



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 06:22 PM GMT

PDB ID : 4KBV  
Title : 70S ribosome translocation intermediate GDPNP-II containing elongation factor EFG/GDPNP, mRNA, and tRNA bound in the pe\*/E state. This entry contains 30S ribosomal subunit B. The full asymmetric unit also contains PDB entries 4KBW (50S subunit B), 4KBT (30S subunit A), and 4KBU (50S subunit A).  
Authors : Zhou, J.; Lancaster, L.; Donohue, J.P.; Noller, H.F.  
Deposited on : 2013-04-23  
Resolution : 3.86 Å(reported)

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

---

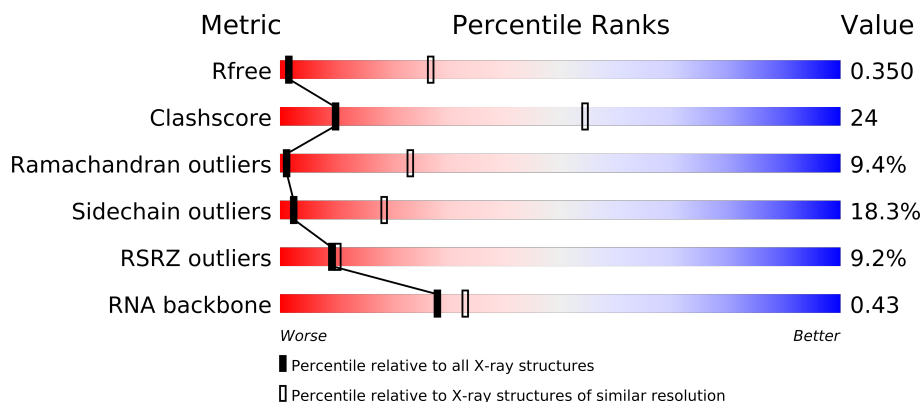
The following versions of software and data (see [references](#)) were used in the production of this report:

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

# 1 Overall quality at a glance

The reported resolution of this entry is 3.86 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1013 (4.30-3.42)
Clashscore	79885	1145 (4.22-3.50)
Ramachandran outliers	78287	1091 (4.22-3.50)
Sidechain outliers	78261	1081 (4.22-3.50)
RSRZ outliers	66119	1014 (4.30-3.42)
RNA backbone	1838	1010 (4.84-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	B	235	
2	C	207	
3	D	208	
4	E	151	
5	F	101	
6	G	155	
7	H	138	
8	I	127	
9	J	99	
10	K	119	
11	L	125	
12	M	125	

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
13	N	60	
14	O	88	
15	P	84	
16	Q	100	
17	R	70	
18	S	79	
19	T	99	
20	A	1511	
21	V	18	
22	W	77	
23	Y	687	
24	U	6	

## 2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 58977 atoms, of which 0 are hydrogen and 0 are deuterium.

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

- Molecule 1 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	235	Total	C	N	O	S	0	0	0
			1910	1218	342	345	5			

- Molecule 2 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	207	Total	C	N	O	S	0	0	0
			1621	1022	315	283	1			

- Molecule 3 is a protein called 30S ribosomal protein S4.

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

- Molecule 4 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	151	Total	C	N	O	S	0	0	0
			1156	729	218	205	4			

- Molecule 5 is a protein called 30S ribosomal protein S6.

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

- Molecule 6 is a protein called 30S ribosomal protein S7.

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

- Molecule 7 is a protein called 30S ribosomal protein S8.

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

- Molecule 8 is a protein called 30S ribosomal protein S9.

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

- Molecule 9 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	99	Total	C	N	O	S	0	0	0
			802	504	157	140	1			

- Molecule 10 is a protein called 30S ribosomal protein S11.

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

- Molecule 11 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	125	Total	C	N	O	S	0	0	0
			976	614	196	165	1			

- Molecule 12 is a protein called 30S ribosomal protein S13.

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

- Molecule 13 is a protein called 30S ribosomal protein S14 type Z.

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

- Molecule 14 is a protein called 30S ribosomal protein S15.

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

- Molecule 15 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	P	84	Total	C	N	O	S	0	0	0
			706	446	140	119	1			

- Molecule 16 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	Q	100	Total	C	N	O	S	0	0	0
			835	534	156	143	2			

- Molecule 17 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	R	70	Total	C	N	O	S	0	0	0
			574	367	112	95				

- Molecule 18 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	S	79	Total	C	N	O	S	0	0	0
			634	405	115	112	2			

- Molecule 19 is a protein called 30S ribosomal protein S20.

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

- Molecule 20 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	A	1511	Total	C	N	O	P	0	0	0
			32474	14455	6015	10494	1510			

- Molecule 21 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	V	18	Total	C	N	O	P	0	0	0
			393	177	81	118	17			

- Molecule 22 is a RNA chain called tRNA-Met.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	W	77	Total	C	N	O	P	0	0	0
			1635	732	291	536	76			

- Molecule 23 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	Y	687	Total	C	N	O	S	0	0	0
			5380	3414	922	1024	20			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	129	LYS	HIS	CONFLICT	UNP Q72I01
Y	226	ASN	HIS	CONFLICT	UNP Q72I01

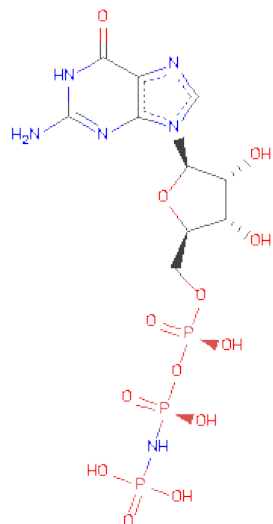
- Molecule 24 is a protein called Viomycin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	U	6	Total	C	N	O	0	0	0
			48	25	13	10			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	Y	1	Total	Mg	0	0
			1	1		

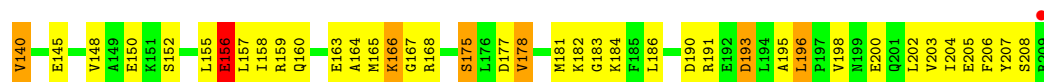
- Molecule 26 is PHOSPHOAMINOPHOSPHONICACID-GUANYLATE ESTER (three-letter code: GNP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>13</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
26	Y	1	32	10	6	13	3	0	0

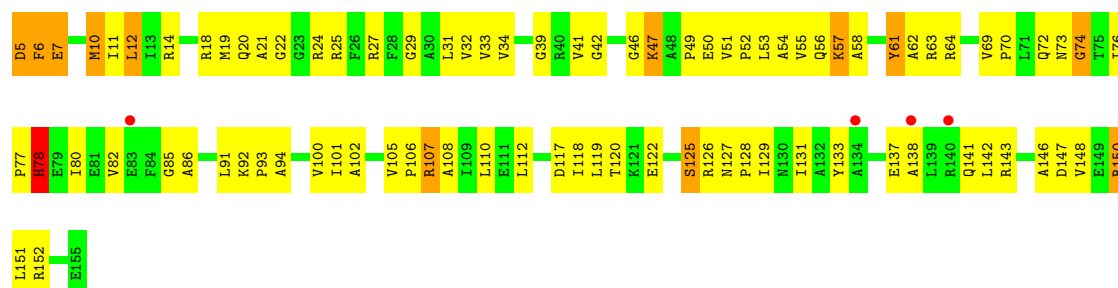






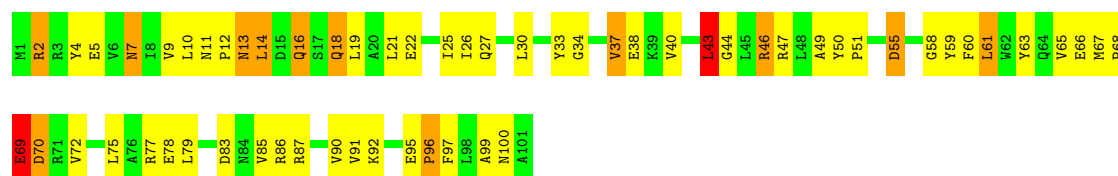
• Molecule 4: 30S ribosomal protein S5

Chain E:



• Molecule 5: 30S ribosomal protein S6

Chain F:



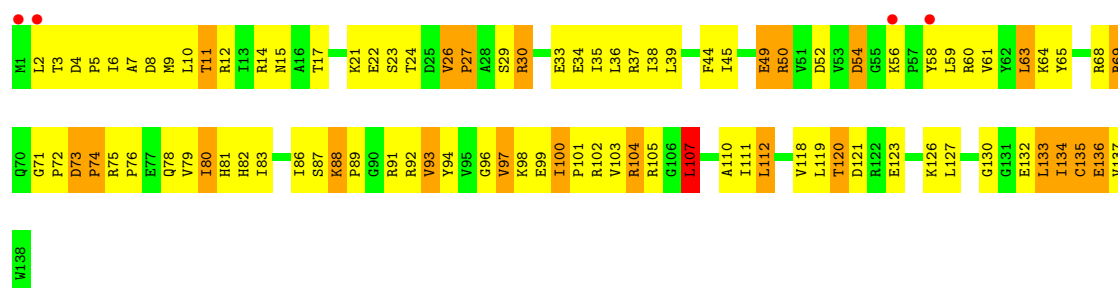
• Molecule 6: 30S ribosomal protein S7

Chain G:



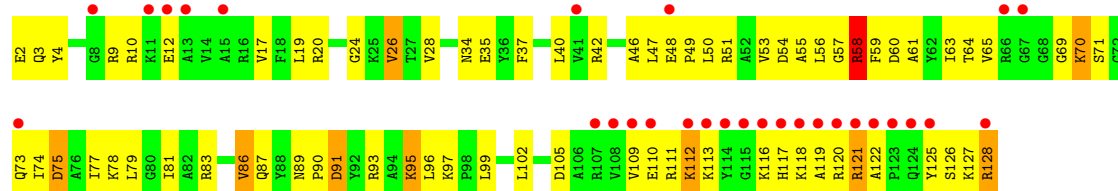
• Molecule 7: 30S ribosomal protein S8

Chain H:



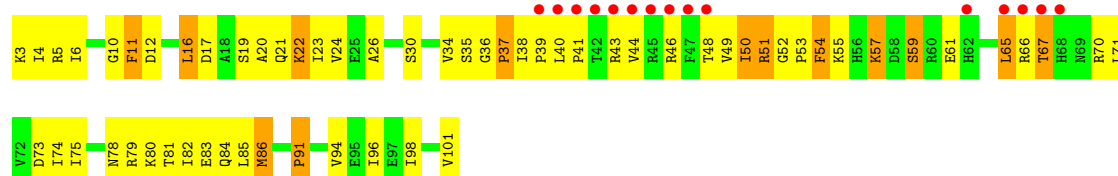
• Molecule 8: 30S ribosomal protein S9

Chain I:



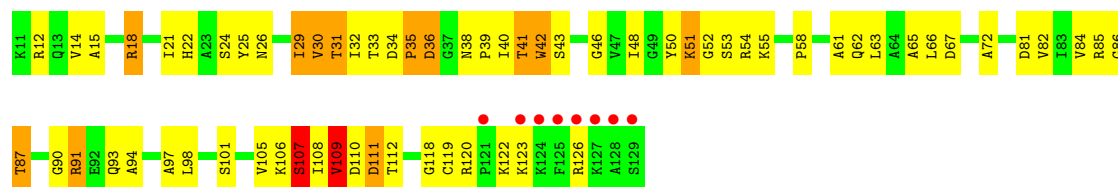
- Molecule 9: 30S ribosomal protein S10

Chain J:



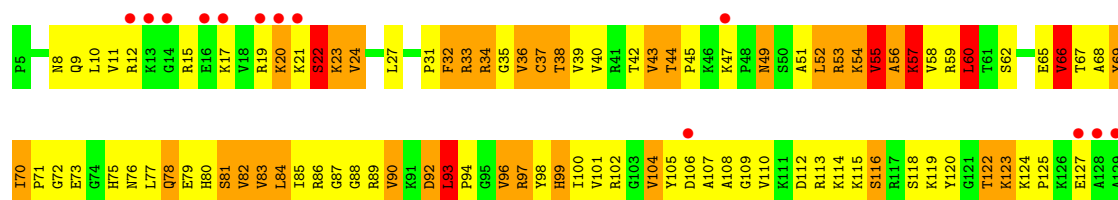
- Molecule 10: 30S ribosomal protein S11

Chain K:



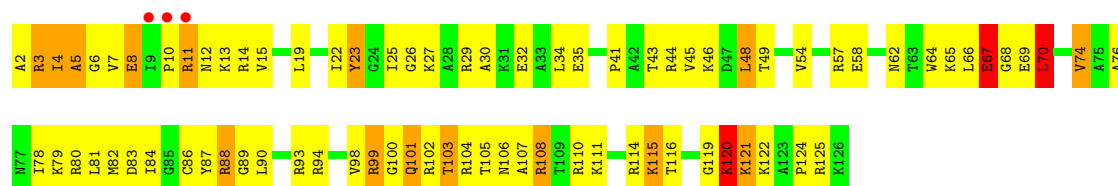
- Molecule 11: 30S ribosomal protein S12

Chain L:



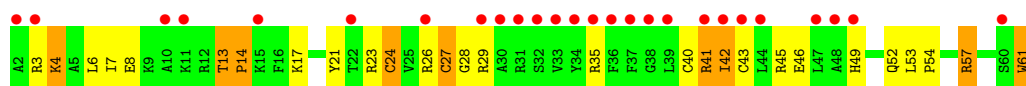
- Molecule 12: 30S ribosomal protein S13

Chain M:



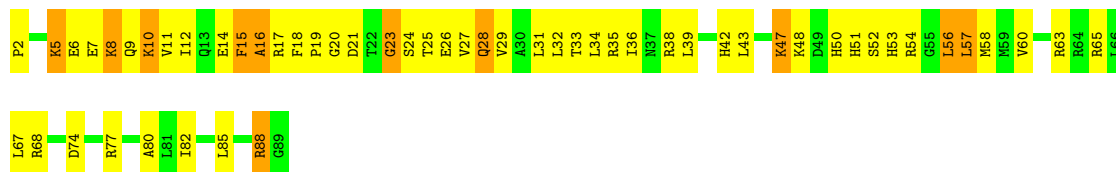
- Molecule 13: 30S ribosomal protein S14 type Z

Chain N:



• Molecule 14: 30S ribosomal protein S15

Chain O:



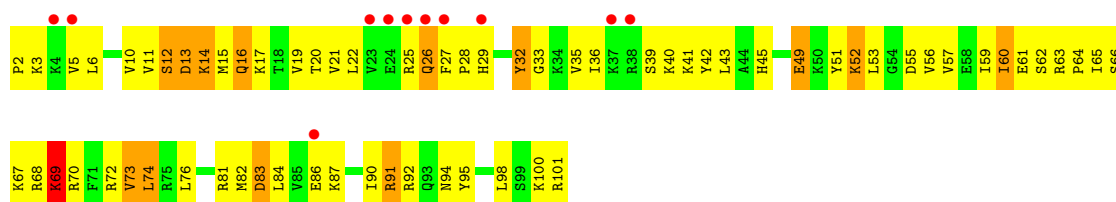
• Molecule 15: 30S ribosomal protein S16

Chain P:



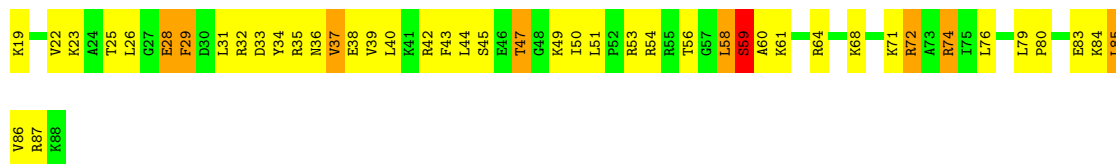
• Molecule 16: 30S ribosomal protein S17

Chain Q:



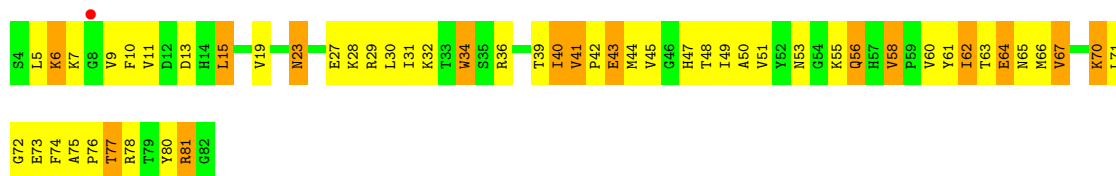
• Molecule 17: 30S ribosomal protein S18

Chain R:



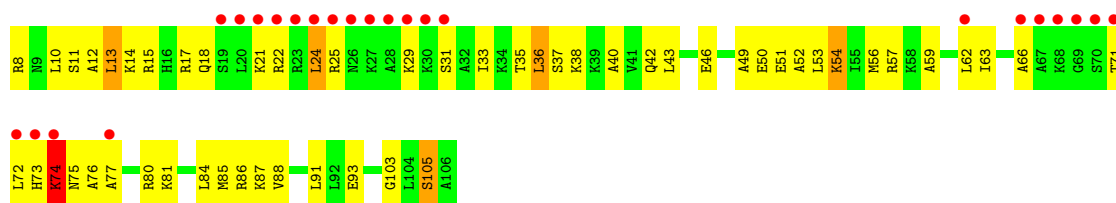
• Molecule 18: 30S ribosomal protein S19

Chain S:



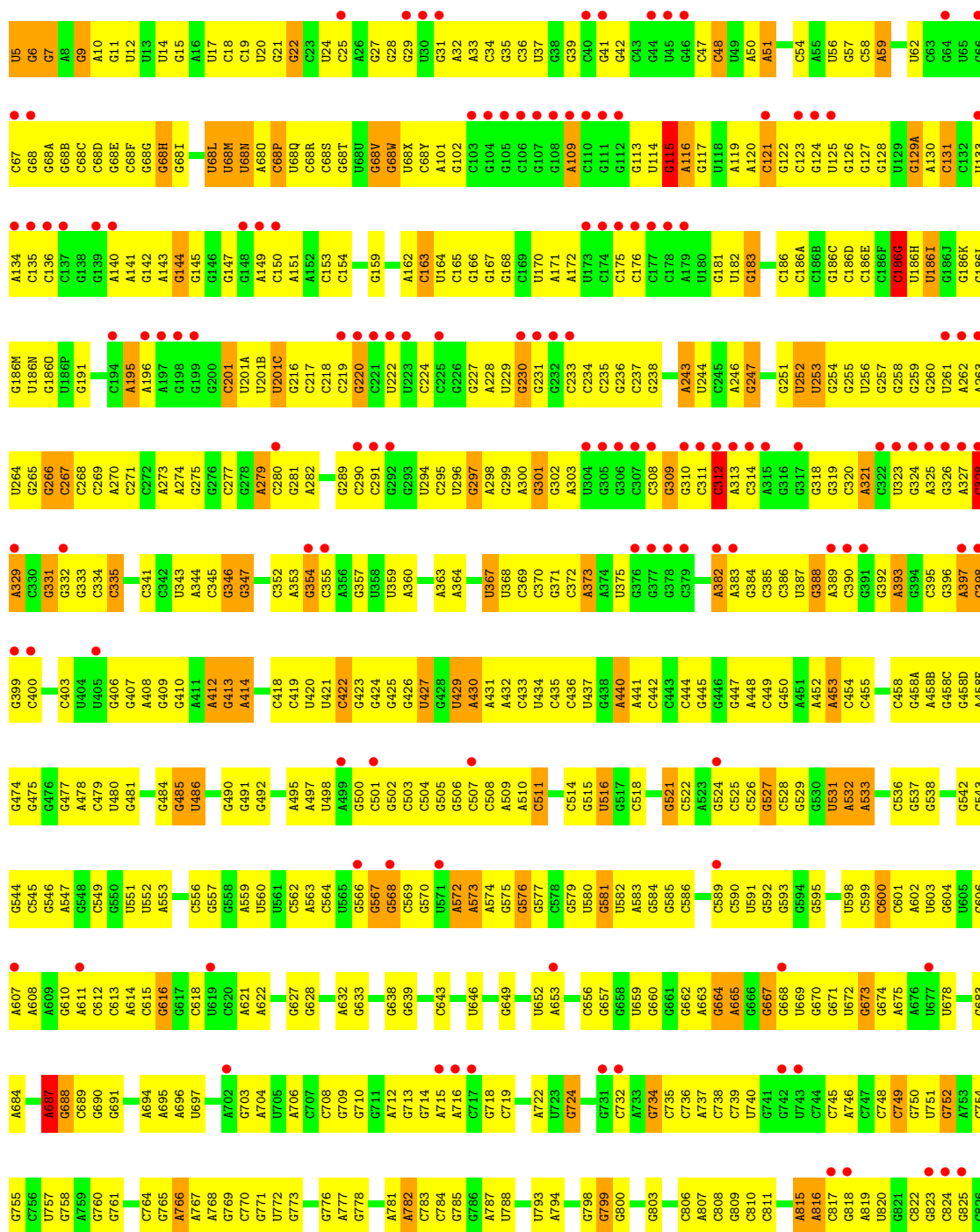
• Molecule 19: 30S ribosomal protein S20

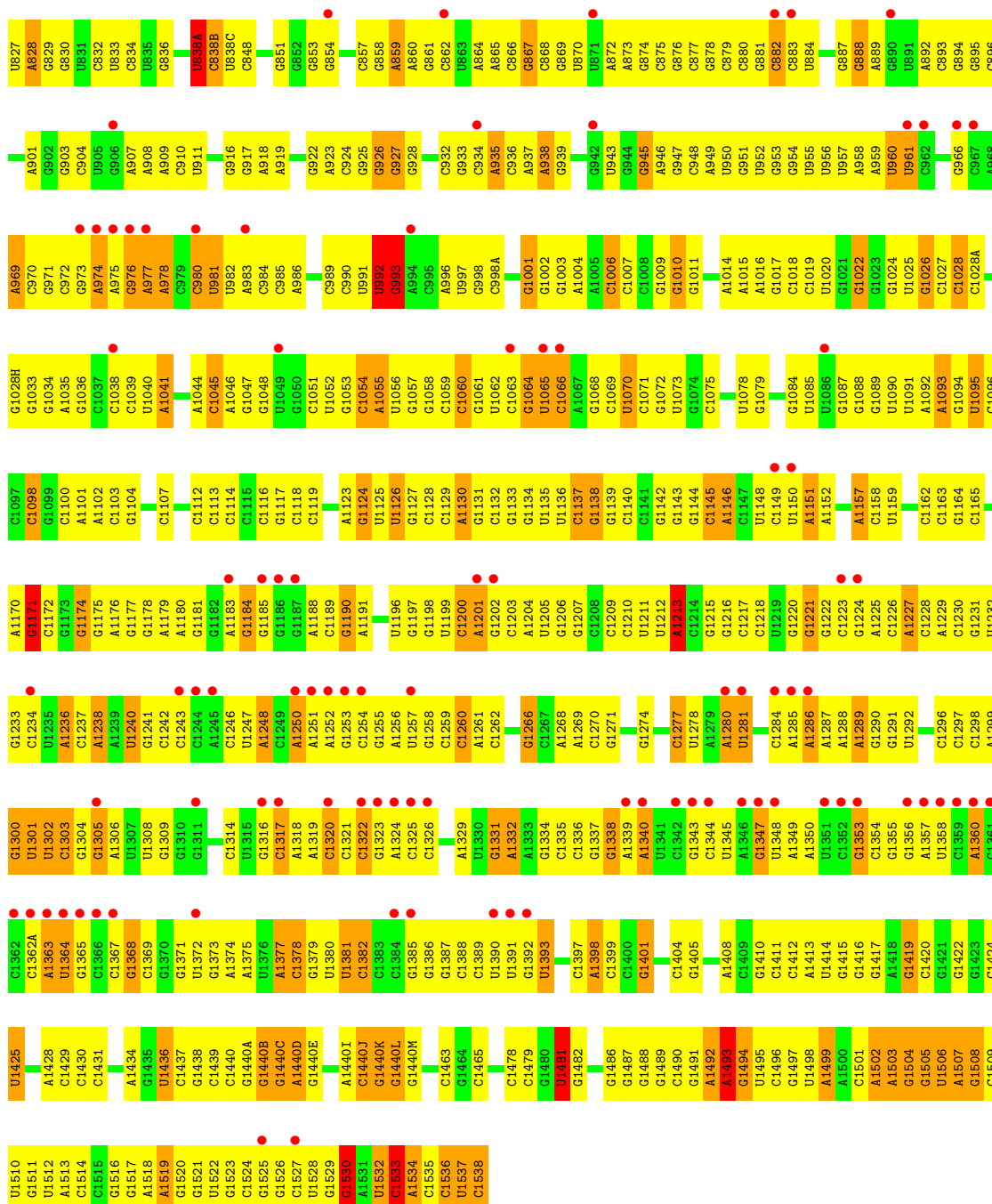
Chain T:



• Molecule 20: 16S ribosomal RNA

Chain A:





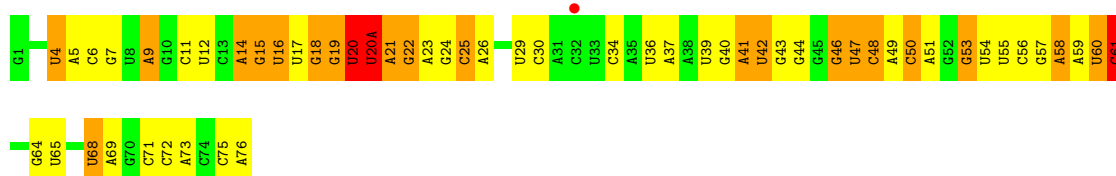
- Molecule 21: messenger RNA

Chain V: 



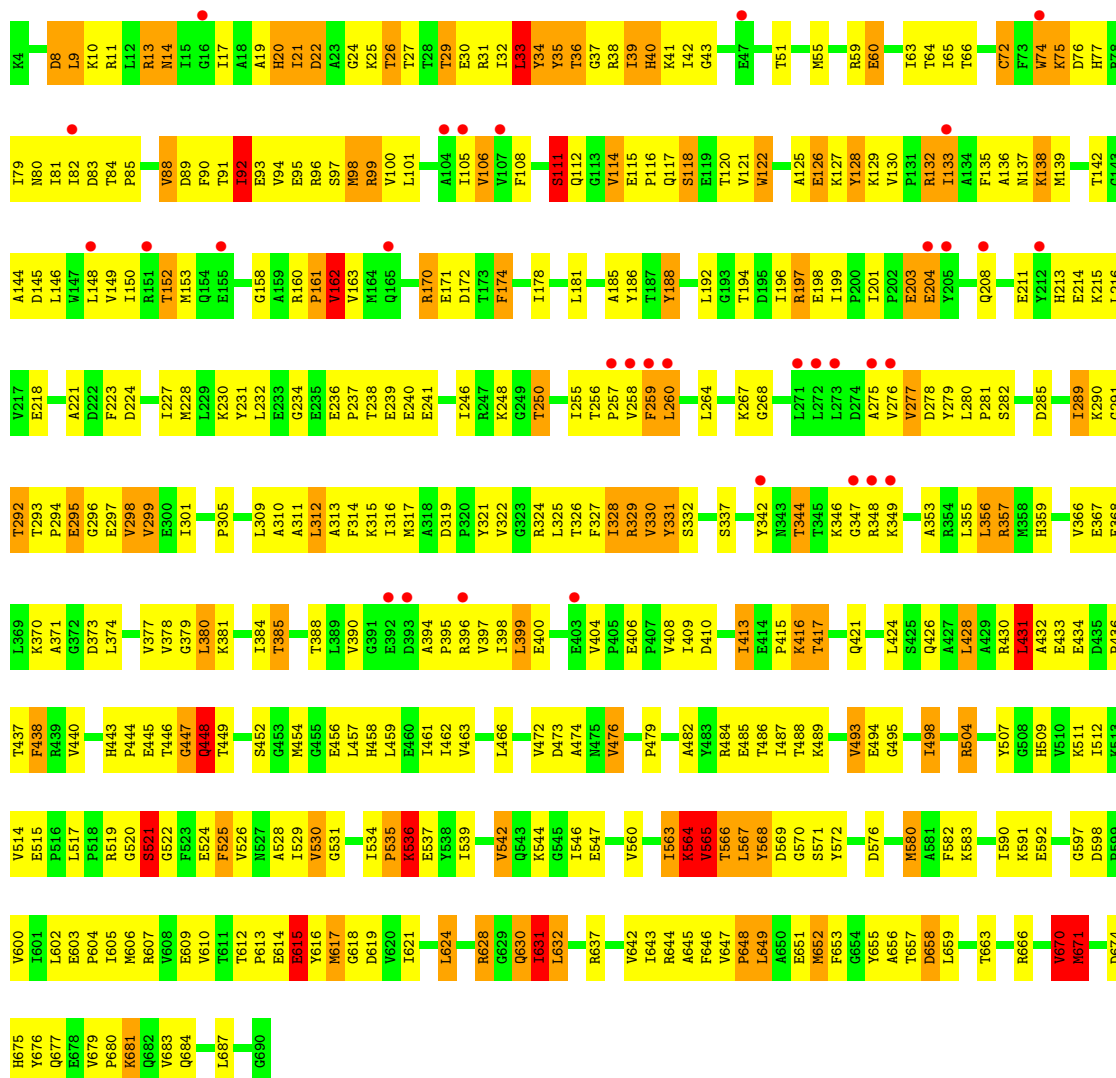
- Molecule 22: tRNA-Met

Chain W:



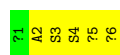
• Molecule 23: Elongation factor G

Chain Y:



• Molecule 24: Viomycin

Chain U:



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	302.39Å 683.92Å 356.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.86 182.04 – 3.87	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.86) 64.4 (182.04-3.87)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.34	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.11 (at 3.89Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.264 , 0.317 0.351 , 0.350	Depositor DCC
$R_{free}$ test set	21649 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	76.3	Xtriage
Anisotropy	0.322	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 289.2	EDS
Estimated twinning fraction	0.320 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.24$ , $\langle L^2 \rangle = 0.09$	Xtriage
Outliers	0 of 432130 reflections	Xtriage
$F_o, F_c$ correlation	0.54	EDS
Total number of atoms	58977	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% of the height of the origin peak. No significant pseudotranslation is detected.*

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



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GNP, DPP, MG, KBE, UAL, 5OH

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	B	0.43	0/1945	0.80	6/2621 (0.2%)
2	C	0.30	0/1645	0.58	0/2216
3	D	0.30	0/1733	0.59	0/2318
4	E	0.30	0/1172	0.58	0/1576
5	F	0.28	0/856	0.56	0/1154
6	G	0.29	0/1276	0.53	0/1709
7	H	0.31	0/1136	0.61	0/1527
8	I	0.32	0/1029	0.56	1/1378 (0.1%)
9	J	0.30	0/815	0.55	0/1095
10	K	0.39	0/900	0.67	0/1213
11	L	0.47	0/992	0.88	2/1327 (0.2%)
12	M	0.27	0/1008	0.59	0/1347
13	N	0.30	0/501	0.49	0/664
14	O	0.32	0/745	0.62	0/992
15	P	0.27	0/722	0.52	0/970
16	Q	0.41	0/848	0.73	0/1131
17	R	0.29	0/579	0.61	0/768
18	S	0.30	0/647	0.61	0/870
19	T	0.33	0/764	0.61	0/1006
20	A	0.38	2/36351 (0.0%)	1.06	96/56736 (0.2%)
21	V	0.29	0/443	0.86	0/691
22	W	0.37	0/1827	1.06	7/2845 (0.2%)
23	Y	0.41	0/5481	0.69	3/7418 (0.0%)
24	U	1.09	0/11	1.84	0/13
All	All	0.37	2/63426 (0.0%)	0.93	115/93585 (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	B	0	3
11	L	0	2
23	Y	0	4
All	All	0	9

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	1393	U	N1-C2	9.25	1.46	1.38
20	A	1393	U	C2-O2	5.28	1.27	1.22

