



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 03:41 AM GMT

PDB ID : 1K8A  
Title : Co-crystal structure of Carbomycin A bound to the 50S ribosomal subunit of *Haloarcula marismortui*  
Authors : Hansen, J.L.; Ippolito, J.A.; Ban, N.; Nissen, P.; Moore, P.B.; Steitz, T.  
Deposited on : 2001-10-23  
Resolution : 3.00 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>

---

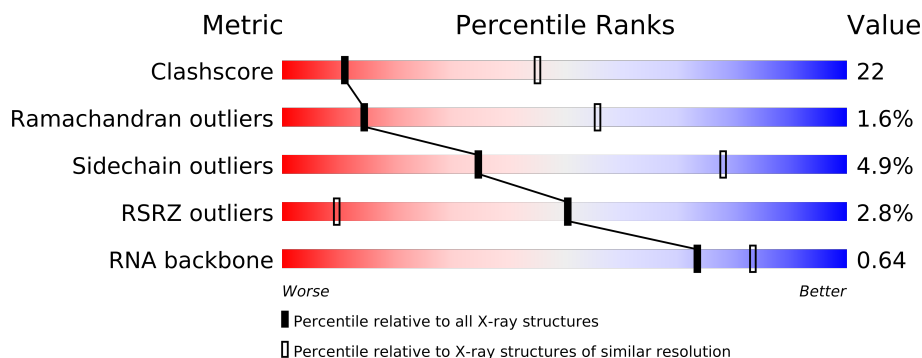
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)
RNA backbone	1838	1070 (3.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	2922	
2	B	122	
3	C	239	
4	D	337	
5	E	246	
6	F	176	
7	G	177	
8	H	119	
9	I	348	
10	J	167	
11	K	145	
12	L	132	
13	M	164	
14	N	194	

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
15	O	186	
16	P	115	
17	Q	148	
18	R	95	
19	S	154	
20	T	84	
21	U	119	
22	V	66	
23	W	70	
24	X	154	
25	Y	91	
26	Z	240	
27	1	73	
28	2	56	
29	3	48	
30	4	92	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
31	CAI	A	4000	-	X
32	MG	A	8022	-	X
32	MG	A	8024	-	X
32	MG	A	8042	-	X
32	MG	A	8044	-	X
32	MG	A	8050	-	X
32	MG	A	8064	-	X
32	MG	A	8067	-	X
32	MG	A	8070	-	X
32	MG	A	8090	-	X
32	MG	A	8092	-	X
32	MG	A	8097	-	X
32	MG	A	8102	-	X
32	MG	A	8103	-	X
32	MG	A	8104	-	X
32	MG	A	8108	-	X
32	MG	A	8116	-	X
32	MG	A	8118	-	X
32	MG	A	8119	-	X
33	NA	A	8301	-	X
33	NA	A	8303	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Geometry	Electron density
33	NA	A	8306	-	X
33	NA	A	8308	-	X
33	NA	A	8310	-	X
33	NA	A	8313	-	X
33	NA	A	8314	-	X
33	NA	A	8316	-	X
33	NA	A	8318	-	X
33	NA	A	8321	-	X
33	NA	A	8323	-	X
33	NA	A	8325	-	X
33	NA	A	8326	-	X
33	NA	A	8329	-	X
33	NA	A	8332	-	X
33	NA	A	8339	-	X
33	NA	A	8340	-	X
33	NA	A	8342	-	X
33	NA	A	8349	-	X
33	NA	A	8350	-	X
33	NA	A	8352	-	X
33	NA	A	8354	-	X
33	NA	A	8355	-	X
33	NA	A	8356	-	X
33	NA	A	8359	-	X
33	NA	A	8360	-	X
33	NA	A	8361	-	X
33	NA	A	8362	-	X
33	NA	A	8363	-	X
33	NA	A	8364	-	X
33	NA	A	8370	-	X
33	NA	A	8371	-	X
33	NA	A	8372	-	X
33	NA	A	8373	-	X
33	NA	A	8374	-	X
33	NA	A	8377	-	X
33	NA	A	8378	-	X
33	NA	A	8379	-	X
33	NA	A	8382	-	X
33	NA	A	8384	-	X
33	NA	A	8385	-	X
33	NA	B	8383	-	X
33	NA	J	8322	-	X
33	NA	N	8365	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Geometry	Electron density
33	NA	S	8337	-	X
33	NA	T	8312	-	X
34	CL	A	8503	-	X
34	CL	A	8505	-	X
34	CL	A	8515	-	X
34	CL	A	8522	-	X
34	CL	A	8523	-	X
34	CL	D	8519	-	X
34	CL	M	8510	-	X
34	CL	P	8508	-	X
34	CL	R	8511	-	X
34	CL	S	8506	-	X
35	K	A	8601	-	X
35	K	A	8603	-	X
36	CD	4	8404	-	X

## 2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 98560 atoms, of which 0 are hydrogen and 0 are deuterium.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2754	Total	C	N	O	P	0	0	0
			59017	26346	10878	19048	2745			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	560	C	U	CONFLICT	? 3377779

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	122	Total	C	N	O	P	0	0	0
			2600	1160	472	847	121			

- Molecule 3 is a protein called RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	237	Total	C	N	O	S	0	0	0
			1754	1072	352	325	5			

- Molecule 4 is a protein called RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	337	Total	C	N	O	S	0	0	0
			2624	1616	493	510	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	PRO	DELETION	UNP P20279
D	310	ARG	PHE	CONFLICT	UNP P20279

- Molecule 5 is a protein called RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	246	Total	C	N	O	S	0	0	0
			1858	1131	344	382	1			

- Molecule 6 is a protein called RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	140	Total	C	N	O	S	0	0	0
			1094	685	195	210	4			

- Molecule 7 is a protein called RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	172	Total	C	N	O	S	0	0	0
			1357	840	224	289	4			

- Molecule 8 is a protein called RIBOSOMAL PROTEIN L7AE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	119	Total	C	N	O	S	0	0	0
			885	552	141	191	1			

- Molecule 9 is a protein called RIBOSOMAL PROTEIN L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	29	Total	C	N	O	S	0	0	0
			240	149	39	51	1			

- Molecule 10 is a protein called RIBOSOMAL PROTEIN L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	156	Total	C	N	O	S	0	0	0
			1215	766	233	212	4			

- Molecule 11 is a protein called RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	142	Total	C	N	O	S	0	0	0
			1119	696	199	221	3			

- Molecule 12 is a protein called RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	132	Total	C	N	O	S	0	0	0
			993	609	189	191	4			

- Molecule 13 is a protein called RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	145	Total	C	N	O	S	0	0	0
			1114	668	222	224				

- Molecule 14 is a protein called RIBOSOMAL PROTEIN L15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	194	Total	C	N	O	S	0	0	0
			1605	988	346	266	5			

- Molecule 15 is a protein called RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	186	Total	C	N	O	S	0	0	0
			1444	895	262	285	2			

- Molecule 16 is a protein called RIBOSOMAL PROTEIN L18E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	115	Total	C	N	O	S	0	0	0
			864	529	161	174				

- Molecule 17 is a protein called RIBOSOMAL PROTEIN L19E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	143	Total	C	N	O	S	0	0	0
			1133	680	230	223				

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	71	LYS	TYR	CONFLICT	UNP P14119

- Molecule 18 is a protein called RIBOSOMAL PROTEIN L21E.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	95	Total	C	N	O			
			734	450	141	143	0	0	0

- Molecule 19 is a protein called RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	S	150	Total	C	N	O	S		
			1149	713	209	223	4	0	0

- Molecule 20 is a protein called RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	T	81	Total	C	N	O	S		
			641	389	111	138	3	0	0

- Molecule 21 is a protein called RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	U	119	Total	C	N	O			
			949	568	180	201		0	0

- Molecule 22 is a protein called RIBOSOMAL PROTEIN L24E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	V	53	Total	C	N	O	S		
			410	244	75	86	5	0	0

- Molecule 23 is a protein called RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	W	65	Total	C	N	O	S		
			499	304	94	100	1	0	0

- Molecule 24 is a protein called RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	X	154	Total	C	N	O	S		
			1195	737	209	243	6	0	0

- Molecule 25 is a protein called RIBOSOMAL PROTEIN L31E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Y	82	Total	C	N	O	S	0	0	0
			654	402	129	122	1			

- Molecule 26 is a protein called RIBOSOMAL PROTEIN L32E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	142	Total	C	N	O		0	0	0
			1130	686	228	216				

- Molecule 27 is a protein called RIBOSOMAL PROTEIN L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	1	73	Total	C	N	O	S	0	0	0
			563	359	111	86	7			

- Molecule 28 is a protein called RIBOSOMAL PROTEIN L37E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	2	56	Total	C	N	O	S	0	0	0
			430	258	86	82	4			

- Molecule 29 is a protein called RIBOSOMAL PROTEIN L39E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	3	46	Total	C	N	O	S	0	0	0
			393	238	86	68	1			

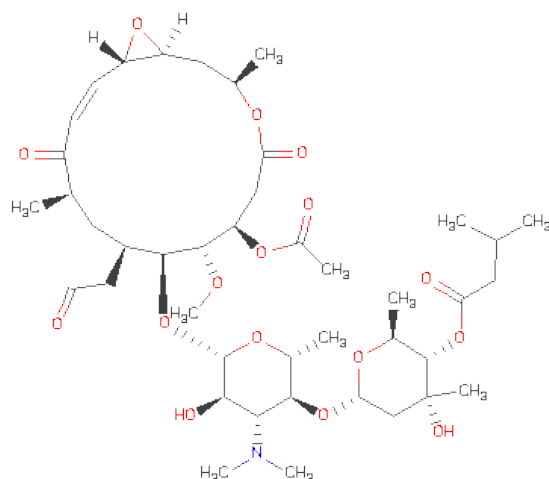
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	?	-	ARG	DELETION	UNP P22452

- Molecule 30 is a protein called RIBOSOMAL PROTEIN L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	4	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 31 is CARBOMYCIN A (three-letter code: CAI) (formula: C<sub>42</sub>H<sub>67</sub>NO<sub>16</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	N	O	0	0
			59	42	1	16		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	D	1	Total	Mg	0	0
			1	1		
32	B	1	Total	Mg	0	0
			1	1		
32	C	2	Total	Mg	0	0
			2	2		
32	Z	1	Total	Mg	0	0
			1	1		
32	A	111	Total	Mg	0	0
			111	111		
32	4	1	Total	Mg	0	0
			1	1		
32	U	1	Total	Mg	0	0
			1	1		
32	L	1	Total	Mg	0	0
			1	1		

- Molecule 33 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	J	2	Total Na 2 2	0	0
33	K	1	Total Na 1 1	0	0
33	E	1	Total Na 1 1	0	0
33	B	2	Total Na 2 2	0	0
33	C	1	Total Na 1 1	0	0
33	A	69	Total Na 69 69	0	0
33	T	1	Total Na 1 1	0	0
33	N	2	Total Na 2 2	0	0
33	U	1	Total Na 1 1	0	0
33	R	1	Total Na 1 1	0	0
33	S	1	Total Na 1 1	0	0
33	M	1	Total Na 1 1	0	0

- Molecule 34 is CHLORIDE ION (three-letter code: CL) (formula: CL).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	P	1	Total Cl 1 1	0	0
34	D	1	Total Cl 1 1	0	0
34	K	3	Total Cl 3 3	0	0
34	C	1	Total Cl 1 1	0	0
34	Z	1	Total Cl 1 1	0	0
34	A	10	Total Cl 10 10	0	0
34	4	1	Total Cl 1 1	0	0
34	N	1	Total Cl 1 1	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	O	1	Total 1	Cl 1	0	0
34	R	1	Total 1	Cl 1	0	0
34	S	1	Total 1	Cl 1	0	0
34	M	1	Total 1	Cl 1	0	0

- Molecule 35 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	A	3	Total 3	K 3	0	0

- Molecule 36 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	P	1	Total 1	Cd 1	0	0
36	2	1	Total 1	Cd 1	0	0
36	1	1	Total 1	Cd 1	0	0
36	4	1	Total 1	Cd 1	0	0
36	V	1	Total 1	Cd 1	0	0

- Molecule 37 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	A	5858	Total 5858	O 5858	0	0
37	B	141	Total 141	O 141	0	0
37	C	138	Total 138	O 138	0	0
37	D	154	Total 154	O 154	0	0
37	E	177	Total 177	O 177	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	F	49	Total 49	O 49	0	0
37	G	44	Total 44	O 44	0	0
37	H	26	Total 26	O 26	0	0
37	I	21	Total 21	O 21	0	0
37	J	79	Total 79	O 79	0	0
37	K	53	Total 53	O 53	0	0
37	L	59	Total 59	O 59	0	0
37	M	87	Total 87	O 87	0	0
37	N	130	Total 130	O 130	0	0
37	O	69	Total 69	O 69	0	0
37	P	44	Total 44	O 44	0	0
37	Q	68	Total 68	O 68	0	0
37	R	51	Total 51	O 51	0	0
37	S	81	Total 81	O 81	0	0
37	T	37	Total 37	O 37	0	0
37	U	37	Total 37	O 37	0	0
37	V	28	Total 28	O 28	0	0
37	W	14	Total 14	O 14	0	0
37	X	69	Total 69	O 69	0	0
37	Y	28	Total 28	O 28	0	0
37	Z	100	Total 100	O 100	0	0

*Continued on next page...*

*Continued from previous page...*

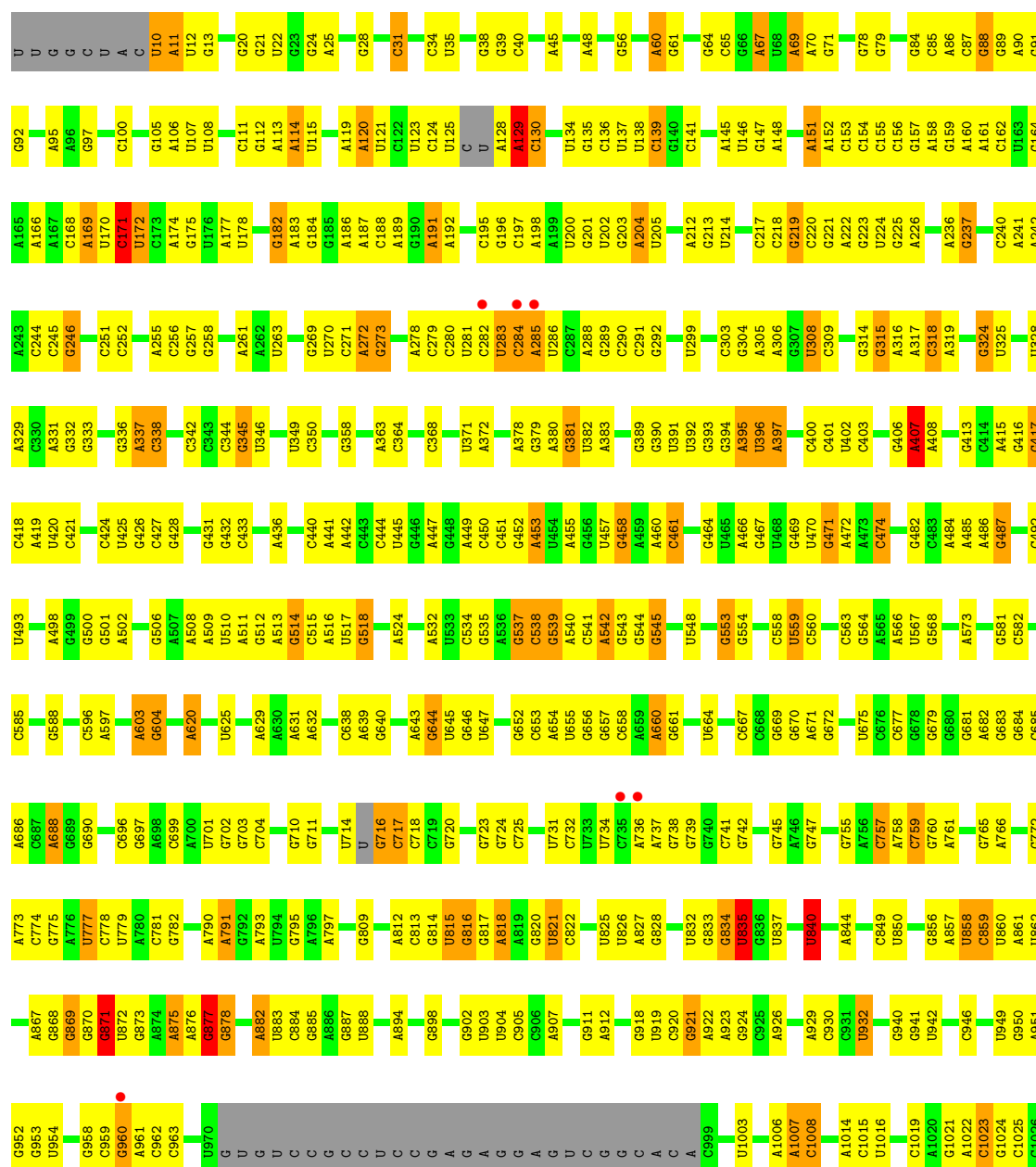
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	1	41	Total 41	O 41	0	0
37	2	58	Total 58	O 58	0	0
37	3	41	Total 41	O 41	0	0
37	4	68	Total 68	O 68	0	0

### 3 Residue-property plots

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

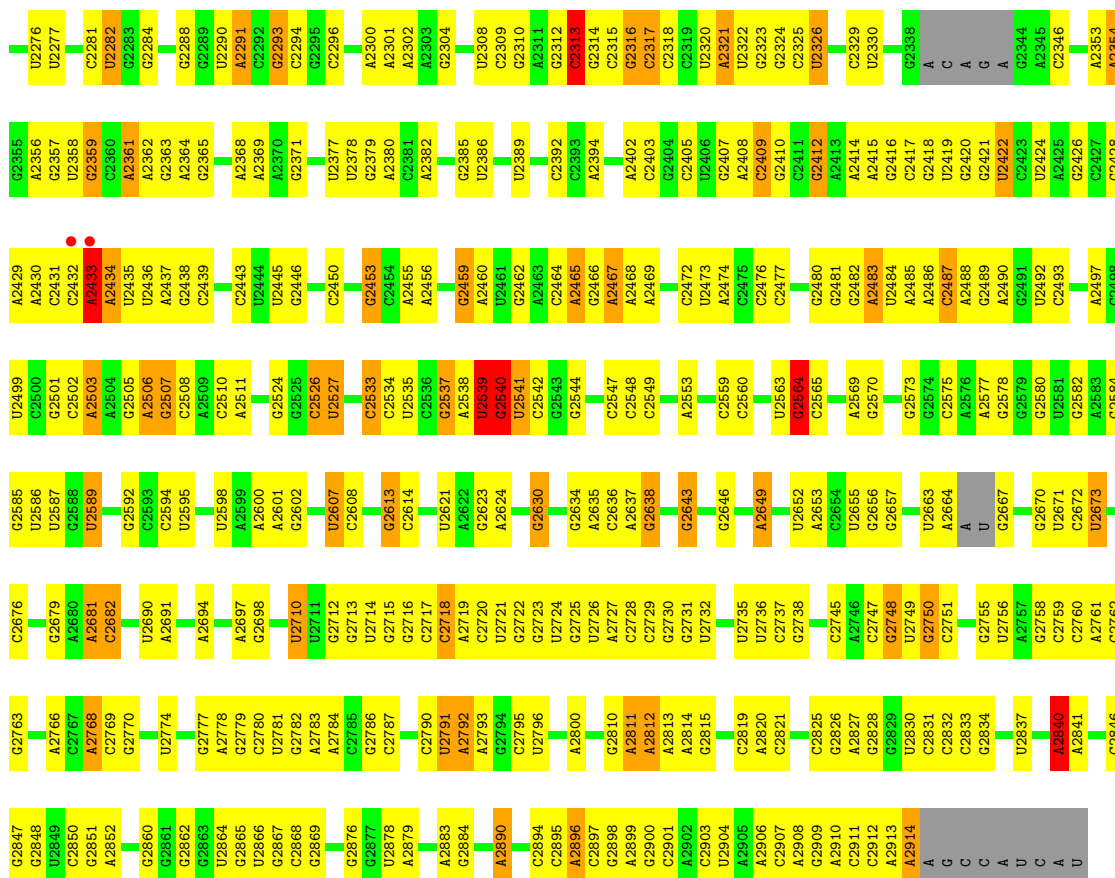
#### • Molecule 1: 23S rRNA

Chain A: 



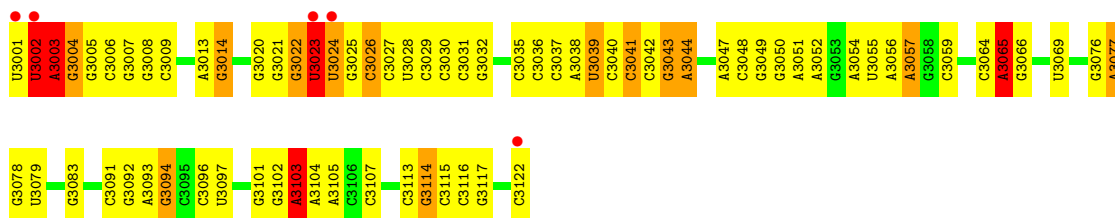


A	G2072	U1980	G1908	C1824	A1729	C1852	A1572	G1387	U1288	A1207	G1027
G	A2073	A1981	A1909	C1825	G1730	U1653	C1483		C1289	C1127	U1028
C		G1982	A1910	C1826	G1731	U1654	G1484	G1391	C1208	U1128	U1029
C		C1983	C1911	G1827	A1732	G1655	A1485	A1392	G1292	C1129	
A	G2079		A1912	G1828	A1733	A1656	A1580	A1393	G1293	G1211	A1032
A	G2080	U1992		C1829	G1734	A1657	U1583	A1487	C1294	C1212	
C	A2081	C1993	A1919	C1830	G1735	A1658		U1489	G1299	C1213	U1041
C	G2082	A1994	C1920	A1736	A1659	G1586	G1586		A1333	A1132	U1042
G	A2083	G1995	A1921	G1833	A1737	G1660	U1587	A1399	G1300	A1133	C1043
U	G2084	U1996	A1922	C1834		G1587	A1494	A1494	G1301	G1135	C1044
C	A2085	A1997	G1923	U1835	U1741	G1588	G1588	A1406	G1302	G1136	G1045
A		G1998	A1924	U1836	U1742	C1866	G1589	A1407	G1302	G1137	
C		A1999	G1925	A1836	G1742	C1867	G1592	U1408	U1306	U1219	G1050
A	G2088	A1999	G1925	A1839	G1742	C1867	G1592	U1408	A1307	G1151	
A	G2089	G2000	G1926	A1840	G1751	U1668	C1593	A1409	A1308	G1051	G1052
U	G2090	G2001	A1931	A1840	G1751	A1669	U1500		A1307	G1221	G1053
C	G2091	C2002	A1931	C1941	G1752	G1670	A1501	A1414	U1309	G1159	G1054
C	G2092	U2003	G1932	G1753	C1752	U1671	G1595	A1502	U1310	C1229	
A	G2093	U2004	G1933	A1845	A1754	U1671	U1596	U1503	G1311	G1160	G1055
U	G2094	G2005	A1934	U1846	A1755	U1672	A1597	U1422	G1312	A1161	U1056
C	A2095	A1946	A1935	A1847	A1755	A1678	U1504	C1423		G1162	U1057
C	A2096	U2008	C1936	A1847	A1759	C1679	U1506	A1424	G1325	G1163	A1058
C	G2097	G2009	U1937	U1850	A1759	C1680	G1601	G1430	A1328	U1164	G1059
C	A2010	G2010	G1938	G1851	U1766	G1681	C1602	G1512	A1329	C1238	C1060
U	A2100	A2011	U1939	A1851	A1767	A1882	A1603	C1513	A1330	A1166	G1861
C	G2102	U2012	C1940	C1856	G1768	A1883	G1604	U1517	A1330	G1167	U1062
G	A2103	G2013	A1941	A1857	C1769	G1684	A1605	U1432	A1331	G1241	G1063
G	A2104	G2014	A1942	A1857	U1770	A1885	G1606	A1433	C1332	C1168	U1064
U	C2104	A2015	A1942	A1857	U1770	A1885	A1607	A1434	A1332	A1242	U1065
C	A2105	U2016	C1943	U1861	G1771	C1686	G1608	U1435	U1333	A1170	U1066
C	C2105	U2016	C1943	U1861	G1771	C1686	G1608	U1435	U1333	A1171	U1066
A	C2106	U2016	C1943	U1861	G1771	C1686	G1608	U1435	U1333	A1171	U1066
A	U2107	G2025	G1946	C1862	G1773	G1688	C1609	A1437	C1335	G1172	A1067
U	A2108	C2026	G1947	G1863	G1774	G1688	G1610	U1525	U1336	C1245	C1068
C	G2109	C2026	G1947	G1863	G1774	C1692	G1610	G1525	A1173	A1246	G1069
C	G2110	U2030	G1951	G1868	G1777	G1697	C1613	U1526	A1337	A1174	
C	G2111	C2031	A	A1869	A1778	U1698	G1614	A1527	G1441	A1247	A1079
C	A2112	U2032	A	C1870	A1779	U1698	G1614	A1528	U1338	A1248	C1080
C	G2113	G2033	C	U1871		C1699	G1618	G1529	A1442	C1176	A1081
G											
G	U2114	U2034	U	G1785	G1785	C1700	G1618	U1531	G1444	C1251	G1076
U	U2115	C2035	U	C1872	C1786	A1701	G1621	U1531	U1446		
U	U2116	C2036	U	U1874	C1787	U1702	G1622	G1535	U1447	C1256	
C	U2117	C2037	U	G1877	U1788	G1706	G1623	C1536	U1347	A1261	
A											
C	A2118	A2038	A	G1877	G1789	G1706	A1624	G1535	A1348	A1261	
C	C2119	A2039	C	G1878	C1790	G1707	U1625	G1543	G1349	A1262	A1079
G	U2120	C2040	C	U1879	U1791	C1708	A1626	U1544	U1350	C1283	C1084
C	G2121		C	U1879	C1798	G1709	G1627	C1545	G1351	C1283	C1085
C	A2122		C	C1882	C1798	A1710	G1630	G1546	C1353	U1266	C1086
C	C2122	G2044	U1964	C		A1711	A1630		U1457	A1189	A1088
G	G2045	G2045	C1965	A1886	A1804	A1712		G1549	C1360	G1268	
U	G2046	G2046	U1966	U1887	G1805	G1713	C1633	U1461	C1361	A1191	A1098
A	G2128	C2047					G1634	C1462	U1362	A1192	G1099
G			A1969	U1890	C1810	A1717	U1635	U1464	G1363	A1193	
G	U2133	G2053	G1970			G1718	G1636		A1372	C1273	U1099
G	G2134	C2054	G1971	C1894	A1815	G1719	U1637		A1274	U1198	G1110
A	A2135	A2055	A1995	A1816	C1720	C1720		U1559	G1375	G1275	
C	G2136		G1896	G1817	G1721	G1721	A1641	A1470	A1471	U1198	
C	A	U2063	C1974	G1818	U1722	U1722	U1561	U1471	A1375	A1199	U1116
C	C	U2064	C1975	G1819	G1723	G1723	U1562	C1472	G1376	A1200	A1117
C	G	U1976	G1976	G1820	U1724	U1724	G1563	C1473	C1377	A1278	A1118
A	U	A1903	G1977	C1821	U1725	U1725	G1564	C1474	C1384	U1279	G1119
C	U	A1904	A1821	A1904	C1725	C1725	U1645		G1384	C1204	U1120
C	G	A1822	A1822	C1822	C1725	C1725	U1645		G1384	C1204	U1120
C	G	A1822	A1822	C1822	C1725	C1725	U1645		G1384	C1204	U1120
C	G	A1822	A1822	C1822	C1725	C1725	U1645		G1384	C1204	U1120
C	G	A1822	A1822	C1822	C1725	C1725	U1645		G1384	C1204	U1120
C	G	A1822	A1822	C1822	C1725	C1725	U1645		G1384	C1204	U1120
C	G	A1822	A1822	C1822	C1725	C1725	U1645		G1384	C1204	U1120
C	G	A1822	A1822	C1822	C1725	C1725	U1645		G1384	C1204	U1120
C	G	A1822	A1822	C1822	C1725	C1725	U1645		G1384	C1204	U1120
C	G	A1822	A1822	C1822	C1725	C1725	U1645		G1384	C1204	U1120
C	G	A1822	A1822	C1822	C1725	C1725	U1645		G1384	C1204	U1120
C	G	A1822	A1822	C1822	C1725	C1725	U1645		G1384	C1204	U1120
C	G	A1822	A1822	C1822	C1725	C1725	U1645		G1384	C1204	U1120
C	G	A1822	A1822	C1822	C1725	C1725	U1645		G1384	C1204	U1120
C	G	A1822	A1822	C1822	C1725	C1725	U1645		G1384	C1204	U1120
C	G	A1822	A1822	C1822	C1725	C1725	U1645		G1384	C1204	U1120
C	G	A1822	A1822	C1822	C1725	C1725	U1645		G1384	C1204	U1120
C	G	A1822	A1822	C1822	C1725	C1725	U1645		G1384	C1204	U1120
C	G	A1822	A1822	C1822	C1725	C1725	U1645		G1384	C1204	U1120
C	G	A1822	A1822	C1822	C1725	C1725	U1645		G1384	C1204	U1120
C	G	A1822	A1822	C1822	C1725	C1725	U1645		G1384	C1204	U1120
C	G	A1822	A1822	C1822	C1725	C1725	U1645		G1384	C1204	U1120
C	G	A1822	A1822	C1822	C1725	C1725	U1645		G1384	C1204	U1120
C	G	A1822	A1822	C1822	C1725	C1725	U1645		G1384	C1204	U1120
C	G	A1822	A1822	C1822	C1725	C1725	U1645		G1384	C1204	U1120
C	G	A1822	A1822	C1822	C1725	C1725	U1645		G1384	C1204	U1120
C	G	A1822	A1822	C1822	C1725	C1725	U1645		G1384	C1204	U1120
C	G	A1822	A1822	C1822	C1725	C1725	U1645		G1384	C1204	U1120
C	G	A1822	A1822	C1822	C1725	C1725	U1645		G1384	C1204	U1120
C	G	A1822	A1822	C1822	C1725	C1725	U1645		G1384	C1204	U1120
C	G	A1822	A1822	C1822	C1725	C1725	U1645		G1384	C1204	U1120
C	G	A1822	A1822	C1822	C1725	C1725	U1645		G1384	C1204	U1120
C	G	A1822	A1822	C1822	C1725	C1725	U1645		G1384	C1204	U1120
C	G	A1822	A1822	C1822	C1725	C1725	U1645		G1384	C1204	U1120
C	G	A1822	A1822	C1822	C1725	C1725	U1645		G1384	C1204	U1120
C	G	A1822	A1822	C1822	C1725	C1725	U1645		G1384	C1204	U1120



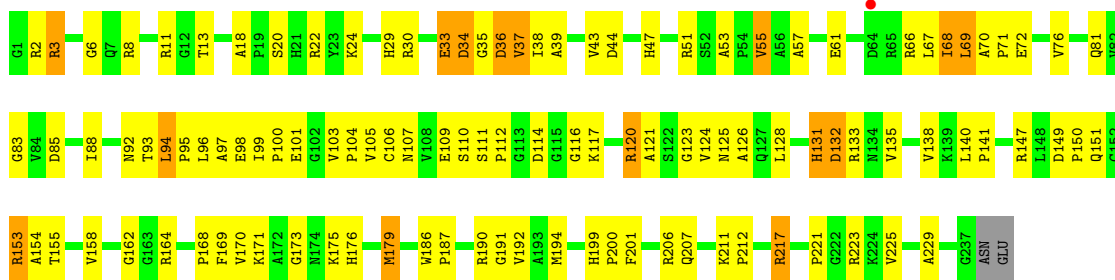
- Molecule 2: 5S rRNA

Chain B:

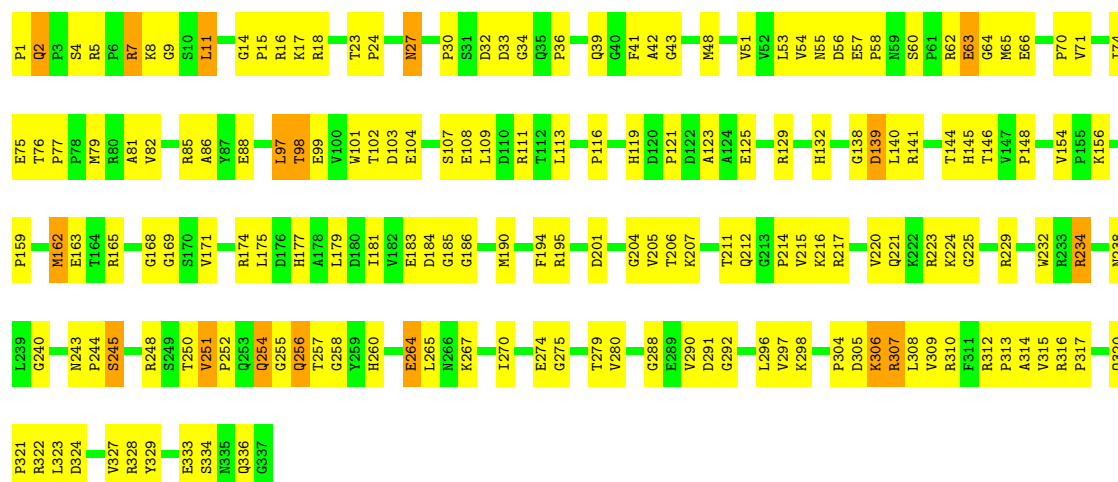


● Molecule 3: RIBOSOMAL PROTEIN L2

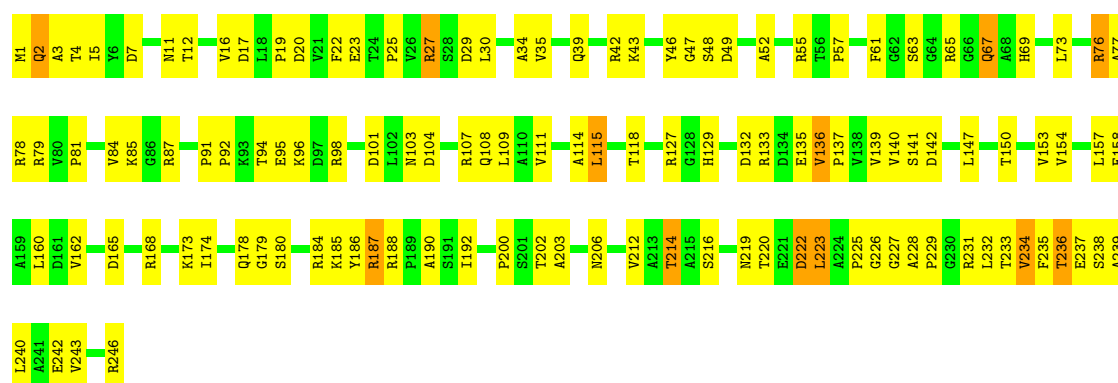
Chain C:



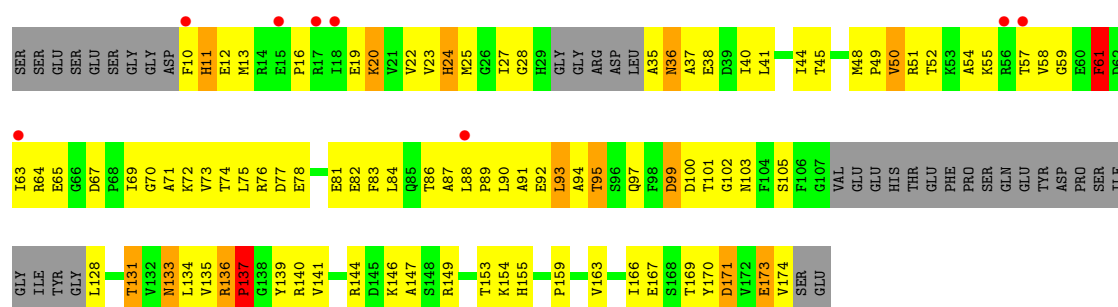
- Molecule 4: RIBOSOMAL PROTEIN L3

Chain D: 

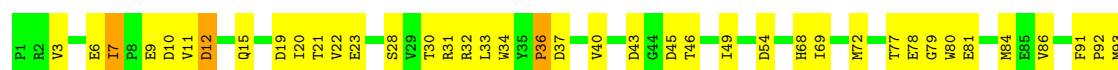
- Molecule 5: RIBOSOMAL PROTEIN L4

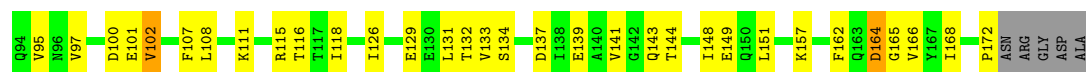
Chain E: 

- Molecule 6: RIBOSOMAL PROTEIN L5

Chain F: 

- Molecule 7: RIBOSOMAL PROTEIN L6

Chain G: 



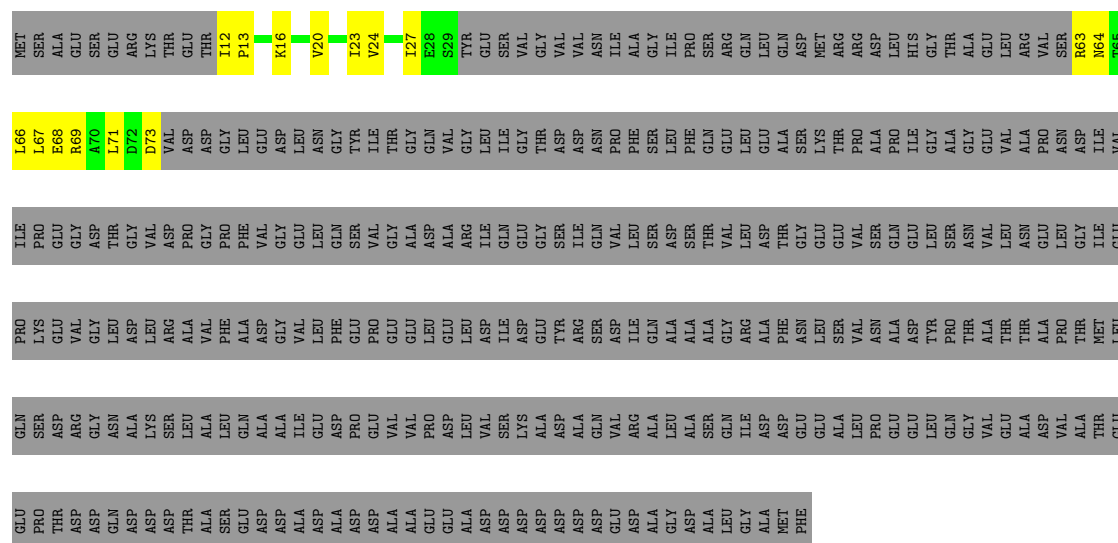
• Molecule 8: RIBOSOMAL PROTEIN L7AE

Chain H:



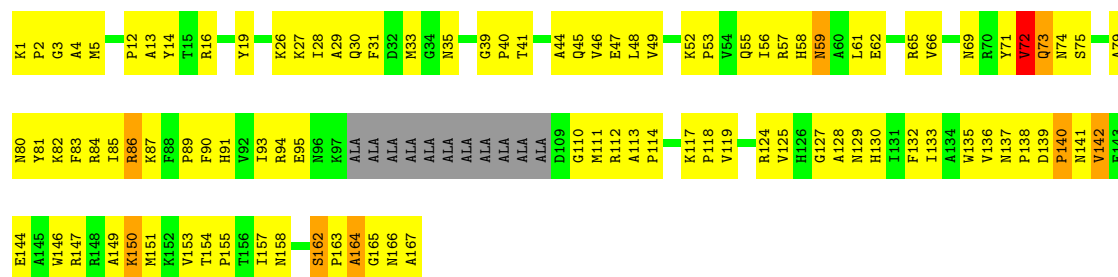
• Molecule 9: RIBOSOMAL PROTEIN L10

Chain I:



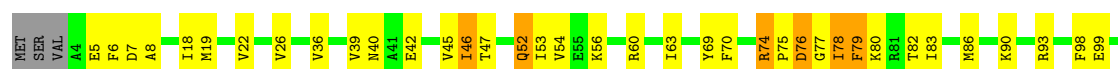
• Molecule 10: RIBOSOMAL PROTEIN L10E

Chain J:



• Molecule 11: RIBOSOMAL PROTEIN L13

Chain K:





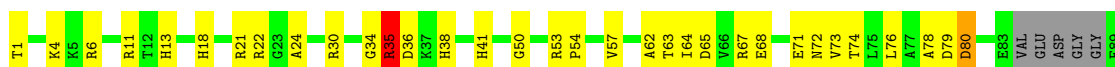
• Molecule 12: RIBOSOMAL PROTEIN L14

Chain L:



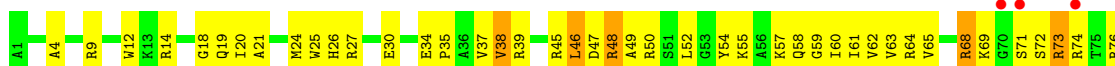
• Molecule 13: RIBOSOMAL PROTEIN L15

Chain M:



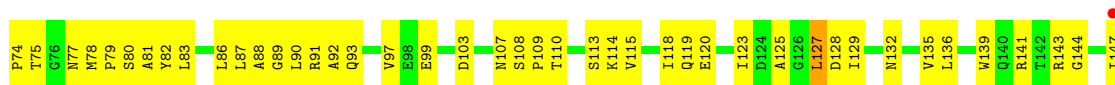
• Molecule 14: RIBOSOMAL PROTEIN L15E

Chain N:



• Molecule 15: RIBOSOMAL PROTEIN L18

Chain O:



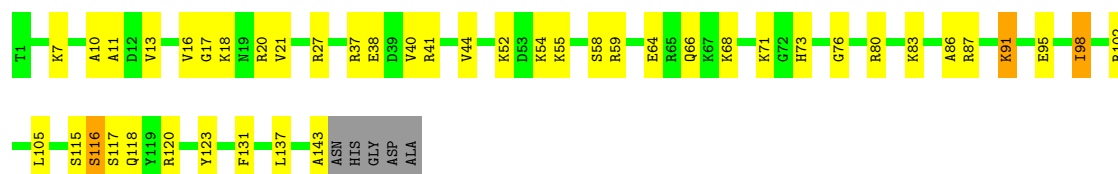
• Molecule 16: RIBOSOMAL PROTEIN L18E

Chain P:



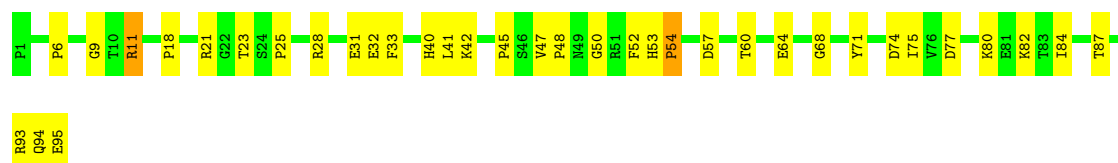
• Molecule 17: RIBOSOMAL PROTEIN L19E

Chain Q:



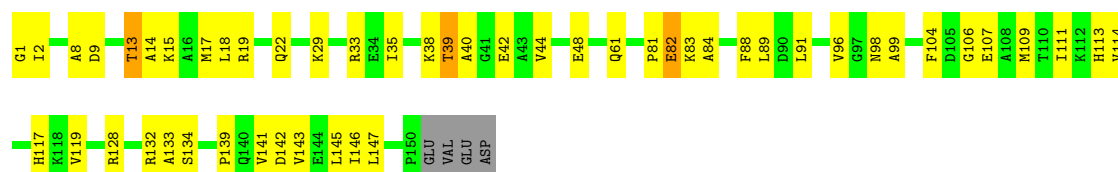
• Molecule 18: RIBOSOMAL PROTEIN L21E

Chain R:



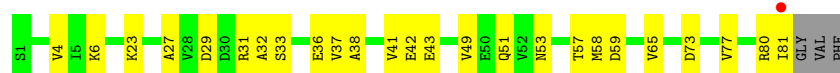
• Molecule 19: RIBOSOMAL PROTEIN L22

Chain S:



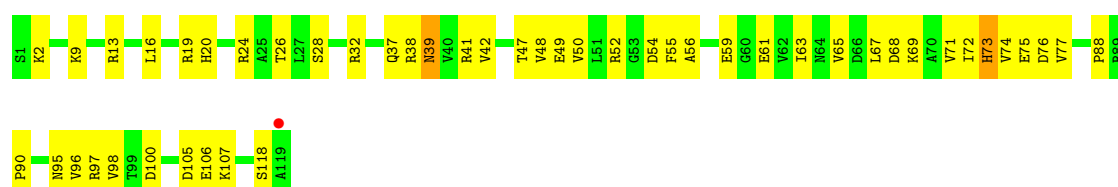
• Molecule 20: RIBOSOMAL PROTEIN L23

Chain T:



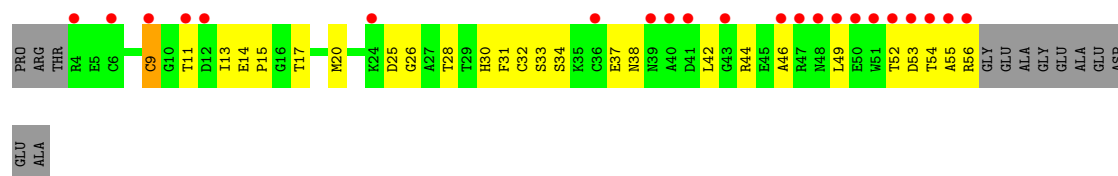
• Molecule 21: RIBOSOMAL PROTEIN L24

Chain U:



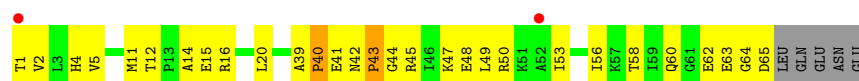
- Molecule 22: RIBOSOMAL PROTEIN L24E

Chain V: 



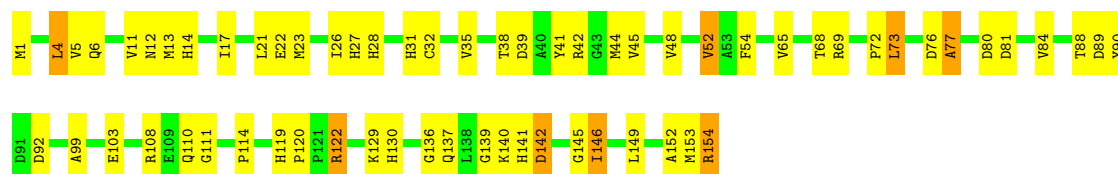
- Molecule 23: RIBOSOMAL PROTEIN L29

Chain W: 



- Molecule 24: RIBOSOMAL PROTEIN L30

Chain X: 



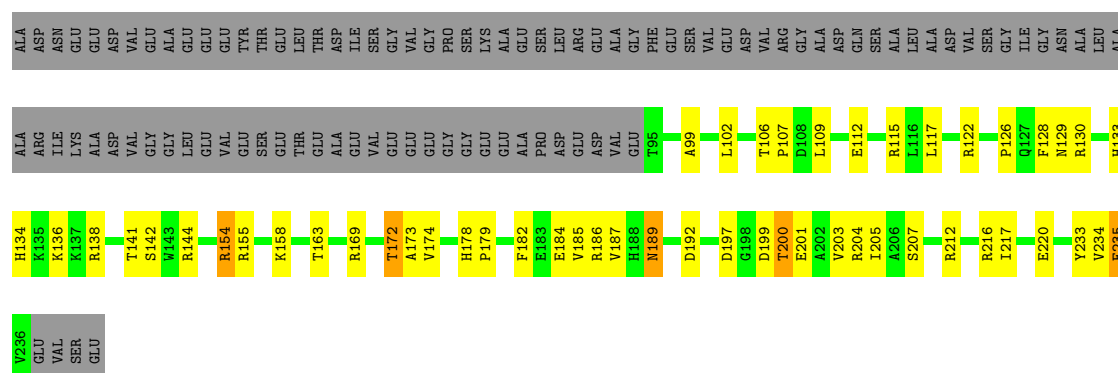
- Molecule 25: RIBOSOMAL PROTEIN L31E

Chain Y: 



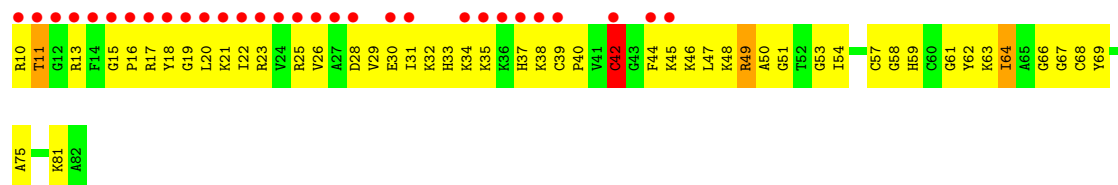
- Molecule 26: RIBOSOMAL PROTEIN L32E

Chain Z: 



- Molecule 27: RIBOSOMAL PROTEIN L37Ae

Chain 1: 



