



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 06:03 am GMT

PDB ID : 1HNX  
Title : STRUCTURE OF THE THERMUS THERMOPHILUS 30S RIBOSOMAL  
SUBUNIT IN COMPLEX WITH PACTAMYCIN  
Authors : Brodersen, D.E.; Clemons Jr., W.M.; Carter, A.P.; Morgan-Warren, R.; Wim-  
berly, B.T.; Ramakrishnan, V.  
Deposited on : 2000-12-08  
Resolution : 3.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

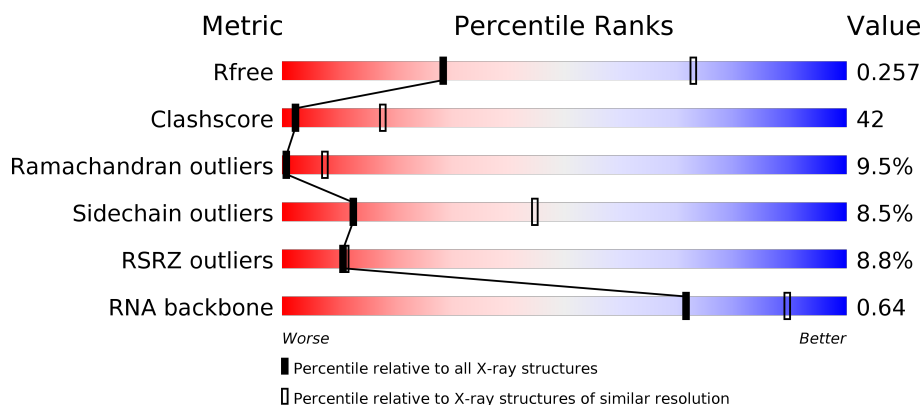
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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))
$R_{free}$	100719	1679 (3.50-3.30)
Clashscore	112137	1832 (3.50-3.30)
Ramachandran outliers	110173	1789 (3.50-3.30)
Sidechain outliers	110143	1789 (3.50-3.30)
RSRZ outliers	101464	1709 (3.50-3.30)
RNA backbone	2435	1009 (3.96-2.84)

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

Mol	Chain	Length	Quality of chain
1	A	1522	<div> <div>14%</div> <div> <div>21%</div> <div>63%</div> <div>14%</div> <div>..</div> </div> </div>
2	X	6	<div> <div>17%</div> <div> <div>33%</div> <div>67%</div> </div> </div>
3	B	256	<div> <div>5%</div> <div> <div>17%</div> <div>58%</div> <div>15%</div> <div>9%</div> <div>.</div> </div> </div>
4	C	239	<div> <div>17%</div> <div> <div>51%</div> <div>17%</div> <div>14%</div> <div>.</div> </div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	D	209	
6	E	162	
7	F	101	
8	G	156	
9	H	138	
10	I	128	
11	J	105	
12	K	129	
13	L	135	
14	M	126	
15	N	61	
16	O	89	
17	P	88	
18	Q	105	
19	R	88	
20	S	93	
21	T	106	
22	V	26	

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
23	MG	A	1546	-	-	-	X
23	MG	A	1553	-	-	-	X
23	MG	A	1557	-	-	-	X
23	MG	A	1560	-	-	-	X
23	MG	A	1562	-	-	-	X
23	MG	A	1566	-	-	-	X
23	MG	A	1586	-	-	-	X

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	MG	A	1593	-	-	-	X
23	MG	A	1595	-	-	-	X
23	MG	A	1600	-	-	-	X
23	MG	A	1606	-	-	-	X
23	MG	A	1626	-	-	-	X
23	MG	A	1629	-	-	-	X

## 2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 51910 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1507	Total	C	N	O	P	22	0	0
			32391	14418	6002	10465	1506			

- Molecule 2 is a RNA chain called FRAGMENT OF MESSENGER RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	6	Total	C	N	O	P	0	0	0
			117	54	14	44	5			

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S4.

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

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	E	150	Total	C	N	O	S	0	0	0
			1146	724	217	201	4			

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S6.

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

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S7.

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

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S8.

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

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	127	Total	C	N	O	S	0	0	0
			1011	639	198	174				

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	98	Total	C	N	O	S	0	0	0
			792	498	156	137	1			

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S11.

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

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	L	124	Total	C	N	O	S	0	0	0
			970	611	195	163	1			

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	M	125	Total	C	N	O	S	0	0	0
			997	617	207	171	2			

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S14.

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

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S15.

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

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	P	88	Total	C	N	O	S	0	0	0
			735	462	147	125	1			

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Q	104	Total	C	N	O	S	0	0	0
			857	547	161	147	2			

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	R	73	Total	C	N	O	0	0	0
			597	380	118	99			

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	S	80	Total	C	N	O	S	0	0	0
			647	414	119	112	2			

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	T	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

- Molecule 22 is a protein called 30S RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	V	24	Total	C	N	O	0	0	0
			208	128	50	30			

- Molecule 23 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

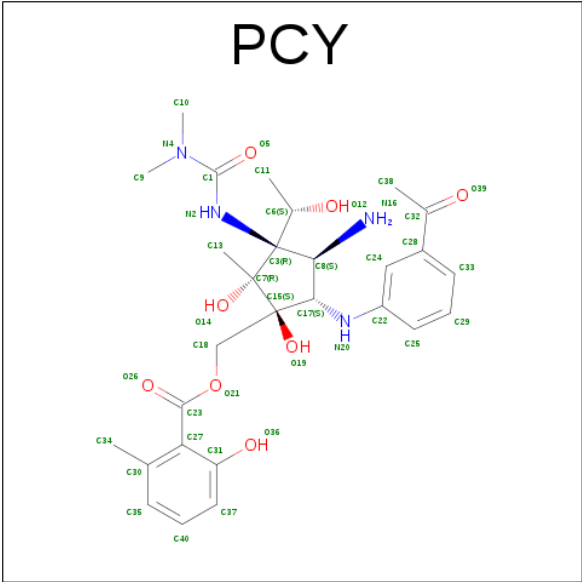
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	H	1	Total	Mg	0	0
			1	1		
23	A	94	Total	Mg	0	0
			94	94		
23	D	1	Total	Mg	0	0
			1	1		

- Molecule 24 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 25 is DE-6-MSA-PACTAMYCIN (three-letter code: PCY) (formula: C<sub>28</sub>H<sub>38</sub>N<sub>4</sub>O<sub>8</sub>).



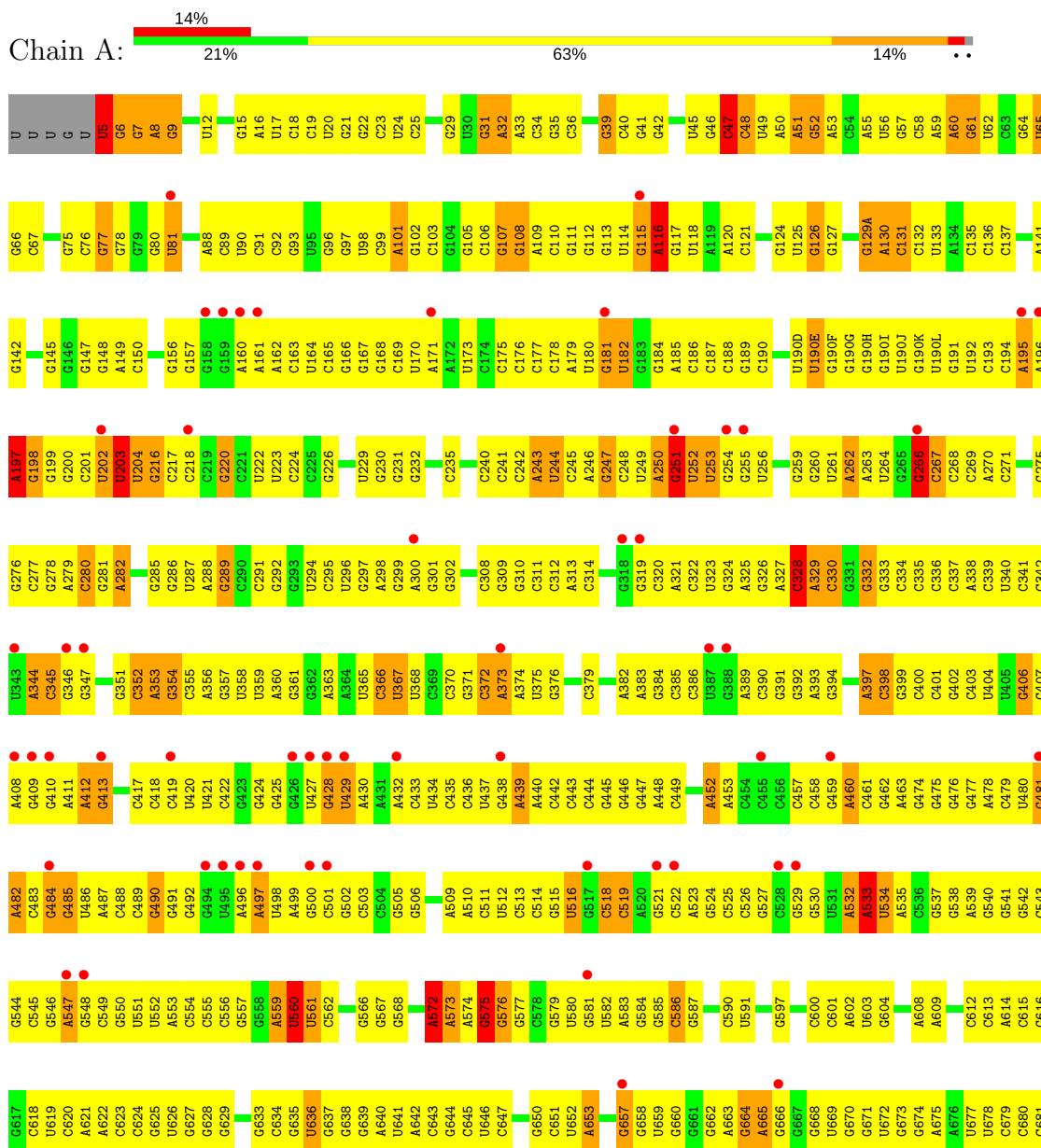


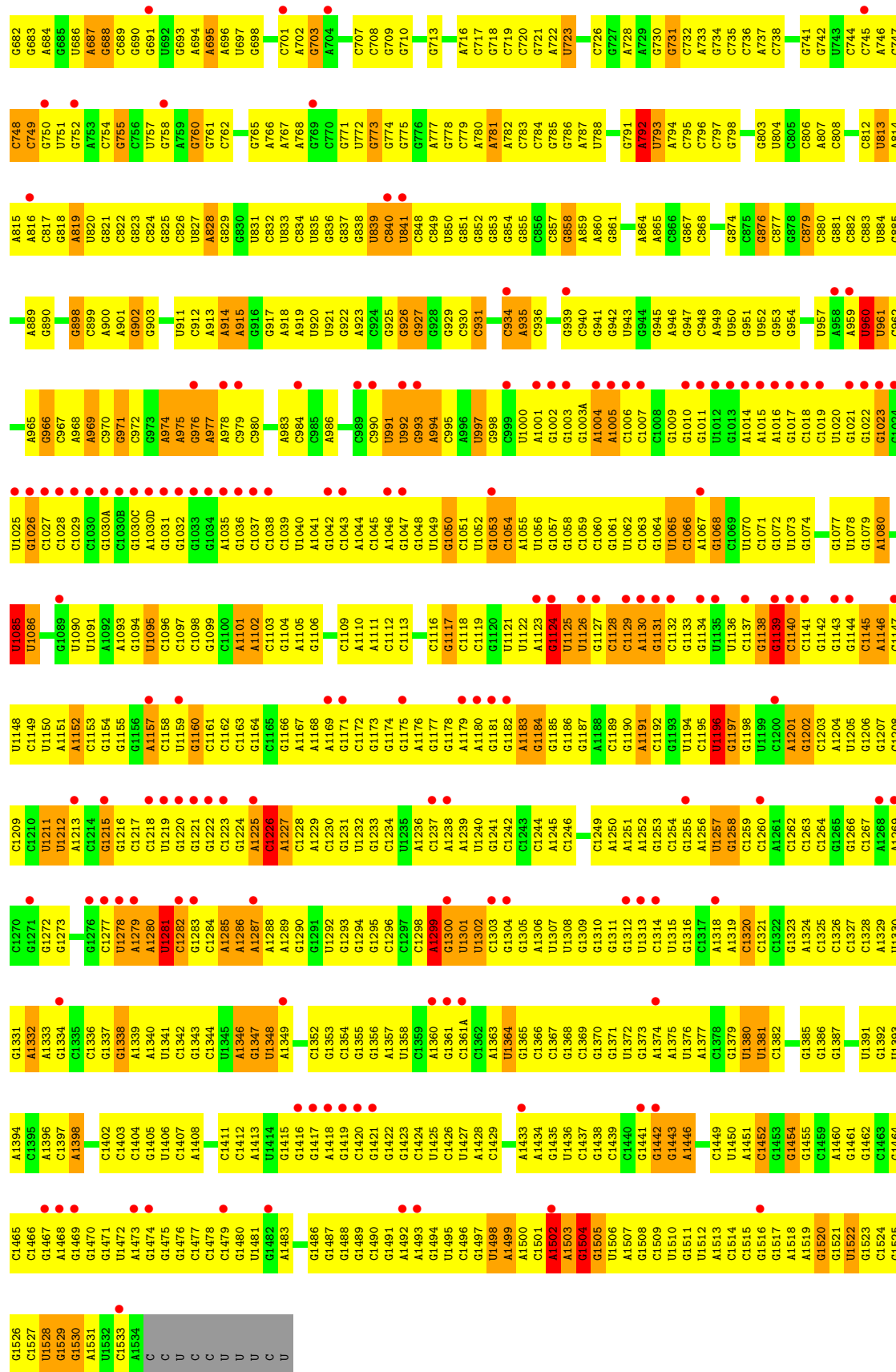
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			40	28	4	8		

### 3 Residue-property plots

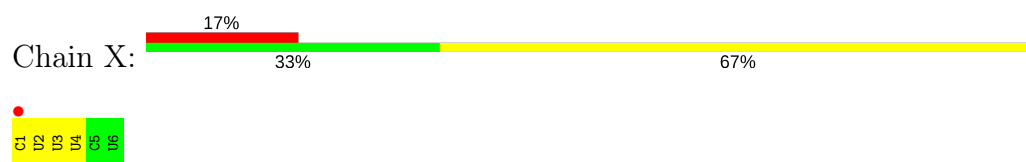
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 ( $\text{RSRZ} > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 16S RIBOSOMAL RNA

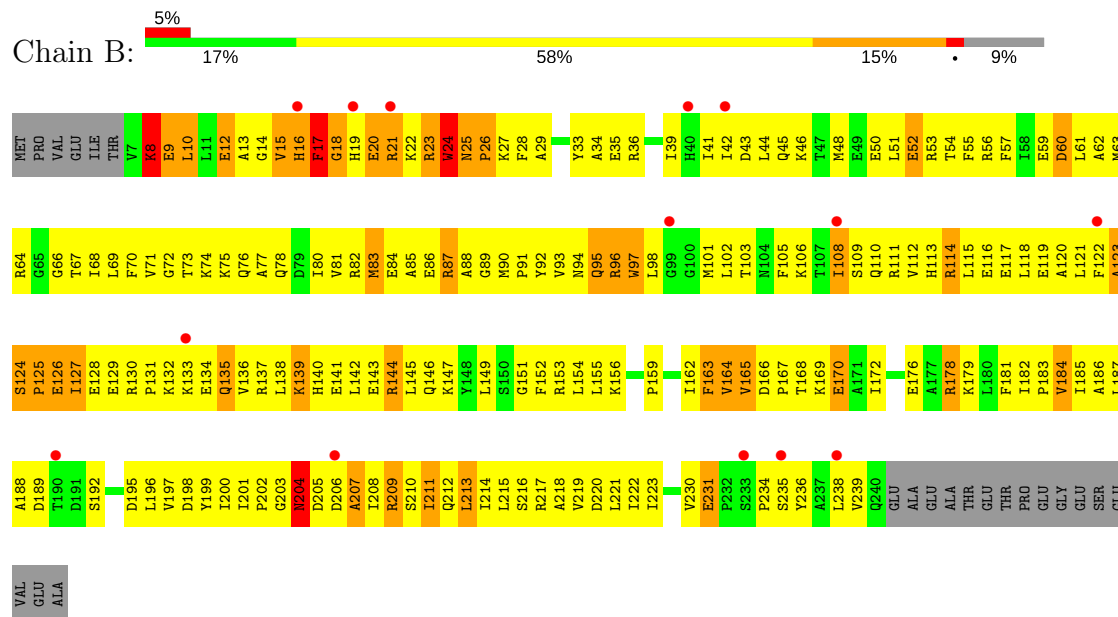




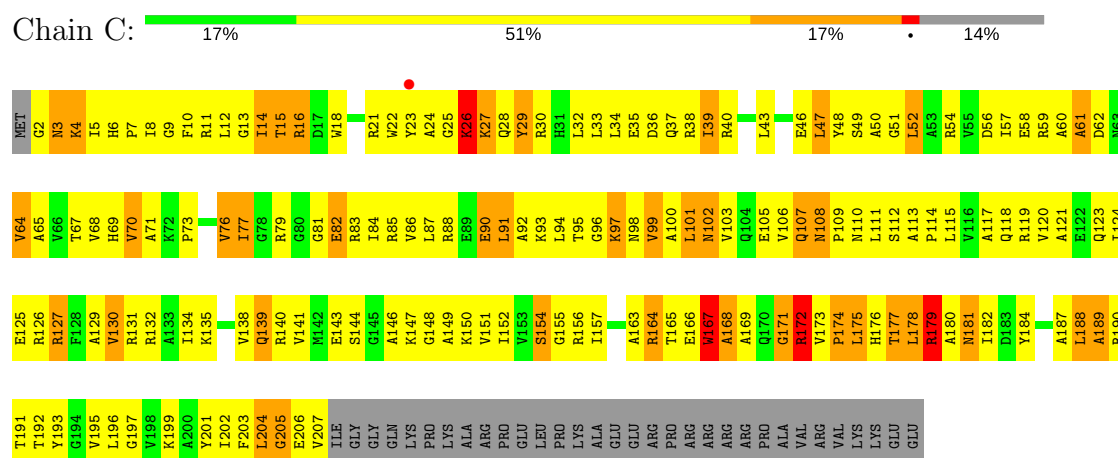
- Molecule 2: FRAGMENT OF MESSENGER RNA



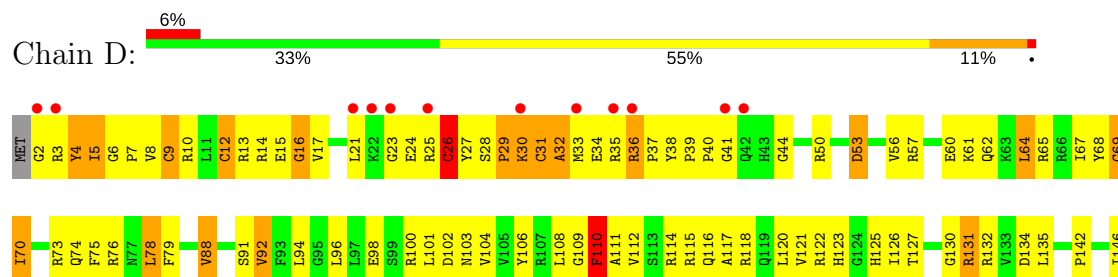
• Molecule 3: 30S RIBOSOMAL PROTEIN S2



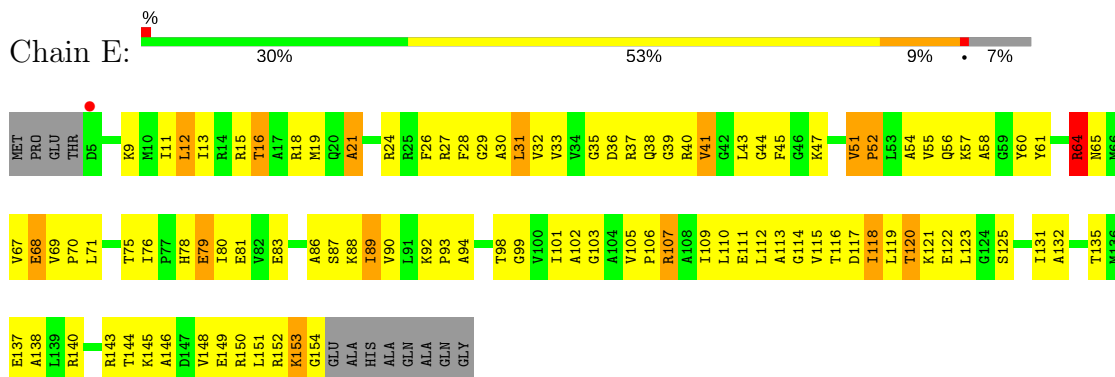
• Molecule 4: 30S RIBOSOMAL PROTEIN S3



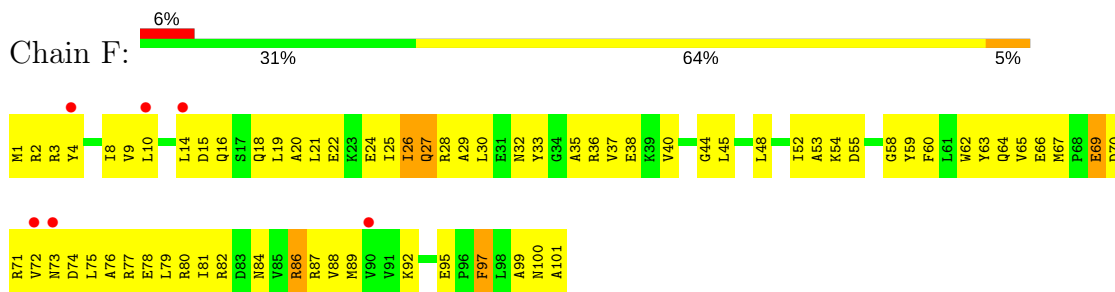
• Molecule 5: 30S RIBOSOMAL PROTEIN S4



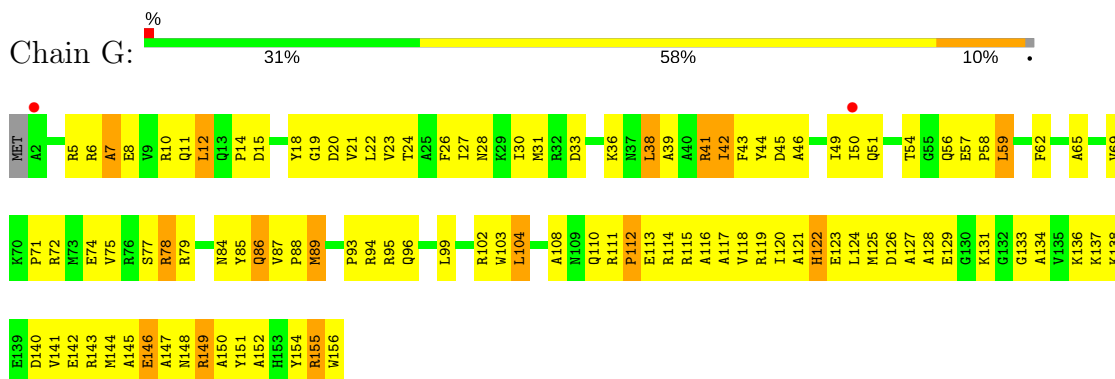
- Molecule 6: 30S RIBOSOMAL PROTEIN S5



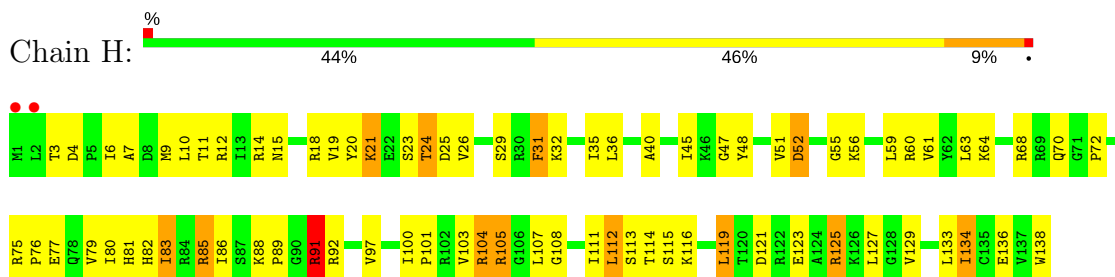
- Molecule 7: 30S RIBOSOMAL PROTEIN S6



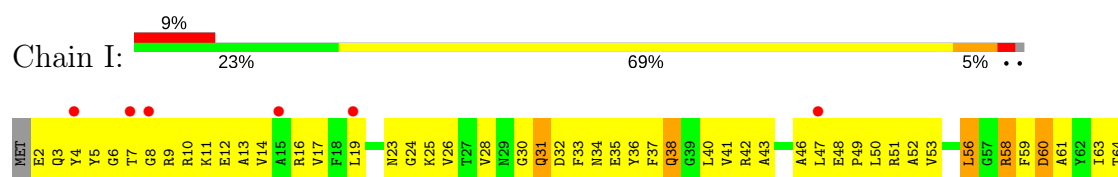
- Molecule 8: 30S RIBOSOMAL PROTEIN S7



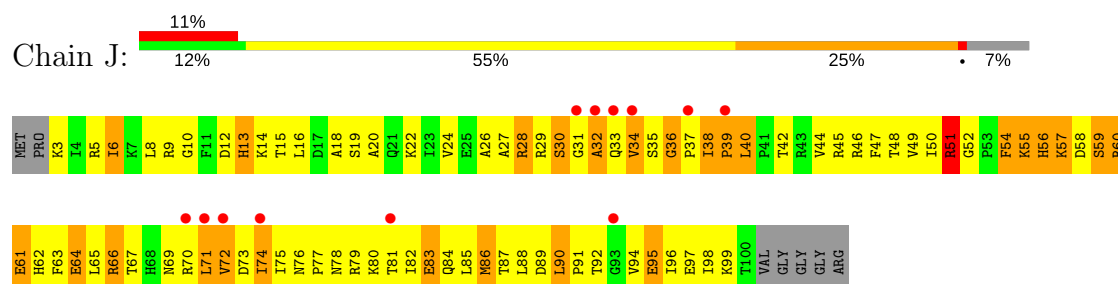
- Molecule 9: 30S RIBOSOMAL PROTEIN S8



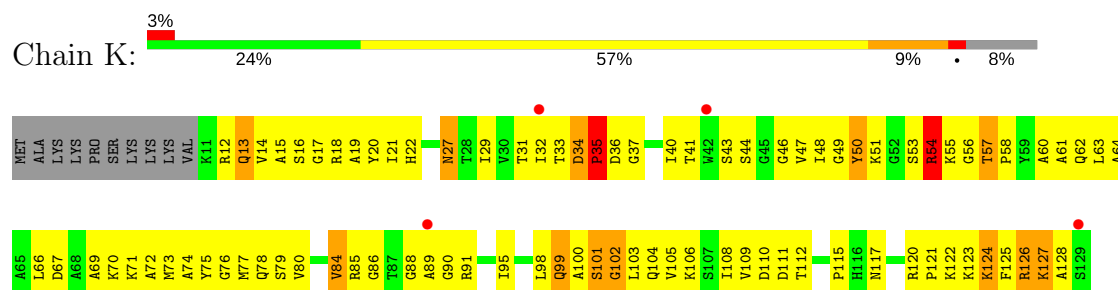
- Molecule 10: 30S RIBOSOMAL PROTEIN S9



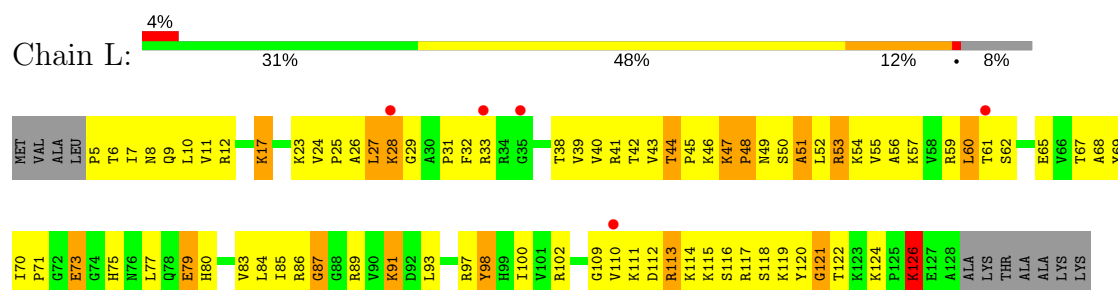
• Molecule 11: 30S RIBOSOMAL PROTEIN S10



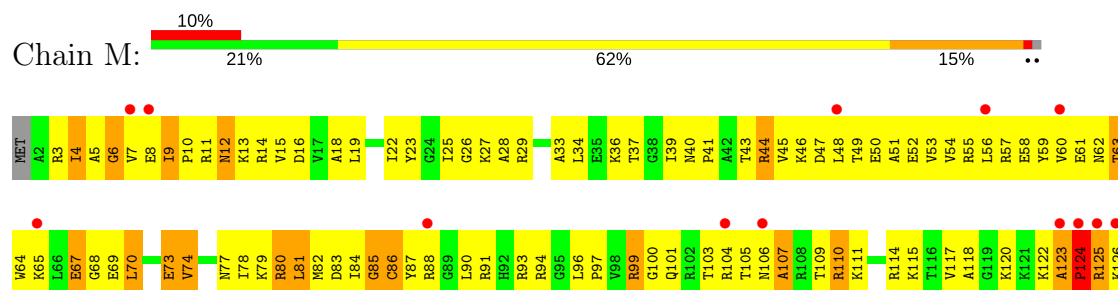
• Molecule 12: 30S RIBOSOMAL PROTEIN S11



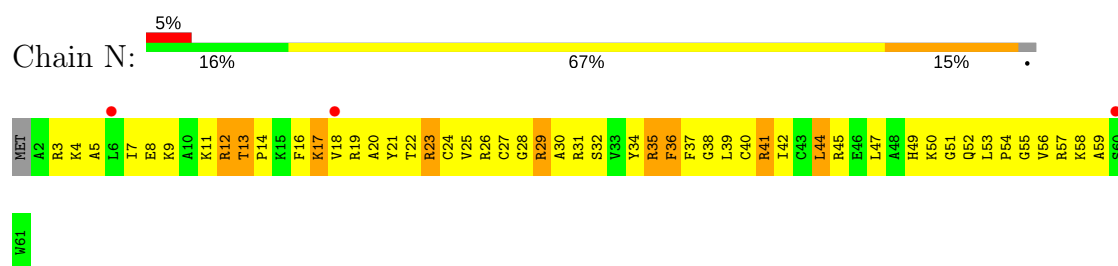
• Molecule 13: 30S RIBOSOMAL PROTEIN S12



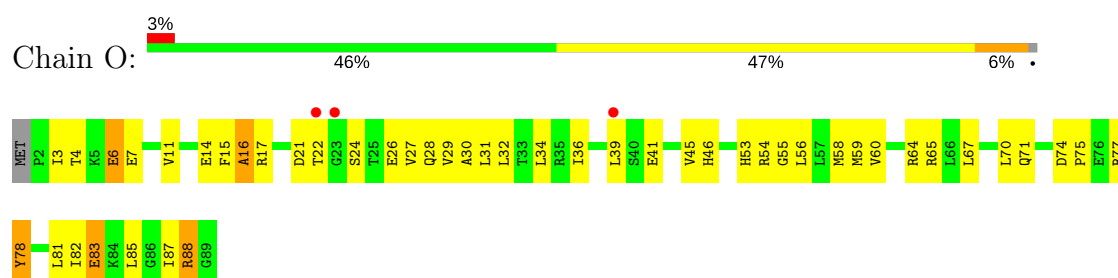
• Molecule 14: 30S RIBOSOMAL PROTEIN S13



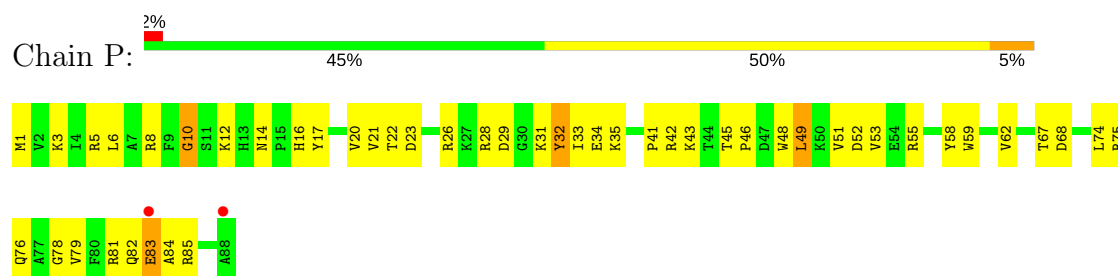
• Molecule 15: 30S RIBOSOMAL PROTEIN S14



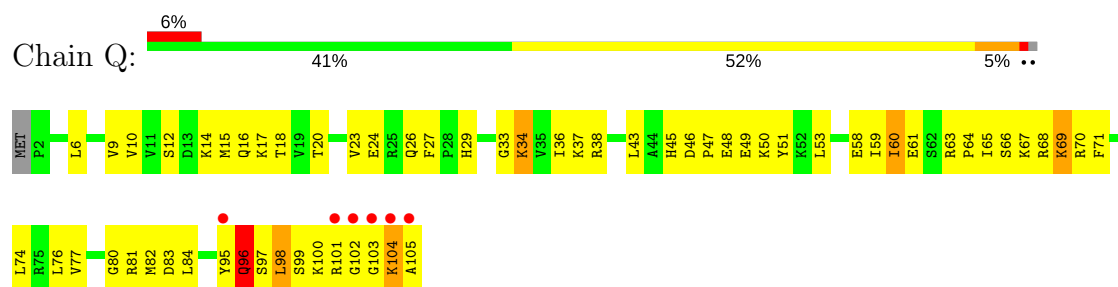
• Molecule 16: 30S RIBOSOMAL PROTEIN S15



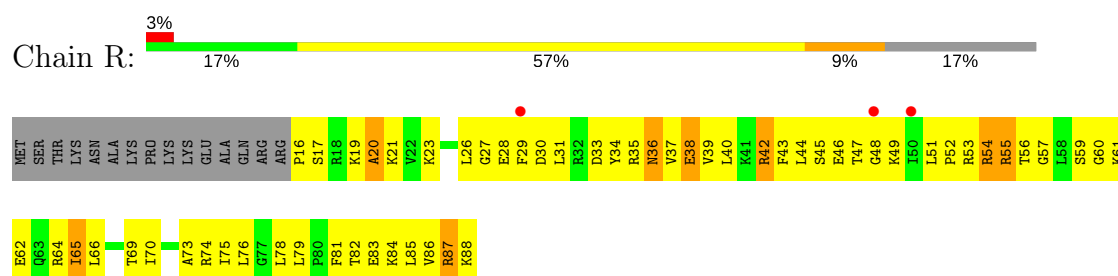
• Molecule 17: 30S RIBOSOMAL PROTEIN S16



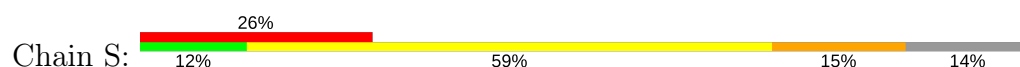
• Molecule 18: 30S RIBOSOMAL PROTEIN S17

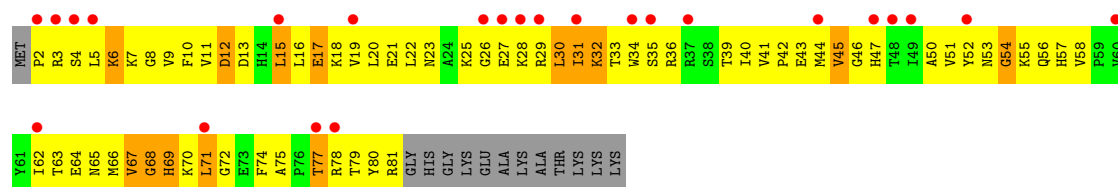


• Molecule 19: 30S RIBOSOMAL PROTEIN S18

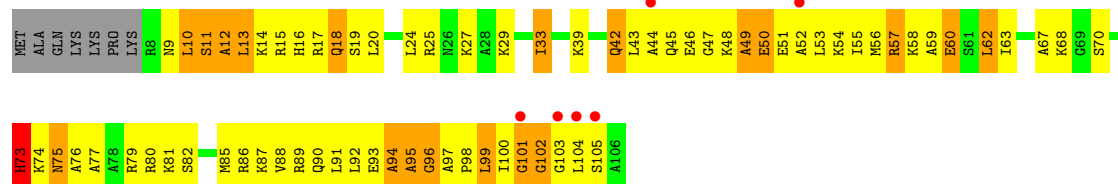


• Molecule 20: 30S RIBOSOMAL PROTEIN S19





● Molecule 21: 30S RIBOSOMAL PROTEIN S20



● Molecule 22: 30S RIBOSOMAL PROTEIN THX





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	401.72Å 401.72Å 177.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	95.34 – 3.40 94.29 – 3.11	Depositor EDS
% Data completeness (in resolution range)	88.9 (95.34-3.40) 83.7 (94.29-3.11)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.74 (at 3.13Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.232 , 0.280 0.213 , 0.257	Depositor DCC
$R_{free}$ test set	8780 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	80.5	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 105.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	51910	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% 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: ZN, PCY, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.53	0/36259	0.75	42/56593 (0.1%)
2	X	0.56	0/128	0.71	0/196
3	B	0.39	0/1935	0.69	0/2609
4	C	0.38	0/1636	0.65	0/2205
5	D	0.43	0/1733	0.71	1/2318 (0.0%)
6	E	0.49	0/1162	0.80	2/1564 (0.1%)
7	F	0.35	0/856	0.65	0/1154
8	G	0.36	0/1276	0.64	0/1709
9	H	0.47	0/1136	0.78	0/1527
10	I	0.35	0/1029	0.66	0/1378
11	J	0.37	0/805	0.68	0/1082
12	K	0.40	0/900	0.75	0/1213
13	L	0.43	0/986	0.75	0/1320
14	M	0.35	0/1008	0.68	0/1347
15	N	0.41	0/501	0.78	0/664
16	O	0.39	0/745	0.64	0/992
17	P	0.46	0/751	0.76	0/1008
18	Q	0.50	0/870	0.78	0/1159
19	R	0.38	0/603	0.65	0/799
20	S	0.35	0/661	0.68	1/890 (0.1%)
21	T	0.38	0/764	0.73	0/1006
22	V	0.50	0/212	0.64	0/277
All	All	0.49	0/55956	0.74	46/83010 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	2	47

There are no bond length outliers.

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1498	U	C2'-C3'-O3'	9.79	131.03	109.50
1	A	1085	U	C2'-C3'-O3'	9.22	129.78	109.50
1	A	60	A	C2'-C3'-O3'	8.05	127.22	109.50
1	A	484	G	C2'-C3'-O3'	7.86	126.78	109.50
1	A	181	G	C2'-C3'-O3'	7.65	126.34	109.50
1	A	243	A	C2'-C3'-O3'	7.49	125.97	109.50
1	A	559	A	C2'-C3'-O3'	7.46	125.92	109.50
1	A	108	G	O4'-C1'-N9	7.26	114.01	108.20
1	A	1346	A	C2'-C3'-O3'	7.25	125.44	109.50
1	A	575	G	C2'-C3'-O3'	7.18	125.29	109.50
1	A	1528	U	C2'-C3'-O3'	7.09	125.09	109.50
1	A	1502	A	N9-C1'-C2'	6.79	122.83	114.00
1	A	792	A	C2'-C3'-O3'	6.65	124.34	113.70
1	A	7	G	C2'-C3'-O3'	6.52	124.13	113.70
1	A	1502	A	C1'-O4'-C4'	-6.46	104.73	109.90
6	E	21	ALA	N-CA-C	-6.44	93.62	111.00
1	A	197	A	N9-C1'-C2'	6.42	122.34	114.00
1	A	372	C	C2'-C3'-O3'	6.37	123.89	113.70
1	A	366	C	C2'-C3'-O3'	6.16	123.56	113.70
1	A	266	G	C2'-C3'-O3'	6.15	123.54	113.70
1	A	1299	A	N9-C1'-C2'	6.00	121.80	114.00
5	D	12	CYS	CA-CB-SG	5.96	124.73	114.00
1	A	1124	G	N9-C1'-C2'	5.89	121.66	114.00
1	A	266	G	O4'-C1'-N9	-5.77	103.59	108.20
1	A	560	U	C2'-C3'-O3'	5.72	122.86	113.70
1	A	107	G	N9-C1'-C2'	-5.62	105.82	112.00
1	A	898	G	N9-C1'-C2'	-5.59	105.85	112.00
1	A	243	A	N9-C1'-C2'	5.55	121.22	114.00
1	A	533	A	N9-C1'-C2'	5.54	121.20	114.00
1	A	1380	U	C2'-C3'-O3'	5.54	122.56	113.70
1	A	1504	G	C2'-C3'-O3'	5.53	122.54	113.70
6	E	64	ARG	N-CA-C	-5.51	96.13	111.00
1	A	533	A	C2'-C3'-O3'	5.46	122.44	113.70
1	A	960	U	C2'-C3'-O3'	5.44	122.41	113.70
1	A	1139	G	N9-C1'-C2'	5.34	120.94	114.00
1	A	760	G	N9-C1'-C2'	-5.34	106.13	112.00
1	A	1528	U	C4'-C3'-C2'	5.33	107.92	102.60
1	A	328	C	C2'-C3'-O3'	5.26	122.11	113.70
1	A	586	C	N1-C1'-C2'	-5.25	106.23	112.00
1	A	220	G	N9-C1'-C2'	-5.22	106.26	112.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	5	U	N1-C1'-C2'	5.20	120.76	114.00
1	A	1281	U	N1-C1'-C2'	5.19	120.75	114.00
1	A	748	C	N1-C1'-C2'	5.07	120.60	114.00
20	S	54	GLY	N-CA-C	-5.07	100.43	113.10
1	A	1145	C	C2'-C3'-O3'	5.06	121.79	113.70
1	A	115	G	C2'-C3'-O3'	5.05	121.78	113.70

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1085	U	C3'
1	A	1498	U	C3'

All (47) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1048	G	Sidechain
1	A	1077	G	Sidechain
1	A	1079	G	Sidechain
1	A	1080	A	Sidechain
1	A	116	A	Sidechain
1	A	1166	G	Sidechain
1	A	1196	U	Sidechain
1	A	1205	U	Sidechain
1	A	1226	C	Sidechain
1	A	126	G	Sidechain
1	A	1281	U	Sidechain
1	A	1299	A	Sidechain
1	A	1393	U	Sidechain
1	A	1396	A	Sidechain
1	A	1454	G	Sidechain
1	A	1522	U	Sidechain
1	A	197	A	Sidechain
1	A	203	U	Sidechain
1	A	226	G	Sidechain
1	A	250	A	Sidechain
1	A	251	G	Sidechain
1	A	253	U	Sidechain
1	A	262	A	Sidechain
1	A	266	G	Sidechain
1	A	47	C	Sidechain
1	A	490	G	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
1	A	5	U	Sidechain
1	A	516	U	Sidechain
1	A	561	U	Sidechain
1	A	572	A	Sidechain
1	A	575	G	Sidechain
1	A	576	G	Sidechain
1	A	597	G	Sidechain
1	A	636	U	Sidechain
1	A	657	G	Sidechain
1	A	664	G	Sidechain
1	A	733	A	Sidechain
1	A	77	G	Sidechain
1	A	773	G	Sidechain
1	A	785	G	Sidechain
1	A	876	G	Sidechain
1	A	879	C	Sidechain
1	A	898	G	Sidechain
1	A	915	A	Sidechain
1	A	931	C	Sidechain
1	A	952	U	Sidechain
1	A	997	U	Sidechain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32391	0	16349	1512	0
2	X	117	0	64	3	0
3	B	1900	0	1951	289	0
4	C	1612	0	1677	276	0
5	D	1703	0	1764	182	0
6	E	1146	0	1207	120	0
7	F	843	0	857	83	0
8	G	1257	0	1296	113	0
9	H	1116	0	1177	96	0
10	I	1011	0	1043	151	0
11	J	792	0	835	158	0
12	K	885	0	904	100	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	L	970	0	1057	125	0
14	M	997	0	1072	142	0
15	N	492	0	529	87	0
16	O	734	0	771	63	0
17	P	735	0	752	67	0
18	Q	857	0	930	104	0
19	R	597	0	668	106	0
20	S	647	0	673	105	0
21	T	762	0	859	106	0
22	V	208	0	221	20	0
23	A	94	0	0	0	0
23	D	1	0	0	0	0
23	H	1	0	0	0	0
24	D	1	0	0	0	0
24	N	1	0	0	0	0
25	A	40	0	38	10	0
All	All	51910	0	36694	3662	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 42.