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	1393	U	N1-C2-O2	12.43	131.50	122.80
20	A	815	A	C5-C6-N6	11.09	132.57	123.70
20	A	815	A	N1-C6-N6	-10.71	112.17	118.60
20	A	1393	U	N3-C4-C5	10.67	121.00	114.60
23	Y	33	LEU	CA-CB-CG	9.39	136.91	115.30
20	A	1465	C	C2-N3-C4	-9.22	115.29	119.90
20	A	815	A	N9-C4-C5	8.55	109.22	105.80
1	B	162	ILE	CB-CA-C	8.50	128.61	111.60
20	A	1393	U	C5-C4-O4	-8.24	120.96	125.90
20	A	1436	U	C2-N3-C4	-7.91	122.25	127.00
20	A	115	G	N3-C4-N9	7.76	130.66	126.00
20	A	687	A	P-O3'-C3'	7.70	128.93	119.70
20	A	754	C	C2-N1-C1'	7.68	127.25	118.80
20	A	115	G	P-O3'-C3'	7.48	128.68	119.70
20	A	1034	G	N3-C4-N9	-7.43	121.54	126.00
20	A	815	A	N3-C4-N9	-7.39	121.48	127.40
20	A	115	G	N3-C4-C5	-7.29	124.95	128.60
20	A	115	G	C4-N9-C1'	7.16	135.81	126.50
20	A	815	A	C6-C5-N7	7.06	137.24	132.30
20	A	1465	C	N3-C4-C5	7.02	124.71	121.90
20	A	1393	U	N3-C2-O2	-6.92	117.36	122.20
20	A	1393	U	C6-N1-C2	6.91	125.15	121.00
20	A	68(E)	G	C5-C6-O6	6.91	132.75	128.60
23	Y	33	LEU	N-CA-C	-6.91	92.35	111.00
20	A	328	C	N1-C2-O2	6.87	123.02	118.90
20	A	618	C	C5-C4-N4	6.81	124.97	120.20
23	Y	33	LEU	CB-CG-CD2	6.81	122.57	111.00
22	W	61	C	N1-C2-O2	6.80	122.98	118.90
22	W	61	C	C2-N1-C1'	6.78	126.26	118.80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	L	55	VAL	CB-CA-C	-6.66	98.75	111.40
20	A	1248	A	N1-C6-N6	-6.66	114.61	118.60
20	A	1436	U	C5-C4-O4	-6.62	121.93	125.90
8	I	58	ARG	NE-CZ-NH1	6.59	123.59	120.30
1	B	163	PHE	N-CA-C	-6.46	93.55	111.00
20	A	1213	A	N1-C6-N6	-6.37	114.78	118.60
20	A	754	C	C6-N1-C2	-6.32	117.77	120.30
20	A	1009	G	O4'-C1'-N9	6.32	113.26	108.20
11	L	60	LEU	CA-CB-CG	6.29	129.76	115.30
20	A	1393	U	N1-C2-N3	-6.28	111.13	114.90
20	A	115	G	C8-N9-C1'	-6.25	118.88	127.00
20	A	68(W)	G	N3-C4-N9	-6.20	122.28	126.00
20	A	68(E)	G	C6-N1-C2	6.19	128.81	125.10
20	A	1213	A	N9-C4-C5	6.17	108.27	105.80
20	A	815	A	C4-C5-N7	-6.14	107.63	110.70
20	A	1393	U	O4'-C1'-N1	6.14	113.11	108.20
20	A	1481	U	N1-C2-O2	-6.08	118.55	122.80
20	A	838(A)	U	C2-N1-C1'	6.06	124.98	117.70
20	A	328	C	C2-N1-C1'	6.03	125.43	118.80
20	A	1213	A	C5-C6-N6	5.99	128.49	123.70
20	A	421	U	C2-N1-C1'	5.98	124.88	117.70
20	A	1170	A	N1-C6-N6	5.96	122.18	118.60
20	A	1493	A	O5'-P-OP2	-5.96	100.33	105.70
20	A	1248	A	C5-C6-N6	5.96	128.47	123.70
20	A	993	G	N3-C4-N9	5.92	129.55	126.00
20	A	68(W)	G	N3-C2-N2	-5.90	115.77	119.90
20	A	1045	C	C2-N1-C1'	5.84	125.23	118.80
22	W	61	C	C6-N1-C1'	-5.79	113.85	120.80
20	A	68(W)	G	N9-C4-C5	5.78	107.71	105.40
20	A	1034	G	N3-C2-N2	-5.74	115.88	119.90
20	A	993	G	N9-C4-C5	-5.73	103.11	105.40
22	W	20(A)	U	P-O3'-C3'	5.71	126.56	119.70
20	A	1508	G	N1-C2-N3	5.70	127.32	123.90
20	A	1009	G	C8-N9-C1'	5.67	134.37	127.00
20	A	687	A	OP2-P-O3'	5.65	117.63	105.20
20	A	1045	C	C6-N1-C1'	-5.63	114.04	120.80
20	A	1281	U	N3-C2-O2	-5.62	118.27	122.20
20	A	1009	G	C4-N9-C1'	-5.61	119.21	126.50
20	A	1248	A	N9-C4-C5	5.60	108.04	105.80
1	B	161	ALA	C-N-CA	-5.59	107.72	121.70
20	A	165	C	N1-C2-O2	-5.58	115.55	118.90
20	A	1054	C	N1-C2-O2	5.56	122.24	118.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	1001	G	N9-C4-C5	5.55	107.62	105.40
20	A	665	A	N1-C6-N6	-5.52	115.29	118.60
22	W	68	U	C2-N1-C1'	-5.51	111.09	117.70
20	A	1010	G	N3-C4-N9	5.50	129.30	126.00
20	A	1171	G	N3-C4-N9	-5.49	122.70	126.00
20	A	186(L)	G	N3-C4-N9	-5.49	122.71	126.00
20	A	1054	C	C2-N1-C1'	5.49	124.84	118.80
20	A	186(G)	C	N3-C2-O2	-5.48	118.06	121.90
20	A	243	A	N1-C6-N6	-5.46	115.33	118.60
20	A	312	C	N3-C2-O2	-5.40	118.12	121.90
20	A	475	G	N3-C4-N9	-5.39	122.76	126.00
1	B	164	VAL	CB-CA-C	-5.34	101.24	111.40
20	A	1001	G	N3-C4-N9	-5.34	122.80	126.00
22	W	68	U	C6-N1-C1'	5.33	128.66	121.20
20	A	115	G	OP2-P-O3'	5.29	116.85	105.20
20	A	1465	C	C5-C4-N4	-5.29	116.50	120.20
20	A	1200	C	C6-N1-C1'	5.26	127.11	120.80
20	A	567	G	N3-C4-N9	5.26	129.15	126.00
20	A	1332	A	C4-C5-C6	5.21	119.61	117.00
20	A	312	C	N1-C2-O2	5.20	122.02	118.90
20	A	328	C	P-O3'-C3'	5.20	125.94	119.70
20	A	1034	G	N3-C4-C5	5.15	131.18	128.60
1	B	163	PHE	O-C-N	5.15	130.93	122.70
20	A	978	A	N1-C6-N6	-5.15	115.51	118.60
22	W	20	U	C2-N1-C1'	5.14	123.87	117.70
20	A	993	G	C8-N9-C1'	-5.14	120.31	127.00
20	A	68(N)	U	O4'-C1'-N1	5.13	112.30	108.20
20	A	201	C	O4'-C1'-N1	5.12	112.30	108.20
20	A	421	U	N1-C2-O2	5.10	126.37	122.80
20	A	1419	G	C6-N1-C2	5.09	128.15	125.10
20	A	992	U	P-O3'-C3'	5.08	125.80	119.70
20	A	1530	G	O4'-C1'-N9	5.08	112.27	108.20
20	A	186(L)	G	N3-C2-N2	-5.07	116.35	119.90
20	A	1508	G	C2-N3-C4	-5.06	109.37	111.90
20	A	1393	U	C4-C5-C6	-5.06	116.66	119.70
20	A	328	C	N3-C2-O2	-5.05	118.36	121.90
20	A	475	G	N3-C2-N2	-5.05	116.36	119.90
20	A	815	A	C8-N9-C1'	5.04	136.77	127.70
20	A	1533	C	O5'-P-OP1	-5.04	101.17	105.70
20	A	618	C	N3-C4-C5	-5.03	119.89	121.90
20	A	1289	A	N1-C6-N6	-5.03	115.58	118.60
20	A	1034	G	C6-C5-N7	5.03	133.42	130.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	1027	C	C6-N1-C2	-5.02	118.29	120.30
1	B	162	ILE	N-CA-C	-5.00	97.50	111.00

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	170	GLU	Peptide
1	B	185	ILE	Peptide
1	B	68	ILE	Peptide
11	L	32	PHE	Peptide
11	L	57	LYS	Peptide
23	Y	162	VAL	Peptide
23	Y	329	ARG	Peptide
23	Y	34	TYR	Peptide
23	Y	564	LYS	Peptide

## 5.2 Close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1910	0	1957	120	0
2	C	1621	0	1688	86	0
3	D	1703	0	1763	116	0
4	E	1156	0	1213	62	0
5	F	843	0	857	46	0
6	G	1257	0	1296	82	0
7	H	1116	0	1177	83	0
8	I	1011	0	1043	58	0
9	J	802	0	849	59	0
10	K	885	0	904	54	0
11	L	976	0	1062	108	0
12	M	997	0	1072	67	0
13	N	492	0	529	24	0
14	O	734	0	771	40	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	P	706	0	725	29	0
16	Q	835	0	906	71	0
17	R	574	0	644	42	0
18	S	634	0	655	41	0
19	T	762	0	859	44	0
20	A	32474	0	16393	1045	0
21	V	393	0	197	14	0
22	W	1635	0	831	66	0
23	Y	5380	0	5436	307	0
24	U	48	0	41	15	0
25	Y	1	0	0	0	0
26	Y	32	0	13	18	0
All	All	58977	0	42881	2409	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 24.

All (2409) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
22:W:50:C:N4	22:W:64:G:H1	1.36	1.22
23:Y:30:GLU:O	23:Y:33:LEU:N	1.79	1.13
20:A:369:C:N4	20:A:392:G:H1	1.46	1.11
20:A:1007:C:N4	20:A:1022:G:H1	1.47	1.10
20:A:815:A:C2	20:A:1527:C:O2	2.03	1.10
11:L:56:ALA:HB3	11:L:68:ALA:HB3	1.35	1.07
20:A:950:U:H3	20:A:1231:G:H1	1.09	1.00
22:W:12:U:H3	22:W:23:A:N6	1.59	1.00
23:Y:163:VAL:HG13	23:Y:258:VAL:HB	1.42	0.99
23:Y:526:VAL:HB	23:Y:566:THR:HG23	1.44	0.99
20:A:1162:C:H42	20:A:1174:G:H1	1.08	0.99
20:A:1056:U:H3	20:A:1204:A:N6	1.61	0.99
20:A:1028:C:H42	20:A:1033:G:H1	1.04	0.99
20:A:514:C:H42	20:A:537:G:H1	1.03	0.98
20:A:1028:C:N3	20:A:1033:G:N2	2.10	0.98
23:Y:22:ASP:O	26:Y:702:GNP:O1B	1.80	0.98
20:A:984:C:H42	20:A:1221:G:H1	1.04	0.98
11:L:33:ARG:HB3	11:L:60:LEU:HD12	1.46	0.98
20:A:418:C:N4	20:A:425:G:H1	1.60	0.98
20:A:862:C:H42	20:A:867:G:H1	1.10	0.97
20:A:131:C:N4	20:A:231:G:H1	1.64	0.95
8:I:55:ALA:HB2	8:I:58:ARG:HH21	1.32	0.95
20:A:27:G:H1	20:A:556:C:H42	1.14	0.95

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:A:1001:G:N2	20:A:1039:C:N3	2.13	0.95
20:A:1116:C:H42	20:A:1184:G:H1	1.15	0.95
20:A:928:G:H1	20:A:1389:C:N4	1.64	0.94
20:A:772:U:H3	20:A:807:A:H61	1.04	0.94
20:A:815:A:H2	20:A:1527:C:O2	1.43	0.94
20:A:1303:C:H42	20:A:1334:G:H1	1.14	0.94
20:A:1491:G:H2'	24:U:6:5OH:HA	1.49	0.93
23:Y:31:ARG:HA	23:Y:33:LEU:HD22	1.50	0.93
20:A:127:G:H1	20:A:234:C:H42	1.13	0.93
23:Y:138:LYS:HG2	26:Y:702:GNP:C6	1.98	0.93
20:A:1001:G:H1	20:A:1039:C:H42	1.04	0.93
11:L:35:GLY:HA3	11:L:83:VAL:HG22	1.50	0.92
20:A:506:G:H1	20:A:525:C:H42	0.97	0.92
20:A:1305:G:N2	20:A:1332:A:N7	2.18	0.92
20:A:570:G:H1	20:A:866:C:H42	1.13	0.92
23:Y:602:LEU:HB3	23:Y:676:TYR:HB3	1.49	0.92
20:A:961:U:O2	20:A:1201:A:N1	2.03	0.91
23:Y:98:MET:HG2	23:Y:125:ALA:HB1	1.51	0.91
20:A:667:G:H1	20:A:739:C:H42	1.18	0.90
20:A:895:G:H1	20:A:904:C:H42	0.95	0.90
22:W:50:C:N3	22:W:64:G:N2	2.20	0.90
20:A:895:G:H1	20:A:904:C:N4	1.70	0.90
20:A:131:C:H42	20:A:231:G:H1	0.90	0.89
22:W:50:C:H42	22:W:64:G:H1	0.89	0.88
20:A:1237:C:H4'	20:A:1334:G:H21	1.37	0.88
20:A:506:G:H1	20:A:525:C:N4	1.72	0.88
20:A:928:G:H1	20:A:1389:C:H42	0.89	0.88
10:K:82:VAL:HB	10:K:108:ILE:HA	1.55	0.88
20:A:514:C:N4	20:A:537:G:H1	1.71	0.88
1:B:69:LEU:H	1:B:162:ILE:HA	1.39	0.88
20:A:442:C:H42	20:A:492:G:H1	1.20	0.88
20:A:1028:C:N4	20:A:1033:G:H1	1.72	0.87
9:J:40:LEU:HD22	9:J:41:PRO:HD2	1.57	0.87
23:Y:329:ARG:HB2	23:Y:374:LEU:HG	1.58	0.86
20:A:1414:U:H2'	20:A:1415:G:H8	1.39	0.86
20:A:657:G:H1	20:A:749:C:H42	1.18	0.86
20:A:369:C:N3	20:A:392:G:N2	2.23	0.86
23:Y:313:ALA:HA	23:Y:328:ILE:HA	1.58	0.85
1:B:171:ALA:HA	1:B:174:VAL:HB	1.59	0.85
20:A:1124:G:H1	20:A:1149:C:H42	1.23	0.85
20:A:923:A:H61	20:A:1393:U:H3	1.23	0.85
3:D:175:SER:HB3	3:D:184:LYS:HB2	1.59	0.85

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
17:R:86:VAL:HG12	17:R:87:ARG:HG3	1.59	0.85
20:A:1350:A:H61	20:A:1372:U:H3	1.18	0.85
20:A:862:C:N3	20:A:867:G:N2	2.25	0.85
20:A:129(A):G:N2	20:A:186(G):C:O2	2.09	0.85
23:Y:95:GLU:HB3	23:Y:99:ARG:HH21	1.42	0.84
1:B:71:VAL:HA	1:B:93:VAL:HB	1.59	0.84
20:A:943:U:O4	20:A:1340:A:N1	2.10	0.84
23:Y:566:THR:HG22	23:Y:567:LEU:H	1.43	0.84
20:A:1056:U:H3	20:A:1204:A:H61	0.85	0.84
20:A:126:G:H1	20:A:235:C:H42	1.21	0.84
11:L:102:ARG:HB3	11:L:109:GLY:H	1.43	0.84
20:A:1261:A:H62	20:A:1274:G:H21	1.25	0.84
2:C:11:ARG:HD2	2:C:15:THR:HB	1.60	0.83
14:O:57:LEU:HD21	20:A:580:U:H4'	1.60	0.83
23:Y:566:THR:O	23:Y:567:LEU:HD23	1.77	0.83
23:Y:63:ILE:HD11	26:Y:702:GNP:O1A	1.78	0.83
7:H:97:VAL:HB	20:A:600:C:H5''	1.59	0.83
20:A:984:C:N4	20:A:1221:G:H1	1.77	0.82
22:W:50:C:N4	22:W:64:G:N1	2.15	0.82
23:Y:484:ARG:HB2	23:Y:602:LEU:HB2	1.59	0.82
12:M:101:GLN:NE2	20:A:949:A:OP1	2.11	0.82
20:A:1414:U:H2'	20:A:1415:G:C8	2.14	0.82
8:I:28:VAL:HG12	8:I:63:ILE:HB	1.62	0.82
20:A:1321:C:H3'	20:A:1322:C:H5''	1.62	0.82
23:Y:63:ILE:HG13	26:Y:702:GNP:O1G	1.80	0.81
23:Y:517:LEU:HD22	23:Y:564:LYS:HB2	1.63	0.81
18:S:62:ILE:HG13	18:S:66:MET:HG3	1.61	0.81
18:S:36:ARG:HH22	18:S:75:ALA:HB3	1.45	0.81
11:L:80:HIS:O	11:L:82:VAL:N	2.14	0.81
23:Y:138:LYS:HG2	26:Y:702:GNP:N1	1.96	0.80
20:A:1001:G:H1	20:A:1039:C:N4	1.79	0.80
20:A:862:C:N4	20:A:867:G:H1	1.79	0.80
11:L:71:PRO:HD3	11:L:100:ILE:HB	1.63	0.80
1:B:83:MET:HB2	1:B:234:PRO:HG3	1.64	0.80
3:D:61:LYS:HG2	3:D:203:VAL:HG13	1.63	0.80
4:E:10:MET:HB3	4:E:32:VAL:HG22	1.61	0.80
7:H:89:PRO:HA	7:H:92:ARG:HH22	1.44	0.80
3:D:57:ARG:HH21	4:E:107:ARG:HH21	1.28	0.80
11:L:53:ARG:HG2	11:L:93:LEU:HD22	1.64	0.80
22:W:11:C:H42	22:W:24:G:H1	1.28	0.79
1:B:70:PHE:O	1:B:93:VAL:N	2.14	0.79
20:A:657:G:H1	20:A:749:C:N4	1.81	0.79

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:A:667:G:H1	20:A:739:C:N4	1.79	0.79
1:B:101:MET:HB2	1:B:102:LEU:HD12	1.65	0.79
20:A:115:G:O2'	20:A:116:A:OP2	2.00	0.78
20:A:570:G:H1	20:A:866:C:N4	1.79	0.78
23:Y:26:THR:OG1	26:Y:702:GNP:O2B	2.02	0.78
9:J:80:LYS:HB3	9:J:84:GLN:HE22	1.48	0.78
23:Y:22:ASP:HB3	26:Y:702:GNP:H5'2	1.65	0.78
23:Y:161:PRO:O	23:Y:256:THR:N	2.17	0.78
20:A:418:C:H42	20:A:425:G:H1	0.85	0.78
15:P:57:ARG:NH2	15:P:81:ARG:O	2.17	0.78
15:P:81:ARG:HH22	20:A:474:G:H5'	1.49	0.78
19:T:66:ALA:HB1	19:T:72:LEU:HB2	1.66	0.78
19:T:75:ASN:HB2	20:A:262:A:H4'	1.67	0.77
20:A:516:U:O2	20:A:533:A:N7	2.17	0.77
11:L:93:LEU:HG	11:L:96:VAL:HG22	1.64	0.77
1:B:169:LYS:O	1:B:172:ILE:N	2.16	0.77
20:A:68(H):G:H1	20:A:68(R):C:H42	1.32	0.77
9:J:16:LEU:HD12	9:J:70:ARG:HH11	1.47	0.77
12:M:114:ARG:HB3	20:A:1228:C:H5''	1.65	0.77
8:I:4:TYR:HB2	8:I:19:LEU:HB2	1.66	0.77
20:A:772:U:H3	20:A:807:A:N6	1.82	0.76
20:A:657:G:N2	20:A:749:C:N3	2.32	0.76
20:A:1162:C:N4	20:A:1174:G:H1	1.83	0.76
23:Y:316:ILE:HD12	23:Y:326:THR:HG22	1.66	0.76
23:Y:246:ILE:O	23:Y:250:THR:OG1	2.03	0.76
20:A:418:C:N3	20:A:425:G:N2	2.32	0.76
22:W:64:G:C2	22:W:65:U:N3	2.54	0.76
20:A:1007:C:N3	20:A:1022:G:N2	2.29	0.76
10:K:81:ASP:OD1	10:K:107:SER:OG	2.04	0.76
9:J:70:ARG:HH21	20:A:1151:A:H4'	1.51	0.76
20:A:1512:U:H2'	20:A:1513:A:C8	2.20	0.76
9:J:49:VAL:HG23	13:N:41:ARG:HB2	1.68	0.76
10:K:118:GLY:HA2	20:A:716:A:H1'	1.68	0.76
23:Y:289:ILE:HD12	23:Y:289:ILE:H	1.50	0.76
23:Y:409:ILE:HG13	23:Y:656:ALA:HB3	1.67	0.76
10:K:123:LYS:HA	10:K:126:ARG:HB3	1.68	0.75
20:A:218:C:H5'	20:A:458(C):G:H1	1.50	0.75
23:Y:163:VAL:HA	23:Y:258:VAL:H	1.50	0.75
20:A:950:U:O2	20:A:1231:G:N2	2.15	0.75
9:J:51:ARG:HB3	20:A:1060:C:H4'	1.67	0.75
20:A:1491:G:H2'	24:U:6:5OH:CA	2.16	0.75
23:Y:98:MET:HG3	23:Y:130:VAL:HG11	1.69	0.75

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:A:925:G:O2'	20:A:927:G:OP1	2.04	0.75
20:A:369:C:H42	20:A:392:G:H1	0.77	0.75
20:A:1303:C:N4	20:A:1334:G:H1	1.85	0.75
4:E:148:VAL:HG13	4:E:152:ARG:HD2	1.67	0.75
3:D:43:HIS:HA	3:D:46:LYS:HD3	1.69	0.74
20:A:923:A:N6	20:A:1393:U:H3	1.85	0.74
10:K:108:ILE:HB	17:R:87:ARG:HA	1.68	0.74
16:Q:45:HIS:HB3	16:Q:72:ARG:HG2	1.68	0.74
16:Q:59:ILE:HA	16:Q:73:VAL:HA	1.68	0.74
1:B:104:ASN:N	1:B:104:ASN:OD1	2.21	0.74
20:A:887:G:H1	20:A:910:C:H42	1.33	0.74
20:A:27:G:H1	20:A:556:C:N4	1.85	0.74
11:L:38:THR:HG23	11:L:57:LYS:HD3	1.70	0.74
23:Y:514:VAL:HA	23:Y:565:VAL:HA	1.69	0.73
23:Y:311:ALA:HA	23:Y:330:VAL:O	1.86	0.73
20:A:672:U:H3	20:A:734:G:H1	1.36	0.73
20:A:1060:C:H2'	20:A:1061:G:H8	1.52	0.73
9:J:57:LYS:HB2	20:A:972:C:H4'	1.69	0.73
12:M:29:ARG:HA	12:M:32:GLU:HG2	1.71	0.73
20:A:869:G:O2'	20:A:872:A:N7	2.20	0.73
12:M:80:ARG:HH11	18:S:65:ASN:HB3	1.54	0.73
9:J:10:GLY:HA3	9:J:16:LEU:HD21	1.71	0.73
2:C:22:TRP:HB3	2:C:59:ARG:H	1.54	0.73
20:A:1248:A:C2	20:A:1289:A:N6	2.57	0.73
20:A:515:G:H1	20:A:536:C:H42	1.33	0.73
4:E:76:ILE:HG12	4:E:78:HIS:H	1.54	0.73
20:A:1026:G:O6	20:A:1035:A:N1	2.20	0.73
20:A:673:G:H2'	20:A:674:G:C8	2.23	0.72
14:O:48:LYS:HB2	20:A:668:G:H4'	1.71	0.72
22:W:41:A:H2'	22:W:42:U:C6	2.24	0.72
20:A:131:C:N3	20:A:231:G:N2	2.33	0.72
20:A:127:G:H1	20:A:234:C:N4	1.85	0.72
12:M:116:THR:HA	20:A:1228:C:H4'	1.72	0.72
20:A:154:C:H42	20:A:167:G:H1	1.37	0.72
22:W:12:U:H3	22:W:23:A:H61	0.82	0.72
11:L:42:THR:HA	11:L:52:LEU:HA	1.71	0.72
23:Y:658:ASP:OD2	23:Y:658:ASP:N	2.21	0.72
23:Y:133:ILE:HD12	23:Y:280:LEU:HD21	1.72	0.72
20:A:552:U:H2'	20:A:553:A:H8	1.54	0.72
22:W:64:G:C6	22:W:65:U:O4	2.42	0.72
8:I:55:ALA:HB2	8:I:58:ARG:NH2	2.04	0.72
20:A:1002:G:H2'	20:A:1003:G:C8	2.24	0.72

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:164:ALA:O	3:D:168:ARG:NH1	2.22	0.72
7:H:89:PRO:HG2	20:A:878:G:H5'	1.70	0.72
20:A:324:G:N1	20:A:327:A:OP2	2.23	0.72
23:Y:276:VAL:HA	23:Y:280:LEU:HD23	1.71	0.71
20:A:62:U:OP1	20:A:385:C:O2'	2.08	0.71
12:M:103:THR:HB	20:A:1226:C:H2'	1.72	0.71
10:K:58:PRO:HB2	10:K:93:GLN:HG3	1.71	0.71
23:Y:456:GLU:HB3	23:Y:657:THR:HG21	1.71	0.71
20:A:1007:C:H42	20:A:1022:G:H1	0.74	0.71
20:A:140:A:H2'	20:A:141:A:C8	2.25	0.71
14:O:53:HIS:HA	14:O:56:LEU:HD23	1.71	0.71
20:A:687:A:O2'	20:A:688:G:OP2	2.07	0.71
23:Y:258:VAL:HG12	23:Y:260:LEU:HD12	1.72	0.71
16:Q:28:PRO:HA	16:Q:35:VAL:HA	1.71	0.71
20:A:581:G:N2	20:A:760:G:N7	2.38	0.71
23:Y:609:GLU:HA	23:Y:643:ILE:O	1.90	0.71
4:E:151:LEU:HB3	7:H:79:VAL:HG22	1.73	0.71
20:A:1123:A:H2	20:A:1150:U:H3	1.38	0.71
23:Y:388:THR:HG21	23:Y:398:ILE:HA	1.70	0.71
20:A:1255:G:O2'	20:A:1258:G:N3	2.21	0.71
5:F:43:LEU:HD23	5:F:60:PHE:HB2	1.73	0.71
9:J:36:GLY:HA3	20:A:1123:A:H4'	1.73	0.71
3:D:57:ARG:NH1	3:D:205:GLU:HB2	2.04	0.70
18:S:11:VAL:HG13	18:S:15:LEU:HD12	1.72	0.70
7:H:34:GLU:HB3	7:H:118:VAL:HG21	1.73	0.70
23:Y:514:VAL:HG13	23:Y:565:VAL:HA	1.72	0.70
4:E:110:LEU:HD13	4:E:118:ILE:HG21	1.72	0.70
20:A:1492:A:H3'	24:U:6:5OH:NP	2.06	0.70
23:Y:293:THR:HA	23:Y:397:VAL:HG12	1.71	0.70
10:K:31:THR:HA	10:K:42:TRP:HA	1.72	0.70
20:A:957:U:O2'	20:A:959:A:N7	2.21	0.70
20:A:806:C:H2'	20:A:807:A:H8	1.57	0.70
17:R:33:ASP:HA	17:R:35:ARG:HH21	1.56	0.70
20:A:175:C:H2'	20:A:176:C:C6	2.26	0.70
23:Y:606:MET:HG3	23:Y:649:LEU:HG	1.73	0.70
22:W:68:U:H2'	22:W:69:A:C8	2.27	0.70
23:Y:59:ARG:HB3	23:Y:64:THR:HA	1.73	0.70
20:A:1116:C:N4	20:A:1184:G:H1	1.87	0.70
2:C:161:GLU:HG3	20:A:1055:A:H4'	1.73	0.70
2:C:58:GLU:H	2:C:65:ALA:HB3	1.57	0.69
11:L:58:VAL:HG21	11:L:85:ILE:HD11	1.73	0.69
23:Y:135:PHE:HA	23:Y:260:LEU:HA	1.74	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:E:102:ALA:HB1	4:E:106:PRO:HB2	1.74	0.69
6:G:87:VAL:HG22	6:G:151:TYR:HB3	1.74	0.69
3:D:127:THR:HA	3:D:132:ARG:HA	1.72	0.69
5:F:50:TYR:OH	17:R:74:ARG:O	2.11	0.69
4:E:125:SER:OG	20:A:19:C:OP1	2.08	0.69
20:A:832:C:O2'	20:A:1538:C:H5'	1.91	0.69
20:A:1040:U:H2'	20:A:1041:A:C8	2.28	0.69
20:A:928:G:N2	20:A:1389:C:N3	2.37	0.69
20:A:442:C:N4	20:A:492:G:H1	1.91	0.69
11:L:15:ARG:NH1	20:A:563:A:N3	2.40	0.69
23:Y:431:LEU:O	23:Y:433:GLU:N	2.26	0.69
1:B:131:PRO:HG2	1:B:134:GLU:HB2	1.74	0.69
20:A:68(A):G:H2'	20:A:68(B):G:H8	1.56	0.69
20:A:521:G:O2'	20:A:536:C:O2'	2.11	0.69
12:M:78:ILE:HD12	12:M:81:LEU:HD22	1.75	0.69
11:L:71:PRO:HG2	11:L:102:ARG:HG2	1.75	0.68
11:L:34:ARG:HG3	11:L:82:VAL:HG13	1.74	0.68
2:C:54:ARG:HB2	2:C:69:HIS:HB2	1.74	0.68
20:A:143:A:H2	20:A:220:G:H22	1.40	0.68
20:A:1350:A:N6	20:A:1372:U:H3	1.89	0.68
22:W:29:U:H2'	22:W:30:C:C6	2.27	0.68
1:B:167:PRO:O	1:B:171:ALA:HB2	1.94	0.68
23:Y:41:LYS:HE2	23:Y:43:GLY:HA3	1.74	0.68
2:C:67:THR:HA	2:C:102:ASN:HB3	1.74	0.68
1:B:71:VAL:HB	1:B:164:VAL:HG13	1.75	0.68
20:A:1522:U:H2'	20:A:1523:G:H8	1.59	0.68
20:A:68(P):C:H2'	20:A:68(Q):U:C6	2.29	0.67
20:A:1065:U:OP2	20:A:1190:G:N2	2.26	0.67
9:J:40:LEU:HD21	20:A:1280:A:H5'	1.76	0.67
4:E:32:VAL:HB	4:E:58:ALA:HB1	1.77	0.67
20:A:126:G:H1	20:A:235:C:N4	1.92	0.67
4:E:50:GLU:HG3	4:E:52:PRO:HD2	1.76	0.67
7:H:30:ARG:NH1	20:A:590:C:OP2	2.28	0.67
3:D:119:GLN:HE22	20:A:406:G:H21	1.42	0.67
20:A:101:A:H2'	20:A:102:G:H8	1.60	0.67
6:G:111:ARG:HB3	6:G:113:GLU:HG2	1.77	0.67
20:A:566:G:H4'	20:A:567:G:H5'	1.75	0.67
10:K:53:SER:HB2	20:A:694:A:H5''	1.76	0.67
20:A:713:G:H2'	20:A:714:G:C8	2.29	0.67
15:P:28:ARG:NH1	20:A:375:U:O2	2.27	0.67
20:A:440:A:H3'	20:A:441:A:C8	2.30	0.67
17:R:45:SER:HB3	17:R:51:LEU:HD11	1.77	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:Y:138:LYS:CG	26:Y:702:GNP:C6	2.71	0.67
20:A:440:A:H3'	20:A:441:A:H8	1.60	0.67
3:D:25:ARG:HB2	20:A:410:G:OP2	1.95	0.67
20:A:610:G:H2'	20:A:611:A:H8	1.60	0.67
20:A:490:G:H2'	20:A:491:G:C8	2.30	0.66
17:R:54:ARG:NH2	20:A:1536:C:O2'	2.27	0.66
10:K:31:THR:HG21	20:A:706:A:O2'	1.96	0.66
23:Y:74:TRP:HD1	23:Y:77:HIS:HD1	1.42	0.66
6:G:36:LYS:HD2	20:A:1373:G:H5''	1.77	0.66
20:A:828:A:H62	20:A:858:G:H21	1.43	0.66
20:A:1385:G:H2'	20:A:1386:G:H8	1.59	0.66
11:L:66:VAL:HB	11:L:98:TYR:HD1	1.60	0.66
20:A:806:C:H2'	20:A:807:A:C8	2.30	0.66
11:L:19:ARG:HG2	11:L:20:LYS:H	1.61	0.66
10:K:81:ASP:HA	10:K:106:LYS:O	1.94	0.66
1:B:91:PRO:HG2	1:B:155:LEU:HD23	1.77	0.66
20:A:1143:G:H2'	20:A:1144:G:C8	2.31	0.66
11:L:34:ARG:HB2	20:A:363:A:OP1	1.96	0.66
22:W:48:C:O2'	22:W:59:A:H4'	1.96	0.66
20:A:123:C:OP1	20:A:311:C:O2'	2.14	0.66
5:F:11:ASN:HD22	5:F:14:LEU:HG	1.61	0.65
20:A:1002:G:H2'	20:A:1003:G:H8	1.58	0.65
23:Y:328:ILE:HD12	23:Y:330:VAL:H	1.60	0.65
20:A:1059:C:H2'	20:A:1060:C:O4'	1.97	0.65
5:F:91:VAL:HG23	20:A:736:C:H5''	1.78	0.65
20:A:678:U:O2'	20:A:778:G:OP1	2.10	0.65
20:A:570:G:N2	20:A:866:C:N3	2.38	0.65
20:A:1300:G:OP2	20:A:1335:C:N4	2.30	0.65
2:C:134:ILE:HD11	2:C:151:VAL:HB	1.77	0.65
20:A:406:G:H1	20:A:436:C:H42	1.44	0.65
20:A:659:U:H2'	20:A:660:G:C8	2.31	0.65
22:W:12:U:O2	22:W:23:A:N1	2.30	0.65
23:Y:329:ARG:HG3	23:Y:374:LEU:CD1	2.27	0.65
19:T:74:LYS:HG2	19:T:75:ASN:H	1.62	0.65
8:I:55:ALA:CB	8:I:58:ARG:HH21	2.09	0.65
23:Y:188:TYR:HA	23:Y:196:ILE:HA	1.76	0.65
14:O:2:PRO:HA	20:A:740:U:OP2	1.97	0.65
20:A:932:C:H2'	20:A:933:G:C8	2.32	0.65
18:S:40:ILE:HG12	18:S:71:LEU:HD23	1.79	0.65
20:A:1491:G:C2'	24:U:6:5OH:HA	2.25	0.65
9:J:61:GLU:OE2	13:N:45:ARG:NH1	2.29	0.65
3:D:13:ARG:HH21	3:D:36:ARG:HG3	1.59	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:A:757:U:H2'	20:A:758:G:O4'	1.97	0.65
23:Y:10:LYS:O	23:Y:13:ARG:NH1	2.28	0.65
20:A:783:C:H42	20:A:799:G:H1	1.45	0.65
20:A:159:G:H1'	20:A:162:A:N6	2.12	0.65
13:N:24:CYS:O	13:N:28:GLY:N	2.29	0.65
20:A:67:C:O2'	20:A:171:A:N3	2.22	0.65
1:B:55:PHE:HA	1:B:58:ILE:HB	1.78	0.65
23:Y:563:ILE:O	23:Y:565:VAL:N	2.27	0.65
22:W:56:C:H2'	22:W:57:G:H8	1.61	0.65
20:A:123:C:H2'	20:A:124:G:C8	2.32	0.65
20:A:1124:G:H1	20:A:1149:C:N4	1.94	0.64
20:A:832:C:H42	20:A:854:G:H1	1.44	0.64
6:G:73:MET:HG2	6:G:90:GLU:HA	1.79	0.64
15:P:42:ARG:NH2	20:A:449:C:O2	2.30	0.64
20:A:62:U:H5'	20:A:385:C:H1'	1.77	0.64
3:D:12:CYS:HA	3:D:19:LEU:HD13	1.79	0.64
22:W:6:C:H2'	22:W:7:G:C8	2.31	0.64
20:A:1492:A:H3'	24:U:6:5OH:HNP	1.60	0.64
1:B:71:VAL:HB	1:B:164:VAL:HA	1.79	0.64
20:A:444:C:H42	20:A:490:G:H1	1.46	0.64
20:A:815:A:H61	20:A:1508:G:H21	1.46	0.64
23:Y:137:ASN:ND2	26:Y:702:GNP:O6	2.30	0.64
20:A:950:U:H2'	20:A:951:G:C8	2.33	0.64
1:B:167:PRO:HD2	1:B:188:ALA:HB2	1.79	0.64
23:Y:14:ASN:ND2	23:Y:80:ASN:HB2	2.13	0.64
20:A:559:A:H4'	20:A:560:U:H5"	1.79	0.64
6:G:29:LYS:HG3	6:G:101:LEU:HD13	1.79	0.64
6:G:156:TRP:HH2	20:A:1378:C:H2'	1.62	0.64
7:H:135:CYS:SG	7:H:136:GLU:N	2.70	0.64
4:E:61:TYR:OH	20:A:1075:C:OP2	2.16	0.64
2:C:86:VAL:HA	2:C:89:GLU:HB2	1.78	0.64
20:A:479:C:H2'	20:A:480:U:C6	2.33	0.64
8:I:20:ARG:O	8:I:60:ASP:N	2.21	0.64
23:Y:293:THR:O	23:Y:295:GLU:N	2.27	0.64
20:A:1297:C:H4'	20:A:1299:A:H2	1.63	0.64
20:A:1248:A:H2	20:A:1289:A:N6	1.96	0.64
20:A:673:G:H2'	20:A:674:G:H8	1.60	0.64
20:A:1522:U:H2'	20:A:1523:G:C8	2.33	0.64
4:E:20:GLN:OE1	4:E:25:ARG:NH2	2.31	0.64
20:A:1503:A:N6	21:V:14:A:H2'	2.12	0.64
23:Y:92:ILE:HG21	23:Y:437:THR:HG21	1.79	0.64
20:A:1225:A:H2'	20:A:1226:C:C5	2.33	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:A:656:C:H42	20:A:750:G:H1	1.46	0.64
23:Y:19:ALA:H	23:Y:25:LYS:HD3	1.64	0.63
16:Q:17:LYS:NZ	20:A:255:G:O2'	2.24	0.63
5:F:37:VAL:HA	5:F:65:VAL:HG12	1.79	0.63
10:K:33:THR:HG22	10:K:39:PRO:HA	1.80	0.63
20:A:827:U:H3	20:A:872:A:H61	1.45	0.63
20:A:123:C:H2'	20:A:124:G:H8	1.63	0.63
20:A:612:C:H42	20:A:628:G:H1	1.46	0.63
6:G:87:VAL:HG21	6:G:154:TYR:HB2	1.78	0.63
2:C:68:VAL:HG12	2:C:70:VAL:HG22	1.79	0.63
23:Y:314:PHE:N	23:Y:327:PHE:O	2.30	0.63
23:Y:213:HIS:O	23:Y:216:LEU:HB3	1.98	0.63
20:A:218:C:H4'	20:A:458(C):G:H22	1.63	0.63
11:L:122:THR:HG22	11:L:125:PRO:HG3	1.80	0.63
20:A:764:C:H2'	20:A:765:G:C8	2.34	0.63
15:P:42:ARG:O	20:A:449:C:O2'	2.16	0.63
7:H:10:LEU:HD22	7:H:83:ILE:HD11	1.79	0.63
8:I:110:GLU:HG2	8:I:113:LYS:HZ1	1.63	0.63
20:A:593:G:H1	20:A:646:U:H3	1.46	0.63
20:A:1010:G:H2'	20:A:1011:G:H8	1.63	0.63
11:L:89:ARG:HA	11:L:96:VAL:HB	1.80	0.63
20:A:1254:C:H2'	20:A:1255:G:H8	1.64	0.63
6:G:118:VAL:O	6:G:122:HIS:ND1	2.32	0.63
11:L:83:VAL:HA	11:L:100:ILE:HG23	1.80	0.63
24:U:3:SER:O	24:U:4:SER:HB3	1.99	0.63
20:A:506:G:N2	20:A:525:C:N3	2.38	0.63
22:W:54:U:H3	22:W:58:A:H62	1.46	0.63
10:K:111:ASP:HA	17:R:84:LYS:HG3	1.80	0.63
23:Y:13:ARG:HH21	23:Y:277:VAL:HG23	1.64	0.63
1:B:92:TYR:HE1	1:B:94:ASN:HB2	1.63	0.63
20:A:1113:C:H2'	20:A:1114:C:H6	1.64	0.63
15:P:26:ARG:HD3	15:P:31:LYS:HB3	1.80	0.63
20:A:600:C:H2'	20:A:601:C:C6	2.33	0.62
12:M:88:ARG:HD3	12:M:88:ARG:H	1.64	0.62
3:D:4:TYR:OH	3:D:10:ARG:NH1	2.32	0.62
23:Y:185:ALA:HB2	23:Y:201:ILE:HG13	1.80	0.62
20:A:770:C:H2'	20:A:771:G:C8	2.35	0.62
7:H:97:VAL:HG13	7:H:98:LYS:H	1.63	0.62
2:C:56:ASP:OD1	2:C:56:ASP:N	2.26	0.62
16:Q:67:LYS:HD2	20:A:266:G:H2'	1.82	0.62
20:A:25:C:H5'	20:A:524:G:H1'	1.81	0.62
20:A:815:A:N6	20:A:1508:G:H21	1.97	0.62

