	0.41
9:H:2:ILE:HB	9:H:45:ALA:HB3	2.02	0.41
9:H:22:ILE:CG2	9:H:52:VAL:HG12	2.45	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:53:ARG:CG	10:I:54:SER:H	2.34	0.41
10:I:55:ARG:HB3	10:I:57:ILE:HG12	2.03	0.41
10:I:76:LYS:HB2	10:I:76:LYS:HE3	1.93	0.41
11:J:17:ARG:NH2	29:X:969:U:O5'	2.54	0.41
12:K:80:MET:O	12:K:85:PRO:HD3	2.21	0.41
13:L:33:ARG:HB2	13:L:33:ARG:CZ	2.51	0.41
15:N:41:ASN:HB3	15:N:45:TYR:HE2	1.86	0.41
17:P:50:VAL:O	17:P:54:GLU:HG3	2.21	0.41
21:T:46:LYS:HB2	21:T:77:ARG:O	2.20	0.41
22:U:48:LYS:HE2	22:U:48:LYS:HB2	1.85	0.41
29:X:71:A:H62	29:X:110:U:H5'	1.85	0.41
29:X:184:A:C6	29:X:185:C:C2	3.09	0.41
29:X:507:A:H2'	29:X:508:G:C8	2.56	0.41
29:X:698:A:C2	29:X:702:A:C5	3.09	0.41
29:X:1047:G:C2	29:X:1131:G:C4	3.09	0.41
29:X:1203:A:N3	29:X:1203:A:H2'	2.35	0.41
29:X:1238:A:O2'	29:X:1239:A:O5'	2.35	0.41
29:X:1300:A:C2	29:X:1301:U:C2	3.09	0.41
29:X:1453:A:H3'	29:X:1454:U:C6	2.55	0.41
29:X:1549:C:H2'	29:X:1550:C:O4'	2.21	0.41
29:X:1554:G:H2'	29:X:1555:A:H8	1.86	0.41
29:X:1724:C:C2	29:X:1747:G:C4	3.09	0.41
29:X:1782:A:N6	29:X:1820:G:O2'	2.54	0.41
29:X:1850:G:O3'	29:X:1851:A:H8	2.04	0.41
29:X:1967:U:H2'	29:X:1968:G:H8	1.86	0.41
29:X:2006:G:H5'	29:X:2596:C:H4'	2.03	0.41
29:X:2038:C:H6	29:X:2038:C:H3'	1.85	0.41
29:X:2230:G:H8	29:X:2230:G:OP2	2.03	0.41
29:X:2265:A:H4'	29:X:2266:A:N9	2.35	0.41
29:X:2411:A:H2'	29:X:2412:A:O4'	2.21	0.41
29:X:2457:A:H3'	29:X:2458:U:H6	1.86	0.41
29:X:2630:C:C2	29:X:2631:C:C5	3.09	0.41
29:X:2662:C:C5	29:X:2663:U:H5	2.39	0.41
1:O:107:ASP:HB3	1:O:108:ALA:H	1.63	0.41
2:A:268:ARG:NH2	29:X:2204:A:OP1	2.54	0.41
3:B:2:LYS:HB2	3:B:200:SER:HB3	2.03	0.41
3:B:170:LEU:HA	3:B:170:LEU:HD23	1.48	0.41
4:C:144:GLY:HA2	4:C:166:TRP:CZ2	2.55	0.41
6:E:156:ALA:HB3	29:X:2509:A:H61	1.85	0.41
9:H:59:ALA:HA	9:H:60:PRO:HD3	1.89	0.41
10:I:18:ARG:NH2	29:X:1262:U:C2	2.89	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:15:ARG:HB3	11:J:16:GLY:H	1.45	0.41
11:J:36:ILE:HG23	11:J:103:VAL:HG22	2.03	0.41
15:N:66:ASN:OD1	15:N:70:ARG:HD2	2.21	0.41
18:Q:39:LYS:NZ	18:Q:50:VAL:HG12	2.36	0.41
22:U:24:ALA:C	22:U:26:ALA:H	2.25	0.41
24:W:21:GLN:C	24:W:23:LEU:H	2.25	0.41
29:X:459:A:H4'	29:X:461:A:N7	2.35	0.41
29:X:465:C:HO2'	29:X:466:A:P	2.42	0.41
29:X:493:A:O2'	29:X:507:A:N1	2.50	0.41
29:X:837:U:H2'	29:X:838:A:H8	1.83	0.41
29:X:858:G:H8	29:X:858:G:P	2.44	0.41
29:X:1059:A:H2'	29:X:1060:C:OP1	2.21	0.41
29:X:1330:G:C4	29:X:1331:G:C8	3.09	0.41
29:X:1354:A:P	29:X:1410:U:H3	2.43	0.41
29:X:2229:G:O2'	29:X:2475:C:OP1	2.36	0.41
29:X:2293:G:H2'	29:X:2294:U:C6	2.56	0.41
29:X:2529:G:C6	29:X:2530:C:N4	2.89	0.41
29:X:2662:C:C4	29:X:2663:U:C5	3.09	0.41
1:O:180:ASN:HA	1:O:183:ALA:HB3	2.04	0.40
2:A:99:ASP:HB2	29:X:1506:C:O2	2.21	0.40
2:A:158:SER:O	2:A:196:VAL:HG11	2.20	0.40
3:B:8:LYS:HD3	3:B:190:GLY:O	2.21	0.40
3:B:27:LEU:HD23	3:B:29:GLY:N	2.32	0.40
3:B:114:GLN:HB2	3:B:160:MET:HB2	2.03	0.40
8:G:43:VAL:HG23	8:G:163:PRO:HB2	2.02	0.40
11:J:27:TYR:HA	11:J:137:VAL:HG21	2.03	0.40
14:M:56:ALA:O	14:M:66:PHE:HA	2.21	0.40
14:M:106:TYR:HD2	14:M:106:TYR:H	1.67	0.40
15:N:55:ARG:HD3	29:X:1166:A:H5''	2.04	0.40
16:O:43:GLU:O	16:O:45:THR:N	2.46	0.40
20:S:71:MET:HA	20:S:78:PRO:HA	2.03	0.40
21:T:21:LEU:HD11	21:T:41:ARG:CZ	2.50	0.40
25:Z:19:ARG:HA	29:X:2029:G:C5'	2.51	0.40
27:2:11:LYS:NZ	29:X:699:G:OP1	2.29	0.40
27:2:29:ASN:O	27:2:33:ARG:HG2	2.21	0.40
28:3:4:MET:CE	29:X:679:C:H1'	2.51	0.40
29:X:484:G:C2	29:X:485:G:N7	2.89	0.40
29:X:611:C:O2	29:X:615:C:H4'	2.20	0.40
29:X:869:C:H42	29:X:933:G:H1	1.69	0.40
29:X:1245:G:C2	29:X:1246:G:C8	3.09	0.40
29:X:1413:U:H2'	29:X:1414:G:H8	1.86	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1659:G:C4	29:X:1660:G:C8	3.09	0.40
29:X:1903:C:O3'	29:X:1904:G:H8	2.04	0.40
29:X:2033:C:N4	29:X:2034:A:C6	2.89	0.40
29:X:2197:U:H2'	29:X:2198:U:H6	1.82	0.40
2:A:24:LEU:HD13	2:A:84:TYR:HB2	2.02	0.40
2:A:53:PHE:CE1	2:A:220:HIS:HA	2.56	0.40
2:A:97:TYR:HB2	2:A:101:GLU:O	2.22	0.40
3:B:144:ARG:NH1	29:X:2551:A:N3	2.70	0.40
5:D:72:LYS:O	5:D:74:ILE:HG13	2.22	0.40
6:E:33:LEU:HD12	6:E:33:LEU:HA	1.89	0.40
7:F:91:PRO:HD2	29:X:1087:C:O2	2.21	0.40
8:G:37:ASP:N	8:G:38:GLU:OE1	2.54	0.40
9:H:50:ILE:HG22	9:H:51:ILE:N	2.36	0.40
12:K:51:LEU:HD23	12:K:66:VAL:HG22	2.03	0.40
14:M:106:TYR:HD1	29:X:1745:C:C4'	2.33	0.40
15:N:6:THR:OG1	15:N:10:ARG:NH2	2.54	0.40
19:R:43:ASP:HB2	19:R:45:LYS:HG3	2.03	0.40
29:X:20:C:H2'	29:X:21:A:C8	2.57	0.40
29:X:174:A:C6	29:X:2409:A:N3	2.89	0.40
29:X:193:A:C8	29:X:445:A:C6	3.08	0.40
29:X:614:G:C6	29:X:636:G:C2	3.10	0.40
29:X:815:A:H3'	29:X:816:U:H6	1.87	0.40
29:X:1135:C:C4	29:X:1136:G:N7	2.89	0.40
29:X:1255:A:C4	29:X:1256:C:C5	3.10	0.40
29:X:1477:C:O2'	29:X:2681:A:H1'	2.21	0.40
29:X:1534:A:H2'	29:X:1535:C:C6	2.56	0.40
29:X:1757:C:C2	29:X:1970:G:C2	3.09	0.40
29:X:2011:U:H2'	29:X:2012:A:C8	2.56	0.40
29:X:2065:A:C2	29:X:2066:G:H1'	2.57	0.40
29:X:2528:G:N3	29:X:2529:G:C8	2.90	0.40
29:X:2590:U:O2	29:X:2590:U:H2'	2.21	0.40
29:X:2617:G:N2	29:X:2755:A:H2'	2.36	0.40
29:X:2697:G:H2'	29:X:2698:G:H8	1.86	0.40
30:Y:3:A:H2'	30:Y:4:C:C6	2.57	0.40
2:A:48:ARG:HE	29:X:791:G:H5''	1.86	0.40
2:A:229:VAL:HG13	2:A:230:ASP:OD2	2.20	0.40
3:B:155:ARG:O	3:B:156:MET:HB3	2.21	0.40
4:C:120:VAL:N	4:C:189:ASP:O	2.43	0.40
5:D:80:ARG:HD3	5:D:83:MET:HB2	2.02	0.40
7:F:63:ARG:HE	7:F:63:ARG:HB2	1.73	0.40
9:H:11:ALA:HB3	9:H:97:VAL:HG23	2.03	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:8:ARG:HB3	12:K:10:LEU:HG	2.03	0.40
17:P:59:PHE:CD1	25:Z:30:LEU:HD11	2.52	0.40
17:P:79:ALA:O	17:P:85:MET:HB2	2.21	0.40
19:R:83:LEU:HD23	19:R:83:LEU:HA	1.92	0.40
22:U:27:ASP:C	22:U:32:ARG:HD3	2.42	0.40
22:U:51:ILE:O	22:U:52:ARG:HD3	2.22	0.40
29:X:67:G:H2'	29:X:68:C:C6	2.54	0.40
29:X:189:A:H2'	29:X:190:A:H8	1.85	0.40
29:X:356:A:H2'	29:X:357:A:C8	2.56	0.40
29:X:404:A:C5	29:X:424:G:C2	3.09	0.40
29:X:486:U:O2'	29:X:515:A:H1'	2.21	0.40
29:X:933:G:H4'	29:X:2248:A:C6	2.56	0.40
29:X:963:G:C6	29:X:964:A:N7	2.89	0.40
29:X:965:G:N3	29:X:2253:A:C2	2.90	0.40
29:X:1326:U:H2'	29:X:1626:A:C2	2.56	0.40
29:X:1504:G:C6	29:X:1505:U:O4	2.75	0.40
29:X:1591:U:H2'	29:X:1592:U:C6	2.57	0.40
29:X:1673:C:H2'	29:X:1674:C:C6	2.56	0.40
29:X:2165:A:H2'	29:X:2166:G:H8	1.87	0.40
29:X:2535:C:H2'	29:X:2536:G:C8	2.56	0.40
29:X:2701:A:C2	29:X:2848:A:C4	3.10	0.40
30:Y:120:G:C2	30:Y:121:G:C5	3.09	0.40
1:O:54:VAL:HG13	1:O:195:ALA:HB2	2.03	0.40
4:C:28:HIS:O	4:C:32:THR:HG23	2.21	0.40
5:D:133:LYS:HB2	5:D:134:GLU:H	1.61	0.40
6:E:12:PRO:HG2	6:E:15:VAL:HG13	2.03	0.40
8:G:98:LYS:HB3	8:G:115:ALA:HB2	2.02	0.40
9:H:129:LEU:HD23	9:H:129:LEU:HA	1.89	0.40
10:I:63:ARG:HB3	28:3:25:PHE:CZ	2.56	0.40
11:J:76:THR:HG22	11:J:91:VAL:HA	2.03	0.40
12:K:46:PRO:HA	12:K:49:GLU:HB2	2.02	0.40
12:K:78:LYS:O	12:K:82:GLU:HB2	2.20	0.40
16:O:53:LYS:H	16:O:53:LYS:HG2	1.67	0.40
28:3:10:ALA:HB1	28:3:14:ILE:HG13	2.02	0.40
29:X:66:U:H2'	29:X:67:G:C8	2.55	0.40
29:X:572:G:H22	29:X:587:A:H2	1.68	0.40
29:X:695:G:N2	29:X:809:C:C2	2.89	0.40
29:X:746:G:C8	29:X:774:A:N6	2.89	0.40
29:X:836:G:O2'	29:X:837:U:H5'	2.22	0.40
29:X:941:U:H2'	29:X:942:U:C6	2.57	0.40
29:X:1079:G:H8	29:X:1079:G:OP2	2.03	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:X:1235:C:C2	29:X:1241:G:N2	2.89	0.40
29:X:1272:G:H2'	29:X:1273:G:C8	2.57	0.40
29:X:2039:G:H2'	29:X:2039:G:N3	2.37	0.40
29:X:2320:G:H2'	29:X:2321:C:C6	2.56	0.40
29:X:2345:A:N6	29:X:2346:G:C2	2.89	0.40
29:X:2559:U:C5	29:X:2560:G:C6	3.10	0.40
29:X:2585:C:C2'	29:X:2586:G:H5'	2.50	0.40
29:X:2666:U:C5	29:X:2667:C:C4	3.09	0.40
29:X:2863:U:N3	29:X:2864:C:C5	2.90	0.40
30:Y:12:C:H42	30:Y:113:G:H1	1.69	0.40
30:Y:35:C:H2'	30:Y:36:A:H8	1.85	0.40
30:Y:94:G:N2	30:Y:95:U:C2	2.89	0.40
1:O:18:ILE:HG12	1:O:185:TYR:HE1	1.85	0.40
3:B:119:ARG:NH1	3:B:158:GLY:HA3	2.36	0.40
9:H:105:PRO:HB2	9:H:107:GLY:H	1.87	0.40
10:I:41:SER:OG	29:X:685:U:OP2	2.33	0.40
14:M:96:ARG:HA	14:M:96:ARG:HD2	1.84	0.40
15:N:91:ASN:HD21	29:X:1007:A:H4'	1.86	0.40
15:N:92:ARG:HG2	29:X:1008:G:OP1	2.21	0.40
24:W:11:GLY:HA2	29:X:980:G:O2'	2.22	0.40
29:X:32:C:H2'	29:X:33:C:C6	2.56	0.40
29:X:654:A:O2'	29:X:655:A:P	2.80	0.40
29:X:697:G:O2'	29:X:801:A:N7	2.46	0.40
29:X:874:A:C2	29:X:875:G:H1'	2.57	0.40
29:X:947:C:C2	29:X:948:C:C5	3.10	0.40
29:X:955:G:H3'	29:X:955:G:C8	2.57	0.40
29:X:1033:G:N2	29:X:1035:G:N2	2.69	0.40
29:X:1080:A:H4'	29:X:1081:A:C8	2.57	0.40
29:X:1265:G:O2'	29:X:1266:G:C8	2.75	0.40
29:X:1320:A:N6	29:X:1622:G:O2'	2.55	0.40
29:X:1359:G:C5	29:X:1360:G:N7	2.90	0.40
29:X:1503:G:C6	29:X:1504:G:C6	3.09	0.40
29:X:2225:G:C4	29:X:2226:A:C8	3.09	0.40
29:X:2262:C:C6	29:X:2368:G:H2'	2.56	0.40
29:X:2302:G:C6	29:X:2303:C:C4	3.10	0.40
29:X:2309:G:N2	29:X:2365:U:C2	2.88	0.40
29:X:2424:G:H2'	29:X:2425:G:C8	2.51	0.40
29:X:2563:U:H2'	29:X:2564:U:H6	1.85	0.40
29:X:2785:A:C8	29:X:2786:G:C8	3.10	0.40
29:X:2856:U:H2'	29:X:2857:C:H6	1.86	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	222/224 (99%)	139 (63%)	58 (26%)	25 (11%)	0	1
2	A	272/274 (99%)	206 (76%)	50 (18%)	16 (6%)	1	7
3	B	203/205 (99%)	152 (75%)	33 (16%)	18 (9%)	0	2
4	C	195/197 (99%)	123 (63%)	50 (26%)	22 (11%)	0	1
5	D	175/177 (99%)	117 (67%)	42 (24%)	16 (9%)	0	2
6	E	169/171 (99%)	119 (70%)	33 (20%)	17 (10%)	0	2
7	F	142/144 (99%)	100 (70%)	27 (19%)	15 (11%)	0	2
8	G	140/142 (99%)	111 (79%)	19 (14%)	10 (7%)	1	4
9	H	132/134 (98%)	96 (73%)	18 (14%)	18 (14%)	0	1
10	I	139/141 (99%)	93 (67%)	30 (22%)	16 (12%)	0	1
11	J	134/136 (98%)	97 (72%)	28 (21%)	9 (7%)	1	5
12	K	111/113 (98%)	81 (73%)	18 (16%)	12 (11%)	0	1
13	L	102/104 (98%)	68 (67%)	18 (18%)	16 (16%)	0	0
14	M	107/109 (98%)	83 (78%)	14 (13%)	10 (9%)	0	2
15	N	115/117 (98%)	90 (78%)	19 (16%)	6 (5%)	1	9
16	O	92/94 (98%)	69 (75%)	13 (14%)	10 (11%)	0	1
17	P	125/127 (98%)	102 (82%)	17 (14%)	6 (5%)	2	11
18	Q	91/93 (98%)	67 (74%)	16 (18%)	8 (9%)	0	3
19	R	108/110 (98%)	63 (58%)	28 (26%)	17 (16%)	0	0
20	S	173/175 (99%)	123 (71%)	32 (18%)	18 (10%)	0	2
21	T	82/84 (98%)	68 (83%)	8 (10%)	6 (7%)	1	4
22	U	70/72 (97%)	39 (56%)	15 (21%)	16 (23%)	0	0
23	V	64/66 (97%)	54 (84%)	9 (14%)	1 (2%)	8	34
24	W	53/55 (96%)	36 (68%)	13 (24%)	4 (8%)	1	4
25	Z	55/57 (96%)	36 (66%)	13 (24%)	6 (11%)	0	1