- Molecule 28: RIBOSOMAL PROTEIN L37E

Chain 2: 



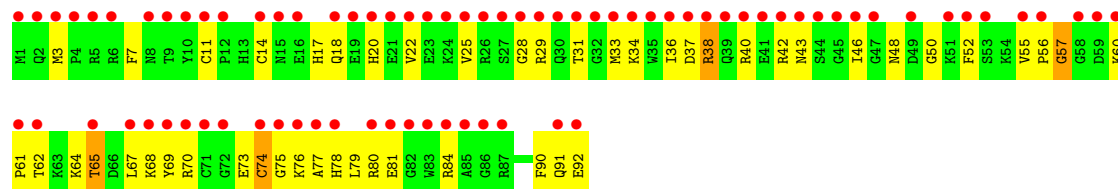
- Molecule 29: RIBOSOMAL PROTEIN L39E

Chain 3: 



- Molecule 30: RIBOSOMAL PROTEIN L44E

Chain 4: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	212.90Å 300.47Å 575.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 49.81 – 2.98	Depositor EDS
% Data completeness (in resolution range)	93.3 (20.00-3.00) 92.3 (49.81-2.98)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.24 (at 2.96Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.227 , 0.265 0.230 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	51.0	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 32.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 367880 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	98560	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.47% 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: MG, CL, NA, K, CD, CAI

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.65	18/66076 (0.0%)	0.79	53/103052 (0.1%)
2	B	0.68	2/2905 (0.1%)	0.87	10/4528 (0.2%)
3	C	0.50	0/1787	0.79	0/2409
4	D	0.50	0/2689	0.73	0/3652
5	E	0.55	0/1883	0.77	0/2551
6	F	0.43	0/1111	0.65	0/1498
7	G	0.49	0/1382	0.66	0/1880
8	H	0.46	0/896	0.66	0/1219
9	I	0.40	0/241	0.56	0/324
10	J	0.52	0/1246	0.83	2/1686 (0.1%)
11	K	0.53	0/1135	0.72	0/1530
12	L	0.51	0/1003	0.77	0/1351
13	M	0.49	0/1126	0.76	0/1504
14	N	0.67	0/1633	0.86	1/2180 (0.0%)
15	O	0.46	0/1473	0.74	0/1999
16	P	0.54	0/873	0.75	0/1181
17	Q	0.50	0/1143	0.67	0/1521
18	R	0.51	0/748	0.77	1/1005 (0.1%)
19	S	0.57	0/1172	0.78	0/1578
20	T	0.43	0/648	0.69	0/875
21	U	0.47	0/957	0.73	0/1289
22	V	0.77	0/417	0.78	0/562
23	W	0.42	0/502	0.62	0/675
24	X	0.55	0/1218	0.75	0/1655
25	Y	0.50	0/664	0.70	0/895
26	Z	0.53	0/1146	0.74	0/1536
27	1	0.89	0/575	0.85	1/763 (0.1%)
28	2	0.57	0/437	0.82	0/578
29	3	0.45	0/398	0.61	0/527
30	4	1.03	0/771	0.79	0/1024
All	All	0.62	20/98255 (0.0%)	0.78	68/147027 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	165
2	B	0	3
All	All	1	168

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2103	A	C5-C4	10.43	1.46	1.38
1	A	2103	A	N7-C5	9.91	1.45	1.39
1	A	2539	U	C5'-C4'	9.04	1.62	1.51
1	A	2486	A	O3'-P	7.36	1.70	1.61
1	A	2105	C	C3'-O3'	6.75	1.51	1.42
2	B	3003	A	C5'-C4'	6.24	1.58	1.51
1	A	2540	G	C5'-C4'	6.13	1.58	1.51
1	A	2105	C	O3'-P	6.00	1.68	1.61
1	A	2539	U	C2'-O2'	5.96	1.49	1.41
2	B	3025	G	O3'-P	-5.84	1.54	1.61
1	A	2103	A	N9-C8	5.82	1.42	1.37
1	A	2106	C	C3'-O3'	-5.67	1.34	1.42
1	A	2539	U	P-OP2	5.64	1.58	1.49
1	A	2433	A	C5-C6	5.30	1.45	1.41
1	A	2103	A	C5-C6	5.30	1.45	1.41
1	A	1206	U	P-OP2	5.24	1.57	1.49
1	A	2540	G	O5'-C5'	5.21	1.52	1.44
1	A	2538	A	O3'-P	-5.21	1.54	1.61
1	A	2106	C	O3'-P	-5.05	1.55	1.61
1	A	2540	G	C2-N3	-5.05	1.28	1.32

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1164	U	OP1-P-O3'	-18.69	64.07	105.20
1	A	1164	U	OP2-P-O3'	-18.22	65.11	105.20
1	A	2540	G	O5'-P-OP1	-13.50	93.55	105.70
1	A	1165	G	O5'-P-OP1	-12.02	94.88	105.70
1	A	1563	G	C2'-C3'-O3'	9.18	129.69	109.50
1	A	1942	A	C5'-C4'-C3'	8.79	130.06	116.00
1	A	2103	A	N1-C2-N3	8.03	133.32	129.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2106	C	N1-C1'-C2'	-8.03	103.17	112.00
1	A	2539	U	P-O3'-C3'	7.92	129.20	119.70
1	A	1942	A	C5'-C4'-O4'	7.76	118.41	109.10
1	A	2106	C	O5'-P-OP2	-7.42	99.03	105.70
1	A	1979	G	C2'-C3'-O3'	7.34	125.64	109.50
2	B	3023	U	OP2-P-O3'	7.08	120.78	105.20
1	A	2540	G	C1'-O4'-C4'	-6.71	104.53	109.90
1	A	2539	U	OP2-P-O3'	6.61	119.73	105.20
2	B	3025	G	O3'-P-O5'	6.57	116.49	104.00
1	A	2103	A	C5'-C4'-O4'	-6.53	101.27	109.10
1	A	2103	A	O4'-C1'-N9	6.46	113.37	108.20
14	N	73	ARG	N-CA-C	-6.41	93.69	111.00
1	A	1165	G	OP1-P-OP2	6.37	129.15	119.60
1	A	2102	G	C5'-C4'-C3'	6.11	125.77	116.00
1	A	2313	C	C5'-C4'-O4'	6.09	116.41	109.10
1	A	2537	G	OP2-P-O3'	6.09	118.61	105.20
1	A	2099	G	OP2-P-O3'	6.09	118.60	105.20
1	A	1165	G	O5'-P-OP2	-6.07	100.23	105.70
1	A	2102	G	C5'-C4'-O4'	6.01	116.32	109.10
1	A	2537	G	O5'-P-OP1	-6.00	100.30	105.70
1	A	2487	C	OP1-P-O3'	6.00	118.39	105.20
1	A	840	U	N1-C1'-C2'	5.99	121.79	114.00
1	A	1283	G	N9-C1'-C2'	-5.92	105.48	112.00
1	A	1504	A	C1'-O4'-C4'	-5.92	105.17	109.90
2	B	3003	A	OP1-P-O3'	5.87	118.11	105.20
1	A	129	A	C2'-C3'-O3'	5.85	123.06	113.70
10	J	74	ASN	N-CA-C	-5.84	95.23	111.00
1	A	2538	A	OP2-P-O3'	5.84	118.05	105.20
1	A	2105	C	OP2-P-O3'	5.76	117.86	105.20
2	B	3039	U	N1-C1'-C2'	5.74	121.45	114.00
1	A	2465	A	N9-C1'-C2'	-5.68	105.75	112.00
1	A	28	G	N9-C1'-C2'	-5.67	105.77	112.00
1	A	1971	G	N9-C1'-C2'	5.63	121.33	114.00
2	B	3023	U	P-O3'-C3'	5.62	126.45	119.70
1	A	2486	A	P-O3'-C3'	5.59	126.41	119.70
1	A	2122	C	OP2-P-O3'	5.54	117.40	105.20
1	A	755	G	O4'-C4'-C3'	-5.50	98.50	104.00
2	B	3003	A	C4'-C3'-C2'	-5.48	97.12	102.60
1	A	1651	C	N1-C1'-C2'	5.40	121.02	114.00
2	B	3004	G	O5'-P-OP1	-5.35	100.89	105.70
1	A	389	G	C5'-C4'-C3'	-5.34	107.45	116.00
1	A	2607	U	N1-C1'-C2'	5.31	120.90	114.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	1	42	CYS	CA-CB-SG	5.31	123.55	114.00
1	A	1683	G	N9-C1'-C2'	5.30	120.89	114.00
10	J	110	GLY	N-CA-C	-5.30	99.85	113.10
1	A	324	G	N9-C1'-C2'	-5.28	106.19	112.00
1	A	407	A	O4'-C4'-C3'	-5.26	98.74	104.00
1	A	171	C	OP2-P-O3'	5.25	116.75	105.20
18	R	68	GLY	N-CA-C	-5.21	100.08	113.10
1	A	1878	G	O4'-C1'-N9	5.19	112.35	108.20
1	A	1204	C	OP2-P-O3'	5.19	116.61	105.20
1	A	2460	A	OP2-P-O3'	5.16	116.55	105.20
1	A	2011	A	C5'-C4'-O4'	5.14	115.27	109.10
1	A	2539	U	O5'-P-OP1	-5.13	101.09	105.70
1	A	1971	G	O4'-C1'-N9	5.09	112.27	108.20
2	B	3002	U	OP2-P-O3'	5.06	116.33	105.20
2	B	3026	C	O3'-P-O5'	5.04	113.57	104.00
1	A	1062	U	N1-C1'-C2'	-5.03	106.47	112.00
1	A	2103	A	N1-C6-N6	5.02	121.61	118.60
1	A	38	G	N9-C1'-C2'	-5.02	106.48	112.00
2	B	3103	A	C5'-C4'-O4'	5.02	115.12	109.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1563	G	C3'

All (168) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1007	A	Sidechain
1	A	1023	C	Sidechain
1	A	1027	G	Sidechain
1	A	1042	U	Sidechain
1	A	1127	C	Sidechain
1	A	1136	U	Sidechain
1	A	1191	A	Sidechain
1	A	1206	U	Sidechain
1	A	1237	U	Sidechain
1	A	1261	A	Sidechain
1	A	1264	U	Sidechain
1	A	1269	G	Sidechain
1	A	1288	U	Sidechain
1	A	1309	U	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
1	A	1336	U	Sidechain
1	A	1347	U	Sidechain
1	A	1376	G	Sidechain
1	A	1387	G	Sidechain
1	A	1408	U	Sidechain
1	A	1430	G	Sidechain
1	A	1432	U	Sidechain
1	A	1447	U	Sidechain
1	A	1458	A	Sidechain
1	A	146	U	Sidechain
1	A	1487	A	Sidechain
1	A	1501	A	Sidechain
1	A	1503	U	Sidechain
1	A	1614	G	Sidechain
1	A	162	C	Sidechain
1	A	1635	U	Sidechain
1	A	1643	C	Sidechain
1	A	1655	G	Sidechain
1	A	1671	U	Sidechain
1	A	1681	G	Sidechain
1	A	1685	A	Sidechain
1	A	1688	G	Sidechain
1	A	170	U	Sidechain
1	A	171	C	Sidechain
1	A	172	U	Sidechain
1	A	1720	C	Sidechain
1	A	1728	G	Sidechain
1	A	1736	A	Sidechain
1	A	174	A	Sidechain
1	A	1777	G	Sidechain
1	A	1819	G	Sidechain
1	A	182	G	Sidechain
1	A	1823	G	Sidechain
1	A	1833	U	Sidechain
1	A	1835	U	Sidechain
1	A	1851	G	Sidechain
1	A	1860	U	Sidechain
1	A	1861	C	Sidechain
1	A	1877	G	Sidechain
1	A	1878	G	Sidechain
1	A	1879	U	Sidechain
1	A	191	A	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
1	A	197	C	Sidechain
1	A	1972	U	Sidechain
1	A	1978	A	Sidechain
1	A	1993	C	Sidechain
1	A	2001	G	Sidechain
1	A	2035	C	Sidechain
1	A	204	A	Sidechain
1	A	2053	G	Sidechain
1	A	2063	U	Sidechain
1	A	2068	G	Sidechain
1	A	2101	A	Sidechain
1	A	2106	C	Sidechain
1	A	2120	U	Sidechain
1	A	2128	G	Sidechain
1	A	2133	U	Sidechain
1	A	22	U	Sidechain
1	A	2266	A	Sidechain
1	A	2282	U	Sidechain
1	A	2288	G	Sidechain
1	A	2293	G	Sidechain
1	A	2304	G	Sidechain
1	A	2308	U	Sidechain
1	A	2312	G	Sidechain
1	A	2313	C	Sidechain
1	A	2316	G	Sidechain
1	A	2326	U	Sidechain
1	A	2358	U	Sidechain
1	A	2359	G	Sidechain
1	A	2364	A	Sidechain
1	A	2378	U	Sidechain
1	A	2394	A	Sidechain
1	A	2409	C	Sidechain
1	A	2412	G	Sidechain
1	A	2433	A	Sidechain
1	A	2434	A	Sidechain
1	A	2436	U	Sidechain
1	A	2439	C	Sidechain
1	A	2453	G	Sidechain
1	A	2459	G	Sidechain
1	A	246	G	Sidechain
1	A	2492	U	Sidechain
1	A	2493	C	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
1	A	2503	A	Sidechain
1	A	2506	A	Sidechain
1	A	2535	U	Sidechain
1	A	2539	U	Sidechain
1	A	2544	G	Sidechain
1	A	2564	G	Sidechain
1	A	2573	G	Sidechain
1	A	2575	C	Sidechain
1	A	261	A	Sidechain
1	A	2630	G	Sidechain
1	A	2643	G	Sidechain
1	A	2655	U	Sidechain
1	A	2663	U	Sidechain
1	A	2673	U	Sidechain
1	A	2710	U	Sidechain
1	A	2774	U	Sidechain
1	A	2790	C	Sidechain
1	A	2793	A	Sidechain
1	A	2810	G	Sidechain
1	A	2811	A	Sidechain
1	A	2840	A	Sidechain
1	A	2864	U	Sidechain
1	A	315	G	Sidechain
1	A	333	G	Sidechain
1	A	395	A	Sidechain
1	A	396	U	Sidechain
1	A	407	A	Sidechain
1	A	436	A	Sidechain
1	A	453	A	Sidechain
1	A	458	G	Sidechain
1	A	460	A	Sidechain
1	A	471	G	Sidechain
1	A	474	C	Sidechain
1	A	48	A	Sidechain
1	A	502	A	Sidechain
1	A	517	U	Sidechain
1	A	518	G	Sidechain
1	A	548	U	Sidechain
1	A	554	G	Sidechain
1	A	720	G	Sidechain
1	A	723	G	Sidechain
1	A	742	G	Sidechain

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Group
1	A	757	C	Sidechain
1	A	759	C	Sidechain
1	A	761	A	Sidechain
1	A	781	C	Sidechain
1	A	782	G	Sidechain
1	A	791	A	Sidechain
1	A	815	U	Sidechain
1	A	816	G	Sidechain
1	A	818	A	Sidechain
1	A	827	A	Sidechain
1	A	835	U	Sidechain
1	A	859	C	Sidechain
1	A	860	U	Sidechain
1	A	867	A	Sidechain
1	A	871	G	Sidechain
1	A	877	G	Sidechain
1	A	882	A	Sidechain
1	A	887	G	Sidechain
1	A	888	U	Sidechain
1	A	904	U	Sidechain
1	A	919	U	Sidechain
1	A	932	U	Sidechain
1	A	946	C	Sidechain
1	A	950	G	Sidechain
1	A	954	U	Sidechain
2	B	3005	G	Sidechain
2	B	3065	A	Sidechain
2	B	3094	G	Sidechain

## 5.2 Close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	59017	0	29799	1358	0
2	B	2600	0	1326	83	0
3	C	1754	0	1763	123	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	2624	0	2533	195	0
5	E	1858	0	1816	151	0
6	F	1094	0	1085	140	0
7	G	1357	0	1266	82	0
8	H	885	0	854	64	0
9	I	240	0	231	20	0
10	J	1215	0	1215	162	0
11	K	1119	0	1098	74	0
12	L	993	0	1027	65	0
13	M	1114	0	1072	78	0
14	N	1605	0	1676	197	0
15	O	1444	0	1401	146	0
16	P	864	0	873	44	0
17	Q	1133	0	1127	60	0
18	R	734	0	728	30	0
19	S	1149	0	1122	61	0
20	T	641	0	605	30	0
21	U	949	0	923	56	0
22	V	410	0	366	38	0
23	W	499	0	511	29	0
24	X	1195	0	1137	92	0
25	Y	654	0	653	48	0
26	Z	1130	0	1133	64	0
27	1	563	0	600	79	0
28	2	430	0	426	26	0
29	3	393	0	406	30	0
30	4	755	0	731	52	0
31	A	59	0	63	4	0
32	4	1	0	0	0	0
32	A	111	0	0	0	0
32	B	1	0	0	0	0
32	C	2	0	0	0	0
32	D	1	0	0	0	0
32	L	1	0	0	0	0
32	U	1	0	0	0	0
32	Z	1	0	0	0	0
33	A	69	0	0	0	0
33	B	2	0	0	0	0
33	C	1	0	0	0	0
33	E	1	0	0	0	0
33	J	2	0	0	0	0
33	K	1	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	M	1	0	0	0	0
33	N	2	0	0	0	0
33	R	1	0	0	0	0
33	S	1	0	0	0	0
33	T	1	0	0	0	0
33	U	1	0	0	0	0
34	4	1	0	0	0	0
34	A	10	0	0	3	0
34	C	1	0	0	0	0
34	D	1	0	0	0	0
34	K	3	0	0	0	0
34	M	1	0	0	0	0
34	N	1	0	0	1	0
34	O	1	0	0	0	0
34	P	1	0	0	0	0
34	R	1	0	0	0	0
34	S	1	0	0	0	0
34	Z	1	0	0	0	0
35	A	3	0	0	0	0
36	1	1	0	0	0	0
36	2	1	0	0	0	0
36	4	1	0	0	0	0
36	P	1	0	0	0	0
36	V	1	0	0	0	0
37	1	41	0	0	17	0
37	2	58	0	0	5	0
37	3	41	0	0	8	0
37	4	68	0	0	11	0
37	A	5858	0	0	321	0
37	B	141	0	0	15	0
37	C	138	0	0	13	0
37	D	154	0	0	32	0
37	E	177	0	0	45	0
37	F	49	0	0	20	0
37	G	44	0	0	13	0
37	H	26	0	0	12	0
37	I	21	0	0	4	0
37	J	79	0	0	23	0
37	K	53	0	0	5	0
37	L	59	0	0	12	0
37	M	87	0	0	22	0
37	N	130	0	0	29	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	O	69	0	0	23	0
37	P	44	0	0	11	0
37	Q	68	0	0	7	0
37	R	51	0	0	5	0
37	S	81	0	0	6	0
37	T	37	0	0	7	0
37	U	37	0	0	4	0
37	V	28	0	0	6	0
37	W	14	0	0	3	0
37	X	69	0	0	7	0
37	Y	28	0	0	10	0
37	Z	100	0	0	18	0
All	All	98560	0	59566	3372	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 22.

All (3372) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:J:86:ARG:NH1	10:J:133:ILE:HG13	1.61	1.15
14:N:52:LEU:HD11	37:N:8615:HOH:O	1.46	1.15
5:E:236:THR:HG22	5:E:239:ALA:H	1.06	1.13
1:A:1160:G:H5'	1:A:1161:A:H5'	1.30	1.11
21:U:71:VAL:HG11	21:U:90:PRO:HB3	1.31	1.11
14:N:87:MET:HG2	30:4:46:ILE:HG21	1.30	1.10
1:A:871:G:H5'	1:A:871:G:H8	1.03	1.10
1:A:2122:C:OP2	37:A:6114:HOH:O	1.69	1.10
1:A:2123:A:OP2	37:A:4844:HOH:O	1.72	1.08
10:J:165:GLY:HA3	37:J:8399:HOH:O	1.53	1.07
24:X:122:ARG:HH21	24:X:154:ARG:HD2	1.13	1.06
27:1:46:LYS:HD3	27:1:59:HIS:HB2	1.37	1.06
1:A:871:G:H5'	1:A:871:G:C8	1.90	1.05
1:A:156:C:H5''	14:N:171:ARG:HD3	1.38	1.05
14:N:35:PRO:HG2	14:N:38:VAL:HG23	1.37	1.04
1:A:1134:G:H4'	10:J:151:MET:HE1	1.39	1.03
25:Y:37:LEU:HD13	25:Y:85:VAL:HG21	1.40	1.03
23:W:12:THR:HG22	23:W:15:GLU:HG3	1.41	1.03
5:E:115:LEU:HD13	5:E:223:LEU:HD21	1.41	1.03
10:J:45:GLN:HB3	10:J:163:PRO:HD2	1.35	1.03
14:N:164:THR:HG22	14:N:167:GLY:H	1.24	1.02
1:A:870:G:H2'	1:A:871:G:H5''	1.37	1.01
24:X:122:ARG:NH2	24:X:154:ARG:HD2	1.77	1.00

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
17:Q:115:SER:H	17:Q:118:GLN:HE21	1.01	0.99
10:J:86:ARG:HH11	10:J:133:ILE:HG13	0.82	0.99
5:E:236:THR:HG21	37:E:8375:HOH:O	1.59	0.99
10:J:26:LYS:HD2	10:J:28:ILE:HD12	1.45	0.99
4:D:86:ALA:HA	37:D:8583:HOH:O	1.62	0.99
6:F:134:LEU:HD11	6:F:166:ILE:HD11	1.41	0.99
14:N:87:MET:CG	30:4:46:ILE:HG21	1.92	0.99
10:J:86:ARG:HH11	10:J:133:ILE:CG1	1.76	0.98
1:A:2717:C:H2'	1:A:2718:C:H5''	1.43	0.98
10:J:162:SER:HB2	10:J:163:PRO:HD3	1.42	0.98
10:J:29:ALA:HB3	10:J:65:ARG:HH12	1.25	0.98
1:A:2121:G:H5''	37:A:3085:HOH:O	1.65	0.97
4:D:264:GLU:HG2	4:D:267:LYS:HE2	1.44	0.97
4:D:62:ARG:HA	4:D:65:MET:HE3	1.46	0.97
12:L:29:LEU:HB3	12:L:55:VAL:HG11	1.46	0.97
1:A:1835:U:H5	1:A:1840:A:N7	1.59	0.97
30:4:70:ARG:HG2	30:4:77:ALA:HB2	1.43	0.97
5:E:5:ILE:HD11	5:E:16:VAL:HG23	1.44	0.96
1:A:542:A:H8	1:A:542:A:H5'	1.29	0.96
24:X:88:THR:HG22	24:X:89:ASP:H	1.31	0.96
1:A:2004:U:H4'	37:A:4862:HOH:O	1.64	0.95
15:O:47:LEU:HD11	15:O:127:LEU:HD21	1.45	0.95
2:B:3006:C:H5''	15:O:37:ARG:NH1	1.80	0.95
1:A:962:C:H1'	15:O:5:ARG:NH1	1.82	0.95
1:A:714:U:H3'	37:A:6481:HOH:O	1.66	0.95
10:J:2:PRO:HB2	37:J:8366:HOH:O	1.67	0.94
6:F:105:SER:HB2	6:F:131:THR:HG23	1.48	0.94
14:N:102:GLU:OE1	14:N:164:THR:HG21	1.67	0.94
37:A:4420:HOH:O	14:N:14:ARG:HG2	1.66	0.94
17:Q:115:SER:OG	17:Q:118:GLN:HG3	1.67	0.93
2:B:3056:A:H2'	2:B:3057:A:H5''	1.49	0.93
1:A:871:G:C5'	1:A:871:G:H8	1.80	0.93
1:A:1242:A:H5'	11:K:82:THR:HG23	1.48	0.93
24:X:88:THR:HB	37:X:6679:HOH:O	1.69	0.93
1:A:1751:G:H2'	1:A:1752:G:H5''	1.48	0.93
14:N:35:PRO:CG	14:N:38:VAL:HG23	1.98	0.93
15:O:7:LYS:HE3	18:R:21:ARG:O	1.68	0.92
4:D:140:LEU:HA	37:D:8583:HOH:O	1.67	0.92
5:E:104:ASP:HA	5:E:107:ARG:HH12	1.35	0.92
12:L:10:GLN:NE2	12:L:10:GLN:H	1.66	0.92
1:A:2121:G:OP2	37:A:3085:HOH:O	1.88	0.92
1:A:2533:C:H5'	1:A:2533:C:H6	1.35	0.91

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
12:L:81:ARG:HB2	12:L:87:ARG:HH11	1.35	0.91
2:B:3076:G:H3'	2:B:3077:A:H5''	1.52	0.91
30:4:25:VAL:HG22	30:4:68:LYS:HG3	1.53	0.91
1:A:1205:U:H2'	1:A:1206:U:H5'	1.51	0.91
1:A:856:G:H2'	37:A:4976:HOH:O	1.67	0.91
13:M:79:ASP:HB3	37:M:8564:HOH:O	1.69	0.90
19:S:99:ALA:HB1	19:S:109:MET:HE1	1.51	0.90
1:A:960:G:H4'	37:A:6965:HOH:O	1.70	0.90
20:T:57:THR:HG22	20:T:59:ASP:H	1.37	0.90
14:N:87:MET:HG2	30:4:46:ILE:CG2	2.00	0.90
26:Z:185:VAL:HA	37:Z:8564:HOH:O	1.72	0.89
10:J:27:LYS:H	10:J:58:HIS:HD2	1.19	0.89
13:M:68:GLU:HA	37:M:8547:HOH:O	1.72	0.89
6:F:25:MET:HE2	6:F:41:LEU:HG	1.54	0.89
19:S:8:ALA:HB1	19:S:13:THR:HG21	1.52	0.89
1:A:1919:A:H4'	37:A:4406:HOH:O	1.72	0.89
1:A:2526:C:O2'	1:A:2527:U:H5'	1.73	0.88
25:Y:25:ARG:HD2	37:Y:3861:HOH:O	1.72	0.88
1:A:2426:G:H1'	37:A:5637:HOH:O	1.73	0.88
4:D:321:PRO:HA	37:D:8664:HOH:O	1.72	0.88
37:A:5838:HOH:O	6:F:99:ASP:HA	1.72	0.88
1:A:2467:A:OP1	37:A:8640:HOH:O	1.89	0.88
10:J:141:ASN:HA	37:J:8367:HOH:O	1.74	0.88
27:1:42:CYS:SG	27:1:44:PHE:HB2	2.14	0.88
1:A:1701:A:H5'	37:A:5826:HOH:O	1.74	0.88
11:K:19:MET:HE3	11:K:132:LEU:HD11	1.54	0.87
27:1:40:PRO:HD3	27:1:47:LEU:HD11	1.53	0.87
15:O:87:LEU:HD12	15:O:186:LEU:HD21	1.55	0.87
37:A:3255:HOH:O	14:N:79:LYS:HD3	1.72	0.87
13:M:133:VAL:HA	37:M:8579:HOH:O	1.73	0.87
12:L:14:LYS:HB2	12:L:45:PRO:HG2	1.57	0.87
15:O:83:LEU:HD13	15:O:175:LEU:HD23	1.56	0.87
3:C:223:ARG:HG3	37:C:8612:HOH:O	1.72	0.87
26:Z:216:ARG:HD3	37:Z:8571:HOH:O	1.74	0.87
10:J:139:ASP:HA	37:J:8371:HOH:O	1.75	0.86
5:E:140:VAL:HB	37:E:8457:HOH:O	1.74	0.86
12:L:10:GLN:HE21	12:L:10:GLN:H	1.18	0.86
13:M:67:ARG:O	13:M:71:GLU:HG3	1.75	0.86
1:A:1667:A:H5'	1:A:1667:A:H8	1.37	0.86
1:A:2506:A:HO2'	1:A:2507:G:H8	0.87	0.86
1:A:1474:C:H6	1:A:1474:C:H5'	1.39	0.86
7:G:97:VAL:HG12	37:G:4191:HOH:O	1.73	0.86

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:E:78:ARG:HG3	5:E:78:ARG:HH11	1.38	0.86
1:A:541:C:H2'	1:A:542:A:H5''	1.55	0.86
16:P:32:ARG:HD3	16:P:32:ARG:O	1.75	0.86
19:S:9:ASP:O	19:S:13:THR:HB	1.76	0.86
29:3:41:HIS:H	29:3:45:ASN:HD22	1.23	0.86
5:E:127:ARG:NH2	5:E:225:PRO:HG2	1.90	0.85
10:J:142:VAL:HG13	37:J:8382:HOH:O	1.76	0.85
3:C:199:HIS:HD2	3:C:201:PHE:HB2	1.40	0.85
1:A:797:A:H4'	27:1:10:ARG:N	1.91	0.85
14:N:87:MET:CB	30:4:46:ILE:HG21	2.07	0.85
26:Z:200:THR:HG22	26:Z:201:GLU:HG3	1.57	0.85
1:A:2717:C:C2'	1:A:2718:C:H5''	2.07	0.85
10:J:55:GLN:HE21	10:J:124:ARG:HE	1.21	0.85
1:A:338:C:H4'	5:E:174:ILE:CD1	2.07	0.84
1:A:1116:U:HO2'	1:A:1118:A:H2	0.88	0.84
1:A:2361:A:H5''	37:A:8604:HOH:O	1.78	0.84
9:I:12:ILE:HA	37:I:4499:HOH:O	1.78	0.84
1:A:870:G:C2'	1:A:871:G:H5''	2.07	0.84
18:R:25:PRO:HB2	37:R:4350:HOH:O	1.76	0.84
37:A:4509:HOH:O	2:B:3103:A:H4'	1.76	0.84
1:A:1184:C:H1'	37:A:7001:HOH:O	1.76	0.84
10:J:162:SER:HB2	10:J:163:PRO:CD	2.06	0.84
26:Z:187:VAL:HG23	26:Z:192:ASP:HB2	1.58	0.84
1:A:172:U:OP2	37:A:5755:HOH:O	1.96	0.84
1:A:2420:G:O2'	1:A:2421:G:H5'	1.77	0.83
11:K:99:GLU:HA	37:K:8572:HOH:O	1.77	0.83
25:Y:78:GLU:HG2	25:Y:79:GLU:H	1.43	0.83
10:J:139:ASP:N	10:J:140:PRO:HD3	1.93	0.83
14:N:84:LYS:HE2	37:N:8575:HOH:O	1.76	0.83
1:A:541:C:C2'	1:A:542:A:H5''	2.08	0.83
17:Q:115:SER:H	17:Q:118:GLN:NE2	1.77	0.83
1:A:1886:A:N3	37:A:4378:HOH:O	2.12	0.83
6:F:20:LYS:HA	6:F:75:LEU:O	1.79	0.83
1:A:1474:C:C6	1:A:1474:C:H5'	2.14	0.83
1:A:797:A:C4'	27:1:10:ARG:N	2.42	0.83
4:D:18:ARG:HG3	4:D:256:GLN:HG3	1.58	0.83
1:A:962:C:H1'	15:O:5:ARG:HH12	1.43	0.82
22:V:9:CYS:HA	22:V:52:THR:HG23	1.59	0.82
10:J:47:GLU:HB3	10:J:133:ILE:CD1	2.08	0.82
14:N:69:LYS:O	14:N:73:ARG:NH2	2.12	0.82
1:A:1666:C:O2'	1:A:1667:A:H5''	1.80	0.82
11:K:26:VAL:HG13	11:K:36:VAL:HG11	1.60	0.82

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:88:ILE:HD13	3:C:100:PRO:HD3	1.61	0.82
1:A:1450:C:H4'	1:A:1451:C:OP2	1.80	0.82
12:L:74:VAL:HG11	12:L:113:ILE:HG12	1.62	0.82
5:E:133:ARG:HD2	37:E:8417:HOH:O	1.80	0.82
15:O:113:SER:HB2	37:O:8561:HOH:O	1.80	0.82
10:J:5:MET:HG3	37:J:8366:HOH:O	1.77	0.81
10:J:26:LYS:HG2	10:J:28:ILE:H	1.45	0.81
10:J:41:THR:HA	37:J:8397:HOH:O	1.80	0.81
24:X:137:GLN:HE21	24:X:141:HIS:HE1	1.28	0.81
1:A:1165:G:H4'	1:A:1174:A:O2'	1.80	0.81
1:A:645:U:OP2	13:M:4:LYS:HE2	1.81	0.81
24:X:88:THR:HG23	24:X:110:GLN:NE2	1.95	0.81
15:O:49:THR:HG22	15:O:56:ASP:HB2	1.63	0.81
18:R:23:THR:HA	37:R:4792:HOH:O	1.80	0.81
1:A:2467:A:H2'	37:A:5005:HOH:O	1.80	0.81
27:1:10:ARG:HA	37:1:8415:HOH:O	1.81	0.81
1:A:2716:G:H5''	4:D:206:THR:HG21	1.62	0.81
9:I:23:ILE:HD13	9:I:67:LEU:HD23	1.63	0.81
37:A:4134:HOH:O	14:N:83:SER:HA	1.79	0.81
5:E:236:THR:HG22	5:E:239:ALA:N	1.91	0.81
15:O:71:TRP:CE3	15:O:175:LEU:HD22	2.16	0.81
5:E:5:ILE:HD11	5:E:16:VAL:CG2	2.12	0.80
8:H:96:ALA:HA	37:H:3111:HOH:O	1.81	0.80
1:A:1353:C:P	37:A:4238:HOH:O	2.40	0.80
15:O:48:VAL:CG1	15:O:55:ASP:HB3	2.11	0.80
23:W:1:THR:HG23	23:W:2:VAL:H	1.45	0.80
26:Z:155:ARG:NH1	37:Z:8558:HOH:O	2.13	0.80
14:N:164:THR:HG23	14:N:165:SER:N	1.96	0.80
1:A:2468:A:H61	30:4:48:ASN:HD21	1.28	0.80
4:D:212:GLN:HB2	4:D:257:THR:HG21	1.62	0.80
1:A:1679:C:H5'	37:A:8908:HOH:O	1.82	0.80
1:A:1166:A:H1'	1:A:1192:A:C2	2.17	0.80
5:E:2:GLN:HB3	37:E:8336:HOH:O	1.80	0.80
24:X:80:ASP:O	24:X:84:VAL:HG23	1.82	0.80
15:O:86:LEU:HD12	15:O:125:ALA:HB2	1.63	0.80
17:Q:143:ALA:HA	37:Q:2178:HOH:O	1.81	0.80
15:O:144:GLY:O	15:O:147:ILE:HG22	1.82	0.80
12:L:74:VAL:HG13	12:L:113:ILE:HG23	1.63	0.79
8:H:46:GLU:O	8:H:73:PRO:HD2	1.83	0.79
2:B:3069:U:OP1	15:O:4:PRO:HG3	1.81	0.79
1:A:2586:U:H3	1:A:2592:G:H22	1.27	0.79
5:E:246:ARG:NH1	5:E:246:ARG:HB3	1.96	0.79

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
29:3:39:ARG:HG2	37:3:3143:HOH:O	1.82	0.79
26:Z:220:GLU:HG2	37:Z:8550:HOH:O	1.82	0.79
1:A:1741:U:H5'	1:A:1742:A:OP1	1.81	0.79
3:C:211:LYS:HB3	3:C:212:PRO:HD2	1.63	0.79
7:G:166:VAL:HG12	37:G:3134:HOH:O	1.80	0.79
22:V:13:ILE:HG12	22:V:32:CYS:CB	2.12	0.79
7:G:20:ILE:HD11	7:G:40:VAL:HG11	1.65	0.79
37:A:6989:HOH:O	4:D:211:THR:HG21	1.83	0.79
20:T:57:THR:HG22	20:T:59:ASP:N	1.98	0.79
10:J:137:ASN:O	10:J:139:ASP:N	2.16	0.79
4:D:238:ASN:HD22	4:D:240:GLY:H	1.31	0.79
14:N:48:ARG:NH2	37:N:8561:HOH:O	2.14	0.79
1:A:1834:C:H2'	1:A:1840:A:N6	1.98	0.78
1:A:2780:C:H1'	7:G:143:GLN:HE21	1.46	0.78
1:A:282:C:H1'	1:A:368:C:N4	1.97	0.78
37:A:4776:HOH:O	12:L:39:GLY:HA2	1.83	0.78
1:A:711:G:H1'	37:A:6631:HOH:O	1.83	0.78
37:A:5341:HOH:O	14:N:170:CYS:SG	2.40	0.78
37:A:3356:HOH:O	14:N:189:VAL:HG21	1.83	0.78
1:A:1244:U:OP1	11:K:18:ILE:HD13	1.83	0.78
4:D:41:PHE:CD1	4:D:79:MET:HE2	2.18	0.78
27:1:11:THR:CG2	27:1:23:ARG:HB2	2.14	0.78
25:Y:71:ARG:HB3	25:Y:88:GLU:OE1	1.83	0.78
1:A:1603:A:H5'	1:A:1605:G:O4'	1.82	0.78
8:H:91:VAL:HG12	8:H:92:GLY:N	1.98	0.78
1:A:1835:U:C5	1:A:1840:A:N7	2.48	0.78
3:C:199:HIS:CD2	3:C:201:PHE:HB2	2.19	0.78
1:A:338:C:H4'	5:E:174:ILE:HD11	1.64	0.78
1:A:1372:A:H3'	37:A:6724:HOH:O	1.82	0.78
11:K:133:GLY:O	11:K:137:GLU:HG3	1.84	0.78
19:S:39:THR:HG22	19:S:42:GLU:H	1.49	0.78
1:A:545:G:H5'	1:A:545:G:H8	1.49	0.78
27:1:39:CYS:SG	27:1:47:LEU:HD21	2.23	0.77
1:A:1118:A:H3'	1:A:1118:A:H8	1.49	0.77
21:U:61:GLU:HG3	37:U:3851:HOH:O	1.83	0.77
2:B:3014:G:H8	2:B:3014:G:H5'	1.49	0.77
7:G:100:ASP:HB2	37:G:2789:HOH:O	1.82	0.77
4:D:201:ASP:HB2	4:D:312:ARG:HD2	1.65	0.77
6:F:27:ILE:HG22	6:F:28:GLY:H	1.49	0.77
1:A:288:A:H61	1:A:364:C:H42	1.32	0.77
1:A:1058:A:H2'	1:A:1060:C:H5''	1.66	0.77
1:A:1187:U:HO2'	1:A:1189:A:H2	1.32	0.77

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:F:154:LYS:H	6:F:154:LYS:HD2	1.49	0.77
1:A:877:G:H5'	1:A:878:G:OP1	1.84	0.77
11:K:19:MET:CE	11:K:132:LEU:HD11	2.14	0.77
1:A:2638:G:H1'	37:A:7297:HOH:O	1.85	0.77
6:F:25:MET:HE1	6:F:37:ALA:HB1	1.65	0.76
29:3:18:ASN:HD21	29:3:40:ARG:H	1.32	0.76
24:X:21:LEU:HD22	24:X:26:ILE:HD11	1.66	0.76
14:N:106:ASN:ND2	34:N:8518:CL:CL	2.55	0.76
19:S:99:ALA:HB1	19:S:109:MET:CE	2.15	0.76
20:T:23:LYS:HE2	37:T:3430:HOH:O	1.86	0.76
1:A:236:A:H4'	1:A:237:G:H5'	1.68	0.76
37:A:6410:HOH:O	14:N:178:LYS:HB2	1.84	0.76
1:A:1116:U:H3	1:A:1246:A:H62	1.31	0.76
27:1:34:LYS:HE2	37:1:8426:HOH:O	1.85	0.76
14:N:164:THR:HG22	14:N:167:GLY:N	1.99	0.76
12:L:10:GLN:HE21	12:L:10:GLN:N	1.84	0.76
1:A:31:C:H4'	37:A:6959:HOH:O	1.85	0.76
5:E:139:VAL:HG13	37:E:8455:HOH:O	1.86	0.76
24:X:68:THR:HG23	24:X:69:ARG:HG2	1.67	0.76
11:K:76:ASP:HA	37:K:8563:HOH:O	1.85	0.76
1:A:2419:U:H5''	1:A:2420:G:H5'	1.68	0.76
19:S:18:LEU:HD12	19:S:143:VAL:HG11	1.66	0.76
1:A:2466:G:OP1	37:A:3220:HOH:O	2.03	0.76
13:M:1:THR:HA	37:M:8525:HOH:O	1.84	0.76
1:A:560:C:H42	1:A:597:A:H61	1.33	0.76
1:A:1209:C:H4'	37:A:4834:HOH:O	1.86	0.76
25:Y:41:PHE:O	25:Y:43:VAL:HG23	1.85	0.76
10:J:59:ASN:HD22	10:J:59:ASN:H	1.33	0.75
1:A:346:U:H4'	37:A:6380:HOH:O	1.86	0.75
30:4:65:THR:HG23	30:4:67:LEU:HG	1.68	0.75
1:A:2506:A:O2'	1:A:2507:G:H8	1.67	0.75
8:H:91:VAL:HG12	8:H:92:GLY:H	1.49	0.75
27:1:18:TYR:HB3	27:1:22:ILE:HG21	1.68	0.75
8:H:63:ILE:HB	8:H:64:PRO:HD3	1.68	0.75
25:Y:15:ARG:HH11	25:Y:15:ARG:HB3	1.51	0.75
10:J:47:GLU:HB3	10:J:133:ILE:HD13	1.66	0.75
2:B:3006:C:OP1	15:O:37:ARG:NH1	2.19	0.75
1:A:1164:U:H3	1:A:1192:A:H2	1.33	0.75
6:F:64:ARG:HG2	6:F:67:ASP:HB3	1.68	0.75
10:J:59:ASN:HD22	10:J:59:ASN:N	1.85	0.75
1:A:289:G:H22	1:A:363:A:H2	1.35	0.75
24:X:4:LEU:HD22	24:X:52:VAL:HG21	1.67	0.75

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
37:A:6959:HOH:O	21:U:9:LYS:HB2	1.85	0.75
1:A:2812:A:H2	1:A:2814:A:H62	1.29	0.75
30:4:74:CYS:SG	30:4:76:LYS:HB2	2.27	0.75
8:H:50:VAL:HG21	8:H:63:ILE:HG21	1.68	0.74
3:C:53:ALA:HB3	37:C:8618:HOH:O	1.87	0.74
14:N:106:ASN:HD22	14:N:114:VAL:HG23	1.51	0.74
1:A:559:U:H6	1:A:559:U:H5'	1.52	0.74
1:A:1120:U:H6	1:A:1120:U:H5''	1.50	0.74
13:M:143:THR:HG22	13:M:144:ASP:N	2.01	0.74
3:C:35:GLY:O	3:C:36:ASP:HB3	1.86	0.74
5:E:78:ARG:HG3	5:E:78:ARG:NH1	2.02	0.74
1:A:2827:A:H2'	1:A:2828:G:O4'	1.87	0.74
14:N:87:MET:HB3	30:4:46:ILE:HD13	1.70	0.74
9:I:12:ILE:N	9:I:13:PRO:HD3	2.02	0.74
1:A:31:C:H2'	37:A:7226:HOH:O	1.87	0.74
1:A:2690:U:O2'	7:G:111:LYS:HE3	1.87	0.74
27:1:38:LYS:HE2	27:1:45:LYS:HE2	1.69	0.74
1:A:1118:A:C8	1:A:1118:A:H3'	2.22	0.74
1:A:21:G:H5'	19:S:2:ILE:HA	1.69	0.74
1:A:1909:A:N1	1:A:2128:G:H1'	2.02	0.74
10:J:150:LYS:HE2	37:J:8384:HOH:O	1.88	0.74
27:1:39:CYS:HA	27:1:47:LEU:HD11	1.70	0.74
1:A:2432:C:O2'	1:A:2433:A:H5'	1.87	0.74
15:O:89:GLY:O	15:O:92:ALA:HB3	1.88	0.74
16:P:47:ARG:HH11	16:P:47:ARG:HG3	1.52	0.74
28:2:10:LYS:HG3	37:2:8433:HOH:O	1.87	0.74
4:D:190:MET:HE2	4:D:194:PHE:CD1	2.22	0.73
27:1:30:GLU:HA	27:1:33:HIS:HB3	1.70	0.73
1:A:2054:A:N3	19:S:128:ARG:NH2	2.36	0.73
5:E:25:PRO:HG2	37:E:8325:HOH:O	1.87	0.73
30:4:40:ARG:HD2	37:4:8548:HOH:O	1.88	0.73
24:X:88:THR:HG22	24:X:89:ASP:N	2.03	0.73
24:X:4:LEU:HD22	24:X:52:VAL:CG2	2.17	0.73
24:X:6:GLN:HB2	24:X:26:ILE:HD12	1.70	0.73
1:A:450:C:OP1	5:E:184:ARG:NH2	2.21	0.73
37:A:3631:HOH:O	4:D:27:ASN:HB2	1.87	0.73
12:L:55:VAL:HG12	12:L:56:SER:N	2.02	0.73
22:V:14:GLU:O	22:V:17:THR:HB	1.89	0.73
1:A:2710:U:H1'	37:A:7159:HOH:O	1.88	0.73
5:E:236:THR:H	5:E:239:ALA:HB3	1.53	0.73
6:F:105:SER:CB	6:F:131:THR:HG23	2.18	0.73
15:O:164:ASP:CG	15:O:167:ASP:HA	2.09	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:F:174:VAL:HG13	37:F:6555:HOH:O	1.88	0.73
23:W:4:HIS:HB3	37:W:6622:HOH:O	1.88	0.73
14:N:169:ARG:HD2	37:N:8589:HOH:O	1.86	0.73
1:A:2421:G:H3'	1:A:2422:U:H5''	1.69	0.73
1:A:1120:U:C6	1:A:1120:U:H5''	2.24	0.73
5:E:104:ASP:HA	5:E:107:ARG:NH1	2.01	0.73
1:A:1118:A:H62	1:A:1244:U:H3	1.35	0.73
7:G:15:GLN:HG3	7:G:20:ILE:HG12	1.69	0.73
27:1:38:LYS:HG2	27:1:45:LYS:HG2	1.70	0.73
1:A:506:G:H22	1:A:509:A:H5'	1.53	0.73
4:D:217:ARG:HG3	4:D:257:THR:HG22	1.70	0.73
7:G:107:PHE:CE2	7:G:108:LEU:HD13	2.23	0.73
25:Y:72:VAL:HG22	25:Y:85:VAL:HG12	1.71	0.72
10:J:162:SER:CB	10:J:163:PRO:HD3	2.18	0.72
15:O:71:TRP:HE3	15:O:175:LEU:HD22	1.55	0.72
26:Z:212:ARG:HD2	37:Z:8605:HOH:O	1.88	0.72
6:F:146:LYS:NZ	15:O:107:ASN:HD21	1.87	0.72
4:D:221:GLN:HE22	12:L:42:ASN:HD22	1.37	0.72
5:E:246:ARG:HH11	5:E:246:ARG:HB3	1.51	0.72
1:A:1209:C:H2'	1:A:1210:G:H8	1.54	0.72
1:A:1160:G:C5'	1:A:1161:A:H5'	2.16	0.72
12:L:81:ARG:HB2	12:L:87:ARG:NH1	2.01	0.72
8:H:99:THR:HA	37:H:3461:HOH:O	1.90	0.72
23:W:39:ALA:N	23:W:40:PRO:HD2	2.05	0.72
7:G:81:GLU:HG2	7:G:134:SER:HB3	1.69	0.72
6:F:19:GLU:O	6:F:20:LYS:HG2	1.90	0.72
11:K:74:ARG:HB3	11:K:74:ARG:HH11	1.53	0.72
1:A:2548:C:OP2	4:D:5:ARG:NH2	2.22	0.72
1:A:1701:A:H4'	1:A:1702:U:H5''	1.72	0.72
22:V:46:ALA:HB1	22:V:52:THR:HG21	1.70	0.72
10:J:33:MET:HB2	10:J:83:PHE:HB3	1.72	0.72
24:X:88:THR:HG23	24:X:110:GLN:HE21	1.54	0.72
6:F:135:VAL:HG22	6:F:136:ARG:H	1.53	0.72
1:A:1594:C:OP2	17:Q:120:ARG:HD2	1.90	0.72
1:A:2281:C:H2'	1:A:2282:U:H5'	1.72	0.72
26:Z:187:VAL:HG23	26:Z:192:ASP:CB	2.20	0.72
10:J:14:TYR:H	10:J:91:HIS:CE1	2.08	0.72
24:X:122:ARG:HG2	24:X:122:ARG:HH11	1.54	0.72
13:M:136:ALA:HB3	37:M:8579:HOH:O	1.89	0.72
22:V:13:ILE:HG12	22:V:32:CYS:HB3	1.71	0.72
1:A:2432:C:O4'	37:A:9316:HOH:O	2.08	0.72
4:D:329:TYR:CE2	22:V:15:PRO:HG2	2.24	0.72