All (3662) 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)
25:A:1632:PCY:C3	25:A:1632:PCY:N2	1.69	1.49
13:L:28:LYS:HD2	13:L:33:ARG:HH22	1.01	1.16
12:K:110:ASP:HB2	19:R:88:LYS:HD2	1.28	1.15
6:E:110:LEU:HD13	6:E:118:ILE:HD12	1.28	1.15
4:C:58:GLU:HB3	11:J:92:THR:HG21	1.29	1.15
1:A:1443:G:H5''	1:A:1446:A:H5'	1.29	1.13
1:A:1256:A:H4'	1:A:1257:U:H5'	1.31	1.12
13:L:41:ARG:HG2	13:L:42:THR:H	1.15	1.12
1:A:1057:G:H5''	4:C:154:SER:HB2	1.33	1.11
5:D:36:ARG:H	5:D:37:PRO:HD3	1.08	1.09
10:I:8:GLY:HA2	10:I:79:LEU:HD12	1.33	1.08
8:G:69:VAL:HG21	8:G:104:LEU:HD21	1.32	1.07
19:R:55:ARG:HB3	19:R:55:ARG:HH11	1.16	1.06
1:A:243:A:H4'	1:A:244:U:H5'	1.34	1.05
4:C:191:THR:HG22	4:C:193:TYR:H	1.19	1.05
6:E:81:GLU:HG2	6:E:90:VAL:HG22	1.39	1.04
1:A:1238:A:H5'	1:A:1336:C:H41	1.20	1.04

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:52:LEU:HD23	4:C:52:LEU:H	1.22	1.04
4:C:172:ARG:HH11	4:C:172:ARG:HB3	1.19	1.03
3:B:77:ALA:HB2	3:B:211:ILE:HD13	1.38	1.02
11:J:51:ARG:HB2	11:J:59:SER:HB3	1.39	1.01
1:A:64:G:H4'	1:A:65:U:O5'	1.57	1.01
8:G:75:VAL:HG11	8:G:86:GLN:HB3	1.43	1.01
4:C:188:LEU:HD13	4:C:189:ALA:H	1.23	1.01
1:A:839:U:H5'	1:A:840:C:H5	1.25	1.00
5:D:150:GLU:H	5:D:150:GLU:CD	1.62	1.00
4:C:14:ILE:HG22	4:C:15:THR:H	1.25	1.00
3:B:80:ILE:HD11	3:B:208:ILE:HG23	1.41	1.00
1:A:1116:C:H2'	1:A:1117:G:H5''	1.42	0.99
6:E:9:LYS:HG3	6:E:112:LEU:HD11	1.44	0.99
1:A:1250:A:H4'	10:I:68:GLY:H	1.29	0.98
1:A:787:A:H2	25:A:1632:PCY:H111	1.24	0.98
12:K:54:ARG:HB3	12:K:54:ARG:HH11	1.29	0.98
1:A:1086:U:H3	1:A:1099:G:H22	1.07	0.98
13:L:60:LEU:HD11	13:L:85:ILE:HD12	1.45	0.98
1:A:80:G:H3'	1:A:81:U:H5''	1.46	0.97
3:B:132:LYS:HA	3:B:135:GLN:HB3	1.43	0.97
13:L:38:THR:HG22	13:L:39:VAL:HG23	1.46	0.97
4:C:94:LEU:HD23	4:C:95:THR:HG23	1.47	0.97
19:R:55:ARG:HB3	19:R:55:ARG:NH1	1.78	0.97
1:A:579:G:H5'	1:A:728:A:H1'	1.47	0.97
14:M:11:ARG:HG2	14:M:12:ASN:H	1.28	0.96
14:M:11:ARG:HG2	14:M:12:ASN:N	1.79	0.96
1:A:1101:A:H4'	1:A:1102:A:O5'	1.59	0.96
1:A:1125:U:H3	11:J:5:ARG:HH21	1.12	0.96
17:P:22:THR:HA	17:P:33:ILE:HD13	1.44	0.96
13:L:27:LEU:HG	13:L:28:LYS:H	1.29	0.95
1:A:141:A:H1'	1:A:182:U:O2	1.66	0.94
3:B:168:THR:OG1	3:B:192:SER:HB3	1.67	0.94
14:M:49:THR:HG22	14:M:51:ALA:H	1.28	0.94
1:A:787:A:C2	25:A:1632:PCY:H111	2.01	0.94
1:A:1366:C:H2'	1:A:1367:C:H6	1.33	0.94
1:A:877:C:O2	9:H:3:THR:HG21	1.68	0.93
4:C:131:ARG:HG2	4:C:135:LYS:HE3	1.50	0.93
1:A:1305:G:O2'	1:A:1306:A:H8	1.50	0.93
1:A:195:A:H4'	21:T:68:LYS:HE2	1.49	0.93
1:A:761:G:H1'	18:Q:104:LYS:O	1.69	0.93
4:C:172:ARG:NH1	4:C:172:ARG:HB3	1.84	0.92

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:29:PRO:O	5:D:30:LYS:HG3	1.69	0.92
8:G:54:THR:HG22	8:G:56:GLN:H	1.34	0.92
12:K:40:ILE:HG22	12:K:41:THR:HG23	1.51	0.92
6:E:80:ILE:HD11	6:E:138:ALA:HB1	1.49	0.91
5:D:57:ARG:HB3	5:D:206:PHE:HB2	1.53	0.91
20:S:55:LYS:HG2	20:S:56:GLN:HE21	1.31	0.91
6:E:43:LEU:HD11	6:E:132:ALA:HB1	1.51	0.91
13:L:24:VAL:HG13	13:L:98:TYR:HE2	1.34	0.91
1:A:1131:G:H1	1:A:1143:G:H21	1.09	0.91
3:B:8:LYS:O	3:B:9:GLU:HB2	1.71	0.91
11:J:31:GLY:HA2	11:J:78:ASN:HD22	1.34	0.90
1:A:371:G:O2'	1:A:372:C:H5'	1.72	0.90
14:M:16:ASP:HB3	14:M:41:PRO:HB3	1.54	0.90
3:B:84:GLU:HB3	3:B:219:VAL:HG21	1.52	0.90
19:R:53:ARG:NH1	19:R:59:SER:HA	1.86	0.90
16:O:56:LEU:HA	16:O:59:MET:HE2	1.52	0.90
21:T:54:LYS:HG3	21:T:100:ILE:HD13	1.53	0.90
1:A:1116:C:C2'	1:A:1117:G:H5''	2.00	0.90
3:B:102:LEU:HD21	3:B:162:ILE:HD11	1.54	0.89
5:D:36:ARG:N	5:D:37:PRO:HD3	1.83	0.89
13:L:28:LYS:HD2	13:L:33:ARG:NH2	1.87	0.89
1:A:351:G:H4'	1:A:352:C:OP1	1.72	0.89
3:B:200:ILE:HG22	3:B:202:PRO:HD3	1.54	0.89
4:C:188:LEU:CD1	4:C:189:ALA:H	1.85	0.89
4:C:34:LEU:HD23	4:C:34:LEU:O	1.73	0.89
1:A:135:C:O2	17:P:1:MET:HB2	1.73	0.89
1:A:1152:A:H5''	11:J:13:HIS:CD2	2.07	0.89
20:S:33:THR:HG22	20:S:35:SER:H	1.38	0.88
20:S:40:ILE:HD13	20:S:62:ILE:HD13	1.54	0.88
13:L:41:ARG:HG2	13:L:42:THR:N	1.89	0.88
4:C:179:ARG:HD3	4:C:206:GLU:HG2	1.56	0.87
4:C:190:ARG:HH11	4:C:190:ARG:HB3	1.40	0.87
5:D:36:ARG:H	5:D:37:PRO:CD	1.88	0.87
10:I:70:LYS:O	10:I:74:ILE:HG13	1.74	0.87
20:S:28:LYS:HG2	20:S:29:ARG:H	1.39	0.87
7:F:36:ARG:HH12	7:F:38:GLU:HG2	1.40	0.87
1:A:447:G:H2'	1:A:485:G:N2	1.90	0.87
7:F:8:ILE:HD11	7:F:79:LEU:HD13	1.56	0.87
3:B:74:LYS:NZ	3:B:206:ASP:HA	1.89	0.87
13:L:75:HIS:HD2	13:L:77:LEU:H	1.18	0.87
5:D:70:ILE:HD11	5:D:100:ARG:CZ	2.05	0.87

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:21:LEU:O	7:F:24:GLU:HB3	1.74	0.87
1:A:761:G:H4'	18:Q:103:GLY:N	1.90	0.87
1:A:1137:C:H4'	1:A:1138:G:C2	2.09	0.87
1:A:1190:G:OP1	4:C:4:LYS:HA	1.74	0.87
6:E:115:VAL:HG11	6:E:118:ILE:HD11	1.57	0.87
12:K:48:ILE:HG22	12:K:49:GLY:H	1.38	0.86
15:N:26:ARG:NH1	15:N:47:LEU:HG	1.90	0.86
21:T:43:LEU:HD13	21:T:51:GLU:HG3	1.55	0.86
1:A:99:C:H2'	1:A:101:A:C8	2.09	0.86
6:E:144:THR:HG22	6:E:146:ALA:H	1.38	0.86
1:A:977:A:H2'	1:A:978:A:H5''	1.55	0.86
4:C:195:VAL:O	4:C:196:LEU:HD23	1.76	0.86
13:L:46:LYS:HG2	13:L:47:LYS:H	1.41	0.86
4:C:179:ARG:HG2	4:C:179:ARG:O	1.75	0.85
11:J:60:ARG:HD2	11:J:60:ARG:N	1.89	0.85
8:G:12:LEU:HD12	8:G:12:LEU:H	1.40	0.85
1:A:1125:U:H3	11:J:5:ARG:NH2	1.72	0.85
4:C:102:ASN:N	4:C:102:ASN:HD22	1.70	0.85
3:B:53:ARG:HH12	3:B:199:TYR:HD2	1.24	0.84
11:J:39:PRO:HA	11:J:70:ARG:NH1	1.91	0.84
12:K:18:ARG:HB2	12:K:33:THR:CG2	2.07	0.84
1:A:250:A:H4'	1:A:251:G:O5'	1.77	0.84
3:B:61:LEU:HD23	3:B:66:GLY:HA3	1.59	0.84
5:D:111:ALA:HB2	5:D:120:LEU:HD12	1.57	0.84
4:C:26:LYS:HE2	4:C:26:LYS:H	1.40	0.84
1:A:1497:G:O2'	1:A:1498:U:H5'	1.76	0.84
1:A:1369:C:H2'	1:A:1370:G:C8	2.12	0.84
3:B:74:LYS:HZ2	3:B:206:ASP:HA	1.40	0.83
13:L:46:LYS:HZ1	13:L:47:LYS:HE3	1.43	0.83
1:A:501:C:H2'	1:A:502:G:H8	1.42	0.83
10:I:8:GLY:CA	10:I:79:LEU:HD12	2.09	0.83
16:O:87:ILE:O	16:O:88:ARG:HB2	1.76	0.83
1:A:1047:G:H5''	15:N:4:LYS:HD2	1.60	0.83
5:D:61:LYS:HD2	5:D:207:TYR:OH	1.78	0.83
4:C:34:LEU:HD12	15:N:25:VAL:HG21	1.59	0.83
13:L:41:ARG:CG	13:L:42:THR:H	1.91	0.83
1:A:1257:U:H4'	1:A:1258:G:O5'	1.78	0.83
21:T:44:ALA:HB2	21:T:88:VAL:HG13	1.60	0.83
3:B:68:ILE:H	3:B:90:MET:CE	1.92	0.83
8:G:71:PRO:HD3	8:G:103:TRP:HZ3	1.42	0.83
8:G:26:PHE:CE2	8:G:30:ILE:HD11	2.14	0.83

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:14:PRO:C	15:N:16:PHE:H	1.80	0.83
20:S:20:LEU:HA	20:S:23:ASN:ND2	1.93	0.83
10:I:26:VAL:HB	10:I:33:PHE:HB2	1.60	0.83
19:R:53:ARG:HH11	19:R:59:SER:HA	1.44	0.83
1:A:1368:G:O2'	1:A:1369:C:H5'	1.79	0.82
3:B:17:PHE:HB3	3:B:44:LEU:HD11	1.59	0.82
4:C:26:LYS:CE	4:C:26:LYS:H	1.92	0.82
9:H:51:VAL:HG12	9:H:52:ASP:H	1.43	0.82
1:A:664:G:H22	1:A:741:G:H1	1.25	0.82
4:C:10:PHE:CE2	4:C:178:LEU:HD13	2.14	0.82
4:C:190:ARG:NH1	4:C:190:ARG:HB3	1.94	0.82
11:J:45:ARG:O	11:J:64:GLU:HA	1.79	0.82
14:M:117:VAL:HG12	14:M:118:ALA:H	1.43	0.82
5:D:32:ALA:C	5:D:34:GLU:H	1.81	0.82
1:A:1025:U:H2'	1:A:1026:G:C8	2.14	0.82
4:C:150:LYS:HE2	4:C:152:ILE:HD11	1.62	0.82
3:B:18:GLY:HA2	3:B:42:ILE:H	1.42	0.82
4:C:174:PRO:HB2	4:C:177:THR:HG22	1.62	0.82
4:C:91:LEU:HD23	4:C:92:ALA:N	1.93	0.82
9:H:51:VAL:HG21	9:H:60:ARG:HG2	1.61	0.82
1:A:701:C:H5'	1:A:703:G:O4'	1.79	0.82
1:A:839:U:H5'	1:A:840:C:C5	2.15	0.82
16:O:26:GLU:OE1	16:O:77:ARG:HD2	1.80	0.81
4:C:84:ILE:O	4:C:88:ARG:HB2	1.79	0.81
8:G:75:VAL:CG1	8:G:86:GLN:HB3	2.10	0.81
1:A:1225:A:H5'	14:M:103:THR:OG1	1.80	0.81
14:M:5:ALA:HB3	14:M:8:GLU:HG3	1.60	0.81
1:A:1056:U:H5'	4:C:163:ALA:HB2	1.63	0.81
5:D:25:ARG:C	5:D:27:TYR:H	1.82	0.81
15:N:27:CYS:SG	15:N:29:ARG:HB2	2.20	0.81
4:C:113:ALA:HB3	4:C:114:PRO:HD3	1.63	0.81
13:L:27:LEU:O	13:L:29:GLY:N	2.12	0.81
13:L:24:VAL:HG13	13:L:98:TYR:CE2	2.14	0.81
1:A:1352:C:H2'	1:A:1353:G:C8	2.16	0.81
5:D:110:PHE:H	5:D:110:PHE:HD1	1.28	0.81
14:M:33:ALA:HA	14:M:59:TYR:HE2	1.45	0.81
1:A:974:A:OP1	15:N:31:ARG:HG2	1.81	0.81
1:A:1236:A:H4'	1:A:1304:G:H4'	1.62	0.81
3:B:72:GLY:HA3	3:B:81:VAL:HG21	1.62	0.81
6:E:41:VAL:HG22	6:E:113:ALA:HA	1.62	0.81
20:S:55:LYS:HG2	20:S:56:GLN:NE2	1.96	0.81

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1238:A:H5'	1:A:1336:C:N4	1.95	0.81
11:J:22:LYS:HE2	11:J:90:LEU:HD12	1.63	0.80
19:R:42:ARG:NH1	19:R:42:ARG:HB3	1.96	0.80
1:A:243:A:C4'	1:A:244:U:H5'	2.11	0.80
1:A:1256:A:H8	4:C:27:LYS:HZ1	1.26	0.80
1:A:328:C:H2'	1:A:328:C:O2	1.82	0.80
1:A:1281:U:H5'	1:A:1282:C:C5	2.17	0.80
19:R:42:ARG:HH11	19:R:42:ARG:HB3	1.46	0.80
1:A:434:U:H2'	1:A:435:C:C6	2.16	0.80
6:E:9:LYS:HD2	6:E:112:LEU:HD21	1.63	0.80
1:A:953:G:H1'	14:M:125:ARG:CB	2.12	0.80
5:D:170:VAL:HG13	5:D:174:LEU:HB2	1.64	0.80
11:J:31:GLY:HA2	11:J:78:ASN:ND2	1.96	0.79
1:A:31:G:N1	1:A:48:C:H5''	1.97	0.79
1:A:80:G:C3'	1:A:81:U:H5''	2.12	0.79
1:A:975:A:H8	1:A:975:A:H5'	1.47	0.79
3:B:55:PHE:HE2	3:B:218:ALA:HA	1.47	0.79
4:C:64:VAL:HG23	4:C:99:VAL:HB	1.63	0.79
17:P:20:VAL:HG11	17:P:32:TYR:CB	2.11	0.79
1:A:1142:G:H2'	1:A:1143:G:O4'	1.82	0.79
1:A:1040:U:H2'	1:A:1041:A:C8	2.17	0.79
5:D:156:GLU:HG2	5:D:160:GLN:HE21	1.48	0.79
1:A:1298:C:H2'	8:G:114:ARG:HH12	1.47	0.79
11:J:16:LEU:HD13	11:J:70:ARG:HG2	1.64	0.79
11:J:35:SER:HB2	11:J:72:VAL:O	1.82	0.79
1:A:948:C:OP1	14:M:109:THR:HG22	1.80	0.79
1:A:1060:C:C5	4:C:2:GLY:HA3	2.17	0.79
1:A:694:A:H3'	1:A:695:A:H5''	1.64	0.79
10:I:46:ALA:HA	10:I:78:LYS:HB2	1.63	0.79
21:T:70:SER:HA	21:T:73:HIS:CD2	2.17	0.79
1:A:1281:U:H5'	1:A:1282:C:H5	1.45	0.79
14:M:14:ARG:HG3	14:M:44:ARG:NH1	1.98	0.79
1:A:1533:C:O2	1:A:1533:C:H2'	1.81	0.79
8:G:71:PRO:HD3	8:G:103:TRP:CZ3	2.17	0.79
1:A:1226:C:H4'	1:A:1227:A:OP1	1.83	0.78
14:M:65:LYS:HG3	14:M:69:GLU:OE2	1.83	0.78
1:A:1241:G:H2'	1:A:1242:C:C6	2.18	0.78
11:J:38:ILE:HG13	11:J:72:VAL:H	1.47	0.78
12:K:18:ARG:HB2	12:K:33:THR:HG23	1.64	0.78
22:V:6:ARG:HD2	22:V:15:ARG:NH1	1.97	0.78
1:A:173:U:H5'	1:A:197:A:O4'	1.84	0.78

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:15:THR:O	4:C:16:ARG:HB2	1.83	0.78
13:L:75:HIS:CD2	13:L:77:LEU:H	2.01	0.78
9:H:19:VAL:HG23	9:H:21:LYS:HD3	1.65	0.78
14:M:79:LYS:HD3	14:M:83:ASP:OD2	1.83	0.78
1:A:1413:A:H2	1:A:1487:G:H22	1.30	0.78
5:D:30:LYS:C	5:D:32:ALA:H	1.85	0.78
1:A:1356:G:H2'	1:A:1357:A:C8	2.19	0.78
5:D:23:GLY:HA3	5:D:112:VAL:HG12	1.65	0.77
12:K:54:ARG:O	12:K:57:THR:HG22	1.84	0.77
14:M:40:ASN:HD22	14:M:41:PRO:CD	1.97	0.77
1:A:31:G:H1	1:A:48:C:H5''	1.50	0.77
17:P:32:TYR:HE2	17:P:35:LYS:HB2	1.48	0.77
21:T:54:LYS:HG3	21:T:100:ILE:CD1	2.14	0.77
1:A:1250:A:H4'	10:I:68:GLY:N	1.98	0.77
3:B:51:LEU:HD22	3:B:55:PHE:HE1	1.50	0.77
4:C:29:TYR:OH	15:N:54:PRO:HG2	1.83	0.77
1:A:1064:G:H4'	1:A:1065:U:H5'	1.65	0.77
3:B:124:SER:HB2	3:B:125:PRO:HD2	1.65	0.77
13:L:25:PRO:C	13:L:27:LEU:H	1.84	0.77
18:Q:27:PHE:CZ	18:Q:36:ILE:HD11	2.20	0.77
20:S:52:TYR:HA	20:S:56:GLN:O	1.85	0.77
1:A:1038:C:H2'	1:A:1039:C:C6	2.19	0.77
17:P:74:LEU:O	17:P:79:VAL:HG23	1.85	0.77
1:A:1497:G:C2'	1:A:1498:U:H5'	2.15	0.77
1:A:926:G:H3'	1:A:1505:G:H21	1.50	0.77
1:A:197:A:H4'	1:A:198:G:O5'	1.84	0.77
1:A:35:G:H2'	1:A:36:C:C6	2.19	0.77
1:A:80:G:H3'	1:A:81:U:C5'	2.14	0.77
1:A:1096:C:H2'	1:A:1097:C:H6	1.49	0.76
1:A:1137:C:H4'	1:A:1138:G:N2	2.00	0.76
11:J:61:GLU:OE1	15:N:45:ARG:HD2	1.84	0.76
1:A:954:G:H21	1:A:1227:A:H62	1.32	0.76
1:A:390:C:O3'	17:P:28:ARG:NH2	2.18	0.76
11:J:44:VAL:HG22	11:J:66:ARG:HB3	1.66	0.76
5:D:187:ARG:NH2	5:D:188:LEU:HD12	2.00	0.76
1:A:107:G:C2'	1:A:108:G:H5'	2.16	0.76
1:A:1241:G:H2'	1:A:1242:C:H6	1.50	0.76
1:A:1254:C:OP1	11:J:45:ARG:HD3	1.85	0.76
4:C:108:ASN:ND2	4:C:111:LEU:HG	2.01	0.76
1:A:1141:C:H2'	1:A:1142:G:H8	1.49	0.76
1:A:1224:G:H2'	20:S:78:ARG:HH22	1.48	0.76

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:781:A:H2'	1:A:782:A:H5'	1.68	0.76
6:E:13:ILE:HG22	6:E:30:ALA:HA	1.68	0.76
19:R:34:TYR:CD1	19:R:35:ARG:HG3	2.20	0.76
21:T:50:GLU:HG2	21:T:100:ILE:HG13	1.67	0.76
1:A:1057:G:H5''	4:C:154:SER:CB	2.14	0.76
1:A:1168:A:H2'	1:A:1169:A:C8	2.21	0.76
11:J:62:HIS:HB3	15:N:59:ALA:HB3	1.65	0.76
13:L:6:THR:OG1	13:L:9:GLN:HG3	1.86	0.76
14:M:3:ARG:HG2	14:M:9:ILE:HG23	1.68	0.76
1:A:502:G:H4'	1:A:550:G:H4'	1.68	0.76
16:O:16:ALA:HB1	16:O:21:ASP:HB3	1.68	0.76
18:Q:45:HIS:NE2	18:Q:47:PRO:HG3	2.00	0.76
4:C:26:LYS:CD	4:C:26:LYS:H	1.99	0.76
6:E:105:VAL:HB	6:E:106:PRO:HD3	1.68	0.76
1:A:1130:A:OP2	1:A:1130:A:H3'	1.85	0.75
1:A:818:G:C3'	1:A:819:A:H5''	2.16	0.75
3:B:55:PHE:CE2	3:B:218:ALA:HA	2.21	0.75
3:B:84:GLU:OE1	3:B:216:SER:HA	1.86	0.75
7:F:26:ILE:HG21	7:F:63:TYR:HE2	1.51	0.75
1:A:1279:A:H5''	1:A:1280:A:OP1	1.85	0.75
14:M:11:ARG:CG	14:M:12:ASN:H	1.99	0.75
18:Q:68:ARG:HH11	18:Q:68:ARG:HG2	1.51	0.75
1:A:1285:A:H4'	1:A:1286:A:O5'	1.87	0.75
1:A:992:U:H4'	1:A:993:G:O5'	1.87	0.75
1:A:1251:A:H2'	1:A:1252:A:C8	2.21	0.75
1:A:502:G:H2'	1:A:503:C:H6	1.51	0.75
4:C:8:ILE:HG23	4:C:16:ARG:HG2	1.68	0.75
1:A:1152:A:H5''	11:J:13:HIS:HD2	1.49	0.75
21:T:39:LYS:HG2	21:T:55:ILE:HD13	1.67	0.75
1:A:1443:G:H5''	1:A:1446:A:C5'	2.12	0.75
3:B:139:LYS:O	3:B:143:GLU:HG2	1.85	0.75
9:H:51:VAL:HG12	9:H:52:ASP:N	2.00	0.75
1:A:1391:U:H2'	1:A:1392:G:C8	2.21	0.75
3:B:28:PHE:CZ	3:B:189:ASP:HA	2.22	0.75
11:J:84:GLN:O	11:J:88:LEU:HD12	1.87	0.75
6:E:115:VAL:HG11	6:E:118:ILE:CD1	2.17	0.74
7:F:33:TYR:HB2	7:F:75:LEU:HD23	1.68	0.74
11:J:8:LEU:HD23	11:J:96:ILE:HG12	1.69	0.74
1:A:1281:U:H4'	1:A:1282:C:OP2	1.87	0.74
4:C:11:ARG:HH12	4:C:179:ARG:H	1.36	0.74
11:J:40:LEU:HD11	11:J:71:LEU:HD23	1.69	0.74

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1229:A:H2'	1:A:1230:C:H6	1.52	0.74
18:Q:24:GLU:OE2	18:Q:37:LYS:HD3	1.86	0.74
21:T:57:ARG:HE	21:T:102:GLY:HA3	1.50	0.74
1:A:1028:C:H2'	1:A:1029:C:C6	2.22	0.74
1:A:1126:U:OP2	1:A:1281:U:O2	2.05	0.74
7:F:4:TYR:OH	7:F:69:GLU:HB3	1.88	0.74
11:J:94:VAL:HG12	11:J:95:GLU:H	1.50	0.74
21:T:50:GLU:O	21:T:100:ILE:HD12	1.88	0.74
10:I:9:ARG:HG2	10:I:14:VAL:HG22	1.69	0.74
9:H:91:ARG:HG2	13:L:7:ILE:HG13	1.68	0.74
21:T:67:ALA:HA	21:T:73:HIS:H	1.53	0.74
1:A:840:C:H5''	1:A:841:U:OP1	1.87	0.74
3:B:188:ALA:O	3:B:202:PRO:HA	1.87	0.74
8:G:79:ARG:HG2	8:G:84:ASN:OD1	1.88	0.74
10:I:4:TYR:CE2	10:I:88:TYR:HA	2.23	0.74
13:L:55:VAL:HG12	13:L:56:ALA:N	2.02	0.74
1:A:1230:C:H1'	14:M:126:LYS:HA	1.70	0.74
1:A:1425:U:H2'	1:A:1426:C:C6	2.23	0.74
3:B:67:THR:HA	3:B:90:MET:HE1	1.67	0.74
4:C:6:HIS:CD2	4:C:8:ILE:HB	2.23	0.74
1:A:129(A):G:O2'	1:A:190(E):U:H2'	1.88	0.74
1:A:447:G:H2'	1:A:485:G:H22	1.50	0.74
4:C:177:THR:HG23	4:C:180:ALA:HB2	1.69	0.74
6:E:11:ILE:HG21	6:E:31:LEU:HD12	1.67	0.74
19:R:39:VAL:HG13	19:R:40:LEU:HD23	1.69	0.74
1:A:1372:U:OP1	10:I:71:SER:HB3	1.88	0.73
3:B:18:GLY:HA3	3:B:41:ILE:HA	1.69	0.73
8:G:122:HIS:HA	8:G:125:MET:HE3	1.70	0.73
1:A:959:A:H3'	1:A:960:U:H5''	1.68	0.73
3:B:137:ARG:HB3	3:B:137:ARG:HH11	1.52	0.73
1:A:1231:G:H4'	10:I:126:SER:HB3	1.67	0.73
1:A:107:G:H2'	1:A:108:G:H5'	1.69	0.73
11:J:8:LEU:HB3	11:J:16:LEU:HD22	1.70	0.73
4:C:32:LEU:HD21	4:C:59:ARG:HD2	1.71	0.73
6:E:76:ILE:HG22	6:E:78:HIS:H	1.53	0.73
14:M:78:ILE:HA	14:M:81:LEU:HD21	1.70	0.73
4:C:193:TYR:HE1	4:C:196:LEU:HD11	1.54	0.73
17:P:21:VAL:HG21	17:P:59:TRP:CD1	2.23	0.73
1:A:738:C:P	7:F:92:LYS:HE3	2.29	0.73
17:P:17:TYR:HE1	17:P:41:PRO:HG2	1.52	0.73
14:M:88:ARG:HD2	20:S:3:ARG:HH21	1.53	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1442:G:H21	1:A:1446:A:H3'	1.51	0.73
1:A:437:U:H5''	5:D:155:LEU:HD22	1.71	0.73
6:E:110:LEU:HD13	6:E:118:ILE:CD1	2.12	0.73
11:J:34:VAL:HG22	11:J:74:ILE:HG23	1.69	0.73
16:O:36:ILE:HG12	16:O:59:MET:HE3	1.70	0.73
1:A:1366:C:H2'	1:A:1367:C:C6	2.21	0.73
11:J:90:LEU:H	11:J:91:PRO:HD2	1.53	0.73
9:H:121:ASP:HB2	9:H:125:ARG:HH21	1.53	0.72
1:A:838:G:H2'	1:A:839:U:H5''	1.70	0.72
1:A:839:U:O2	1:A:839:U:H2'	1.88	0.72
3:B:91:PRO:HB3	3:B:154:LEU:HB2	1.69	0.72
17:P:8:ARG:HB2	17:P:28:ARG:NH1	2.04	0.72
1:A:1208:C:H2'	1:A:1209:C:H6	1.53	0.72
1:A:1426:C:H2'	1:A:1427:U:C6	2.25	0.72
1:A:344:A:H4'	1:A:345:C:OP2	1.87	0.72
3:B:88:ALA:HB2	3:B:219:VAL:HG13	1.70	0.72
14:M:40:ASN:HD22	14:M:41:PRO:HD2	1.53	0.72
1:A:1000:U:H2'	1:A:1001:A:C8	2.25	0.72
1:A:1222:G:OP1	20:S:77:THR:HG21	1.88	0.72
1:A:1065:U:H4'	1:A:1066:C:O5'	1.87	0.72
1:A:1149:C:H2'	1:A:1150:U:C6	2.24	0.72
1:A:1356:G:H2'	1:A:1357:A:H8	1.53	0.72
6:E:51:VAL:O	6:E:55:VAL:HG23	1.89	0.72
14:M:34:LEU:CD1	14:M:41:PRO:HA	2.19	0.72
4:C:188:LEU:HD13	4:C:189:ALA:N	2.04	0.72
14:M:14:ARG:HB3	14:M:16:ASP:OD1	1.90	0.72
17:P:20:VAL:CG1	17:P:32:TYR:HB2	2.19	0.72
1:A:1003(A):G:C2	1:A:1004:A:H1'	2.24	0.72
11:J:8:LEU:HB2	11:J:70:ARG:HB2	1.71	0.72
1:A:101:A:O2'	1:A:102:G:H5'	1.90	0.72
1:A:1442:G:N2	1:A:1446:A:H3'	2.03	0.72
1:A:113:G:H1'	1:A:354:G:H5'	1.70	0.72
1:A:977:A:C2'	1:A:978:A:H5''	2.20	0.72
3:B:51:LEU:HD22	3:B:55:PHE:CE1	2.25	0.72
7:F:10:LEU:HD12	7:F:59:TYR:HB3	1.71	0.72
3:B:23:ARG:NH1	3:B:24:TRP:HA	2.05	0.71
4:C:14:ILE:HG22	4:C:15:THR:N	2.04	0.71
5:D:162:LEU:HD13	5:D:181:MET:HG2	1.72	0.71
1:A:737:A:H1'	7:F:73:ASN:HD21	1.55	0.71
21:T:57:ARG:NE	21:T:102:GLY:HA3	2.05	0.71
1:A:1064:G:H4'	1:A:1065:U:C5'	2.20	0.71

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1323:G:H2'	1:A:1324:A:C8	2.26	0.71
1:A:448:A:OP2	1:A:485:G:N2	2.23	0.71
1:A:818:G:O2'	1:A:819:A:H5''	1.89	0.71
3:B:16:HIS:NE2	3:B:214:ILE:HG12	2.05	0.71
4:C:64:VAL:HB	4:C:99:VAL:HG21	1.71	0.71
11:J:49:VAL:O	11:J:60:ARG:HA	1.89	0.71
1:A:975:A:C8	1:A:975:A:H5'	2.25	0.71
1:A:1298:C:C5	8:G:114:ARG:HD3	2.24	0.71
10:I:78:LYS:HD3	10:I:101:PHE:HD2	1.54	0.71
11:J:38:ILE:HG13	11:J:71:LEU:HB3	1.70	0.71
14:M:81:LEU:HD12	14:M:88:ARG:HD3	1.72	0.71
22:V:10:ARG:HA	22:V:13:ILE:HD12	1.72	0.71
1:A:189:G:H2'	1:A:190:C:C6	2.25	0.71
1:A:650:G:O2'	1:A:651:C:H5'	1.90	0.71
6:E:92:LYS:O	6:E:118:ILE:HG22	1.91	0.71
12:K:51:LYS:O	12:K:55:LYS:HE3	1.90	0.71
1:A:1475:G:H2'	1:A:1476:G:H8	1.54	0.71
5:D:32:ALA:C	5:D:34:GLU:N	2.43	0.71
15:N:14:PRO:HB2	15:N:16:PHE:O	1.90	0.71
1:A:818:G:C2'	1:A:819:A:H5''	2.21	0.71
1:A:882:C:O2'	1:A:883:C:H5'	1.90	0.71
13:L:83:VAL:HG22	13:L:84:LEU:H	1.56	0.71
18:Q:59:ILE:HG23	18:Q:71:PHE:HB3	1.70	0.71
1:A:1053:G:C3'	1:A:1054:C:H5'	2.21	0.71
1:A:1443:G:C5'	1:A:1446:A:H5'	2.16	0.71
1:A:266:G:C8	1:A:266:G:H5''	2.25	0.71
13:L:55:VAL:HG12	13:L:56:ALA:H	1.55	0.71
3:B:15:VAL:CG1	3:B:209:ARG:HG3	2.20	0.71
19:R:36:ASN:ND2	19:R:38:GLU:HG2	2.05	0.71
4:C:52:LEU:HD21	4:C:118:GLN:HE22	1.55	0.71
6:E:120:THR:HG23	6:E:121:LYS:N	2.04	0.71
1:A:1316:G:H4'	15:N:18:VAL:HG11	1.73	0.71
1:A:1182:G:H4'	1:A:1183:A:H5''	1.73	0.70
12:K:43:SER:HA	12:K:47:VAL:HG21	1.73	0.70
1:A:524:G:H2'	1:A:525:C:C6	2.25	0.70
3:B:218:ALA:O	3:B:222:ILE:HG13	1.91	0.70
14:M:29:ARG:HB3	14:M:64:TRP:CH2	2.27	0.70
17:P:67:THR:HG22	17:P:68:ASP:N	2.06	0.70
1:A:1072:G:H2'	1:A:1073:U:C6	2.25	0.70
1:A:922:G:H5'	6:E:19:MET:O	1.89	0.70
7:F:69:GLU:HA	7:F:72:VAL:HG23	1.72	0.70

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1117:G:H4'	10:I:104:ARG:NH1	2.07	0.70
1:A:1256:A:C4'	1:A:1257:U:H5'	2.16	0.70
1:A:1487:G:O2'	1:A:1488:G:H5'	1.90	0.70
1:A:976:G:OP2	1:A:1358:U:H1'	1.91	0.70
4:C:91:LEU:HD11	4:C:99:VAL:HG13	1.73	0.70
1:A:939:G:H5''	8:G:102:ARG:NH2	2.07	0.70
11:J:56:HIS:O	11:J:58:ASP:N	2.24	0.70
19:R:48:GLY:H	19:R:82:THR:HA	1.57	0.70
1:A:1493:A:O2'	1:A:1494:G:H5'	1.90	0.70
1:A:822:C:O2'	1:A:823:G:H5'	1.92	0.70
5:D:173:TRP:HB2	5:D:187:ARG:O	1.91	0.70
1:A:1347:G:C8	10:I:107:ARG:HB3	2.26	0.70
3:B:23:ARG:N	3:B:23:ARG:HD3	2.06	0.70
14:M:11:ARG:CG	14:M:12:ASN:N	2.55	0.70
1:A:1238:A:C8	1:A:1303:C:H1'	2.26	0.70
1:A:17:U:H2'	1:A:18:C:C6	2.25	0.70
1:A:353:A:H5'	1:A:353:A:H8	1.57	0.70
1:A:1343:G:H1'	10:I:121:ARG:HH12	1.56	0.70
15:N:11:LYS:O	15:N:13:THR:N	2.25	0.70
20:S:16:LEU:O	20:S:19:VAL:HG12	1.91	0.70
4:C:134:ILE:HG23	4:C:151:VAL:HB	1.73	0.70
5:D:152:SER:HB3	5:D:155:LEU:HD12	1.73	0.70
8:G:149:ARG:O	8:G:149:ARG:HD2	1.91	0.70
1:A:953:G:H1'	14:M:125:ARG:HB3	1.74	0.70
1:A:1124:G:H3'	1:A:1145:C:H41	1.55	0.70
1:A:1495:U:H2'	1:A:1496:C:C6	2.26	0.70
1:A:481:G:O2'	1:A:482:A:N7	2.24	0.70
1:A:646:U:H2'	1:A:647:C:C6	2.26	0.70
11:J:8:LEU:HD12	11:J:20:ALA:HB2	1.72	0.70
14:M:49:THR:HG22	14:M:51:ALA:N	2.04	0.70
14:M:50:GLU:O	14:M:54:VAL:HG23	1.92	0.70
10:I:97:LYS:HG3	10:I:102:LEU:HD12	1.72	0.69
13:L:126:LYS:N	13:L:126:LYS:HD2	2.07	0.69
14:M:33:ALA:HA	14:M:59:TYR:CE2	2.27	0.69
1:A:501:C:H2'	1:A:502:G:C8	2.27	0.69
6:E:15:ARG:HD3	6:E:26:PHE:CD2	2.25	0.69
13:L:42:THR:CG2	13:L:52:LEU:HB3	2.22	0.69
1:A:518:C:O2'	13:L:50:SER:HB3	1.92	0.69
7:F:26:ILE:HG21	7:F:63:TYR:CE2	2.26	0.69
11:J:94:VAL:HG12	11:J:95:GLU:N	2.07	0.69
1:A:382:A:H2'	1:A:383:A:C8	2.27	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:87:VAL:HG13	8:G:88:PRO:HD2	1.73	0.69
14:M:52:GLU:HG2	14:M:55:ARG:HH21	1.56	0.69
1:A:440:A:H5'	1:A:442:C:OP2	1.91	0.69
4:C:180:ALA:O	4:C:181:ASN:HB3	1.93	0.69
5:D:187:ARG:HH21	5:D:188:LEU:HD12	1.58	0.69
1:A:1438:G:H2'	1:A:1439:C:C6	2.28	0.69
8:G:116:ALA:HA	8:G:119:ARG:NH2	2.08	0.69
1:A:1030(A):G:N2	1:A:1030(C):G:H3'	2.07	0.69
3:B:19:HIS:HD2	3:B:205:ASP:OD1	1.76	0.69
5:D:187:ARG:HH21	5:D:188:LEU:HB2	1.57	0.69
5:D:187:ARG:NE	5:D:188:LEU:H	1.90	0.69
1:A:923:A:OP1	6:E:21:ALA:HB2	1.91	0.69
12:K:44:SER:H	12:K:47:VAL:HB	1.57	0.69
13:L:27:LEU:HG	13:L:28:LYS:N	2.05	0.69
14:M:117:VAL:HG12	14:M:118:ALA:N	2.07	0.69
1:A:1003(A):G:H2'	1:A:1004:A:H4'	1.73	0.69
1:A:1038:C:H2'	1:A:1039:C:H6	1.56	0.69
1:A:1035:A:H2'	1:A:1036:G:H8	1.58	0.69
1:A:192:U:H2'	1:A:193:C:H6	1.58	0.69
3:B:71:VAL:O	3:B:165:VAL:HG23	1.93	0.69
8:G:85:TYR:O	8:G:87:VAL:HG23	1.93	0.69
12:K:86:GLY:H	12:K:112:THR:HG23	1.58	0.69
17:P:17:TYR:CE1	17:P:41:PRO:HG2	2.28	0.69
19:R:26:LEU:HD11	19:R:39:VAL:HG23	1.74	0.69
1:A:502:G:H2'	1:A:503:C:C6	2.28	0.68
7:F:100:ASN:HD22	19:R:23:LYS:HG2	1.58	0.68
1:A:1128:C:H4'	10:I:16:ARG:HH12	1.58	0.68
1:A:287:U:O2'	1:A:288:A:H5'	1.92	0.68
4:C:52:LEU:CD2	4:C:52:LEU:H	2.01	0.68
7:F:19:LEU:HD23	7:F:19:LEU:C	2.13	0.68
13:L:47:LYS:HB2	13:L:48:PRO:CD	2.23	0.68
18:Q:59:ILE:HG22	18:Q:71:PHE:CD1	2.29	0.68
1:A:406:G:H5'	5:D:5:ILE:HD13	1.74	0.68
1:A:437:U:O2'	1:A:438:G:H5'	1.94	0.68
1:A:926:G:H5'	1:A:927:G:O5'	1.93	0.68
6:E:75:THR:HG23	6:E:76:ILE:N	2.09	0.68
1:A:255:G:H1'	18:Q:16:GLN:NE2	2.09	0.68
1:A:659:U:O2'	1:A:660:G:H5'	1.93	0.68
22:V:6:ARG:NH1	22:V:15:ARG:HH12	1.92	0.68
1:A:1229:A:OP2	14:M:114:ARG:HD3	1.93	0.68
1:A:1316:G:H4'	15:N:18:VAL:CG1	2.24	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:164:ARG:HH11	4:C:164:ARG:HB3	1.59	0.68
5:D:150:GLU:CD	5:D:150:GLU:N	2.42	0.68
10:I:48:GLU:N	10:I:49:PRO:HD2	2.07	0.68
13:L:47:LYS:CB	13:L:48:PRO:HD3	2.24	0.68
1:A:1148:U:H2'	1:A:1149:C:O4'	1.94	0.68
4:C:14:ILE:O	4:C:16:ARG:N	2.27	0.68
12:K:124:LYS:HB3	12:K:125:PHE:CD1	2.29	0.68
16:O:60:VAL:O	16:O:64:ARG:HG2	1.94	0.68
1:A:673:G:H2'	1:A:674:G:C8	2.27	0.68
8:G:145:ALA:C	8:G:147:ALA:H	1.97	0.68
18:Q:74:LEU:HD23	18:Q:74:LEU:C	2.13	0.68
1:A:1223:C:OP1	1:A:1224:G:H3'	1.93	0.68
4:C:175:LEU:HD11	4:C:201:TYR:HE2	1.58	0.68
21:T:45:GLN:HA	21:T:91:LEU:HD22	1.74	0.68
1:A:1277:C:H2'	1:A:1278:U:H5'	1.76	0.68
1:A:1392:G:N2	1:A:1502:A:H8	1.92	0.68
1:A:186:C:O3'	21:T:82:SER:HB3	1.94	0.68
1:A:922:G:H2'	1:A:923:A:C8	2.29	0.68
5:D:98:GLU:HG2	5:D:189:PRO:HG3	1.75	0.68
1:A:371:G:C2'	1:A:372:C:H5'	2.23	0.68
18:Q:97:SER:HB2	18:Q:102:GLY:C	2.14	0.68
3:B:134:GLU:C	3:B:136:VAL:H	1.96	0.67
3:B:209:ARG:HE	3:B:239:VAL:HG11	1.59	0.67
17:P:81:ARG:CG	17:P:83:GLU:HG2	2.24	0.67
1:A:477:G:H2'	1:A:478:A:H8	1.59	0.67
3:B:61:LEU:CD2	3:B:66:GLY:HA3	2.23	0.67
17:P:43:LYS:HG3	17:P:48:TRP:CE3	2.30	0.67
3:B:200:ILE:HG22	3:B:202:PRO:CD	2.24	0.67
4:C:38:ARG:HH11	4:C:38:ARG:HG3	1.59	0.67
4:C:35:GLU:HG3	4:C:95:THR:HG21	1.76	0.67
1:A:1006:C:H2'	1:A:1007:C:H6	1.59	0.67
1:A:1131:G:H1	1:A:1143:G:N2	1.90	0.67
1:A:149:A:H2'	1:A:150:C:C6	2.29	0.67
3:B:68:ILE:H	3:B:90:MET:HE1	1.57	0.67
4:C:34:LEU:HD23	4:C:34:LEU:C	2.14	0.67
11:J:51:ARG:H	11:J:59:SER:CB	2.08	0.67
13:L:83:VAL:CG2	13:L:100:ILE:HG23	2.24	0.67
16:O:17:ARG:HH11	16:O:17:ARG:HG3	1.59	0.67
1:A:838:G:C2'	1:A:839:U:H5''	2.23	0.67
1:A:1226:C:H5''	14:M:103:THR:OG1	1.95	0.67
4:C:52:LEU:HD23	4:C:52:LEU:N	2.04	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:111:ARG:HD3	10:I:112:LYS:N	2.10	0.67
11:J:72:VAL:O	11:J:73:ASP:HB2	1.92	0.67
1:A:538:G:H2'	1:A:539:A:H8	1.60	0.67
3:B:101:MET:HG2	3:B:108:ILE:HD13	1.77	0.67
3:B:114:ARG:NH1	3:B:118:LEU:HD21	2.10	0.67
4:C:191:THR:HG21	4:C:193:TYR:CZ	2.29	0.67
6:E:12:LEU:C	6:E:12:LEU:HD22	2.14	0.67
7:F:95:GLU:H	7:F:95:GLU:CD	1.97	0.67
1:A:130:A:C8	18:Q:63:ARG:HG3	2.30	0.67
19:R:74:ARG:HB3	19:R:81:PHE:CE1	2.30	0.67
19:R:86:VAL:O	19:R:87:ARG:HB2	1.95	0.67
1:A:1319:A:H5'	1:A:1320:C:OP1	1.94	0.67
1:A:657:G:H4'	16:O:28:GLN:HG2	1.75	0.67
5:D:8:VAL:O	5:D:10:ARG:N	2.28	0.67
10:I:118:LYS:O	10:I:119:ALA:HB3	1.94	0.67
10:I:26:VAL:CG1	10:I:28:VAL:HG23	2.24	0.67
17:P:34:GLU:OE2	17:P:55:ARG:HD3	1.95	0.67
1:A:1238:A:N7	1:A:1303:C:H1'	2.10	0.67
1:A:560:U:H5'	1:A:566:G:N2	2.10	0.67
1:A:939:G:H5''	8:G:102:ARG:HH22	1.60	0.67
6:E:15:ARG:O	6:E:27:ARG:O	2.12	0.67
13:L:53:ARG:CB	13:L:93:LEU:HD11	2.25	0.67
1:A:376:G:OP2	17:P:67:THR:HG21	1.95	0.67
1:A:1086:U:H3	1:A:1099:G:N2	1.86	0.66
1:A:1133:G:H2'	1:A:1134:G:H8	1.59	0.66
1:A:1329:A:P	14:M:28:ALA:HB3	2.34	0.66
4:C:102:ASN:N	4:C:102:ASN:ND2	2.40	0.66
4:C:188:LEU:CD1	4:C:195:VAL:HG13	2.26	0.66
1:A:429:U:H2'	5:D:25:ARG:HH12	1.58	0.66
9:H:119:LEU:HD23	9:H:119:LEU:N	2.10	0.66
10:I:26:VAL:HG12	10:I:28:VAL:HG23	1.77	0.66
20:S:11:VAL:HG22	20:S:39:THR:O	1.95	0.66
21:T:85:MET:HE3	21:T:103:GLY:O	1.95	0.66
8:G:116:ALA:HA	8:G:119:ARG:CZ	2.25	0.66
20:S:40:ILE:HD11	20:S:71:LEU:HD23	1.75	0.66
8:G:23:VAL:O	8:G:27:ILE:HG13	1.95	0.66
10:I:97:LYS:CG	10:I:102:LEU:HD12	2.25	0.66
19:R:45:SER:C	19:R:47:THR:H	1.99	0.66
1:A:1515:C:O2'	1:A:1516:G:H5'	1.95	0.66
17:P:20:VAL:HG11	17:P:32:TYR:HB2	1.77	0.66
1:A:1128:C:H1'	1:A:1146:A:H61	1.61	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1117:G:H4'	10:I:104:ARG:HH11	1.60	0.66
12:K:110:ASP:HB2	19:R:88:LYS:CD	2.17	0.66
1:A:1244:C:H2'	1:A:1245:A:C8	2.31	0.66
1:A:189:G:H2'	1:A:190:C:H6	1.60	0.66
3:B:53:ARG:NH1	3:B:199:TYR:HD2	1.92	0.66
4:C:77:ILE:HA	4:C:84:ILE:HB	1.77	0.66
6:E:101:ILE:O	6:E:120:THR:HB	1.95	0.66
11:J:49:VAL:HG13	15:N:41:ARG:HB2	1.77	0.66
15:N:41:ARG:HG3	15:N:42:ILE:N	2.10	0.66
18:Q:101:ARG:HE	18:Q:101:ARG:HA	1.60	0.66
1:A:1338:G:H2'	1:A:1339:A:C8	2.30	0.66
1:A:190(J):U:H2'	1:A:190(K):G:C8	2.31	0.66
7:F:44:GLY:HA2	7:F:59:TYR:CE1	2.31	0.66
1:A:1124:G:H5'	11:J:35:SER:O	1.95	0.66
11:J:78:ASN:O	11:J:80:LYS:N	2.29	0.66
1:A:1117:G:H5'	1:A:1117:G:H8	1.60	0.66
1:A:269:C:H2'	1:A:270:A:C8	2.31	0.66
4:C:191:THR:CG2	4:C:192:THR:N	2.59	0.66
4:C:46:GLU:O	4:C:48:TYR:N	2.29	0.66
7:F:69:GLU:HA	7:F:72:VAL:CG2	2.26	0.66
1:A:1263:C:H2'	1:A:1264:C:C6	2.31	0.66
1:A:1292:U:H5'	10:I:38:GLN:HE22	1.61	0.66
1:A:246:A:N6	1:A:281:G:H1'	2.11	0.66
1:A:853:G:O2'	1:A:854:G:H5'	1.95	0.66
19:R:48:GLY:O	19:R:74:ARG:NH2	2.29	0.66
1:A:1095:U:H2'	1:A:1096:C:C6	2.30	0.65
1:A:328:C:H4'	1:A:329:A:O5'	1.95	0.65
5:D:25:ARG:C	5:D:27:TYR:N	2.48	0.65
1:A:1057:G:O2'	1:A:1058:G:H5'	1.97	0.65
7:F:4:TYR:CZ	7:F:72:VAL:HG21	2.31	0.65
1:A:883:C:O2'	1:A:884:U:H5'	1.96	0.65
4:C:190:ARG:HH11	4:C:190:ARG:CB	2.08	0.65
5:D:148:VAL:CG1	5:D:158:ILE:HD13	2.27	0.65
13:L:45:PRO:HD3	13:L:51:ALA:O	1.96	0.65
1:A:1195:C:H2'	1:A:1197:G:H5'	1.77	0.65
4:C:107:GLN:H	4:C:107:GLN:CD	2.00	0.65
18:Q:95:TYR:C	18:Q:97:SER:H	1.99	0.65
1:A:452:A:HO2'	1:A:453:A:H8	1.45	0.65
8:G:146:GLU:HA	8:G:149:ARG:HB2	1.78	0.65
14:M:54:VAL:O	14:M:58:GLU:HG2	1.96	0.65
18:Q:24:GLU:CD	18:Q:37:LYS:HD3	2.17	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:U:C2'	1:A:438:G:H5'	2.26	0.65
4:C:175:LEU:HD21	4:C:201:TYR:CD2	2.31	0.65
4:C:64:VAL:HB	4:C:99:VAL:CG2	2.27	0.65
5:D:187:ARG:HE	5:D:188:LEU:H	1.45	0.65
11:J:38:ILE:CD1	11:J:71:LEU:HB3	2.26	0.65
11:J:26:ALA:HB1	11:J:84:GLN:HB3	1.79	0.65
13:L:47:LYS:HB2	13:L:48:PRO:HD3	1.77	0.65
18:Q:60:ILE:HD13	18:Q:61:GLU:N	2.12	0.65
20:S:51:VAL:HB	20:S:75:ALA:HB2	1.77	0.65
1:A:723:U:O2	1:A:723:U:H2'	1.95	0.65
3:B:217:ARG:HA	3:B:220:ASP:OD2	1.96	0.65
12:K:57:THR:HG23	12:K:60:ALA:H	1.61	0.65
15:N:9:LYS:HD3	15:N:9:LYS:O	1.96	0.65
20:S:64:GLU:O	20:S:67:VAL:HG23	1.97	0.65
1:A:1278:U:H5''	1:A:1279:A:O4'	1.95	0.65
1:A:1435:G:H2'	1:A:1436:U:C6	2.31	0.65
8:G:50:ILE:O	8:G:54:THR:HB	1.96	0.65
12:K:80:VAL:HG21	12:K:103:LEU:HD13	1.77	0.65
15:N:26:ARG:HH12	15:N:47:LEU:HG	1.62	0.65
19:R:87:ARG:HG2	19:R:87:ARG:HH11	1.61	0.65
20:S:13:ASP:HA	20:S:16:LEU:HB3	1.78	0.65
1:A:267:C:H2'	1:A:268:C:H6	1.62	0.65
3:B:118:LEU:HB2	3:B:142:LEU:HD21	1.79	0.65
5:D:127:THR:HB	5:D:147:ALA:HB3	1.79	0.65
1:A:835:U:OP1	19:R:64:ARG:NH2	2.30	0.65
1:A:1369:C:H2'	1:A:1370:G:H8	1.60	0.65
1:A:1490:C:O2'	1:A:1491:G:H5'	1.97	0.65
3:B:54:THR:HG23	3:B:199:TYR:HB3	1.78	0.65
5:D:28:SER:O	5:D:30:LYS:N	2.30	0.65
9:H:111:ILE:C	9:H:112:LEU:HD23	2.18	0.65
11:J:5:ARG:O	11:J:98:ILE:HG23	1.97	0.65
13:L:27:LEU:C	13:L:29:GLY:H	2.00	0.65
1:A:1163:C:H2'	1:A:1164:G:H8	1.61	0.64
1:A:1529:G:H5'	1:A:1529:G:N3	2.13	0.64
1:A:818:G:H3'	1:A:819:A:C5'	2.27	0.64
3:B:95:GLN:HA	3:B:95:GLN:OE1	1.97	0.64
4:C:59:ARG:HG2	4:C:64:VAL:HG13	1.78	0.64
11:J:55:LYS:O	11:J:56:HIS:HB2	1.97	0.64
21:T:42:GLN:O	21:T:45:GLN:HB3	1.97	0.64
20:S:40:ILE:HB	20:S:67:VAL:O	1.97	0.64
1:A:1355:G:O2'	1:A:1356:G:H5'	1.97	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:U:H2'	1:A:253:U:C6	2.33	0.64
1:A:533:A:H2'	1:A:535:A:OP2	1.98	0.64
6:E:102:ALA:CB	6:E:120:THR:HG21	2.28	0.64
6:E:64:ARG:O	6:E:65:ASN:HB3	1.97	0.64
12:K:14:VAL:HG21	12:K:40:ILE:HD11	1.78	0.64
18:Q:95:TYR:O	18:Q:97:SER:N	2.29	0.64
1:A:1499:A:O2'	1:A:1500:A:H5'	1.98	0.64
1:A:321:A:O2'	1:A:322:C:H5'	1.96	0.64
1:A:370:C:O2'	1:A:371:G:H5'	1.97	0.64
3:B:68:ILE:H	3:B:90:MET:HE2	1.60	0.64
4:C:179:ARG:CG	4:C:179:ARG:O	2.45	0.64
13:L:83:VAL:HG22	13:L:84:LEU:N	2.11	0.64
14:M:22:ILE:HD12	14:M:25:ILE:HD12	1.78	0.64
1:A:1300:G:O2'	1:A:1301:U:H6	1.80	0.64
4:C:188:LEU:HD11	4:C:195:VAL:HG13	1.80	0.64
1:A:587:G:OP1	9:H:89:PRO:HB3	1.97	0.64
13:L:33:ARG:HD3	13:L:62:SER:HB3	1.80	0.64
1:A:255:G:H1'	18:Q:16:GLN:HE22	1.62	0.64
1:A:1527:C:O2'	1:A:1528:U:H5'	1.98	0.64
4:C:177:THR:O	4:C:177:THR:HG23	1.97	0.64
4:C:77:ILE:HG22	4:C:81:GLY:HA2	1.80	0.64
5:D:148:VAL:HG11	5:D:158:ILE:HD13	1.79	0.64
5:D:187:ARG:HE	5:D:188:LEU:N	1.95	0.64
10:I:108:VAL:HG12	10:I:109:VAL:N	2.12	0.64
14:M:4:ILE:HG22	14:M:5:ALA:N	2.13	0.64
22:V:9:ARG:NH1	22:V:22:ARG:HA	2.12	0.64
1:A:1064:G:C4'	1:A:1065:U:H5'	2.28	0.64
1:A:1478:C:H2'	1:A:1479:C:H6	1.62	0.64
1:A:428:G:H4'	1:A:429:U:O5'	1.98	0.64
1:A:664:G:OP1	19:R:64:ARG:HD2	1.97	0.64
4:C:110:ASN:ND2	4:C:140:ARG:HB3	2.12	0.64
4:C:7:PRO:HG2	4:C:184:TYR:HB2	1.80	0.64
1:A:969:A:N6	14:M:124:PRO:HB3	2.13	0.64
1:A:1160:G:O2'	1:A:1161:C:H5'	1.98	0.64
1:A:1278:U:H5''	1:A:1279:A:C5'	2.27	0.64
1:A:1000:U:H2'	1:A:1001:A:H8	1.62	0.64
7:F:80:ARG:NH1	7:F:88:VAL:HB	2.12	0.64
9:H:101:PRO:HG3	9:H:133:LEU:HD11	1.80	0.64
3:B:92:TYR:CE1	3:B:151:GLY:HA3	2.33	0.64
3:B:95:GLN:O	3:B:96:ARG:HD2	1.97	0.64
8:G:18:TYR:HD2	8:G:59:LEU:HD22	1.63	0.64