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	1	52/54 (96%)	31 (60%)	13 (25%)	8 (15%)	0	0
27	2	45/47 (96%)	38 (84%)	6 (13%)	1 (2%)	5	27
28	3	63/65 (97%)	38 (60%)	17 (27%)	8 (13%)	0	1
All	All	3431/3487 (98%)	2439 (71%)	657 (19%)	335 (10%)	0	2

All (335) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	17	SER
1	0	61	PRO
1	0	157	ILE
1	0	216	PRO
2	A	25	ALA
2	A	111	LEU
2	A	202	LYS
3	B	34	VAL
3	B	85	ALA
3	B	86	PRO
3	B	117	MET
3	B	123	ALA
3	B	133	LYS
3	B	180	ASN
4	C	9	GLN
4	C	20	PRO
4	C	51	VAL
4	C	52	SER
4	C	54	THR
4	C	97	ARG
4	C	126	ALA
4	C	172	VAL
4	C	174	GLY
5	D	40	LEU
5	D	134	GLU
6	E	24	PHE
6	E	42	THR
6	E	55	PRO
6	E	58	ALA
6	E	65	HIS
6	E	112	PRO
6	E	126	PRO
6	E	165	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
7	F	23	VAL
7	F	50	ASP
7	F	74	MET
7	F	116	ASN
8	G	37	ASP
8	G	66	HIS
8	G	110	LEU
9	H	5	GLN
9	H	29	ILE
9	H	41	ASN
9	H	47	VAL
9	H	61	ARG
9	H	84	ALA
9	H	116	ARG
10	I	29	THR
10	I	78	SER
10	I	82	ASP
10	I	110	ALA
10	I	111	SER
11	J	21	ASP
11	J	23	LYS
11	J	135	ARG
12	K	4	GLY
12	K	11	ASN
12	K	13	ASN
12	K	20	LEU
12	K	32	GLY
12	K	88	ALA
12	K	100	VAL
13	L	10	LYS
13	L	21	THR
13	L	33	ARG
13	L	45	ASP
13	L	53	ALA
14	M	25	PRO
14	M	43	ASN
14	M	83	PHE
15	N	5	LYS
15	N	7	GLY
15	N	27	SER
16	O	24	SER
16	O	29	ALA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
17	P	49	SER
17	P	50	VAL
17	P	81	HIS
17	P	82	ASN
17	P	87	GLU
19	R	11	ASN
19	R	51	VAL
19	R	58	VAL
19	R	60	PRO
19	R	78	ALA
19	R	93	ARG
19	R	110	SER
20	S	91	PRO
20	S	124	ALA
20	S	169	VAL
21	T	30	VAL
21	T	64	ASP
21	T	74	LYS
22	U	14	VAL
22	U	15	VAL
22	U	18	VAL
22	U	25	ARG
22	U	55	GLY
22	U	60	VAL
22	U	76	LYS
24	W	36	ASP
24	W	38	PRO
25	Z	34	PRO
26	1	40	TYR
26	1	44	ALA
28	3	53	ALA
1	0	62	HIS
1	0	87	ALA
1	0	100	ALA
1	0	108	ALA
1	0	137	LYS
2	A	41	GLY
2	A	125	PRO
2	A	169	GLU
2	A	239	ARG
3	B	60	ASN
3	B	71	GLY

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	B	118	LYS
4	C	11	GLY
4	C	22	VAL
4	C	37	SER
4	C	43	ALA
4	C	56	ARG
4	C	75	PRO
4	C	178	TYR
5	D	33	LYS
5	D	42	SER
5	D	122	PHE
5	D	132	ILE
5	D	133	LYS
6	E	18	ASN
6	E	100	GLY
6	E	173	ALA
7	F	14	ALA
7	F	22	PRO
7	F	82	ALA
8	G	38	GLU
8	G	77	GLY
8	G	94	LYS
9	H	4	PRO
9	H	22	ILE
9	H	42	LYS
9	H	66	ALA
9	H	69	VAL
9	H	79	HIS
10	I	41	SER
10	I	44	GLY
10	I	57	ILE
10	I	86	THR
10	I	99	VAL
11	J	13	GLN
11	J	26	ASP
11	J	98	VAL
12	K	40	LYS
12	K	103	ARG
13	L	20	THR
13	L	55	SER
13	L	56	SER
13	L	59	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
13	L	61	SER
13	L	93	SER
13	L	96	TYR
14	M	16	ILE
14	M	17	GLU
14	M	26	ASP
16	O	16	GLU
18	Q	3	HIS
18	Q	59	PRO
18	Q	61	LYS
18	Q	67	ARG
19	R	25	LEU
19	R	79	SER
20	S	26	LYS
22	U	10	LYS
22	U	29	GLY
22	U	32	ARG
22	U	63	SER
25	Z	36	CYS
26	1	30	ASN
28	3	12	ARG
28	3	34	THR
28	3	51	ALA
1	0	28	LEU
1	0	33	PHE
1	0	45	ILE
1	0	102	GLY
1	0	146	ALA
1	0	203	VAL
2	A	187	SER
2	A	198	ASN
2	A	241	GLY
2	A	246	PRO
3	B	17	ASN
3	B	127	ALA
3	B	155	ARG
4	C	83	ALA
4	C	171	PRO
5	D	71	LYS
5	D	80	ARG
6	E	7	GLN
6	E	41	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
6	E	172	LYS
7	F	47	ASP
8	G	65	LYS
8	G	113	GLU
9	H	28	GLY
9	H	71	LYS
10	I	65	PHE
10	I	68	VAL
10	I	81	GLN
11	J	11	ARG
12	K	56	LYS
13	L	26	LYS
14	M	46	ARG
14	M	47	SER
15	N	73	GLY
15	N	103	PRO
16	O	45	THR
18	Q	8	GLN
19	R	20	ASP
19	R	87	GLU
20	S	7	PRO
20	S	14	LEU
20	S	51	LEU
20	S	58	GLY
20	S	63	PRO
20	S	94	VAL
20	S	156	GLU
21	T	83	ALA
22	U	17	SER
22	U	27	ASP
22	U	47	HIS
24	W	17	VAL
24	W	22	ALA
25	Z	21	SER
26	1	28	ARG
26	1	46	HIS
26	1	48	VAL
27	2	17	GLY
28	3	46	LYS
1	0	6	LEU
1	0	139	GLY
1	0	158	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	0	197	PRO
2	A	45	ASN
3	B	66	HIS
3	B	73	ALA
3	B	144	ARG
3	B	154	LYS
4	C	90	SER
5	D	20	PHE
5	D	35	VAL
5	D	77	PHE
7	F	19	PRO
7	F	25	PRO
7	F	70	LYS
7	F	83	GLY
8	G	140	GLN
10	I	116	ARG
12	K	102	THR
13	L	68	ALA
13	L	97	HIS
14	M	74	GLY
16	O	20	ILE
16	O	40	VAL
16	O	44	GLN
18	Q	84	GLU
19	R	52	ASN
19	R	64	ASN
19	R	102	LYS
20	S	37	LYS
20	S	57	GLU
20	S	88	TYR
20	S	122	ILE
20	S	128	ARG
21	T	8	GLY
23	V	3	PRO
25	Z	24	ALA
2	A	228	PRO
3	B	131	SER
4	C	15	ILE
4	C	27	LEU
4	C	41	GLY
5	D	29	PRO
5	D	44	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
6	E	23	VAL
7	F	113	PRO
9	H	70	VAL
9	H	124	MET
11	J	81	GLU
11	J	133	VAL
12	K	57	GLY
16	O	31	ASP
19	R	65	PRO
25	Z	4	HIS
25	Z	20	ARG
26	1	51	ALA
28	3	63	PRO
1	0	67	SER
1	0	120	GLY
2	A	201	HIS
5	D	21	GLY
5	D	113	ASP
6	E	92	VAL
8	G	165	VAL
13	L	84	ILE
16	O	60	VAL
19	R	31	GLY
19	R	100	ASP
20	S	35	ASP
22	U	12	ASN
22	U	41	VAL
1	0	89	VAL
2	A	165	VAL
7	F	52	ILE
10	I	24	GLY
14	M	7	ILE
15	N	88	ILE
20	S	125	PRO
26	1	43	VAL
16	O	17	GLY
18	Q	9	ALA
18	Q	29	VAL
21	T	31	VAL
28	3	16	ILE
1	0	86	GLY
1	0	165	GLY

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	A	229	VAL
9	H	40	GLY
17	P	35	PRO
10	I	10	PRO
28	3	28	GLY
1	0	91	GLY
6	E	76	VAL
7	F	96	VAL

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	167/167 (100%)	150 (90%)	17 (10%)	6	24
2	A	214/214 (100%)	177 (83%)	37 (17%)	1	8
3	B	155/155 (100%)	123 (79%)	32 (21%)	1	5
4	C	157/157 (100%)	117 (74%)	40 (26%)	0	2
5	D	153/153 (100%)	126 (82%)	27 (18%)	1	8
6	E	136/136 (100%)	111 (82%)	25 (18%)	1	7
7	F	107/107 (100%)	94 (88%)	13 (12%)	4	18
8	G	118/118 (100%)	97 (82%)	21 (18%)	1	8
9	H	103/103 (100%)	73 (71%)	30 (29%)	0	1
10	I	108/108 (100%)	88 (82%)	20 (18%)	1	7
11	J	110/110 (100%)	82 (74%)	28 (26%)	0	2
12	K	90/90 (100%)	68 (76%)	22 (24%)	0	3
13	L	74/74 (100%)	46 (62%)	28 (38%)	0	0
14	M	92/92 (100%)	58 (63%)	34 (37%)	0	0
15	N	96/96 (100%)	82 (85%)	14 (15%)	2	12
16	O	75/75 (100%)	59 (79%)	16 (21%)	1	4
17	P	109/109 (100%)	85 (78%)	24 (22%)	1	4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	Q	75/75 (100%)	57 (76%)	18 (24%)	0	3
19	R	91/91 (100%)	71 (78%)	20 (22%)	1	4
20	S	149/149 (100%)	119 (80%)	30 (20%)	1	5
21	T	62/62 (100%)	42 (68%)	20 (32%)	0	1
22	U	57/57 (100%)	38 (67%)	19 (33%)	0	1
23	V	54/54 (100%)	45 (83%)	9 (17%)	2	9
24	W	48/48 (100%)	38 (79%)	10 (21%)	1	5
25	Z	51/51 (100%)	43 (84%)	8 (16%)	2	10
26	1	38/38 (100%)	33 (87%)	5 (13%)	3	15
27	2	40/40 (100%)	32 (80%)	8 (20%)	1	5
28	3	51/51 (100%)	34 (67%)	17 (33%)	0	1
All	All	2780/2780 (100%)	2188 (79%)	592 (21%)	1	4