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
15:O:159:TYR:HB3	15:O:162:ASP:HB2	1.72	0.72
1:A:506:G:H22	1:A:509:A:C5'	2.02	0.72
14:N:78:ASN:ND2	37:N:8646:HOH:O	2.22	0.72
14:N:81:ARG:HG3	14:N:85:ARG:HB2	1.72	0.72
10:J:71:TYR:C	10:J:73:GLN:H	1.93	0.72
14:N:173:LEU:HD23	14:N:183:VAL:HG12	1.72	0.72
1:A:544:G:H2'	1:A:545:G:H5''	1.72	0.71
14:N:172:GLY:O	14:N:183:VAL:HG11	1.90	0.71
5:E:27:ARG:HG3	5:E:29:ASP:OD1	1.90	0.71
24:X:22:GLU:HG2	24:X:27:HIS:CD2	2.25	0.71
14:N:87:MET:HB3	30:4:46:ILE:HG21	1.72	0.71
14:N:91:ILE:HA	37:N:8644:HOH:O	1.89	0.71
14:N:38:VAL:O	14:N:63:VAL:HG13	1.89	0.71
1:A:2281:C:C2'	1:A:2282:U:H5'	2.20	0.71
1:A:2459:G:OP2	30:4:64:LYS:HD2	1.90	0.71
14:N:87:MET:CB	30:4:46:ILE:HD13	2.20	0.71
27:1:37:HIS:HB2	27:1:47:LEU:HB2	1.72	0.71
5:E:76:ARG:HD2	37:E:8440:HOH:O	1.91	0.71
17:Q:115:SER:N	17:Q:118:GLN:HE21	1.85	0.71
1:A:2363:G:O3'	18:R:11:ARG:NH1	2.24	0.71
4:D:62:ARG:CA	4:D:65:MET:HE3	2.20	0.71
17:Q:98:ILE:HD12	17:Q:102:ARG:NE	2.06	0.71
2:B:3056:A:C2'	2:B:3057:A:H5''	2.20	0.71
1:A:1485:A:H4'	37:A:9859:HOH:O	1.89	0.71
24:X:72:PRO:HG2	24:X:77:ALA:HB3	1.71	0.71
6:F:88:LEU:HB2	6:F:89:PRO:HD3	1.73	0.71
10:J:26:LYS:HD2	10:J:28:ILE:CD1	2.20	0.71
10:J:56:ILE:HG22	10:J:61:LEU:HD22	1.73	0.71
1:A:111:C:O2'	28:2:20:ARG:HG2	1.91	0.71
7:G:11:VAL:HG12	7:G:12:ASP:N	2.06	0.71
17:Q:59:ARG:NH2	17:Q:66:GLN:HE22	1.89	0.71
1:A:1625:U:H4'	37:A:4226:HOH:O	1.90	0.70
37:A:7092:HOH:O	30:4:60:LYS:HG3	1.89	0.70
4:D:62:ARG:HA	4:D:65:MET:CE	2.19	0.70
1:A:541:C:H2'	1:A:542:A:C5'	2.20	0.70
1:A:1119:G:H2'	11:K:52:GLN:NE2	2.06	0.70
1:A:284:C:H4'	1:A:285:A:O5'	1.90	0.70
1:A:263:U:O4'	8:H:59:ILE:HD13	1.90	0.70
1:A:2346:C:O2'	6:F:52:THR:HG21	1.91	0.70
23:W:42:ASN:HB3	37:W:7247:HOH:O	1.91	0.70
1:A:1080:C:H4'	1:A:1081:A:OP1	1.90	0.70
2:B:3006:C:C5'	15:O:37:ARG:NH1	2.54	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2533:C:H5'	1:A:2533:C:C6	2.23	0.70
12:L:22:ASP:HB2	37:L:5264:HOH:O	1.92	0.70
1:A:1187:U:H2'	37:A:6434:HOH:O	1.91	0.70
28:2:8:GLN:HE22	28:2:11:LYS:NZ	1.89	0.70
10:J:163:PRO:HG2	37:J:8338:HOH:O	1.89	0.70
25:Y:76:ARG:HH11	25:Y:76:ARG:HG3	1.55	0.70
1:A:1116:U:O2'	1:A:1118:A:H2	1.70	0.70
22:V:9:CYS:CA	22:V:52:THR:HG23	2.21	0.70
1:A:204:A:H2'	1:A:205:U:H5'	1.72	0.70
14:N:64:ARG:HD2	37:N:8584:HOH:O	1.91	0.70
3:C:200:PRO:HD3	37:C:8520:HOH:O	1.91	0.70
1:A:625:U:H5'	37:A:9757:HOH:O	1.92	0.70
2:B:3048:C:H4'	15:O:141:ARG:HH21	1.57	0.70
23:W:12:THR:HG22	23:W:15:GLU:CG	2.21	0.70
1:A:1334:C:OP2	37:A:3583:HOH:O	2.10	0.70
11:K:93:ARG:HH11	11:K:93:ARG:HB3	1.55	0.70
14:N:74:ARG:NH2	37:N:8629:HOH:O	2.23	0.70
8:H:104:ALA:HA	37:H:6617:HOH:O	1.91	0.70
7:G:43:ASP:HA	37:G:5864:HOH:O	1.92	0.70
1:A:542:A:H5'	1:A:542:A:C8	2.19	0.69
24:X:21:LEU:HD22	24:X:26:ILE:CD1	2.22	0.69
14:N:89:ASN:HA	37:N:8554:HOH:O	1.92	0.69
1:A:396:U:H4'	37:4:8529:HOH:O	1.92	0.69
16:P:87:THR:O	16:P:91:GLN:HG3	1.92	0.69
24:X:5:VAL:HG22	24:X:32:CYS:HB2	1.75	0.69
3:C:121:ALA:O	3:C:124:VAL:HG22	1.91	0.69
28:2:1:THR:HB	37:2:8457:HOH:O	1.90	0.69
21:U:55:PHE:HB2	37:U:6384:HOH:O	1.90	0.69
1:A:281:U:H2'	1:A:282:C:O4'	1.92	0.69
27:1:30:GLU:HA	27:1:33:HIS:CB	2.23	0.69
1:A:447:A:OP1	21:U:2:LYS:HG2	1.93	0.69
4:D:307:ARG:HH11	4:D:307:ARG:HB2	1.56	0.69
1:A:182:G:H4'	14:N:157:LEU:HD13	1.72	0.69
14:N:61:ILE:HG13	37:N:8622:HOH:O	1.92	0.69
1:A:1119:G:N2	1:A:1246:A:C2	2.60	0.69
4:D:162:MET:HE3	4:D:308:LEU:HD21	1.73	0.69
3:C:199:HIS:CD2	3:C:201:PHE:H	2.11	0.69
1:A:1771:U:H4'	27:1:20:LEU:HD21	1.72	0.69
1:A:1751:G:C2'	1:A:1752:G:H5''	2.22	0.69
1:A:1666:C:H2'	1:A:1667:A:H5'	1.73	0.69
1:A:1667:A:H5'	1:A:1667:A:C8	2.25	0.69
5:E:98:ARG:O	37:E:8347:HOH:O	2.09	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2316:G:H8	37:A:5201:HOH:O	1.76	0.69
15:O:183:ASP:OD2	15:O:186:LEU:HD12	1.92	0.69
2:B:3013:A:O2'	2:B:3014:G:H5''	1.92	0.69
24:X:21:LEU:HD21	24:X:48:VAL:HG11	1.75	0.69
26:Z:141:THR:HG23	37:Z:8592:HOH:O	1.92	0.69
1:A:2456:A:H5'	37:A:5241:HOH:O	1.92	0.69
11:K:107:ASN:ND2	11:K:109:TYR:H	1.91	0.69
4:D:258:GLY:H	4:D:260:HIS:CE1	2.10	0.69
24:X:65:VAL:HA	24:X:68:THR:HG22	1.75	0.69
2:B:3039:U:H1'	2:B:3044:A:H61	1.56	0.69
5:E:162:VAL:HG13	5:E:232:LEU:HD21	1.75	0.69
26:Z:235:GLU:CD	26:Z:235:GLU:H	1.95	0.68
3:C:101:GLU:OE2	3:C:131:HIS:HB2	1.93	0.68
5:E:107:ARG:NH1	5:E:107:ARG:HB3	2.08	0.68
17:Q:58:SER:HB3	37:Q:4744:HOH:O	1.94	0.68
4:D:141:ARG:HD2	4:D:163:GLU:OE2	1.92	0.68
1:A:2359:G:O5'	37:A:5237:HOH:O	2.12	0.68
1:A:2271:G:P	37:A:9011:HOH:O	2.50	0.68
14:N:186:SER:O	14:N:189:VAL:HG12	1.93	0.68
6:F:54:ALA:HB2	6:F:69:ILE:HD12	1.75	0.68
1:A:2912:C:OP2	37:A:5101:HOH:O	2.11	0.68
1:A:2768:A:H2'	1:A:2769:C:O4'	1.92	0.68
1:A:631:A:N3	1:A:2073:G:O2'	2.26	0.68
1:A:2635:A:O2'	1:A:2636:C:H5'	1.94	0.68
6:F:41:LEU:HA	6:F:44:ILE:HG22	1.76	0.68
4:D:145:HIS:HD2	4:D:146:THR:O	1.76	0.68
1:A:544:G:C2'	1:A:545:G:H5''	2.24	0.68
14:N:139:PRO:O	14:N:140:ALA:HB3	1.92	0.68
10:J:127:GLY:O	10:J:128:ALA:HB3	1.93	0.68
1:A:242:A:O2'	37:A:9373:HOH:O	2.11	0.68
1:A:951:A:C2'	1:A:952:G:H5'	2.24	0.68
24:X:110:GLN:HA	24:X:110:GLN:NE2	2.09	0.68
1:A:1191:A:H3'	1:A:1192:A:H5''	1.74	0.68
1:A:2506:A:H1'	37:A:5601:HOH:O	1.92	0.68
26:Z:200:THR:HG22	26:Z:201:GLU:CG	2.22	0.68
27:1:29:VAL:O	27:1:33:HIS:HB2	1.94	0.68
27:1:49:ARG:HD2	37:1:8430:HOH:O	1.93	0.68
1:A:1249:U:H2'	1:A:1250:C:C6	2.28	0.68
3:C:192:VAL:HB	37:C:8605:HOH:O	1.92	0.68
15:O:48:VAL:HG11	15:O:55:ASP:HB3	1.75	0.68
25:Y:18:ARG:NH1	37:Y:4132:HOH:O	2.27	0.68
1:A:656:G:OP2	16:P:37:ARG:HD2	1.93	0.68

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:J:57:ARG:HG3	37:J:8354:HOH:O	1.94	0.67
1:A:2755:G:H1'	37:A:4242:HOH:O	1.94	0.67
1:A:2676:C:H4'	11:K:70:PHE:CE1	2.29	0.67
1:A:558:C:H5'	37:A:4812:HOH:O	1.92	0.67
29:3:22:PRO:HG2	29:3:25:VAL:HG23	1.76	0.67
1:A:516:A:OP2	37:A:5193:HOH:O	2.11	0.67
14:N:68:ARG:HD3	14:N:68:ARG:O	1.94	0.67
19:S:39:THR:HB	19:S:42:GLU:HG3	1.75	0.67
6:F:64:ARG:CG	6:F:67:ASP:HB3	2.24	0.67
27:1:62:TYR:CE2	27:1:64:ILE:HG23	2.30	0.67
27:1:75:ALA:HB3	37:1:8439:HOH:O	1.93	0.67
13:M:21:ARG:N	37:M:8535:HOH:O	2.27	0.67
24:X:4:LEU:O	24:X:32:CYS:HA	1.94	0.67
4:D:214:PRO:HD2	37:D:8520:HOH:O	1.95	0.67
19:S:106:GLY:HA2	19:S:109:MET:HE3	1.76	0.67
6:F:23:VAL:HG23	6:F:23:VAL:O	1.95	0.67
1:A:1878:G:H1'	37:A:5666:HOH:O	1.95	0.67
1:A:2897:C:O2'	1:A:2898:G:H5'	1.95	0.67
1:A:299:U:H5'	37:A:6872:HOH:O	1.94	0.67
1:A:2291:A:C8	1:A:2309:C:H5'	2.29	0.67
29:3:41:HIS:N	29:3:45:ASN:HD22	1.90	0.67
11:K:131:THR:HG22	11:K:134:GLU:H	1.60	0.67
23:W:64:GLY:O	23:W:65:ASP:HB2	1.94	0.67
15:O:164:ASP:OD2	15:O:167:ASP:HA	1.94	0.67
16:P:42:GLU:HB2	37:P:2176:HOH:O	1.93	0.67
7:G:79:GLY:HA3	37:G:7046:HOH:O	1.94	0.67
4:D:179:LEU:O	4:D:183:GLU:HG2	1.95	0.67
4:D:7:ARG:HD3	4:D:9:GLY:O	1.95	0.67
1:A:2276:U:H2'	1:A:2277:U:C6	2.30	0.67
1:A:2508:C:H2'	37:A:6288:HOH:O	1.95	0.67
1:A:2466:G:H5''	37:A:3220:HOH:O	1.95	0.66
1:A:941:G:O2'	1:A:942:U:H5'	1.94	0.66
1:A:383:A:OP2	37:A:9352:HOH:O	2.12	0.66
1:A:2123:A:H5'	14:N:89:ASN:HD21	1.60	0.66
14:N:164:THR:CG2	14:N:165:SER:N	2.58	0.66
1:A:1614:G:H2'	37:A:4187:HOH:O	1.94	0.66
1:A:2301:A:H5''	1:A:2302:A:H5'	1.76	0.66
10:J:3:GLY:HA2	10:J:57:ARG:HH12	1.60	0.66
10:J:140:PRO:HB3	37:J:8382:HOH:O	1.95	0.66
3:C:36:ASP:OD2	3:C:85:ASP:HB2	1.95	0.66
1:A:204:A:C2'	1:A:205:U:H5'	2.24	0.66
14:N:138:HIS:ND1	14:N:139:PRO:O	2.28	0.66

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
31:A:4000:CAI:H21A	34:A:8523:CL:CL	2.31	0.66
8:H:105:ALA:HB2	37:H:5522:HOH:O	1.94	0.66
5:E:1:MET:HG2	5:E:2:GLN:H	1.60	0.66
1:A:1159:G:P	37:A:3858:HOH:O	2.53	0.66
1:A:21:G:C5'	19:S:2:ILE:HA	2.25	0.66
27:1:61:GLY:HA3	37:1:8427:HOH:O	1.94	0.66
1:A:338:C:H5''	37:E:8427:HOH:O	1.96	0.66
1:A:282:C:H1'	1:A:368:C:H42	1.58	0.66
1:A:2408:A:H2	37:A:9671:HOH:O	1.77	0.66
4:D:24:PRO:CG	4:D:204:GLY:HA2	2.26	0.66
1:A:1735:C:O2'	1:A:1736:A:H5'	1.95	0.66
1:A:1857:A:N6	1:A:2247:C:H1'	2.11	0.66
1:A:2434:A:O3'	30:4:28:GLY:HA3	1.94	0.66
37:A:3295:HOH:O	14:N:157:LEU:HD11	1.95	0.66
1:A:2578:G:H5'	1:A:2578:G:H8	1.61	0.66
6:F:69:ILE:O	6:F:69:ILE:HG22	1.95	0.66
1:A:2064:U:H5'	1:A:2652:U:O3'	1.96	0.66
1:A:2748:G:H2'	37:A:7077:HOH:O	1.96	0.66
37:B:5071:HOH:O	15:O:23:ARG:HD3	1.95	0.66
2:B:3006:C:H5''	15:O:37:ARG:HH12	1.59	0.66
28:2:25:LYS:HE2	37:3:7213:HOH:O	1.96	0.66
17:Q:71:LYS:O	17:Q:71:LYS:HG3	1.96	0.66
14:N:38:VAL:C	14:N:63:VAL:HG13	2.17	0.66
1:A:2505:G:O2'	1:A:2506:A:H5'	1.96	0.66
11:K:103:VAL:HG12	37:K:8563:HOH:O	1.95	0.66
15:O:61:ALA:HB3	15:O:88:ALA:HB2	1.78	0.66
37:A:4082:HOH:O	14:N:94:LYS:HE3	1.95	0.66
3:C:164:ARG:NE	37:C:8597:HOH:O	2.28	0.66
1:A:1766:U:O2	1:A:1778:A:H5'	1.96	0.66
1:A:2851:G:O2'	1:A:2852:A:H5'	1.96	0.66
3:C:100:PRO:HG2	3:C:103:VAL:HG21	1.76	0.65
6:F:95:THR:O	6:F:97:GLN:N	2.25	0.65
1:A:581:G:H5'	37:A:7220:HOH:O	1.96	0.65
1:A:2813:A:OP2	37:A:3849:HOH:O	2.14	0.65
1:A:160:A:C4	1:A:177:A:C2	2.84	0.65
10:J:46:VAL:O	10:J:146:TRP:HH2	1.79	0.65
8:H:110:GLU:HG2	37:H:6926:HOH:O	1.95	0.65
20:T:51:GLN:HE21	20:T:53:ASN:HD21	1.45	0.65
1:A:1328:A:OP1	26:Z:169:ARG:HD2	1.96	0.65
10:J:111:MET:O	10:J:114:PRO:HD3	1.96	0.65
1:A:188:C:H5''	14:N:163:LEU:HD21	1.77	0.65
1:A:2064:U:H4'	1:A:2653:A:OP1	1.96	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2320:U:H4'	1:A:2321:A:O4'	1.96	0.65
26:Z:117:LEU:HD12	26:Z:174:VAL:HG11	1.79	0.65
1:A:871:G:C5'	1:A:871:G:C8	2.65	0.65
1:A:1845:A:OP2	3:C:190:ARG:NH1	2.30	0.65
5:E:178:GLN:OE1	37:E:8473:HOH:O	2.13	0.65
5:E:16:VAL:HG12	5:E:17:ASP:N	2.11	0.65
1:A:469:G:O2'	37:A:9628:HOH:O	2.14	0.65
24:X:130:HIS:O	24:X:136:GLY:HA3	1.97	0.65
1:A:485:A:O2'	1:A:487:G:H5'	1.97	0.65
6:F:97:GLN:O	6:F:97:GLN:HG2	1.96	0.65
1:A:2346:C:H6	1:A:2346:C:O5'	1.79	0.65
1:A:2096:A:H2'	1:A:2539:U:H1'	1.77	0.65
1:A:1160:G:H5'	1:A:1161:A:C5'	2.16	0.65
10:J:84:ARG:NH2	10:J:135:TRP:HH2	1.95	0.65
4:D:162:MET:CE	4:D:308:LEU:HD21	2.26	0.65
4:D:175:LEU:C	4:D:175:LEU:HD23	2.17	0.64
10:J:27:LYS:N	10:J:58:HIS:HD2	1.93	0.64
10:J:58:HIS:HA	10:J:61:LEU:HD23	1.78	0.64
24:X:13:MET:HE3	24:X:17:ILE:HG22	1.79	0.64
13:M:143:THR:HG22	13:M:145:LEU:H	1.60	0.64
1:A:134:U:C2	1:A:145:A:C2	2.86	0.64
1:A:820:G:O2'	1:A:856:G:H4'	1.98	0.64
3:C:88:ILE:O	3:C:88:ILE:HG22	1.96	0.64
4:D:207:LYS:HG2	4:D:304:PRO:HB3	1.77	0.64
14:N:113:ARG:NH2	14:N:156:ARG:HG2	2.12	0.64
2:B:3020:G:H3'	37:B:2984:HOH:O	1.96	0.64
37:A:5232:HOH:O	15:O:21:HIS:HE1	1.81	0.64
10:J:136:VAL:HG23	37:J:8343:HOH:O	1.95	0.64
10:J:139:ASP:H	10:J:140:PRO:HD3	1.62	0.64
17:Q:38:GLU:HA	17:Q:41:ARG:HH11	1.61	0.64
1:A:2392:C:N3	37:A:4408:HOH:O	2.29	0.64
1:A:2421:G:H3'	1:A:2422:U:C5'	2.28	0.64
11:K:107:ASN:HD21	11:K:109:TYR:HB2	1.62	0.64
37:A:3128:HOH:O	14:N:152:ARG:HG3	1.97	0.64
21:U:37:GLN:OE1	21:U:118:SER:HA	1.97	0.64
21:U:63:ILE:HD11	21:U:75:GLU:HB2	1.80	0.64
1:A:1741:U:O2'	1:A:2723:G:H4'	1.97	0.64
4:D:221:GLN:HE22	12:L:42:ASN:ND2	1.95	0.64
5:E:129:HIS:CE1	5:E:231:ARG:HA	2.33	0.64
1:A:1847:A:OP1	3:C:175:LYS:HG3	1.96	0.64
1:A:1256:C:OP2	37:A:6690:HOH:O	2.15	0.64
14:N:52:LEU:HD13	14:N:116:ASN:HB3	1.80	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
37:A:9768:HOH:O	13:M:4:LYS:HG3	1.96	0.64
3:C:76:VAL:HG23	27:1:63:LYS:HB3	1.79	0.64
16:P:44:ASN:OD1	16:P:65:LEU:HB2	1.98	0.64
2:B:3001:U:O3'	2:B:3003:A:H5''	1.98	0.64
25:Y:31:ILE:O	25:Y:35:GLU:HG3	1.98	0.64
15:O:37:ARG:NE	37:O:8533:HOH:O	2.31	0.64
1:A:1119:G:H22	1:A:1246:A:H2	1.43	0.64
1:A:282:C:O2'	1:A:283:U:H5'	1.98	0.64
3:C:37:VAL:HG22	37:C:8607:HOH:O	1.98	0.64
13:M:22:ARG:HG2	37:M:8527:HOH:O	1.96	0.64
13:M:53:ARG:HH22	13:M:57:VAL:HG12	1.63	0.64
1:A:2502:C:C2'	1:A:2503:A:H5'	2.28	0.64
10:J:27:LYS:H	10:J:58:HIS:CD2	2.10	0.64
2:B:3014:G:H5'	2:B:3014:G:C8	2.31	0.64
1:A:1187:U:O2'	1:A:1189:A:H2	1.81	0.64
3:C:94:LEU:N	3:C:94:LEU:HD23	2.12	0.64
27:1:53:GLY:HA2	27:1:67:GLY:O	1.98	0.64
5:E:115:LEU:O	5:E:118:THR:HB	1.98	0.63
9:I:12:ILE:N	9:I:13:PRO:CD	2.61	0.63
22:V:9:CYS:HA	22:V:52:THR:CG2	2.28	0.63
1:A:2094:G:H4'	4:D:245:SER:HB3	1.79	0.63
26:Z:109:LEU:HA	37:Z:8573:HOH:O	1.98	0.63
5:E:242:GLU:HG3	37:E:8383:HOH:O	1.97	0.63
21:U:47:THR:HB	21:U:100:ASP:HB3	1.80	0.63
26:Z:144:ARG:CZ	37:Z:8616:HOH:O	2.45	0.63
4:D:305:ASP:O	4:D:306:LYS:HB2	1.98	0.63
1:A:821:U:H2'	1:A:822:C:H6	1.62	0.63
1:A:2361:A:H2'	1:A:2362:A:C8	2.33	0.63
27:1:30:GLU:HB3	27:1:34:LYS:HE3	1.80	0.63
37:A:5791:HOH:O	22:V:56:ARG:HB3	1.97	0.63
14:N:114:VAL:HG21	14:N:159:THR:HG21	1.80	0.63
8:H:50:VAL:HG13	8:H:60:VAL:HG11	1.80	0.63
13:M:148:GLU:HA	37:M:8578:HOH:O	1.97	0.63
12:L:115:ARG:HG3	12:L:116:GLU:N	2.14	0.63
1:A:873:G:H2'	1:A:875:A:N7	2.14	0.63
14:N:34:GLU:HB3	14:N:35:PRO:HD2	1.80	0.63
3:C:88:ILE:HD13	3:C:100:PRO:CD	2.29	0.63
11:K:75:PRO:HG2	11:K:105:LEU:HD21	1.80	0.63
10:J:28:ILE:HA	10:J:62:GLU:OE1	1.98	0.63
1:A:281:U:H3'	37:A:6740:HOH:O	1.99	0.63
1:A:1311:G:C2	1:A:1312:G:C8	2.87	0.63
14:N:59:GLY:HA3	14:N:141:ILE:CD1	2.28	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1170:U:O2'	1:A:1172:G:N7	2.29	0.63
1:A:1730:G:H5'	1:A:1731:C:C5	2.34	0.63
15:O:12:ARG:HD3	15:O:18:THR:OG1	1.98	0.63
19:S:39:THR:HG23	19:S:107:GLU:O	1.97	0.63
3:C:105:VAL:HG11	3:C:154:ALA:HB1	1.80	0.63
1:A:681:G:N3	1:A:681:G:H5'	2.14	0.63
3:C:69:LEU:HD21	3:C:120:ARG:HB3	1.81	0.63
2:B:3009:C:OP2	37:B:466:HOH:O	2.16	0.63
1:A:154:C:H2'	1:A:155:C:H6	1.63	0.63
1:A:2082:G:O2'	1:A:2083:A:H5'	1.98	0.63
15:O:4:PRO:HD2	37:O:8559:HOH:O	1.99	0.63
2:B:3029:C:H2'	2:B:3030:C:H5'	1.79	0.63
1:A:2502:C:H2'	1:A:2503:A:H5'	1.81	0.63
1:A:2890:A:H1'	22:V:56:ARG:NH2	2.14	0.63
1:A:1130:U:H2'	1:A:1131:G:O4'	1.99	0.63
1:A:603:A:H5''	1:A:604:G:OP1	1.97	0.63
1:A:168:C:O2'	1:A:169:A:H5'	1.98	0.63
5:E:142:ASP:OD2	5:E:238:SER:OG	2.16	0.62
1:A:1134:G:H4'	10:J:151:MET:CE	2.24	0.62
1:A:1834:C:H2'	1:A:1840:A:H62	1.63	0.62
6:F:35:ALA:N	37:F:5576:HOH:O	2.31	0.62
13:M:114:VAL:HG11	37:M:8579:HOH:O	1.98	0.62
1:A:184:G:H5''	14:N:153:THR:HG22	1.81	0.62
1:A:157:G:H4'	14:N:95:LYS:HE3	1.81	0.62
37:A:4392:HOH:O	11:K:47:THR:HB	1.99	0.62
15:O:80:SER:HB2	37:O:8536:HOH:O	1.99	0.62
26:Z:115:ARG:NE	37:Z:8556:HOH:O	2.31	0.62
14:N:30:GLU:O	14:N:34:GLU:HG3	1.99	0.62
12:L:74:VAL:O	12:L:74:VAL:HG12	1.99	0.62
14:N:157:LEU:HB3	14:N:160:PHE:HD1	1.64	0.62
25:Y:75:ALA:O	25:Y:83:ALA:HA	1.99	0.62
1:A:2613:G:O2'	1:A:2614:C:H5'	2.00	0.62
15:O:119:GLN:O	15:O:123:ILE:HG13	1.99	0.62
16:P:39:THR:O	16:P:115:ARG:NH2	2.32	0.62
5:E:84:VAL:O	5:E:85:LYS:HB2	1.99	0.62
10:J:55:GLN:NE2	10:J:124:ARG:HE	1.92	0.62
1:A:1773:G:C8	27:1:16:PRO:HA	2.34	0.62
5:E:12:THR:HB	37:E:8448:HOH:O	1.97	0.62
4:D:248:ARG:O	4:D:251:VAL:CG1	2.48	0.62
1:A:318:C:O2	37:A:3372:HOH:O	2.13	0.62
15:O:169:PRO:O	15:O:172:PHE:HB3	2.00	0.62
7:G:6:GLU:HA	7:G:46:THR:HG22	1.81	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:E:118:THR:O	5:E:136:VAL:HG13	1.99	0.62
12:L:30:LYS:O	12:L:55:VAL:HG13	1.98	0.62
1:A:1119:G:H8	11:K:52:GLN:HE22	1.46	0.62
12:L:74:VAL:HG12	12:L:75:ARG:HG3	1.81	0.62
19:S:18:LEU:HB2	19:S:143:VAL:HG12	1.80	0.62
1:A:2433:A:H2'	1:A:2434:A:C8	2.34	0.62
2:B:3039:U:H1'	2:B:3044:A:N6	2.13	0.62
1:A:2472:C:O2'	1:A:2634:G:H4'	1.98	0.62
8:H:2:VAL:HG22	8:H:57:GLU:OE1	1.99	0.62
1:A:2908:A:H2'	1:A:2909:G:O4'	1.99	0.62
4:D:82:VAL:HG12	4:D:82:VAL:O	1.98	0.62
15:O:157:PRO:HA	37:O:8526:HOH:O	1.98	0.62
12:L:32:ILE:HD11	12:L:56:SER:HB3	1.80	0.62
26:Z:187:VAL:CG2	26:Z:192:ASP:HB2	2.30	0.62
11:K:74:ARG:O	11:K:78:ILE:HG12	1.98	0.62
4:D:51:VAL:CG2	4:D:327:VAL:HG13	2.29	0.62
19:S:82:GLU:HG3	19:S:83:LYS:H	1.65	0.62
1:A:1700:C:OP2	37:A:5580:HOH:O	2.15	0.62
7:G:69:ILE:HA	7:G:72:MET:CE	2.30	0.62
15:O:73:ALA:N	37:O:8568:HOH:O	2.33	0.62
30:4:7:PHE:HE2	30:4:22:VAL:HG21	1.65	0.62
26:Z:178:HIS:CG	26:Z:179:PRO:HD2	2.35	0.62
25:Y:78:GLU:CG	25:Y:79:GLU:H	2.12	0.62
13:M:53:ARG:NH2	13:M:57:VAL:HG12	2.14	0.62
1:A:2314:G:C2'	1:A:2315:C:H5'	2.30	0.62
1:A:2047:C:H5'	37:A:9397:HOH:O	1.99	0.62
3:C:33:GLU:O	3:C:34:ASP:HB2	1.99	0.62
1:A:1684:A:H1'	29:3:43:ARG:HH22	1.65	0.62
1:A:1116:U:O2'	1:A:1118:A:C2	2.49	0.62
5:E:246:ARG:NE	37:E:8430:HOH:O	2.32	0.62
23:W:39:ALA:C	23:W:41:GLU:H	2.03	0.62
6:F:135:VAL:HG22	6:F:136:ARG:N	2.14	0.62
24:X:81:ASP:OD1	24:X:92:ASP:HB2	1.99	0.62
27:1:31:ILE:O	27:1:35:LYS:HG3	1.99	0.62
21:U:48:VAL:HG22	21:U:97:ARG:O	1.99	0.62
5:E:61:PHE:HB3	37:E:8451:HOH:O	1.99	0.62
1:A:1819:G:H2'	1:A:1820:G:H4'	1.80	0.62
26:Z:172:THR:HG22	26:Z:173:ALA:N	2.14	0.62
1:A:272:A:H5'	1:A:273:G:OP2	1.99	0.62
1:A:1634:G:H3'	37:A:3463:HOH:O	1.99	0.62
5:E:214:THR:HG21	37:E:8408:HOH:O	1.99	0.62
1:A:2502:C:H4'	10:J:151:MET:HG2	1.82	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
21:U:9:LYS:HE3	21:U:13:ARG:NH1	2.15	0.62
1:A:2324:G:H4'	1:A:2418:G:O2'	1.99	0.62
6:F:25:MET:CE	6:F:37:ALA:HB1	2.29	0.62
6:F:38:GLU:HB3	6:F:49:PRO:HG2	1.82	0.62
19:S:18:LEU:HD12	19:S:143:VAL:CG1	2.30	0.62
1:A:1269:G:O2'	1:A:1270:U:H5'	2.00	0.62
4:D:55:ASN:HB3	4:D:63:GLU:HA	1.80	0.62
10:J:46:VAL:HG12	10:J:146:TRP:HZ3	1.65	0.61
4:D:195:ARG:HG2	4:D:323:LEU:HD22	1.81	0.61
1:A:1923:G:H4'	30:4:31:THR:O	2.00	0.61
12:L:62:PRO:HG3	12:L:65:ARG:HH21	1.65	0.61
6:F:99:ASP:CB	6:F:103:ASN:H	2.14	0.61
17:Q:10:ALA:HA	17:Q:13:VAL:HG12	1.82	0.61
13:M:104:ASP:HB3	37:M:8570:HOH:O	2.00	0.61
27:1:46:LYS:HB3	37:1:8442:HOH:O	2.00	0.61
6:F:25:MET:CE	6:F:41:LEU:HG	2.30	0.61
1:A:921:G:H4'	1:A:924:G:C6	2.35	0.61
17:Q:13:VAL:HG21	17:Q:41:ARG:HG2	1.83	0.61
26:Z:189:ASN:ND2	26:Z:192:ASP:H	1.97	0.61
1:A:2241:C:O2'	1:A:2242:U:H5'	1.99	0.61
15:O:154:LEU:O	15:O:155:GLU:HB3	2.01	0.61
1:A:1197:G:N2	37:A:5777:HOH:O	2.33	0.61
1:A:2414:A:H2'	1:A:2415:A:C8	2.35	0.61
14:N:74:ARG:HH11	14:N:74:ARG:HG3	1.65	0.61
5:E:103:ASN:HB3	37:E:8309:HOH:O	2.00	0.61
6:F:54:ALA:CB	6:F:69:ILE:HD12	2.30	0.61
1:A:2577:A:H5'	37:A:7289:HOH:O	1.98	0.61
37:A:8976:HOH:O	14:N:94:LYS:HE2	1.99	0.61
14:N:166:ALA:HB1	37:N:8542:HOH:O	2.01	0.61
25:Y:25:ARG:HG2	37:Y:5356:HOH:O	1.98	0.61
6:F:95:THR:C	6:F:97:GLN:H	2.03	0.61
1:A:2769:C:H2'	1:A:2770:G:O4'	2.01	0.61
17:Q:38:GLU:HA	17:Q:41:ARG:NH1	2.15	0.61
1:A:272:A:H3'	37:A:7066:HOH:O	2.01	0.61
1:A:2079:G:O6	37:A:7403:HOH:O	2.12	0.61
4:D:71:VAL:HG11	4:D:296:LEU:HB3	1.82	0.61
14:N:154:ARG:HG3	37:N:8612:HOH:O	1.99	0.61
1:A:1086:A:C6	24:X:11:VAL:HG11	2.35	0.61
6:F:99:ASP:HB2	6:F:103:ASN:HB2	1.83	0.61
6:F:38:GLU:OE2	6:F:51:ARG:CZ	2.49	0.61
19:S:82:GLU:HG3	19:S:83:LYS:N	2.15	0.61
1:A:669:G:O2'	1:A:670:G:H5'	2.01	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
22:V:49:LEU:HD11	37:V:3805:HOH:O	2.01	0.61
1:A:1205:U:H2'	1:A:1206:U:C5'	2.29	0.61
15:O:86:LEU:O	15:O:90:LEU:HG	2.01	0.61
1:A:1086:A:N6	24:X:11:VAL:HG11	2.15	0.61
4:D:168:GLY:N	4:D:174:ARG:HD3	2.15	0.61
37:A:5862:HOH:O	6:F:55:LYS:HB2	1.99	0.61
14:N:139:PRO:O	14:N:140:ALA:CB	2.48	0.61
11:K:75:PRO:HG2	11:K:105:LEU:CD2	2.30	0.61
4:D:248:ARG:NH1	37:D:8619:HOH:O	2.30	0.61
1:A:20:G:H21	19:S:117:HIS:HD2	1.48	0.61
29:3:35:ARG:HB2	37:3:2691:HOH:O	2.00	0.61
4:D:264:GLU:HG2	4:D:267:LYS:CE	2.26	0.61
9:I:63:ARG:N	37:I:2569:HOH:O	2.34	0.61
7:G:20:ILE:CD1	7:G:40:VAL:HG11	2.30	0.61
13:M:143:THR:CG2	13:M:144:ASP:N	2.63	0.61
4:D:42:ALA:HB1	4:D:308:LEU:HD11	1.83	0.61
5:E:162:VAL:HG12	5:E:192:ILE:HD11	1.83	0.61
1:A:2787:C:H5	37:A:4192:HOH:O	1.84	0.61
8:H:53:ASP:OD1	8:H:80:GLN:HB2	2.00	0.61
1:A:2637:A:H5'	37:A:8860:HOH:O	2.01	0.61
1:A:214:U:H5'	37:A:5686:HOH:O	2.00	0.61
5:E:16:VAL:HG12	5:E:17:ASP:H	1.66	0.60
28:2:8:GLN:HE22	28:2:11:LYS:HZ2	1.49	0.60
3:C:94:LEU:HG	3:C:99:ILE:HD11	1.82	0.60
1:A:2748:G:H5'	37:A:7077:HOH:O	2.01	0.60
1:A:2878:U:H2'	1:A:2879:A:O4'	2.01	0.60
4:D:2:GLN:HA	37:D:8625:HOH:O	2.00	0.60
4:D:66:GLU:OE1	4:D:328:ARG:HD2	2.01	0.60
27:1:39:CYS:CB	27:1:47:LEU:HD21	2.31	0.60
1:A:2359:G:H3'	37:A:5237:HOH:O	2.01	0.60
1:A:2096:A:H2'	1:A:2539:U:C1'	2.30	0.60
5:E:55:ARG:HB2	37:E:8311:HOH:O	1.99	0.60
10:J:75:SER:O	10:J:79:ALA:HB2	2.01	0.60
10:J:48:LEU:HG	10:J:157:ILE:HG21	1.83	0.60
12:L:81:ARG:HD3	12:L:87:ARG:NH1	2.17	0.60
22:V:9:CYS:SG	22:V:11:THR:HG23	2.40	0.60
4:D:217:ARG:HG3	4:D:257:THR:CG2	2.31	0.60
3:C:190:ARG:NH2	3:C:207:GLN:OE1	2.34	0.60
22:V:30:HIS:HB3	37:V:6215:HOH:O	2.01	0.60
1:A:2587:U:H2'	1:A:2589:U:H5''	1.83	0.60
24:X:119:HIS:HD2	24:X:120:PRO:O	1.85	0.60
5:E:235:PHE:HE2	5:E:243:VAL:HG21	1.66	0.60

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1192:A:O2'	1:A:1193:A:OP1	2.19	0.60
1:A:1151:G:OP1	9:I:16:LYS:NZ	2.33	0.60
2:B:3028:U:H2'	2:B:3029:C:C6	2.36	0.60
1:A:1713:G:H1'	37:A:4626:HOH:O	2.00	0.60
19:S:44:VAL:O	19:S:48:GLU:HG3	2.01	0.60
10:J:150:LYS:HB2	10:J:157:ILE:HD12	1.83	0.60
25:Y:78:GLU:HG2	25:Y:79:GLU:N	2.14	0.60
24:X:21:LEU:HD21	24:X:48:VAL:CG1	2.32	0.60
4:D:329:TYR:HE2	22:V:15:PRO:HG2	1.64	0.60
21:U:48:VAL:HG22	21:U:97:ARG:C	2.20	0.60
1:A:2766:A:O2'	4:D:265:LEU:O	2.18	0.60
10:J:130:HIS:CD2	10:J:133:ILE:HD11	2.36	0.60
4:D:140:LEU:HD23	37:D:8583:HOH:O	2.00	0.60
26:Z:189:ASN:HD22	26:Z:189:ASN:C	2.03	0.60
1:A:558:C:C2'	1:A:559:U:H5''	2.32	0.60
6:F:64:ARG:CD	6:F:67:ASP:HB3	2.32	0.60
37:A:7116:HOH:O	27:1:31:ILE:HG13	2.01	0.60
1:A:69:A:H5'	1:A:69:A:C8	2.36	0.60
1:A:1123:A:C6	1:A:1238:C:H5'	2.37	0.60
14:N:87:MET:HB2	14:N:91:ILE:HD11	1.83	0.60
6:F:163:VAL:HA	37:F:6326:HOH:O	2.02	0.60
2:B:3076:G:C3'	2:B:3077:A:H5''	2.31	0.60
5:E:127:ARG:HD2	5:E:229:PRO:O	2.01	0.60
1:A:2453:G:H3'	37:A:5467:HOH:O	2.00	0.60
23:W:5:VAL:HG23	37:W:2271:HOH:O	2.02	0.60
1:A:1681:G:H5''	1:A:1682:A:H5'	1.83	0.60
6:F:57:THR:HG23	6:F:63:ILE:HG22	1.83	0.60
14:N:74:ARG:O	14:N:88:VAL:HG13	2.01	0.60
2:B:3049:G:H5''	37:B:4707:HOH:O	2.02	0.60
8:H:28:ALA:HB3	8:H:99:THR:O	2.02	0.60
15:O:151:ASP:O	15:O:154:LEU:HB2	2.02	0.60
15:O:22:GLN:HG2	15:O:26:LEU:HD22	1.82	0.60
1:A:2284:G:H1'	37:A:9149:HOH:O	2.01	0.60
13:M:30:ARG:NH2	37:M:8523:HOH:O	2.26	0.60
1:A:816:G:H5'	1:A:1598:A:H4'	1.84	0.60
1:A:1743:G:H1'	37:A:4449:HOH:O	2.00	0.60
1:A:1474:C:H6	1:A:1474:C:C5'	2.13	0.60
14:N:172:GLY:C	14:N:183:VAL:HG11	2.23	0.60
1:A:2768:A:O2'	1:A:2769:C:H5'	2.02	0.60
2:B:3003:A:N6	2:B:3022:G:H1'	2.17	0.60
3:C:179:MET:HG2	3:C:186:TRP:CB	2.32	0.60
1:A:513:A:N3	37:A:3234:HOH:O	2.30	0.60

