



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 08:29 am GMT

PDB ID : 3CC2  
Title : The Refined Crystal Structure of the Haloarcula Marismortui Large Ribosomal Subunit at 2.4 Angstrom Resolution with rrnA Sequence for the 23S rRNA and Genome-derived Sequences for r-Proteins  
Authors : Gurel, G.; Blaha, G.  
Deposited on : 2008-02-23  
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

---

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

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

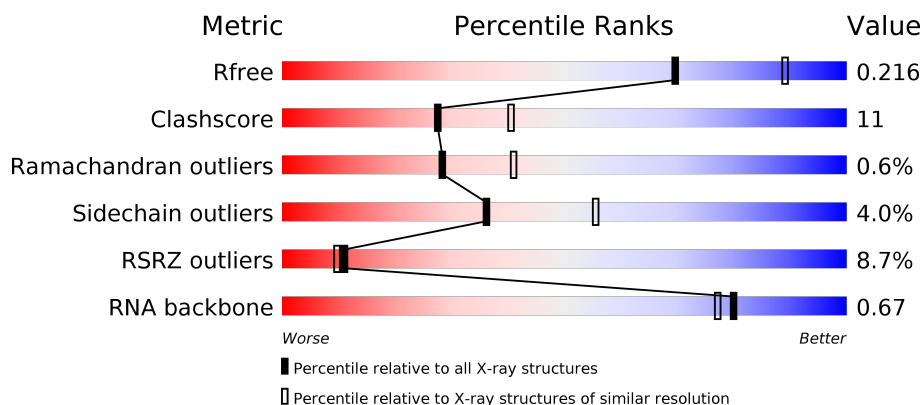
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)
RNA backbone	2435	1034 (2.86-1.94)

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

Mol	Chain	Length	Quality of chain
1	A	240	<div> <div>9%</div> <div>70%</div> <div>26%</div> <div>..</div> </div>
2	B	338	<div> <div>12%</div> <div>71%</div> <div>25%</div> <div>.</div> </div>
3	C	246	<div> <div>6%</div> <div>75%</div> <div>21%</div> <div>.</div> </div>
4	D	177	<div> <div>49%</div> <div>47%</div> <div>29%</div> <div>21%</div> </div>

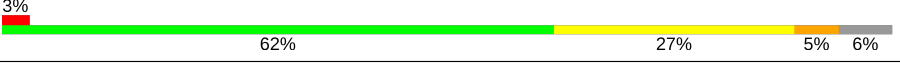

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	178	
6	F	120	
7	G	348	
8	H	177	
9	I	162	
10	J	145	
11	K	132	
12	L	165	
13	M	196	
14	N	187	
15	O	116	
16	P	149	
17	Q	96	
18	R	155	
19	S	85	
20	T	120	
21	U	67	
22	V	71	
23	W	154	
24	X	92	
25	Y	241	
26	Z	116	
27	1	57	
28	2	50	
29	3	92	

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
30	0	2923	
31	9	122	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	MG	0	8060	-	-	-	X
32	MG	0	8064	-	-	-	X
32	MG	0	8066	-	-	-	X
34	NA	0	8302	-	-	-	X
34	NA	0	8303	-	-	-	X
34	NA	0	8305	-	-	-	X
34	NA	0	8320	-	-	-	X
34	NA	0	8323	-	-	-	X
34	NA	0	8325	-	-	-	X
34	NA	0	8326	-	-	-	X
34	NA	0	8327	-	-	-	X
34	NA	0	8331	-	-	-	X
34	NA	0	8335	-	-	-	X
34	NA	0	8340	-	-	-	X
34	NA	0	8350	-	-	-	X
34	NA	0	8356	-	-	-	X
34	NA	0	8359	-	-	-	X
34	NA	0	8362	-	-	-	X
34	NA	0	8364	-	-	-	X
34	NA	0	8366	-	-	-	X
34	NA	0	8368	-	-	-	X
34	NA	0	8371	-	-	-	X
34	NA	0	8372	-	-	-	X
34	NA	0	8374	-	-	-	X
34	NA	0	8376	-	-	-	X
34	NA	0	8378	-	-	-	X
34	NA	0	8379	-	-	-	X
34	NA	R	8386	-	-	-	X

## 2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 99049 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L2P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	0	0
			1753	1072	352	324	5			

- Molecule 2 is a protein called 50S ribosomal protein L3P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	337	Total	C	N	O	S	0	0	0
			2625	1616	493	511	5			

- Molecule 3 is a protein called 50S ribosomal protein L4P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	246	Total	C	N	O	S	0	0	0
			1860	1130	345	384	1			

- Molecule 4 is a protein called 50S ribosomal protein L5P.

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

- Molecule 5 is a protein called 50S ribosomal protein L6P.

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

- Molecule 6 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	119	Total	C	N	O	S	0	0	0
			890	551	141	197	1			

- Molecule 7 is a protein called 50S ribosomal protein L10E.

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

- Molecule 8 is a protein called 50S ribosomal protein L10e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	160	Total	C	N	O	S	0	0	0
			1282	798	240	238	6			

- Molecule 9 is a protein called 50S ribosomal protein L11P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	70	Total	C	N	O	S	0	0	0
			519	323	81	114	1			

- Molecule 10 is a protein called 50S ribosomal protein L13P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	142	Total	C	N	O	S	0	0	0
			1120	696	199	222	3			

- Molecule 11 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	132	Total	C	N	O	S	0	0	0
			994	609	189	192	4			

- Molecule 12 is a protein called 50S ribosomal protein L15P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	L	145	Total	C	N	O	0	0	0
			1118	670	222	226			

- Molecule 13 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	194	Total	C	N	O	S	0	0	0
			1558	943	333	281	1			

- Molecule 14 is a protein called 50S ribosomal protein L18P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	186	Total	C	N	O	S	0	0	0
			1445	895	262	286	2			

- Molecule 15 is a protein called 50S ribosomal protein L18e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	115	Total	C	N	O		0	0	0
			865	529	161	175				

- Molecule 16 is a protein called 50S ribosomal protein L19e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	143	Total	C	N	O		0	0	0
			1136	683	229	224				

- Molecule 17 is a protein called 50S ribosomal protein L21e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	95	Total	C	N	O		0	0	0
			735	450	141	144				

- Molecule 18 is a protein called 50S ribosomal protein L22P.

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

- Molecule 19 is a protein called 50S ribosomal protein L23P.

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

- Molecule 20 is a protein called 50S ribosomal protein L24P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	119	Total	C	N	O		0	0	0
			950	568	180	202				

- Molecule 21 is a protein called 50S ribosomal protein L24e.

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

- Molecule 22 is a protein called 50S ribosomal protein L29P.

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

- Molecule 23 is a protein called 50S ribosomal protein L30P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	W	154	Total	C	N	O	S	0	0	0
			1196	737	209	244	6			

- Molecule 24 is a protein called 50S ribosomal protein L31e.

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

- Molecule 25 is a protein called 50S ribosomal protein L32e.

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

- Molecule 26 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	73	Total	C	N	O	S	0	0	0
			573	343	113	112	5			

- Molecule 27 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 28 is a protein called 50S ribosomal protein L39e.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 29 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 30 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	0	2754	Total	C	N	O	P	0	0	0
			59021	26349	10873	19054	2745			

- Molecule 31 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	9	122	Total	C	N	O	P	0	0	0
			2599	1160	471	847	121			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	0	109	Total	Mg	0	0
			109	109		
32	9	1	Total	Mg	0	0
			1	1		
32	K	1	Total	Mg	0	0
			1	1		
32	B	1	Total	Mg	0	0
			1	1		
32	A	1	Total	Mg	0	0
			1	1		
32	T	1	Total	Mg	0	0
			1	1		
32	Y	1	Total	Mg	0	0
			1	1		
32	3	1	Total	Mg	0	0
			1	1		

- Molecule 33 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	0	2	Total K 2 2	0	0

- Molecule 34 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	0	73	Total Na 73 73	0	0
34	J	1	Total Na 1 1	0	0
34	Q	1	Total Na 1 1	0	0
34	H	1	Total Na 1 1	0	0
34	C	1	Total Na 1 1	0	0
34	A	1	Total Na 1 1	0	0
34	R	2	Total Na 2 2	0	0
34	9	3	Total Na 3 3	0	0
34	L	1	Total Na 1 1	0	0
34	S	1	Total Na 1 1	0	0
34	M	1	Total Na 1 1	0	0

- Molecule 35 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	10	Total Cl 10 10	0	0
35	J	3	Total Cl 3 3	0	0
35	B	1	Total Cl 1 1	0	0
35	A	1	Total Cl 1 1	0	0
35	N	1	Total Cl 1 1	0	0
35	O	1	Total Cl 1 1	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	R	1	Total 1	Cl 1	0	0
35	Y	1	Total 1	Cl 1	0	0
35	L	1	Total 1	Cl 1	0	0
35	3	1	Total 1	Cl 1	0	0
35	M	1	Total 1	Cl 1	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	O	1	Total 1	Cd 1	0	0
36	Z	1	Total 1	Cd 1	0	0
36	1	1	Total 1	Cd 1	0	0
36	3	1	Total 1	Cd 1	0	0
36	U	1	Total 1	Cd 1	0	0

- Molecule 37 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	0	5949	Total 5949	O 5949	0	0
37	A	117	Total 117	O 117	0	0
37	B	146	Total 146	O 146	0	0
37	C	170	Total 170	O 170	0	0
37	D	47	Total 47	O 47	0	0
37	E	42	Total 42	O 42	0	0
37	F	24	Total 24	O 24	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	G	19	Total 19	O 19	0	0
37	H	72	Total 72	O 72	0	0
37	I	9	Total 9	O 9	0	0
37	J	51	Total 51	O 51	0	0
37	K	56	Total 56	O 56	0	0
37	L	72	Total 72	O 72	0	0
37	M	119	Total 119	O 119	0	0
37	N	65	Total 65	O 65	0	0
37	O	39	Total 39	O 39	0	0
37	P	63	Total 63	O 63	0	0
37	Q	52	Total 52	O 52	0	0
37	R	80	Total 80	O 80	0	0
37	S	33	Total 33	O 33	0	0
37	T	38	Total 38	O 38	0	0
37	U	27	Total 27	O 27	0	0
37	V	14	Total 14	O 14	0	0
37	W	66	Total 66	O 66	0	0
37	X	29	Total 29	O 29	0	0
37	Y	94	Total 94	O 94	0	0
37	Z	26	Total 26	O 26	0	0
37	1	53	Total 53	O 53	0	0

*Continued on next page...*

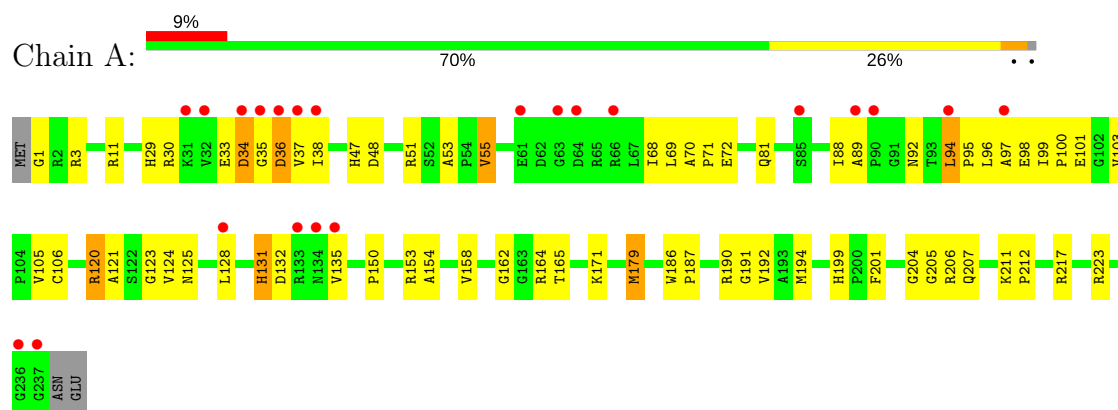
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	2	40	Total 40	O 40	0	0
37	3	72	Total 72	O 72	0	0
37	9	139	Total 139	O 139	0	0

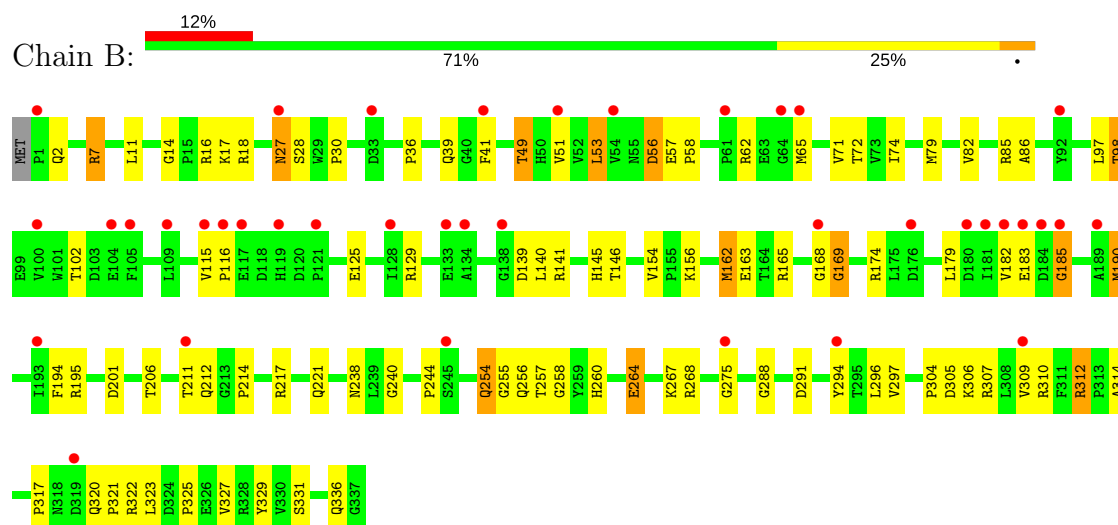
### 3 Residue-property plots [i](#)

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

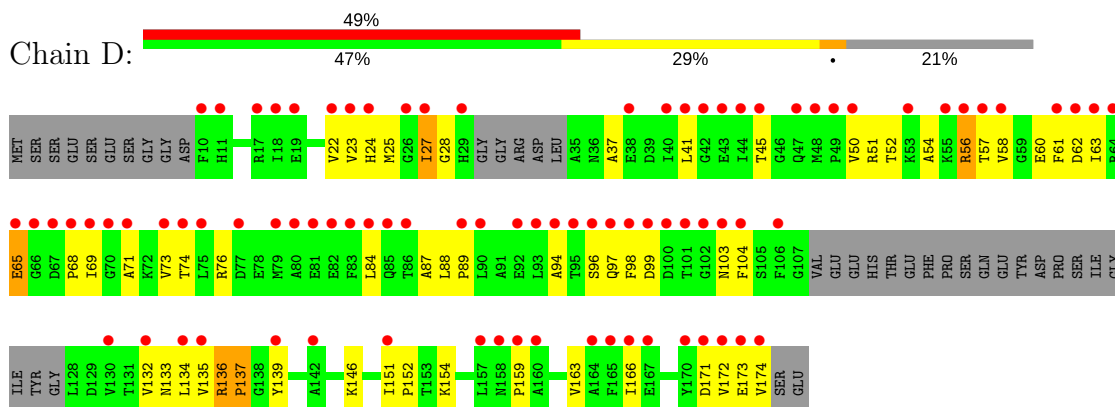
#### • Molecule 1: 50S ribosomal protein L2P



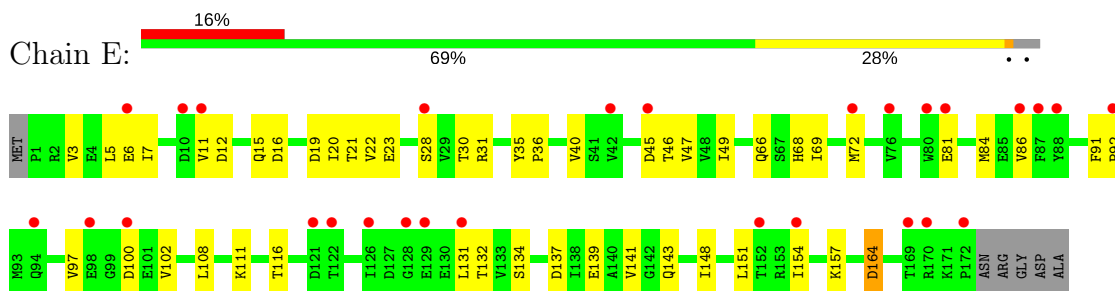
#### • Molecule 2: 50S ribosomal protein L3P



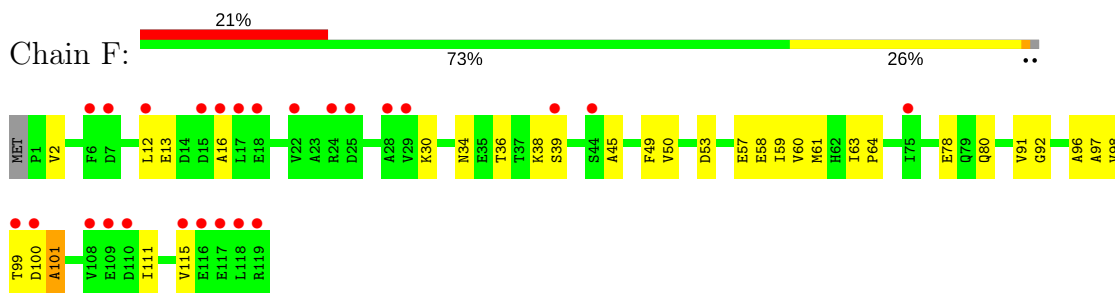
- Molecule 4: 50S ribosomal protein L5P



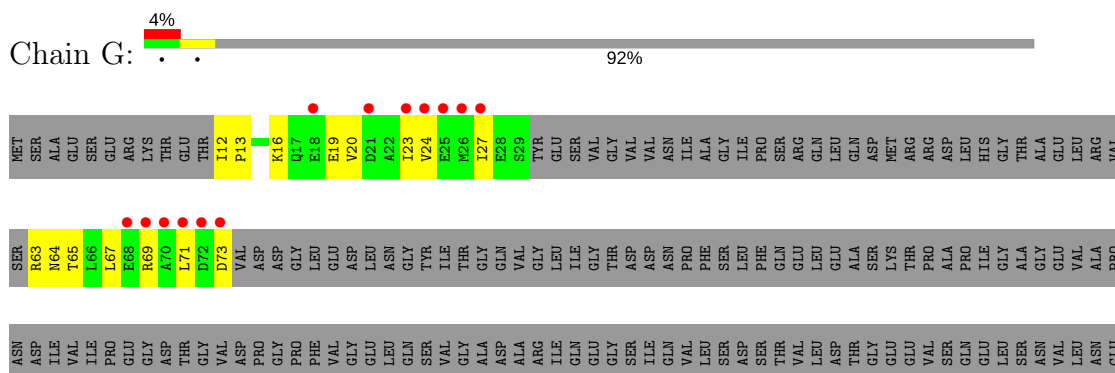
- Molecule 5: 50S ribosomal protein L6P

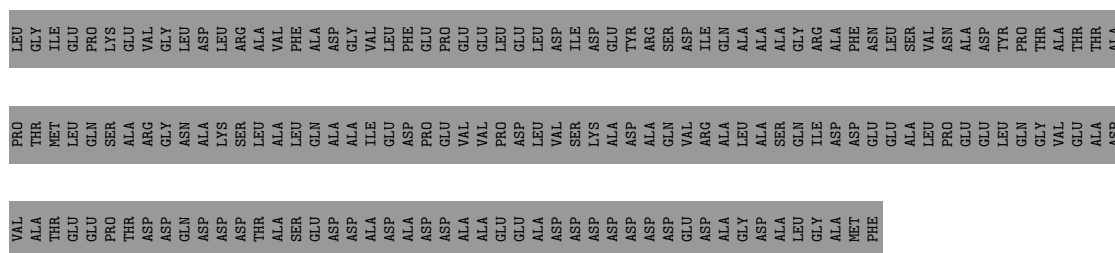


- Molecule 6: 50S ribosomal protein L7Ae

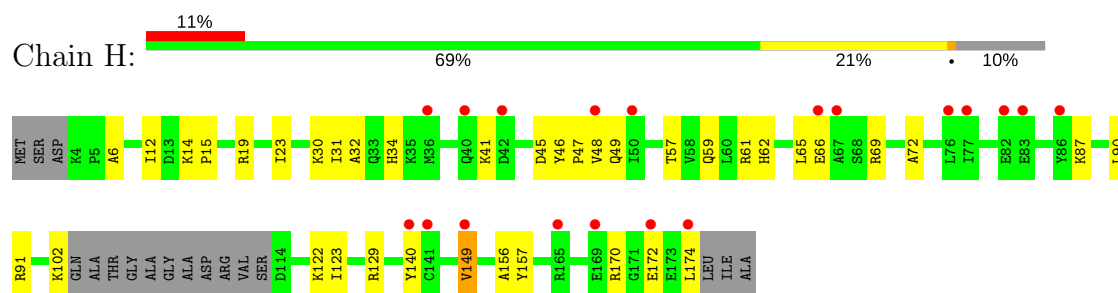


- Molecule 7: 50S ribosomal protein L10E

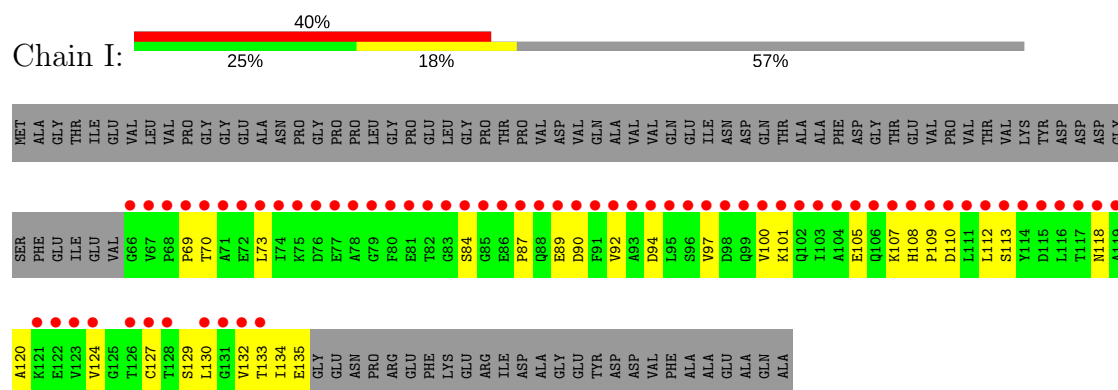




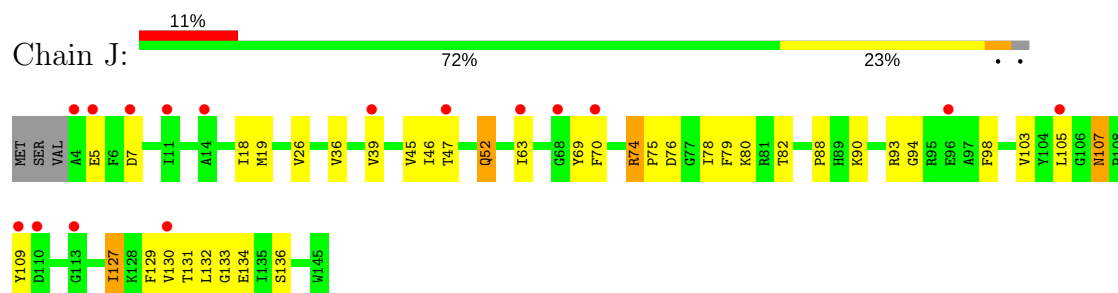
- Molecule 8: 50S ribosomal protein L10e



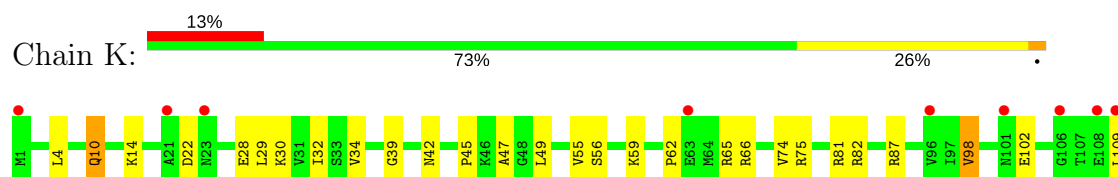
- Molecule 9: 50S ribosomal protein L11P



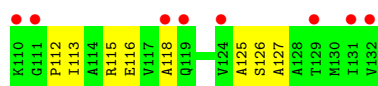
- Molecule 10: 50S ribosomal protein L13P



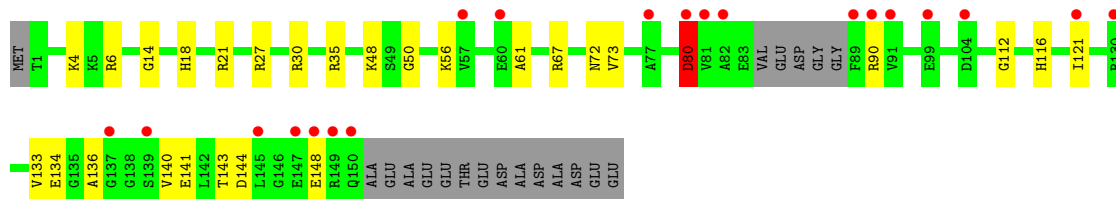
- Molecule 11: 50S ribosomal protein L14P



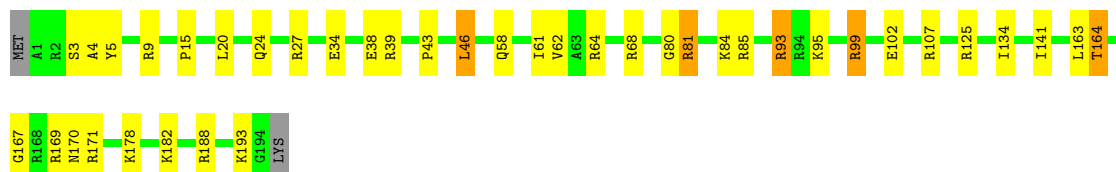




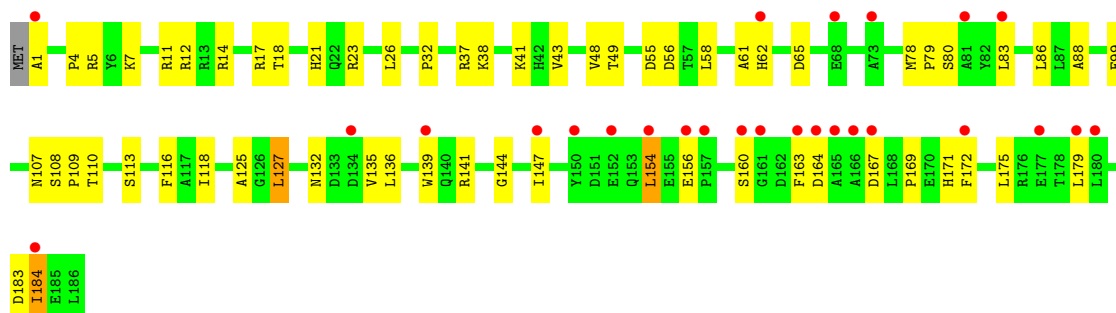
- Molecule 12: 50S ribosomal protein L15P



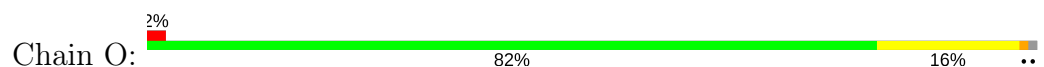
- Molecule 13: 50S ribosomal protein L15e



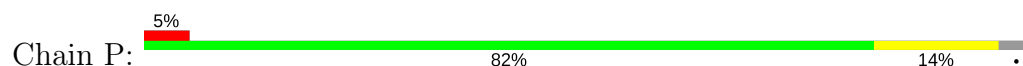
- Molecule 14: 50S ribosomal protein L18P