All (592) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	16	TYR
1	0	24	LEU
1	0	26	LYS
1	0	38	GLU
1	0	64	THR
1	0	70	VAL
1	0	95	LEU
1	0	110	VAL
1	0	112	THR
1	0	114	ASP
1	0	121	GLN
1	0	137	LYS
1	0	152	LEU
1	0	157	ILE
1	0	166	VAL
1	0	168	HIS
1	0	212	THR
2	A	7	LYS
2	A	10	THR
2	A	13	ARG
2	A	21	PHE
2	A	35	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	A	40	THR
2	A	49	ILE
2	A	59	LYS
2	A	63	ARG
2	A	66	ASP
2	A	68	LYS
2	A	70	ARG
2	A	82	ILE
2	A	88	ARG
2	A	91	ARG
2	A	96	HIS
2	A	113	VAL
2	A	116	THR
2	A	117	VAL
2	A	118	ASN
2	A	138	VAL
2	A	142	VAL
2	A	145	LEU
2	A	148	VAL
2	A	163	VAL
2	A	165	VAL
2	A	169	GLU
2	A	190	TYR
2	A	204	ILE
2	A	239	ARG
2	A	246	PRO
2	A	247	VAL
2	A	252	LYS
2	A	270	LEU
2	A	271	VAL
2	A	273	ARG
2	A	274	ARG
3	B	11	MET
3	B	12	THR
3	B	14	ILE
3	B	19	ARG
3	B	38	THR
3	B	40	GLN
3	B	41	THR
3	B	49	ILE
3	B	66	HIS
3	B	72	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	B	76	ARG
3	B	79	ARG
3	B	84	PHE
3	B	87	ASP
3	B	90	SER
3	B	92	ASN
3	B	93	VAL
3	B	94	ASP
3	B	116	VAL
3	B	117	MET
3	B	126	PRO
3	B	132	LYS
3	B	136	ARG
3	B	141	ILE
3	B	145	LYS
3	B	152	LYS
3	B	167	VAL
3	B	176	ARG
3	B	182	ILE
3	B	192	ASN
3	B	199	ARG
3	B	200	SER
4	C	7	ILE
4	C	10	ASN
4	C	13	ARG
4	C	16	GLU
4	C	21	GLU
4	C	22	VAL
4	C	28	HIS
4	C	31	VAL
4	C	37	SER
4	C	38	ARG
4	C	42	THR
4	C	47	THR
4	C	50	GLN
4	C	51	VAL
4	C	52	SER
4	C	59	TYR
4	C	68	ARG
4	C	76	THR
4	C	87	LYS
4	C	92	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
4	C	97	ARG
4	C	98	GLN
4	C	99	VAL
4	C	106	MET
4	C	112	GLN
4	C	113	GLU
4	C	121	ASP
4	C	124	ASP
4	C	131	LYS
4	C	140	ASN
4	C	143	ASP
4	C	150	LEU
4	C	153	ASP
4	C	155	GLU
4	C	162	ARG
4	C	163	ASN
4	C	167	VAL
4	C	169	VAL
4	C	172	VAL
4	C	181	LEU
5	D	9	ASN
5	D	25	VAL
5	D	46	ASP
5	D	61	THR
5	D	66	ILE
5	D	68	THR
5	D	72	LYS
5	D	80	ARG
5	D	85	VAL
5	D	89	VAL
5	D	92	ARG
5	D	106	ILE
5	D	115	ARG
5	D	117	ILE
5	D	123	ASP
5	D	125	ARG
5	D	127	ASN
5	D	128	TYR
5	D	136	LEU
5	D	142	THR
5	D	143	TYR
5	D	147	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
5	D	148	LYS
5	D	150	ARG
5	D	156	ILE
5	D	158	THR
5	D	159	THR
6	E	6	LYS
6	E	11	VAL
6	E	20	GLN
6	E	33	LEU
6	E	35	VAL
6	E	38	ASN
6	E	40	GLU
6	E	41	LEU
6	E	42	THR
6	E	43	VAL
6	E	44	ARG
6	E	48	ASP
6	E	61	HIS
6	E	67	LEU
6	E	69	ARG
6	E	84	THR
6	E	109	TYR
6	E	111	HIS
6	E	115	ILE
6	E	121	VAL
6	E	122	THR
6	E	134	SER
6	E	140	LEU
6	E	152	ARG
6	E	165	VAL
7	F	2	ARG
7	F	10	LEU
7	F	23	VAL
7	F	33	ASN
7	F	59	ILE
7	F	63	ARG
7	F	84	ILE
7	F	99	LEU
7	F	102	ASP
7	F	112	MET
7	F	121	GLU
7	F	134	MET

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
7	F	137	THR
8	G	31	THR
8	G	38	GLU
8	G	40	ASN
8	G	42	VAL
8	G	53	ARG
8	G	54	LEU
8	G	65	LYS
8	G	73	ASN
8	G	82	VAL
8	G	83	ILE
8	G	99	VAL
8	G	101	THR
8	G	102	ARG
8	G	114	THR
8	G	140	GLN
8	G	150	VAL
8	G	154	GLU
8	G	155	THR
8	G	156	HIS
8	G	159	SER
8	G	167	LYS
9	H	3	MET
9	H	8	LEU
9	H	9	ASP
9	H	10	VAL
9	H	18	GLU
9	H	19	ILE
9	H	35	THR
9	H	36	THR
9	H	41	ASN
9	H	43	ARG
9	H	46	HIS
9	H	51	ILE
9	H	57	ASP
9	H	65	LYS
9	H	73	VAL
9	H	74	VAL
9	H	78	SER
9	H	82	LYS
9	H	83	ARG
9	H	89	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
9	H	90	ARG
9	H	93	ARG
9	H	104	GLU
9	H	109	ARG
9	H	117	GLU
9	H	121	ARG
9	H	122	ARG
9	H	124	MET
9	H	126	ILE
9	H	127	VAL
10	I	4	HIS
10	I	6	LEU
10	I	18	ARG
10	I	19	VAL
10	I	28	LYS
10	I	45	LYS
10	I	48	PHE
10	I	53	ARG
10	I	65	PHE
10	I	74	VAL
10	I	81	GLN
10	I	82	ASP
10	I	91	ASP
10	I	96	TYR
10	I	99	VAL
10	I	109	LEU
10	I	120	VAL
10	I	121	HIS
10	I	133	VAL
10	I	142	LEU
11	J	11	ARG
11	J	12	LYS
11	J	15	ARG
11	J	17	ARG
11	J	26	ASP
11	J	27	TYR
11	J	35	LEU
11	J	45	SER
11	J	47	GLN
11	J	48	ILE
11	J	49	GLU
11	J	52	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
11	J	60	ARG
11	J	64	LYS
11	J	68	ARG
11	J	72	ASP
11	J	73	LYS
11	J	82	THR
11	J	84	MET
11	J	93	TYR
11	J	102	ARG
11	J	106	GLU
11	J	130	THR
11	J	132	MET
11	J	133	VAL
11	J	137	VAL
11	J	139	ASP
11	J	140	GLU
12	K	11	ASN
12	K	14	SER
12	K	20	LEU
12	K	26	THR
12	K	33	ARG
12	K	35	GLN
12	K	36	THR
12	K	51	LEU
12	K	52	ILE
12	K	53	THR
12	K	59	ASP
12	K	64	ARG
12	K	65	LEU
12	K	73	LYS
12	K	75	VAL
12	K	83	VAL
12	K	89	GLU
12	K	94	TYR
12	K	95	THR
12	K	99	ARG
12	K	113	ILE
12	K	114	GLU
13	L	11	LEU
13	L	12	ARG
13	L	13	THR
13	L	15	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
13	L	17	VAL
13	L	20	THR
13	L	24	SER
13	L	29	LEU
13	L	31	VAL
13	L	33	ARG
13	L	35	SER
13	L	36	LYS
13	L	37	HIS
13	L	38	ILE
13	L	39	TYR
13	L	43	ILE
13	L	60	LYS
13	L	66	ASP
13	L	71	VAL
13	L	82	LYS
13	L	85	LYS
13	L	91	ARG
13	L	93	SER
13	L	95	LYS
13	L	97	HIS
13	L	99	ARG
13	L	108	ARG
13	L	109	GLU
14	M	2	GLN
14	M	9	ARG
14	M	12	LEU
14	M	13	LEU
14	M	14	ARG
14	M	19	ASP
14	M	21	THR
14	M	22	ARG
14	M	23	GLN
14	M	28	ARG
14	M	29	PRO
14	M	32	THR
14	M	37	THR
14	M	40	ARG
14	M	44	ARG
14	M	51	GLU
14	M	54	VAL
14	M	57	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
14	M	60	SER
14	M	62	SER
14	M	63	ARG
14	M	68	VAL
14	M	69	ARG
14	M	70	LYS
14	M	72	SER
14	M	77	VAL
14	M	78	GLU
14	M	91	VAL
14	M	95	GLU
14	M	96	ARG
14	M	99	VAL
14	M	101	ARG
14	M	103	LYS
14	M	106	TYR
15	N	5	LYS
15	N	9	VAL
15	N	17	VAL
15	N	34	ASN
15	N	36	PHE
15	N	51	ARG
15	N	63	GLN
15	N	77	SER
15	N	80	ILE
15	N	85	ARG
15	N	93	LYS
15	N	102	GLU
15	N	113	SER
15	N	118	GLN
16	O	7	THR
16	O	10	LYS
16	O	11	GLN
16	O	14	VAL
16	O	18	ASP
16	O	31	ASP
16	O	32	LYS
16	O	35	LEU
16	O	38	LEU
16	O	47	PHE
16	O	55	THR
16	O	65	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
16	O	69	ILE
16	O	72	ARG
16	O	78	VAL
16	O	83	ARG
17	P	16	GLN
17	P	17	GLN
17	P	21	ARG
17	P	25	PHE
17	P	31	VAL
17	P	36	ARG
17	P	40	LEU
17	P	41	VAL
17	P	42	VAL
17	P	50	VAL
17	P	63	SER
17	P	66	GLU
17	P	84	GLU
17	P	88	ASP
17	P	91	PHE
17	P	96	TYR
17	P	98	ASP
17	P	103	LEU
17	P	105	ARG
17	P	109	ARG
17	P	115	ASN
17	P	117	ILE
17	P	124	ILE
17	P	126	ILE
18	Q	5	ASP
18	Q	6	ILE
18	Q	26	SER
18	Q	27	PHE
18	Q	30	SER
18	Q	40	ASP
18	Q	48	VAL
18	Q	57	ASN
18	Q	64	ARG
18	Q	65	VAL
18	Q	67	ARG
18	Q	75	ARG
18	Q	80	VAL
18	Q	81	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
18	Q	82	LEU
18	Q	84	GLU
18	Q	88	ILE
18	Q	91	LEU
19	R	9	HIS
19	R	22	VAL
19	R	23	ILE
19	R	32	GLN
19	R	43	ASP
19	R	44	GLN
19	R	46	VAL
19	R	48	VAL
19	R	51	VAL
19	R	53	VAL
19	R	56	LYS
19	R	57	ASN
19	R	66	GLN
19	R	73	GLU
19	R	74	LEU
19	R	80	LYS
19	R	84	VAL
19	R	90	LYS
19	R	104	VAL
19	R	106	VAL
20	S	3	LEU
20	S	13	LYS
20	S	15	ASP
20	S	18	MET
20	S	22	VAL
20	S	24	TYR
20	S	26	LYS
20	S	35	ASP
20	S	37	LYS
20	S	48	THR
20	S	55	THR
20	S	57	GLU
20	S	70	GLN
20	S	72	ASP
20	S	73	LYS
20	S	87	THR
20	S	95	SER
20	S	96	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
20	S	99	HIS
20	S	100	THR
20	S	108	VAL
20	S	109	GLN
20	S	112	LEU
20	S	120	LEU
20	S	128	ARG
20	S	139	THR
20	S	151	ASP
20	S	156	GLU
20	S	159	THR
20	S	166	LEU
21	T	4	LYS
21	T	5	LYS
21	T	7	VAL
21	T	10	SER
21	T	11	LYS
21	T	12	ASN
21	T	19	LYS
21	T	21	LEU
21	T	29	GLU
21	T	37	LEU
21	T	41	ARG
21	T	43	THR
21	T	49	GLN
21	T	62	LEU
21	T	64	ASP
21	T	70	ILE
21	T	77	ARG
21	T	79	ILE
21	T	81	ILE
21	T	82	GLU
22	U	8	THR
22	U	10	LYS
22	U	12	ASN
22	U	14	VAL
22	U	15	VAL
22	U	19	ILE
22	U	20	ARG
22	U	21	ARG
22	U	23	LYS
22	U	32	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
22	U	33	LYS
22	U	37	ILE
22	U	40	ARG
22	U	49	LYS
22	U	57	VAL
22	U	63	SER
22	U	67	ILE
22	U	69	THR
22	U	76	LYS
23	V	12	THR
23	V	16	LYS
23	V	21	ARG
23	V	25	LEU
23	V	26	MET
23	V	46	LEU
23	V	53	LEU
23	V	55	THR
23	V	63	LYS
24	W	3	ILE
24	W	6	VAL
24	W	10	ILE
24	W	26	ARG
24	W	34	VAL
24	W	37	THR
24	W	46	THR
24	W	51	LEU
24	W	52	GLU
24	W	53	VAL
25	Z	9	LYS
25	Z	25	LEU
25	Z	26	THR
25	Z	34	PRO
25	Z	44	HIS
25	Z	48	ASN
25	Z	52	TYR
25	Z	57	VAL
26	1	10	VAL
26	1	15	SER
26	1	24	THR
26	1	37	LEU
26	1	46	HIS
27	2	4	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
27	2	12	ARG
27	2	21	ARG
27	2	24	THR
27	2	26	SER
27	2	28	ARG
27	2	29	ASN
27	2	42	LEU
28	3	7	HIS
28	3	9	MET
28	3	13	ARG
28	3	14	ILE
28	3	19	THR
28	3	21	LYS
28	3	22	VAL
28	3	26	LYS
28	3	29	LYS
28	3	30	ARG
28	3	31	HIS
28	3	34	THR
28	3	39	ASP
28	3	46	LYS
28	3	55	TRP
28	3	62	LEU
28	3	64	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	186	GLN
2	A	129	ASN
2	A	227	ASN
3	B	60	ASN
3	B	192	ASN
4	C	132	ASN
6	E	139	GLN
7	F	11	GLN
13	L	37	HIS
14	M	48	GLN
15	N	37	GLN
16	O	57	GLN
20	S	109	GLN
23	V	52	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
26	1	30	ASN
26	1	46	HIS
28	3	7	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
29	X	2776/2881 (96%)	839 (30%)	30 (1%)
30	Y	121/122 (99%)	35 (28%)	1 (0%)
All	All	2897/3003 (96%)	874 (30%)	31 (1%)