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:J:85:ILE:HB	10:J:132:PHE:CE2	2.37	0.60
14:N:74:ARG:HG3	14:N:74:ARG:NH1	2.17	0.60
14:N:104:ARG:O	14:N:108:LYS:HG2	2.02	0.60
23:W:39:ALA:O	23:W:41:GLU:N	2.35	0.60
1:A:2897:C:H2'	1:A:2898:G:H8	1.66	0.60
14:N:46:LEU:HG	37:N:8621:HOH:O	2.02	0.60
4:D:30:PRO:HB2	4:D:39:GLN:NE2	2.16	0.60
19:S:132:ARG:HG2	19:S:133:ALA:N	2.17	0.60
20:T:43:GLU:HB3	37:T:7106:HOH:O	2.01	0.60
7:G:15:GLN:NE2	7:G:40:VAL:O	2.35	0.59
3:C:131:HIS:O	3:C:132:ASP:HB2	2.00	0.59
1:A:1377:C:H5'	1:A:1377:C:H6	1.66	0.59
3:C:153:ARG:HB2	3:C:153:ARG:HH11	1.67	0.59
16:P:59:VAL:HG23	16:P:111:VAL:HG23	1.83	0.59
37:A:5067:HOH:O	4:D:298:LYS:HD3	2.01	0.59
10:J:49:VAL:O	10:J:157:ILE:HG23	2.03	0.59
1:A:2506:A:C1'	37:A:5601:HOH:O	2.50	0.59
1:A:1029:U:O2'	1:A:1273:C:OP1	2.19	0.59
23:W:58:THR:O	23:W:62:GLU:HG3	2.02	0.59
6:F:50:VAL:O	6:F:71:ALA:HA	2.02	0.59
1:A:1641:A:H2'	1:A:1642:A:H5'	1.84	0.59
1:A:381:G:H5''	37:A:3882:HOH:O	2.01	0.59
3:C:223:ARG:NH1	37:C:8518:HOH:O	2.36	0.59
8:H:100:ASP:HB3	37:H:5691:HOH:O	2.02	0.59
1:A:2676:C:H4'	11:K:70:PHE:HE1	1.66	0.59
30:4:3:MET:O	30:4:90:PHE:HA	2.02	0.59
1:A:349:U:O2'	1:A:350:C:H5'	2.02	0.59
18:R:50:GLY:HA3	18:R:87:THR:OG1	2.02	0.59
1:A:739:G:C5	37:A:7079:HOH:O	2.51	0.59
27:1:47:LEU:HD23	27:1:57:CYS:HB2	1.85	0.59
1:A:2503:A:OP1	10:J:147:ARG:NH2	2.35	0.59
1:A:545:G:C8	1:A:545:G:H5'	2.36	0.59
1:A:1810:C:OP1	22:V:44:ARG:NE	2.22	0.59
18:R:75:ILE:CD1	18:R:84:ILE:HD11	2.33	0.59
28:2:28:HIS:CE1	28:2:31:LYS:HE2	2.38	0.59
37:E:8357:HOH:O	16:P:3:THR:HG21	2.03	0.59
1:A:189:A:OP1	14:N:171:ARG:NH2	2.36	0.59
37:A:4103:HOH:O	10:J:151:MET:HE2	2.02	0.59
5:E:127:ARG:HG2	5:E:127:ARG:HH11	1.67	0.59
27:1:25:ARG:O	27:1:29:VAL:HG23	2.03	0.59
1:A:2064:U:H5'	1:A:2652:U:H4'	1.83	0.59
1:A:2310:G:OP2	10:J:114:PRO:HD2	2.01	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2093:G:H5''	37:A:9058:HOH:O	2.00	0.59
1:A:2559:C:H4'	37:A:6790:HOH:O	2.02	0.59
1:A:1176:C:H1'	37:A:3499:HOH:O	2.02	0.59
15:O:58:LEU:HD12	15:O:58:LEU:N	2.17	0.59
1:A:2433:A:H2'	1:A:2434:A:H8	1.68	0.59
1:A:1393:A:H2'	1:A:1394:C:C6	2.38	0.59
1:A:2251:G:H4'	37:A:6944:HOH:O	2.03	0.59
1:A:926:A:O2'	13:M:41:HIS:HD2	1.86	0.59
4:D:280:VAL:CG1	4:D:334:SER:HA	2.32	0.59
24:X:88:THR:CG2	24:X:89:ASP:H	2.11	0.59
4:D:146:THR:O	4:D:159:PRO:HB3	2.03	0.59
21:U:75:GLU:O	21:U:76:ASP:HB2	2.02	0.59
5:E:85:LYS:NZ	37:E:8328:HOH:O	2.13	0.59
6:F:65:GLU:HG3	37:F:6752:HOH:O	2.01	0.59
21:U:52:ARG:HB2	21:U:95:ASN:HB3	1.85	0.59
1:A:1657:A:H2'	1:A:1658:A:C8	2.38	0.59
1:A:470:U:O2'	28:2:16:HIS:HD2	1.85	0.59
4:D:154:VAL:HG12	4:D:156:LYS:HG2	1.85	0.59
12:L:55:VAL:HG12	12:L:56:SER:H	1.67	0.59
1:A:280:C:H2'	1:A:281:U:O4'	2.03	0.59
23:W:39:ALA:N	23:W:40:PRO:CD	2.65	0.59
4:D:195:ARG:HD2	4:D:324:ASP:OD1	2.03	0.59
26:Z:126:PRO:HG2	26:Z:128:PHE:CE1	2.38	0.59
27:1:48:LYS:HG2	37:1:8433:HOH:O	2.01	0.59
1:A:125:U:H2'	37:A:3336:HOH:O	2.02	0.59
1:A:661:G:C5	1:A:686:A:C2	2.90	0.59
21:U:71:VAL:CG1	21:U:90:PRO:HB3	2.20	0.59
1:A:2121:G:O2'	1:A:2122:C:H5'	2.03	0.59
5:E:77:ALA:O	5:E:78:ARG:HG3	2.03	0.59
1:A:285:A:H2'	1:A:286:U:O4'	2.03	0.59
4:D:51:VAL:HG23	4:D:329:TYR:O	2.02	0.59
1:A:182:G:H5'	37:A:4711:HOH:O	2.02	0.59
4:D:24:PRO:HG3	4:D:204:GLY:HA2	1.85	0.59
1:A:1204:C:H1'	37:A:4303:HOH:O	2.03	0.59
3:C:18:ALA:O	3:C:20:SER:N	2.33	0.59
1:A:1477:C:O2'	1:A:1478:U:H5'	2.02	0.59
7:G:101:GLU:HB2	7:G:116:THR:O	2.02	0.59
5:E:142:ASP:OD1	5:E:236:THR:HG23	2.02	0.58
14:N:104:ARG:O	14:N:108:LYS:HE2	2.03	0.58
14:N:185:PRO:HG2	14:N:189:VAL:HG11	1.85	0.58
4:D:333:GLU:HB2	22:V:14:GLU:OE2	2.03	0.58
4:D:125:GLU:O	4:D:129:ARG:HG3	2.02	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1234:U:N3	4:D:244:PRO:HB3	2.18	0.58
11:K:74:ARG:CB	11:K:74:ARG:HH11	2.16	0.58
1:A:407:A:H5'	37:A:5570:HOH:O	2.03	0.58
1:A:485:A:N3	1:A:487:G:H5"	2.18	0.58
6:F:55:LYS:HA	37:F:6752:HOH:O	2.04	0.58
10:J:35:ASN:ND2	10:J:80:ASN:HA	2.18	0.58
10:J:3:GLY:HA2	10:J:57:ARG:NH1	2.18	0.58
3:C:105:VAL:CG1	3:C:154:ALA:HB1	2.33	0.58
3:C:192:VAL:CG1	3:C:207:GLN:HB3	2.33	0.58
29:3:24:TRP:CD1	37:3:6863:HOH:O	2.52	0.58
1:A:1861:C:H4'	3:C:6:GLY:O	2.03	0.58
1:A:1265:G:H1'	37:A:4558:HOH:O	2.02	0.58
1:A:960:G:N3	1:A:960:G:H2'	2.19	0.58
6:F:19:GLU:HG3	37:F:6165:HOH:O	2.04	0.58
1:A:553:G:P	26:Z:204:ARG:HH22	2.26	0.58
12:L:62:PRO:HG3	12:L:65:ARG:NH2	2.18	0.58
7:G:93:MET:HE1	7:G:165:GLY:N	2.19	0.58
11:K:22:VAL:O	11:K:26:VAL:HG23	2.04	0.58
13:M:148:GLU:HB2	37:M:8594:HOH:O	2.01	0.58
20:T:51:GLN:HE21	20:T:53:ASN:ND2	2.00	0.58
15:O:143:ARG:HA	15:O:172:PHE:CD2	2.39	0.58
4:D:36:PRO:HA	4:D:168:GLY:CA	2.33	0.58
16:P:14:LEU:HD23	16:P:102:ILE:HD11	1.84	0.58
1:A:39:G:N2	1:A:444:C:C2	2.72	0.58
37:B:5851:HOH:O	15:O:113:SER:HB3	2.03	0.58
2:B:3055:U:H4'	2:B:3056:A:C8	2.39	0.58
1:A:797:A:O4'	27:1:10:ARG:N	2.36	0.58
27:1:11:THR:OG1	27:1:23:ARG:HB2	2.04	0.58
20:T:4:VAL:HG23	37:T:2334:HOH:O	2.01	0.58
6:F:170:TYR:O	6:F:171:ASP:HB3	2.03	0.58
1:A:958:G:O2'	1:A:959:C:H5'	2.02	0.58
5:E:79:ARG:O	5:E:87:ARG:HG2	2.03	0.58
1:A:564:G:H1'	37:A:5852:HOH:O	2.04	0.58
7:G:15:GLN:HG2	7:G:19:ASP:O	2.04	0.58
24:X:4:LEU:HD23	24:X:54:PHE:HB3	1.85	0.58
1:A:21:G:H4'	19:S:2:ILE:HG22	1.86	0.58
15:O:163:PHE:HA	37:O:8519:HOH:O	2.04	0.58
20:T:6:LYS:HB2	20:T:27:ALA:O	2.03	0.58
6:F:22:VAL:HG22	6:F:74:THR:HG22	1.86	0.58
10:J:44:ALA:HA	10:J:163:PRO:O	2.04	0.58
1:A:820:G:OP1	27:1:17:ARG:NH2	2.30	0.58
1:A:283:U:H5"	1:A:284:C:P	2.44	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1406:A:N1	37:A:5580:HOH:O	2.32	0.58
22:V:20:MET:HE1	37:V:7438:HOH:O	2.04	0.58
1:A:151:A:C2	1:A:442:A:C8	2.92	0.58
1:A:2718:C:H6	1:A:2718:C:H5'	1.69	0.58
1:A:1185:U:H2'	1:A:1186:C:C6	2.39	0.58
1:A:2634:G:O2'	1:A:2635:A:H5'	2.04	0.58
1:A:1505:U:H6	1:A:1505:U:H5'	1.68	0.58
37:A:6992:HOH:O	5:E:188:ARG:CD	2.52	0.58
23:W:56:ILE:O	23:W:60:GLN:HG3	2.04	0.58
1:A:828:G:N7	37:A:5406:HOH:O	2.32	0.58
19:S:104:PHE:HB2	19:S:109:MET:HE1	1.86	0.57
26:Z:216:ARG:CD	37:Z:8571:HOH:O	2.43	0.57
1:A:2506:A:O2'	1:A:2507:G:O5'	2.22	0.57
13:M:145:LEU:O	13:M:148:GLU:HG3	2.04	0.57
23:W:44:GLY:O	23:W:48:GLU:HG2	2.04	0.57
4:D:248:ARG:NH2	37:D:8525:HOH:O	2.36	0.57
1:A:2729:C:O2'	1:A:2730:G:H5'	2.03	0.57
1:A:461:C:H2'	37:A:3568:HOH:O	2.03	0.57
10:J:56:ILE:HG22	10:J:61:LEU:CD2	2.33	0.57
6:F:44:ILE:HG23	6:F:45:THR:HG23	1.86	0.57
4:D:312:ARG:HD3	4:D:315:VAL:HG13	1.86	0.57
1:A:558:C:O2'	1:A:559:U:H5''	2.05	0.57
4:D:141:ARG:HG2	4:D:165:ARG:HA	1.85	0.57
3:C:164:ARG:HB2	27:1:68:CYS:SG	2.43	0.57
1:A:113:A:OP2	1:A:114:A:H2'	2.03	0.57
17:Q:18:LYS:O	17:Q:21:VAL:HG22	2.03	0.57
19:S:17:MET:HE1	19:S:19:ARG:NH2	2.19	0.57
15:O:49:THR:CG2	15:O:56:ASP:HB2	2.32	0.57
14:N:47:ASP:CG	14:N:48:ARG:N	2.57	0.57
4:D:305:ASP:O	4:D:306:LYS:CB	2.51	0.57
4:D:54:VAL:HB	37:D:8615:HOH:O	2.03	0.57
37:A:8711:HOH:O	14:N:82:ARG:HD2	2.05	0.57
1:A:2540:G:O2'	1:A:2541:U:H5''	2.04	0.57
4:D:74:ILE:HG13	37:D:8607:HOH:O	2.04	0.57
6:F:23:VAL:HG22	6:F:73:VAL:HB	1.86	0.57
10:J:13:ALA:HA	10:J:91:HIS:CE1	2.40	0.57
25:Y:71:ARG:HB2	37:Y:6590:HOH:O	2.04	0.57
15:O:141:ARG:N	37:O:8571:HOH:O	2.36	0.57
2:B:3044:A:O4'	6:F:76:ARG:NE	2.37	0.57
5:E:233:THR:HG22	5:E:234:VAL:N	2.18	0.57
3:C:2:ARG:NH1	37:C:8516:HOH:O	2.27	0.57
1:A:2694:A:H4'	7:G:91:PHE:CE1	2.39	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1559:A:H1'	37:A:5413:HOH:O	2.04	0.57
5:E:236:THR:HA	37:E:8457:HOH:O	2.03	0.57
9:I:12:ILE:HG22	9:I:12:ILE:O	2.04	0.57
24:X:137:GLN:HE21	24:X:141:HIS:CE1	2.15	0.57
1:A:1589:G:N2	1:A:1605:G:H1'	2.20	0.57
1:A:558:C:H2'	1:A:559:U:C5'	2.34	0.57
3:C:105:VAL:HG12	3:C:106:CYS:N	2.19	0.57
15:O:184:ILE:HG22	15:O:185:GLU:HG3	1.86	0.57
13:M:125:PHE:CZ	13:M:140:VAL:HG13	2.39	0.57
26:Z:186:ARG:HH11	26:Z:186:ARG:HG2	1.70	0.57
4:D:24:PRO:HG2	4:D:204:GLY:HA2	1.86	0.57
1:A:69:A:H8	1:A:69:A:H5'	1.70	0.57
1:A:1041:U:H2'	1:A:1042:U:H5'	1.86	0.57
1:A:2497:A:OP2	37:A:3560:HOH:O	2.17	0.57
1:A:1925:G:O2'	1:A:1926:G:H5'	2.05	0.57
8:H:100:ASP:O	8:H:101:ALA:O	2.23	0.57
29:3:22:PRO:HG2	29:3:25:VAL:CG2	2.33	0.57
1:A:1269:G:H2'	1:A:1270:U:C6	2.39	0.57
1:A:1947:G:N2	1:A:1966:U:C2	2.73	0.57
1:A:136:C:H2'	1:A:137:U:O4'	2.04	0.57
1:A:2443:C:H3'	37:A:3048:HOH:O	2.04	0.57
1:A:629:A:C2	1:A:2074:A:C2	2.93	0.57
14:N:37:VAL:HG21	14:N:108:LYS:HG3	1.87	0.57
13:M:120:LEU:HD12	13:M:133:VAL:HG21	1.85	0.57
12:L:37:TYR:CD2	37:L:7169:HOH:O	2.53	0.57
1:A:2507:G:H2'	1:A:2510:C:H42	1.70	0.57
24:X:48:VAL:O	24:X:48:VAL:HG12	2.03	0.57
24:X:48:VAL:O	24:X:48:VAL:CG1	2.51	0.57
20:T:81:ILE:HG23	37:T:4527:HOH:O	2.05	0.57
1:A:1723:G:H2'	37:A:9203:HOH:O	2.03	0.57
11:K:19:MET:HE2	11:K:79:PHE:HA	1.85	0.57
1:A:2256:G:H2'	1:A:2257:G:H5'	1.87	0.57
10:J:136:VAL:HG22	10:J:137:ASN:O	2.04	0.57
10:J:139:ASP:N	10:J:140:PRO:CD	2.67	0.57
24:X:141:HIS:HB2	24:X:146:ILE:HG12	1.85	0.57
10:J:71:TYR:C	10:J:73:GLN:N	2.56	0.57
3:C:192:VAL:HG12	3:C:207:GLN:HB3	1.87	0.57
1:A:1329:A:H2	37:A:4243:HOH:O	1.88	0.57
1:A:2001:G:O2'	1:A:2002:C:H5'	2.05	0.57
1:A:538:C:H5''	1:A:539:G:C8	2.40	0.57
10:J:48:LEU:HD13	10:J:146:TRP:HB3	1.87	0.56
4:D:190:MET:HE2	4:D:194:PHE:HD1	1.67	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:816:G:C6	1:A:817:G:N1	2.73	0.56
37:A:9345:HOH:O	13:M:41:HIS:HE1	1.88	0.56
1:A:105:G:O2'	1:A:106:A:H5'	2.05	0.56
13:M:138:GLY:HA3	37:M:8558:HOH:O	2.04	0.56
10:J:47:GLU:CB	10:J:133:ILE:HD13	2.34	0.56
6:F:37:ALA:O	6:F:40:ILE:HG12	2.06	0.56
10:J:69:ASN:O	10:J:72:VAL:HG12	2.06	0.56
1:A:474:C:O3'	5:E:73:LEU:HD21	2.05	0.56
7:G:37:ASP:OD1	11:K:125:SER:HB3	2.05	0.56
2:B:3055:U:H4'	2:B:3056:A:H8	1.70	0.56
1:A:1205:U:C2'	1:A:1206:U:H5'	2.29	0.56
27:1:11:THR:HG21	27:1:23:ARG:HB2	1.86	0.56
1:A:183:A:H5'	14:N:157:LEU:HD12	1.87	0.56
4:D:7:ARG:NH1	4:D:11:LEU:HD22	2.21	0.56
2:B:3003:A:H2'	37:B:2430:HOH:O	2.04	0.56
30:4:73:GLU:HB2	37:4:8525:HOH:O	2.04	0.56
19:S:119:VAL:HG21	19:S:142:ASP:CG	2.26	0.56
1:A:1523:G:H2'	1:A:1524:U:C6	2.40	0.56
1:A:2405:C:H5'	37:A:6132:HOH:O	2.04	0.56
11:K:45:VAL:HG23	11:K:130:VAL:O	2.04	0.56
8:H:50:VAL:CG2	8:H:63:ILE:HG21	2.36	0.56
4:D:307:ARG:HH11	4:D:307:ARG:CB	2.18	0.56
1:A:383:A:H4'	37:A:4881:HOH:O	2.04	0.56
4:D:16:ARG:NH1	37:D:8620:HOH:O	2.37	0.56
1:A:2326:U:H4'	1:A:2412:G:H4'	1.86	0.56
27:1:54:ILE:HD12	37:1:8416:HOH:O	2.05	0.56
1:A:2906:A:H5'	1:A:2907:C:O4'	2.04	0.56
1:A:2464:C:H5''	1:A:2465:A:OP1	2.05	0.56
1:A:1528:A:H2'	1:A:1529:G:O4'	2.06	0.56
1:A:12:U:H2'	1:A:13:G:H5'	1.86	0.56
1:A:56:G:H5''	23:W:50:ARG:NH1	2.21	0.56
25:Y:37:LEU:CD1	25:Y:85:VAL:HG21	2.26	0.56
25:Y:15:ARG:HH11	25:Y:15:ARG:CB	2.18	0.56
13:M:57:VAL:HG12	13:M:57:VAL:O	2.04	0.56
1:A:2326:U:H4'	1:A:2412:G:C4'	2.36	0.56
1:A:1687:C:O2	28:2:9:GLY:HA2	2.05	0.56
4:D:297:VAL:HB	37:D:8607:HOH:O	2.06	0.56
1:A:2000:G:O2'	1:A:2001:G:H5'	2.06	0.56
1:A:679:G:OP2	37:A:4001:HOH:O	2.17	0.56
1:A:221:G:H2'	1:A:222:A:C8	2.40	0.56
1:A:415:A:O2'	1:A:416:G:H5'	2.06	0.56
3:C:81:GLN:HB2	3:C:92:ASN:ND2	2.20	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2896:A:H2'	1:A:2896:A:N3	2.21	0.56
1:A:920:C:H5'	1:A:921:G:C4	2.41	0.56
11:K:126:ASN:O	11:K:129:PHE:HE2	1.89	0.56
8:H:107:VAL:HG23	37:H:6617:HOH:O	2.04	0.56
23:W:64:GLY:O	23:W:65:ASP:CB	2.54	0.56
15:O:152:GLU:C	15:O:154:LEU:H	2.07	0.56
2:B:3002:U:H4'	2:B:3002:U:OP2	2.05	0.56
15:O:78:MET:HB2	15:O:79:PRO:HD3	1.87	0.56
7:G:172:PRO:HB3	37:G:6931:HOH:O	2.06	0.56
1:A:2582:G:H4'	37:L:4440:HOH:O	2.06	0.56
5:E:141:SER:HA	37:E:8381:HOH:O	2.05	0.56
6:F:27:ILE:HD11	6:F:37:ALA:CB	2.35	0.56
1:A:2524:G:H21	1:A:2526:C:N4	2.03	0.56
7:G:23:GLU:HG2	7:G:28:SER:HB3	1.88	0.56
1:A:251:C:O2'	1:A:252:C:H5'	2.06	0.56
13:M:149:ARG:O	13:M:150:GLN:HB2	2.06	0.56
1:A:1181:A:H2'	1:A:1182:C:O4'	2.05	0.56
20:T:51:GLN:NE2	20:T:53:ASN:HD21	2.04	0.56
2:B:3041:C:O4'	6:F:50:VAL:HG23	2.06	0.56
1:A:1441:G:O2'	1:A:1442:A:H5'	2.06	0.56
1:A:1165:G:H3'	1:A:1165:G:OP1	2.06	0.56
27:1:23:ARG:NH1	37:1:8404:HOH:O	2.39	0.56
11:K:46:ILE:HA	37:K:8527:HOH:O	2.05	0.56
1:A:1450:C:C4'	1:A:1451:C:OP2	2.54	0.56
7:G:68:HIS:O	7:G:72:MET:HG3	2.06	0.56
1:A:1057:A:C6	1:A:1058:A:C6	2.94	0.56
4:D:7:ARG:NH1	4:D:11:LEU:CD2	2.69	0.56
1:A:926:A:O2'	13:M:41:HIS:CD2	2.59	0.56
37:L:1387:HOH:O	22:V:20:MET:HE3	2.05	0.56
1:A:2081:A:H4'	11:K:69:TYR:CE1	2.40	0.56
2:B:3107:C:H5	37:B:3167:HOH:O	1.89	0.56
5:E:115:LEU:HD21	5:E:243:VAL:HG13	1.87	0.55
37:A:6979:HOH:O	19:S:132:ARG:NH2	2.39	0.55
37:A:6992:HOH:O	5:E:188:ARG:HD3	2.05	0.55
1:A:1527:A:H1'	1:A:1528:A:C8	2.41	0.55
1:A:1787:C:OP1	17:Q:68:LYS:HE2	2.06	0.55
1:A:45:A:N6	1:A:147:G:C4	2.74	0.55
30:4:62:THR:HB	37:4:8550:HOH:O	2.05	0.55
1:A:684:G:H2'	1:A:685:C:C6	2.40	0.55
14:N:55:LYS:HB2	14:N:60:ILE:CD1	2.37	0.55
12:L:9:THR:O	12:L:10:GLN:C	2.44	0.55
17:Q:120:ARG:NH2	17:Q:123:TYR:CD2	2.75	0.55

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2256:G:C2'	1:A:2257:G:H5'	2.36	0.55
1:A:88:G:H8	1:A:88:G:H5'	1.71	0.55
5:E:7:ASP:OD1	5:E:11:ASN:O	2.23	0.55
1:A:542:A:H2'	1:A:543:G:O4'	2.06	0.55
20:T:57:THR:HG22	20:T:59:ASP:HB2	1.87	0.55
37:A:9374:HOH:O	12:L:39:GLY:HA3	2.05	0.55
4:D:79:MET:HE3	4:D:144:THR:HG21	1.87	0.55
24:X:5:VAL:O	24:X:52:VAL:HG22	2.05	0.55
1:A:484:A:N1	1:A:506:G:H4'	2.21	0.55
1:A:2791:U:H1'	1:A:2792:A:H5''	1.89	0.55
15:O:38:LYS:HD2	15:O:114:LYS:HE3	1.88	0.55
26:Z:99:ALA:HB2	26:Z:233:TYR:CZ	2.41	0.55
3:C:72:GLU:HG3	27:1:66:GLY:HA2	1.88	0.55
25:Y:66:THR:HG23	25:Y:67:PRO:HD2	1.88	0.55
5:E:118:THR:CG2	5:E:137:PRO:HB3	2.37	0.55
15:O:5:ARG:HG3	18:R:18:PRO:CB	2.36	0.55
9:I:12:ILE:HD12	37:I:692:HOH:O	2.05	0.55
12:L:74:VAL:O	12:L:74:VAL:CG1	2.54	0.55
24:X:26:ILE:O	24:X:26:ILE:HG13	2.06	0.55
10:J:127:GLY:O	10:J:128:ALA:CB	2.54	0.55
10:J:75:SER:HB3	10:J:79:ALA:HB1	1.88	0.55
1:A:539:G:H2'	1:A:540:A:C8	2.41	0.55
1:A:2429:A:H2'	1:A:2430:A:C8	2.41	0.55
19:S:14:ALA:HB3	19:S:147:LEU:HB2	1.89	0.55
9:I:64:ASN:N	9:I:64:ASN:HD22	2.04	0.55
37:A:8806:HOH:O	3:C:11:ARG:HD3	2.05	0.55
27:1:46:LYS:O	27:1:57:CYS:HA	2.07	0.55
14:N:37:VAL:HG21	14:N:108:LYS:CG	2.36	0.55
1:A:2526:C:C2'	1:A:2527:U:H5'	2.36	0.55
10:J:71:TYR:O	10:J:73:GLN:N	2.38	0.55
11:K:107:ASN:C	11:K:107:ASN:HD22	2.10	0.55
1:A:920:C:H4'	1:A:921:G:C2	2.42	0.55
1:A:396:U:OP2	30:4:38:ARG:NH1	2.39	0.55
1:A:2769:C:C2'	1:A:2770:G:H5'	2.37	0.55
14:N:59:GLY:HA3	14:N:141:ILE:HD12	1.89	0.55
1:A:119:A:H2'	1:A:120:A:H5''	1.88	0.55
1:A:1711:A:O2'	1:A:1712:A:H5'	2.06	0.55
18:R:32:GLU:HA	18:R:71:TYR:OH	2.07	0.55
1:A:2402:A:H1'	37:A:9731:HOH:O	2.06	0.55
6:F:25:MET:HE1	6:F:37:ALA:O	2.05	0.55
4:D:238:ASN:HD22	4:D:240:GLY:N	2.02	0.55
19:S:39:THR:HB	19:S:42:GLU:CG	2.36	0.55

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:F:64:ARG:O	6:F:67:ASP:OD2	2.23	0.55
1:A:1909:A:H2'	1:A:1910:A:C8	2.41	0.55
8:H:107:VAL:O	8:H:111:ILE:HG13	2.05	0.55
4:D:248:ARG:O	4:D:251:VAL:HG12	2.06	0.55
1:A:212:A:O4'	1:A:214:U:C6	2.60	0.55
34:A:8513:CL:CL	37:A:4243:HOH:O	2.56	0.55
28:2:21:ARG:HD2	28:2:37:CYS:SG	2.46	0.55
24:X:149:LEU:HG	24:X:153:MET:HE2	1.89	0.55
10:J:166:ASN:N	10:J:166:ASN:HD22	2.03	0.55
1:A:2780:C:H1'	7:G:143:GLN:NE2	2.18	0.55
1:A:152:A:O2'	1:A:153:C:H5'	2.07	0.55
17:Q:16:VAL:HG12	17:Q:17:GLY:N	2.21	0.55
11:K:39:VAL:HG12	11:K:40:ASN:ND2	2.22	0.55
1:A:902:G:N7	13:M:18:HIS:HD2	2.04	0.55
24:X:108:ARG:HE	24:X:114:PRO:HG3	1.71	0.55
6:F:101:THR:HG22	37:F:7400:HOH:O	2.07	0.55
1:A:2123:A:H5'	14:N:89:ASN:ND2	2.22	0.55
12:L:34:VAL:HB	37:L:7169:HOH:O	2.07	0.55
6:F:136:ARG:HD2	6:F:155:HIS:O	2.07	0.55
24:X:76:ASP:O	24:X:77:ALA:C	2.46	0.55
18:R:40:HIS:CE1	18:R:94:GLN:HA	2.42	0.55
1:A:1127:C:H2'	1:A:1128:U:H5'	1.88	0.55
7:G:21:THR:HG23	7:G:30:THR:OG1	2.07	0.55
1:A:1003:U:O2	10:J:90:PHE:CZ	2.59	0.55
10:J:65:ARG:CZ	37:J:8386:HOH:O	2.55	0.55
5:E:118:THR:HG22	5:E:137:PRO:HB3	1.89	0.55
20:T:57:THR:C	20:T:59:ASP:H	2.10	0.55
1:A:2459:G:P	30:4:64:LYS:HB2	2.47	0.55
31:A:4000:CAI:H2B1	31:A:4000:CAI:H6A3	1.89	0.55
3:C:164:ARG:CZ	37:C:8597:HOH:O	2.55	0.55
1:A:2729:C:H2'	1:A:2730:G:H8	1.72	0.55
1:A:1887:U:OP1	27:1:21:LYS:HE3	2.07	0.55
24:X:38:THR:HG22	24:X:39:ASP:N	2.22	0.55
10:J:86:ARG:HD3	10:J:130:HIS:HD2	1.72	0.54
5:E:98:ARG:NH1	37:E:8356:HOH:O	2.39	0.54
7:G:23:GLU:HG2	7:G:28:SER:CB	2.37	0.54
1:A:182:G:O2'	1:A:183:A:H5'	2.07	0.54
1:A:155:C:OP2	14:N:188:ARG:HD3	2.07	0.54
17:Q:80:ARG:HG2	17:Q:87:ARG:CZ	2.37	0.54
1:A:289:G:N2	1:A:363:A:H2	2.03	0.54
1:A:559:U:C6	1:A:559:U:H5'	2.40	0.54
1:A:1894:C:C2	1:A:1939:U:C4	2.94	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1308:A:H5'	37:A:6473:HOH:O	2.07	0.54
2:B:3035:C:H5''	37:B:4078:HOH:O	2.07	0.54
1:A:1008:C:H5''	10:J:16:ARG:HH12	1.72	0.54
24:X:122:ARG:NH2	24:X:154:ARG:CD	2.62	0.54
10:J:26:LYS:HD2	10:J:28:ILE:HB	1.89	0.54
12:L:55:VAL:CG1	12:L:56:SER:N	2.71	0.54
30:4:48:ASN:ND2	30:4:50:GLY:H	2.05	0.54
29:3:41:HIS:H	29:3:45:ASN:ND2	1.97	0.54
26:Z:154:ARG:NH1	26:Z:155:ARG:HG3	2.22	0.54
14:N:47:ASP:CG	14:N:48:ARG:H	2.10	0.54
9:I:64:ASN:O	9:I:68:GLU:HG3	2.07	0.54
1:A:1753:C:O2	4:D:229:ARG:NH2	2.40	0.54
11:K:142:ASN:O	11:K:144:THR:N	2.40	0.54
1:A:306:A:P	21:U:38:ARG:HH21	2.30	0.54
1:A:1007:A:H2'	10:J:19:TYR:CZ	2.43	0.54
7:G:157:LYS:NZ	37:G:2401:HOH:O	2.39	0.54
14:N:155:HIS:O	14:N:158:ARG:HG2	2.07	0.54
1:A:1174:A:C5	1:A:1201:C:H4'	2.42	0.54
8:H:99:THR:HG23	8:H:99:THR:O	2.07	0.54
28:2:25:LYS:O	28:2:25:LYS:HG2	2.07	0.54
15:O:155:GLU:O	15:O:156:GLU:HG3	2.08	0.54
16:P:25:VAL:HG23	16:P:26:TRP:N	2.22	0.54
23:W:49:LEU:O	23:W:53:ILE:HG13	2.07	0.54
1:A:1434:A:H2'	1:A:1436:C:C5	2.42	0.54
3:C:140:LEU:HB3	3:C:141:PRO:HD2	1.89	0.54
30:4:55:VAL:HG22	37:4:8509:HOH:O	2.07	0.54
1:A:921:G:H4'	1:A:924:G:N1	2.23	0.54
1:A:2100:A:C2	31:A:4000:CAI:H201	2.43	0.54
21:U:48:VAL:HG23	21:U:98:VAL:HA	1.88	0.54
5:E:47:GLY:HA2	5:E:92:PRO:HB2	1.90	0.54
1:A:1659:A:H2'	1:A:1660:G:O4'	2.08	0.54
1:A:1669:A:H2'	1:A:1670:G:C8	2.43	0.54
1:A:2445:U:H2'	1:A:2446:G:C8	2.42	0.54
28:2:2:GLY:O	28:2:6:PRO:HG2	2.08	0.54
1:A:929:A:C8	1:A:930:C:C5	2.96	0.54
14:N:60:ILE:C	14:N:61:ILE:HD12	2.28	0.54
1:A:541:C:O2'	1:A:542:A:H5''	2.07	0.54
6:F:41:LEU:HA	6:F:44:ILE:CG2	2.37	0.54
16:P:35:LYS:O	16:P:40:HIS:NE2	2.41	0.54
1:A:1119:G:H2'	11:K:52:GLN:HE22	1.71	0.54
1:A:1209:C:H2'	1:A:1210:G:C8	2.39	0.54
1:A:2638:G:H5'	37:A:4487:HOH:O	2.07	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:E:129:HIS:HE1	5:E:231:ARG:HA	1.72	0.54
1:A:951:A:H2'	1:A:952:G:H5'	1.88	0.54
2:B:3020:G:O2'	2:B:3021:G:H5'	2.07	0.54
1:A:1351:G:OP1	5:E:96:LYS:NZ	2.35	0.54
4:D:85:ARG:NH1	37:D:8641:HOH:O	2.40	0.54
1:A:2860:G:H1'	37:A:6337:HOH:O	2.08	0.54
13:M:65:ASP:HA	13:M:109:LEU:O	2.07	0.54
14:N:52:LEU:HD21	37:N:8615:HOH:O	2.08	0.54
6:F:99:ASP:HB3	6:F:103:ASN:H	1.72	0.54
2:B:3054:A:O2'	2:B:3055:U:H5'	2.08	0.54
29:3:18:ASN:ND2	29:3:40:ARG:H	2.01	0.54
4:D:254:GLN:HG2	4:D:255:GLY:N	2.23	0.54
1:A:2779:G:H21	7:G:143:GLN:NE2	2.05	0.54
4:D:314:ALA:HB3	4:D:317:PRO:HG3	1.89	0.54
25:Y:43:VAL:HG12	25:Y:44:ASP:N	2.22	0.54
14:N:155:HIS:CE1	14:N:158:ARG:HE	2.26	0.54
14:N:123:ASP:C	14:N:123:ASP:OD1	2.46	0.54
1:A:1504:A:OP2	37:A:7351:HOH:O	2.18	0.54
13:M:13:HIS:NE2	37:M:8521:HOH:O	2.34	0.54
14:N:72:SER:OG	14:N:74:ARG:HB2	2.08	0.54
14:N:39:ARG:HA	14:N:63:VAL:HG22	1.90	0.54
14:N:164:THR:HB	37:N:8520:HOH:O	2.07	0.54
1:A:1182:C:H1'	1:A:1192:A:H8	1.73	0.54
1:A:1118:A:C8	1:A:1118:A:C3'	2.85	0.54
8:H:46:GLU:N	37:H:3461:HOH:O	2.41	0.54
11:K:107:ASN:HD22	11:K:109:TYR:H	1.54	0.54
26:Z:144:ARG:NE	37:Z:8616:HOH:O	2.41	0.54
1:A:2314:G:O2'	1:A:2315:C:H5'	2.07	0.54
30:4:75:GLY:HA2	37:4:8558:HOH:O	2.08	0.54
1:A:1768:C:H2'	1:A:1769:C:O4'	2.07	0.54
1:A:1972:U:H2'	1:A:1973:A:H5'	1.89	0.54
1:A:2089:A:C2'	1:A:2090:G:H5'	2.37	0.54
1:A:534:C:N4	37:A:7113:HOH:O	2.31	0.54
2:B:3023:U:H5''	2:B:3024:U:OP2	2.07	0.54
7:G:69:ILE:HA	7:G:72:MET:HE2	1.90	0.54
6:F:86:THR:O	6:F:90:LEU:HG	2.08	0.54
4:D:251:VAL:HG23	4:D:252:PRO:HD2	1.89	0.54
21:U:48:VAL:CG2	21:U:98:VAL:HA	2.37	0.54
18:R:75:ILE:HD13	18:R:84:ILE:HD11	1.89	0.54
1:A:918:G:C2	1:A:926:A:C2	2.96	0.54
1:A:240:C:H4'	14:N:146:GLN:NE2	2.22	0.54
20:T:29:ASP:OD1	20:T:31:ARG:HG3	2.06	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
24:X:6:GLN:HB2	24:X:26:ILE:CD1	2.37	0.54
1:A:1333:U:H2'	1:A:1334:C:C6	2.43	0.54
1:A:1878:G:C1'	37:A:5666:HOH:O	2.55	0.54
10:J:112:ARG:O	10:J:113:ALA:C	2.46	0.54
13:M:104:ASP:O	13:M:105:TYR:HB3	2.07	0.54
10:J:117:LYS:O	10:J:119:VAL:HG13	2.08	0.54
1:A:652:G:H8	37:A:9583:HOH:O	1.90	0.54
5:E:219:ASN:O	5:E:222:ASP:OD1	2.26	0.53
12:L:74:VAL:CG1	12:L:113:ILE:HG12	2.36	0.53
7:G:81:GLU:HG2	7:G:134:SER:CB	2.35	0.53
13:M:54:PRO:HG2	13:M:57:VAL:CG2	2.38	0.53
18:R:40:HIS:HD2	18:R:60:THR:OG1	1.91	0.53
1:A:1391:G:H2'	1:A:1392:A:H5'	1.91	0.53
16:P:38:ARG:NH1	37:P:7674:HOH:O	2.40	0.53
5:E:236:THR:O	5:E:237:GLU:C	2.46	0.53
10:J:57:ARG:O	10:J:61:LEU:HD22	2.07	0.53
1:A:1119:G:H8	11:K:52:GLN:NE2	2.06	0.53
1:A:877:G:H3'	37:A:9683:HOH:O	2.07	0.53
13:M:143:THR:HG22	13:M:144:ASP:H	1.73	0.53
4:D:307:ARG:HH11	4:D:307:ARG:CG	2.21	0.53
4:D:36:PRO:HA	4:D:168:GLY:HA3	1.90	0.53
4:D:14:GLY:HA2	4:D:15:PRO:C	2.28	0.53
1:A:703:G:O2'	1:A:704:C:H5'	2.08	0.53
2:B:3031:C:O2'	2:B:3032:G:H5'	2.08	0.53
1:A:738:G:H3'	37:A:6584:HOH:O	2.07	0.53
1:A:778:C:C4	1:A:779:U:C4	2.96	0.53
1:A:2862:G:H4'	4:D:336:GLN:O	2.08	0.53
11:K:130:VAL:HG12	11:K:131:THR:N	2.22	0.53
11:K:6:PHE:O	11:K:8:ALA:N	2.41	0.53
1:A:1551:C:O2	1:A:1634:G:N2	2.36	0.53
1:A:2251:G:H2'	1:A:2252:A:C8	2.44	0.53
10:J:72:VAL:HG11	10:J:81:TYR:CZ	2.44	0.53
1:A:2649:A:H8	1:A:2649:A:H5'	1.73	0.53
1:A:2630:G:O6	3:C:206:ARG:NH2	2.42	0.53
3:C:24:LYS:NZ	3:C:47:HIS:O	2.39	0.53
1:A:1299:G:O6	13:M:6:ARG:HD3	2.09	0.53
15:O:34:LEU:HA	15:O:47:LEU:HD23	1.90	0.53
1:A:820:G:C6	3:C:171:LYS:HB2	2.44	0.53
6:F:23:VAL:HG21	6:F:45:THR:HG21	1.90	0.53
1:A:281:U:O2'	1:A:282:C:H5'	2.09	0.53
15:O:151:ASP:HB3	37:O:8528:HOH:O	2.07	0.53
3:C:173:GLY:O	3:C:176:HIS:HB3	2.08	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:3064:C:H2'	2:B:3065:A:H5'	1.90	0.53
6:F:10:PHE:CG	6:F:11:HIS:N	2.76	0.53
1:A:2371:G:H5'	37:A:4565:HOH:O	2.07	0.53
1:A:25:A:H5'	37:A:8713:HOH:O	2.09	0.53
1:A:1636:G:O2'	1:A:1637:A:H5'	2.08	0.53
8:H:34:ASN:O	8:H:38:LYS:HG3	2.08	0.53
10:J:45:GLN:HG3	10:J:135:TRP:NE1	2.24	0.53
15:O:47:LEU:HD13	15:O:97:VAL:HG11	1.91	0.53
37:A:9275:HOH:O	4:D:254:GLN:HG3	2.08	0.53
7:G:31:ARG:NH1	37:G:5919:HOH:O	2.40	0.53
3:C:200:PRO:HG2	3:C:225:VAL:HG21	1.89	0.53
1:A:2329:C:O2'	1:A:2330:U:H5'	2.08	0.53
1:A:2266:A:P	37:A:5407:HOH:O	2.65	0.53
8:H:21:GLU:O	8:H:24:ARG:HG3	2.07	0.53
2:B:3059:C:H5'	37:B:5233:HOH:O	2.08	0.53
1:A:2467:A:H3'	37:A:5005:HOH:O	2.08	0.53
4:D:240:GLY:HA3	37:D:8529:HOH:O	2.07	0.53
1:A:2379:G:H4'	1:A:2380:A:H5''	1.91	0.53
1:A:766:A:H5'	37:A:4212:HOH:O	2.09	0.53
1:A:1066:U:H2'	1:A:1067:A:C8	2.43	0.53
1:A:1168:C:H2'	1:A:1169:U:O4'	2.07	0.53
1:A:1183:C:N4	37:A:3962:HOH:O	2.38	0.53
10:J:59:ASN:ND2	10:J:59:ASN:H	2.06	0.53
37:A:3236:HOH:O	14:N:79:LYS:HD2	2.09	0.53
1:A:1159:G:H21	1:A:1189:A:H8	1.55	0.53
1:A:1874:U:H2'	3:C:120:ARG:HG3	1.90	0.53
10:J:53:PRO:HG3	10:J:127:GLY:H	1.73	0.53
4:D:7:ARG:HG2	4:D:7:ARG:HH11	1.73	0.53
21:U:48:VAL:CG1	21:U:96:VAL:HG13	2.39	0.53
1:A:2089:A:O2'	1:A:2090:G:H5'	2.09	0.53
1:A:1654:U:H2'	3:C:47:HIS:HD2	1.74	0.53
1:A:390:G:N7	37:A:9613:HOH:O	2.34	0.53
1:A:585:C:H6	37:A:5640:HOH:O	1.90	0.53
1:A:175:G:H2'	14:N:192:ALA:HB3	1.90	0.53
1:A:2719:A:C2	4:D:70:PRO:HG3	2.44	0.53
4:D:138:GLY:O	4:D:139:ASP:O	2.26	0.53
12:L:101:ASN:O	12:L:102:GLU:HB2	2.08	0.53
14:N:115:LEU:O	14:N:116:ASN:HB2	2.08	0.53
10:J:163:PRO:O	10:J:164:ALA:HB2	2.08	0.53
1:A:2720:C:O2	12:L:87:ARG:NH2	2.41	0.53
4:D:7:ARG:CD	4:D:9:GLY:O	2.56	0.53
4:D:82:VAL:HG12	4:D:101:TRP:CE3	2.44	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:J:75:SER:C	10:J:79:ALA:HB2	2.29	0.53
30:4:18:GLN:OE1	30:4:73:GLU:HB3	2.08	0.53
1:A:1697:G:H1'	37:A:6813:HOH:O	2.08	0.53
15:O:64:SER:C	15:O:66:LEU:H	2.13	0.53
1:A:1349:G:H5''	37:A:3359:HOH:O	2.08	0.53
27:1:58:GLY:HA3	37:1:8442:HOH:O	2.08	0.53
27:1:19:GLY:O	27:1:23:ARG:HG2	2.09	0.53
1:A:2421:G:H4'	37:A:4339:HOH:O	2.08	0.53
15:O:61:ALA:CB	15:O:88:ALA:HB2	2.39	0.53
1:A:1787:C:H4'	1:A:2883:A:O4'	2.09	0.53
1:A:2382:A:H5'	37:A:4302:HOH:O	2.08	0.53
30:4:11:CYS:HB2	30:4:20:HIS:CE1	2.44	0.53
1:A:1951:G:N2	37:A:5804:HOH:O	2.42	0.53
1:A:2760:C:H5''	37:A:4880:HOH:O	2.08	0.53
27:1:59:HIS:CE1	37:1:8441:HOH:O	2.62	0.53
1:A:2502:C:C4'	10:J:151:MET:HG2	2.38	0.53
1:A:1166:A:H1'	1:A:1192:A:N1	2.23	0.53
2:B:3103:A:O2'	2:B:3104:A:H5'	2.08	0.53
21:U:9:LYS:HE3	21:U:13:ARG:HH11	1.74	0.53
5:E:162:VAL:HG12	5:E:162:VAL:O	2.09	0.53
13:M:24:ALA:HB2	13:M:30:ARG:HD2	1.90	0.53
1:A:514:G:OP1	1:A:514:G:H2'	2.09	0.53
24:X:41:TYR:O	24:X:45:VAL:HG13	2.09	0.53
3:C:95:PRO:HG2	3:C:98:GLU:HG2	1.91	0.53
1:A:371:U:H2'	1:A:372:A:H8	1.74	0.53
10:J:84:ARG:CZ	10:J:135:TRP:HH2	2.21	0.52
1:A:1058:A:H2'	1:A:1060:C:C5'	2.38	0.52
1:A:2405:C:C5'	37:A:6132:HOH:O	2.56	0.52
20:T:29:ASP:OD1	20:T:31:ARG:NH1	2.43	0.52
19:S:114:VAL:O	19:S:114:VAL:HG13	2.08	0.52
1:A:1213:C:O2'	1:A:1214:G:H5'	2.09	0.52
4:D:75:GLU:C	4:D:77:PRO:HD3	2.30	0.52
1:A:453:A:H4'	1:A:455:A:N7	2.24	0.52
1:A:646:G:H2'	1:A:647:U:C6	2.44	0.52
15:O:34:LEU:HD13	15:O:47:LEU:HD21	1.91	0.52
2:B:3006:C:P	15:O:37:ARG:NH1	2.82	0.52
7:G:143:GLN:CG	37:G:2113:HOH:O	2.57	0.52
7:G:143:GLN:HG2	37:G:2113:HOH:O	2.08	0.52
4:D:168:GLY:H	4:D:174:ARG:HD3	1.73	0.52
13:M:73:VAL:HG23	13:M:74:THR:H	1.73	0.52
6:F:58:VAL:HG12	6:F:59:GLY:N	2.24	0.52
11:K:77:GLY:O	11:K:80:LYS:N	2.42	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:111:C:OP1	37:A:3446:HOH:O	2.19	0.52
15:O:80:SER:CB	37:O:8536:HOH:O	2.57	0.52
4:D:55:ASN:HB3	4:D:64:GLY:H	1.74	0.52
7:G:77:THR:OG1	7:G:78:GLU:N	2.41	0.52
26:Z:122:ARG:NH2	37:Z:8533:HOH:O	2.42	0.52
14:N:134:ILE:O	14:N:136:PRO:HD3	2.10	0.52
3:C:217:ARG:CG	3:C:217:ARG:HH11	2.22	0.52
37:A:5737:HOH:O	29:3:44:ARG:HG2	2.09	0.52
19:S:29:LYS:HB3	37:S:8533:HOH:O	2.09	0.52
1:A:834:G:H5''	1:A:835:U:O5'	2.09	0.52
10:J:47:GLU:CB	10:J:133:ILE:CD1	2.84	0.52
17:Q:115:SER:O	17:Q:117:SER:N	2.43	0.52
1:A:1164:U:C4'	1:A:1165:G:OP1	2.51	0.52
6:F:35:ALA:HB1	37:F:3279:HOH:O	2.09	0.52
1:A:2269:C:C2'	1:A:2270:G:H5'	2.39	0.52
1:A:2435:U:H1'	37:A:4978:HOH:O	2.10	0.52
22:V:14:GLU:OE1	22:V:15:PRO:HD2	2.09	0.52
8:H:110:GLU:O	8:H:114:LYS:HG3	2.09	0.52
1:A:159:G:H2'	1:A:175:G:H22	1.73	0.52
1:A:1497:G:H4'	1:A:1627:G:O2'	2.09	0.52
1:A:2724:U:H2'	1:A:2725:G:O4'	2.09	0.52
29:3:48:ASP:O	29:3:49:GLU:HB2	2.09	0.52
24:X:110:GLN:HE21	24:X:110:GLN:HA	1.72	0.52
1:A:1701:A:H4'	1:A:1702:U:C5'	2.39	0.52
1:A:2270:G:H4'	3:C:223:ARG:HH12	1.75	0.52
10:J:13:ALA:HA	10:J:91:HIS:HE1	1.74	0.52
1:A:219:G:O5'	1:A:220:C:H5''	2.09	0.52
1:A:660:A:H4'	1:A:661:G:O5'	2.10	0.52
13:M:90:ARG:NH2	13:M:121:ILE:HD11	2.25	0.52
26:Z:107:PRO:HB3	26:Z:182:PHE:CE2	2.45	0.52
1:A:812:A:H1'	37:A:3527:HOH:O	2.09	0.52
5:E:111:VAL:HB	37:E:8324:HOH:O	2.09	0.52
6:F:166:ILE:HD12	37:F:6326:HOH:O	2.09	0.52
12:L:82:ARG:NH2	12:L:115:ARG:HG2	2.25	0.52
1:A:1969:A:O2'	1:A:1970:G:H5'	2.08	0.52
18:R:28:ARG:HD3	37:R:6206:HOH:O	2.10	0.52
18:R:93:ARG:HH11	18:R:93:ARG:HG3	1.74	0.52
14:N:12:TRP:CE2	14:N:20:ILE:HD11	2.44	0.52
1:A:2119:C:O2'	1:A:2120:U:H5'	2.10	0.52
20:T:57:THR:CG2	20:T:59:ASP:HB2	2.39	0.52
1:A:1701:A:H5''	1:A:1702:U:H3'	1.92	0.52
15:O:182:GLY:N	37:O:8572:HOH:O	2.43	0.52

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:558:C:H2'	1:A:559:U:H5'	1.92	0.52
7:G:11:VAL:CG1	7:G:12:ASP:N	2.71	0.52
2:B:3008:G:P	37:B:5071:HOH:O	2.67	0.52
14:N:59:GLY:HA3	14:N:141:ILE:HD11	1.90	0.52
1:A:201:G:N2	1:A:202:U:C2	2.78	0.52
12:L:34:VAL:HG22	12:L:47:ALA:HB2	1.91	0.52
19:S:18:LEU:HG	19:S:91:LEU:HD13	1.91	0.52
25:Y:43:VAL:CG1	25:Y:47:ALA:HB3	2.39	0.52
16:P:47:ARG:NH1	16:P:47:ARG:HG3	2.23	0.52
21:U:49:GLU:OE2	21:U:97:ARG:HD2	2.09	0.52
1:A:1477:C:H5'	1:A:1868:G:C5'	2.40	0.52
1:A:2540:G:H2'	1:A:2541:U:H5'	1.91	0.52
18:R:33:PHE:N	18:R:71:TYR:OH	2.38	0.52
1:A:1003:U:O2	10:J:90:PHE:HZ	1.92	0.52
24:X:31:HIS:HB3	37:X:5420:HOH:O	2.09	0.52
1:A:1666:C:C2'	1:A:1667:A:C5'	2.88	0.52
7:G:69:ILE:HA	7:G:72:MET:HE3	1.92	0.52
8:H:91:VAL:CG1	8:H:92:GLY:N	2.69	0.52
3:C:36:ASP:HA	3:C:83:GLY:HA3	1.92	0.52
28:2:1:THR:HA	37:2:8411:HOH:O	2.10	0.52
5:E:160:LEU:O	5:E:162:VAL:HG23	2.09	0.52
6:F:11:HIS:C	6:F:13:MET:H	2.13	0.52
3:C:55:VAL:HG22	3:C:68:ILE:O	2.10	0.52
3:C:96:LEU:HD22	3:C:128:LEU:HD13	1.91	0.52
1:A:2483:A:HO2'	1:A:2484:U:H5	1.57	0.52
27:1:39:CYS:HA	27:1:47:LEU:CD1	2.37	0.52
1:A:2487:C:H2'	1:A:2488:A:H5'	1.90	0.52
1:A:1180:U:H2'	1:A:1181:A:O4'	2.10	0.52
10:J:56:ILE:HG21	10:J:61:LEU:HD13	1.92	0.52
5:E:76:ARG:HD3	37:E:8367:HOH:O	2.10	0.52
1:A:1189:A:O2'	1:A:1208:C:H2'	2.10	0.52
13:M:143:THR:CG2	13:M:144:ASP:H	2.23	0.52
6:F:59:GLY:C	6:F:61:PHE:H	2.14	0.52
1:A:849:C:O2'	1:A:850:U:H5'	2.10	0.52
5:E:35:VAL:HG21	5:E:227:GLY:HA2	1.91	0.52
1:A:2563:U:H2'	1:A:2565:C:O5'	2.10	0.52
10:J:62:GLU:O	10:J:66:VAL:HG23	2.10	0.51
15:O:5:ARG:HG3	18:R:18:PRO:HB3	1.92	0.51
3:C:199:HIS:HD2	3:C:201:PHE:H	1.59	0.51
24:X:21:LEU:HB3	24:X:26:ILE:HG12	1.92	0.51
24:X:6:GLN:HA	24:X:52:VAL:HG23	1.91	0.51
5:E:139:VAL:CG1	37:E:8455:HOH:O	2.54	0.51