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:41:VAL:HG23	20:S:43:GLU:HG2	1.79	0.64
1:A:735:C:O2'	1:A:736:C:H5'	1.99	0.63
4:C:11:ARG:NH1	4:C:179:ARG:H	1.95	0.63
5:D:127:THR:HG23	5:D:130:GLY:O	1.98	0.63
14:M:62:ASN:O	14:M:63:THR:HB	1.97	0.63
20:S:62:ILE:HD12	20:S:66:MET:HG3	1.80	0.63
1:A:1229:A:H2'	1:A:1230:C:C6	2.32	0.63
11:J:3:LYS:HA	11:J:75:ILE:HA	1.80	0.63
13:L:97:ARG:HB2	13:L:98:TYR:CE1	2.33	0.63
1:A:1239:A:H62	1:A:1299:A:H62	1.46	0.63
1:A:539:A:OP1	13:L:114:LYS:HE2	1.98	0.63
1:A:646:U:H2'	1:A:647:C:H6	1.62	0.63
1:A:677:U:H3	1:A:713:G:H22	1.45	0.63
1:A:806:C:O2'	1:A:807:A:H5'	1.98	0.63
3:B:223:ILE:HG21	3:B:230:VAL:HG23	1.80	0.63
6:E:51:VAL:O	6:E:54:ALA:HB3	1.98	0.63
6:E:99:GLY:O	6:E:117:ASP:HA	1.98	0.63
11:J:3:LYS:N	11:J:77:PRO:HD3	2.14	0.63
3:B:19:HIS:CD2	3:B:205:ASP:OD1	2.51	0.63
1:A:1256:A:H8	4:C:27:LYS:NZ	1.97	0.63
11:J:8:LEU:CD2	11:J:96:ILE:HG12	2.29	0.63
19:R:33:ASP:OD2	19:R:36:ASN:HB2	1.98	0.63
12:K:84:VAL:HG21	19:R:88:LYS:HD3	1.79	0.63
20:S:53:ASN:N	20:S:53:ASN:HD22	1.95	0.63
1:A:334:C:H2'	1:A:335:C:C6	2.33	0.63
1:A:627:G:O2'	1:A:628:G:H5'	1.98	0.63
1:A:1112:C:O2	4:C:179:ARG:HB3	1.99	0.63
8:G:136:LYS:HG2	8:G:140:ASP:OD1	1.97	0.63
15:N:12:ARG:O	15:N:14:PRO:N	2.31	0.63
1:A:1189:C:OP1	11:J:51:ARG:NH2	2.29	0.63
1:A:1425:U:H2'	1:A:1426:C:H6	1.64	0.63
3:B:124:SER:HB2	3:B:125:PRO:CD	2.27	0.63
6:E:41:VAL:CG2	6:E:113:ALA:HA	2.29	0.63
1:A:1042:G:O2'	1:A:1043:C:H5'	1.98	0.63
1:A:1305:G:N2	1:A:1331:G:O2'	2.32	0.63
1:A:254:G:OP1	18:Q:67:LYS:O	2.17	0.63
3:B:84:GLU:HB3	3:B:219:VAL:CG2	2.28	0.63
4:C:110:ASN:HD21	4:C:140:ARG:HB3	1.62	0.63
1:A:8:A:N6	5:D:209:ARG:HB2	2.14	0.63
12:K:48:ILE:HG22	12:K:49:GLY:N	2.13	0.63
13:L:28:LYS:CD	13:L:33:ARG:HH22	1.95	0.63

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Q:67:LYS:HA	18:Q:70:ARG:HH12	1.63	0.63
19:R:36:ASN:HD22	19:R:38:GLU:HG2	1.63	0.63
19:R:55:ARG:CB	19:R:55:ARG:HH11	2.02	0.63
19:R:52:PRO:O	19:R:56:THR:HG23	1.99	0.63
1:A:163:C:O2'	1:A:164:U:H5'	1.99	0.63
1:A:913:A:H1'	1:A:914:A:O4'	1.99	0.63
3:B:184:VAL:HG12	3:B:198:ASP:H	1.64	0.63
4:C:130:VAL:O	4:C:134:ILE:HG13	1.99	0.63
1:A:1149:C:H2'	1:A:1150:U:H6	1.63	0.63
1:A:1231:G:C4'	10:I:126:SER:HB3	2.28	0.63
5:D:174:LEU:O	5:D:186:LEU:HD11	1.99	0.63
13:L:47:LYS:CB	13:L:48:PRO:CD	2.75	0.63
1:A:1016:A:H2'	1:A:1017:G:O4'	1.98	0.62
1:A:1030(C):G:H2'	1:A:1030(D):A:C8	2.33	0.62
1:A:115:G:H1'	1:A:116:A:N7	2.14	0.62
1:A:1391:U:H2'	1:A:1392:G:H8	1.64	0.62
13:L:27:LEU:C	13:L:29:GLY:N	2.52	0.62
14:M:8:GLU:OE1	14:M:22:ILE:HA	1.99	0.62
17:P:20:VAL:HG11	17:P:32:TYR:HB3	1.80	0.62
9:H:48:TYR:HB2	9:H:60:ARG:O	1.99	0.62
14:M:57:ARG:HG2	14:M:61:GLU:OE2	1.99	0.62
11:J:81:THR:O	11:J:85:LEU:HG	1.99	0.62
14:M:3:ARG:HA	14:M:8:GLU:O	1.99	0.62
21:T:53:LEU:HD13	21:T:101:GLY:N	2.14	0.62
1:A:424:G:H2'	1:A:425:G:H8	1.64	0.62
1:A:939:G:H2'	1:A:940:C:C6	2.34	0.62
11:J:62:HIS:CB	15:N:59:ALA:HB3	2.28	0.62
1:A:188:C:C4'	21:T:89:ARG:NH1	2.62	0.62
1:A:434:U:H2'	1:A:435:C:H6	1.64	0.62
1:A:490:G:H2'	1:A:491:G:H8	1.64	0.62
3:B:118:LEU:HD11	3:B:141:GLU:OE1	1.98	0.62
4:C:191:THR:HG21	4:C:193:TYR:CE1	2.34	0.62
4:C:35:GLU:CG	4:C:59:ARG:HH22	2.13	0.62
4:C:70:VAL:C	4:C:106:VAL:HG23	2.20	0.62
5:D:187:ARG:HH21	5:D:188:LEU:CG	2.13	0.62
8:G:21:VAL:HG23	8:G:22:LEU:N	2.13	0.62
11:J:37:PRO:HA	11:J:72:VAL:HG22	1.80	0.62
1:A:254:G:O2'	1:A:255:G:H5'	1.99	0.62
3:B:137:ARG:HB3	3:B:137:ARG:NH1	2.14	0.62
3:B:119:GLU:CD	3:B:153:ARG:HH22	2.02	0.62
6:E:116:THR:HG23	6:E:117:ASP:OD2	2.00	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:877:C:H1'	9:H:3:THR:CG2	2.30	0.62
10:I:28:VAL:HG21	10:I:33:PHE:HD1	1.64	0.62
11:J:28:ARG:HH12	11:J:33:GLN:HG2	1.63	0.62
1:A:352:C:H4'	1:A:354:G:OP1	1.99	0.62
1:A:761:G:H4'	18:Q:102:GLY:C	2.19	0.62
11:J:30:SER:O	11:J:78:ASN:HB2	2.00	0.62
20:S:7:LYS:HG3	20:S:7:LYS:O	2.00	0.62
21:T:11:SER:C	21:T:13:LEU:H	2.03	0.62
1:A:1221:G:O2'	1:A:1222:G:H5'	1.98	0.62
1:A:719:C:H3'	1:A:720:C:C6	2.34	0.62
3:B:25:ASN:C	3:B:25:ASN:HD22	2.03	0.62
1:A:738:C:OP1	7:F:92:LYS:HE3	2.00	0.62
10:I:106:ALA:O	10:I:108:VAL:HG23	2.00	0.62
1:A:1307:U:H5'	14:M:109:THR:HG21	1.80	0.62
16:O:29:VAL:HG12	16:O:85:LEU:CD1	2.30	0.62
19:R:60:GLY:O	19:R:64:ARG:HB2	1.99	0.62
21:T:53:LEU:HD23	21:T:56:MET:HE3	1.81	0.62
1:A:1428:A:H2'	1:A:1429:C:C6	2.35	0.62
1:A:540:G:H2'	1:A:541:G:H8	1.65	0.62
4:C:181:ASN:HD21	4:C:204:LEU:HD12	1.63	0.62
5:D:36:ARG:N	5:D:37:PRO:CD	2.57	0.62
6:E:78:HIS:HD2	9:H:107:LEU:HD12	1.64	0.62
8:G:18:TYR:CD2	8:G:59:LEU:HB2	2.35	0.62
9:H:138:TRP:OXT	9:H:138:TRP:HE3	1.82	0.62
12:K:88:GLY:O	12:K:90:GLY:N	2.32	0.62
16:O:27:VAL:O	16:O:30:ALA:HB3	1.99	0.62
17:P:52:ASP:OD2	17:P:52:ASP:O	2.17	0.62
18:Q:81:ARG:HG3	18:Q:81:ARG:O	2.00	0.62
20:S:40:ILE:HG21	20:S:62:ILE:CD1	2.29	0.62
1:A:1314:C:OP2	20:S:6:LYS:HG2	2.00	0.62
1:A:397:A:H5'	1:A:398:C:OP1	2.00	0.62
3:B:140:HIS:HA	3:B:143:GLU:CG	2.30	0.62
3:B:16:HIS:NE2	3:B:214:ILE:CG1	2.63	0.62
10:I:78:LYS:HD3	10:I:101:PHE:CD2	2.35	0.62
12:K:108:ILE:O	12:K:109:VAL:HG23	2.00	0.62
1:A:190(F):G:H4'	1:A:190(G):G:OP2	2.00	0.61
1:A:382:A:H2'	1:A:383:A:H8	1.65	0.61
4:C:191:THR:HG22	4:C:193:TYR:N	2.03	0.61
5:D:111:ALA:HB3	5:D:117:ALA:HB2	1.82	0.61
11:J:30:SER:OG	11:J:81:THR:HA	2.00	0.61
12:K:15:ALA:O	12:K:78:GLN:N	2.31	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:42:THR:HG23	13:L:52:LEU:HB3	1.81	0.61
21:T:39:LYS:CD	21:T:55:ILE:HD13	2.30	0.61
1:A:190(E):U:O2'	18:Q:63:ARG:NH2	2.33	0.61
1:A:476:G:O2'	1:A:477:G:H5'	2.01	0.61
6:E:103:GLY:O	6:E:106:PRO:HD2	1.99	0.61
15:N:29:ARG:HH11	15:N:29:ARG:HG2	1.65	0.61
17:P:52:ASP:OD2	17:P:55:ARG:HB2	2.00	0.61
1:A:1300:G:HO2'	1:A:1301:U:H6	1.45	0.61
1:A:1053:G:C4'	1:A:1054:C:H5'	2.30	0.61
1:A:1407:C:O2'	1:A:1408:A:H5'	2.00	0.61
1:A:1392:G:H21	1:A:1502:A:H8	1.46	0.61
1:A:539:A:H2'	1:A:540:G:C8	2.35	0.61
3:B:178:ARG:HH11	3:B:178:ARG:HG3	1.63	0.61
7:F:2:ARG:CD	7:F:69:GLU:HG2	2.30	0.61
9:H:60:ARG:HG3	9:H:60:ARG:HH11	1.64	0.61
1:A:1250:A:C4'	10:I:68:GLY:H	2.10	0.61
11:J:96:ILE:HG22	11:J:97:GLU:H	1.64	0.61
1:A:129(A):G:N3	1:A:190(E):U:H5'	2.16	0.61
1:A:474:G:H2'	1:A:475:G:H8	1.64	0.61
1:A:974:A:P	15:N:31:ARG:HG2	2.41	0.61
4:C:191:THR:HG22	4:C:192:THR:N	2.14	0.61
1:A:1006:C:H2'	1:A:1007:C:C6	2.36	0.61
1:A:1132:C:H2'	1:A:1133:G:C8	2.36	0.61
1:A:255:G:H2'	1:A:256:U:C6	2.34	0.61
1:A:301:G:O2'	1:A:302:G:H5'	2.00	0.61
21:T:53:LEU:O	21:T:57:ARG:HD3	2.00	0.61
1:A:1157:A:H4'	1:A:1158:C:O5'	2.00	0.61
1:A:1278:U:H5''	1:A:1279:A:H5'	1.83	0.61
1:A:926:G:H3'	1:A:1505:G:N2	2.15	0.61
1:A:235:C:H1'	18:Q:61:GLU:OE1	2.01	0.61
1:A:411:A:C4	1:A:413:G:H1'	2.35	0.61
4:C:6:HIS:CD2	4:C:8:ILE:H	2.19	0.61
5:D:151:LYS:HD2	5:D:151:LYS:H	1.66	0.61
8:G:85:TYR:HD1	8:G:154:TYR:HE1	1.48	0.61
1:A:1231:G:H4'	10:I:126:SER:CB	2.30	0.61
17:P:1:MET:HE3	17:P:3:LYS:HG2	1.82	0.61
17:P:82:GLN:O	17:P:84:ALA:N	2.34	0.61
1:A:435:C:H2'	1:A:436:C:H6	1.64	0.61
1:A:538:G:H2'	1:A:539:A:C8	2.36	0.61
1:A:746:A:O2'	1:A:747:C:H5'	2.01	0.61
1:A:818:G:C3'	1:A:819:A:C5'	2.79	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:849:C:H2'	1:A:850:U:H6	1.65	0.61
3:B:77:ALA:HB2	3:B:211:ILE:CD1	2.22	0.61
4:C:107:GLN:O	4:C:108:ASN:HB3	2.01	0.61
8:G:42:ILE:HG22	8:G:120:ILE:HD12	1.82	0.61
20:S:20:LEU:HD12	20:S:21:GLU:N	2.16	0.61
1:A:481:G:H2'	1:A:483:C:N4	2.15	0.61
8:G:146:GLU:CA	8:G:149:ARG:HB2	2.31	0.61
10:I:31:GLN:HB3	10:I:35:GLU:HB3	1.83	0.61
13:L:126:LYS:H	13:L:126:LYS:CD	2.13	0.61
1:A:178:C:O2'	1:A:179:A:H5'	2.01	0.61
1:A:518:C:H4'	1:A:519:C:O5'	2.00	0.61
3:B:129:GLU:O	3:B:130:ARG:HB2	2.01	0.61
3:B:136:VAL:HA	3:B:139:LYS:HB2	1.83	0.61
5:D:189:PRO:HB2	5:D:194:LEU:HD21	1.82	0.61
9:H:14:ARG:O	9:H:18:ARG:HD3	2.01	0.61
21:T:39:LYS:CG	21:T:55:ILE:HD13	2.30	0.61
21:T:56:MET:HE2	21:T:88:VAL:HG11	1.83	0.61
1:A:1182:G:O2'	1:A:1183:A:OP2	2.18	0.60
1:A:1262:C:H2'	1:A:1263:C:C6	2.36	0.60
1:A:1405:G:O2'	1:A:1406:U:H5'	2.00	0.60
1:A:1502:A:H2	1:A:1505:G:N1	1.99	0.60
1:A:624:C:O2'	1:A:625:G:H5'	2.00	0.60
6:E:120:THR:CG2	6:E:121:LYS:N	2.64	0.60
1:A:1343:G:H1'	10:I:121:ARG:NH1	2.15	0.60
13:L:115:LYS:C	13:L:117:ARG:H	2.05	0.60
19:R:34:TYR:HA	19:R:69:THR:HG23	1.83	0.60
19:R:53:ARG:HH11	19:R:59:SER:CA	2.14	0.60
1:A:156:G:O2'	1:A:157:G:H5'	2.00	0.60
25:A:1632:PCY:H102	25:A:1632:PCY:O19	2.01	0.60
4:C:7:PRO:O	4:C:11:ARG:HD2	1.99	0.60
7:F:25:ILE:HD12	7:F:82:ARG:HD2	1.83	0.60
20:S:31:ILE:HG22	20:S:32:LYS:H	1.66	0.60
1:A:1031:G:H2'	1:A:1032:G:H8	1.67	0.60
1:A:959:A:C2	1:A:1222:G:O4'	2.54	0.60
1:A:357:G:O2'	1:A:358:U:H5'	2.01	0.60
3:B:62:ALA:C	3:B:64:ARG:H	2.04	0.60
1:A:407:G:O2'	5:D:116:GLN:HG3	2.01	0.60
13:L:45:PRO:HG3	13:L:53:ARG:HD3	1.82	0.60
14:M:81:LEU:CD2	14:M:81:LEU:N	2.64	0.60
15:N:14:PRO:C	15:N:16:PHE:N	2.51	0.60
1:A:1310:G:O6	20:S:2:PRO:HB3	2.01	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:C:O2'	1:A:177:C:H5'	2.00	0.60
1:A:188:C:H4'	21:T:89:ARG:NH1	2.17	0.60
1:A:411:A:N9	1:A:413:G:H1'	2.16	0.60
3:B:18:GLY:CA	3:B:41:ILE:HA	2.30	0.60
4:C:67:THR:O	4:C:69:HIS:CD2	2.54	0.60
5:D:88:VAL:O	5:D:92:VAL:HG23	2.02	0.60
13:L:46:LYS:NZ	13:L:47:LYS:HG3	2.16	0.60
1:A:1347:G:N2	1:A:1373:G:H2'	2.17	0.60
1:A:269:C:H2'	1:A:270:A:H8	1.66	0.60
1:A:858:G:O2'	1:A:859:A:H5'	2.02	0.60
14:M:6:GLY:O	14:M:7:VAL:HG22	2.02	0.60
18:Q:97:SER:CB	18:Q:103:GLY:HA2	2.32	0.60
1:A:1475:G:H2'	1:A:1476:G:C8	2.36	0.60
4:C:30:ARG:HH11	4:C:30:ARG:HG2	1.67	0.60
15:N:8:GLU:O	15:N:11:LYS:HB2	2.01	0.60
15:N:9:LYS:C	15:N:9:LYS:HD3	2.22	0.60
1:A:1257:U:H4'	1:A:1258:G:C5'	2.32	0.60
1:A:1510:U:H2'	1:A:1511:G:C8	2.36	0.60
3:B:23:ARG:HH12	3:B:24:TRP:HA	1.67	0.60
4:C:60:ALA:O	4:C:61:ALA:HB2	2.02	0.60
11:J:38:ILE:CG1	11:J:71:LEU:HB3	2.31	0.60
20:S:32:LYS:O	20:S:32:LYS:HG3	2.00	0.60
1:A:949:A:N7	14:M:106:ASN:ND2	2.50	0.60
4:C:7:PRO:CG	4:C:184:TYR:HB2	2.32	0.60
11:J:12:ASP:HB3	11:J:15:THR:HB	1.82	0.60
1:A:537:G:OP1	13:L:113:ARG:NH2	2.35	0.60
14:M:10:PRO:HB2	14:M:18:ALA:HB1	1.82	0.60
22:V:2:GLY:O	22:V:4:GLY:N	2.35	0.60
1:A:683:G:H2'	1:A:684:A:C8	2.37	0.60
3:B:73:THR:HB	3:B:170:GLU:OE2	2.02	0.60
5:D:191:ARG:HD2	5:D:191:ARG:O	2.01	0.60
6:E:35:GLY:HA3	6:E:112:LEU:HB3	1.84	0.60
21:T:44:ALA:CB	21:T:88:VAL:HG13	2.32	0.60
1:A:1412:C:H2'	1:A:1413:A:C8	2.37	0.60
1:A:1426:C:H2'	1:A:1427:U:H6	1.65	0.60
1:A:130:A:OP2	1:A:190(E):U:H2'	2.02	0.60
1:A:204:U:H4'	1:A:216:G:O5'	2.02	0.60
3:B:140:HIS:HA	3:B:143:GLU:HG2	1.84	0.60
7:F:53:ALA:C	7:F:55:ASP:H	2.05	0.60
10:I:100:GLY:O	10:I:102:LEU:N	2.35	0.60
11:J:64:GLU:HG2	15:N:59:ALA:HB2	1.83	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1091:U:O2	1:A:1093:A:C8	2.55	0.59
1:A:620:C:N1	5:D:135:LEU:HD13	2.16	0.59
11:J:51:ARG:H	11:J:59:SER:HB3	1.67	0.59
1:A:376:G:H5''	17:P:5:ARG:HD2	1.82	0.59
7:F:60:PHE:CE2	19:R:78:LEU:HD21	2.37	0.59
1:A:877:C:H5''	9:H:88:LYS:HD3	1.84	0.59
6:E:12:LEU:HD13	6:E:31:LEU:HB2	1.84	0.59
12:K:48:ILE:HD13	12:K:63:LEU:HB2	1.83	0.59
14:M:40:ASN:ND2	14:M:41:PRO:HD2	2.17	0.59
17:P:28:ARG:HG3	17:P:29:ASP:OD2	2.00	0.59
21:T:76:ALA:O	21:T:80:ARG:HG2	2.02	0.59
1:A:1129:C:O2'	1:A:1130:A:OP2	2.20	0.59
1:A:1403:C:H1'	1:A:1500:A:N1	2.16	0.59
1:A:953:G:O4'	14:M:125:ARG:HA	2.03	0.59
3:B:124:SER:O	3:B:127:ILE:HG13	2.01	0.59
4:C:102:ASN:O	4:C:103:VAL:HG23	2.03	0.59
9:H:113:SER:HB2	9:H:134:ILE:HD11	1.84	0.59
10:I:112:LYS:HD3	10:I:112:LYS:C	2.22	0.59
11:J:30:SER:HB3	11:J:80:LYS:HG3	1.83	0.59
21:T:10:LEU:HD12	21:T:12:ALA:HB3	1.82	0.59
3:B:51:LEU:HD21	3:B:201:ILE:HG23	1.83	0.59
3:B:223:ILE:HD13	3:B:230:VAL:HG21	1.84	0.59
4:C:130:VAL:HG21	4:C:157:ILE:HG23	1.85	0.59
10:I:10:ARG:HG2	10:I:75:ASP:HB2	1.85	0.59
10:I:81:ILE:O	10:I:85:LEU:HB2	2.02	0.59
13:L:32:PHE:HB3	13:L:84:LEU:HD11	1.83	0.59
14:M:40:ASN:HB3	14:M:43:THR:HG23	1.83	0.59
1:A:1208:C:H2'	1:A:1209:C:C6	2.34	0.59
1:A:1225:A:H2'	1:A:1225:A:N3	2.17	0.59
1:A:452:A:O2'	1:A:453:A:H8	1.85	0.59
1:A:613:C:O2'	1:A:614:A:H5'	2.03	0.59
1:A:697:U:H2'	1:A:698:G:H5'	1.84	0.59
1:A:1287:A:H2	1:A:1353:G:N3	2.00	0.59
3:B:98:LEU:N	3:B:98:LEU:HD23	2.17	0.59
4:C:36:ASP:HB3	4:C:40:ARG:HH12	1.67	0.59
3:B:130:ARG:HB3	3:B:131:PRO:HD2	1.84	0.59
5:D:199:ASN:ND2	5:D:201:GLN:HB3	2.18	0.59
19:R:16:PRO:O	19:R:17:SER:HB3	2.02	0.59
20:S:18:LYS:O	20:S:22:LEU:HG	2.02	0.59
1:A:1176:A:H2'	1:A:1177:G:C8	2.38	0.59
1:A:812:C:O2'	1:A:813:U:P	2.60	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:112:SER:HB2	4:C:115:LEU:HD12	1.84	0.59
14:M:3:ARG:CG	14:M:9:ILE:HG23	2.32	0.59
18:Q:15:MET:HE1	18:Q:43:LEU:HD22	1.84	0.59
1:A:266:G:O3'	18:Q:67:LYS:HB2	2.02	0.59
1:A:1182:G:H4'	1:A:1183:A:C5'	2.32	0.59
1:A:1256:A:H61	1:A:1278:U:H1'	1.68	0.59
1:A:1367:C:H5'	11:J:60:ARG:NH1	2.16	0.59
1:A:1493:A:C2'	1:A:1494:G:H5'	2.33	0.59
1:A:195:A:H4'	21:T:68:LYS:CE	2.31	0.59
1:A:202:U:H4'	1:A:203:U:OP1	2.03	0.59
1:A:96:G:O2'	1:A:97:G:H5'	2.03	0.59
9:H:112:LEU:N	9:H:112:LEU:HD23	2.16	0.59
10:I:121:ARG:HH11	10:I:121:ARG:HG2	1.67	0.59
10:I:114:TYR:CE1	11:J:60:ARG:HB2	2.38	0.59
22:V:6:ARG:HD2	22:V:15:ARG:HH12	1.66	0.59
1:A:1296:C:H4'	1:A:1302:U:C5	2.38	0.59
1:A:1381:U:O2'	1:A:1382:C:H5'	2.03	0.59
1:A:1472:U:O2'	1:A:1473:A:H5'	2.02	0.59
3:B:124:SER:CB	3:B:125:PRO:HD2	2.33	0.59
3:B:144:ARG:HG3	3:B:145:LEU:N	2.18	0.59
10:I:17:VAL:HG11	10:I:81:ILE:HA	1.85	0.59
13:L:25:PRO:C	13:L:27:LEU:N	2.57	0.59
14:M:15:VAL:HG23	14:M:43:THR:O	2.03	0.59
6:E:151:LEU:HD11	9:H:77:GLU:OE2	2.02	0.58
7:F:33:TYR:HA	7:F:71:ARG:NH2	2.17	0.58
12:K:48:ILE:HD11	12:K:64:ALA:N	2.18	0.58
13:L:75:HIS:HD2	13:L:77:LEU:N	1.93	0.58
18:Q:74:LEU:HD23	18:Q:74:LEU:O	2.02	0.58
1:A:1287:A:H2'	1:A:1288:A:C8	2.37	0.58
1:A:279:A:H5'	1:A:281:G:O4'	2.03	0.58
1:A:521:G:O2'	1:A:522:C:H5'	2.02	0.58
1:A:824:C:H2'	1:A:825:G:H8	1.68	0.58
1:A:926:G:H5'	1:A:927:G:C5'	2.33	0.58
10:I:11:LYS:O	10:I:11:LYS:HG2	2.03	0.58
10:I:79:LEU:O	10:I:79:LEU:HD13	2.03	0.58
12:K:101:SER:OG	12:K:102:GLY:N	2.35	0.58
13:L:46:LYS:NZ	13:L:47:LYS:HE3	2.17	0.58
20:S:42:PRO:O	20:S:45:VAL:HG23	2.01	0.58
1:A:1263:C:H2'	1:A:1264:C:H6	1.67	0.58
1:A:1412:C:H2'	1:A:1413:A:H8	1.68	0.58
1:A:277:C:H5''	18:Q:68:ARG:NH2	2.19	0.58

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:C:H2'	1:A:515:G:H8	1.67	0.58
1:A:900:A:H2'	1:A:901:A:C8	2.37	0.58
3:B:16:HIS:CE1	3:B:214:ILE:HG12	2.38	0.58
3:B:23:ARG:O	3:B:24:TRP:O	2.21	0.58
5:D:187:ARG:HH21	5:D:188:LEU:CB	2.16	0.58
1:A:954:G:H5''	14:M:120:LYS:HD3	1.86	0.58
14:M:9:ILE:N	14:M:9:ILE:HD12	2.17	0.58
1:A:1020:U:H2'	1:A:1021:G:H8	1.69	0.58
1:A:1346:A:H2'	8:G:10:ARG:HH22	1.68	0.58
1:A:1423:G:O2'	1:A:1424:C:H5'	2.03	0.58
3:B:133:LYS:O	3:B:137:ARG:HG3	2.04	0.58
3:B:103:THR:N	3:B:176:GLU:OE1	2.31	0.58
4:C:195:VAL:C	4:C:196:LEU:HD23	2.24	0.58
4:C:6:HIS:CD2	4:C:9:GLY:H	2.22	0.58
5:D:3:ARG:NH2	5:D:74:GLN:OE1	2.36	0.58
5:D:64:LEU:O	5:D:64:LEU:HD22	2.04	0.58
7:F:27:GLN:HA	7:F:30:LEU:HD12	1.85	0.58
1:A:881:G:P	13:L:12:ARG:HH22	2.26	0.58
20:S:16:LEU:C	20:S:18:LYS:H	2.07	0.58
1:A:259:G:O2'	1:A:260:G:H5'	2.03	0.58
1:A:33:A:H2'	1:A:34:C:C6	2.38	0.58
1:A:353:A:H5'	1:A:353:A:C8	2.39	0.58
1:A:407:G:H2'	1:A:408:A:H8	1.69	0.58
10:I:48:GLU:HA	10:I:51:ARG:NH1	2.18	0.58
1:A:1110:A:H8	1:A:1110:A:O5'	1.85	0.58
1:A:1411:C:H2'	1:A:1412:C:C6	2.39	0.58
1:A:621:A:H2'	1:A:622:A:C8	2.38	0.58
1:A:953:G:H2'	1:A:954:G:O4'	2.04	0.58
1:A:993:G:H4'	1:A:994:A:OP2	2.02	0.58
4:C:83:ARG:C	4:C:85:ARG:H	2.06	0.58
4:C:47:LEU:HD11	4:C:87:LEU:HD13	1.85	0.58
5:D:130:GLY:O	5:D:131:ARG:C	2.42	0.58
6:E:13:ILE:HA	6:E:29:GLY:O	2.04	0.58
11:J:5:ARG:HA	11:J:73:ASP:OD1	2.03	0.58
11:J:63:PHE:CZ	15:N:45:ARG:HG3	2.38	0.58
14:M:87:TYR:CZ	14:M:91:ARG:HD3	2.39	0.58
14:M:97:PRO:HB2	14:M:101:GLN:OE1	2.04	0.58
12:K:111:ASP:OD1	19:R:84:LYS:HE2	2.04	0.58
1:A:1216:G:H5''	15:N:5:ALA:CB	2.33	0.58
1:A:393:A:O2'	1:A:394:G:H5'	2.04	0.58
10:I:49:PRO:HD3	10:I:78:LYS:HG2	1.85	0.58