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:Y:63:ILE:HG23	26:Y:702:GNP:O1G	1.99	0.62
20:A:149:A:H2'	20:A:150:C:C6	2.34	0.62
20:A:1507:A:H2'	20:A:1508:G:H8	1.62	0.62
19:T:76:ALA:HB2	20:A:262:A:H5''	1.79	0.62
23:Y:388:THR:HG23	23:Y:399:LEU:HD22	1.82	0.62
20:A:1070:U:H2'	20:A:1071:C:H6	1.65	0.62
3:D:165:MET:HA	3:D:168:ARG:HD2	1.79	0.62
10:K:86:GLY:HA2	10:K:112:THR:HG23	1.81	0.62
3:D:115:ARG:NH1	20:A:407:G:OP1	2.33	0.62
3:D:26:CYS:HA	3:D:31:CYS:HA	1.81	0.62
1:B:155:LEU:HD11	1:B:159:PRO:HG3	1.82	0.62
20:A:1010:G:H2'	20:A:1011:G:C8	2.35	0.62
23:Y:160:ARG:HG2	23:Y:162:VAL:HG23	1.80	0.62
20:A:833:U:H2'	20:A:834:C:C6	2.35	0.62
3:D:157:LEU:HA	3:D:160:GLN:HB2	1.82	0.62
12:M:76:ALA:HA	12:M:79:LYS:HG3	1.80	0.62
12:M:83:ASP:OD1	12:M:84:ILE:N	2.33	0.62
4:E:27:ARG:HE	4:E:49:PRO:HD3	1.65	0.62
20:A:526:C:H2'	20:A:527:G:H4'	1.82	0.62
18:S:31:ILE:HD11	18:S:49:ILE:HG12	1.81	0.62
4:E:5:ASP:OD1	4:E:5:ASP:N	2.33	0.62
22:W:21:A:N6	22:W:46:G:H2'	2.15	0.62
20:A:1415:G:H2'	20:A:1416:G:O4'	2.00	0.62
10:K:120:ARG:HH12	20:A:1524:C:H5''	1.65	0.62
20:A:1357:A:H61	20:A:1365:G:H1	1.47	0.61
20:A:985:C:H2'	20:A:986:A:C8	2.35	0.61
20:A:671:G:H1	20:A:735:C:H42	1.48	0.61
20:A:133:U:H3	20:A:229:U:H3	1.48	0.61
1:B:164:VAL:HB	1:B:186:ALA:HA	1.81	0.61
20:A:68(O):A:C8	20:A:68(P):C:H1'	2.35	0.61
23:Y:27:THR:O	23:Y:30:GLU:HG2	2.00	0.61
22:W:11:C:N4	22:W:24:G:H1	1.97	0.61
20:A:600:C:H2'	20:A:601:C:H6	1.64	0.61
9:J:39:PRO:HB2	20:A:1151:A:H5'	1.81	0.61
5:F:9:VAL:HB	5:F:87:ARG:HB2	1.82	0.61
16:Q:100:LYS:HB2	20:A:246:A:H3'	1.80	0.61
23:Y:100:VAL:HG23	23:Y:329:ARG:HD2	1.81	0.61
20:A:521:G:O6	20:A:528:C:N3	2.33	0.61
6:G:78:ARG:HB3	6:G:85:TYR:HB2	1.81	0.61
23:Y:114:VAL:HG23	23:Y:116:PRO:HD3	1.82	0.61
19:T:54:LYS:HE3	19:T:57:ARG:HH21	1.64	0.61
20:A:186(G):C:H1'	20:A:186(K):G:C2	2.35	0.61

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
22:W:54:U:O4	22:W:58:A:N7	2.34	0.61
20:A:627:G:H2'	20:A:628:G:C8	2.36	0.61
23:Y:415:PRO:HB3	23:Y:474:ALA:HA	1.82	0.61
20:A:143:A:H5'	20:A:196:A:N1	2.15	0.61
20:A:1128:C:O2'	20:A:1130:A:N7	2.26	0.61
20:A:745:C:H2'	20:A:746:A:C8	2.35	0.61
14:O:54:ARG:HE	20:A:579:G:HO2'	1.48	0.61
20:A:1306:A:H61	20:A:1331:G:H1'	1.64	0.61
20:A:1145:C:O2'	20:A:1146:A:O5'	2.17	0.61
19:T:86:ARG:NH2	20:A:258:G:OP1	2.31	0.61
20:A:41:G:H2'	20:A:42:G:H8	1.66	0.61
20:A:1291:G:H2'	20:A:1292:U:C6	2.35	0.61
3:D:20:TYR:O	3:D:22:LYS:N	2.27	0.61
23:Y:679:VAL:O	23:Y:681:LYS:N	2.33	0.61
20:A:1254:C:H2'	20:A:1255:G:C8	2.36	0.61
4:E:20:GLN:O	4:E:22:GLY:N	2.34	0.61
19:T:81:LYS:HG2	19:T:85:MET:HE2	1.83	0.61
23:Y:292:THR:HG23	23:Y:297:GLU:H	1.66	0.61
20:A:1305:G:O2'	20:A:1331:G:N2	2.34	0.60
3:D:32:ALA:HB1	20:A:429:U:H5'	1.83	0.60
20:A:309:G:H2'	20:A:310:G:C8	2.36	0.60
1:B:19:HIS:HB2	1:B:204:ASN:HD22	1.65	0.60
10:K:108:ILE:HD13	17:R:87:ARG:HG2	1.82	0.60
20:A:515:G:H1	20:A:536:C:N4	1.99	0.60
12:M:119:GLY:O	12:M:120:LYS:HB2	2.00	0.60
6:G:95:ARG:HH12	20:A:938:A:H4'	1.66	0.60
23:Y:542:VAL:HG23	23:Y:582:PHE:HB3	1.82	0.60
23:Y:546:ILE:HG23	23:Y:590:ILE:HG13	1.83	0.60
20:A:186(D):C:H2'	20:A:186(E):C:C6	2.36	0.60
20:A:68(D):C:N3	20:A:68(V):G:O6	2.34	0.60
7:H:33:GLU:OE1	7:H:50:ARG:NH2	2.34	0.60
1:B:106:LYS:HD2	1:B:106:LYS:H	1.66	0.60
19:T:33:ILE:HD11	19:T:62:LEU:HB3	1.83	0.60
20:A:1355:G:H2'	20:A:1356:G:C8	2.36	0.60
6:G:12:LEU:HD13	6:G:25:ALA:HB2	1.82	0.60
4:E:101:ILE:O	4:E:120:THR:OG1	2.18	0.60
20:A:1306:A:N6	20:A:1331:G:H1'	2.17	0.60
20:A:1131:G:H2'	20:A:1132:C:C6	2.37	0.60
23:Y:357:ARG:NH1	23:Y:373:ASP:OD2	2.35	0.60
20:A:237:C:H2'	20:A:238:G:H8	1.67	0.60
23:Y:529:ILE:HD12	23:Y:539:ILE:HD11	1.83	0.60
1:B:153:ARG:O	1:B:156:LYS:NZ	2.24	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
16:Q:95:TYR:OH	20:A:279:A:OP2	2.11	0.60
20:A:115:G:HO2'	20:A:116:A:P	2.24	0.60
6:G:79:ARG:HB2	20:A:1381:U:C2	2.36	0.60
20:A:832:C:H4'	20:A:1538:C:H5"	1.82	0.60
20:A:757:U:O2'	20:A:879:C:O2	2.19	0.60
11:L:123:LYS:HA	20:A:36:C:H5"	1.84	0.60
11:L:58:VAL:CG2	11:L:85:ILE:HD11	2.31	0.60
4:E:105:VAL:HB	4:E:106:PRO:HD3	1.84	0.60
12:M:74:VAL:O	12:M:78:ILE:HG12	2.02	0.60
3:D:14:ARG:HA	3:D:40:PRO:HD2	1.81	0.60
20:A:573:A:N3	20:A:883:C:O2'	2.35	0.60
14:O:24:SER:HA	20:A:751:U:H1'	1.84	0.60
23:Y:507:TYR:HB2	23:Y:576:ASP:HB3	1.84	0.60
1:B:184:VAL:H	1:B:198:ASP:HB2	1.67	0.59
2:C:156:ARG:HH21	2:C:161:GLU:HA	1.65	0.59
21:V:6:G:H2'	21:V:7:G:C8	2.37	0.59
20:A:908:A:H2'	20:A:909:A:C8	2.37	0.59
23:Y:485:GLU:HB2	23:Y:560:VAL:HG22	1.84	0.59
11:L:100:ILE:HG22	11:L:101:VAL:H	1.67	0.59
20:A:490:G:H2'	20:A:491:G:H8	1.65	0.59
7:H:111:ILE:HB	7:H:135:CYS:H	1.67	0.59
20:A:41:G:H2'	20:A:42:G:C8	2.37	0.59
20:A:1224:G:N2	20:A:1362(A):C:N3	2.50	0.59
20:A:1343:G:H2'	20:A:1344:C:C6	2.37	0.59
7:H:94:TYR:CG	20:A:598:U:H4'	2.37	0.59
18:S:76:PRO:HB3	18:S:81:ARG:HH22	1.66	0.59
12:M:115:LYS:NZ	20:A:1228:C:OP1	2.35	0.59
23:Y:227:ILE:HD11	23:Y:241:GLU:HG3	1.82	0.59
10:K:32:ILE:HD12	10:K:72:ALA:HB2	1.84	0.59
5:F:26:ILE:O	5:F:30:LEU:HG	2.02	0.59
23:Y:117:GLN:O	23:Y:120:THR:OG1	2.13	0.59
20:A:879:C:H2'	20:A:880:C:C6	2.37	0.59
20:A:1513:A:H2'	20:A:1514:C:C6	2.36	0.59
17:R:74:ARG:NH1	20:A:718:G:O6	2.36	0.59
20:A:201(B):U:H5"	20:A:201(C):U:OP1	2.01	0.59
22:W:9:A:H8	22:W:12:U:O4	1.85	0.59
2:C:163:ALA:HB3	20:A:1056:U:H4'	1.83	0.59
20:A:1388:C:H2'	20:A:1389:C:H6	1.67	0.59
20:A:1385:G:H2'	20:A:1386:G:C8	2.38	0.59
20:A:977:A:H8	20:A:1223:C:C4	2.20	0.59
21:V:17:U:H2'	21:V:18:G:C8	2.38	0.59
20:A:114:U:O4	20:A:313:A:N1	2.36	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
12:M:45:VAL:HG23	12:M:48:LEU:HD12	1.84	0.59
1:B:208:ILE:HB	1:B:239:VAL:HG22	1.84	0.59
22:W:20(A):U:O2'	22:W:21:A:O5'	2.17	0.59
23:Y:111:SER:OG	23:Y:112:GLN:N	2.33	0.59
20:A:1001:G:N2	20:A:1039:C:C2	2.65	0.59
12:M:84:ILE:HD11	18:S:63:THR:HG23	1.84	0.59
11:L:37:CYS:SG	11:L:38:THR:N	2.75	0.59
20:A:1354:C:H2'	20:A:1355:G:C8	2.38	0.59
20:A:985:C:H2'	20:A:986:A:H8	1.67	0.59
8:I:118:LYS:O	8:I:120:ARG:N	2.36	0.59
3:D:96:LEU:HG	3:D:139:ARG:NH2	2.18	0.59
20:A:313:A:H2'	20:A:314:C:C6	2.37	0.59
20:A:1356:G:H2'	20:A:1357:A:C8	2.36	0.59
20:A:1271:G:H5'	20:A:1314:C:H5'	1.85	0.59
23:Y:82:ILE:HB	23:Y:101:LEU:HD21	1.84	0.59
11:L:90:VAL:H	11:L:96:VAL:HG21	1.67	0.59
23:Y:223:PHE:HB3	23:Y:248:LYS:HD3	1.85	0.59
5:F:13:ASN:ND2	5:F:55:ASP:OD2	2.35	0.59
6:G:32:ARG:HG2	20:A:1240:U:C2	2.38	0.59
20:A:861:G:HO2'	20:A:874:G:HO2'	1.24	0.58
9:J:55:LYS:HG3	20:A:973:G:O4'	2.02	0.58
6:G:79:ARG:HD3	6:G:79:ARG:H	1.66	0.58
16:Q:13:ASP:O	16:Q:15:MET:N	2.34	0.58
11:L:35:GLY:HA2	11:L:58:VAL:HG13	1.85	0.58
20:A:601:C:H2'	20:A:602:A:H8	1.68	0.58
20:A:1412:C:H2'	20:A:1413:A:C8	2.38	0.58
20:A:1039:C:H2'	20:A:1040:U:C6	2.38	0.58
20:A:431:A:H2'	20:A:432:A:H8	1.68	0.58
20:A:1440(J):C:O2'	20:A:1440(K):G:H5''	2.02	0.58
24:U:5:UAL:C	24:U:6:5OH:HS	2.33	0.58
2:C:119:ARG:HG2	2:C:140:ARG:HH22	1.69	0.58
18:S:39:THR:HA	18:S:70:LYS:HA	1.86	0.58
9:J:39:PRO:HA	9:J:70:ARG:HG3	1.85	0.58
20:A:1528:U:O2'	20:A:1530:G:H5'	2.03	0.58
20:A:1237:C:H4'	20:A:1334:G:N2	2.13	0.58
18:S:53:ASN:HB2	18:S:58:VAL:HG22	1.86	0.58
20:A:938:A:H2'	20:A:939:G:O4'	2.03	0.58
20:A:201(A):U:O2'	20:A:201(B):U:H5'	2.04	0.58
22:W:6:C:H2'	22:W:7:G:H8	1.69	0.58
20:A:903:G:H2'	20:A:904:C:C6	2.38	0.58
20:A:892:A:O2'	20:A:1415:G:O2'	2.20	0.58
20:A:1261:A:H62	20:A:1274:G:N2	1.97	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:I:17:VAL:HA	8:I:63:ILE:HG23	1.85	0.58
1:B:101:MET:HA	1:B:108:ILE:HG12	1.86	0.58
20:A:68(H):G:H1	20:A:68(R):C:N4	1.98	0.58
20:A:687:A:N3	20:A:688:G:H1'	2.18	0.58
20:A:652:U:O4	20:A:752:G:O2'	2.21	0.58
9:J:35:SER:HB3	9:J:73:ASP:HB2	1.85	0.58
23:Y:91:THR:O	23:Y:93:GLU:N	2.37	0.58
11:L:84:LEU:HB2	11:L:104:VAL:HG11	1.85	0.58
20:A:584:G:H2'	20:A:585:G:C8	2.39	0.58
3:D:8:VAL:HG11	3:D:115:ARG:HD3	1.86	0.58
20:A:1251:A:N3	20:A:1369:C:O2'	2.36	0.58
20:A:1071:C:N3	20:A:1104:G:O6	2.37	0.58
2:C:130:VAL:HG21	2:C:157:ILE:HG22	1.86	0.58
20:A:1126:U:H2'	20:A:1127:G:O4'	2.04	0.58
10:K:30:VAL:HG21	10:K:65:ALA:HA	1.86	0.58
20:A:1231:G:H2'	20:A:1232:U:C6	2.38	0.58
16:Q:10:VAL:HA	16:Q:21:VAL:HG22	1.86	0.58
4:E:29:GLY:HA2	4:E:46:GLY:O	2.04	0.58
3:D:65:ARG:HB3	3:D:75:PHE:CE2	2.39	0.58
20:A:59:A:H3'	20:A:331:G:H22	1.69	0.58
20:A:662:G:H2'	20:A:663:A:C8	2.38	0.58
23:Y:30:GLU:HB2	23:Y:51:THR:HG22	1.85	0.58
11:L:33:ARG:O	11:L:85:ILE:HD13	2.03	0.58
12:M:78:ILE:HA	12:M:81:LEU:HB2	1.86	0.58
20:A:1367:C:H2'	20:A:1368:G:O4'	2.04	0.58
22:W:14:A:H2'	22:W:15:G:O4'	2.04	0.58
1:B:77:ALA:O	1:B:81:VAL:HG13	2.04	0.58
23:Y:616:TYR:HB3	23:Y:663:THR:HA	1.85	0.58
20:A:1534:A:H1'	21:V:12:A:H61	1.69	0.58
20:A:560:U:H5'	20:A:566:G:N2	2.19	0.57
20:A:68(A):G:H2'	20:A:68(B):G:C8	2.37	0.57
22:W:39:U:H2'	22:W:40:G:C8	2.39	0.57
20:A:195:A:N3	20:A:222:U:O2'	2.33	0.57
2:C:120:VAL:HA	2:C:123:GLN:HG3	1.84	0.57
4:E:146:ALA:HB1	4:E:150:ARG:HH22	1.69	0.57
23:Y:514:VAL:HA	23:Y:565:VAL:CA	2.35	0.57
24:U:6:5OH:HS	24:U:6:5OH:N	2.19	0.57
20:A:892:A:H2'	20:A:893:C:C6	2.39	0.57
20:A:130:A:N1	20:A:233:C:H1'	2.19	0.57
20:A:1338:G:N2	22:W:41:A:H1'	2.20	0.57
10:K:122:LYS:NZ	20:A:798:G:OP2	2.36	0.57
13:N:23:ARG:HH11	13:N:29:ARG:HA	1.70	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:Y:130:VAL:O	23:Y:132:ARG:HD3	2.04	0.57
3:D:56:VAL:HA	3:D:59:ARG:HB2	1.84	0.57
20:A:1224:G:H1	20:A:1362(A):C:H42	1.50	0.57
3:D:166:LYS:HE2	3:D:178:VAL:HB	1.87	0.57
20:A:614:A:H2'	20:A:615:C:C6	2.39	0.57
23:Y:83:ASP:N	23:Y:83:ASP:OD1	2.36	0.57
20:A:62:U:C5'	20:A:385:C:H1'	2.35	0.57
1:B:92:TYR:CE1	1:B:94:ASN:HB2	2.39	0.57
1:B:79:ASP:O	1:B:82:ARG:HG2	2.04	0.57
14:O:63:ARG:O	14:O:67:LEU:HG	2.04	0.57
12:M:19:LEU:HD13	12:M:22:ILE:HD12	1.86	0.57
11:L:102:ARG:NH2	11:L:109:GLY:O	2.37	0.57
20:A:442:C:N3	20:A:492:G:N2	2.45	0.57
20:A:1143:G:H2'	20:A:1144:G:H8	1.68	0.57
23:Y:188:TYR:OH	23:Y:268:GLY:N	2.37	0.57
16:Q:21:VAL:HG11	16:Q:59:ILE:HD11	1.86	0.57
20:A:674:G:H2'	20:A:675:A:C8	2.39	0.57
23:Y:227:ILE:HA	23:Y:230:LYS:HB2	1.87	0.57
23:Y:612:THR:OG1	23:Y:616:TYR:HB2	2.03	0.57
5:F:97:PHE:HB3	17:R:31:LEU:HD12	1.86	0.57
20:A:10:A:H61	20:A:24:U:H3	1.51	0.57
4:E:72:GLN:O	4:E:74:GLY:N	2.33	0.57
20:A:354:G:N2	20:A:388:G:O2'	2.35	0.57
22:W:64:G:H2'	22:W:65:U:C6	2.40	0.57
20:A:1513:A:H2'	20:A:1514:C:H6	1.69	0.57
20:A:454:C:N4	20:A:479:C:N3	2.53	0.57
18:S:41:VAL:O	18:S:43:GLU:N	2.37	0.57
11:L:124:LYS:HE2	20:A:500:G:H5'	1.86	0.57
20:A:1202:G:H2'	20:A:1203:C:O4'	2.05	0.57
23:Y:631:ILE:HA	23:Y:645:ALA:HA	1.86	0.57
3:D:120:LEU:HA	3:D:123:HIS:HB2	1.87	0.57
9:J:48:THR:OG1	20:A:975:A:N6	2.37	0.57
20:A:1388:C:H2'	20:A:1389:C:C6	2.40	0.57
20:A:68(Q):U:H2'	20:A:68(R):C:O4'	2.05	0.57
9:J:50:ILE:HG12	13:N:41:ARG:NH1	2.20	0.57
6:G:118:VAL:HG13	6:G:122:HIS:CE1	2.40	0.57
23:Y:20:HIS:HD2	23:Y:117:GLN:HB2	1.69	0.57
15:P:72:ARG:HH11	20:A:453:A:H1'	1.70	0.57
23:Y:138:LYS:HE2	26:Y:702:GNP:C4	2.35	0.56
23:Y:519:ARG:HD3	23:Y:677:GLN:HA	1.87	0.56
23:Y:311:ALA:HA	23:Y:330:VAL:C	2.24	0.56
9:J:50:ILE:HG23	13:N:41:ARG:HH12	1.70	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:66:VAL:O	2:C:102:ASN:N	2.38	0.56
1:B:189:ASP:OD1	1:B:189:ASP:N	2.29	0.56
20:A:667:G:N2	20:A:739:C:N3	2.47	0.56
19:T:36:LEU:HD12	19:T:59:ALA:HB2	1.86	0.56
20:A:695:A:H2'	20:A:696:A:C8	2.40	0.56
15:P:66:PRO:HG2	15:P:71:ARG:HH22	1.70	0.56
4:E:93:PRO:HG3	7:H:105:ARG:HG2	1.86	0.56
23:Y:33:LEU:HD23	23:Y:34:TYR:H	1.69	0.56
22:W:22:G:H2'	22:W:23:A:H8	1.69	0.56
23:Y:514:VAL:CG1	23:Y:565:VAL:HA	2.35	0.56
1:B:162:ILE:HG12	1:B:164:VAL:HG22	1.87	0.56
12:M:80:ARG:HA	12:M:83:ASP:HB3	1.85	0.56
11:L:34:ARG:NH1	20:A:363:A:OP2	2.38	0.56
16:Q:13:ASP:OD1	16:Q:13:ASP:N	2.33	0.56
20:A:1440(J):C:O2'	20:A:1440(K):G:N3	2.38	0.56
14:O:43:LEU:O	14:O:47:LYS:HB3	2.04	0.56
16:Q:5:VAL:HG12	16:Q:60:ILE:HG13	1.86	0.56
20:A:408:A:H2'	20:A:409:G:C8	2.39	0.56
20:A:1233:G:H2'	20:A:1234:C:C6	2.40	0.56
17:R:25:THR:HG22	17:R:42:ARG:HH11	1.69	0.56
20:A:422:C:O2	20:A:423:G:N2	2.37	0.56
20:A:1436:U:H2'	20:A:1437:C:C6	2.40	0.56
20:A:669:U:H2'	20:A:670:G:C8	2.41	0.56
20:A:551:U:H2'	20:A:552:U:C6	2.41	0.56
20:A:308:C:H2'	20:A:309:G:H8	1.70	0.56
20:A:1355:G:H2'	20:A:1356:G:H8	1.69	0.56
19:T:11:SER:HA	19:T:13:LEU:HG	1.87	0.56
20:A:181:G:O2'	20:A:183:G:N7	2.38	0.56
19:T:43:LEU:HB3	19:T:52:ALA:HB2	1.87	0.56
20:A:397:A:O2'	20:A:399:G:OP2	2.12	0.56
11:L:113:ARG:NH1	20:A:537:G:OP1	2.34	0.56
20:A:895:G:N2	20:A:904:C:N3	2.43	0.56
20:A:1510:U:H2'	20:A:1511:G:C8	2.41	0.56
16:Q:57:VAL:HB	16:Q:73:VAL:HG11	1.87	0.56
23:Y:670:VAL:O	23:Y:671:MET:HB3	2.05	0.56
20:A:509:A:N3	20:A:543:C:O2'	2.31	0.56
4:E:101:ILE:HD12	20:A:7:G:H3'	1.87	0.56
10:K:21:ILE:HG12	10:K:30:VAL:HG12	1.88	0.56
20:A:1201:A:H4'	20:A:1202:G:H5''	1.88	0.56
23:Y:312:LEU:HD23	23:Y:313:ALA:H	1.71	0.56
18:S:53:ASN:N	18:S:56:GLN:O	2.36	0.56
10:K:48:ILE:HD11	10:K:67:ASP:HB2	1.86	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:A:816:A:OP2	20:A:1526:G:O2'	2.23	0.56
20:A:1486:G:H2'	20:A:1487:G:O4'	2.06	0.56
20:A:1204:A:H3'	20:A:1205:U:C6	2.41	0.56
1:B:102:LEU:HD23	1:B:177:ALA:HB2	1.87	0.56
1:B:22:LYS:HE2	20:A:830:G:H5''	1.88	0.56
20:A:1142:G:H2'	20:A:1143:G:O4'	2.06	0.56
23:Y:325:LEU:HD21	23:Y:356:LEU:HD22	1.87	0.56
9:J:43:ARG:HB2	9:J:67:THR:HB	1.87	0.56
9:J:34:VAL:HG22	9:J:74:ILE:HG22	1.86	0.56
23:Y:221:ALA:HB1	23:Y:228:MET:HG3	1.88	0.56
7:H:54:ASP:O	7:H:56:LYS:NZ	2.39	0.56
22:W:64:G:C2	22:W:65:U:C4	2.93	0.56
11:L:32:PHE:O	11:L:84:LEU:HD12	2.06	0.56
20:A:298:A:H2'	20:A:299:G:O4'	2.06	0.56
20:A:308:C:H2'	20:A:309:G:C8	2.41	0.56
16:Q:43:LEU:HB2	16:Q:70:ARG:O	2.05	0.56
20:A:1131:G:H2'	20:A:1132:C:H6	1.70	0.56
21:V:8:A:H2'	21:V:9:G:C8	2.41	0.56
23:Y:617:MET:O	23:Y:621:ILE:HG12	2.05	0.56
20:A:1072:G:H2'	20:A:1073:U:C6	2.41	0.56
20:A:1391:U:H2'	20:A:1392:G:H8	1.70	0.56
20:A:1492:A:H2'	24:U:6:5OH:NQ	2.20	0.56
12:M:87:TYR:CE2	20:A:1321:C:H4'	2.40	0.56
18:S:29:ARG:HA	18:S:47:HIS:NE2	2.21	0.56
20:A:385:C:H2'	20:A:386:C:C6	2.41	0.56
20:A:917:G:H2'	20:A:918:A:C8	2.40	0.56
5:F:44:GLY:HA2	5:F:59:TYR:CE2	2.40	0.56
20:A:1481:U:H2'	20:A:1482:G:C8	2.41	0.56
11:L:42:THR:HG23	11:L:43:VAL:H	1.71	0.56
20:A:1229:A:H2'	20:A:1230:C:C6	2.40	0.56
6:G:36:LYS:HB3	20:A:1373:G:H5''	1.88	0.56
10:K:97:ALA:O	10:K:101:SER:OG	2.23	0.56
20:A:121:C:N4	20:A:236:G:N7	2.53	0.56
20:A:1149:C:H2'	20:A:1150:U:C6	2.41	0.55
8:I:120:ARG:HH11	20:A:1345:U:H5''	1.71	0.55
3:D:190:ASP:H	3:D:193:ASP:HB2	1.70	0.55
12:M:26:GLY:N	20:A:1329:A:H5''	2.21	0.55
1:B:53:ARG:O	1:B:56:ARG:HB2	2.06	0.55
11:L:34:ARG:HG3	11:L:82:VAL:CG1	2.37	0.55
12:M:32:GLU:HA	12:M:35:GLU:HB3	1.88	0.55
20:A:219:C:H2'	20:A:220:G:O4'	2.06	0.55
17:R:22:VAL:H	17:R:56:THR:HA	1.70	0.55

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:Y:342:TYR:HA	23:Y:349:LYS:HA	1.88	0.55
20:A:383:A:O5'	20:A:383:A:H8	1.89	0.55
14:O:33:THR:HA	14:O:36:ILE:HD12	1.87	0.55
19:T:73:HIS:NE2	20:A:325:A:H5''	2.21	0.55
14:O:7:GLU:O	14:O:10:LYS:HG3	2.07	0.55
20:A:667:G:H2'	20:A:668:G:C8	2.41	0.55
1:B:175:ARG:NH2	20:A:1075:C:O3'	2.39	0.55
3:D:53:ASP:HB2	4:E:107:ARG:HH22	1.71	0.55
9:J:51:ARG:HG2	9:J:59:SER:O	2.06	0.55
23:Y:59:ARG:HD3	23:Y:65:ILE:H	1.70	0.55
2:C:66:VAL:HB	2:C:101:LEU:HA	1.89	0.55
17:R:74:ARG:HA	17:R:79:LEU:HB3	1.88	0.55
4:E:119:LEU:HD11	20:A:6:G:C5	2.42	0.55
20:A:227:G:H2'	20:A:228:A:H8	1.71	0.55
7:H:119:LEU:HD13	7:H:127:LEU:HD23	1.87	0.55
9:J:24:VAL:HG21	9:J:37:PRO:HG3	1.88	0.55
23:Y:448:GLN:HE22	23:Y:479:PRO:HA	1.71	0.55
23:Y:607:ARG:HA	23:Y:645:ALA:O	2.06	0.55
12:M:11:ARG:O	12:M:13:LYS:N	2.40	0.55
2:C:37:GLN:HA	2:C:40:ARG:HD2	1.88	0.55
8:I:17:VAL:HG13	8:I:63:ILE:HD12	1.88	0.55
20:A:1246:C:H42	20:A:1291:G:H1	1.53	0.55
20:A:881:G:H2'	20:A:882:C:C6	2.42	0.55
5:F:12:PRO:HD2	5:F:86:ARG:NH1	2.21	0.55
23:Y:438:PHE:H	23:Y:438:PHE:HD2	1.55	0.55
4:E:100:VAL:HG23	4:E:107:ARG:HD3	1.88	0.55
19:T:18:GLN:O	19:T:22:ARG:HG3	2.06	0.55
8:I:111:ARG:HG3	20:A:1369:C:P	2.47	0.55
19:T:13:LEU:O	19:T:17:ARG:HG3	2.07	0.55
20:A:1236:A:H4'	20:A:1304:G:H4'	1.89	0.55
11:L:85:ILE:HG23	11:L:98:TYR:HB3	1.89	0.55
20:A:296:U:O2'	20:A:556:C:O2	2.24	0.55
20:A:1491:G:H2'	24:U:6:5OH:C	2.37	0.55
1:B:161:ALA:HA	1:B:183:PRO:O	2.07	0.55
20:A:458(A):G:O6	20:A:458(C):G:H5''	2.07	0.55
20:A:291:C:H42	20:A:309:G:H1	1.53	0.55
20:A:255:G:N1	20:A:271:C:O2	2.34	0.55
7:H:120:THR:OG1	7:H:121:ASP:N	2.39	0.55
16:Q:40:LYS:HB3	16:Q:42:TYR:HE1	1.71	0.55
2:C:88:ARG:HA	2:C:91:LEU:HG	1.88	0.55
20:A:864:A:H2'	20:A:865:A:C8	2.42	0.55
14:O:18:PHE:O	14:O:20:GLY:N	2.40	0.55