- Molecule 15: 50S ribosomal protein L18e

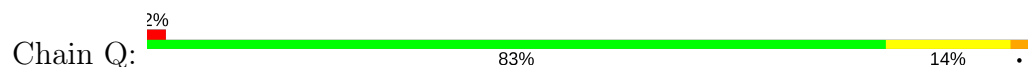


- Molecule 16: 50S ribosomal protein L19e

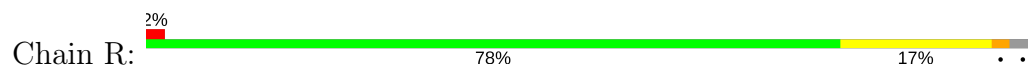




- Molecule 17: 50S ribosomal protein L21e

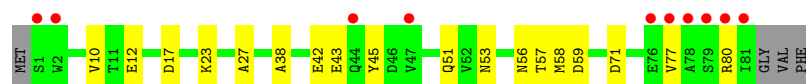


- Molecule 18: 50S ribosomal protein L22P

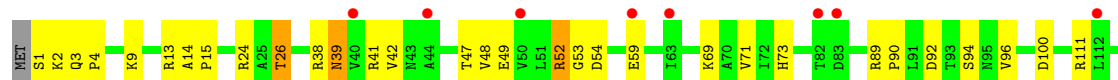


ASP

- Molecule 19: 50S ribosomal protein L23P



- Molecule 20: 50S ribosomal protein L24P

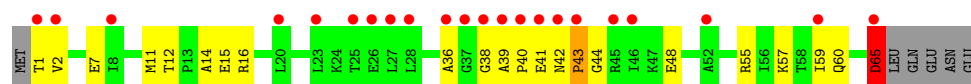


- Molecule 21: 50S ribosomal protein L24e

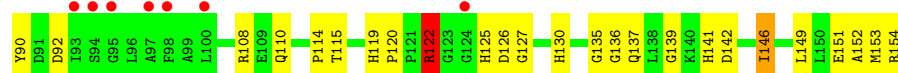


- Molecule 22: 50S ribosomal protein L29P

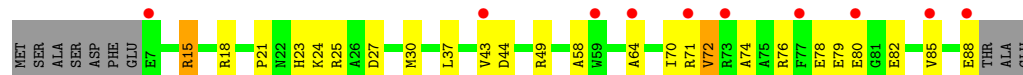




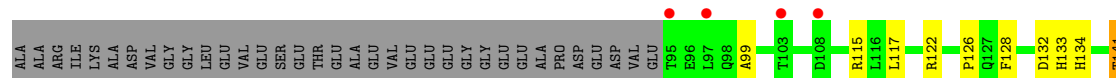
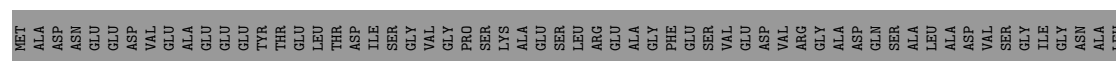
• Molecule 23: 50S ribosomal protein L30P



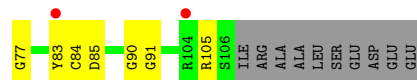
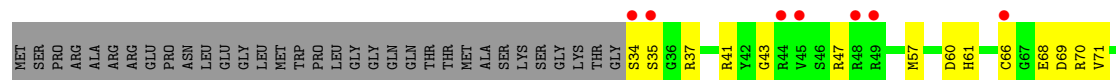
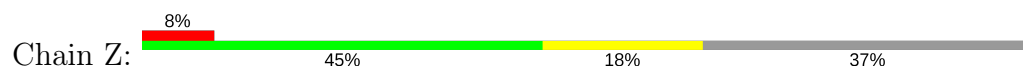
• Molecule 24: 50S ribosomal protein L31e



• Molecule 25: 50S ribosomal protein L32e



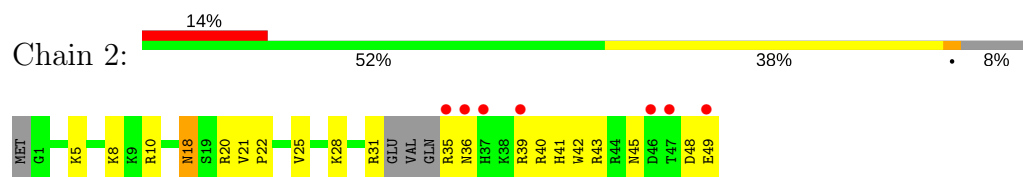
• Molecule 26: 50S ribosomal protein L37Ae



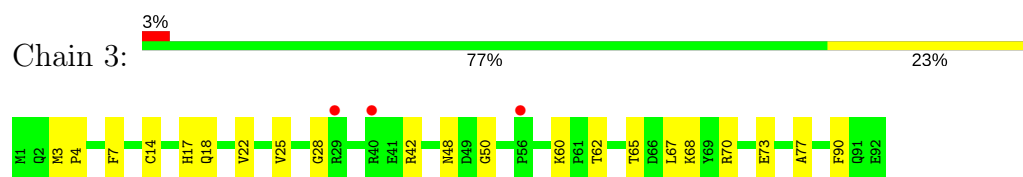
• Molecule 27: 50S ribosomal protein L37e



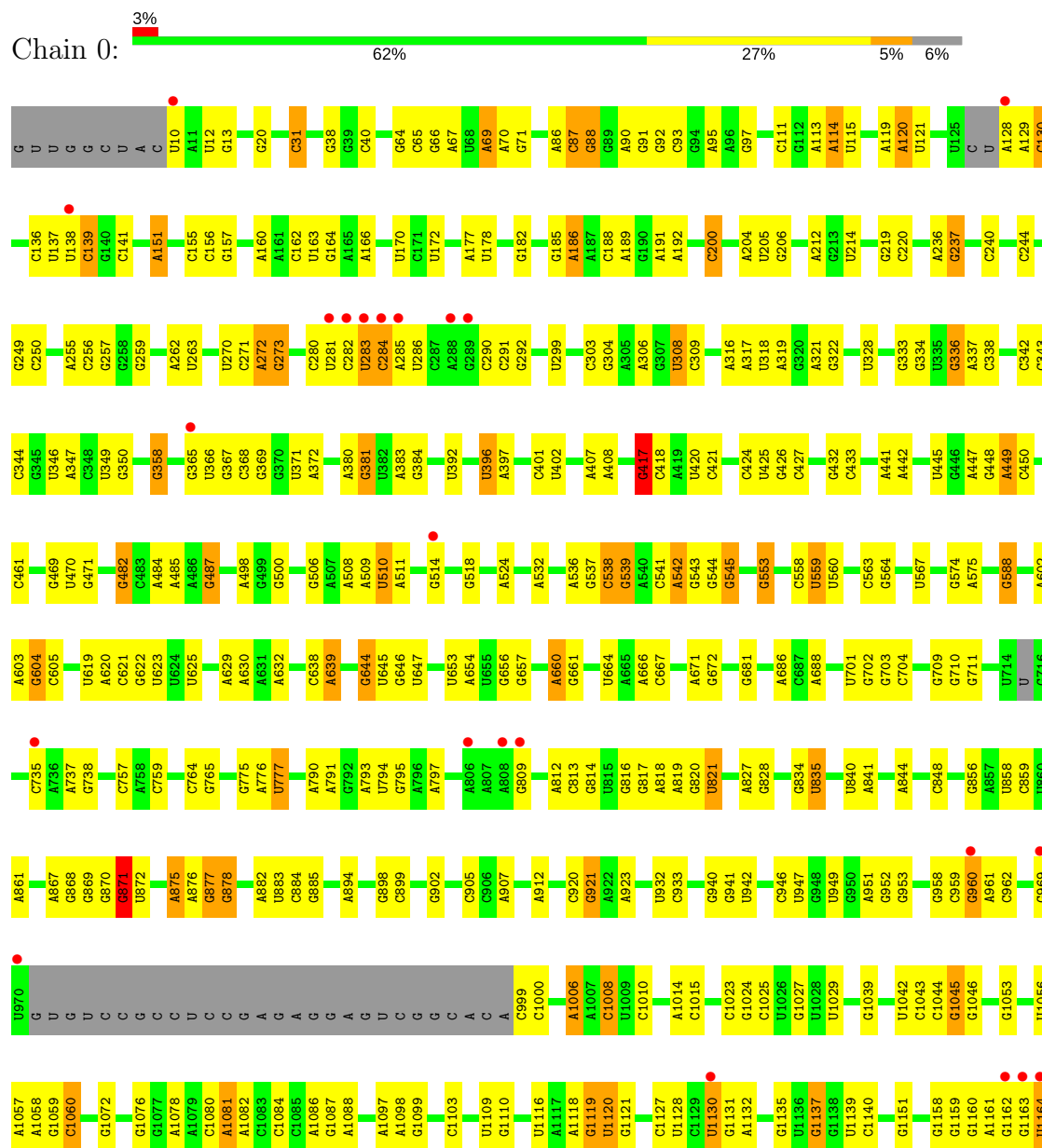
- Molecule 28: 50S ribosomal protein L39e



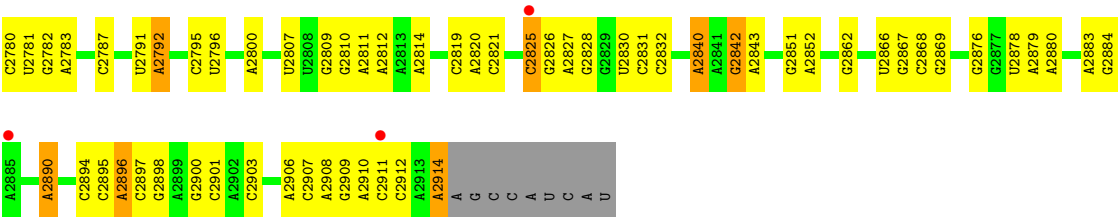
- Molecule 29: 50S ribosomal protein L44E



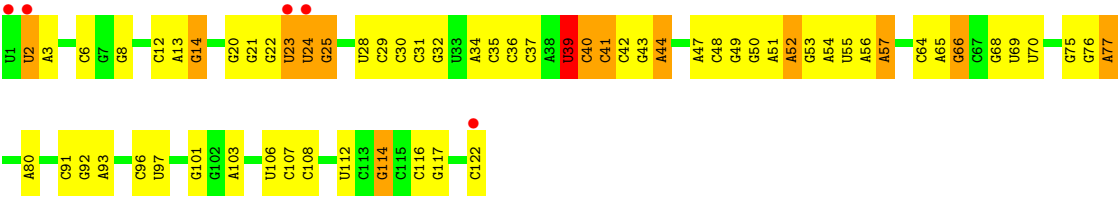
- Molecule 30: 23S RIBOSOMAL RNA



C2667	G2537	G2453	G2338	A	G1971	G1848	A1716	A1597	C1462	A1341	G1235	G1165
G2668	A2538	A2456	A	C	U1972	C1856	A1717	A1598	U1463	C1342	A1236	A1166
U2669	U2541	U2457	C	A	A1973	C1863	U1722	A1603	A1470	C1343	U1237	G1167
U2670	C2542	U2457	G	C	G1976	G1867	U1723	G1604	U1350	U1350	C1238	C1168
C2671	G2543	U2457	A	C	U1977	G1868	U1724	G1605	C1474	U1351	G1239	U1170
U2672	G2543	U2457	A	C	A1978	G1867	C1725	G1611	U1352	A1352	G1240	U1171
C2676	C2542	U2457	A	C	G1979	G1868	U1725	G1612	C1477	C1353	G1241	G1172
A2681	A2465	A2465	A	C	U1980	G1868	U1726	A1613	A1482	C1360	C1242	A1173
C2682	A2466	A2466	A	C	U1985	G1867	U1727	G1614	A1483	C1360	C1243	A1174
U2690	A2467	A2467	A	C	U1988	G1867	U1728	G1615	G1484	A1367	C1245	G1175
A2691	A2468	A2468	A	C	U1992	G1867	U1729	U1624	A1485	U1368	A1246	G1176
C2692	A2469	A2469	A	C	C1993	G1867	U1730	U1625	A1493	A1369	U1249	G1177
U2698	C2472	C2472	A	C	C1994	G1867	U1731	U1626	A1493	U1370	C1250	G1178
A2694	C2476	C2476	A	C	U1995	G1867	U1732	U1627	G1497	A1372	C1251	U1180
C2697	C2477	C2477	A	C	G1996	G1867	U1733	U1628	G1497	A1372	C1252	A1181
C2698	U2478	U2478	A	C	U1997	G1867	U1734	U1629	U1500	C1377	C1253	C1182
U2710	A2479	A2479	A	C	G2001	G1867	U1735	U1630	U1503	C1384	G1257	C1183
C2711	C2480	C2480	A	C	C2002	G1867	U1736	U1631	U1504	C1384	G1258	U1185
G2712	A2483	A2483	A	C	U2003	G1867	U1737	U1632	U1505	A1393	U1266	C1186
G2716	C2487	C2487	A	C	G2005	G1867	U1738	U1633	U1506	C1394	C1267	A1188
C2717	U2488	U2488	A	C	U2008	G1867	U1739	U1634	G1521	A1406	G1268	A1189
A2719	U2489	U2489	A	C	G2009	G1867	U1740	U1635	U1524	A1407	G1269	G1190
C2720	C2490	C2490	A	C	A2010	G1867	U1741	U1636	U1525	A1408	A1278	A1191
U2721	U2491	U2491	A	C	U2011	G1867	U1742	U1637	A1526	G1409	U1279	A1192
C2722	U2492	U2492	A	C	U2012	G1867	U1743	U1638	A1527	A1413	C1289	A1193
G2723	U2493	U2493	A	C	G2013	G1867	U1744	U1639	A1528	A1414	G1290	A1194
U2724	A2502	A2502	A	C	U2014	G1867	U1745	U1640	A1529	A1417	A1291	G1195
C2725	C2503	C2503	A	C	G2015	G1867	U1746	U1641	G1535	U1418	C1294	G1196
U2726	A2504	A2504	A	C	U2016	G1867	U1747	U1642	C1536	U1419	G1295	G1197
C2729	U2505	U2505	A	C	A2019	G1867	U1748	U1643	G1545	C1420	G1299	A1199
G2730	A2506	A2506	A	C	C2031	G1867	U1749	U1644	U1546	C1423	G1300	C1201
C2738	U2507	U2507	A	C	U2032	G1867	U1750	U1645	G1556	A1424	U1304	A1202
C2747	C2508	C2508	A	C	G2033	G1867	U1751	U1646	G1557	A1427	C1305	G1203
G2748	U2509	U2509	A	C	U2034	G1867	U1752	U1647	G1558	U1428	U1306	U1205
U2749	A2511	A2511	A	C	G2044	G1867	U1753	U1648	U1559	U1429	U1307	U1206
C2750	C2515	C2515	A	C	U2045	G1867	U1754	U1649	U1560	U1430	A1313	A1207
A2653	U2516	U2516	A	C	A2054	G1867	U1755	U1650	U1561	G1433	U1314	C1208
C2654	C2517	C2517	A	C	C2061	G1867	U1756	U1651	C1562	U1434	U1315	C1209
G2655	U2518	U2518	A	C	U2062	G1867	U1757	U1652	U1563	U1435	G1316	G1210
C2656	C2519	C2519	A	C	A2063	G1867	U1758	U1653	U1564	C1436	G1317	C1211
U2754	A2521	A2521	A	C	U2064	G1867	U1759	U1654	U1565	U1437	G1318	C1212
G2755	C2522	C2522	A	C	G2070	G1867	U1760	U1655	U1566	U1438	G1319	C1213
U2756	U2523	U2523	A	C	C2071	G1867	U1761	U1656	U1567	U1439	G1320	G1214
C2762	A2524	A2524	A	C	U2072	G1867	U1762	U1657	U1568	U1440	A1328	A1215
A2768	C2525	C2525	A	C	G2073	G1867	U1763	U1658	U1569	U1441	U1329	G1216
C2769	U2526	U2526	A	C	A2074	G1867	U1764	U1659	U1570	U1442	U1330	G1217
G2770	C2527	C2527	A	C	C2075	G1867	U1765	U1660	U1571	A1443	U1331	U1219
C2777	U2528	U2528	A	C	U2076	G1867	U1766	U1661	U1572	C1450	U1332	C1229
A2778	A2529	A2529	A	C	G2077	G1867	U1767	U1662	U1573	C1451	C1333	A1230
G2779	C2530	C2530	A	C	C2078	G1867	U1768	U1663	U1574	C1452	C1334	U1234



● Molecule 31: 5S RIBOSOMAL RNA



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	211.65Å 299.67Å 573.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.95 – 2.40 85.47 – 2.40	Depositor EDS
% Data completeness (in resolution range)	90.5 (49.95-2.40) 90.6 (85.47-2.40)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.37 (at 2.40Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.199 , 0.231 0.183 , 0.216	Depositor DCC
$R_{free}$ test set	6200 reflections (0.98%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.9	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 48.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	99049	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.49% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, OMG, CL, NA, K, CD, OMU, UR3, 1MA, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.33	0/1786	0.66	0/2408
2	B	0.32	0/2690	0.64	0/3652
3	C	0.36	0/1885	0.64	0/2552
4	D	0.32	0/1111	0.56	0/1498
5	E	0.31	0/1382	0.56	0/1880
6	F	0.32	0/901	0.54	0/1224
7	G	0.42	0/241	0.74	0/324
8	H	0.39	0/1302	0.68	0/1743
9	I	0.34	0/526	0.53	0/716
10	J	0.33	0/1136	0.58	0/1530
11	K	0.32	0/1004	0.65	0/1351
12	L	0.34	0/1130	0.65	0/1509
13	M	0.33	0/1582	0.62	0/2116
14	N	0.28	0/1474	0.61	0/1999
15	O	0.32	0/874	0.59	1/1181 (0.1%)
16	P	0.32	0/1147	0.52	0/1528
17	Q	0.33	0/749	0.67	0/1005
18	R	1.31	7/1172 (0.6%)	1.13	5/1578 (0.3%)
19	S	0.33	0/648	0.59	1/875 (0.1%)
20	T	0.31	0/958	0.62	1/1289 (0.1%)
21	U	0.36	0/417	0.60	0/562
22	V	0.36	0/502	0.68	1/675 (0.1%)
23	W	0.33	0/1219	0.65	1/1655 (0.1%)
24	X	0.36	0/664	0.59	0/895
25	Y	0.36	0/1146	0.62	0/1536
26	Z	0.34	0/584	0.66	0/781
27	1	0.42	0/438	0.65	0/578
28	2	0.33	0/401	0.56	0/529
29	3	0.36	0/771	0.59	0/1024
30	0	0.33	0/65958	0.69	21/102869 (0.0%)
31	9	0.29	0/2904	0.69	1/4526 (0.0%)
All	All	0.36	7/98702 (0.0%)	0.68	32/147588 (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
18	R	1	0
30	0	0	39
31	9	0	1
All	All	1	40

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	150	PRO	CA-C	-29.63	0.93	1.52
18	R	150	PRO	CB-CG	16.19	2.31	1.50
18	R	150	PRO	N-CA	14.71	1.72	1.47
18	R	150	PRO	CA-CB	12.12	1.77	1.53
18	R	150	PRO	CG-CD	11.79	1.89	1.50
18	R	150	PRO	C-O	11.61	1.46	1.23
18	R	150	PRO	N-CD	9.24	1.60	1.47

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	R	150	PRO	N-CA-C	-24.01	49.68	112.10
18	R	150	PRO	CB-CA-C	-19.94	62.16	112.00
18	R	150	PRO	CA-C-O	-16.63	80.28	120.20
30	0	1942	A	C5'-C4'-C3'	8.15	129.05	116.00
18	R	150	PRO	CA-N-CD	7.93	122.80	111.70
22	V	65	ASP	CB-CG-OD1	7.92	125.43	118.30
30	0	871	G	C5'-C4'-O4'	-7.20	100.46	109.10
18	R	150	PRO	N-CA-CB	6.86	111.54	103.30
30	0	1819	G	C5'-C4'-C3'	6.74	126.79	116.00
30	0	1504	A	C1'-O4'-C4'	-6.54	104.67	109.90
31	9	39	U	N1-C1'-C2'	6.47	122.41	114.00
30	0	2316	G	C5'-C4'-C3'	-6.43	105.71	116.00
30	0	1979	G	C2'-C3'-O3'	6.36	123.87	113.70
30	0	1878	G	N9-C1'-C2'	-6.28	105.09	112.00
30	0	1942	A	C5'-C4'-O4'	6.20	116.54	109.10
30	0	2467	A	C1'-O4'-C4'	-6.18	104.95	109.90
30	0	206	G	C5'-C4'-C3'	-6.05	106.32	116.00
30	0	2291	A	N9-C1'-C2'	5.93	121.71	114.00
30	0	1829	A	N9-C1'-C2'	-5.85	105.56	112.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	1592	G	N9-C1'-C2'	5.66	121.36	114.00
30	0	1942	A	C4'-C3'-C2'	-5.44	97.16	102.60
30	0	1942	A	C1'-O4'-C4'	-5.30	105.66	109.90
23	W	122	ARG	NE-CZ-NH1	5.27	122.94	120.30
30	0	1504	A	N9-C1'-C2'	5.25	120.83	114.00
30	0	2313	C	C5'-C4'-O4'	5.25	115.40	109.10
30	0	841	A	C1'-O4'-C4'	-5.23	105.72	109.90
15	O	66	GLY	N-CA-C	5.16	126.01	113.10
30	0	777	U	O4'-C1'-N1	5.15	112.32	108.20
19	S	27	ALA	N-CA-C	-5.09	97.27	111.00
20	T	52	ARG	N-CA-C	5.06	124.66	111.00
30	0	1819	G	C4'-C3'-C2'	-5.05	97.55	102.60
30	0	1120	U	C5'-C4'-C3'	-5.02	107.97	116.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	R	150	PRO	CA

All (40) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	1039	G	Sidechain
30	0	1078	A	Sidechain
30	0	1237	U	Sidechain
30	0	1340	G	Sidechain
30	0	1342	C	Sidechain
30	0	1417	G	Sidechain
30	0	1450	C	Sidechain
30	0	1829	A	Sidechain
30	0	1845	A	Sidechain
30	0	1848	G	Sidechain
30	0	1863	G	Sidechain
30	0	1867	G	Sidechain
30	0	1877	G	Sidechain
30	0	1878	G	Sidechain
30	0	1972	U	Sidechain
30	0	2103	A	Sidechain
30	0	2316	G	Sidechain
30	0	2465	A	Sidechain
30	0	2493	C	Sidechain
30	0	2503	A	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
30	0	2506	A	Sidechain
30	0	2543	G	Sidechain
30	0	2552	C	Sidechain
30	0	2564	G	Sidechain
30	0	2607	U	Sidechain
30	0	2630	G	Sidechain
30	0	270	U	Sidechain
30	0	2842	G	Sidechain
30	0	396	U	Sidechain
30	0	417	G	Sidechain
30	0	449	A	Sidechain
30	0	469	G	Sidechain
30	0	471	G	Sidechain
30	0	482	G	Sidechain
30	0	518	G	Sidechain
30	0	619	U	Sidechain
30	0	639	A	Sidechain
30	0	795	G	Sidechain
30	0	867	A	Sidechain
31	9	39	U	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1753	0	1766	74	0
2	B	2625	0	2533	80	0
3	C	1860	0	1813	65	0
4	D	1094	0	1085	45	0
5	E	1357	0	1266	42	0
6	F	890	0	843	26	0
7	G	240	0	231	11	0
8	H	1282	0	1292	34	0
9	I	519	0	500	23	0
10	J	1120	0	1098	39	0
11	K	994	0	1027	40	0
12	L	1118	0	1076	26	0
13	M	1558	0	1572	44	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	N	1445	0	1401	55	0
15	O	865	0	873	19	0
16	P	1136	0	1123	20	0
17	Q	735	0	728	11	0
18	R	1149	0	1122	31	0
19	S	641	0	605	13	0
20	T	950	0	923	24	0
21	U	410	0	364	16	0
22	V	499	0	511	19	0
23	W	1196	0	1137	66	0
24	X	654	0	653	21	0
25	Y	1130	0	1133	30	0
26	Z	573	0	532	14	0
27	1	431	0	426	17	0
28	2	396	0	413	24	0
29	3	755	0	728	16	0
30	0	59021	0	29809	870	0
31	9	2599	0	1325	72	0
32	0	109	0	0	0	0
32	3	1	0	0	0	0
32	9	1	0	0	0	0
32	A	1	0	0	0	0
32	B	1	0	0	0	0
32	K	1	0	0	0	0
32	T	1	0	0	0	0
32	Y	1	0	0	0	0
33	0	2	0	0	0	0
34	0	73	0	0	0	0
34	9	3	0	0	0	0
34	A	1	0	0	0	0
34	C	1	0	0	0	0
34	H	1	0	0	0	0
34	J	1	0	0	0	0
34	L	1	0	0	0	0
34	M	1	0	0	0	0
34	Q	1	0	0	0	0
34	R	2	0	0	0	0
34	S	1	0	0	0	0
35	0	10	0	0	0	0
35	3	1	0	0	0	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	J	3	0	0	1	0
35	L	1	0	0	0	0
35	M	1	0	0	0	0
35	N	1	0	0	0	0
35	O	1	0	0	0	0
35	R	1	0	0	0	0
35	Y	1	0	0	0	0
36	1	1	0	0	0	0
36	3	1	0	0	0	0
36	O	1	0	0	0	0
36	U	1	0	0	0	0
36	Z	1	0	0	0	0
37	0	5949	0	0	149	0
37	1	53	0	0	2	0
37	2	40	0	0	4	0
37	3	72	0	0	6	0
37	9	139	0	0	7	0
37	A	117	0	0	14	0
37	B	146	0	0	13	0
37	C	170	0	0	18	0
37	D	47	0	0	5	0
37	E	42	0	0	4	0
37	F	24	0	0	2	0
37	G	19	0	0	1	0
37	H	72	0	0	5	0
37	I	9	0	0	3	0
37	J	51	0	0	2	0
37	K	56	0	0	5	0
37	L	72	0	0	9	0
37	M	119	0	0	9	0
37	N	65	0	0	10	0
37	O	39	0	0	3	0
37	P	63	0	0	1	0
37	Q	52	0	0	3	0
37	R	80	0	0	2	0
37	S	33	0	0	2	0
37	T	38	0	0	2	0
37	U	27	0	0	1	0
37	V	14	0	0	1	0
37	W	66	0	0	5	0
37	X	29	0	0	5	0
37	Y	94	0	0	10	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	Z	26	0	0	2	0
All	All	99049	0	59908	1694	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (1694) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:150:PRO:CG	18:R:150:PRO:CD	1.89	1.50
14:N:37:ARG:NH1	31:9:6:C:H5''	1.61	1.14
30:0:871:G:C8	30:0:871:G:H5'	1.86	1.10
30:0:960:G:H4'	37:0:6980:HOH:O	1.49	1.09
18:R:150:PRO:CG	18:R:150:PRO:CB	2.30	1.08
18:R:150:PRO:CG	18:R:150:PRO:C	2.21	1.08
30:0:1160:G:C5'	30:0:1161:A:H5'	1.85	1.06
15:O:3:THR:HG22	30:0:656:G:H5'	1.38	1.06
10:J:82:THR:HG23	30:0:1242:A:H5'	1.37	1.05
13:M:171:ARG:HD3	30:0:156:C:H5''	1.37	1.05
30:0:2812:A:H2	30:0:2814:A:H62	1.08	1.02
30:0:1160:G:H5'	30:0:1161:A:H5'	1.02	1.01
31:9:56:A:H2'	31:9:57:A:H5''	1.42	1.01
30:0:1372:A:H3'	37:0:6737:HOH:O	1.60	1.00
30:0:1160:G:H5'	30:0:1161:A:C5'	1.91	1.00
30:0:2717:C:H2'	30:0:2718:C:H5''	1.43	0.99
11:K:29:LEU:HB3	11:K:55:VAL:HG11	1.44	0.99
31:9:76:G:H3'	31:9:77:A:H5''	1.44	0.98
30:0:2710:U:H1'	37:0:7172:HOH:O	1.62	0.98
30:0:1474:C:H6	30:0:1474:C:H5'	1.30	0.97
24:X:37:LEU:HD13	24:X:85:VAL:HG21	1.46	0.96
30:0:542:A:H5'	30:0:542:A:H8	1.28	0.96
30:0:871:G:H8	30:0:871:G:H5'	1.25	0.95
30:0:2717:C:C2'	30:0:2718:C:H5''	1.96	0.95
28:2:41:HIS:H	28:2:45:ASN:HD22	1.11	0.95
4:D:134:LEU:HD11	4:D:166:ILE:HD11	1.49	0.94
30:0:214:U:H5'	37:0:5687:HOH:O	1.67	0.94
30:0:541:C:H2'	30:0:542:A:H5''	1.50	0.94
11:K:10:GLN:H	11:K:10:GLN:HE21	0.96	0.93
30:0:1835:U:H5	30:0:1840:A:N7	1.66	0.93
30:0:1625:U:H4'	37:0:4207:HOH:O	1.68	0.93
3:C:236:THR:HG22	3:C:239:ALA:H	1.30	0.93