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:C:H5'	18:Q:70:ARG:HG2	1.84	0.58
1:A:1466:C:H2'	1:A:1467:G:O4'	2.04	0.58
1:A:1502:A:C2	1:A:1505:G:N1	2.70	0.58
1:A:791:G:H2'	1:A:792:A:H5'	1.84	0.58
1:A:930:C:O2'	1:A:931:C:H5'	2.04	0.58
11:J:39:PRO:HA	11:J:70:ARG:HH11	1.69	0.58
1:A:1262:C:H2'	1:A:1263:C:H6	1.68	0.58
1:A:19:C:H2'	1:A:20:U:H6	1.68	0.58
1:A:983:A:H5'	1:A:984:C:OP2	2.04	0.58
4:C:171:GLY:O	4:C:173:VAL:HG23	2.03	0.58
5:D:187:ARG:HH21	5:D:188:LEU:CD1	2.17	0.58
10:I:8:GLY:HA2	10:I:79:LEU:CD1	2.22	0.58
11:J:42:THR:HG23	11:J:67:THR:O	2.03	0.58
13:L:6:THR:HG1	13:L:9:GLN:HG3	1.68	0.58
1:A:1309:G:N7	14:M:99:ARG:NH2	2.52	0.58
15:N:26:ARG:HH11	15:N:47:LEU:HG	1.69	0.58
15:N:24:CYS:HB3	15:N:28:GLY:H	1.69	0.58
1:A:1256:A:H5'	1:A:1258:G:O4'	2.04	0.58
1:A:1438:G:H2'	1:A:1439:C:H6	1.69	0.58
1:A:961:U:C2'	1:A:962:C:H5'	2.34	0.58
3:B:111:ARG:HB3	3:B:149:LEU:HD11	1.86	0.58
4:C:110:ASN:O	4:C:111:LEU:HD23	2.03	0.58
1:A:1251:A:H4'	10:I:12:GLU:OE2	2.04	0.58
1:A:1367:C:H4'	11:J:48:THR:HG21	1.85	0.58
13:L:115:LYS:O	13:L:117:ARG:N	2.35	0.58
13:L:126:LYS:H	13:L:126:LYS:HD2	1.68	0.58
13:L:43:VAL:HG12	13:L:44:THR:N	2.19	0.58
1:A:1220:G:N2	20:S:54:GLY:O	2.34	0.58
1:A:1096:C:H2'	1:A:1097:C:C6	2.36	0.57
1:A:838:G:C3'	1:A:839:U:H5''	2.34	0.57
8:G:145:ALA:O	8:G:147:ALA:N	2.37	0.57
8:G:51:GLN:OE1	8:G:51:GLN:HA	2.04	0.57
11:J:38:ILE:HG22	11:J:39:PRO:HD2	1.86	0.57
13:L:50:SER:O	13:L:51:ALA:HB2	2.04	0.57
16:O:4:THR:O	16:O:7:GLU:HB2	2.04	0.57
17:P:21:VAL:HG21	17:P:59:TRP:NE1	2.19	0.57
20:S:47:HIS:O	20:S:62:ILE:HG22	2.04	0.57
1:A:1347:G:O2'	1:A:1348:U:P	2.61	0.57
1:A:398:C:O2'	1:A:399:G:H5'	2.03	0.57
1:A:443:C:H2'	1:A:444:C:H6	1.69	0.57
3:B:33:TYR:HB3	3:B:41:ILE:O	2.04	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:76:GLN:HG3	3:B:206:ASP:OD1	2.04	0.57
5:D:70:ILE:HD11	5:D:100:ARG:NH1	2.20	0.57
14:M:81:LEU:HA	14:M:84:ILE:HG12	1.86	0.57
14:M:87:TYR:HA	14:M:90:LEU:HD12	1.86	0.57
20:S:15:LEU:HD12	20:S:16:LEU:N	2.19	0.57
1:A:1292:U:C5'	10:I:38:GLN:HE22	2.17	0.57
1:A:1346:A:C2'	8:G:10:ARG:HH22	2.17	0.57
1:A:1513:A:H2'	1:A:1514:C:C6	2.40	0.57
1:A:551:U:H2'	1:A:552:U:C6	2.40	0.57
1:A:628:G:H2'	1:A:629:G:H8	1.70	0.57
1:A:657:G:O2'	1:A:658:G:H5'	2.05	0.57
1:A:690:G:H2'	1:A:691:G:O4'	2.04	0.57
1:A:867:G:O2'	1:A:868:C:H5'	2.03	0.57
4:C:71:ALA:HA	4:C:106:VAL:HB	1.86	0.57
5:D:7:PRO:HG2	5:D:10:ARG:HD2	1.86	0.57
13:L:38:THR:HG22	13:L:39:VAL:CG2	2.27	0.57
14:M:81:LEU:HD22	14:M:81:LEU:H	1.69	0.57
14:M:81:LEU:CD2	14:M:81:LEU:H	2.18	0.57
4:C:29:TYR:CZ	15:N:54:PRO:HG2	2.40	0.57
1:A:1015:A:H2'	1:A:1016:A:C8	2.40	0.57
1:A:105:G:H2'	1:A:106:C:C6	2.39	0.57
1:A:1303:C:H2'	1:A:1304:G:H5'	1.86	0.57
1:A:1497:G:H2'	1:A:1498:U:H5'	1.87	0.57
3:B:71:VAL:HB	3:B:164:VAL:HG23	1.87	0.57
10:I:50:LEU:C	10:I:52:ALA:H	2.07	0.57
1:A:865:A:H5'	1:A:1078:U:O4	2.04	0.57
5:D:104:VAL:HG11	5:D:146:ILE:HD12	1.85	0.57
11:J:6:ILE:HA	11:J:98:ILE:HG12	1.85	0.57
13:L:69:TYR:HE2	13:L:71:PRO:HA	1.70	0.57
14:M:49:THR:CG2	14:M:51:ALA:H	2.12	0.57
19:R:53:ARG:NH1	19:R:59:SER:CA	2.66	0.57
1:A:1161:C:H2'	1:A:1162:C:H6	1.69	0.57
1:A:334:C:H2'	1:A:335:C:H6	1.68	0.57
1:A:849:C:O2'	1:A:850:U:H5'	2.04	0.57
4:C:148:GLY:HA3	4:C:172:ARG:O	2.04	0.57
8:G:72:ARG:HG2	8:G:142:GLU:OE1	2.04	0.57
13:L:83:VAL:HG21	13:L:100:ILE:HG23	1.85	0.57
1:A:1190:G:HO2'	1:A:1191:A:P	2.27	0.57
1:A:1260:C:O5'	1:A:1284:C:H4'	2.04	0.57
1:A:975:A:H4'	1:A:976:G:H5'	1.87	0.57
1:A:992:U:O2'	1:A:993:G:OP2	2.21	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1056:U:C5'	4:C:163:ALA:HB2	2.33	0.57
5:D:199:ASN:HD21	5:D:201:GLN:CB	2.17	0.57
6:E:89:ILE:HD13	6:E:90:VAL:H	1.70	0.57
1:A:1054:C:OP1	1:A:1197:G:OP1	2.23	0.57
1:A:229:U:O2'	1:A:230:G:H5'	2.04	0.57
1:A:457:C:H2'	1:A:458:C:H6	1.69	0.57
1:A:514:C:H2'	1:A:515:G:C8	2.40	0.57
1:A:860:A:H2'	1:A:861:G:O4'	2.04	0.57
4:C:156:ARG:H	4:C:163:ALA:HA	1.68	0.57
4:C:52:LEU:CD2	4:C:118:GLN:HE22	2.17	0.57
9:H:29:SER:OG	9:H:32:LYS:HB2	2.04	0.57
9:H:31:PHE:CE1	9:H:35:ILE:HD11	2.40	0.57
12:K:27:ASN:HA	12:K:56:GLY:HA2	1.85	0.57
1:A:1508:G:O2'	1:A:1509:C:H5'	2.03	0.57
1:A:997:U:H2'	1:A:998:G:O4'	2.05	0.57
5:D:173:TRP:CD2	5:D:189:PRO:HB3	2.40	0.57
13:L:117:ARG:HD2	13:L:122:THR:OG1	2.05	0.57
15:N:21:TYR:CE2	15:N:23:ARG:HG3	2.38	0.57
17:P:22:THR:CA	17:P:33:ILE:HD13	2.29	0.57
21:T:63:ILE:HD13	21:T:80:ARG:HB3	1.87	0.57
1:A:1320:C:H2'	1:A:1321:C:O4'	2.05	0.56
1:A:1488:G:H2'	1:A:1489:G:C8	2.40	0.56
1:A:477:G:H2'	1:A:478:A:C8	2.39	0.56
1:A:545:C:O2'	1:A:546:G:H5'	2.05	0.56
3:B:15:VAL:HG11	3:B:209:ARG:HG3	1.86	0.56
8:G:78:ARG:HB2	8:G:156:TRP:CZ3	2.40	0.56
19:R:34:TYR:HD1	19:R:35:ARG:HG3	1.70	0.56
1:A:1056:U:H5'	4:C:163:ALA:CB	2.32	0.56
1:A:1289:A:H2'	1:A:1290:G:H5'	1.87	0.56
1:A:390:C:H2'	1:A:391:G:C8	2.41	0.56
1:A:581:G:O2'	18:Q:105:ALA:HB1	2.04	0.56
3:B:164:VAL:HG12	3:B:186:ALA:HB2	1.87	0.56
4:C:26:LYS:HE2	4:C:26:LYS:N	2.16	0.56
5:D:64:LEU:HB2	5:D:198:VAL:HG11	1.86	0.56
8:G:95:ARG:HG2	8:G:99:LEU:HD11	1.87	0.56
9:H:48:TYR:CD1	9:H:48:TYR:C	2.79	0.56
15:N:23:ARG:NH1	15:N:30:ALA:HB2	2.20	0.56
16:O:3:ILE:N	16:O:3:ILE:HD12	2.19	0.56
20:S:40:ILE:HG21	20:S:62:ILE:HD11	1.85	0.56
1:A:1380:U:O2'	1:A:1381:U:OP2	2.20	0.56
1:A:627:G:H2'	1:A:628:G:H8	1.71	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:114:ARG:HH11	3:B:118:LEU:HD21	1.69	0.56
3:B:93:VAL:HG11	3:B:97:TRP:CD1	2.40	0.56
6:E:110:LEU:O	6:E:115:VAL:HB	2.04	0.56
1:A:1179:A:H2'	1:A:1180:A:O4'	2.06	0.56
1:A:202:U:H5''	1:A:203:U:OP2	2.04	0.56
1:A:90:U:H2'	1:A:91:C:C6	2.39	0.56
10:I:50:LEU:C	10:I:52:ALA:N	2.56	0.56
12:K:69:ALA:O	12:K:73:MET:HG2	2.05	0.56
16:O:29:VAL:HG12	16:O:85:LEU:HD12	1.87	0.56
21:T:96:GLY:O	21:T:97:ALA:HB3	2.05	0.56
1:A:1502:A:H5''	1:A:1503:A:OP2	2.06	0.56
1:A:538:G:O2'	1:A:539:A:H5'	2.06	0.56
1:A:828:A:H2'	1:A:829:G:O4'	2.06	0.56
3:B:12:GLU:C	3:B:14:GLY:N	2.57	0.56
4:C:99:VAL:CG2	4:C:100:ALA:N	2.67	0.56
5:D:112:VAL:N	5:D:116:GLN:OE1	2.37	0.56
12:K:48:ILE:HD13	12:K:63:LEU:CB	2.35	0.56
18:Q:97:SER:CB	18:Q:103:GLY:CA	2.84	0.56
1:A:1056:U:O2'	1:A:1057:G:H5'	2.06	0.56
1:A:1333:A:H2'	1:A:1334:G:O4'	2.04	0.56
1:A:165:C:H2'	1:A:166:G:H8	1.70	0.56
3:B:8:LYS:O	3:B:9:GLU:CB	2.51	0.56
4:C:108:ASN:HD21	4:C:111:LEU:HG	1.71	0.56
4:C:120:VAL:O	4:C:124:ILE:HG13	2.05	0.56
4:C:36:ASP:O	4:C:39:ILE:HB	2.05	0.56
4:C:43:LEU:O	4:C:47:LEU:HB2	2.06	0.56
5:D:199:ASN:HD22	5:D:199:ASN:C	2.09	0.56
1:A:1130:A:N6	1:A:1144:G:H21	2.04	0.56
1:A:586:C:O2'	1:A:587:G:H5'	2.05	0.56
1:A:750:G:H1'	16:O:22:THR:OG1	2.06	0.56
1:A:920:U:H2'	1:A:921:U:C6	2.40	0.56
1:A:959:A:H2'	1:A:960:U:O4'	2.05	0.56
1:A:969:A:H61	14:M:124:PRO:HB3	1.70	0.56
5:D:114:ARG:HG3	5:D:114:ARG:HH11	1.69	0.56
8:G:62:PHE:O	8:G:65:ALA:HB3	2.06	0.56
8:G:93:PRO:HG2	8:G:94:ARG:H	1.70	0.56
10:I:47:LEU:C	10:I:49:PRO:HD2	2.26	0.56
11:J:12:ASP:OD1	11:J:14:LYS:N	2.37	0.56
11:J:96:ILE:HG22	11:J:97:GLU:N	2.20	0.56
17:P:81:ARG:HG3	17:P:83:GLU:HG2	1.88	0.56
22:V:6:ARG:CZ	22:V:15:ARG:HH12	2.19	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:662:G:O2'	1:A:836:G:H5''	2.05	0.56
1:A:731:G:OP1	1:A:766:A:H1'	2.06	0.56
1:A:990:C:H2'	1:A:991:U:O4'	2.05	0.56
4:C:22:TRP:CE3	4:C:32:LEU:HD22	2.40	0.56
5:D:12:CYS:SG	5:D:31:CYS:SG	3.04	0.56
8:G:155:ARG:O	8:G:156:TRP:CB	2.54	0.56
9:H:51:VAL:CG1	9:H:52:ASP:H	2.15	0.56
1:A:689:C:P	12:K:46:GLY:HA3	2.45	0.56
12:K:54:ARG:HB3	12:K:54:ARG:NH1	2.10	0.56
13:L:55:VAL:CG1	13:L:56:ALA:H	2.19	0.56
11:J:64:GLU:HG2	15:N:59:ALA:CB	2.36	0.56
21:T:67:ALA:HB2	21:T:77:ALA:HB2	1.87	0.56
1:A:1184:G:H2'	1:A:1185:G:H8	1.70	0.56
1:A:1294:G:O2'	1:A:1295:G:H5'	2.05	0.56
1:A:1312:G:O2'	1:A:1313:U:H5'	2.06	0.56
1:A:555:C:H2'	1:A:556:C:C6	2.41	0.56
1:A:807:A:H2'	1:A:808:C:C6	2.41	0.56
3:B:17:PHE:HD1	3:B:17:PHE:C	2.09	0.56
9:H:20:TYR:CE1	9:H:76:PRO:HD2	2.41	0.56
9:H:6:ILE:HD12	9:H:35:ILE:HD12	1.86	0.56
9:H:9:MET:CE	9:H:32:LYS:HG2	2.36	0.56
10:I:48:GLU:HA	10:I:51:ARG:HH11	1.71	0.56
11:J:82:ILE:O	11:J:86:MET:HB2	2.05	0.56
13:L:26:ALA:O	13:L:27:LEU:O	2.23	0.56
13:L:54:LYS:HB3	13:L:70:ILE:HD12	1.88	0.56
21:T:100:ILE:HG22	21:T:102:GLY:H	1.71	0.56
1:A:1250:A:H2'	1:A:1251:A:C8	2.40	0.56
1:A:222:U:H2'	1:A:223:U:C6	2.41	0.56
1:A:828:A:H5''	1:A:859:A:C2	2.41	0.56
4:C:92:ALA:C	4:C:94:LEU:H	2.09	0.56
8:G:15:ASP:OD2	8:G:44:TYR:OH	2.24	0.56
11:J:27:ALA:C	11:J:29:ARG:H	2.08	0.56
15:N:41:ARG:HG3	15:N:42:ILE:H	1.71	0.56
21:T:82:SER:O	21:T:86:ARG:HB2	2.06	0.56
1:A:1035:A:H2'	1:A:1036:G:C8	2.40	0.56
1:A:22:G:H4'	1:A:885:G:C8	2.41	0.56
9:H:19:VAL:CG2	9:H:21:LYS:HD3	2.36	0.56
12:K:58:PRO:O	12:K:61:ALA:HB3	2.06	0.56
13:L:7:ILE:O	13:L:11:VAL:HG23	2.05	0.56
13:L:120:TYR:O	13:L:122:THR:HG23	2.06	0.56
14:M:22:ILE:HB	14:M:25:ILE:HD12	1.88	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:46:LYS:HE2	14:M:47:ASP:OD1	2.05	0.56
19:R:74:ARG:HA	19:R:79:LEU:O	2.06	0.56
19:R:86:VAL:O	19:R:87:ARG:CB	2.54	0.56
1:A:47:C:H6	1:A:365:U:H2'	1.71	0.55
1:A:539:A:H2'	1:A:540:G:H8	1.70	0.55
1:A:686:U:O2'	1:A:687:A:H8	1.88	0.55
10:I:26:VAL:HA	10:I:61:ALA:O	2.06	0.55
11:J:91:PRO:HB2	11:J:94:VAL:HG23	1.89	0.55
12:K:85:ARG:HH11	12:K:85:ARG:HG3	1.71	0.55
17:P:26:ARG:HE	17:P:31:LYS:HB3	1.72	0.55
18:Q:101:ARG:NE	18:Q:101:ARG:HA	2.21	0.55
20:S:30:LEU:HD23	20:S:31:ILE:N	2.21	0.55
20:S:43:GLU:H	20:S:43:GLU:CD	2.08	0.55
1:A:1014:A:H2'	1:A:1015:A:C8	2.41	0.55
1:A:1070:U:H2'	1:A:1071:C:H6	1.71	0.55
1:A:1360:A:H2'	1:A:1361:G:O4'	2.06	0.55
1:A:1411:C:H2'	1:A:1412:C:H6	1.71	0.55
1:A:168:G:O2'	1:A:169:C:H5'	2.07	0.55
3:B:83:MET:HG3	3:B:238:LEU:HD12	1.88	0.55
4:C:193:TYR:CE1	4:C:196:LEU:HD11	2.36	0.55
4:C:70:VAL:O	4:C:106:VAL:HG23	2.06	0.55
17:P:1:MET:O	17:P:3:LYS:HG3	2.05	0.55
1:A:1480:G:H2'	1:A:1481:U:H6	1.71	0.55
3:B:239:VAL:HG12	3:B:239:VAL:O	2.06	0.55
4:C:177:THR:CG2	4:C:180:ALA:HB2	2.36	0.55
5:D:170:VAL:CG1	5:D:174:LEU:HB2	2.34	0.55
5:D:180:GLY:HA3	5:D:182:LYS:HE2	1.87	0.55
10:I:108:VAL:HG12	10:I:109:VAL:H	1.70	0.55
11:J:39:PRO:O	11:J:40:LEU:HB2	2.06	0.55
16:O:4:THR:OG1	16:O:6:GLU:HG2	2.06	0.55
1:A:341:C:H2'	1:A:342:C:C6	2.42	0.55
1:A:45:U:H2'	1:A:46:G:C8	2.41	0.55
3:B:77:ALA:CB	3:B:211:ILE:HD13	2.25	0.55
4:C:36:ASP:HA	4:C:39:ILE:HD12	1.87	0.55
4:C:6:HIS:HD2	4:C:8:ILE:H	1.54	0.55
8:G:85:TYR:HD1	8:G:154:TYR:CE1	2.25	0.55
11:J:32:ALA:HB2	11:J:75:ILE:O	2.07	0.55
21:T:50:GLU:C	21:T:100:ILE:HD12	2.27	0.55
1:A:1441:G:H4'	1:A:1442:G:N7	2.21	0.55
1:A:1451:A:OP2	1:A:1452:C:H5	1.89	0.55
1:A:253:U:H2'	1:A:254:G:C8	2.42	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:A:H2'	1:A:89:C:O4'	2.07	0.55
3:B:164:VAL:HG12	3:B:186:ALA:CB	2.37	0.55
3:B:189:ASP:OD1	3:B:205:ASP:HB3	2.06	0.55
4:C:134:ILE:CG2	4:C:151:VAL:HB	2.37	0.55
6:E:19:MET:HE1	6:E:24:ARG:NH1	2.21	0.55
1:A:1346:A:C4	8:G:10:ARG:NH2	2.75	0.55
10:I:64:THR:O	10:I:65:VAL:HG23	2.07	0.55
1:A:1326:C:OP1	22:V:12:LYS:NZ	2.36	0.55
1:A:324:G:N2	1:A:327:A:C8	2.75	0.55
1:A:579:G:H2'	1:A:580:U:C6	2.41	0.55
1:A:625:G:H2'	1:A:626:U:C6	2.42	0.55
4:C:138:VAL:HG22	4:C:151:VAL:HG23	1.87	0.55
6:E:93:PRO:CG	9:H:105:ARG:HE	2.19	0.55
8:G:15:ASP:O	8:G:19:GLY:HA2	2.07	0.55
9:H:51:VAL:HG21	9:H:60:ARG:CG	2.32	0.55
10:I:117:HIS:C	10:I:118:LYS:HG3	2.26	0.55
10:I:121:ARG:C	10:I:121:ARG:HD3	2.26	0.55
13:L:55:VAL:CG1	13:L:56:ALA:N	2.70	0.55
1:A:1306:A:O2'	14:M:109:THR:HG21	2.07	0.55
19:R:36:ASN:C	19:R:36:ASN:HD22	2.10	0.55
20:S:44:MET:O	20:S:47:HIS:HB2	2.07	0.55
21:T:56:MET:CE	21:T:88:VAL:HG11	2.35	0.55
1:A:1172:C:O2'	1:A:1173:G:H5'	2.07	0.55
1:A:285:G:O2'	1:A:286:G:H5'	2.07	0.55
4:C:178:LEU:O	4:C:179:ARG:CB	2.54	0.55
5:D:109:GLY:O	5:D:111:ALA:N	2.39	0.55
1:A:542:G:OP1	5:D:10:ARG:NH2	2.40	0.55
6:E:45:PHE:CD2	6:E:47:LYS:HE3	2.41	0.55
8:G:145:ALA:C	8:G:147:ALA:N	2.60	0.55
10:I:24:GLY:HA2	10:I:59:PHE:O	2.05	0.55
1:A:1277:C:C2'	1:A:1278:U:H5'	2.36	0.55
1:A:92:C:O2'	1:A:93:G:H5'	2.07	0.55
4:C:123:GLN:HE22	4:C:140:ARG:HH22	1.54	0.55
7:F:22:GLU:OE1	7:F:82:ARG:HD3	2.07	0.55
8:G:30:ILE:HD13	8:G:120:ILE:HD13	1.87	0.55
8:G:75:VAL:HA	8:G:87:VAL:O	2.07	0.55
11:J:12:ASP:O	11:J:15:THR:HG22	2.07	0.55
12:K:40:ILE:HG23	12:K:75:TYR:CD2	2.41	0.55
14:M:78:ILE:O	14:M:82:MET:HB2	2.07	0.55
15:N:44:LEU:C	15:N:44:LEU:HD12	2.27	0.55
18:Q:103:GLY:O	18:Q:104:LYS:O	2.24	0.55

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:13:ASP:O	20:S:17:GLU:HG2	2.07	0.55
1:A:1038:C:H2'	1:A:1039:C:C5	2.41	0.55
1:A:1470:G:O2'	1:A:1471:G:H5'	2.07	0.55
1:A:393:A:OP2	17:P:12:LYS:HE2	2.07	0.55
3:B:12:GLU:C	3:B:14:GLY:H	2.10	0.55
3:B:142:LEU:HB3	3:B:146:GLN:NE2	2.22	0.55
3:B:223:ILE:HG21	3:B:230:VAL:CG2	2.37	0.55
4:C:174:PRO:HB2	4:C:177:THR:CG2	2.33	0.55
8:G:30:ILE:HD13	8:G:120:ILE:CD1	2.37	0.55
9:H:7:ALA:HB2	9:H:85:ARG:HD2	1.89	0.55
12:K:15:ALA:HA	12:K:76:GLY:O	2.07	0.55
14:M:84:ILE:O	14:M:86:CYS:N	2.39	0.55
16:O:39:LEU:HD23	16:O:39:LEU:C	2.27	0.55
18:Q:59:ILE:CG2	18:Q:71:PHE:HB3	2.37	0.55
12:K:84:VAL:CG2	19:R:88:LYS:HD3	2.37	0.55
1:A:957:U:H4'	20:S:79:THR:HB	1.88	0.55
21:T:86:ARG:O	21:T:90:GLN:HG3	2.06	0.55
1:A:1004:A:H3'	1:A:1025:U:O4	2.07	0.55
1:A:1044:A:H2'	1:A:1045:C:O4'	2.07	0.55
1:A:1442:G:H2'	1:A:1442:G:N3	2.21	0.55
1:A:1521:G:H2'	1:A:1522:U:C6	2.42	0.55
1:A:513:C:O2'	1:A:514:C:H5'	2.07	0.55
1:A:684:A:O3'	12:K:12:ARG:NH2	2.39	0.55
1:A:797:C:O2'	1:A:798:G:H5'	2.06	0.55
3:B:34:ALA:O	3:B:41:ILE:N	2.36	0.55
11:J:12:ASP:OD1	11:J:14:LYS:HB2	2.07	0.55
11:J:8:LEU:CD1	11:J:20:ALA:HB2	2.37	0.55
11:J:85:LEU:O	11:J:87:THR:N	2.40	0.55
12:K:84:VAL:HG11	12:K:95:ILE:HD11	1.88	0.55
13:L:53:ARG:HD2	13:L:53:ARG:N	2.22	0.55
18:Q:15:MET:CE	18:Q:43:LEU:HD22	2.37	0.55
19:R:19:LYS:O	19:R:20:ALA:HB3	2.06	0.55
20:S:30:LEU:HD23	20:S:31:ILE:H	1.71	0.55
1:A:29:G:H5'	1:A:296:U:OP1	2.07	0.54
1:A:513:C:H2'	1:A:514:C:C6	2.43	0.54
4:C:70:VAL:O	4:C:106:VAL:N	2.39	0.54
4:C:23:TYR:CD2	4:C:24:ALA:N	2.75	0.54
4:C:33:LEU:HD11	15:N:53:LEU:CD2	2.37	0.54
5:D:15:GLU:O	5:D:17:VAL:N	2.39	0.54
5:D:24:GLU:HG2	5:D:25:ARG:N	2.21	0.54
5:D:30:LYS:O	5:D:32:ALA:N	2.39	0.54

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:29:ALA:O	7:F:30:LEU:C	2.46	0.54
1:A:1250:A:H5''	10:I:68:GLY:N	2.22	0.54
11:J:51:ARG:H	11:J:59:SER:HB2	1.72	0.54
20:S:30:LEU:HD21	20:S:50:ALA:HB2	1.89	0.54
1:A:708:C:H2'	1:A:709:G:H8	1.71	0.54
1:A:765:G:H1	1:A:812:C:H2'	1.72	0.54
3:B:102:LEU:HD21	3:B:162:ILE:CD1	2.34	0.54
3:B:10:LEU:C	3:B:12:GLU:H	2.10	0.54
3:B:132:LYS:HG2	3:B:135:GLN:OE1	2.07	0.54
3:B:27:LYS:HD3	3:B:195:ASP:OD2	2.07	0.54
3:B:33:TYR:HB2	3:B:43:ASP:HB2	1.88	0.54
5:D:174:LEU:O	5:D:186:LEU:CD1	2.55	0.54
5:D:26:CYS:HA	5:D:31:CYS:HB2	1.89	0.54
8:G:54:THR:CG2	8:G:56:GLN:HE21	2.21	0.54
10:I:48:GLU:N	10:I:49:PRO:CD	2.70	0.54
10:I:4:TYR:CD2	10:I:88:TYR:HA	2.42	0.54
13:L:55:VAL:CG1	13:L:67:THR:HG23	2.38	0.54
15:N:54:PRO:O	15:N:56:VAL:HG23	2.06	0.54
16:O:87:ILE:HG22	16:O:88:ARG:N	2.22	0.54
18:Q:26:GLN:O	18:Q:27:PHE:HB3	2.07	0.54
21:T:33:ILE:HD13	21:T:63:ILE:HG12	1.88	0.54
1:A:1019:C:H2'	1:A:1020:U:O4'	2.08	0.54
3:B:178:ARG:HH21	3:B:196:LEU:HA	1.73	0.54
5:D:13:ARG:NH2	5:D:40:PRO:HA	2.22	0.54
5:D:98:GLU:OE1	5:D:194:LEU:HD11	2.07	0.54
6:E:11:ILE:HG12	6:E:33:VAL:HG23	1.89	0.54
20:S:31:ILE:O	20:S:32:LYS:HB3	2.07	0.54
21:T:14:LYS:O	21:T:17:ARG:HB2	2.06	0.54
1:A:109:A:H2'	1:A:326:G:N2	2.22	0.54
1:A:1116:C:H2'	1:A:1117:G:C5'	2.26	0.54
1:A:1141:C:H2'	1:A:1142:G:C8	2.36	0.54
1:A:1163:C:H2'	1:A:1164:G:C8	2.41	0.54
1:A:1173:G:O2'	1:A:1174:G:H5'	2.06	0.54
1:A:1514:C:H2'	1:A:1515:C:C6	2.42	0.54
1:A:160:A:H2'	1:A:161:A:O4'	2.08	0.54
1:A:17:U:H2'	1:A:18:C:H6	1.72	0.54
5:D:103:ASN:O	5:D:106:TYR:HB3	2.07	0.54
1:A:409:G:OP1	5:D:24:GLU:O	2.26	0.54
7:F:53:ALA:O	7:F:55:ASP:N	2.39	0.54
8:G:129:GLU:CB	8:G:131:LYS:HE2	2.37	0.54
6:E:93:PRO:HG2	9:H:105:ARG:HE	1.72	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:33:THR:HG1	12:K:37:GLY:C	2.10	0.54
16:O:55:GLY:O	16:O:59:MET:HG3	2.07	0.54
1:A:1021:G:H2'	1:A:1022:G:O4'	2.07	0.54
1:A:612:C:H2'	1:A:613:C:C6	2.43	0.54
1:A:731:G:O2'	1:A:732:C:H5'	2.08	0.54
1:A:7:G:H5'	1:A:298:A:O4'	2.06	0.54
3:B:17:PHE:CD1	3:B:17:PHE:C	2.81	0.54
4:C:52:LEU:HD21	4:C:118:GLN:NE2	2.21	0.54
6:E:43:LEU:HD23	6:E:44:GLY:N	2.22	0.54
9:H:45:ILE:HG13	9:H:47:GLY:N	2.23	0.54
15:N:44:LEU:O	15:N:44:LEU:HD12	2.08	0.54
18:Q:17:LYS:HD3	18:Q:47:PRO:HA	1.90	0.54
1:A:1003(A):G:H2'	1:A:1004:A:C4'	2.36	0.54
1:A:1044:A:H2'	1:A:1045:C:C4'	2.37	0.54
1:A:148:G:O2'	1:A:149:A:H5'	2.08	0.54
1:A:478:A:O2'	1:A:479:C:H5'	2.08	0.54
1:A:64:G:C4'	1:A:65:U:O5'	2.44	0.54
1:A:722:A:H4'	1:A:723:U:C5	2.43	0.54
1:A:665:A:N3	1:A:732:C:H2'	2.23	0.54
1:A:961:U:O2'	1:A:962:C:H5'	2.07	0.54
1:A:979:C:H2'	1:A:980:C:H5'	1.89	0.54
3:B:124:SER:CB	3:B:125:PRO:CD	2.86	0.54
3:B:213:LEU:HD23	3:B:213:LEU:C	2.28	0.54
5:D:25:ARG:O	5:D:27:TYR:N	2.41	0.54
13:L:24:VAL:HG12	13:L:24:VAL:O	2.07	0.54
22:V:17:THR:O	22:V:22:ARG:HD3	2.07	0.54
1:A:1148:U:O2'	1:A:1149:C:H5'	2.08	0.54
1:A:1149:C:OP1	10:I:9:ARG:HD3	2.07	0.54
1:A:403:C:O2'	1:A:404:U:H5'	2.08	0.54
1:A:457:C:H2'	1:A:458:C:C6	2.43	0.54
1:A:625:G:H4'	17:P:16:HIS:CD2	2.43	0.54
1:A:643:C:H2'	1:A:644:G:H8	1.73	0.54
4:C:47:LEU:CD2	4:C:68:VAL:HG11	2.38	0.54
5:D:100:ARG:O	5:D:104:VAL:HG23	2.08	0.54
6:E:102:ALA:HB1	6:E:120:THR:HG21	1.88	0.54
10:I:65:VAL:HG21	10:I:77:ILE:HD11	1.90	0.54
1:A:357:G:OP1	1:A:367:U:H2'	2.08	0.54
1:A:407:G:H2'	1:A:408:A:C8	2.42	0.54
12:K:108:ILE:HB	19:R:87:ARG:O	2.08	0.54
14:M:81:LEU:O	14:M:86:CYS:HB3	2.07	0.54
17:P:43:LYS:HG3	17:P:48:TRP:CD2	2.43	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1381:U:H2'	1:A:1382:C:H6	1.72	0.54
1:A:142:G:O2'	1:A:196:A:N1	2.31	0.54
1:A:620:C:H2'	1:A:621:A:O4'	2.07	0.54
4:C:167:TRP:O	4:C:168:ALA:HB3	2.07	0.54
14:M:52:GLU:HG2	14:M:55:ARG:NH2	2.22	0.54
14:M:36:LYS:HD2	14:M:59:TYR:CZ	2.43	0.54
18:Q:76:LEU:C	18:Q:76:LEU:HD23	2.28	0.54
18:Q:97:SER:HB2	18:Q:102:GLY:O	2.08	0.54
1:A:1415:G:H2'	1:A:1416:G:H8	1.72	0.54
1:A:1468:A:H2'	1:A:1469:G:O4'	2.07	0.54
1:A:1509:C:O2'	1:A:1510:U:H5'	2.08	0.54
1:A:175:C:H2'	1:A:176:C:H6	1.71	0.54
1:A:682:G:O2'	1:A:683:G:H5'	2.07	0.54
1:A:767:A:O2'	1:A:768:A:H5'	2.08	0.54
4:C:28:GLN:O	4:C:30:ARG:N	2.41	0.54
4:C:35:GLU:CG	4:C:95:THR:HG21	2.38	0.54
5:D:64:LEU:HG	5:D:198:VAL:HG11	1.90	0.54
3:B:181:PHE:CD2	9:H:70:GLN:HB3	2.43	0.54
10:I:25:LYS:HG3	10:I:60:ASP:OD1	2.08	0.54
13:L:89:ARG:HG2	13:L:97:ARG:HA	1.89	0.54
13:L:53:ARG:HB3	13:L:93:LEU:HD11	1.90	0.54
21:T:53:LEU:HD13	21:T:101:GLY:H	1.73	0.54
1:A:248:C:O2'	1:A:249:U:H5'	2.08	0.53
1:A:487:A:H2'	1:A:488:C:O4'	2.08	0.53
1:A:540:G:H2'	1:A:541:G:C8	2.42	0.53
1:A:719:C:H3'	1:A:720:C:H6	1.71	0.53
4:C:33:LEU:HD11	15:N:53:LEU:HD22	1.90	0.53
4:C:3:ASN:C	4:C:4:LYS:HG2	2.28	0.53
11:J:29:ARG:HB2	11:J:84:GLN:HE22	1.72	0.53
13:L:40:VAL:O	13:L:40:VAL:HG12	2.08	0.53
14:M:5:ALA:HB3	14:M:8:GLU:CG	2.34	0.53
1:A:976:G:OP1	15:N:32:SER:HA	2.08	0.53
16:O:26:GLU:HA	16:O:81:LEU:HD11	1.90	0.53
1:A:1245:A:H2'	1:A:1246:C:C6	2.44	0.53
1:A:615:C:O2'	1:A:616:G:H5'	2.07	0.53
4:C:30:ARG:HG2	4:C:30:ARG:NH1	2.23	0.53
5:D:25:ARG:HE	5:D:30:LYS:HD3	1.71	0.53
12:K:109:VAL:HG22	19:R:86:VAL:HA	1.90	0.53
15:N:29:ARG:HB3	15:N:40:CYS:HB3	1.90	0.53
20:S:12:ASP:HB2	20:S:35:SER:OG	2.08	0.53
21:T:56:MET:O	21:T:59:ALA:HB3	2.08	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1225:A:H5'	14:M:103:THR:HG1	1.74	0.53
1:A:75:G:H2'	1:A:76:C:H6	1.73	0.53
1:A:922:G:N3	1:A:1398:A:H2	2.06	0.53
1:A:950:U:H2'	1:A:951:G:C8	2.42	0.53
3:B:134:GLU:C	3:B:136:VAL:N	2.61	0.53
1:A:877:C:H1'	9:H:3:THR:HG21	1.90	0.53
18:Q:97:SER:OG	18:Q:103:GLY:HA3	2.09	0.53
1:A:1518:A:H2'	1:A:1519:A:C8	2.43	0.53
1:A:554:C:H2'	1:A:555:C:H6	1.74	0.53
1:A:792:A:H4'	1:A:793:U:H5''	1.90	0.53
3:B:200:ILE:HG22	3:B:201:ILE:N	2.24	0.53
6:E:102:ALA:HA	6:E:120:THR:CG2	2.38	0.53
7:F:3:ARG:HH21	7:F:64:GLN:NE2	2.06	0.53
8:G:141:VAL:O	8:G:144:MET:HB2	2.08	0.53
12:K:22:HIS:HB3	12:K:29:ILE:HG23	1.90	0.53
18:Q:97:SER:HB2	18:Q:103:GLY:HA2	1.91	0.53
1:A:1480:G:H2'	1:A:1481:U:C6	2.42	0.53
1:A:15:G:H1'	6:E:19:MET:HE2	1.91	0.53
1:A:264:U:H4'	18:Q:63:ARG:HD3	1.91	0.53
1:A:433:C:H2'	1:A:434:U:H6	1.73	0.53
4:C:43:LEU:HD13	4:C:68:VAL:CG2	2.39	0.53
4:C:79:ARG:HG2	4:C:82:GLU:HG2	1.89	0.53
11:J:80:LYS:HA	11:J:83:GLU:HB2	1.90	0.53
15:N:23:ARG:HG2	15:N:23:ARG:HH11	1.74	0.53
4:C:12:LEU:HD11	15:N:51:GLY:CA	2.39	0.53
21:T:43:LEU:HD11	21:T:55:ILE:HD12	1.91	0.53
1:A:1260:C:H4'	1:A:1284:C:H5'	1.91	0.53
1:A:75:G:H2'	1:A:76:C:C6	2.44	0.53
3:B:74:LYS:HZ1	3:B:206:ASP:HA	1.72	0.53
5:D:109:GLY:O	5:D:110:PHE:C	2.47	0.53
12:K:72:ALA:HB1	12:K:77:MET:HG3	1.90	0.53
14:M:77:ASN:O	14:M:80:ARG:HB3	2.07	0.53
14:M:96:LEU:O	14:M:110:ARG:NH1	2.42	0.53
18:Q:18:THR:HG23	18:Q:69:LYS:HE3	1.89	0.53
1:A:129(A):G:C2	1:A:190(E):U:H5'	2.44	0.53
1:A:1347:G:C2'	1:A:1348:U:OP2	2.57	0.53
1:A:1420:C:H2'	1:A:1421:G:C8	2.43	0.53
1:A:1461:G:O2'	1:A:1462:G:H5'	2.09	0.53
1:A:791:G:H2'	1:A:792:A:C5'	2.39	0.53
1:A:834:C:H2'	1:A:835:U:H6	1.73	0.53
3:B:101:MET:N	3:B:108:ILE:HD12	2.24	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:88:ALA:O	3:B:90:MET:N	2.42	0.53
5:D:199:ASN:HD21	5:D:201:GLN:HB3	1.74	0.53
7:F:14:LEU:HB2	7:F:19:LEU:HB2	1.89	0.53
7:F:36:ARG:HH11	7:F:36:ARG:HG2	1.74	0.53
8:G:110:GLN:OE1	8:G:110:GLN:HA	2.09	0.53
9:H:9:MET:HE2	9:H:32:LYS:HG2	1.89	0.53
11:J:18:ALA:O	11:J:22:LYS:HG3	2.08	0.53
1:A:1150:U:O2	11:J:39:PRO:HG3	2.08	0.53
12:K:100:ALA:O	12:K:102:GLY:N	2.42	0.53
18:Q:82:MET:O	18:Q:83:ASP:C	2.47	0.53
21:T:24:LEU:HD12	21:T:27:LYS:HD3	1.90	0.53
1:A:1236:A:H2'	1:A:1237:C:C6	2.43	0.53
1:A:132:C:O2'	1:A:133:U:H5'	2.08	0.53
1:A:216:G:H2'	1:A:217:C:C6	2.44	0.53
1:A:781:A:H2	1:A:1514:C:C4'	2.22	0.53
1:A:946:A:H2'	1:A:947:G:C8	2.44	0.53
3:B:126:GLU:O	3:B:129:GLU:HB2	2.09	0.53
3:B:152:PHE:CE1	3:B:155:LEU:HD12	2.43	0.53
3:B:23:ARG:H	3:B:23:ARG:HD3	1.71	0.53
3:B:67:THR:CA	3:B:90:MET:HE1	2.39	0.53
4:C:157:ILE:HD11	4:C:166:GLU:HB2	1.90	0.53
8:G:18:TYR:CD2	8:G:59:LEU:HD22	2.42	0.53
14:M:122:LYS:O	14:M:123:ALA:HB2	2.09	0.53
4:C:13:GLY:HA3	15:N:57:ARG:CZ	2.38	0.53
16:O:41:GLU:OE2	16:O:41:GLU:HA	2.09	0.53
18:Q:97:SER:HB2	18:Q:103:GLY:CA	2.38	0.53
18:Q:68:ARG:HH11	18:Q:68:ARG:CG	2.22	0.53
19:R:40:LEU:CB	19:R:79:LEU:HD11	2.38	0.53
1:A:1066:C:O2'	1:A:1067:A:H5'	2.08	0.53
1:A:1404:C:H2'	1:A:1405:G:C8	2.44	0.53
1:A:399:G:O2'	1:A:400:C:H5'	2.08	0.53
1:A:930:C:C2'	1:A:931:C:H5'	2.39	0.53
3:B:115:LEU:O	3:B:119:GLU:HG3	2.08	0.53
3:B:140:HIS:O	3:B:143:GLU:HB2	2.08	0.53
4:C:22:TRP:CZ3	4:C:32:LEU:HD22	2.43	0.53
9:H:82:HIS:O	9:H:83:ILE:HB	2.09	0.53
11:J:50:ILE:HG22	11:J:52:GLY:O	2.09	0.53
13:L:11:VAL:HG21	18:Q:34:LYS:HG2	1.91	0.53
14:M:37:THR:O	14:M:37:THR:HG22	2.08	0.53
19:R:87:ARG:HG2	19:R:87:ARG:NH1	2.24	0.53
1:A:102:G:H2'	1:A:103:C:H6	1.73	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1154:G:H2'	1:A:1155:G:H8	1.74	0.53
1:A:1343:G:H2'	1:A:1344:C:C6	2.44	0.53
1:A:927:G:H4'	1:A:1503:A:N7	2.24	0.53
1:A:21:G:H2'	1:A:22:G:C8	2.44	0.53
1:A:281:G:O2'	1:A:282:A:OP2	2.24	0.53
1:A:39:G:O2'	1:A:40:C:H5'	2.09	0.53
4:C:139:GLN:O	4:C:143:GLU:N	2.39	0.53
10:I:48:GLU:OE1	10:I:51:ARG:HD2	2.09	0.53
11:J:81:THR:C	11:J:83:GLU:H	2.10	0.53
14:M:34:LEU:HD13	14:M:41:PRO:HA	1.90	0.53
1:A:1348:U:H2'	1:A:1349:A:H8	1.74	0.52
1:A:164:U:H2'	1:A:165:C:C6	2.44	0.52
1:A:966:G:H2'	1:A:967:C:C6	2.44	0.52
3:B:143:GLU:O	3:B:147:LYS:HG3	2.08	0.52
4:C:73:PRO:HD3	4:C:105:GLU:HG3	1.92	0.52
7:F:19:LEU:HD23	7:F:20:ALA:N	2.24	0.52
8:G:108:ALA:O	8:G:119:ARG:HD2	2.09	0.52
11:J:16:LEU:HD23	11:J:94:VAL:HG13	1.90	0.52
16:O:64:ARG:HH11	16:O:64:ARG:HG3	1.74	0.52
1:A:1305:G:H2'	1:A:1331:G:N2	2.24	0.52
1:A:170:U:O2'	1:A:171:A:H5'	2.09	0.52
1:A:500:G:N2	1:A:546:G:H1'	2.24	0.52
4:C:119:ARG:HG2	4:C:140:ARG:NH1	2.25	0.52
4:C:173:VAL:O	4:C:173:VAL:HG12	2.08	0.52
4:C:91:LEU:HD21	4:C:99:VAL:HG13	1.90	0.52
6:E:15:ARG:O	6:E:16:THR:O	2.27	0.52
11:J:75:ILE:HG22	11:J:76:ASN:N	2.24	0.52
18:Q:69:LYS:C	18:Q:70:ARG:HD2	2.29	0.52
18:Q:98:LEU:O	18:Q:98:LEU:HD12	2.08	0.52
20:S:22:LEU:CD2	20:S:28:LYS:HD2	2.38	0.52
1:A:1005:A:C2'	1:A:1006:C:H5'	2.38	0.52
1:A:518:C:H5'	1:A:530:G:O4'	2.09	0.52
1:A:757:U:H2'	1:A:758:G:O4'	2.10	0.52
1:A:77:G:O2'	1:A:78:G:H5'	2.09	0.52
4:C:138:VAL:CG2	4:C:151:VAL:HG23	2.39	0.52
5:D:30:LYS:C	5:D:32:ALA:N	2.57	0.52
1:A:600:C:OP1	9:H:97:VAL:HG12	2.09	0.52
11:J:20:ALA:O	11:J:24:VAL:HG23	2.10	0.52
13:L:33:ARG:CD	13:L:62:SER:HB3	2.39	0.52
13:L:98:TYR:N	13:L:98:TYR:CD1	2.77	0.52
15:N:37:PHE:CE2	15:N:53:LEU:HD13	2.44	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:48:TRP:O	17:P:49:LEU:HB2	2.10	0.52
1:A:1207:G:O2'	1:A:1208:C:H5'	2.09	0.52
1:A:1347:G:H3'	10:I:108:VAL:O	2.09	0.52
1:A:401:C:H2'	1:A:402:G:H8	1.74	0.52
3:B:119:GLU:OE2	3:B:153:ARG:NH2	2.42	0.52
5:D:151:LYS:CD	5:D:151:LYS:H	2.22	0.52
5:D:33:MET:O	5:D:37:PRO:HG3	2.09	0.52
6:E:36:ASP:CG	6:E:40:ARG:HB2	2.29	0.52
6:E:81:GLU:OE1	6:E:88:LYS:HE2	2.09	0.52
12:K:34:ASP:O	12:K:36:ASP:N	2.43	0.52
17:P:75:ARG:O	17:P:78:GLY:N	2.41	0.52
1:A:1195:C:H3'	1:A:1196:U:C5'	2.39	0.52
1:A:1288:A:H1'	1:A:1353:G:O4'	2.09	0.52
1:A:1478:C:H2'	1:A:1479:C:C6	2.44	0.52
3:B:53:ARG:NH1	3:B:199:TYR:CD2	2.73	0.52
4:C:58:GLU:H	4:C:65:ALA:HB3	1.74	0.52
5:D:96:LEU:CD1	5:D:96:LEU:N	2.73	0.52
6:E:51:VAL:HB	6:E:52:PRO:HD3	1.92	0.52
11:J:89:ASP:O	11:J:90:LEU:HD23	2.09	0.52
1:A:1228:C:OP1	14:M:115:LYS:HD3	2.10	0.52
16:O:70:LEU:HD12	16:O:78:TYR:HB2	1.91	0.52
19:R:53:ARG:NH1	19:R:60:GLY:N	2.57	0.52
21:T:43:LEU:HD13	21:T:51:GLU:CG	2.35	0.52
21:T:56:MET:HE2	21:T:88:VAL:CG1	2.39	0.52
1:A:794:A:H2'	1:A:795:C:C6	2.45	0.52
3:B:149:LEU:O	3:B:153:ARG:HG2	2.09	0.52
6:E:80:ILE:C	6:E:80:ILE:HD12	2.30	0.52
7:F:45:LEU:HA	7:F:58:GLY:O	2.10	0.52
8:G:21:VAL:CG2	8:G:22:LEU:N	2.72	0.52
18:Q:97:SER:OG	18:Q:98:LEU:N	2.40	0.52
1:A:1061:G:O2'	1:A:1062:U:H5'	2.10	0.52
1:A:1125:U:OP2	1:A:1145:C:N4	2.43	0.52
1:A:180:U:H2'	1:A:181:G:H5'	1.91	0.52
1:A:579:G:H2'	1:A:580:U:H6	1.75	0.52
3:B:200:ILE:CG2	3:B:201:ILE:N	2.72	0.52
1:A:1112:C:N3	4:C:178:LEU:N	2.58	0.52
4:C:48:TYR:HA	4:C:52:LEU:HD22	1.91	0.52
7:F:74:ASP:OD1	7:F:77:ARG:CZ	2.57	0.52
10:I:95:LYS:O	10:I:99:LEU:HD23	2.09	0.52
1:A:1117:G:O3'	10:I:104:ARG:HD2	2.10	0.52
1:A:385:C:H2'	1:A:386:C:C6	2.45	0.52

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:A:O2'	1:A:409:G:H5'	2.09	0.52
1:A:624:C:H2'	1:A:625:G:H8	1.74	0.52
1:A:429:U:C2'	5:D:25:ARG:HH12	2.23	0.52
5:D:29:PRO:O	5:D:30:LYS:CG	2.51	0.52
5:D:60:GLU:HA	5:D:60:GLU:OE1	2.10	0.52
14:M:82:MET:O	14:M:93:ARG:NH2	2.43	0.52
18:Q:74:LEU:CD2	18:Q:74:LEU:C	2.77	0.52
1:A:187:C:O2	21:T:105:SER:HB3	2.08	0.52
1:A:103:C:P	21:T:17:ARG:HH11	2.33	0.52
21:T:94:ALA:O	21:T:95:ALA:HB3	2.10	0.52
1:A:774:G:O2'	1:A:775:G:H5'	2.10	0.52
1:A:972:C:H4'	11:J:57:LYS:HB3	1.91	0.52
4:C:82:GLU:O	4:C:86:VAL:HG23	2.10	0.52
5:D:61:LYS:HD2	5:D:207:TYR:CZ	2.44	0.52
5:D:31:CYS:C	5:D:33:MET:H	2.13	0.52
1:A:1298:C:C6	8:G:114:ARG:NH1	2.78	0.52
8:G:15:ASP:HB3	8:G:19:GLY:N	2.24	0.52
10:I:110:GLU:OE2	10:I:113:LYS:NZ	2.43	0.52
1:A:1123:A:O3'	11:J:36:GLY:HA3	2.09	0.52
11:J:65:LEU:C	11:J:65:LEU:HD23	2.30	0.52
14:M:107:ALA:O	14:M:111:LYS:HB2	2.10	0.52
18:Q:95:TYR:C	18:Q:97:SER:N	2.62	0.52
1:A:147:G:O2'	1:A:148:G:H5'	2.10	0.52
1:A:229:U:O2'	17:P:23:ASP:HB2	2.09	0.52
1:A:253:U:H2'	1:A:254:G:H8	1.75	0.52
1:A:435:C:H2'	1:A:436:C:C6	2.45	0.52
1:A:19:C:O2	1:A:572:A:H2	1.92	0.52
1:A:586:C:O3'	9:H:89:PRO:HB2	2.11	0.52
5:D:151:LYS:N	5:D:151:LYS:HD2	2.24	0.52
12:K:21:ILE:HD12	12:K:95:ILE:HG12	1.90	0.52
13:L:83:VAL:HG21	13:L:100:ILE:CG2	2.39	0.52
1:A:612:C:H2'	1:A:613:C:H6	1.74	0.51
4:C:174:PRO:CB	4:C:177:THR:HG22	2.38	0.51
4:C:47:LEU:HD23	4:C:68:VAL:HG11	1.92	0.51
8:G:154:TYR:O	8:G:156:TRP:N	2.43	0.51
14:M:109:THR:HG23	14:M:110:ARG:N	2.24	0.51
17:P:67:THR:CG2	17:P:68:ASP:N	2.73	0.51
18:Q:97:SER:O	18:Q:99:SER:N	2.44	0.51
20:S:63:THR:HB	20:S:65:ASN:OD1	2.09	0.51
1:A:1063:C:H3'	1:A:1064:G:H2'	1.92	0.51
1:A:1240:U:H4'	1:A:1241:G:OP2	2.09	0.51