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:187:ALA:HB3	2:C:198:VAL:HB	1.88	0.55
20:A:1028:C:C2	20:A:1033:G:N2	2.63	0.55
23:Y:25:LYS:HE3	26:Y:702:GNP:O1B	2.07	0.55
20:A:1305:G:H1	20:A:1331:G:H2'	1.72	0.55
20:A:947:G:H2'	20:A:948:C:C6	2.42	0.55
20:A:892:A:HO2'	20:A:1415:G:HO2'	1.52	0.55
20:A:18:C:N3	20:A:917:G:O6	2.40	0.55
22:W:47:U:H4'	22:W:48:C:H5''	1.89	0.55
5:F:5:GLU:HB2	5:F:91:VAL:HG12	1.89	0.55
20:A:5:U:O2'	20:A:6:G:O5'	2.18	0.55
20:A:431:A:H2'	20:A:432:A:C8	2.42	0.55
16:Q:101:ARG:HG2	20:A:247:G:OP2	2.07	0.55
16:Q:56:VAL:HG23	16:Q:81:ARG:HG3	1.88	0.55
20:A:879:C:H2'	20:A:880:C:H6	1.72	0.54
20:A:1060:C:H2'	20:A:1061:G:C8	2.38	0.54
23:Y:257:PRO:HB2	23:Y:259:PHE:CZ	2.42	0.54
23:Y:456:GLU:HA	23:Y:459:LEU:HD12	1.89	0.54
14:O:54:ARG:NE	20:A:579:G:O2'	2.30	0.54
2:C:123:GLN:HE21	2:C:133:ALA:HB1	1.71	0.54
21:V:8:A:H2'	21:V:9:G:H8	1.71	0.54
6:G:58:PRO:O	6:G:62:PHE:HB2	2.07	0.54
20:A:1498:U:H1'	20:A:1499:A:N7	2.22	0.54
23:Y:33:LEU:HD23	23:Y:34:TYR:N	2.22	0.54
20:A:1507:A:H2'	20:A:1508:G:C8	2.42	0.54
9:J:55:LYS:O	20:A:972:C:O2'	2.22	0.54
23:Y:624:LEU:HD21	23:Y:643:ILE:HG21	1.90	0.54
16:Q:66:SER:HB3	16:Q:69:LYS:HB2	1.89	0.54
3:D:191:ARG:HH12	3:D:195:ALA:HA	1.71	0.54
20:A:504:C:H2'	20:A:511:C:H5	1.73	0.54
20:A:1504:G:H4'	20:A:1505:G:O4'	2.06	0.54
20:A:444:C:H2'	20:A:445:G:H8	1.72	0.54
20:A:1251:A:H2'	20:A:1252:A:C8	2.42	0.54
20:A:1070:U:H2'	20:A:1071:C:C6	2.43	0.54
20:A:782:A:H62	20:A:800:G:H21	1.55	0.54
20:A:1213:A:O2'	20:A:1215:G:N7	2.35	0.54
20:A:367:U:H3	20:A:393:A:H61	1.54	0.54
1:B:166:ASP:HA	1:B:188:ALA:HB2	1.89	0.54
1:B:162:ILE:HG23	1:B:184:VAL:HG13	1.89	0.54
11:L:49:ASN:OD1	11:L:49:ASN:N	2.39	0.54
20:A:627:G:H2'	20:A:628:G:H8	1.72	0.54
20:A:243:A:H4'	20:A:244:U:H3'	1.88	0.54
16:Q:81:ARG:HB3	16:Q:84:LEU:HD12	1.88	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:A:1211:U:H1'	20:A:1213:A:C2	2.42	0.54
20:A:434:U:H2'	20:A:435:C:C6	2.42	0.54
23:Y:24:GLY:HA2	26:Y:702:GNP:H8	1.90	0.54
20:A:924:C:O2'	20:A:1502:A:N1	2.37	0.54
20:A:101:A:H2'	20:A:102:G:C8	2.40	0.54
16:Q:63:ARG:HE	20:A:130:A:H5'	1.72	0.54
23:Y:163:VAL:HG22	23:Y:258:VAL:CG2	2.38	0.54
23:Y:344:THR:HB	23:Y:398:ILE:HG12	1.88	0.54
4:E:52:PRO:O	4:E:56:GLN:HG2	2.05	0.54
16:Q:68:ARG:O	16:Q:70:ARG:N	2.34	0.54
3:D:65:ARG:HB3	3:D:75:PHE:CZ	2.43	0.54
8:I:46:ALA:HB2	8:I:74:ILE:HG22	1.87	0.54
3:D:86:LYS:HE2	3:D:87:GLY:N	2.22	0.54
22:W:9:A:C8	22:W:12:U:O4	2.61	0.54
23:Y:482:ALA:HB1	23:Y:484:ARG:HH11	1.73	0.54
7:H:89:PRO:O	20:A:586:C:H4'	2.08	0.54
3:D:12:CYS:HB3	3:D:33:MET:HG2	1.88	0.54
23:Y:390:VAL:HG21	23:Y:396:ARG:HA	1.90	0.54
6:G:74:GLU:HB3	6:G:91:VAL:HG21	1.90	0.54
23:Y:29:THR:HG21	23:Y:81:ILE:HG21	1.90	0.54
23:Y:136:ALA:HB3	23:Y:260:LEU:HB2	1.90	0.54
11:L:40:VAL:HA	11:L:54:LYS:HA	1.89	0.54
11:L:31:PRO:HB2	20:A:552:U:O2'	2.08	0.54
3:D:9:CYS:HB3	3:D:32:ALA:HB3	1.89	0.54
17:R:53:ARG:HH21	17:R:59:SER:HA	1.72	0.54
6:G:140:ASP:HA	6:G:143:ARG:HH21	1.73	0.54
20:A:320:C:H2'	20:A:321:A:C8	2.43	0.54
20:A:1405:G:H1	20:A:1496:C:H42	1.56	0.54
16:Q:51:TYR:HE1	16:Q:76:LEU:HB2	1.72	0.54
20:A:1347:G:N2	20:A:1373:G:H2'	2.23	0.54
20:A:1356:G:H2'	20:A:1357:A:H8	1.71	0.54
23:Y:11:ARG:HB2	23:Y:76:ASP:O	2.08	0.54
14:O:16:ALA:HB1	14:O:21:ASP:HB3	1.90	0.54
20:A:1018:C:H2'	20:A:1019:C:C6	2.42	0.54
20:A:1162:C:N3	20:A:1174:G:N2	2.42	0.54
6:G:111:ARG:HE	6:G:123:GLU:HB2	1.72	0.54
20:A:246:A:C2	20:A:282:A:C4	2.95	0.54
20:A:1134:G:C2	20:A:1135:U:H1'	2.43	0.54
12:M:67:GLU:OE1	12:M:68:GLY:N	2.39	0.54
11:L:84:LEU:HB2	11:L:104:VAL:CG1	2.38	0.53
20:A:570:G:O5'	20:A:570:G:H8	1.90	0.53
6:G:113:GLU:HB2	6:G:119:ARG:HG2	1.89	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
15:P:42:ARG:HA	20:A:450:G:H5'	1.90	0.53
2:C:40:ARG:HH12	13:N:52:GLN:HB3	1.73	0.53
20:A:318:G:H2'	20:A:319:G:C8	2.43	0.53
5:F:7:ASN:ND2	5:F:61:LEU:O	2.38	0.53
6:G:38:LEU:HA	6:G:41:ARG:HD3	1.88	0.53
20:A:1438:G:H1	20:A:1463:C:H42	1.56	0.53
23:Y:313:ALA:HA	23:Y:328:ILE:CA	2.36	0.53
20:A:584:G:H2'	20:A:585:G:H8	1.74	0.53
20:A:887:G:H1	20:A:910:C:N4	2.04	0.53
12:M:122:LYS:HA	20:A:954:G:H5'	1.89	0.53
1:B:146:GLN:O	1:B:150:SER:OG	2.26	0.53
14:O:47:LYS:H	14:O:47:LYS:HD3	1.73	0.53
20:A:989:C:H2'	20:A:990:C:H6	1.72	0.53
20:A:1176:A:H2'	20:A:1177:G:O4'	2.09	0.53
20:A:722:A:H2'	20:A:724:G:C8	2.43	0.53
12:M:102:ARG:CZ	12:M:104:ARG:HB3	2.39	0.53
1:B:198:ASP:OD2	7:H:68:ARG:NH2	2.41	0.53
20:A:892:A:H2'	20:A:893:C:H6	1.73	0.53
4:E:100:VAL:HG12	4:E:118:ILE:HG22	1.88	0.53
3:D:15:GLU:HG2	3:D:59:ARG:HH22	1.72	0.53
7:H:71:GLY:O	7:H:73:ASP:N	2.41	0.53
7:H:8:ASP:OD2	7:H:12:ARG:NH2	2.42	0.53
23:Y:9:LEU:O	23:Y:282:SER:OG	2.26	0.53
11:L:58:VAL:HG12	11:L:60:LEU:H	1.73	0.53
23:Y:514:VAL:HA	23:Y:565:VAL:O	2.08	0.53
20:A:955:U:H2'	20:A:956:U:O4'	2.08	0.53
20:A:621:A:H2'	20:A:622:A:C8	2.43	0.53
20:A:1224:G:N2	20:A:1362(A):C:C2	2.77	0.53
12:M:26:GLY:H	20:A:1329:A:H5''	1.73	0.53
8:I:65:VAL:HG11	8:I:77:ILE:HD11	1.91	0.53
10:K:24:SER:OG	10:K:25:TYR:N	2.41	0.53
16:Q:86:GLU:O	16:Q:90:ILE:HG13	2.08	0.53
20:A:1504:G:OP1	20:A:1507:A:O2'	2.15	0.53
23:Y:311:ALA:CB	23:Y:330:VAL:HA	2.38	0.53
20:A:68(R):C:H2'	20:A:68(S):C:C5	2.43	0.53
20:A:1179:A:H2'	20:A:1180:A:O4'	2.08	0.53
23:Y:139:MET:HB3	23:Y:174:PHE:HE1	1.74	0.53
2:C:6:HIS:HD2	2:C:8:ILE:HB	1.73	0.53
20:A:186(N):U:H2'	20:A:186(O):G:C8	2.43	0.53
1:B:211:ILE:O	1:B:215:LEU:HB2	2.09	0.53
11:L:17:LYS:NZ	20:A:303:A:H5'	2.23	0.53
23:Y:356:LEU:HB2	23:Y:378:VAL:HG23	1.90	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:H:12:ARG:NH2	20:A:825:G:O2'	2.41	0.53
23:Y:511:LYS:HB3	23:Y:568:TYR:CZ	2.43	0.53
20:A:1419:G:H2'	20:A:1420:C:C6	2.43	0.53
8:I:42:ARG:HD2	8:I:71:SER:HB2	1.90	0.53
4:E:108:ALA:O	4:E:112:LEU:HG	2.09	0.53
12:M:2:ALA:O	12:M:4:ILE:N	2.41	0.53
20:A:810:C:H2'	20:A:811:C:O4'	2.07	0.53
20:A:12:U:O2	20:A:22:G:O6	2.27	0.53
5:F:69:GLU:O	5:F:72:VAL:HG12	2.09	0.53
8:I:2:GLU:HG3	8:I:3:GLN:HG3	1.89	0.53
23:Y:30:GLU:O	23:Y:31:ARG:C	2.47	0.53
23:Y:150:ILE:HG23	23:Y:161:PRO:HG3	1.91	0.53
13:N:42:ILE:HD13	13:N:45:ARG:HD3	1.90	0.53
23:Y:133:ILE:HB	23:Y:259:PHE:HE1	1.74	0.53
16:Q:67:LYS:HB3	20:A:254:G:OP2	2.09	0.53
20:A:1251:A:H2'	20:A:1252:A:H8	1.74	0.53
10:K:21:ILE:HD11	10:K:98:LEU:HD11	1.90	0.53
20:A:1404:C:H2'	20:A:1405:G:C8	2.43	0.53
16:Q:90:ILE:HG21	20:A:583:A:H5'	1.90	0.53
20:A:501:C:H2'	20:A:502:G:C8	2.43	0.53
1:B:35:GLU:H	1:B:36:ARG:NH2	2.06	0.53
23:Y:214:GLU:O	23:Y:218:GLU:N	2.36	0.53
11:L:113:ARG:HH21	11:L:115:LYS:HB2	1.74	0.53
18:S:78:ARG:HE	20:A:1222:G:H5''	1.74	0.53
20:A:312:C:H2'	20:A:313:A:C8	2.44	0.53
20:A:444:C:H2'	20:A:445:G:C8	2.44	0.53
20:A:736:C:H2'	20:A:737:A:C8	2.44	0.53
7:H:83:ILE:HB	7:H:137:VAL:HG22	1.91	0.53
23:Y:390:VAL:HB	23:Y:394:ALA:HB3	1.91	0.53
11:L:36:VAL:H	11:L:58:VAL:HA	1.74	0.53
11:L:85:ILE:HG13	11:L:98:TYR:HB3	1.90	0.53
1:B:167:PRO:HD2	1:B:188:ALA:CB	2.38	0.53
11:L:45:PRO:HA	11:L:92:ASP:HB3	1.90	0.53
6:G:87:VAL:HG13	6:G:151:TYR:HB3	1.91	0.53
6:G:94:ARG:NH1	20:A:1377:A:OP1	2.42	0.53
20:A:1436:U:H2'	20:A:1437:C:H6	1.73	0.53
7:H:87:SER:HB3	7:H:132:GLU:OE2	2.10	0.53
10:K:40:ILE:HG22	10:K:41:THR:HG23	1.91	0.53
20:A:175:C:H2'	20:A:176:C:H6	1.72	0.52
7:H:6:ILE:O	7:H:10:LEU:HG	2.09	0.52
23:Y:346:LYS:O	23:Y:348:ARG:N	2.43	0.52
1:B:135:GLN:O	1:B:139:LYS:HG3	2.09	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:A:1088:G:H2'	20:A:1089:G:C8	2.43	0.52
20:A:1006:C:H2'	20:A:1007:C:C6	2.45	0.52
23:Y:63:ILE:CG1	26:Y:702:GNP:O1G	2.55	0.52
23:Y:301:ILE:HG21	23:Y:331:TYR:HB3	1.91	0.52
3:D:64:LEU:HD22	3:D:203:VAL:HG11	1.90	0.52
17:R:74:ARG:HH12	20:A:719:C:H42	1.56	0.52
23:Y:394:ALA:O	23:Y:396:ARG:N	2.43	0.52
20:A:1323:G:H2'	20:A:1324:A:C8	2.43	0.52
10:K:34:ASP:O	10:K:36:ASP:N	2.34	0.52
20:A:572:A:HO2'	20:A:916:G:HO2'	1.47	0.52
23:Y:108:PHE:HD1	23:Y:115:GLU:HG3	1.75	0.52
20:A:772:U:H2'	20:A:773:G:C8	2.44	0.52
20:A:68(H):G:N2	20:A:68(R):C:N3	2.46	0.52
20:A:827:U:H3	20:A:872:A:N6	2.06	0.52
20:A:552:U:H2'	20:A:553:A:C8	2.39	0.52
10:K:85:ARG:HA	10:K:110:ASP:O	2.09	0.52
20:A:1440(J):C:H1'	20:A:1440(K):G:C2	2.45	0.52
23:Y:630:GLN:O	23:Y:646:PHE:HB2	2.08	0.52
19:T:50:GLU:HG2	19:T:51:GLU:H	1.74	0.52
3:D:34:GLU:HA	3:D:37:PRO:HG3	1.91	0.52
8:I:50:LEU:HD23	8:I:53:VAL:HG23	1.90	0.52
11:L:69:TYR:CG	11:L:70:ILE:N	2.77	0.52
3:D:15:GLU:HB3	3:D:63:LYS:HE2	1.92	0.52
20:A:163:C:H2'	20:A:164:U:C6	2.44	0.52
6:G:94:ARG:NH2	6:G:95:ARG:HB2	2.25	0.52
12:M:3:ARG:HH21	12:M:7:VAL:HG22	1.74	0.52
3:D:152:SER:HA	3:D:155:LEU:HD12	1.91	0.52
23:Y:208:GLN:O	23:Y:211:GLU:HG2	2.08	0.52
16:Q:22:LEU:HD13	16:Q:41:LYS:HG2	1.91	0.52
23:Y:602:LEU:HA	23:Y:677:GLN:O	2.10	0.52
3:D:62:GLN:NE2	20:A:544:G:OP1	2.33	0.52
7:H:111:ILE:O	7:H:134:ILE:N	2.42	0.52
1:B:81:VAL:O	1:B:85:ALA:N	2.38	0.52
7:H:5:PRO:HA	7:H:8:ASP:HB3	1.91	0.52
3:D:118:ARG:HG3	3:D:136:PRO:HG2	1.91	0.52
22:W:72:C:H2'	22:W:73:A:O4'	2.10	0.52
16:Q:83:ASP:N	16:Q:83:ASP:OD1	2.41	0.52
4:E:57:LYS:HB3	4:E:57:LYS:HZ3	1.73	0.52
20:A:1237:C:H42	20:A:1337:G:H1	1.57	0.52
20:A:1338:G:H21	22:W:41:A:H1'	1.74	0.52
20:A:1381:U:H2'	20:A:1382:C:H5'	1.92	0.52
23:Y:534:ILE:HD11	23:Y:570:GLY:HA3	1.92	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
22:W:39:U:H2'	22:W:40:G:H8	1.75	0.52
23:Y:535:PRO:O	23:Y:537:GLU:N	2.43	0.52
15:P:27:LYS:HG3	15:P:30:GLY:HA3	1.91	0.52
19:T:14:LYS:HG3	19:T:17:ARG:NH2	2.25	0.52
20:A:395:C:H2'	20:A:396:G:H8	1.74	0.52
14:O:33:THR:O	14:O:36:ILE:HB	2.10	0.52
23:Y:628:ARG:HE	23:Y:648:PRO:HG2	1.74	0.52
20:A:1507:A:OP2	21:V:15:A:N6	2.40	0.52
20:A:861:G:H1	20:A:868:C:H42	1.56	0.52
20:A:58:C:H2'	20:A:59:A:O4'	2.09	0.52
12:M:8:GLU:HG2	12:M:22:ILE:HG23	1.91	0.52
20:A:947:G:O2'	20:A:1306:A:H4'	2.09	0.52
3:D:61:LYS:HG3	3:D:206:PHE:HD2	1.74	0.52
20:A:1230:C:H5'	22:W:30:C:H5''	1.91	0.52
20:A:1247:U:H3	20:A:1290:G:H1	1.58	0.52
2:C:119:ARG:HD3	2:C:140:ARG:HH12	1.74	0.52
20:A:1137:C:H4'	20:A:1138:G:C2	2.45	0.52
23:Y:379:GLY:O	23:Y:380:LEU:HB2	2.09	0.52
20:A:1493:A:P	24:U:2:DPP:HB3	2.49	0.52
20:A:1504:G:H4'	20:A:1505:G:O5'	2.09	0.52
11:L:34:ARG:CG	11:L:82:VAL:HG13	2.40	0.52
20:A:154:C:N4	20:A:167:G:H1	2.05	0.52
22:W:58:A:O2'	22:W:60:U:OP2	2.28	0.52
20:A:1113:C:H2'	20:A:1114:C:C6	2.44	0.52
1:B:208:ILE:HD13	1:B:239:VAL:HA	1.92	0.52
16:Q:11:VAL:HG23	16:Q:20:THR:HB	1.92	0.52
11:L:76:ASN:H	11:L:77:LEU:HD12	1.75	0.52
23:Y:163:VAL:HG22	23:Y:258:VAL:HG21	1.92	0.51
20:A:217:C:H2'	20:A:218:C:H6	1.75	0.51
3:D:165:MET:O	3:D:167:GLY:N	2.43	0.51
20:A:1225:A:H2'	20:A:1226:C:C6	2.45	0.51
16:Q:68:ARG:C	16:Q:70:ARG:H	2.13	0.51
20:A:1175:G:H2'	20:A:1176:A:O4'	2.10	0.51
16:Q:22:LEU:HD11	16:Q:39:SER:HB2	1.93	0.51
6:G:42:ILE:HG21	6:G:116:ALA:HB3	1.91	0.51
20:A:1494:G:H2'	20:A:1495:U:H6	1.75	0.51
20:A:1505:G:H5'	20:A:1506:U:H5''	1.90	0.51
1:B:168:THR:C	1:B:171:ALA:H	2.13	0.51
3:D:61:LYS:HD3	3:D:207:TYR:CZ	2.45	0.51
12:M:122:LYS:HB3	20:A:953:G:O2'	2.10	0.51
20:A:974:A:H4'	20:A:975:A:H3'	1.91	0.51
1:B:19:HIS:CG	1:B:20:GLU:N	2.79	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:A:1266:G:N2	20:A:1268:A:H3'	2.25	0.51
12:M:58:GLU:O	12:M:62:ASN:ND2	2.43	0.51
20:A:1511:G:H2'	20:A:1512:U:O4'	2.10	0.51
3:D:165:MET:O	3:D:168:ARG:N	2.43	0.51
12:M:88:ARG:HH11	20:A:1320:C:H4'	1.76	0.51
2:C:48:TYR:O	2:C:50:ALA:N	2.43	0.51
2:C:63:ASN:HA	2:C:98:ASN:HB2	1.92	0.51
1:B:223:ILE:O	1:B:228:GLY:N	2.41	0.51
20:A:1316:G:N1	20:A:1319:A:OP2	2.39	0.51
23:Y:331:TYR:O	23:Y:371:ALA:HB1	2.09	0.51
8:I:61:ALA:O	8:I:63:ILE:HG12	2.11	0.51
20:A:1537:U:O2'	20:A:1538:C:OP1	2.27	0.51
10:K:84:VAL:N	10:K:109:VAL:O	2.43	0.51
20:A:1440(K):G:H2'	20:A:1440(L):G:O4'	2.10	0.51
23:Y:305:PRO:HB2	23:Y:370:LYS:HD2	1.92	0.51
1:B:164:VAL:CG1	1:B:170:GLU:HB3	2.39	0.51
3:D:61:LYS:O	3:D:64:LEU:HB3	2.10	0.51
22:W:42:U:H2'	22:W:43:G:O4'	2.10	0.51
20:A:1298:C:H5'	20:A:1299:A:N3	2.24	0.51
9:J:44:VAL:HA	9:J:65:LEU:O	2.10	0.51
12:M:102:ARG:NH2	20:A:952:U:O4	2.42	0.51
20:A:1016:A:O5'	20:A:1016:A:H8	1.93	0.51
20:A:945:G:C2	20:A:946:A:C8	2.98	0.51
20:A:294:U:OP1	20:A:610:G:O2'	2.28	0.51
20:A:299:G:H2'	20:A:300:A:C8	2.46	0.51
20:A:808:C:H2'	20:A:809:G:C8	2.46	0.51
5:F:46:ARG:HB3	5:F:60:PHE:CE1	2.45	0.51
20:A:151:A:N7	20:A:170:U:O4	2.43	0.51
20:A:10:A:H2'	20:A:11:G:C8	2.46	0.51
20:A:1088:G:H2'	20:A:1089:G:H8	1.76	0.51
20:A:545:C:O2'	20:A:549:C:H5'	2.11	0.51
14:O:8:LYS:HE3	14:O:12:ILE:HD11	1.93	0.51
11:L:113:ARG:NH2	11:L:115:LYS:HB2	2.26	0.51
23:Y:63:ILE:CG2	26:Y:702:GNP:O1G	2.58	0.51
20:A:757:U:H5''	20:A:822:C:O2'	2.10	0.51
11:L:31:PRO:HB3	20:A:553:A:O4'	2.10	0.51
8:I:110:GLU:HG2	8:I:113:LYS:NZ	2.25	0.51
20:A:989:C:H2'	20:A:990:C:C6	2.45	0.51
10:K:82:VAL:N	10:K:107:SER:O	2.44	0.51
23:Y:330:VAL:O	23:Y:331:TYR:CG	2.63	0.51
3:D:15:GLU:OE1	3:D:66:ARG:HG3	2.11	0.51
23:Y:315:LYS:NZ	23:Y:434:GLU:OE2	2.42	0.51

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:A:5:U:HO2'	20:A:6:G:P	2.33	0.51
20:A:1116:C:N3	20:A:1184:G:N2	2.49	0.51
20:A:1389:C:H2'	20:A:1390:U:H6	1.75	0.51
1:B:170:GLU:O	1:B:174:VAL:HG23	2.11	0.51
13:N:45:ARG:HG3	13:N:49:HIS:CE1	2.46	0.51
16:Q:51:TYR:CE1	16:Q:76:LEU:HB2	2.46	0.51
20:A:1026:G:H1	20:A:1035:A:H2	1.58	0.51
20:A:576:G:H8	20:A:881:G:HO2'	1.58	0.51
20:A:1440(L):G:H2'	20:A:1440(M):G:H8	1.76	0.51
23:Y:85:PRO:HB3	23:Y:94:VAL:HG22	1.93	0.51
1:B:68:ILE:HG22	1:B:163:PHE:N	2.26	0.51
1:B:183:PRO:HA	1:B:198:ASP:OD1	2.11	0.51
20:A:869:G:H4'	20:A:872:A:C8	2.45	0.51
20:A:656:C:N4	20:A:750:G:H1	2.08	0.51
20:A:1136:U:H5''	20:A:1137:C:C5	2.46	0.51
20:A:582:U:H3'	20:A:583:A:H8	1.76	0.51
7:H:91:ARG:HB3	7:H:93:VAL:HG23	1.93	0.51
5:F:96:PRO:HA	17:R:32:ARG:HB2	1.93	0.51
12:M:34:LEU:HD13	12:M:41:PRO:HA	1.93	0.51
1:B:71:VAL:HG21	1:B:162:ILE:HD11	1.92	0.50
9:J:55:LYS:HE3	20:A:973:G:H1'	1.92	0.50
23:Y:291:GLY:HA3	23:Y:399:LEU:HA	1.93	0.50
12:M:98:VAL:N	20:A:1308:U:OP1	2.44	0.50
19:T:105:SER:N	20:A:186(A):C:O2	2.36	0.50
6:G:47:CYS:O	6:G:50:ILE:HB	2.10	0.50
12:M:89:GLY:O	12:M:93:ARG:HG3	2.11	0.50
1:B:46:LYS:O	1:B:50:GLU:HG2	2.11	0.50
23:Y:137:ASN:CG	26:Y:702:GNP:O6	2.50	0.50
20:A:1391:U:H2'	20:A:1392:G:C8	2.45	0.50
20:A:126:G:N2	20:A:235:C:N3	2.52	0.50
20:A:687:A:H62	20:A:703:G:H21	1.59	0.50
7:H:30:ARG:NH2	20:A:643:C:OP1	2.44	0.50
3:D:13:ARG:HH11	3:D:40:PRO:HB3	1.75	0.50
16:Q:92:ARG:O	16:Q:95:TYR:HB2	2.11	0.50
20:A:368:U:OP2	23:Y:353:ALA:HA	2.10	0.50
19:T:84:LEU:O	19:T:88:VAL:HG23	2.11	0.50
23:Y:14:ASN:HD21	23:Y:374:LEU:HD22	1.77	0.50
20:A:323:U:H2'	20:A:324:G:O4'	2.10	0.50
6:G:78:ARG:HD2	6:G:79:ARG:H	1.76	0.50
1:B:55:PHE:HE1	1:B:218:ALA:HA	1.76	0.50
23:Y:238:THR:HG22	23:Y:241:GLU:HG2	1.94	0.50
20:A:21:G:H2'	20:A:22:G:C8	2.47	0.50