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:59:GLN:HE21	8:H:129:ARG:HE	1.17	0.92
30:0:381:G:H5''	37:0:3859:HOH:O	1.67	0.92
13:M:164:THR:HG22	13:M:167:GLY:H	1.33	0.92
30:0:282:C:H1'	30:0:368:C:N4	1.85	0.91
30:0:871:G:H8	30:0:871:G:C5'	1.83	0.91
20:T:71:VAL:HG11	20:T:90:PRO:HB3	1.53	0.90
30:0:1184:C:H1'	37:0:7015:HOH:O	1.70	0.90
30:0:870:G:H2'	30:0:871:G:H5''	1.51	0.90
30:0:2291:A:C8	30:0:2309:C:H5'	2.06	0.90
21:U:52:THR:HG22	21:U:54:THR:H	1.35	0.90
30:0:1116:U:O2'	30:0:1118:A:H2	1.55	0.89
30:0:1667:A:H8	30:0:1667:A:H5'	1.36	0.89
30:0:2748:G:H2'	37:0:7089:HOH:O	1.72	0.89
2:B:212:GLN:HB2	2:B:257:THR:HG21	1.54	0.89
30:0:1666:C:O2'	30:0:1667:A:H5''	1.70	0.89
30:0:1701:A:H4'	30:0:1702:U:H5''	1.53	0.89
30:0:236:A:H4'	30:0:237:G:H5'	1.55	0.87
30:0:541:C:C2'	30:0:542:A:H5''	2.03	0.87
2:B:140:LEU:HA	37:B:8581:HOH:O	1.74	0.87
11:K:39:GLY:HA2	37:0:4763:HOH:O	1.73	0.87
30:0:871:G:C8	30:0:871:G:C5'	2.58	0.87
30:0:1116:U:H3	30:0:1246:A:H62	1.23	0.86
16:P:115:SER:H	16:P:118:GLN:HE21	1.19	0.86
30:0:69:A:H5'	30:0:69:A:C8	2.10	0.86
4:D:154:LYS:HD2	4:D:154:LYS:H	1.38	0.86
23:W:137:GLN:HE21	23:W:141:HIS:HE1	1.19	0.86
30:0:2506:A:O2'	30:0:2507:G:H8	1.59	0.86
23:W:6:GLN:HB2	23:W:26:ILE:HD12	1.55	0.85
30:0:1300:G:H1'	37:0:4223:HOH:O	1.77	0.85
14:N:37:ARG:HH12	31:9:6:C:H5''	1.39	0.85
1:A:223:ARG:HH12	30:0:2270:G:H4'	1.42	0.85
31:9:39:U:H1'	31:9:44:A:H61	1.42	0.85
30:0:282:C:O2'	30:0:283:U:H5'	1.77	0.84
26:Z:70:ARG:HD2	26:Z:83:TYR:HB2	1.58	0.84
30:0:545:G:H8	30:0:545:G:H5'	1.40	0.84
23:W:88:THR:HB	37:W:6679:HOH:O	1.77	0.84
30:0:506:G:H22	30:0:509:A:C5'	1.91	0.83
30:0:1119:G:N2	30:0:1246:A:C2	2.46	0.83
30:0:69:A:H5'	30:0:69:A:H8	1.42	0.83
31:9:14:G:H5'	31:9:14:G:H8	1.43	0.83
2:B:206:THR:HG21	30:0:2716:G:H5''	1.60	0.83

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1730:G:H5'	30:0:1731:C:C5	2.14	0.82
26:Z:34:SER:HB2	37:Z:8414:HOH:O	1.77	0.82
30:0:1862:C:H1'	37:0:6768:HOH:O	1.80	0.82
30:0:2586:U:H3	30:0:2592:G:H22	1.28	0.82
30:0:1118:A:H3'	30:0:1118:A:H8	1.44	0.82
30:0:272:A:H3'	37:0:7079:HOH:O	1.79	0.81
30:0:2769:C:C2'	30:0:2770:G:H5'	2.10	0.81
37:I:5128:HOH:O	30:0:1168:C:H4'	1.81	0.81
25:Y:200:THR:HG22	25:Y:201:GLU:HG3	1.61	0.81
18:R:99:ALA:HB1	18:R:109:MET:HE1	1.63	0.81
30:0:506:G:H22	30:0:509:A:H5''	1.45	0.81
30:0:564:G:H1'	37:0:5857:HOH:O	1.81	0.81
30:0:346:U:H4'	37:0:6392:HOH:O	1.80	0.81
2:B:221:GLN:HE22	11:K:42:ASN:HD22	1.26	0.81
30:0:2851:G:O2'	30:0:2852:A:H5'	1.81	0.81
11:K:10:GLN:N	11:K:10:GLN:HE21	1.79	0.81
18:R:8:ALA:HB1	18:R:13:THR:HG21	1.63	0.81
8:H:170:ARG:HD2	37:H:8342:HOH:O	1.79	0.80
31:9:56:A:C2'	31:9:57:A:H5''	2.11	0.80
23:W:88:THR:HG23	23:W:110:GLN:HE21	1.46	0.80
21:U:46:ALA:HB1	21:U:52:THR:HG21	1.63	0.80
30:0:1474:C:C6	30:0:1474:C:H5'	2.17	0.80
30:0:1973:A:H5'	30:0:1973:A:H8	1.47	0.80
30:0:2908:A:H2'	30:0:2909:G:O4'	1.82	0.80
30:0:1118:A:H3'	30:0:1118:A:C8	2.16	0.80
14:N:83:LEU:HD13	14:N:175:LEU:HD23	1.63	0.80
30:0:2637:A:H5'	37:0:8794:HOH:O	1.80	0.79
1:A:199:HIS:HD2	1:A:201:PHE:H	1.27	0.79
2:B:238:ASN:HD22	2:B:240:GLY:H	1.26	0.79
3:C:127:ARG:NH2	3:C:225:PRO:HG2	1.98	0.79
2:B:307:ARG:HG3	2:B:307:ARG:HH11	1.47	0.79
30:0:544:G:H2'	30:0:545:G:H5''	1.65	0.78
31:9:29:C:H2'	31:9:30:C:H5'	1.66	0.78
30:0:1119:G:H22	30:0:1246:A:H2	1.32	0.78
30:0:541:C:H2'	30:0:542:A:C5'	2.14	0.78
15:O:3:THR:CG2	30:0:656:G:H5'	2.12	0.78
13:M:102:GLU:OE1	13:M:164:THR:HG21	1.83	0.78
11:K:81:ARG:HB2	11:K:87:ARG:HH11	1.49	0.78
23:W:122:ARG:NH2	23:W:154:ARG:HB3	1.99	0.78
30:0:182:G:H5'	37:0:4697:HOH:O	1.83	0.78
8:H:59:GLN:NE2	8:H:129:ARG:HE	1.81	0.77

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:30:LYS:H	8:H:62:HIS:HD2	1.31	0.77
30:0:1919:A:H4'	37:0:4389:HOH:O	1.85	0.77
30:0:2896:A:H5''	37:0:5645:HOH:O	1.84	0.77
3:C:1:MET:HG2	3:C:2:GLN:H	1.49	0.77
30:0:1206:U:H6	30:0:1206:U:H5'	1.50	0.76
30:0:1165:G:H4'	30:0:1174:A:O2'	1.86	0.76
1:A:100:PRO:HG2	1:A:103:VAL:HG21	1.67	0.76
30:0:1080:C:H4'	30:0:1081:A:OP1	1.84	0.76
22:V:1:THR:HG23	22:V:2:VAL:H	1.50	0.76
23:W:4:LEU:HD22	23:W:52:VAL:HG21	1.68	0.76
30:0:2004:U:H4'	37:0:4853:HOH:O	1.85	0.76
30:0:542:A:H5'	30:0:542:A:C8	2.18	0.76
14:N:144:GLY:O	14:N:147:ILE:HG22	1.85	0.76
30:0:603:A:H5''	30:0:604:G:OP1	1.86	0.75
6:F:50:VAL:HG13	6:F:60:VAL:HG11	1.66	0.75
30:0:2769:C:H2'	30:0:2770:G:H5'	1.68	0.75
30:0:2506:A:HO2'	30:0:2507:G:H8	0.81	0.75
30:0:1701:A:H4'	30:0:1702:U:C5'	2.16	0.75
10:J:19:MET:HE3	10:J:132:LEU:HD21	1.69	0.75
14:N:37:ARG:NH1	31:9:6:C:C5'	2.48	0.75
2:B:321:PRO:HA	37:B:8656:HOH:O	1.85	0.75
30:0:877:G:H5'	30:0:878:G:OP1	1.86	0.74
29:3:65:THR:HG22	29:3:67:LEU:HG	1.69	0.74
30:0:2635:A:O2'	30:0:2636:C:H5'	1.88	0.74
30:0:559:U:H5'	30:0:559:U:H6	1.53	0.74
30:0:870:G:C2'	30:0:871:G:H5''	2.18	0.74
4:D:99:ASP:HB3	4:D:103:ASN:H	1.53	0.74
31:9:39:U:H1'	31:9:44:A:N6	2.03	0.74
2:B:86:ALA:HA	37:B:8581:HOH:O	1.87	0.73
30:0:1603:A:H5'	30:0:1605:G:O4'	1.88	0.73
2:B:74:ILE:HD13	2:B:309:VAL:HG21	1.69	0.73
37:B:8634:HOH:O	30:0:2672:C:H1'	1.87	0.73
30:0:2323:G:H5''	37:0:4318:HOH:O	1.88	0.73
5:E:143:GLN:NE2	30:0:2779:G:H21	1.86	0.73
30:0:558:C:O2'	30:0:559:U:H5''	1.89	0.73
14:N:113:SER:HB2	37:N:8558:HOH:O	1.87	0.73
30:0:1497:G:H4'	30:0:1627:G:O2'	1.88	0.72
9:I:73:LEU:HD12	9:I:107:LYS:HZ2	1.53	0.72
30:0:1666:C:H2'	30:0:1667:A:H5'	1.70	0.72
1:A:35:GLY:O	1:A:36:ASP:HB3	1.90	0.72
30:0:1130:U:H5'	37:0:7223:HOH:O	1.89	0.72

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:201:ASP:HB2	2:B:312:ARG:HD2	1.71	0.72
30:0:2505:G:O2'	30:0:2506:A:H5'	1.89	0.72
3:C:174:ILE:CD1	30:0:338:C:H4'	2.19	0.72
15:O:3:THR:HG22	30:0:656:G:C5'	2.18	0.72
30:0:2507:G:H2'	30:0:2510:C:H42	1.55	0.72
30:0:1180:U:H1'	37:0:9766:HOH:O	1.90	0.71
4:D:25:MET:HE3	4:D:37:ALA:HB1	1.71	0.71
14:N:23:ARG:HD3	37:N:8546:HOH:O	1.90	0.71
9:I:127:CYS:HB3	9:I:132:VAL:HB	1.71	0.71
11:K:14:LYS:HB2	11:K:45:PRO:HG2	1.71	0.71
11:K:10:GLN:H	11:K:10:GLN:NE2	1.80	0.71
30:0:2756:U:H3	30:0:2896:A:H2	1.34	0.71
1:A:211:LYS:HB2	37:A:8612:HOH:O	1.91	0.71
4:D:28:GLY:HA2	4:D:69:ILE:HG23	1.71	0.71
21:U:9:CYS:HA	21:U:52:THR:HG23	1.73	0.71
26:Z:34:SER:OG	30:0:797:A:H4'	1.90	0.71
1:A:51:ARG:HB2	37:A:8599:HOH:O	1.91	0.71
30:0:1667:A:C8	30:0:1667:A:H5'	2.25	0.70
30:0:299:U:H5'	37:0:6885:HOH:O	1.91	0.70
28:2:41:HIS:N	28:2:45:ASN:HD22	1.88	0.70
30:0:1835:U:C5	30:0:1840:A:N7	2.56	0.70
30:0:1634:G:H3'	37:0:3430:HOH:O	1.90	0.70
30:0:1166:A:H61	30:0:1180:U:H3	1.38	0.70
30:0:1183:C:N4	30:0:1184:C:H41	1.90	0.70
30:0:558:C:C2'	30:0:559:U:H5''	2.21	0.70
31:9:14:G:H5'	31:9:14:G:C8	2.26	0.70
2:B:36:PRO:HA	2:B:168:GLY:HA3	1.73	0.70
16:P:59:ARG:NH2	16:P:66:GLN:HE22	1.90	0.70
9:I:97:VAL:HG12	9:I:101:LYS:HE3	1.74	0.70
13:M:171:ARG:CD	30:0:156:C:H5''	2.19	0.69
18:R:128:ARG:NH2	30:0:2054:A:N3	2.40	0.69
30:0:2426:G:H1'	37:0:5638:HOH:O	1.92	0.69
30:0:2533:C:H5'	30:0:2533:C:H6	1.57	0.69
28:2:39:ARG:HG2	37:2:3143:HOH:O	1.92	0.69
13:M:178:LYS:HB2	37:0:6424:HOH:O	1.90	0.69
1:A:223:ARG:NH1	30:0:2270:G:H4'	2.07	0.69
2:B:41:PHE:CD1	2:B:79:MET:HE2	2.27	0.69
30:0:281:U:H2'	30:0:282:C:O4'	1.91	0.69
30:0:951:A:C2'	30:0:952:G:H5'	2.22	0.69
1:A:191:GLY:HA2	1:A:194:MET:CE	2.22	0.69
10:J:76:ASP:HA	37:J:5907:HOH:O	1.93	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1603:A:H5''	30:0:1605:G:H5'	1.75	0.69
30:0:536:A:H3'	37:0:4588:HOH:O	1.92	0.69
5:E:20:ILE:HD11	5:E:40:VAL:HG11	1.74	0.69
30:0:558:C:H2'	30:0:559:U:C5'	2.23	0.69
30:0:1058:A:H2'	30:0:1060:C:H5''	1.74	0.68
30:0:1632:A:H2'	30:0:1633:C:H5'	1.74	0.68
30:0:2812:A:C2	30:0:2814:A:N6	2.59	0.68
11:K:98:VAL:HG13	11:K:102:GLU:HA	1.74	0.68
30:0:2756:U:N3	30:0:2896:A:C2	2.59	0.68
2:B:211:THR:HG21	37:0:7003:HOH:O	1.92	0.68
30:0:2769:C:H2'	30:0:2770:G:C5'	2.23	0.68
30:0:2787:C:H5	37:0:4174:HOH:O	1.76	0.68
30:0:1166:A:H1'	30:0:1192:A:C2	2.28	0.68
30:0:1730:G:C5'	30:0:1731:C:C6	2.77	0.68
28:2:41:HIS:H	28:2:45:ASN:ND2	1.89	0.68
3:C:76:ARG:HG2	3:C:78:ARG:NH1	2.08	0.68
1:A:191:GLY:HA2	1:A:194:MET:HE3	1.76	0.68
30:0:1766:U:O2	30:0:1778:A:H5'	1.94	0.68
25:Y:169:ARG:HD2	30:0:1328:A:OP1	1.94	0.67
30:0:1701:A:H5'	37:0:5830:HOH:O	1.93	0.67
30:0:1730:G:H5'	30:0:1731:C:H5	1.58	0.67
11:K:34:VAL:HG22	11:K:47:ALA:HB2	1.76	0.67
11:K:74:VAL:HG11	11:K:113:ILE:HG12	1.76	0.67
30:0:1189:A:H3'	37:0:7231:HOH:O	1.93	0.67
30:0:1878:G:H1'	37:0:5667:HOH:O	1.94	0.67
19:S:57:THR:HG22	19:S:59:ASP:H	1.58	0.67
30:0:1441:G:O2'	30:0:1442:A:H5'	1.94	0.67
30:0:272:A:H5'	30:0:273:G:OP2	1.94	0.67
18:R:98:ASN:HD21	30:0:500:G:H21	1.41	0.67
23:W:125:HIS:HD2	23:W:127:GLY:H	1.42	0.67
3:C:140:VAL:HB	37:C:8449:HOH:O	1.93	0.67
30:0:2064:U:H5'	30:0:2652:U:O3'	1.94	0.67
30:0:1377:C:H6	30:0:1377:C:H5'	1.60	0.67
30:0:1187:U:O2'	30:0:1189:A:H2	1.77	0.67
10:J:74:ARG:HB3	10:J:74:ARG:HH11	1.58	0.67
30:0:1819:G:H2'	30:0:1820:G:H4'	1.76	0.67
29:3:48:ASN:HD21	30:0:2468:A:H61	1.41	0.67
8:H:6:ALA:HA	8:H:61:ARG:NH1	2.10	0.67
11:K:81:ARG:HB2	11:K:87:ARG:NH1	2.09	0.66
30:0:2827:A:H2'	30:0:2828:G:O4'	1.95	0.66
30:0:31:C:H4'	37:0:6974:HOH:O	1.94	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:856:G:H2'	37:0:4975:HOH:O	1.94	0.66
1:A:199:HIS:CD2	1:A:201:PHE:H	2.11	0.66
23:W:141:HIS:HB2	23:W:146:ILE:HG12	1.78	0.66
6:F:91:VAL:HG12	6:F:92:GLY:H	1.60	0.66
22:V:12:THR:HG22	22:V:15:GLU:HG3	1.78	0.66
21:U:56:ARG:NH2	30:0:2890:A:H1'	2.11	0.66
30:0:545:G:C8	30:0:545:G:H5'	2.27	0.66
23:W:21:LEU:HD22	23:W:26:ILE:HD11	1.77	0.66
10:J:52:GLN:HE22	30:0:1119:G:H8	1.42	0.66
30:0:711:G:H1'	37:0:6640:HOH:O	1.95	0.66
30:0:1205:U:H2'	30:0:1206:U:C5'	2.25	0.66
3:C:115:LEU:HD13	3:C:223:LEU:HD21	1.77	0.66
3:C:139:VAL:HG13	37:C:8446:HOH:O	1.95	0.66
30:0:1209:C:H2'	30:0:1210:G:H8	1.61	0.66
30:0:2783:A:H3'	37:0:4774:HOH:O	1.95	0.66
3:C:236:THR:HG21	37:C:8373:HOH:O	1.96	0.66
30:0:1185:U:H2'	30:0:1186:C:C6	2.31	0.66
30:0:544:G:C2'	30:0:545:G:H5''	2.24	0.66
3:C:236:THR:HG22	3:C:239:ALA:N	2.08	0.66
4:D:135:VAL:HG22	4:D:136:ARG:H	1.60	0.66
30:0:1205:U:H2'	30:0:1206:U:H5''	1.76	0.65
12:L:30:ARG:HD3	30:0:164:G:H4'	1.78	0.65
22:V:1:THR:HB	30:0:93:C:H5''	1.76	0.65
23:W:6:GLN:HB2	23:W:26:ILE:CD1	2.26	0.65
30:0:2414:A:H2'	30:0:2415:A:C8	2.31	0.65
30:0:856:G:C8	37:0:4975:HOH:O	2.48	0.65
14:N:49:THR:HG22	14:N:56:ASP:HB2	1.78	0.65
23:W:122:ARG:HH11	23:W:122:ARG:CG	2.08	0.65
23:W:21:LEU:HD22	23:W:26:ILE:CD1	2.26	0.65
31:9:64:C:H2'	31:9:65:A:H5'	1.79	0.65
30:0:1741:U:H5'	30:0:1742:A:OP1	1.96	0.65
14:N:5:ARG:NH1	30:0:962:C:H1'	2.10	0.65
31:9:54:A:O2'	31:9:55:U:H5'	1.96	0.65
3:C:5:ILE:HD11	3:C:16:VAL:HG23	1.78	0.65
23:W:4:LEU:HD23	23:W:54:PHE:HB3	1.78	0.65
18:R:29:LYS:HE2	30:0:524:A:C5'	2.26	0.65
3:C:5:ILE:HD11	3:C:16:VAL:CG2	2.27	0.65
6:F:96:ALA:HA	37:F:3111:HOH:O	1.97	0.65
16:P:59:ARG:HH22	16:P:66:GLN:HE22	1.42	0.65
23:W:88:THR:HG23	23:W:110:GLN:NE2	2.11	0.65
30:0:1878:G:O2'	30:0:1879:U:C6	2.48	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:185:GLY:HA2	37:B:8633:HOH:O	1.97	0.65
16:P:117:SER:HB3	30:0:1593:C:OP1	1.98	0.64
30:0:2608:C:H2'	37:0:3110:HOH:O	1.96	0.64
4:D:54:ALA:HB2	4:D:69:ILE:HD12	1.78	0.64
5:E:97:VAL:HG12	37:E:4191:HOH:O	1.97	0.64
12:L:133:VAL:HA	37:L:8562:HOH:O	1.95	0.64
12:L:18:HIS:HD2	30:0:902:G:N7	1.95	0.64
22:V:42:ASN:HB3	37:V:7247:HOH:O	1.97	0.64
30:0:1632:A:C2'	30:0:1633:C:H5'	2.28	0.64
27:1:16:HIS:HD2	30:0:470:U:O2'	1.81	0.64
23:W:137:GLN:HE21	23:W:141:HIS:CE1	2.09	0.64
30:0:31:C:H2'	37:0:7238:HOH:O	1.97	0.64
30:0:1666:C:C2'	30:0:1667:A:H5''	2.27	0.64
8:H:49:GLN:HE21	8:H:140:TYR:HE2	1.46	0.64
30:0:1666:C:H2'	30:0:1667:A:C5'	2.27	0.64
14:N:4:PRO:HG3	31:9:69:U:OP1	1.98	0.63
9:I:73:LEU:HD12	9:I:107:LYS:NZ	2.12	0.63
30:0:1641:A:H2'	30:0:1642:A:H5'	1.79	0.63
10:J:69:TYR:CE1	30:0:2081:A:H4'	2.34	0.63
2:B:41:PHE:HB3	2:B:190:MET:HE3	1.80	0.63
19:S:51:GLN:HE21	19:S:53:ASN:HD21	1.45	0.63
30:0:2649:A:H5'	30:0:2649:A:H8	1.63	0.63
30:0:2717:C:H2'	30:0:2718:C:C5'	2.24	0.63
11:K:32:ILE:HD11	11:K:56:SER:HB3	1.78	0.63
13:M:99:ARG:HH21	13:M:170:ASN:HD22	1.45	0.63
30:0:1330:A:H2	37:0:4223:HOH:O	1.81	0.63
30:0:2769:C:O2'	30:0:2770:G:H5'	1.97	0.63
5:E:139:GLU:OE2	30:0:2781:U:H1'	1.99	0.63
25:Y:141:THR:HG23	37:Y:8586:HOH:O	1.99	0.63
23:W:21:LEU:HD21	23:W:48:VAL:HG11	1.81	0.63
25:Y:187:VAL:HG12	25:Y:205:ILE:HA	1.81	0.63
3:C:47:GLY:HA2	3:C:92:PRO:HB2	1.81	0.63
30:0:281:U:O2'	30:0:282:C:H5'	1.99	0.63
30:0:558:C:H2'	30:0:559:U:H5'	1.81	0.63
30:0:506:G:H22	30:0:509:A:H5'	1.64	0.62
18:R:39:THR:HG23	18:R:107:GLU:O	1.98	0.62
20:T:9:LYS:HB2	37:0:6974:HOH:O	1.98	0.62
27:1:20:ARG:HG2	30:0:111:C:O2'	1.99	0.62
10:J:70:PHE:CE1	30:0:2676:C:H4'	2.34	0.62
27:1:25:LYS:HE2	37:2:7213:HOH:O	1.98	0.62
30:0:2832:C:H5	37:0:6762:HOH:O	1.82	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:185:VAL:HG12	37:Y:8567:HOH:O	1.99	0.62
28:2:43:ARG:HH22	30:0:1684:A:H1'	1.64	0.62
9:I:120:ALA:O	9:I:124:VAL:HG23	1.99	0.62
26:Z:60:ASP:HB3	26:Z:69:ASP:HB3	1.80	0.62
1:A:192:VAL:HB	37:A:8587:HOH:O	1.99	0.62
2:B:7:ARG:HG2	2:B:7:ARG:HH11	1.65	0.62
30:0:138:U:H5''	30:0:139:C:OP2	1.99	0.62
30:0:1666:C:C2'	30:0:1667:A:C5'	2.78	0.62
30:0:2717:C:O2'	30:0:2718:C:H5''	1.99	0.62
30:0:2768:A:H2'	30:0:2769:C:O4'	1.99	0.62
2:B:195:ARG:HG2	2:B:323:LEU:HD22	1.81	0.62
4:D:57:THR:HG23	4:D:63:ILE:HA	1.82	0.62
5:E:3:VAL:HG22	5:E:49:ILE:HB	1.80	0.62
10:J:47:THR:HB	37:0:4375:HOH:O	2.00	0.62
30:0:1730:G:H5''	30:0:1731:C:H6	1.65	0.62
2:B:145:HIS:HD2	2:B:146:THR:O	1.83	0.62
4:D:99:ASP:HA	37:0:5842:HOH:O	2.00	0.62
30:0:1118:A:C8	30:0:1118:A:C3'	2.79	0.61
29:3:25:VAL:HG22	29:3:68:LYS:HG3	1.82	0.61
29:3:73:GLU:HB3	37:3:8559:HOH:O	2.00	0.61
31:9:2:U:OP2	31:9:3:A:H5'	2.00	0.61
31:9:29:C:C2'	31:9:30:C:H5'	2.30	0.61
30:0:1130:U:H2'	30:0:1131:G:O4'	2.00	0.61
2:B:211:THR:HG23	30:0:2840:A:OP1	2.00	0.61
30:0:396:U:O2'	30:0:418:C:H4'	2.00	0.61
2:B:179:LEU:O	2:B:183:GLU:HG2	1.99	0.61
6:F:91:VAL:HG12	6:F:92:GLY:N	2.14	0.61
12:L:136:ALA:HB3	37:L:8562:HOH:O	1.99	0.61
13:M:80:GLY:O	13:M:81:ARG:HD3	1.99	0.61
30:0:1778:A:H2'	30:0:1779:A:H5'	1.82	0.61
30:0:2346:C:O5'	30:0:2346:C:H6	1.83	0.61
30:0:2533:C:C6	30:0:2533:C:H5'	2.34	0.61
3:C:236:THR:H	3:C:239:ALA:HB3	1.65	0.61
18:R:39:THR:HG22	18:R:42:GLU:H	1.65	0.61
30:0:1189:A:H1'	30:0:1209:C:H1'	1.83	0.61
5:E:49:ILE:HD11	5:E:69:ILE:HD12	1.83	0.61
2:B:16:ARG:NH1	37:B:8617:HOH:O	2.34	0.61
3:C:96:LYS:NZ	30:0:1351:G:OP1	2.33	0.61
30:0:1201:C:H2'	30:0:1202:A:H5'	1.82	0.61
30:0:951:A:O2'	30:0:952:G:H5'	2.01	0.61
30:0:960:G:H2'	30:0:960:G:N3	2.16	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1189:A:H1'	30:0:1209:C:C1'	2.30	0.61
30:0:2502:C:C2'	30:0:2503:A:H5'	2.30	0.61
15:O:42:GLU:HB2	37:O:2176:HOH:O	2.00	0.61
31:9:13:A:O2'	31:9:14:G:H5''	2.00	0.61
26:Z:35:SER:HB3	26:Z:47:ARG:HB2	1.81	0.61
10:J:82:THR:HG23	30:0:1242:A:C5'	2.24	0.60
2:B:238:ASN:HD22	2:B:240:GLY:N	1.98	0.60
12:L:143:THR:HG22	12:L:144:ASP:N	2.16	0.60
4:D:163:VAL:HA	37:D:6326:HOH:O	2.02	0.60
11:K:118:ALA:HA	11:K:125:ALA:HB2	1.81	0.60
23:W:21:LEU:HB3	23:W:26:ILE:HG12	1.82	0.60
8:H:6:ALA:HA	8:H:61:ARG:HH12	1.67	0.60
13:M:61:ILE:HG13	37:M:8617:HOH:O	1.99	0.60
20:T:24:ARG:HH21	20:T:39:ASN:HD22	1.46	0.60
8:H:19:ARG:HH12	30:0:1008:C:H5''	1.65	0.60
30:0:2587:OMU:H2'	30:0:2589:U:H5''	1.83	0.60
1:A:105:VAL:CG1	1:A:154:ALA:HB1	2.31	0.60
1:A:48:ASP:HB3	37:A:8599:HOH:O	2.02	0.60
12:L:4:LYS:HE2	30:0:645:U:OP2	2.01	0.60
30:0:2415:A:H2'	30:0:2416:G:H5'	1.82	0.60
9:I:110:ASP:O	30:0:1163:G:H5'	2.02	0.60
14:N:37:ARG:NH1	31:9:6:C:OP1	2.34	0.60
30:0:2768:A:O2'	30:0:2769:C:H5'	2.01	0.60
30:0:1528:A:H2'	30:0:1529:G:O4'	2.01	0.60
30:0:1172:G:H5''	37:0:6809:HOH:O	2.01	0.60
30:0:1377:C:H5'	30:0:1377:C:C6	2.37	0.60
30:0:1559:A:H1'	37:0:5413:HOH:O	2.02	0.60
18:R:117:HIS:HD2	30:0:20:G:H21	1.50	0.60
2:B:267:LYS:HD3	37:B:8526:HOH:O	2.01	0.60
23:W:88:THR:HG22	23:W:89:ASP:N	2.17	0.60
25:Y:235:GLU:H	25:Y:235:GLU:CD	2.05	0.60
30:0:1205:U:C2'	30:0:1206:U:H5''	2.32	0.59
30:0:1350:U:H4'	37:0:4662:HOH:O	2.02	0.59
30:0:2670:G:O2'	30:0:2671:U:H5'	2.02	0.59
30:0:2578:G:H5'	30:0:2578:G:H8	1.67	0.59
2:B:212:GLN:HB2	2:B:257:THR:CG2	2.29	0.59
10:J:18:ILE:HD13	30:0:1244:U:OP1	2.02	0.59
25:Y:133:HIS:HD2	37:Y:8579:HOH:O	1.85	0.59
30:0:1175:G:H1'	30:0:1193:A:H2'	1.84	0.59
30:0:2488:A:H2	37:0:6826:HOH:O	1.84	0.59
14:N:48:VAL:CG1	14:N:55:ASP:HB3	2.32	0.59