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1372:U:C2'	1:A:1373:G:H5'	2.40	0.51
1:A:1427:U:H2'	1:A:1428:A:C8	2.44	0.51
1:A:788:U:O3'	25:A:1632:PCY:H25	2.10	0.51
1:A:190(I):G:O2'	1:A:190(J):U:H5'	2.09	0.51
1:A:382:A:C2	1:A:383:A:C4	2.98	0.51
1:A:939:G:H2'	1:A:940:C:H6	1.74	0.51
3:B:17:PHE:CD1	3:B:18:GLY:N	2.78	0.51
4:C:64:VAL:CG2	4:C:99:VAL:HB	2.36	0.51
5:D:132:ARG:O	5:D:132:ARG:HG3	2.11	0.51
8:G:51:GLN:HG2	8:G:58:PRO:HD3	1.93	0.51
8:G:87:VAL:HG12	8:G:88:PRO:O	2.10	0.51
11:J:38:ILE:CG1	11:J:72:VAL:H	2.18	0.51
13:L:112:ASP:O	13:L:114:LYS:HG3	2.10	0.51
20:S:5:LEU:O	20:S:6:LYS:CB	2.59	0.51
1:A:1142:G:C2	1:A:1143:G:H1'	2.45	0.51
4:C:83:ARG:C	4:C:85:ARG:N	2.64	0.51
8:G:18:TYR:HB3	8:G:59:LEU:HD22	1.92	0.51
17:P:6:LEU:HB3	17:P:17:TYR:HD2	1.75	0.51
1:A:1216:G:H5''	15:N:5:ALA:HB2	1.91	0.51
1:A:1257:U:O2'	1:A:1258:G:OP2	2.27	0.51
1:A:129(A):G:O2'	1:A:130:A:OP2	2.29	0.51
1:A:760:G:H2'	1:A:761:G:H5'	1.92	0.51
1:A:960:U:O2	1:A:960:U:H5'	2.10	0.51
1:A:974:A:OP2	15:N:41:ARG:NH1	2.43	0.51
3:B:101:MET:HG2	3:B:108:ILE:CD1	2.40	0.51
3:B:62:ALA:O	3:B:64:ARG:N	2.35	0.51
6:E:135:THR:O	6:E:138:ALA:HB3	2.10	0.51
9:H:104:ARG:NH2	9:H:138:TRP:CH2	2.78	0.51
9:H:51:VAL:CG1	9:H:52:ASP:N	2.70	0.51
9:H:83:ILE:O	9:H:83:ILE:HG23	2.10	0.51
12:K:33:THR:OG1	12:K:34:ASP:N	2.44	0.51
16:O:31:LEU:HD12	16:O:31:LEU:H	1.75	0.51
1:A:281:G:O2'	1:A:282:A:C8	2.64	0.51
1:A:390:C:H2'	1:A:391:G:H8	1.74	0.51
1:A:974:A:H8	1:A:974:A:OP1	1.93	0.51
5:D:187:ARG:NE	5:D:188:LEU:N	2.56	0.51
7:F:86:ARG:O	7:F:87:ARG:HG2	2.11	0.51
1:A:1368:G:P	10:I:112:LYS:O	2.68	0.51
10:I:4:TYR:CE1	10:I:88:TYR:HD1	2.28	0.51
1:A:1152:A:C5'	11:J:13:HIS:HD2	2.18	0.51
21:T:57:ARG:HH21	21:T:100:ILE:CG2	2.23	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:T:56:MET:HE2	21:T:88:VAL:CB	2.40	0.51
1:A:1039:C:O2'	1:A:1040:U:H5'	2.11	0.51
1:A:1279:A:O2'	1:A:1281:U:OP2	2.26	0.51
1:A:1420:C:H2'	1:A:1421:G:H8	1.75	0.51
1:A:1522:U:O2'	1:A:1523:G:H5'	2.10	0.51
1:A:255:G:H2'	1:A:256:U:H6	1.75	0.51
1:A:734:G:H21	19:R:75:ILE:HD11	1.75	0.51
4:C:40:ARG:HG3	4:C:40:ARG:HH11	1.76	0.51
6:E:24:ARG:HG2	6:E:24:ARG:HH11	1.76	0.51
11:J:3:LYS:HG2	11:J:75:ILE:HG23	1.92	0.51
12:K:19:ALA:HB2	12:K:80:VAL:HG11	1.91	0.51
12:K:95:ILE:O	12:K:99:GLN:HG3	2.10	0.51
18:Q:10:VAL:O	18:Q:53:LEU:HD12	2.10	0.51
21:T:79:ARG:O	21:T:80:ARG:C	2.47	0.51
1:A:1036:G:H2'	1:A:1037:C:O4'	2.10	0.51
1:A:459:G:H3'	1:A:460:A:H5''	1.91	0.51
1:A:628:G:H2'	1:A:629:G:C8	2.46	0.51
1:A:942:G:N2	1:A:943:U:H1'	2.26	0.51
3:B:125:PRO:HG2	3:B:126:GLU:H	1.75	0.51
3:B:142:LEU:HB3	3:B:146:GLN:HE22	1.75	0.51
3:B:35:GLU:HA	3:B:39:ILE:O	2.10	0.51
3:B:80:ILE:HD13	3:B:212:GLN:HB2	1.92	0.51
4:C:152:ILE:HB	4:C:199:LYS:HB2	1.93	0.51
1:A:542:G:H5'	5:D:41:GLY:HA3	1.91	0.51
5:D:78:LEU:HD21	5:D:96:LEU:HB3	1.93	0.51
7:F:48:LEU:HD13	7:F:52:ILE:CG1	2.41	0.51
12:K:48:ILE:HD11	12:K:64:ALA:CA	2.41	0.51
18:Q:66:SER:O	18:Q:70:ARG:NH1	2.43	0.51
19:R:21:LYS:HG3	19:R:57:GLY:HA3	1.91	0.51
20:S:40:ILE:CD1	20:S:62:ILE:HD13	2.32	0.51
1:A:1070:U:H2'	1:A:1071:C:C6	2.45	0.51
1:A:1095:U:H2'	1:A:1096:C:H6	1.76	0.51
1:A:1161:C:H2'	1:A:1162:C:C6	2.46	0.51
1:A:47:C:C6	1:A:365:U:H2'	2.46	0.51
1:A:505:G:H2'	1:A:506:G:H8	1.75	0.51
1:A:761:G:H2'	1:A:762:C:C6	2.46	0.51
1:A:780:A:O2'	1:A:781:A:H5''	2.11	0.51
3:B:15:VAL:CG2	3:B:209:ARG:HG3	2.41	0.51
4:C:22:TRP:NE1	4:C:36:ASP:OD1	2.40	0.51
4:C:83:ARG:HA	4:C:86:VAL:HG23	1.93	0.51
14:M:8:GLU:HG3	14:M:22:ILE:HG23	1.93	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:81:LEU:HD23	14:M:81:LEU:N	2.26	0.51
21:T:47:GLY:O	21:T:49:ALA:N	2.44	0.51
1:A:217:C:O2'	1:A:218:C:H5'	2.11	0.51
1:A:332:G:O2'	1:A:333:G:H5'	2.11	0.51
1:A:543:C:O2'	1:A:544:G:H5'	2.10	0.51
1:A:57:G:H2'	1:A:58:C:C6	2.45	0.51
3:B:80:ILE:HD13	3:B:212:GLN:CA	2.40	0.51
6:E:15:ARG:CD	6:E:26:PHE:CD2	2.94	0.51
9:H:61:VAL:O	9:H:63:LEU:HD13	2.11	0.51
10:I:3:GLN:HG2	10:I:4:TYR:N	2.26	0.51
11:J:34:VAL:HG12	11:J:36:GLY:H	1.76	0.51
12:K:104:GLN:OE1	12:K:106:LYS:HE2	2.11	0.51
12:K:74:ALA:C	12:K:76:GLY:H	2.14	0.51
13:L:110:VAL:O	13:L:122:THR:HG21	2.10	0.51
14:M:96:LEU:HB3	14:M:97:PRO:HD2	1.93	0.51
17:P:32:TYR:H	17:P:32:TYR:HD1	1.59	0.51
1:A:1041:A:H2'	1:A:1042:G:H8	1.76	0.51
1:A:1167:A:H2'	1:A:1168:A:C8	2.46	0.51
1:A:1250:A:H5'	10:I:68:GLY:O	2.11	0.51
1:A:1346:A:H61	1:A:1374:A:H3'	1.74	0.51
1:A:1426:C:O2'	1:A:1427:U:H5'	2.10	0.51
1:A:243:A:C2	1:A:246:A:C8	2.98	0.51
1:A:309:G:H2'	1:A:310:G:H8	1.76	0.51
1:A:644:G:O2'	1:A:645:C:H5'	2.10	0.51
1:A:953:G:N7	14:M:104:ARG:NH2	2.56	0.51
10:I:58:ARG:CG	10:I:58:ARG:HH11	2.24	0.51
12:K:62:GLN:O	12:K:66:LEU:HG	2.11	0.51
18:Q:76:LEU:HD23	18:Q:77:VAL:N	2.26	0.51
1:A:1005:A:H2'	1:A:1006:C:H5'	1.93	0.50
1:A:1010:G:O2'	1:A:1011:G:H5'	2.12	0.50
1:A:1041:A:H2'	1:A:1042:G:C8	2.45	0.50
1:A:1102:A:H2'	1:A:1103:C:H6	1.76	0.50
1:A:1418:A:H2'	1:A:1419:G:O4'	2.11	0.50
1:A:541:G:O2'	1:A:542:G:H5'	2.11	0.50
1:A:825:G:O2'	1:A:826:C:H5'	2.11	0.50
1:A:98:U:O2'	1:A:99:C:H5'	2.11	0.50
3:B:184:VAL:N	3:B:198:ASP:OD2	2.41	0.50
6:E:81:GLU:CG	6:E:90:VAL:HG22	2.28	0.50
8:G:113:GLU:HG2	8:G:119:ARG:HG2	1.93	0.50
11:J:6:ILE:HG23	11:J:98:ILE:CD1	2.41	0.50
20:S:22:LEU:HD13	20:S:28:LYS:HB2	1.92	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:G:H2'	1:A:106:C:H6	1.75	0.50
1:A:1138:G:H3'	1:A:1138:G:N3	2.27	0.50
1:A:1342:C:H5''	10:I:125:TYR:CE1	2.46	0.50
1:A:1386:G:O2'	1:A:1387:G:H5'	2.10	0.50
1:A:1397:C:H4'	1:A:1398:A:OP2	2.10	0.50
1:A:991:U:O2'	1:A:992:U:H5'	2.10	0.50
4:C:141:VAL:HG11	4:C:202:ILE:HG12	1.93	0.50
5:D:205:GLU:O	5:D:208:SER:HB2	2.10	0.50
6:E:115:VAL:HG11	6:E:118:ILE:CG1	2.40	0.50
13:L:33:ARG:HH11	13:L:62:SER:HB3	1.75	0.50
22:V:2:GLY:C	22:V:4:GLY:N	2.64	0.50
1:A:1249:C:H2'	1:A:1250:A:H5'	1.93	0.50
3:B:36:ARG:HD2	3:B:41:ILE:CD1	2.41	0.50
4:C:121:ALA:O	4:C:125:GLU:HG3	2.11	0.50
4:C:182:ILE:HG12	4:C:203:PHE:HD1	1.74	0.50
8:G:69:VAL:HG21	8:G:104:LEU:CD2	2.23	0.50
10:I:111:ARG:HD3	10:I:112:LYS:C	2.32	0.50
10:I:46:ALA:HB1	10:I:77:ILE:HG22	1.93	0.50
11:J:5:ARG:C	11:J:98:ILE:HG23	2.31	0.50
12:K:13:GLN:HA	12:K:75:TYR:O	2.12	0.50
13:L:71:PRO:O	13:L:102:ARG:HD2	2.11	0.50
20:S:15:LEU:O	20:S:19:VAL:N	2.44	0.50
1:A:671:G:H2'	1:A:672:U:O4'	2.11	0.50
4:C:91:LEU:CD1	4:C:99:VAL:HG13	2.41	0.50
5:D:103:ASN:O	5:D:106:TYR:N	2.44	0.50
7:F:9:VAL:HB	7:F:87:ARG:HB2	1.93	0.50
8:G:71:PRO:O	8:G:96:GLN:HG2	2.11	0.50
3:B:179:LYS:HA	9:H:72:PRO:HD3	1.92	0.50
10:I:93:ARG:O	10:I:95:LYS:N	2.45	0.50
15:N:21:TYR:HE2	15:N:23:ARG:HG3	1.77	0.50
16:O:4:THR:H	16:O:7:GLU:HG3	1.75	0.50
19:R:34:TYR:CE1	19:R:35:ARG:HG3	2.46	0.50
1:A:1130:A:OP2	1:A:1131:G:OP2	2.30	0.50
1:A:1258:G:O2'	1:A:1259:C:H5'	2.12	0.50
1:A:393:A:C2'	1:A:394:G:H5'	2.40	0.50
1:A:437:U:H2'	1:A:438:G:H5'	1.93	0.50
1:A:961:U:H2'	1:A:962:C:H5'	1.93	0.50
3:B:60:ASP:CG	3:B:64:ARG:NH2	2.64	0.50
3:B:57:PHE:O	3:B:60:ASP:HB3	2.11	0.50
4:C:34:LEU:HD21	4:C:38:ARG:CZ	2.42	0.50
4:C:8:ILE:O	4:C:11:ARG:N	2.44	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:149:ALA:HB3	5:D:152:SER:OG	2.12	0.50
7:F:65:VAL:HG23	7:F:66:GLU:N	2.27	0.50
9:H:56:LYS:N	9:H:56:LYS:HD2	2.25	0.50
3:B:181:PHE:HD2	9:H:70:GLN:HB3	1.76	0.50
1:A:881:G:OP2	13:L:12:ARG:NH2	2.44	0.50
1:A:1070:U:O2'	1:A:1071:C:H5'	2.12	0.50
1:A:270:A:H2'	1:A:271:C:C6	2.46	0.50
1:A:313:A:H2'	1:A:314:C:C6	2.47	0.50
1:A:475:G:H2'	1:A:476:G:H8	1.76	0.50
1:A:818:G:H3'	1:A:819:A:H5''	1.88	0.50
1:A:824:C:O2'	1:A:825:G:H5'	2.10	0.50
1:A:899:C:H2'	1:A:900:A:C8	2.47	0.50
1:A:913:A:O2'	1:A:914:A:P	2.70	0.50
3:B:184:VAL:CG1	3:B:197:VAL:HA	2.42	0.50
3:B:230:VAL:HG13	3:B:231:GLU:OE2	2.12	0.50
3:B:17:PHE:HA	3:B:44:LEU:HD21	1.92	0.50
4:C:7:PRO:HG2	4:C:184:TYR:CB	2.41	0.50
5:D:117:ALA:O	5:D:121:VAL:HG23	2.12	0.50
10:I:4:TYR:CZ	10:I:88:TYR:HD1	2.30	0.50
11:J:45:ARG:NH2	15:N:36:PHE:CE2	2.76	0.50
18:Q:68:ARG:NH1	18:Q:68:ARG:HG2	2.24	0.50
1:A:1054:C:O2'	1:A:1055:A:H5''	2.12	0.50
1:A:149:A:O2'	1:A:150:C:H5'	2.12	0.50
1:A:650:G:C2'	1:A:651:C:H5'	2.41	0.50
5:D:157:LEU:C	5:D:157:LEU:HD13	2.32	0.50
1:A:921:U:O2	6:E:19:MET:HB2	2.12	0.50
7:F:2:ARG:HG3	7:F:69:GLU:HG2	1.93	0.50
9:H:36:LEU:CD1	9:H:59:LEU:HD13	2.41	0.50
9:H:64:LYS:HG2	9:H:79:VAL:HG21	1.94	0.50
10:I:17:VAL:CG2	10:I:80:GLY:HA3	2.41	0.50
11:J:51:ARG:CB	11:J:59:SER:HB3	2.28	0.50
15:N:29:ARG:HB3	15:N:40:CYS:CB	2.40	0.50
16:O:87:ILE:O	16:O:88:ARG:CB	2.53	0.50
21:T:45:GLN:CA	21:T:91:LEU:HD22	2.42	0.50
22:V:9:ARG:HH11	22:V:22:ARG:HA	1.76	0.50
1:A:1217:C:O2'	1:A:1218:C:H5'	2.11	0.50
1:A:1370:G:O2'	1:A:1371:G:H5'	2.12	0.50
1:A:1402:C:H2'	1:A:1403:C:O4'	2.12	0.50
1:A:299:G:C6	1:A:300:A:N1	2.80	0.50
1:A:446:G:O2'	1:A:447:G:H5'	2.12	0.50
3:B:15:VAL:HG11	3:B:210:SER:N	2.26	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:102:ASN:ND2	4:C:102:ASN:H	2.09	0.50
7:F:18:GLN:O	7:F:21:LEU:HB3	2.12	0.50
7:F:75:LEU:HD13	7:F:75:LEU:C	2.32	0.50
9:H:119:LEU:HB2	9:H:123:GLU:HB3	1.93	0.50
11:J:47:PHE:CE2	15:N:37:PHE:HE1	2.29	0.50
11:J:54:PHE:O	11:J:55:LYS:HG2	2.11	0.50
1:A:1053:G:H4'	1:A:1054:C:H5'	1.93	0.50
1:A:1234:C:H1'	1:A:1364:U:O2	2.12	0.50
1:A:644:G:C5	1:A:645:C:C5	3.00	0.50
3:B:17:PHE:CA	3:B:44:LEU:HD21	2.41	0.50
6:E:115:VAL:HG12	6:E:116:THR:N	2.25	0.50
8:G:38:LEU:O	8:G:38:LEU:HD12	2.12	0.50
9:H:7:ALA:CB	9:H:85:ARG:HG3	2.42	0.50
1:A:1348:U:H4'	10:I:120:ARG:HD2	1.94	0.50
13:L:17:LYS:HA	13:L:17:LYS:HE3	1.94	0.50
14:M:90:LEU:HD23	14:M:93:ARG:HH11	1.77	0.50
7:F:101:ALA:HB1	19:R:28:GLU:OE2	2.12	0.50
21:T:15:ARG:HA	21:T:18:GLN:HG3	1.93	0.50
21:T:57:ARG:HG2	21:T:57:ARG:NH1	2.27	0.50
1:A:1277:C:H1'	1:A:1282:C:O2	2.12	0.49
1:A:1308:U:H2'	1:A:1309:G:C8	2.47	0.49
1:A:1367:C:H5'	11:J:60:ARG:HH12	1.76	0.49
1:A:1434:A:O2'	1:A:1435:G:H5'	2.11	0.49
1:A:590:C:O2'	1:A:591:U:H5'	2.12	0.49
1:A:637:G:O2'	1:A:638:G:H5'	2.12	0.49
1:A:849:C:H2'	1:A:850:U:C6	2.46	0.49
3:B:197:VAL:HB	3:B:200:ILE:CG1	2.42	0.49
5:D:3:ARG:NH2	5:D:74:GLN:CD	2.65	0.49
7:F:95:GLU:N	7:F:95:GLU:CD	2.66	0.49
1:A:1298:C:C4	8:G:114:ARG:HD3	2.46	0.49
15:N:23:ARG:HA	15:N:30:ALA:HA	1.94	0.49
18:Q:97:SER:HB2	18:Q:103:GLY:N	2.27	0.49
19:R:36:ASN:ND2	19:R:39:VAL:H	2.10	0.49
20:S:28:LYS:CG	20:S:29:ARG:H	2.17	0.49
1:A:1206:G:C6	1:A:1207:G:C5	3.00	0.49
1:A:1293:G:O2'	1:A:1294:G:H5'	2.12	0.49
1:A:197:A:H1'	1:A:198:G:O4'	2.12	0.49
1:A:384:G:H2'	1:A:385:C:C6	2.47	0.49
1:A:621:A:H2'	1:A:622:A:H8	1.76	0.49
1:A:820:U:H4'	1:A:821:G:OP2	2.12	0.49
5:D:68:TYR:O	5:D:69:GLY:C	2.50	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:148:ASN:C	8:G:150:ALA:H	2.15	0.49
11:J:3:LYS:HG2	11:J:75:ILE:HG12	1.95	0.49
14:M:86:CYS:SG	14:M:88:ARG:HB3	2.52	0.49
15:N:57:ARG:HG2	15:N:58:LYS:N	2.27	0.49
17:P:67:THR:HG22	17:P:68:ASP:H	1.75	0.49
1:A:1311:G:N7	20:S:2:PRO:HA	2.26	0.49
1:A:1044:A:H2'	1:A:1045:C:C5'	2.42	0.49
1:A:1060:C:O2'	1:A:1061:G:H5'	2.13	0.49
1:A:1346:A:N1	1:A:1374:A:H5''	2.28	0.49
1:A:294:U:H2'	1:A:295:C:C6	2.47	0.49
1:A:358:U:H2'	1:A:359:U:C6	2.48	0.49
1:A:760:G:C2	18:Q:103:GLY:O	2.64	0.49
1:A:918:A:H2'	1:A:919:A:C8	2.48	0.49
3:B:208:ILE:O	3:B:210:SER:N	2.46	0.49
4:C:6:HIS:NE2	4:C:8:ILE:HB	2.27	0.49
5:D:190:ASP:O	5:D:194:LEU:HD23	2.12	0.49
6:E:19:MET:CE	6:E:24:ARG:NH1	2.75	0.49
8:G:143:ARG:O	8:G:145:ALA:O	2.30	0.49
1:A:1367:C:H5''	10:I:114:TYR:HB2	1.94	0.49
12:K:122:LYS:O	12:K:123:LYS:C	2.50	0.49
12:K:14:VAL:O	12:K:15:ALA:HB3	2.12	0.49
19:R:62:GLU:O	19:R:65:ILE:HG13	2.12	0.49
1:A:1010:G:H2'	1:A:1011:G:H8	1.78	0.49
1:A:1005:A:C1'	1:A:1036:G:H22	2.25	0.49
1:A:1112:C:O2	4:C:178:LEU:O	2.30	0.49
1:A:1221:G:C2'	1:A:1222:G:H5'	2.43	0.49
1:A:1283:G:O2'	1:A:1284:C:H5'	2.12	0.49
1:A:165:C:O2'	1:A:166:G:H5'	2.12	0.49
1:A:403:C:H2'	1:A:404:U:H6	1.77	0.49
3:B:156:LYS:O	3:B:156:LYS:HD3	2.12	0.49
5:D:70:ILE:HD11	5:D:100:ARG:NE	2.27	0.49
7:F:99:ALA:O	7:F:100:ASN:C	2.50	0.49
11:J:19:SER:HB2	11:J:91:PRO:HG3	1.94	0.49
11:J:98:ILE:HG22	11:J:99:LYS:N	2.27	0.49
13:L:46:LYS:O	13:L:47:LYS:C	2.50	0.49
14:M:3:ARG:HG2	14:M:9:ILE:CG2	2.38	0.49
16:O:53:HIS:O	16:O:56:LEU:HB3	2.12	0.49
20:S:31:ILE:HG22	20:S:32:LYS:N	2.27	0.49
1:A:1314:C:C5	20:S:6:LYS:HE2	2.48	0.49
1:A:1366:C:C2	1:A:1367:C:C5	3.00	0.49
1:A:192:U:O4'	21:T:103:GLY:HA2	2.13	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:A:H2'	1:A:301:G:O4'	2.11	0.49
1:A:627:G:H2'	1:A:628:G:C8	2.47	0.49
1:A:666:G:H5'	1:A:726:C:H1'	1.94	0.49
1:A:761:G:H2'	1:A:762:C:H6	1.78	0.49
7:F:36:ARG:NH1	7:F:36:ARG:HG2	2.26	0.49
7:F:3:ARG:HH21	7:F:64:GLN:HE22	1.61	0.49
1:A:643:C:H4'	9:H:31:PHE:CE2	2.48	0.49
12:K:67:ASP:OD2	12:K:71:LYS:HE3	2.12	0.49
15:N:12:ARG:O	15:N:13:THR:C	2.50	0.49
17:P:28:ARG:NH1	17:P:29:ASP:OD2	2.45	0.49
17:P:42:ARG:O	17:P:43:LYS:C	2.51	0.49
1:A:1044:A:C2'	1:A:1045:C:H5'	2.43	0.49
1:A:1216:G:H2'	1:A:1217:C:H6	1.77	0.49
1:A:1329:A:O2'	1:A:1330:U:H5'	2.12	0.49
1:A:1347:G:O2'	1:A:1348:U:OP2	2.26	0.49
1:A:255:G:O6	1:A:266:G:O6	2.31	0.49
1:A:339:C:H2'	1:A:340:U:C6	2.48	0.49
3:B:144:ARG:HG3	3:B:145:LEU:H	1.76	0.49
3:B:83:MET:CE	3:B:234:PRO:HG2	2.42	0.49
3:B:92:TYR:CD1	3:B:151:GLY:HA3	2.48	0.49
4:C:131:ARG:CG	4:C:135:LYS:HE3	2.31	0.49
4:C:77:ILE:O	4:C:84:ILE:N	2.43	0.49
5:D:199:ASN:C	5:D:199:ASN:ND2	2.65	0.49
5:D:209:ARG:HG2	5:D:209:ARG:HH11	1.77	0.49
5:D:3:ARG:HH22	5:D:74:GLN:CD	2.15	0.49
10:I:63:ILE:HG22	10:I:64:THR:O	2.13	0.49
11:J:63:PHE:HZ	15:N:45:ARG:HG3	1.78	0.49
21:T:57:ARG:HH11	21:T:57:ARG:CG	2.25	0.49
22:V:2:GLY:C	22:V:4:GLY:H	2.15	0.49
1:A:1152:A:O2'	1:A:1153:C:H5'	2.12	0.49
1:A:296:U:H1'	1:A:556:C:H1'	1.95	0.49
1:A:308:C:H2'	1:A:309:G:C8	2.48	0.49
1:A:417:C:H2'	1:A:418:C:H6	1.76	0.49
1:A:420:U:H2'	1:A:422:C:C5	2.47	0.49
1:A:826:C:H2'	1:A:827:U:H6	1.78	0.49
3:B:122:PHE:O	3:B:123:ALA:HB2	2.13	0.49
4:C:148:GLY:HA3	4:C:203:PHE:HB3	1.95	0.49
6:E:83:GLU:HA	6:E:87:SER:O	2.12	0.49
8:G:45:ASP:O	8:G:49:ILE:HG13	2.13	0.49
13:L:70:ILE:HD13	13:L:77:LEU:HD12	1.93	0.49
14:M:94:ARG:NH2	20:S:81:ARG:HD3	2.27	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Q:67:LYS:O	18:Q:68:ARG:C	2.51	0.49
19:R:36:ASN:CG	19:R:39:VAL:HG12	2.33	0.49
1:A:1211:U:H1'	1:A:1213:A:C2	2.48	0.49
1:A:382:A:O2'	1:A:383:A:H5'	2.13	0.49
1:A:547:A:H4'	1:A:548:G:O5'	2.12	0.49
3:B:169:LYS:O	3:B:169:LYS:HD3	2.13	0.49
3:B:204:ASN:HB3	3:B:210:SER:OG	2.12	0.49
3:B:61:LEU:HD23	3:B:61:LEU:O	2.13	0.49
4:C:59:ARG:CG	4:C:64:VAL:HG13	2.42	0.49
5:D:6:GLY:O	5:D:7:PRO:C	2.51	0.49
10:I:100:GLY:C	10:I:102:LEU:N	2.66	0.49
14:M:22:ILE:CD1	14:M:25:ILE:HD12	2.42	0.49
4:C:34:LEU:CD1	15:N:25:VAL:HG21	2.37	0.49
16:O:45:VAL:HG12	16:O:46:HIS:H	1.78	0.49
1:A:375:U:H4'	17:P:17:TYR:CE2	2.47	0.49
20:S:31:ILE:O	20:S:32:LYS:CB	2.61	0.49
1:A:192:U:C1'	21:T:103:GLY:HA2	2.43	0.49
21:T:58:LYS:O	21:T:62:LEU:HD23	2.13	0.49
1:A:1184:G:OP1	1:A:1184:G:H3'	2.12	0.49
1:A:1202:G:O2'	1:A:1203:C:H5'	2.12	0.49
1:A:1278:U:C5'	1:A:1279:A:O4'	2.61	0.49
1:A:203:U:H5''	1:A:204:U:OP1	2.13	0.49
1:A:247:G:OP2	18:Q:100:LYS:HG3	2.12	0.49
4:C:134:ILE:HG22	4:C:168:ALA:HB3	1.94	0.49
4:C:149:ALA:HA	4:C:201:TYR:O	2.13	0.49
4:C:180:ALA:O	4:C:181:ASN:CB	2.61	0.49
4:C:35:GLU:HG2	4:C:59:ARG:HH22	1.76	0.49
5:D:62:GLN:HE22	5:D:65:ARG:HH12	1.59	0.49
8:G:138:LYS:C	8:G:138:LYS:HD3	2.34	0.49
6:E:78:HIS:CD2	9:H:107:LEU:HD12	2.45	0.49
10:I:19:LEU:HB3	10:I:59:PHE:CE2	2.48	0.49
11:J:24:VAL:HG21	11:J:37:PRO:HD3	1.94	0.49
1:A:1305:G:H2'	1:A:1331:G:H22	1.78	0.49
1:A:1528:U:O2'	1:A:1530:G:H5'	2.12	0.49
1:A:556:C:O2'	1:A:557:G:H5'	2.13	0.49
3:B:19:HIS:CG	3:B:20:GLU:H	2.31	0.49
3:B:17:PHE:H	3:B:44:LEU:HD21	1.77	0.49
5:D:121:VAL:O	5:D:134:ASP:HA	2.13	0.49
12:K:110:ASP:HB3	19:R:85:LEU:HB3	1.95	0.49
14:M:81:LEU:HD23	14:M:82:MET:N	2.28	0.49
16:O:17:ARG:NH1	16:O:77:ARG:NH1	2.60	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:26:ARG:HH21	17:P:31:LYS:HE2	1.77	0.49
17:P:52:ASP:OD2	17:P:55:ARG:CB	2.61	0.49
18:Q:59:ILE:CG2	18:Q:71:PHE:CD1	2.96	0.49
20:S:67:VAL:HG12	20:S:68:GLY:N	2.27	0.49
20:S:74:PHE:N	20:S:74:PHE:CD1	2.80	0.49
20:S:80:TYR:CG	20:S:81:ARG:N	2.81	0.49
1:A:113:G:C1'	1:A:354:G:H5'	2.39	0.48
1:A:1325:C:O2'	1:A:1326:C:H5'	2.13	0.48
1:A:194:C:O2'	21:T:68:LYS:HD3	2.13	0.48
1:A:325:A:H2'	1:A:326:G:C8	2.48	0.48
1:A:437:U:O2'	5:D:123:HIS:CD2	2.66	0.48
1:A:567:G:H2'	1:A:568:G:O4'	2.12	0.48
1:A:694:A:C3'	1:A:695:A:H5''	2.40	0.48
1:A:754:C:H3'	1:A:754:C:O2	2.13	0.48
3:B:23:ARG:N	3:B:23:ARG:CD	2.71	0.48
4:C:167:TRP:O	4:C:168:ALA:CB	2.61	0.48
6:E:39:GLY:HA2	6:E:69:VAL:HB	1.94	0.48
11:J:55:LYS:O	11:J:56:HIS:CB	2.61	0.48
13:L:43:VAL:CG2	13:L:55:VAL:HG21	2.43	0.48
17:P:20:VAL:CG1	17:P:32:TYR:CB	2.82	0.48
18:Q:66:SER:HB3	18:Q:69:LYS:HD3	1.95	0.48
20:S:20:LEU:O	20:S:23:ASN:HB2	2.12	0.48
21:T:50:GLU:HG3	21:T:99:LEU:HD12	1.95	0.48
1:A:1068:G:N3	1:A:1191:A:C2	2.81	0.48
1:A:132:C:H2'	1:A:133:U:H6	1.78	0.48
1:A:459:G:H3'	1:A:460:A:C5'	2.43	0.48
1:A:490:G:H2'	1:A:491:G:C8	2.48	0.48
1:A:515:G:O2'	1:A:516:U:H5'	2.14	0.48
1:A:80:G:C2'	1:A:81:U:H5''	2.43	0.48
3:B:51:LEU:O	3:B:52:GLU:C	2.52	0.48
4:C:97:LYS:O	4:C:98:ASN:HB3	2.12	0.48
7:F:52:ILE:O	7:F:53:ALA:HB3	2.13	0.48
9:H:51:VAL:CG2	9:H:60:ARG:HG2	2.40	0.48
10:I:9:ARG:CG	10:I:14:VAL:HG22	2.41	0.48
10:I:26:VAL:HG11	10:I:28:VAL:HG23	1.95	0.48
12:K:27:ASN:OD1	12:K:55:LYS:HG2	2.13	0.48
12:K:34:ASP:HB2	12:K:35:PRO:HD2	1.95	0.48
1:A:502:G:OP1	13:L:118:SER:CB	2.61	0.48
20:S:50:ALA:HA	20:S:58:VAL:O	2.12	0.48
21:T:60:GLU:HG3	21:T:81:LYS:HE3	1.94	0.48
1:A:926:G:H1'	2:X:3:U:O4	2.13	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1167:A:C6	1:A:1168:A:C6	3.02	0.48
1:A:1244:C:H2'	1:A:1245:A:H8	1.74	0.48
1:A:389:A:H2'	1:A:390:C:C5'	2.43	0.48
1:A:831:U:H2'	1:A:832:C:C6	2.48	0.48
1:A:832:C:O2'	1:A:833:U:H5'	2.13	0.48
3:B:90:MET:HE3	3:B:91:PRO:HD3	1.94	0.48
5:D:110:PHE:N	5:D:110:PHE:CD1	2.71	0.48
1:A:1187:G:OP1	10:I:113:LYS:HE2	2.13	0.48
12:K:84:VAL:HG23	12:K:110:ASP:HA	1.95	0.48
1:A:1230:C:O2'	14:M:126:LYS:HA	2.13	0.48
20:S:23:ASN:HA	20:S:26:GLY:O	2.13	0.48
1:A:1003:G:N2	1:A:1039:C:C2	2.81	0.48
1:A:1095:U:H5''	1:A:1109:C:O2	2.13	0.48
1:A:1301:U:O2'	1:A:1302:U:OP1	2.31	0.48
1:A:1288:A:O4'	1:A:1353:G:H4'	2.13	0.48
3:B:51:LEU:CD2	3:B:201:ILE:HG23	2.44	0.48
8:G:74:GLU:O	8:G:88:PRO:HA	2.13	0.48
9:H:108:GLY:HA3	9:H:138:TRP:HB3	1.93	0.48
10:I:127:LYS:HD2	10:I:127:LYS:N	2.28	0.48
13:L:28:LYS:HG3	13:L:33:ARG:HH12	1.78	0.48
15:N:25:VAL:HG12	15:N:38:GLY:O	2.14	0.48
20:S:53:ASN:N	20:S:53:ASN:ND2	2.59	0.48
21:T:56:MET:HE2	21:T:88:VAL:HB	1.95	0.48
1:A:1342:C:O2'	1:A:1343:G:H5'	2.13	0.48
1:A:443:C:H2'	1:A:444:C:C6	2.47	0.48
1:A:545:C:O2'	1:A:549:C:OP1	2.31	0.48
4:C:105:GLU:O	4:C:107:GLN:NE2	2.44	0.48
4:C:67:THR:O	4:C:69:HIS:HD2	1.95	0.48
11:J:65:LEU:HD12	15:N:56:VAL:HG22	1.95	0.48
7:F:97:PHE:N	19:R:30:ASP:OD1	2.47	0.48
20:S:20:LEU:HA	20:S:23:ASN:HD22	1.73	0.48
1:A:1020:U:H2'	1:A:1021:G:C8	2.49	0.48
1:A:1190:G:O2'	1:A:1191:A:P	2.70	0.48
1:A:1489:G:O2'	1:A:1490:C:H5'	2.13	0.48
1:A:376:G:P	17:P:67:THR:HG21	2.54	0.48
3:B:117:GLU:O	3:B:120:ALA:HB3	2.13	0.48
3:B:87:ARG:HB3	3:B:219:VAL:HG11	1.95	0.48
4:C:175:LEU:HD21	4:C:201:TYR:CE2	2.47	0.48
4:C:204:LEU:O	4:C:205:GLY:O	2.32	0.48
5:D:32:ALA:O	5:D:34:GLU:N	2.45	0.48
13:L:117:ARG:CZ	13:L:124:LYS:HA	2.44	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:70:LEU:HD11	16:O:78:TYR:N	2.29	0.48
21:T:43:LEU:HD12	21:T:52:ALA:HA	1.96	0.48
1:A:262:A:H4'	21:T:75:ASN:ND2	2.28	0.48
1:A:1511:G:O2'	1:A:1512:U:H5'	2.14	0.48
1:A:173:U:H5	1:A:198:G:HO2'	1.57	0.48
1:A:262:A:C6	1:A:263:A:C6	3.02	0.48
1:A:356:A:O2'	1:A:357:G:H5'	2.14	0.48
1:A:979:C:O2	15:N:19:ARG:HG2	2.14	0.48
4:C:173:VAL:N	4:C:174:PRO:CD	2.75	0.48
4:C:181:ASN:ND2	4:C:204:LEU:HD12	2.28	0.48
4:C:90:GLU:O	4:C:93:LYS:HB2	2.14	0.48
5:D:104:VAL:HG11	5:D:146:ILE:CD1	2.42	0.48
7:F:75:LEU:HD13	7:F:75:LEU:O	2.13	0.48
8:G:18:TYR:CD1	8:G:18:TYR:N	2.82	0.48
9:H:11:THR:HG22	9:H:15:ASN:ND2	2.29	0.48
9:H:23:SER:O	9:H:24:THR:HB	2.13	0.48
10:I:36:TYR:CD2	10:I:37:PHE:CE2	3.02	0.48
1:A:1152:A:OP1	11:J:13:HIS:HB2	2.13	0.48
14:M:23:TYR:CD2	14:M:70:LEU:HD13	2.49	0.48
19:R:27:GLY:O	19:R:29:PHE:HD2	1.95	0.48
20:S:5:LEU:O	20:S:6:LYS:HB2	2.13	0.48
1:A:1442:G:C2'	1:A:1442:G:N3	2.76	0.48
1:A:248:C:C2'	1:A:249:U:H5'	2.44	0.48
1:A:333:G:O2'	1:A:334:C:H5'	2.14	0.48
1:A:585:G:C5	1:A:586:C:C5	3.02	0.48
1:A:60:A:H4'	1:A:61:G:O5'	2.14	0.48
1:A:618:C:N3	1:A:622:A:N6	2.61	0.48
3:B:206:ASP:O	3:B:207:ALA:HB3	2.13	0.48
4:C:108:ASN:OD1	4:C:110:ASN:HB2	2.14	0.48
4:C:180:ALA:HB3	4:C:182:ILE:HG13	1.94	0.48
5:D:126:ILE:HG22	5:D:127:THR:N	2.28	0.48
12:K:110:ASP:OD2	19:R:88:LYS:NZ	2.47	0.48
19:R:19:LYS:O	19:R:20:ALA:CB	2.62	0.48
1:A:1102:A:H2'	1:A:1103:C:C6	2.49	0.48
1:A:116:A:H8	1:A:116:A:O5'	1.97	0.48
1:A:162:A:H2'	1:A:163:C:O4'	2.12	0.48
1:A:192:U:O2'	1:A:193:C:H5'	2.14	0.48
3:B:208:ILE:O	3:B:209:ARG:C	2.52	0.48
3:B:187:LEU:HD23	3:B:214:ILE:HG21	1.96	0.48
4:C:164:ARG:HH11	4:C:164:ARG:CB	2.25	0.48
5:D:120:LEU:HD23	5:D:125:HIS:HD2	1.78	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:14:ARG:C	5:D:16:GLY:H	2.17	0.48
5:D:194:LEU:HD22	5:D:194:LEU:N	2.29	0.48
6:E:93:PRO:HG2	9:H:105:ARG:HH21	1.79	0.48
11:J:60:ARG:O	11:J:61:GLU:CB	2.62	0.48
11:J:71:LEU:O	11:J:72:VAL:HB	2.13	0.48
17:P:84:ALA:O	17:P:85:ARG:C	2.52	0.48
18:Q:12:SER:HB3	18:Q:20:THR:HB	1.95	0.48
1:A:1312:G:N7	20:S:4:SER:HB3	2.29	0.48
1:A:1308:U:H2'	1:A:1309:G:H8	1.79	0.48
1:A:67:C:O2'	1:A:171:A:H1'	2.13	0.48
1:A:188:C:H4'	21:T:89:ARG:HH11	1.76	0.48
1:A:190(H):G:O2'	1:A:190(I):G:H5'	2.14	0.48
1:A:194:C:H2'	1:A:195:A:H5''	1.95	0.48
1:A:614:A:H2'	1:A:615:C:C6	2.49	0.48
1:A:622:A:C8	1:A:623:C:C5	3.02	0.48
1:A:812:C:O2'	1:A:813:U:OP2	2.31	0.48
3:B:121:LEU:O	3:B:123:ALA:N	2.46	0.48
3:B:144:ARG:O	3:B:147:LYS:N	2.45	0.48
3:B:68:ILE:O	3:B:91:PRO:HD2	2.14	0.48
5:D:38:TYR:HB2	5:D:39:PRO:HD2	1.96	0.48
9:H:104:ARG:HG3	9:H:138:TRP:CD2	2.49	0.48
10:I:93:ARG:CZ	10:I:97:LYS:HZ1	2.27	0.48
18:Q:67:LYS:CA	18:Q:70:ARG:HH12	2.27	0.48
1:A:1331:G:O2'	1:A:1332:A:P	2.71	0.47
1:A:418:C:H2'	1:A:419:C:H6	1.78	0.47
1:A:444:C:O2'	1:A:445:G:H5'	2.14	0.47
6:E:112:LEU:HD23	6:E:112:LEU:N	2.29	0.47
7:F:36:ARG:O	7:F:36:ARG:HG2	2.13	0.47
1:A:1178:G:P	10:I:97:LYS:HZ3	2.37	0.47
17:P:32:TYR:CE2	17:P:35:LYS:HB2	2.39	0.47
20:S:55:LYS:CG	20:S:56:GLN:HE21	2.17	0.47
21:T:92:LEU:O	21:T:94:ALA:N	2.47	0.47
1:A:1061:G:C2'	1:A:1062:U:H5'	2.44	0.47
1:A:1139:G:O2'	1:A:1140:C:P	2.72	0.47
1:A:1218:C:H2'	1:A:1219:U:C6	2.49	0.47
1:A:1227:A:H2'	1:A:1228:C:O5'	2.14	0.47
25:A:1632:PCY:H133	25:A:1632:PCY:H103	1.95	0.47
1:A:346:G:C2'	1:A:347:G:H5'	2.43	0.47
1:A:479:C:H2'	1:A:480:U:O4'	2.14	0.47
1:A:439:A:C4	1:A:497:A:C2	3.02	0.47
1:A:554:C:H2'	1:A:555:C:C6	2.48	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:575:G:OP1	1:A:575:G:H4'	2.14	0.47
1:A:935:A:H2'	1:A:936:C:H6	1.80	0.47
3:B:132:LYS:O	3:B:136:VAL:HG23	2.14	0.47
3:B:21:ARG:NH1	3:B:23:ARG:HG2	2.29	0.47
5:D:176:LEU:HA	5:D:183:GLY:HA2	1.96	0.47
8:G:77:SER:O	8:G:156:TRP:CH2	2.67	0.47
9:H:119:LEU:HB2	9:H:123:GLU:CB	2.43	0.47
11:J:90:LEU:N	11:J:91:PRO:HD2	2.25	0.47
13:L:43:VAL:HG23	13:L:55:VAL:HG21	1.96	0.47
14:M:39:ILE:HD13	14:M:52:GLU:HB3	1.97	0.47
20:S:67:VAL:O	20:S:69:HIS:N	2.47	0.47
1:A:1003:G:C6	1:A:1003(A):G:C6	3.02	0.47
1:A:162:A:C5	1:A:163:C:H1'	2.50	0.47
1:A:512:U:H2'	1:A:513:C:C6	2.49	0.47
1:A:680:C:O2'	1:A:681:C:H5'	2.14	0.47
1:A:716:A:O2'	1:A:717:C:H5'	2.13	0.47
1:A:939:G:C6	1:A:940:C:N4	2.83	0.47
3:B:96:ARG:O	3:B:98:LEU:HD23	2.14	0.47
12:K:66:LEU:HB3	12:K:70:LYS:HE3	1.95	0.47
14:M:73:GLU:O	14:M:74:VAL:C	2.51	0.47
14:M:94:ARG:HH22	20:S:81:ARG:HD3	1.79	0.47
16:O:45:VAL:HG12	16:O:46:HIS:N	2.30	0.47
1:A:580:U:H5''	16:O:58:MET:HG2	1.96	0.47
17:P:51:VAL:HG12	17:P:51:VAL:O	2.13	0.47
1:A:255:G:C1'	18:Q:16:GLN:NE2	2.76	0.47
18:Q:6:LEU:HD13	18:Q:23:VAL:HG11	1.95	0.47
1:A:1128:C:H2'	1:A:1129:C:H5''	1.96	0.47
1:A:1068:G:N2	1:A:1191:A:N3	2.62	0.47
1:A:1256:A:H4'	1:A:1257:U:C5'	2.23	0.47
1:A:1314:C:H2'	1:A:1315:U:C6	2.50	0.47
1:A:341:C:H2'	1:A:342:C:H6	1.79	0.47
1:A:686:U:O2'	1:A:687:A:C8	2.63	0.47
1:A:926:G:N2	1:A:1505:G:H2'	2.29	0.47
3:B:122:PHE:HE2	3:B:139:LYS:HG2	1.79	0.47
3:B:166:ASP:OD1	3:B:205:ASP:HB2	2.14	0.47
3:B:43:ASP:OD1	3:B:43:ASP:C	2.52	0.47
4:C:123:GLN:NE2	4:C:140:ARG:HH22	2.12	0.47
6:E:15:ARG:HD3	6:E:26:PHE:HB3	1.97	0.47
6:E:40:ARG:HG2	6:E:68:GLU:OE2	2.14	0.47
8:G:23:VAL:HG13	8:G:43:PHE:CE2	2.48	0.47
12:K:50:TYR:HD1	12:K:60:ALA:HB2	1.80	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:R:26:LEU:HD23	19:R:29:PHE:CZ	2.49	0.47
19:R:59:SER:OG	19:R:62:GLU:HG3	2.14	0.47
1:A:1136:U:H5''	1:A:1137:C:OP2	2.14	0.47
1:A:1331:G:O2'	1:A:1332:A:OP2	2.28	0.47
1:A:1454:G:H2'	1:A:1455:G:H8	1.79	0.47
1:A:199:G:O2'	1:A:200:G:H5'	2.15	0.47
1:A:411:A:C6	1:A:429:U:C4	3.02	0.47
1:A:600:C:O2'	1:A:601:C:H5'	2.13	0.47
1:A:773:G:O2'	1:A:774:G:H5'	2.15	0.47
3:B:45:GLN:O	3:B:48:MET:HB2	2.14	0.47
3:B:98:LEU:HB2	3:B:108:ILE:HD11	1.95	0.47
4:C:39:ILE:HG21	4:C:57:ILE:HD11	1.96	0.47
7:F:67:MET:CE	7:F:72:VAL:HA	2.45	0.47
20:S:28:LYS:HG2	20:S:29:ARG:N	2.19	0.47
1:A:1216:G:H2'	1:A:1217:C:C6	2.49	0.47
1:A:124:G:C6	1:A:125:U:C4	3.02	0.47
1:A:124:G:C5	1:A:125:U:C4	3.03	0.47
1:A:127:G:OP1	1:A:635:G:H1'	2.15	0.47
1:A:252:U:H2'	1:A:253:U:H6	1.75	0.47
1:A:308:C:H2'	1:A:309:G:H8	1.80	0.47
1:A:458:C:H2'	1:A:459:G:O4'	2.15	0.47
1:A:491:G:H2'	1:A:492:G:H8	1.79	0.47
1:A:942:G:C2	1:A:943:U:C6	3.02	0.47
1:A:961:U:H2'	1:A:962:C:C5'	2.45	0.47
1:A:976:G:C8	1:A:1358:U:C2	3.02	0.47
3:B:112:VAL:O	3:B:115:LEU:HB3	2.14	0.47
6:E:28:PHE:O	6:E:47:LYS:HA	2.13	0.47
7:F:10:LEU:CD1	7:F:59:TYR:HB3	2.43	0.47
9:H:114:THR:C	9:H:116:LYS:H	2.17	0.47
11:J:12:ASP:OD1	11:J:15:THR:N	2.45	0.47
13:L:87:GLY:H	13:L:98:TYR:HB3	1.78	0.47
19:R:65:ILE:O	19:R:66:LEU:C	2.52	0.47
2:X:1:C:H2'	2:X:2:U:H5'	1.95	0.47
1:A:1194:U:O2'	1:A:1195:C:H5'	2.13	0.47
1:A:1300:G:O2'	1:A:1301:U:P	2.73	0.47
3:B:127:ILE:HB	3:B:128:GLU:OE1	2.14	0.47
3:B:182:ILE:O	3:B:183:PRO:C	2.52	0.47
3:B:17:PHE:HD1	3:B:18:GLY:N	2.12	0.47
3:B:67:THR:HG23	3:B:90:MET:CE	2.45	0.47
3:B:88:ALA:C	3:B:90:MET:H	2.18	0.47
3:B:68:ILE:N	3:B:90:MET:HE1	2.27	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:U:OP1	5:D:13:ARG:NH2	2.47	0.47
10:I:100:GLY:C	10:I:102:LEU:H	2.18	0.47
10:I:117:HIS:HB2	10:I:121:ARG:HD2	1.96	0.47
15:N:27:CYS:SG	15:N:29:ARG:CB	2.98	0.47
17:P:20:VAL:CG1	17:P:21:VAL:N	2.77	0.47
17:P:45:THR:HB	17:P:46:PRO:HD2	1.96	0.47
18:Q:97:SER:OG	18:Q:103:GLY:CA	2.63	0.47
20:S:7:LYS:CG	20:S:7:LYS:O	2.63	0.47
1:A:1051:C:O2'	1:A:1052:U:H5'	2.14	0.47
1:A:1152:A:H2'	1:A:1153:C:C6	2.50	0.47
1:A:1202:G:C2'	1:A:1203:C:H5'	2.45	0.47
1:A:1520:G:H2'	1:A:1521:G:H8	1.79	0.47
1:A:185:A:H2'	1:A:186:C:C6	2.49	0.47
1:A:636:U:H2'	1:A:637:G:H8	1.79	0.47
3:B:130:ARG:HH22	4:C:207:VAL:CG2	2.28	0.47
4:C:191:THR:HG21	4:C:193:TYR:CE2	2.48	0.47
4:C:6:HIS:HD2	4:C:8:ILE:N	2.12	0.47
5:D:3:ARG:NH1	5:D:118:ARG:HH12	2.13	0.47
6:E:146:ALA:O	6:E:149:GLU:HB3	2.15	0.47
6:E:15:ARG:HD2	6:E:15:ARG:C	2.35	0.47
8:G:111:ARG:HB3	8:G:113:GLU:OE2	2.15	0.47
8:G:18:TYR:CE2	8:G:59:LEU:HB2	2.49	0.47
9:H:114:THR:OG1	9:H:119:LEU:HD21	2.14	0.47
10:I:111:ARG:NH1	10:I:111:ARG:HG3	2.29	0.47
11:J:12:ASP:C	11:J:14:LYS:H	2.18	0.47
15:N:57:ARG:HG2	15:N:58:LYS:H	1.79	0.47
17:P:6:LEU:HB3	17:P:17:TYR:CD2	2.50	0.47
18:Q:84:LEU:HA	18:Q:84:LEU:HD23	1.70	0.47
1:A:1326:C:H5''	22:V:12:LYS:NZ	2.30	0.47
1:A:106:C:O2'	1:A:379:C:H5''	2.15	0.47
1:A:1126:U:H6	1:A:1126:U:P	2.37	0.47
1:A:1256:A:N6	1:A:1278:U:H1'	2.29	0.47