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:A:1440(C):G:H2'	20:A:1440(D):A:C2	2.47	0.50
9:J:78:ASN:O	9:J:81:THR:OG1	2.29	0.50
9:J:38:ILE:HG23	9:J:71:LEU:HB3	1.92	0.50
23:Y:329:ARG:CB	23:Y:374:LEU:HG	2.36	0.50
20:A:1417:G:H2'	20:A:1482:G:N2	2.27	0.50
6:G:87:VAL:HG12	6:G:155:ARG:HG2	1.93	0.50
6:G:29:LYS:HE3	6:G:101:LEU:HD11	1.92	0.50
14:O:38:ARG:HB3	20:A:740:U:OP1	2.11	0.50
21:V:13:A:H5''	21:V:14:A:OP2	2.11	0.50
20:A:395:C:H2'	20:A:396:G:C8	2.46	0.50
6:G:47:CYS:HA	6:G:50:ILE:HD12	1.93	0.50
20:A:888:G:H3'	20:A:889:A:H2'	1.93	0.50
23:Y:30:GLU:O	23:Y:32:ILE:N	2.44	0.50
11:L:45:PRO:CA	11:L:92:ASP:HB3	2.41	0.50
20:A:385:C:H2'	20:A:386:C:H6	1.77	0.50
23:Y:55:MET:H	23:Y:59:ARG:HB2	1.76	0.50
14:O:23:GLY:HA3	20:A:750:G:N3	2.26	0.50
14:O:50:HIS:CG	20:A:764:C:H5''	2.46	0.50
23:Y:162:VAL:HB	23:Y:255:ILE:HG13	1.93	0.50
1:B:156:LYS:O	1:B:157:ARG:HB2	2.10	0.50
23:Y:11:ARG:HD3	23:Y:40:HIS:CE1	2.46	0.50
20:A:1145:C:HO2'	20:A:1146:A:P	2.34	0.50
20:A:543:C:H2'	20:A:544:G:C8	2.46	0.50
23:Y:315:LYS:H	23:Y:327:PHE:HB2	1.75	0.50
23:Y:443:HIS:CE1	23:Y:445:GLU:HB2	2.46	0.50
23:Y:101:LEU:O	23:Y:128:TYR:OH	2.24	0.50
9:J:80:LYS:HB3	9:J:84:GLN:NE2	2.22	0.50
7:H:15:ASN:ND2	20:A:827:U:O4'	2.36	0.50
7:H:83:ILE:HA	7:H:136:GLU:O	2.12	0.50
20:A:1135:U:O2	20:A:1138:G:N2	2.33	0.50
7:H:44:PHE:HD2	7:H:80:ILE:HG13	1.76	0.50
3:D:204:ILE:O	3:D:208:SER:N	2.41	0.50
22:W:22:G:H2'	22:W:23:A:C8	2.47	0.50
1:B:174:VAL:HG22	1:B:184:VAL:HG11	1.92	0.50
9:J:52:GLY:HA2	20:A:1059:C:O2'	2.12	0.50
3:D:22:LYS:HB3	3:D:26:CYS:HB2	1.92	0.50
10:K:84:VAL:HG23	10:K:110:ASP:HA	1.92	0.50
12:M:48:LEU:HD23	12:M:49:THR:H	1.77	0.50
23:Y:511:LYS:HB2	23:Y:569:ASP:O	2.10	0.50
20:A:1494:G:H2'	20:A:1495:U:C6	2.46	0.50
11:L:22:SER:O	11:L:24:VAL:N	2.33	0.50
3:D:74:GLN:O	3:D:78:LEU:HG	2.12	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:G:69:VAL:HG13	6:G:138:LYS:HB2	1.94	0.50
12:M:94:ARG:CZ	18:S:81:ARG:HG3	2.41	0.50
20:A:1306:A:H1'	20:A:1332:A:N1	2.26	0.50
20:A:1047:G:H1	20:A:1210:C:H42	1.59	0.50
18:S:19:VAL:O	18:S:23:ASN:HB3	2.12	0.50
2:C:95:THR:OG1	2:C:95:THR:O	2.26	0.50
20:A:1277:C:H2'	20:A:1278:U:H5'	1.93	0.50
2:C:160:ALA:O	2:C:162:GLN:N	2.44	0.50
15:P:18:ARG:HG2	15:P:20:VAL:HG12	1.94	0.50
20:A:1221:G:H2'	20:A:1222:G:O4'	2.11	0.49
3:D:53:ASP:OD1	3:D:53:ASP:N	2.45	0.49
11:L:88:GLY:O	11:L:99:HIS:NE2	2.45	0.49
9:J:10:GLY:HA3	9:J:16:LEU:CD2	2.42	0.49
16:Q:45:HIS:CB	16:Q:72:ARG:HG2	2.37	0.49
23:Y:609:GLU:HG2	23:Y:644:ARG:HA	1.94	0.49
20:A:976:G:OP2	20:A:1358:U:O2'	2.29	0.49
1:B:217:ARG:O	1:B:221:LEU:HB2	2.12	0.49
20:A:301:G:H2'	20:A:302:G:C8	2.46	0.49
20:A:1440(A):G:H5"	20:A:1440(B):G:O5'	2.12	0.49
11:L:36:VAL:N	11:L:58:VAL:HA	2.26	0.49
1:B:187:LEU:HD23	1:B:201:ILE:HG22	1.94	0.49
20:A:129(A):G:H5'	20:A:186(K):G:H5'	1.94	0.49
14:O:65:ARG:O	14:O:68:ARG:HB3	2.11	0.49
1:B:33:TYR:O	1:B:34:ALA:O	2.31	0.49
23:Y:32:ILE:HA	23:Y:34:TYR:O	2.13	0.49
1:B:164:VAL:HG12	1:B:165:VAL:N	2.26	0.49
20:A:757:U:H4'	20:A:822:C:O2	2.13	0.49
6:G:87:VAL:HG11	6:G:154:TYR:C	2.32	0.49
3:D:119:GLN:HG2	3:D:120:LEU:HG	1.94	0.49
22:W:71:C:H2'	22:W:72:C:C6	2.47	0.49
7:H:80:ILE:H	7:H:80:ILE:HD12	1.76	0.49
23:Y:580:MET:O	23:Y:583:LYS:HB3	2.12	0.49
9:J:17:ASP:HA	9:J:20:ALA:HB3	1.93	0.49
20:A:1399:C:H42	20:A:1504:G:H1	1.60	0.49
20:A:828:A:H2'	20:A:829:G:O4'	2.12	0.49
20:A:767:A:H2'	20:A:768:A:O4'	2.13	0.49
20:A:408:A:H2'	20:A:409:G:H8	1.76	0.49
20:A:396:G:OP1	23:Y:349:LYS:NZ	2.45	0.49
23:Y:144:ALA:HB3	23:Y:170:ARG:HG3	1.94	0.49
20:A:1062:U:H2'	20:A:1063:C:C6	2.48	0.49
9:J:19:SER:O	9:J:23:ILE:HG12	2.11	0.49
20:A:31:G:N2	20:A:48:C:H5"	2.26	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:31:HIS:HA	2:C:34:LEU:HD12	1.93	0.49
3:D:61:LYS:HA	3:D:203:VAL:HG22	1.94	0.49
11:L:38:THR:CG2	11:L:57:LYS:HB2	2.41	0.49
20:A:828:A:H62	20:A:858:G:N2	2.10	0.49
10:K:110:ASP:O	10:K:112:THR:N	2.45	0.49
23:Y:238:THR:OG1	23:Y:239:GLU:N	2.46	0.49
16:Q:13:ASP:HA	16:Q:19:VAL:HG12	1.94	0.49
7:H:69:ARG:NH2	7:H:74:PRO:O	2.45	0.49
20:A:186:C:H2'	20:A:186(A):C:C6	2.48	0.49
3:D:88:VAL:O	3:D:90:GLY:N	2.45	0.49
23:Y:118:SER:HA	23:Y:121:VAL:HG22	1.94	0.49
3:D:31:CYS:H	3:D:33:MET:HB2	1.76	0.49
20:A:124:G:H2'	20:A:125:U:O4'	2.12	0.49
16:Q:17:LYS:HD2	20:A:255:G:H4'	1.95	0.49
1:B:150:SER:O	1:B:153:ARG:HB3	2.13	0.49
20:A:783:C:H2'	20:A:784:C:H6	1.78	0.49
23:Y:223:PHE:O	23:Y:248:LYS:NZ	2.41	0.49
10:K:29:ILE:HG12	10:K:30:VAL:N	2.27	0.49
15:P:45:THR:HG21	20:A:616:G:O2'	2.12	0.49
20:A:1411:C:H42	20:A:1489:G:H1	1.61	0.49
19:T:87:LYS:O	19:T:91:LEU:HG	2.13	0.49
20:A:485:G:H4'	20:A:486:U:H6	1.78	0.49
11:L:101:VAL:HB	11:L:104:VAL:HG13	1.93	0.49
23:Y:526:VAL:N	23:Y:566:THR:HA	2.27	0.49
9:J:51:ARG:CB	20:A:1060:C:H4'	2.38	0.49
23:Y:74:TRP:HB3	23:Y:77:HIS:HB2	1.95	0.49
20:A:882:C:O2'	20:A:883:C:H5'	2.13	0.49
8:I:70:LYS:O	8:I:73:GLN:HB2	2.13	0.49
2:C:39:ILE:O	2:C:43:LEU:HG	2.12	0.49
13:N:57:ARG:HH11	13:N:57:ARG:HB3	1.76	0.49
22:W:50:C:H2'	22:W:51:A:O4'	2.13	0.49
20:A:738:C:H2'	20:A:739:C:H6	1.77	0.49
20:A:124:G:H5''	20:A:310:G:H21	1.77	0.49
5:F:90:VAL:O	20:A:736:C:H4'	2.13	0.49
6:G:67:GLU:HA	6:G:70:LYS:HD2	1.95	0.49
4:E:133:TYR:HE1	20:A:1078:U:HO2'	1.59	0.49
20:A:260:G:N2	20:A:265:G:N7	2.57	0.49
20:A:363:A:H2'	20:A:364:A:C8	2.48	0.49
2:C:59:ARG:HG2	2:C:64:VAL:HA	1.95	0.49
20:A:1253:G:H2'	20:A:1254:C:C6	2.47	0.49
22:W:19:G:H22	22:W:56:C:H42	1.59	0.49
20:A:975:A:H4'	20:A:976:G:H5''	1.95	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
19:T:31:SER:OG	20:A:1440(M):G:H5''	2.13	0.49
10:K:62:GLN:HG3	10:K:97:ALA:HB2	1.95	0.49
7:H:110:ALA:HB3	7:H:121:ASP:HB3	1.94	0.49
20:A:1419:G:H2'	20:A:1420:C:H6	1.77	0.49
6:G:127:ALA:HA	6:G:135:VAL:HG21	1.95	0.49
23:Y:96:ARG:NH1	23:Y:385:THR:OG1	2.46	0.49
20:A:838(A):U:O2'	20:A:838(B):C:H5''	2.11	0.49
8:I:57:GLY:C	8:I:59:PHE:H	2.17	0.48
23:Y:259:PHE:CZ	23:Y:275:ALA:HB1	2.48	0.48
20:A:595:G:H22	20:A:643:C:H42	1.61	0.48
5:F:12:PRO:O	5:F:13:ASN:ND2	2.46	0.48
20:A:1134:G:H2'	20:A:1135:U:O4'	2.13	0.48
3:D:155:LEU:HB3	3:D:158:ILE:HD13	1.94	0.48
20:A:301:G:H2'	20:A:302:G:H8	1.77	0.48
20:A:1389:C:H2'	20:A:1390:U:C6	2.48	0.48
20:A:943:U:C4	20:A:1340:A:N1	2.79	0.48
20:A:109:A:H62	20:A:324:G:H21	1.60	0.48
23:Y:610:VAL:HG13	23:Y:643:ILE:HB	1.94	0.48
4:E:151:LEU:O	7:H:64:LYS:NZ	2.46	0.48
4:E:127:ASN:O	4:E:131:ILE:HG12	2.12	0.48
3:D:31:CYS:N	3:D:33:MET:HB2	2.29	0.48
3:D:10:ARG:HH21	20:A:542:G:H5''	1.78	0.48
20:A:1297:C:H4'	20:A:1299:A:C2	2.43	0.48
19:T:63:ILE:HB	19:T:81:LYS:HD3	1.94	0.48
16:Q:25:ARG:O	16:Q:26:GLN:NE2	2.45	0.48
23:Y:8:ASP:HB3	23:Y:11:ARG:H	1.77	0.48
3:D:101:LEU:HD13	3:D:138:TYR:HD2	1.78	0.48
11:L:87:GLY:HA2	11:L:98:TYR:H	1.78	0.48
20:A:1028(H):G:H2'	20:A:1033:G:O4'	2.13	0.48
20:A:1415:G:C5	20:A:1416:G:C8	3.01	0.48
20:A:1321:C:H3'	20:A:1322:C:C5'	2.36	0.48
11:L:69:TYR:HB3	11:L:99:HIS:ND1	2.29	0.48
1:B:97:TRP:CE3	1:B:172:ILE:HG13	2.48	0.48
20:A:140:A:H2'	20:A:141:A:H8	1.73	0.48
5:F:46:ARG:HB3	5:F:60:PHE:CD1	2.48	0.48
20:A:243:A:C2	20:A:282:A:N6	2.78	0.48
20:A:1532:U:H1'	20:A:1533:C:OP1	2.13	0.48
11:L:100:ILE:HG22	11:L:101:VAL:N	2.28	0.48
20:A:1238:A:C8	20:A:1303:C:H1'	2.49	0.48
5:F:43:LEU:HD21	5:F:46:ARG:HD2	1.94	0.48
18:S:31:ILE:HG12	18:S:48:THR:O	2.13	0.48
16:Q:40:LYS:HB3	16:Q:42:TYR:CE1	2.46	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:A:504:C:H2'	20:A:511:C:C5	2.49	0.48
23:Y:108:PHE:CD1	23:Y:115:GLU:HG3	2.49	0.48
11:L:33:ARG:HG2	11:L:60:LEU:HB3	1.96	0.48
8:I:121:ARG:HG3	20:A:1350:A:OP1	2.13	0.48
11:L:86:ARG:HB3	11:L:99:HIS:HB2	1.95	0.48
16:Q:57:VAL:HG12	16:Q:76:LEU:HA	1.94	0.48
20:A:1230:C:H5'	22:W:30:C:C5'	2.42	0.48
20:A:953:G:H2'	20:A:954:G:O4'	2.13	0.48
20:A:543:C:H2'	20:A:544:G:H8	1.78	0.48
20:A:1019:C:H2'	20:A:1020:U:O4'	2.14	0.48
20:A:448:A:OP2	20:A:485:G:N2	2.37	0.48
20:A:507:C:H3'	20:A:508:C:H2'	1.96	0.48
9:J:6:ILE:HG22	9:J:98:ILE:HA	1.96	0.48
20:A:738:C:H2'	20:A:739:C:C6	2.49	0.48
3:D:57:ARG:NH1	3:D:202:LEU:HA	2.29	0.48
20:A:1511:G:H1	20:A:1524:C:H42	1.60	0.48
9:J:49:VAL:HG12	9:J:61:GLU:O	2.13	0.48
20:A:1064:G:O2'	20:A:1065:U:OP2	2.32	0.48
10:K:85:ARG:HH22	20:A:708:C:P	2.37	0.48
16:Q:63:ARG:HG3	20:A:130:A:C8	2.49	0.48
19:T:53:LEU:O	19:T:56:MET:HB2	2.12	0.48
1:B:33:TYR:O	1:B:41:ILE:HB	2.14	0.48
3:D:101:LEU:O	3:D:105:VAL:HG23	2.14	0.48
11:L:11:VAL:HG22	16:Q:29:HIS:CD2	2.49	0.48
10:K:50:TYR:CG	10:K:54:ARG:HB3	2.49	0.48
18:S:77:THR:OG1	20:A:958:A:N6	2.47	0.48
21:V:18:G:H2'	21:V:19:G:O4'	2.13	0.48
18:S:41:VAL:C	18:S:43:GLU:H	2.17	0.48
21:V:8:A:HO2'	21:V:9:G:P	2.37	0.48
20:A:144:G:H2'	20:A:145:G:O4'	2.13	0.48
1:B:67:THR:HA	1:B:90:MET:SD	2.54	0.48
3:D:73:ARG:HB2	20:A:546:G:OP1	2.14	0.48
20:A:1040:U:H2'	20:A:1041:A:H8	1.78	0.48
20:A:758:G:H5'	20:A:880:C:H1'	1.95	0.48
17:R:71:LYS:O	17:R:74:ARG:HG3	2.14	0.48
20:A:201:C:O2'	20:A:201(A):U:H2'	2.13	0.48
6:G:103:TRP:HZ3	6:G:138:LYS:HA	1.77	0.48
2:C:35:GLU:HG2	2:C:39:ILE:HD11	1.96	0.48
20:A:1188:A:H2'	20:A:1189:C:O4'	2.13	0.48
20:A:1492:A:H2'	24:U:6:5OH:HNQ	1.77	0.48
20:A:522:C:O4'	20:A:536:C:H4'	2.14	0.48
13:N:41:ARG:HD2	13:N:42:ILE:N	2.29	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:A:975:A:C8	20:A:1357:A:H2	2.32	0.48
8:I:111:ARG:HB3	8:I:113:LYS:HZ2	1.78	0.48
20:A:1343:G:H2'	20:A:1344:C:H6	1.78	0.48
20:A:355:C:H1'	20:A:388:G:H1'	1.96	0.48
20:A:325:A:H2'	20:A:326:G:O4'	2.13	0.48
5:F:18:GLN:O	5:F:21:LEU:HB3	2.14	0.48
19:T:37:SER:O	19:T:40:ALA:HB3	2.14	0.48
20:A:632:A:H2'	20:A:633:G:O4'	2.14	0.48
10:K:31:THR:CA	10:K:42:TRP:HA	2.42	0.48
7:H:10:LEU:O	7:H:14:ARG:HG3	2.13	0.48
20:A:266:G:O2'	20:A:268:C:OP2	2.18	0.48
14:O:32:LEU:O	14:O:36:ILE:HG13	2.14	0.48
23:Y:448:GLN:HB2	23:Y:448:GLN:HE21	1.51	0.48
23:Y:148:LEU:O	23:Y:152:THR:OG1	2.27	0.48
14:O:77:ARG:HA	14:O:80:ALA:HB3	1.96	0.48
6:G:30:ILE:HG22	6:G:39:ALA:HB1	1.95	0.48
23:Y:192:LEU:HG	23:Y:194:THR:HG23	1.96	0.48
20:A:1095:U:H2'	20:A:1096:C:C6	2.49	0.48
20:A:68(L):U:H5''	20:A:68(M):U:OP2	2.13	0.48
14:O:5:LYS:O	14:O:9:GLN:HG2	2.13	0.48
18:S:63:THR:OG1	18:S:66:MET:SD	2.64	0.47
20:A:585:G:H2'	20:A:586:C:C6	2.49	0.47
20:A:62:U:H5'	20:A:385:C:O2	2.13	0.47
20:A:595:G:H22	20:A:643:C:N4	2.12	0.47
23:Y:509:HIS:HB3	23:Y:571:SER:OG	2.14	0.47
20:A:1224:G:H1	20:A:1362(A):C:N4	2.11	0.47
8:I:91:ASP:N	8:I:91:ASP:OD1	2.47	0.47
15:P:25:ARG:NH2	20:A:230:G:O4'	2.47	0.47
2:C:16:ARG:NH2	2:C:183:ASP:OD1	2.47	0.47
11:L:118:SER:O	20:A:35:G:H1'	2.13	0.47
4:E:126:ARG:HA	4:E:131:ILE:HD11	1.95	0.47
20:A:19:C:H2'	20:A:20:U:C6	2.49	0.47
20:A:783:C:H2'	20:A:784:C:C6	2.49	0.47
17:R:60:ALA:O	17:R:64:ARG:HG3	2.14	0.47
20:A:1290:G:H3'	20:A:1291:G:C8	2.49	0.47
10:K:26:ASN:O	10:K:55:LYS:HB2	2.13	0.47
7:H:44:PHE:CD2	7:H:80:ILE:HG13	2.49	0.47
20:A:1424:C:H2'	20:A:1425:U:C6	2.49	0.47
22:W:49:A:C6	22:W:50:C:N4	2.82	0.47
20:A:28:G:O2'	20:A:296:U:H5''	2.14	0.47
2:C:70:VAL:HG23	2:C:104:GLN:H	1.78	0.47
20:A:745:C:H2'	20:A:746:A:H8	1.78	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:123:GLN:NE2	2:C:133:ALA:HB1	2.29	0.47
20:A:1015:A:H2'	20:A:1016:A:C8	2.49	0.47
16:Q:29:HIS:CG	16:Q:32:TYR:HB2	2.49	0.47
7:H:36:LEU:HD22	7:H:61:VAL:HG11	1.97	0.47
23:Y:33:LEU:HG	23:Y:34:TYR:CD2	2.49	0.47
2:C:59:ARG:HD2	2:C:64:VAL:HG22	1.97	0.47
20:A:327:A:O2'	20:A:328:C:O4'	2.29	0.47
1:B:51:LEU:HD22	1:B:55:PHE:HE2	1.78	0.47
6:G:156:TRP:HZ3	20:A:1379:G:H4'	1.79	0.47
20:A:42:G:N3	20:A:622:A:H2	2.12	0.47
6:G:42:ILE:HD12	6:G:115:ARG:HH21	1.79	0.47
23:Y:493:VAL:HG21	23:Y:592:GLU:HB3	1.96	0.47
3:D:79:PHE:CE2	3:D:207:TYR:HB3	2.49	0.47
22:W:18:G:H2'	22:W:57:G:N2	2.30	0.47
20:A:266:G:O2'	20:A:267:C:O5'	2.33	0.47
3:D:96:LEU:HG	3:D:139:ARG:HH22	1.78	0.47
6:G:30:ILE:HD12	6:G:43:PHE:HB2	1.95	0.47
3:D:196:LEU:HD13	3:D:198:VAL:HB	1.96	0.47
14:O:39:LEU:HD12	14:O:56:LEU:HD22	1.95	0.47
3:D:175:SER:O	3:D:183:GLY:HA2	2.15	0.47
23:Y:276:VAL:O	23:Y:280:LEU:HB2	2.15	0.47
17:R:74:ARG:HB3	17:R:79:LEU:HD22	1.96	0.47
23:Y:77:HIS:CE1	23:Y:277:VAL:HG21	2.50	0.47
7:H:14:ARG:NH1	20:A:875:C:O2'	2.46	0.47
12:M:19:LEU:HD12	12:M:25:ILE:HG21	1.97	0.47
20:A:10:A:H2'	20:A:11:G:H8	1.80	0.47
21:V:8:A:O2'	21:V:9:G:OP1	2.27	0.47
20:A:227:G:H2'	20:A:228:A:C8	2.49	0.47
23:Y:149:VAL:O	23:Y:153:MET:HG3	2.14	0.47
9:J:26:ALA:HB1	9:J:85:LEU:CD2	2.45	0.47
12:M:86:CYS:O	12:M:90:LEU:N	2.41	0.47
15:P:25:ARG:NH2	20:A:229:U:O2'	2.32	0.47
20:A:300:A:H8	20:A:300:A:O5'	1.97	0.47
4:E:11:ILE:HG22	4:E:12:LEU:HD12	1.96	0.47
20:A:115:G:H1'	20:A:116:A:C8	2.50	0.47
1:B:169:LYS:O	1:B:172:ILE:HG12	2.14	0.47
22:W:43:G:H2'	22:W:44:G:H8	1.80	0.47
10:K:46:GLY:HA3	10:K:55:LYS:HG2	1.97	0.47
20:A:399:G:H2'	20:A:400:C:C6	2.49	0.47
2:C:61:ALA:C	2:C:63:ASN:H	2.18	0.47
7:H:88:LYS:HB3	20:A:877:C:H5''	1.96	0.47
18:S:6:LYS:HG2	18:S:7:LYS:H	1.80	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:Y:203:GLU:HB3	23:Y:204:GLU:H	1.42	0.47
23:Y:446:THR:OG1	23:Y:447:GLY:N	2.47	0.47
16:Q:45:HIS:HB3	16:Q:72:ARG:HA	1.97	0.47
20:A:832:C:O2'	20:A:1538:C:C5'	2.61	0.47
1:B:92:TYR:CE2	1:B:151:GLY:HA3	2.49	0.47
20:A:593:G:O6	20:A:646:U:O4	2.33	0.47
20:A:1291:G:H2'	20:A:1292:U:C5	2.50	0.47
8:I:69:GLY:HA3	20:A:1371:G:O3'	2.15	0.47
23:Y:106:VAL:HB	23:Y:108:PHE:CZ	2.50	0.47
20:A:252:U:H2'	20:A:253:U:C5	2.49	0.47
20:A:256:U:O4	20:A:270:A:N1	2.48	0.47
20:A:859:A:H2'	20:A:860:A:C8	2.49	0.47
11:L:109:GLY:HA3	11:L:120:TYR:C	2.34	0.47
20:A:186(G):C:H1'	20:A:186(K):G:N1	2.29	0.47
20:A:68(O):A:H3'	20:A:68(P):C:C4'	2.45	0.47
23:Y:257:PRO:HB2	23:Y:259:PHE:CE1	2.50	0.47
20:A:712:A:H2'	20:A:713:G:O4'	2.15	0.47
1:B:103:THR:C	1:B:105:PHE:H	2.18	0.47
20:A:1440(L):G:H2'	20:A:1440(M):G:C8	2.50	0.47
4:E:46:GLY:HA3	4:E:54:ALA:HB1	1.96	0.47
7:H:86:ILE:HG13	7:H:133:LEU:HD22	1.96	0.47
20:A:607:A:H2'	20:A:608:A:O4'	2.14	0.47
20:A:346:G:H5'	20:A:347:G:OP2	2.15	0.47
2:C:83:ARG:O	2:C:87:LEU:HD23	2.14	0.47
9:J:82:ILE:O	9:J:86:MET:HG2	2.14	0.47
23:Y:466:LEU:HG	23:Y:472:VAL:HB	1.95	0.47
20:A:947:G:H2'	20:A:948:C:H6	1.78	0.47
11:L:52:LEU:HD12	11:L:54:LYS:NZ	2.29	0.47
16:Q:21:VAL:CG1	16:Q:59:ILE:HD11	2.44	0.47
16:Q:45:HIS:CB	16:Q:72:ARG:HA	2.44	0.47
20:A:1252:A:H61	20:A:1285:A:H61	1.63	0.47
20:A:237:C:H2'	20:A:238:G:C8	2.49	0.47
11:L:123:LYS:HD2	20:A:37:U:OP2	2.15	0.47
20:A:1223:C:OP2	20:A:1224:G:H2'	2.15	0.47
20:A:1270:C:H2'	20:A:1271:G:H8	1.80	0.47
12:M:19:LEU:HA	12:M:22:ILE:HD12	1.97	0.47
2:C:121:ALA:HB2	2:C:187:ALA:HB1	1.97	0.47
7:H:87:SER:HB2	7:H:93:VAL:HB	1.97	0.47
3:D:135:LEU:HD12	20:A:403:C:H5'	1.97	0.47
3:D:100:ARG:O	3:D:104:VAL:HG23	2.15	0.47
5:F:21:LEU:O	5:F:25:ILE:HG12	2.14	0.47
6:G:72:ARG:HA	6:G:96:GLN:NE2	2.30	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:I:116:LYS:HG2	8:I:122:ALA:HA	1.97	0.47
20:A:437:U:H3	20:A:495:A:H62	1.63	0.47
23:Y:197:ARG:HG3	23:Y:198:GLU:H	1.80	0.47
11:L:104:VAL:HG23	11:L:105:TYR:H	1.80	0.46
20:A:949:A:H2'	20:A:950:U:C6	2.51	0.46
20:A:294:U:H2'	20:A:295:C:C6	2.50	0.46
10:K:107:SER:HA	17:R:86:VAL:HG13	1.97	0.46
23:Y:14:ASN:HD22	23:Y:80:ASN:HB2	1.79	0.46
23:Y:290:LYS:HB3	23:Y:298:VAL:HG22	1.97	0.46
17:R:33:ASP:HB3	17:R:36:ASN:ND2	2.29	0.46
23:Y:41:LYS:HG2	23:Y:43:GLY:H	1.78	0.46
3:D:62:GLN:O	3:D:66:ARG:HG2	2.15	0.46
3:D:14:ARG:NH2	3:D:40:PRO:HG2	2.30	0.46
17:R:60:ALA:HB2	20:A:834:C:H5''	1.96	0.46
20:A:396:G:H2'	20:A:398:C:H5	1.79	0.46
8:I:73:GLN:O	8:I:77:ILE:HG13	2.15	0.46
1:B:139:LYS:O	1:B:143:GLU:HG2	2.14	0.46
2:C:72:LYS:HE3	2:C:74:GLY:H	1.81	0.46
3:D:102:ASP:HA	3:D:121:VAL:HG21	1.96	0.46
5:F:75:LEU:O	5:F:79:LEU:HG	2.15	0.46
20:A:1068:G:H1	20:A:1107:C:H42	1.63	0.46
15:P:5:ARG:HH12	15:P:24:ALA:HA	1.79	0.46
3:D:13:ARG:NH1	3:D:40:PRO:HB3	2.29	0.46
20:A:1292:U:O5'	20:A:1292:U:H6	1.98	0.46
8:I:69:GLY:O	8:I:73:GLN:HG3	2.15	0.46
3:D:122:ARG:HH21	20:A:403:C:H4'	1.80	0.46
23:Y:145:ASP:OD2	23:Y:148:LEU:N	2.46	0.46
20:A:1518:A:H2'	20:A:1519:A:C8	2.50	0.46
1:B:149:LEU:HD22	1:B:152:PHE:HD1	1.79	0.46
20:A:866:C:H4'	20:A:919:A:H5'	1.97	0.46
8:I:63:ILE:HG22	8:I:64:THR:H	1.80	0.46
4:E:50:GLU:CG	4:E:52:PRO:HD2	2.43	0.46
23:Y:507:TYR:HE1	23:Y:571:SER:HG	1.63	0.46
20:A:142:G:O2'	20:A:195:A:N6	2.46	0.46
7:H:91:ARG:HH22	20:A:564:C:H4'	1.80	0.46
7:H:100:ILE:HA	7:H:101:PRO:HD3	1.82	0.46
23:Y:530:VAL:HG13	23:Y:531:GLY:H	1.81	0.46
17:R:44:LEU:HG	17:R:50:ILE:HA	1.96	0.46
20:A:807:A:H2'	20:A:808:C:H5'	1.97	0.46
20:A:127:G:N2	20:A:234:C:N3	2.51	0.46
6:G:87:VAL:HG22	6:G:151:TYR:CG	2.50	0.46
18:S:73:GLU:HA	20:A:1320:C:H1'	1.98	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:A:1298:C:H5'	20:A:1299:A:C2	2.50	0.46
19:T:56:MET:HE1	19:T:88:VAL:HG21	1.98	0.46
20:A:447:G:N1	20:A:485:G:H1'	2.31	0.46
3:D:121:VAL:HA	3:D:126:ILE:HG13	1.96	0.46
1:B:200:ILE:HG22	1:B:202:PRO:HD3	1.97	0.46
20:A:113:G:H2'	20:A:114:U:C6	2.51	0.46
1:B:54:THR:O	1:B:58:ILE:HG12	2.15	0.46
23:Y:314:PHE:CE1	23:Y:327:PHE:HB3	2.50	0.46
20:A:1355:G:H1	20:A:1367:C:H42	1.64	0.46
9:J:46:ARG:HD2	13:N:61:TRP:CH2	2.50	0.46
23:Y:162:VAL:HB	23:Y:255:ILE:CG1	2.45	0.46
2:C:5:ILE:HD13	2:C:6:HIS:H	1.79	0.46
15:P:48:TRP:CE3	15:P:49:LEU:HB2	2.50	0.46
5:F:100:ASN:HA	17:R:23:LYS:HE3	1.97	0.46
23:Y:17:ILE:HG22	23:Y:25:LYS:HG2	1.98	0.46
20:A:1001:G:H2'	20:A:1002:G:C8	2.50	0.46
20:A:922:G:H2'	20:A:923:A:H8	1.79	0.46
1:B:162:ILE:O	1:B:185:ILE:O	2.34	0.46
4:E:106:PRO:O	4:E:110:LEU:HG	2.16	0.46
17:R:74:ARG:HE	17:R:79:LEU:HD22	1.80	0.46
10:K:18:ARG:HG2	10:K:33:THR:O	2.16	0.46
23:Y:600:VAL:HG23	23:Y:684:GLN:HE22	1.81	0.46
17:R:53:ARG:NH2	17:R:59:SER:HA	2.30	0.46
20:A:186(N):U:H2'	20:A:186(O):G:H8	1.80	0.46
23:Y:628:ARG:HG3	23:Y:651:GLU:HG2	1.96	0.46
20:A:888:G:H5''	20:A:889:A:H3'	1.97	0.46
20:A:252:U:O2'	20:A:275:G:N2	2.46	0.46
7:H:35:ILE:HA	7:H:35:ILE:HD13	1.78	0.46
18:S:77:THR:O	18:S:77:THR:OG1	2.23	0.46
20:A:150:C:H2'	20:A:151:A:O4'	2.16	0.46
4:E:19:MET:SD	20:A:15:G:H1'	2.56	0.46
20:A:974:A:H8	20:A:974:A:OP1	1.98	0.46
20:A:833:U:H2'	20:A:834:C:H6	1.79	0.46
23:Y:536:LYS:HE3	23:Y:536:LYS:N	2.31	0.46
11:L:66:VAL:HB	11:L:98:TYR:CD1	2.46	0.46
20:A:950:U:H2'	20:A:951:G:H8	1.79	0.46
23:Y:63:ILE:HG13	26:Y:702:GNP:PG	2.55	0.46
11:L:47:LYS:HE3	20:A:1492:A:H5''	1.98	0.46
12:M:125:ARG:HD2	20:A:969:A:C6	2.51	0.46
4:E:51:VAL:HB	4:E:52:PRO:HD3	1.98	0.46
20:A:663:A:H2'	20:A:664:G:O4'	2.16	0.46
3:D:100:ARG:HH12	3:D:118:ARG:NH2	2.13	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:F:33:TYR:CD2	5:F:75:LEU:HB2	2.50	0.46
7:H:39:LEU:HB3	7:H:45:ILE:H	1.81	0.46
20:A:1124:G:O2'	20:A:1145:C:N4	2.48	0.46
11:L:9:GLN:NE2	20:A:880:C:H3'	2.31	0.46
4:E:78:HIS:CE1	4:E:143:ARG:H	2.34	0.46
7:H:14:ARG:HG2	7:H:83:ILE:HG23	1.98	0.46
20:A:612:C:N4	20:A:628:G:H1	2.12	0.46
20:A:68(V):G:C2	20:A:68(W):G:H1'	2.51	0.46
20:A:1412:C:H2'	20:A:1413:A:H8	1.81	0.46
10:K:65:ALA:HB3	10:K:97:ALA:HB3	1.98	0.46
7:H:112:LEU:HG	7:H:119:LEU:O	2.15	0.46
20:A:1242:C:H2'	20:A:1243:C:C6	2.51	0.46
20:A:1430:C:H2'	20:A:1431:C:C6	2.50	0.46
10:K:63:LEU:O	10:K:66:LEU:HB2	2.15	0.46
20:A:901:A:H8	20:A:901:A:O5'	1.98	0.46
11:L:102:ARG:C	11:L:104:VAL:H	2.19	0.46
11:L:56:ALA:HB3	11:L:68:ALA:CB	2.26	0.46
23:Y:512:ILE:HG22	23:Y:567:LEU:HB3	1.97	0.46
20:A:297:G:H4'	20:A:557:G:O2'	2.14	0.46
20:A:667:G:H2'	20:A:668:G:H8	1.81	0.46
23:Y:310:ALA:O	23:Y:331:TYR:HB2	2.16	0.46
18:S:77:THR:HG1	20:A:958:A:H62	1.62	0.46
8:I:57:GLY:O	8:I:59:PHE:N	2.48	0.46
23:Y:291:GLY:O	23:Y:299:VAL:HG12	2.15	0.46
20:A:697:U:O2	20:A:785:G:N2	2.38	0.46
20:A:691:G:H1'	20:A:696:A:N6	2.30	0.46
7:H:69:ARG:HG3	7:H:69:ARG:H	1.59	0.46
7:H:9:MET:O	7:H:12:ARG:N	2.49	0.46
2:C:35:GLU:O	2:C:38:ARG:N	2.50	0.46
3:D:121:VAL:HA	3:D:126:ILE:CG1	2.46	0.46
8:I:48:GLU:N	8:I:49:PRO:HD2	2.31	0.46
20:A:1303:C:N3	20:A:1334:G:N2	2.41	0.45
20:A:68(N):U:H3'	20:A:68(O):A:C8	2.51	0.45
20:A:166:G:H2'	20:A:167:G:O4'	2.16	0.45
23:Y:631:ILE:C	23:Y:645:ALA:HA	2.36	0.45
20:A:683:G:H2'	20:A:684:A:C8	2.52	0.45
16:Q:64:PRO:HB3	16:Q:70:ARG:NH2	2.30	0.45
9:J:46:ARG:HD2	13:N:61:TRP:CZ3	2.50	0.45
7:H:93:VAL:O	7:H:132:GLU:HA	2.16	0.45
18:S:10:PHE:CG	20:A:1318:A:H4'	2.51	0.45
20:A:1488:G:H2'	20:A:1489:G:O4'	2.15	0.45
20:A:413:G:H4'	20:A:414:A:H5'	1.98	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:103:ASN:HA	3:D:106:TYR:HB3	1.98	0.45
7:H:7:ALA:O	7:H:11:THR:OG1	2.30	0.45
20:A:862:C:C2	20:A:867:G:N2	2.74	0.45
20:A:18:C:O2	20:A:917:G:N1	2.37	0.45
11:L:15:ARG:HH12	20:A:563:A:H2'	1.81	0.45
6:G:111:ARG:HB2	6:G:119:ARG:HD2	1.99	0.45
4:E:94:ALA:HA	20:A:6:G:O6	2.15	0.45
12:M:102:ARG:HH21	12:M:105:THR:HG23	1.81	0.45
20:A:1316:G:H1'	20:A:1360:A:H2	1.80	0.45
5:F:4:TYR:CD1	5:F:92:LYS:HA	2.51	0.45
18:S:27:GLU:HB3	18:S:28:LYS:H	1.47	0.45
20:A:591:U:H2'	20:A:592:G:C8	2.51	0.45
20:A:56:U:H2'	20:A:57:G:H8	1.81	0.45
1:B:74:LYS:H	1:B:74:LYS:HD2	1.81	0.45
18:S:78:ARG:O	18:S:81:ARG:NH1	2.48	0.45
19:T:72:LEU:HB3	19:T:77:ALA:HB2	1.98	0.45
20:A:1357:A:N6	20:A:1365:G:H1	2.13	0.45
20:A:1015:A:C6	20:A:1016:A:C6	3.04	0.45
3:D:72:GLU:CD	20:A:545:C:H5''	2.36	0.45
20:A:992:U:H1'	20:A:993:G:OP2	2.17	0.45
16:Q:12:SER:HB2	16:Q:14:LYS:HE2	1.99	0.45
20:A:359:U:H2'	20:A:360:A:C8	2.51	0.45
3:D:93:PHE:O	3:D:97:LEU:HG	2.16	0.45
23:Y:413:ILE:HA	23:Y:476:VAL:HA	1.98	0.45
20:A:776:G:HO2'	20:A:777:A:H8	1.63	0.45
23:Y:136:ALA:H	23:Y:260:LEU:HA	1.81	0.45
23:Y:21:ILE:HG13	23:Y:22:ASP:N	2.32	0.45
20:A:230:G:H2'	20:A:231:G:O4'	2.17	0.45
8:I:53:VAL:O	8:I:55:ALA:N	2.49	0.45
20:A:894:G:H2'	20:A:895:G:O4'	2.17	0.45
14:O:28:GLN:HB3	20:A:657:G:H4'	1.98	0.45
20:A:34:C:H2'	20:A:35:G:C8	2.51	0.45
15:P:81:ARG:HA	20:A:458(E):A:H4'	1.98	0.45
20:A:68(X):U:H2'	20:A:68(Y):C:C6	2.52	0.45
3:D:14:ARG:NH2	20:A:542:G:O3'	2.50	0.45
20:A:151:A:H62	20:A:170:U:H3	1.65	0.45
8:I:111:ARG:NH1	20:A:1368:G:OP1	2.50	0.45
6:G:95:ARG:HE	6:G:99:LEU:HD11	1.82	0.45
20:A:1224:G:C2	20:A:1362(A):C:N3	2.85	0.45
20:A:1089:G:H2'	20:A:1090:U:O4'	2.16	0.45
23:Y:462:ILE:O	23:Y:466:LEU:HB2	2.16	0.45
1:B:75:LYS:O	1:B:78:GLN:HB3	2.17	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:Y:632:LEU:N	23:Y:644:ARG:O	2.50	0.45
20:A:254:G:H2'	20:A:255:G:H8	1.82	0.45
20:A:612:C:H2'	20:A:613:C:O4'	2.15	0.45
2:C:136:GLN:O	2:C:140:ARG:HG3	2.16	0.45
20:A:1090:U:H2'	20:A:1091:U:C6	2.52	0.45
18:S:5:LEU:HD23	18:S:10:PHE:HB2	1.98	0.45
20:A:269:C:H2'	20:A:270:A:C8	2.52	0.45
2:C:109:PRO:HG2	2:C:110:ASN:OD1	2.17	0.45
20:A:1084:G:N7	20:A:1085:U:N3	2.64	0.45
20:A:936:C:H2'	20:A:937:A:O4'	2.16	0.45
6:G:107:ALA:HB3	6:G:134:ALA:HB2	1.99	0.45
20:A:234:C:H2'	20:A:235:C:H6	1.82	0.45
1:B:162:ILE:HG12	1:B:164:VAL:CG2	2.47	0.45
1:B:165:VAL:O	1:B:187:LEU:N	2.46	0.45
1:B:108:ILE:O	1:B:112:VAL:HG23	2.16	0.45
9:J:50:ILE:HG12	13:N:41:ARG:HH12	1.81	0.45
20:A:581:G:H8	20:A:581:G:OP2	1.99	0.45
20:A:254:G:H2'	20:A:255:G:C8	2.52	0.45
20:A:1440(J):C:H1'	20:A:1440(K):G:N2	2.31	0.45
12:M:66:LEU:O	12:M:68:GLY:N	2.50	0.45
7:H:88:LYS:H	7:H:88:LYS:HG3	1.55	0.45
9:J:53:PRO:HG3	20:A:1058:G:N2	2.31	0.45
15:P:51:VAL:HG12	15:P:52:ASP:H	1.81	0.45
19:T:103:GLY:C	20:A:191:G:H21	2.20	0.45
23:Y:526:VAL:H	23:Y:566:THR:HA	1.81	0.45
11:L:93:LEU:HD11	11:L:96:VAL:HG13	1.99	0.45
20:A:781:A:H2	20:A:1514:C:H1'	1.80	0.45
23:Y:325:LEU:HD13	23:Y:327:PHE:HE2	1.82	0.45
23:Y:356:LEU:HB2	23:Y:378:VAL:CG2	2.47	0.45
23:Y:322:VAL:HB	23:Y:378:VAL:HG13	1.99	0.45
13:N:61:TRP:CZ2	20:A:1368:G:H4'	2.50	0.45
19:T:36:LEU:HG	19:T:62:LEU:HD12	1.98	0.45
7:H:120:THR:H	7:H:123:GLU:HB2	1.82	0.45
7:H:119:LEU:HB3	7:H:123:GLU:HB3	1.98	0.45
6:G:138:LYS:O	6:G:142:GLU:HG2	2.16	0.45
2:C:83:ARG:NH1	2:C:87:LEU:HD21	2.32	0.45
20:A:134:A:H2'	20:A:135:C:C6	2.52	0.45
4:E:39:GLY:O	4:E:69:VAL:N	2.50	0.45
5:F:99:ALA:N	17:R:29:PHE:O	2.43	0.45
2:C:139:GLN:O	2:C:143:GLU:HG3	2.17	0.45
20:A:1478:C:H2'	20:A:1479:C:H6	1.81	0.45
11:L:58:VAL:CG1	11:L:60:LEU:HD13	2.46	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:A:584:G:H1	20:A:757:U:H3	1.62	0.45
23:Y:133:ILE:HB	23:Y:259:PHE:CE1	2.51	0.45
2:C:84:ILE:HG13	2:C:101:LEU:HD13	1.99	0.45
2:C:65:ALA:O	2:C:67:THR:N	2.50	0.45
6:G:89:MET:HA	6:G:155:ARG:HD2	1.97	0.45
5:F:49:ALA:HB1	17:R:80:PRO:HB3	1.98	0.45
12:M:122:LYS:NZ	12:M:125:ARG:HH21	2.14	0.45
3:D:21:LEU:HD11	3:D:66:ARG:O	2.16	0.45
14:O:35:ARG:O	14:O:38:ARG:HB2	2.17	0.45
20:A:1213:A:O2'	20:A:1215:G:C8	2.70	0.45
23:Y:170:ARG:HB3	23:Y:171:GLU:H	1.58	0.45
20:A:1440(D):A:H2'	20:A:1440(D):A:N3	2.32	0.45
4:E:34:VAL:HG11	4:E:63:ARG:HG2	1.99	0.45
20:A:996:A:H2'	20:A:997:U:H6	1.82	0.45
6:G:97:GLN:O	6:G:100:ALA:HB3	2.17	0.45
15:P:54:GLU:H	15:P:54:GLU:HG3	1.47	0.45
23:Y:25:LYS:NZ	23:Y:84:THR:HG23	2.31	0.45
1:B:101:MET:HG3	1:B:101:MET:H	1.58	0.45
20:A:255:G:O6	20:A:271:C:N3	2.49	0.45
23:Y:616:TYR:CE1	23:Y:666:ARG:HD3	2.52	0.45
16:Q:63:ARG:NH2	20:A:186(I):U:H1'	2.32	0.45
5:F:19:LEU:HD11	5:F:59:TYR:CE1	2.52	0.45
16:Q:83:ASP:O	16:Q:87:LYS:HG3	2.17	0.45
6:G:26:PHE:CE2	6:G:30:ILE:HD11	2.51	0.45
18:S:7:LYS:HA	18:S:7:LYS:HD3	1.73	0.45
20:A:1516:G:H2'	20:A:1518:A:OP2	2.16	0.45
13:N:43:CYS:O	13:N:46:GLU:HG2	2.17	0.45
7:H:60:ARG:NH1	7:H:60:ARG:HB2	2.32	0.45
12:M:120:LYS:HG2	20:A:955:U:H5'	2.00	0.45
19:T:56:MET:SD	19:T:88:VAL:HG21	2.57	0.45
20:A:419:C:H2'	20:A:420:U:O4'	2.17	0.45
22:W:75:C:O3'	22:W:76:A:H8	1.98	0.45
19:T:25:ARG:HG3	19:T:29:LYS:HE3	1.99	0.45
11:L:78:GLN:H	11:L:78:GLN:HG2	1.56	0.45
11:L:60:LEU:HB2	11:L:62:SER:H	1.80	0.44
20:A:984:C:N3	20:A:1221:G:N2	2.47	0.44
20:A:867:G:H2'	20:A:868:C:C6	2.52	0.44
15:P:81:ARG:HH11	15:P:81:ARG:HB2	1.82	0.44
20:A:124:G:OP1	20:A:310:G:N2	2.50	0.44
18:S:49:ILE:HG22	18:S:51:VAL:HG13	1.98	0.44
19:T:14:LYS:HA	19:T:17:ARG:NE	2.32	0.44
23:Y:342:TYR:N	23:Y:390:VAL:O	2.39	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:A:186(C):G:C6	20:A:186(O):G:C6	3.05	0.44
2:C:72:LYS:HA	2:C:72:LYS:HD2	1.83	0.44
2:C:110:ASN:OD1	2:C:110:ASN:N	2.49	0.44
20:A:997:U:H3	20:A:1044:A:H2	1.64	0.44
7:H:104:ARG:HB3	7:H:107:LEU:HG	1.99	0.44
20:A:1428:A:H2'	20:A:1429:C:H6	1.82	0.44
6:G:23:VAL:O	6:G:27:ILE:HG13	2.16	0.44
7:H:21:LYS:N	7:H:65:TYR:OH	2.50	0.44
23:Y:683:VAL:HG12	23:Y:687:LEU:HG	1.98	0.44
11:L:104:VAL:HG23	11:L:106:ASP:H	1.82	0.44
8:I:117:HIS:HB2	8:I:121:ARG:HB3	1.98	0.44
20:A:217:C:H2'	20:A:218:C:C6	2.52	0.44
9:J:16:LEU:HA	9:J:16:LEU:HD22	1.79	0.44
20:A:567:G:C2	20:A:568:G:H1'	2.51	0.44
2:C:54:ARG:HB3	2:C:56:ASP:OD1	2.17	0.44
3:D:15:GLU:OE1	3:D:63:LYS:HG3	2.17	0.44
16:Q:69:LYS:HG3	20:A:254:G:H5''	1.99	0.44
15:P:31:LYS:HB3	15:P:31:LYS:HE2	1.78	0.44
5:F:40:VAL:HG23	5:F:63:TYR:CD1	2.53	0.44
14:O:68:ARG:NH1	20:A:583:A:OP1	2.50	0.44
2:C:6:HIS:HB3	2:C:9:GLY:H	1.82	0.44
1:B:207:ALA:O	1:B:211:ILE:HG12	2.18	0.44
20:A:31:G:H22	20:A:48:C:H5''	1.82	0.44
12:M:120:LYS:O	12:M:121:LYS:HB2	2.18	0.44
23:Y:41:LYS:HG2	23:Y:43:GLY:N	2.32	0.44
20:A:1347:G:H4'	20:A:1348:U:H6	1.82	0.44
23:Y:188:TYR:CD2	23:Y:267:LYS:HG2	2.53	0.44
15:P:40:ASP:OD2	15:P:42:ARG:HG2	2.17	0.44
16:Q:66:SER:OG	16:Q:67:LYS:N	2.51	0.44
3:D:156:GLU:HB3	3:D:157:LEU:HD12	1.99	0.44
20:A:6:G:O2'	20:A:7:G:H5''	2.17	0.44
12:M:5:ALA:O	12:M:7:VAL:N	2.47	0.44
2:C:4:LYS:HA	2:C:4:LYS:HZ3	1.81	0.44
1:B:123:ALA:HA	1:B:127:ILE:HD11	1.99	0.44
6:G:15:ASP:HB2	6:G:20:ASP:O	2.16	0.44
17:R:47:THR:HG23	17:R:49:LYS:H	1.82	0.44
3:D:29:PRO:HG2	3:D:30:LYS:HZ3	1.82	0.44
20:A:1401:G:H1	20:A:1501:C:H42	1.64	0.44
22:W:64:G:N1	22:W:65:U:O4	2.50	0.44
11:L:70:ILE:HB	11:L:72:GLY:H	1.82	0.44
22:W:19:G:OP1	22:W:59:A:N6	2.50	0.44
16:Q:41:LYS:HE3	20:A:277:C:OP1	2.17	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:J:22:LYS:NZ	9:J:26:ALA:HB2	2.33	0.44
20:A:996:A:H2'	20:A:997:U:C6	2.52	0.44
20:A:1428:A:H2'	20:A:1429:C:C6	2.52	0.44
1:B:12:GLU:HB3	1:B:44:LEU:HD13	2.00	0.44
14:O:17:ARG:NE	14:O:17:ARG:HA	2.33	0.44
20:A:369:C:N4	20:A:392:G:N1	2.23	0.44
20:A:1507:A:P	21:V:15:A:H61	2.41	0.44
23:Y:631:ILE:HA	23:Y:645:ALA:CA	2.47	0.44
20:A:68(Y):C:H2'	20:A:101:A:O4'	2.16	0.44
20:A:1374:A:H2'	20:A:1375:A:C8	2.52	0.44
2:C:151:VAL:O	2:C:168:ALA:HB3	2.17	0.44
20:A:1299:A:H2'	20:A:1301:U:C6	2.52	0.44
20:A:1284:C:OP2	20:A:1285:A:O2'	2.32	0.44
1:B:105:PHE:HB3	1:B:106:LYS:NZ	2.33	0.44
15:P:67:THR:O	15:P:71:ARG:NH1	2.50	0.44
20:A:1178:G:N2	20:A:1180:A:H3'	2.33	0.44
3:D:122:ARG:HD3	3:D:136:PRO:HD3	1.99	0.44
20:A:1495:U:OP2	23:Y:504:ARG:NH1	2.44	0.44
3:D:30:LYS:HE2	3:D:30:LYS:N	2.33	0.44
20:A:335:C:H1'	20:A:1434:A:H1'	1.99	0.44
16:Q:52:LYS:HE3	16:Q:52:LYS:HB3	1.82	0.44
23:Y:514:VAL:HA	23:Y:565:VAL:C	2.37	0.44
20:A:1238:A:H2	20:A:1241:G:H21	1.65	0.44
1:B:158:LEU:HA	1:B:159:PRO:HD3	1.80	0.44
6:G:25:ALA:O	6:G:28:ASN:HB2	2.18	0.44
20:A:582:U:H2'	20:A:583:A:O4'	2.17	0.44
6:G:70:LYS:H	6:G:138:LYS:HE3	1.82	0.44
2:C:110:ASN:HB3	2:C:141:VAL:HA	2.00	0.44
20:A:477:G:H2'	20:A:478:A:O4'	2.18	0.44
16:Q:94:ASN:O	16:Q:98:LEU:HD12	2.17	0.44
20:A:1508:G:H2'	20:A:1509:C:O4'	2.18	0.44
20:A:1056:U:H2'	20:A:1057:G:C8	2.53	0.44
5:F:87:ARG:CZ	20:A:673:G:H4'	2.47	0.44
20:A:406:G:H1	20:A:436:C:N4	2.12	0.44
7:H:4:ASP:OD2	7:H:6:ILE:HB	2.17	0.44
10:K:94:ALA:O	10:K:98:LEU:HG	2.17	0.44
7:H:112:LEU:HB3	7:H:133:LEU:HA	1.99	0.44
20:A:1177:G:H2'	20:A:1178:G:O4'	2.17	0.44
3:D:28:SER:HB2	3:D:29:PRO:HD3	2.00	0.44
6:G:13:GLN:O	6:G:24:THR:OG1	2.17	0.44
20:A:998:G:H2'	20:A:998(A):C:C6	2.53	0.44
11:L:56:ALA:O	11:L:58:VAL:HG23	2.17	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:57:ARG:HG3	3:D:202:LEU:O	2.18	0.44
10:K:120:ARG:NH1	20:A:1524:C:H5'	2.31	0.44
19:T:22:ARG:HB2	20:A:323:U:H4'	2.00	0.44
4:E:86:ALA:HB1	4:E:125:SER:HB3	2.00	0.44
20:A:503:C:O2	20:A:510:A:H2	2.00	0.44
2:C:50:ALA:O	2:C:71:ALA:HB3	2.17	0.44
9:J:26:ALA:HB1	9:J:85:LEU:HD22	1.99	0.44
23:Y:544:LYS:HA	23:Y:547:GLU:HB3	1.99	0.44
19:T:12:ALA:O	19:T:15:ARG:HB2	2.18	0.44
13:N:13:THR:HA	13:N:14:PRO:HD2	1.91	0.44
23:Y:512:ILE:HA	23:Y:567:LEU:HA	1.99	0.44
1:B:162:ILE:HG23	1:B:184:VAL:HA	2.00	0.44
11:L:57:LYS:HA	11:L:65:GLU:O	2.18	0.44
20:A:559:A:H4'	20:A:560:U:H3'	2.00	0.44
23:Y:13:ARG:HD3	23:Y:79:ILE:HG12	2.00	0.44
20:A:1374:A:H2'	20:A:1375:A:H8	1.82	0.44
20:A:426:G:H2'	20:A:427:U:O4'	2.18	0.44
20:A:149:A:H2'	20:A:150:C:H6	1.81	0.44
9:J:44:VAL:O	9:J:46:ARG:HD3	2.18	0.44
14:O:36:ILE:CD1	14:O:60:VAL:HG22	2.48	0.44
10:K:34:ASP:OD2	10:K:38:ASN:N	2.51	0.44
6:G:15:ASP:HB3	6:G:19:GLY:N	2.33	0.44
20:A:709:G:H2'	20:A:710:G:H8	1.82	0.44
3:D:159:ARG:O	3:D:163:GLU:HB2	2.18	0.44
1:B:187:LEU:HD22	1:B:188:ALA:N	2.32	0.43
11:L:73:GLU:HA	20:A:521:G:OP1	2.18	0.43
20:A:68(S):C:C4	20:A:68(T):G:N7	2.86	0.43
4:E:18:ARG:NH2	4:E:25:ARG:HD2	2.32	0.43
20:A:1130:A:N6	20:A:1131:G:O6	2.50	0.43
5:F:12:PRO:HD2	5:F:86:ARG:HH11	1.83	0.43
7:H:120:THR:N	7:H:123:GLU:HB2	2.33	0.43
7:H:9:MET:HG3	7:H:26:VAL:HG11	2.00	0.43
23:Y:139:MET:SD	23:Y:144:ALA:HB1	2.58	0.43
22:W:36:U:C4	22:W:37:A:C5	3.06	0.43
2:C:33:LEU:HA	2:C:36:ASP:HB3	1.99	0.43
17:R:85:LEU:H	17:R:85:LEU:HD12	1.83	0.43
23:Y:75:LYS:HB3	23:Y:75:LYS:HE3	1.61	0.43
1:B:182:ILE:O	1:B:184:VAL:HG23	2.18	0.43
1:B:185:ILE:HG23	1:B:199:TYR:HB2	1.99	0.43
20:A:328:C:H4'	20:A:329:A:H5'	2.00	0.43
7:H:14:ARG:HH12	20:A:876:G:H4'	1.82	0.43
6:G:11:GLN:CD	6:G:12:LEU:H	2.22	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:Y:529:ILE:HD13	23:Y:534:ILE:HB	2.00	0.43
16:Q:92:ARG:HA	16:Q:95:TYR:CD2	2.53	0.43
12:M:23:TYR:CE1	12:M:70:LEU:HD23	2.53	0.43
14:O:8:LYS:O	14:O:12:ILE:HG13	2.18	0.43
23:Y:683:VAL:O	23:Y:687:LEU:N	2.51	0.43
20:A:120:A:H2'	20:A:122:G:N7	2.33	0.43
20:A:531:U:H4'	20:A:532:A:O5'	2.18	0.43
20:A:1363:A:H4'	20:A:1364:U:H5''	2.00	0.43
23:Y:90:PHE:CD1	23:Y:458:HIS:HB2	2.53	0.43
13:N:17:LYS:N	20:A:1317:C:OP1	2.49	0.43
23:Y:128:TYR:CE2	23:Y:130:VAL:HB	2.54	0.43
14:O:56:LEU:HG	14:O:57:LEU:N	2.33	0.43
20:A:910:C:H2'	20:A:911:U:C6	2.53	0.43
20:A:683:G:C6	20:A:684:A:C6	3.06	0.43
20:A:123:C:O2'	20:A:290:C:H1'	2.19	0.43
5:F:69:GLU:HB2	5:F:70:ASP:H	1.42	0.43
20:A:257:G:H1	20:A:269:C:H42	1.66	0.43
23:Y:603:GLU:HB2	23:Y:604:PRO:HD2	2.00	0.43
1:B:24:TRP:HB2	1:B:25:ASN:H	1.63	0.43
20:A:50:A:H4'	20:A:51:A:H5'	2.00	0.43
2:C:167:TRP:CE3	2:C:167:TRP:HA	2.52	0.43
20:A:295:C:H2'	20:A:296:U:O4'	2.18	0.43
23:Y:330:VAL:O	23:Y:331:TYR:CB	2.66	0.43
20:A:218:C:H5'	20:A:458(C):G:N1	2.26	0.43
19:T:74:LYS:N	19:T:74:LYS:HD3	2.32	0.43
8:I:19:LEU:HB3	8:I:59:PHE:HD2	1.84	0.43
20:A:581:G:N2	20:A:761:G:O6	2.51	0.43
3:D:55:ALA:HB2	20:A:509:A:H5'	2.00	0.43
2:C:3:ASN:ND2	20:A:1062:U:O4	2.51	0.43
3:D:125:HIS:HE1	20:A:437:U:O3'	2.01	0.43
17:R:68:LYS:HB3	17:R:72:ARG:HH22	1.82	0.43
23:Y:565:VAL:HB	23:Y:566:THR:H	1.55	0.43
24:U:4:SER:HB3	24:U:6:5OH:NQ	2.33	0.43
20:A:1349:A:H2'	20:A:1350:A:O4'	2.19	0.43
20:A:601:C:H2'	20:A:602:A:C8	2.50	0.43
18:S:53:ASN:ND2	18:S:77:THR:HG22	2.33	0.43
19:T:80:ARG:NH2	20:A:261:U:OP1	2.51	0.43
12:M:111:LYS:NZ	20:A:1228:C:OP2	2.47	0.43
3:D:41:GLY:HA2	20:A:542:G:H5'	1.99	0.43
20:A:1296:C:H4'	20:A:1302:U:C4	2.54	0.43
2:C:70:VAL:O	2:C:105:GLU:HA	2.17	0.43
20:A:1103:C:H2'	20:A:1104:G:O4'	2.18	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:A:1132:C:H2'	20:A:1133:G:C8	2.54	0.43
20:A:1534:A:O5'	20:A:1534:A:H8	2.01	0.43
16:Q:62:SER:HA	20:A:186(I):U:O4	2.18	0.43
7:H:69:ARG:NH2	7:H:73:ASP:O	2.52	0.43
23:Y:528:ALA:HB3	23:Y:568:TYR:HA	2.00	0.43
20:A:269:C:H2'	20:A:270:A:H8	1.82	0.43
20:A:606:G:H3'	20:A:607:A:H5'	2.00	0.43
11:L:113:ARG:NH2	20:A:538:G:OP2	2.51	0.43
8:I:9:ARG:NH2	20:A:1149:C:OP1	2.52	0.43
11:L:52:LEU:HD12	11:L:54:LYS:HZ1	1.84	0.43
11:L:70:ILE:HD12	11:L:72:GLY:CA	2.49	0.43
19:T:72:LEU:HD11	19:T:80:ARG:HD2	2.00	0.43
20:A:328:C:O2	20:A:328:C:H2'	2.18	0.43
3:D:60:GLU:HA	3:D:63:LYS:HB2	2.01	0.43
15:P:28:ARG:HD2	20:A:389:A:H2	1.84	0.43
20:A:444:C:N4	20:A:490:G:H1	2.13	0.43
1:B:91:PRO:HA	1:B:151:GLY:O	2.19	0.43
22:W:59:A:H2'	22:W:60:U:O4'	2.19	0.43
20:A:123:C:H5''	20:A:311:C:O2'	2.17	0.43
10:K:18:ARG:HD3	10:K:35:PRO:HA	2.00	0.43
6:G:32:ARG:HA	6:G:32:ARG:HD3	1.70	0.43
19:T:10:LEU:C	19:T:12:ALA:H	2.21	0.43
1:B:124:SER:C	1:B:126:GLU:H	2.21	0.43
13:N:26:ARG:O	13:N:27:CYS:HB3	2.18	0.43
11:L:107:ALA:O	11:L:109:GLY:N	2.51	0.43
23:Y:484:ARG:O	23:Y:602:LEU:N	2.52	0.43
11:L:52:LEU:HD21	20:A:521:G:OP2	2.19	0.43
20:A:261:U:N3	20:A:264:U:OP2	2.41	0.43
19:T:74:LYS:HG2	19:T:75:ASN:N	2.30	0.43
23:Y:276:VAL:HG13	23:Y:280:LEU:HG	1.99	0.43
22:W:15:G:H3'	22:W:16:U:C5'	2.48	0.43
4:E:150:ARG:H	4:E:150:ARG:HG2	1.48	0.43
20:A:186(M):G:H2'	20:A:186(N):U:C6	2.54	0.43
20:A:259:G:H2'	20:A:260:G:O4'	2.18	0.43
23:Y:428:LEU:HD22	23:Y:440:VAL:HG11	2.01	0.43
19:T:35:THR:HA	19:T:38:LYS:HB2	2.00	0.43
6:G:8:GLU:HB2	6:G:9:VAL:H	1.63	0.43
20:A:769:G:OP2	20:A:803:G:O2'	2.34	0.43
20:A:1390:U:H2'	20:A:1391:U:O4'	2.18	0.43
20:A:1238:A:N7	20:A:1303:C:H1'	2.34	0.43
11:L:8:ASN:ND2	20:A:880:C:OP1	2.51	0.43
12:M:115:LYS:HD2	20:A:1227:A:H4'	2.00	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:N:53:LEU:HA	13:N:54:PRO:HD3	1.72	0.43
23:Y:291:GLY:O	23:Y:397:VAL:HB	2.19	0.43
20:A:832:C:N4	20:A:854:G:H1	2.14	0.43
20:A:68(B):G:H2'	20:A:68(C):C:O4'	2.18	0.43
20:A:503:C:H42	20:A:542:G:H1	1.67	0.43
12:M:14:ARG:HD2	20:A:1296:C:H5'	2.00	0.43
2:C:50:ALA:HB3	2:C:76:VAL:HG11	2.01	0.43
5:F:12:PRO:HB3	5:F:58:GLY:HA2	2.01	0.43
10:K:40:ILE:HG22	10:K:41:THR:CG2	2.49	0.43
23:Y:121:VAL:HG23	23:Y:122:TRP:H	1.83	0.43
22:W:53:G:H1	22:W:61:C:H42	1.67	0.43
4:E:122:GLU:HB3	20:A:9:G:OP1	2.18	0.43
12:M:99:ARG:HA	12:M:99:ARG:NE	2.33	0.43
1:B:21:ARG:HG2	1:B:21:ARG:H	1.61	0.43
11:L:45:PRO:HB2	11:L:49:ASN:OD1	2.19	0.43
11:L:44:THR:HA	11:L:45:PRO:HD3	1.88	0.43
23:Y:280:LEU:HA	23:Y:281:PRO:HD2	1.80	0.43
4:E:127:ASN:HA	4:E:128:PRO:HD3	1.87	0.43
6:G:78:ARG:HD3	6:G:154:TYR:O	2.19	0.43
3:D:9:CYS:O	3:D:12:CYS:HB2	2.18	0.43
10:K:84:VAL:HG22	10:K:109:VAL:O	2.19	0.43
20:A:59:A:H3'	20:A:331:G:N2	2.33	0.43
6:G:59:LEU:HD12	6:G:62:PHE:HB3	2.00	0.43
5:F:61:LEU:HD22	5:F:63:TYR:OH	2.18	0.43
20:A:572:A:O2'	20:A:916:G:O2'	2.24	0.43
19:T:50:GLU:HG2	19:T:51:GLU:N	2.33	0.43
22:W:71:C:H2'	22:W:72:C:H6	1.84	0.43
20:A:1493:A:OP2	24:U:2:DPP:HB3	2.19	0.43
23:Y:197:ARG:NE	23:Y:197:ARG:HA	2.33	0.43
20:A:1157:A:H4'	20:A:1158:C:O5'	2.19	0.43
20:A:823:G:H2'	20:A:824:C:C6	2.53	0.43
17:R:61:LYS:HE3	17:R:61:LYS:HB2	1.85	0.43
20:A:186(G):C:H3'	20:A:186(H):U:H6	1.83	0.43
20:A:599:C:H2'	20:A:600:C:C6	2.53	0.43
4:E:100:VAL:HA	4:E:118:ILE:HG22	2.00	0.43
9:J:51:ARG:HB2	9:J:52:GLY:H	1.59	0.43
23:Y:459:LEU:O	23:Y:463:VAL:HG23	2.19	0.43
20:A:832:C:H1'	20:A:1538:C:H4'	2.00	0.43
20:A:429:U:H4'	20:A:430:A:OP1	2.19	0.43
3:D:19:LEU:HB3	3:D:21:LEU:HG	2.01	0.43
1:B:28:PHE:O	1:B:31:TYR:HB2	2.19	0.43
8:I:112:LYS:HZ1	8:I:116:LYS:HB2	1.84	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:I:83:ARG:O	8:I:86:VAL:HG12	2.19	0.43
23:Y:457:LEU:O	23:Y:461:ILE:HG12	2.19	0.43
23:Y:488:THR:OG1	23:Y:489:LYS:N	2.52	0.43
23:Y:35:TYR:CD1	23:Y:36:THR:N	2.87	0.42
22:W:20(A):U:HO2'	22:W:21:A:P	2.40	0.42
11:L:113:ARG:HE	11:L:114:LYS:H	1.66	0.42
20:A:923:A:H2'	20:A:924:C:O4'	2.18	0.42
20:A:441:A:H3'	20:A:442:C:H6	1.84	0.42
9:J:52:GLY:C	9:J:54:PHE:H	2.21	0.42
20:A:328:C:H4'	20:A:329:A:C5'	2.49	0.42
7:H:79:VAL:O	7:H:81:HIS:N	2.51	0.42
6:G:151:TYR:HA	6:G:154:TYR:CD1	2.54	0.42
17:R:79:LEU:HA	17:R:80:PRO:HD2	1.90	0.42
3:D:5:ILE:HD13	20:A:406:G:H4'	2.01	0.42
6:G:101:LEU:HD12	6:G:102:ARG:N	2.34	0.42
20:A:159:G:H1'	20:A:162:A:H61	1.79	0.42
9:J:4:ILE:HB	9:J:74:ILE:HG12	2.01	0.42
14:O:36:ILE:HG12	14:O:60:VAL:HG22	2.00	0.42
1:B:74:LYS:HE2	1:B:74:LYS:HB3	1.83	0.42
1:B:84:GLU:OE1	1:B:87:ARG:NH1	2.52	0.42
1:B:138:LEU:HA	1:B:141:GLU:OE1	2.19	0.42
1:B:231:GLU:HA	1:B:232:PRO:HD3	1.73	0.42
18:S:32:LYS:HA	18:S:50:ALA:O	2.19	0.42
1:B:17:PHE:CD2	1:B:17:PHE:N	2.88	0.42
23:Y:32:ILE:C	23:Y:34:TYR:N	2.68	0.42
20:A:1507:A:C2	20:A:1530:G:H1'	2.54	0.42
20:A:299:G:C6	20:A:300:A:C6	3.08	0.42
1:B:171:ALA:O	1:B:175:ARG:HB2	2.18	0.42
4:E:11:ILE:HD12	4:E:105:VAL:HG22	2.02	0.42
6:G:78:ARG:N	6:G:85:TYR:O	2.48	0.42
3:D:19:LEU:O	3:D:21:LEU:HB2	2.19	0.42
6:G:36:LYS:HB3	20:A:1373:G:C5'	2.49	0.42
22:W:19:G:H5'	22:W:20:U:O5'	2.19	0.42
20:A:124:G:H4'	20:A:291:C:O2'	2.19	0.42
20:A:171:A:H2'	20:A:172:A:C8	2.54	0.42
2:C:104:GLN:HB3	2:C:105:GLU:H	1.63	0.42
20:A:431:A:C4	20:A:432:A:C8	3.07	0.42
23:Y:348:ARG:HG3	23:Y:349:LYS:N	2.34	0.42
20:A:1138:G:C5	20:A:1140:C:H1'	2.53	0.42
6:G:46:ALA:O	6:G:50:ILE:HG13	2.19	0.42
1:B:124:SER:HB3	1:B:125:PRO:HD2	1.99	0.42
20:A:603:U:H2'	20:A:604:G:H8	1.84	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:A:343:U:O2'	20:A:344:A:H2'	2.19	0.42
8:I:95:LYS:HE2	8:I:95:LYS:HB2	1.86	0.42
18:S:34:TRP:HB3	20:A:1014:A:H1'	2.01	0.42
2:C:154:SER:O	2:C:197:GLY:N	2.50	0.42
3:D:145:GLU:OE1	3:D:182:LYS:HB3	2.19	0.42
2:C:193:TYR:C	20:A:1206:G:H4'	2.40	0.42
9:J:11:PHE:HD2	9:J:11:PHE:HA	1.70	0.42
2:C:11:ARG:HB3	2:C:16:ARG:HB2	2.01	0.42
7:H:15:ASN:HD21	20:A:827:U:C4'	2.33	0.42
10:K:58:PRO:O	10:K:61:ALA:HB3	2.20	0.42
20:A:687:A:C2	20:A:704:A:C6	3.07	0.42
6:G:29:LYS:HE2	20:A:1375:A:H5''	2.01	0.42
4:E:24:ARG:HH12	20:A:15:G:H4'	1.84	0.42
20:A:266:G:H5'	20:A:268:C:H41	1.85	0.42
20:A:1246:C:N3	20:A:1291:G:N2	2.63	0.42
8:I:120:ARG:NH1	20:A:1345:U:H5''	2.33	0.42
20:A:59:A:N3	20:A:59:A:H2'	2.35	0.42
3:D:108:LEU:HD23	3:D:110:PHE:HD2	1.84	0.42
10:K:51:LYS:H	10:K:54:ARG:HB2	1.84	0.42
20:A:603:U:H2'	20:A:604:G:C8	2.54	0.42
3:D:177:ASP:O	3:D:181:MET:N	2.52	0.42
20:A:1171:G:H2'	20:A:1172:C:H6	1.84	0.42
20:A:273:A:N6	20:A:274:A:C6	2.87	0.42
19:T:21:LYS:O	19:T:24:LEU:HB3	2.18	0.42
14:O:25:THR:OG1	14:O:26:GLU:OE2	2.37	0.42
1:B:133:LYS:HD3	1:B:133:LYS:HA	1.78	0.42
20:A:1028:C:N3	20:A:1033:G:C2	2.85	0.42
1:B:166:ASP:O	1:B:170:GLU:HB2	2.18	0.42
1:B:71:VAL:O	1:B:165:VAL:HG23	2.19	0.42
11:L:49:ASN:HB3	20:A:529:G:O6	2.19	0.42
15:P:81:ARG:NH2	20:A:474:G:H5'	2.26	0.42
20:A:1525:G:C4	20:A:1526:G:C8	3.08	0.42
6:G:137:LYS:O	6:G:140:ASP:HB3	2.19	0.42
1:B:49:GLU:O	1:B:52:GLU:HB3	2.19	0.42
3:D:105:VAL:HG12	3:D:110:PHE:HB2	2.00	0.42
5:F:100:ASN:HB2	17:R:28:GLU:H	1.85	0.42
23:Y:521:SER:HB2	23:Y:522:GLY:H	1.60	0.42
20:A:333:G:H2'	20:A:334:C:H6	1.84	0.42
15:P:70:ALA:O	15:P:74:LEU:HG	2.19	0.42
15:P:83:GLU:HB3	15:P:84:ALA:H	1.60	0.42
20:A:689:C:H2'	20:A:690:G:O4'	2.19	0.42
13:N:4:LYS:O	13:N:8:GLU:HG2	2.20	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
12:M:46:LYS:HD3	12:M:46:LYS:C	2.40	0.42
20:A:926:G:H21	20:A:1505:G:H2'	1.83	0.42
12:M:108:ARG:HB2	20:A:948:C:OP2	2.18	0.42
9:J:36:GLY:O	9:J:38:ILE:N	2.53	0.42
18:S:47:HIS:H	18:S:62:ILE:HG23	1.84	0.42
1:B:100:GLY:HA2	1:B:104:ASN:CG	2.39	0.42
9:J:57:LYS:NZ	20:A:972:C:H5'	2.34	0.42
2:C:22:TRP:HB3	2:C:59:ARG:N	2.29	0.42
20:A:829:G:H2'	20:A:830:G:C8	2.53	0.42
1:B:51:LEU:O	1:B:55:PHE:HD2	2.03	0.42
11:L:123:LYS:HD2	20:A:37:U:P	2.59	0.42
1:B:208:ILE:O	1:B:212:GLN:HB2	2.19	0.42
20:A:10:A:N6	20:A:24:U:H3	2.16	0.42
10:K:26:ASN:O	10:K:55:LYS:HE3	2.20	0.42
20:A:1087:G:O6	20:A:1098:C:N3	2.52	0.42
23:Y:60:GLU:H	23:Y:60:GLU:HG2	1.57	0.42
23:Y:136:ALA:H	23:Y:260:LEU:CB	2.32	0.42
14:O:42:HIS:HD2	20:A:739:C:O2'	2.02	0.42
11:L:53:ARG:HG2	11:L:93:LEU:CD2	2.43	0.42
23:Y:610:VAL:HG22	23:Y:643:ILE:HG13	2.01	0.42
17:R:74:ARG:CA	17:R:79:LEU:HB3	2.50	0.42
23:Y:72:CYS:HB3	23:Y:79:ILE:O	2.20	0.42
1:B:111:ARG:NH2	20:A:1104:G:OP1	2.52	0.42
5:F:2:ARG:NH1	5:F:69:GLU:OE2	2.53	0.42
8:I:48:GLU:HA	8:I:51:ARG:HB2	2.02	0.42
2:C:178:LEU:HD23	20:A:1112:C:N3	2.34	0.42
5:F:16:GLN:CD	5:F:16:GLN:H	2.22	0.42
23:Y:416:LYS:HB3	23:Y:417:THR:H	1.65	0.42
22:W:5:A:H2'	22:W:6:C:C6	2.54	0.42
16:Q:91:ARG:NH1	20:A:584:G:OP1	2.52	0.42
2:C:32:LEU:HD22	2:C:59:ARG:NH2	2.33	0.42
23:Y:631:ILE:HG12	23:Y:644:ARG:O	2.18	0.42
23:Y:649:LEU:HA	23:Y:652:MET:HB3	2.00	0.42
23:Y:317:MET:HB3	23:Y:325:LEU:HB2	2.02	0.42
5:F:86:ARG:H	5:F:86:ARG:HG2	1.74	0.42
20:A:697:U:H3	20:A:798:G:H1'	1.84	0.42
20:A:1046:A:H3'	20:A:1047:G:H8	1.83	0.42
20:A:980:C:H5'	20:A:981:U:C5	2.55	0.42
17:R:37:VAL:HG23	17:R:38:GLU:H	1.85	0.42
12:M:54:VAL:O	12:M:57:ARG:HG2	2.20	0.42
23:Y:309:LEU:HA	23:Y:332:SER:O	2.20	0.42
23:Y:526:VAL:HB	23:Y:566:THR:CG2	2.31	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:A:1065:U:H4'	20:A:1066:C:H5'	2.02	0.42
20:A:328:C:H1'	20:A:329:A:OP2	2.20	0.42
6:G:89:MET:HA	6:G:155:ARG:HH11	1.85	0.42
11:L:10:LEU:HD21	11:L:15:ARG:HH21	1.84	0.42
7:H:14:ARG:HH12	20:A:876:G:C4'	2.32	0.42
20:A:1100:C:N4	20:A:1103:C:OP1	2.53	0.42
3:D:96:LEU:HG	3:D:139:ARG:CZ	2.50	0.42
7:H:123:GLU:O	7:H:126:LYS:HB3	2.19	0.42
8:I:77:ILE:O	8:I:81:ILE:HG13	2.20	0.42
20:A:1018:C:H2'	20:A:1019:C:H6	1.85	0.42
2:C:43:LEU:O	2:C:47:LEU:HB3	2.20	0.42
22:W:25:C:C4	22:W:26:A:N7	2.88	0.42
23:Y:34:TYR:O	23:Y:35:TYR:HD2	2.03	0.42
11:L:81:SER:OG	11:L:106:ASP:OD2	2.30	0.42
9:J:50:ILE:HG13	9:J:51:ARG:N	2.34	0.42
20:A:966:G:H1'	22:W:34:C:H4'	2.02	0.42
3:D:113:SER:O	3:D:115:ARG:N	2.52	0.42
3:D:8:VAL:HG23	3:D:9:CYS:H	1.85	0.42
20:A:1378:C:H6	20:A:1378:C:O5'	2.02	0.42
16:Q:43:LEU:HD23	16:Q:43:LEU:HA	1.71	0.42
16:Q:63:ARG:HH22	20:A:186(I):U:H1'	1.84	0.42
10:K:52:GLY:HA2	20:A:691:G:O6	2.20	0.42
19:T:14:LYS:HG3	19:T:17:ARG:HH21	1.85	0.42
6:G:69:VAL:HG22	6:G:135:VAL:HG22	2.02	0.42
17:R:40:LEU:HA	17:R:43:PHE:HD1	1.85	0.42
2:C:92:ALA:HB2	2:C:99:VAL:HG21	2.02	0.42
20:A:1092:A:N7	20:A:1093:A:N6	2.67	0.42
6:G:88:PRO:HD3	6:G:148:ASN:HB3	2.02	0.42
23:Y:482:ALA:HB1	23:Y:484:ARG:NH1	2.34	0.42
18:S:58:VAL:HG21	18:S:75:ALA:CB	2.49	0.42
11:L:90:VAL:HG23	11:L:92:ASP:OD1	2.20	0.42
20:A:17:U:H2'	20:A:18:C:O4'	2.20	0.42
12:M:121:LYS:HD3	12:M:121:LYS:N	2.35	0.42
3:D:25:ARG:C	3:D:27:TYR:H	2.24	0.42
18:S:71:LEU:O	18:S:73:GLU:N	2.53	0.42
23:Y:681:LYS:O	23:Y:684:GLN:N	2.45	0.42
20:A:573:A:H2'	20:A:574:A:C8	2.55	0.42
20:A:399:G:H2'	20:A:400:C:H6	1.83	0.42
23:Y:11:ARG:HD3	23:Y:40:HIS:HE1	1.84	0.42
2:C:13:GLY:HA2	13:N:57:ARG:HH21	1.85	0.42
16:Q:29:HIS:HB3	16:Q:33:GLY:N	2.35	0.42
7:H:96:GLY:O	7:H:100:ILE:HG13	2.20	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:A:935:A:H2'	20:A:936:C:C6	2.54	0.42
4:E:6:PHE:O	4:E:7:GLU:HB2	2.20	0.42
8:I:10:ARG:HG3	8:I:105:ASP:CB	2.49	0.42
23:Y:605:ILE:O	23:Y:674:ASP:HB3	2.20	0.42
14:O:15:PHE:HD2	14:O:15:PHE:HA	1.68	0.42
20:A:861:G:H1	20:A:868:C:N4	2.18	0.41
11:L:53:ARG:N	11:L:53:ARG:HE	2.18	0.41
20:A:1510:U:H2'	20:A:1511:G:H8	1.81	0.41
20:A:911:U:O2'	20:A:1490:C:H5'	2.20	0.41
20:A:960:U:C5	20:A:1225:A:C8	3.07	0.41
4:E:14:ARG:NH2	20:A:1079:G:O3'	2.53	0.41
3:D:36:ARG:NH2	20:A:427:U:OP2	2.52	0.41
20:A:1301:U:H3'	20:A:1302:U:H5''	2.01	0.41
8:I:111:ARG:HH11	20:A:1368:G:H5''	1.85	0.41
23:Y:617:MET:SD	23:Y:618:GLY:N	2.93	0.41
23:Y:342:TYR:HD1	23:Y:349:LYS:HG2	1.85	0.41
20:A:447:G:C6	20:A:485:G:H1'	2.55	0.41
19:T:10:LEU:O	19:T:12:ALA:N	2.52	0.41
20:A:787:A:H2'	20:A:788:U:C6	2.54	0.41
8:I:126:SER:O	8:I:128:ARG:HD3	2.20	0.41
20:A:1269:A:H1'	20:A:1326:C:H1'	2.01	0.41
23:Y:34:TYR:O	23:Y:35:TYR:CD2	2.73	0.41
11:L:36:VAL:HG23	11:L:58:VAL:O	2.20	0.41
22:W:23:A:C4	22:W:24:G:C8	3.07	0.41
24:U:6:5OH:CS	24:U:6:5OH:N	2.83	0.41
14:O:39:LEU:O	14:O:42:HIS:N	2.53	0.41
23:Y:326:THR:O	23:Y:328:ILE:HG23	2.21	0.41
23:Y:250:THR:HG21	23:Y:279:TYR:HB3	2.01	0.41
9:J:55:LYS:N	9:J:55:LYS:HD2	2.35	0.41
2:C:32:LEU:HD22	2:C:59:ARG:HH22	1.85	0.41
23:Y:606:MET:CG	23:Y:649:LEU:HG	2.48	0.41
22:W:4:U:O4	22:W:69:A:N1	2.54	0.41
20:A:563:A:O4'	20:A:566:G:N2	2.53	0.41
20:A:590:C:H42	20:A:649:G:H1	1.68	0.41
23:Y:590:ILE:HA	23:Y:590:ILE:HD13	1.92	0.41
7:H:8:ASP:O	7:H:12:ARG:HG3	2.19	0.41
23:Y:215:LYS:O	23:Y:218:GLU:HB3	2.20	0.41
9:J:17:ASP:O	9:J:21:GLN:N	2.47	0.41
20:A:1171:G:H2'	20:A:1172:C:C6	2.55	0.41
20:A:153:C:H42	20:A:168:G:H1	1.67	0.41
20:A:1048:G:H1	20:A:1209:C:H42	1.66	0.41
20:A:836:G:C6	20:A:851:G:C6	3.08	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:35:ARG:HB3	20:A:412:A:C2	2.55	0.41
20:A:1148:U:H2'	20:A:1149:C:O4'	2.20	0.41
23:Y:326:THR:OG1	23:Y:377:VAL:HG13	2.21	0.41
23:Y:409:ILE:HG13	23:Y:656:ALA:CB	2.43	0.41
2:C:22:TRP:CZ2	13:N:54:PRO:HG2	2.56	0.41
5:F:46:ARG:HG2	5:F:47:ARG:N	2.35	0.41
7:H:34:GLU:CB	7:H:118:VAL:HG21	2.44	0.41
6:G:87:VAL:HG22	6:G:151:TYR:CB	2.45	0.41
20:A:853:G:H2'	20:A:854:G:O4'	2.20	0.41
20:A:373:A:H4'	20:A:480:U:O2'	2.20	0.41
20:A:1503:A:H61	21:V:14:A:H2'	1.85	0.41
18:S:49:ILE:HG13	18:S:60:VAL:O	2.21	0.41
20:A:1440(K):G:N2	20:A:1440(L):G:C5	2.88	0.41
16:Q:32:TYR:HA	16:Q:32:TYR:HD2	1.74	0.41
15:P:5:ARG:NH2	15:P:23:ASP:O	2.53	0.41
8:I:75:ASP:O	8:I:78:LYS:HB3	2.19	0.41
23:Y:655:TYR:O	23:Y:659:LEU:N	2.46	0.41
5:F:10:LEU:HG	5:F:85:VAL:HG22	2.01	0.41
23:Y:319:ASP:OD2	23:Y:321:TYR:HB2	2.21	0.41
1:B:174:VAL:O	1:B:175:ARG:C	2.57	0.41
20:A:1416:G:H2'	20:A:1417:G:O4'	2.20	0.41
7:H:98:LYS:NZ	20:A:632:A:OP1	2.53	0.41
7:H:97:VAL:HG12	20:A:600:C:OP1	2.21	0.41
23:Y:609:GLU:H	23:Y:670:VAL:HG23	1.86	0.41
3:D:15:GLU:CG	3:D:59:ARG:HH22	2.34	0.41
6:G:108:ALA:O	6:G:119:ARG:HB3	2.20	0.41
22:W:55:U:O2'	22:W:57:G:O6	2.35	0.41
6:G:76:ARG:HD3	6:G:156:TRP:HE1	1.86	0.41
4:E:20:GLN:H	4:E:24:ARG:HA	1.85	0.41
16:Q:43:LEU:HD12	16:Q:69:LYS:HA	2.01	0.41
23:Y:486:THR:O	23:Y:600:VAL:N	2.53	0.41
17:R:53:ARG:HG3	17:R:58:LEU:O	2.21	0.41
8:I:102:LEU:HD22	20:A:1179:A:H5''	2.02	0.41
6:G:26:PHE:HE2	6:G:30:ILE:HD11	1.86	0.41
8:I:10:ARG:HG3	8:I:105:ASP:HB2	2.03	0.41
20:A:1325:C:H2'	20:A:1326:C:C6	2.56	0.41
8:I:47:LEU:HD23	8:I:56:LEU:HD11	2.01	0.41
23:Y:637:ARG:HG3	23:Y:642:VAL:HG23	2.01	0.41
23:Y:406:GLU:O	23:Y:454:MET:HG2	2.20	0.41
7:H:17:THR:HB	7:H:78:GLN:CD	2.41	0.41
16:Q:6:LEU:HA	16:Q:6:LEU:HD23	1.92	0.41
22:W:7:G:C2	22:W:49:A:H1'	2.55	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:167:PRO:HA	1:B:170:GLU:C	2.41	0.41
20:A:715:A:H2'	20:A:716:A:O4'	2.20	0.41
11:L:17:LYS:HG2	11:L:19:ARG:H	1.85	0.41
20:A:765:G:O2'	20:A:766:A:H5'	2.21	0.41
23:Y:612:THR:HA	23:Y:613:PRO:HD3	1.89	0.41
20:A:1215:G:H2'	20:A:1216:G:H8	1.86	0.41
3:D:135:LEU:H	3:D:135:LEU:HD22	1.84	0.41
20:A:1266:G:H22	20:A:1268:A:H3'	1.84	0.41
20:A:1259:C:H5''	20:A:1260:C:OP2	2.20	0.41
9:J:91:PRO:HB2	9:J:94:VAL:HB	2.03	0.41
4:E:47:LYS:HE2	4:E:47:LYS:HB2	1.75	0.41
22:W:49:A:N1	22:W:65:U:O4	2.53	0.41
14:O:39:LEU:HD22	14:O:42:HIS:HB3	2.01	0.41
20:A:895:G:H2'	20:A:896:C:C6	2.56	0.41
23:Y:312:LEU:O	23:Y:328:ILE:HB	2.20	0.41
23:Y:289:ILE:CD1	23:Y:289:ILE:H	2.20	0.41
16:Q:59:ILE:HG23	16:Q:72:ARG:O	2.21	0.41
2:C:24:ALA:HB1	2:C:29:TYR:HA	2.03	0.41
7:H:34:GLU:O	7:H:38:ILE:HG12	2.20	0.41
6:G:80:VAL:HG21	6:G:85:TYR:CE1	2.55	0.41
11:L:10:LEU:HA	11:L:10:LEU:HD23	1.93	0.41
3:D:17:VAL:O	3:D:19:LEU:HD12	2.20	0.41
2:C:134:ILE:O	2:C:138:VAL:HG23	2.21	0.41
20:A:171:A:H2'	20:A:172:A:H8	1.86	0.41
7:H:82:HIS:O	7:H:137:VAL:HA	2.20	0.41
3:D:156:GLU:HB3	3:D:157:LEU:H	1.69	0.41
3:D:65:ARG:HD3	3:D:75:PHE:CD2	2.56	0.41
17:R:56:THR:OG1	17:R:58:LEU:HD22	2.21	0.41
20:A:367:U:H3	20:A:393:A:N6	2.17	0.41
20:A:1408:A:C2	20:A:1494:G:C5	3.09	0.41
12:M:30:ALA:O	12:M:34:LEU:HG	2.21	0.41
20:A:998:G:H2'	20:A:998(A):C:H6	1.85	0.41
20:A:370:C:H2'	20:A:371:G:H8	1.85	0.41
20:A:1123:A:N1	20:A:1150:U:O4	2.54	0.41
12:M:119:GLY:N	22:W:29:U:OP1	2.54	0.41
20:A:1521:G:H2'	20:A:1522:U:O4'	2.20	0.41
1:B:111:ARG:HH12	20:A:1104:G:H4'	1.86	0.41
12:M:45:VAL:HA	12:M:48:LEU:HD12	2.03	0.41
5:F:95:GLU:O	5:F:97:PHE:N	2.54	0.41
9:J:43:ARG:HD3	9:J:43:ARG:HA	1.76	0.41
5:F:44:GLY:HA2	5:F:59:TYR:CZ	2.55	0.41
3:D:74:GLN:HA	3:D:77:ASN:OD1	2.21	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:4:LYS:NZ	20:A:1191:A:H5''	2.36	0.41
18:S:30:LEU:HD13	18:S:32:LYS:HD2	2.01	0.41
11:L:21:LYS:HE3	11:L:23:LYS:HB2	2.02	0.41
6:G:3:ARG:HG3	20:A:1380:U:C5	2.56	0.41
20:A:68(F):C:H2'	20:A:68(G):G:H8	1.85	0.41
12:M:108:ARG:N	12:M:108:ARG:HD2	2.36	0.41
20:A:33:A:H2'	20:A:34:C:O4'	2.20	0.41
20:A:33:A:H4'	20:A:364:A:H1'	2.02	0.41
4:E:127:ASN:HD21	20:A:18:C:P	2.44	0.41
20:A:954:G:H2'	20:A:955:U:C6	2.55	0.41
20:A:406:G:H2'	20:A:407:G:O4'	2.21	0.41
21:V:13:A:H3'	21:V:14:A:O4'	2.20	0.41
16:Q:16:GLN:CD	20:A:254:G:H21	2.24	0.41
20:A:766:A:H2'	20:A:767:A:O4'	2.21	0.41
20:A:1250:A:H3'	20:A:1251:A:C8	2.56	0.41
20:A:59:A:O3'	20:A:387:U:H4'	2.20	0.41
17:R:22:VAL:N	17:R:56:THR:HA	2.35	0.41
20:A:1439:C:H2'	20:A:1440:C:C6	2.55	0.41
23:Y:487:ILE:HB	23:Y:597:GLY:O	2.20	0.41
13:N:6:LEU:HD11	20:A:982:U:OP2	2.21	0.41
23:Y:615:GLU:H	23:Y:615:GLU:HG3	1.64	0.41
16:Q:3:LYS:HE3	20:A:128:G:O3'	2.21	0.41
8:I:28:VAL:HA	8:I:63:ILE:O	2.21	0.41
20:A:116:A:H2'	20:A:117:G:O4'	2.21	0.41
1:B:172:ILE:HG12	1:B:173:ALA:H	1.84	0.41
9:J:51:ARG:HE	9:J:59:SER:HB3	1.86	0.41
20:A:1338:G:C2	20:A:1339:A:C4	3.08	0.41
10:K:90:GLY:HA2	10:K:93:GLN:HB2	2.01	0.41
12:M:125:ARG:O	20:A:966:G:H5'	2.21	0.41
4:E:51:VAL:O	4:E:55:VAL:HG23	2.21	0.41
17:R:45:SER:HB3	17:R:51:LEU:CD1	2.49	0.41
18:S:73:GLU:HB3	18:S:74:PHE:CD2	2.56	0.41
1:B:111:ARG:HD2	20:A:1103:C:O2'	2.20	0.41
14:O:54:ARG:NE	20:A:579:G:HO2'	2.13	0.41
20:A:1290:G:H3'	20:A:1291:G:H8	1.86	0.41
16:Q:25:ARG:NH2	20:A:238:G:OP1	2.54	0.41
20:A:382:A:H2'	20:A:383:A:C8	2.56	0.41
7:H:12:ARG:HD2	7:H:26:VAL:HG23	2.03	0.41
1:B:219:VAL:O	1:B:223:ILE:HG13	2.21	0.41
23:Y:443:HIS:C	23:Y:445:GLU:H	2.24	0.41
20:A:1410:G:H2'	20:A:1411:C:H6	1.85	0.41
4:E:6:PHE:HB2	4:E:63:ARG:NH2	2.35	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:I:95:LYS:O	8:I:99:LEU:HD23	2.20	0.41
20:A:1206:G:H2'	20:A:1207:G:C8	2.55	0.41
20:A:333:G:H2'	20:A:334:C:C6	2.55	0.41
12:M:57:ARG:HB3	12:M:57:ARG:HE	1.78	0.41
8:I:10:ARG:HD3	8:I:75:ASP:HB2	2.03	0.41
4:E:42:GLY:HA3	4:E:62:ALA:O	2.20	0.41
4:E:82:VAL:HG21	4:E:138:ALA:HA	2.02	0.41
19:T:42:GLN:O	19:T:46:GLU:HG2	2.21	0.41
8:I:96:LEU:HA	8:I:96:LEU:HD12	1.81	0.41
20:A:1286:A:H3'	20:A:1286:A:N3	2.35	0.41
23:Y:524:GLU:O	23:Y:525:PHE:HB3	2.21	0.41
23:Y:494:GLU:HG2	23:Y:495:GLY:N	2.35	0.41
2:C:114:PRO:HA	2:C:185:GLY:HA3	2.03	0.41
7:H:49:GLU:O	7:H:59:LEU:HD23	2.21	0.41
16:Q:65:ILE:HA	16:Q:65:ILE:HD13	1.88	0.41
11:L:33:ARG:CB	11:L:60:LEU:HD12	2.34	0.41
8:I:50:LEU:HD23	8:I:50:LEU:HA	1.87	0.41
20:A:922:G:H21	20:A:1398:A:H2	1.69	0.41
1:B:68:ILE:HA	1:B:161:ALA:O	2.20	0.41
23:Y:14:ASN:ND2	23:Y:374:LEU:HD13	2.36	0.41
1:B:172:ILE:HG12	1:B:173:ALA:N	2.36	0.41
23:Y:289:ILE:HG22	23:Y:290:LYS:H	1.85	0.41
19:T:22:ARG:HD3	20:A:323:U:H4'	2.03	0.41
6:G:151:TYR:HA	6:G:154:TYR:HD1	1.85	0.41
20:A:1386:G:H2'	20:A:1387:G:H8	1.86	0.41
8:I:120:ARG:O	20:A:1344:C:H5'	2.21	0.41
15:P:69:THR:O	15:P:72:ARG:HB3	2.20	0.41
10:K:52:GLY:N	10:K:55:LYS:HG3	2.36	0.41
12:M:23:TYR:O	12:M:66:LEU:HD23	2.20	0.41
1:B:31:TYR:CE1	1:B:46:LYS:HG2	2.56	0.41
23:Y:145:ASP:CG	23:Y:146:LEU:H	2.24	0.41
10:K:63:LEU:HA	10:K:66:LEU:HD12	2.03	0.41
20:A:1051:C:H2'	20:A:1052:U:C6	2.55	0.41
20:A:1163:C:H2'	20:A:1164:G:H8	1.85	0.41
20:A:1198:G:H2'	20:A:1199:U:C6	2.55	0.41
23:Y:22:ASP:C	26:Y:702:GNP:O1B	2.54	0.40
20:A:27:G:H2'	20:A:28:G:C8	2.56	0.40
1:B:182:ILE:HA	1:B:182:ILE:HD13	1.88	0.40
11:L:116:SER:C	11:L:118:SER:H	2.24	0.40
11:L:53:ARG:H	11:L:54:LYS:HZ1	1.68	0.40
20:A:114:U:H2'	20:A:115:G:C8	2.56	0.40
9:J:57:LYS:CB	20:A:972:C:H4'	2.45	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:157:ILE:HG13	2:C:157:ILE:H	1.56	0.40
5:F:97:PHE:O	17:R:31:LEU:N	2.52	0.40
8:I:37:PHE:CE2	8:I:70:LYS:HG3	2.56	0.40
20:A:1316:G:N2	20:A:1318:A:H3'	2.35	0.40
1:B:46:LYS:HD2	1:B:49:GLU:OE2	2.20	0.40
2:C:35:GLU:O	2:C:39:ILE:HG13	2.20	0.40
20:A:1068:G:H2'	20:A:1069:C:C6	2.56	0.40
7:H:21:LYS:O	7:H:23:SER:N	2.55	0.40
6:G:121:ALA:O	6:G:125:MET:HG2	2.21	0.40
8:I:90:PRO:O	8:I:93:ARG:HB3	2.21	0.40
20:A:1217:C:H2'	20:A:1218:C:C6	2.56	0.40
20:A:1217:C:H2'	20:A:1218:C:H6	1.86	0.40
20:A:638:G:H2'	20:A:639:G:O4'	2.21	0.40
4:E:77:PRO:HG2	4:E:142:LEU:HD22	2.02	0.40
7:H:24:THR:HG23	7:H:63:LEU:CD1	2.51	0.40
20:A:1288:A:H1'	20:A:1353:G:H4'	2.03	0.40
12:M:64:TRP:HB2	12:M:65:LYS:H	1.74	0.40
6:G:114:ARG:HA	6:G:114:ARG:HD3	1.95	0.40
20:A:556:C:H2'	20:A:557:G:O4'	2.21	0.40
16:Q:2:PRO:N	20:A:127:G:HO2'	2.20	0.40
20:A:14:U:N3	20:A:17:U:OP2	2.43	0.40
2:C:123:GLN:O	2:C:128:PHE:HB2	2.21	0.40
20:A:889:A:H61	20:A:907:A:H3'	1.85	0.40
20:A:1014:A:H8	20:A:1014:A:O5'	2.05	0.40
23:Y:637:ARG:HG3	23:Y:642:VAL:CG2	2.51	0.40
16:Q:2:PRO:HA	20:A:128:G:H5'	2.04	0.40
23:Y:97:SER:O	23:Y:101:LEU:HG	2.20	0.40
23:Y:100:VAL:O	23:Y:329:ARG:NH1	2.55	0.40
3:D:79:PHE:CZ	3:D:207:TYR:HB3	2.57	0.40
20:A:1151:A:H1'	20:A:1152:A:C8	2.55	0.40
3:D:43:HIS:O	3:D:45:GLN:N	2.53	0.40
6:G:79:ARG:HB2	20:A:1381:U:N1	2.36	0.40
20:A:1347:G:N1	20:A:1374:A:OP2	2.43	0.40
22:W:57:G:H2'	22:W:57:G:N3	2.37	0.40
18:S:73:GLU:HG3	20:A:1320:C:H1'	2.02	0.40
20:A:434:U:H2'	20:A:435:C:H6	1.84	0.40
2:C:95:THR:O	2:C:97:LYS:N	2.54	0.40
1:B:34:ALA:O	1:B:41:ILE:HG13	2.21	0.40
7:H:96:GLY:HA2	7:H:130:GLY:HA3	2.03	0.40
14:O:25:THR:O	14:O:29:VAL:HG23	2.20	0.40
9:J:5:ARG:NH1	9:J:101:VAL:HG11	2.36	0.40
23:Y:126:GLU:C	23:Y:129:LYS:H	2.25	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:A:1118:C:H2'	20:A:1119:C:C6	2.57	0.40
20:A:926:G:N2	20:A:1505:G:H2'	2.37	0.40
20:A:1184:G:H2'	20:A:1185:G:H8	1.86	0.40
20:A:667:G:P	20:A:732:C:HO2'	2.44	0.40
18:S:63:THR:OG1	18:S:64:GLU:N	2.55	0.40
3:D:57:ARG:HH21	4:E:107:ARG:NH2	2.06	0.40
11:L:53:ARG:HG3	11:L:69:TYR:CD1	2.56	0.40
22:W:41:A:H2'	22:W:42:U:H6	1.78	0.40
5:F:50:TYR:HA	5:F:51:PRO:HD2	1.88	0.40
6:G:101:LEU:O	6:G:105:VAL:HG23	2.21	0.40
20:A:162:A:H3'	20:A:163:C:O4'	2.21	0.40
12:M:14:ARG:HG2	12:M:44:ARG:NH1	2.36	0.40
2:C:157:ILE:HG12	2:C:164:ARG:HH21	1.86	0.40
16:Q:60:ILE:HG23	16:Q:61:GLU:O	2.20	0.40
23:Y:142:THR:HA	23:Y:171:GLU:HG3	2.03	0.40
5:F:67:MET:HB2	5:F:68:PRO:HD2	2.03	0.40
11:L:27:LEU:HA	11:L:27:LEU:HD23	1.89	0.40
20:A:951:G:H1'	20:A:970:C:O2'	2.22	0.40
12:M:90:LEU:HD23	12:M:94:ARG:HE	1.85	0.40
23:Y:517:LEU:HD12	23:Y:517:LEU:HA	1.93	0.40
3:D:61:LYS:HG3	3:D:206:PHE:CD2	2.54	0.40
20:A:263:A:H2'	20:A:264:U:C6	2.57	0.40
2:C:29:TYR:O	2:C:32:LEU:HB2	2.22	0.40
2:C:19:GLU:O	2:C:56:ASP:HA	2.21	0.40
2:C:70:VAL:HG12	2:C:71:ALA:H	1.87	0.40
16:Q:92:ARG:HD2	16:Q:95:TYR:CD2	2.57	0.40
7:H:121:ASP:N	7:H:121:ASP:OD1	2.54	0.40
8:I:70:LYS:O	8:I:74:ILE:HG13	2.21	0.40
20:A:1308:U:H2'	20:A:1309:G:H8	1.87	0.40
6:G:27:ILE:HG21	6:G:40:ALA:HB2	2.02	0.40
23:Y:37:GLY:O	23:Y:38:ARG:HG3	2.21	0.40
14:O:11:VAL:HA	14:O:14:GLU:HB2	2.02	0.40
7:H:27:PRO:HD3	7:H:58:TYR:CE2	2.57	0.40
2:C:27:LYS:H	2:C:27:LYS:HG2	1.56	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	233/235 (99%)	164 (70%)	49 (21%)	20 (9%)	1	26
2	C	205/207 (99%)	136 (66%)	47 (23%)	22 (11%)	1	17
3	D	206/208 (99%)	140 (68%)	49 (24%)	17 (8%)	1	27
4	E	149/151 (99%)	125 (84%)	16 (11%)	8 (5%)	3	41
5	F	99/101 (98%)	81 (82%)	10 (10%)	8 (8%)	1	28
6	G	153/155 (99%)	116 (76%)	24 (16%)	13 (8%)	1	26
7	H	136/138 (99%)	90 (66%)	29 (21%)	17 (12%)	1	14
8	I	125/127 (98%)	100 (80%)	16 (13%)	9 (7%)	2	32
9	J	97/99 (98%)	71 (73%)	20 (21%)	6 (6%)	2	37
10	K	117/119 (98%)	82 (70%)	22 (19%)	13 (11%)	1	17
11	L	123/125 (98%)	54 (44%)	41 (33%)	28 (23%)	0	2
12	M	123/125 (98%)	85 (69%)	22 (18%)	16 (13%)	0	13
13	N	58/60 (97%)	45 (78%)	8 (14%)	5 (9%)	1	26
14	O	86/88 (98%)	60 (70%)	20 (23%)	6 (7%)	2	33
15	P	82/84 (98%)	59 (72%)	20 (24%)	3 (4%)	5	53
16	Q	98/100 (98%)	72 (74%)	17 (17%)	9 (9%)	1	24
17	R	68/70 (97%)	49 (72%)	16 (24%)	3 (4%)	4	47
18	S	77/79 (98%)	38 (49%)	29 (38%)	10 (13%)	0	13
19	T	97/99 (98%)	79 (81%)	14 (14%)	4 (4%)	4	49
23	Y	685/687 (100%)	476 (70%)	143 (21%)	66 (10%)	1	22
24	U	2/6 (33%)	2 (100%)	0	0	100	100
All	All	3019/3063 (99%)	2124 (70%)	612 (20%)	283 (9%)	1	23