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
25:Y:15:ARG:NH1	25:Y:15:ARG:HB3	2.21	0.51
6:F:86:THR:HG23	37:F:7477:HOH:O	2.08	0.51
7:G:7:ILE:HD11	7:G:11:VAL:C	2.30	0.51
8:H:105:ALA:CB	37:H:5522:HOH:O	2.56	0.51
1:A:1778:A:H2'	1:A:1779:A:H5'	1.91	0.51
19:S:119:VAL:O	19:S:119:VAL:HG12	2.09	0.51
8:H:117:GLU:C	8:H:119:ARG:H	2.13	0.51
6:F:153:THR:HG22	37:F:5234:HOH:O	2.10	0.51
1:A:1996:U:O2'	1:A:1997:A:H5'	2.10	0.51
10:J:83:PHE:HZ	10:J:146:TRP:HE1	1.56	0.51
1:A:1593:C:OP1	17:Q:117:SER:CB	2.58	0.51
15:O:37:ARG:NH2	37:O:8533:HOH:O	2.44	0.51
1:A:1192:A:H3'	1:A:1193:A:H5'	1.91	0.51
10:J:14:TYR:N	10:J:91:HIS:CE1	2.76	0.51
1:A:952:G:H4'	37:A:3596:HOH:O	2.09	0.51
1:A:2851:G:C2'	1:A:2852:A:H5'	2.40	0.51
23:W:20:LEU:HD22	23:W:60:GLN:HE22	1.75	0.51
1:A:538:C:OP2	26:Z:134:HIS:HE1	1.94	0.51
1:A:2055:A:H5'	19:S:134:SER:HB2	1.92	0.51
1:A:256:C:H2'	1:A:257:G:O4'	2.10	0.51
5:E:43:LYS:NZ	37:E:8392:HOH:O	2.42	0.51
1:A:2570:G:H5''	37:A:4472:HOH:O	2.11	0.51
8:H:39:SER:HB3	8:H:45:ALA:HB2	1.91	0.51
14:N:39:ARG:NE	37:N:8622:HOH:O	2.43	0.51
11:K:45:VAL:HG22	11:K:46:ILE:N	2.24	0.51
4:D:41:PHE:HB3	4:D:190:MET:HE1	1.91	0.51
25:Y:76:ARG:NH1	25:Y:76:ARG:HG3	2.24	0.51
1:A:1332:C:O2'	1:A:1333:U:H5'	2.10	0.51
26:Z:144:ARG:NH2	37:Z:8616:HOH:O	2.42	0.51
19:S:111:ILE:HG23	19:S:145:LEU:HD11	1.92	0.51
21:U:24:ARG:HH21	21:U:39:ASN:HD22	1.57	0.51
1:A:2821:C:H4'	4:D:116:PRO:HB3	1.91	0.51
15:O:170:GLU:O	15:O:174:GLU:HG3	2.10	0.51
1:A:2269:C:H2'	1:A:2270:G:H5'	1.91	0.51
3:C:132:ASP:OD1	3:C:133:ARG:N	2.41	0.51
1:A:1500:U:P	17:Q:41:ARG:HH22	2.33	0.51
37:A:9534:HOH:O	30:4:84:ARG:HB2	2.09	0.51
21:U:28:SER:O	21:U:32:ARG:HG3	2.10	0.51
5:E:39:GLN:O	5:E:43:LYS:HD3	2.11	0.51
1:A:1422:U:H2'	1:A:1423:C:C6	2.45	0.51
8:H:19:ALA:O	8:H:22:VAL:HG22	2.10	0.51
1:A:724:G:O2'	1:A:725:C:H5'	2.11	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
24:X:90:TYR:CE2	24:X:99:ALA:HB2	2.45	0.51
8:H:58:GLU:HA	8:H:61:MET:HG3	1.93	0.51
12:L:27:ARG:HD2	37:L:4747:HOH:O	2.10	0.51
15:O:32:PRO:HD2	15:O:99:GLU:O	2.11	0.51
1:A:1470:A:OP1	14:N:93:ARG:HD2	2.11	0.51
10:J:154:THR:HB	10:J:155:PRO:HD3	1.93	0.51
10:J:150:LYS:HA	10:J:153:VAL:HG22	1.93	0.51
26:Z:187:VAL:HB	37:Z:8572:HOH:O	2.10	0.51
6:F:49:PRO:HG3	37:F:5828:HOH:O	2.09	0.51
6:F:19:GLU:O	6:F:133:ASN:HB3	2.11	0.51
8:H:91:VAL:CG1	8:H:92:GLY:H	2.19	0.51
16:P:47:ARG:NH2	37:P:510:HOH:O	2.43	0.51
4:D:162:MET:HG3	4:D:310:ARG:NH1	2.26	0.51
1:A:1262:C:H1'	24:X:120:PRO:HG3	1.92	0.51
20:T:73:ASP:O	20:T:77:VAL:HG23	2.10	0.51
1:A:1719:G:H1'	37:A:3297:HOH:O	2.10	0.51
14:N:87:MET:SD	37:N:8532:HOH:O	2.59	0.51
14:N:27:ARG:O	14:N:30:GLU:N	2.44	0.51
10:J:26:LYS:HD3	10:J:89:PRO:HG3	1.92	0.51
8:H:28:ALA:CB	8:H:99:THR:HG23	2.40	0.51
7:G:31:ARG:NH1	7:G:68:HIS:CG	2.79	0.51
24:X:26:ILE:O	24:X:26:ILE:CG1	2.58	0.51
17:Q:98:ILE:HD12	17:Q:102:ARG:CZ	2.40	0.51
1:A:516:A:P	37:A:5193:HOH:O	2.67	0.51
1:A:157:G:OP2	37:A:9059:HOH:O	2.19	0.51
3:C:109:GLU:HG2	3:C:116:GLY:H	1.76	0.51
3:C:109:GLU:HG2	3:C:116:GLY:N	2.26	0.51
1:A:440:C:H2'	1:A:441:A:C8	2.46	0.51
1:A:535:G:H8	37:A:4691:HOH:O	1.92	0.51
15:O:43:VAL:HG11	15:O:81:ALA:HA	1.93	0.51
22:V:52:THR:HG22	22:V:54:THR:HB	1.93	0.51
7:G:32:ARG:O	7:G:33:LEU:HD23	2.10	0.51
37:A:5409:HOH:O	11:K:74:ARG:HD3	2.10	0.51
11:K:93:ARG:HB3	11:K:93:ARG:NH1	2.23	0.51
1:A:875:A:C2	3:C:194:MET:SD	3.04	0.51
1:A:1130:U:H5'	37:A:7209:HOH:O	2.10	0.51
12:L:101:ASN:O	12:L:102:GLU:CB	2.59	0.51
15:O:50:LEU:HB2	37:O:8523:HOH:O	2.11	0.51
8:H:79:GLN:HB2	37:H:5498:HOH:O	2.10	0.51
1:A:1882:C:O2'	1:A:2012:U:OP2	2.27	0.51
37:A:4843:HOH:O	24:X:154:ARG:C	2.49	0.51
1:A:1166:A:H61	1:A:1180:U:H3	1.58	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:E:1:MET:HG2	5:E:2:GLN:N	2.24	0.51
1:A:283:U:H5''	1:A:284:C:OP2	2.11	0.51
1:A:1189:A:H1'	1:A:1209:C:C1'	2.41	0.51
30:4:7:PHE:HE2	30:4:22:VAL:CG2	2.23	0.51
1:A:2256:G:H2'	1:A:2257:G:C5'	2.41	0.51
13:M:134:GLU:HA	13:M:138:GLY:O	2.11	0.51
1:A:929:A:O5'	1:A:929:A:H8	1.93	0.51
1:A:449:A:N7	5:E:43:LYS:HG2	2.26	0.51
1:A:1850:U:H2'	1:A:1851:G:H8	1.75	0.51
10:J:129:ASN:HD22	10:J:129:ASN:N	2.09	0.51
1:A:303:C:O2'	1:A:304:G:H5'	2.11	0.51
10:J:130:HIS:CG	10:J:133:ILE:HD11	2.45	0.51
14:N:35:PRO:HD2	14:N:38:VAL:HG21	1.92	0.51
1:A:962:C:C1'	15:O:5:ARG:NH1	2.66	0.51
10:J:139:ASP:OD2	37:J:8394:HOH:O	2.19	0.51
1:A:2459:G:C8	37:A:6544:HOH:O	2.54	0.51
1:A:402:U:H2'	1:A:403:C:C6	2.45	0.51
1:A:130:C:H5'	37:A:4768:HOH:O	2.10	0.51
6:F:44:ILE:HG12	6:F:83:PHE:HE1	1.74	0.50
5:E:246:ARG:NH2	37:E:8430:HOH:O	2.43	0.50
4:D:27:ASN:HD22	4:D:27:ASN:H	1.57	0.50
1:A:1044:C:H5''	37:A:8623:HOH:O	2.10	0.50
1:A:2909:G:O2'	1:A:2910:A:H5'	2.12	0.50
1:A:894:A:C2	5:E:87:ARG:NH2	2.79	0.50
15:O:176:ARG:O	15:O:180:LEU:HG	2.11	0.50
15:O:139:TRP:HA	15:O:139:TRP:CE3	2.46	0.50
1:A:138:U:H5''	1:A:139:C:OP2	2.11	0.50
1:A:2623:G:O2'	1:A:2624:A:H5'	2.10	0.50
1:A:1921:A:C6	1:A:1922:A:C2	2.99	0.50
1:A:2866:U:H4'	1:A:2867:G:H5'	1.93	0.50
1:A:820:G:C5	3:C:171:LYS:HB2	2.47	0.50
1:A:1495:C:H1'	1:A:1573:A:H1'	1.93	0.50
1:A:2314:G:H2'	1:A:2315:C:H5'	1.92	0.50
1:A:1483:C:O2'	1:A:1484:G:H5'	2.11	0.50
5:E:150:THR:HA	5:E:203:ALA:O	2.11	0.50
5:E:132:ASP:HB3	37:E:8363:HOH:O	2.09	0.50
8:H:101:ALA:HB2	8:H:108:LEU:HD22	1.93	0.50
14:N:114:VAL:HG21	14:N:159:THR:CG2	2.40	0.50
1:A:1250:C:O2'	1:A:1251:C:H5'	2.12	0.50
4:D:204:GLY:C	37:D:8660:HOH:O	2.49	0.50
1:A:2694:A:H4'	7:G:91:PHE:HE1	1.76	0.50
1:A:1444:G:O2'	1:A:1445:G:H5'	2.11	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
37:B:7568:HOH:O	15:O:107:ASN:HB3	2.11	0.50
16:P:44:ASN:HA	16:P:65:LEU:O	2.11	0.50
37:A:7083:HOH:O	4:D:2:GLN:HG3	2.10	0.50
1:A:317:A:H5''	21:U:52:ARG:HD2	1.92	0.50
17:Q:7:LYS:CD	17:Q:21:VAL:CG2	2.90	0.50
21:U:32:ARG:NH1	21:U:38:ARG:HH12	2.10	0.50
13:M:72:ASN:O	13:M:76:LEU:HG	2.11	0.50
21:U:77:VAL:HB	37:U:4584:HOH:O	2.11	0.50
1:A:2815:G:H2'	37:A:5264:HOH:O	2.09	0.50
1:A:2598:U:H5''	12:L:36:GLY:HA2	1.93	0.50
23:W:12:THR:CG2	23:W:15:GLU:HG3	2.30	0.50
1:A:2004:U:H2'	1:A:2004:U:O2	2.11	0.50
19:S:96:VAL:HG13	19:S:106:GLY:HA3	1.93	0.50
26:Z:154:ARG:HH12	26:Z:155:ARG:HG3	1.75	0.50
1:A:2911:C:H2'	1:A:2912:C:C6	2.47	0.50
1:A:1172:G:H1'	37:A:4531:HOH:O	2.11	0.50
1:A:2368:A:N6	15:O:18:THR:O	2.45	0.50
14:N:154:ARG:CZ	37:N:8642:HOH:O	2.59	0.50
1:A:702:G:O2'	1:A:703:G:H5'	2.12	0.50
29:3:49:GLU:O	37:3:131:HOH:O	2.19	0.50
14:N:65:VAL:HG21	14:N:105:ALA:HB2	1.94	0.50
3:C:135:VAL:HG21	3:C:147:ARG:NH1	2.26	0.50
4:D:8:LYS:HG3	4:D:220:VAL:HG12	1.92	0.50
27:1:47:LEU:CD2	27:1:57:CYS:HB2	2.41	0.50
24:X:90:TYR:N	24:X:90:TYR:CD1	2.79	0.50
6:F:41:LEU:CA	6:F:44:ILE:HG22	2.40	0.50
1:A:431:G:P	14:N:48:ARG:HH12	2.34	0.50
25:Y:9:VAL:HG13	25:Y:88:GLU:OE2	2.12	0.50
5:E:168:ARG:NH2	5:E:190:ALA:O	2.44	0.50
14:N:95:LYS:HG2	14:N:99:ARG:HB3	1.92	0.50
1:A:1595:G:O2'	1:A:1596:U:H5'	2.11	0.50
19:S:132:ARG:NH1	37:S:8558:HOH:O	2.43	0.50
20:T:29:ASP:CG	20:T:31:ARG:NH1	2.65	0.50
6:F:11:HIS:O	6:F:12:GLU:HB3	2.11	0.50
1:A:2904:U:H4'	25:Y:8:ARG:NH1	2.26	0.50
5:E:237:GLU:HB2	37:E:8437:HOH:O	2.11	0.50
14:N:63:VAL:O	14:N:130:GLU:HA	2.12	0.50
1:A:1205:U:C2'	1:A:1206:U:C5'	2.89	0.50
1:A:2467:A:P	37:A:8640:HOH:O	2.63	0.50
1:A:338:C:H4'	5:E:174:ILE:HD12	1.92	0.50
14:N:122:GLU:OE2	14:N:127:LYS:HE2	2.12	0.50
1:A:677:C:H4'	5:E:246:ARG:NH2	2.27	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:661:G:C4	1:A:686:A:C2	3.00	0.50
1:A:1525:G:H5'	1:A:1526:A:OP2	2.12	0.50
2:B:3091:C:H2'	2:B:3092:G:O4'	2.11	0.50
1:A:1804:A:H2'	1:A:1805:G:C8	2.45	0.50
4:D:234:ARG:NH1	37:D:8623:HOH:O	2.44	0.50
1:A:2036:C:OP1	37:A:6235:HOH:O	2.20	0.50
10:J:132:PHE:O	10:J:133:ILE:HD13	2.11	0.50
14:N:35:PRO:CG	14:N:38:VAL:CG2	2.81	0.50
25:Y:72:VAL:HG22	25:Y:85:VAL:CG1	2.41	0.50
4:D:320:GLN:HG3	4:D:321:PRO:HD2	1.93	0.50
1:A:797:A:H5'	27:1:10:ARG:HG2	1.94	0.50
1:A:1942:A:O2'	1:A:1943:C:H5'	2.12	0.50
8:H:50:VAL:CG1	8:H:60:VAL:HG11	2.42	0.50
2:B:3008:G:O6	15:O:11:ARG:NH1	2.44	0.50
17:Q:13:VAL:HG11	17:Q:40:VAL:CG1	2.41	0.50
27:1:50:ALA:HB3	27:1:54:ILE:HG22	1.93	0.50
1:A:1654:U:H2'	3:C:47:HIS:CD2	2.47	0.50
1:A:514:G:O5'	1:A:514:G:H8	1.95	0.50
1:A:1828:G:H2'	1:A:1829:A:H5'	1.92	0.50
3:C:13:THR:HB	37:C:8543:HOH:O	2.12	0.50
10:J:26:LYS:HD2	10:J:28:ILE:CG1	2.41	0.50
1:A:1056:U:H2'	1:A:1057:A:O4'	2.12	0.50
14:N:80:GLY:O	14:N:81:ARG:HD3	2.12	0.50
3:C:93:THR:C	3:C:94:LEU:HD23	2.32	0.50
13:M:53:ARG:NH2	13:M:57:VAL:CG1	2.75	0.50
1:A:168:C:C2'	1:A:169:A:H5'	2.41	0.50
1:A:1503:U:H2'	1:A:1504:A:O4'	2.12	0.50
8:H:79:GLN:HG3	8:H:82:ASP:OD2	2.11	0.50
1:A:710:G:OP1	16:P:24:ALA:HB3	2.12	0.50
37:A:4634:HOH:O	4:D:216:LYS:HA	2.11	0.50
14:N:61:ILE:N	14:N:61:ILE:HD12	2.27	0.49
15:O:87:LEU:CD1	15:O:186:LEU:HD21	2.36	0.49
22:V:52:THR:HG22	22:V:54:THR:H	1.77	0.49
5:E:246:ARG:CB	5:E:246:ARG:HH11	2.24	0.49
37:A:3328:HOH:O	21:U:9:LYS:CD	2.59	0.49
5:E:25:PRO:HD2	37:E:8435:HOH:O	2.11	0.49
2:B:3042:C:H2'	37:B:6700:HOH:O	2.12	0.49
14:N:68:ARG:CD	14:N:68:ARG:O	2.59	0.49
2:B:3029:C:C2'	2:B:3030:C:H5'	2.42	0.49
24:X:149:LEU:HG	24:X:153:MET:CE	2.42	0.49
21:U:38:ARG:HG3	21:U:38:ARG:HH11	1.76	0.49
1:A:78:G:C6	1:A:79:G:C6	3.00	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
21:U:50:VAL:HG12	21:U:56:ALA:HA	1.93	0.49
10:J:59:ASN:ND2	10:J:59:ASN:N	2.57	0.49
10:J:141:ASN:CA	37:J:8367:HOH:O	2.45	0.49
27:1:30:GLU:O	27:1:33:HIS:HB3	2.12	0.49
19:S:18:LEU:HB2	19:S:143:VAL:CG1	2.41	0.49
3:C:36:ASP:O	3:C:38:ILE:N	2.45	0.49
1:A:2321:A:O2'	1:A:2322:U:H3'	2.12	0.49
16:P:14:LEU:CD2	16:P:102:ILE:HD11	2.42	0.49
1:A:1896:G:H1'	37:A:3823:HOH:O	2.11	0.49
22:V:33:SER:O	22:V:37:GLU:HG3	2.12	0.49
6:F:27:ILE:HG22	6:F:28:GLY:N	2.21	0.49
4:D:240:GLY:HA3	37:D:8662:HOH:O	2.12	0.49
1:A:220:C:P	37:A:5602:HOH:O	2.69	0.49
1:A:1268:C:H2'	1:A:1269:G:H8	1.77	0.49
3:C:194:MET:HE1	37:C:8517:HOH:O	2.11	0.49
14:N:59:GLY:C	14:N:141:ILE:HD11	2.33	0.49
6:F:57:THR:HG23	6:F:63:ILE:CB	2.42	0.49
30:4:17:HIS:O	30:4:18:GLN:HG3	2.12	0.49
1:A:2756:U:H3	1:A:2896:A:H2	1.56	0.49
1:A:159:G:H2'	1:A:175:G:N2	2.26	0.49
1:A:371:U:H2'	1:A:372:A:C8	2.48	0.49
2:B:3096:C:H2'	2:B:3097:U:C6	2.47	0.49
1:A:95:A:H5''	1:A:97:G:O4'	2.12	0.49
14:N:52:LEU:HD13	14:N:116:ASN:CB	2.42	0.49
27:1:59:HIS:HA	37:1:8444:HOH:O	2.12	0.49
1:A:2763:G:OP1	12:L:9:THR:OG1	2.19	0.49
14:N:114:VAL:HB	14:N:159:THR:HG23	1.95	0.49
6:F:84:LEU:C	6:F:86:THR:H	2.15	0.49
15:O:11:ARG:O	15:O:15:GLU:HG3	2.12	0.49
5:E:84:VAL:O	5:E:85:LYS:CB	2.59	0.49
1:A:1127:C:C5	1:A:1128:U:C4	2.99	0.49
21:U:20:HIS:ND1	21:U:41:ARG:NE	2.56	0.49
24:X:142:ASP:HB3	24:X:145:GLY:H	1.76	0.49
5:E:20:ASP:O	5:E:23:GLU:HB2	2.13	0.49
1:A:1052:G:H2'	1:A:1052:G:N3	2.26	0.49
1:A:394:G:H1	14:N:181:GLU:CD	2.16	0.49
5:E:104:ASP:O	5:E:108:GLN:HG3	2.13	0.49
6:F:23:VAL:CG2	6:F:23:VAL:O	2.59	0.49
4:D:43:GLY:O	4:D:308:LEU:HD12	2.12	0.49
2:B:3042:C:O2	6:F:76:ARG:NH1	2.45	0.49
1:A:2271:G:H2'	1:A:2271:G:N3	2.27	0.49
1:A:2064:U:H2'	1:A:2065:C:H6	1.78	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
22:V:49:LEU:CD1	37:V:3805:HOH:O	2.60	0.49
4:D:1:PRO:O	4:D:2:GLN:HB2	2.12	0.49
1:A:737:A:H2'	1:A:738:G:O4'	2.12	0.49
2:B:3092:G:H2'	2:B:3093:A:C8	2.47	0.49
1:A:1717:A:H5''	17:Q:54:LYS:HB2	1.94	0.49
5:E:65:ARG:HG3	5:E:67:GLN:HB2	1.95	0.49
14:N:39:ARG:NH2	37:N:8622:HOH:O	2.46	0.49
23:W:12:THR:HG23	23:W:14:ALA:H	1.76	0.49
19:S:39:THR:CG2	19:S:42:GLU:HG3	2.42	0.49
1:A:1334:C:H2'	1:A:1335:C:H6	1.76	0.49
1:A:952:G:OP1	18:R:42:LYS:HE2	2.12	0.49
26:Z:115:ARG:CZ	37:Z:8556:HOH:O	2.61	0.49
30:4:73:GLU:HB3	37:4:8559:HOH:O	2.12	0.49
1:A:88:G:N7	29:3:28:LYS:HD2	2.27	0.49
2:B:3031:C:H2'	2:B:3032:G:O4'	2.12	0.49
17:Q:27:ARG:HA	37:Q:3969:HOH:O	2.12	0.49
1:A:432:G:O2'	1:A:433:C:H5'	2.12	0.49
1:A:2777:G:O2'	1:A:2778:A:H5'	2.12	0.49
12:L:76:GLN:HB2	37:L:1433:HOH:O	2.13	0.49
1:A:2533:C:H6	1:A:2533:C:C5'	2.18	0.49
1:A:544:G:H2'	1:A:545:G:C5'	2.43	0.49
1:A:418:C:OP2	37:A:5329:HOH:O	2.19	0.49
1:A:1730:G:H5'	1:A:1731:C:C6	2.47	0.49
1:A:1644:C:C2	1:A:1645:U:C6	3.01	0.49
1:A:1592:G:O2'	1:A:1593:C:O4'	2.29	0.49
17:Q:115:SER:HG	17:Q:118:GLN:HG3	1.76	0.49
6:F:99:ASP:O	6:F:159:PRO:HG3	2.12	0.49
24:X:139:GLY:O	24:X:141:HIS:HD2	1.95	0.49
1:A:2812:A:C2	1:A:2814:A:N6	2.74	0.49
4:D:304:PRO:HD2	4:D:307:ARG:HD2	1.95	0.49
14:N:68:ARG:O	14:N:68:ARG:CG	2.58	0.49
1:A:2276:U:H2'	1:A:2277:U:H6	1.78	0.49
17:Q:38:GLU:N	37:Q:3178:HOH:O	2.43	0.49
37:A:7217:HOH:O	14:N:154:ARG:HB2	2.12	0.49
6:F:65:GLU:HA	37:F:6752:HOH:O	2.11	0.49
2:B:3041:C:C6	6:F:50:VAL:HG21	2.48	0.49
1:A:2403:C:H5'	37:A:5571:HOH:O	2.13	0.49
1:A:775:G:OP1	28:2:16:HIS:HE1	1.96	0.49
1:A:2256:G:O2'	1:A:2257:G:H5'	2.12	0.49
30:4:91:GLN:O	30:4:92:GLU:HB2	2.12	0.49
30:4:81:GLU:HB2	37:4:8540:HOH:O	2.11	0.49
16:P:88:LYS:HB3	37:P:7061:HOH:O	2.12	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
17:Q:83:LYS:NZ	37:Q:6315:HOH:O	2.45	0.49
1:A:2121:G:C2'	1:A:2122:C:H5'	2.42	0.49
1:A:1151:G:OP1	9:I:63:ARG:NH1	2.46	0.49
19:S:39:THR:CB	19:S:42:GLU:HG3	2.43	0.49
1:A:625:U:H5''	1:A:1044:C:N4	2.27	0.49
1:A:1773:G:O2'	27:1:15:GLY:HA2	2.12	0.49
12:L:125:ALA:C	12:L:127:ALA:H	2.16	0.49
1:A:84:G:O2'	1:A:85:C:H5'	2.13	0.49
8:H:13:GLU:OE2	8:H:78:GLU:HG2	2.12	0.49
26:Z:136:LYS:HE2	26:Z:138:ARG:NH1	2.28	0.49
1:A:903:U:C2	13:M:11:ARG:O	2.66	0.49
1:A:2115:U:H2'	1:A:2116:U:C6	2.48	0.49
1:A:1825:U:O2'	1:A:1826:C:H5'	2.13	0.49
6:F:99:ASP:HB2	6:F:103:ASN:H	1.78	0.49
1:A:2488:A:H2	37:A:6812:HOH:O	1.96	0.49
1:A:1594:C:O2'	1:A:1607:A:H4'	2.13	0.49
3:C:186:TRP:CG	3:C:187:PRO:HA	2.48	0.49
21:U:41:ARG:HG2	21:U:41:ARG:HH11	1.78	0.49
1:A:644:G:H5'	1:A:644:G:N3	2.28	0.49
1:A:1618:G:H5'	37:A:3540:HOH:O	2.12	0.49
6:F:36:ASN:HA	37:F:7500:HOH:O	2.13	0.49
10:J:166:ASN:N	10:J:166:ASN:ND2	2.61	0.48
15:O:90:LEU:HB2	15:O:186:LEU:HD22	1.94	0.48
12:L:75:ARG:CZ	37:L:4172:HOH:O	2.60	0.48
1:A:558:C:H2'	1:A:559:U:H5''	1.94	0.48
27:1:38:LYS:HG3	37:1:8431:HOH:O	2.11	0.48
1:A:760:G:C6	1:A:894:A:N6	2.81	0.48
26:Z:99:ALA:HB2	26:Z:233:TYR:CE2	2.48	0.48
1:A:858:U:H2'	1:A:859:C:C6	2.47	0.48
1:A:224:U:H1'	37:A:9469:HOH:O	2.12	0.48
14:N:74:ARG:HD3	14:N:91:ILE:HD12	1.94	0.48
1:A:1164:U:O4'	1:A:1165:G:OP1	2.30	0.48
5:E:127:ARG:HG2	5:E:127:ARG:NH1	2.26	0.48
17:Q:98:ILE:CD1	17:Q:102:ARG:NE	2.76	0.48
1:A:1249:U:H2'	1:A:1250:C:H6	1.76	0.48
24:X:13:MET:HE3	24:X:17:ILE:CG2	2.43	0.48
1:A:1819:G:H2'	1:A:1820:G:C5'	2.43	0.48
1:A:739:G:N7	37:A:7079:HOH:O	2.45	0.48
27:1:51:GLY:HA3	37:1:8416:HOH:O	2.12	0.48
1:A:2672:C:O2'	1:A:2673:U:H5'	2.13	0.48
5:E:154:VAL:O	5:E:158:GLU:HG3	2.13	0.48
4:D:119:HIS:O	4:D:121:PRO:HD3	2.12	0.48