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:49:G:O2'	31:9:50:G:H5'	2.01	0.59
1:A:190:ARG:NH2	1:A:207:GLN:OE1	2.35	0.59
23:W:4:LEU:O	23:W:32:CYS:HA	2.03	0.59
23:W:88:THR:HG22	23:W:89:ASP:H	1.67	0.59
30:0:2756:U:N3	30:0:2896:A:H2	1.98	0.59
31:9:23:U:O2'	31:9:24:U:H4'	2.02	0.59
23:W:84:VAL:HG12	37:W:6679:HOH:O	2.02	0.59
30:0:567:U:H5''	37:0:5949:HOH:O	2.01	0.59
30:0:2420:G:O2'	30:0:2421:G:H5'	2.02	0.59
3:C:27:ARG:NH2	30:0:657:G:OP1	2.31	0.59
10:J:107:ASN:HD21	10:J:109:TYR:HB2	1.68	0.59
23:W:139:GLY:O	23:W:141:HIS:HD2	1.85	0.59
30:0:1159:G:H1	30:0:1208:C:H42	1.50	0.59
30:0:204:A:C2'	30:0:205:U:H5'	2.32	0.59
30:0:2649:A:H5'	30:0:2649:A:C8	2.38	0.59
30:0:1120:U:H5''	30:0:1120:U:C6	2.37	0.58
11:K:87:ARG:HG3	30:0:2721:U:H4'	1.85	0.58
9:I:112:LEU:HD11	30:0:1162:G:H1'	1.84	0.58
11:K:109:LEU:HD13	11:K:113:ILE:HD11	1.85	0.58
23:W:122:ARG:HH11	23:W:122:ARG:HG2	1.68	0.58
30:0:1182:C:H1'	30:0:1192:A:H8	1.68	0.58
30:0:1667:A:H2'	30:0:1668:U:C6	2.38	0.58
30:0:2316:G:H4'	37:0:5638:HOH:O	2.03	0.58
31:9:64:C:C2'	31:9:65:A:H5'	2.33	0.58
18:R:17:MET:SD	37:R:8542:HOH:O	2.57	0.58
31:9:75:G:H1	31:9:106:U:H3	1.51	0.58
8:H:48:VAL:HA	8:H:170:ARG:O	2.03	0.58
18:R:29:LYS:HE2	30:0:524:A:H5'	1.85	0.58
30:0:1730:G:C5'	30:0:1731:C:H6	2.16	0.58
30:0:2604:A:H5'	37:0:5339:HOH:O	2.04	0.58
3:C:236:THR:CG2	3:C:239:ALA:H	2.11	0.58
18:R:99:ALA:HB1	18:R:109:MET:CE	2.32	0.58
20:T:52:ARG:HD2	30:0:317:A:H5''	1.84	0.58
1:A:211:LYS:HB3	1:A:212:PRO:HD2	1.84	0.58
3:C:76:ARG:HD3	37:C:8366:HOH:O	2.04	0.58
5:E:100:ASP:HB2	37:E:2789:HOH:O	2.03	0.58
23:W:64:THR:O	23:W:68:THR:HG22	2.04	0.58
23:W:80:ASP:O	23:W:84:VAL:HG23	2.02	0.58
30:0:2320:U:H4'	30:0:2321:A:O4'	2.03	0.58
30:0:2718:C:H6	30:0:2718:C:H5'	1.69	0.58
4:D:146:LYS:NZ	14:N:107:ASN:HD21	2.01	0.58

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:134:HIS:HE1	30:0:538:C:OP2	1.87	0.58
14:N:80:SER:HB2	37:N:8535:HOH:O	2.02	0.58
19:S:51:GLN:NE2	19:S:53:ASN:HD21	2.02	0.58
30:0:1118:A:H8	30:0:1119:G:H5''	1.67	0.58
31:9:92:G:H2'	31:9:93:A:C8	2.39	0.58
12:L:148:GLU:HA	37:L:8561:HOH:O	2.04	0.58
14:N:43:VAL:HG13	14:N:118:ILE:HD11	1.84	0.58
30:0:2064:U:H4'	30:0:2653:A:OP1	2.04	0.57
29:3:60:LYS:HG3	37:0:7104:HOH:O	2.04	0.57
31:9:20:G:O2'	31:9:21:G:H5'	2.04	0.57
10:J:107:ASN:ND2	10:J:109:TYR:H	2.01	0.57
30:0:2878:U:H2'	30:0:2879:A:O4'	2.04	0.57
31:9:35:C:H5''	37:9:8455:HOH:O	2.04	0.57
3:C:78:ARG:HG3	3:C:78:ARG:HH11	1.67	0.57
16:P:10:ALA:HA	16:P:13:VAL:HG12	1.86	0.57
18:R:29:LYS:HE2	30:0:524:A:H5''	1.87	0.57
3:C:76:ARG:HG2	3:C:78:ARG:HH12	1.68	0.57
4:D:103:ASN:ND2	4:D:134:LEU:H	2.02	0.57
30:0:1119:G:N2	30:0:1246:A:H2	1.95	0.57
31:9:28:U:H2'	31:9:29:C:C6	2.39	0.57
2:B:162:MET:HE2	2:B:310:ARG:HD3	1.87	0.57
19:S:57:THR:HG22	19:S:59:ASP:N	2.18	0.57
30:0:1819:G:H5'	37:0:4250:HOH:O	2.05	0.57
30:0:1972:U:H2'	30:0:1973:A:H5''	1.85	0.57
23:W:38:THR:HG22	37:W:3580:HOH:O	2.03	0.57
30:0:1679:C:H5'	37:0:8846:HOH:O	2.04	0.57
30:0:1701:A:H5''	30:0:1702:U:H3'	1.86	0.57
30:0:1834:C:H2'	30:0:1840:A:N6	2.18	0.57
30:0:432:G:O2'	30:0:433:C:H5'	2.05	0.57
30:0:1289:C:O2'	30:0:1290:G:H5'	2.05	0.57
30:0:2064:U:H5'	30:0:2652:U:H4'	1.85	0.57
12:L:6:ARG:HD3	30:0:1299:G:O6	2.04	0.57
30:0:1730:G:C5'	30:0:1731:C:C5	2.87	0.57
30:0:558:C:C2'	30:0:559:U:C5'	2.82	0.57
3:C:115:LEU:HD21	3:C:243:VAL:HG13	1.87	0.57
23:W:125:HIS:CD2	23:W:127:GLY:H	2.23	0.57
30:0:558:C:H2'	30:0:559:U:H5''	1.86	0.56
30:0:681:G:N3	30:0:681:G:H5'	2.20	0.56
1:A:121:ALA:O	1:A:124:VAL:HG22	2.04	0.56
6:F:50:VAL:CG1	6:F:60:VAL:HG11	2.35	0.56
13:M:182:LYS:HE2	30:0:392:U:O2'	2.05	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:24:GLN:NE2	13:M:27:ARG:HH11	2.03	0.56
25:Y:144:ARG:NH1	37:Y:8573:HOH:O	2.37	0.56
30:0:1181:A:C2'	30:0:1182:C:H5'	2.36	0.56
30:0:2467:A:H1'	37:0:4272:HOH:O	2.04	0.56
30:0:282:C:O2'	30:0:283:U:C5'	2.51	0.56
27:1:42:SER:HB2	37:1:8409:HOH:O	2.05	0.56
30:0:703:G:O2'	30:0:704:C:H5'	2.06	0.56
13:M:24:GLN:HE21	13:M:27:ARG:HH11	1.53	0.56
14:N:7:LYS:HE3	17:Q:21:ARG:O	2.05	0.56
21:U:14:GLU:O	21:U:17:THR:HB	2.05	0.56
25:Y:204:ARG:HH22	30:0:553:G:P	2.28	0.56
30:0:1878:G:O2'	30:0:1879:U:H6	1.89	0.56
30:0:2435:U:H1'	37:0:4978:HOH:O	2.06	0.56
1:A:192:VAL:HG13	37:A:8553:HOH:O	2.05	0.56
10:J:103:VAL:HG12	37:J:5907:HOH:O	2.04	0.56
19:S:43:GLU:HB3	37:S:7106:HOH:O	2.05	0.56
30:0:2488:A:H61	30:0:2534:C:H42	1.53	0.56
30:0:2851:G:C2'	30:0:2852:A:H5'	2.35	0.56
3:C:162:VAL:HG22	3:C:232:LEU:HD21	1.86	0.56
3:C:1:MET:HG2	3:C:2:GLN:N	2.20	0.56
30:0:2300:A:H4'	30:0:2301:A:O5'	2.06	0.56
16:P:143:ALA:HA	37:P:184:HOH:O	2.03	0.56
30:0:1118:A:H62	30:0:1244:U:H3	1.54	0.56
6:F:38:LYS:HE3	30:0:244:C:OP2	2.06	0.56
30:0:282:C:H1'	30:0:368:C:H42	1.70	0.56
1:A:153:ARG:HH11	1:A:153:ARG:HB2	1.71	0.56
10:J:107:ASN:HD22	10:J:109:TYR:H	1.53	0.56
30:0:1278:A:H4'	30:0:1279:U:C4	2.41	0.56
2:B:139:ASP:HB2	2:B:165:ARG:HE	1.70	0.56
11:K:34:VAL:CG2	11:K:47:ALA:HB2	2.36	0.56
22:V:39:ALA:N	22:V:40:PRO:HD2	2.21	0.56
30:0:1477:C:H5'	30:0:1868:G:C5'	2.35	0.56
30:0:899:C:H5'	37:0:9733:HOH:O	2.05	0.56
30:0:2251:G:H2'	30:0:2252:A:C8	2.41	0.56
27:1:8:GLN:HE22	27:1:11:LYS:NZ	2.04	0.56
1:A:223:ARG:HG3	37:A:8595:HOH:O	2.05	0.56
5:E:143:GLN:HE21	30:0:2780:C:H1'	1.71	0.56
11:K:55:VAL:HG12	11:K:56:SER:N	2.21	0.56
13:M:95:LYS:HE2	30:0:157:G:H4'	1.88	0.56
14:N:37:ARG:NE	37:N:8533:HOH:O	2.39	0.56
30:0:2502:C:H2'	30:0:2503:A:H5'	1.87	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:50:VAL:HG22	31:9:41:C:O4'	2.05	0.56
2:B:320:GLN:HE21	2:B:321:PRO:HD2	1.70	0.56
30:0:1120:U:H5'	30:0:1121:G:OP2	2.05	0.55
30:0:1250:C:O2'	30:0:1251:C:H5'	2.05	0.55
30:0:2825:C:H4'	30:0:2826:G:O5'	2.06	0.55
30:0:396:U:H1'	37:0:7180:HOH:O	2.06	0.55
31:9:91:C:H2'	31:9:92:G:O4'	2.05	0.55
20:T:53:GLY:HA3	37:T:6384:HOH:O	2.05	0.55
16:P:120:ARG:HD2	30:0:1594:C:OP2	2.07	0.55
30:0:2361:A:H5''	37:0:8523:HOH:O	2.07	0.55
37:N:8545:HOH:O	31:9:49:G:H5''	2.05	0.55
1:A:96:LEU:HD22	1:A:128:LEU:HD13	1.87	0.55
5:E:68:HIS:O	5:E:72:MET:HG3	2.06	0.55
5:E:81:GLU:HG2	5:E:134:SER:HB3	1.86	0.55
11:K:98:VAL:CG1	11:K:102:GLU:HA	2.35	0.55
21:U:37:GLU:HB3	37:U:408:HOH:O	2.06	0.55
4:D:25:MET:CE	4:D:37:ALA:HB1	2.36	0.55
14:N:110:THR:HB	14:N:113:SER:OG	2.06	0.55
14:N:141:ARG:HH21	31:9:48:C:H4'	1.71	0.55
30:0:1783:A:O2'	30:0:1784:U:H5'	2.06	0.55
30:0:88:G:H5'	30:0:88:G:H8	1.72	0.55
23:W:115:THR:HG23	37:W:5420:HOH:O	2.06	0.55
23:W:21:LEU:HD21	23:W:48:VAL:CG1	2.36	0.55
13:M:188:ARG:HD3	30:0:155:C:OP2	2.06	0.55
30:0:204:A:H2'	30:0:205:U:H5'	1.88	0.55
11:K:74:VAL:HG12	11:K:75:ARG:HG3	1.87	0.55
18:R:25:PHE:CE2	18:R:29:LYS:HE3	2.41	0.55
30:0:1636:G:O2'	30:0:1637:A:H5'	2.07	0.55
3:C:129:HIS:CE1	3:C:231:ARG:HA	2.42	0.55
6:F:13:GLU:OE2	6:F:78:GLU:HG2	2.07	0.55
13:M:99:ARG:HD2	13:M:167:GLY:HA2	1.87	0.55
23:W:122:ARG:HG3	23:W:152:ALA:O	2.06	0.55
5:E:91:PHE:CE1	30:0:2694:A:H4'	2.41	0.55
22:V:39:ALA:C	22:V:41:GLU:H	2.09	0.55
30:0:1595:G:O2'	30:0:1596:U:H5'	2.07	0.55
27:1:16:HIS:HE1	30:0:775:G:OP1	1.90	0.55
28:2:22:PRO:HG2	28:2:25:VAL:HG23	1.88	0.55
2:B:17:LYS:O	2:B:260:HIS:HD2	1.90	0.55
11:K:74:VAL:CG1	11:K:113:ILE:HG12	2.36	0.55
13:M:134:ILE:HG23	13:M:141:ILE:HD13	1.89	0.55
30:0:1135:G:H5'	37:0:5475:HOH:O	2.05	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1165:G:O2'	30:0:1174:A:H1'	2.07	0.54
30:0:661:G:C5	30:0:686:A:C2	2.95	0.54
13:M:84:LYS:HE2	37:M:8571:HOH:O	2.06	0.54
14:N:11:ARG:HG3	14:N:14:ARG:NH1	2.22	0.54
14:N:41:LYS:HD3	37:9:8439:HOH:O	2.08	0.54
25:Y:169:ARG:HD3	30:0:1328:A:C8	2.43	0.54
30:0:1972:U:H2'	30:0:1973:A:C5'	2.37	0.54
30:0:2467:A:O2'	30:0:2468:A:H2'	2.06	0.54
10:J:70:PHE:HE1	30:0:2676:C:H4'	1.72	0.54
30:0:1181:A:H2'	30:0:1182:C:H5'	1.89	0.54
30:0:2419:U:H5''	30:0:2420:G:H5'	1.89	0.54
30:0:485:A:N3	30:0:487:G:H5''	2.22	0.54
2:B:125:GLU:O	2:B:129:ARG:HG3	2.07	0.54
30:0:1158:G:O2'	30:0:1159:G:H5'	2.08	0.54
30:0:2712:G:H5'	37:0:4763:HOH:O	2.07	0.54
3:C:79:ARG:O	3:C:87:ARG:HG2	2.08	0.54
9:I:100:VAL:HG11	9:I:124:VAL:HG22	1.89	0.54
11:K:29:LEU:HB3	11:K:55:VAL:CG1	2.28	0.54
13:M:34:GLU:HB3	13:M:38:GLU:HG3	1.88	0.54
18:R:17:MET:HE1	37:0:3769:HOH:O	2.06	0.54
30:0:1299:G:H5'	37:0:3611:HOH:O	2.06	0.54
30:0:1926:G:H2'	30:0:1927:A:C8	2.43	0.54
30:0:2524:G:H21	30:0:2526:C:N4	2.05	0.54
30:0:343:C:O2'	30:0:344:C:H5'	2.06	0.54
31:9:76:G:C3'	31:9:77:A:H5''	2.28	0.54
2:B:18:ARG:HG3	2:B:256:GLN:HG3	1.89	0.54
2:B:254:GLN:HG3	37:0:9223:HOH:O	2.08	0.54
9:I:69:PRO:HA	30:0:1164:U:OP1	2.08	0.54
30:0:1615:A:H5'	37:0:3722:HOH:O	2.06	0.54
30:0:200:C:H2'	37:0:9976:HOH:O	2.08	0.54
3:C:115:LEU:O	3:C:118:THR:HB	2.08	0.54
4:D:159:PRO:O	4:D:163:VAL:HG23	2.07	0.54
25:Y:187:VAL:HG22	25:Y:192:ASP:HB2	1.89	0.54
30:0:1279:U:O2	30:0:1279:U:H2'	2.06	0.54
30:0:644:G:N3	30:0:644:G:H5'	2.22	0.54
4:D:23:VAL:HG21	4:D:45:THR:HG21	1.88	0.54
11:K:82:ARG:NH2	11:K:115:ARG:HG2	2.23	0.54
30:0:1268:C:O2'	30:0:1269:G:H5'	2.07	0.54
30:0:1973:A:H5'	30:0:1973:A:C8	2.35	0.54
30:0:2638:G:H5'	37:0:4469:HOH:O	2.08	0.54
24:X:43:VAL:HG12	24:X:44:ASP:N	2.23	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1972:U:C2'	30:0:1973:A:H5''	2.37	0.54
30:0:280:C:H2'	30:0:281:U:O4'	2.08	0.54
17:Q:95:GLU:HA	30:0:949:U:H4'	1.89	0.54
2:B:51:VAL:CG2	2:B:327:VAL:HG13	2.38	0.54
4:D:54:ALA:CB	4:D:69:ILE:HD12	2.38	0.54
12:L:80:ASP:HB2	12:L:90:ARG:O	2.08	0.54
9:I:87:PRO:C	9:I:89:GLU:H	2.10	0.53
2:B:336:GLN:O	30:0:2862:G:H4'	2.07	0.53
24:X:25:ARG:HD2	37:X:3861:HOH:O	2.07	0.53
3:C:184:ARG:HD2	30:0:1306:U:OP1	2.08	0.53
14:N:160:SER:HB3	31:9:51:A:H5'	1.89	0.53
14:N:4:PRO:HD2	37:0:6319:HOH:O	2.08	0.53
23:W:88:THR:HG23	23:W:110:GLN:HB3	1.89	0.53
9:I:113:SER:HB2	9:I:118:ASN:HB2	1.89	0.53
13:M:169:ARG:HD2	37:M:8587:HOH:O	2.08	0.53
30:0:1730:G:H5''	30:0:1731:C:C6	2.41	0.53
30:0:2001:G:O2'	30:0:2002:C:H5'	2.08	0.53
30:0:95:A:H5''	30:0:97:G:O4'	2.08	0.53
1:A:36:ASP:O	1:A:38:ILE:N	2.34	0.53
5:E:11:VAL:HG12	5:E:12:ASP:N	2.23	0.53
20:T:1:SER:HB2	30:0:447:A:OP2	2.08	0.53
10:J:75:PRO:HG2	10:J:105:LEU:HD21	1.89	0.53
2:B:329:TYR:CE2	21:U:15:PRO:HG2	2.44	0.53
30:0:814:G:H4'	37:0:9664:HOH:O	2.08	0.53
27:1:21:ARG:HD2	27:1:37:CYS:SG	2.48	0.53
1:A:88:ILE:HD13	1:A:100:PRO:HD3	1.90	0.53
8:H:32:ALA:HB3	8:H:69:ARG:HH12	1.73	0.53
1:A:105:VAL:HG11	1:A:154:ALA:HB1	1.90	0.53
21:U:39:ASN:ND2	21:U:44:ARG:HH11	2.06	0.53
30:0:1116:U:O2'	30:0:1118:A:C2	2.40	0.53
30:0:172:U:H5'	37:0:3697:HOH:O	2.09	0.53
31:9:24:U:H3'	31:9:25:G:H5'	1.90	0.53
1:A:97:ALA:HB2	1:A:150:PRO:HB2	1.91	0.53
2:B:51:VAL:HG23	2:B:329:TYR:O	2.09	0.53
4:D:135:VAL:HG21	4:D:139:TYR:CD1	2.43	0.53
5:E:69:ILE:HA	5:E:72:MET:HE3	1.90	0.53
6:F:101:ALA:HA	37:F:5413:HOH:O	2.09	0.53
13:M:81:ARG:HG3	13:M:85:ARG:HB2	1.91	0.53
30:0:2563:U:H2'	30:0:2565:C:O5'	2.08	0.52
13:M:58:GLN:NE2	30:0:259:G:H21	2.08	0.52
31:9:107:C:H5	37:9:8435:HOH:O	1.91	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:73:HIS:HE1	30:0:1789:G:O6	1.91	0.52
30:0:1189:A:H1'	30:0:1209:C:O4'	2.09	0.52
30:0:1525:G:H5'	30:0:1526:A:OP2	2.09	0.52
29:3:17:HIS:O	29:3:18:GLN:HG3	2.10	0.52
2:B:307:ARG:HG3	2:B:307:ARG:NH1	2.20	0.52
6:F:58:GLU:HA	6:F:61:MET:HE2	1.90	0.52
14:N:163:PHE:HZ	14:N:171:HIS:HD1	1.55	0.52
22:V:57:LYS:HA	22:V:60:GLN:HE21	1.74	0.52
30:0:2866:U:H4'	30:0:2867:G:H5'	1.90	0.52
6:F:39:SER:HB3	6:F:45:ALA:HB2	1.91	0.52
7:G:64:ASN:N	7:G:64:ASN:HD22	2.06	0.52
14:N:12:ARG:HD3	14:N:18:THR:OG1	2.09	0.52
16:P:83:LYS:HG2	30:0:793:A:H5''	1.92	0.52
17:Q:40:HIS:HE1	30:0:949:U:O2'	1.92	0.52
30:0:2256:G:H2'	30:0:2257:G:C5'	2.39	0.52
1:A:81:GLN:HB2	1:A:92:ASN:ND2	2.23	0.52
6:F:53:ASP:OD1	6:F:80:GLN:HB2	2.09	0.52
16:P:41:ARG:HH22	30:0:1500:U:P	2.32	0.52
18:R:18:LEU:HG	18:R:91:LEU:HD13	1.90	0.52
30:0:2241:C:O2'	30:0:2242:U:H5'	2.09	0.52
30:0:794:U:H3	30:0:819:A:H61	1.57	0.52
4:D:135:VAL:HG22	4:D:136:ARG:N	2.24	0.52
30:0:1211:G:O2'	30:0:1212:C:H5'	2.10	0.52
13:M:163:LEU:HD21	30:0:188:C:H5''	1.91	0.52
1:A:123:GLY:HA3	1:A:162:GLY:HA2	1.92	0.52
3:C:246:ARG:NH1	37:C:8369:HOH:O	2.42	0.52
17:Q:25:PRO:HB2	37:Q:4350:HOH:O	2.10	0.52
23:W:151:GLU:O	23:W:154:ARG:HB2	2.09	0.52
1:A:95:PRO:HG2	1:A:98:GLU:HG2	1.91	0.52
15:O:47:ARG:HG3	15:O:47:ARG:HH11	1.75	0.52
25:Y:132:ASP:OD2	30:0:621:C:H5'	2.10	0.52
5:E:69:ILE:HA	5:E:72:MET:CE	2.40	0.52
6:F:63:ILE:HB	6:F:64:PRO:HD3	1.92	0.52
23:W:130:HIS:O	23:W:136:GLY:HA3	2.10	0.52
8:H:15:PRO:HG3	30:0:1053:G:OP1	2.10	0.52
30:0:319:A:H4'	30:0:338:C:C4	2.45	0.52
20:T:1:SER:HB2	30:0:447:A:P	2.50	0.52
30:0:65:C:O2'	30:0:66:G:H5'	2.09	0.52
30:0:820:G:O2'	30:0:856:G:H4'	2.10	0.52
14:N:11:ARG:NH1	31:9:8:G:O6	2.42	0.52
1:A:47:HIS:HD2	30:0:1654:U:H2'	1.74	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:MET:HG2	1:A:186:TRP:CB	2.40	0.51
9:I:108:HIS:N	9:I:109:PRO:HD2	2.25	0.51
30:0:1118:A:C8	30:0:1119:G:H5''	2.45	0.51
30:0:1120:U:H6	30:0:1120:U:H5''	1.75	0.51
30:0:2329:C:O2'	30:0:2330:U:H5'	2.10	0.51
30:0:291:C:H2'	30:0:292:G:O4'	2.11	0.51
10:J:19:MET:HE2	10:J:132:LEU:HD11	1.92	0.51
26:Z:61:HIS:HB2	26:Z:71:VAL:HB	1.91	0.51
30:0:1406:A:H4'	30:0:1407:A:H5''	1.92	0.51
30:0:2507:G:H2'	30:0:2510:C:N4	2.23	0.51
30:0:256:C:H2'	30:0:257:G:O4'	2.11	0.51
15:O:25:VAL:HG12	30:0:709:G:O2'	2.10	0.51
2:B:305:ASP:O	2:B:306:LYS:HB2	2.11	0.51
8:H:66:GLU:HA	37:H:8381:HOH:O	2.09	0.51
17:Q:11:ARG:HD3	37:Q:5620:HOH:O	2.09	0.51
19:S:51:GLN:HE21	19:S:53:ASN:ND2	2.08	0.51
24:X:71:ARG:HD3	37:X:2171:HOH:O	2.10	0.51
25:Y:187:VAL:HB	25:Y:203:VAL:HG22	1.91	0.51
30:0:1165:G:O2'	30:0:1174:A:C1'	2.59	0.51
30:0:1942:A:H3'	37:0:6896:HOH:O	2.11	0.51
30:0:1996:U:O2'	30:0:1997:A:H5'	2.11	0.51
30:0:2769:C:H2'	30:0:2770:G:O4'	2.11	0.51
30:0:951:A:H2'	30:0:952:G:H5'	1.92	0.51
28:2:31:ARG:NH2	37:2:7177:HOH:O	2.43	0.51
3:C:236:THR:HA	37:C:8449:HOH:O	2.10	0.51
9:I:124:VAL:O	9:I:124:VAL:HG12	2.11	0.51
25:Y:169:ARG:HB2	30:0:1268:C:O2'	2.11	0.51
30:0:2795:C:O2'	30:0:2796:U:H5'	2.09	0.51
30:0:920:C:H5'	30:0:921:G:C4	2.45	0.51
8:H:12:ILE:HG23	8:H:129:ARG:CZ	2.41	0.51
14:N:48:VAL:HG11	14:N:55:ASP:HB3	1.93	0.51
30:0:1527:A:H1'	30:0:1528:A:C8	2.45	0.51
30:0:2072:G:C6	30:0:2533:C:H1'	2.46	0.51
30:0:969:G:H1	30:0:999:C:H42	1.59	0.51
1:A:192:VAL:HG12	1:A:207:GLN:HB3	1.91	0.51
1:A:191:GLY:HA2	1:A:194:MET:HE2	1.93	0.51
19:S:10:VAL:HG11	22:V:36:ALA:HA	1.92	0.51
30:0:1342:C:O2'	30:0:1343:C:H5'	2.10	0.51
30:0:2830:U:H3'	37:0:4770:HOH:O	2.09	0.51
30:0:90:A:H2'	30:0:91:G:O4'	2.11	0.51
29:3:48:ASN:ND2	29:3:50:GLY:H	2.09	0.51