1:A:851:G:H2'	1:A:852:G:H8	1.79	0.47
1:A:950:U:H2'	1:A:951:G:H8	1.80	0.47
1:A:9:G:OP1	6:E:122:GLU:HB2	2.15	0.47
3:B:16:HIS:CD2	3:B:210:SER:OG	2.67	0.47
3:B:62:ALA:C	3:B:64:ARG:N	2.68	0.47
3:B:73:THR:HG22	3:B:169:LYS:HE3	1.97	0.47
3:B:82:ARG:O	3:B:86:GLU:HG3	2.15	0.47
4:C:6:HIS:HD2	4:C:9:GLY:H	1.61	0.47
11:J:39:PRO:O	11:J:69:ASN:O	2.33	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Q:104:LYS:O	18:Q:105:ALA:HB2	2.15	0.47
12:K:110:ASP:CB	19:R:88:LYS:HD2	2.20	0.47
1:A:1096:C:O2'	1:A:1097:C:H5'	2.15	0.47
1:A:1147:C:O2'	10:I:16:ARG:HD3	2.15	0.47
1:A:344:A:H5''	1:A:345:C:H5	1.80	0.47
1:A:532:A:H2'	1:A:532:A:N3	2.30	0.47
1:A:552:U:O2'	1:A:553:A:H5'	2.15	0.47
3:B:125:PRO:HG2	3:B:126:GLU:HG3	1.97	0.47
3:B:118:LEU:HB2	3:B:142:LEU:CD2	2.45	0.47
1:A:1111:A:N6	4:C:177:THR:HA	2.30	0.47
4:C:39:ILE:HG22	4:C:40:ARG:N	2.28	0.47
5:D:192:GLU:OE1	5:D:192:GLU:N	2.48	0.47
5:D:8:VAL:CG1	5:D:21:LEU:HD13	2.44	0.47
8:G:137:LYS:O	8:G:141:VAL:HG23	2.15	0.47
1:A:521:G:OP1	13:L:73:GLU:O	2.32	0.47
14:M:26:GLY:O	14:M:28:ALA:N	2.48	0.47
15:N:9:LYS:HG3	15:N:21:TYR:O	2.15	0.47
19:R:40:LEU:N	19:R:40:LEU:HD23	2.29	0.47
20:S:39:THR:HA	20:S:70:LYS:HG2	1.97	0.47
22:V:9:ARG:HG3	22:V:13:ILE:HD11	1.96	0.47
1:A:1009:G:C6	1:A:1021:G:C6	3.04	0.47
25:A:1632:PCY:C8	25:A:1632:PCY:N2	2.71	0.47
1:A:184:G:C4'	1:A:224:C:H4'	2.44	0.47
1:A:33:A:H2'	1:A:34:C:H6	1.77	0.47
1:A:413:G:N3	1:A:413:G:H2'	2.30	0.47
1:A:52:G:O2'	1:A:53:A:H5'	2.14	0.47
1:A:547:A:OP2	5:D:2:GLY:N	2.48	0.47
1:A:302:G:N3	1:A:556:C:H4'	2.30	0.47
1:A:708:C:H2'	1:A:709:G:C8	2.49	0.47
1:A:848:C:H2'	1:A:849:C:C6	2.50	0.47
7:F:76:ALA:O	7:F:77:ARG:C	2.53	0.47
12:K:124:LYS:HB3	12:K:125:PHE:CE1	2.49	0.47
13:L:111:LYS:O	13:L:112:ASP:HB2	2.15	0.47
14:M:78:ILE:O	14:M:81:LEU:HD23	2.15	0.47
16:O:15:PHE:O	16:O:16:ALA:C	2.52	0.47
20:S:51:VAL:HG12	20:S:52:TYR:N	2.29	0.47
1:A:1301:U:O2'	1:A:1302:U:P	2.72	0.46
1:A:1411:C:O2'	1:A:1412:C:H5'	2.14	0.46
1:A:17:U:H4'	1:A:1080:A:O4'	2.15	0.46
1:A:281:G:C2'	1:A:282:A:OP2	2.63	0.46
1:A:46:G:H2'	1:A:366:C:H41	1.80	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:573:A:C2	1:A:574:A:C2	3.03	0.46
1:A:663:A:O2'	1:A:664:G:H5'	2.15	0.46
1:A:730:G:N2	1:A:765:G:H5''	2.30	0.46
3:B:84:GLU:HA	3:B:87:ARG:HB2	1.96	0.46
3:B:90:MET:CE	3:B:90:MET:HA	2.45	0.46
5:D:157:LEU:CD2	5:D:161:ASN:HD21	2.28	0.46
6:E:153:LYS:HB3	6:E:154:GLY:H	1.58	0.46
10:I:113:LYS:HD3	10:I:119:ALA:HA	1.97	0.46
10:I:128:ARG:OXT	10:I:128:ARG:CG	2.63	0.46
11:J:27:ALA:HB2	11:J:85:LEU:HD21	1.97	0.46
12:K:99:GLN:HA	12:K:105:VAL:HG21	1.98	0.46
1:A:539:A:OP2	13:L:115:LYS:HE2	2.15	0.46
16:O:39:LEU:HD13	16:O:59:MET:CE	2.45	0.46
19:R:51:LEU:HB2	19:R:56:THR:HG22	1.97	0.46
20:S:41:VAL:HB	20:S:43:GLU:OE2	2.16	0.46
21:T:53:LEU:HD23	21:T:56:MET:CE	2.45	0.46
1:A:1285:A:O2'	1:A:1286:A:OP2	2.30	0.46
3:B:124:SER:O	3:B:127:ILE:CD1	2.64	0.46
3:B:201:ILE:HG21	3:B:214:ILE:HG21	1.96	0.46
4:C:76:VAL:HG11	4:C:103:VAL:HG21	1.97	0.46
7:F:48:LEU:HD13	7:F:52:ILE:HG13	1.96	0.46
8:G:41:ARG:O	8:G:42:ILE:C	2.54	0.46
10:I:118:LYS:O	10:I:119:ALA:CB	2.59	0.46
11:J:94:VAL:CG1	11:J:95:GLU:N	2.77	0.46
1:A:523:A:C2	13:L:91:LYS:HB3	2.50	0.46
11:J:49:VAL:CG1	15:N:41:ARG:HB2	2.45	0.46
1:A:761:G:H1'	18:Q:103:GLY:O	2.16	0.46
20:S:16:LEU:O	20:S:20:LEU:HG	2.15	0.46
1:A:1057:G:H2'	1:A:1058:G:O4'	2.15	0.46
1:A:1520:G:O2'	1:A:1521:G:H5'	2.15	0.46
1:A:266:G:O2'	1:A:267:C:P	2.74	0.46
1:A:383:A:H2'	1:A:384:G:H5'	1.96	0.46
1:A:55:A:H2'	1:A:56:U:H6	1.81	0.46
1:A:659:U:C2'	1:A:660:G:H5'	2.45	0.46
1:A:737:A:H1'	7:F:73:ASN:ND2	2.26	0.46
1:A:854:G:C6	1:A:855:G:N7	2.84	0.46
1:A:857:C:H2'	1:A:858:G:O4'	2.15	0.46
3:B:18:GLY:CA	3:B:42:ILE:H	2.19	0.46
6:E:71:LEU:HD21	6:E:115:VAL:HG22	1.96	0.46
6:E:79:GLU:C	6:E:80:ILE:HG23	2.36	0.46
10:I:5:TYR:HA	10:I:17:VAL:O	2.14	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1249:C:O2'	10:I:73:GLN:NE2	2.48	0.46
12:K:126:ARG:O	12:K:127:LYS:C	2.54	0.46
16:O:58:MET:HE2	16:O:58:MET:HB2	1.69	0.46
1:A:1372:U:H2'	1:A:1373:G:H5'	1.97	0.46
1:A:1372:U:H2'	1:A:1373:G:C5'	2.45	0.46
1:A:278:G:O4'	1:A:282:A:H1'	2.15	0.46
1:A:428:G:C2	1:A:430:A:N6	2.83	0.46
1:A:674:G:H2'	1:A:675:A:H8	1.80	0.46
1:A:960:U:O2'	1:A:1223:C:H4'	2.14	0.46
1:A:968:A:OP2	10:I:128:ARG:NH2	2.48	0.46
3:B:15:VAL:HG13	3:B:209:ARG:HG3	1.97	0.46
10:I:30:GLY:O	10:I:31:GLN:O	2.34	0.46
12:K:106:LYS:HD3	12:K:106:LYS:HA	1.74	0.46
12:K:16:SER:HA	12:K:79:SER:O	2.15	0.46
13:L:83:VAL:CG2	13:L:84:LEU:H	2.25	0.46
20:S:81:ARG:O	20:S:81:ARG:HG2	2.16	0.46
21:T:45:GLN:HA	21:T:91:LEU:CD2	2.44	0.46
1:A:1022:G:N2	1:A:1023:G:N7	2.62	0.46
1:A:1349:A:H1'	1:A:1374:A:N6	2.30	0.46
1:A:16:A:O2'	1:A:17:U:H5'	2.15	0.46
1:A:188:C:O4'	21:T:89:ARG:NH1	2.48	0.46
1:A:513:C:H2'	1:A:514:C:H6	1.80	0.46
1:A:687:A:H4'	1:A:688:G:O5'	2.16	0.46
1:A:848:C:O2'	1:A:849:C:H5'	2.16	0.46
3:B:221:LEU:C	3:B:221:LEU:HD13	2.36	0.46
5:D:158:ILE:HG22	5:D:181:MET:HE2	1.98	0.46
5:D:78:LEU:HA	5:D:78:LEU:HD23	1.69	0.46
1:A:921:U:O2'	6:E:19:MET:O	2.30	0.46
8:G:138:LYS:HE2	8:G:142:GLU:OE1	2.15	0.46
8:G:38:LEU:O	8:G:42:ILE:HG13	2.15	0.46
9:H:75:ARG:HA	9:H:76:PRO:HD3	1.64	0.46
20:S:80:TYR:CE2	20:S:81:ARG:HB2	2.50	0.46
21:T:10:LEU:O	21:T:12:ALA:N	2.49	0.46
1:A:1014:A:C2	20:S:34:TRP:NE1	2.84	0.46
1:A:1128:C:H4'	10:I:16:ARG:NH1	2.29	0.46
1:A:1203:C:O2'	1:A:1204:A:H5'	2.15	0.46
1:A:1480:G:O2'	1:A:1481:U:H5'	2.15	0.46
1:A:1533:C:O2	1:A:1533:C:C2'	2.55	0.46
1:A:319:G:O2'	1:A:320:C:H5'	2.16	0.46
1:A:738:C:OP2	7:F:92:LYS:HE3	2.15	0.46
3:B:15:VAL:HG11	3:B:209:ARG:C	2.36	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:14:ILE:CG2	4:C:15:THR:H	2.05	0.46
4:C:79:ARG:C	4:C:81:GLY:H	2.19	0.46
4:C:96:GLY:O	4:C:98:ASN:N	2.48	0.46
5:D:111:ALA:HB2	5:D:120:LEU:CD1	2.39	0.46
6:E:119:LEU:HD23	6:E:119:LEU:HA	1.67	0.46
6:E:143:ARG:NH1	9:H:77:GLU:CD	2.69	0.46
21:T:43:LEU:CD1	21:T:55:ILE:HD12	2.46	0.46
1:A:934:C:H5	1:A:1344:C:H2'	1.81	0.46
1:A:1498:U:H4'	1:A:1519:A:C2	2.51	0.46
1:A:259:G:C2'	1:A:260:G:H5'	2.46	0.46
1:A:707:C:H2'	1:A:708:C:C6	2.50	0.46
3:B:116:GLU:HA	3:B:119:GLU:OE1	2.16	0.46
3:B:69:LEU:HB2	3:B:159:PRO:HB3	1.97	0.46
1:A:877:C:H1'	9:H:3:THR:HG23	1.97	0.46
10:I:120:ARG:O	10:I:121:ARG:C	2.54	0.46
12:K:48:ILE:HD11	12:K:63:LEU:C	2.36	0.46
14:M:109:THR:CG2	14:M:110:ARG:N	2.79	0.46
14:M:40:ASN:ND2	14:M:41:PRO:CD	2.73	0.46
16:O:54:ARG:O	16:O:55:GLY:C	2.51	0.46
1:A:1320:C:N3	20:S:36:ARG:HG3	2.31	0.46
21:T:42:GLN:HE21	21:T:42:GLN:C	2.19	0.46
1:A:1021:G:C2	1:A:1022:G:H1'	2.51	0.46
1:A:1238:A:N7	1:A:1303:C:C1'	2.78	0.46
1:A:5:U:HO2'	1:A:6:G:P	2.39	0.46
1:A:669:U:H2'	1:A:670:G:C8	2.50	0.46
1:A:694:A:H5'	12:K:53:SER:HB2	1.96	0.46
3:B:14:GLY:O	3:B:15:VAL:HG22	2.16	0.46
4:C:109:PRO:HA	4:C:115:LEU:HD12	1.98	0.46
4:C:64:VAL:O	4:C:99:VAL:HG23	2.16	0.46
6:E:31:LEU:CD2	6:E:43:LEU:HD21	2.46	0.46
8:G:42:ILE:HG23	8:G:117:ALA:HA	1.97	0.46
13:L:83:VAL:CG2	13:L:84:LEU:N	2.79	0.46
14:M:58:GLU:OE2	14:M:58:GLU:HA	2.16	0.46
15:N:25:VAL:HG12	15:N:39:LEU:HD23	1.97	0.46
15:N:3:ARG:O	15:N:4:LYS:C	2.53	0.46
16:O:11:VAL:O	16:O:14:GLU:HB3	2.15	0.46
19:R:40:LEU:HB3	19:R:79:LEU:HD11	1.97	0.46
19:R:44:LEU:CD1	19:R:79:LEU:HD22	2.46	0.46
1:A:1121:U:H2'	1:A:1122:U:C6	2.51	0.46
1:A:125:U:H2'	1:A:126:G:C8	2.51	0.46
1:A:1375:A:H2'	1:A:1376:U:O4'	2.15	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:A:H2'	1:A:163:C:C4'	2.46	0.46
1:A:232:G:H1'	1:A:262:A:N1	2.30	0.46
1:A:62:U:H5''	1:A:385:C:O2	2.16	0.46
1:A:603:U:O2'	1:A:604:G:H5'	2.15	0.46
3:B:21:ARG:HH12	3:B:23:ARG:HG2	1.80	0.46
5:D:149:ALA:HB3	5:D:152:SER:CB	2.46	0.46
7:F:76:ALA:O	7:F:80:ARG:HG3	2.16	0.46
7:F:9:VAL:HG22	7:F:60:PHE:CD2	2.51	0.46
6:E:143:ARG:NH1	9:H:77:GLU:OE2	2.49	0.46
11:J:10:GLY:N	11:J:16:LEU:HD21	2.31	0.46
12:K:54:ARG:CB	12:K:54:ARG:HH11	2.14	0.46
14:M:90:LEU:HD23	14:M:93:ARG:NH1	2.31	0.46
21:T:14:LYS:HA	21:T:17:ARG:CZ	2.45	0.46
1:A:1460:A:P	21:T:27:LYS:NZ	2.89	0.46
21:T:53:LEU:HD21	21:T:104:LEU:HD12	1.97	0.46
1:A:1065:U:O2'	1:A:1066:C:OP2	2.29	0.46
1:A:1132:C:H2'	1:A:1133:G:H8	1.79	0.46
1:A:1145:C:O2'	1:A:1146:A:O5'	2.33	0.46
1:A:1279:A:O2'	1:A:1282:C:N4	2.49	0.46
1:A:166:G:H2'	1:A:167:G:H8	1.81	0.46
1:A:505:G:H2'	1:A:506:G:C8	2.50	0.46
1:A:745:C:O2'	1:A:746:A:H5'	2.15	0.46
1:A:879:C:O2'	1:A:880:C:H5'	2.16	0.46
3:B:12:GLU:CG	3:B:213:LEU:HD11	2.46	0.46
4:C:150:LYS:HG3	4:C:169:ALA:HB2	1.98	0.46
5:D:152:SER:CB	5:D:155:LEU:HD12	2.43	0.46
13:L:46:LYS:HZ1	13:L:47:LYS:CE	2.22	0.46
16:O:75:PRO:O	16:O:78:TYR:HB3	2.16	0.46
16:O:82:ILE:O	16:O:83:GLU:C	2.53	0.46
1:A:761:G:C4'	18:Q:103:GLY:N	2.72	0.46
1:A:187:C:C2	21:T:105:SER:HB3	2.51	0.46
1:A:311:C:H2'	1:A:312:C:H6	1.81	0.45
1:A:814:A:N7	1:A:816:A:C4	2.84	0.45
3:B:53:ARG:O	3:B:56:ARG:HB3	2.16	0.45
6:E:122:GLU:O	6:E:123:LEU:HD23	2.16	0.45
7:F:33:TYR:CB	7:F:75:LEU:HD23	2.42	0.45
9:H:97:VAL:HA	9:H:100:ILE:HD11	1.97	0.45
9:H:80:ILE:O	9:H:80:ILE:HG22	2.14	0.45
10:I:9:ARG:HA	10:I:13:ALA:O	2.16	0.45
11:J:94:VAL:CG1	11:J:95:GLU:H	2.23	0.45
14:M:39:ILE:O	14:M:40:ASN:C	2.54	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:45:VAL:HG12	20:S:46:GLY:N	2.31	0.45
21:T:14:LYS:O	21:T:18:GLN:HG2	2.15	0.45
1:A:1073:U:H2'	1:A:1074:G:H8	1.81	0.45
1:A:1186:G:N2	1:A:1187:G:H1'	2.31	0.45
1:A:1316:G:N2	1:A:1318:A:H3'	2.32	0.45
1:A:1111:A:H61	4:C:177:THR:HA	1.81	0.45
4:C:34:LEU:CD2	4:C:34:LEU:C	2.84	0.45
4:C:84:ILE:O	4:C:84:ILE:HG12	2.17	0.45
5:D:76:ARG:O	5:D:79:PHE:HB3	2.16	0.45
8:G:54:THR:HG21	8:G:56:GLN:HE21	1.79	0.45
14:M:37:THR:HG23	14:M:55:ARG:HB3	1.98	0.45
16:O:4:THR:OG1	16:O:7:GLU:HG2	2.16	0.45
1:A:102:G:H2'	1:A:103:C:C6	2.50	0.45
1:A:1477:C:H2'	1:A:1478:C:C6	2.52	0.45
1:A:1531:A:O5'	1:A:1531:A:H8	2.00	0.45
1:A:965:A:O2'	1:A:966:G:OP2	2.33	0.45
4:C:43:LEU:N	4:C:43:LEU:HD23	2.31	0.45
5:D:199:ASN:ND2	5:D:201:GLN:CB	2.78	0.45
5:D:35:ARG:O	5:D:36:ARG:HB2	2.16	0.45
7:F:101:ALA:CB	19:R:28:GLU:HG2	2.46	0.45
11:J:9:ARG:HG3	11:J:9:ARG:O	2.16	0.45
17:P:51:VAL:O	17:P:52:ASP:C	2.55	0.45
1:A:1125:U:O4	11:J:5:ARG:NE	2.47	0.45
1:A:130:A:H5'	18:Q:63:ARG:NE	2.32	0.45
1:A:276:G:O2'	1:A:277:C:H5'	2.16	0.45
1:A:663:A:H2'	1:A:664:G:O4'	2.16	0.45
3:B:16:HIS:O	3:B:17:PHE:O	2.34	0.45
5:D:120:LEU:HD23	5:D:125:HIS:CD2	2.51	0.45
5:D:65:ARG:HG3	5:D:75:PHE:CD1	2.52	0.45
6:E:33:VAL:HG11	6:E:109:ILE:HA	1.98	0.45
7:F:2:ARG:CG	7:F:69:GLU:HG2	2.47	0.45
8:G:54:THR:HG22	8:G:56:GLN:HG3	1.98	0.45
9:H:116:LYS:NZ	9:H:127:LEU:HD12	2.31	0.45
9:H:116:LYS:HD2	9:H:129:VAL:HG11	1.98	0.45
9:H:3:THR:HG23	9:H:4:ASP:N	2.31	0.45
10:I:112:LYS:O	10:I:112:LYS:HD3	2.15	0.45
10:I:42:ARG:O	10:I:43:ALA:C	2.54	0.45
14:M:36:LYS:HD2	14:M:59:TYR:OH	2.16	0.45
18:Q:59:ILE:HD13	18:Q:59:ILE:HA	1.72	0.45
20:S:27:GLU:HA	20:S:47:HIS:HE1	1.81	0.45
1:A:1104:G:O2'	1:A:1105:A:H5'	2.17	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1191:A:H2'	1:A:1192:C:C6	2.52	0.45
1:A:1385:G:O2'	1:A:1386:G:H5'	2.16	0.45
1:A:1435:G:H8	1:A:1435:G:O5'	2.00	0.45
25:A:1632:PCY:C6	25:A:1632:PCY:N2	2.71	0.45
1:A:66:G:H4'	1:A:173:U:C5	2.52	0.45
1:A:197:A:N1	1:A:220:G:O2'	2.48	0.45
1:A:417:C:H2'	1:A:418:C:C6	2.51	0.45
3:B:178:ARG:NH1	3:B:178:ARG:HG3	2.30	0.45
3:B:69:LEU:HD23	3:B:70:PHE:N	2.31	0.45
4:C:60:ALA:O	4:C:61:ALA:CB	2.65	0.45
5:D:114:ARG:CG	5:D:114:ARG:HH11	2.30	0.45
14:M:57:ARG:O	14:M:61:GLU:HG3	2.15	0.45
19:R:88:LYS:HG2	19:R:88:LYS:OXT	2.16	0.45
1:A:1113:C:H6	1:A:1113:C:O5'	2.00	0.45
1:A:1305:G:O2'	1:A:1306:A:C8	2.35	0.45
1:A:1347:G:C6	10:I:107:ARG:NH1	2.85	0.45
1:A:1353:G:O2'	1:A:1354:C:H5'	2.17	0.45
3:B:109:SER:O	3:B:112:VAL:N	2.49	0.45
3:B:90:MET:HE3	3:B:90:MET:HA	1.98	0.45
4:C:100:ALA:O	4:C:101:LEU:HB2	2.15	0.45
5:D:94:LEU:HD22	5:D:196:LEU:CD1	2.46	0.45
6:E:60:TYR:CE1	6:E:64:ARG:CZ	3.00	0.45
10:I:6:GLY:N	10:I:84:ALA:HB2	2.32	0.45
11:J:26:ALA:HB1	11:J:84:GLN:CB	2.45	0.45
11:J:30:SER:HB2	11:J:81:THR:N	2.31	0.45
11:J:6:ILE:CG2	11:J:98:ILE:HG12	2.46	0.45
12:K:29:ILE:HG13	12:K:43:SER:O	2.16	0.45
14:M:5:ALA:O	14:M:6:GLY:C	2.55	0.45
14:M:60:VAL:O	14:M:63:THR:HG22	2.17	0.45
20:S:32:LYS:HA	20:S:50:ALA:O	2.17	0.45
1:A:1132:C:H42	1:A:1142:G:H1	1.64	0.45
1:A:1337:G:H5''	1:A:1338:G:OP1	2.17	0.45
1:A:118:U:O4	1:A:288:A:H2'	2.17	0.45
3:B:73:THR:HG23	3:B:96:ARG:HD2	1.99	0.45
6:E:18:ARG:HG2	6:E:19:MET:N	2.31	0.45
6:E:45:PHE:CE2	6:E:47:LYS:HE3	2.52	0.45
7:F:69:GLU:N	7:F:69:GLU:OE1	2.50	0.45
6:E:143:ARG:HH12	9:H:77:GLU:CD	2.20	0.45
11:J:5:ARG:HG3	11:J:73:ASP:OD1	2.16	0.45
15:N:14:PRO:O	15:N:16:PHE:N	2.47	0.45
19:R:36:ASN:ND2	19:R:38:GLU:CG	2.76	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:25:LYS:HD2	20:S:25:LYS:H	1.81	0.45
20:S:33:THR:HG22	20:S:34:TRP:N	2.32	0.45
20:S:3:ARG:O	20:S:4:SER:HB3	2.15	0.45
20:S:70:LYS:O	20:S:72:GLY:N	2.50	0.45
1:A:1106:G:OP1	4:C:172:ARG:HD3	2.17	0.45
1:A:1267:C:O2	22:V:20:LYS:HD3	2.17	0.45
1:A:160:A:H1'	1:A:344:A:C5	2.52	0.45
1:A:190(L):U:H3	21:T:105:SER:HG	1.65	0.45
1:A:192:U:H2'	1:A:193:C:C6	2.45	0.45
1:A:243:A:N6	1:A:281:G:O2'	2.50	0.45
1:A:412:A:N6	5:D:35:ARG:HD3	2.31	0.45
1:A:542:G:H2'	1:A:543:C:H6	1.82	0.45
1:A:633:G:H2'	1:A:634:C:C6	2.52	0.45
3:B:213:LEU:C	3:B:213:LEU:CD2	2.85	0.45
4:C:11:ARG:HH11	4:C:11:ARG:HG2	1.82	0.45
4:C:129:ALA:HB3	4:C:132:ARG:HD2	1.99	0.45
5:D:101:LEU:O	5:D:102:ASP:C	2.55	0.45
5:D:163:GLU:C	5:D:165:MET:N	2.69	0.45
6:E:107:ARG:NH1	6:E:107:ARG:HB2	2.32	0.45
9:H:103:VAL:O	9:H:104:ARG:C	2.54	0.45
11:J:44:VAL:HG13	11:J:64:GLU:HB2	1.99	0.45
15:N:17:LYS:HE2	15:N:17:LYS:HB2	1.74	0.45
15:N:50:LYS:HD3	15:N:52:GLN:HE21	1.81	0.45
19:R:36:ASN:C	19:R:36:ASN:ND2	2.70	0.45
19:R:36:ASN:HD21	19:R:38:GLU:HB2	1.82	0.45
20:S:25:LYS:N	20:S:25:LYS:HD2	2.31	0.45
1:A:1129:C:HO2'	1:A:1130:A:P	2.39	0.45
1:A:1288:A:H1'	1:A:1352:C:O2'	2.17	0.45
1:A:179:A:O2'	1:A:180:U:H5'	2.17	0.45
1:A:24:U:H2'	1:A:25:C:C6	2.52	0.45
1:A:448:A:H2'	1:A:449:C:C6	2.52	0.45
7:F:25:ILE:CD1	7:F:82:ARG:HD2	2.47	0.45
10:I:111:ARG:O	10:I:119:ALA:HB2	2.17	0.45
21:T:54:LYS:HE3	21:T:100:ILE:HD11	1.98	0.45
21:T:57:ARG:HH21	21:T:100:ILE:HG23	1.82	0.45
1:A:1195:C:H3'	1:A:1196:U:H5''	1.98	0.45
1:A:1256:A:O2'	1:A:1257:U:P	2.75	0.45
1:A:1367:C:C2	1:A:1368:G:C8	3.05	0.45
1:A:246:A:C2	1:A:282:A:C5	3.05	0.45
1:A:358:U:H2'	1:A:359:U:H6	1.82	0.45
1:A:409:G:H2'	1:A:410:G:O4'	2.17	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:639:G:O2'	1:A:640:A:H5'	2.16	0.45
1:A:645:C:O2'	1:A:646:U:H5'	2.16	0.45
1:A:678:U:O2'	1:A:679:C:H5'	2.17	0.45
1:A:761:G:C1'	18:Q:103:GLY:O	2.65	0.45
3:B:120:ALA:O	3:B:124:SER:HB3	2.17	0.45
8:G:46:ALA:O	8:G:50:ILE:HG13	2.17	0.45
11:J:51:ARG:HG2	11:J:51:ARG:HH11	1.82	0.45
1:A:552:U:H4'	13:L:86:ARG:O	2.17	0.45
1:A:1202:G:C2	15:N:42:ILE:HG21	2.51	0.45
16:O:17:ARG:NH1	16:O:17:ARG:HG3	2.28	0.45
1:A:1225:A:N3	1:A:1225:A:C2'	2.80	0.44
1:A:475:G:O2'	1:A:476:G:H5'	2.16	0.44
1:A:601:C:O2'	1:A:602:A:H5'	2.17	0.44
1:A:771:G:H2'	1:A:772:U:C6	2.52	0.44
3:B:125:PRO:HG2	3:B:126:GLU:N	2.32	0.44
3:B:215:LEU:HD23	3:B:215:LEU:HA	1.84	0.44
4:C:110:ASN:HB3	4:C:144:SER:OG	2.16	0.44
4:C:147:LYS:HE2	4:C:205:GLY:HA2	1.99	0.44
4:C:38:ARG:HG3	4:C:38:ARG:NH1	2.29	0.44
5:D:57:ARG:NH2	6:E:107:ARG:HE	2.15	0.44
6:E:143:ARG:HD3	6:E:143:ARG:HA	1.68	0.44
6:E:57:LYS:HG2	6:E:61:TYR:CE2	2.52	0.44
9:H:40:ALA:HA	9:H:45:ILE:HG12	1.99	0.44
12:K:127:LYS:HD3	12:K:127:LYS:HA	1.71	0.44
19:R:47:THR:HG22	19:R:48:GLY:N	2.32	0.44
1:A:1025:U:H4'	1:A:1025:U:OP1	2.17	0.44
1:A:1221:G:O4'	20:S:54:GLY:HA3	2.17	0.44
1:A:1238:A:H2	1:A:1241:G:N3	2.14	0.44
1:A:1367:C:H5''	10:I:114:TYR:CB	2.47	0.44
1:A:550:G:O2'	1:A:551:U:H5'	2.17	0.44
1:A:619:U:N3	5:D:134:ASP:OD1	2.50	0.44
1:A:635:G:O2'	1:A:636:U:H5'	2.17	0.44
1:A:833:U:H2'	1:A:834:C:C6	2.52	0.44
1:A:876:G:H2'	1:A:877:C:C6	2.52	0.44
1:A:90:U:H2'	1:A:91:C:H6	1.83	0.44
1:A:976:G:OP1	15:N:31:ARG:O	2.35	0.44
1:A:995:C:H2'	1:A:995:C:O2	2.17	0.44
3:B:59:GLU:O	3:B:60:ASP:C	2.56	0.44
4:C:3:ASN:N	4:C:3:ASN:ND2	2.64	0.44
4:C:77:ILE:O	4:C:83:ARG:HB3	2.17	0.44
8:G:129:GLU:HG3	8:G:131:LYS:HE2	1.99	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1119:C:OP2	10:I:9:ARG:NH2	2.50	0.44
11:J:60:ARG:H	11:J:60:ARG:HD2	1.78	0.44
12:K:125:PHE:CD1	12:K:125:PHE:N	2.85	0.44
13:L:54:LYS:N	13:L:54:LYS:HD2	2.31	0.44
1:A:953:G:C1'	14:M:125:ARG:HA	2.47	0.44
11:J:45:ARG:NH1	15:N:36:PHE:CE2	2.81	0.44
17:P:6:LEU:N	17:P:6:LEU:HD12	2.31	0.44
18:Q:45:HIS:CD2	18:Q:47:PRO:HG3	2.51	0.44
1:A:103:C:OP1	21:T:17:ARG:HD2	2.17	0.44
1:A:112:G:H2'	1:A:113:G:H5'	2.00	0.44
1:A:1142:G:O2'	1:A:1143:G:H5'	2.17	0.44
1:A:1183:A:O2'	1:A:1184:G:P	2.75	0.44
1:A:1327:C:O2'	1:A:1328:C:H5'	2.18	0.44
1:A:551:U:H2'	1:A:552:U:H6	1.82	0.44
1:A:824:C:H2'	1:A:825:G:C8	2.51	0.44
1:A:970:C:O2	14:M:126:LYS:C	2.56	0.44
1:A:950:U:H4'	1:A:971:G:C2	2.53	0.44
3:B:91:PRO:CA	3:B:154:LEU:HD12	2.47	0.44
3:B:172:ILE:O	3:B:172:ILE:HG22	2.16	0.44
3:B:184:VAL:HG12	3:B:197:VAL:HA	2.00	0.44
4:C:46:GLU:C	4:C:48:TYR:H	2.19	0.44
5:D:200:GLU:O	5:D:203:VAL:N	2.51	0.44
7:F:2:ARG:NE	7:F:69:GLU:HG2	2.32	0.44
10:I:69:GLY:O	10:I:73:GLN:HG3	2.18	0.44
10:I:85:LEU:O	10:I:92:TYR:CD1	2.70	0.44
14:M:53:VAL:O	14:M:57:ARG:HB2	2.17	0.44
19:R:39:VAL:HG13	19:R:40:LEU:N	2.31	0.44
19:R:47:THR:HA	19:R:83:GLU:HB2	1.99	0.44
1:A:1221:G:H4'	20:S:77:THR:OG1	2.17	0.44
1:A:960:U:H1'	1:A:1223:C:H5'	1.99	0.44
1:A:1292:U:O2'	1:A:1293:G:H5'	2.18	0.44
1:A:165:C:H2'	1:A:166:G:C8	2.50	0.44
1:A:291:C:O2'	1:A:292:G:H5'	2.17	0.44
1:A:744:C:H2'	1:A:745:C:C6	2.52	0.44
9:H:60:ARG:HH11	9:H:60:ARG:CG	2.26	0.44
10:I:79:LEU:HD13	10:I:83:ARG:HG3	1.99	0.44
10:I:97:LYS:O	10:I:100:GLY:N	2.48	0.44
14:M:81:LEU:HD23	14:M:82:MET:H	1.82	0.44
15:N:23:ARG:HG2	15:N:30:ALA:HB2	2.00	0.44
20:S:16:LEU:C	20:S:18:LYS:N	2.70	0.44
20:S:31:ILE:CG2	20:S:32:LYS:H	2.28	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:U:H2'	1:A:115:G:C8	2.53	0.44
1:A:991:U:O4	1:A:1212:U:H1'	2.17	0.44
1:A:1232:U:H2'	1:A:1233:G:O4'	2.18	0.44
1:A:1511:G:H2'	1:A:1512:U:O4'	2.17	0.44
4:C:39:ILE:HD12	4:C:57:ILE:HD13	1.98	0.44
7:F:19:LEU:C	7:F:19:LEU:CD2	2.83	0.44
7:F:69:GLU:O	7:F:72:VAL:HG23	2.18	0.44
8:G:121:ALA:O	8:G:125:MET:HG3	2.18	0.44
10:I:50:LEU:HG	10:I:81:ILE:HG21	1.99	0.44
10:I:50:LEU:O	10:I:52:ALA:N	2.50	0.44
12:K:60:ALA:O	12:K:61:ALA:C	2.56	0.44
15:N:41:ARG:HG2	15:N:41:ARG:HH11	1.83	0.44
16:O:6:GLU:O	16:O:7:GLU:C	2.55	0.44
19:R:45:SER:C	19:R:47:THR:N	2.69	0.44
1:A:1040:U:H2'	1:A:1041:A:H8	1.77	0.44
1:A:1085:U:H3'	1:A:1086:U:C5	2.52	0.44
1:A:1127:G:H21	1:A:1146:A:H62	1.66	0.44
1:A:1238:A:C2	1:A:1241:G:N3	2.86	0.44
1:A:1272:G:O2'	1:A:1273:G:H5'	2.17	0.44
1:A:1372:U:O2'	1:A:1373:G:H5'	2.18	0.44
1:A:1449:C:H2'	1:A:1450:U:H6	1.81	0.44
1:A:41:G:H2'	1:A:42:G:H8	1.81	0.44
1:A:709:G:O2'	1:A:710:G:H5'	2.17	0.44
1:A:582:U:C2	1:A:760:G:C6	3.06	0.44
1:A:781:A:C2'	1:A:782:A:H5'	2.43	0.44
1:A:899:C:O5'	1:A:899:C:H6	1.99	0.44
3:B:10:LEU:C	3:B:12:GLU:N	2.70	0.44
4:C:112:SER:HB2	4:C:115:LEU:CD1	2.47	0.44
4:C:34:LEU:HD12	15:N:25:VAL:CG2	2.38	0.44
4:C:77:ILE:CG2	4:C:81:GLY:HA2	2.45	0.44
4:C:77:ILE:HD13	4:C:84:ILE:HD12	1.99	0.44
4:C:91:LEU:CG	4:C:99:VAL:HG13	2.47	0.44
5:D:142:PRO:HA	5:D:185:PHE:HD2	1.83	0.44
12:K:99:GLN:HA	12:K:105:VAL:CG2	2.47	0.44
13:L:109:GLY:HA3	13:L:121:GLY:O	2.18	0.44
13:L:47:LYS:HB3	13:L:48:PRO:HD3	1.98	0.44
14:M:77:ASN:O	14:M:80:ARG:N	2.50	0.44
18:Q:45:HIS:CD2	18:Q:65:ILE:HD13	2.53	0.44
7:F:89:MET:HE1	19:R:76:LEU:HG	1.99	0.44
19:R:81:PHE:O	19:R:82:THR:HB	2.17	0.44
1:A:1231:G:H5''	10:I:126:SER:CB	2.48	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:C:H2'	1:A:434:U:C6	2.50	0.44
1:A:972:C:OP1	11:J:57:LYS:NZ	2.37	0.44
3:B:209:ARG:HG2	3:B:209:ARG:HH11	1.83	0.44
3:B:25:ASN:O	3:B:26:PRO:C	2.56	0.44
4:C:164:ARG:NH1	4:C:164:ARG:CB	2.81	0.44
4:C:178:LEU:O	4:C:179:ARG:HB3	2.17	0.44
4:C:35:GLU:CD	4:C:95:THR:HG21	2.38	0.44
9:H:111:ILE:O	9:H:134:ILE:HB	2.18	0.44
10:I:64:THR:HG22	10:I:65:VAL:H	1.83	0.44
10:I:71:SER:O	10:I:74:ILE:HB	2.17	0.44
18:Q:96:GLN:O	18:Q:96:GLN:HG2	2.17	0.44
1:A:1017:G:O2'	1:A:1018:C:H5'	2.18	0.44
1:A:1121:U:H2'	1:A:1122:U:H6	1.83	0.44
1:A:1509:C:H2'	1:A:1510:U:O4'	2.18	0.44
1:A:179:A:H2'	1:A:180:U:C6	2.53	0.44
1:A:748:C:O2'	1:A:749:C:OP2	2.32	0.44
1:A:889:A:H4'	1:A:890:G:OP1	2.18	0.44
1:A:925:G:O2'	1:A:926:G:H5''	2.18	0.44
3:B:12:GLU:HG3	3:B:213:LEU:HD11	1.99	0.44
3:B:60:ASP:CG	3:B:64:ARG:HH22	2.21	0.44
3:B:80:ILE:CD1	3:B:212:GLN:HB2	2.48	0.44
8:G:88:PRO:O	8:G:89:MET:CB	2.66	0.44
10:I:8:GLY:O	10:I:76:ALA:HB1	2.17	0.44
12:K:46:GLY:O	12:K:48:ILE:O	2.36	0.44
12:K:85:ARG:NH1	12:K:85:ARG:HG3	2.31	0.44
13:L:23:LYS:O	13:L:24:VAL:HG23	2.17	0.44
14:M:29:ARG:HB3	14:M:64:TRP:CZ3	2.52	0.44
18:Q:45:HIS:HB2	18:Q:69:LYS:HE2	2.00	0.44
1:A:1058:G:H2'	1:A:1059:C:O4'	2.18	0.44
1:A:1065:U:C5	1:A:1190:G:C4	3.06	0.44
1:A:118:U:O4	1:A:289:G:H4'	2.18	0.44
1:A:1226:C:H5''	14:M:103:THR:HG1	1.83	0.44
1:A:1441:G:H4'	1:A:1442:G:C5	2.53	0.44
1:A:1492:A:H2'	1:A:1493:A:C8	2.53	0.44
1:A:1501:C:OP2	1:A:1504:G:H2'	2.18	0.44
1:A:336:C:O2'	1:A:337:C:H5'	2.17	0.44
1:A:401:C:H1'	1:A:622:A:H1'	1.99	0.44
1:A:911:U:H2'	1:A:912:C:C6	2.53	0.44
3:B:110:GLN:HA	3:B:113:HIS:HD2	1.83	0.44
3:B:112:VAL:O	3:B:113:HIS:C	2.55	0.44
3:B:19:HIS:CG	3:B:20:GLU:N	2.86	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:83:MET:HE1	3:B:234:PRO:HG2	2.00	0.44
3:B:22:LYS:HD2	3:B:35:GLU:CD	2.38	0.44
3:B:50:GLU:O	3:B:51:LEU:C	2.56	0.44
4:C:35:GLU:OE2	4:C:97:LYS:HG3	2.17	0.44
5:D:28:SER:O	5:D:29:PRO:C	2.57	0.44
10:I:46:ALA:O	10:I:81:ILE:HD12	2.17	0.44
13:L:38:THR:HB	13:L:57:LYS:HB2	1.99	0.44
1:A:970:C:O2	14:M:126:LYS:OXT	2.36	0.44
17:P:17:TYR:N	17:P:17:TYR:CD1	2.86	0.44
18:Q:68:ARG:O	18:Q:69:LYS:HB2	2.18	0.44
19:R:34:TYR:CD1	19:R:34:TYR:C	2.92	0.44
20:S:42:PRO:HA	20:S:45:VAL:HG23	2.00	0.44
1:A:192:U:H1'	21:T:103:GLY:HA2	2.00	0.44
21:T:16:HIS:CE1	21:T:20:LEU:HD11	2.53	0.44
21:T:93:GLU:OE2	21:T:93:GLU:HA	2.17	0.44
1:A:1305:G:H5''	22:V:4:GLY:C	2.38	0.44
1:A:1057:G:H4'	4:C:197:GLY:H	1.83	0.43
1:A:1091:U:O2	1:A:1093:A:H8	1.99	0.43
1:A:373:A:O2'	1:A:374:A:H5'	2.18	0.43
1:A:542:G:H2'	1:A:543:C:C6	2.53	0.43
1:A:625:G:H2'	1:A:626:U:H6	1.81	0.43
1:A:640:A:O2'	1:A:641:U:H5'	2.18	0.43
1:A:653:A:N3	1:A:653:A:H2'	2.33	0.43
5:D:31:CYS:O	5:D:33:MET:N	2.42	0.43
8:G:133:GLY:O	8:G:137:LYS:HG3	2.18	0.43
8:G:28:ASN:OD1	8:G:36:LYS:NZ	2.51	0.43
11:J:80:LYS:O	11:J:83:GLU:HB3	2.18	0.43
12:K:91:ARG:CZ	19:R:88:LYS:HE2	2.48	0.43
13:L:48:PRO:HG2	13:L:49:ASN:H	1.82	0.43
15:N:54:PRO:C	15:N:56:VAL:H	2.21	0.43
1:A:1057:G:C2'	1:A:1058:G:H5'	2.48	0.43
1:A:1064:G:C2	1:A:1066:C:N4	2.86	0.43
1:A:110:C:C4	1:A:111:G:C5	3.06	0.43
1:A:1139:G:HO2'	1:A:1140:C:P	2.41	0.43
1:A:1175:G:O2'	1:A:1176:A:H5'	2.18	0.43
1:A:1196:U:H4'	1:A:1197:G:OP2	2.17	0.43
1:A:1306:A:N6	1:A:1331:G:H1'	2.32	0.43
1:A:1415:G:H2'	1:A:1416:G:C8	2.53	0.43
1:A:1488:G:H2'	1:A:1489:G:H8	1.82	0.43
1:A:182:U:O4	1:A:223:U:H1'	2.18	0.43
1:A:7:G:H5'	1:A:298:A:H5'	1.99	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:A:N6	1:A:361:G:C4'	2.81	0.43
1:A:580:U:H2'	1:A:581:G:O4'	2.18	0.43
1:A:748:C:H1'	1:A:749:C:H5	1.83	0.43
1:A:783:C:O2'	1:A:784:C:H5'	2.18	0.43
1:A:836:G:C6	1:A:851:G:C6	3.06	0.43
1:A:575:G:C5	1:A:881:G:C2	3.06	0.43
3:B:167:PRO:HG3	3:B:188:ALA:CB	2.48	0.43
4:C:134:ILE:CD1	4:C:166:GLU:HB3	2.47	0.43
4:C:83:ARG:HE	4:C:87:LEU:HD11	1.83	0.43
5:D:108:LEU:HD23	5:D:108:LEU:HA	1.82	0.43
5:D:3:ARG:NH1	5:D:118:ARG:NH1	2.65	0.43
6:E:110:LEU:CD1	6:E:118:ILE:HD12	2.20	0.43
6:E:12:LEU:C	6:E:12:LEU:CD2	2.86	0.43
6:E:79:GLU:O	6:E:80:ILE:CG2	2.66	0.43
7:F:32:ASN:N	7:F:32:ASN:ND2	2.66	0.43
9:H:10:LEU:HD22	9:H:83:ILE:HD11	2.00	0.43
9:H:7:ALA:HB2	9:H:85:ARG:HG3	2.00	0.43
10:I:40:LEU:O	10:I:42:ARG:N	2.51	0.43
11:J:9:ARG:C	11:J:16:LEU:HD21	2.38	0.43
11:J:9:ARG:CB	11:J:9:ARG:NH1	2.81	0.43
14:M:74:VAL:O	14:M:77:ASN:N	2.48	0.43
4:C:12:LEU:HD11	15:N:51:GLY:HA2	2.00	0.43
1:A:101:A:H2'	1:A:102:G:H8	1.83	0.43
1:A:1110:A:N6	1:A:1111:A:C6	2.86	0.43
1:A:1255:G:H3'	1:A:1279:A:N6	2.33	0.43
1:A:1313:U:O2'	1:A:1314:C:H5'	2.18	0.43
1:A:1353:G:H2'	1:A:1354:C:H6	1.82	0.43
1:A:162:A:H8	1:A:162:A:O5'	2.01	0.43
1:A:22:G:O2'	1:A:23:C:H5'	2.18	0.43
1:A:363:A:C2	13:L:31:PRO:HG2	2.53	0.43
1:A:389:A:H2'	1:A:390:C:H5'	2.00	0.43
1:A:424:G:H2'	1:A:425:G:C8	2.50	0.43
1:A:432:A:N7	1:A:433:C:C4	2.86	0.43
1:A:518:C:O2'	1:A:519:C:OP2	2.33	0.43
1:A:522:C:H41	13:L:53:ARG:HH22	1.66	0.43
1:A:662:G:O2'	1:A:836:G:C5'	2.66	0.43
5:D:100:ARG:NH2	5:D:118:ARG:HH22	2.16	0.43
7:F:24:GLU:OE2	7:F:28:ARG:NH1	2.51	0.43
9:H:138:TRP:OXT	9:H:138:TRP:CE3	2.68	0.43
10:I:19:LEU:HB3	10:I:59:PHE:CD2	2.52	0.43
21:T:39:LYS:HD3	21:T:55:ILE:HD13	2.00	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1231:G:O2'	1:A:1232:U:H5'	2.18	0.43
1:A:179:A:H2'	1:A:180:U:H6	1.84	0.43
1:A:186:C:H2'	1:A:187:C:H6	1.83	0.43
1:A:190(L):U:O2'	1:A:191:G:H5'	2.18	0.43
1:A:393:A:H2'	1:A:394:G:H5'	2.00	0.43
1:A:826:C:H2'	1:A:827:U:C6	2.54	0.43
1:A:920:U:H2'	1:A:921:U:H6	1.82	0.43
1:A:965:A:C2	1:A:969:A:C2	3.06	0.43
3:B:73:THR:CG2	3:B:96:ARG:CZ	2.96	0.43
3:B:98:LEU:HB2	3:B:108:ILE:CD1	2.49	0.43
4:C:154:SER:OG	4:C:155:GLY:N	2.49	0.43
4:C:174:PRO:O	4:C:177:THR:HG22	2.19	0.43
7:F:14:LEU:HD21	7:F:84:ASN:OD1	2.18	0.43
8:G:33:ASP:N	8:G:33:ASP:OD1	2.51	0.43
10:I:108:VAL:CG1	10:I:109:VAL:N	2.80	0.43
11:J:46:ARG:HH11	11:J:64:GLU:CB	2.31	0.43
11:J:81:THR:C	11:J:83:GLU:N	2.72	0.43
11:J:87:THR:O	11:J:88:LEU:HG	2.19	0.43
11:J:22:LYS:CE	11:J:90:LEU:HD12	2.41	0.43
12:K:121:PRO:HG2	12:K:126:ARG:HG2	1.99	0.43
13:L:117:ARG:O	13:L:119:LYS:O	2.36	0.43
19:R:47:THR:C	19:R:49:LYS:H	2.21	0.43
1:A:1026:G:H2'	1:A:1027:C:H5'	2.01	0.43
1:A:1253:G:N1	1:A:1285:A:N6	2.66	0.43
1:A:1292:U:H5'	10:I:38:GLN:NE2	2.29	0.43
1:A:136:C:H2'	1:A:137:C:H6	1.83	0.43
1:A:16:A:C2'	1:A:17:U:H5'	2.48	0.43
1:A:489:C:H2'	1:A:490:G:H8	1.83	0.43
1:A:696:A:O5'	1:A:696:A:H8	2.01	0.43
1:A:929:G:O2'	1:A:930:C:H5'	2.18	0.43
3:B:105:PHE:O	3:B:106:LYS:C	2.56	0.43
3:B:126:GLU:HA	3:B:129:GLU:OE1	2.18	0.43
3:B:154:LEU:O	3:B:155:LEU:C	2.57	0.43
3:B:166:ASP:HB3	3:B:169:LYS:HB3	2.01	0.43
5:D:156:GLU:O	5:D:160:GLN:HG3	2.19	0.43
5:D:91:SER:O	5:D:92:VAL:C	2.56	0.43
6:E:94:ALA:CB	6:E:98:THR:HG21	2.48	0.43
8:G:30:ILE:CD1	8:G:120:ILE:HD13	2.48	0.43
8:G:88:PRO:O	8:G:89:MET:HB3	2.18	0.43
10:I:32:ASP:O	10:I:35:GLU:N	2.50	0.43
10:I:58:ARG:NH1	10:I:58:ARG:CG	2.81	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:21:ASP:OD1	16:O:24:SER:OG	2.31	0.43
19:R:40:LEU:HB2	19:R:79:LEU:HD11	2.00	0.43
19:R:46:GLU:N	19:R:46:GLU:CD	2.72	0.43
19:R:43:PHE:C	19:R:51:LEU:HD12	2.39	0.43
1:A:1181:G:H4'	1:A:1184:G:H5'	2.01	0.43
1:A:1213:A:C6	1:A:1215:G:H1'	2.54	0.43
1:A:1346:A:N9	8:G:10:ARG:NH2	2.66	0.43
1:A:145:G:H1	1:A:177:C:H42	1.67	0.43
1:A:279:A:H5''	1:A:280:C:H3'	2.00	0.43
1:A:668:G:H1'	16:O:46:HIS:HD2	1.83	0.43
1:A:6:G:C4	6:E:119:LEU:HD11	2.53	0.43
1:A:755:G:OP2	16:O:65:ARG:HD2	2.19	0.43
3:B:197:VAL:HB	3:B:200:ILE:HG12	1.99	0.43
3:B:23:ARG:NH1	3:B:24:TRP:CA	2.79	0.43
5:D:96:LEU:N	5:D:96:LEU:HD12	2.34	0.43
8:G:20:ASP:HB3	8:G:23:VAL:HG23	2.01	0.43
15:N:24:CYS:HB3	15:N:28:GLY:N	2.32	0.43
16:O:71:GLN:HB2	16:O:78:TYR:CD1	2.54	0.43
18:Q:9:VAL:HG21	18:Q:84:LEU:CD1	2.49	0.43
18:Q:9:VAL:HG21	18:Q:84:LEU:HD13	2.00	0.43
19:R:26:LEU:HD23	19:R:29:PHE:CE2	2.53	0.43
19:R:61:LYS:O	19:R:65:ILE:HG12	2.19	0.43
20:S:27:GLU:HA	20:S:47:HIS:CE1	2.54	0.43
1:A:1220:G:H1'	20:S:52:TYR:CD2	2.53	0.43
1:A:1251:A:H2'	1:A:1252:A:H8	1.81	0.43
1:A:251:G:H4'	1:A:252:U:O5'	2.17	0.43