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2015:A:H2'	1:A:2016:U:O4'	2.13	0.48
10:J:84:ARG:CZ	10:J:135:TRP:CH2	2.97	0.48
1:A:821:U:O2'	1:A:822:C:H5'	2.13	0.48
1:A:2781:U:H1'	7:G:139:GLU:OE2	2.13	0.48
7:G:3:VAL:HG22	7:G:49:ILE:HB	1.95	0.48
13:M:148:GLU:CG	37:M:8556:HOH:O	2.60	0.48
1:A:1306:U:OP1	5:E:184:ARG:HD2	2.14	0.48
1:A:506:G:H22	1:A:509:A:H5''	1.75	0.48
4:D:205:VAL:O	4:D:307:ARG:NE	2.46	0.48
1:A:2898:G:O2'	1:A:2899:A:H5'	2.13	0.48
24:X:119:HIS:CD2	24:X:120:PRO:O	2.65	0.48
1:A:2649:A:C8	1:A:2649:A:H5'	2.48	0.48
10:J:144:GLU:OE1	10:J:144:GLU:HA	2.13	0.48
37:A:5165:HOH:O	17:Q:55:LYS:HA	2.12	0.48
1:A:164:G:N7	37:A:3207:HOH:O	2.35	0.48
16:P:77:ALA:HA	16:P:96:VAL:O	2.13	0.48
1:A:2713:G:O2'	1:A:2714:U:H5'	2.12	0.48
1:A:920:C:H4'	1:A:921:G:N2	2.28	0.48
5:E:76:ARG:HG2	5:E:78:ARG:NH1	2.27	0.48
29:3:40:ARG:HH11	29:3:40:ARG:HG2	1.78	0.48
11:K:131:THR:HG22	11:K:133:GLY:N	2.28	0.48
9:I:63:ARG:O	9:I:67:LEU:HG	2.13	0.48
11:K:77:GLY:O	11:K:78:ILE:C	2.50	0.48
1:A:2432:C:Cl'	37:A:3646:HOH:O	2.62	0.48
1:A:251:C:H1'	14:N:58:GLN:HE22	1.77	0.48
4:D:2:GLN:CD	37:D:8625:HOH:O	2.50	0.48
1:A:2672:C:H1'	37:D:8641:HOH:O	2.13	0.48
1:A:2598:U:O2	1:A:2600:A:H8	1.96	0.48
14:N:174:ARG:HG3	37:N:8522:HOH:O	2.13	0.48
3:C:97:ALA:HB2	3:C:150:PRO:HB2	1.94	0.48
8:H:27:GLY:HA3	37:H:5413:HOH:O	2.14	0.48
20:T:37:VAL:O	20:T:41:VAL:HG23	2.13	0.48
1:A:2594:C:O2'	1:A:2595:U:H5'	2.13	0.48
37:A:4843:HOH:O	24:X:122:ARG:NH2	2.46	0.48
2:B:3057:A:C8	6:F:141:VAL:HG21	2.49	0.48
22:V:52:THR:CG2	22:V:54:THR:HB	2.44	0.48
8:H:47:LEU:HB2	8:H:108:LEU:HD11	1.96	0.48
6:F:146:LYS:NZ	15:O:107:ASN:ND2	2.60	0.48
6:F:146:LYS:HZ3	15:O:107:ASN:HD21	1.60	0.48
1:A:92:G:H4'	23:W:44:GLY:HA3	1.95	0.48
15:O:141:ARG:HB3	37:O:8571:HOH:O	2.13	0.48
1:A:2084:C:O2'	1:A:2085:A:H5'	2.14	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:305:A:C5	1:A:329:A:C2	3.01	0.48
1:A:1982:C:OP2	37:A:3844:HOH:O	2.20	0.48
1:A:2044:G:OP1	25:Y:23:HIS:HE1	1.96	0.48
1:A:1653:A:N6	37:A:3828:HOH:O	2.46	0.48
14:N:55:LYS:O	14:N:60:ILE:HD12	2.13	0.48
27:1:10:ARG:HG3	27:1:11:THR:N	2.29	0.48
5:E:133:ARG:NH2	37:E:8432:HOH:O	2.47	0.48
1:A:317:A:C2	1:A:337:A:C5	3.01	0.48
21:U:38:ARG:HG3	21:U:38:ARG:NH1	2.28	0.48
6:F:59:GLY:O	6:F:61:PHE:N	2.36	0.48
15:O:33:ARG:NH1	15:O:103:ASP:OD2	2.42	0.48
1:A:1862:C:H1'	37:A:6753:HOH:O	2.14	0.48
1:A:1292:G:HO2'	1:A:1293:U:H6	1.61	0.48
1:A:1592:G:O2'	1:A:1593:C:O5'	2.31	0.48
12:L:37:TYR:CE2	12:L:45:PRO:HA	2.48	0.48
1:A:1666:C:O2'	1:A:1667:A:C5'	2.57	0.48
13:M:146:GLY:C	13:M:148:GLU:H	2.17	0.48
26:Z:117:LEU:HD12	26:Z:174:VAL:CG1	2.44	0.48
21:U:48:VAL:HG11	21:U:96:VAL:CG1	2.44	0.48
4:D:76:THR:N	4:D:77:PRO:HD3	2.29	0.48
22:V:31:PHE:CG	22:V:37:GLU:HG2	2.49	0.48
1:A:1862:C:C2'	1:A:1863:G:H5'	2.44	0.48
1:A:2783:A:H3'	37:A:4786:HOH:O	2.12	0.48
20:T:32:ALA:HA	20:T:36:GLU:OE1	2.13	0.48
1:A:870:G:C3'	1:A:871:G:H5''	2.44	0.48
15:O:91:ARG:HG3	15:O:186:LEU:HD23	1.96	0.48
1:A:1189:A:H1'	1:A:1209:C:H1'	1.96	0.48
37:A:3328:HOH:O	21:U:9:LYS:HD2	2.11	0.48
24:X:76:ASP:O	24:X:77:ALA:O	2.32	0.48
1:A:512:G:O3'	1:A:513:A:H8	1.97	0.48
24:X:38:THR:HG22	24:X:39:ASP:H	1.79	0.48
1:A:1669:A:H2'	1:A:1670:G:H8	1.79	0.48
20:T:29:ASP:OD2	20:T:31:ARG:NH1	2.46	0.48
5:E:49:ASP:HB3	5:E:52:ALA:HB2	1.95	0.48
1:A:1173:A:H2'	37:A:3911:HOH:O	2.14	0.48
1:A:128:A:H3'	1:A:128:A:C8	2.48	0.48
2:B:3051:A:H5'	15:O:160:SER:HB3	1.96	0.48
16:P:32:ARG:HB2	37:P:4656:HOH:O	2.13	0.48
10:J:118:PRO:HD2	37:J:8339:HOH:O	2.14	0.48
1:A:2118:A:O2'	1:A:2119:C:H5'	2.14	0.48
7:G:86:VAL:CG1	7:G:129:GLU:HA	2.44	0.48
1:A:1407:A:O2'	1:A:1408:U:H3'	2.13	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:379:G:OP1	37:A:9129:HOH:O	2.20	0.48
3:C:168:PRO:O	3:C:170:VAL:HG23	2.14	0.48
10:J:46:VAL:O	10:J:146:TRP:CH2	2.63	0.48
1:A:2721:U:H4'	12:L:87:ARG:HG3	1.96	0.48
5:E:107:ARG:CB	5:E:107:ARG:HH11	2.27	0.48
1:A:1666:C:C2'	1:A:1667:A:H5'	2.42	0.48
15:O:58:LEU:CD1	15:O:58:LEU:N	2.77	0.48
1:A:2780:C:H2'	1:A:2781:U:C6	2.49	0.48
1:A:2781:U:H2'	1:A:2782:G:H5'	1.95	0.48
1:A:559:U:H2'	1:A:560:C:O4'	2.14	0.48
7:G:11:VAL:HG12	7:G:12:ASP:H	1.79	0.48
1:A:1333:U:H2'	1:A:1334:C:H6	1.79	0.48
4:D:162:MET:HG3	4:D:310:ARG:CZ	2.44	0.48
1:A:177:A:H2'	1:A:178:U:O4'	2.14	0.48
1:A:1269:G:H2'	1:A:1270:U:H6	1.78	0.48
24:X:13:MET:CE	24:X:17:ILE:HG22	2.43	0.48
13:M:140:VAL:O	13:M:140:VAL:HG12	2.13	0.48
16:P:10:LEU:HD13	16:P:99:GLU:HG3	1.96	0.48
1:A:837:U:H4'	37:A:9970:HOH:O	2.12	0.48
1:A:542:A:H1'	37:A:4236:HOH:O	2.13	0.47
15:O:37:ARG:CZ	37:O:8533:HOH:O	2.62	0.47
10:J:57:ARG:C	10:J:59:ASN:N	2.66	0.47
1:A:1733:A:H4'	4:D:212:GLN:HA	1.95	0.47
1:A:2781:U:C2'	1:A:2782:G:H5'	2.44	0.47
1:A:21:G:H5''	19:S:1:GLY:O	2.14	0.47
1:A:220:C:O5'	37:A:5602:HOH:O	2.20	0.47
6:F:95:THR:OG1	6:F:174:VAL:HG22	2.14	0.47
19:S:22:GLN:HA	19:S:139:PRO:O	2.14	0.47
6:F:144:ARG:NH2	37:F:3839:HOH:O	2.43	0.47
16:P:80:ASP:OD1	16:P:81:PHE:N	2.46	0.47
1:A:1907:U:O2	1:A:1933:G:C2	2.67	0.47
10:J:157:ILE:CG2	10:J:158:ASN:N	2.76	0.47
15:O:47:LEU:CD1	15:O:97:VAL:HG11	2.43	0.47
1:A:920:C:H5''	1:A:921:G:O5'	2.13	0.47
17:Q:143:ALA:HA	37:Q:5521:HOH:O	2.14	0.47
1:A:1060:C:H6	1:A:1060:C:H5'	1.79	0.47
14:N:173:LEU:HD23	14:N:183:VAL:CG1	2.43	0.47
1:A:907:A:H4'	1:A:1328:A:C2	2.49	0.47
1:A:187:A:H3'	1:A:188:C:H6	1.79	0.47
15:O:154:LEU:HG	15:O:155:GLU:H	1.79	0.47
15:O:154:LEU:O	15:O:155:GLU:CB	2.63	0.47
4:D:243:ASN:HA	4:D:244:PRO:C	2.34	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:M:149:ARG:N	37:M:8575:HOH:O	2.47	0.47
16:P:25:VAL:HG23	16:P:26:TRP:H	1.79	0.47
5:E:95:GLU:N	5:E:95:GLU:OE1	2.44	0.47
1:A:417:G:P	37:A:6953:HOH:O	2.71	0.47
1:A:2830:U:H3'	37:A:4782:HOH:O	2.12	0.47
1:A:1555:G:H4'	1:A:1630:A:H2	1.79	0.47
14:N:55:LYS:O	14:N:57:LYS:N	2.47	0.47
1:A:2004:U:H5''	1:A:2005:G:C8	2.49	0.47
1:A:1242:A:H5'	11:K:82:THR:CG2	2.33	0.47
6:F:35:ALA:O	6:F:37:ALA:N	2.47	0.47
12:L:14:LYS:HB2	12:L:45:PRO:CG	2.37	0.47
12:L:109:LEU:HD13	12:L:113:ILE:HD11	1.96	0.47
37:B:4707:HOH:O	15:O:147:ILE:HD12	2.14	0.47
37:A:6563:HOH:O	3:C:211:LYS:HG2	2.13	0.47
14:N:186:SER:OG	14:N:189:VAL:HG12	2.14	0.47
13:M:143:THR:HG21	37:M:8543:HOH:O	2.14	0.47
7:G:7:ILE:HG22	7:G:45:ASP:O	2.14	0.47
1:A:445:U:H1'	37:A:6872:HOH:O	2.14	0.47
5:E:178:GLN:C	5:E:180:SER:N	2.66	0.47
14:N:149:TRP:O	14:N:152:ARG:HG2	2.13	0.47
1:A:2079:G:C6	1:A:2080:G:C6	3.02	0.47
19:S:40:ALA:O	19:S:44:VAL:HG23	2.14	0.47
1:A:2445:U:H2'	1:A:2446:G:H8	1.76	0.47
5:E:147:LEU:HA	37:E:8421:HOH:O	2.15	0.47
1:A:10:U:H5'	37:A:5583:HOH:O	2.14	0.47
1:A:278:A:H2'	1:A:279:C:O4'	2.15	0.47
1:A:1677:U:OP2	29:3:8:LYS:NZ	2.46	0.47
29:3:39:ARG:NH1	37:3:6391:HOH:O	2.48	0.47
1:A:2435:U:P	30:4:28:GLY:HA3	2.54	0.47
4:D:53:LEU:HD21	4:D:270:ILE:HD12	1.96	0.47
1:A:2459:G:OP1	30:4:64:LYS:N	2.25	0.47
3:C:94:LEU:HG	3:C:99:ILE:CD1	2.44	0.47
8:H:110:GLU:HA	8:H:113:ASP:OD2	2.15	0.47
1:A:154:C:H2'	1:A:155:C:C6	2.45	0.47
7:G:9:GLU:HG3	7:G:10:ASP:N	2.29	0.47
1:A:2831:C:H2'	1:A:2832:C:H5'	1.97	0.47
1:A:814:G:H4'	37:A:9704:HOH:O	2.14	0.47
1:A:1545:C:H2'	1:A:1546:G:O4'	2.14	0.47
10:J:26:LYS:CD	10:J:28:ILE:HB	2.44	0.47
11:K:19:MET:CE	11:K:132:LEU:CD1	2.90	0.47
11:K:52:GLN:HG3	11:K:53:ILE:N	2.29	0.47
1:A:2420:G:H4'	37:A:3662:HOH:O	2.15	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:88:ILE:CD1	3:C:100:PRO:HD3	2.38	0.47
1:A:840:U:H2'	19:S:128:ARG:NH1	2.30	0.47
37:A:8906:HOH:O	27:1:16:PRO:HG3	2.14	0.47
1:A:1819:G:H2'	1:A:1820:G:C4'	2.45	0.47
4:D:54:VAL:O	4:D:55:ASN:C	2.52	0.47
26:Z:186:ARG:NH1	26:Z:186:ARG:HG2	2.30	0.47
14:N:12:TRP:HB2	37:N:8601:HOH:O	2.14	0.47
13:M:78:ALA:N	37:M:8534:HOH:O	2.47	0.47
37:A:3579:HOH:O	4:D:48:MET:N	2.45	0.47
15:O:132:ASN:O	15:O:135:VAL:HG12	2.15	0.47
4:D:108:GLU:HB3	4:D:111:ARG:HD2	1.96	0.47
1:A:2834:G:OP1	25:Y:39:LYS:HE2	2.14	0.47
1:A:2103:A:H5'	37:A:5551:HOH:O	2.14	0.47
1:A:328:U:O4'	5:E:202:THR:HG22	2.14	0.47
1:A:2112:A:H2'	1:A:2113:G:C8	2.50	0.47
1:A:2499:U:H1'	37:A:9007:HOH:O	2.14	0.47
24:X:122:ARG:HH22	24:X:154:ARG:C	2.18	0.47
1:A:380:A:OP2	14:N:9:ARG:HD2	2.15	0.47
37:A:8973:HOH:O	27:1:34:LYS:HD3	2.14	0.47
4:D:195:ARG:NH1	4:D:324:ASP:OD1	2.46	0.47
5:E:55:ARG:N	37:E:8311:HOH:O	2.37	0.47
1:A:2032:U:O2'	1:A:2033:G:H5''	2.14	0.47
14:N:37:VAL:HG13	14:N:63:VAL:HG11	1.97	0.47
17:Q:115:SER:C	17:Q:117:SER:H	2.18	0.47
1:A:1592:G:HO2'	1:A:1593:C:C4'	2.28	0.47
1:A:2005:G:O2'	1:A:2008:U:OP2	2.16	0.47
25:Y:25:ARG:CZ	37:Y:3861:HOH:O	2.63	0.47
10:J:39:GLY:O	10:J:41:THR:N	2.48	0.47
5:E:246:ARG:CZ	37:E:8430:HOH:O	2.61	0.47
3:C:211:LYS:HB3	3:C:212:PRO:CD	2.40	0.47
7:G:20:ILE:CD1	7:G:33:LEU:HD12	2.45	0.47
7:G:49:ILE:HD11	7:G:69:ILE:HD12	1.96	0.47
4:D:315:VAL:HG23	4:D:316:ARG:HG2	1.97	0.47
1:A:1189:A:H1'	1:A:1209:C:O4'	2.15	0.47
27:1:26:VAL:O	27:1:30:GLU:HG3	2.15	0.47
11:K:80:LYS:HE2	11:K:98:PHE:CZ	2.49	0.47
1:A:450:C:H4'	5:E:46:TYR:CE1	2.50	0.47
6:F:93:LEU:HB3	6:F:97:GLN:OE1	2.15	0.47
1:A:2769:C:O2'	1:A:2770:G:H5'	2.15	0.47
29:3:22:PRO:HB2	29:3:24:TRP:CD1	2.49	0.47
1:A:2415:A:N3	15:O:26:LEU:HD13	2.29	0.47
1:A:2079:G:C6	1:A:2080:G:C5	3.03	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
37:A:6979:HOH:O	19:S:132:ARG:CZ	2.62	0.47
1:A:106:A:H1'	37:A:9077:HOH:O	2.15	0.47
1:A:56:G:H5''	23:W:50:ARG:HH12	1.80	0.47
1:A:120:A:H2'	1:A:120:A:N3	2.29	0.47
37:A:4784:HOH:O	16:P:38:ARG:HG2	2.14	0.47
1:A:2819:C:H2'	1:A:2820:A:C8	2.49	0.47
1:A:303:C:H2'	1:A:304:G:O4'	2.14	0.47
21:U:74:VAL:HB	21:U:77:VAL:HG21	1.97	0.47
3:C:169:PHE:O	3:C:170:VAL:HB	2.15	0.47
1:A:1992:U:H2'	1:A:1994:A:OP2	2.14	0.47
1:A:639:A:H2'	1:A:640:G:C8	2.48	0.47
1:A:324:G:O2'	1:A:325:U:H5'	2.15	0.47
1:A:426:G:C2	1:A:427:C:C2	3.02	0.47
1:A:2894:C:O2'	1:A:2895:C:H5'	2.14	0.47
4:D:123:ALA:O	37:D:8650:HOH:O	2.21	0.47
1:A:1055:G:OP2	10:J:94:ARG:NH1	2.48	0.47
1:A:1375:A:H4'	37:A:6783:HOH:O	2.14	0.47
1:A:1450:C:O2'	1:A:1494:A:H5'	2.14	0.47
2:B:3049:G:H2'	2:B:3050:G:O4'	2.15	0.47
6:F:86:THR:C	6:F:89:PRO:HD2	2.35	0.47
2:B:3047:A:C2	2:B:3048:C:C2	3.02	0.47
1:A:2100:A:N3	31:A:4000:CAI:H201	2.29	0.47
1:A:603:A:H4'	1:A:604:G:O5'	2.14	0.47
1:A:929:A:N7	1:A:930:C:C5	2.82	0.47
1:A:1473:U:C2	28:2:42:SER:HB2	2.50	0.47
1:A:2088:C:H1'	1:A:2841:A:N1	2.29	0.47
1:A:316:A:H5'	21:U:54:ASP:OD2	2.13	0.47
1:A:2533:C:O2'	1:A:2534:C:H5'	2.15	0.47
6:F:49:PRO:HA	6:F:73:VAL:HG22	1.97	0.47
1:A:2426:G:H5'	37:A:8817:HOH:O	2.14	0.47
15:O:110:THR:HB	15:O:113:SER:OG	2.15	0.47
21:U:9:LYS:CE	21:U:13:ARG:NH1	2.78	0.47
1:A:407:A:C2	1:A:408:A:C4	3.03	0.47
1:A:1634:G:H2'	1:A:1635:U:C6	2.50	0.47
1:A:2416:G:H2'	1:A:2417:C:C6	2.50	0.47
1:A:1132:A:N6	1:A:1229:C:H2'	2.30	0.47
9:I:66:LEU:O	9:I:69:ARG:HB3	2.14	0.47
1:A:288:A:H2'	1:A:289:G:C8	2.50	0.47
1:A:558:C:C2'	1:A:559:U:C5'	2.92	0.47
37:A:3923:HOH:O	16:P:37:ARG:HG3	2.15	0.47
4:D:175:LEU:O	4:D:175:LEU:HD23	2.14	0.47
1:A:470:U:O2'	28:2:16:HIS:CD2	2.66	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:151:A:H2'	1:A:152:A:O4'	2.15	0.47
1:A:120:A:C6	28:2:17:THR:HG21	2.50	0.47
1:A:1887:U:OP1	27:1:21:LYS:HG3	2.15	0.47
1:A:1829:A:H2'	1:A:1830:C:H5'	1.97	0.47
13:M:112:GLY:O	13:M:132:LYS:NZ	2.34	0.47
1:A:2795:C:O2'	1:A:2796:U:H5'	2.15	0.47
16:P:49:GLU:HG2	37:P:5191:HOH:O	2.14	0.47
16:P:7:LEU:HD22	37:P:5650:HOH:O	2.14	0.47
1:A:1218:U:H2'	1:A:1219:U:C6	2.50	0.47
1:A:2501:G:H1'	37:A:4103:HOH:O	2.14	0.46
6:F:25:MET:SD	6:F:40:ILE:HD11	2.55	0.46
1:A:920:C:N4	1:A:2467:A:C4	2.83	0.46
1:A:1667:A:H2'	1:A:1668:U:C6	2.50	0.46
24:X:54:PHE:CZ	24:X:140:LYS:HB2	2.50	0.46
24:X:65:VAL:HA	24:X:68:THR:CG2	2.44	0.46
1:A:2293:G:C5	1:A:2294:C:C5	3.04	0.46
13:M:73:VAL:HG23	13:M:74:THR:N	2.30	0.46
1:A:2011:A:P	37:A:5505:HOH:O	2.73	0.46
1:A:1850:U:H2'	1:A:1851:G:C8	2.50	0.46
15:O:180:LEU:O	15:O:181:ASP:HB3	2.14	0.46
1:A:858:U:H2'	1:A:859:C:H6	1.80	0.46
15:O:62:HIS:HB3	15:O:65:ASP:OD1	2.15	0.46
1:A:2473:U:O3'	1:A:2474:A:H3'	2.14	0.46
4:D:148:PRO:HD2	37:D:8584:HOH:O	2.14	0.46
14:N:108:LYS:N	14:N:108:LYS:HD3	2.30	0.46
10:J:26:LYS:HG2	10:J:28:ILE:N	2.24	0.46
1:A:1116:U:H3	1:A:1246:A:N6	2.05	0.46
19:S:39:THR:HB	19:S:42:GLU:CD	2.34	0.46
1:A:111:C:H2'	1:A:112:G:O4'	2.15	0.46
1:A:2271:G:OP2	37:A:9011:HOH:O	2.21	0.46
4:D:248:ARG:O	4:D:251:VAL:HG13	2.16	0.46
10:J:35:ASN:ND2	10:J:79:ALA:O	2.48	0.46
1:A:1265:G:C1'	37:A:4558:HOH:O	2.62	0.46
2:B:3064:C:C2'	2:B:3065:A:H5'	2.45	0.46
1:A:202:U:O2'	1:A:203:G:H5'	2.15	0.46
21:U:106:GLU:HG3	37:U:4913:HOH:O	2.15	0.46
2:B:3117:G:C2'	37:B:2118:HOH:O	2.63	0.46
1:A:731:U:O2'	1:A:732:C:H5'	2.16	0.46
14:N:52:LEU:HD13	14:N:116:ASN:CG	2.36	0.46
37:A:6839:HOH:O	14:N:39:ARG:CD	2.64	0.46
7:G:95:VAL:O	7:G:126:ILE:HD13	2.16	0.46
15:O:82:TYR:C	15:O:82:TYR:CD2	2.88	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:710:G:P	16:P:24:ALA:HB3	2.56	0.46
1:A:2134:G:C6	1:A:2258:A:C8	3.04	0.46
1:A:2133:U:H4'	1:A:2134:G:H5'	1.97	0.46
4:D:177:HIS:O	4:D:181:ILE:HG13	2.16	0.46
25:Y:12:ILE:HD12	25:Y:36:HIS:ND1	2.31	0.46
21:U:73:HIS:CD2	21:U:88:PRO:HG3	2.50	0.46
1:A:2107:U:O2'	1:A:2108:A:H5'	2.15	0.46
1:A:1562:C:H2'	1:A:1562:C:O2	2.15	0.46
6:F:99:ASP:CB	6:F:103:ASN:HB2	2.45	0.46
4:D:144:THR:HG22	4:D:145:HIS:N	2.30	0.46
5:E:216:SER:OG	37:E:8408:HOH:O	2.20	0.46
1:A:88:G:H2'	1:A:89:G:C8	2.50	0.46
24:X:28:HIS:CD2	24:X:31:HIS:CE1	3.04	0.46
37:L:408:HOH:O	22:V:37:GLU:HB3	2.16	0.46
1:A:2657:G:OP1	4:D:17:LYS:HB2	2.16	0.46
19:S:35:ILE:O	19:S:38:LYS:HB2	2.14	0.46
13:M:34:GLY:C	13:M:36:ASP:H	2.18	0.46
1:A:2111:G:C2	1:A:2477:C:C2	3.04	0.46
26:Z:187:VAL:HG12	26:Z:205:ILE:HA	1.97	0.46
6:F:35:ALA:C	6:F:37:ALA:N	2.67	0.46
22:V:9:CYS:O	22:V:52:THR:HG23	2.14	0.46
15:O:159:TYR:HE2	15:O:163:PHE:HE2	1.63	0.46
6:F:52:THR:N	6:F:70:GLY:O	2.48	0.46
3:C:93:THR:HG23	3:C:154:ALA:O	2.16	0.46
1:A:2826:G:C6	1:A:2913:A:N6	2.84	0.46
10:J:53:PRO:HA	10:J:125:VAL:O	2.15	0.46
14:N:113:ARG:NH1	14:N:152:ARG:O	2.47	0.46
2:B:3030:C:OP1	6:F:137:PRO:O	2.33	0.46
4:D:55:ASN:HB3	4:D:64:GLY:N	2.30	0.46
15:O:154:LEU:HG	15:O:155:GLU:N	2.30	0.46
3:C:29:HIS:CE1	3:C:107:ASN:ND2	2.84	0.46
1:A:1308:A:O4'	5:E:226:GLY:HA3	2.16	0.46
1:A:1699:C:H4'	37:A:5982:HOH:O	2.16	0.46
1:A:135:G:O2'	14:N:135:ASP:OD2	2.24	0.46
1:A:1079:A:N1	1:A:2068:G:O2'	2.45	0.46
1:A:682:A:H3'	1:A:683:G:H8	1.80	0.46
1:A:464:G:N7	37:A:5000:HOH:O	2.36	0.46
10:J:46:VAL:HG12	10:J:146:TRP:CZ3	2.48	0.46
11:K:45:VAL:HG21	11:K:129:PHE:CD1	2.51	0.46
11:K:131:THR:HB	11:K:134:GLU:HG3	1.96	0.46
11:K:46:ILE:HG12	11:K:53:ILE:HD13	1.96	0.46
4:D:280:VAL:HG13	4:D:334:SER:HA	1.97	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1041:U:H2'	1:A:1042:U:C5'	2.46	0.46
13:M:73:VAL:HG21	13:M:116:HIS:CD2	2.51	0.46
18:R:93:ARG:NH1	18:R:93:ARG:HG3	2.31	0.46
1:A:1023:C:H2'	1:A:1024:G:O4'	2.15	0.46
1:A:790:A:H1'	1:A:1710:A:H2'	1.97	0.46
4:D:275:GLY:O	4:D:291:ASP:HA	2.16	0.46
4:D:56:ASP:OD1	4:D:322:ARG:HB3	2.14	0.46
16:P:60:VAL:O	16:P:62:GLY:N	2.38	0.46
1:A:765:G:O3'	5:E:69:HIS:HB3	2.15	0.46
1:A:458:G:H5'	37:E:8372:HOH:O	2.15	0.46
10:J:65:ARG:HB3	37:J:8386:HOH:O	2.15	0.46
2:B:3006:C:C5'	15:O:37:ARG:HH12	2.24	0.46
15:O:5:ARG:O	37:O:8555:HOH:O	2.21	0.46
26:Z:189:ASN:HA	26:Z:217:ILE:HD11	1.97	0.46
1:A:2467:A:C2'	37:A:5005:HOH:O	2.50	0.46
29:3:24:TRP:NE1	37:3:6863:HOH:O	2.47	0.46
26:Z:112:GLU:CD	26:Z:115:ARG:NH1	2.69	0.46
27:1:28:ASP:O	27:1:31:ILE:HG22	2.16	0.46
21:U:48:VAL:HG13	21:U:49:GLU:N	2.29	0.46
1:A:113:A:H3'	1:A:114:A:H5''	1.98	0.46
10:J:81:TYR:CD1	10:J:81:TYR:C	2.88	0.46
1:A:2365:G:H4'	18:R:45:PRO:O	2.15	0.46
1:A:1535:G:H2'	1:A:1536:C:C6	2.51	0.46
1:A:2296:C:H5	37:R:5998:HOH:O	1.98	0.46
1:A:1785:G:OP1	17:Q:76:GLY:HA3	2.16	0.46
18:R:77:ASP:OD2	18:R:82:LYS:NZ	2.40	0.46
20:T:58:MET:SD	29:3:8:LYS:HE3	2.56	0.46
6:F:41:LEU:O	6:F:44:ILE:HG22	2.16	0.46
11:K:79:PHE:O	11:K:79:PHE:HD2	1.97	0.46
1:A:319:A:H4'	1:A:338:C:C4	2.50	0.46
13:M:148:GLU:HG3	37:M:8556:HOH:O	2.15	0.46
10:J:112:ARG:C	10:J:114:PRO:HD3	2.35	0.46
1:A:1773:G:H8	27:1:16:PRO:HA	1.81	0.46
1:A:524:A:H5'	19:S:29:LYS:HE2	1.98	0.46
4:D:215:VAL:HB	4:D:234:ARG:HH12	1.81	0.46
1:A:1862:C:O2'	1:A:1863:G:H5'	2.16	0.46
1:A:818:A:C2	27:1:13:ARG:HA	2.51	0.46
23:W:45:ARG:C	23:W:47:LYS:N	2.69	0.46
11:K:54:VAL:HG11	11:K:138:THR:HG21	1.98	0.46
14:N:91:ILE:HG23	37:N:8644:HOH:O	2.15	0.46
14:N:37:VAL:CG1	14:N:63:VAL:HG11	2.46	0.46
10:J:33:MET:SD	10:J:65:ARG:HD2	2.56	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:F:51:ARG:HD3	37:F:7636:HOH:O	2.16	0.46
4:D:217:ARG:CG	4:D:257:THR:HG22	2.43	0.46
2:B:3049:G:O2'	2:B:3050:G:H5'	2.16	0.46
1:A:2910:A:H5''	37:A:3697:HOH:O	2.15	0.46
6:F:57:THR:HG23	6:F:63:ILE:CG2	2.45	0.46
4:D:279:THR:CG2	4:D:280:VAL:N	2.78	0.46
6:F:10:PHE:CD1	6:F:11:HIS:N	2.84	0.46
1:A:257:G:O2'	1:A:258:G:H5'	2.16	0.46
4:D:88:GLU:HG3	4:D:88:GLU:O	2.15	0.46
3:C:3:ARG:HB2	3:C:8:ARG:HE	1.81	0.46
30:4:57:GLY:HA2	37:4:8524:HOH:O	2.16	0.46
1:A:382:U:C5	1:A:406:G:N2	2.84	0.46
10:J:31:PHE:HA	10:J:85:ILE:CG2	2.46	0.46
30:4:69:TYR:O	30:4:77:ALA:HA	2.16	0.46
2:B:3057:A:H8	6:F:141:VAL:HG21	1.80	0.46
1:A:960:G:N3	1:A:960:G:C2'	2.78	0.46
24:X:4:LEU:HD21	24:X:52:VAL:HG11	1.98	0.46
8:H:16:ALA:HA	8:H:111:ILE:HD13	1.98	0.46
14:N:68:ARG:HG2	14:N:68:ARG:O	2.16	0.46
1:A:1947:G:N2	1:A:1966:U:O2	2.48	0.46
1:A:643:A:N1	1:A:902:G:O2'	2.41	0.46
1:A:949:U:O2'	18:R:40:HIS:HE1	1.99	0.46
1:A:451:C:N4	1:A:452:G:C6	2.84	0.46
1:A:269:G:C2	1:A:270:U:O4	2.69	0.46
24:X:129:LYS:HG2	37:X:1990:HOH:O	2.15	0.46
15:O:37:ARG:HD3	15:O:37:ARG:HA	1.81	0.45
1:A:1159:G:H1	1:A:1208:C:H42	1.64	0.45
7:G:80:TRP:O	7:G:134:SER:HA	2.15	0.45
1:A:182:G:O3'	14:N:157:LEU:CD1	2.64	0.45
1:A:1613:C:H2'	1:A:1614:G:O4'	2.16	0.45
4:D:36:PRO:HA	4:D:168:GLY:HA2	1.98	0.45
1:A:1423:C:O2'	1:A:1424:A:H5'	2.16	0.45
4:D:81:ALA:O	4:D:186:GLY:HA3	2.16	0.45
8:H:48:VAL:CG2	8:H:74:PHE:HB3	2.45	0.45
19:S:84:ALA:O	19:S:88:PHE:HD1	1.99	0.45
1:A:825:U:H5''	1:A:826:U:OP1	2.15	0.45
1:A:653:C:H2'	1:A:654:A:C8	2.50	0.45
10:J:157:ILE:HG22	10:J:158:ASN:N	2.30	0.45
24:X:139:GLY:O	24:X:141:HIS:CD2	2.69	0.45
5:E:46:TYR:CE2	5:E:98:ARG:NH1	2.84	0.45
15:O:73:ALA:HB2	15:O:163:PHE:CZ	2.51	0.45
7:G:126:ILE:HB	7:G:131:LEU:CD2	2.45	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:E:192:ILE:CG2	5:E:234:VAL:HG12	2.46	0.45
3:C:192:VAL:O	3:C:192:VAL:HG12	2.16	0.45
1:A:2064:U:H2'	1:A:2065:C:C6	2.52	0.45
15:O:21:HIS:HB3	37:O:8566:HOH:O	2.16	0.45
1:A:2430:A:H8	1:A:2430:A:O5'	1.99	0.45
10:J:95:GLU:HB3	10:J:119:VAL:HG11	1.98	0.45
6:F:58:VAL:CG1	6:F:59:GLY:N	2.78	0.45
3:C:217:ARG:HG2	3:C:229:ALA:HB2	1.98	0.45
21:U:41:ARG:NH1	21:U:42:VAL:O	2.49	0.45
13:M:35:ARG:O	13:M:35:ARG:NH1	2.48	0.45
13:M:98:GLU:O	13:M:99:GLU:CB	2.64	0.45
1:A:500:G:H21	19:S:98:ASN:HD21	1.63	0.45
1:A:413:G:N2	1:A:428:G:C4	2.84	0.45
5:E:76:ARG:HG2	5:E:78:ARG:HH12	1.82	0.45
9:I:16:LYS:O	9:I:20:VAL:HG23	2.17	0.45
8:H:28:ALA:HB3	8:H:99:THR:HG23	1.99	0.45
24:X:4:LEU:HD22	24:X:52:VAL:HG22	1.96	0.45
7:G:108:LEU:HD11	7:G:164:ASP:HB2	1.99	0.45
25:Y:76:ARG:O	25:Y:77:PHE:HB3	2.16	0.45
1:A:2094:G:C2	1:A:2652:U:O2	2.69	0.45
1:A:1506:U:H6	1:A:1506:U:H5'	1.81	0.45
24:X:41:TYR:CD2	24:X:44:MET:HE3	2.51	0.45
1:A:2820:A:H2'	1:A:2821:C:C6	2.52	0.45
13:M:91:VAL:O	13:M:91:VAL:HG13	2.16	0.45
1:A:424:C:H2'	1:A:425:U:C6	2.50	0.45
1:A:1463:A:C6	1:A:1464:U:C4	3.04	0.45
1:A:962:C:H5''	37:A:4474:HOH:O	2.17	0.45
6:F:23:VAL:HG21	6:F:45:THR:CG2	2.46	0.45
11:K:79:PHE:O	11:K:83:ILE:HG13	2.16	0.45
1:A:283:U:H5	1:A:284:C:N4	2.14	0.45
8:H:58:GLU:HA	8:H:61:MET:HE2	1.98	0.45
27:1:38:LYS:HE2	27:1:45:LYS:CE	2.44	0.45
5:E:25:PRO:HA	37:E:8355:HOH:O	2.17	0.45
1:A:86:A:C2	29:3:25:VAL:HG13	2.52	0.45
1:A:1268:C:O2'	1:A:1269:G:H5'	2.16	0.45
13:M:54:PRO:HG2	13:M:57:VAL:HG21	1.97	0.45
21:U:96:VAL:HG13	21:U:97:ARG:N	2.31	0.45
4:D:139:ASP:HB3	37:D:8550:HOH:O	2.16	0.45
1:A:202:U:C2'	1:A:203:G:H5'	2.47	0.45
15:O:75:THR:CG2	37:O:8538:HOH:O	2.64	0.45
1:A:1902:G:H2'	1:A:1903:U:O4'	2.16	0.45
1:A:2580:G:H4'	37:A:6303:HOH:O	2.17	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1471:A:H5''	37:N:8577:HOH:O	2.15	0.45
10:J:86:ARG:NH1	10:J:130:HIS:CD2	2.85	0.45
1:A:2488:A:OP1	37:A:4244:HOH:O	2.20	0.45
16:P:32:ARG:HE	16:P:35:LYS:HD2	1.82	0.45
11:K:42:GLU:O	11:K:131:THR:HG23	2.16	0.45
24:X:21:LEU:HB3	24:X:26:ILE:CG1	2.47	0.45
6:F:94:ALA:HB3	6:F:174:VAL:HA	1.99	0.45
1:A:2073:G:OP2	1:A:2490:A:H5'	2.16	0.45
1:A:1878:G:C4'	37:A:5666:HOH:O	2.64	0.45
21:U:49:GLU:HB3	21:U:59:GLU:CG	2.46	0.45
1:A:2541:U:O2'	1:A:2542:C:H5'	2.16	0.45
1:A:2832:C:H5	37:A:6747:HOH:O	1.98	0.45
1:A:2353:A:H4'	1:A:2354:A:O5'	2.16	0.45
1:A:1706:G:C5	1:A:1707:G:C6	3.05	0.45
25:Y:21:PRO:HD3	37:Y:6179:HOH:O	2.17	0.45
10:J:48:LEU:CD1	10:J:157:ILE:HG21	2.46	0.45
5:E:104:ASP:N	37:E:8309:HOH:O	2.49	0.45
12:L:10:GLN:NE2	12:L:10:GLN:N	2.47	0.45
1:A:820:G:H5'	1:A:821:U:H5'	1.98	0.45
16:P:32:ARG:HD3	16:P:32:ARG:C	2.37	0.45
1:A:2723:G:H1'	37:A:4397:HOH:O	2.15	0.45
1:A:1594:C:C2	1:A:1601:G:C2	3.05	0.45
5:E:180:SER:HB2	37:E:8452:HOH:O	2.17	0.45
1:A:1266:U:H4'	26:Z:115:ARG:HH21	1.81	0.45
26:Z:112:GLU:HA	26:Z:112:GLU:OE1	2.17	0.45
22:V:44:ARG:CB	37:V:3805:HOH:O	2.64	0.45
1:A:1682:A:H5''	37:A:9032:HOH:O	2.17	0.45
15:O:184:ILE:HG22	15:O:185:GLU:N	2.32	0.45
13:M:90:ARG:NH1	13:M:119:THR:HG21	2.32	0.45
1:A:329:A:OP2	5:E:206:ASN:HB2	2.17	0.45
1:A:424:C:H2'	1:A:425:U:H6	1.82	0.45
13:M:101:ASP:C	13:M:103:ALA:H	2.18	0.45
37:A:7070:HOH:O	30:4:79:LEU:HD22	2.16	0.45
1:A:2621:U:H5	37:A:9557:HOH:O	2.00	0.45
5:E:185:LYS:HD3	5:E:186:TYR:CE1	2.52	0.45
1:A:24:G:N2	1:A:518:G:H1'	2.31	0.45
20:T:38:ALA:O	20:T:42:GLU:HG3	2.16	0.45
10:J:30:GLN:H	10:J:65:ARG:NH1	2.15	0.45
10:J:29:ALA:N	10:J:62:GLU:OE1	2.47	0.45
10:J:62:GLU:OE2	10:J:66:VAL:CG2	2.65	0.45
1:A:1593:C:OP1	17:Q:117:SER:HB3	2.17	0.45
16:P:32:ARG:NH1	37:P:2336:HOH:O	2.49	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:3078:G:O2'	2:B:3079:U:P	2.75	0.45
22:V:11:THR:HG22	22:V:53:ASP:OD2	2.17	0.45
7:G:31:ARG:HH12	7:G:68:HIS:CE1	2.35	0.45
4:D:41:PHE:CD2	4:D:190:MET:HE3	2.51	0.45
7:G:7:ILE:HD11	7:G:11:VAL:O	2.17	0.45
1:A:2837:U:H1'	4:D:307:ARG:HH12	1.82	0.45
1:A:2769:C:H2'	1:A:2770:G:C5'	2.46	0.45
14:N:138:HIS:C	14:N:139:PRO:O	2.49	0.45
21:U:96:VAL:CG1	21:U:97:ARG:N	2.80	0.45
22:V:20:MET:CG	22:V:28:THR:HG23	2.47	0.45
17:Q:7:LYS:CD	17:Q:21:VAL:HG21	2.47	0.45
24:X:28:HIS:HD2	24:X:31:HIS:CE1	2.34	0.45
1:A:255:A:H2'	1:A:256:C:C6	2.52	0.45
8:H:79:GLN:HB2	8:H:82:ASP:OD2	2.17	0.45
4:D:322:ARG:HB2	37:D:8609:HOH:O	2.17	0.45
1:A:883:U:O2	1:A:883:U:C2'	2.65	0.45
1:A:1135:G:H5'	37:A:5475:HOH:O	2.17	0.45
26:Z:133:HIS:HD2	37:Z:8585:HOH:O	2.00	0.45
23:W:16:ARG:NH2	23:W:63:GLU:HG3	2.31	0.45
3:C:57:ALA:HA	3:C:67:LEU:HD23	1.98	0.45
14:N:18:GLY:O	14:N:21:ALA:HB3	2.17	0.45
3:C:125:ASN:HB3	3:C:158:VAL:HG12	1.98	0.45
14:N:62:VAL:C	14:N:63:VAL:HG23	2.37	0.45
14:N:14:ARG:HB3	37:N:8593:HOH:O	2.16	0.45
5:E:107:ARG:CB	5:E:107:ARG:NH1	2.79	0.45
1:A:2505:G:C2'	1:A:2506:A:H5'	2.47	0.45
1:A:1185:U:H5'	37:A:7001:HOH:O	2.17	0.45
1:A:2852:A:H5''	37:A:4787:HOH:O	2.16	0.45
17:Q:10:ALA:HA	17:Q:13:VAL:CG1	2.45	0.45
14:N:59:GLY:CA	14:N:141:ILE:HD11	2.47	0.45
1:A:2453:G:H5'	37:A:4251:HOH:O	2.17	0.45
37:A:5571:HOH:O	18:R:50:GLY:HA2	2.17	0.45
28:2:28:HIS:HD2	28:2:30:LYS:H	1.65	0.45
1:A:812:A:H2'	1:A:813:C:O4'	2.17	0.45
1:A:2011:A:H4'	1:A:2012:U:O5'	2.17	0.45
6:F:140:ARG:O	6:F:144:ARG:HG2	2.16	0.45
1:A:682:A:H2'	1:A:683:G:O4'	2.17	0.45
1:A:818:A:H2	27:1:13:ARG:HA	1.81	0.45
3:C:30:ARG:HB3	3:C:30:ARG:HE	1.61	0.45
3:C:123:GLY:HA3	3:C:162:GLY:HA2	1.99	0.45
26:Z:189:ASN:HD22	26:Z:192:ASP:H	1.65	0.45
1:A:2269:C:H2'	1:A:2270:G:C5'	2.47	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1119:G:N2	1:A:1246:A:H2	2.10	0.45
7:G:31:ARG:HH12	7:G:68:HIS:CD2	2.35	0.45
15:O:163:PHE:O	15:O:164:ASP:O	2.34	0.45
1:A:183:A:C5'	14:N:157:LEU:HD12	2.47	0.45
1:A:1845:A:P	3:C:190:ARG:HH11	2.39	0.45
15:O:11:ARG:HG3	15:O:14:ARG:NH1	2.31	0.45
3:C:29:HIS:HB2	3:C:153:ARG:HH12	1.82	0.45
7:G:101:GLU:OE2	7:G:115:ARG:NH1	2.49	0.45
10:J:72:VAL:CG1	10:J:81:TYR:CZ	3.00	0.45
8:H:21:GLU:HA	8:H:24:ARG:HE	1.81	0.45
1:A:524:A:C5'	19:S:29:LYS:HE2	2.46	0.45
26:Z:106:THR:HG23	26:Z:107:PRO:HD2	1.98	0.45
26:Z:107:PRO:HD3	26:Z:182:PHE:CE1	2.52	0.45
1:A:1409:G:H5'	37:A:3297:HOH:O	2.16	0.45
8:H:78:GLU:CB	37:H:2750:HOH:O	2.64	0.45
1:A:324:G:C6	1:A:325:U:C5	3.05	0.45
15:O:1:ALA:HB3	37:O:8576:HOH:O	2.16	0.45
1:A:667:C:H5'	37:A:9605:HOH:O	2.16	0.45
1:A:1362:U:H5'	37:A:9838:HOH:O	2.17	0.45
1:A:241:A:C2	1:A:378:A:H4'	2.52	0.45
1:A:567:U:H5''	37:X:5817:HOH:O	2.17	0.45
22:V:52:THR:HG22	22:V:54:THR:N	2.32	0.45
7:G:84:MET:HE1	7:G:133:VAL:HG21	1.98	0.45
4:D:74:ILE:HD13	4:D:309:VAL:HG21	1.99	0.45
1:A:2679:G:H2'	1:A:2681:A:OP2	2.17	0.45
3:C:3:ARG:HB2	3:C:8:ARG:NE	2.32	0.45
1:A:1583:U:H1'	37:A:9552:HOH:O	2.16	0.45
21:U:19:ARG:NH1	21:U:68:ASP:O	2.50	0.45
1:A:2123:A:OP1	14:N:89:ASN:ND2	2.50	0.44
5:E:223:LEU:HD12	5:E:223:LEU:HA	1.79	0.44
10:J:4:ALA:HB3	37:J:8366:HOH:O	2.17	0.44
12:L:37:TYR:HE2	12:L:45:PRO:HA	1.81	0.44
4:D:41:PHE:CZ	4:D:79:MET:HG3	2.52	0.44
1:A:657:G:OP1	5:E:27:ARG:NH2	2.40	0.44
17:Q:13:VAL:HG11	17:Q:40:VAL:HG11	1.98	0.44
24:X:108:ARG:O	24:X:111:GLY:N	2.41	0.44
19:S:145:LEU:HD12	19:S:146:ILE:H	1.82	0.44
1:A:1375:A:C2'	1:A:1376:G:H5'	2.47	0.44
1:A:486:A:H1'	37:A:6311:HOH:O	2.17	0.44
1:A:963:C:O5'	1:A:963:C:H6	2.00	0.44
1:A:1609:C:H2'	1:A:1610:G:H8	1.81	0.44
28:2:52:SER:HA	37:2:8443:HOH:O	2.17	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
25:Y:30:MET:CE	25:Y:58:ALA:HB3	2.47	0.44
5:E:142:ASP:OD1	5:E:237:GLU:HB3	2.18	0.44
9:I:23:ILE:O	9:I:27:ILE:HG13	2.16	0.44
3:C:51:ARG:HB2	37:C:8618:HOH:O	2.15	0.44
15:O:73:ALA:HB1	15:O:74:PRO:CD	2.47	0.44
1:A:777:U:O2'	28:2:11:LYS:HG2	2.17	0.44
11:K:6:PHE:HB3	11:K:109:TYR:OH	2.17	0.44
5:E:129:HIS:CE1	5:E:232:LEU:H	2.35	0.44
1:A:2909:G:H2'	1:A:2910:A:H8	1.82	0.44
24:X:11:VAL:O	24:X:12:ASN:HB2	2.17	0.44
1:A:779:U:H5'	1:A:1836:A:C2	2.52	0.44
3:C:217:ARG:NH1	3:C:217:ARG:CG	2.80	0.44
1:A:814:G:H8	37:A:6743:HOH:O	2.00	0.44
1:A:911:G:H5'	1:A:932:U:OP1	2.17	0.44
1:A:1302:G:C5'	1:A:1331:A:O3'	2.65	0.44
37:A:5827:HOH:O	26:Z:158:LYS:HD3	2.17	0.44
4:D:132:HIS:CE1	4:D:171:VAL:HG21	2.52	0.44
24:X:84:VAL:HG12	37:X:6679:HOH:O	2.16	0.44
1:A:2840:A:OP1	4:D:211:THR:HG23	2.18	0.44
1:A:553:G:O4'	1:A:1325:G:H5'	2.18	0.44
1:A:1743:G:N7	37:A:8844:HOH:O	2.36	0.44
1:A:926:A:H1'	13:M:38:HIS:O	2.18	0.44
1:A:128:A:O2'	1:A:129:A:H5'	2.17	0.44
1:A:2727:A:H2'	1:A:2728:C:H5'	1.99	0.44
1:A:121:U:OP2	29:3:10:ARG:NH2	2.47	0.44
3:C:43:VAL:O	3:C:44:ASP:HB2	2.17	0.44
1:A:815:U:OP1	37:A:9239:HOH:O	2.20	0.44
10:J:31:PHE:HE2	10:J:87:LYS:O	2.00	0.44
5:E:141:SER:HB3	37:E:8424:HOH:O	2.18	0.44
1:A:2715:G:N2	4:D:264:GLU:OE1	2.51	0.44
30:4:69:TYR:HB2	30:4:78:HIS:CE1	2.53	0.44
15:O:182:GLY:O	15:O:183:ASP:O	2.36	0.44
9:I:12:ILE:HB	37:I:4714:HOH:O	2.17	0.44
8:H:101:ALA:HB2	8:H:108:LEU:CD2	2.47	0.44
6:F:154:LYS:H	6:F:154:LYS:CD	2.24	0.44
25:Y:43:VAL:CG1	25:Y:44:ASP:N	2.80	0.44
23:W:39:ALA:C	23:W:41:GLU:N	2.70	0.44
3:C:105:VAL:HG13	3:C:155:THR:O	2.18	0.44
1:A:1878:G:O2'	1:A:1879:U:C6	2.67	0.44
1:A:1543:G:N1	1:A:1641:A:OP2	2.39	0.44
4:D:279:THR:OG1	4:D:290:VAL:HB	2.18	0.44
17:Q:7:LYS:HD3	17:Q:21:VAL:HG21	1.99	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2791:U:C1'	1:A:2792:A:H5''	2.47	0.44
1:A:158:A:O2'	1:A:159:G:H5'	2.18	0.44
1:A:2012:U:H6	37:A:3110:HOH:O	2.00	0.44
25:Y:12:ILE:HG23	25:Y:36:HIS:CG	2.53	0.44
8:H:48:VAL:HG23	8:H:74:PHE:CB	2.48	0.44
21:U:19:ARG:HD3	21:U:67:LEU:O	2.18	0.44
6:F:91:ALA:HB1	37:F:5198:HOH:O	2.17	0.44
1:A:1786:C:O2'	37:A:6875:HOH:O	2.21	0.44
26:Z:130:ARG:HB2	26:Z:142:SER:O	2.18	0.44
1:A:1414:A:H2'	1:A:1415:G:O4'	2.18	0.44
21:U:65:VAL:HG22	21:U:72:ILE:HG22	2.00	0.44
1:A:1512:G:N2	1:A:1513:C:H1'	2.31	0.44
26:Z:187:VAL:O	26:Z:187:VAL:HG13	2.17	0.44
1:A:2467:A:C3'	37:A:5005:HOH:O	2.65	0.44
1:A:282:C:H2'	1:A:283:U:O4'	2.17	0.44
1:A:204:A:H2'	1:A:205:U:C5'	2.45	0.44
4:D:175:LEU:C	4:D:175:LEU:CD2	2.84	0.44
1:A:1730:G:C5'	1:A:1731:C:C6	3.00	0.44
1:A:563:C:H2'	1:A:564:G:O4'	2.18	0.44
1:A:1523:G:C6	1:A:1524:U:O4	2.70	0.44
37:A:9465:HOH:O	8:H:34:ASN:HB2	2.17	0.44
8:H:21:GLU:O	8:H:24:ARG:CG	2.65	0.44
1:A:1050:G:C6	1:A:1051:C:C4	3.06	0.44
1:A:1302:G:H5'	1:A:1331:A:O3'	2.18	0.44
1:A:2317:C:C4	1:A:2318:C:C4	3.05	0.44
1:A:2045:G:H2'	1:A:2046:G:O4'	2.17	0.44
26:Z:102:LEU:HA	37:Z:8525:HOH:O	2.18	0.44
1:A:1871:U:O4'	1:A:1873:G:C8	2.71	0.44
1:A:1386:G:N3	37:A:9760:HOH:O	2.36	0.44
27:1:47:LEU:HD23	27:1:57:CYS:CB	2.46	0.44
10:J:149:ALA:C	10:J:151:MET:H	2.20	0.44
6:F:81:GLU:O	6:F:83:PHE:N	2.51	0.44
29:3:40:ARG:NH1	29:3:40:ARG:HG2	2.32	0.44
2:B:3104:A:O2'	2:B:3105:A:H5'	2.18	0.44
1:A:1494:A:C4	1:A:1495:C:C5	3.06	0.44
1:A:645:U:H4'	37:E:8335:HOH:O	2.16	0.44
1:A:2779:G:O2'	1:A:2780:C:H5'	2.18	0.44
3:C:76:VAL:CG2	27:1:63:LYS:HB3	2.47	0.44
4:D:82:VAL:CG1	4:D:82:VAL:O	2.63	0.44
22:V:49:LEU:O	22:V:55:ALA:CB	2.66	0.44
6:F:59:GLY:C	6:F:61:PHE:N	2.71	0.44
1:A:420:U:H2'	1:A:421:C:C6	2.52	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1307:A:H1'	37:A:4452:HOH:O	2.17	0.44
4:D:225:GLY:HA3	37:D:8571:HOH:O	2.17	0.44
3:C:149:ASP:OD1	3:C:151:GLN:HB2	2.17	0.44
24:X:88:THR:CG2	24:X:110:GLN:NE2	2.76	0.44
10:J:136:VAL:HA	37:J:8343:HOH:O	2.18	0.44
14:N:45:ARG:CZ	14:N:48:ARG:HG3	2.48	0.44
15:O:167:ASP:O	15:O:168:LEU:HD23	2.18	0.44
17:Q:98:ILE:HD13	17:Q:98:ILE:O	2.18	0.44
1:A:2898:G:H4'	4:D:288:GLY:HA2	1.99	0.44
20:T:80:ARG:NH1	37:T:7263:HOH:O	2.50	0.44
1:A:793:A:H5''	17:Q:83:LYS:HG2	2.00	0.44
1:A:2656:G:O2'	1:A:2657:G:H5'	2.17	0.44
1:A:1940:C:H4'	37:A:6881:HOH:O	2.17	0.44
5:E:187:ARG:O	5:E:187:ARG:HG3	2.17	0.44
1:A:148:A:H5''	28:2:44:LYS:HG2	2.00	0.44
4:D:102:THR:HG22	37:D:8617:HOH:O	2.17	0.44
19:S:33:ARG:HG3	37:S:8565:HOH:O	2.17	0.44
17:Q:131:PHE:CD1	17:Q:137:LEU:HD13	2.52	0.44
10:J:150:LYS:HE2	37:J:8380:HOH:O	2.18	0.44
10:J:26:LYS:HD3	10:J:89:PRO:CG	2.48	0.44
5:E:219:ASN:O	5:E:223:LEU:HB2	2.18	0.44
4:D:41:PHE:HB3	4:D:190:MET:CE	2.47	0.44
3:C:51:ARG:NH1	3:C:120:ARG:O	2.50	0.44
15:O:72:GLU:H	15:O:171:HIS:CE1	2.35	0.44
6:F:94:ALA:O	6:F:95:THR:O	2.36	0.44
5:E:27:ARG:HG2	5:E:30:LEU:HG	1.99	0.44
1:A:183:A:O2'	1:A:184:G:H5'	2.17	0.44
1:A:160:A:C5	1:A:177:A:C2	3.05	0.44
1:A:795:G:N3	1:A:817:G:C2	2.86	0.44
16:P:26:TRP:N	37:P:3062:HOH:O	2.49	0.44
18:R:31:GLU:CD	18:R:93:ARG:HH12	2.21	0.44
1:A:1644:C:H2'	1:A:1645:U:H6	1.83	0.44
6:F:140:ARG:HG3	6:F:140:ARG:HH11	1.83	0.44
1:A:639:A:C2	1:A:1363:G:C2	3.06	0.44
1:A:135:G:H1'	14:N:135:ASP:OD2	2.18	0.44
1:A:2409:C:O2'	1:A:2410:G:H5'	2.18	0.44
3:C:110:SER:N	3:C:114:ASP:OD2	2.51	0.44
14:N:137:ASP:C	14:N:142:LYS:HE3	2.38	0.44
37:A:9809:HOH:O	3:C:221:PRO:HA	2.18	0.44
1:A:861:A:H2'	1:A:862:U:C6	2.52	0.44
1:A:1098:A:H2'	1:A:1099:G:O4'	2.18	0.44
4:D:97:LEU:HD21	37:D:8648:HOH:O	2.18	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:E:34:ALA:HB3	5:E:220:THR:HG21	2.00	0.44
12:L:30:LYS:C	12:L:55:VAL:HG13	2.38	0.44
1:A:1164:U:C1'	1:A:1165:G:OP1	2.66	0.44
15:O:175:LEU:HD12	15:O:175:LEU:HA	1.87	0.44
1:A:1119:G:C8	11:K:52:GLN:NE2	2.86	0.44
7:G:139:GLU:CG	37:G:5919:HOH:O	2.65	0.44
1:A:1057:A:N6	1:A:1058:A:N6	2.65	0.44
1:A:596:C:H2'	1:A:597:A:C8	2.53	0.44
6:F:173:GLU:HG3	6:F:174:VAL:N	2.33	0.44
1:A:1335:C:OP2	26:Z:207:SER:CB	2.66	0.44
5:E:129:HIS:HD2	5:E:165:ASP:OD2	2.00	0.44
4:D:23:THR:HA	4:D:24:PRO:HD3	1.84	0.44
1:A:1268:C:O2'	26:Z:169:ARG:HB2	2.18	0.44
19:S:141:VAL:HG12	19:S:142:ASP:O	2.18	0.44
16:P:4:ASN:HB3	16:P:7:LEU:HB3	2.00	0.44
1:A:1609:C:H2'	1:A:1610:G:C8	2.53	0.44
1:A:392:U:C5'	14:N:193:LYS:HB3	2.48	0.44
5:E:19:PRO:HG2	5:E:22:PHE:CD1	2.53	0.44
7:G:118:ILE:HG23	7:G:144:THR:HG21	2.00	0.44
1:A:1241:G:N3	11:K:86:MET:HE2	2.33	0.44
1:A:1014:A:H5''	2:B:3101:G:O2'	2.17	0.44
22:V:38:ASN:O	22:V:42:LEU:HG	2.17	0.44
24:X:1:MET:HB2	24:X:103:GLU:HG2	1.98	0.44
1:A:1823:G:C6	1:A:1824:C:C4	3.06	0.44
5:E:140:VAL:HG12	5:E:141:SER:N	2.33	0.43
5:E:114:ALA:HB1	5:E:223:LEU:HB3	2.00	0.43
4:D:60:SER:C	4:D:62:ARG:H	2.20	0.43
5:E:107:ARG:HH11	5:E:107:ARG:HB3	1.79	0.43
1:A:2526:C:H5'	1:A:2526:C:C6	2.52	0.43
25:Y:25:ARG:CG	37:Y:5356:HOH:O	2.64	0.43
7:G:20:ILE:HD12	7:G:33:LEU:HD12	2.00	0.43
1:A:1589:G:H22	1:A:1605:G:H1'	1.82	0.43
3:C:101:GLU:HG2	3:C:131:HIS:ND1	2.33	0.43
37:A:6992:HOH:O	5:E:188:ARG:HD2	2.17	0.43
17:Q:7:LYS:HD2	17:Q:21:VAL:CG2	2.47	0.43
1:A:2293:G:H1'	1:A:2464:C:C2	2.53	0.43
1:A:222:A:H2'	1:A:223:G:O4'	2.18	0.43
13:M:34:GLY:O	13:M:36:ASP:N	2.51	0.43
20:T:42:GLU:HG2	20:T:49:VAL:HG23	1.99	0.43
1:A:1301:C:O2'	1:A:1331:A:H4'	2.18	0.43
1:A:1912:A:O5'	1:A:1912:A:H8	2.01	0.43
13:M:64:ILE:O	13:M:64:ILE:HG23	2.17	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
15:O:108:SER:HA	15:O:109:PRO:HD3	1.78	0.43
1:A:537:G:C6	1:A:620:A:C8	3.06	0.43
7:G:36:PRO:HD3	11:K:127:ILE:HD12	2.00	0.43
7:G:34:TRP:O	11:K:127:ILE:HD11	2.17	0.43
1:A:2584:G:C2	1:A:2585:G:N7	2.86	0.43
10:J:47:GLU:HG2	10:J:133:ILE:HD12	1.99	0.43
1:A:1161:A:O5'	1:A:1161:A:H8	2.01	0.43
10:J:65:ARG:NH2	10:J:66:VAL:HG22	2.33	0.43
27:1:11:THR:HG23	27:1:23:ARG:HB2	1.97	0.43
1:A:1246:A:O2'	1:A:1247:A:H3'	2.19	0.43
11:K:46:ILE:O	11:K:46:ILE:HG12	2.18	0.43
14:N:97:ILE:HD13	14:N:127:LYS:HD2	1.98	0.43
15:O:171:HIS:CE1	37:O:8568:HOH:O	2.70	0.43
8:H:111:ILE:O	8:H:115:VAL:HG23	2.17	0.43
1:A:2455:A:H2'	1:A:2456:A:O4'	2.18	0.43
3:C:192:VAL:O	3:C:192:VAL:CG1	2.66	0.43
1:A:485:A:OP2	37:A:3543:HOH:O	2.21	0.43
1:A:154:C:O2'	1:A:155:C:H5'	2.18	0.43
22:V:44:ARG:HB3	37:V:3805:HOH:O	2.18	0.43
1:A:958:G:H2'	1:A:959:C:C6	2.52	0.43
1:A:1562:C:H42	1:A:2738:G:H1	1.65	0.43
3:C:8:ARG:HG2	37:C:8554:HOH:O	2.18	0.43
5:E:153:VAL:O	5:E:157:LEU:HG	2.18	0.43
1:A:40:C:O5'	1:A:40:C:H6	2.01	0.43
1:A:1336:U:C2	1:A:1337:A:C8	3.05	0.43
1:A:1211:G:O2'	1:A:1212:C:H5'	2.18	0.43
2:B:3114:G:H2'	2:B:3115:C:C6	2.54	0.43
4:D:223:ARG:HG3	4:D:232:TRP:O	2.18	0.43
18:R:64:GLU:HG3	18:R:74:ASP:OD2	2.18	0.43
2:B:3006:C:P	15:O:37:ARG:HH11	2.40	0.43
1:A:1943:C:O4'	3:C:212:PRO:HA	2.17	0.43
7:G:107:PHE:CZ	7:G:108:LEU:HD13	2.51	0.43
6:F:84:LEU:HA	6:F:87:ALA:HB3	2.01	0.43
12:L:6:ALA:HB3	12:L:116:GLU:HG2	2.01	0.43
12:L:65:ARG:O	12:L:66:ARG:HB2	2.18	0.43
21:U:26:THR:HA	21:U:39:ASN:HB3	1.99	0.43
1:A:426:G:O2'	1:A:427:C:H5'	2.18	0.43
1:A:2317:C:C5	1:A:2318:C:C4	3.06	0.43
1:A:344:C:H2'	1:A:345:G:O4'	2.17	0.43
30:4:43:ASN:ND2	37:4:8506:HOH:O	2.29	0.43
24:X:122:ARG:CG	24:X:122:ARG:HH11	2.24	0.43
10:J:147:ARG:HA	10:J:150:LYS:NZ	2.34	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
25:Y:74:ALA:CB	25:Y:85:VAL:HG22	2.48	0.43
23:W:1:THR:HG23	23:W:2:VAL:N	2.23	0.43
8:H:99:THR:O	8:H:100:ASP:HB2	2.18	0.43
1:A:1741:U:HO2'	1:A:2723:G:H4'	1.82	0.43
1:A:236:A:O5'	1:A:236:A:H2'	2.18	0.43
27:1:33:HIS:HE1	27:1:49:ARG:NE	2.17	0.43
1:A:1044:C:C5'	37:A:8623:HOH:O	2.67	0.43
1:A:396:U:O2'	1:A:418:C:H4'	2.18	0.43
26:Z:129:ASN:OD1	26:Z:141:THR:OG1	2.32	0.43
11:K:70:PHE:O	11:K:70:PHE:CD2	2.71	0.43
4:D:7:ARG:NH2	4:D:250:THR:O	2.52	0.43
1:A:134:U:O2	1:A:145:A:C2	2.70	0.43
1:A:1773:G:H2'	1:A:1774:G:H5'	2.00	0.43
1:A:113:A:OP2	1:A:114:A:H5''	2.18	0.43
17:Q:16:VAL:CG1	17:Q:20:ARG:HB2	2.48	0.43
10:J:117:LYS:HB2	37:J:8339:HOH:O	2.19	0.43
1:A:1969:A:N7	1:A:1970:G:C6	2.86	0.43
1:A:2325:C:H1'	37:A:3713:HOH:O	2.17	0.43
7:G:132:THR:HB	37:G:2227:HOH:O	2.18	0.43
1:A:123:U:H2'	1:A:124:C:H6	1.84	0.43
1:A:832:U:H2'	1:A:833:G:C8	2.54	0.43
7:G:102:VAL:HG11	7:G:148:ILE:HD11	2.00	0.43
1:A:2123:A:P	14:N:89:ASN:HD22	2.41	0.43
1:A:1593:C:H5'	17:Q:116:SER:O	2.18	0.43
12:L:55:VAL:CG1	12:L:56:SER:H	2.29	0.43
1:A:821:U:H2'	1:A:822:C:C6	2.47	0.43
2:B:3078:G:N2	2:B:3103:A:OP2	2.49	0.43
4:D:316:ARG:N	4:D:317:PRO:HD3	2.34	0.43
24:X:5:VAL:O	24:X:52:VAL:CG2	2.66	0.43
1:A:2432:C:H4'	30:4:36:ILE:HG12	2.00	0.43
11:K:93:ARG:HH11	11:K:93:ARG:CB	2.26	0.43
3:C:99:ILE:O	3:C:131:HIS:CE1	2.71	0.43
1:A:2769:C:H2'	1:A:2770:G:H5'	2.01	0.43
1:A:251:C:H4'	14:N:140:ALA:HB2	2.01	0.43
1:A:1238:C:H4'	37:A:5565:HOH:O	2.17	0.43
37:A:4024:HOH:O	14:N:146:GLN:HG2	2.17	0.43
1:A:244:C:H6	1:A:244:C:O5'	2.01	0.43
8:H:34:ASN:HA	14:N:4:ALA:HB2	2.01	0.43
1:A:2265:U:H2'	1:A:2266:A:C8	2.54	0.43
18:R:77:ASP:N	18:R:80:LYS:O	2.52	0.43
1:A:1241:G:N2	11:K:86:MET:HE1	2.33	0.43
8:H:12:LEU:HD23	8:H:12:LEU:O	2.18	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
16:P:54:GLU:HG2	16:P:73:ASP:O	2.19	0.43
19:S:15:LYS:HE3	37:S:8577:HOH:O	2.18	0.43
1:A:2745:C:H5	37:A:5432:HOH:O	2.01	0.43
1:A:2481:G:H3'	1:A:2482:G:H5''	2.00	0.43
14:N:87:MET:HG3	14:N:87:MET:H	1.48	0.43
27:1:42:CYS:SG	27:1:44:PHE:N	2.81	0.43
1:A:1246:A:C4	1:A:1248:A:C8	3.07	0.43
24:X:21:LEU:HD13	24:X:26:ILE:HD11	2.00	0.43
8:H:58:GLU:HG3	8:H:61:MET:HE1	2.00	0.43
37:A:4287:HOH:O	15:O:21:HIS:HD2	2.01	0.43
16:P:59:VAL:CG2	16:P:111:VAL:HG23	2.49	0.43
1:A:2730:G:O2'	1:A:2731:G:H5'	2.19	0.43
4:D:16:ARG:NE	37:D:8556:HOH:O	2.28	0.43
1:A:2883:A:H2'	1:A:2884:G:O4'	2.19	0.43
1:A:1398:G:H2'	1:A:1399:A:C8	2.54	0.43
29:3:11:LEU:HD23	29:3:11:LEU:HA	1.80	0.43
1:A:1574:C:H6	1:A:1574:C:O5'	2.01	0.43
15:O:120:GLU:HG3	15:O:136:LEU:HD13	2.00	0.43
5:E:3:ALA:HA	37:E:8459:HOH:O	2.19	0.43
1:A:1890:U:H4'	1:A:2010:A:C6	2.54	0.43
14:N:25:TRP:HE3	14:N:26:HIS:HD2	1.66	0.43
1:A:1461:U:H2'	1:A:1462:C:C6	2.54	0.43
1:A:1191:A:N1	1:A:1206:U:O4	2.51	0.43
1:A:1191:A:C3'	1:A:1192:A:H5''	2.44	0.43
12:L:37:TYR:HD2	37:L:7169:HOH:O	1.92	0.43
11:K:130:VAL:CG1	11:K:131:THR:N	2.82	0.43
1:A:1189:A:N3	37:A:7218:HOH:O	2.48	0.43
11:K:74:ARG:NH1	11:K:76:ASP:HB2	2.33	0.43
1:A:2911:C:H2'	1:A:2912:C:H6	1.83	0.43
1:A:2064:U:H4'	1:A:2653:A:P	2.59	0.43
10:J:113:ALA:N	10:J:114:PRO:CD	2.82	0.43
17:Q:41:ARG:O	17:Q:44:VAL:HB	2.18	0.43
1:A:308:U:C4	1:A:342:C:H1'	2.53	0.43
15:O:154:LEU:HD12	15:O:156:GLU:O	2.19	0.43
1:A:1041:U:C2'	1:A:1042:U:H5'	2.49	0.43
1:A:1970:G:C5'	37:A:6606:HOH:O	2.66	0.43
1:A:2681:A:N6	1:A:2714:U:H4'	2.33	0.43
1:A:426:G:H2'	1:A:427:C:O4'	2.18	0.43
37:A:3701:HOH:O	25:Y:59:TRP:HB2	2.18	0.43
1:A:123:U:O2'	1:A:124:C:H5'	2.19	0.43
1:A:107:U:H2'	1:A:108:U:H5'	2.00	0.43
1:A:1586:G:O2'	1:A:1587:U:H5'	2.18	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:N:76:ARG:HG2	14:N:76:ARG:HH11	1.82	0.43
4:D:274:GLU:HA	4:D:292:GLY:O	2.18	0.43
1:A:745:G:O6	16:P:68:GLY:HA3	2.19	0.43
10:J:48:LEU:CG	10:J:157:ILE:HG21	2.47	0.43
23:W:12:THR:HG23	23:W:14:ALA:N	2.34	0.43
1:A:2526:C:H5'	37:A:7143:HOH:O	2.17	0.43
2:B:3078:G:O2'	2:B:3079:U:OP2	2.35	0.43
1:A:236:A:O5'	1:A:236:A:C2'	2.66	0.43
1:A:922:A:N7	1:A:2281:C:H5'	2.33	0.43
3:C:105:VAL:CG1	3:C:106:CYS:N	2.81	0.43
1:A:941:G:C5	1:A:942:U:C4	3.06	0.43
2:B:3007:G:OP1	15:O:23:ARG:HD2	2.17	0.43
1:A:1730:G:H5'	1:A:1731:C:H5	1.80	0.43
21:U:48:VAL:HG13	21:U:96:VAL:HG13	2.01	0.43
1:A:2428:G:C6	1:A:2464:C:H1'	2.54	0.43
26:Z:107:PRO:HB3	26:Z:182:PHE:CD2	2.54	0.43
25:Y:8:ARG:NH1	37:Y:2479:HOH:O	2.51	0.43
1:A:1706:G:C6	1:A:1707:G:C6	3.06	0.43
1:A:1937:U:O2'	1:A:1938:G:H5'	2.18	0.43
15:O:115:VAL:O	15:O:118:ILE:HB	2.18	0.43
17:Q:64:GLU:HG2	37:Q:2495:HOH:O	2.18	0.43
1:A:2488:A:O2'	1:A:2489:G:H5'	2.19	0.43
1:A:1572:A:H2'	1:A:1573:A:C8	2.53	0.43
9:I:20:VAL:O	9:I:24:VAL:HG23	2.19	0.43
7:G:20:ILE:HD12	7:G:33:LEU:CD1	2.49	0.43
1:A:220:C:OP2	1:A:2431:C:H1'	2.19	0.43
1:A:2073:G:C6	1:A:2607:U:C2	3.06	0.43
4:D:248:ARG:HG2	37:K:8540:HOH:O	2.19	0.43
1:A:1299:G:N7	13:M:6:ARG:NH1	2.66	0.43
12:L:99:ASP:OD1	12:L:101:ASN:N	2.51	0.43
14:N:137:ASP:O	14:N:142:LYS:HE3	2.19	0.43
7:G:137:ASP:O	7:G:141:VAL:HG23	2.19	0.43
1:A:1221:G:N7	37:A:3410:HOH:O	2.37	0.43
5:E:200:PRO:HB3	5:E:212:VAL:HG23	2.01	0.43
1:A:466:A:H2'	1:A:467:G:O4'	2.19	0.43
1:A:2038:A:OP2	4:D:224:LYS:NZ	2.45	0.43
1:A:2468:A:H1'	37:A:3402:HOH:O	2.18	0.43
29:3:36:ASN:HB3	29:3:39:ARG:NE	2.34	0.43
7:G:31:ARG:HH12	7:G:68:HIS:CG	2.36	0.43
8:H:60:VAL:O	8:H:61:MET:C	2.57	0.43
8:H:63:ILE:HB	8:H:64:PRO:CD	2.45	0.43
7:G:11:VAL:HG13	7:G:23:GLU:O	2.18	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2290:U:H4'	1:A:2291:A:OP1	2.17	0.43
15:O:149:GLU:O	15:O:152:GLU:HB2	2.18	0.43
1:A:1596:U:H2'	1:A:1598:A:OP2	2.19	0.43
1:A:1925:G:OP1	30:4:29:ARG:NH2	2.52	0.43
1:A:1167:G:O2'	1:A:1168:C:H5'	2.19	0.43
19:S:113:HIS:O	19:S:145:LEU:HD12	2.19	0.43
17:Q:105:LEU:CD2	17:Q:137:LEU:HD21	2.49	0.43
1:A:64:G:H2'	1:A:65:C:O4'	2.19	0.43
1:A:2262:C:O5'	1:A:2262:C:H6	2.02	0.43
6:F:128:LEU:HD23	6:F:128:LEU:C	2.39	0.43
3:C:70:ALA:HA	3:C:71:PRO:HD3	1.81	0.43
4:D:104:GLU:HG3	37:D:8594:HOH:O	2.19	0.43
1:A:1869:A:H2'	1:A:1870:C:O4'	2.18	0.43
14:N:87:MET:HB2	14:N:91:ILE:CD1	2.49	0.42
24:X:122:ARG:CG	24:X:122:ARG:NH1	2.81	0.42
17:Q:115:SER:C	17:Q:117:SER:N	2.72	0.42
1:A:2812:A:N7	37:A:7054:HOH:O	2.36	0.42
13:M:145:LEU:HB2	37:M:8543:HOH:O	2.18	0.42
4:D:51:VAL:HG13	4:D:53:LEU:HD13	2.01	0.42
7:G:11:VAL:CG1	7:G:12:ASP:H	2.32	0.42
4:D:204:GLY:HA3	37:D:8660:HOH:O	2.18	0.42
1:A:1268:C:H2'	1:A:1269:G:C8	2.54	0.42
1:A:686:A:O2'	1:A:747:G:H4'	2.19	0.42
13:M:125:PHE:CE1	13:M:140:VAL:HG13	2.54	0.42
1:A:221:G:C6	1:A:222:A:C6	3.07	0.42
16:P:26:TRP:HA	16:P:26:TRP:CE3	2.54	0.42
1:A:1504:A:O2'	1:A:1506:U:OP2	2.33	0.42
19:S:111:ILE:HG23	19:S:145:LEU:CD1	2.49	0.42
1:A:2821:C:H4'	4:D:116:PRO:CB	2.49	0.42
2:B:3092:G:C6	2:B:3093:A:C6	3.08	0.42
10:J:167:ALA:HA	37:J:8373:HOH:O	2.19	0.42
7:G:162:PHE:CD1	7:G:162:PHE:N	2.86	0.42
24:X:73:LEU:HD12	24:X:73:LEU:HA	1.85	0.42
25:Y:70:ILE:HG23	25:Y:70:ILE:O	2.19	0.42
29:3:19:SER:HB3	37:3:4479:HOH:O	2.18	0.42
3:C:39:ALA:HB3	3:C:61:GLU:OE2	2.19	0.42
3:C:126:ALA:HB1	3:C:138:VAL:CG1	2.48	0.42
1:A:161:A:H3'	37:A:8917:HOH:O	2.18	0.42
1:A:1278:A:H4'	1:A:1279:U:C4	2.54	0.42
1:A:1199:A:C5	1:A:1200:A:C5	3.07	0.42
25:Y:7:GLU:HA	25:Y:74:ALA:O	2.18	0.42
20:T:57:THR:HG22	20:T:59:ASP:CB	2.49	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
15:O:71:TRP:CE3	15:O:175:LEU:CD2	2.96	0.42
13:M:145:LEU:HD23	13:M:145:LEU:O	2.18	0.42
6:F:146:LYS:HZ1	15:O:107:ASN:HD21	1.64	0.42
4:D:4:SER:O	4:D:5:ARG:HB2	2.20	0.42
4:D:260:HIS:HA	37:D:8633:HOH:O	2.18	0.42
6:F:76:ARG:O	6:F:77:ASP:HB2	2.19	0.42
3:C:192:VAL:O	3:C:207:GLN:HG2	2.19	0.42
1:A:2890:A:H2'	37:A:4745:HOH:O	2.19	0.42
3:C:191:GLY:HA2	3:C:194:MET:CE	2.50	0.42
37:A:9642:HOH:O	19:S:83:LYS:HB3	2.19	0.42
1:A:1634:G:H2'	1:A:1635:U:H6	1.84	0.42
1:A:1123:A:C2	1:A:1129:C:H4'	2.54	0.42
17:Q:16:VAL:CG1	17:Q:17:GLY:N	2.82	0.42
1:A:2569:A:H2'	1:A:2570:G:O5'	2.19	0.42
1:A:419:A:H1'	1:A:1921:A:C2	2.54	0.42
1:A:2598:U:O2	1:A:2600:A:C8	2.72	0.42
1:A:2108:A:O2'	1:A:2110:G:H5''	2.19	0.42
1:A:1707:G:N2	1:A:1709:G:H3'	2.34	0.42
1:A:123:U:H2'	1:A:124:C:C6	2.54	0.42
14:N:49:ALA:C	14:N:54:TYR:HB3	2.39	0.42
1:A:492:C:C2	1:A:501:G:N2	2.87	0.42
8:H:26:THR:HB	8:H:102:GLY:HA3	2.01	0.42
1:A:2846:C:H2'	1:A:2847:G:H8	1.83	0.42
4:D:98:THR:O	4:D:99:GLU:HG3	2.19	0.42
12:L:118:ALA:C	12:L:120:ARG:H	2.23	0.42
24:X:122:ARG:HG2	24:X:152:ALA:O	2.18	0.42
10:J:150:LYS:NZ	37:J:8380:HOH:O	2.48	0.42
1:A:1592:G:C5	1:A:1593:C:C4	3.06	0.42
29:3:40:ARG:HG3	29:3:45:ASN:CB	2.49	0.42
14:N:71:SER:O	14:N:73:ARG:NH1	2.49	0.42
27:1:30:GLU:CA	27:1:33:HIS:HB3	2.45	0.42
23:W:42:ASN:O	23:W:44:GLY:N	2.52	0.42
2:B:3048:C:H4'	15:O:141:ARG:NH2	2.29	0.42
4:D:304:PRO:HA	37:D:8536:HOH:O	2.19	0.42
1:A:951:A:O2'	1:A:952:G:H5'	2.19	0.42
2:B:3008:G:C6	2:B:3009:C:C4	3.07	0.42
1:A:1500:U:OP2	17:Q:41:ARG:NH2	2.52	0.42
1:A:816:G:C5	1:A:817:G:C6	3.08	0.42
3:C:179:MET:HG2	3:C:186:TRP:HB2	2.00	0.42
1:A:470:U:H2'	1:A:471:G:O4'	2.19	0.42
37:A:3971:HOH:O	3:C:11:ARG:NE	2.52	0.42
1:A:1825:U:O4'	1:A:1999:C:H5''	2.18	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2016:U:H6	1:A:2016:U:O5'	2.02	0.42
1:A:1754:A:H2'	1:A:1755:A:O4'	2.20	0.42
1:A:1790:C:H2'	1:A:1791:U:H6	1.84	0.42
1:A:1978:A:HO2'	1:A:1980:U:H6	1.66	0.42
1:A:940:G:O2'	1:A:1032:A:N1	2.51	0.42
12:L:58:THR:HG22	12:L:59:LYS:HG3	2.01	0.42
1:A:291:C:H2'	1:A:292:G:O4'	2.19	0.42
15:O:127:LEU:HA	15:O:127:LEU:HD12	1.85	0.42
1:A:236:A:H4'	1:A:237:G:OP1	2.19	0.42
4:D:53:LEU:HD11	4:D:327:VAL:HG22	2.02	0.42
4:D:221:GLN:NE2	12:L:42:ASN:HD22	2.10	0.42
1:A:182:G:O3'	14:N:157:LEU:HD13	2.18	0.42
1:A:407:A:H2'	1:A:408:A:C8	2.55	0.42
20:T:53:ASN:ND2	37:T:2190:HOH:O	2.53	0.42
1:A:2096:A:H2'	1:A:2539:U:O4'	2.20	0.42
17:Q:10:ALA:CA	17:Q:13:VAL:HG12	2.47	0.42
17:Q:11:ALA:HB2	17:Q:18:LYS:HA	2.01	0.42
1:A:1524:U:O2'	1:A:1525:G:P	2.77	0.42
1:A:929:A:N7	1:A:930:C:C4	2.87	0.42
1:A:392:U:H4'	14:N:193:LYS:HB3	2.02	0.42
37:A:5786:HOH:O	3:C:22:ARG:HG2	2.19	0.42
1:A:1931:A:H8	1:A:1931:A:O5'	2.02	0.42
1:A:2356:A:H2'	1:A:2357:G:O4'	2.19	0.42
4:D:57:GLU:HA	4:D:58:PRO:HD2	1.91	0.42
1:A:1338:U:H2'	1:A:1339:G:O4'	2.19	0.42
1:A:716:G:H2'	1:A:717:C:O5'	2.20	0.42
14:N:19:GLN:N	37:N:8563:HOH:O	2.52	0.42
14:N:63:VAL:HG21	14:N:109:PHE:CE1	2.55	0.42
30:4:65:THR:HG23	30:4:67:LEU:CG	2.42	0.42
1:A:2431:C:O2'	1:A:2432:C:H5'	2.19	0.42
6:F:95:THR:C	6:F:97:GLN:N	2.68	0.42
7:G:22:VAL:O	7:G:28:SER:HA	2.19	0.42
1:A:1069:C:H4'	1:A:1081:A:O2'	2.19	0.42
25:Y:76:ARG:HA	25:Y:82:GLU:O	2.19	0.42
1:A:515:C:H3'	37:A:5193:HOH:O	2.18	0.42
5:E:178:GLN:O	5:E:179:GLY:C	2.58	0.42
1:A:154:C:P	14:N:188:ARG:HH12	2.42	0.42
24:X:38:THR:O	24:X:42:ARG:HB2	2.20	0.42
1:A:2107:U:H6	1:A:2107:U:O5'	2.02	0.42
1:A:1471:A:H2'	1:A:1472:C:C6	2.54	0.42
5:E:173:LYS:HB3	5:E:187:ARG:HG3	2.01	0.42
1:A:1236:A:H2'	1:A:1237:U:O4'	2.19	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:F:35:ALA:HB2	37:F:5858:HOH:O	2.20	0.42
6:F:35:ALA:C	6:F:37:ALA:H	2.22	0.42
3:C:199:HIS:HD2	3:C:201:PHE:CB	2.22	0.42
10:J:55:GLN:HE22	10:J:91:HIS:CD2	2.38	0.42
1:A:1450:C:O2'	1:A:1493:A:H2'	2.20	0.42
1:A:1189:A:H3'	37:A:7218:HOH:O	2.20	0.42
15:O:77:ASN:OD1	15:O:80:SER:HB2	2.19	0.42
1:A:2382:A:OP1	30:4:80:ARG:HG2	2.19	0.42
1:A:844:A:C6	1:A:882:A:C5	3.07	0.42
1:A:690:G:H4'	1:A:741:C:O2	2.20	0.42
1:A:1789:G:O6	17:Q:73:HIS:HE1	2.02	0.42
1:A:2560:C:O2	37:A:9455:HOH:O	2.22	0.42
18:R:47:VAL:HA	18:R:48:PRO:HD3	1.82	0.42
1:A:2670:G:O2'	1:A:2671:U:H5'	2.20	0.42
14:N:115:LEU:HD13	14:N:116:ASN:HB2	2.00	0.42
1:A:2779:G:H1'	37:A:5650:HOH:O	2.19	0.42
1:A:711:G:C2	1:A:718:C:C2	3.07	0.42
1:A:1209:C:C2	1:A:1210:G:C8	3.07	0.42
12:L:106:GLY:HA3	37:L:5264:HOH:O	2.19	0.42
30:4:31:THR:HB	30:4:33:MET:CE	2.50	0.42
1:A:2453:G:H4'	13:M:50:GLY:C	2.40	0.42
3:C:153:ARG:CB	3:C:153:ARG:HH11	2.32	0.42
4:D:279:THR:HG22	4:D:280:VAL:N	2.34	0.42
1:A:1973:A:H5'	1:A:1973:A:H8	1.85	0.42
1:A:2090:G:H2'	1:A:2091:G:C8	2.55	0.42
1:A:2118:A:H2'	1:A:2119:C:H6	1.85	0.42
1:A:413:G:N3	1:A:428:G:C2	2.88	0.42
1:A:2377:U:H6	1:A:2377:U:O5'	2.02	0.42
1:A:226:A:H1'	1:A:393:G:C5	2.54	0.42
1:A:2263:G:C6	1:A:2264:A:C5	3.08	0.42
15:O:93:GLN:HG2	37:O:8558:HOH:O	2.19	0.42
5:E:57:PRO:HA	37:E:8317:HOH:O	2.19	0.42
2:B:3038:A:H2	2:B:3043:G:H5''	1.84	0.42
12:L:72:VAL:HG11	12:L:121:PHE:CD1	2.54	0.42
23:W:11:MET:HB3	23:W:15:GLU:HB2	2.00	0.42
15:O:86:LEU:HD12	15:O:125:ALA:CB	2.42	0.42
16:P:35:LYS:HD3	37:P:3360:HOH:O	2.20	0.42
5:E:127:ARG:NE	5:E:228:ALA:O	2.42	0.42
14:N:45:ARG:HB3	14:N:48:ARG:HB2	2.02	0.42
1:A:31:C:C2	37:A:5697:HOH:O	2.56	0.42
1:A:218:C:OP2	1:A:220:C:N4	2.47	0.42
1:A:657:G:H2'	1:A:658:C:C6	2.55	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
29:3:25:VAL:O	29:3:29:THR:HG23	2.20	0.42
12:L:66:ARG:HG2	12:L:66:ARG:HH11	1.85	0.42
19:S:17:MET:HE1	37:S:8530:HOH:O	2.18	0.42
1:A:1973:A:H2'	1:A:1974:G:O4'	2.20	0.42
13:M:73:VAL:HG11	13:M:118:LEU:HD21	2.01	0.42
1:A:1501:A:C6	1:A:1502:A:C6	3.07	0.42
1:A:1934:A:C8	1:A:1935:C:C5	3.08	0.42
1:A:1053:G:OP1	10:J:12:PRO:HG3	2.19	0.42
1:A:696:C:HO2'	1:A:697:G:H5'	1.84	0.42
9:I:71:LEU:C	9:I:73:ASP:H	2.22	0.42
1:A:2758:G:H2'	1:A:2759:C:C6	2.55	0.42
1:A:1456:C:H2'	1:A:1457:U:C6	2.55	0.42
1:A:472:A:O4'	1:A:774:C:H4'	2.19	0.42
15:O:49:THR:CG2	15:O:58:LEU:HD11	2.50	0.42
8:H:46:GLU:OE1	8:H:100:ASP:HA	2.19	0.42
1:A:2712:G:P	37:A:4776:HOH:O	2.78	0.42
1:A:1589:G:H4'	37:A:6394:HOH:O	2.20	0.42
1:A:1158:G:O2'	1:A:1159:G:H5'	2.20	0.42
6:F:94:ALA:HB3	6:F:174:VAL:CA	2.50	0.42
7:G:126:ILE:HB	7:G:131:LEU:HD23	2.01	0.42
1:A:332:G:H4'	21:U:2:LYS:O	2.19	0.42
3:C:105:VAL:HG11	3:C:154:ALA:CB	2.48	0.42
1:A:1730:G:C5'	1:A:1731:C:H6	2.32	0.42
1:A:1820:G:C6	1:A:2030:A:C2	3.08	0.42
26:Z:126:PRO:HG2	26:Z:128:PHE:CZ	2.54	0.42
6:F:169:THR:O	6:F:170:TYR:HB2	2.19	0.42
1:A:2564:G:OP2	1:A:2565:C:H5''	2.20	0.42
1:A:400:C:O2'	1:A:401:C:H5'	2.20	0.42
21:U:105:ASP:OD1	21:U:107:LYS:N	2.52	0.42
20:T:33:SER:OG	20:T:36:GLU:HG3	2.20	0.42
13:M:62:ALA:HB2	13:M:103:ALA:CB	2.50	0.42
17:Q:105:LEU:HD21	17:Q:137:LEU:HD21	2.01	0.42
19:S:61:GLN:CD	37:S:8541:HOH:O	2.57	0.42
1:A:1015:C:H2'	1:A:1016:U:C6	2.55	0.42
1:A:213:G:N2	1:A:225:G:H2'	2.35	0.42
1:A:217:C:OP1	1:A:395:A:O2'	2.30	0.42
1:A:1166:A:H2'	1:A:1166:A:N3	2.35	0.42
26:Z:185:VAL:HG12	37:Z:8572:HOH:O	2.19	0.42
6:F:48:MET:HA	6:F:49:PRO:HD3	1.77	0.42
15:O:67:ALA:C	15:O:69:TYR:N	2.73	0.42
1:A:840:U:H2'	19:S:128:ARG:HH12	1.83	0.42
6:F:93:LEU:HG	37:F:3862:HOH:O	2.20	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
17:Q:37:ARG:O	17:Q:41:ARG:HG3	2.20	0.42
1:A:1634:G:C6	1:A:1635:U:C4	3.07	0.42
5:E:55:ARG:NH2	28:2:56:GLU:OE2	2.34	0.42
1:A:2428:G:O6	1:A:2464:C:H1'	2.20	0.42
1:A:1549:C:N3	1:A:1637:A:C2	2.88	0.42
1:A:2623:G:C2'	1:A:2624:A:H5'	2.50	0.42
1:A:1804:A:H2'	1:A:1805:G:H8	1.85	0.42
1:A:315:G:C6	1:A:316:A:C6	3.08	0.42
1:A:2737:C:H2'	37:A:5688:HOH:O	2.19	0.42
27:1:46:LYS:NZ	37:1:8444:HOH:O	2.53	0.41
14:N:62:VAL:O	14:N:63:VAL:CG2	2.68	0.41
6:F:159:PRO:O	6:F:163:VAL:HG23	2.19	0.41
1:A:920:C:C4	1:A:2467:A:C5	3.07	0.41
12:L:45:PRO:HB2	37:L:7169:HOH:O	2.20	0.41
15:O:67:ALA:HA	15:O:71:TRP:HB3	2.02	0.41
20:T:23:LYS:HD3	20:T:65:VAL:HG12	2.01	0.41
6:F:67:ASP:O	6:F:69:ILE:HG13	2.19	0.41
6:F:92:GLU:O	6:F:93:LEU:O	2.38	0.41
1:A:331:A:C6	1:A:332:G:C4	3.07	0.41
6:F:77:ASP:HB3	6:F:78:GLU:H	1.59	0.41
1:A:177:A:C8	1:A:178:U:C5	3.08	0.41
37:A:3971:HOH:O	3:C:11:ARG:CZ	2.68	0.41
1:A:1788:U:C2	1:A:1805:G:N2	2.87	0.41
1:A:97:G:C2	21:U:107:LYS:HD2	2.55	0.41
37:A:5739:HOH:O	14:N:174:ARG:HD3	2.20	0.41
1:A:790:A:H2'	1:A:791:A:O4'	2.20	0.41
13:M:63:THR:HA	13:M:107:LYS:O	2.20	0.41
1:A:573:A:P	37:A:6582:HOH:O	2.78	0.41
1:A:397:A:P	37:A:3908:HOH:O	2.77	0.41
1:A:60:A:O2'	1:A:61:G:H5'	2.20	0.41
1:A:671:A:O2'	1:A:672:G:H2'	2.19	0.41
3:C:66:ARG:HB2	3:C:66:ARG:HH11	1.84	0.41
5:E:109:LEU:HD12	5:E:109:LEU:O	2.20	0.41
1:A:1815:A:H4'	1:A:2751:C:O4'	2.20	0.41
14:N:98:GLN:NE2	14:N:117:SER:O	2.52	0.41
1:A:2502:C:H2'	1:A:2503:A:C5'	2.49	0.41
1:A:1593:C:OP1	17:Q:117:SER:HB2	2.21	0.41
8:H:62:HIS:O	8:H:63:ILE:C	2.58	0.41
1:A:2547:C:OP2	4:D:5:ARG:NH1	2.53	0.41
26:Z:129:ASN:CG	26:Z:141:THR:OG1	2.58	0.41
1:A:445:U:C1'	37:A:6872:HOH:O	2.67	0.41
1:A:2300:A:H4'	1:A:2301:A:O5'	2.20	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
15:O:143:ARG:NH1	15:O:173:ASP:OD2	2.44	0.41
1:A:553:G:O2'	26:Z:179:PRO:HG3	2.21	0.41
1:A:2415:A:H2'	1:A:2416:G:H5'	2.01	0.41
28:2:21:ARG:HD2	28:2:39:PHE:HB2	2.02	0.41
2:B:3116:C:O2'	2:B:3117:G:H5'	2.21	0.41
1:A:1384:C:H5'	25:Y:30:MET:HG2	2.02	0.41
7:G:132:THR:HG23	7:G:132:THR:O	2.20	0.41
1:A:1339:G:C6	1:A:1340:G:N1	2.88	0.41
1:A:2697:A:H2'	1:A:2698:G:O4'	2.19	0.41
30:4:34:LYS:HB2	30:4:37:ASP:OD2	2.20	0.41
1:A:1759:A:N3	1:A:1818:C:H2'	2.35	0.41
10:J:85:ILE:O	10:J:85:ILE:HG23	2.20	0.41
10:J:86:ARG:H	10:J:86:ARG:HG2	1.44	0.41
14:N:88:VAL:O	14:N:88:VAL:HG12	2.20	0.41
1:A:2721:U:C4	1:A:2722:G:N7	2.89	0.41
4:D:60:SER:C	4:D:62:ARG:N	2.73	0.41
15:O:67:ALA:HA	15:O:71:TRP:H	1.85	0.41
1:A:319:A:H4'	1:A:338:C:C5	2.54	0.41
1:A:380:A:H5''	14:N:48:ARG:NH2	2.35	0.41
30:4:74:CYS:SG	30:4:76:LYS:CB	3.05	0.41
1:A:2911:C:H3'	37:A:5101:HOH:O	2.20	0.41
26:Z:184:GLU:OE1	26:Z:204:ARG:NH1	2.53	0.41
1:A:734:U:O2'	1:A:737:A:N6	2.53	0.41
1:A:1654:U:OP1	37:A:6956:HOH:O	2.22	0.41
13:M:98:GLU:O	13:M:99:GLU:HB2	2.19	0.41
3:C:114:ASP:HB2	3:C:117:LYS:HE2	2.01	0.41
1:A:482:G:H4'	1:A:508:A:N1	2.35	0.41
15:O:19:ASP:C	15:O:19:ASP:OD1	2.57	0.41
1:A:2424:U:H4'	18:R:6:PRO:HD2	2.02	0.41
1:A:2025:G:C6	1:A:2026:C:C4	3.08	0.41
1:A:195:C:H2'	1:A:196:G:H5'	2.02	0.41
11:K:135:ILE:O	11:K:139:LEU:HG	2.20	0.41
15:O:34:LEU:HD22	15:O:129:ILE:CD1	2.50	0.41
9:I:12:ILE:O	9:I:13:PRO:C	2.58	0.41
4:D:238:ASN:ND2	4:D:240:GLY:H	2.09	0.41
1:A:2781:U:H2'	1:A:2782:G:C5'	2.50	0.41
27:1:22:ILE:O	27:1:26:VAL:HG23	2.21	0.41
37:A:3328:HOH:O	21:U:9:LYS:HD3	2.21	0.41
1:A:263:U:C2	8:H:59:ILE:HD12	2.55	0.41
3:C:191:GLY:HA2	3:C:194:MET:HE3	2.03	0.41
28:2:28:HIS:O	28:2:32:LYS:N	2.49	0.41
1:A:655:U:O2'	16:P:3:THR:HB	2.20	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
37:A:9345:HOH:O	13:M:41:HIS:CE1	2.66	0.41
1:A:2405:C:P	37:A:6132:HOH:O	2.77	0.41
2:B:3093:A:C5	2:B:3094:G:H1'	2.56	0.41
1:A:2481:G:C3'	1:A:2482:G:H5''	2.51	0.41
1:A:757:C:H2'	1:A:758:A:C8	2.56	0.41
1:A:1059:G:C2	1:A:2072:G:N7	2.89	0.41
14:N:131:VAL:O	14:N:133:LEU:HD12	2.20	0.41
1:A:2385:G:H2'	1:A:2386:U:C6	2.56	0.41
1:A:1275:C:C2'	1:A:1276:U:H5'	2.50	0.41
1:A:912:A:C4	1:A:1294:A:C2	3.09	0.41
10:J:26:LYS:HD2	10:J:28:ILE:CB	2.50	0.41
1:A:2488:A:H61	1:A:2534:C:H42	1.69	0.41
6:F:81:GLU:C	6:F:83:PHE:N	2.74	0.41
25:Y:25:ARG:NH1	37:Y:3861:HOH:O	2.53	0.41
1:A:920:C:H5'	1:A:921:G:N3	2.35	0.41
1:A:2506:A:O2'	1:A:2507:G:P	2.79	0.41
11:K:46:ILE:O	11:K:46:ILE:CG1	2.65	0.41
1:A:2362:A:H2'	1:A:2363:G:C8	2.55	0.41
14:N:185:PRO:CG	14:N:189:VAL:HG11	2.49	0.41
1:A:1187:U:C3'	37:A:6434:HOH:O	2.68	0.41
30:4:40:ARG:HG3	30:4:52:PHE:CD2	2.55	0.41
14:N:85:ARG:NE	37:N:8519:HOH:O	2.47	0.41
1:A:2646:G:H1'	34:A:8523:CL:CL	2.57	0.41
21:U:63:ILE:HG22	21:U:63:ILE:O	2.20	0.41
1:A:2083:A:N6	11:K:90:LYS:HE2	2.35	0.41
1:A:2549:C:H1'	4:D:248:ARG:NH2	2.35	0.41
1:A:1019:C:P	37:A:3516:HOH:O	2.78	0.41
30:4:11:CYS:HB2	30:4:20:HIS:HE1	1.84	0.41
10:J:154:THR:HB	10:J:155:PRO:CD	2.50	0.41
1:A:2865:G:HO2'	1:A:2866:U:H5	1.69	0.41
1:A:10:U:O4	1:A:532:A:OP2	2.38	0.41
1:A:638:C:H2'	1:A:639:A:C8	2.55	0.41
25:Y:21:PRO:HG2	25:Y:24:LYS:HD3	2.03	0.41
1:A:290:C:O2'	1:A:291:C:H5'	2.20	0.41
1:A:696:C:C2'	1:A:697:G:H5'	2.50	0.41
11:K:56:LYS:HE2	11:K:60:ARG:NH2	2.36	0.41
1:A:2833:C:C2	1:A:2848:G:N2	2.89	0.41
1:A:772:G:H2'	1:A:773:A:O4'	2.21	0.41
10:J:165:GLY:C	10:J:166:ASN:HD22	2.24	0.41
24:X:122:ARG:CZ	37:X:5817:HOH:O	2.69	0.41
5:E:16:VAL:CG1	5:E:17:ASP:N	2.80	0.41
1:A:2467:A:O2'	1:A:2468:A:H2'	2.20	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1494:A:C2	1:A:1495:C:C4	3.08	0.41
6:F:67:ASP:N	6:F:67:ASP:OD1	2.53	0.41
6:F:167:GLU:OE2	6:F:173:GLU:HG2	2.19	0.41
6:F:173:GLU:O	6:F:174:VAL:C	2.59	0.41
6:F:135:VAL:HG21	6:F:139:TYR:CD1	2.56	0.41
14:N:81:ARG:HB3	14:N:86:MET:HG2	2.02	0.41
14:N:173:LEU:HA	14:N:183:VAL:HG11	2.03	0.41
1:A:2346:C:H4'	6:F:52:THR:HG22	2.03	0.41
1:A:134:U:N3	1:A:145:A:N1	2.68	0.41
5:E:214:THR:HG23	37:E:8443:HOH:O	2.21	0.41
1:A:1656:A:H2'	1:A:1657:A:O4'	2.21	0.41
1:A:1019:C:O2	18:R:94:GLN:NE2	2.54	0.41
1:A:1391:G:C5	1:A:1435:U:C4	3.08	0.41
1:A:244:C:OP2	8:H:38:LYS:HE3	2.21	0.41
1:A:1829:A:C2'	1:A:1830:C:H5'	2.50	0.41
15:O:33:ARG:NH2	37:O:8554:HOH:O	2.41	0.41
13:M:126:SER:O	13:M:127:GLU:C	2.57	0.41
1:A:2750:G:O5'	1:A:2750:G:H8	2.04	0.41
16:P:21:SER:OG	16:P:106:PRO:HB2	2.20	0.41
12:L:19:THR:HG22	12:L:20:CYS:N	2.35	0.41
1:A:245:C:H2'	1:A:246:G:H5'	2.01	0.41
1:A:2868:C:H2'	1:A:2869:G:O4'	2.21	0.41
1:A:567:U:O2'	1:A:568:G:H5'	2.20	0.41
10:J:56:ILE:HG21	10:J:61:LEU:CD1	2.51	0.41
6:F:23:VAL:CG2	6:F:73:VAL:HB	2.49	0.41
13:M:148:GLU:HG2	37:M:8556:HOH:O	2.20	0.41
1:A:2690:U:H4'	7:G:111:LYS:NZ	2.35	0.41
10:J:73:GLN:OE1	10:J:73:GLN:CA	2.68	0.41
1:A:2346:C:H4'	6:F:52:THR:CG2	2.50	0.41
1:A:383:A:C2	1:A:407:A:C4	3.08	0.41
1:A:2241:C:H2'	1:A:2242:U:C6	2.55	0.41
1:A:661:G:C6	1:A:686:A:C2	3.09	0.41
37:A:3756:HOH:O	26:Z:186:ARG:HD2	2.20	0.41
1:A:240:C:H2'	1:A:240:C:O2	2.21	0.41
17:Q:83:LYS:O	17:Q:86:ALA:HB3	2.21	0.41
1:A:314:G:N2	1:A:316:A:H3'	2.35	0.41
1:A:245:C:C2'	1:A:246:G:H5'	2.51	0.41
12:L:90:PHE:CD1	12:L:90:PHE:N	2.89	0.41
6:F:24:HIS:HB2	6:F:72:LYS:CB	2.51	0.41
1:A:1440:U:P	37:A:4027:HOH:O	2.79	0.41
2:B:3026:C:O2'	2:B:3027:C:H5'	2.20	0.41
1:A:2389:U:H4'	18:R:53:HIS:CD2	2.55	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
17:Q:91:LYS:O	17:Q:95:GLU:HG3	2.20	0.41
15:O:25:ARG:HA	15:O:28:LYS:HG3	2.02	0.41
37:A:9735:HOH:O	14:N:87:MET:HE3	2.20	0.41
1:A:566:A:H2'	1:A:567:U:O4'	2.21	0.41
24:X:154:ARG:HE	24:X:154:ARG:HB3	1.65	0.41
1:A:2004:U:H2'	1:A:2005:G:OP1	2.20	0.41
2:B:3040:C:N4	6:F:51:ARG:HB2	2.35	0.41
1:A:391:U:OP2	14:N:84:LYS:NZ	2.49	0.41
1:A:1187:U:H3'	37:A:6434:HOH:O	2.20	0.41
27:1:38:LYS:HD3	37:1:8425:HOH:O	2.20	0.41
15:O:74:PRO:HG2	15:O:159:TYR:CZ	2.56	0.41
5:E:165:ASP:O	5:E:168:ARG:HB3	2.21	0.41
4:D:7:ARG:NH1	4:D:11:LEU:HD21	2.36	0.41
24:X:14:HIS:HB2	24:X:17:ILE:HG13	2.02	0.41
1:A:1377:C:C6	1:A:1377:C:H5'	2.51	0.41
7:G:116:THR:HG22	7:G:151:LEU:HD22	2.03	0.41
14:N:20:ILE:O	14:N:24:MET:HG2	2.21	0.41
1:A:1444:G:O2'	1:A:1502:A:N1	2.44	0.41
13:M:72:ASN:HB2	37:M:8587:HOH:O	2.20	0.41
1:A:1051:C:H2'	1:A:1052:G:O4'	2.21	0.41
1:A:492:C:O2'	1:A:493:U:H5'	2.21	0.41
1:A:582:C:N4	37:A:5985:HOH:O	2.54	0.41
1:A:2450:C:H6	1:A:2450:C:O5'	2.03	0.41
3:C:111:SER:O	3:C:112:PRO:C	2.59	0.41
1:A:2735:U:H2'	1:A:2736:U:C6	2.55	0.41
1:A:198:A:H2'	37:A:5442:HOH:O	2.20	0.41
14:N:115:LEU:O	14:N:116:ASN:CB	2.68	0.41
1:A:2121:G:P	37:A:3085:HOH:O	2.67	0.41
27:1:46:LYS:HB2	27:1:57:CYS:SG	2.61	0.41
14:N:61:ILE:HA	37:N:8622:HOH:O	2.20	0.41
10:J:45:GLN:CB	10:J:163:PRO:HD2	2.25	0.41
6:F:102:GLY:O	6:F:134:LEU:HD12	2.21	0.41
1:A:1840:A:H4'	1:A:1841:C:O5'	2.21	0.41
15:O:47:LEU:HD23	15:O:47:LEU:HA	1.79	0.41
25:Y:25:ARG:CD	37:Y:3861:HOH:O	2.46	0.41
15:O:186:LEU:HD23	15:O:186:LEU:HA	1.88	0.41
11:K:45:VAL:CG2	11:K:46:ILE:N	2.83	0.41
1:A:171:C:OP2	14:N:84:LYS:HG3	2.21	0.41
14:N:69:LYS:HG2	14:N:127:LYS:HG3	2.01	0.41
3:C:103:VAL:HA	3:C:104:PRO:HD3	1.86	0.41
1:A:1188:A:C5	1:A:1189:A:C2	3.09	0.41
14:N:68:ARG:N	37:N:8544:HOH:O	2.51	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:941:G:C6	1:A:942:U:C4	3.08	0.41
1:A:2577:A:H4'	1:A:2578:G:C8	2.55	0.41
1:A:1773:G:C8	27:1:16:PRO:CA	3.04	0.41
1:A:308:U:H5'	21:U:97:ARG:NH2	2.36	0.41
7:G:91:PHE:HA	7:G:92:PRO:HD3	1.90	0.41
20:T:80:ARG:HG2	37:T:4527:HOH:O	2.20	0.41
1:A:2255:A:C6	1:A:2256:G:C5	3.08	0.41
9:I:64:ASN:N	9:I:64:ASN:ND2	2.67	0.41
1:A:1127:C:C2'	1:A:1128:U:H5'	2.50	0.41
1:A:1517:U:C2	1:A:1670:G:N2	2.89	0.41
1:A:834:G:H3'	1:A:835:U:H4'	2.03	0.41
1:A:432:G:N2	1:A:433:C:C2	2.89	0.41
1:A:128:A:C3'	1:A:128:A:C8	3.03	0.41
1:A:1565:C:O4'	1:A:2738:G:H1'	2.21	0.41
22:V:34:SER:O	22:V:38:ASN:ND2	2.54	0.41
4:D:224:LYS:HD3	4:D:224:LYS:HA	1.76	0.41
1:A:696:C:O2'	1:A:697:G:H5'	2.20	0.41
1:A:60:A:C2	1:A:61:G:C8	3.09	0.41
1:A:2039:A:H2'	1:A:2040:C:C6	2.56	0.41
19:S:89:LEU:HA	19:S:89:LEU:HD23	1.86	0.41
25:Y:27:ASP:N	25:Y:27:ASP:OD2	2.52	0.41
1:A:2900:G:H2'	1:A:2901:C:O4'	2.21	0.41
1:A:1624:A:H5'	1:A:1626:A:O4'	2.21	0.41
1:A:1821:A:O2'	1:A:1822:A:H5'	2.21	0.41
12:L:130:MET:SD	22:V:25:ASP:O	2.79	0.41
12:L:130:MET:SD	22:V:26:GLY:HA3	2.60	0.41
1:A:1021:G:O2'	1:A:1022:A:H5'	2.21	0.41
37:A:6119:HOH:O	2:B:3083:G:H4'	2.21	0.41
1:A:2691:A:H8	1:A:2691:A:OP1	2.04	0.41
1:A:2437:A:H2'	1:A:2438:G:C8	2.56	0.41
1:A:1064:U:H2'	1:A:1065:G:C8	2.56	0.41
1:A:1839:A:H5'	1:A:2643:G:H4'	2.03	0.41
21:U:69:LYS:O	21:U:71:VAL:HG23	2.21	0.41
1:A:542:A:C8	1:A:542:A:C5'	2.99	0.41
12:L:14:LYS:HD2	12:L:45:PRO:HG3	2.03	0.41
1:A:1666:C:H2'	1:A:1667:A:H8	1.86	0.41
11:K:46:ILE:CG1	11:K:53:ILE:HD13	2.51	0.41
1:A:1886:A:H4'	37:1:8405:HOH:O	2.21	0.41
4:D:312:ARG:HG2	4:D:313:PRO:O	2.20	0.41
4:D:51:VAL:HG21	4:D:327:VAL:HG13	2.03	0.41
1:A:157:G:H4'	14:N:95:LYS:CE	2.48	0.41
1:A:816:G:C6	1:A:817:G:C6	3.09	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2251:G:H2'	1:A:2252:A:H8	1.86	0.41
1:A:113:A:H3'	1:A:114:A:C5'	2.51	0.41
1:A:629:A:N7	37:A:9435:HOH:O	2.37	0.41
30:4:84:ARG:HB3	37:4:8550:HOH:O	2.21	0.41
1:A:2791:U:H4'	1:A:2792:A:OP1	2.21	0.41
1:A:646:G:H2'	1:A:647:U:H6	1.84	0.41
37:A:3579:HOH:O	4:D:48:MET:HB2	2.21	0.41
1:A:1339:G:C5	1:A:1340:G:C6	3.09	0.41
1:A:716:G:C2'	1:A:717:C:O5'	2.69	0.41
1:A:2323:G:H5'	37:A:6557:HOH:O	2.20	0.41
1:A:1946:C:H2'	1:A:1971:G:C8	2.56	0.41
1:A:1235:G:C1'	11:K:63:ILE:HG23	2.50	0.41
1:A:1976:G:O2'	1:A:1977:U:H5'	2.21	0.41
14:N:147:LEU:O	14:N:148:SER:C	2.60	0.41
1:A:2105:C:O2	1:A:2485:A:C6	2.74	0.41
1:A:34:C:C4	1:A:35:U:C4	3.09	0.41
14:N:35:PRO:HD2	14:N:38:VAL:CG2	2.51	0.40
14:N:39:ARG:CZ	37:N:8622:HOH:O	2.68	0.40
1:A:1751:G:C3'	1:A:1752:G:H5''	2.51	0.40
19:S:106:GLY:HA2	19:S:109:MET:CE	2.49	0.40
1:A:869:G:OP1	14:N:79:LYS:HE2	2.21	0.40
15:O:71:TRP:N	37:O:8539:HOH:O	2.54	0.40
7:G:143:GLN:NE2	37:G:2113:HOH:O	2.53	0.40
1:A:876:A:N7	1:A:878:G:H1'	2.36	0.40
7:G:84:MET:HB2	7:G:131:LEU:HB2	2.03	0.40
4:D:162:MET:CE	4:D:310:ARG:HD3	2.52	0.40
1:A:299:U:C5'	37:A:6872:HOH:O	2.63	0.40
1:A:2407:G:O2'	1:A:2408:A:H5'	2.21	0.40
28:2:28:HIS:CD2	28:2:30:LYS:HB2	2.55	0.40
1:A:1436:C:O2'	1:A:1437:A:H5'	2.21	0.40
1:A:2569:A:O5'	1:A:2569:A:H8	2.04	0.40
1:A:401:C:H2'	1:A:402:U:C6	2.56	0.40
16:P:96:VAL:HG13	16:P:100:GLN:HB2	2.03	0.40
1:A:2783:A:O2'	1:A:2784:A:H5'	2.20	0.40
25:Y:30:MET:HE3	25:Y:59:TRP:HE1	1.85	0.40
1:A:1241:G:H21	11:K:86:MET:CE	2.34	0.40
14:N:49:ALA:HB1	14:N:54:TYR:CB	2.51	0.40
1:A:1815:A:H2'	1:A:1816:C:O4'	2.21	0.40
1:A:100:C:H4'	21:U:16:LEU:HB2	2.03	0.40
1:A:675:U:O2'	5:E:42:ARG:NH1	2.53	0.40
4:D:109:LEU:HG	4:D:113:LEU:HD12	2.03	0.40
1:A:2667:G:H1'	1:A:2914:A:N3	2.35	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
18:R:41:LEU:HB3	18:R:52:PHE:CZ	2.56	0.40
1:A:1531:U:O2	1:A:1661:A:C2	2.74	0.40
25:Y:51:ASP:OD2	25:Y:52:PRO:HD2	2.21	0.40
5:E:136:VAL:HG22	5:E:137:PRO:HA	2.02	0.40
20:T:57:THR:CG2	20:T:58:MET:N	2.85	0.40
1:A:2422:U:OP1	37:A:6479:HOH:O	2.21	0.40
14:N:77:PHE:CD2	14:N:86:MET:HA	2.56	0.40
30:4:60:LYS:HG3	30:4:61:PRO:HD2	2.03	0.40
15:O:50:LEU:HA	15:O:50:LEU:HD12	1.84	0.40
1:A:1828:G:C2'	1:A:1829:A:H5'	2.51	0.40
5:E:95:GLU:H	5:E:95:GLU:CD	2.24	0.40
4:D:32:ASP:HA	37:D:8577:HOH:O	2.21	0.40
7:G:149:GLU:OE1	7:G:168:ILE:HG12	2.21	0.40
1:A:1352:A:N1	5:E:48:SER:HB3	2.36	0.40
1:A:2101:A:H5'	5:E:63:SER:HB3	2.04	0.40
2:B:3036:C:C5	2:B:3037:C:C5	3.09	0.40
24:X:122:ARG:HG2	24:X:122:ARG:NH1	2.27	0.40
15:O:35:VAL:HG12	15:O:37:ARG:HG2	2.02	0.40
2:B:3076:G:H2'	2:B:3077:A:OP1	2.21	0.40
29:3:41:HIS:O	29:3:45:ASN:HB2	2.20	0.40
4:D:255:GLY:O	4:D:257:THR:HG23	2.21	0.40
7:G:81:GLU:HA	7:G:133:VAL:O	2.20	0.40
1:A:2547:C:H2'	1:A:2548:C:H6	1.85	0.40
3:C:164:ARG:HA	27:1:69:TYR:CE1	2.57	0.40
1:A:664:U:O4	1:A:681:G:H5''	2.20	0.40
10:J:35:ASN:HD21	10:J:80:ASN:HA	1.84	0.40
14:N:46:LEU:HD22	14:N:50:ARG:HG3	2.02	0.40
10:J:72:VAL:HG13	10:J:72:VAL:O	2.20	0.40
1:A:2266:A:C5'	37:A:5407:HOH:O	2.68	0.40
15:O:82:TYR:OH	15:O:176:ARG:NH1	2.54	0.40
2:B:3092:G:H22	10:J:52:LYS:NZ	2.19	0.40
1:A:2681:A:H4'	1:A:2682:C:H5'	2.03	0.40
1:A:90:A:H2'	1:A:91:G:O4'	2.22	0.40
1:A:1076:G:C2	1:A:1084:C:C2	3.09	0.40
2:B:3113:C:H5''	37:B:2295:HOH:O	2.21	0.40
18:R:9:GLY:HA2	37:R:6663:HOH:O	2.20	0.40
24:X:90:TYR:N	37:X:6679:HOH:O	2.54	0.40
1:A:920:C:N4	1:A:2467:A:C8	2.89	0.40
4:D:145:HIS:CD2	4:D:146:THR:O	2.64	0.40
22:V:14:GLU:HA	22:V:15:PRO:HD2	1.94	0.40
4:D:307:ARG:CG	4:D:307:ARG:NH1	2.83	0.40
26:Z:234:VAL:HG12	26:Z:235:GLU:N	2.36	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2912:C:H2'	1:A:2913:A:O4'	2.22	0.40
1:A:2379:G:N7	1:A:2408:A:N1	2.70	0.40
2:B:3003:A:H61	2:B:3022:G:H1'	1.86	0.40
1:A:67:A:H5''	1:A:69:A:C8	2.57	0.40
1:A:1123:A:N6	1:A:1238:C:H5'	2.36	0.40
1:A:1522:A:H2'	1:A:1523:G:H5'	2.02	0.40
5:E:203:ALA:C	37:E:8423:HOH:O	2.60	0.40
1:A:10:U:HO2'	1:A:11:A:P	2.45	0.40
1:A:1983:C:O5'	1:A:1983:C:H6	2.05	0.40
16:P:41:ALA:HA	37:P:5104:HOH:O	2.21	0.40
1:A:1621:G:O2'	1:A:1622:G:H5'	2.22	0.40
1:A:1267:C:OP2	37:A:3759:HOH:O	2.22	0.40
15:O:44:ARG:HG3	15:O:45:ALA:N	2.36	0.40
26:Z:197:ASP:OD1	26:Z:199:ASP:HB2	2.21	0.40
27:1:39:CYS:HA	27:1:47:LEU:CG	2.51	0.40
27:1:57:CYS:O	27:1:61:GLY:N	2.52	0.40
14:N:61:ILE:CG2	14:N:62:VAL:N	2.84	0.40
6:F:27:ILE:HD11	6:F:37:ALA:HB3	2.03	0.40
2:B:3078:G:N2	2:B:3102:G:H2'	2.36	0.40
15:O:74:PRO:CD	15:O:159:TYR:CE2	3.04	0.40
6:F:86:THR:CG2	37:F:7477:HOH:O	2.69	0.40
2:B:3044:A:H1'	6:F:76:ARG:NH2	2.36	0.40
1:A:2379:G:H4'	1:A:2380:A:C5'	2.51	0.40
1:A:1652:C:O2	3:C:164:ARG:HD2	2.22	0.40
1:A:2731:G:H2'	1:A:2732:U:O4'	2.21	0.40
1:A:736:A:H2'	1:A:737:A:O4'	2.21	0.40
19:S:145:LEU:HD12	19:S:146:ILE:N	2.35	0.40
1:A:1025:C:H5'	24:X:23:MET:O	2.21	0.40
28:2:22:CYS:HB2	37:2:8423:HOH:O	2.22	0.40
5:E:4:THR:HB	5:E:135:GLU:OE1	2.21	0.40
1:A:688:A:H62	13:M:111:ALA:HB2	1.85	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	235/239 (98%)	207 (88%)	25 (11%)	3 (1%)	18	62
4	D	335/337 (99%)	303 (90%)	24 (7%)	8 (2%)	9	42
5	E	244/246 (99%)	224 (92%)	20 (8%)	0	100	100
6	F	134/176 (76%)	95 (71%)	27 (20%)	12 (9%)	1	5
7	G	170/177 (96%)	160 (94%)	10 (6%)	0	100	100
8	H	117/119 (98%)	103 (88%)	11 (9%)	3 (3%)	8	39
9	I	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
10	J	152/167 (91%)	132 (87%)	14 (9%)	6 (4%)	5	26
11	K	140/145 (97%)	131 (94%)	5 (4%)	4 (3%)	7	35
12	L	130/132 (98%)	120 (92%)	8 (6%)	2 (2%)	15	58
13	M	141/164 (86%)	118 (84%)	21 (15%)	2 (1%)	16	60
14	N	192/194 (99%)	170 (88%)	20 (10%)	2 (1%)	22	70
15	O	184/186 (99%)	163 (89%)	15 (8%)	6 (3%)	6	32
16	P	113/115 (98%)	106 (94%)	7 (6%)	0	100	100
17	Q	141/148 (95%)	137 (97%)	3 (2%)	1 (1%)	30	78
18	R	93/95 (98%)	84 (90%)	8 (9%)	1 (1%)	21	67
19	S	148/154 (96%)	138 (93%)	9 (6%)	1 (1%)	30	78
20	T	79/84 (94%)	73 (92%)	6 (8%)	0	100	100
21	U	117/119 (98%)	110 (94%)	7 (6%)	0	100	100
22	V	51/66 (77%)	47 (92%)	4 (8%)	0	100	100
23	W	63/70 (90%)	58 (92%)	3 (5%)	2 (3%)	6	33
24	X	152/154 (99%)	145 (95%)	6 (4%)	1 (1%)	30	78
25	Y	80/91 (88%)	70 (88%)	8 (10%)	2 (2%)	9	40
26	Z	140/240 (58%)	137 (98%)	3 (2%)	0	100	100
27	1	71/73 (97%)	62 (87%)	8 (11%)	1 (1%)	16	60
28	2	54/56 (96%)	50 (93%)	4 (7%)	0	100	100
29	3	42/48 (88%)	42 (100%)	0	0	100	100
30	4	90/92 (98%)	86 (96%)	2 (2%)	2 (2%)	10	45
All	All	3633/4235 (86%)	3295 (91%)	279 (8%)	59 (2%)	14	56