All (283) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	20	GLU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	B	34	ALA
1	B	67	THR
1	B	76	GLN
1	B	103	THR
1	B	157	ARG
1	B	186	ALA
2	C	36	ASP
2	C	49	SER
2	C	60	ALA
2	C	161	GLU
2	C	207	VAL
3	D	5	ILE
3	D	84	LYS
3	D	89	THR
3	D	114	ARG
3	D	156	GLU
3	D	166	LYS
4	E	6	PHE
4	E	7	GLU
4	E	21	ALA
5	F	13	ASN
5	F	69	GLU
6	G	6	ARG
6	G	8	GLU
6	G	15	ASP
7	H	22	GLU
7	H	26	VAL
7	H	27	PRO
7	H	93	VAL
7	H	99	GLU
7	H	100	ILE
8	I	54	ASP
8	I	119	ALA
9	J	51	ARG
9	J	57	LYS
9	J	83	GLU
9	J	91	PRO
10	K	12	ARG
10	K	42	TRP
10	K	87	THR
10	K	91	ARG
10	K	107	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
10	K	109	VAL
10	K	111	ASP
11	L	34	ARG
11	L	37	CYS
11	L	39	VAL
11	L	55	VAL
11	L	66	VAL
11	L	81	SER
11	L	104	VAL
11	L	108	ALA
11	L	123	LYS
12	M	12	ASN
12	M	67	GLU
13	N	14	PRO
13	N	27	CYS
16	Q	53	LEU
16	Q	74	LEU
17	R	37	VAL
18	S	70	LYS
19	T	74	LYS
23	Y	35	TYR
23	Y	39	ILE
23	Y	88	VAL
23	Y	92	ILE
23	Y	331	TYR
23	Y	347	GLY
23	Y	380	LEU
23	Y	400	GLU
23	Y	431	LEU
23	Y	432	ALA
23	Y	498	ILE
23	Y	536	LYS
23	Y	564	LYS
23	Y	631	ILE
23	Y	671	MET
1	B	17	PHE
1	B	95	GLN
1	B	105	PHE
1	B	165	VAL
2	C	14	ILE
2	C	45	LYS
2	C	47	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	C	66	VAL
2	C	130	VAL
2	C	157	ILE
2	C	178	LEU
3	D	20	TYR
3	D	21	LEU
3	D	44	GLY
3	D	186	LEU
5	F	34	GLY
6	G	4	ARG
6	G	5	ARG
6	G	90	GLU
6	G	120	ILE
7	H	74	PRO
7	H	97	VAL
7	H	134	ILE
8	I	24	GLY
8	I	26	VAL
10	K	43	SER
11	L	43	VAL
11	L	94	PRO
11	L	96	VAL
11	L	97	ARG
11	L	99	HIS
11	L	119	LYS
12	M	3	ARG
12	M	6	GLY
12	M	10	PRO
12	M	99	ARG
12	M	101	GLN
12	M	107	ALA
12	M	120	LYS
14	O	19	PRO
16	Q	49	GLU
16	Q	55	ASP
16	Q	69	LYS
16	Q	73	VAL
17	R	28	GLU
18	S	9	VAL
18	S	42	PRO
18	S	45	VAL
19	T	71	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
19	T	105	SER
23	Y	21	ILE
23	Y	22	ASP
23	Y	36	THR
23	Y	75	LYS
23	Y	111	SER
23	Y	161	PRO
23	Y	162	VAL
23	Y	292	THR
23	Y	324	ARG
23	Y	330	VAL
23	Y	395	PRO
23	Y	416	LYS
23	Y	447	GLY
23	Y	448	GLN
23	Y	565	VAL
23	Y	566	THR
23	Y	568	TYR
23	Y	614	GLU
23	Y	652	MET
1	B	191	ASP
1	B	230	VAL
1	B	235	SER
1	B	237	ALA
2	C	85	ARG
2	C	96	GLY
2	C	112	SER
2	C	180	ALA
3	D	28	SER
4	E	73	ASN
4	E	78	HIS
5	F	70	ASP
5	F	96	PRO
6	G	7	ALA
6	G	19	GLY
6	G	37	ASN
7	H	2	LEU
7	H	72	PRO
7	H	76	PRO
7	H	107	LEU
8	I	35	GLU
8	I	58	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
9	J	37	PRO
10	K	15	ALA
11	L	23	LYS
11	L	36	VAL
11	L	51	ALA
11	L	56	ALA
11	L	79	GLU
13	N	13	THR
14	O	16	ALA
14	O	23	GLY
15	P	28	ARG
15	P	43	LYS
16	Q	12	SER
18	S	15	LEU
18	S	55	LYS
18	S	67	VAL
18	S	80	TYR
23	Y	74	TRP
23	Y	138	LYS
23	Y	204	GLU
23	Y	234	GLY
23	Y	359	HIS
23	Y	417	THR
23	Y	520	GLY
23	Y	521	SER
23	Y	525	PHE
23	Y	632	LEU
23	Y	653	PHE
23	Y	680	PRO
23	Y	681	LYS
1	B	129	GLU
1	B	229	VAL
2	C	26	LYS
2	C	35	GLU
2	C	51	GLY
3	D	47	ARG
3	D	73	ARG
4	E	70	PRO
8	I	87	GLN
8	I	127	LYS
9	J	59	SER
10	K	36	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
10	K	105	VAL
11	L	22	SER
12	M	5	ALA
12	M	11	ARG
12	M	70	LEU
13	N	24	CYS
16	Q	82	MET
17	R	59	SER
18	S	40	ILE
19	T	49	ALA
23	Y	89	ASP
23	Y	181	LEU
23	Y	615	GLU
23	Y	628	ARG
23	Y	648	PRO
23	Y	649	LEU
23	Y	670	VAL
1	B	128	GLU
1	B	130	ARG
2	C	61	ALA
4	E	74	GLY
5	F	38	GLU
6	G	31	MET
7	H	80	ILE
7	H	103	VAL
7	H	120	THR
11	L	12	ARG
11	L	93	LEU
11	L	112	ASP
11	L	127	GLU
12	M	124	PRO
13	N	3	ARG
14	O	6	GLU
14	O	88	ARG
15	P	46	PRO
16	Q	14	LYS
23	Y	14	ASN
23	Y	294	PRO
3	D	75	PHE
5	F	14	LEU
5	F	43	LEU
6	G	18	TYR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
6	G	88	PRO
8	I	89	ASN
11	L	69	TYR
12	M	74	VAL
23	Y	296	GLY
23	Y	493	VAL
2	C	74	GLY
3	D	29	PRO
12	M	100	GLY
14	O	27	VAL
23	Y	158	GLY
23	Y	384	ILE
23	Y	535	PRO
2	C	80	GLY
3	D	88	VAL
3	D	140	VAL
7	H	75	ARG
12	M	4	ILE
23	Y	444	PRO
1	B	66	GLY
10	K	14	VAL
10	K	35	PRO
18	S	72	GLY
23	Y	366	VAL
4	E	85	GLY
11	L	82	VAL
11	L	83	VAL
23	Y	42	ILE
23	Y	530	VAL
23	Y	436	PRO