All (874) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
29	X	8	A
29	X	13	A
29	X	15	G
29	X	54	G
29	X	63	A
29	X	66	U
29	X	70	A
29	X	73	A
29	X	74	G
29	X	75	C
29	X	88	G
29	X	89	A
29	X	90	G
29	X	91	A
29	X	92	U
29	X	100	G
29	X	101	A
29	X	102	C
29	X	107	G
29	X	116	A
29	X	117	A
29	X	118	U
29	X	120	G
29	X	123	A
29	X	129	A
29	X	135	U
29	X	136	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
29	X	138	G
29	X	144	U
29	X	147	G
29	X	158	A
29	X	159	A
29	X	170	U
29	X	173	A
29	X	175	C
29	X	176	A
29	X	177	U
29	X	180	C
29	X	181	A
29	X	182	G
29	X	192	G
29	X	193	A
29	X	199	A
29	X	200	A
29	X	201	G
29	X	202	A
29	X	203	G
29	X	205	A
29	X	206	U
29	X	207	U
29	X	209	G
29	X	218	A
29	X	219	G
29	X	221	A
29	X	222	G
29	X	225	G
29	X	226	C
29	X	227	G
29	X	228	A
29	X	229	G
29	X	238	G
29	X	243	G
29	X	245	C
29	X	248	A
29	X	305	A
29	X	308	C
29	X	309	G
29	X	310	A
29	X	321	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
29	X	322	A
29	X	323	G
29	X	324	C
29	X	335	A
29	X	340	G
29	X	341	A
29	X	342	G
29	X	343	A
29	X	346	C
29	X	354	C
29	X	356	A
29	X	357	A
29	X	361	G
29	X	396	U
29	X	397	U
29	X	399	G
29	X	400	U
29	X	403	A
29	X	404	A
29	X	408	U
29	X	409	G
29	X	412	U
29	X	413	G
29	X	414	A
29	X	415	A
29	X	418	C
29	X	424	G
29	X	425	A
29	X	453	U
29	X	455	A
29	X	458	G
29	X	459	A
29	X	463	C
29	X	466	A
29	X	467	U
29	X	469	G
29	X	475	U
29	X	476	G
29	X	478	G
29	X	479	G
29	X	481	A
29	X	483	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
29	X	486	U
29	X	492	G
29	X	494	A
29	X	500	G
29	X	504	G
29	X	506	G
29	X	511	A
29	X	512	A
29	X	514	G
29	X	515	A
29	X	516	G
29	X	518	A
29	X	519	C
29	X	520	C
29	X	521	U
29	X	532	A
29	X	534	U
29	X	539	A
29	X	540	G
29	X	541	C
29	X	542	A
29	X	543	G
29	X	545	C
29	X	554	U
29	X	555	U
29	X	556	A
29	X	557	U
29	X	558	G
29	X	559	C
29	X	560	G
29	X	564	U
29	X	569	C
29	X	571	U
29	X	572	G
29	X	580	A
29	X	582	G
29	X	583	C
29	X	584	A
29	X	587	A
29	X	591	G
29	X	594	G
29	X	595	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
29	X	601	A
29	X	602	C
29	X	604	U
29	X	609	U
29	X	610	G
29	X	611	C
29	X	613	A
29	X	616	U
29	X	620	G
29	X	624	A
29	X	625	A
29	X	626	A
29	X	627	A
29	X	628	A
29	X	631	G
29	X	633	G
29	X	637	G
29	X	638	A
29	X	645	G
29	X	648	A
29	X	655	A
29	X	656	U
29	X	657	A
29	X	663	G
29	X	664	C
29	X	666	U
29	X	668	A
29	X	672	C
29	X	673	G
29	X	682	G
29	X	683	A
29	X	689	A
29	X	695	G
29	X	699	G
29	X	712	A
29	X	714	G
29	X	727	U
29	X	728	G
29	X	729	A
29	X	730	C
29	X	731	A
29	X	732	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
29	X	739	G
29	X	740	A
29	X	741	G
29	X	743	A
29	X	754	G
29	X	758	G
29	X	760	U
29	X	765	C
29	X	773	G
29	X	776	G
29	X	778	G
29	X	787	A
29	X	789	G
29	X	790	A
29	X	795	A
29	X	797	A
29	X	798	G
29	X	805	G
29	X	807	A
29	X	815	A
29	X	816	U
29	X	818	G
29	X	821	A
29	X	824	U
29	X	825	C
29	X	831	G
29	X	832	A
29	X	834	A
29	X	836	G
29	X	838	A
29	X	840	U
29	X	841	G
29	X	848	A
29	X	851	C
29	X	852	U
29	X	857	U
29	X	858	G
29	X	859	U
29	X	869	C
29	X	872	G
29	X	879	A
29	X	880	C

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
29	X	912	A
29	X	914	C
29	X	922	A
29	X	924	C
29	X	926	C
29	X	927	C
29	X	931	G
29	X	937	C
29	X	939	C
29	X	940	G
29	X	943	U
29	X	946	U
29	X	947	C
29	X	950	G
29	X	955	G
29	X	956	A
29	X	957	G
29	X	964	A
29	X	967	G
29	X	969	U
29	X	972	C
29	X	975	C
29	X	976	C
29	X	982	C
29	X	984	A
29	X	985	G
29	X	992	A
29	X	994	A
29	X	1001	A
29	X	1005	U
29	X	1007	A
29	X	1013	G
29	X	1015	U
29	X	1016	C
29	X	1017	C
29	X	1018	C
29	X	1020	A
29	X	1022	A
29	X	1023	U
29	X	1024	G
29	X	1028	G
29	X	1029	C

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
29	X	1033	G
29	X	1034	U
29	X	1036	G
29	X	1037	U
29	X	1044	U
29	X	1047	G
29	X	1055	A
29	X	1056	U
29	X	1058	G
29	X	1059	A
29	X	1060	C
29	X	1061	A
29	X	1066	G
29	X	1068	A
29	X	1069	G
29	X	1071	U
29	X	1072	U
29	X	1079	G
29	X	1080	A
29	X	1081	A
29	X	1082	G
29	X	1084	A
29	X	1086	C
29	X	1089	C
29	X	1096	A
29	X	1097	A
29	X	1098	G
29	X	1099	A
29	X	1100	G
29	X	1101	U
29	X	1102	G
29	X	1104	G
29	X	1107	A
29	X	1108	U
29	X	1111	C
29	X	1112	U
29	X	1113	C
29	X	1114	A
29	X	1119	U
29	X	1120	C
29	X	1121	G
29	X	1122	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
29	X	1123	G
29	X	1124	U
29	X	1128	G
29	X	1137	A
29	X	1138	A
29	X	1139	A
29	X	1140	A
29	X	1141	U
29	X	1142	G
29	X	1143	A
29	X	1145	C
29	X	1146	G
29	X	1149	G
29	X	1151	U
29	X	1152	C
29	X	1153	A
29	X	1154	A
29	X	1158	A
29	X	1162	A
29	X	1165	G
29	X	1166	A
29	X	1168	G
29	X	1178	C
29	X	1179	A
29	X	1185	C
29	X	1187	A
29	X	1189	G
29	X	1195	U
29	X	1199	U
29	X	1200	G
29	X	1209	G
29	X	1218	C
29	X	1220	G
29	X	1223	G
29	X	1225	G
29	X	1226	A
29	X	1233	A
29	X	1235	C
29	X	1236	G
29	X	1238	A
29	X	1240	G
29	X	1246	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
29	X	1247	U
29	X	1250	A
29	X	1255	A
29	X	1256	C
29	X	1261	G
29	X	1266	G
29	X	1269	G
29	X	1271	C
29	X	1275	A
29	X	1277	G
29	X	1280	U
29	X	1281	A
29	X	1284	G
29	X	1285	A
29	X	1286	U
29	X	1288	A
29	X	1290	A
29	X	1291	G
29	X	1299	A
29	X	1302	C
29	X	1307	U
29	X	1313	U
29	X	1314	A
29	X	1322	G
29	X	1326	U
29	X	1331	G
29	X	1334	A
29	X	1342	U
29	X	1346	C
29	X	1347	C
29	X	1351	G
29	X	1354	A
29	X	1359	G
29	X	1365	U
29	X	1370	U
29	X	1378	A
29	X	1381	G
29	X	1391	A
29	X	1392	U
29	X	1393	G
29	X	1395	A
29	X	1398	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
29	X	1403	U
29	X	1404	C
29	X	1408	A
29	X	1409	U
29	X	1425	G
29	X	1427	G
29	X	1428	G
29	X	1433	A
29	X	1435	G
29	X	1442	C
29	X	1454	U
29	X	1459	U
29	X	1460	G
29	X	1468	A
29	X	1469	U
29	X	1470	G
29	X	1475	U
29	X	1490	U
29	X	1498	G
29	X	1505	U
29	X	1506	C
29	X	1507	A
29	X	1512	A
29	X	1517	C
29	X	1518	C
29	X	1522	C
29	X	1523	A
29	X	1524	C
29	X	1525	A
29	X	1527	G
29	X	1541	G
29	X	1543	G
29	X	1544	A
29	X	1545	G
29	X	1552	C
29	X	1553	G
29	X	1562	G
29	X	1563	U
29	X	1564	U
29	X	1574	A
29	X	1575	C
29	X	1582	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
29	X	1585	A
29	X	1586	A
29	X	1601	U
29	X	1602	G
29	X	1603	A
29	X	1616	C
29	X	1618	U
29	X	1619	A
29	X	1622	G
29	X	1624	A
29	X	1625	A
29	X	1626	A
29	X	1628	C
29	X	1631	C
29	X	1643	A
29	X	1651	U
29	X	1653	C
29	X	1656	U
29	X	1662	G
29	X	1663	C
29	X	1665	C
29	X	1666	G
29	X	1668	G
29	X	1669	A
29	X	1670	G
29	X	1677	C
29	X	1678	G
29	X	1680	U
29	X	1688	U
29	X	1690	U
29	X	1691	G
29	X	1692	C
29	X	1696	C
29	X	1697	U
29	X	1699	A
29	X	1707	A
29	X	1711	C
29	X	1714	A
29	X	1717	A
29	X	1718	A
29	X	1722	G
29	X	1733	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
29	X	1734	C
29	X	1735	G
29	X	1741	G
29	X	1747	G
29	X	1749	G
29	X	1750	A
29	X	1751	A
29	X	1755	G
29	X	1760	G
29	X	1764	A
29	X	1766	U
29	X	1772	C
29	X	1775	A
29	X	1776	A
29	X	1777	A
29	X	1778	U
29	X	1779	C
29	X	1782	A
29	X	1788	C
29	X	1791	C
29	X	1799	A
29	X	1800	A
29	X	1808	C
29	X	1811	A
29	X	1812	U
29	X	1819	U
29	X	1821	A
29	X	1825	C
29	X	1829	C
29	X	1846	A
29	X	1849	G
29	X	1854	G
29	X	1859	A
29	X	1867	A
29	X	1869	A
29	X	1872	A
29	X	1875	C
29	X	1883	A
29	X	1884	A
29	X	1886	G
29	X	1889	G
29	X	1890	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
29	X	1891	C
29	X	1893	G
29	X	1896	A
29	X	1898	U
29	X	1900	U
29	X	1904	G
29	X	1906	U
29	X	1907	C
29	X	1909	U
29	X	1910	A
29	X	1913	G
29	X	1914	U
29	X	1918	G
29	X	1919	A
29	X	1920	A
29	X	1921	A
29	X	1923	U
29	X	1924	C
29	X	1926	U
29	X	1927	U
29	X	1928	G
29	X	1938	U
29	X	1949	A
29	X	1950	C
29	X	1953	A
29	X	1955	G
29	X	1975	G
29	X	1976	U
29	X	1979	C
29	X	1980	A
29	X	1995	G
29	X	1999	U
29	X	2001	G
29	X	2004	U
29	X	2006	G
29	X	2009	U
29	X	2014	A
29	X	2018	G
29	X	2026	C
29	X	2028	C
29	X	2029	G
29	X	2032	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
29	X	2033	C
29	X	2034	A
29	X	2038	C
29	X	2039	G
29	X	2043	A
29	X	2044	G
29	X	2045	A
29	X	2047	C
29	X	2052	G
29	X	2058	U
29	X	2059	U
29	X	2063	A
29	X	2074	U
29	X	2075	U
29	X	2076	G
29	X	2091	C
29	X	2093	G
29	X	2094	C
29	X	2097	A
29	X	2099	G
29	X	2100	A
29	X	2101	U
29	X	2103	G
29	X	2104	G
29	X	2107	G
29	X	2108	G
29	X	2110	G
29	X	2111	C
29	X	2115	C
29	X	2116	G
29	X	2117	A
29	X	2118	A
29	X	2120	C
29	X	2122	G
29	X	2123	G
29	X	2124	C
29	X	2126	U
29	X	2127	U
29	X	2128	U
29	X	2129	U
29	X	2131	G
29	X	2135	C

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
29	X	2141	A
29	X	2142	G
29	X	2147	C
29	X	2152	A
29	X	2153	A
29	X	2154	A
29	X	2156	A
29	X	2157	C
29	X	2158	C
29	X	2162	C
29	X	2164	G
29	X	2171	U
29	X	2173	G
29	X	2180	U
29	X	2181	A
29	X	2182	A
29	X	2188	A
29	X	2189	A
29	X	2190	A
29	X	2191	A
29	X	2192	U
29	X	2193	C
29	X	2196	U
29	X	2199	C
29	X	2200	G
29	X	2204	A
29	X	2206	C
29	X	2217	G
29	X	2228	U
29	X	2230	G
29	X	2234	G
29	X	2243	C
29	X	2247	A
29	X	2252	A
29	X	2262	C
29	X	2266	A
29	X	2267	A
29	X	2268	G
29	X	2269	G
29	X	2278	A
29	X	2283	G
29	X	2284	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
29	X	2285	U
29	X	2286	G
29	X	2287	G
29	X	2288	A
29	X	2290	A
29	X	2298	U
29	X	2300	G
29	X	2301	A
29	X	2303	C
29	X	2304	G
29	X	2305	C
29	X	2306	A
29	X	2312	A
29	X	2313	G
29	X	2314	A
29	X	2315	A
29	X	2319	G
29	X	2324	G
29	X	2326	C
29	X	2327	U
29	X	2329	C
29	X	2333	A
29	X	2335	U
29	X	2355	A
29	X	2357	A
29	X	2358	C
29	X	2361	G
29	X	2362	G
29	X	2363	G
29	X	2364	C
29	X	2368	G
29	X	2369	U
29	X	2375	G
29	X	2379	G
29	X	2386	G
29	X	2389	G
29	X	2398	U
29	X	2399	C
29	X	2402	U
29	X	2407	G
29	X	2408	G
29	X	2409	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
29	X	2410	U
29	X	2418	A
29	X	2419	C
29	X	2420	C
29	X	2424	G
29	X	2426	G
29	X	2427	A
29	X	2428	U
29	X	2431	C
29	X	2432	A
29	X	2438	A
29	X	2441	U
29	X	2447	G
29	X	2448	A
29	X	2452	U
29	X	2453	C
29	X	2455	A
29	X	2457	A
29	X	2458	U
29	X	2461	G
29	X	2463	G
29	X	2466	G
29	X	2468	G
29	X	2470	U
29	X	2471	U
29	X	2473	G
29	X	2477	C
29	X	2478	C
29	X	2479	U
29	X	2481	G
29	X	2482	A
29	X	2484	G
29	X	2486	C
29	X	2492	G
29	X	2494	C
29	X	2497	A
29	X	2501	U
29	X	2504	G
29	X	2516	U
29	X	2521	A
29	X	2522	G
29	X	2533	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
29	X	2538	C
29	X	2545	A
29	X	2546	G
29	X	2550	C
29	X	2551	A
29	X	2552	C
29	X	2557	G
29	X	2559	U
29	X	2560	G
29	X	2564	U
29	X	2565	C
29	X	2571	G
29	X	2579	A
29	X	2581	A
29	X	2582	G
29	X	2589	C
29	X	2590	U
29	X	2591	C
29	X	2594	U
29	X	2600	A
29	X	2609	G
29	X	2613	A
29	X	2617	G
29	X	2625	U
29	X	2633	A
29	X	2639	A
29	X	2640	G
29	X	2642	G
29	X	2643	G
29	X	2651	U
29	X	2653	A
29	X	2657	G
29	X	2661	G
29	X	2663	U
29	X	2666	U
29	X	2668	U
29	X	2674	C
29	X	2678	C
29	X	2687	G
29	X	2691	C
29	X	2692	A
29	X	2693	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
29	X	2694	G
29	X	2698	G
29	X	2701	A
29	X	2702	G
29	X	2703	C
29	X	2706	U
29	X	2713	A
29	X	2718	A
29	X	2719	U
29	X	2724	G
29	X	2728	A
29	X	2732	C
29	X	2737	A
29	X	2743	G
29	X	2744	A
29	X	2745	A
29	X	2746	G
29	X	2751	C
29	X	2758	A
29	X	2759	U
29	X	2760	G
29	X	2769	C
29	X	2771	C
29	X	2774	U
29	X	2775	U
29	X	2777	A
29	X	2778	U
29	X	2779	C
29	X	2780	A
29	X	2791	C
29	X	2793	G
29	X	2795	A
29	X	2796	A
29	X	2797	G
29	X	2800	C
29	X	2808	U
29	X	2809	A
29	X	2810	A
29	X	2811	G
29	X	2815	C
29	X	2823	G
29	X	2824	C