1:A:312:C:H2'	1:A:313:A:C8	2.53	0.43
1:A:496:A:C2	1:A:497:A:C5	3.06	0.43
1:A:782:A:H4'	1:A:1514:C:O2'	2.19	0.43
1:A:437:U:C5'	5:D:155:LEU:HD22	2.46	0.43
6:E:86:ALA:C	6:E:125:SER:HB3	2.39	0.43
10:I:121:ARG:NH1	10:I:121:ARG:HG2	2.31	0.43
1:A:1152:A:O3'	11:J:13:HIS:CD2	2.72	0.43
11:J:28:ARG:C	11:J:29:ARG:HG3	2.39	0.43
14:M:125:ARG:HH11	14:M:125:ARG:HG3	1.84	0.43
15:N:3:ARG:O	15:N:7:ILE:HG13	2.18	0.43
15:N:24:CYS:HB2	15:N:40:CYS:HB3	2.00	0.43
16:O:34:LEU:HD23	16:O:34:LEU:O	2.19	0.43
1:A:1028:C:H2'	1:A:1029:C:H6	1.80	0.43
1:A:1374:A:O2'	1:A:1375:A:H5'	2.19	0.43
1:A:1520:G:H2'	1:A:1521:G:C8	2.54	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:922:G:O2'	1:A:923:A:H5'	2.19	0.43
4:C:112:SER:O	4:C:113:ALA:C	2.57	0.43
15:N:21:TYR:HE2	15:N:23:ARG:NE	2.17	0.43
1:A:1028:C:O5'	1:A:1028:C:H6	2.01	0.43
1:A:110:C:H2'	1:A:111:G:O4'	2.19	0.43
1:A:1133:G:H2'	1:A:1134:G:C8	2.47	0.43
1:A:1486:G:H2'	1:A:1487:G:O4'	2.18	0.43
1:A:385:C:O2'	1:A:386:C:H5'	2.18	0.43
1:A:5:U:O2'	1:A:6:G:P	2.77	0.43
1:A:761:G:O4'	18:Q:103:GLY:O	2.37	0.43
1:A:930:C:H2'	1:A:931:C:H5'	2.01	0.43
3:B:134:GLU:O	3:B:136:VAL:N	2.52	0.43
4:C:32:LEU:O	4:C:32:LEU:HD23	2.18	0.43
5:D:29:PRO:C	5:D:30:LYS:HG3	2.36	0.43
5:D:39:PRO:HG2	5:D:44:GLY:HA2	2.01	0.43
6:E:137:GLU:O	6:E:140:ARG:HB2	2.18	0.43
6:E:148:VAL:O	6:E:152:ARG:HG3	2.18	0.43
11:J:49:VAL:HG12	11:J:50:ILE:O	2.19	0.43
14:M:74:VAL:HA	14:M:77:ASN:HD22	1.83	0.43
16:O:6:GLU:CD	16:O:6:GLU:H	2.21	0.43
16:O:74:ASP:OD2	16:O:77:ARG:HG3	2.19	0.43
19:R:44:LEU:HD12	19:R:79:LEU:HD22	2.01	0.43
20:S:41:VAL:CG2	20:S:43:GLU:HG2	2.47	0.43
21:T:45:GLN:C	21:T:47:GLY:H	2.22	0.43
1:A:1327:C:OP1	22:V:20:LYS:N	2.51	0.43
1:A:1002:G:H2'	1:A:1003:G:C8	2.54	0.43
1:A:1072:G:H2'	1:A:1073:U:H6	1.82	0.43
1:A:1229:A:OP2	14:M:114:ARG:CD	2.64	0.43
1:A:971:G:C8	1:A:1365:G:H4'	2.54	0.43
1:A:1433:A:O2'	1:A:1434:A:H5'	2.19	0.43
1:A:533:A:O2'	1:A:534:U:P	2.77	0.43
1:A:579:G:H5'	1:A:728:A:C1'	2.33	0.43
1:A:608:A:H2'	1:A:609:A:O4'	2.19	0.43
3:B:83:MET:HE2	3:B:235:SER:HA	2.01	0.43
7:F:75:LEU:O	7:F:79:LEU:HG	2.19	0.43
9:H:45:ILE:HG13	9:H:47:GLY:H	1.82	0.43
16:O:87:ILE:CG2	16:O:88:ARG:N	2.82	0.43
19:R:73:ALA:HB3	19:R:79:LEU:HD12	2.01	0.43
1:A:1118:C:H1'	1:A:1179:A:C4	2.54	0.42
1:A:1402:C:C5	1:A:1403:C:C5	3.07	0.42
1:A:1422:G:H2'	1:A:1423:G:H8	1.83	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:117:ALA:HB1	4:C:187:ALA:HB2	2.01	0.42
4:C:82:GLU:O	4:C:85:ARG:HB3	2.18	0.42
6:E:31:LEU:HD23	6:E:45:PHE:CD1	2.54	0.42
7:F:19:LEU:C	7:F:21:LEU:H	2.22	0.42
10:I:111:ARG:HH11	10:I:111:ARG:HG3	1.84	0.42
10:I:5:TYR:C	10:I:84:ALA:HB2	2.39	0.42
13:L:46:LYS:CG	13:L:47:LYS:H	2.15	0.42
14:M:26:GLY:C	14:M:28:ALA:N	2.73	0.42
15:N:34:TYR:O	15:N:35:ARG:C	2.57	0.42
16:O:29:VAL:HG11	16:O:67:LEU:HD21	2.00	0.42
19:R:21:LYS:HG3	19:R:57:GLY:CA	2.48	0.42
20:S:16:LEU:HA	20:S:19:VAL:HG12	2.00	0.42
1:A:1058:G:C6	1:A:1059:C:N3	2.87	0.42
1:A:1305:G:N2	1:A:1331:G:HO2'	2.16	0.42
1:A:1347:G:HO2'	1:A:1348:U:P	2.37	0.42
1:A:542:G:O2'	1:A:543:C:H5'	2.18	0.42
1:A:585:G:C6	1:A:586:C:C4	3.07	0.42
1:A:636:U:H2'	1:A:637:G:C8	2.54	0.42
1:A:986:A:H1'	20:S:54:GLY:O	2.18	0.42
4:C:167:TRP:HB3	4:C:168:ALA:H	1.43	0.42
6:E:111:GLU:C	6:E:113:ALA:N	2.73	0.42
6:E:32:VAL:HB	6:E:58:ALA:HB1	2.01	0.42
8:G:115:ARG:O	8:G:118:VAL:HB	2.20	0.42
8:G:104:LEU:HD23	8:G:134:ALA:HB1	2.01	0.42
8:G:151:TYR:N	8:G:151:TYR:CD1	2.87	0.42
8:G:152:ALA:C	8:G:154:TYR:H	2.23	0.42
10:I:92:TYR:O	10:I:93:ARG:C	2.57	0.42
12:K:115:PRO:C	12:K:117:ASN:H	2.21	0.42
19:R:29:PHE:CE1	19:R:31:LEU:HD21	2.54	0.42
21:T:89:ARG:HH21	21:T:104:LEU:HB3	1.84	0.42
1:A:1324:A:O4'	1:A:1361(A):C:H4'	2.19	0.42
1:A:1474:G:O2'	1:A:1475:G:H5'	2.19	0.42
1:A:328:C:C2'	1:A:328:C:O2	2.56	0.42
1:A:384:G:O2'	1:A:385:C:H5'	2.19	0.42
1:A:390:C:O5'	1:A:390:C:H6	2.03	0.42
1:A:41:G:O2'	1:A:42:G:H5'	2.20	0.42
1:A:502:G:C1'	1:A:550:G:H5'	2.49	0.42
1:A:642:A:N7	9:H:115:SER:HA	2.34	0.42
1:A:644:G:C6	1:A:645:C:C5	3.07	0.42
1:A:694:A:N1	1:A:787:A:O2'	2.50	0.42
1:A:778:G:O2'	1:A:779:C:H5'	2.18	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:794:A:C6	1:A:795:C:C4	3.07	0.42
1:A:914:A:O2'	1:A:915:A:H5'	2.19	0.42
1:A:994:A:H8	1:A:994:A:OP1	2.02	0.42
4:C:34:LEU:CD2	4:C:38:ARG:HG2	2.49	0.42
5:D:98:GLU:CG	5:D:189:PRO:HG3	2.47	0.42
5:D:7:PRO:HG2	5:D:10:ARG:CD	2.49	0.42
10:I:127:LYS:HB2	14:M:126:LYS:NZ	2.34	0.42
11:J:80:LYS:HD3	11:J:83:GLU:HB3	2.01	0.42
12:K:98:LEU:O	12:K:99:GLN:C	2.57	0.42
13:L:43:VAL:CG1	13:L:44:THR:N	2.82	0.42
16:O:81:LEU:CD2	16:O:85:LEU:HD12	2.48	0.42
19:R:66:LEU:HG	19:R:70:ILE:CD1	2.50	0.42
1:A:1136:U:O5'	1:A:1136:U:H6	2.03	0.42
1:A:1256:A:H2	1:A:1258:G:N1	2.17	0.42
1:A:1300:G:C2'	1:A:1301:U:OP2	2.67	0.42
1:A:1376:U:H2'	1:A:1377:A:C8	2.55	0.42
1:A:1397:C:HO2'	1:A:1398:A:P	2.42	0.42
1:A:281:G:O2'	1:A:282:A:P	2.77	0.42
1:A:392:G:H2'	1:A:393:A:H8	1.85	0.42
1:A:436:C:H2'	1:A:437:U:H6	1.84	0.42
1:A:437:U:H2'	1:A:438:G:C5'	2.50	0.42
1:A:482:A:C2	1:A:483:C:H1'	2.54	0.42
1:A:658:G:O2'	1:A:659:U:H5'	2.19	0.42
1:A:913:A:O2'	1:A:914:A:O4'	2.31	0.42
1:A:959:A:C3'	1:A:960:U:H5''	2.45	0.42
3:B:13:ALA:C	3:B:15:VAL:N	2.72	0.42
3:B:145:LEU:HD22	3:B:149:LEU:HD12	2.01	0.42
3:B:168:THR:HG1	3:B:192:SER:HB3	1.77	0.42
3:B:19:HIS:O	3:B:20:GLU:O	2.37	0.42
3:B:76:GLN:OE1	3:B:76:GLN:HA	2.18	0.42
10:I:79:LEU:CD1	10:I:83:ARG:HD2	2.50	0.42
11:J:60:ARG:CD	11:J:60:ARG:N	2.73	0.42
1:A:954:G:C5'	14:M:120:LYS:HD3	2.49	0.42
14:M:52:GLU:HA	14:M:55:ARG:HE	1.83	0.42
11:J:63:PHE:CE1	15:N:45:ARG:HG3	2.54	0.42
1:A:275:G:H5'	18:Q:14:LYS:HB3	2.01	0.42
19:R:42:ARG:HH11	19:R:42:ARG:CB	2.23	0.42
1:A:1055:A:C2	1:A:1056:U:H1'	2.54	0.42
1:A:1253:G:H2'	1:A:1254:C:C6	2.54	0.42
1:A:131:C:H2'	1:A:132:C:C6	2.54	0.42
1:A:243:A:C2	1:A:245:C:C2	3.07	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:C:O2'	1:A:278:G:H5'	2.20	0.42
1:A:327:A:HO2'	1:A:328:C:H6	1.62	0.42
1:A:515:G:C5	1:A:516:U:C5	3.07	0.42
1:A:533:A:O2'	1:A:534:U:OP1	2.33	0.42
1:A:582:U:O4'	18:Q:105:ALA:HA	2.20	0.42
1:A:781:A:C2	1:A:1514:C:H4'	2.55	0.42
1:A:902:G:O2'	1:A:903:G:H5'	2.19	0.42
3:B:167:PRO:HG3	3:B:188:ALA:HB2	2.00	0.42
3:B:69:LEU:C	3:B:69:LEU:HD23	2.40	0.42
3:B:130:ARG:HH22	4:C:207:VAL:HG23	1.84	0.42
5:D:115:ARG:O	5:D:118:ARG:HB3	2.20	0.42
7:F:15:ASP:H	7:F:18:GLN:NE2	2.17	0.42
8:G:121:ALA:O	8:G:124:LEU:HB2	2.19	0.42
10:I:93:ARG:NH1	10:I:97:LYS:NZ	2.67	0.42
1:A:538:G:P	13:L:115:LYS:HG3	2.60	0.42
13:L:50:SER:O	13:L:51:ALA:CB	2.68	0.42
1:A:751:U:H4'	16:O:24:SER:HA	2.01	0.42
1:A:449:C:O2	17:P:42:ARG:HD2	2.19	0.42
1:A:1131:G:HO2'	1:A:1132:C:H6	1.67	0.42
1:A:1253:G:C2	1:A:1254:C:C2	3.07	0.42
1:A:930:C:H2'	1:A:931:C:C5'	2.50	0.42
3:B:80:ILE:HD13	3:B:212:GLN:N	2.34	0.42
4:C:204:LEU:O	4:C:205:GLY:C	2.57	0.42
4:C:39:ILE:CD1	4:C:57:ILE:HD13	2.49	0.42
5:D:24:GLU:HG2	5:D:25:ARG:H	1.83	0.42
8:G:31:MET:HB2	8:G:39:ALA:HB2	2.02	0.42
9:H:6:ILE:HD12	9:H:35:ILE:CD1	2.48	0.42
11:J:9:ARG:HB2	11:J:9:ARG:HH11	1.83	0.42
13:L:59:ARG:HD3	13:L:65:GLU:OE2	2.19	0.42
9:H:91:ARG:CG	13:L:7:ILE:HG13	2.45	0.42
14:M:6:GLY:O	14:M:7:VAL:CG2	2.68	0.42
18:Q:76:LEU:HD23	18:Q:77:VAL:C	2.40	0.42
21:T:11:SER:C	21:T:13:LEU:N	2.71	0.42
1:A:1049:U:O2'	1:A:1050:G:OP2	2.30	0.42
1:A:1191:A:H2'	1:A:1192:C:H6	1.83	0.42
1:A:1227:A:C2'	1:A:1228:C:O5'	2.67	0.42
1:A:1262:C:H42	1:A:1273:G:H1	1.66	0.42
1:A:1449:C:H2'	1:A:1450:U:C6	2.55	0.42
1:A:1490:C:H2'	1:A:1491:G:O4'	2.20	0.42
1:A:186:C:H2'	1:A:187:C:C6	2.55	0.42
1:A:184:G:O4'	1:A:224:C:H4'	2.19	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:A:H4'	1:A:330:C:OP1	2.20	0.42
1:A:338:A:H2'	1:A:339:C:C6	2.55	0.42
1:A:446:G:C2'	1:A:447:G:H5'	2.50	0.42
1:A:499:A:H4'	1:A:500:G:OP1	2.19	0.42
1:A:796:C:H6	1:A:796:C:O5'	2.03	0.42
1:A:803:G:H2'	1:A:804:U:C6	2.55	0.42
3:B:101:MET:CA	3:B:108:ILE:HD12	2.50	0.42
3:B:125:PRO:C	3:B:127:ILE:H	2.23	0.42
3:B:138:LEU:O	3:B:139:LYS:C	2.58	0.42
3:B:69:LEU:C	3:B:69:LEU:CD2	2.88	0.42
4:C:107:GLN:H	4:C:107:GLN:NE2	2.17	0.42
5:D:23:GLY:HA3	5:D:112:VAL:CG1	2.45	0.42
7:F:1:MET:HE3	7:F:66:GLU:HG2	2.02	0.42
12:K:33:THR:OG1	12:K:37:GLY:C	2.58	0.42
13:L:10:LEU:HD23	13:L:10:LEU:HA	1.79	0.42
13:L:5:PRO:HA	13:L:9:GLN:OE1	2.20	0.42
14:M:23:TYR:HB2	14:M:67:GLU:OE2	2.20	0.42
17:P:20:VAL:HG13	17:P:32:TYR:HB2	1.99	0.42
17:P:43:LYS:N	17:P:43:LYS:HD2	2.35	0.42
1:A:761:G:O2'	18:Q:104:LYS:HA	2.20	0.42
18:Q:68:ARG:NH1	18:Q:68:ARG:CG	2.79	0.42
22:V:10:ARG:O	22:V:11:GLY:C	2.57	0.42
1:A:1339:A:H2'	1:A:1340:A:O4'	2.20	0.42
1:A:1347:G:C5	10:I:107:ARG:NH1	2.87	0.42
1:A:1509:C:C2'	1:A:1510:U:H5'	2.49	0.42
25:A:1632:PCY:H17	25:A:1632:PCY:H24	1.89	0.42
1:A:301:G:H2'	1:A:302:G:H8	1.85	0.42
1:A:436:C:H2'	1:A:437:U:C6	2.55	0.42
1:A:502:G:H1'	1:A:550:G:H5'	2.00	0.42
1:A:781:A:H2	1:A:1514:C:O4'	2.02	0.42
4:C:22:TRP:O	4:C:22:TRP:CE3	2.71	0.42
4:C:3:ASN:H	4:C:3:ASN:ND2	2.17	0.42
5:D:170:VAL:O	5:D:171:GLY:C	2.58	0.42
5:D:194:LEU:CD2	5:D:194:LEU:N	2.83	0.42
5:D:53:ASP:O	5:D:57:ARG:HD3	2.19	0.42
6:E:11:ILE:HG22	6:E:12:LEU:N	2.34	0.42
10:I:5:TYR:CG	10:I:6:GLY:N	2.88	0.42
11:J:46:ARG:HH11	11:J:64:GLU:HB3	1.84	0.42
13:L:7:ILE:O	13:L:8:ASN:C	2.57	0.42
17:P:49:LEU:HG	17:P:49:LEU:O	2.19	0.42
18:Q:53:LEU:HD12	18:Q:53:LEU:HA	1.88	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:30:LEU:C	20:S:31:ILE:HD13	2.39	0.42
21:T:51:GLU:HA	21:T:54:LYS:HB2	2.02	0.42
1:A:1004:A:C8	1:A:1037:C:O2	2.73	0.42
1:A:260:G:H2'	1:A:261:U:C6	2.55	0.42
1:A:51:A:H4'	1:A:52:G:C5'	2.49	0.42
1:A:642:A:C8	9:H:115:SER:HA	2.55	0.42
1:A:968:A:H8	1:A:968:A:OP1	2.02	0.42
4:C:26:LYS:CD	4:C:26:LYS:N	2.71	0.42
4:C:70:VAL:HG21	4:C:76:VAL:HG21	2.01	0.42
1:A:620:C:C2	5:D:135:LEU:HD13	2.54	0.42
6:E:37:ARG:HA	6:E:114:GLY:CA	2.50	0.42
6:E:30:ALA:O	6:E:45:PHE:HA	2.20	0.42
7:F:97:PHE:C	7:F:97:PHE:CD2	2.93	0.42
10:I:64:THR:HG22	10:I:65:VAL:N	2.34	0.42
11:J:6:ILE:HG23	11:J:98:ILE:HG12	2.02	0.42
12:K:40:ILE:HG23	12:K:75:TYR:CE2	2.55	0.42
13:L:32:PHE:HE1	13:L:86:ARG:HB2	1.84	0.42
16:O:39:LEU:CD2	16:O:56:LEU:HB2	2.50	0.42
21:T:100:ILE:O	21:T:102:GLY:N	2.53	0.42
21:T:25:ARG:O	21:T:29:LYS:HG3	2.18	0.42
1:A:1005:A:H2'	1:A:1006:C:C5'	2.50	0.42
1:A:1085:U:H3'	1:A:1086:U:H5	1.85	0.42
1:A:1124:G:C8	1:A:1145:C:C5	3.08	0.42
1:A:1255:G:H2'	1:A:1279:A:H62	1.83	0.42
1:A:1256:A:H2	1:A:1258:G:C2	2.38	0.42
1:A:12:U:H4'	1:A:526:C:H4'	2.02	0.42
1:A:1417:G:O2'	1:A:1483:A:N6	2.53	0.42
1:A:1521:G:H2'	1:A:1522:U:H6	1.83	0.42
1:A:301:G:H2'	1:A:302:G:C8	2.55	0.42
1:A:373:A:C4	1:A:482:A:N7	2.88	0.42
1:A:918:A:H2'	1:A:919:A:O4'	2.19	0.42
3:B:25:ASN:O	3:B:27:LYS:N	2.53	0.42
4:C:180:ALA:HB1	4:C:203:PHE:CE1	2.55	0.42
5:D:50:ARG:C	5:D:50:ARG:HD2	2.41	0.42
6:E:102:ALA:CA	6:E:120:THR:HG21	2.49	0.42
7:F:69:GLU:C	7:F:71:ARG:H	2.24	0.42
8:G:77:SER:O	8:G:156:TRP:HH2	2.03	0.42
10:I:7:THR:HG22	10:I:8:GLY:N	2.35	0.42
10:I:99:LEU:HD22	10:I:99:LEU:N	2.35	0.42
14:M:105:THR:O	14:M:106:ASN:C	2.57	0.42
17:P:51:VAL:CG1	17:P:51:VAL:O	2.68	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:T:18:GLN:O	21:T:19:SER:C	2.58	0.42
21:T:53:LEU:O	21:T:57:ARG:CD	2.66	0.42
1:A:1151:A:HO2'	1:A:1152:A:P	2.43	0.41
1:A:1046:A:H61	1:A:1213:A:H61	1.67	0.41
1:A:1405:G:O4'	1:A:1519:A:H4'	2.20	0.41
1:A:1497:G:H1'	1:A:1518:A:C2	2.55	0.41
1:A:356:A:H1'	1:A:368:U:O2'	2.20	0.41
1:A:392:G:H2'	1:A:393:A:C8	2.54	0.41
1:A:56:U:O2'	1:A:57:G:H5'	2.19	0.41
1:A:803:G:H2'	1:A:804:U:H6	1.84	0.41
1:A:994:A:C8	1:A:994:A:OP1	2.72	0.41
1:A:1104:G:OP1	3:B:111:ARG:HD2	2.20	0.41
3:B:124:SER:O	3:B:127:ILE:CG1	2.66	0.41
3:B:118:LEU:CD1	3:B:141:GLU:HB3	2.50	0.41
3:B:17:PHE:N	3:B:44:LEU:HD21	2.35	0.41
4:C:12:LEU:HA	4:C:12:LEU:HD23	1.74	0.41
5:D:127:THR:CB	5:D:147:ALA:HB3	2.48	0.41
6:E:13:ILE:HG22	6:E:30:ALA:CA	2.45	0.41
12:K:99:GLN:HG2	12:K:105:VAL:HG21	2.01	0.41
13:L:113:ARG:HB2	13:L:122:THR:HG21	2.00	0.41
14:M:94:ARG:HA	14:M:94:ARG:HD3	1.85	0.41
16:O:34:LEU:HD23	16:O:34:LEU:C	2.41	0.41
16:O:39:LEU:HD22	16:O:56:LEU:HD13	2.01	0.41
16:O:85:LEU:HD23	16:O:85:LEU:HA	1.73	0.41
1:A:463:A:C4'	17:P:82:GLN:HE21	2.32	0.41
7:F:100:ASN:ND2	19:R:23:LYS:HG2	2.29	0.41
21:T:57:ARG:CG	21:T:57:ARG:NH1	2.82	0.41
21:T:60:GLU:O	21:T:63:ILE:HB	2.20	0.41
1:A:1060:C:H4'	11:J:52:GLY:N	2.35	0.41
25:A:1632:PCY:H342	2:X:2:U:C5'	2.50	0.41
1:A:200:G:H2'	1:A:201:C:O4'	2.20	0.41
1:A:359:U:O2'	1:A:360:A:H5'	2.20	0.41
1:A:370:C:C2'	1:A:371:G:H5'	2.50	0.41
1:A:374:A:C6	1:A:375:U:C4	3.07	0.41
1:A:652:U:H2'	1:A:752:G:N1	2.35	0.41
3:B:75:LYS:O	3:B:75:LYS:HD3	2.19	0.41
4:C:172:ARG:NH1	4:C:174:PRO:HG3	2.35	0.41
4:C:47:LEU:CD1	4:C:47:LEU:H	2.33	0.41
5:D:56:VAL:HG12	5:D:202:LEU:HD13	2.03	0.41
6:E:144:THR:HG22	6:E:145:LYS:N	2.35	0.41
7:F:4:TYR:OH	7:F:72:VAL:HG21	2.20	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:60:ARG:NH1	9:H:60:ARG:CG	2.78	0.41
10:I:17:VAL:HG11	10:I:81:ILE:CA	2.50	0.41
12:K:109:VAL:HG13	19:R:85:LEU:O	2.19	0.41
13:L:69:TYR:CE2	13:L:71:PRO:HA	2.53	0.41
1:A:264:U:O2'	18:Q:64:PRO:HB2	2.21	0.41
18:Q:66:SER:HB3	18:Q:69:LYS:HB3	2.02	0.41
19:R:85:LEU:HD12	19:R:86:VAL:H	1.85	0.41
1:A:1178:G:P	10:I:97:LYS:NZ	2.93	0.41
1:A:1346:A:C8	8:G:10:ARG:NH2	2.89	0.41
1:A:22:G:H2'	1:A:23:C:C6	2.55	0.41
1:A:267:C:H2'	1:A:268:C:C6	2.47	0.41
1:A:300:A:H2'	1:A:301:G:H5'	2.02	0.41
1:A:401:C:H2'	1:A:402:G:C8	2.54	0.41
1:A:696:A:H1'	1:A:786:G:O2'	2.19	0.41
3:B:164:VAL:O	3:B:186:ALA:HA	2.21	0.41
3:B:19:HIS:CD2	3:B:20:GLU:HG2	2.55	0.41
4:C:83:ARG:O	4:C:86:VAL:N	2.53	0.41
6:E:102:ALA:HA	6:E:120:THR:HG21	2.01	0.41
7:F:101:ALA:HB2	19:R:28:GLU:HA	2.01	0.41
7:F:78:GLU:HA	7:F:81:ILE:HD12	2.02	0.41
8:G:112:PRO:HD2	8:G:113:GLU:OE2	2.20	0.41
8:G:124:LEU:O	8:G:127:ALA:HB3	2.20	0.41
9:H:104:ARG:HG3	9:H:138:TRP:CG	2.55	0.41
12:K:100:ALA:O	12:K:101:SER:C	2.59	0.41
13:L:11:VAL:HG13	18:Q:29:HIS:CD2	2.54	0.41
13:L:79:GLU:O	13:L:80:HIS:CG	2.73	0.41
16:O:70:LEU:HD12	16:O:78:TYR:CB	2.50	0.41
17:P:20:VAL:HG12	17:P:21:VAL:O	2.19	0.41
18:Q:60:ILE:HB	18:Q:74:LEU:HB2	2.02	0.41
19:R:40:LEU:C	19:R:42:ARG:N	2.74	0.41
20:S:51:VAL:O	20:S:57:HIS:HA	2.20	0.41
1:A:1125:U:H5''	1:A:1126:U:H5	1.85	0.41
1:A:1341:U:H6	1:A:1341:U:O5'	2.03	0.41
1:A:1366:C:C6	1:A:1367:C:H5	2.38	0.41
1:A:1460:A:H2'	1:A:1461:G:O4'	2.20	0.41
1:A:240:C:O2'	1:A:241:C:H5'	2.20	0.41
1:A:496:A:H4'	1:A:497:A:OP1	2.20	0.41
1:A:766:A:C8	1:A:814:A:C6	3.08	0.41
1:A:960:U:O2	1:A:960:U:H2'	2.18	0.41
1:A:971:G:OP1	1:A:972:C:H5''	2.20	0.41
3:B:108:ILE:O	3:B:108:ILE:CG2	2.65	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:59:GLU:O	3:B:62:ALA:HB3	2.20	0.41
4:C:91:LEU:HD23	4:C:92:ALA:CA	2.49	0.41
5:D:4:TYR:O	5:D:5:ILE:HB	2.21	0.41
8:G:125:MET:O	8:G:128:ALA:N	2.53	0.41
1:A:1251:A:H4'	10:I:12:GLU:CD	2.40	0.41
11:J:44:VAL:HG21	11:J:66:ARG:HH21	1.85	0.41
12:K:66:LEU:O	12:K:69:ALA:N	2.54	0.41
14:M:122:LYS:O	14:M:123:ALA:CB	2.67	0.41
14:M:19:LEU:HD21	14:M:56:LEU:CD2	2.50	0.41
19:R:47:THR:HG21	19:R:49:LYS:HE3	2.03	0.41
19:R:53:ARG:NH1	19:R:60:GLY:H	2.18	0.41
1:A:1138:G:C6	1:A:1140:C:H1'	2.55	0.41
1:A:1152:A:H2'	1:A:1153:C:H6	1.86	0.41
1:A:1307:U:H2'	1:A:1308:U:C6	2.56	0.41
1:A:1419:G:O2'	1:A:1420:C:H5'	2.21	0.41
1:A:1498:U:H4'	1:A:1519:A:H2	1.85	0.41
1:A:22:G:H2'	1:A:23:C:H6	1.85	0.41
1:A:50:A:N6	1:A:361:G:H4'	2.35	0.41
1:A:482:A:H2'	1:A:483:C:O4'	2.20	0.41
1:A:485:G:C2'	1:A:486:U:OP2	2.68	0.41
1:A:568:G:N2	1:A:883:C:C2	2.88	0.41
1:A:60:A:C2	1:A:107:G:N3	2.89	0.41
1:A:707:C:H2'	1:A:708:C:H6	1.85	0.41
1:A:792:A:C5	1:A:794:A:N6	2.89	0.41
1:A:80:G:C3'	1:A:81:U:C5'	2.89	0.41
1:A:948:C:O2'	1:A:949:A:H5'	2.20	0.41
3:B:236:TYR:O	3:B:236:TYR:CD2	2.73	0.41
4:C:99:VAL:HG23	4:C:100:ALA:N	2.36	0.41
6:E:41:VAL:O	6:E:67:VAL:N	2.50	0.41
9:H:100:ILE:HG23	9:H:112:LEU:HD11	2.02	0.41
10:I:65:VAL:HG12	10:I:65:VAL:O	2.21	0.41
11:J:72:VAL:HG12	11:J:73:ASP:N	2.34	0.41
1:A:1524:C:OP1	12:K:120:ARG:NH1	2.53	0.41
14:M:74:VAL:O	14:M:77:ASN:HB2	2.21	0.41
17:P:10:GLY:HA3	17:P:14:ASN:O	2.21	0.41
17:P:42:ARG:C	17:P:43:LYS:HD2	2.40	0.41
1:A:1030(A):G:H22	1:A:1030(C):G:H3'	1.82	0.41
1:A:1289:A:C2'	1:A:1290:G:H5'	2.50	0.41
1:A:1333:A:H2'	1:A:1334:G:C5'	2.51	0.41
1:A:1525:G:O2'	1:A:1526:G:H5'	2.19	0.41
1:A:242:C:H2'	1:A:243:A:H5'	2.02	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:C:H2'	1:A:490:G:C8	2.55	0.41
1:A:566:G:H4'	1:A:567:G:OP1	2.21	0.41
1:A:55:A:H2'	1:A:56:U:C6	2.55	0.41
1:A:803:G:C5	1:A:804:U:C5	3.09	0.41
1:A:823:G:O2'	1:A:824:C:H5'	2.20	0.41
4:C:25:GLY:CA	4:C:26:LYS:HE2	2.50	0.41
6:E:15:ARG:CZ	6:E:26:PHE:CE2	3.04	0.41
10:I:93:ARG:CZ	10:I:97:LYS:NZ	2.84	0.41
11:J:38:ILE:HG13	11:J:71:LEU:CB	2.46	0.41
11:J:38:ILE:HG13	11:J:72:VAL:N	2.26	0.41
12:K:57:THR:O	12:K:57:THR:HG23	2.20	0.41
18:Q:6:LEU:O	18:Q:58:GLU:HA	2.21	0.41
1:A:267:C:OP2	18:Q:67:LYS:HD2	2.21	0.41
20:S:42:PRO:HD2	20:S:43:GLU:OE2	2.20	0.41
1:A:1327:C:OP1	22:V:21:TYR:HD1	2.03	0.41
1:A:19:C:H2'	1:A:20:U:C6	2.52	0.41
1:A:229:U:C2'	1:A:230:G:H5'	2.51	0.41
1:A:299:G:C6	1:A:300:A:C2	3.09	0.41
1:A:418:C:H2'	1:A:419:C:C6	2.54	0.41
1:A:669:U:H2'	1:A:670:G:H8	1.84	0.41
1:A:742:G:C5'	16:O:58:MET:HE1	2.51	0.41
1:A:754:C:C3'	1:A:754:C:O2	2.68	0.41
3:B:189:ASP:HB3	3:B:203:GLY:O	2.20	0.41
6:E:79:GLU:C	6:E:80:ILE:CG2	2.89	0.41
6:E:90:VAL:HB	6:E:121:LYS:HB3	2.03	0.41
7:F:53:ALA:C	7:F:55:ASP:N	2.73	0.41
9:H:11:THR:O	9:H:12:ARG:C	2.58	0.41
9:H:121:ASP:HB2	9:H:125:ARG:NH2	2.28	0.41
12:K:50:TYR:CD1	12:K:60:ALA:HB2	2.56	0.41
12:K:69:ALA:O	12:K:72:ALA:HB3	2.20	0.41
13:L:60:LEU:HD11	13:L:85:ILE:CD1	2.34	0.41
14:M:123:ALA:O	14:M:124:PRO:C	2.59	0.41
16:O:70:LEU:HD12	16:O:78:TYR:CA	2.51	0.41
16:O:78:TYR:CZ	16:O:82:ILE:HD11	2.56	0.41
18:Q:67:LYS:HG2	18:Q:68:ARG:N	2.36	0.41
19:R:44:LEU:HA	19:R:49:LYS:O	2.20	0.41
20:S:22:LEU:CD1	20:S:28:LYS:HD2	2.50	0.41
1:A:1031:G:H2'	1:A:1032:G:C8	2.50	0.41
1:A:1164:G:C6	1:A:1173:G:C6	3.09	0.41
1:A:1213:A:N1	1:A:1215:G:H1'	2.36	0.41
1:A:1504:G:OP2	1:A:1504:G:H3'	2.20	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:A:H4'	1:A:413:G:H8	1.86	0.41
1:A:760:G:H2'	1:A:761:G:C5'	2.50	0.41
1:A:794:A:C5	1:A:795:C:C4	3.09	0.41
1:A:818:G:H3'	1:A:819:A:H5'	2.01	0.41
3:B:230:VAL:CG1	3:B:231:GLU:N	2.83	0.41
4:C:154:SER:OG	4:C:196:LEU:HA	2.21	0.41
4:C:34:LEU:HD23	4:C:38:ARG:HG2	2.02	0.41
5:D:15:GLU:C	5:D:17:VAL:N	2.74	0.41
8:G:15:ASP:HB3	8:G:19:GLY:H	1.85	0.41
8:G:6:ARG:O	8:G:7:ALA:C	2.59	0.41
9:H:55:GLY:C	9:H:56:LYS:HD2	2.41	0.41
9:H:63:LEU:N	9:H:63:LEU:CD1	2.83	0.41
18:Q:27:PHE:C	18:Q:27:PHE:CD1	2.94	0.41
19:R:21:LYS:C	19:R:23:LYS:H	2.24	0.41
1:A:187:C:N3	21:T:105:SER:HB3	2.35	0.41
1:A:1128:C:O2	1:A:1144:G:N2	2.54	0.41
1:A:115:G:O2'	1:A:116:A:OP2	2.35	0.41
1:A:1266:G:N2	1:A:1269:A:OP2	2.50	0.41
1:A:190(I):G:H2'	1:A:190(J):U:O4'	2.21	0.41
1:A:428:G:OP2	5:D:7:PRO:HG3	2.21	0.41
1:A:613:C:H2'	1:A:614:A:H8	1.85	0.41
1:A:913:A:O2'	1:A:914:A:OP2	2.38	0.41
1:A:979:C:C2'	1:A:980:C:H5'	2.51	0.41
3:B:70:PHE:O	3:B:92:TYR:HA	2.20	0.41
4:C:14:ILE:O	4:C:15:THR:C	2.59	0.41
4:C:10:PHE:CZ	4:C:178:LEU:HD13	2.55	0.41
4:C:5:ILE:HD12	4:C:5:ILE:O	2.21	0.41
5:D:92:VAL:O	5:D:96:LEU:HD13	2.19	0.41
10:I:30:GLY:O	10:I:31:GLN:C	2.59	0.41
11:J:75:ILE:CG2	11:J:76:ASN:N	2.84	0.41
17:P:82:GLN:O	17:P:83:GLU:C	2.59	0.41
18:Q:33:GLY:O	18:Q:34:LYS:C	2.57	0.41
18:Q:17:LYS:HA	18:Q:46:ASP:O	2.20	0.41
1:A:1157:A:O4'	1:A:1158:C:C2	2.74	0.41
1:A:1227:A:OP1	20:S:80:TYR:OH	2.28	0.41
1:A:1464:G:O2'	1:A:1465:C:H5'	2.21	0.41
1:A:583:A:H2'	1:A:584:G:O4'	2.20	0.41
1:A:966:G:H2'	1:A:967:C:H6	1.86	0.41
3:B:137:ARG:CB	3:B:137:ARG:NH1	2.82	0.41
3:B:166:ASP:OD2	3:B:169:LYS:HB2	2.21	0.41
3:B:26:PRO:O	3:B:29:ALA:HB2	2.20	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:42:ILE:HD11	3:B:189:ASP:HB2	2.02	0.41
3:B:82:ARG:O	3:B:83:MET:C	2.59	0.41
5:D:162:LEU:HA	5:D:165:MET:HB2	2.03	0.41
5:D:57:ARG:NH2	5:D:205:GLU:OE2	2.54	0.41
6:E:15:ARG:HD2	6:E:15:ARG:O	2.20	0.41
6:E:69:VAL:HA	6:E:70:PRO:HD3	1.84	0.41
14:M:39:ILE:HG21	14:M:48:LEU:HD21	2.02	0.41
14:M:67:GLU:HB3	14:M:68:GLY:H	1.59	0.41
19:R:54:ARG:H	19:R:54:ARG:HG3	1.41	0.41
19:R:85:LEU:HD12	19:R:86:VAL:N	2.36	0.41
20:S:10:PHE:HE2	20:S:12:ASP:OD1	2.04	0.41
21:T:19:SER:OG	21:T:20:LEU:N	2.54	0.41
1:A:1001:A:C2	1:A:1041:A:C2	3.09	0.41
1:A:1190:G:C2'	1:A:1191:A:OP2	2.69	0.41
1:A:1436:U:O2'	1:A:1437:C:H5'	2.21	0.41
1:A:262:A:H4'	21:T:75:ASN:HD22	1.86	0.41
1:A:309:G:O2'	1:A:310:G:H5'	2.21	0.41
1:A:366:C:H1'	1:A:367:U:OP1	2.21	0.41
1:A:487:A:H2'	1:A:488:C:H6	1.86	0.41
1:A:501:C:O2'	1:A:502:G:H5'	2.21	0.41
1:A:941:G:O2'	1:A:942:G:H5'	2.21	0.41
1:A:1104:G:P	3:B:111:ARG:HD2	2.61	0.41
3:B:163:PHE:HA	3:B:185:ILE:HB	2.02	0.41
3:B:51:LEU:HD21	3:B:201:ILE:CG2	2.49	0.41
3:B:8:LYS:CD	3:B:9:GLU:N	2.84	0.41
4:C:23:TYR:CG	4:C:24:ALA:N	2.89	0.41
4:C:51:GLY:O	4:C:70:VAL:HA	2.21	0.41
5:D:209:ARG:NH1	5:D:209:ARG:HG2	2.36	0.41
8:G:31:MET:HB2	8:G:39:ALA:CB	2.51	0.41
12:K:17:GLY:O	12:K:80:VAL:HA	2.20	0.41
1:A:707:C:OP1	12:K:85:ARG:NH1	2.54	0.41
14:M:13:LYS:O	14:M:45:VAL:HG23	2.21	0.41
1:A:1329:A:C5'	14:M:29:ARG:HD2	2.51	0.41
14:M:8:GLU:C	14:M:9:ILE:HG13	2.41	0.41
16:O:32:LEU:HA	16:O:32:LEU:HD23	1.87	0.41
18:Q:48:GLU:C	18:Q:50:LYS:N	2.74	0.41
18:Q:95:TYR:CD1	18:Q:95:TYR:N	2.89	0.41
20:S:30:LEU:O	20:S:31:ILE:HD13	2.21	0.41
21:T:87:LYS:O	21:T:91:LEU:HD12	2.21	0.41
1:A:1053:G:C3'	1:A:1054:C:C5'	2.96	0.40
1:A:116:A:H2'	1:A:117:G:H8	1.86	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1171:G:O2'	1:A:1172:C:H5'	2.20	0.40
1:A:1049:U:H1'	1:A:1201:A:N7	2.36	0.40
1:A:32:A:H2'	1:A:33:A:C8	2.56	0.40
1:A:35:G:H2'	1:A:36:C:H6	1.80	0.40
1:A:55:A:O2'	1:A:56:U:H5'	2.21	0.40
1:A:837:G:H2'	1:A:838:G:C8	2.56	0.40
3:B:142:LEU:O	3:B:143:GLU:C	2.60	0.40
3:B:97:TRP:HH2	3:B:176:GLU:CD	2.23	0.40
4:C:48:TYR:C	4:C:50:ALA:H	2.25	0.40
6:E:115:VAL:HG11	6:E:118:ILE:HG12	2.02	0.40
6:E:12:LEU:HD22	6:E:13:ILE:N	2.36	0.40
6:E:122:GLU:HG2	6:E:131:ILE:HD12	2.02	0.40
7:F:30:LEU:C	7:F:35:ALA:HB3	2.41	0.40
11:J:45:ARG:HH22	15:N:36:PHE:HE2	1.58	0.40
13:L:26:ALA:C	13:L:27:LEU:O	2.60	0.40
13:L:79:GLU:O	13:L:80:HIS:ND1	2.54	0.40
1:A:1329:A:OP1	14:M:29:ARG:HG3	2.21	0.40
14:M:85:GLY:O	14:M:86:CYS:C	2.60	0.40
19:R:59:SER:O	19:R:60:GLY:C	2.59	0.40
19:R:61:LYS:O	19:R:64:ARG:HB3	2.21	0.40
21:T:46:GLU:H	21:T:46:GLU:HG3	1.60	0.40
1:A:1003(A):G:C6	1:A:1004:A:N3	2.89	0.40
1:A:1504:G:OP1	1:A:1507:A:H4'	2.22	0.40
1:A:275:G:C2	1:A:276:G:C8	3.10	0.40
1:A:663:A:H5''	19:R:61:LYS:HE3	2.03	0.40
1:A:864:A:H2	1:A:917:G:N3	2.20	0.40
3:B:46:LYS:C	3:B:48:MET:N	2.74	0.40
4:C:112:SER:HB2	4:C:115:LEU:CG	2.51	0.40
5:D:149:ALA:HB3	5:D:152:SER:HB2	2.03	0.40
5:D:163:GLU:C	5:D:165:MET:H	2.25	0.40
7:F:40:VAL:HG23	7:F:62:TRP:O	2.20	0.40
10:I:32:ASP:HB3	10:I:35:GLU:HB2	2.02	0.40
11:J:32:ALA:CB	11:J:75:ILE:O	2.69	0.40
12:K:20:TYR:HE2	12:K:85:ARG:NH2	2.19	0.40
12:K:32:ILE:HG22	12:K:77:MET:HE2	2.03	0.40
16:O:27:VAL:HG12	16:O:31:LEU:CD1	2.51	0.40
16:O:31:LEU:N	16:O:31:LEU:HD12	2.36	0.40
17:P:20:VAL:HG12	17:P:21:VAL:N	2.35	0.40
19:R:66:LEU:HG	19:R:70:ILE:HD11	2.02	0.40
20:S:22:LEU:HD13	20:S:28:LYS:CB	2.51	0.40
21:T:67:ALA:O	21:T:73:HIS:ND1	2.54	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:T:44:ALA:HB1	21:T:92:LEU:HG	2.02	0.40
1:A:1003:G:N1	1:A:1003(A):G:C6	2.89	0.40
1:A:112:G:C2'	1:A:113:G:H5'	2.50	0.40
1:A:1347:G:HO2'	1:A:1373:G:H1	1.69	0.40
1:A:1504:G:H3'	1:A:1504:G:P	2.61	0.40
1:A:297:G:N2	1:A:299:G:H3'	2.37	0.40
1:A:112:G:H21	1:A:354:G:C4'	2.34	0.40
1:A:58:C:O2'	1:A:59:A:H5'	2.22	0.40
1:A:638:G:O2'	1:A:639:G:H5'	2.21	0.40
1:A:695:A:H2'	1:A:696:A:C8	2.57	0.40
1:A:693:G:O6	1:A:788:U:H4'	2.21	0.40
1:A:792:A:H1'	1:A:794:A:N7	2.37	0.40
1:A:792:A:H4'	1:A:793:U:C5'	2.51	0.40
1:A:8:A:H5'	6:E:101:ILE:HG22	2.03	0.40
3:B:16:HIS:CD2	3:B:210:SER:HG	2.39	0.40
3:B:73:THR:CG2	3:B:169:LYS:HE3	2.51	0.40
3:B:85:ALA:O	3:B:88:ALA:O	2.39	0.40
4:C:126:ARG:O	4:C:127:ARG:HB2	2.22	0.40
4:C:157:ILE:CD1	4:C:166:GLU:HB2	2.51	0.40
4:C:85:ARG:O	4:C:85:ARG:HD2	2.21	0.40
8:G:144:MET:O	8:G:148:ASN:ND2	2.50	0.40
8:G:54:THR:HG21	8:G:56:GLN:NE2	2.36	0.40
9:H:86:ILE:HD12	9:H:133:LEU:HD22	2.04	0.40
10:I:17:VAL:HG21	10:I:80:GLY:HA3	2.03	0.40
12:K:67:ASP:OD1	12:K:71:LYS:HE3	2.21	0.40
13:L:68:ALA:HB1	13:L:100:ILE:HG13	2.03	0.40
13:L:85:ILE:HG23	13:L:98:TYR:CB	2.50	0.40
14:M:79:LYS:O	14:M:83:ASP:OD2	2.40	0.40
15:N:28:GLY:O	15:N:30:ALA:N	2.55	0.40
15:N:41:ARG:NH1	15:N:41:ARG:HG2	2.37	0.40
21:T:100:ILE:O	21:T:101:GLY:C	2.60	0.40
21:T:90:GLN:HA	21:T:93:GLU:HG2	2.03	0.40
22:V:6:ARG:CD	22:V:15:ARG:HH12	2.32	0.40
1:A:1023:G:H2'	1:A:1023:G:N3	2.37	0.40
1:A:1051:C:H2'	1:A:1052:U:H6	1.87	0.40
1:A:1197:G:O2'	1:A:1198:G:H5'	2.21	0.40
1:A:166:G:O2'	1:A:167:G:H5'	2.22	0.40
1:A:294:U:H2'	1:A:295:C:H6	1.84	0.40
1:A:334:C:O2'	1:A:335:C:H5'	2.19	0.40
1:A:640:A:C2'	1:A:641:U:H5'	2.51	0.40
1:A:781:A:H2	1:A:1514:C:H4'	1.86	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:55:VAL:O	6:E:58:ALA:HB3	2.21	0.40
9:H:114:THR:C	9:H:116:LYS:N	2.75	0.40
9:H:119:LEU:HD12	9:H:123:GLU:C	2.42	0.40
9:H:25:ASP:OD1	9:H:60:ARG:NE	2.53	0.40
10:I:120:ARG:O	10:I:122:ALA:N	2.54	0.40
12:K:86:GLY:H	12:K:112:THR:CG2	2.31	0.40
1:A:979:C:C2	15:N:19:ARG:HG2	2.56	0.40
17:P:55:ARG:O	17:P:58:TYR:HB3	2.21	0.40
18:Q:51:TYR:N	18:Q:51:TYR:CD1	2.88	0.40
19:R:21:LYS:C	19:R:23:LYS:N	2.73	0.40
21:T:92:LEU:HA	21:T:92:LEU:HD23	1.90	0.40
1:A:1090:U:O2'	1:A:1091:U:H5'	2.22	0.40
1:A:1097:C:H2'	1:A:1098:C:C6	2.56	0.40
1:A:1346:A:C4	1:A:1348:U:C4	3.09	0.40
1:A:136:C:H2'	1:A:137:C:C6	2.57	0.40
1:A:161:A:H2'	1:A:162:A:C8	2.57	0.40
1:A:322:C:O2'	1:A:323:U:H5'	2.21	0.40
1:A:355:C:C4	1:A:356:A:N7	2.90	0.40
1:A:437:U:H5''	5:D:155:LEU:CD2	2.47	0.40
1:A:529:G:H5'	1:A:533:A:C2	2.57	0.40
1:A:919:A:O2'	1:A:920:U:H5'	2.22	0.40
1:A:922:G:H2'	1:A:923:A:H8	1.81	0.40
3:B:78:GLN:O	3:B:94:ASN:OD1	2.40	0.40
4:C:40:ARG:NH1	4:C:40:ARG:HG3	2.36	0.40
4:C:18:TRP:O	4:C:54:ARG:NH2	2.54	0.40
5:D:9:CYS:SG	5:D:12:CYS:SG	3.19	0.40
8:G:113:GLU:HG3	8:G:118:VAL:HG12	2.04	0.40
8:G:123:GLU:OE1	8:G:134:ALA:HB2	2.22	0.40
8:G:95:ARG:HG2	8:G:99:LEU:CD1	2.52	0.40
9:H:68:ARG:HH11	9:H:68:ARG:HG2	1.86	0.40
1:A:1367:C:C5'	11:J:60:ARG:NH1	2.84	0.40
12:K:54:ARG:HG2	12:K:54:ARG:H	1.62	0.40
14:M:19:LEU:HD21	14:M:56:LEU:HD21	2.03	0.40
15:N:18:VAL:C	15:N:20:ALA:H	2.24	0.40
18:Q:48:GLU:O	18:Q:49:GLU:C	2.58	0.40
19:R:16:PRO:O	19:R:17:SER:CB	2.69	0.40
20:S:41:VAL:HG23	20:S:44:MET:HG3	2.03	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	B	232/256 (91%)	155 (67%)	49 (21%)	28 (12%)	0	4
4	C	204/239 (85%)	120 (59%)	52 (26%)	32 (16%)	0	2
5	D	206/209 (99%)	146 (71%)	41 (20%)	19 (9%)	1	8
6	E	148/162 (91%)	126 (85%)	18 (12%)	4 (3%)	6	37
7	F	99/101 (98%)	75 (76%)	18 (18%)	6 (6%)	2	17
8	G	153/156 (98%)	114 (74%)	24 (16%)	15 (10%)	1	7
9	H	136/138 (99%)	122 (90%)	10 (7%)	4 (3%)	5	36
10	I	125/128 (98%)	90 (72%)	28 (22%)	7 (6%)	2	19
11	J	96/105 (91%)	58 (60%)	20 (21%)	18 (19%)	0	1
12	K	117/129 (91%)	87 (74%)	16 (14%)	14 (12%)	0	4
13	L	122/135 (90%)	91 (75%)	19 (16%)	12 (10%)	1	7
14	M	123/126 (98%)	84 (68%)	23 (19%)	16 (13%)	0	3
15	N	58/61 (95%)	40 (69%)	10 (17%)	8 (14%)	0	3
16	O	86/89 (97%)	63 (73%)	20 (23%)	3 (4%)	4	32
17	P	86/88 (98%)	66 (77%)	17 (20%)	3 (4%)	4	32
18	Q	102/105 (97%)	84 (82%)	13 (13%)	5 (5%)	2	22
19	R	71/88 (81%)	51 (72%)	18 (25%)	2 (3%)	6	37
20	S	78/93 (84%)	52 (67%)	15 (19%)	11 (14%)	0	3
21	T	97/106 (92%)	61 (63%)	19 (20%)	17 (18%)	0	1
22	V	22/26 (85%)	17 (77%)	4 (18%)	1 (4%)	3	24
All	All	2361/2540 (93%)	1702 (72%)	434 (18%)	225 (10%)	1	7