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:23:VAL:HG21	4:D:45:THR:CG2	2.41	0.51
30:0:2301:A:H5''	30:0:2302:A:H5'	1.91	0.51
30:0:2591:C:H2'	30:0:2592:G:O4'	2.11	0.51
24:X:15:ARG:NH1	30:0:2896:A:OP1	2.44	0.51
30:0:848:C:H5'	37:0:6823:HOH:O	2.10	0.51
31:9:49:G:H2'	31:9:50:G:O4'	2.11	0.51
4:D:104:PHE:CE2	4:D:132:VAL:HB	2.46	0.51
4:D:84:LEU:HA	4:D:87:ALA:HB3	1.93	0.51
5:E:23:GLU:HG2	5:E:28:SER:HB3	1.93	0.51
10:J:75:PRO:HG2	10:J:105:LEU:CD2	2.41	0.51
12:L:30:ARG:HD2	37:0:8538:HOH:O	2.11	0.51
22:V:55:ARG:O	22:V:59:ILE:HG12	2.11	0.51
1:A:53:ALA:HB3	37:A:8599:HOH:O	2.10	0.51
23:W:65:VAL:HA	23:W:68:THR:HG22	1.92	0.51
30:0:1180:U:H2'	30:0:1181:A:C8	2.46	0.51
30:0:2478:U:O2'	30:0:2479:A:H5'	2.10	0.51
11:K:30:LYS:O	11:K:55:VAL:HG13	2.11	0.51
21:U:33:SER:O	21:U:37:GLU:HG3	2.10	0.51
30:0:1333:U:H2'	30:0:1334:C:C6	2.46	0.50
30:0:1503:U:H2'	30:0:1504:A:O4'	2.12	0.50
30:0:2445:U:H2'	30:0:2446:G:C8	2.46	0.50
30:0:2756:U:C2	30:0:2896:A:H2	2.28	0.50
30:0:960:G:N3	30:0:960:G:C2'	2.74	0.50
31:9:56:A:C3'	31:9:57:A:H5''	2.40	0.50
3:C:214:THR:HG23	37:C:8435:HOH:O	2.10	0.50
4:D:25:MET:HE2	4:D:41:LEU:HG	1.93	0.50
25:Y:126:PRO:HG2	25:Y:128:PHE:CE1	2.46	0.50
30:0:2265:U:H2'	30:0:2266:A:C8	2.47	0.50
28:2:35:ARG:HB2	37:2:2691:HOH:O	2.11	0.50
2:B:264:GLU:HG2	2:B:267:LYS:CE	2.41	0.50
30:0:1741:U:O2'	30:0:2723:G:H4'	2.11	0.50
2:B:288:GLY:HA2	30:0:2898:G:H4'	1.93	0.50
27:1:28:HIS:HE1	30:0:776:A:OP1	1.94	0.50
2:B:212:GLN:HA	30:0:1733:A:H4'	1.92	0.50
7:G:16:LYS:O	7:G:20:VAL:HG23	2.12	0.50
8:H:41:LYS:HE2	8:H:45:ASP:HB3	1.93	0.50
8:H:6:ALA:HB3	30:0:2521:A:OP2	2.10	0.50
16:P:54:LYS:HB2	30:0:1717:A:H5''	1.94	0.50
30:0:2415:A:C2'	30:0:2416:G:H5'	2.41	0.50
30:0:2472:C:O2'	30:0:2634:G:H4'	2.12	0.50
9:I:112:LEU:CD1	30:0:1162:G:H1'	2.41	0.50