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
29	X	2832	G
29	X	2836	U
29	X	2847	G
29	X	2848	A
29	X	2849	C
29	X	2851	G
29	X	2854	G
29	X	2861	A
29	X	2862	G
29	X	2865	G
29	X	2866	A
29	X	2867	G
29	X	2868	G
29	X	2869	U
30	Y	11	G
30	Y	14	C
30	Y	15	A
30	Y	16	U
30	Y	17	A
30	Y	20	A
30	Y	27	A
30	Y	28	A
30	Y	29	C
30	Y	37	C
30	Y	39	C
30	Y	40	C
30	Y	43	G
30	Y	44	C
30	Y	46	G
30	Y	47	A
30	Y	49	C
30	Y	51	G
30	Y	52	G
30	Y	53	G
30	Y	55	C
30	Y	59	A
30	Y	63	A
30	Y	70	C
30	Y	75	A
30	Y	76	U
30	Y	86	A
30	Y	99	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
30	Y	108	G
30	Y	112	A
30	Y	114	C
30	Y	115	G
30	Y	121	G
30	Y	122	U
30	Y	123	U

All (31) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
29	X	459	A
29	X	465	C
29	X	475	U
29	X	511	A
29	X	518	A
29	X	654	A
29	X	655	A
29	X	813	A
29	X	939	C
29	X	940	G
29	X	1000	G
29	X	1123	G
29	X	1138	A
29	X	1225	G
29	X	1506	C
29	X	1526	U
29	X	1601	U
29	X	1602	G
29	X	1690	U
29	X	1715	A
29	X	1777	A
29	X	2044	G
29	X	2228	U
29	X	2550	C
29	X	2551	A
29	X	2592	U
29	X	2736	U
29	X	2758	A
29	X	2823	G
29	X	2854	G
30	Y	16	U

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 187 ligands modelled in this entry, 186 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$
32	HGR	X	6178	-	39,39,39	1.81	7 (17%)	50,58,58	1.72	9 (18%)

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
32	HGR	X	6178	-	-	4/20/79/79	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	X	6178	HGR	C5-C6	-4.19	1.42	1.50
32	X	6178	HGR	C1-C6	4.15	1.41	1.35
32	X	6178	HGR	C12-C14	4.14	1.43	1.33
32	X	6178	HGR	C12-C6	3.87	1.55	1.44
32	X	6178	HGR	C3-C2	-3.78	1.41	1.48
32	X	6178	HGR	C5-C4	-3.34	1.43	1.49
32	X	6178	HGR	C17-N1	2.12	1.49	1.45

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	X	6178	HGR	C10-O3-C3	4.73	126.09	115.36
32	X	6178	HGR	C4-C5-C6	4.24	121.49	112.36
32	X	6178	HGR	C23-O8-C18	-4.00	100.22	106.31
32	X	6178	HGR	C4-C3-C2	-3.98	118.17	121.83
32	X	6178	HGR	O3-C3-C2	3.09	118.43	112.56
32	X	6178	HGR	O1-C10-C9	-2.72	101.47	104.98
32	X	6178	HGR	O10-C19-C17	2.58	114.88	109.66
32	X	6178	HGR	C1-C2-C3	2.52	120.84	115.99
32	X	6178	HGR	C5-C6-C1	-2.46	116.95	121.34

There are no chirality outliers.

All (4) torsion outliers are listed below:

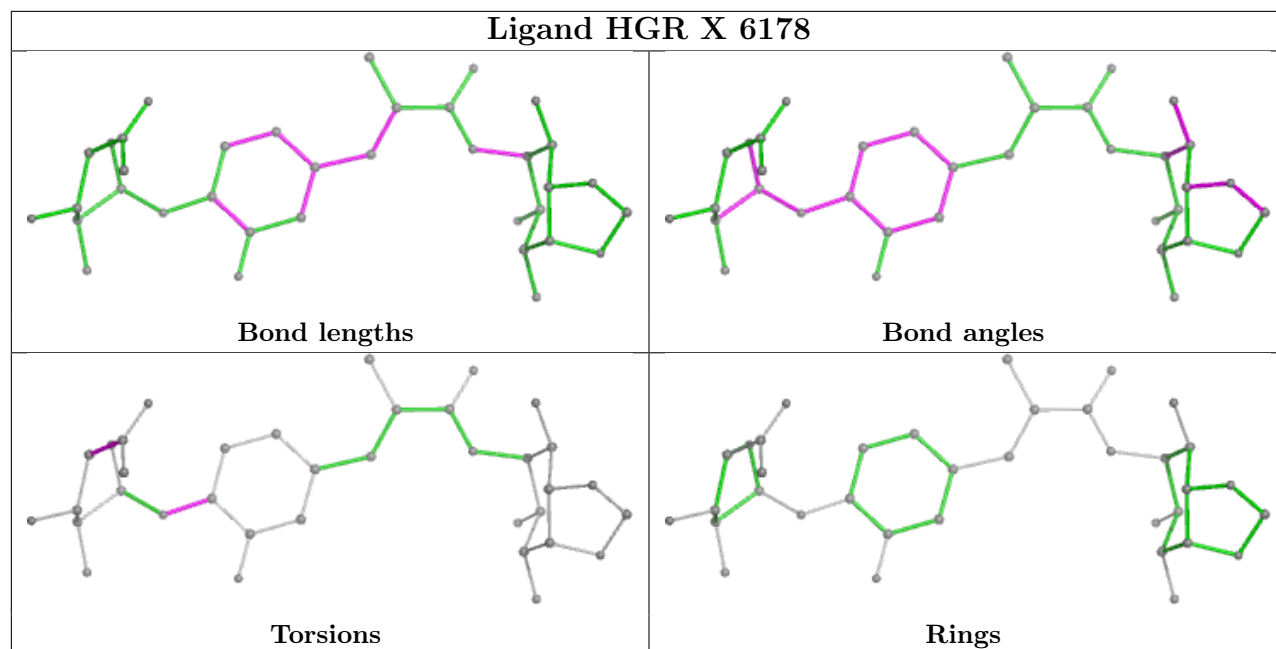
Mol	Chain	Res	Type	Atoms
32	X	6178	HGR	C2-C3-O3-C10
32	X	6178	HGR	C13-C11-C7-O1
32	X	6178	HGR	C13-C11-C7-C8
32	X	6178	HGR	O6-C11-C7-C8

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	X	6178	HGR	2	0

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



## 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	0	224/224 (100%)	1.56	64 (28%) 1 2	291, 311, 319, 322	0
2	A	274/274 (100%)	1.54	88 (32%) 1 1	108, 151, 172, 185	0
3	B	205/205 (100%)	1.04	31 (15%) 6 4	67, 102, 129, 146	0
4	C	197/197 (100%)	0.95	24 (12%) 10 6	93, 133, 158, 177	0
5	D	177/177 (100%)	1.00	30 (16%) 5 3	165, 183, 200, 214	0
6	E	171/171 (100%)	0.84	19 (11%) 12 7	116, 167, 191, 198	0
7	F	144/144 (100%)	1.26	32 (22%) 3 2	233, 259, 275, 281	0
8	G	142/142 (100%)	0.93	19 (13%) 8 5	87, 125, 139, 169	0
9	H	134/134 (100%)	0.87	14 (10%) 13 7	70, 92, 108, 118	0
10	I	141/141 (100%)	1.86	59 (41%) 1 1	98, 150, 173, 182	0
11	J	136/136 (100%)	1.61	41 (30%) 1 1	107, 126, 156, 159	0
12	K	113/113 (100%)	1.19	21 (18%) 4 3	63, 82, 95, 99	0
13	L	104/104 (100%)	2.01	43 (41%) 1 1	126, 147, 162, 173	0
14	M	109/109 (100%)	0.84	14 (12%) 9 5	72, 89, 117, 147	0
15	N	117/117 (100%)	1.17	25 (21%) 3 2	90, 118, 144, 153	0
16	O	94/94 (100%)	0.92	14 (14%) 7 4	103, 129, 156, 173	0
17	P	127/127 (100%)	0.85	18 (14%) 7 4	81, 96, 120, 180	0
18	Q	93/93 (100%)	1.19	13 (13%) 7 4	108, 137, 160, 176	0
19	R	110/110 (100%)	1.14	23 (20%) 3 2	111, 131, 166, 180	0
20	S	175/175 (100%)	0.99	18 (10%) 13 8	134, 167, 185, 193	0
21	T	84/84 (100%)	1.74	29 (34%) 1 1	111, 130, 148, 171	0
22	U	72/72 (100%)	2.80	42 (58%) 0 0	134, 163, 177, 182	0
23	V	66/66 (100%)	1.84	23 (34%) 1 1	147, 163, 190, 201	0
24	W	55/55 (100%)	1.02	7 (12%) 9 5	112, 124, 142, 157	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	Z	57/57 (100%)	0.95	10 (17%) 5 3	82, 97, 120, 130	0
26	1	54/54 (100%)	1.87	21 (38%) 1 1	140, 153, 179, 189	0
27	2	47/47 (100%)	1.74	19 (40%) 1 1	108, 121, 132, 134	0
28	3	65/65 (100%)	2.25	29 (44%) 1 1	115, 132, 143, 153	0
29	X	2780/2881 (96%)	0.65	228 (8%) 19 10	59, 127, 241, 397	0
30	Y	122/122 (100%)	0.69	10 (8%) 19 10	110, 157, 182, 203	0
All	All	6389/6490 (98%)	1.00	1028 (16%) 5 4	59, 134, 276, 397	0

All (1028) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
29	X	2116	G	12.4
22	U	27	ASP	10.7
29	X	2127	U	10.4
13	L	12	ARG	10.0
30	Y	43	G	9.8
22	U	8	THR	9.2
29	X	731	A	9.1
29	X	730	C	8.6
22	U	13	LEU	8.4
20	S	74	ARG	8.2
23	V	3	PRO	7.9
11	J	21	ASP	7.8
29	X	2125	C	7.5
29	X	2115	C	7.5
1	0	159	PHE	7.5
1	0	162	ASP	7.5
23	V	2	LYS	7.4
13	L	34	SER	7.2
5	D	81	GLN	7.2
21	T	2	ALA	7.2
30	Y	123	U	7.1
2	A	265	THR	7.0
10	I	74	VAL	7.0
13	L	9	ARG	6.9
13	L	94	TYR	6.9
10	I	67	ASN	6.9
10	I	69	GLY	6.9
10	I	103	ASN	6.9
13	L	36	LYS	6.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
10	I	33	GLY	6.8
13	L	93	SER	6.8
22	U	26	ALA	6.8
3	B	205	SER	6.7
13	L	8	ARG	6.6
15	N	48	ARG	6.5
23	V	6	MET	6.5
22	U	16	ASN	6.4
11	J	99	LYS	6.4
18	Q	32	LYS	6.4
11	J	22	ALA	6.3
12	K	69	ASP	6.3
10	I	68	VAL	6.3
11	J	100	PRO	6.3
1	O	158	GLU	6.2
4	C	88	PRO	6.1
12	K	22	ARG	6.1
22	U	25	ARG	6.1
20	S	15	ASP	6.0
2	A	32	ALA	6.0
29	X	1086	C	6.0
2	A	255	LYS	6.0
5	D	72	LYS	6.0
1	O	163	LYS	6.0
2	A	35	GLU	5.9
6	E	173	ALA	5.9
22	U	15	VAL	5.9
29	X	1901	A	5.8
20	S	75	LYS	5.8
29	X	1900	U	5.8
20	S	68	ALA	5.8
2	A	231	HIS	5.8
18	Q	62	ARG	5.8
2	A	241	GLY	5.8
20	S	73	LYS	5.7
29	X	2133	G	5.7
11	J	37	ALA	5.7
29	X	1085	G	5.7
2	A	51	SER	5.7
11	J	16	GLY	5.6
29	X	834	A	5.6
28	3	23	MET	5.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
29	X	2120	C	5.6
7	F	115	LEU	5.6
10	I	79	GLN	5.6
29	X	1139	A	5.6
13	L	31	VAL	5.6
29	X	2092	U	5.6
15	N	20	ARG	5.6
14	M	99	VAL	5.6
28	3	37	SER	5.5
16	O	5	ILE	5.5
29	X	2126	U	5.5
29	X	2121	U	5.5
29	X	1902	A	5.4
26	1	23	THR	5.4
13	L	24	SER	5.4
29	X	2776	U	5.4
22	U	12	ASN	5.4
2	A	223	GLY	5.3
2	A	36	ALA	5.3
29	X	1897	C	5.3
21	T	3	HIS	5.3
22	U	28	GLY	5.3
29	X	1090	C	5.2
29	X	1102	G	5.2
10	I	45	LYS	5.2
20	S	92	VAL	5.2
14	M	53	VAL	5.2
12	K	7	GLY	5.2
20	S	72	ASP	5.1
13	L	53	ALA	5.1
2	A	268	ARG	5.1
29	X	2274	C	5.1
16	O	74	TYR	5.1
4	C	91	TYR	5.1
19	R	43	ASP	5.1
10	I	75	VAL	5.1
15	N	53	LYS	5.1
16	O	81	ARG	5.0
28	3	46	LYS	5.0
22	U	51	ILE	5.0
28	3	54	GLU	5.0
18	Q	8	GLN	5.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
11	J	98	VAL	5.0
13	L	33	ARG	5.0
13	L	40	ALA	4.9
29	X	2114	G	4.9
4	C	38	ARG	4.9
10	I	66	ASN	4.9
13	L	20	THR	4.9
29	X	1525	A	4.9
11	J	97	VAL	4.9
26	1	53	ALA	4.9
29	X	1187	A	4.8
11	J	23	LYS	4.8
29	X	1552	C	4.8
29	X	728	G	4.8
11	J	20	GLY	4.8
29	X	2275	U	4.8
28	3	64	ARG	4.8
29	X	1899	A	4.7
19	R	4	PRO	4.7
2	A	237	GLU	4.7
29	X	2128	U	4.7
29	X	1101	U	4.7
10	I	37	GLN	4.7
2	A	55	GLY	4.7
22	U	52	ARG	4.7
28	3	12	ARG	4.7
29	X	2103	G	4.6
26	1	22	TYR	4.6
2	A	239	ARG	4.6
28	3	11	LYS	4.6
23	V	1	MET	4.6
29	X	2124	C	4.6
1	0	218	ILE	4.6
21	T	5	LYS	4.6
1	0	169	ALA	4.6
29	X	1922	U	4.6
29	X	1524	C	4.5
29	X	1089	C	4.5
21	T	74	LYS	4.5
19	R	12	ASP	4.4
1	0	54	VAL	4.4
5	D	103	LEU	4.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
7	F	23	VAL	4.4
29	X	2777	A	4.4
29	X	1797	C	4.4
22	U	40	ARG	4.4
2	A	71	ASP	4.4
1	0	43	LEU	4.4
8	G	99	VAL	4.4
30	Y	42	U	4.4
11	J	101	GLY	4.4
2	A	104	TYR	4.3
2	A	254	THR	4.3
15	N	57	PHE	4.3
22	U	47	HIS	4.3
20	S	93	GLU	4.3
24	W	15	ASN	4.3
2	A	251	GLY	4.3
1	0	25	VAL	4.2
4	C	2	ALA	4.2
14	M	106	TYR	4.2
21	T	24	LYS	4.2
12	K	68	GLN	4.2
23	V	4	SER	4.2
22	U	46	LEU	4.2
10	I	44	GLY	4.2
29	X	2109	A	4.1
29	X	2385	U	4.1
10	I	50	GLU	4.1
21	T	76	ALA	4.1
11	J	48	ILE	4.1
3	B	54	LYS	4.1
11	J	26	ASP	4.1
22	U	30	VAL	4.1
26	1	33	ALA	4.1
28	3	32	GLN	4.1
26	1	9	ILE	4.1
10	I	38	LYS	4.1
29	X	1753	A	4.1
7	F	18	THR	4.1
6	E	172	LYS	4.1
16	O	83	ARG	4.1
29	X	1189	G	4.1
25	Z	42	SER	4.1