All (59) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	139	ASP
6	F	93	LEU
6	F	95	THR
6	F	137	PRO
6	F	173	GLU
8	H	101	ALA
10	J	162	SER
11	K	7	ASP
11	K	143	LYS
13	M	80	ASP
15	O	154	LEU
15	O	164	ASP
15	O	183	ASP
24	X	77	ALA
3	C	34	ASP
3	C	37	VAL
4	D	34	GLY
4	D	169	GLY
6	F	11	HIS
6	F	20	LYS
6	F	171	ASP
10	J	72	VAL
10	J	138	PRO
10	J	164	ALA
11	K	5	GLU
15	O	162	ASP
17	Q	116	SER
23	W	43	PRO
30	4	57	GLY
3	C	132	ASP
4	D	184	ASP
6	F	16	PRO
6	F	36	ASN
6	F	82	GLU
8	H	64	PRO
12	L	119	GLN
13	M	35	ARG
14	N	140	ALA
15	O	167	ASP
15	O	181	ASP
25	Y	77	PHE
27	1	81	LYS
30	4	56	PRO

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
6	F	61	PHE
6	F	147	ALA
8	H	61	MET
10	J	40	PRO
12	L	126	SER
4	D	185	GLY
4	D	2	GLN
4	D	107	SER
4	D	306	LYS
14	N	165	SER
23	W	40	PRO
11	K	78	ILE
18	R	54	PRO
10	J	140	PRO
19	S	81	PRO
25	Y	70	ILE

### 5.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	179/181 (99%)	167 (93%)	12 (7%)	23	64
4	D	282/282 (100%)	266 (94%)	16 (6%)	29	71
5	E	193/193 (100%)	176 (91%)	17 (9%)	14	48
6	F	117/147 (80%)	107 (92%)	10 (8%)	15	51
7	G	152/155 (98%)	146 (96%)	6 (4%)	43	85
8	H	92/92 (100%)	92 (100%)	0	100	100
9	I	27/283 (10%)	27 (100%)	0	100	100
10	J	122/122 (100%)	113 (93%)	9 (7%)	20	58
11	K	118/121 (98%)	107 (91%)	11 (9%)	13	45
12	L	106/106 (100%)	103 (97%)	3 (3%)	56	91
13	M	112/126 (89%)	109 (97%)	3 (3%)	57	91
14	N	166/166 (100%)	157 (95%)	9 (5%)	31	74
15	O	149/149 (100%)	143 (96%)	6 (4%)	42	84

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	P	93/93 (100%)	91 (98%)	2 (2%)	64	93
17	Q	113/116 (97%)	110 (97%)	3 (3%)	57	91
18	R	79/79 (100%)	75 (95%)	4 (5%)	33	76
19	S	117/121 (97%)	114 (97%)	3 (3%)	59	91
20	T	71/73 (97%)	71 (100%)	0	100	100
21	U	105/105 (100%)	103 (98%)	2 (2%)	69	94
22	V	44/52 (85%)	43 (98%)	1 (2%)	63	93
23	W	51/56 (91%)	50 (98%)	1 (2%)	68	94
24	X	130/130 (100%)	122 (94%)	8 (6%)	26	67
25	Y	66/73 (90%)	62 (94%)	4 (6%)	26	68
26	Z	120/195 (62%)	113 (94%)	7 (6%)	28	71
27	1	56/56 (100%)	51 (91%)	5 (9%)	14	48
28	2	46/46 (100%)	46 (100%)	0	100	100
29	3	42/44 (96%)	41 (98%)	1 (2%)	61	92
30	4	79/79 (100%)	74 (94%)	5 (6%)	25	66
All	All	3027/3441 (88%)	2879 (95%)	148 (5%)	35	78

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	3	ARG
3	C	33	GLU
3	C	36	ASP
3	C	55	VAL
3	C	68	ILE
3	C	69	LEU
3	C	94	LEU
3	C	120	ARG
3	C	131	HIS
3	C	153	ARG
3	C	179	MET
3	C	217	ARG
4	D	7	ARG
4	D	11	LEU
4	D	27	ASN
4	D	33	ASP
4	D	63	GLU

Continued on next page...