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1603:A:C5'	30:0:1605:G:O4'	2.60	0.50
30:0:1921:A:C6	30:0:1922:A:C2	3.00	0.50
30:0:2842:G:H2'	30:0:2843:A:H5'	1.93	0.50
30:0:447:A:O2'	30:0:448:G:H5'	2.12	0.50
4:D:76:ARG:NE	31:9:44:A:O4'	2.45	0.50
2:B:214:PRO:HD2	37:B:8521:HOH:O	2.12	0.50
5:E:15:GLN:HG2	5:E:19:ASP:O	2.12	0.50
14:N:86:LEU:HD12	14:N:125:ALA:HB2	1.94	0.50
23:W:122:ARG:NH2	37:0:4835:HOH:O	2.45	0.50
24:X:76:ARG:HH11	24:X:76:ARG:HG3	1.74	0.50
3:C:174:ILE:HD11	30:0:338:C:H4'	1.94	0.50
10:J:45:VAL:HG21	10:J:129:PHE:CD1	2.46	0.50
20:T:24:ARG:HH21	20:T:39:ASN:ND2	2.09	0.50
30:0:1342:C:C2'	30:0:1343:C:H5'	2.42	0.50
30:0:1419:U:H5'	30:0:1420:C:OP2	2.11	0.50
30:0:861:A:C8	37:0:5228:HOH:O	2.55	0.50
28:2:8:LYS:NZ	30:0:1677:U:OP2	2.43	0.50
29:3:62:THR:HB	37:3:8549:HOH:O	2.10	0.50
20:T:38:ARG:NH1	37:T:6217:HOH:O	2.44	0.50
25:Y:187:VAL:HG23	37:Y:8567:HOH:O	2.11	0.50
30:0:2505:G:C2'	30:0:2506:A:H5'	2.41	0.50
30:0:308:U:C4	30:0:342:C:H1'	2.46	0.50
30:0:702:G:O2'	30:0:703:G:H5'	2.12	0.50
2:B:254:GLN:HG2	2:B:255:GLY:N	2.25	0.50
22:V:44:GLY:HA3	30:0:92:G:H4'	1.94	0.50
6:F:59:ILE:HD13	30:0:263:U:O4'	2.11	0.50
29:3:3:MET:O	29:3:90:PHE:HA	2.12	0.50
8:H:14:LYS:HE2	37:0:3382:HOH:O	2.11	0.50
8:H:49:GLN:HG3	8:H:140:TYR:CE2	2.47	0.50
11:K:62:PRO:HG3	11:K:65:ARG:NH2	2.26	0.50
26:Z:77:GLY:HA2	26:Z:91:GLY:O	2.12	0.50
10:J:52:GLN:NE2	30:0:1119:G:H8	2.06	0.49
17:Q:15:LYS:HD3	30:0:2364:A:H5''	1.93	0.49
1:A:179:MET:HA	1:A:179:MET:CE	2.42	0.49
1:A:3:ARG:HD3	30:0:870:G:OP2	2.11	0.49
37:R:8545:HOH:O	30:0:1370:G:H5''	2.12	0.49
30:0:2256:G:H2'	30:0:2257:G:H5'	1.95	0.49
2:B:102:THR:HG21	2:B:182:VAL:O	2.11	0.49
3:C:98:ARG:NH1	37:C:8355:HOH:O	2.44	0.49
8:H:72:ALA:HB2	8:H:156:ALA:HB2	1.94	0.49
14:N:179:LEU:HA	14:N:184:ILE:HD12	1.93	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:13:MET:CE	23:W:17:ILE:HG22	2.42	0.49
30:0:185:G:H4'	30:0:186:A:H4'	1.94	0.49
30:0:2061:C:C2'	30:0:2062:A:H5'	2.42	0.49
30:0:542:A:H2'	30:0:543:G:O4'	2.13	0.49
1:A:128:LEU:HG	37:A:8568:HOH:O	2.11	0.49
2:B:102:THR:HG23	2:B:182:VAL:HG12	1.95	0.49
7:G:20:VAL:O	7:G:24:VAL:HG23	2.12	0.49
13:M:164:THR:HG22	13:M:167:GLY:N	2.14	0.49
23:W:11:VAL:HG11	30:0:1086:A:C6	2.46	0.49
30:0:1127:C:C5	30:0:1128:U:C4	3.00	0.49
25:Y:115:ARG:HH21	30:0:1266:U:H4'	1.76	0.49
27:1:16:HIS:CD2	30:0:470:U:O2'	2.65	0.49
30:0:602:A:O2'	30:0:605:C:H4'	2.11	0.49
30:0:941:G:O2'	30:0:942:U:H5'	2.12	0.49
1:A:47:HIS:CD2	30:0:1654:U:H2'	2.47	0.49
15:O:24:ALA:HB3	30:0:710:G:OP1	2.11	0.49
20:T:49:GLU:HB3	20:T:59:GLU:HG2	1.95	0.49
23:W:68:THR:HG23	23:W:69:ARG:HG2	1.94	0.49
30:0:1137:G:H1'	37:0:3414:HOH:O	2.12	0.49
30:0:1206:U:H2'	30:0:1207:A:O4'	2.13	0.49
30:0:858:U:C6	37:0:4975:HOH:O	2.66	0.49
3:C:43:LYS:HG2	30:0:449:A:N7	2.27	0.49
4:D:154:LYS:H	4:D:154:LYS:CD	2.18	0.49
22:V:16:ARG:NH1	22:V:65:ASP:O	2.46	0.49
30:0:1189:A:O2'	30:0:1208:C:H2'	2.11	0.49
30:0:1819:G:H2'	30:0:1820:G:C4'	2.43	0.49
30:0:2010:A:H2'	37:0:5505:HOH:O	2.11	0.49
30:0:1787:C:H4'	30:0:2883:A:O4'	2.12	0.49
3:C:233:THR:HG22	3:C:234:VAL:N	2.26	0.49
1:A:211:LYS:O	30:0:1943:C:H4'	2.13	0.49
30:0:407:A:H5'	37:0:5572:HOH:O	2.13	0.49
4:D:23:VAL:HG22	4:D:73:VAL:HB	1.95	0.49
26:Z:37:ARG:NH1	37:Z:8419:HOH:O	2.45	0.49
30:0:1205:U:H2'	30:0:1206:U:H5'	1.95	0.49
28:2:22:PRO:HG2	28:2:25:VAL:CG2	2.42	0.49
4:D:65:GLU:HG3	37:D:6752:HOH:O	2.12	0.49
30:0:1641:A:C2'	30:0:1642:A:H5'	2.43	0.49
28:2:5:LYS:HD2	30:0:1675:C:H5''	1.95	0.49
30:0:2289:G:N2	30:0:2291:A:C2	2.71	0.49
30:0:441:A:H1'	30:0:442:A:N7	2.28	0.49
31:9:20:G:H3'	37:9:8434:HOH:O	2.13	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1167:G:H2'	30:0:1168:C:O4'	2.13	0.49
30:0:2089:A:O2'	30:0:2090:G:H5'	2.13	0.49
30:0:2896:A:N3	30:0:2896:A:H2'	2.28	0.49
30:0:482:G:H4'	30:0:508:A:N1	2.28	0.49
22:V:1:THR:CB	30:0:93:C:H5''	2.43	0.49
1:A:194:MET:SD	30:0:875:A:C2	3.06	0.49
2:B:221:GLN:HE22	11:K:42:ASN:ND2	2.03	0.49
3:C:78:ARG:HG3	3:C:78:ARG:NH1	2.27	0.49
8:H:49:GLN:NE2	8:H:140:TYR:HE2	2.11	0.49
10:J:88:PRO:O	10:J:94:GLY:HA3	2.13	0.49
30:0:1314:U:H5''	30:0:1316:G:O4'	2.13	0.48
30:0:559:U:H2'	30:0:560:U:O4'	2.13	0.48
30:0:871:G:H4'	37:0:3951:HOH:O	2.12	0.48
24:X:80:GLU:HB3	37:X:5564:HOH:O	2.12	0.48
30:0:1291:A:H2	37:0:4838:HOH:O	1.96	0.48
10:J:19:MET:CE	10:J:132:LEU:HD11	2.43	0.48
30:0:1730:G:H5'	30:0:1731:C:C6	2.43	0.48
30:0:737:A:H2'	30:0:738:G:O4'	2.13	0.48
2:B:154:VAL:HG12	2:B:156:LYS:HG2	1.96	0.48
30:0:1014:A:H2'	30:0:1015:C:H5'	1.95	0.48
30:0:1506:U:H6	30:0:1506:U:H5'	1.79	0.48
12:L:18:HIS:CD2	30:0:902:G:N7	2.79	0.48
2:B:304:PRO:HD2	2:B:307:ARG:NE	2.29	0.48
2:B:62:ARG:HA	2:B:65:MET:CE	2.43	0.48
3:C:129:HIS:HE1	3:C:231:ARG:HA	1.79	0.48
7:G:12:ILE:N	7:G:13:PRO:HD3	2.28	0.48
30:0:1339:G:C6	30:0:1340:G:N1	2.80	0.48
30:0:1667:A:H2'	30:0:1668:U:H6	1.77	0.48
5:E:91:PHE:HE1	30:0:2694:A:H4'	1.78	0.48
30:0:2911:C:H2'	30:0:2912:C:C6	2.49	0.48
2:B:264:GLU:HG2	2:B:267:LYS:HE2	1.95	0.48
2:B:297:VAL:HB	37:B:8606:HOH:O	2.12	0.48
13:M:107:ARG:NH1	37:M:8573:HOH:O	2.46	0.48
16:P:81:LYS:HG2	37:0:9060:HOH:O	2.14	0.48
30:0:1044:C:H3'	30:0:1045:G:H5''	1.95	0.48
30:0:1377:C:C5'	30:0:1377:C:H6	2.25	0.48
30:0:1588:G:C6	30:0:1589:G:N1	2.82	0.48
30:0:2314:G:C2'	30:0:2315:C:H5'	2.43	0.48
1:A:125:ASN:HB3	1:A:158:VAL:HG12	1.95	0.48
14:N:58:LEU:N	14:N:58:LEU:HD12	2.29	0.48
18:R:18:LEU:HB2	18:R:143:VAL:CG1	2.43	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:39:ALA:N	22:V:40:PRO:CD	2.77	0.48
30:0:1159:G:H21	30:0:1189:A:H8	1.62	0.48
30:0:1772:C:H5'	30:0:1773:G:C5	2.49	0.48
30:0:2421:G:H4'	37:0:4318:HOH:O	2.13	0.48
30:0:871:G:H8	30:0:871:G:H5''	1.74	0.48
31:9:2:U:OP2	31:9:2:U:H4'	2.14	0.48
2:B:82:VAL:HG12	2:B:82:VAL:O	2.12	0.48
2:B:85:ARG:NH1	37:B:8634:HOH:O	2.46	0.48
4:D:166:ILE:HD12	37:D:6326:HOH:O	2.13	0.48
13:M:99:ARG:HH21	13:M:170:ASN:ND2	2.11	0.48
24:X:23:HIS:HE1	30:0:2044:G:OP1	1.96	0.48
30:0:1409:G:H5'	37:0:3263:HOH:O	2.14	0.48
30:0:255:A:H2'	30:0:256:C:C6	2.49	0.48
30:0:2754:G:C2'	30:0:2755:G:H5'	2.44	0.48
31:9:55:U:H4'	31:9:56:A:C8	2.48	0.48
1:A:29:HIS:HB2	1:A:153:ARG:HH12	1.79	0.48
2:B:268:ARG:NH2	2:B:325:PRO:HG3	2.28	0.48
3:C:12:THR:HB	37:C:8439:HOH:O	2.13	0.48
4:D:137:PRO:O	31:9:30:C:OP1	2.32	0.48
10:J:74:ARG:NH1	10:J:76:ASP:HB2	2.28	0.48
12:L:67:ARG:HB2	12:L:112:GLY:HA3	1.95	0.48
13:M:15:PRO:HA	13:M:20:LEU:HD23	1.95	0.48
23:W:108:ARG:HE	23:W:114:PRO:HG3	1.78	0.48
24:X:25:ARG:HG2	37:X:5356:HOH:O	2.13	0.48
30:0:1202:A:C2'	30:0:1203:G:H5'	2.44	0.48
30:0:1419:U:H2'	30:0:1685:A:C2	2.49	0.48
30:0:2134:G:C6	30:0:2258:A:C8	3.01	0.48
30:0:236:A:C4'	30:0:237:G:H5'	2.38	0.48
30:0:2909:G:H2'	30:0:2910:A:H8	1.78	0.48
14:N:11:ARG:HD3	31:9:114:G:O6	2.13	0.48
3:C:27:ARG:HG3	3:C:29:ASP:OD1	2.14	0.48
18:R:29:LYS:HD3	37:0:4262:HOH:O	2.14	0.48
30:0:1484:G:H2'	37:0:8620:HOH:O	2.14	0.48
11:K:87:ARG:NH2	30:0:2720:C:O2	2.47	0.48
13:M:125:ARG:HD3	37:0:4520:HOH:O	2.13	0.48
23:W:154:ARG:NH1	30:0:588:G:O6	2.46	0.48
23:W:38:THR:HG22	23:W:39:ASP:N	2.29	0.48
26:Z:35:SER:CB	26:Z:47:ARG:HB2	2.44	0.48
30:0:10:U:O4	30:0:532:A:OP2	2.31	0.47
30:0:2668:G:H2'	30:0:2669:U:C6	2.49	0.47
30:0:2768:A:H5''	37:0:3966:HOH:O	2.13	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:PRO:HB2	37:A:8556:HOH:O	2.14	0.47
3:C:87:ARG:NH2	30:0:894:A:C2	2.82	0.47
14:N:4:PRO:HB2	30:0:1010:C:H4'	1.96	0.47
30:0:1202:A:H2'	30:0:1203:G:H5'	1.96	0.47
30:0:1735:C:O2'	30:0:1736:A:H5'	2.12	0.47
30:0:1883:U:O2'	30:0:1884:G:H5'	2.13	0.47
30:0:2487:C:H5	37:0:4427:HOH:O	1.97	0.47
30:0:764:C:H2'	30:0:765:G:O4'	2.14	0.47
5:E:111:LYS:HE3	30:0:2690:U:O2'	2.14	0.47
8:H:6:ALA:CA	8:H:61:ARG:HH12	2.26	0.47
14:N:132:ASN:O	14:N:135:VAL:HG12	2.13	0.47
16:P:115:SER:OG	16:P:118:GLN:HG3	2.15	0.47
23:W:149:LEU:HG	23:W:153:MET:CE	2.44	0.47
30:0:1474:C:C5'	30:0:1474:C:H6	2.15	0.47
30:0:1878:G:O2'	30:0:1879:U:P	2.73	0.47
30:0:285:A:H2'	30:0:286:U:O4'	2.14	0.47
30:0:920:C:H5''	30:0:921:G:O5'	2.14	0.47
9:I:84:SER:HB3	9:I:92:VAL:CG2	2.44	0.47
10:J:45:VAL:HG23	10:J:130:VAL:O	2.14	0.47
10:J:131:THR:HG22	10:J:134:GLU:H	1.79	0.47
17:Q:66:LYS:HB2	17:Q:70:ALA:O	2.14	0.47
23:W:38:THR:O	23:W:42:ARG:HB2	2.14	0.47
23:W:4:LEU:HD22	23:W:52:VAL:CG2	2.40	0.47
23:W:72:PRO:HG2	23:W:77:ALA:HB3	1.97	0.47
30:0:1450:C:H4'	30:0:1493:A:C5	2.49	0.47
30:0:407:A:H8	37:0:4000:HOH:O	1.96	0.47
30:0:816:G:C6	30:0:817:G:N1	2.82	0.47
1:A:164:ARG:NE	37:A:8580:HOH:O	2.47	0.47
23:W:38:THR:HG22	23:W:39:ASP:H	1.79	0.47
30:0:2724:U:H2'	30:0:2725:G:O4'	2.14	0.47
30:0:426:G:H2'	30:0:427:C:O4'	2.14	0.47
30:0:834:G:H4'	30:0:835:U:OP2	2.15	0.47
29:3:70:ARG:HD3	37:3:8571:HOH:O	2.14	0.47
18:R:14:ALA:HB3	18:R:147:LEU:HB2	1.97	0.47
21:U:17:THR:HG22	21:U:18:GLY:N	2.29	0.47
30:0:1006:A:N1	30:0:2311:A:H1'	2.29	0.47
30:0:1116:U:HO2'	30:0:1118:A:H2	0.72	0.47
30:0:1187:U:HO2'	30:0:1188:A:H8	1.60	0.47
30:0:1132:A:N6	30:0:1229:C:H2'	2.30	0.47
30:0:603:A:H4'	30:0:604:G:O5'	2.15	0.47
1:A:211:LYS:HD3	37:A:8604:HOH:O	2.14	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:87:ARG:NH1	37:K:4066:HOH:O	2.47	0.47
15:O:14:LEU:HD23	15:O:102:ILE:HD11	1.96	0.47
22:V:12:THR:HG23	22:V:14:ALA:H	1.80	0.47
25:Y:189:ASN:HA	25:Y:217:ILE:HD11	1.94	0.47
30:0:506:G:N2	30:0:509:A:H5''	2.22	0.47
5:E:84:MET:HE1	5:E:148:ILE:HD12	1.97	0.47
13:M:107:ARG:HH11	13:M:107:ARG:HG3	1.80	0.47
13:M:61:ILE:HA	37:M:8617:HOH:O	2.15	0.47
25:Y:144:ARG:NE	37:Y:8610:HOH:O	2.47	0.47
30:0:1056:U:H2'	30:0:1057:A:O4'	2.15	0.47
30:0:162:C:H2'	30:0:163:U:H5'	1.96	0.47
30:0:1681:G:H5''	30:0:1682:A:H5'	1.96	0.47
30:0:2900:G:H2'	30:0:2901:C:O4'	2.15	0.47
3:C:214:THR:HB	37:0:9200:HOH:O	2.13	0.47
4:D:94:ALA:HB3	4:D:97:GLN:HG3	1.96	0.47
25:Y:122:ARG:NH2	37:Y:8535:HOH:O	2.48	0.47
30:0:2291:A:N9	30:0:2309:C:H5'	2.29	0.47
30:0:2831:C:C2'	30:0:2832:C:H5'	2.45	0.47
5:E:132:THR:HB	37:E:2227:HOH:O	2.14	0.47
5:E:35:TYR:HA	10:J:127:ILE:HD12	1.96	0.47
14:N:1:ALA:HB2	31:9:14:G:O2'	2.15	0.47
20:T:71:VAL:HG11	20:T:90:PRO:CB	2.36	0.47
30:0:1181:A:H2'	30:0:1182:C:C5'	2.45	0.47
30:0:2019:A:H5'	37:0:4079:HOH:O	2.15	0.47
30:0:2506:A:O2'	30:0:2507:G:O5'	2.33	0.47
10:J:75:PRO:HD3	10:J:136:SER:OG	2.15	0.47
30:0:1562:C:O2	30:0:1562:C:H2'	2.14	0.47
30:0:1657:A:H2'	30:0:1658:A:C8	2.50	0.47
11:K:66:ARG:HD2	30:0:1992:U:OP2	2.15	0.47
30:0:417:G:P	37:0:6968:HOH:O	2.71	0.47
31:9:24:U:H3'	31:9:25:G:C5'	2.45	0.47
30:0:1205:U:C2'	30:0:1206:U:C5'	2.93	0.46
30:0:1213:C:O2'	30:0:1214:G:H5'	2.15	0.46
30:0:1353:C:P	37:0:4219:HOH:O	2.73	0.46
30:0:2361:A:H2'	30:0:2362:A:C8	2.50	0.46
4:D:172:VAL:HG12	4:D:173:GLU:N	2.30	0.46
14:N:38:LYS:HE2	14:N:107:ASN:ND2	2.30	0.46
30:0:2256:G:C2'	30:0:2257:G:H5'	2.44	0.46
30:0:2419:U:H5''	30:0:2420:G:C5'	2.45	0.46
30:0:920:C:H4'	30:0:921:G:C2	2.49	0.46
31:9:31:C:H2'	31:9:32:G:O4'	2.16	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:ALA:HA	1:A:71:PRO:HD3	1.76	0.46
2:B:27:ASN:HB2	37:0:3602:HOH:O	2.16	0.46
6:F:30:LYS:HE2	6:F:99:THR:HG21	1.97	0.46
20:T:54:ASP:OD2	30:0:316:A:H5'	2.16	0.46
20:T:92:ASP:OD1	20:T:94:SER:HB3	2.16	0.46
25:Y:189:ASN:ND2	25:Y:192:ASP:H	2.14	0.46
26:Z:41:ARG:NH1	30:0:821:U:H4'	2.31	0.46
30:0:1441:G:H1'	37:0:7314:HOH:O	2.15	0.46
12:L:73:VAL:HG21	12:L:116:HIS:CD2	2.50	0.46
14:N:147:ILE:HB	37:N:8545:HOH:O	2.14	0.46
21:U:14:GLU:OE1	21:U:15:PRO:HD2	2.16	0.46
30:0:1200:A:H4'	37:0:6890:HOH:O	2.14	0.46
30:0:2112:A:H2'	30:0:2113:G:C8	2.51	0.46
30:0:2456:A:H5'	37:0:5242:HOH:O	2.15	0.46
30:0:445:U:H1'	37:0:6885:HOH:O	2.14	0.46
4:D:27:ILE:HD11	4:D:37:ALA:HB3	1.98	0.46
7:G:19:GLU:O	7:G:23:ILE:HG13	2.15	0.46
15:O:87:THR:O	15:O:91:GLN:HG3	2.16	0.46
20:T:111:ARG:HB3	20:T:119:ALA:HB2	1.98	0.46
30:0:1044:C:H5	37:0:6150:HOH:O	1.96	0.46
30:0:1174:A:C5	30:0:1201:C:H4'	2.50	0.46
30:0:136:C:H2'	30:0:137:U:O4'	2.15	0.46
30:0:1625:U:H5''	37:0:5568:HOH:O	2.15	0.46
30:0:69:A:H8	30:0:69:A:C5'	2.20	0.46
31:9:31:C:C2	31:9:50:G:N2	2.84	0.46
12:L:61:ALA:HA	37:L:8553:HOH:O	2.15	0.46
16:P:41:ARG:NH2	30:0:1500:U:OP2	2.48	0.46
19:S:56:ASN:O	28:2:8:LYS:NZ	2.46	0.46
20:T:9:LYS:HE3	20:T:13:ARG:NH1	2.30	0.46
24:X:30:MET:HE1	24:X:58:ALA:HB3	1.97	0.46
30:0:2010:A:C2'	37:0:5505:HOH:O	2.62	0.46
30:0:2256:G:O2'	30:0:2257:G:H5'	2.16	0.46
30:0:284:C:H4'	30:0:285:A:H8	1.80	0.46
30:0:538:C:H5''	30:0:539:G:C8	2.50	0.46
27:1:8:GLN:HE22	27:1:11:LYS:HZ2	1.62	0.46
31:9:55:U:H4'	31:9:56:A:H8	1.78	0.46
7:G:23:ILE:O	7:G:27:ILE:HG13	2.15	0.46
30:0:1181:A:N1	30:0:1192:A:O2'	2.48	0.46
30:0:1252:A:H2'	30:0:1253:C:O4'	2.15	0.46
30:0:1947:G:H2'	30:0:1948:G:H8	1.81	0.46
30:0:821:U:H5''	37:0:9582:HOH:O	2.15	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:118:THR:O	3:C:136:VAL:HG13	2.16	0.46
24:X:30:MET:HG2	30:0:1384:C:H5'	1.98	0.46
30:0:1393:A:H2'	30:0:1394:C:C6	2.51	0.46
5:E:143:GLN:HE22	30:0:2779:G:H21	1.59	0.46
30:0:876:A:N3	30:0:876:A:H2'	2.31	0.46
6:F:2:VAL:HG22	6:F:57:GLU:OE1	2.15	0.46
20:T:69:LYS:O	20:T:71:VAL:HG23	2.16	0.46
25:Y:220:GLU:HG3	37:Y:8546:HOH:O	2.15	0.46
30:0:1592:G:O2'	30:0:1593:C:O5'	2.34	0.46
30:0:2570:G:H5''	37:0:4452:HOH:O	2.15	0.46
30:0:304:G:H1'	30:0:347:A:N6	2.31	0.46
31:9:36:C:C5	31:9:37:C:C5	3.04	0.46
1:A:88:ILE:HG22	1:A:88:ILE:O	2.16	0.46
3:C:104:ASP:HA	3:C:107:ARG:NH1	2.31	0.46
4:D:22:VAL:HG22	4:D:74:THR:HG22	1.96	0.46
8:H:102:LYS:HD3	8:H:122:LYS:HD3	1.97	0.46
5:E:36:PRO:HD3	10:J:127:ILE:HD12	1.97	0.46
11:K:81:ARG:HD3	11:K:87:ARG:NH1	2.31	0.46
23:W:3:ALA:O	23:W:54:PHE:HA	2.16	0.46
24:X:21:PRO:HG2	24:X:24:LYS:HD3	1.96	0.46
30:0:1249:U:H2'	30:0:1250:C:C6	2.51	0.46
30:0:2672:C:O2'	30:0:2673:U:H5'	2.16	0.46
30:0:2831:C:H2'	30:0:2832:C:H5'	1.97	0.46
30:0:1314:U:H2'	37:0:5422:HOH:O	2.15	0.45
30:0:2726:U:O2	30:0:2749:U:O5'	2.34	0.45
30:0:574:G:O2'	30:0:575:A:H5'	2.16	0.45
1:A:192:VAL:CG1	1:A:207:GLN:HB3	2.46	0.45
13:M:99:ARG:CD	13:M:167:GLY:HA2	2.46	0.45
14:N:164:ASP:OD1	14:N:167:ASP:HA	2.15	0.45
30:0:119:A:H2'	30:0:120:A:H5''	1.96	0.45
30:0:138:U:OP2	30:0:139:C:H5	1.98	0.45
30:0:2716:G:O2'	30:0:2717:C:H5'	2.17	0.45
2:B:98:THR:HG22	30:0:2820:A:OP1	2.16	0.45
30:0:69:A:C8	30:0:69:A:C5'	2.92	0.45
31:9:52:A:H2'	31:9:53:G:O4'	2.16	0.45
14:N:154:LEU:C	14:N:156:GLU:H	2.19	0.45
19:S:45:TYR:HD2	37:S:4527:HOH:O	1.99	0.45
20:T:3:GLN:HA	20:T:4:PRO:HD3	1.82	0.45
30:0:1119:G:C6	30:0:1244:U:C5	3.04	0.45
30:0:1559:A:C1'	37:0:5413:HOH:O	2.62	0.45
30:0:2061:C:H2'	30:0:2062:A:H5'	1.98	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:168:ARG:NH2	3:C:190:ALA:O	2.49	0.45
14:N:61:ALA:HB3	14:N:88:ALA:HB2	1.98	0.45
37:C:8357:HOH:O	15:O:3:THR:HG21	2.15	0.45
30:0:1183:C:H42	30:0:1184:C:H41	1.62	0.45
30:0:130:C:H5'	37:0:4755:HOH:O	2.16	0.45
3:C:58:ALA:HA	3:C:73:GLN:HE21	1.81	0.45
5:E:31:ARG:NH1	37:E:5919:HOH:O	2.49	0.45
14:N:164:ASP:CG	14:N:167:ASP:HA	2.37	0.45
19:S:38:ALA:O	19:S:42:GLU:HG3	2.15	0.45
28:2:41:HIS:HE1	30:0:1439:C:OP1	1.99	0.45
30:0:1878:G:O2'	30:0:1879:U:C5	2.67	0.45
20:T:2:LYS:HG2	30:0:447:A:OP1	2.17	0.45
30:0:844:A:C6	30:0:882:A:C5	3.04	0.45
5:E:7:ILE:HG22	5:E:45:ASP:O	2.16	0.45
8:H:69:ARG:HD3	37:H:8381:HOH:O	2.16	0.45
14:N:108:SER:HA	14:N:109:PRO:HD3	1.76	0.45
15:O:35:LYS:HD3	37:0:4157:HOH:O	2.17	0.45
16:P:16:VAL:CG1	16:P:20:ARG:HB2	2.46	0.45
30:0:1505:U:H1'	37:0:7139:HOH:O	2.16	0.45
13:M:171:ARG:NH2	30:0:189:A:OP1	2.49	0.45
30:0:1925:G:O2'	30:0:1926:G:H5'	2.17	0.45
30:0:2289:G:N2	30:0:2291:A:H2	2.13	0.45
30:0:2326:C:H4'	30:0:2412:G:H4'	1.99	0.45
14:N:127:LEU:HD13	37:N:8556:HOH:O	2.16	0.45
16:P:115:SER:H	16:P:118:GLN:NE2	2.00	0.45
26:Z:84:CYS:O	26:Z:85:ASP:HB2	2.15	0.45
30:0:1188:A:N7	30:0:1189:A:C2	2.85	0.45
30:0:1545:C:H2'	30:0:1546:G:O4'	2.17	0.45
30:0:2526:C:H5'	30:0:2526:C:C6	2.51	0.45
30:0:816:G:H5'	30:0:1598:A:H4'	1.98	0.45
3:C:104:ASP:HA	3:C:107:ARG:HH12	1.80	0.45
5:E:5:LEU:HD21	5:E:66:GLN:HG3	1.99	0.45
10:J:107:ASN:C	10:J:107:ASN:HD22	2.20	0.45
30:0:1060:C:H6	30:0:1060:C:H5'	1.82	0.45
30:0:1200:A:H3'	37:0:5302:HOH:O	2.16	0.45
30:0:1596:U:H2'	30:0:1598:A:OP2	2.16	0.45
18:R:80:TYR:O	30:0:2050:G:H5''	2.17	0.45
30:0:2667:G:H1'	30:0:2914:A:N3	2.31	0.45
1:A:100:PRO:HG2	1:A:103:VAL:CG2	2.44	0.45
2:B:72:THR:HB	37:B:8606:HOH:O	2.16	0.45
3:C:127:ARG:CZ	3:C:225:PRO:HG2	2.45	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:133:THR:HG22	9:I:134:ILE:N	2.32	0.45
15:O:96:VAL:HG13	15:O:100:GLN:HB2	1.98	0.45
16:P:13:VAL:HG21	16:P:41:ARG:HG2	1.99	0.45
30:0:1183:C:H2'	37:0:5790:HOH:O	2.17	0.45
1:A:1:GLY:HA2	30:0:2114:C:OP1	2.17	0.45
4:D:52:THR:HG21	30:0:2346:C:O2'	2.16	0.45
30:0:2361:A:H8	30:0:2361:A:H5'	1.82	0.45
30:0:2509:A:OP2	30:0:2510:C:H5	2.00	0.45
30:0:2515:C:H2'	30:0:2516:G:O4'	2.16	0.45
30:0:2781:U:C2'	30:0:2782:G:H5'	2.46	0.45
30:0:484:A:N1	30:0:506:G:H4'	2.32	0.45
30:0:541:C:C2'	30:0:542:A:C5'	2.82	0.45
1:A:33:GLU:CD	1:A:33:GLU:H	2.20	0.45
6:F:60:VAL:HG12	6:F:60:VAL:O	2.17	0.45
13:M:134:ILE:CG2	13:M:141:ILE:HD13	2.47	0.45
15:O:39:THR:O	15:O:115:ARG:NH2	2.49	0.45
19:S:17:ASP:HB3	19:S:23:LYS:HB2	1.99	0.45
30:0:1209:C:H2'	30:0:1210:G:C8	2.48	0.45
12:L:14:GLY:O	30:0:1295:G:H5''	2.17	0.45
30:0:2883:A:H2'	30:0:2884:G:O4'	2.17	0.45
30:0:999:C:O2'	30:0:1000:C:H5'	2.18	0.44
30:0:1979:G:O2'	30:0:1980:U:OP1	2.29	0.44
27:1:10:LYS:HG3	37:1:8431:HOH:O	2.17	0.44
2:B:141:ARG:HD2	2:B:163:GLU:OE2	2.16	0.44
4:D:51:ARG:HH11	4:D:68:PRO:HB3	1.81	0.44
6:F:16:ALA:HA	6:F:111:ILE:HD13	1.99	0.44
8:H:23:ILE:HG23	8:H:123:ILE:HD11	1.99	0.44
8:H:61:ARG:HH11	8:H:61:ARG:HG3	1.82	0.44
11:K:74:VAL:HG13	11:K:113:ILE:HG23	1.98	0.44
30:0:1044:C:H5''	37:0:8543:HOH:O	2.17	0.44
30:0:1058:A:H2'	30:0:1060:C:C5'	2.44	0.44
37:I:5128:HOH:O	30:0:1168:C:C5'	2.64	0.44
28:2:42:TRP:HB3	30:0:1418:U:OP1	2.18	0.44
30:0:1942:A:O2'	30:0:1943:C:H5'	2.18	0.44
30:0:2553:A:H2'	30:0:2553:A:N3	2.31	0.44
30:0:2781:U:H2'	30:0:2782:G:H5'	2.00	0.44
30:0:316:A:N3	30:0:336:G:O2'	2.43	0.44
30:0:292:G:H2'	30:0:358:G:N2	2.33	0.44
29:3:70:ARG:HG2	29:3:77:ALA:HB2	1.99	0.44
3:C:16:VAL:HG12	3:C:17:ASP:H	1.81	0.44
11:K:75:ARG:HD3	11:K:112:PRO:O	2.16	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:164:THR:HB	37:M:8519:HOH:O	2.17	0.44
13:M:167:GLY:O	13:M:171:ARG:HG3	2.17	0.44
15:O:37:ARG:HD2	30:O:656:G:OP2	2.17	0.44
30:O:1477:C:H5'	30:O:1868:G:H5''	1.98	0.44
30:O:2090:G:H2'	30:O:2091:G:C8	2.51	0.44
30:O:2103:A:N7	30:O:2538:A:N6	2.65	0.44
30:O:212:A:O4'	30:O:214:U:C6	2.71	0.44
30:O:2135:A:O2'	30:O:2136:G:H5'	2.16	0.44
30:O:2642:G:H2'	30:O:2643:G:O4'	2.17	0.44
30:O:2712:G:P	37:O:4763:HOH:O	2.75	0.44
30:O:2791:U:H1'	30:O:2792:A:H5''	1.99	0.44
30:O:958:G:H2'	30:O:959:C:C6	2.52	0.44
27:1:25:LYS:HD2	28:2:48:ASP:HA	1.98	0.44
31:9:57:A:N6	37:9:8441:HOH:O	2.47	0.44
3:C:25:PRO:HG2	37:C:8322:HOH:O	2.17	0.44
8:H:59:GLN:HE21	8:H:129:ARG:NE	2.00	0.44
18:R:128:ARG:HH22	30:O:2054:A:H2	1.61	0.44
30:O:2812:A:N7	37:O:7067:HOH:O	2.36	0.44
31:9:2:U:C4'	37:9:8480:HOH:O	2.66	0.44
3:C:236:THR:HG22	3:C:239:ALA:CB	2.47	0.44
4:D:88:LEU:HB2	4:D:89:PRO:HD3	1.98	0.44
5:E:3:VAL:CG2	5:E:49:ILE:HB	2.48	0.44
10:J:90:LYS:HB2	35:J:8502:CL:CL	2.54	0.44
10:J:93:ARG:HH11	10:J:93:ARG:HB3	1.81	0.44
12:L:21:ARG:N	37:L:8524:HOH:O	2.50	0.44
15:O:14:LEU:CD2	15:O:102:ILE:HD11	2.48	0.44
17:Q:26:PRO:O	17:Q:30:VAL:HG23	2.17	0.44
18:R:111:ILE:HG23	18:R:145:LEU:CD1	2.48	0.44
25:Y:144:ARG:NH2	37:Y:8610:HOH:O	2.49	0.44
30:O:2115:U:H2'	30:O:2116:U:C6	2.53	0.44
30:O:281:U:H3'	37:O:6755:HOH:O	2.17	0.44
2:B:244:PRO:HB3	30:O:1234:U:N3	2.32	0.44
3:C:2:GLN:HB3	37:C:8333:HOH:O	2.17	0.44
3:C:2:GLN:HB3	37:C:8384:HOH:O	2.18	0.44
4:D:50:VAL:O	4:D:71:ALA:HA	2.18	0.44
4:D:56:ARG:N	37:D:6752:HOH:O	2.50	0.44
8:H:62:HIS:HA	8:H:65:LEU:HD23	1.99	0.44
12:L:133:VAL:HB	37:L:8547:HOH:O	2.17	0.44
18:R:106:GLY:HA2	18:R:109:MET:CE	2.47	0.44
30:O:1014:A:H5''	31:9:101:G:O2'	2.18	0.44
30:O:1940:C:H4'	37:O:6896:HOH:O	2.16	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1948:G:H2'	30:0:1949:G:O4'	2.18	0.44
30:0:2004:U:H2'	30:0:2005:G:OP1	2.16	0.44
30:0:559:U:H5'	30:0:559:U:C6	2.42	0.44
30:0:834:G:H3'	30:0:835:U:H4'	1.99	0.44
29:3:28:GLY:HA3	30:0:2434:A:O3'	2.17	0.44
2:B:57:GLU:HA	2:B:58:PRO:HD2	1.89	0.44
3:C:153:VAL:O	3:C:157:LEU:HG	2.18	0.44
5:E:116:THR:HG22	5:E:151:LEU:HD22	2.00	0.44
13:M:193:LYS:HB3	30:0:392:U:C5'	2.48	0.44
22:V:7:GLU:O	22:V:11:MET:HG3	2.18	0.44
30:0:1423:C:O2'	30:0:1424:A:H5'	2.18	0.44
30:0:2353:A:H4'	30:0:2354:A:O5'	2.17	0.44
30:0:737:A:H2	37:0:6249:HOH:O	1.98	0.44
27:1:28:HIS:CD2	27:1:30:LYS:HB2	2.52	0.44
2:B:71:VAL:HG11	2:B:296:LEU:HD22	1.99	0.44
3:C:140:VAL:HG12	3:C:141:SER:N	2.33	0.44
7:G:63:ARG:NH1	30:0:1151:G:OP1	2.50	0.44
11:K:45:PRO:HB2	37:0:6920:HOH:O	2.17	0.44
21:U:13:ILE:HG12	21:U:32:CYS:HB3	1.99	0.44
30:0:113:A:OP2	30:0:114:A:H2'	2.17	0.44
30:0:1299:G:N2	37:0:4223:HOH:O	2.49	0.44
3:C:184:ARG:NH2	30:0:450:C:OP1	2.35	0.44
30:0:660:A:H4'	30:0:661:G:O5'	2.18	0.44
14:N:160:SER:CB	31:9:51:A:H5'	2.48	0.44
3:C:237:GLU:HB2	37:C:8428:HOH:O	2.16	0.44
3:C:235:PHE:HE2	3:C:243:VAL:HG21	1.82	0.44
5:E:31:ARG:NH1	5:E:68:HIS:CG	2.86	0.44
8:H:172:GLU:HB3	37:H:8392:HOH:O	2.18	0.44
12:L:143:THR:HG22	12:L:144:ASP:H	1.78	0.44
30:0:2403:C:H2'	30:0:2404:G:O5'	2.17	0.44
29:3:14:CYS:SG	37:3:8559:HOH:O	2.62	0.44
31:9:34:A:H2'	31:9:35:C:O4'	2.18	0.44
30:0:2031:C:H2'	30:0:2032:U:O4'	2.17	0.43
30:0:2326:C:H4'	30:0:2412:G:C4'	2.48	0.43
30:0:2401:A:H5'	37:0:9014:HOH:O	2.18	0.43
30:0:240:C:O2	30:0:240:C:H2'	2.18	0.43
1:A:171:LYS:HB2	30:0:820:G:C5	2.53	0.43
31:9:49:G:C2'	31:9:50:G:H5'	2.48	0.43
8:H:41:LYS:HE2	8:H:45:ASP:CB	2.47	0.43
14:N:139:TRP:HA	14:N:139:TRP:CE3	2.53	0.43
14:N:169:PRO:O	14:N:172:PHE:HB3	2.18	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:12:THR:HG22	22:V:15:GLU:CG	2.46	0.43
23:W:137:GLN:NE2	23:W:141:HIS:HE1	1.99	0.43
30:0:1592:G:O2'	30:0:1593:C:O4'	2.34	0.43
30:0:2820:A:H2'	30:0:2821:C:O4'	2.18	0.43
30:0:653:U:H2'	30:0:654:A:C8	2.53	0.43
12:L:27:ARG:HD2	30:0:757:C:OP1	2.18	0.43
28:2:20:ARG:HG2	28:2:21:VAL:N	2.33	0.43
2:B:41:PHE:CD2	2:B:190:MET:HE3	2.53	0.43
3:C:107:ARG:NH1	37:C:8429:HOH:O	2.51	0.43
5:E:20:ILE:CD1	5:E:40:VAL:HG11	2.44	0.43
22:V:44:GLY:O	22:V:48:GLU:HG2	2.18	0.43
23:W:125:HIS:HE1	37:W:3071:HOH:O	2.01	0.43
23:W:5:VAL:HG11	23:W:153:MET:HE3	1.98	0.43
24:X:74:ALA:HB2	24:X:85:VAL:HG13	2.00	0.43
30:0:1825:U:O2'	30:0:1826:C:H5'	2.18	0.43
30:0:2073:G:OP2	30:0:2490:A:H5'	2.19	0.43
30:0:2508:C:H2'	37:0:6301:HOH:O	2.17	0.43
30:0:2697:A:H2'	30:0:2698:G:O4'	2.18	0.43
30:0:333:G:O2'	30:0:334:G:H5'	2.19	0.43
30:0:510:U:H6	37:0:6987:HOH:O	2.01	0.43
2:B:14:GLY:HA3	37:B:8609:HOH:O	2.17	0.43
2:B:62:ARG:HA	2:B:65:MET:HE2	2.01	0.43
13:M:64:ARG:HD2	37:M:8581:HOH:O	2.17	0.43
14:N:116:PHE:HB3	14:N:136:LEU:HD23	2.00	0.43
30:0:1367:A:H2'	30:0:1368:U:O4'	2.18	0.43
30:0:1684:A:O2'	30:0:1685:A:H5''	2.18	0.43
30:0:2754:G:O2'	30:0:2755:G:H5'	2.17	0.43
30:0:2768:A:H3'	37:0:3966:HOH:O	2.17	0.43
28:2:48:ASP:O	28:2:49:GLU:HB2	2.18	0.43
31:9:80:A:C2	31:9:103:A:C4	3.07	0.43
31:9:65:A:N6	31:9:112:U:C6	2.86	0.43
2:B:30:PRO:HB2	2:B:39:GLN:NE2	2.33	0.43
3:C:242:GLU:HG3	37:C:8381:HOH:O	2.19	0.43
7:G:12:ILE:HA	37:0:5006:HOH:O	2.17	0.43
15:O:38:ARG:NH1	37:O:7674:HOH:O	2.50	0.43
21:U:9:CYS:CA	21:U:52:THR:HG23	2.47	0.43
23:W:88:THR:HG22	23:W:90:TYR:HD1	1.82	0.43
30:0:2464:C:H5''	30:0:2465:A:OP1	2.18	0.43
30:0:941:G:C5	30:0:942:U:C4	3.06	0.43
31:9:39:U:HO2'	31:9:42:C:H5	1.58	0.43
1:A:33:GLU:O	1:A:34:ASP:HB2	2.18	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:74:ARG:O	10:J:78:ILE:HG12	2.18	0.43
13:M:39:ARG:NH2	37:M:8617:HOH:O	2.51	0.43
18:R:111:ILE:HG23	18:R:145:LEU:HD11	2.01	0.43
20:T:41:ARG:NH1	20:T:42:VAL:O	2.51	0.43
30:0:1406:A:H4'	30:0:1407:A:C5'	2.49	0.43
30:0:2072:G:H3'	30:0:2073:G:C5'	2.49	0.43
30:0:2269:C:C2'	30:0:2270:G:H5'	2.49	0.43
1:A:206:ARG:NH2	30:0:2630:G:O6	2.48	0.43
30:0:380:A:H4'	30:0:381:G:OP1	2.19	0.43
30:0:876:A:N3	30:0:876:A:C2'	2.82	0.43
1:A:153:ARG:HD3	37:A:8528:HOH:O	2.18	0.43
2:B:314:ALA:HB3	2:B:317:PRO:HG3	2.00	0.43
5:E:137:ASP:O	5:E:141:VAL:HG23	2.19	0.43
13:M:9:ARG:HD2	30:0:380:A:OP2	2.18	0.43
14:N:11:ARG:NH2	37:N:8519:HOH:O	2.51	0.43
16:P:80:ARG:HG2	16:P:87:ARG:CZ	2.48	0.43
23:W:119:HIS:HD2	23:W:120:PRO:O	2.01	0.43
24:X:43:VAL:HG22	24:X:76:ARG:NH1	2.32	0.43
25:Y:117:LEU:HA	25:Y:174:VAL:HG11	2.01	0.43
26:Z:37:ARG:HD3	30:0:818:A:O2'	2.19	0.43
30:0:1535:G:H2'	30:0:1536:C:C6	2.54	0.43
30:0:249:G:O2'	30:0:250:C:H5'	2.18	0.43
6:F:59:ILE:CD1	30:0:263:U:C2	3.01	0.43
5:E:31:ARG:HH12	5:E:68:HIS:CG	2.36	0.43
9:I:84:SER:HB2	9:I:90:ASP:HB2	1.99	0.43
11:K:28:GLU:HB3	11:K:59:LYS:HB2	2.00	0.43
19:S:57:THR:CG2	19:S:58:MET:N	2.82	0.43
23:W:108:ARG:HE	23:W:114:PRO:CG	2.32	0.43
23:W:126:ASP:HB3	23:W:135:GLY:O	2.18	0.43
24:X:25:ARG:HD3	24:X:64:ALA:O	2.18	0.43
30:0:1556:G:O2'	30:0:1557:G:H5'	2.18	0.43
30:0:1701:A:H1'	37:0:5924:HOH:O	2.18	0.43
30:0:2456:A:H2'	30:0:2457:U:C6	2.53	0.43
30:0:567:U:C5'	37:0:5949:HOH:O	2.65	0.43
1:A:105:VAL:HG12	1:A:106:CYS:N	2.33	0.43
6:F:36:THR:HG23	6:F:97:ALA:HB2	2.00	0.43
18:R:132:ARG:HG2	18:R:133:ALA:N	2.34	0.43
22:V:1:THR:HG23	22:V:2:VAL:N	2.28	0.43
30:0:1098:A:H2'	30:0:1099:G:O4'	2.19	0.43
30:0:1163:G:H2'	30:0:1164:U:C5	2.54	0.43
30:0:1771:U:O2'	30:0:1773:G:N7	2.51	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2842:G:C2'	30:0:2843:A:H5'	2.48	0.43
30:0:2868:C:H2'	30:0:2869:G:O4'	2.19	0.43
30:0:303:C:H2'	30:0:304:G:O4'	2.19	0.43
5:E:11:VAL:HG13	5:E:23:GLU:O	2.19	0.43
20:T:14:ALA:HA	20:T:15:PRO:HD3	1.91	0.43
30:0:1883:U:C2'	30:0:1884:G:H5'	2.49	0.43
30:0:407:A:H2'	30:0:408:A:C8	2.54	0.43
27:1:28:HIS:HD2	27:1:30:LYS:H	1.65	0.43
1:A:171:LYS:HB2	30:0:820:G:C6	2.54	0.43
1:A:186:TRP:CG	1:A:187:PRO:HA	2.54	0.43
2:B:36:PRO:HA	2:B:168:GLY:CA	2.46	0.43
4:D:58:VAL:CG1	4:D:60:GLU:HG2	2.48	0.43
6:F:50:VAL:CG2	6:F:63:ILE:HG21	2.49	0.43
8:H:149:VAL:HG22	37:H:8378:HOH:O	2.18	0.43
11:K:125:ALA:C	11:K:127:ALA:H	2.23	0.43
12:L:50:GLY:C	30:0:2453:G:H4'	2.39	0.43
17:Q:45:PRO:O	30:0:2365:G:H4'	2.18	0.43
37:Q:5998:HOH:O	30:0:2296:C:H5	2.01	0.42
30:0:283:U:C5	30:0:284:C:N3	2.87	0.42
30:0:559:U:C5'	30:0:559:U:H6	2.28	0.42
30:0:818:A:H5''	37:0:6135:HOH:O	2.18	0.42
28:2:28:LYS:O	30:0:87:C:H2'	2.19	0.42
28:2:40:ARG:HG3	28:2:45:ASN:CB	2.49	0.42
1:A:55:VAL:HG22	1:A:68:ILE:O	2.19	0.42
2:B:190:MET:HE1	2:B:194:PHE:CD1	2.54	0.42
2:B:49:THR:HG21	2:B:331:SER:O	2.19	0.42
9:I:129:SER:O	9:I:130:LEU:HD23	2.19	0.42
12:L:143:THR:CG2	12:L:144:ASP:N	2.80	0.42
14:N:62:HIS:HB3	14:N:65:ASP:OD1	2.19	0.42
37:I:3512:HOH:O	30:0:1163:G:N2	2.52	0.42
30:0:1165:G:H1'	30:0:1174:A:H1'	2.01	0.42
30:0:1202:A:H2'	30:0:1203:G:C5'	2.50	0.42
30:0:128:A:O2'	30:0:129:A:H5'	2.19	0.42
30:0:1427:A:H61	30:0:1440:U:H1'	1.84	0.42
30:0:1562:C:H42	30:0:2738:G:H1	1.67	0.42
30:0:946:C:H2'	30:0:947:U:C6	2.54	0.42
27:1:28:HIS:CD2	27:1:31:LYS:HG3	2.53	0.42
29:3:3:MET:HG3	29:3:4:PRO:HD2	2.01	0.42
1:A:11:ARG:HD3	37:0:8736:HOH:O	2.19	0.42
12:L:72:ASN:HB2	37:L:8570:HOH:O	2.17	0.42
13:M:81:ARG:HD2	30:0:160:A:O3'	2.19	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:119:HIS:HE1	37:0:9078:HOH:O	2.02	0.42
24:X:74:ALA:CB	24:X:85:VAL:HG22	2.49	0.42
23:W:23:MET:O	30:0:1025:C:H5'	2.19	0.42
30:0:1641:A:H2'	30:0:1642:A:C5'	2.48	0.42
30:0:907:A:H4'	30:0:1328:A:C2	2.54	0.42
4:D:173:GLU:HG3	4:D:174:VAL:HG23	2.02	0.42
6:F:91:VAL:HG11	30:0:262:A:OP2	2.19	0.42
6:F:49:PHE:HE1	6:F:98:VAL:HG23	1.84	0.42
8:H:34:HIS:HD2	8:H:90:LEU:O	2.01	0.42
30:0:1183:C:N4	30:0:1184:C:N4	2.64	0.42
30:0:1980:U:O2	30:0:2008:U:H4'	2.19	0.42
30:0:2290:U:H2'	37:0:6681:HOH:O	2.18	0.42
30:0:2372:A:H2'	30:0:2373:U:C6	2.55	0.42
30:0:2493:C:O2	30:0:2493:C:H2'	2.17	0.42
30:0:2526:C:O2'	30:0:2527:U:H5'	2.19	0.42
4:D:76:ARG:NH1	31:9:42:C:O2	2.51	0.42
5:E:21:THR:HG23	5:E:30:THR:OG1	2.19	0.42
14:N:32:PRO:HD2	14:N:99:GLU:O	2.20	0.42
17:Q:33:PHE:HE2	17:Q:93:ARG:HG3	1.83	0.42
23:W:11:VAL:HG11	30:0:1086:A:N6	2.34	0.42
30:0:1462:C:O2'	30:0:1463:U:H5'	2.19	0.42
30:0:1701:A:H4'	30:0:1702:U:O5'	2.18	0.42
1:A:187:PRO:HB2	30:0:1845:A:O3'	2.20	0.42
5:E:6:GLU:HG2	5:E:46:THR:HG22	2.01	0.42
10:J:130:VAL:HG12	10:J:131:THR:N	2.35	0.42
23:W:41:TYR:HA	23:W:44:MET:HE3	2.01	0.42
23:W:73:LEU:HA	23:W:73:LEU:HD12	1.77	0.42
24:X:18:ARG:NH1	37:X:4132:HOH:O	2.52	0.42
30:0:1433:G:O2'	30:0:1434:A:H5'	2.20	0.42
30:0:2243:C:H5''	37:0:3288:HOH:O	2.19	0.42
30:0:2323:G:H5'	37:0:6566:HOH:O	2.19	0.42
37:3:8515:HOH:O	30:0:2408:A:H2	2.02	0.42
30:0:2421:G:H3'	30:0:2422:U:C5'	2.50	0.42
30:0:2769:C:C2'	30:0:2770:G:C5'	2.86	0.42
30:0:349:U:O2'	30:0:350:G:H5'	2.20	0.42
30:0:366:U:H2'	30:0:367:G:O4'	2.19	0.42
30:0:912:A:C4	30:0:1294:A:C2	3.08	0.42
29:3:18:GLN:HG2	37:3:8514:HOH:O	2.19	0.42
31:9:116:C:O2'	31:9:117:G:H5'	2.20	0.42
31:9:39:U:C2'	31:9:40:C:OP1	2.68	0.42
4:D:166:ILE:HB	37:D:6326:HOH:O	2.18	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:43:PRO:HG3	13:M:62:VAL:HG21	2.00	0.42
24:X:43:VAL:HG12	24:X:44:ASP:H	1.84	0.42
24:X:72:VAL:HG22	24:X:85:VAL:HG12	2.01	0.42
25:Y:208:LYS:O	30:0:1313:A:H5'	2.19	0.42
30:0:1482:A:O2'	30:0:1483:C:H5'	2.20	0.42
30:0:1624:A:H4'	30:0:1625:U:H5'	2.02	0.42
30:0:177:A:H2'	30:0:178:U:O4'	2.19	0.42
30:0:1878:G:O2'	30:0:1879:U:OP2	2.37	0.42
30:0:2271:G:N3	30:0:2271:G:H2'	2.34	0.42
30:0:2831:C:H2'	30:0:2832:C:C5'	2.49	0.42
30:0:2894:C:O2'	30:0:2895:C:H5'	2.19	0.42
30:0:790:A:H2'	30:0:791:A:O4'	2.20	0.42
2:B:258:GLY:H	2:B:260:HIS:CE1	2.36	0.42
3:C:133:ARG:NH1	37:C:8406:HOH:O	2.51	0.42
3:C:202:THR:HG22	30:0:328:U:O4'	2.20	0.42
9:I:101:LYS:O	9:I:105:GLU:HG3	2.19	0.42
13:M:5:TYR:HE2	13:M:46:LEU:HD13	1.84	0.42
14:N:23:ARG:NH1	37:N:8546:HOH:O	2.52	0.42
18:R:18:LEU:HD12	18:R:143:VAL:CG1	2.49	0.42
30:0:1042:U:O2'	30:0:1043:C:H5'	2.20	0.42
30:0:1565:C:O4'	30:0:2738:G:H1'	2.20	0.42
30:0:1589:G:N2	30:0:1605:G:H1'	2.35	0.42
16:P:88:GLN:HE22	30:0:1799:G:H21	1.67	0.42
30:0:282:C:O2'	30:0:283:U:C4'	2.68	0.42
30:0:420:U:H2'	30:0:421:C:C6	2.55	0.42
30:0:441:A:H8	30:0:441:A:O5'	2.03	0.42
1:A:132:ASP:HB3	1:A:135:VAL:H	1.85	0.42
1:A:199:HIS:HE1	30:0:1881:A:OP1	2.02	0.42
5:E:84:MET:HB2	5:E:131:LEU:HB2	2.01	0.42
8:H:46:TYR:HA	8:H:47:PRO:HD3	1.76	0.42
8:H:30:LYS:N	8:H:62:HIS:HD2	2.07	0.42
10:J:131:THR:HG22	10:J:133:GLY:N	2.35	0.42
30:0:1119:G:N2	30:0:1246:A:N1	2.67	0.42
30:0:1304:U:H2'	30:0:1305:C:C6	2.55	0.42
30:0:1453:G:N2	30:0:1675:C:C2	2.88	0.42
30:0:2909:G:O2'	30:0:2910:A:H5'	2.20	0.42
30:0:870:G:C3'	30:0:871:G:H5''	2.50	0.42
30:0:883:U:C2'	30:0:883:U:O2	2.68	0.42
31:9:65:A:O2'	31:9:66:G:P	2.78	0.42
2:B:115:VAL:HA	2:B:116:PRO:HD3	1.87	0.42
12:L:134:GLU:HG3	37:L:8547:HOH:O	2.18	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:84:ALA:O	18:R:88:PHE:HD1	2.02	0.42
30:0:1218:U:H2'	30:0:1219:U:C6	2.54	0.42
30:0:12:U:H2'	30:0:13:G:H5'	2.02	0.42
30:0:1634:G:H2'	30:0:1635:U:C6	2.54	0.42
30:0:2070:G:H5''	37:0:3318:HOH:O	2.20	0.42
30:0:2403:C:C2'	30:0:2404:G:O5'	2.68	0.42
37:L:8533:HOH:O	30:0:2453:G:H5''	2.19	0.42
30:0:2491:G:H1'	37:0:6418:HOH:O	2.19	0.42
30:0:2559:C:H4'	37:0:6805:HOH:O	2.19	0.42
30:0:2664:A:OP1	30:0:2664:A:H8	2.03	0.42
21:U:50:GLU:HB3	30:0:2866:U:C4	2.55	0.42
30:0:2879:A:H2'	30:0:2880:A:O4'	2.20	0.42
30:0:290:C:O2'	30:0:291:C:H5'	2.20	0.42
30:0:151:A:C2	30:0:442:A:C8	3.08	0.42
3:C:118:THR:CG2	3:C:137:PRO:HB3	2.50	0.42
20:T:26:THR:HA	20:T:39:ASN:HB3	2.01	0.42
21:U:31:PHE:CG	21:U:37:GLU:HG2	2.55	0.42
30:0:1131:G:C6	30:0:1230:A:C4	3.07	0.41
30:0:1613:C:H2'	30:0:1614:G:O4'	2.19	0.41
30:0:1615:A:H4'	37:0:5434:HOH:O	2.20	0.41
30:0:1697:G:O2'	30:0:1698:U:H5'	2.20	0.41
30:0:1947:G:H2'	30:0:1948:G:C8	2.54	0.41
30:0:1993:C:C4	30:0:1994:A:C6	3.08	0.41
30:0:2777:G:O2'	30:0:2778:A:H5'	2.19	0.41
30:0:383:A:H2'	30:0:384:G:O4'	2.20	0.41
30:0:638:C:H2'	30:0:639:A:C8	2.54	0.41
27:1:28:HIS:HD2	27:1:31:LYS:H	1.68	0.41
28:2:18:ASN:HD21	28:2:40:ARG:H	1.68	0.41
28:2:36:ASN:HB3	28:2:39:ARG:HG3	2.01	0.41
1:A:11:ARG:HA	37:0:6768:HOH:O	2.20	0.41
2:B:294:TYR:HE2	37:B:8649:HOH:O	2.02	0.41
3:C:133:ARG:NE	3:C:138:VAL:HG22	2.35	0.41
7:G:67:LEU:O	7:G:71:LEU:HG	2.20	0.41
12:L:56:LYS:HE3	30:0:2443:C:O3'	2.20	0.41
13:M:93:ARG:HD2	30:0:1470:A:OP1	2.20	0.41
30:0:1842:A:C4	30:0:1979:G:C6	3.09	0.41
30:0:1946:C:H2'	30:0:1971:G:C8	2.55	0.41
30:0:1985:U:C2	30:0:1996:U:O4'	2.73	0.41
30:0:1909:A:N1	30:0:2128:G:H1'	2.34	0.41
30:0:2356:A:H2'	30:0:2357:G:O4'	2.19	0.41
30:0:2385:G:H2'	30:0:2386:U:C6	2.56	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2388:C:O2'	30:0:2389:U:H5'	2.21	0.41
30:0:284:C:N4	37:0:6734:HOH:O	2.52	0.41
31:9:47:A:C2	31:9:48:C:C2	3.08	0.41
11:K:4:LEU:HD22	11:K:116:GLU:HB3	2.02	0.41
30:0:1103:C:C2	30:0:1241:G:N2	2.88	0.41
30:0:2312:G:H2'	30:0:2313:C:H5'	2.02	0.41
5:E:143:GLN:NE2	30:0:2780:C:H1'	2.34	0.41
30:0:283:U:H5	30:0:284:C:N3	2.18	0.41
30:0:321:A:O2'	30:0:322:G:H5'	2.20	0.41
30:0:542:A:C5'	30:0:542:A:C8	2.99	0.41
30:0:629:A:H2'	30:0:630:A:O4'	2.21	0.41
30:0:827:A:H2'	30:0:828:G:O4'	2.20	0.41
30:0:932:U:H2'	30:0:933:C:C6	2.55	0.41
31:9:65:A:C2'	31:9:66:G:OP2	2.67	0.41
1:A:153:ARG:NH1	1:A:153:ARG:HB2	2.35	0.41
1:A:89:ALA:HB3	37:A:8616:HOH:O	2.19	0.41
23:W:21:LEU:HD13	23:W:26:ILE:HD11	2.02	0.41
30:0:1257:C:H2'	30:0:1258:G:O4'	2.20	0.41
30:0:1819:G:H2'	30:0:1820:G:C5'	2.51	0.41
30:0:2518:C:H2'	30:0:2519:C:O4'	2.20	0.41
30:0:2809:G:H2'	30:0:2810:G:O4'	2.21	0.41
18:R:98:ASN:ND2	30:0:500:G:H21	2.14	0.41
30:0:664:U:O4	30:0:681:G:H5'	2.20	0.41
28:2:18:ASN:ND2	28:2:40:ARG:H	2.17	0.41
1:A:94:LEU:HG	1:A:99:ILE:CD1	2.50	0.41
5:E:108:LEU:HD11	5:E:164:ASP:HB2	2.02	0.41
7:G:65:THR:O	7:G:69:ARG:HB2	2.19	0.41
18:R:119:VAL:HG21	18:R:142:ASP:CG	2.40	0.41
30:0:1171:A:H2'	30:0:1172:G:H5'	2.02	0.41
30:0:1926:G:H2'	30:0:1927:A:H8	1.82	0.41
30:0:2003:U:H4'	30:0:2004:U:H5	1.84	0.41
27:1:2:GLY:O	27:1:6:PRO:HG2	2.20	0.41
7:G:63:ARG:N	37:G:2569:HOH:O	2.53	0.41
20:T:2:LYS:HE2	37:0:6955:HOH:O	2.20	0.41
23:W:81:ASP:OD1	23:W:92:ASP:HB2	2.19	0.41
30:0:1185:U:H2'	30:0:1186:C:H6	1.82	0.41
30:0:1413:A:H2'	30:0:1414:A:O4'	2.20	0.41
12:L:48:LYS:HE2	30:0:220:C:C2	2.56	0.41
1:A:204:GLY:N	30:0:2634:G:OP2	2.41	0.41
30:0:2729:C:O2'	30:0:2730:G:H5'	2.20	0.41
30:0:2897:C:H2'	30:0:2898:G:H8	1.85	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:371:U:H2'	30:0:372:A:H8	1.86	0.41
30:0:666:A:H2'	30:0:667:C:O4'	2.21	0.41
29:3:7:PHE:HE2	29:3:22:VAL:HG21	1.86	0.41
31:9:107:C:H2'	31:9:108:C:C6	2.55	0.41
31:9:68:G:C6	31:9:69:U:C4	3.08	0.41
1:A:101:GLU:OE2	1:A:131:HIS:HB2	2.20	0.41
2:B:217:ARG:HG3	2:B:257:THR:HG22	2.01	0.41
5:E:154:ILE:HD11	5:E:157:LYS:HE2	2.03	0.41
9:I:94:ASP:OD1	9:I:133:THR:HB	2.21	0.41
10:J:52:GLN:NE2	30:0:1119:G:C8	2.87	0.41
11:K:65:ARG:HD3	37:K:5358:HOH:O	2.20	0.41
16:P:59:ARG:HH22	16:P:66:GLN:NE2	2.16	0.41
22:V:38:GLY:C	22:V:40:PRO:HD2	2.41	0.41
25:Y:186:ARG:HG2	25:Y:186:ARG:HH11	1.86	0.41
26:Z:43:GLY:O	26:Z:47:ARG:HG2	2.21	0.41
30:0:940:G:C5	30:0:1027:G:C2	3.08	0.41
30:0:1172:G:H1'	37:0:4513:HOH:O	2.20	0.41
30:0:2015:A:H2'	30:0:2016:U:O4'	2.21	0.41
30:0:255:A:H2'	30:0:256:C:H6	1.84	0.41
30:0:401:C:H2'	30:0:402:U:C6	2.55	0.41
30:0:558:C:H5'	37:0:4803:HOH:O	2.20	0.41
30:0:625:U:H5''	30:0:1044:C:N4	2.35	0.41
1:A:95:PRO:HA	1:A:153:ARG:HA	2.02	0.41
4:D:96:SER:C	4:D:98:PHE:H	2.23	0.41
5:E:47:VAL:HG11	5:E:69:ILE:HD13	2.03	0.41
15:O:25:VAL:HG23	15:O:26:TRP:N	2.36	0.41
30:0:1529:G:H5'	37:0:6937:HOH:O	2.20	0.41
30:0:1626:A:H2'	30:0:1627:G:O4'	2.20	0.41
30:0:1815:A:H2'	30:0:1816:C:O4'	2.21	0.41
30:0:368:C:H2'	30:0:369:G:H5'	2.02	0.41
30:0:646:G:H2'	30:0:647:U:C6	2.56	0.41
3:C:214:THR:HG21	37:C:8399:HOH:O	2.20	0.41
4:D:151:ILE:HA	4:D:152:PRO:HD3	1.95	0.41
12:L:121:ILE:HG12	12:L:141:GLU:HB2	2.01	0.41
30:0:1023:C:H2'	30:0:1024:G:O4'	2.20	0.41
30:0:2718:C:H5'	30:0:2718:C:C6	2.53	0.41
2:B:28:SER:HB2	30:0:2807:U:OP2	2.21	0.41
30:0:2756:U:O2	30:0:2896:A:H2	2.03	0.41
30:0:2906:A:H5'	30:0:2907:C:O4'	2.21	0.41
30:0:38:G:N2	37:0:6885:HOH:O	2.54	0.41
30:0:424:C:H2'	30:0:425:U:C6	2.55	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:THR:HG22	37:A:8611:HOH:O	2.21	0.41
3:C:46:TYR:CE2	3:C:98:ARG:NH1	2.89	0.41
6:F:111:ILE:O	6:F:115:VAL:HG23	2.20	0.41
6:F:34:ASN:HA	13:M:4:ALA:HB2	2.03	0.41
9:I:133:THR:HG22	9:I:134:ILE:H	1.86	0.41
13:M:169:ARG:NH2	37:M:8548:HOH:O	2.51	0.41
20:T:47:THR:HB	20:T:100:ASP:HB3	2.01	0.41
37:K:7438:HOH:O	21:U:20:MET:HE1	2.21	0.41
30:0:1611:G:O2'	30:0:1612:A:H5'	2.21	0.41
30:0:1883:U:H5'	30:0:2012:U:OP2	2.20	0.41
30:0:282:C:C2'	30:0:283:U:H5'	2.51	0.41
30:0:290:C:H1'	37:0:5650:HOH:O	2.20	0.41
30:0:365:G:C6	30:0:366:U:C4	3.09	0.41
30:0:603:A:H1'	30:0:605:C:C2	2.56	0.41
1:A:205:GLY:HA3	37:0:5905:HOH:O	2.21	0.41
10:J:26:VAL:HG13	10:J:36:VAL:HG11	2.02	0.41
10:J:63:ILE:HD11	30:0:1236:A:C8	2.56	0.41
11:K:22:ASP:HB2	37:K:5264:HOH:O	2.21	0.41
14:N:171:HIS:CE1	37:N:8566:HOH:O	2.74	0.41
20:T:38:ARG:HH21	30:0:306:A:P	2.44	0.41
30:0:1139:U:H2'	30:0:1140:C:C6	2.56	0.41
30:0:1159:G:H1	30:0:1208:C:N4	2.18	0.41
30:0:1429:U:C2'	30:0:1430:G:H5'	2.51	0.41
30:0:2362:A:H2'	30:0:2363:G:C8	2.56	0.41
30:0:661:G:C6	30:0:686:A:C2	3.08	0.41
31:9:96:C:H2'	31:9:97:U:C6	2.56	0.41
8:H:31:ILE:HA	8:H:66:GLU:OE1	2.20	0.41
6:F:38:LYS:NZ	13:M:3:SER:HA	2.36	0.41
25:Y:99:ALA:HB2	25:Y:233:TYR:CZ	2.55	0.41
1:A:72:GLU:HG3	26:Z:90:GLY:HA2	2.03	0.41
30:0:1080:C:O5'	30:0:1080:C:H6	2.03	0.40
30:0:2237:G:H1'	37:0:4393:HOH:O	2.20	0.40
30:0:2691:A:OP1	30:0:2691:A:H8	2.04	0.40
30:0:812:A:H2'	30:0:813:C:O4'	2.20	0.40
30:0:999:C:H2'	30:0:1000:C:O4'	2.21	0.40
31:9:12:C:H5'	31:9:70:U:O4'	2.21	0.40
1:A:211:LYS:HB3	1:A:212:PRO:CD	2.50	0.40
2:B:116:PRO:HG3	30:0:2821:C:H4'	2.03	0.40
9:I:87:PRO:C	9:I:89:GLU:N	2.75	0.40
10:J:80:LYS:HE2	10:J:98:PHE:CE1	2.56	0.40
15:O:26:TRP:HB2	37:O:3062:HOH:O	2.19	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:149:LEU:HG	23:W:153:MET:HE1	2.03	0.40
25:Y:155:ARG:NH1	37:Y:8556:HOH:O	2.53	0.40
30:0:1076:G:C2	30:0:1084:C:C2	3.09	0.40
30:0:1191:A:H2'	30:0:1193:A:H5'	2.03	0.40
30:0:1976:G:O2'	30:0:1977:U:H5'	2.21	0.40
30:0:2103:A:O2'	30:0:2104:C:H5'	2.21	0.40
30:0:2819:C:H2'	30:0:2820:A:C8	2.56	0.40
30:0:40:C:H6	30:0:40:C:O5'	2.04	0.40
11:K:115:ARG:NH2	37:K:3160:HOH:O	2.53	0.40
11:K:62:PRO:HG3	11:K:65:ARG:HH21	1.85	0.40
17:Q:25:PRO:HA	17:Q:26:PRO:HD3	1.77	0.40
23:W:125:HIS:CE1	30:0:1097:A:H5''	2.55	0.40
30:0:1181:A:O2'	30:0:1182:C:H5'	2.20	0.40
28:2:10:ARG:NH2	30:0:121:U:OP2	2.40	0.40
30:0:1632:A:H2'	30:0:1633:C:C5'	2.46	0.40
30:0:1714:C:O2'	30:0:1715:C:H5'	2.21	0.40
10:J:70:PHE:CD1	30:0:2676:C:H4'	2.56	0.40
30:0:383:A:C2	30:0:407:A:C4	3.09	0.40
30:0:64:G:H2'	30:0:65:C:O4'	2.22	0.40
30:0:858:U:H2'	30:0:859:C:C6	2.56	0.40
31:9:107:C:O2'	31:9:108:C:H5'	2.22	0.40
1:A:69:LEU:HD21	1:A:120:ARG:HB3	2.03	0.40
2:B:141:ARG:HG2	2:B:165:ARG:HA	2.03	0.40
2:B:56:ASP:OD1	2:B:322:ARG:HB3	2.21	0.40
4:D:58:VAL:HB	4:D:62:ASP:HB3	2.02	0.40
5:E:91:PHE:HA	5:E:92:PRO:HD3	1.92	0.40
8:H:12:ILE:HD12	8:H:57:THR:HG22	2.03	0.40
23:W:35:VAL:HA	23:W:36:PRO:HD3	1.78	0.40
23:W:5:VAL:HG11	23:W:153:MET:CE	2.51	0.40
24:X:78:GLU:HG2	24:X:79:GLU:H	1.86	0.40
25:Y:184:GLU:OE1	25:Y:204:ARG:NH1	2.55	0.40
30:0:1046:G:N3	30:0:1082:A:H2	2.19	0.40
30:0:1434:A:H2'	30:0:1436:C:C5	2.56	0.40
30:0:2314:G:H2'	30:0:2315:C:H5'	2.03	0.40
30:0:10:U:C4	30:0:532:A:N7	2.89	0.40
28:2:40:ARG:HG3	28:2:45:ASN:HB2	2.04	0.40
31:9:2:U:H4'	37:9:8480:HOH:O	2.20	0.40
1:A:153:ARG:CB	1:A:153:ARG:HH11	2.33	0.40
2:B:53:LEU:HD11	2:B:327:VAL:HG22	2.03	0.40
6:F:91:VAL:CG1	6:F:92:GLY:N	2.84	0.40
9:I:70:THR:OG1	9:I:107:LYS:HE2	2.22	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:37:ARG:HH12	31:9:6:C:C5'	2.23	0.40
14:N:78:MET:HB2	14:N:79:PRO:HD3	2.02	0.40
24:X:30:MET:CE	24:X:58:ALA:HB3	2.52	0.40
30:0:553:G:O4'	30:0:1325:G:H5'	2.20	0.40
30:0:1333:U:H2'	30:0:1334:C:H6	1.86	0.40
30:0:1571:G:C2'	30:0:1626:A:H61	2.34	0.40
30:0:1656:A:H2'	30:0:1657:A:O4'	2.21	0.40
30:0:2002:C:H2'	30:0:2003:U:H5'	2.03	0.40
30:0:2575:C:H2'	30:0:2576:A:O4'	2.21	0.40
30:0:563:C:H2'	30:0:564:G:O4'	2.22	0.40
30:0:622:G:O2'	30:0:623:U:H5'	2.21	0.40
15:O:38:ARG:HD3	30:0:654:A:OP2	2.22	0.40
30:0:671:A:O2'	30:0:672:G:H2'	2.22	0.40
2:B:36:PRO:HG3	2:B:169:GLY:H	1.86	0.40
2:B:275:GLY:O	2:B:291:ASP:HA	2.21	0.40
2:B:41:PHE:CZ	2:B:79:MET:HG3	2.56	0.40
3:C:138:VAL:O	3:C:234:VAL:HA	2.21	0.40
5:E:22:VAL:O	5:E:28:SER:HA	2.22	0.40
14:N:21:HIS:HD2	37:0:4268:HOH:O	2.05	0.40
14:N:38:LYS:HB2	14:N:38:LYS:HE3	1.81	0.40
19:S:77:VAL:O	19:S:80:ARG:HG2	2.22	0.40
23:W:88:THR:CG2	23:W:89:ASP:H	2.34	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	235/240 (98%)	220 (94%)	13 (6%)	2 (1%)	20	29
2	B	335/338 (99%)	315 (94%)	17 (5%)	3 (1%)	20	29
3	C	244/246 (99%)	231 (95%)	13 (5%)	0	100	100