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
29	X	833	A	4.1
29	X	984	A	4.0
22	U	43	ARG	4.0
5	D	3	GLN	4.0
11	J	131	LYS	4.0
16	O	73	LYS	4.0
22	U	34	THR	4.0
29	X	2117	A	4.0
22	U	10	LYS	4.0
29	X	1103	C	4.0
22	U	75	TYR	3.9
15	N	21	ALA	3.9
18	Q	9	ALA	3.9
2	A	226	MET	3.9
21	T	15	ASP	3.9
14	M	104	LEU	3.9
2	A	64	ILE	3.9
28	3	45	GLY	3.9
26	1	26	LYS	3.9
1	0	195	ALA	3.8
13	L	10	LYS	3.8
29	X	1920	A	3.8
21	T	75	GLY	3.8
11	J	117	GLU	3.8
27	2	47	GLU	3.8
2	A	61	LEU	3.8
29	X	1114	A	3.8
2	A	262	LYS	3.8
16	O	80	TYR	3.8
28	3	66	LYS	3.8
16	O	72	ARG	3.8
18	Q	37	GLU	3.8
29	X	2104	G	3.8
2	A	60	ARG	3.8
2	A	242	ALA	3.8
2	A	267	ASP	3.8
29	X	2774	U	3.8
4	C	41	GLY	3.8
9	H	11	ALA	3.8
13	L	30	SER	3.7
15	N	39	LEU	3.7
10	I	101	ARG	3.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
19	R	42	ARG	3.7
29	X	1523	A	3.7
29	X	2015	G	3.7
7	F	123	ALA	3.7
5	D	99	PHE	3.7
17	P	8	PHE	3.7
6	E	168	GLN	3.7
2	A	238	GLY	3.7
7	F	24	GLY	3.7
25	Z	56	GLN	3.7
2	A	250	TRP	3.7
6	E	111	HIS	3.7
29	X	2108	G	3.7
29	X	715	U	3.6
13	L	96	TYR	3.6
20	S	69	VAL	3.6
29	X	774	A	3.6
2	A	56	GLY	3.6
14	M	30	GLY	3.6
21	T	73	GLY	3.6
1	0	205	LEU	3.6
2	A	222	ARG	3.6
23	V	7	ARG	3.6
29	X	601	A	3.6
12	K	43	GLU	3.6
2	A	259	THR	3.6
28	3	6	THR	3.6
22	U	42	GLN	3.6
12	K	15	SER	3.6
10	I	104	ARG	3.6
29	X	1138	A	3.6
1	0	171	ILE	3.6
5	D	67	ILE	3.6
3	B	118	LYS	3.6
22	U	23	LYS	3.6
11	J	139	ASP	3.6
10	I	31	GLY	3.6
10	I	46	GLY	3.6
5	D	32	GLU	3.6
28	3	63	PRO	3.6
22	U	29	GLY	3.5
10	I	48	PHE	3.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
11	J	96	SER	3.5
27	2	10	ARG	3.5
26	1	1	ALA	3.5
26	1	5	ALA	3.5
29	X	436	A	3.5
29	X	2119	A	3.5
29	X	1037	U	3.5
29	X	2129	U	3.5
28	3	36	LYS	3.5
29	X	2049	C	3.5
28	3	65	GLY	3.5
28	3	3	LYS	3.5
28	3	16	ILE	3.5
2	A	266	SER	3.5
18	Q	2	SER	3.5
16	O	70	TYR	3.5
27	2	29	ASN	3.5
2	A	106	LEU	3.5
1	0	166	VAL	3.5
16	O	79	GLN	3.5
30	Y	2	C	3.5
22	U	62	LEU	3.5
29	X	2313	G	3.5
2	A	68	LYS	3.5
2	A	230	ASP	3.5
22	U	44	ALA	3.4
22	U	45	ASN	3.4
26	1	0	ALA	3.4
1	0	37	VAL	3.4
13	L	89	PHE	3.4
15	N	49	ASP	3.4
13	L	55	SER	3.4
12	K	18	VAL	3.4
26	1	11	LYS	3.4
26	1	28	ARG	3.4
29	X	1409	U	3.4
29	X	2152	A	3.4
29	X	2153	A	3.4
19	R	15	HIS	3.4
23	V	59	GLU	3.4
11	J	18	MET	3.4
10	I	71	THR	3.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	A	65	ILE	3.4
3	B	137	ARG	3.4
29	X	1319	C	3.4
10	I	58	ALA	3.4
1	0	39	VAL	3.4
13	L	17	VAL	3.4
29	X	2132	G	3.4
3	B	133	LYS	3.4
13	L	95	LYS	3.4
4	C	31	VAL	3.4
11	J	40	PRO	3.4
2	A	57	GLY	3.4
2	A	217	ARG	3.4
1	0	170	PRO	3.3
6	E	5	GLY	3.3
19	R	14	LEU	3.3
29	X	1921	A	3.3
29	X	2045	A	3.3
29	X	2733	A	3.3
7	F	77	LEU	3.3
29	X	727	U	3.3
3	B	76	ARG	3.3
9	H	127	VAL	3.3
23	V	30	PHE	3.3
15	N	2	PRO	3.3
2	A	220	HIS	3.3
12	K	3	HIS	3.3
21	T	20	TYR	3.3
8	G	168	THR	3.3
9	H	43	ARG	3.3
27	2	1	MET	3.3
29	X	2557	G	3.3
29	X	1526	U	3.3
11	J	36	ILE	3.3
2	A	215	LEU	3.3
29	X	1188	A	3.3
4	C	147	LYS	3.3
6	E	175	LYS	3.3
3	B	136	ARG	3.3
1	0	5	ALA	3.3
29	X	1551	U	3.3
6	E	60	LYS	3.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
29	X	1091	C	3.2
2	A	261	ARG	3.2
3	B	165	VAL	3.2
12	K	23	ALA	3.2
5	D	31	ILE	3.2
22	U	63	SER	3.2
27	2	22	MET	3.2
29	X	1808	C	3.2
30	Y	62	C	3.2
14	M	54	VAL	3.2
3	B	123	ALA	3.2
1	0	47	PRO	3.2
4	C	19	LEU	3.2
16	O	41	GLY	3.2
15	N	34	ASN	3.2
19	R	11	ASN	3.2
11	J	38	MET	3.2
22	U	14	VAL	3.2
2	A	252	LYS	3.2
6	E	64	LEU	3.2
29	X	2161	C	3.2
29	X	843	G	3.2
2	A	224	SER	3.2
2	A	211	ARG	3.2
2	A	213	ARG	3.2
21	T	77	ARG	3.2
2	A	62	TYR	3.2
5	D	173	MET	3.2
2	A	31	LYS	3.2
13	L	16	LYS	3.2
1	0	210	LEU	3.2
26	1	21	TYR	3.2
4	C	196	VAL	3.2
11	J	119	PHE	3.2
11	J	17	ARG	3.1
12	K	14	SER	3.1
3	B	163	GLU	3.1
10	I	102	LYS	3.1
3	B	52	ALA	3.1
29	X	2091	C	3.1
1	0	160	ARG	3.1
28	3	20	GLY	3.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
10	I	15	ASP	3.1
6	E	17	VAL	3.1
23	V	57	LYS	3.1
1	0	132	LEU	3.1
7	F	113	PRO	3.1
29	X	2314	A	3.1
29	X	222	G	3.1
29	X	2099	G	3.1
3	B	204	ALA	3.1
22	U	21	ARG	3.1
2	A	216	GLY	3.1
15	N	5	LYS	3.1
13	L	87	VAL	3.1
7	F	99	LEU	3.1
23	V	37	LEU	3.1
17	P	98	ASP	3.1
10	I	13	ARG	3.1
13	L	14	ARG	3.1
21	T	55	ARG	3.1
7	F	125	ASN	3.1
2	A	253	PRO	3.1
20	S	87	THR	3.1
29	X	413	G	3.1
29	X	424	G	3.1
19	R	13	LYS	3.1
7	F	68	ILE	3.1
11	J	102	ARG	3.1
29	X	1252	C	3.1
13	L	81	GLU	3.0
8	G	35	LYS	3.0
21	T	44	LYS	3.0
27	2	25	LYS	3.0
13	L	27	LEU	3.0
2	A	43	ARG	3.0
29	X	1798	G	3.0
10	I	72	TYR	3.0
1	0	9	LYS	3.0
5	D	71	LYS	3.0
22	U	11	LYS	3.0
10	I	36	GLY	3.0
10	I	54	SER	3.0
29	X	1801	C	3.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
12	K	29	LEU	3.0
2	A	53	PHE	3.0
12	K	71	HIS	3.0
12	K	9	LYS	3.0
29	X	983	G	3.0
29	X	2687	G	3.0
2	A	229	VAL	3.0
11	J	19	THR	3.0
15	N	52	ASN	3.0
22	U	18	VAL	3.0
14	M	28	ARG	3.0
29	X	2779	C	3.0
1	0	157	ILE	3.0
3	B	159	HIS	3.0
29	X	1434	U	3.0
29	X	1676	U	3.0
5	D	143	TYR	3.0
8	G	37	ASP	3.0
29	X	1734	C	3.0
29	X	1671	A	3.0
1	0	147	GLY	3.0
28	3	40	GLU	3.0
29	X	1923	U	3.0
29	X	2105	U	3.0
7	F	127	VAL	3.0
13	L	11	LEU	3.0
28	3	4	MET	2.9
29	X	1063	C	2.9
29	X	123	A	2.9
29	X	248	A	2.9
29	X	407	A	2.9
29	X	846	A	2.9
29	X	2004	U	2.9
29	X	2590	U	2.9
19	R	21	THR	2.9
19	R	79	SER	2.9
27	2	23	LYS	2.9
1	0	131	GLY	2.9
6	E	112	PRO	2.9
10	I	76	LYS	2.9
29	X	778	G	2.9
29	X	1223	G	2.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
30	Y	9	G	2.9
10	I	59	ARG	2.9
1	O	155	GLY	2.9
9	H	44	TYR	2.9
21	T	22	GLY	2.9
11	J	106	GLU	2.9
7	F	126	THR	2.9
27	2	15	THR	2.9
1	O	69	ARG	2.9
9	H	26	ASN	2.9
29	X	2249	U	2.9
29	X	2326	C	2.9
9	H	1	MET	2.9
28	3	60	LEU	2.9
3	B	125	GLY	2.9
11	J	103	VAL	2.9
4	C	20	PRO	2.9
2	A	59	LYS	2.9
10	I	35	LYS	2.9
5	D	74	ILE	2.9
1	O	164	THR	2.9
21	T	58	THR	2.9
8	G	97	ASP	2.9
7	F	104	VAL	2.9
8	G	111	LYS	2.9
29	X	729	A	2.9
10	I	70	THR	2.8
2	A	33	LEU	2.8
19	R	74	LEU	2.8
7	F	21	PRO	2.8
15	N	35	ALA	2.8
13	L	19	THR	2.8
23	V	9	LEU	2.8
19	R	108	VAL	2.8
29	X	1553	G	2.8
10	I	25	GLY	2.8
7	F	52	ILE	2.8
10	I	49	PHE	2.8
1	O	192	LEU	2.8
2	A	245	VAL	2.8
15	N	9	VAL	2.8
21	T	7	VAL	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
6	E	61	HIS	2.8
21	T	56	ASP	2.8
1	0	48	ARG	2.8
11	J	15	ARG	2.8
12	K	19	ALA	2.8
29	X	637	G	2.8
29	X	1222	G	2.8
29	X	2250	G	2.8
13	L	60	LYS	2.8
26	1	34	LYS	2.8
3	B	113	THR	2.8
26	1	24	THR	2.8
4	C	79	GLY	2.8
6	E	174	GLY	2.8
1	0	106	PHE	2.8
8	G	72	PRO	2.8
13	L	15	ARG	2.8
29	X	242	A	2.8
29	X	402	A	2.8
7	F	20	ALA	2.8
13	L	57	ALA	2.8
19	R	75	ALA	2.8
23	V	28	LEU	2.8
26	1	13	GLU	2.8
26	1	12	MET	2.8
29	X	1186	G	2.8
10	I	26	THR	2.8
19	R	68	GLY	2.8
29	X	835	U	2.7
3	B	120	TRP	2.7
2	A	151	LYS	2.7
10	I	62	LYS	2.7
19	R	5	SER	2.7
29	X	972	C	2.7
5	D	101	GLU	2.7
7	F	78	ILE	2.7
3	B	187	ALA	2.7
29	X	2122	G	2.7
1	0	24	LEU	2.7
10	I	80	LEU	2.7
15	N	47	TYR	2.7
21	T	51	VAL	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
29	X	1799	A	2.7
29	X	1954	A	2.7
1	0	42	ARG	2.7
2	A	240	THR	2.7
27	2	24	THR	2.7
1	0	68	VAL	2.7
1	0	161	ASN	2.7
11	J	39	GLU	2.7
5	D	156	ILE	2.7
29	X	2118	A	2.7
29	X	2692	A	2.7
1	0	40	HIS	2.7
23	V	38	ALA	2.7
17	P	106	LEU	2.7
6	E	26	VAL	2.7
2	A	204	ILE	2.7
5	D	154	ILE	2.7
29	X	339	U	2.7
23	V	61	ALA	2.7
29	X	957	G	2.7
1	0	156	ARG	2.7
15	N	12	ARG	2.7
29	X	975	C	2.7
7	F	107	ILE	2.6
1	0	207	SER	2.6
2	A	212	SER	2.6
22	U	9	GLY	2.6
25	Z	59	ALA	2.6
5	D	146	VAL	2.6
8	G	93	LYS	2.6
27	2	14	LYS	2.6
22	U	22	GLY	2.6
1	0	67	SER	2.6
29	X	2670	C	2.6
22	U	65	ASN	2.6
4	C	101	GLN	2.6
7	F	120	VAL	2.6
1	0	209	TYR	2.6
25	Z	3	LYS	2.6
1	0	41	PHE	2.6
2	A	249	PRO	2.6
29	X	514	G	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
29	X	955	G	2.6
1	0	213	THR	2.6
13	L	13	THR	2.6
26	1	31	THR	2.6
5	D	157	VAL	2.6
24	W	40	VAL	2.6
17	P	30	TYR	2.6
1	0	188	LEU	2.6
1	0	108	ALA	2.6
23	V	33	ALA	2.6
10	I	34	HIS	2.6
20	S	67	LYS	2.6
29	X	1285	A	2.6
15	N	25	TRP	2.6
21	T	36	ILE	2.6
29	X	33	C	2.6
27	2	5	TYR	2.6
29	X	578	U	2.6
29	X	1019	U	2.6
21	T	39	ARG	2.6
3	B	131	SER	2.6
7	F	119	SER	2.6
22	U	49	LYS	2.6
26	1	8	ILE	2.5
1	0	28	LEU	2.5
29	X	921	A	2.5
2	A	236	GLY	2.5
10	I	24	GLY	2.5
12	K	4	GLY	2.5
23	V	47	ARG	2.5
29	X	519	C	2.5
10	I	43	ALA	2.5
23	V	5	GLU	2.5
26	1	36	GLU	2.5
29	X	1249	G	2.5
29	X	2093	G	2.5
29	X	2297	G	2.5
18	Q	34	THR	2.5
19	R	8	SER	2.5
10	I	65	PHE	2.5
3	B	155	ARG	2.5
27	2	12	ARG	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
29	X	524	A	2.5
29	X	1796	A	2.5
17	P	18	VAL	2.5
22	U	35	THR	2.5
29	X	768	U	2.5
29	X	26	G	2.5
2	A	52	ARG	2.5
2	A	256	GLY	2.5
11	J	11	ARG	2.5
22	U	36	GLY	2.5
10	I	17	LYS	2.5
9	H	114	VAL	2.5
2	A	37	LEU	2.5
9	H	8	LEU	2.5
21	T	45	PHE	2.5
22	U	17	SER	2.5
29	X	1792	C	2.5
13	L	41	GLN	2.5
2	A	258	LYS	2.5
5	D	49	ALA	2.5
15	N	54	LYS	2.5
18	Q	39	LYS	2.5
10	I	118	VAL	2.5
17	P	116	ILE	2.5
5	D	130	LEU	2.5
10	I	98	LEU	2.5
23	V	48	ARG	2.5
4	C	50	GLN	2.5
13	L	86	GLN	2.5
24	W	8	SER	2.5
29	X	583	C	2.5
29	X	803	C	2.5
20	S	66	VAL	2.5
22	U	67	ILE	2.4
4	C	35	LEU	2.4
29	X	2522	G	2.4
1	0	56	GLY	2.4
3	B	140	SER	2.4
3	B	121	ASN	2.4
8	G	106	TYR	2.4
29	X	408	U	2.4
15	N	8	ILE	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	0	126	LEU	2.4
10	I	55	ARG	2.4
15	N	36	PHE	2.4
8	G	98	LYS	2.4
10	I	14	LYS	2.4
13	L	26	LYS	2.4
1	0	57	THR	2.4
21	T	13	GLY	2.4
21	T	65	GLY	2.4
16	O	14	VAL	2.4
17	P	97	VAL	2.4
22	U	60	VAL	2.4
29	X	1913	G	2.4
29	X	2095	G	2.4
2	A	54	ILE	2.4
2	A	69	ARG	2.4
2	A	257	LEU	2.4
7	F	34	ILE	2.4
10	I	53	ARG	2.4
15	N	18	LEU	2.4
3	B	132	LYS	2.4
29	X	1202	U	2.4
3	B	142	GLY	2.4
24	W	13	PRO	2.4
4	C	66	ASN	2.4
13	L	59	LEU	2.4
2	A	67	PHE	2.4
2	A	233	HIS	2.4
2	A	248	THR	2.4
19	R	107	ALA	2.4
14	M	57	ILE	2.4
17	P	11	LYS	2.4
18	Q	40	ASP	2.4
28	3	38	GLY	2.4
2	A	214	TRP	2.4
20	S	123	VAL	2.4
29	X	1062	G	2.4
15	N	63	GLN	2.4
29	X	2100	A	2.4
25	Z	8	LYS	2.3
27	2	8	ASN	2.3
29	X	1903	C	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
6	E	167	GLU	2.3
10	I	73	GLU	2.3
3	B	129	HIS	2.3
6	E	170	ALA	2.3
24	W	6	VAL	2.3
20	S	8	ARG	2.3
23	V	42	ARG	2.3
28	3	26	LYS	2.3
29	X	396	U	2.3
29	X	542	A	2.3
29	X	636	G	2.3
29	X	1251	G	2.3
29	X	2123	G	2.3
29	X	2587	G	2.3
29	X	2847	G	2.3
10	I	39	SER	2.3
10	I	41	SER	2.3
5	D	105	ASN	2.3
12	K	89	GLU	2.3
1	0	148	MET	2.3
28	3	35	GLY	2.3
9	H	134	LEU	2.3
10	I	108	LEU	2.3
7	F	19	PRO	2.3
9	H	6	SER	2.3
29	X	1770	U	2.3
7	F	116	ASN	2.3
8	G	73	ASN	2.3
29	X	387	A	2.3
29	X	404	A	2.3
1	0	109	VAL	2.3
10	I	40	ARG	2.3
24	W	22	ALA	2.3
28	3	53	ALA	2.3
2	A	264	LYS	2.3
8	G	137	LYS	2.3
28	3	7	HIS	2.3
29	X	361	G	2.3
29	X	958	G	2.3
9	H	81	ILE	2.3
29	X	405	C	2.3
29	X	769	C	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
27	2	19	ARG	2.3
4	C	90	SER	2.3
2	A	234	GLY	2.3
17	P	29	LYS	2.3
24	W	45	LYS	2.3
10	I	4	HIS	2.3
10	I	83	LEU	2.3
25	Z	58	LEU	2.3
29	X	1778	U	2.3
29	X	2327	U	2.3
17	P	107	ILE	2.3
29	X	2521	A	2.3
2	A	34	THR	2.3
17	P	102	THR	2.3
21	T	18	PRO	2.3
4	C	84	PHE	2.3
29	X	1284	G	2.3
29	X	1963	G	2.3
29	X	2044	G	2.3
29	X	2750	G	2.3
29	X	1623	C	2.3
2	A	70	ARG	2.3
19	R	106	VAL	2.3
28	3	29	LYS	2.3
7	F	124	ALA	2.3
10	I	22	GLY	2.3
11	J	45	SER	2.3
21	T	63	SER	2.3
1	0	88	ASP	2.2
15	N	56	ASP	2.2
13	L	21	THR	2.2
29	X	1895	A	2.2
29	X	2581	A	2.2
8	G	74	MET	2.2