All (225) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	8	LYS

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
3	B	9	GLU
3	B	15	VAL
3	B	16	HIS
3	B	17	PHE
3	B	20	GLU
3	B	21	ARG
3	B	24	TRP
3	B	123	ALA
3	B	124	SER
4	C	4	LYS
4	C	15	THR
4	C	16	ARG
4	C	26	LYS
4	C	29	TYR
4	C	47	LEU
4	C	61	ALA
4	C	77	ILE
4	C	101	LEU
4	C	171	GLY
4	C	179	ARG
5	D	4	TYR
5	D	29	PRO
5	D	36	ARG
5	D	110	PHE
6	E	16	THR
8	G	7	ALA
8	G	155	ARG
9	H	83	ILE
9	H	134	ILE
10	I	31	GLN
10	I	41	VAL
11	J	57	LYS
11	J	61	GLU
11	J	79	ARG
11	J	86	MET
12	K	35	PRO
12	K	89	ALA
12	K	101	SER
13	L	27	LEU
13	L	28	LYS
13	L	47	LYS
14	M	63	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
14	M	67	GLU
14	M	107	ALA
14	M	123	ALA
14	M	124	PRO
15	N	22	THR
17	P	49	LEU
17	P	83	GLU
18	Q	96	GLN
18	Q	98	LEU
18	Q	104	LYS
19	R	87	ARG
20	S	6	LYS
20	S	32	LYS
20	S	69	HIS
20	S	71	LEU
21	T	73	HIS
3	B	18	GLY
3	B	60	ASP
3	B	83	MET
3	B	89	GLY
4	C	49	SER
4	C	97	LYS
4	C	154	SER
4	C	168	ALA
4	C	172	ARG
4	C	181	ASN
4	C	189	ALA
4	C	205	GLY
5	D	16	GLY
5	D	32	ALA
5	D	88	VAL
5	D	92	VAL
6	E	153	LYS
7	F	26	ILE
8	G	5	ARG
8	G	42	ILE
8	G	89	MET
9	H	24	THR
9	H	91	ARG
10	I	94	ALA
10	I	101	PHE
11	J	30	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
11	J	34	VAL
11	J	54	PHE
11	J	56	HIS
11	J	72	VAL
12	K	27	ASN
12	K	126	ARG
12	K	127	LYS
12	K	128	ALA
13	L	51	ALA
13	L	73	GLU
13	L	79	GLU
13	L	91	LYS
13	L	116	SER
13	L	121	GLY
14	M	6	GLY
14	M	12	ASN
14	M	74	VAL
14	M	85	GLY
14	M	100	GLY
15	N	29	ARG
15	N	35	ARG
15	N	36	PHE
15	N	55	GLY
16	O	88	ARG
18	Q	80	GLY
20	S	45	VAL
20	S	68	GLY
21	T	11	SER
21	T	49	ALA
21	T	102	GLY
22	V	3	LYS
3	B	52	GLU
3	B	63	MET
3	B	165	VAL
3	B	209	ARG
4	C	39	ILE
4	C	146	ALA
5	D	30	LYS
5	D	31	CYS
5	D	69	GLY
5	D	131	ARG
5	D	153	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
6	E	107	ARG
11	J	13	HIS
11	J	32	ALA
11	J	36	GLY
11	J	59	SER
11	J	90	LEU
12	K	54	ARG
12	K	57	THR
12	K	124	LYS
13	L	48	PRO
14	M	27	LYS
14	M	80	ARG
14	M	86	CYS
15	N	12	ARG
15	N	13	THR
17	P	10	GLY
18	Q	69	LYS
19	R	20	ALA
21	T	48	LYS
21	T	50	GLU
21	T	74	LYS
21	T	99	LEU
3	B	126	GLU
3	B	135	GLN
3	B	204	ASN
3	B	213	LEU
4	C	167	TRP
4	C	174	PRO
4	C	177	THR
4	C	178	LEU
5	D	26	CYS
5	D	73	ARG
5	D	175	SER
5	D	179	GLU
7	F	16	GLN
7	F	70	ASP
8	G	14	PRO
8	G	41	ARG
8	G	78	ARG
8	G	86	GLN
8	G	112	PRO
8	G	146	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
8	G	149	ARG
10	I	56	LEU
10	I	111	ARG
11	J	28	ARG
11	J	40	LEU
11	J	51	ARG
12	K	99	GLN
13	L	126	LYS
14	M	73	GLU
14	M	99	ARG
15	N	23	ARG
16	O	16	ALA
20	S	9	VAL
20	S	17	GLU
21	T	9	ASN
21	T	98	PRO
3	B	26	PRO
3	B	95	GLN
3	B	125	PRO
4	C	76	VAL
4	C	108	ASN
4	C	127	ARG
4	C	130	VAL
5	D	5	ILE
5	D	9	CYS
7	F	27	GLN
8	G	59	LEU
8	G	122	HIS
12	K	13	GLN
12	K	50	TYR
12	K	102	GLY
16	O	78	TYR
20	S	31	ILE
21	T	60	GLU
21	T	95	ALA
21	T	96	GLY
3	B	127	ILE
3	B	207	ALA
4	C	27	LYS
4	C	62	ASP
7	F	54	LYS
8	G	104	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
11	J	39	PRO
21	T	12	ALA
21	T	94	ALA
10	I	65	VAL
20	S	8	GLY
7	F	37	VAL
13	L	87	GLY
3	B	211	ILE
6	E	52	PRO
21	T	33	ILE
4	C	14	ILE
14	M	4	ILE
21	T	101	GLY
20	S	67	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	B	202/220 (92%)	181 (90%)	21 (10%)	8	34
4	C	160/188 (85%)	136 (85%)	24 (15%)	3	18
5	D	180/181 (99%)	168 (93%)	12 (7%)	19	57
6	E	115/123 (94%)	102 (89%)	13 (11%)	7	29
7	F	90/90 (100%)	87 (97%)	3 (3%)	43	76
8	G	126/127 (99%)	119 (94%)	7 (6%)	25	62
9	H	119/119 (100%)	105 (88%)	14 (12%)	6	27
10	I	98/99 (99%)	86 (88%)	12 (12%)	6	26
11	J	87/92 (95%)	76 (87%)	11 (13%)	5	25
12	K	90/99 (91%)	85 (94%)	5 (6%)	25	62
13	L	104/111 (94%)	96 (92%)	8 (8%)	15	49
14	M	100/101 (99%)	93 (93%)	7 (7%)	18	55
15	N	49/50 (98%)	45 (92%)	4 (8%)	13	47

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	O	79/80 (99%)	77 (98%)	2 (2%)	53	81
17	P	74/74 (100%)	70 (95%)	4 (5%)	26	63
18	Q	96/97 (99%)	92 (96%)	4 (4%)	34	70
19	R	64/77 (83%)	57 (89%)	7 (11%)	7	32
20	S	71/80 (89%)	67 (94%)	4 (6%)	25	62
21	T	76/82 (93%)	68 (90%)	8 (10%)	8	34
22	V	19/21 (90%)	19 (100%)	0	100	100
All	All	1999/2111 (95%)	1829 (92%)	170 (8%)	12	45

All (170) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	8	LYS
3	B	10	LEU
3	B	12	GLU
3	B	17	PHE
3	B	23	ARG
3	B	24	TRP
3	B	25	ASN
3	B	87	ARG
3	B	96	ARG
3	B	97	TRP
3	B	108	ILE
3	B	114	ARG
3	B	139	LYS
3	B	144	ARG
3	B	163	PHE
3	B	164	VAL
3	B	170	GLU
3	B	178	ARG
3	B	184	VAL
3	B	204	ASN
3	B	231	GLU
4	C	3	ASN
4	C	21	ARG
4	C	26	LYS
4	C	37	GLN
4	C	52	LEU
4	C	56	ASP
4	C	64	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
4	C	70	VAL
4	C	82	GLU
4	C	90	GLU
4	C	91	LEU
4	C	99	VAL
4	C	102	ASN
4	C	107	GLN
4	C	139	GLN
4	C	164	ARG
4	C	165	THR
4	C	167	TRP
4	C	172	ARG
4	C	175	LEU
4	C	176	HIS
4	C	179	ARG
4	C	188	LEU
4	C	204	LEU
5	D	26	CYS
5	D	53	ASP
5	D	64	LEU
5	D	67	ILE
5	D	70	ILE
5	D	78	LEU
5	D	110	PHE
5	D	122	ARG
5	D	170	VAL
5	D	179	GLU
5	D	192	GLU
5	D	199	ASN
6	E	12	LEU
6	E	31	LEU
6	E	38	GLN
6	E	41	VAL
6	E	51	VAL
6	E	56	GLN
6	E	64	ARG
6	E	68	GLU
6	E	79	GLU
6	E	89	ILE
6	E	118	ILE
6	E	120	THR
6	E	150	ARG

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
7	F	69	GLU
7	F	86	ARG
7	F	97	PHE
8	G	8	GLU
8	G	11	GLN
8	G	12	LEU
8	G	24	THR
8	G	38	LEU
8	G	57	GLU
8	G	126	ASP
9	H	21	LYS
9	H	26	VAL
9	H	31	PHE
9	H	52	ASP
9	H	81	HIS
9	H	85	ARG
9	H	91	ARG
9	H	92	ARG
9	H	104	ARG
9	H	105	ARG
9	H	112	LEU
9	H	119	LEU
9	H	125	ARG
9	H	136	GLU
10	I	2	GLU
10	I	23	ASN
10	I	34	ASN
10	I	38	GLN
10	I	53	VAL
10	I	56	LEU
10	I	58	ARG
10	I	60	ASP
10	I	65	VAL
10	I	91	ASP
10	I	111	ARG
10	I	121	ARG
11	J	6	ILE
11	J	38	ILE
11	J	51	ARG
11	J	55	LYS
11	J	60	ARG
11	J	64	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
11	J	66	ARG
11	J	71	LEU
11	J	74	ILE
11	J	83	GLU
11	J	95	GLU
12	K	31	THR
12	K	34	ASP
12	K	35	PRO
12	K	54	ARG
12	K	84	VAL
13	L	17	LYS
13	L	44	THR
13	L	53	ARG
13	L	60	LEU
13	L	61	THR
13	L	98	TYR
13	L	113	ARG
13	L	126	LYS
14	M	9	ILE
14	M	44	ARG
14	M	70	LEU
14	M	81	LEU
14	M	110	ARG
14	M	124	PRO
14	M	125	ARG
15	N	17	LYS
15	N	41	ARG
15	N	44	LEU
15	N	49	HIS
16	O	6	GLU
16	O	83	GLU
17	P	32	TYR
17	P	53	VAL
17	P	62	VAL
17	P	76	GLN
18	Q	34	LYS
18	Q	38	ARG
18	Q	60	ILE
18	Q	96	GLN
19	R	36	ASN
19	R	37	VAL
19	R	38	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
19	R	42	ARG
19	R	54	ARG
19	R	55	ARG
19	R	65	ILE
20	S	12	ASP
20	S	15	LEU
20	S	30	LEU
20	S	77	THR
21	T	10	LEU
21	T	13	LEU
21	T	18	GLN
21	T	42	GLN
21	T	57	ARG
21	T	62	LEU
21	T	73	HIS
21	T	75	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
3	B	19	HIS
3	B	25	ASN
3	B	40	HIS
3	B	113	HIS
3	B	140	HIS
3	B	146	GLN
3	B	204	ASN
4	C	3	ASN
4	C	6	HIS
4	C	31	HIS
4	C	69	HIS
4	C	102	ASN
4	C	104	GLN
4	C	118	GLN
4	C	123	GLN
4	C	139	GLN
4	C	170	GLN
4	C	181	ASN
5	D	62	GLN
5	D	123	HIS
5	D	160	GLN
5	D	161	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
5	D	199	ASN
6	E	20	GLN
6	E	73	ASN
7	F	18	GLN
7	F	27	GLN
7	F	32	ASN
7	F	57	GLN
7	F	64	GLN
7	F	73	ASN
7	F	94	GLN
7	F	100	ASN
8	G	37	ASN
8	G	56	GLN
8	G	68	ASN
8	G	106	GLN
10	I	38	GLN
10	I	73	GLN
11	J	56	HIS
11	J	62	HIS
11	J	78	ASN
11	J	84	GLN
12	K	22	HIS
12	K	38	ASN
12	K	117	ASN
13	L	49	ASN
13	L	75	HIS
14	M	12	ASN
14	M	40	ASN
14	M	62	ASN
14	M	77	ASN
15	N	49	HIS
16	O	13	GLN
16	O	37	ASN
18	Q	16	GLN
19	R	36	ASN
20	S	53	ASN
20	S	56	GLN
21	T	16	HIS
21	T	42	GLN
21	T	75	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1506/1522 (98%)	220 (14%)	0
2	X	5/6 (83%)	1 (20%)	0
All	All	1511/1528 (98%)	221 (14%)	0

All (221) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	8	A
1	A	9	G
1	A	31	G
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	49	U
1	A	51	A
1	A	52	G
1	A	61	G
1	A	65	U
1	A	81	U
1	A	101	A
1	A	116	A
1	A	120	A
1	A	121	C
1	A	129(A)	G
1	A	130	A
1	A	131	C
1	A	182	U
1	A	190(D)	U
1	A	190(E)	U
1	A	195	A
1	A	197	A
1	A	198	G
1	A	202	U
1	A	203	U
1	A	204	U
1	A	216	G
1	A	231	G
1	A	244	U
1	A	247	G
1	A	251	G
1	A	252	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	266	G
1	A	267	C
1	A	280	C
1	A	282	A
1	A	289	G
1	A	328	C
1	A	329	A
1	A	330	C
1	A	332	G
1	A	344	A
1	A	345	C
1	A	352	C
1	A	353	A
1	A	354	G
1	A	367	U
1	A	373	A
1	A	397	A
1	A	398	C
1	A	406	G
1	A	412	A
1	A	413	G
1	A	421	U
1	A	428	G
1	A	429	U
1	A	439	A
1	A	452	A
1	A	460	A
1	A	461	C
1	A	462	G
1	A	481	G
1	A	482	A
1	A	484	G
1	A	485	G
1	A	497	A
1	A	498	U
1	A	509	A
1	A	510	A
1	A	511	C
1	A	518	C
1	A	519	C
1	A	527	G
1	A	532	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	533	A
1	A	534	U
1	A	547	A
1	A	559	A
1	A	560	U
1	A	561	U
1	A	562	C
1	A	572	A
1	A	573	A
1	A	575	G
1	A	576	G
1	A	577	G
1	A	653	A
1	A	665	A
1	A	687	A
1	A	688	G
1	A	695	A
1	A	702	A
1	A	703	G
1	A	718	G
1	A	721	G
1	A	723	U
1	A	731	G
1	A	749	C
1	A	755	G
1	A	777	A
1	A	781	A
1	A	792	A
1	A	793	U
1	A	813	U
1	A	815	A
1	A	817	C
1	A	819	A
1	A	828	A
1	A	839	U
1	A	840	C
1	A	841	U
1	A	858	G
1	A	874	G
1	A	902	G
1	A	914	A
1	A	926	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	927	G
1	A	934	C
1	A	935	A
1	A	945	G
1	A	960	U
1	A	961	U
1	A	966	G
1	A	969	A
1	A	971	G
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	991	U
1	A	992	U
1	A	993	G
1	A	994	A
1	A	1004	A
1	A	1005	A
1	A	1023	G
1	A	1026	G
1	A	1050	G
1	A	1053	G
1	A	1054	C
1	A	1065	U
1	A	1066	C
1	A	1068	G
1	A	1085	U
1	A	1086	U
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1102	A
1	A	1117	G
1	A	1124	G
1	A	1125	U
1	A	1126	U
1	A	1128	C
1	A	1129	C
1	A	1130	A
1	A	1131	G
1	A	1138	G

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	1139	G
1	A	1140	C
1	A	1146	A
1	A	1152	A
1	A	1157	A
1	A	1159	U
1	A	1160	G
1	A	1183	A
1	A	1184	G
1	A	1191	A
1	A	1196	U
1	A	1197	G
1	A	1201	A
1	A	1202	G
1	A	1211	U
1	A	1212	U
1	A	1215	G
1	A	1225	A
1	A	1226	C
1	A	1227	A
1	A	1257	U
1	A	1258	G
1	A	1278	U
1	A	1279	A
1	A	1280	A
1	A	1281	U
1	A	1282	C
1	A	1285	A
1	A	1286	A
1	A	1287	A
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1320	C
1	A	1332	A
1	A	1338	G
1	A	1347	G
1	A	1348	U
1	A	1363	A
1	A	1364	U
1	A	1379	G
1	A	1381	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	1394	A
1	A	1398	A
1	A	1442	G
1	A	1443	G
1	A	1446	A
1	A	1452	C
1	A	1499	A
1	A	1502	A
1	A	1503	A
1	A	1504	G
1	A	1505	G
1	A	1506	U
1	A	1517	G
1	A	1520	G
1	A	1529	G
1	A	1530	G
2	X	4	U

There are no RNA pucker outliers to report.

## 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 99 ligands modelled in this entry, 98 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
25	PCY	A	1632	-	37,42,42	7.63	37 (100%)	40,65,65	1.53	7 (17%)

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
25	PCY	A	1632	-	-	0/33/67/67	0/3/3/3

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	1632	PCY	C38-C32	2.29	1.56	1.49
25	A	1632	PCY	C15-C17	3.20	1.65	1.54
25	A	1632	PCY	C27-C23	3.53	1.59	1.50
25	A	1632	PCY	C17-C8	4.11	1.64	1.51
25	A	1632	PCY	C10-N4	4.67	1.62	1.46
25	A	1632	PCY	O12-C6	5.19	1.57	1.43
25	A	1632	PCY	C9-N4	5.31	1.64	1.46
25	A	1632	PCY	O26-C23	5.44	1.37	1.22
25	A	1632	PCY	O19-C15	5.60	1.53	1.44
25	A	1632	PCY	C11-C6	5.64	1.68	1.52
25	A	1632	PCY	O21-C18	5.64	1.55	1.45
25	A	1632	PCY	C35-C30	6.38	1.53	1.39
25	A	1632	PCY	C28-C32	6.39	1.61	1.49
25	A	1632	PCY	C13-C7	6.82	1.69	1.52
25	A	1632	PCY	O5-C1	7.17	1.36	1.23
25	A	1632	PCY	C8-N16	7.29	1.62	1.47
25	A	1632	PCY	C27-C31	7.39	1.54	1.41
25	A	1632	PCY	C24-C28	7.62	1.50	1.39
25	A	1632	PCY	C29-C25	8.10	1.54	1.38
25	A	1632	PCY	C1-N2	8.12	1.52	1.37
25	A	1632	PCY	C37-C31	8.13	1.54	1.39
25	A	1632	PCY	O14-C7	8.22	1.59	1.44
25	A	1632	PCY	O21-C23	8.42	1.53	1.33
25	A	1632	PCY	C22-N20	8.45	1.55	1.39
25	A	1632	PCY	C33-C28	8.64	1.53	1.39
25	A	1632	PCY	O39-C32	8.66	1.51	1.22
25	A	1632	PCY	C34-C30	8.74	1.68	1.51
25	A	1632	PCY	C40-C37	8.87	1.55	1.38
25	A	1632	PCY	C29-C33	8.88	1.55	1.38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	1632	PCY	C25-C22	9.08	1.54	1.39
25	A	1632	PCY	C3-C8	9.22	1.69	1.54
25	A	1632	PCY	O36-C31	9.25	1.55	1.36
25	A	1632	PCY	C40-C35	9.41	1.56	1.38
25	A	1632	PCY	C27-C30	9.51	1.53	1.40
25	A	1632	PCY	C24-C22	9.99	1.56	1.39
25	A	1632	PCY	C1-N4	10.67	1.54	1.36
25	A	1632	PCY	C17-N20	11.21	1.59	1.45

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	1632	PCY	C22-N20-C17	-5.14	112.19	123.18
25	A	1632	PCY	O5-C1-N4	-2.11	118.48	122.09
25	A	1632	PCY	C38-C32-C28	-2.06	115.03	119.27
25	A	1632	PCY	O39-C32-C28	2.41	124.84	119.72
25	A	1632	PCY	C3-N2-C1	3.01	132.93	124.50
25	A	1632	PCY	C18-O21-C23	3.12	123.03	116.52
25	A	1632	PCY	C31-C27-C30	3.42	122.01	118.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	A	1632	PCY	10	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	1506/1522 (98%)	1.16	210 (13%) 3 4	37, 70, 161, 199	0
2	X	6/6 (100%)	1.00	1 (16%) 2 2	62, 79, 117, 151	0
3	B	234/256 (91%)	0.23	14 (5%) 23 22	34, 87, 162, 199	0
4	C	206/239 (86%)	0.07	1 (0%) 90 88	41, 91, 153, 179	0
5	D	208/209 (99%)	0.28	12 (5%) 24 23	35, 71, 128, 191	0
6	E	150/162 (92%)	0.10	1 (0%) 87 85	34, 58, 111, 168	0
7	F	101/101 (100%)	0.46	6 (5%) 23 22	56, 95, 147, 167	0
8	G	155/156 (99%)	0.03	2 (1%) 77 73	47, 85, 147, 175	0
9	H	138/138 (100%)	0.05	2 (1%) 75 71	21, 52, 92, 139	0
10	I	127/128 (99%)	0.44	12 (9%) 9 10	37, 96, 140, 181	0
11	J	98/105 (93%)	0.67	12 (12%) 5 5	50, 119, 184, 199	0
12	K	119/129 (92%)	0.30	4 (3%) 46 41	41, 73, 137, 178	0
13	L	124/135 (91%)	0.34	5 (4%) 39 35	30, 72, 131, 180	0
14	M	125/126 (99%)	0.66	13 (10%) 7 7	56, 89, 153, 188	0
15	N	60/61 (98%)	0.45	3 (5%) 30 27	50, 86, 157, 170	0
16	O	88/89 (98%)	0.25	3 (3%) 46 41	38, 70, 136, 186	0
17	P	88/88 (100%)	0.28	2 (2%) 61 56	35, 63, 164, 198	0
18	Q	104/105 (99%)	0.62	6 (5%) 24 23	35, 62, 137, 199	0
19	R	73/88 (82%)	0.25	3 (4%) 38 34	43, 75, 154, 194	0
20	S	80/93 (86%)	1.65	24 (30%) 1 1	66, 110, 158, 199	0
21	T	99/106 (93%)	0.36	6 (6%) 22 21	44, 72, 133, 194	0
22	V	24/26 (92%)	0.58	2 (8%) 12 13	44, 79, 128, 149	0
All	All	3913/4068 (96%)	0.66	344 (8%) 11 11	21, 75, 155, 199	0

All (344) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
18	Q	105	ALA	15.8
20	S	3	ARG	15.2
18	Q	103	GLY	13.2
14	M	124	PRO	13.0
18	Q	102	GLY	10.7
18	Q	104	LYS	9.9
1	A	1129	C	8.7
14	M	125	ARG	8.4
21	T	103	GLY	7.6
20	S	4	SER	6.8
1	A	1036	G	6.5
1	A	1006	C	6.4
1	A	1005	A	6.2
14	M	123	ALA	6.0
1	A	1024	G	5.8
20	S	2	PRO	5.6
1	A	1023	G	5.6
12	K	89	ALA	5.5
21	T	104	LEU	5.5
1	A	1222	G	5.3
20	S	49	ILE	5.3
1	A	1037	C	5.1
20	S	77	THR	5.1
1	A	1144	G	4.9
1	A	1035	A	4.9
5	D	42	GLN	4.8
1	A	1017	G	4.8
1	A	1124	G	4.8
20	S	52	TYR	4.7
1	A	993	G	4.7
7	F	14	LEU	4.7
1	A	1220	G	4.6
14	M	7	VAL	4.6
14	M	126	LYS	4.6
5	D	23	GLY	4.5
20	S	27	GLU	4.4
1	A	1004	A	4.4
1	A	1029	C	4.4
1	A	1011	G	4.4
16	O	23	GLY	4.4
20	S	34	TRP	4.3
21	T	105	SER	4.3
1	A	1277	C	4.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
15	N	6	LEU	4.2
1	A	1022	G	4.2
1	A	1030(A)	G	4.2
1	A	1139	G	4.1
1	A	1025	U	4.1
20	S	37	ARG	4.1
5	D	22	LYS	4.1
20	S	35	SER	4.0
1	A	1221	G	4.0
1	A	978	A	4.0
1	A	1492	A	4.0
5	D	25	ARG	4.0
1	A	1018	C	4.0
1	A	266	G	4.0
10	I	7	THR	4.0
1	A	1441	G	3.9
1	A	160	A	3.9
22	V	6	ARG	3.9
5	D	2	GLY	3.8
1	A	1159	U	3.8
1	A	1123	A	3.8
1	A	1140	C	3.8
16	O	22	THR	3.8
1	A	1001	A	3.8
1	A	1032	G	3.8
5	D	41	GLY	3.8
1	A	1053	G	3.8
3	B	122	PHE	3.8
1	A	529	G	3.7
1	A	1171	G	3.7
18	Q	101	ARG	3.7
20	S	78	ARG	3.7
11	J	33	GLN	3.7
1	A	1200	C	3.7
1	A	1141	C	3.6
1	A	1030(B)	C	3.6
9	H	1	MET	3.6
3	B	16	HIS	3.6
1	A	1279	A	3.6
1	A	1026	G	3.6
1	A	1038	C	3.6
5	D	33	MET	3.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	1002	G	3.6
1	A	1033	G	3.5
1	A	1268	A	3.5
1	A	1034	G	3.5
1	A	1143	G	3.5
7	F	73	ASN	3.5
1	A	1318	A	3.5
1	A	1468	A	3.5
20	S	60	VAL	3.5
1	A	1467	G	3.5
1	A	373	A	3.5
1	A	1482	G	3.4
1	A	1014	A	3.4
5	D	35	ARG	3.4
20	S	19	VAL	3.4
1	A	81	U	3.4
1	A	1131	G	3.4
1	A	1215	G	3.4
1	A	1180	A	3.4
3	B	233	SER	3.4
1	A	990	C	3.4
1	A	1030	C	3.4
1	A	1042	G	3.4
10	I	102	LEU	3.3
1	A	494	G	3.3
1	A	343	U	3.3
3	B	238	LEU	3.3
1	A	388	G	3.3
1	A	426	G	3.3
1	A	1127	G	3.3
1	A	1031	G	3.3
1	A	1019	C	3.2
1	A	1313	U	3.2
1	A	1043	C	3.2
1	A	1361(A)	C	3.2
1	A	992	U	3.2
1	A	1283	G	3.2
14	M	106	ASN	3.2
20	S	47	HIS	3.2
12	K	129	SER	3.2
1	A	1027	C	3.1
18	Q	95	TYR	3.1

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
11	J	70	ARG	3.1
10	I	15	ALA	3.1
1	A	195	A	3.1
1	A	1030(D)	A	3.0
1	A	410	G	3.0
1	A	1419	G	3.0
1	A	1013	G	3.0
1	A	1010	G	3.0
1	A	429	U	3.0
10	I	19	LEU	3.0
1	A	251	G	3.0
8	G	2	ALA	2.9
15	N	18	VAL	2.9
1	A	1361	G	2.9
20	S	31	ILE	2.9
11	J	81	THR	2.9
17	P	83	GLU	2.9
2	X	1	C	2.9
12	K	42	TRP	2.9
1	A	548	G	2.9
1	A	481	G	2.9
13	L	35	GLY	2.9
20	S	28	LYS	2.9
1	A	161	A	2.9
1	A	438	G	2.9
17	P	88	ALA	2.9
11	J	72	VAL	2.8
10	I	70	LYS	2.8
1	A	1135	U	2.8
6	E	5	ASP	2.8
1	A	1015	A	2.8
1	A	1442	G	2.8
5	D	3	ARG	2.8
1	A	427	U	2.8
1	A	1237	C	2.8
11	J	71	LEU	2.8
1	A	666	G	2.8
3	B	190	THR	2.8
13	L	28	LYS	2.8
1	A	159	G	2.8
14	M	104	ARG	2.7
1	A	1417	G	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
20	S	44	MET	2.7
11	J	93	GLY	2.7
11	J	32	ALA	2.7
1	A	1433	A	2.7
1	A	255	G	2.7
1	A	984	C	2.7
1	A	1003	G	2.7
1	A	1334	G	2.7
1	A	1157	A	2.7
20	S	29	ARG	2.7
1	A	528	C	2.6
1	A	484	G	2.6
1	A	521	G	2.6
1	A	750	G	2.6
1	A	254	G	2.6
5	D	30	LYS	2.6
3	B	21	ARG	2.6
1	A	1147	C	2.6
15	N	60	SER	2.6
13	L	33	ARG	2.6
1	A	1175	G	2.6
1	A	1269	A	2.6
1	A	1028	C	2.6
1	A	1479	C	2.6
1	A	495	U	2.6
21	T	44	ALA	2.6
1	A	1282	C	2.6
1	A	1181	G	2.6
1	A	745	C	2.6
11	J	31	GLY	2.6
14	M	65	LYS	2.5
1	A	408	A	2.5
1	A	547	A	2.5
1	A	1473	A	2.5
1	A	1213	A	2.5
7	F	10	LEU	2.5
11	J	34	VAL	2.5
1	A	346	G	2.5
1	A	1304	G	2.5
14	M	48	LEU	2.5
1	A	1287	A	2.5
1	A	1493	A	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	B	40	HIS	2.5
20	S	62	ILE	2.5
1	A	181	G	2.5
1	A	1012	U	2.4
1	A	347	G	2.4
1	A	1089	G	2.4
1	A	691	G	2.4
3	B	42	ILE	2.4
1	A	1219	U	2.4
19	R	29	PHE	2.4
7	F	72	VAL	2.4
1	A	1278	U	2.4
1	A	158	G	2.4
14	M	8	GLU	2.4
1	A	840	C	2.4
1	A	1303	C	2.4
1	A	1416	G	2.4
1	A	999	C	2.4
21	T	52	ALA	2.3
1	A	1260	C	2.3
1	A	409	G	2.3
1	A	1223	C	2.3
1	A	1420	C	2.3
14	M	88	ARG	2.3
14	M	56	LEU	2.3
1	A	496	A	2.3
1	A	1046	A	2.3
1	A	1418	A	2.3
3	B	133	LYS	2.3
1	A	701	C	2.3
1	A	939	G	2.3
1	A	1474	G	2.3
1	A	1360	A	2.3
7	F	4	TYR	2.3
21	T	101	GLY	2.3
20	S	5	LEU	2.3
1	A	319	G	2.3
1	A	1182	G	2.3
1	A	1374	A	2.3
19	R	50	ILE	2.3
1	A	196	A	2.3
1	A	318	G	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	1134	G	2.3
8	G	50	ILE	2.3
10	I	97	LYS	2.3
1	A	1218	C	2.2
22	V	20	LYS	2.2
1	A	202	U	2.2
11	J	39	PRO	2.2
1	A	1179	A	2.2
1	A	841	U	2.2
1	A	501	C	2.2
1	A	704	A	2.2
1	A	1502	A	2.2
1	A	428	G	2.2
1	A	758	G	2.2
1	A	934	C	2.2
13	L	61	THR	2.2
1	A	1016	A	2.2
12	K	32	ILE	2.2
10	I	8	GLY	2.2
1	A	522	C	2.2
1	A	1007	C	2.2
1	A	1030(C)	G	2.2
20	S	48	THR	2.2
1	A	455	C	2.2
1	A	1021	G	2.2
1	A	1276	G	2.2
10	I	92	TYR	2.2
1	A	517	G	2.2
1	A	1047	G	2.2
3	B	108	ILE	2.2
1	A	1314	C	2.1
1	A	976	G	2.1
1	A	497	A	2.1
1	A	959	A	2.1
20	S	71	LEU	2.1
1	A	989	C	2.1
1	A	171	A	2.1
1	A	413	G	2.1
1	A	581	G	2.1
1	A	958	A	2.1
1	A	1132	C	2.1
10	I	4	TYR	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
7	F	90	VAL	2.1
1	A	752	G	2.1
1	A	1067	A	2.1
1	A	1130	A	2.1
1	A	1169	A	2.1
1	A	1469	G	2.1
1	A	1137	C	2.1
5	D	36	ARG	2.1
11	J	74	ILE	2.1
10	I	47	LEU	2.1
4	C	23	TYR	2.1
1	A	500	G	2.1
1	A	657	G	2.1
1	A	1516	G	2.1
1	A	979	C	2.1
1	A	1533	C	2.1
1	A	300	A	2.1
1	A	115	G	2.1
1	A	1300	G	2.1
1	A	1421	G	2.1
10	I	85	LEU	2.1
20	S	15	LEU	2.1
14	M	60	VAL	2.1
1	A	387	U	2.1
10	I	96	LEU	2.1
16	O	39	LEU	2.1
1	A	419	C	2.1
1	A	1255	G	2.1
1	A	1271	G	2.1
3	B	19	HIS	2.1
1	A	432	A	2.1
5	D	21	LEU	2.1
19	R	48	GLY	2.1
11	J	37	PRO	2.1
1	A	459	G	2.0
1	A	1312	G	2.0
13	L	110	VAL	2.0
1	A	816	A	2.0
1	A	769	G	2.0
20	S	26	GLY	2.0
3	B	206	ASP	2.0
1	A	1225	A	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	1349	A	2.0
3	B	235	SER	2.0
9	H	2	LEU	2.0
1	A	1238	A	2.0
3	B	99	GLY	2.0
1	A	1126	U	2.0
1	A	218	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
23	MG	A	1562	1/1	0.96	0.65	44.99	45,45,45,45	0
23	MG	A	1557	1/1	0.98	0.43	9.85	45,45,45,45	0
23	MG	A	1553	1/1	0.96	0.40	8.11	45,45,45,45	0
23	MG	A	1626	1/1	0.91	0.30	6.57	45,45,45,45	1
23	MG	A	1629	1/1	0.95	0.71	6.53	45,45,45,45	1
23	MG	A	1606	1/1	0.94	0.52	5.73	45,45,45,45	0
23	MG	A	1586	1/1	0.93	0.38	5.41	45,45,45,45	0
23	MG	A	1566	1/1	0.75	0.40	4.98	45,45,45,45	0
23	MG	A	1600	1/1	0.95	0.38	4.87	45,45,45,45	0
23	MG	A	1595	1/1	0.97	0.35	4.49	45,45,45,45	0
23	MG	A	1593	1/1	0.95	0.32	3.61	45,45,45,45	0
23	MG	A	1560	1/1	0.93	0.30	2.39	45,45,45,45	0
23	MG	A	1546	1/1	0.95	0.38	2.32	45,45,45,45	0
23	MG	A	1614	1/1	0.72	0.28	1.91	45,45,45,45	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
25	PCY	A	1632	40/40	0.91	0.34	1.43	28,28,28,28	0
23	MG	A	1619	1/1	0.71	0.23	1.29	45,45,45,45	1
23	MG	D	215	1/1	0.92	0.31	1.11	45,45,45,45	0
23	MG	A	211	1/1	0.91	0.33	1.10	45,45,45,45	0
23	MG	A	1579	1/1	0.97	0.28	0.46	45,45,45,45	0
23	MG	A	1588	1/1	0.95	0.29	0.32	45,45,45,45	0
23	MG	A	1607	1/1	0.94	0.29	-0.08	45,45,45,45	0
24	ZN	D	300	1/1	0.99	0.34	-0.23	53,53,53,53	0
24	ZN	N	190	1/1	1.00	0.22	-0.27	53,53,53,53	1
23	MG	A	1599	1/1	0.91	0.28	-0.54	45,45,45,45	0
23	MG	A	1577	1/1	0.96	0.25	-0.68	45,45,45,45	0
23	MG	A	1613	1/1	0.71	0.27	-0.81	45,45,45,45	1
23	MG	A	1604	1/1	0.90	0.21	-1.14	45,45,45,45	1
23	MG	A	1576	1/1	0.93	0.20	-1.21	45,45,45,45	0
23	MG	A	1611	1/1	0.84	0.20	-1.23	45,45,45,45	1
23	MG	A	1625	1/1	0.99	0.19	-1.24	45,45,45,45	1
23	MG	A	1620	1/1	0.88	0.19	-1.27	45,45,45,45	0
23	MG	A	1581	1/1	0.83	0.23	-1.29	45,45,45,45	1
23	MG	A	1601	1/1	0.93	0.17	-1.64	45,45,45,45	0
23	MG	A	1603	1/1	0.95	0.20	-1.83	45,45,45,45	0
23	MG	A	1575	1/1	0.89	0.13	-1.94	45,45,45,45	1
23	MG	A	1609	1/1	0.88	0.16	-2.49	45,45,45,45	0
23	MG	A	1605	1/1	0.83	0.11	-3.51	45,45,45,45	0
23	MG	A	1592	1/1	0.89	0.12	-6.39	45,45,45,45	0
23	MG	A	1627	1/1	0.99	0.39	-	45,45,45,45	1
23	MG	A	1612	1/1	0.89	0.31	-	45,45,45,45	0
23	MG	A	1621	1/1	0.95	0.57	-	45,45,45,45	1
23	MG	A	1584	1/1	0.98	0.47	-	45,45,45,45	0
23	MG	A	86	1/1	0.92	0.40	-	45,45,45,45	0
23	MG	A	1608	1/1	0.98	0.07	-	45,45,45,45	0
23	MG	A	1563	1/1	0.94	0.22	-	45,45,45,45	0
23	MG	A	1616	1/1	0.92	0.18	-	45,45,45,45	0
23	MG	A	1618	1/1	0.68	0.80	-	45,45,45,45	1
23	MG	A	1552	1/1	0.97	0.20	-	45,45,45,45	0
23	MG	A	1610	1/1	0.92	0.18	-	45,45,45,45	0
23	MG	A	1550	1/1	0.53	0.74	-	45,45,45,45	1
23	MG	A	1578	1/1	0.87	0.33	-	45,45,45,45	0
23	MG	A	1590	1/1	0.79	0.34	-	45,45,45,45	0
23	MG	A	1565	1/1	0.93	0.67	-	45,45,45,45	0
23	MG	A	1561	1/1	0.95	0.73	-	45,45,45,45	0
23	MG	A	1547	1/1	0.97	0.50	-	45,45,45,45	0
23	MG	A	1574	1/1	0.90	0.29	-	45,45,45,45	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
23	MG	A	1598	1/1	0.96	0.23	-	45,45,45,45	1
23	MG	A	1558	1/1	0.82	0.30	-	45,45,45,45	0
23	MG	A	1597	1/1	0.89	0.12	-	45,45,45,45	0
23	MG	A	1567	1/1	0.88	0.59	-	45,45,45,45	0
23	MG	A	1594	1/1	0.94	0.35	-	45,45,45,45	0
23	MG	A	1549	1/1	0.83	0.17	-	45,45,45,45	1
23	MG	A	1628	1/1	0.99	0.26	-	45,45,45,45	1
23	MG	A	1568	1/1	0.78	0.57	-	45,45,45,45	0
23	MG	A	71	1/1	0.86	0.47	-	45,45,45,45	0
23	MG	A	1596	1/1	0.93	0.40	-	45,45,45,45	1
23	MG	A	1623	1/1	0.87	0.43	-	45,45,45,45	1
23	MG	A	1569	1/1	0.95	1.06	-	45,45,45,45	1
23	MG	A	1571	1/1	0.91	0.24	-	45,45,45,45	0
23	MG	A	1624	1/1	0.95	0.50	-	45,45,45,45	1
23	MG	A	1572	1/1	0.96	0.61	-	45,45,45,45	0
23	MG	A	1622	1/1	0.97	0.51	-	45,45,45,45	1
23	MG	A	1591	1/1	0.90	0.51	-	45,45,45,45	0
23	MG	A	1573	1/1	0.97	0.47	-	45,45,45,45	0
23	MG	A	1570	1/1	0.90	0.31	-	45,45,45,45	1
23	MG	A	1617	1/1	0.97	0.40	-	45,45,45,45	1
23	MG	A	1582	1/1	0.92	0.32	-	45,45,45,45	1
23	MG	A	1585	1/1	0.77	0.42	-	45,45,45,45	1
23	MG	A	1564	1/1	0.77	0.22	-	45,45,45,45	0
23	MG	A	1551	1/1	0.93	0.36	-	45,45,45,45	0
23	MG	A	1631	1/1	0.99	0.55	-	45,45,45,45	1
23	MG	A	210	1/1	0.64	0.37	-	45,45,45,45	1
23	MG	A	1587	1/1	0.90	0.36	-	45,45,45,45	0
23	MG	A	214	1/1	0.90	0.16	-	45,45,45,45	0
23	MG	A	212	1/1	0.77	0.95	-	45,45,45,45	1
23	MG	A	1630	1/1	0.96	1.31	-	45,45,45,45	1
23	MG	A	1559	1/1	0.93	0.42	-	45,45,45,45	0
23	MG	A	87	1/1	0.92	0.24	-	45,45,45,45	1
23	MG	A	1545	1/1	0.83	0.11	-	45,45,45,45	0
23	MG	A	1589	1/1	0.98	0.32	-	45,45,45,45	0
23	MG	H	213	1/1	0.64	1.00	-	45,45,45,45	1
23	MG	A	1555	1/1	0.97	0.32	-	45,45,45,45	0
23	MG	A	1554	1/1	0.98	0.51	-	45,45,45,45	0
23	MG	A	1615	1/1	0.78	0.96	-	45,45,45,45	1
23	MG	A	1548	1/1	0.73	0.30	-	45,45,45,45	0
23	MG	A	1580	1/1	0.90	0.17	-	45,45,45,45	0
23	MG	A	1602	1/1	0.95	0.37	-	45,45,45,45	0
23	MG	A	1583	1/1	0.94	0.12	-	45,45,45,45	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
23	MG	A	1556	1/1	0.67	0.27	-	45,45,45,45	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.