*Continued from previous page...*

Mol	Chain	Res	Type
4	D	97	LEU
4	D	98	THR
4	D	103	ASP
4	D	162	MET
4	D	234	ARG
4	D	245	SER
4	D	251	VAL
4	D	254	GLN
4	D	256	GLN
4	D	264	GLU
4	D	307	ARG
5	E	2	GLN
5	E	27	ARG
5	E	67	GLN
5	E	76	ARG
5	E	81	PRO
5	E	91	PRO
5	E	94	THR
5	E	101	ASP
5	E	115	LEU
5	E	136	VAL
5	E	187	ARG
5	E	214	THR
5	E	222	ASP
5	E	223	LEU
5	E	234	VAL
5	E	236	THR
5	E	240	LEU
6	F	24	HIS
6	F	50	VAL
6	F	61	PHE
6	F	99	ASP
6	F	100	ASP
6	F	131	THR
6	F	133	ASN
6	F	136	ARG
6	F	137	PRO
6	F	149	ARG
7	G	7	ILE
7	G	12	ASP
7	G	36	PRO
7	G	54	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
7	G	102	VAL
7	G	164	ASP
10	J	1	LYS
10	J	59	ASN
10	J	72	VAL
10	J	73	GLN
10	J	82	LYS
10	J	86	ARG
10	J	93	ILE
10	J	142	VAL
10	J	150	LYS
11	K	46	ILE
11	K	52	GLN
11	K	74	ARG
11	K	76	ASP
11	K	79	PHE
11	K	107	ASN
11	K	112	ASP
11	K	120	SER
11	K	125	SER
11	K	127	ILE
11	K	131	THR
12	L	7	ASP
12	L	10	GLN
12	L	98	VAL
13	M	35	ARG
13	M	80	ASP
13	M	117	GLU
14	N	38	VAL
14	N	46	LEU
14	N	48	ARG
14	N	68	ARG
14	N	81	ARG
14	N	87	MET
14	N	93	ARG
14	N	99	ARG
14	N	164	THR
15	O	26	LEU
15	O	43	VAL
15	O	127	LEU
15	O	128	ASP
15	O	152	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
15	O	163	PHE
16	P	3	THR
16	P	111	VAL
17	Q	52	LYS
17	Q	91	LYS
17	Q	98	ILE
18	R	11	ARG
18	R	54	PRO
18	R	57	ASP
18	R	95	GLU
19	S	13	THR
19	S	39	THR
19	S	82	GLU
21	U	39	ASN
21	U	73	HIS
22	V	9	CYS
23	W	43	PRO
24	X	4	LEU
24	X	35	VAL
24	X	52	VAL
24	X	73	LEU
24	X	122	ARG
24	X	142	ASP
24	X	146	ILE
24	X	154	ARG
25	Y	15	ARG
25	Y	27	ASP
25	Y	44	ASP
25	Y	72	VAL
26	Z	154	ARG
26	Z	163	THR
26	Z	172	THR
26	Z	189	ASN
26	Z	200	THR
26	Z	203	VAL
26	Z	235	GLU
27	1	11	THR
27	1	32	LYS
27	1	42	CYS
27	1	49	ARG
27	1	64	ILE
29	3	18	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
30	4	14	CYS
30	4	38	ARG
30	4	42	ARG
30	4	65	THR
30	4	74	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (88) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	47	HIS
3	C	92	ASN
3	C	127	GLN
3	C	199	HIS
4	D	27	ASN
4	D	145	HIS
4	D	191	ASN
4	D	238	ASN
4	D	260	HIS
4	D	332	ASN
5	E	2	GLN
5	E	39	GLN
5	E	129	HIS
6	F	47	GLN
6	F	103	ASN
6	F	133	ASN
7	G	106	ASN
7	G	143	GLN
8	H	80	GLN
9	I	17	GLN
9	I	64	ASN
10	J	8	ASN
10	J	35	ASN
10	J	55	GLN
10	J	58	HIS
10	J	59	ASN
10	J	69	ASN
10	J	74	ASN
10	J	80	ASN
10	J	91	HIS
10	J	129	ASN
10	J	130	HIS
10	J	137	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
10	J	166	ASN
11	K	52	GLN
11	K	107	ASN
11	K	126	ASN
12	L	10	GLN
12	L	42	ASN
13	M	18	HIS
13	M	41	HIS
13	M	58	GLN
13	M	116	HIS
14	N	26	HIS
14	N	58	GLN
14	N	89	ASN
14	N	176	GLN
15	O	107	ASN
15	O	140	GLN
15	O	153	GLN
17	Q	50	GLN
17	Q	66	GLN
17	Q	73	HIS
17	Q	118	GLN
18	R	16	ASN
18	R	40	HIS
19	S	61	GLN
19	S	94	ASN
19	S	98	ASN
19	S	113	HIS
19	S	117	HIS
19	S	123	GLN
20	T	53	ASN
21	U	39	ASN
22	V	38	ASN
22	V	39	ASN
23	W	60	GLN
24	X	27	HIS
24	X	28	HIS
24	X	87	HIS
24	X	110	GLN
24	X	119	HIS
24	X	125	HIS
24	X	141	HIS
25	Y	23	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
26	Z	134	HIS
26	Z	149	GLN
26	Z	189	ASN
28	2	8	GLN
28	2	16	HIS
28	2	28	HIS
29	3	16	ASN
29	3	18	ASN
29	3	41	HIS
29	3	45	ASN
30	4	13	HIS
30	4	30	GLN
30	4	48	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2747/2922 (94%)	247 (8%)	35 (1%)
2	B	121/122 (99%)	15 (12%)	6 (4%)
All	All	2868/3044 (94%)	262 (9%)	41 (1%)

All (262) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	11	A
1	A	31	C
1	A	60	A
1	A	67	A
1	A	69	A
1	A	70	A
1	A	71	G
1	A	87	C
1	A	88	G
1	A	114	A
1	A	115	U
1	A	120	A
1	A	130	C
1	A	139	C
1	A	141	C
1	A	151	A
1	A	166	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	169	A
1	A	186	A
1	A	191	A
1	A	192	A
1	A	200	U
1	A	219	G
1	A	237	G
1	A	271	C
1	A	272	A
1	A	273	G
1	A	283	U
1	A	284	C
1	A	285	A
1	A	308	U
1	A	309	C
1	A	318	C
1	A	336	G
1	A	337	A
1	A	345	G
1	A	358	G
1	A	381	G
1	A	397	A
1	A	417	G
1	A	457	U
1	A	461	C
1	A	487	G
1	A	498	A
1	A	510	U
1	A	511	A
1	A	514	G
1	A	537	G
1	A	538	C
1	A	539	G
1	A	542	A
1	A	545	G
1	A	553	G
1	A	559	U
1	A	588	G
1	A	604	G
1	A	620	A
1	A	632	A
1	A	644	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	660	A
1	A	688	A
1	A	701	U
1	A	717	C
1	A	759	C
1	A	777	U
1	A	809	G
1	A	821	U
1	A	835	U
1	A	840	U
1	A	858	U
1	A	868	G
1	A	869	G
1	A	871	G
1	A	872	U
1	A	875	A
1	A	877	G
1	A	878	G
1	A	884	C
1	A	885	G
1	A	898	G
1	A	905	C
1	A	921	G
1	A	923	A
1	A	953	G
1	A	960	G
1	A	961	A
1	A	1006	A
1	A	1008	C
1	A	1029	U
1	A	1045	G
1	A	1059	G
1	A	1060	C
1	A	1072	G
1	A	1081	A
1	A	1087	G
1	A	1088	A
1	A	1109	U
1	A	1110	G
1	A	1119	G
1	A	1130	U
1	A	1137	G

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	1151	G
1	A	1161	A
1	A	1162	G
1	A	1164	U
1	A	1165	G
1	A	1166	A
1	A	1171	A
1	A	1174	A
1	A	1175	G
1	A	1177	A
1	A	1185	U
1	A	1192	A
1	A	1193	A
1	A	1206	U
1	A	1208	C
1	A	1216	G
1	A	1237	U
1	A	1238	C
1	A	1239	G
1	A	1279	U
1	A	1289	C
1	A	1342	C
1	A	1353	C
1	A	1360	C
1	A	1377	C
1	A	1407	A
1	A	1451	C
1	A	1474	C
1	A	1485	A
1	A	1488	U
1	A	1505	U
1	A	1506	U
1	A	1524	U
1	A	1525	G
1	A	1526	A
1	A	1528	A
1	A	1564	C
1	A	1580	A
1	A	1592	G
1	A	1625	U
1	A	1626	A
1	A	1633	C

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	1634	G
1	A	1656	A
1	A	1667	A
1	A	1682	A
1	A	1684	A
1	A	1685	A
1	A	1692	C
1	A	1701	A
1	A	1710	A
1	A	1722	U
1	A	1723	G
1	A	1725	C
1	A	1731	C
1	A	1737	A
1	A	1752	G
1	A	1778	A
1	A	1798	C
1	A	1820	G
1	A	1829	A
1	A	1856	C
1	A	1879	U
1	A	1904	A
1	A	1919	A
1	A	1942	A
1	A	1943	C
1	A	1971	G
1	A	1973	A
1	A	1974	G
1	A	1978	A
1	A	1980	U
1	A	1982	C
1	A	1996	U
1	A	2008	U
1	A	2011	A
1	A	2012	U
1	A	2013	G
1	A	2033	G
1	A	2034	U
1	A	2064	U
1	A	2072	G
1	A	2073	G
1	A	2074	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	2096	A
1	A	2101	A
1	A	2102	G
1	A	2103	A
1	A	2104	C
1	A	2110	G
1	A	2238	A
1	A	2258	A
1	A	2271	G
1	A	2272	G
1	A	2291	A
1	A	2317	C
1	A	2321	A
1	A	2354	A
1	A	2361	A
1	A	2369	A
1	A	2422	U
1	A	2462	G
1	A	2467	A
1	A	2469	A
1	A	2476	C
1	A	2480	G
1	A	2483	A
1	A	2507	G
1	A	2511	A
1	A	2527	U
1	A	2533	C
1	A	2537	G
1	A	2540	G
1	A	2541	U
1	A	2553	A
1	A	2564	G
1	A	2589	U
1	A	2601	A
1	A	2602	G
1	A	2608	C
1	A	2613	G
1	A	2638	G
1	A	2649	A
1	A	2664	A
1	A	2681	A
1	A	2682	C

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	2726	U
1	A	2747	C
1	A	2748	G
1	A	2749	U
1	A	2750	G
1	A	2762	C
1	A	2768	A
1	A	2786	G
1	A	2792	A
1	A	2800	A
1	A	2811	A
1	A	2812	A
1	A	2825	C
1	A	2840	A
1	A	2850	C
1	A	2876	G
1	A	2890	A
1	A	2896	A
1	A	2903	C
1	A	2914	A
2	B	3002	U
2	B	3003	A
2	B	3004	G
2	B	3014	G
2	B	3022	G
2	B	3024	U
2	B	3041	C
2	B	3043	G
2	B	3044	A
2	B	3052	A
2	B	3057	A
2	B	3066	G
2	B	3077	A
2	B	3114	G
2	B	3122	C

All (41) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	10	U
1	A	129	A
1	A	284	C

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	338	C
1	A	603	A
1	A	644	G
1	A	699	C
1	A	716	G
1	A	834	G
1	A	857	A
1	A	871	G
1	A	877	G
1	A	898	G
1	A	1080	C
1	A	1164	U
1	A	1237	U
1	A	1246	A
1	A	1352	A
1	A	1377	C
1	A	1450	C
1	A	1563	G
1	A	1667	A
1	A	1856	C
1	A	1942	A
1	A	1979	G
1	A	2011	A
1	A	2102	G
1	A	2103	A
1	A	2313	C
1	A	2467	A
1	A	2526	C
1	A	2649	A
1	A	2718	C
1	A	2761	A
1	A	2791	U
2	B	3002	U
2	B	3003	A
2	B	3023	U
2	B	3043	G
2	B	3065	A
2	B	3103	A

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 234 ligands modelled in this entry, 233 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
31	CAI	A	4000	1	62,62,62	2.78	21 (33%)	90,90,90	1.80	28 (31%)

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
31	CAI	A	4000	1	-	0/66/110/110	0/2/4/4

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	4000	CAI	C2-C3	-12.70	1.29	1.53
31	A	4000	CAI	C6-C5	-6.37	1.40	1.52
31	A	4000	CAI	C20-C21	5.62	1.71	1.49
31	A	4000	CAI	O3-C3	5.35	1.55	1.46
31	A	4000	CAI	C2A-C3A	4.65	1.62	1.53
31	A	4000	CAI	O21-C21	4.58	1.52	1.19
31	A	4000	CAI	C4A-C5A	4.36	1.60	1.52
31	A	4000	CAI	O4B-C4B	3.80	1.52	1.45
31	A	4000	CAI	C5-C4	3.43	1.58	1.52
31	A	4000	CAI	C2-C1	-3.41	1.43	1.50
31	A	4000	CAI	C6A-C5A	-3.21	1.43	1.51
31	A	4000	CAI	C8-C9	-3.08	1.46	1.50
31	A	4000	CAI	C4A-C3A	-2.67	1.47	1.53

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	4000	CAI	O12-C13	2.58	1.49	1.45
31	A	4000	CAI	O3-C17	2.58	1.41	1.35
31	A	4000	CAI	O3B-C3B	2.47	1.49	1.44
31	A	4000	CAI	O1A-C1A	2.45	1.48	1.41
31	A	4000	CAI	C13-C12	2.44	1.52	1.46
31	A	4000	CAI	C4-C3	-2.42	1.47	1.52
31	A	4000	CAI	C12-C11	2.37	1.58	1.50
31	A	4000	CAI	O5B-C1B	2.25	1.48	1.42

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	4000	CAI	O21-C21-C20	-5.29	102.86	125.14
31	A	4000	CAI	C5-C4-C3	4.43	121.25	113.33
31	A	4000	CAI	C7-C6-C5	3.84	121.51	111.58
31	A	4000	CAI	C19-O4-C4	-3.50	105.09	114.56
31	A	4000	CAI	C3C-C2C-C1C	-3.31	107.78	114.19
31	A	4000	CAI	C4A-C3A-N3A	-3.27	103.71	111.70
31	A	4000	CAI	O3-C17-O17	-3.24	116.34	122.90
31	A	4000	CAI	C15-O15-C1	-2.96	114.19	117.98
31	A	4000	CAI	O5A-C5A-C6A	-2.85	100.42	106.70
31	A	4000	CAI	O1B-C4A-C5A	2.81	114.03	106.75
31	A	4000	CAI	O4B-C1C-O1C	2.65	130.75	123.65
31	A	4000	CAI	O4B-C1C-C2C	-2.63	106.36	111.43
31	A	4000	CAI	C22-C8-C7	-2.62	106.12	111.45
31	A	4000	CAI	C1B-O1B-C4A	-2.61	109.33	114.67
31	A	4000	CAI	O3-C3-C2	2.60	113.42	106.67
31	A	4000	CAI	O3B-C3B-C2B	2.54	113.98	108.03
31	A	4000	CAI	C3-C2-C1	2.50	119.30	112.60
31	A	4000	CAI	C12-C11-C10	-2.47	119.64	125.14
31	A	4000	CAI	C3B-C4B-C5B	2.44	115.58	111.16
31	A	4000	CAI	C6-C20-C21	-2.35	107.39	116.25
31	A	4000	CAI	C20-C6-C5	2.29	117.15	110.77
31	A	4000	CAI	C6-C5-C4	2.27	117.24	113.59
31	A	4000	CAI	C22-C8-C9	2.18	113.20	109.65
31	A	4000	CAI	C15-C14-C13	-2.17	109.53	114.45
31	A	4000	CAI	O1B-C4A-C3A	-2.14	103.56	108.73
31	A	4000	CAI	C1A-O5A-C5A	-2.07	110.10	113.55
31	A	4000	CAI	C3-O3-C17	2.06	120.84	117.47
31	A	4000	CAI	C2-C3-C4	2.01	121.53	113.68

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	2754/2922 (94%)	-0.24	25 (0%) 81 24	25, 51, 97, 142	0
2	B	122/122 (100%)	0.03	5 (4%) 35 7	33, 69, 99, 152	0
3	C	237/239 (99%)	-0.04	1 (0%) 90 41	30, 64, 95, 112	0
4	D	337/337 (100%)	-0.20	0 100 100	24, 57, 84, 96	0
5	E	246/246 (100%)	-0.24	0 100 100	23, 50, 74, 84	0
6	F	140/176 (79%)	0.67	8 (5%) 23 5	63, 104, 122, 128	0
7	G	172/177 (97%)	0.12	0 100 100	41, 68, 90, 94	0
8	H	119/119 (100%)	0.33	1 (0%) 83 26	63, 81, 102, 108	0
9	I	29/348 (8%)	0.73	0 100 100	77, 93, 100, 104	0
10	J	156/167 (93%)	-0.04	0 100 100	36, 57, 84, 93	0
11	K	142/145 (97%)	-0.18	0 100 100	30, 50, 75, 84	0
12	L	132/132 (100%)	-0.18	0 100 100	34, 56, 79, 85	0
13	M	145/164 (88%)	0.16	0 100 100	30, 75, 106, 114	0
14	N	194/194 (100%)	0.04	8 (4%) 35 7	36, 56, 95, 105	0
15	O	186/186 (100%)	0.34	9 (4%) 29 6	45, 74, 112, 124	0
16	P	115/115 (100%)	-0.09	0 100 100	40, 57, 75, 79	0
17	Q	143/148 (96%)	0.05	0 100 100	40, 61, 77, 84	0
18	R	95/95 (100%)	-0.22	0 100 100	36, 50, 65, 79	0
19	S	150/154 (97%)	-0.24	0 100 100	31, 45, 67, 75	0
20	T	81/84 (96%)	0.04	1 (1%) 75 20	48, 66, 86, 89	0
21	U	119/119 (100%)	0.07	1 (0%) 83 26	44, 62, 88, 100	0
22	V	53/66 (80%)	1.66	22 (41%) 1 0	84, 96, 103, 112	0
23	W	65/70 (92%)	0.47	2 (3%) 47 9	56, 81, 111, 116	0
24	X	154/154 (100%)	-0.25	0 100 100	32, 46, 65, 74	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	Y	82/91 (90%)	0.06	0 <span>100</span> <span>100</span>	41, 59, 85, 100	0
26	Z	142/240 (59%)	-0.16	0 <span>100</span> <span>100</span>	27, 46, 69, 87	0
27	1	73/73 (100%)	1.87	30 (41%) <span>1</span> <span>0</span>	82, 97, 105, 106	0
28	2	56/56 (100%)	-0.38	0 <span>100</span> <span>100</span>	28, 38, 45, 49	0
29	3	46/48 (95%)	0.02	0 <span>100</span> <span>100</span>	38, 68, 89, 104	0
30	4	92/92 (100%)	3.31	77 (83%) <span>0</span> <span>0</span>	94, 109, 114, 119	0
All	All	6577/7279 (90%)	-0.02	190 (2%) <span>50</span> <span>9</span>	23, 57, 104, 152	0

All (190) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
30	4	37	ASP	8.4
30	4	38	ARG	7.6
30	4	41	GLU	7.1
2	B	3001	U	6.8
27	1	11	THR	6.5
30	4	11	CYS	6.2
27	1	12	GLY	5.7
30	4	39	GLN	5.7
27	1	21	LYS	5.5
30	4	32	GLY	5.5
1	A	735	C	5.4
27	1	23	ARG	5.3
30	4	34	LYS	5.2
27	1	15	GLY	5.2
30	4	31	THR	5.2
30	4	33	MET	5.1
30	4	30	GLN	5.1
1	A	1173	A	5.1
30	4	84	ARG	5.0
30	4	71	CYS	5.0
1	A	1171	A	4.9
27	1	26	VAL	4.8
30	4	77	ALA	4.8
30	4	35	TRP	4.7
30	4	40	ARG	4.7
30	4	76	LYS	4.7
14	N	70	GLY	4.6
27	1	25	ARG	4.6
30	4	56	PRO	4.6

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
27	1	20	LEU	4.5
30	4	20	HIS	4.5
30	4	29	ARG	4.5
30	4	42	ARG	4.4
30	4	23	GLU	4.4
23	W	1	THR	4.4
14	N	71	SER	4.3
27	1	13	ARG	4.2
30	4	14	CYS	4.2
27	1	22	ILE	4.2
30	4	68	LYS	4.2
27	1	19	GLY	4.1
1	A	1172	G	4.1
27	1	45	LYS	4.1
30	4	26	ARG	4.1
30	4	62	THR	4.1
1	A	1199	A	4.1
27	1	30	GLU	4.0
27	1	31	ILE	4.0
30	4	81	GLU	4.0
27	1	10	ARG	3.9
30	4	22	VAL	3.9
30	4	82	GLY	3.9
1	A	1198	U	3.9
30	4	21	GLU	3.9
30	4	47	GLY	3.9
27	1	16	PRO	3.8
30	4	45	GLY	3.8
30	4	8	ASN	3.8
27	1	18	TYR	3.7
30	4	83	TRP	3.7
30	4	67	LEU	3.7
30	4	91	GLN	3.7
27	1	34	LYS	3.7
30	4	51	LYS	3.5
27	1	35	LYS	3.5
27	1	44	PHE	3.3
30	4	9	THR	3.3
1	A	1175	G	3.3
30	4	58	GLY	3.3
1	A	736	A	3.3
14	N	89	ASN	3.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
30	4	16	GLU	3.3
27	1	27	ALA	3.2
30	4	36	ILE	3.2
15	O	179	LEU	3.2
27	1	24	VAL	3.2
30	4	1	MET	3.2
22	V	55	ALA	3.2
30	4	74	CYS	3.2
27	1	17	ARG	3.2
30	4	59	ASP	3.2
30	4	10	TYR	3.2
8	H	90	GLU	3.2
27	1	39	CYS	3.2
30	4	6	ARG	3.1
30	4	78	HIS	3.1
30	4	24	LYS	3.1
30	4	61	PRO	3.1
22	V	52	THR	3.0
22	V	4	ARG	3.0
22	V	51	TRP	3.0
30	4	18	GLN	3.0
30	4	60	LYS	3.0
30	4	27	SER	3.0
30	4	28	GLY	3.0
14	N	90	ARG	2.9
30	4	3	MET	2.9
30	4	75	GLY	2.9
22	V	48	ASN	2.9
6	F	63	ILE	2.9
6	F	57	THR	2.8
22	V	47	ARG	2.8
1	A	1951	G	2.8
22	V	49	LEU	2.8
2	B	3024	U	2.8
27	1	38	LYS	2.8
1	A	1169	U	2.8
27	1	28	ASP	2.8
1	A	1170	U	2.7
27	1	14	PHE	2.7
30	4	53	SER	2.7
15	O	186	LEU	2.7
30	4	12	PRO	2.7

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
21	U	119	ALA	2.7
1	A	2004	U	2.7
30	4	46	ILE	2.7
14	N	81	ARG	2.7
22	V	41	ASP	2.7
2	B	3002	U	2.6
22	V	12	ASP	2.6
30	4	85	ALA	2.6
30	4	86	GLY	2.6
15	O	184	ILE	2.6
22	V	9	CYS	2.6
30	4	2	GLN	2.6
3	C	64	ASP	2.6
30	4	65	THR	2.6
30	4	43	ASN	2.6
30	4	4	PRO	2.6
22	V	50	GLU	2.6
27	1	37	HIS	2.5
30	4	52	PHE	2.5
30	4	15	ASN	2.5
27	1	42	CYS	2.5
22	V	11	THR	2.5
30	4	44	SER	2.5
22	V	40	ALA	2.5
6	F	88	LEU	2.4
30	4	5	ARG	2.4
1	A	1177	A	2.4
1	A	1168	C	2.4
30	4	80	ARG	2.4
15	O	152	GLU	2.3
22	V	53	ASP	2.3
22	V	54	THR	2.3
6	F	18	ILE	2.3
22	V	24	LYS	2.3
6	F	56	ARG	2.3
1	A	1279	U	2.3
30	4	72	GLY	2.3
6	F	15	GLU	2.3
30	4	55	VAL	2.3
1	A	284	C	2.3
30	4	19	GLU	2.3
14	N	74	ARG	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
6	F	17	ARG	2.2
1	A	282	C	2.2
27	1	36	LYS	2.2
22	V	36	CYS	2.2
30	4	49	ASP	2.2
14	N	80	GLY	2.2
30	4	70	ARG	2.2
6	F	10	PHE	2.2
22	V	46	ALA	2.2
15	O	178	THR	2.2
15	O	147	ILE	2.2
2	B	3122	C	2.2
2	B	3023	U	2.2
30	4	25	VAL	2.1
15	O	150	TYR	2.1
1	A	2433	A	2.1
15	O	155	GLU	2.1
1	A	2432	C	2.1
1	A	960	G	2.1
22	V	6	CYS	2.1
22	V	56	ARG	2.1
30	4	87	ARG	2.1
1	A	2237	G	2.1
20	T	81	ILE	2.1
1	A	285	A	2.1
30	4	92	GLU	2.1
1	A	1925	G	2.1
15	O	181	ASP	2.1
14	N	82	ARG	2.1
30	4	69	TYR	2.1
22	V	43	GLY	2.0
1	A	1181	A	2.0
22	V	39	ASN	2.0
1	A	1190	G	2.0
23	W	52	ALA	2.0

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

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

## 6.3 Carbohydrates

There are no carbohydrates in this entry.

## 6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
33	NA	A	8384	1/1	2.21	65.65	109,109,109,109	0
33	NA	A	8363	1/1	0.52	61.40	56,56,56,56	0
35	K	A	8603	1/1	0.39	44.64	67,67,67,67	0
33	NA	A	8360	1/1	0.57	43.83	36,36,36,36	0
32	MG	A	8092	1/1	0.48	33.75	115,115,115,115	0
33	NA	B	8383	1/1	0.82	32.84	103,103,103,103	0
33	NA	A	8310	1/1	0.40	30.13	42,42,42,42	0
32	MG	A	8090	1/1	0.25	26.22	67,67,67,67	0
33	NA	A	8371	1/1	0.35	25.78	56,56,56,56	0
33	NA	A	8364	1/1	0.40	25.20	53,53,53,53	0
34	CL	A	8515	1/1	0.35	24.11	92,92,92,92	0
33	NA	A	8370	1/1	0.27	21.90	39,39,39,39	0
32	MG	A	8024	1/1	0.56	21.53	81,81,81,81	0
32	MG	A	8104	1/1	0.28	21.43	54,54,54,54	0
33	NA	A	8306	1/1	0.28	21.40	65,65,65,65	0
33	NA	A	8374	1/1	0.60	19.65	75,75,75,75	0
33	NA	A	8377	1/1	0.27	18.09	71,71,71,71	0
33	NA	A	8372	1/1	0.68	17.77	71,71,71,71	0
32	MG	A	8022	1/1	0.53	17.05	56,56,56,56	0
33	NA	A	8373	1/1	0.60	17.04	71,71,71,71	0
33	NA	A	8385	1/1	0.23	16.99	34,34,34,34	0
33	NA	A	8379	1/1	0.34	16.33	44,44,44,44	0
35	K	A	8601	1/1	0.34	16.04	62,62,62,62	0
33	NA	A	8318	1/1	0.34	14.61	42,42,42,42	0
33	NA	A	8378	1/1	0.53	14.47	37,37,37,37	0
33	NA	A	8329	1/1	0.24	14.33	64,64,64,64	0
34	CL	A	8523	1/1	0.27	13.89	56,56,56,56	0
32	MG	A	8103	1/1	0.28	13.36	57,57,57,57	0
33	NA	A	8356	1/1	0.34	13.13	52,52,52,52	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
33	NA	J	8322	1/1	0.42	13.00	59,59,59,59	0
34	CL	A	8503	1/1	0.32	12.98	63,63,63,63	0
33	NA	A	8342	1/1	0.20	12.59	60,60,60,60	0
33	NA	A	8354	1/1	0.28	12.27	44,44,44,44	0
32	MG	A	8070	1/1	0.37	11.44	62,62,62,62	0
32	MG	A	8064	1/1	0.31	11.19	23,23,23,23	0
33	NA	A	8313	1/1	0.27	10.62	75,75,75,75	0
32	MG	A	8042	1/1	0.26	9.51	46,46,46,46	0
33	NA	A	8361	1/1	0.29	9.05	63,63,63,63	0
34	CL	S	8506	1/1	0.28	8.86	48,48,48,48	0
33	NA	A	8362	1/1	0.27	8.76	56,56,56,56	0
32	MG	A	8119	1/1	0.23	8.63	19,19,19,19	0
34	CL	D	8519	1/1	0.42	7.99	71,71,71,71	0
33	NA	A	8359	1/1	0.39	7.93	64,64,64,64	0
32	MG	A	8118	1/1	0.32	7.51	22,22,22,22	0
33	NA	A	8314	1/1	0.27	7.42	35,35,35,35	0
33	NA	A	8340	1/1	0.28	7.42	42,42,42,42	0
33	NA	N	8365	1/1	0.45	7.09	50,50,50,50	0
33	NA	A	8350	1/1	0.21	6.84	38,38,38,38	0
34	CL	A	8505	1/1	0.40	6.80	95,95,95,95	0
33	NA	A	8326	1/1	0.40	6.11	61,61,61,61	0
33	NA	A	8316	1/1	0.21	5.99	53,53,53,53	0
34	CL	A	8522	1/1	0.31	5.83	83,83,83,83	0
33	NA	A	8323	1/1	0.23	5.76	53,53,53,53	0
33	NA	A	8321	1/1	0.27	5.71	50,50,50,50	0
33	NA	A	8303	1/1	0.21	5.62	43,43,43,43	0
33	NA	A	8339	1/1	0.24	5.21	33,33,33,33	0
33	NA	A	8355	1/1	0.34	4.94	54,54,54,54	0
31	CAI	A	4000	59/59	0.22	4.86	40,47,60,62	0
32	MG	A	8097	1/1	0.19	4.57	29,29,29,29	0
32	MG	A	8116	1/1	0.25	4.48	85,85,85,85	0
32	MG	A	8050	1/1	0.26	4.40	85,85,85,85	0
33	NA	A	8352	1/1	0.24	4.28	46,46,46,46	0
33	NA	A	8382	1/1	0.21	4.19	59,59,59,59	0
32	MG	A	8044	1/1	0.23	4.11	70,70,70,70	0
33	NA	A	8332	1/1	0.23	3.82	57,57,57,57	0
34	CL	R	8511	1/1	0.39	3.19	84,84,84,84	0
34	CL	M	8510	1/1	0.56	3.18	108,108,108,108	0
33	NA	A	8349	1/1	0.18	2.96	56,56,56,56	0
32	MG	A	8102	1/1	0.56	2.60	109,109,109,109	0
33	NA	A	8301	1/1	0.18	2.58	19,19,19,19	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
34	CL	P	8508	1/1	0.33	2.52	91,91,91,91	0
33	NA	T	8312	1/1	0.30	2.49	61,61,61,61	0
33	NA	A	8308	1/1	0.18	2.46	53,53,53,53	0
33	NA	A	8325	1/1	0.17	2.37	60,60,60,60	0
32	MG	A	8108	1/1	0.20	2.29	67,67,67,67	0
33	NA	S	8337	1/1	0.30	2.28	40,40,40,40	0
32	MG	A	8067	1/1	0.19	2.04	57,57,57,57	0
32	MG	A	8091	1/1	0.18	1.96	53,53,53,53	0
32	MG	A	8089	1/1	0.18	1.90	64,64,64,64	0
33	NA	A	8328	1/1	0.18	1.46	47,47,47,47	0
33	NA	A	8327	1/1	0.17	1.42	27,27,27,27	0
32	MG	A	8041	1/1	0.19	1.24	68,68,68,68	0
32	MG	A	8114	1/1	0.45	1.12	97,97,97,97	0
32	MG	A	8047	1/1	0.17	1.09	41,41,41,41	0
32	MG	A	8049	1/1	0.23	1.04	81,81,81,81	0
33	NA	A	8341	1/1	0.20	0.96	44,44,44,44	0
33	NA	A	8331	1/1	0.17	0.65	46,46,46,46	0
33	NA	A	8375	1/1	0.24	0.56	54,54,54,54	0
34	CL	A	8512	1/1	0.18	0.50	39,39,39,39	0
32	MG	A	8060	1/1	0.16	0.36	62,62,62,62	0
32	MG	A	8013	1/1	0.16	0.35	56,56,56,56	0
33	NA	A	8307	1/1	0.14	0.27	34,34,34,34	0
33	NA	A	8319	1/1	0.28	0.25	49,49,49,49	0
32	MG	A	8075	1/1	0.15	0.20	33,33,33,33	0
32	MG	A	8098	1/1	0.18	0.15	23,23,23,23	0
33	NA	A	8335	1/1	0.16	0.15	61,61,61,61	0
32	MG	A	8040	1/1	0.16	0.06	124,124,124,124	0
35	K	A	8602	1/1	0.21	0.06	69,69,69,69	0
33	NA	A	8367	1/1	0.13	-0.01	50,50,50,50	0
33	NA	A	8369	1/1	0.31	-0.09	60,60,60,60	0
34	CL	A	8516	1/1	0.18	-0.10	43,43,43,43	0
32	MG	C	8105	1/1	0.36	-0.12	40,40,40,40	0
32	MG	A	8106	1/1	0.16	-0.12	59,59,59,59	0
33	NA	A	8338	1/1	0.17	-0.15	79,79,79,79	0
34	CL	C	8509	1/1	0.20	-0.21	82,82,82,82	0
32	MG	A	8093	1/1	0.14	-0.38	37,37,37,37	0
33	NA	A	8366	1/1	0.13	-0.44	45,45,45,45	0
33	NA	A	8324	1/1	0.14	-0.49	61,61,61,61	0
32	MG	A	8088	1/1	0.15	-0.51	24,24,24,24	0
36	CD	4	8404	1/1	0.75	-0.51	202,202,202,202	0
34	CL	K	8521	1/1	0.14	-0.64	43,43,43,43	0
32	MG	A	8100	1/1	0.12	-0.70	65,65,65,65	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
34	CL	A	8514	1/1	0.14	-0.72	57,57,57,57	0
32	MG	4	8078	1/1	0.49	-0.82	74,74,74,74	0
33	NA	A	8302	1/1	0.13	-0.92	27,27,27,27	0
32	MG	A	8086	1/1	0.11	-0.93	44,44,44,44	0
32	MG	A	8011	1/1	0.12	-0.95	24,24,24,24	0
34	CL	A	8517	1/1	0.17	-1.02	52,52,52,52	0
33	NA	A	8333	1/1	0.12	-1.14	37,37,37,37	0
33	NA	E	8304	1/1	0.13	-1.19	43,43,43,43	0
33	NA	K	8346	1/1	0.14	-1.22	27,27,27,27	0
32	MG	A	8101	1/1	0.14	-1.26	59,59,59,59	0
34	CL	K	8501	1/1	0.12	-1.28	50,50,50,50	0
33	NA	M	8380	1/1	0.13	-1.30	52,52,52,52	0
32	MG	A	8081	1/1	0.14	-1.40	44,44,44,44	0
34	CL	O	8507	1/1	0.17	-1.43	58,58,58,58	0
32	MG	A	8043	1/1	0.13	-1.47	52,52,52,52	0
32	MG	A	8074	1/1	0.07	-1.53	12,12,12,12	0
32	MG	A	8087	1/1	0.11	-1.56	41,41,41,41	0
33	NA	A	8334	1/1	0.09	-1.58	30,30,30,30	0
34	CL	N	8518	1/1	0.17	-1.66	51,51,51,51	0
33	NA	J	8309	1/1	0.08	-1.68	21,21,21,21	0
34	CL	4	8504	1/1	0.36	-1.70	98,98,98,98	0
36	CD	1	8403	1/1	0.20	-1.71	180,180,180,180	0
32	MG	A	8107	1/1	0.07	-1.73	40,40,40,40	0
32	MG	Z	8109	1/1	0.13	-1.75	42,42,42,42	0
32	MG	D	8055	1/1	0.08	-1.76	77,77,77,77	0
32	MG	U	8073	1/1	0.15	-1.84	40,40,40,40	0
34	CL	A	8513	1/1	0.12	-1.85	60,60,60,60	0
33	NA	A	8320	1/1	0.12	-1.86	35,35,35,35	0
32	MG	A	8068	1/1	0.05	-1.90	52,52,52,52	0
33	NA	A	8330	1/1	0.09	-1.93	39,39,39,39	0
32	MG	A	8003	1/1	0.12	-2.01	14,14,14,14	0
36	CD	2	8402	1/1	0.06	-2.11	60,60,60,60	0
33	NA	B	8351	1/1	0.09	-2.24	44,44,44,44	0
32	MG	A	8012	1/1	0.09	-2.39	25,25,25,25	0
36	CD	V	8401	1/1	0.34	-2.39	202,202,202,202	0
33	NA	A	8317	1/1	0.09	-2.43	27,27,27,27	0
33	NA	A	8336	1/1	0.15	-2.56	49,49,49,49	0
32	MG	A	8066	1/1	0.07	-2.58	66,66,66,66	0
33	NA	A	8353	1/1	0.09	-2.58	32,32,32,32	0
33	NA	C	8345	1/1	0.14	-2.63	43,43,43,43	0
32	MG	A	8053	1/1	0.12	-2.65	45,45,45,45	0
32	MG	A	8037	1/1	0.11	-2.69	30,30,30,30	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
34	CL	K	8502	1/1	0.09	-2.91	48,48,48,48	0
32	MG	A	8094	1/1	0.13	-2.92	63,63,63,63	0
32	MG	A	8001	1/1	0.11	-2.94	30,30,30,30	0
33	NA	A	8305	1/1	0.09	-2.98	20,20,20,20	0
33	NA	A	8381	1/1	0.11	-3.02	42,42,42,42	0
32	MG	A	8099	1/1	0.10	-3.06	51,51,51,51	0
32	MG	A	8079	1/1	0.11	-3.10	56,56,56,56	0
32	MG	A	8117	1/1	0.10	-3.23	17,17,17,17	0
32	MG	A	8056	1/1	0.07	-3.24	40,40,40,40	0
32	MG	A	8082	1/1	0.13	-3.29	63,63,63,63	0
32	MG	A	8058	1/1	0.10	-3.30	57,57,57,57	0
32	MG	C	8065	1/1	0.05	-3.47	48,48,48,48	0
33	NA	R	8348	1/1	0.07	-3.54	23,23,23,23	0
32	MG	A	8039	1/1	0.08	-3.55	76,76,76,76	0
32	MG	A	8062	1/1	0.11	-3.80	80,80,80,80	0
32	MG	A	8111	1/1	0.11	-3.81	47,47,47,47	0
33	NA	A	8311	1/1	0.08	-3.81	34,34,34,34	0
32	MG	A	8005	1/1	0.11	-3.85	41,41,41,41	0
33	NA	A	8315	1/1	0.12	-3.87	40,40,40,40	0
32	MG	A	8002	1/1	0.09	-3.88	25,25,25,25	0
32	MG	A	8057	1/1	0.10	-3.92	48,48,48,48	0
32	MG	A	8063	1/1	0.09	-3.93	67,67,67,67	0
33	NA	A	8357	1/1	0.07	-3.97	60,60,60,60	0
33	NA	A	8368	1/1	0.09	-3.99	41,41,41,41	0
32	MG	A	8027	1/1	0.05	-4.06	69,69,69,69	0
32	MG	A	8046	1/1	0.07	-4.07	48,48,48,48	0
32	MG	A	8014	1/1	0.10	-4.15	14,14,14,14	0
34	CL	Z	8520	1/1	0.12	-4.17	39,39,39,39	0
32	MG	A	8015	1/1	0.10	-4.17	43,43,43,43	0
33	NA	N	8347	1/1	0.10	-4.21	25,25,25,25	0
32	MG	A	8076	1/1	0.08	-4.39	76,76,76,76	0
32	MG	A	8030	1/1	0.09	-4.47	19,19,19,19	0
32	MG	A	8038	1/1	0.06	-4.49	33,33,33,33	0
32	MG	A	8051	1/1	0.07	-4.59	57,57,57,57	0
33	NA	U	8343	1/1	0.06	-4.84	18,18,18,18	0
32	MG	A	8006	1/1	0.06	-4.91	61,61,61,61	0
32	MG	A	8032	1/1	0.05	-5.18	23,23,23,23	0
32	MG	A	8008	1/1	0.05	-5.32	46,46,46,46	0
32	MG	A	8048	1/1	0.07	-5.41	54,54,54,54	0
32	MG	A	8007	1/1	0.10	-5.54	25,25,25,25	0
32	MG	A	8035	1/1	0.06	-5.58	49,49,49,49	0
32	MG	A	8010	1/1	0.07	-5.71	48,48,48,48	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
36	CD	P	8405	1/1	0.07	-5.87	136,136,136,136	0
32	MG	A	8033	1/1	0.04	-5.89	19,19,19,19	0
32	MG	L	8069	1/1	0.05	-6.08	78,78,78,78	0
32	MG	A	8019	1/1	0.05	-6.15	34,34,34,34	0
32	MG	A	8080	1/1	0.05	-6.20	31,31,31,31	0
32	MG	A	8059	1/1	0.10	-6.21	35,35,35,35	0
32	MG	A	8045	1/1	0.10	-6.32	50,50,50,50	0
32	MG	A	8061	1/1	0.05	-6.43	33,33,33,33	0
32	MG	A	8018	1/1	0.09	-6.50	43,43,43,43	0
32	MG	A	8110	1/1	0.07	-6.57	41,41,41,41	0
32	MG	A	8115	1/1	0.12	-6.60	47,47,47,47	0
32	MG	A	8004	1/1	0.05	-6.70	52,52,52,52	0
33	NA	A	8344	1/1	0.05	-6.73	24,24,24,24	0
32	MG	A	8112	1/1	0.07	-6.75	52,52,52,52	0
32	MG	A	8021	1/1	0.07	-6.78	19,19,19,19	0
32	MG	A	8071	1/1	0.08	-6.97	66,66,66,66	0
32	MG	A	8031	1/1	0.05	-7.40	32,32,32,32	0
32	MG	A	8017	1/1	0.04	-7.50	24,24,24,24	0
32	MG	A	8096	1/1	0.08	-7.53	48,48,48,48	0
32	MG	A	8072	1/1	0.10	-7.57	83,83,83,83	0
32	MG	A	8020	1/1	0.06	-7.68	33,33,33,33	0
32	MG	A	8028	1/1	0.04	-7.79	34,34,34,34	0
32	MG	A	8085	1/1	0.10	-7.98	77,77,77,77	0
32	MG	A	8025	1/1	0.03	-8.43	41,41,41,41	0
32	MG	A	8054	1/1	0.09	-8.92	42,42,42,42	0
32	MG	A	8009	1/1	0.05	-9.28	24,24,24,24	0
32	MG	A	8077	1/1	0.07	-9.86	21,21,21,21	0
32	MG	A	8016	1/1	0.11	-10.27	59,59,59,59	0
32	MG	A	8034	1/1	0.04	-10.66	15,15,15,15	0
32	MG	A	8029	1/1	0.12	-10.87	36,36,36,36	0
32	MG	A	8052	1/1	0.08	-10.90	43,43,43,43	0
32	MG	A	8023	1/1	0.07	-11.32	29,29,29,29	0
32	MG	A	8026	1/1	0.04	-11.69	12,12,12,12	0
32	MG	A	8083	1/1	0.07	-12.63	44,44,44,44	0
32	MG	A	8084	1/1	0.06	-13.51	40,40,40,40	0
32	MG	B	8095	1/1	0.07	-15.53	67,67,67,67	0
32	MG	A	8036	1/1	0.06	-18.56	28,28,28,28	0
32	MG	A	8113	1/1	0.31	-	45,45,45,45	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.