1	0	44	GLY	2.2
2	A	25	ALA	2.2
7	F	26	ALA	2.2
20	S	124	ALA	2.2
26	1	35	LEU	2.2
29	X	395	G	2.2
29	X	682	G	2.2
29	X	1396	C	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	0	107	ASP	2.2
22	U	61	TRP	2.2
1	0	61	PRO	2.2
7	F	22	PRO	2.2
25	Z	11	THR	2.2
6	E	95	ARG	2.2
10	I	16	ARG	2.2
29	X	577	U	2.2
5	D	148	LYS	2.2
1	0	167	VAL	2.2
11	J	133	VAL	2.2
13	L	88	VAL	2.2
8	G	90	LEU	2.2
10	I	109	LEU	2.2
11	J	41	ALA	2.2
13	L	58	ALA	2.2
29	X	1259	A	2.2
3	B	161	GLY	2.2
1	0	189	ILE	2.2
2	A	82	ILE	2.2
15	N	29	SER	2.2
5	D	84	PRO	2.2
29	X	434	C	2.2
29	X	1214	C	2.2
17	P	105	ARG	2.2
19	R	30	LYS	2.2
29	X	758	G	2.2
29	X	950	G	2.2
29	X	1554	G	2.2
16	O	6	GLN	2.2
28	3	61	MET	2.2
12	K	6	ALA	2.2
13	L	79	ALA	2.2
20	S	161	ALA	2.2
28	3	43	GLY	2.2
3	B	188	ILE	2.2
18	Q	53	ILE	2.2
18	Q	28	TRP	2.2
21	T	16	SER	2.2
8	G	30	LYS	2.2
3	B	143	GLN	2.2
6	E	109	TYR	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
11	J	121	LEU	2.2
2	A	153	ALA	2.2
19	R	109	ALA	2.2
29	X	74	G	2.2
29	X	338	G	2.2
29	X	1228	G	2.2
29	X	2106	G	2.2
3	B	149	ARG	2.2
14	M	100	ARG	2.2
23	V	29	ARG	2.2
14	M	29	PRO	2.2
17	P	61	PRO	2.2
13	L	56	SER	2.2
29	X	1215	A	2.2
29	X	2248	A	2.2
2	A	45	ASN	2.2
16	O	78	VAL	2.2
17	P	41	VAL	2.2
1	0	185	TYR	2.2
8	G	100	TYR	2.2
12	K	16	ALA	2.1
14	M	2	GLN	2.2
2	A	243	GLY	2.1
9	H	28	GLY	2.1
29	X	1950	C	2.1
29	X	1966	C	2.1
29	X	2135	C	2.1
12	K	8	ARG	2.1
21	T	41	ARG	2.1
8	G	70	PHE	2.1
25	Z	4	HIS	2.1
7	F	25	PRO	2.1
28	3	2	PRO	2.1
29	X	786	U	2.1
29	X	1898	U	2.1
29	X	1755	G	2.1
29	X	2221	G	2.1
1	0	127	LEU	2.1
4	C	177	VAL	2.1
19	R	48	VAL	2.1
23	V	60	LEU	2.1
7	F	108	ALA	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
9	H	49	ASP	2.1
7	F	7	ILE	2.1
5	D	69	LYS	2.1
11	J	105	PHE	2.1
23	V	14	PHE	2.1
11	J	71	PRO	2.1
2	A	16	MET	2.1
4	C	166	TRP	2.1
20	S	71	MET	2.1
20	S	166	LEU	2.1
29	X	2483	U	2.1
30	Y	10	U	2.1
5	D	73	SER	2.1
23	V	32	ALA	2.1
5	D	97	TYR	2.1
21	T	8	GLY	2.1
29	X	2018	G	2.1
17	P	15	LYS	2.1
25	Z	13	LYS	2.1
27	2	18	PHE	2.1
30	Y	47	A	2.1
2	A	181	GLU	2.1
19	R	84	VAL	2.1
2	A	19	ALA	2.1
27	2	32	ALA	2.1
29	X	223	C	2.1
29	X	2558	C	2.1
1	0	30	THR	2.1
5	D	66	ILE	2.1
7	F	137	THR	2.1
26	1	25	THR	2.1
2	A	46	ARG	2.1
3	B	139	GLY	2.1
12	K	40	LYS	2.1
18	Q	47	GLY	2.1
19	R	28	LYS	2.1
27	2	6	GLN	2.1
29	X	973	U	2.1
4	C	123	PHE	2.1
14	M	66	PHE	2.1
5	D	91	LEU	2.1
29	X	11	G	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
29	X	200	A	2.1
1	0	84	ALA	2.1
21	T	83	ALA	2.1
22	U	24	ALA	2.1
1	0	45	ILE	2.1
2	A	102	LYS	2.1
8	G	147	ARG	2.1
4	C	81	GLY	2.1
10	I	51	GLY	2.1
11	J	62	GLY	2.1
25	Z	26	THR	2.1
27	2	43	THR	2.1
4	C	3	GLN	2.1
12	K	24	GLN	2.1
7	F	114	ASP	2.1
13	L	90	ASP	2.1
29	X	2048	C	2.1
29	X	34	U	2.1
29	X	775	U	2.1
29	X	845	U	2.1
5	D	57	LEU	2.1
6	E	105	MET	2.1
1	0	58	VAL	2.1
15	N	17	VAL	2.1
14	M	78	GLU	2.1
2	A	103	ARG	2.0
5	D	53	ALA	2.0
10	I	28	LYS	2.0
17	P	32	ARG	2.0
17	P	124	ILE	2.0
22	U	39	LYS	2.0
27	2	33	ARG	2.0
13	L	38	ILE	2.0
29	X	2014	A	2.0
29	X	337	G	2.0
29	X	487	G	2.0
29	X	2010	G	2.0
4	C	64	THR	2.0
2	A	8	PRO	2.0
29	X	127	C	2.0
29	X	1092	U	2.0
29	X	2364	C	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
30	Y	32	C	2.0
4	C	39	ARG	2.0
16	O	82	ARG	2.0
17	P	111	ARG	2.0
15	N	23	GLY	2.0
7	F	66	THR	2.0
8	G	146	THR	2.0
2	A	15	GLN	2.0
6	E	171	LEU	2.0
9	H	27	SER	2.0
29	X	1896	A	2.0
30	Y	61	A	2.0
11	J	132	MET	2.0
1	O	46	ASP	2.0
5	D	147	ASP	2.0
10	I	123	ASP	2.0
18	Q	74	ASP	2.0
29	X	965	G	2.0
29	X	1761	G	2.0
3	B	152	LYS	2.0
11	J	60	ARG	2.0
11	J	134	LYS	2.0
13	L	99	ARG	2.0
2	A	225	ALA	2.0
3	B	55	ALA	2.0
11	J	69	ILE	2.0
14	M	55	ILE	2.0
29	X	12	U	2.0
1	O	65	GLY	2.0
29	X	1115	C	2.0
29	X	1795	C	2.0
29	X	2273	C	2.0
29	X	2601	C	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	B-factors(Å <sup>2</sup> )	Q<0.9
31	MG	X	6135	1/1	0.12	0.84	129,129,129,129	0
31	MG	X	6152	1/1	0.16	0.34	158,158,158,158	0
31	MG	X	6116	1/1	0.31	0.98	99,99,99,99	0
31	MG	X	6101	1/1	0.35	1.00	138,138,138,138	0
31	MG	X	6103	1/1	0.37	0.28	126,126,126,126	0
31	MG	X	6142	1/1	0.39	0.57	106,106,106,106	0
31	MG	X	6130	1/1	0.46	0.39	132,132,132,132	0
31	MG	X	6125	1/1	0.47	0.55	109,109,109,109	0
31	MG	X	6159	1/1	0.48	0.53	109,109,109,109	0
31	MG	X	6162	1/1	0.48	0.63	104,104,104,104	0
31	MG	X	6177	1/1	0.48	0.53	125,125,125,125	0
31	MG	Y	204	1/1	0.49	0.49	116,116,116,116	0
31	MG	X	6137	1/1	0.51	0.40	136,136,136,136	0
31	MG	X	6079	1/1	0.53	0.38	99,99,99,99	0
31	MG	X	6176	1/1	0.54	0.40	73,73,73,73	0
31	MG	X	6100	1/1	0.54	0.48	111,111,111,111	0
31	MG	X	6117	1/1	0.54	0.42	130,130,130,130	0
31	MG	X	6114	1/1	0.55	0.67	93,93,93,93	0
31	MG	X	6003	1/1	0.56	0.41	72,72,72,72	0
31	MG	X	6046	1/1	0.56	0.57	76,76,76,76	0
31	MG	X	6147	1/1	0.56	0.80	93,93,93,93	0
31	MG	Y	203	1/1	0.57	0.62	96,96,96,96	0
31	MG	X	6087	1/1	0.57	0.54	85,85,85,85	0
31	MG	X	6051	1/1	0.58	0.46	83,83,83,83	0
31	MG	X	6060	1/1	0.59	1.14	80,80,80,80	0
31	MG	X	6167	1/1	0.61	0.76	97,97,97,97	0
31	MG	X	6022	1/1	0.61	0.47	92,92,92,92	0
31	MG	X	6153	1/1	0.61	0.44	114,114,114,114	0
31	MG	X	6093	1/1	0.61	0.38	96,96,96,96	0
31	MG	X	6148	1/1	0.61	0.28	104,104,104,104	0
31	MG	X	6006	1/1	0.62	0.69	70,70,70,70	0
31	MG	X	6175	1/1	0.62	0.54	121,121,121,121	0
31	MG	X	6029	1/1	0.63	0.36	82,82,82,82	0
31	MG	X	6149	1/1	0.63	0.43	99,99,99,99	0
31	MG	X	6132	1/1	0.63	0.54	84,84,84,84	0
31	MG	X	6141	1/1	0.64	0.42	87,87,87,87	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
31	MG	X	6133	1/1	0.64	0.56	91,91,91,91	0
31	MG	X	6139	1/1	0.64	0.32	113,113,113,113	0
31	MG	X	6096	1/1	0.65	0.26	99,99,99,99	0
31	MG	X	6020	1/1	0.65	0.38	76,76,76,76	0
31	MG	X	6018	1/1	0.65	0.52	86,86,86,86	0
31	MG	X	6076	1/1	0.65	0.43	73,73,73,73	0
31	MG	X	6174	1/1	0.65	0.34	117,117,117,117	0
31	MG	X	6160	1/1	0.66	0.67	108,108,108,108	0
31	MG	X	6124	1/1	0.66	0.42	100,100,100,100	0
31	MG	X	6052	1/1	0.66	0.49	86,86,86,86	0
31	MG	X	6057	1/1	0.67	0.66	92,92,92,92	0
31	MG	X	6165	1/1	0.67	0.34	88,88,88,88	0
31	MG	X	6017	1/1	0.67	0.34	54,54,54,54	0
31	MG	X	6049	1/1	0.68	0.57	91,91,91,91	0
31	MG	X	6025	1/1	0.68	0.58	76,76,76,76	0
31	MG	X	6001	1/1	0.69	0.54	67,67,67,67	0
31	MG	X	6158	1/1	0.69	0.26	76,76,76,76	0
31	MG	X	6099	1/1	0.69	0.59	120,120,120,120	0
31	MG	X	6106	1/1	0.69	0.38	100,100,100,100	0
31	MG	X	6150	1/1	0.69	0.48	97,97,97,97	0
31	MG	X	6163	1/1	0.69	0.27	82,82,82,82	0
31	MG	X	6073	1/1	0.69	0.23	105,105,105,105	0
31	MG	X	6092	1/1	0.70	0.49	97,97,97,97	0
31	MG	X	6048	1/1	0.70	0.44	66,66,66,66	0
31	MG	X	6168	1/1	0.70	0.44	100,100,100,100	0
31	MG	Y	205	1/1	0.70	0.39	123,123,123,123	0
31	MG	X	6123	1/1	0.71	0.41	89,89,89,89	0
31	MG	X	6072	1/1	0.71	0.54	101,101,101,101	0
31	MG	X	6155	1/1	0.71	0.45	108,108,108,108	0
31	MG	X	6042	1/1	0.71	0.74	96,96,96,96	0
31	MG	X	6043	1/1	0.71	0.27	106,106,106,106	0
31	MG	X	6013	1/1	0.71	0.69	76,76,76,76	0
31	MG	X	6170	1/1	0.72	0.41	97,97,97,97	0
31	MG	X	6120	1/1	0.72	0.34	78,78,78,78	0
31	MG	X	6053	1/1	0.72	0.67	85,85,85,85	0
31	MG	X	6115	1/1	0.72	0.22	133,133,133,133	0
31	MG	X	6045	1/1	0.73	0.53	94,94,94,94	0
31	MG	X	6089	1/1	0.73	0.44	89,89,89,89	0
31	MG	X	6113	1/1	0.73	0.33	143,143,143,143	0
31	MG	Y	201	1/1	0.74	0.46	96,96,96,96	0
31	MG	X	6019	1/1	0.74	0.30	75,75,75,75	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
31	MG	X	6112	1/1	0.75	0.27	80,80,80,80	0
31	MG	X	6156	1/1	0.75	0.29	91,91,91,91	0
31	MG	X	6157	1/1	0.75	0.42	96,96,96,96	0
31	MG	X	6097	1/1	0.75	0.32	122,122,122,122	0
31	MG	X	6058	1/1	0.75	0.27	70,70,70,70	0
31	MG	H	201	1/1	0.76	0.21	104,104,104,104	0
31	MG	X	6033	1/1	0.76	0.60	76,76,76,76	0
31	MG	X	6172	1/1	0.76	0.23	88,88,88,88	0
31	MG	X	6173	1/1	0.76	0.20	87,87,87,87	0
31	MG	X	6083	1/1	0.76	0.32	83,83,83,83	0
31	MG	X	6127	1/1	0.76	0.45	81,81,81,81	0
31	MG	A	301	1/1	0.77	0.38	108,108,108,108	0
31	MG	X	6129	1/1	0.77	0.50	89,89,89,89	0
31	MG	X	6146	1/1	0.77	0.24	125,125,125,125	0
31	MG	X	6105	1/1	0.77	0.43	86,86,86,86	0
31	MG	X	6031	1/1	0.77	0.49	85,85,85,85	0
31	MG	X	6111	1/1	0.77	0.41	98,98,98,98	0
31	MG	X	6074	1/1	0.77	0.48	89,89,89,89	0
31	MG	X	6027	1/1	0.77	0.63	65,65,65,65	0
31	MG	X	6061	1/1	0.77	0.24	100,100,100,100	0
31	MG	X	6140	1/1	0.77	0.23	97,97,97,97	0
31	MG	X	6169	1/1	0.77	0.43	91,91,91,91	0
31	MG	X	6118	1/1	0.78	0.30	82,82,82,82	0
31	MG	X	6010	1/1	0.78	0.45	64,64,64,64	0
31	MG	X	6062	1/1	0.78	1.04	87,87,87,87	0
31	MG	X	6091	1/1	0.78	0.44	72,72,72,72	0
31	MG	X	6068	1/1	0.78	0.30	111,111,111,111	0
31	MG	X	6134	1/1	0.78	0.13	100,100,100,100	0
31	MG	X	6154	1/1	0.79	0.49	96,96,96,96	0
31	MG	X	6011	1/1	0.79	0.29	104,104,104,104	0
31	MG	X	6015	1/1	0.79	0.27	74,74,74,74	0
31	MG	Y	202	1/1	0.79	0.18	130,130,130,130	0
31	MG	X	6030	1/1	0.79	0.29	101,101,101,101	0
31	MG	X	6024	1/1	0.79	0.25	100,100,100,100	0
31	MG	X	6016	1/1	0.79	0.38	74,74,74,74	0
31	MG	X	6014	1/1	0.80	0.38	99,99,99,99	0
31	MG	X	6004	1/1	0.80	0.24	93,93,93,93	0
31	MG	X	6090	1/1	0.80	0.52	72,72,72,72	0
31	MG	X	6077	1/1	0.80	0.40	80,80,80,80	0
31	MG	X	6002	1/1	0.80	0.23	91,91,91,91	0
31	MG	X	6007	1/1	0.80	0.38	78,78,78,78	0
31	MG	X	6085	1/1	0.80	0.44	66,66,66,66	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
31	MG	X	6082	1/1	0.81	0.51	105,105,105,105	0
31	MG	X	6066	1/1	0.81	0.21	105,105,105,105	0
31	MG	X	6055	1/1	0.81	0.34	85,85,85,85	0
31	MG	X	6037	1/1	0.81	0.50	65,65,65,65	0
31	MG	X	6151	1/1	0.81	0.52	88,88,88,88	0
31	MG	X	6078	1/1	0.81	0.38	89,89,89,89	0
31	MG	X	6035	1/1	0.81	0.60	80,80,80,80	0
31	MG	X	6080	1/1	0.81	0.77	82,82,82,82	0
31	MG	X	6054	1/1	0.82	0.45	79,79,79,79	0
31	MG	X	6075	1/1	0.82	0.15	85,85,85,85	0
31	MG	X	6126	1/1	0.82	0.34	114,114,114,114	0
31	MG	X	6171	1/1	0.82	0.35	118,118,118,118	0
31	MG	X	6161	1/1	0.82	0.33	113,113,113,113	0
31	MG	X	6023	1/1	0.83	0.42	83,83,83,83	0
31	MG	X	6104	1/1	0.83	0.44	89,89,89,89	0
31	MG	X	6108	1/1	0.83	0.37	108,108,108,108	0
31	MG	X	6144	1/1	0.84	0.36	132,132,132,132	0
31	MG	X	6094	1/1	0.84	0.35	95,95,95,95	0
31	MG	X	6081	1/1	0.84	0.32	90,90,90,90	0
31	MG	X	6143	1/1	0.84	0.50	99,99,99,99	0
31	MG	X	6039	1/1	0.85	0.19	79,79,79,79	0
31	MG	X	6095	1/1	0.85	0.37	78,78,78,78	0
31	MG	X	6164	1/1	0.85	0.31	86,86,86,86	0
31	MG	X	6110	1/1	0.85	0.40	84,84,84,84	0
31	MG	X	6145	1/1	0.85	0.25	84,84,84,84	0
31	MG	X	6047	1/1	0.86	0.23	79,79,79,79	0
31	MG	N	201	1/1	0.86	0.27	74,74,74,74	0
31	MG	X	6063	1/1	0.86	0.41	87,87,87,87	0
31	MG	X	6065	1/1	0.86	0.20	93,93,93,93	0
31	MG	X	6138	1/1	0.86	0.26	86,86,86,86	0
31	MG	X	6040	1/1	0.86	0.53	63,63,63,63	0
31	MG	X	6050	1/1	0.86	0.53	91,91,91,91	0
31	MG	X	6069	1/1	0.86	0.32	65,65,65,65	0
31	MG	X	6109	1/1	0.87	0.30	92,92,92,92	0
31	MG	X	6102	1/1	0.87	0.21	98,98,98,98	0
31	MG	X	6128	1/1	0.87	0.21	131,131,131,131	0
31	MG	X	6032	1/1	0.87	0.32	86,86,86,86	0
31	MG	X	6098	1/1	0.87	0.21	71,71,71,71	0
31	MG	X	6122	1/1	0.87	0.43	84,84,84,84	0
31	MG	X	6084	1/1	0.87	0.22	124,124,124,124	0
31	MG	X	6059	1/1	0.87	0.27	88,88,88,88	0
31	MG	X	6026	1/1	0.87	0.24	79,79,79,79	0