### 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
1	B	203/203 (100%)	165 (81%)	38 (19%)	<b>2</b> <b>18</b>
2	C	161/161 (100%)	121 (75%)	40 (25%)	<b>1</b> <b>8</b>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	180/180 (100%)	149 (83%)	31 (17%)	3	22
4	E	116/116 (100%)	93 (80%)	23 (20%)	2	15
5	F	90/90 (100%)	74 (82%)	16 (18%)	2	20
6	G	126/126 (100%)	106 (84%)	20 (16%)	4	28
7	H	119/119 (100%)	99 (83%)	20 (17%)	3	24
8	I	98/98 (100%)	82 (84%)	16 (16%)	3	26
9	J	89/89 (100%)	74 (83%)	15 (17%)	3	24
10	K	90/90 (100%)	78 (87%)	12 (13%)	6	37
11	L	104/104 (100%)	77 (74%)	27 (26%)	1	7
12	M	100/100 (100%)	82 (82%)	18 (18%)	2	19
13	N	49/49 (100%)	40 (82%)	9 (18%)	2	18
14	O	79/79 (100%)	62 (78%)	17 (22%)	1	11
15	P	72/72 (100%)	60 (83%)	12 (17%)	3	25
16	Q	95/95 (100%)	82 (86%)	13 (14%)	5	35
17	R	61/61 (100%)	48 (79%)	13 (21%)	1	12
18	S	69/69 (100%)	54 (78%)	15 (22%)	1	11
19	T	76/76 (100%)	69 (91%)	7 (9%)	13	56
23	Y	579/579 (100%)	472 (82%)	107 (18%)	2	18
24	U	2/2 (100%)	2 (100%)	0	100	100
All	All	2558/2558 (100%)	2089 (82%)	469 (18%)	2	18