Continued on next page...



Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	134/177 (76%)	115 (86%)	15 (11%)	4 (3%)	5	4
5	E	170/178 (96%)	165 (97%)	5 (3%)	0	100	100
6	F	117/120 (98%)	106 (91%)	9 (8%)	2 (2%)	11	13
7	G	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
8	H	156/177 (88%)	148 (95%)	8 (5%)	0	100	100
9	I	68/162 (42%)	57 (84%)	11 (16%)	0	100	100
10	J	140/145 (97%)	132 (94%)	7 (5%)	1 (1%)	25	37
11	K	130/132 (98%)	124 (95%)	5 (4%)	1 (1%)	22	33
12	L	141/165 (86%)	126 (89%)	14 (10%)	1 (1%)	25	37
13	M	192/196 (98%)	187 (97%)	5 (3%)	0	100	100
14	N	184/187 (98%)	170 (92%)	11 (6%)	3 (2%)	11	15
15	O	113/116 (97%)	111 (98%)	2 (2%)	0	100	100
16	P	141/149 (95%)	140 (99%)	1 (1%)	0	100	100
17	Q	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
18	R	148/155 (96%)	144 (97%)	4 (3%)	0	100	100
19	S	79/85 (93%)	75 (95%)	4 (5%)	0	100	100
20	T	117/120 (98%)	112 (96%)	5 (4%)	0	100	100
21	U	51/67 (76%)	48 (94%)	2 (4%)	1 (2%)	9	10
22	V	63/71 (89%)	60 (95%)	2 (3%)	1 (2%)	11	15
23	W	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	25	37
24	X	80/92 (87%)	74 (92%)	5 (6%)	1 (1%)	14	19
25	Y	140/241 (58%)	140 (100%)	0	0	100	100
26	Z	71/116 (61%)	63 (89%)	6 (8%)	2 (3%)	6	5
27	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
28	2	42/50 (84%)	42 (100%)	0	0	100	100
29	3	90/92 (98%)	87 (97%)	3 (3%)	0	100	100
All	All	3705/4472 (83%)	3505 (95%)	177 (5%)	23 (1%)	28	41

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	VAL
6	F	101	ALA

Continued on next page...