*Continued on next page...*

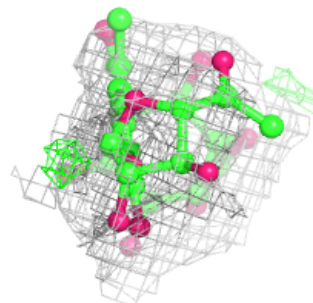
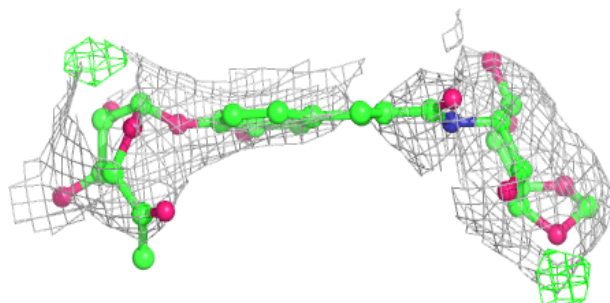
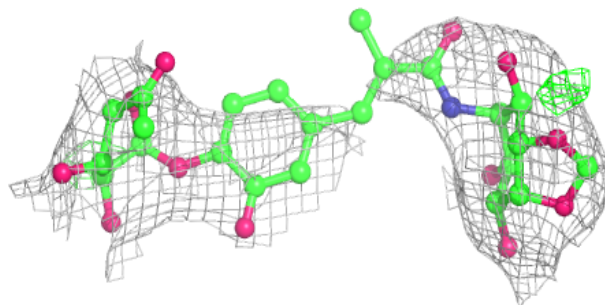
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
31	MG	X	6119	1/1	0.88	0.49	89,89,89,89	0
31	MG	X	6028	1/1	0.88	0.22	75,75,75,75	0
31	MG	X	6131	1/1	0.88	0.36	80,80,80,80	0
31	MG	X	6070	1/1	0.88	0.34	69,69,69,69	0
31	MG	M	201	1/1	0.89	0.54	71,71,71,71	0
31	MG	X	6009	1/1	0.89	0.22	50,50,50,50	0
31	MG	X	6038	1/1	0.89	0.11	82,82,82,82	0
31	MG	X	6056	1/1	0.89	0.24	81,81,81,81	0
31	MG	X	6071	1/1	0.89	0.38	99,99,99,99	0
31	MG	X	6064	1/1	0.90	0.52	77,77,77,77	0
31	MG	X	6166	1/1	0.90	0.24	76,76,76,76	0
31	MG	X	6136	1/1	0.90	0.36	84,84,84,84	0
31	MG	X	6107	1/1	0.91	0.22	76,76,76,76	0
31	MG	X	6008	1/1	0.91	0.23	58,58,58,58	0
31	MG	X	6012	1/1	0.91	0.26	78,78,78,78	0
31	MG	X	6041	1/1	0.91	0.35	64,64,64,64	0
31	MG	X	6034	1/1	0.91	0.15	69,69,69,69	0
31	MG	X	6036	1/1	0.92	0.28	70,70,70,70	0
31	MG	X	6044	1/1	0.92	0.29	66,66,66,66	0
32	HGR	X	6178	36/36	0.92	0.15	79,99,109,111	0
31	MG	X	6021	1/1	0.93	0.14	91,91,91,91	0
31	MG	X	6005	1/1	0.94	0.52	58,58,58,58	0
31	MG	X	6088	1/1	0.94	0.21	88,88,88,88	0
31	MG	X	6121	1/1	0.95	0.68	85,85,85,85	0
31	MG	X	6086	1/1	0.96	0.08	104,104,104,104	0
31	MG	X	6067	1/1	0.96	0.12	72,72,72,72	0

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

**Electron density around HGR X 6178:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.