All (469) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	7	VAL
1	B	9	GLU
1	B	15	VAL
1	B	16	HIS
1	B	17	PHE
1	B	21	ARG
1	B	28	PHE
1	B	32	ILE
1	B	36	ARG
1	B	49	GLU
1	B	69	LEU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	B	74	LYS
1	B	81	VAL
1	B	101	MET
1	B	103	THR
1	B	104	ASN
1	B	109	SER
1	B	134	GLU
1	B	141	GLU
1	B	145	LEU
1	B	154	LEU
1	B	155	LEU
1	B	162	ILE
1	B	163	PHE
1	B	168	THR
1	B	172	ILE
1	B	175	ARG
1	B	185	ILE
1	B	187	LEU
1	B	189	ASP
1	B	190	THR
1	B	208	ILE
1	B	212	GLN
1	B	213	LEU
1	B	221	LEU
1	B	226	ARG
1	B	230	VAL
1	B	236	TYR
2	C	4	LYS
2	C	5	ILE
2	C	6	HIS
2	C	15	THR
2	C	19	GLU
2	C	22	TRP
2	C	39	ILE
2	C	47	LEU
2	C	48	TYR
2	C	52	LEU
2	C	55	VAL
2	C	56	ASP
2	C	57	ILE
2	C	67	THR
2	C	70	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	C	75	VAL
2	C	84	ILE
2	C	86	VAL
2	C	99	VAL
2	C	101	LEU
2	C	102	ASN
2	C	110	ASN
2	C	118	GLN
2	C	119	ARG
2	C	123	GLN
2	C	124	ILE
2	C	127	ARG
2	C	128	PHE
2	C	132	ARG
2	C	134	ILE
2	C	142	MET
2	C	152	ILE
2	C	157	ILE
2	C	164	ARG
2	C	167	TRP
2	C	176	HIS
2	C	179	ARG
2	C	184	TYR
2	C	188	LEU
2	C	208	ILE
3	D	3	ARG
3	D	5	ILE
3	D	9	CYS
3	D	13	ARG
3	D	21	LEU
3	D	24	GLU
3	D	28	SER
3	D	30	LYS
3	D	54	TYR
3	D	56	VAL
3	D	57	ARG
3	D	60	GLU
3	D	61	LYS
3	D	63	LYS
3	D	67	ILE
3	D	72	GLU
3	D	83	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	D	86	LYS
3	D	107	ARG
3	D	114	ARG
3	D	127	THR
3	D	132	ARG
3	D	140	VAL
3	D	148	VAL
3	D	150	GLU
3	D	156	GLU
3	D	175	SER
3	D	178	VAL
3	D	193	ASP
3	D	196	LEU
3	D	200	GLU
4	E	5	ASP
4	E	10	MET
4	E	12	LEU
4	E	31	LEU
4	E	33	VAL
4	E	41	VAL
4	E	47	LYS
4	E	53	LEU
4	E	57	LYS
4	E	61	TYR
4	E	64	ARG
4	E	78	HIS
4	E	80	ILE
4	E	91	LEU
4	E	92	LYS
4	E	107	ARG
4	E	117	ASP
4	E	125	SER
4	E	129	ILE
4	E	137	GLU
4	E	141	GLN
4	E	147	ASP
4	E	150	ARG
5	F	2	ARG
5	F	7	ASN
5	F	16	GLN
5	F	18	GLN
5	F	22	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
5	F	27	GLN
5	F	37	VAL
5	F	43	LEU
5	F	46	ARG
5	F	55	ASP
5	F	61	LEU
5	F	66	GLU
5	F	69	GLU
5	F	77	ARG
5	F	78	GLU
5	F	83	ASP
6	G	10	ARG
6	G	11	GLN
6	G	12	LEU
6	G	18	TYR
6	G	21	VAL
6	G	24	THR
6	G	32	ARG
6	G	35	LYS
6	G	36	LYS
6	G	54	THR
6	G	67	GLU
6	G	74	GLU
6	G	76	ARG
6	G	79	ARG
6	G	94	ARG
6	G	97	GLN
6	G	104	LEU
6	G	106	GLN
6	G	115	ARG
6	G	149	ARG
7	H	3	THR
7	H	11	THR
7	H	29	SER
7	H	30	ARG
7	H	37	ARG
7	H	49	GLU
7	H	50	ARG
7	H	52	ASP
7	H	54	ASP
7	H	63	LEU
7	H	69	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
7	H	73	ASP
7	H	88	LYS
7	H	102	ARG
7	H	104	ARG
7	H	107	LEU
7	H	112	LEU
7	H	133	LEU
7	H	135	CYS
7	H	136	GLU
8	I	12	GLU
8	I	26	VAL
8	I	34	ASN
8	I	40	LEU
8	I	70	LYS
8	I	75	ASP
8	I	79	LEU
8	I	86	VAL
8	I	91	ASP
8	I	95	LYS
8	I	97	LYS
8	I	109	VAL
8	I	112	LYS
8	I	121	ARG
8	I	125	TYR
8	I	128	ARG
9	J	3	LYS
9	J	11	PHE
9	J	12	ASP
9	J	16	LEU
9	J	22	LYS
9	J	30	SER
9	J	50	ILE
9	J	54	PHE
9	J	65	LEU
9	J	66	ARG
9	J	67	THR
9	J	75	ILE
9	J	79	ARG
9	J	86	MET
9	J	96	ILE
10	K	18	ARG
10	K	22	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
10	K	29	ILE
10	K	30	VAL
10	K	31	THR
10	K	41	THR
10	K	51	LYS
10	K	87	THR
10	K	91	ARG
10	K	107	SER
10	K	109	VAL
10	K	119	CYS
11	L	20	LYS
11	L	22	SER
11	L	24	VAL
11	L	33	ARG
11	L	38	THR
11	L	44	THR
11	L	49	ASN
11	L	52	LEU
11	L	53	ARG
11	L	54	LYS
11	L	55	VAL
11	L	57	LYS
11	L	59	ARG
11	L	60	LEU
11	L	66	VAL
11	L	67	THR
11	L	70	ILE
11	L	75	HIS
11	L	78	GLN
11	L	84	LEU
11	L	90	VAL
11	L	92	ASP
11	L	93	LEU
11	L	97	ARG
11	L	110	VAL
11	L	116	SER
11	L	122	THR
12	M	8	GLU
12	M	15	VAL
12	M	23	TYR
12	M	27	LYS
12	M	43	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
12	M	48	LEU
12	M	67	GLU
12	M	69	GLU
12	M	70	LEU
12	M	82	MET
12	M	88	ARG
12	M	103	THR
12	M	106	ASN
12	M	108	ARG
12	M	110	ARG
12	M	115	LYS
12	M	120	LYS
12	M	121	LYS
13	N	4	LYS
13	N	7	ILE
13	N	21	TYR
13	N	35	ARG
13	N	40	CYS
13	N	41	ARG
13	N	42	ILE
13	N	57	ARG
13	N	61	TRP
14	O	5	LYS
14	O	8	LYS
14	O	10	LYS
14	O	15	PHE
14	O	28	GLN
14	O	31	LEU
14	O	34	LEU
14	O	47	LYS
14	O	51	HIS
14	O	52	SER
14	O	56	LEU
14	O	57	LEU
14	O	58	MET
14	O	74	ASP
14	O	82	ILE
14	O	85	LEU
14	O	88	ARG
15	P	23	ASP
15	P	32	TYR
15	P	36	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
15	P	43	LYS
15	P	45	THR
15	P	54	GLU
15	P	57	ARG
15	P	68	ASP
15	P	69	THR
15	P	71	ARG
15	P	80	PHE
15	P	81	ARG
16	Q	13	ASP
16	Q	16	GLN
16	Q	26	GLN
16	Q	27	PHE
16	Q	32	TYR
16	Q	36	ILE
16	Q	49	GLU
16	Q	52	LYS
16	Q	60	ILE
16	Q	69	LYS
16	Q	74	LEU
16	Q	83	ASP
16	Q	91	ARG
17	R	19	LYS
17	R	26	LEU
17	R	29	PHE
17	R	34	TYR
17	R	39	VAL
17	R	47	THR
17	R	58	LEU
17	R	59	SER
17	R	72	ARG
17	R	74	ARG
17	R	76	LEU
17	R	83	GLU
17	R	85	LEU
18	S	6	LYS
18	S	13	ASP
18	S	23	ASN
18	S	34	TRP
18	S	41	VAL
18	S	43	GLU
18	S	44	MET

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
18	S	56	GLN
18	S	58	VAL
18	S	61	TYR
18	S	62	ILE
18	S	64	GLU
18	S	67	VAL
18	S	77	THR
18	S	81	ARG
19	T	8	ARG
19	T	13	LEU
19	T	24	LEU
19	T	36	LEU
19	T	54	LYS
19	T	74	LYS
19	T	93	GLU
23	Y	8	ASP
23	Y	9	LEU
23	Y	13	ARG
23	Y	20	HIS
23	Y	26	THR
23	Y	29	THR
23	Y	33	LEU
23	Y	39	ILE
23	Y	40	HIS
23	Y	60	GLU
23	Y	66	THR
23	Y	72	CYS
23	Y	88	VAL
23	Y	92	ILE
23	Y	98	MET
23	Y	99	ARG
23	Y	105	ILE
23	Y	106	VAL
23	Y	111	SER
23	Y	114	VAL
23	Y	118	SER
23	Y	122	TRP
23	Y	126	GLU
23	Y	127	LYS
23	Y	128	TYR
23	Y	132	ARG
23	Y	133	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
23	Y	152	THR
23	Y	170	ARG
23	Y	172	ASP
23	Y	174	PHE
23	Y	178	ILE
23	Y	186	TYR
23	Y	188	TYR
23	Y	197	ARG
23	Y	199	ILE
23	Y	203	GLU
23	Y	224	ASP
23	Y	231	TYR
23	Y	232	LEU
23	Y	236	GLU
23	Y	237	PRO
23	Y	240	GLU
23	Y	250	THR
23	Y	259	PHE
23	Y	260	LEU
23	Y	264	LEU
23	Y	277	VAL
23	Y	278	ASP
23	Y	285	ASP
23	Y	289	ILE
23	Y	295	GLU
23	Y	298	VAL
23	Y	299	VAL
23	Y	312	LEU
23	Y	328	ILE
23	Y	337	SER
23	Y	344	THR
23	Y	355	LEU
23	Y	356	LEU
23	Y	357	ARG
23	Y	367	GLU
23	Y	368	GLU
23	Y	381	LYS
23	Y	385	THR
23	Y	399	LEU
23	Y	404	VAL
23	Y	408	VAL
23	Y	410	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
23	Y	413	ILE
23	Y	421	GLN
23	Y	424	LEU
23	Y	426	GLN
23	Y	428	LEU
23	Y	430	ARG
23	Y	431	LEU
23	Y	438	PHE
23	Y	448	GLN
23	Y	449	THR
23	Y	452	SER
23	Y	473	ASP
23	Y	476	VAL
23	Y	498	ILE
23	Y	504	ARG
23	Y	515	GLU
23	Y	521	SER
23	Y	536	LYS
23	Y	542	VAL
23	Y	563	ILE
23	Y	564	LYS
23	Y	565	VAL
23	Y	567	LEU
23	Y	572	TYR
23	Y	580	MET
23	Y	591	LYS
23	Y	598	ASP
23	Y	615	GLU
23	Y	617	MET
23	Y	619	ASP
23	Y	624	LEU
23	Y	630	GLN
23	Y	631	ILE
23	Y	647	VAL
23	Y	658	ASP
23	Y	670	VAL
23	Y	671	MET
23	Y	675	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	6	HIS
2	C	123	GLN
2	C	136	GLN
2	C	181	ASN
3	D	119	GLN
3	D	123	HIS
3	D	125	HIS
4	E	78	HIS
4	E	127	ASN
5	F	11	ASN
6	G	37	ASN
7	H	78	GLN
8	I	124	GLN
9	J	76	ASN
9	J	84	GLN
10	K	116	HIS
14	O	42	HIS
16	Q	26	GLN
17	R	36	ASN
23	Y	14	ASN
23	Y	20	HIS
23	Y	40	HIS
23	Y	137	ASN
23	Y	362	HIS
23	Y	448	GLN
23	Y	684	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
20	A	1511/1511 (100%)	304 (20%)	18 (1%)
21	V	17/18 (94%)	8 (47%)	1 (5%)
22	W	76/77 (98%)	22 (28%)	2 (2%)
All	All	1604/1606 (99%)	334 (20%)	21 (1%)

All (334) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
20	A	6	G
20	A	7	G
20	A	9	G
20	A	22	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
20	A	29	G
20	A	32	A
20	A	39	G
20	A	47	C
20	A	48	C
20	A	51	A
20	A	54	C
20	A	59	A
20	A	68	G
20	A	68(H)	G
20	A	68(I)	G
20	A	68(L)	U
20	A	68(M)	U
20	A	68(P)	C
20	A	68(V)	G
20	A	109	A
20	A	115	G
20	A	116	A
20	A	119	A
20	A	121	C
20	A	129(A)	G
20	A	131	C
20	A	136	C
20	A	144	G
20	A	147	G
20	A	163	C
20	A	182	U
20	A	183	G
20	A	186(G)	C
20	A	186(I)	U
20	A	195	A
20	A	201(C)	U
20	A	216	G
20	A	220	G
20	A	224	C
20	A	230	G
20	A	247	G
20	A	251	G
20	A	252	U
20	A	253	U
20	A	267	C
20	A	279	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
20	A	280	C
20	A	281	G
20	A	289	G
20	A	297	G
20	A	301	G
20	A	309	G
20	A	312	C
20	A	321	A
20	A	328	C
20	A	329	A
20	A	331	G
20	A	332	G
20	A	335	C
20	A	341	C
20	A	345	C
20	A	346	G
20	A	347	G
20	A	352	C
20	A	353	A
20	A	354	G
20	A	357	G
20	A	367	U
20	A	372	C
20	A	373	A
20	A	382	A
20	A	384	G
20	A	388	G
20	A	390	C
20	A	393	A
20	A	397	A
20	A	398	C
20	A	412	A
20	A	413	G
20	A	414	A
20	A	422	C
20	A	424	G
20	A	427	U
20	A	430	A
20	A	433	C
20	A	440	A
20	A	452	A
20	A	453	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
20	A	455	C
20	A	458	C
20	A	458(B)	A
20	A	458(D)	G
20	A	481	G
20	A	485	G
20	A	486	U
20	A	497	A
20	A	498	U
20	A	505	G
20	A	511	C
20	A	516	U
20	A	518	C
20	A	521	G
20	A	527	G
20	A	531	U
20	A	532	A
20	A	533	A
20	A	547	A
20	A	562	C
20	A	568	G
20	A	569	C
20	A	572	A
20	A	573	A
20	A	575	G
20	A	576	G
20	A	577	G
20	A	581	G
20	A	589	C
20	A	600	C
20	A	616	G
20	A	653	A
20	A	664	G
20	A	665	A
20	A	667	G
20	A	673	G
20	A	687	A
20	A	688	G
20	A	724	G
20	A	734	G
20	A	749	C
20	A	752	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
20	A	755	G
20	A	766	A
20	A	782	A
20	A	793	U
20	A	794	A
20	A	799	G
20	A	816	A
20	A	817	C
20	A	818	G
20	A	819	A
20	A	820	U
20	A	828	A
20	A	838(A)	U
20	A	838(B)	C
20	A	838(C)	U
20	A	848	C
20	A	857	C
20	A	859	A
20	A	867	G
20	A	870	U
20	A	873	A
20	A	882	C
20	A	884	U
20	A	888	G
20	A	926	G
20	A	927	G
20	A	934	C
20	A	935	A
20	A	938	A
20	A	945	G
20	A	960	U
20	A	961	U
20	A	969	A
20	A	971	G
20	A	974	A
20	A	976	G
20	A	977	A
20	A	978	A
20	A	980	C
20	A	981	U
20	A	983	A
20	A	991	U

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
20	A	992	U
20	A	993	G
20	A	1004	A
20	A	1006	C
20	A	1017	G
20	A	1022	G
20	A	1024	G
20	A	1025	U
20	A	1026	G
20	A	1028	C
20	A	1028(A)	C
20	A	1036	G
20	A	1038	C
20	A	1041	A
20	A	1045	C
20	A	1053	G
20	A	1054	C
20	A	1055	A
20	A	1060	C
20	A	1064	G
20	A	1065	U
20	A	1066	C
20	A	1070	U
20	A	1093	A
20	A	1094	G
20	A	1095	U
20	A	1098	C
20	A	1101	A
20	A	1102	A
20	A	1117	G
20	A	1124	G
20	A	1125	U
20	A	1126	U
20	A	1129	C
20	A	1130	A
20	A	1137	C
20	A	1138	G
20	A	1139	G
20	A	1145	C
20	A	1146	A
20	A	1151	A
20	A	1157	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
20	A	1159	U
20	A	1165	C
20	A	1171	G
20	A	1174	G
20	A	1181	G
20	A	1183	A
20	A	1184	G
20	A	1190	G
20	A	1196	U
20	A	1197	G
20	A	1200	C
20	A	1201	A
20	A	1212	U
20	A	1213	A
20	A	1220	G
20	A	1221	G
20	A	1227	A
20	A	1236	A
20	A	1238	A
20	A	1240	U
20	A	1250	A
20	A	1256	A
20	A	1257	U
20	A	1260	C
20	A	1262	C
20	A	1266	G
20	A	1277	C
20	A	1280	A
20	A	1281	U
20	A	1286	A
20	A	1287	A
20	A	1300	G
20	A	1301	U
20	A	1302	U
20	A	1303	C
20	A	1305	G
20	A	1317	C
20	A	1320	C
20	A	1322	C
20	A	1331	G
20	A	1336	C
20	A	1338	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
20	A	1340	A
20	A	1347	G
20	A	1353	G
20	A	1360	A
20	A	1363	A
20	A	1364	U
20	A	1368	G
20	A	1377	A
20	A	1378	C
20	A	1381	U
20	A	1382	C
20	A	1397	C
20	A	1398	A
20	A	1401	G
20	A	1422	G
20	A	1425	U
20	A	1440(B)	G
20	A	1440(C)	G
20	A	1440(D)	A
20	A	1440(E)	G
20	A	1440(I)	A
20	A	1440(J)	C
20	A	1440(K)	G
20	A	1440(L)	G
20	A	1481	U
20	A	1492	A
20	A	1493	A
20	A	1494	G
20	A	1497	G
20	A	1499	A
20	A	1502	A
20	A	1503	A
20	A	1504	G
20	A	1505	G
20	A	1506	U
20	A	1507	A
20	A	1517	G
20	A	1519	A
20	A	1520	G
20	A	1529	G
20	A	1530	G
20	A	1532	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
20	A	1533	C
20	A	1534	A
20	A	1535	C
20	A	1536	C
20	A	1537	U
20	A	1538	C
21	V	5	A
21	V	9	G
21	V	11	U
21	V	12	A
21	V	13	A
21	V	14	A
21	V	15	A
21	V	21	A
22	W	4	U
22	W	9	A
22	W	14	A
22	W	15	G
22	W	16	U
22	W	17	U
22	W	18	G
22	W	19	G
22	W	20	U
22	W	20(A)	U
22	W	21	A
22	W	22	G
22	W	25	C
22	W	42	U
22	W	46	G
22	W	47	U
22	W	48	C
22	W	50	C
22	W	53	G
22	W	58	A
22	W	60	U
22	W	61	C

All (21) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
20	A	5	U
20	A	115	G

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type
20	A	251	G
20	A	266	G
20	A	328	C
20	A	429	U
20	A	484	G
20	A	531	U
20	A	687	A
20	A	748	C
20	A	992	U
20	A	1064	G
20	A	1101	A
20	A	1145	C
20	A	1200	C
20	A	1504	G
20	A	1532	U
20	A	1537	U
21	V	8	A
22	W	20(A)	U
22	W	41	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
24	KBE	U	1	24	8,8,9	8.66	1 (12%)	6,8,10	1.01	1 (16%)
24	DPP	U	2	24	5,5,6	6.98	1 (20%)	3,5,7	2.65	2 (66%)
24	UAL	U	5	24	7,8,9	1.43	1 (14%)	6,9,11	1.03	0
24	5OH	U	6	24	12,12,13	6.58	3 (25%)	13,16,18	0.85	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means

no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	KBE	U	1	24	-	0/6/7/8	0/0/0/0
24	DPP	U	2	24	-	0/2/4/6	0/0/0/0
24	UAL	U	5	24	-	0/3/7/9	0/0/0/0
24	5OH	U	6	24	-	0/2/18/20	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	U	1	KBE	O-C	24.35	1.28	1.11
24	U	6	5OH	O-C	22.02	1.26	1.11
24	U	2	DPP	O-C	15.38	1.22	1.11
24	U	6	5OH	CQ-NP	5.08	1.40	1.34
24	U	6	5OH	CQ-NR	2.40	1.40	1.32
24	U	5	UAL	CA-N	-2.24	1.31	1.35

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	U	2	DPP	C-CA-N	3.85	117.68	113.83
24	U	2	DPP	CB-CA-N	-2.48	103.17	111.50
24	U	1	KBE	CG-CB-CA	2.13	115.07	111.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is 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	$\# Z  > 2$
26	GNP	Y	702	25	34,34,34	1.72	6 (17%)	50,54,54	5.62	14 (28%)

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
26	GNP	Y	702	25	-	0/18/38/38	0/1/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	Y	702	GNP	PG-O1G	6.13	1.53	1.46
26	Y	702	GNP	PB-N3B	-4.52	1.60	1.64
26	Y	702	GNP	PA-O3A	-2.67	1.55	1.59
26	Y	702	GNP	PB-O3A	-2.30	1.55	1.59
26	Y	702	GNP	PA-O2A	-2.15	1.45	1.55
26	Y	702	GNP	PG-N3B	-2.07	1.62	1.64

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Y	702	GNP	C6-C5-N7	-37.55	129.08	134.14
26	Y	702	GNP	PA-O3A-PB	-4.60	116.10	131.81
26	Y	702	GNP	C2-N3-C4	-3.75	109.82	115.09
26	Y	702	GNP	C4'-O4'-C1'	-3.69	105.75	109.75
26	Y	702	GNP	C4-C5-N7	3.50	112.52	109.52
26	Y	702	GNP	C5-C4-N3	3.32	130.76	125.94
26	Y	702	GNP	C6-N1-C2	3.19	125.09	119.51
26	Y	702	GNP	O2B-PB-O1B	3.17	117.21	109.89
26	Y	702	GNP	O3G-PG-O2G	3.07	116.45	107.66
26	Y	702	GNP	O3G-PG-O1G	-2.98	105.95	113.60
26	Y	702	GNP	PB-N3B-PG	-2.88	125.23	130.07
26	Y	702	GNP	O1B-PB-N3B	2.73	115.95	111.83
26	Y	702	GNP	O1G-PG-N3B	-2.15	108.57	111.83
26	Y	702	GNP	C5'-C4'-C3'	-2.10	106.82	115.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	B	235/235 (100%)	-0.38	0 100 100	26, 78, 150, 182	0
2	C	207/207 (100%)	-0.15	1 (0%) 88 76	33, 66, 122, 164	0
3	D	208/208 (100%)	0.29	9 (4%) 34 26	16, 79, 141, 186	0
4	E	151/151 (100%)	-0.07	4 (2%) 53 39	23, 71, 126, 185	0
5	F	101/101 (100%)	-0.37	0 100 100	29, 64, 127, 176	0
6	G	155/155 (100%)	-0.10	3 (1%) 64 47	39, 86, 144, 209	0
7	H	138/138 (100%)	-0.15	4 (2%) 49 36	33, 67, 126, 179	0
8	I	127/127 (100%)	1.03	29 (22%) 1 2	16, 69, 128, 177	0
9	J	99/99 (100%)	0.55	15 (15%) 3 4	24, 81, 132, 167	0
10	K	119/119 (100%)	0.01	8 (6%) 17 16	37, 83, 128, 165	0
11	L	125/125 (100%)	0.26	13 (10%) 7 9	21, 72, 139, 179	0
12	M	125/125 (100%)	-0.24	3 (2%) 56 41	58, 97, 159, 195	0
13	N	60/60 (100%)	1.90	26 (43%) 1 1	30, 54, 113, 147	0
14	O	88/88 (100%)	-0.27	0 100 100	32, 73, 127, 165	0
15	P	84/84 (100%)	0.76	13 (15%) 3 4	29, 73, 132, 175	0
16	Q	100/100 (100%)	0.37	11 (11%) 6 8	42, 74, 130, 159	0
17	R	70/70 (100%)	-0.18	0 100 100	26, 69, 132, 198	0
18	S	79/79 (100%)	-0.11	1 (1%) 74 57	26, 89, 165, 199	0
19	T	99/99 (100%)	1.03	24 (24%) 1 2	27, 80, 144, 169	0
20	A	1511/1511 (100%)	0.67	224 (14%) 3 4	6, 84, 166, 265	0
21	V	18/18 (100%)	1.62	6 (33%) 1 2	33, 135, 179, 181	0
22	W	77/77 (100%)	-0.21	1 (1%) 74 57	43, 116, 183, 208	0
23	Y	687/687 (100%)	0.01	33 (4%) 29 23	25, 86, 158, 217	0
24	U	2/6 (33%)	-0.25	0 100 100	66, 66, 66, 66	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	4665/4669 (99%)	0.29	428 (9%) 9 10	6, 81, 156, 265	0

All (428) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	A	134	A	17.1
20	A	135	C	13.0
20	A	325	A	11.4
20	A	328	C	10.4
8	I	124	GLN	9.5
20	A	110	C	9.5
20	A	1363	A	9.3
20	A	1244	C	9.3
20	A	1364	U	8.8
20	A	197	A	8.7
20	A	136	C	8.6
15	P	25	ARG	8.2
20	A	133	U	8.1
10	K	127	LYS	7.8
20	A	173	U	7.8
20	A	824	C	7.7
20	A	109	A	7.5
20	A	221	C	7.5
19	T	72	LEU	7.4
20	A	882	C	7.4
19	T	23	ARG	7.3
20	A	825	G	7.3
8	I	128	ARG	7.0
20	A	231	G	6.8
20	A	1253	G	6.8
20	A	818	G	6.8
20	A	976	G	6.8
20	A	1251	A	6.6
9	J	42	THR	6.6
20	A	1362(A)	C	6.6
20	A	220	G	6.5
8	I	120	ARG	6.5
20	A	326	G	6.5
20	A	377	G	6.5
20	A	823	G	6.4
19	T	69	GLY	6.4
20	A	174	C	6.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
20	A	1348	U	6.3
20	A	1357	A	6.1
20	A	1243	C	6.1
16	Q	38	ARG	6.0
19	T	73	HIS	6.0
13	N	30	ALA	5.9
8	I	117	HIS	5.8
20	A	977	A	5.8
20	A	376	G	5.8
20	A	232	G	5.8
20	A	230	G	5.8
21	V	8	A	5.8
20	A	45	U	5.7
8	I	123	PRO	5.6
8	I	122	ALA	5.6
21	V	7	G	5.6
15	P	24	ALA	5.5
11	L	129	ALA	5.4
20	A	111	G	5.4
20	A	324	G	5.3
20	A	619	U	5.3
15	P	27	LYS	5.3
20	A	1352	C	5.3
20	A	125	U	5.2
20	A	1365	G	5.2
20	A	311	C	5.2
20	A	354	G	5.2
20	A	292	G	5.1
20	A	1358	U	5.1
8	I	119	ALA	5.1
10	K	128	ALA	5.1
20	A	378	G	5.1
20	A	149	A	5.1
13	N	31	ARG	5.0
20	A	323	U	5.0
20	A	329	A	5.0
9	J	66	ARG	5.0
9	J	47	PHE	4.9
20	A	607	A	4.9
20	A	1066	C	4.9
20	A	291	C	4.9
20	A	1252	A	4.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
20	A	1325	C	4.9
9	J	41	PRO	4.8
19	T	24	LEU	4.8
20	A	1285	A	4.8
19	T	66	ALA	4.8
20	A	1186	G	4.8
20	A	975	A	4.8
15	P	26	ARG	4.8
9	J	43	ARG	4.8
21	V	12	A	4.7
8	I	113	LYS	4.7
20	A	108	G	4.7
20	A	124	G	4.7
11	L	20	LYS	4.7
21	V	11	U	4.7
13	N	2	ALA	4.6
20	A	104	G	4.5
20	A	743	U	4.5
3	D	131	ARG	4.5
20	A	137	C	4.5
20	A	1359	C	4.5
19	T	71	THR	4.5
19	T	22	ARG	4.5
20	A	1343	G	4.5
20	A	1362	C	4.4
20	A	1323	G	4.4
13	N	11	LYS	4.4
20	A	1342	C	4.4
20	A	1185	G	4.4
8	I	116	LYS	4.4
20	A	1305	G	4.4
20	A	1353	G	4.4
15	P	70	ALA	4.3
16	Q	86	GLU	4.3
12	M	11	ARG	4.3
20	A	390	C	4.3
8	I	108	VAL	4.3
20	A	391	G	4.3
2	C	45	LYS	4.2
20	A	716	A	4.2
20	A	66	G	4.2
13	N	35	ARG	4.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
10	K	129	SER	4.2
8	I	115	GLY	4.2
20	A	105	G	4.2
23	Y	165	GLN	4.1
13	N	39	LEU	4.1
23	Y	259	PHE	4.1
23	Y	258	VAL	4.1
23	Y	403	GLU	4.1
16	Q	26	GLN	4.1
20	A	732	C	4.1
20	A	702	A	4.1
20	A	1187	G	4.1
23	Y	105	ILE	4.0
20	A	314	C	4.0
11	L	16	GLU	4.0
20	A	310	G	4.0
10	K	126	ARG	4.0
10	K	123	LYS	4.0
8	I	112	LYS	4.0
20	A	307	C	3.9
9	J	40	LEU	3.9
19	T	68	LYS	3.9
16	Q	25	ARG	3.8
20	A	611	A	3.8
13	N	33	VAL	3.8
20	A	175	C	3.8
20	A	308	C	3.8
20	A	312	C	3.8
20	A	1385	G	3.8
20	A	233	C	3.8
20	A	322	C	3.8
20	A	962	C	3.7
16	Q	37	LYS	3.7
20	A	1049	U	3.7
20	A	1224	G	3.7
20	A	196	A	3.7
20	A	1311	G	3.7
15	P	1	MET	3.7
9	J	45	ARG	3.7
8	I	125	TYR	3.7
20	A	524	G	3.7
20	A	389	A	3.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
23	Y	260	LEU	3.7
20	A	198	G	3.7
9	J	44	VAL	3.6
20	A	112	G	3.6
20	A	123	C	3.6
20	A	46	G	3.6
11	L	12	ARG	3.6
11	L	13	LYS	3.6
3	D	118	ARG	3.6
20	A	355	C	3.6
20	A	1201	A	3.6
15	P	28	ARG	3.6
20	A	1356	G	3.5
3	D	136	PRO	3.5
19	T	20	LEU	3.5
13	N	34	TYR	3.5
20	A	1150	U	3.5
20	A	1361	G	3.5
20	A	1367	C	3.5
13	N	49	HIS	3.5
20	A	121	C	3.5
23	Y	393	ASP	3.5
20	A	261	U	3.5
20	A	262	A	3.5
20	A	176	C	3.5
13	N	38	GLY	3.5
20	A	44	G	3.5
20	A	399	G	3.5
15	P	23	ASP	3.5
20	A	225	C	3.4
20	A	1324	A	3.4
13	N	32	SER	3.4
20	A	106	C	3.4
20	A	974	A	3.4
20	A	1391	U	3.4
23	Y	392	GLU	3.4
20	A	1351	U	3.4
20	A	1286	A	3.4
13	N	42	ILE	3.4
20	A	1347	G	3.4
20	A	1366	C	3.4
8	I	107	ARG	3.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
19	T	29	LYS	3.3
23	Y	342	TYR	3.3
20	A	890	G	3.3
20	A	1339	A	3.3
23	Y	148	LEU	3.3
19	T	28	ALA	3.3
20	A	1322	C	3.3
3	D	209	ARG	3.3
20	A	219	C	3.3
20	A	400	C	3.3
20	A	1527	C	3.3
20	A	1250	A	3.3
20	A	906	G	3.3
23	Y	208	GLN	3.3
19	T	21	LYS	3.2
16	Q	23	VAL	3.2
20	A	967	C	3.2
20	A	1234	C	3.2
11	L	47	LYS	3.2
13	N	29	ARG	3.2
19	T	25	ARG	3.2
20	A	222	U	3.1
13	N	37	PHE	3.1
20	A	148	G	3.1
19	T	67	ALA	3.1
13	N	47	LEU	3.1
20	A	1392	G	3.1
3	D	80	GLU	3.1
16	Q	27	PHE	3.1
20	A	290	C	3.1
20	A	1326	C	3.1
20	A	64	G	3.1
8	I	110	GLU	3.1
9	J	48	THR	3.0
20	A	327	A	3.0
20	A	1280	A	3.0
20	A	178	C	3.0
20	A	668	G	3.0
11	L	127	GLU	3.0
8	I	13	ALA	3.0
20	A	1245	A	3.0
10	K	124	LYS	3.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
20	A	731	G	3.0
8	I	11	LYS	3.0
13	N	41	ARG	3.0
20	A	1525	G	3.0
8	I	118	LYS	3.0
8	I	66	ARG	3.0
19	T	31	SER	3.0
20	A	40	C	3.0
13	N	43	CYS	2.9
15	P	55	ARG	2.9
20	A	817	C	2.9
20	A	1086	U	2.9
19	T	26	ASN	2.9
20	A	942	G	2.9
23	Y	275	ALA	2.9
20	A	107	G	2.9
20	A	313	A	2.9
7	H	1	MET	2.9
23	Y	47	GLU	2.9
20	A	1038	C	2.9
20	A	199	G	2.9
23	Y	204	GLU	2.9
3	D	76	ARG	2.9
20	A	1281	U	2.8
9	J	67	THR	2.8
20	A	382	A	2.8
20	A	1257	U	2.8
11	L	21	LYS	2.8
3	D	138	TYR	2.8
20	A	379	C	2.8
21	V	9	G	2.8
20	A	871	U	2.8
23	Y	272	LEU	2.8
13	N	3	ARG	2.8
20	A	30	U	2.7
20	A	223	U	2.7
9	J	65	LEU	2.7
13	N	48	ALA	2.7
20	A	1384	C	2.7
8	I	121	ARG	2.7
13	N	36	PHE	2.7
9	J	46	ARG	2.7

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
12	M	10	PRO	2.7
20	A	589	C	2.7
23	Y	107	VAL	2.7
13	N	44	LEU	2.7
4	E	140	ARG	2.7
16	Q	4	LYS	2.7
23	Y	396	ARG	2.7
20	A	883	C	2.7
20	A	1344	C	2.7
20	A	305	G	2.7
23	Y	74	TRP	2.7
19	T	74	LYS	2.7
15	P	8	ARG	2.7
23	Y	82	ILE	2.7
23	Y	349	LYS	2.6
20	A	1390	U	2.6
20	A	717	C	2.6
20	A	677	U	2.6
20	A	1372	U	2.6
20	A	973	G	2.6
20	A	140	A	2.6
20	A	31	G	2.5
20	A	1149	C	2.5
20	A	1063	C	2.5
20	A	397	A	2.5
20	A	177	C	2.5
11	L	19	ARG	2.5
20	A	398	C	2.5
9	J	68	HIS	2.5
19	T	77	ALA	2.5
11	L	128	ALA	2.5
7	H	2	LEU	2.5
23	Y	151	ARG	2.5
20	A	566	G	2.5
4	E	134	ALA	2.5
8	I	114	TYR	2.5
23	Y	276	VAL	2.5
3	D	139	ARG	2.4
20	A	742	G	2.4
6	G	14	PRO	2.4
20	A	1202	G	2.4
22	W	32	C	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
8	I	67	GLY	2.4
16	Q	5	VAL	2.4
20	A	934	C	2.4
20	A	1254	C	2.4
6	G	41	ARG	2.4
10	K	121	PRO	2.4
16	Q	24	GLU	2.4
23	Y	133	ILE	2.4
6	G	82	GLY	2.4
20	A	68	G	2.4
8	I	8	GLY	2.4
20	A	317	G	2.4
19	T	70	SER	2.4
21	V	13	A	2.4
19	T	19	SER	2.4
20	A	1183	A	2.4
8	I	41	VAL	2.3
20	A	332	G	2.3
20	A	966	G	2.3
23	Y	212	TYR	2.3
7	H	58	TYR	2.3
20	A	1065	U	2.3
20	A	499	A	2.3
4	E	83	GLU	2.3
15	P	31	LYS	2.3
20	A	1346	A	2.3
20	A	150	C	2.3
11	L	17	LYS	2.3
20	A	862	C	2.3
19	T	30	LYS	2.3
20	A	1320	C	2.3
20	A	29	G	2.3
20	A	67	C	2.3
3	D	103	ASN	2.2
23	Y	16	GLY	2.2
7	H	56	LYS	2.2
20	A	306	G	2.2
10	K	125	PHE	2.2
20	A	1360	A	2.2
23	Y	257	PRO	2.2
13	N	15	LYS	2.2
13	N	26	ARG	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
20	A	1340	A	2.2
23	Y	205	TYR	2.2
20	A	280	C	2.2
20	A	1284	C	2.2
20	A	961	U	2.2
20	A	507	C	2.2
20	A	980	C	2.2
20	A	1317	C	2.2
20	A	263	A	2.2
20	A	571	U	2.2
12	M	9	ILE	2.2
9	J	39	PRO	2.2
20	A	653	A	2.2
23	Y	271	LEU	2.2
8	I	73	GLN	2.2
20	A	1223	C	2.1
23	Y	273	LEU	2.1
11	L	14	GLY	2.1
18	S	8	GLY	2.1
20	A	41	G	2.1
13	N	10	ALA	2.1
11	L	106	ASP	2.1
23	Y	155	GLU	2.1
23	Y	347	GLY	2.1
20	A	501	C	2.1
9	J	62	HIS	2.1
20	A	994	A	2.1
8	I	48	GLU	2.1
20	A	194	C	2.1
20	A	139	G	2.1
20	A	568	G	2.1
20	A	103	C	2.1
20	A	25	C	2.1
8	I	109	VAL	2.1
8	I	15	ALA	2.1
20	A	179	A	2.1
20	A	383	A	2.1
20	A	304	U	2.1
20	A	315	A	2.0
20	A	983	A	2.0
8	I	12	GLU	2.0
23	Y	348	ARG	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
4	E	138	ALA	2.0
15	P	65	GLN	2.0
15	P	7	ALA	2.0
20	A	405	U	2.0
20	A	854	G	2.0
20	A	1316	G	2.0
19	T	27	LYS	2.0
13	N	60	SER	2.0
20	A	715	A	2.0
23	Y	104	ALA	2.0
13	N	22	THR	2.0
16	Q	29	HIS	2.0
19	T	62	LEU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
24	DPP	U	2	6/7	0.15	-	65,65,65,65	0
24	UAL	U	5	9/10	0.13	-	65,65,65,65	0
24	KBE	U	1	9/10	0.17	-	65,65,65,65	0
24	5OH	U	6	12/13	0.32	-	99,101,102,102	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
25	MG	Y	701	1/1	0.14	-	104,104,104,104	0
26	GNP	Y	702	32/32	0.23	-	58,71,81,83	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.