*Continued from previous page...*

Mol	Chain	Res	Type
10	J	5	GLU
12	L	80	ASP
14	N	154	LEU
14	N	184	ILE
4	D	27	ILE
14	N	183	ASP
22	V	43	PRO
23	W	77	ALA
26	Z	105	ARG
2	B	185	GLY
4	D	56	ARG
4	D	65	GLU
21	U	55	ALA
26	Z	66	CYS
1	A	34	ASP
4	D	171	ASP
2	B	169	GLY
11	K	126	SER
6	F	100	ASP
2	B	2	GLN
24	X	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	
1	A	179/182 (98%)	171 (96%)	8 (4%)	32	50
2	B	282/283 (100%)	268 (95%)	14 (5%)	28	45
3	C	193/193 (100%)	179 (93%)	14 (7%)	16	26
4	D	117/148 (79%)	112 (96%)	5 (4%)	33	52
5	E	152/156 (97%)	148 (97%)	4 (3%)	51	72
6	F	93/94 (99%)	92 (99%)	1 (1%)	78	90
7	G	27/282 (10%)	26 (96%)	1 (4%)	39	59
8	H	134/145 (92%)	129 (96%)	5 (4%)	39	59

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	I	58/130 (45%)	57 (98%)	1 (2%)	66	82
10	J	118/121 (98%)	110 (93%)	8 (7%)	18	29
11	K	106/106 (100%)	103 (97%)	3 (3%)	49	70
12	L	113/127 (89%)	110 (97%)	3 (3%)	50	71
13	M	158/160 (99%)	152 (96%)	6 (4%)	38	58
14	N	149/150 (99%)	146 (98%)	3 (2%)	60	79
15	O	93/94 (99%)	90 (97%)	3 (3%)	44	65
16	P	113/117 (97%)	111 (98%)	2 (2%)	64	81
17	Q	79/80 (99%)	75 (95%)	4 (5%)	28	44
18	R	117/122 (96%)	115 (98%)	2 (2%)	66	82
19	S	71/74 (96%)	69 (97%)	2 (3%)	49	70
20	T	105/106 (99%)	98 (93%)	7 (7%)	19	30
21	U	44/53 (83%)	44 (100%)	0	100	100
22	V	51/57 (90%)	49 (96%)	2 (4%)	37	56
23	W	130/130 (100%)	123 (95%)	7 (5%)	26	41
24	X	66/74 (89%)	60 (91%)	6 (9%)	11	16
25	Y	120/196 (61%)	112 (93%)	8 (7%)	19	30
26	Z	60/94 (64%)	58 (97%)	2 (3%)	43	64
27	1	46/47 (98%)	46 (100%)	0	100	100
28	2	42/46 (91%)	41 (98%)	1 (2%)	54	74
29	3	79/79 (100%)	78 (99%)	1 (1%)	73	87
All	All	3095/3646 (85%)	2972 (96%)	123 (4%)	36	55

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ARG
1	A	36	ASP
1	A	55	VAL
1	A	94	LEU
1	A	120	ARG
1	A	131	HIS
1	A	179	MET
1	A	217	ARG
2	B	7	ARG

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	11	LEU
2	B	27	ASN
2	B	49	THR
2	B	53	LEU
2	B	56	ASP
2	B	97	LEU
2	B	98	THR
2	B	162	MET
2	B	174	ARG
2	B	190	MET
2	B	254	GLN
2	B	264	GLU
2	B	312	ARG
3	C	2	GLN
3	C	27	ARG
3	C	67	GLN
3	C	94	THR
3	C	136	VAL
3	C	162	VAL
3	C	187	ARG
3	C	214	THR
3	C	222	ASP
3	C	223	LEU
3	C	234	VAL
3	C	236	THR
3	C	240	LEU
3	C	243	VAL
4	D	24	HIS
4	D	61	PHE
4	D	133	ASN
4	D	136	ARG
4	D	137	PRO
5	E	16	ASP
5	E	86	VAL
5	E	102	VAL
5	E	164	ASP
6	F	12	LEU
7	G	73	ASP
8	H	87	LYS
8	H	91	ARG
8	H	149	VAL
8	H	157	TYR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
8	H	174	LEU
9	I	135	GLU
10	J	7	ASP
10	J	39	VAL
10	J	46	ILE
10	J	52	GLN
10	J	74	ARG
10	J	79	PHE
10	J	107	ASN
10	J	127	ILE
11	K	10	GLN
11	K	49	LEU
11	K	98	VAL
12	L	35	ARG
12	L	80	ASP
12	L	140	VAL
13	M	46	LEU
13	M	68	ARG
13	M	81	ARG
13	M	93	ARG
13	M	99	ARG
13	M	164	THR
14	N	17	ARG
14	N	26	LEU
14	N	127	LEU
15	O	3	THR
15	O	98	LEU
15	O	111	VAL
16	P	91	LYS
16	P	98	ILE
17	Q	11	ARG
17	Q	16	ASN
17	Q	57	ASP
17	Q	95	GLU
18	R	13	THR
18	R	39	THR
19	S	12	GLU
19	S	71	ASP
20	T	26	THR
20	T	39	ASN
20	T	48	VAL
20	T	73	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
20	T	89	ARG
20	T	96	VAL
20	T	115	GLU
22	V	43	PRO
22	V	65	ASP
23	W	26	ILE
23	W	35	VAL
23	W	52	VAL
23	W	73	LEU
23	W	122	ARG
23	W	142	ASP
23	W	146	ILE
24	X	15	ARG
24	X	27	ASP
24	X	49	ARG
24	X	72	VAL
24	X	82	GLU
24	X	88	GLU
25	Y	141	THR
25	Y	154	ARG
25	Y	172	THR
25	Y	187	VAL
25	Y	189	ASN
25	Y	200	THR
25	Y	203	VAL
25	Y	220	GLU
26	Z	57	MET
26	Z	68	GLU
28	2	18	ASN
29	3	42	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	199	HIS
2	B	27	ASN
2	B	145	HIS
2	B	221	GLN
2	B	238	ASN
2	B	256	GLN
2	B	260	HIS
2	B	320	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	332	ASN
3	C	39	GLN
3	C	73	GLN
3	C	129	HIS
3	C	151	GLN
3	C	163	HIS
4	D	103	ASN
4	D	133	ASN
5	E	106	ASN
5	E	119	HIS
5	E	143	GLN
7	G	17	GLN
7	G	64	ASN
8	H	34	HIS
8	H	59	GLN
8	H	62	HIS
8	H	73	ASN
10	J	52	GLN
10	J	107	ASN
10	J	126	ASN
11	K	10	GLN
11	K	44	HIS
12	L	18	HIS
12	L	41	HIS
13	M	24	GLN
13	M	58	GLN
13	M	137	ASN
13	M	170	ASN
14	N	21	HIS
14	N	107	ASN
16	P	50	GLN
16	P	66	GLN
16	P	73	HIS
16	P	88	GLN
16	P	118	GLN
17	Q	40	HIS
18	R	61	GLN
18	R	94	ASN
18	R	98	ASN
18	R	113	HIS
18	R	117	HIS
19	S	9	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
19	S	51	GLN
20	T	39	ASN
21	U	39	ASN
21	U	48	ASN
22	V	60	GLN
23	W	110	GLN
23	W	119	HIS
23	W	125	HIS
23	W	141	HIS
24	X	23	HIS
25	Y	133	HIS
25	Y	134	HIS
25	Y	149	GLN
25	Y	189	ASN
27	1	8	GLN
27	1	16	HIS
27	1	28	HIS
28	2	16	ASN
28	2	18	ASN
28	2	41	HIS
28	2	45	ASN
29	3	2	GLN
29	3	15	ASN
29	3	48	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	224 (8%)	0
31	9	121/122 (99%)	16 (13%)	0
All	All	2866/3045 (94%)	240 (8%)	0

All (240) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
30	0	31	C
30	0	67	A
30	0	69	A
30	0	70	A
30	0	71	G
30	0	86	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
30	0	87	C
30	0	88	G
30	0	114	A
30	0	115	U
30	0	120	A
30	0	130	C
30	0	139	C
30	0	141	C
30	0	151	A
30	0	166	A
30	0	170	U
30	0	186	A
30	0	191	A
30	0	192	A
30	0	200	C
30	0	219	G
30	0	237	G
30	0	271	C
30	0	272	A
30	0	273	G
30	0	283	U
30	0	284	C
30	0	308	U
30	0	309	C
30	0	318	U
30	0	336	G
30	0	337	A
30	0	358	G
30	0	381	G
30	0	397	A
30	0	417	G
30	0	461	C
30	0	487	G
30	0	498	A
30	0	510	U
30	0	511	A
30	0	514	G
30	0	537	G
30	0	538	C
30	0	539	G
30	0	542	A
30	0	545	G

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
30	0	553	G
30	0	559	U
30	0	588	G
30	0	604	G
30	0	620	A
30	0	632	A
30	0	644	G
30	0	660	A
30	0	688	A
30	0	701	U
30	0	735	C
30	0	759	C
30	0	777	U
30	0	809	G
30	0	821	U
30	0	835	U
30	0	840	U
30	0	868	G
30	0	869	G
30	0	871	G
30	0	872	U
30	0	875	A
30	0	877	G
30	0	878	G
30	0	884	C
30	0	885	G
30	0	898	G
30	0	905	C
30	0	921	G
30	0	923	A
30	0	953	G
30	0	960	G
30	0	961	A
30	0	1006	A
30	0	1008	C
30	0	1029	U
30	0	1045	G
30	0	1059	G
30	0	1060	C
30	0	1072	G
30	0	1081	A
30	0	1087	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
30	0	1088	A
30	0	1109	U
30	0	1110	G
30	0	1119	G
30	0	1130	U
30	0	1137	G
30	0	1164	U
30	0	1165	G
30	0	1166	A
30	0	1174	A
30	0	1175	G
30	0	1185	U
30	0	1192	A
30	0	1193	A
30	0	1206	U
30	0	1216	G
30	0	1238	C
30	0	1239	G
30	0	1279	U
30	0	1289	C
30	0	1342	C
30	0	1353	C
30	0	1360	C
30	0	1377	C
30	0	1407	A
30	0	1409	G
30	0	1474	C
30	0	1485	A
30	0	1505	U
30	0	1506	U
30	0	1524	U
30	0	1525	G
30	0	1526	A
30	0	1528	A
30	0	1592	G
30	0	1603	A
30	0	1625	U
30	0	1626	A
30	0	1634	G
30	0	1656	A
30	0	1667	A
30	0	1682	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
30	0	1684	A
30	0	1685	A
30	0	1692	C
30	0	1701	A
30	0	1722	U
30	0	1723	G
30	0	1725	C
30	0	1731	C
30	0	1752	G
30	0	1778	A
30	0	1779	A
30	0	1798	C
30	0	1820	G
30	0	1829	A
30	0	1856	C
30	0	1879	U
30	0	1919	A
30	0	1942	A
30	0	1943	C
30	0	1971	G
30	0	1973	A
30	0	1978	A
30	0	1979	G
30	0	1980	U
30	0	1996	U
30	0	2008	U
30	0	2011	A
30	0	2012	U
30	0	2013	G
30	0	2033	G
30	0	2034	U
30	0	2064	U
30	0	2072	G
30	0	2073	G
30	0	2074	A
30	0	2096	A
30	0	2101	A
30	0	2102	G
30	0	2103	A
30	0	2104	C
30	0	2110	G
30	0	2243	C

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
30	0	2258	A
30	0	2271	G
30	0	2272	G
30	0	2291	A
30	0	2317	C
30	0	2321	A
30	0	2354	A
30	0	2361	A
30	0	2369	A
30	0	2422	U
30	0	2462	G
30	0	2469	A
30	0	2476	C
30	0	2480	G
30	0	2483	A
30	0	2507	G
30	0	2509	A
30	0	2511	A
30	0	2533	C
30	0	2537	G
30	0	2541	U
30	0	2553	A
30	0	2564	G
30	0	2589	U
30	0	2601	A
30	0	2602	G
30	0	2608	C
30	0	2613	G
30	0	2649	A
30	0	2664	A
30	0	2681	A
30	0	2682	C
30	0	2719	A
30	0	2726	U
30	0	2747	C
30	0	2748	G
30	0	2749	U
30	0	2750	G
30	0	2762	C
30	0	2768	A
30	0	2792	A
30	0	2800	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
30	0	2811	A
30	0	2825	C
30	0	2840	A
30	0	2876	G
30	0	2890	A
30	0	2896	A
30	0	2903	C
30	0	2914	A
31	9	2	U
31	9	14	G
31	9	22	G
31	9	23	U
31	9	24	U
31	9	25	G
31	9	40	C
31	9	41	C
31	9	43	G
31	9	44	A
31	9	52	A
31	9	57	A
31	9	66	G
31	9	77	A
31	9	114	G
31	9	122	C

There are no RNA pucker outliers to report.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
30	OMU	0	2587	30	14,22,23	0.98	1 (7%)	18,31,34	3.64	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
30	OMG	0	2588	30	18,26,27	1.04	2 (11%)	22,38,41	2.48	4 (18%)
30	UR3	0	2619	30	14,22,23	0.72	0	16,32,35	0.74	0
30	PSU	0	2621	30	16,21,22	1.58	3 (18%)	20,30,33	6.13	4 (20%)
30	1MA	0	628	30,34	16,25,26	1.01	1 (6%)	13,37,40	1.20	1 (7%)

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
30	OMU	0	2587	30	-	0/5/27/28	0/2/2/2
30	OMG	0	2588	30	-	0/5/27/28	0/3/3/3
30	UR3	0	2619	30	-	0/3/25/26	0/2/2/2
30	PSU	0	2621	30	-	0/7/25/26	0/2/2/2
30	1MA	0	628	30,34	-	0/3/25/26	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2621	PSU	C5-C1'	-4.79	1.48	1.52
30	0	2588	OMG	C8-N7	-2.03	1.30	1.34
30	0	2621	PSU	C2-N1	2.52	1.43	1.38
30	0	2587	OMU	C4-N3	2.67	1.37	1.33
30	0	2621	PSU	C4-N3	2.73	1.38	1.33
30	0	628	1MA	C6-N6	2.73	1.33	1.27
30	0	2588	OMG	C6-N1	3.35	1.39	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2621	PSU	N1-C2-N3	-19.33	114.50	128.40
30	0	2621	PSU	C5-C4-N3	-12.89	114.85	125.43
30	0	2588	OMG	C5-C6-N1	-8.36	111.57	123.48
30	0	628	1MA	C2-N3-C4	-3.75	110.65	116.41
30	0	2587	OMU	C5-C4-N3	-3.54	114.66	123.12
30	0	2588	OMG	C2-N3-C4	-2.87	111.81	115.16
30	0	2588	OMG	N3-C2-N1	-2.41	123.94	127.46
30	0	2621	PSU	C6-N1-C2	2.97	120.12	115.36
30	0	2588	OMG	C6-N1-C2	6.39	125.25	116.06
30	0	2621	PSU	C4-N3-C2	13.75	127.18	115.16

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2587	OMU	C4-N3-C2	14.93	126.96	114.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	0	2587	OMU	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 231 ligands modelled in this entry, 231 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	237/240 (98%)	0.81	22 (9%) 9 8	19, 38, 77, 98	0
2	B	337/338 (99%)	1.01	39 (11%) 5 5	21, 46, 74, 84	0
3	C	246/246 (100%)	0.68	14 (5%) 24 23	15, 36, 60, 71	0
4	D	140/177 (79%)	2.73	86 (61%) 0 0	47, 90, 115, 123	0
5	E	172/178 (96%)	1.15	28 (16%) 2 2	39, 61, 81, 85	0
6	F	119/120 (99%)	1.03	25 (21%) 1 1	34, 61, 90, 104	0
7	G	29/348 (8%)	2.34	13 (44%) 0 0	69, 86, 95, 98	0
8	H	160/177 (90%)	1.03	19 (11%) 5 4	30, 48, 83, 90	0
9	I	70/162 (43%)	5.01	65 (92%) 0 0	122, 136, 154, 155	0
10	J	142/145 (97%)	1.05	16 (11%) 6 5	29, 43, 66, 89	0
11	K	132/132 (100%)	1.07	17 (12%) 4 3	27, 42, 65, 77	0
12	L	145/165 (87%)	0.99	20 (13%) 3 3	18, 55, 101, 117	0
13	M	194/196 (98%)	0.21	0 100 100	20, 31, 47, 55	0
14	N	186/187 (99%)	1.01	26 (13%) 3 3	32, 53, 102, 112	0
15	O	115/116 (99%)	0.25	2 (1%) 70 68	29, 45, 62, 70	0
16	P	143/149 (95%)	0.78	7 (4%) 30 29	31, 45, 57, 68	0
17	Q	95/96 (98%)	0.53	2 (2%) 64 61	26, 35, 54, 66	0
18	R	150/155 (96%)	0.69	3 (2%) 65 63	22, 37, 58, 71	0
19	S	81/85 (95%)	0.89	10 (12%) 5 4	31, 48, 72, 82	0
20	T	119/120 (99%)	0.74	9 (7%) 15 13	29, 46, 78, 98	0
21	U	53/67 (79%)	0.96	5 (9%) 9 8	34, 48, 66, 76	0
22	V	65/71 (91%)	2.07	22 (33%) 0 0	40, 62, 106, 113	0
23	W	154/154 (100%)	0.77	11 (7%) 17 15	28, 42, 59, 71	0
24	X	82/92 (89%)	1.15	10 (12%) 5 4	36, 50, 78, 94	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	142/241 (58%)	0.46	8 (5%) 25 24	22, 36, 60, 80	0
26	Z	73/116 (62%)	0.92	9 (12%) 5 4	34, 48, 68, 87	0
27	1	56/57 (98%)	0.74	0 100 100	19, 24, 31, 40	0
28	2	46/50 (92%)	1.02	7 (15%) 2 2	26, 50, 75, 89	0
29	3	92/92 (100%)	0.51	3 (3%) 47 45	22, 45, 62, 76	0
30	0	2749/2923 (94%)	0.24	78 (2%) 53 51	16, 36, 81, 155	0
31	9	122/122 (100%)	0.13	5 (4%) 38 36	31, 54, 77, 138	0
All	All	6646/7517 (88%)	0.67	581 (8%) 11 10	15, 42, 89, 155	0

All (581) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	V	1	THR	15.0
9	I	91	PHE	12.4
14	N	166	ALA	11.4
4	D	63	ILE	10.1
9	I	88	GLN	9.8
9	I	80	PHE	9.6
22	V	39	ALA	8.9
4	D	10	PHE	8.9
9	I	128	THR	8.5
9	I	97	VAL	8.3
9	I	83	GLY	8.3
22	V	40	PRO	8.2
9	I	66	GLY	7.9
9	I	74	ILE	7.8
9	I	108	HIS	7.8
1	A	237	GLY	7.8
9	I	109	PRO	7.5
19	S	81	ILE	7.5
9	I	90	ASP	7.4
9	I	79	GLY	7.4
9	I	132	VAL	7.2
9	I	112	LEU	7.2
9	I	70	THR	7.1
9	I	76	ASP	7.0
4	D	61	PHE	6.7
24	X	88	GLU	6.7
9	I	106	GLN	6.7
7	G	23	ILE	6.6

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
9	I	99	GLN	6.4
11	K	118	ALA	6.3
8	H	174	LEU	6.3
9	I	100	VAL	6.2
9	I	71	ALA	6.1
9	I	78	ALA	6.1
9	I	68	PRO	6.1
4	D	11	HIS	6.1
30	0	1198	U	6.0
4	D	44	ILE	6.0
22	V	38	GLY	6.0
4	D	57	THR	5.9
9	I	82	THR	5.9
9	I	72	GLU	5.7
4	D	170	TYR	5.7
30	0	1171	A	5.6
1	A	35	GLY	5.5
4	D	18	ILE	5.5
9	I	116	LEU	5.5
9	I	73	LEU	5.5
4	D	75	LEU	5.5
9	I	84	SER	5.4
30	0	1202	A	5.4
31	9	1	U	5.4
9	I	92	VAL	5.4
9	I	111	LEU	5.4
9	I	102	GLN	5.4
9	I	130	LEU	5.4
7	G	24	VAL	5.3
9	I	113	SER	5.2
9	I	114	TYR	5.2
9	I	119	ALA	5.2
9	I	89	GLU	5.1
4	D	171	ASP	5.1
4	D	85	GLN	5.0
4	D	99	ASP	5.0
9	I	104	ALA	5.0
25	Y	235	GLU	5.0
4	D	84	LEU	5.0
9	I	98	ASP	5.0
9	I	110	ASP	4.9
4	D	58	VAL	4.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
4	D	106	PHE	4.9
4	D	134	LEU	4.8
9	I	86	GLU	4.8
4	D	165	PHE	4.8
4	D	40	ILE	4.8
19	S	1	SER	4.8
14	N	73	ALA	4.8
12	L	80	ASP	4.8
6	F	119	ARG	4.7
4	D	68	PRO	4.7
22	V	43	PRO	4.7
31	9	24	U	4.7
30	0	1199	A	4.6
30	0	1172	G	4.6
4	D	98	PHE	4.6
9	I	118	ASN	4.6
4	D	69	ILE	4.6
9	I	105	GLU	4.6
1	A	37	VAL	4.6
5	E	87	PHE	4.6
4	D	166	ILE	4.5
8	H	50	ILE	4.5
8	H	169	GLU	4.5
9	I	131	GLY	4.5
4	D	64	ARG	4.5
10	J	4	ALA	4.5
4	D	81	GLU	4.4
26	Z	34	SER	4.4
4	D	157	LEU	4.4
4	D	172	VAL	4.4
30	0	1200	A	4.2
4	D	173	GLU	4.2
28	2	49	GLU	4.2
30	0	1173	A	4.2
4	D	92	GLU	4.2
9	I	69	PRO	4.2
9	I	103	ILE	4.2
30	0	1174	A	4.2
14	N	161	GLY	4.1
4	D	23	VAL	4.1
30	0	2237	G	4.1
9	I	81	GLU	4.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
12	L	150	GLN	4.1
6	F	117	GLU	4.0
2	B	1	PRO	4.0
7	G	71	LEU	4.0
1	A	31	LYS	4.0
4	D	67	ASP	4.0
9	I	67	VAL	4.0
4	D	70	GLY	4.0
3	C	135	GLU	3.9
30	0	282	C	3.9
4	D	132	VAL	3.9
25	Y	236	VAL	3.9
30	0	960	G	3.9
31	9	23	U	3.8
19	S	76	GLU	3.8
4	D	83	PHE	3.8
8	H	48	VAL	3.8
30	0	1203	G	3.8
30	0	284	C	3.8
30	0	10	U	3.8
2	B	61	PRO	3.8
22	V	41	GLU	3.8
4	D	95	THR	3.8
30	0	2238	A	3.7
30	0	1525	G	3.7
14	N	152	GLU	3.7
10	J	14	ALA	3.7
1	A	36	ASP	3.7
4	D	62	ASP	3.7
4	D	26	GLY	3.7
30	0	1180	U	3.7
4	D	66	GLY	3.7
14	N	68	GLU	3.7
4	D	101	THR	3.7
30	0	1201	C	3.7
4	D	104	PHE	3.6
25	Y	108	ASP	3.6
19	S	77	VAL	3.6
4	D	86	THR	3.6
23	W	95	GLY	3.6
2	B	309	VAL	3.6
22	V	65	ASP	3.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
30	0	1625	U	3.6
1	A	85	SER	3.6
30	0	1179	C	3.6
4	D	17	ARG	3.5
23	W	93	ILE	3.5
30	0	1177	A	3.5
11	K	119	GLN	3.5
8	H	36	MET	3.5
19	S	78	ALA	3.5
4	D	102	GLY	3.5
8	H	40	GLN	3.5
9	I	77	GLU	3.5
9	I	95	LEU	3.5
4	D	74	THR	3.4
4	D	164	ALA	3.4
22	V	25	THR	3.4
1	A	90	PRO	3.4
11	K	129	THR	3.4
1	A	64	ASP	3.4
2	B	133	GLU	3.4
24	X	7	GLU	3.4
4	D	93	LEU	3.4
4	D	43	GLU	3.4
14	N	139	TRP	3.4
22	V	46	ILE	3.4
30	0	970	U	3.4
22	V	37	GLY	3.4
5	E	10	ASP	3.4
4	D	130	VAL	3.3
9	I	96	SER	3.3
30	0	1163	G	3.3
5	E	11	VAL	3.3
23	W	97	ALA	3.3
4	D	53	LYS	3.3
12	L	81	VAL	3.3
24	X	85	VAL	3.3
30	0	1948	G	3.2
9	I	126	THR	3.2
7	G	73	ASP	3.2
9	I	94	ASP	3.2
14	N	134	ASP	3.2
21	U	47	ARG	3.2

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
14	N	180	LEU	3.2
30	0	1167	G	3.2
30	0	1175	G	3.2
10	J	130	VAL	3.2
16	P	77	ALA	3.2
1	A	128	LEU	3.2
4	D	65	GLU	3.2
4	D	73	VAL	3.2
9	I	123	VAL	3.2
3	C	132	ASP	3.1
5	E	169	THR	3.1
30	0	1197	G	3.1
4	D	41	LEU	3.1
14	N	81	ALA	3.1
12	L	121	ILE	3.1
14	N	184	ILE	3.1
30	0	1192	A	3.1
30	0	1165	G	3.1
4	D	94	ALA	3.1
14	N	83	LEU	3.1
23	W	38	THR	3.1
30	0	1951	G	3.1
30	0	1170	U	3.1
9	I	101	LYS	3.1
30	0	1196	C	3.1
4	D	29	HIS	3.1
2	B	184	ASP	3.0
9	I	122	GLU	3.0
4	D	79	MET	3.0
8	H	77	ILE	3.0
4	D	103	ASN	3.0
6	F	12	LEU	3.0
4	D	135	VAL	3.0
9	I	85	GLY	3.0
4	D	56	ARG	3.0
24	X	71	ARG	3.0
3	C	8	LEU	3.0
4	D	55	LYS	3.0
4	D	24	HIS	3.0
30	0	2103	A	3.0
1	A	135	VAL	3.0
1	A	236	GLY	3.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
8	H	86	TYR	3.0
9	I	75	LYS	3.0
25	Y	95	THR	3.0
7	G	27	ILE	2.9
7	G	70	ALA	2.9
9	I	87	PRO	2.9
17	Q	95	GLU	2.9
6	F	18	GLU	2.9
5	E	170	ARG	2.9
22	V	45	ARG	2.9
2	B	104	GLU	2.9
24	X	80	GLU	2.9
4	D	89	PRO	2.9
4	D	160	ALA	2.9
18	R	150	PRO	2.9
30	0	281	U	2.9
10	J	110	ASP	2.9
11	K	109	LEU	2.9
6	F	116	GLU	2.9
21	U	9	CYS	2.9
6	F	29	VAL	2.9
7	G	26	MET	2.9
30	0	1929	G	2.9
4	D	49	PRO	2.9
8	H	172	GLU	2.9
23	W	61	THR	2.9
30	0	2769	C	2.9
8	H	149	VAL	2.9
11	K	132	VAL	2.9
15	O	1	SER	2.9
30	0	283	U	2.9
19	S	2	TRP	2.9
12	L	60	GLU	2.8
1	A	38	ILE	2.8
30	0	1162	G	2.8
7	G	18	GLU	2.8
11	K	63	GLU	2.8
16	P	45	ASP	2.8
22	V	42	ASN	2.8
29	3	56	PRO	2.8
4	D	139	TYR	2.8
14	N	157	PRO	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
9	I	127	CYS	2.8
1	A	63	GLY	2.8
4	D	167	GLU	2.8
12	L	82	ALA	2.8
30	O	2508	C	2.8
19	S	79	SER	2.8
2	B	51	VAL	2.8
6	F	108	VAL	2.8
6	F	100	ASP	2.8
30	O	1169	U	2.8
11	K	111	GLY	2.8
1	A	133	ARG	2.8
16	P	22	TRP	2.8
6	F	16	ALA	2.8
30	O	735	C	2.8
26	Z	104	ARG	2.8
2	B	65	MET	2.8
2	B	181	ILE	2.7
20	T	82	THR	2.7
22	V	8	ILE	2.7
30	O	138	U	2.7
4	D	80	ALA	2.7
14	N	154	LEU	2.7
30	O	1965	C	2.7
4	D	174	VAL	2.7
5	E	128	GLY	2.7
14	N	163	PHE	2.7
8	H	76	LEU	2.7
11	K	108	GLU	2.7
26	Z	35	SER	2.7
28	2	39	ARG	2.7
1	A	34	ASP	2.7
4	D	158	ASN	2.7
16	P	76	GLY	2.7
2	B	100	VAL	2.7
4	D	97	GLN	2.7
5	E	154	ILE	2.7
9	I	115	ASP	2.7
23	W	94	SER	2.7
30	O	1967	U	2.7
3	C	64	GLY	2.7
11	K	101	ASN	2.7

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
4	D	77	ASP	2.7
3	C	138	VAL	2.6
10	J	39	VAL	2.6
22	V	2	VAL	2.6
30	O	1208	C	2.6
2	B	116	PRO	2.6
6	F	15	ASP	2.6
8	H	66	GLU	2.6
12	L	77	ALA	2.6
20	T	119	ALA	2.6
21	U	55	ALA	2.6
11	K	96	VAL	2.6
30	O	365	G	2.6
4	D	45	THR	2.6
23	W	86	GLU	2.6
5	E	126	ILE	2.6
31	9	122	C	2.6
4	D	47	GLN	2.6
4	D	90	LEU	2.6
10	J	5	GLU	2.6
30	O	1950	G	2.6
12	L	137	GLY	2.6
23	W	124	GLY	2.6
4	D	142	ALA	2.6
5	E	100	ASP	2.6
6	F	25	ASP	2.6
26	Z	83	TYR	2.6
12	L	91	VAL	2.5
22	V	23	LEU	2.5
7	G	21	ASP	2.5
10	J	7	ASP	2.5
30	O	1949	G	2.5
14	N	167	ASP	2.5
5	E	28	SER	2.5
7	G	68	GLU	2.5
30	O	2825	C	2.5
2	B	119	HIS	2.5
16	P	67	LYS	2.5
2	B	121	PRO	2.5
2	B	189	ALA	2.5
4	D	82	GLU	2.5
4	D	100	ASP	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
4	D	27	ILE	2.5
20	T	50	VAL	2.5
14	N	62	HIS	2.5
1	A	66	ARG	2.5
2	B	117	GLU	2.5
19	S	80	ARG	2.5
24	X	77	PHE	2.5
5	E	72	MET	2.5
28	2	35	ARG	2.5
30	0	1178	G	2.5
6	F	115	VAL	2.5
30	0	1521	C	2.5
15	O	23	GLY	2.5
22	V	28	LEU	2.4
5	E	88	TYR	2.4
9	I	121	LYS	2.4
7	G	72	ASP	2.4
12	L	148	GLU	2.4
14	N	177	GLU	2.4
4	D	71	ALA	2.4
24	X	73	ARG	2.4
3	C	243	VAL	2.4
5	E	86	VAL	2.4
20	T	63	ILE	2.4
9	I	107	LYS	2.4
6	F	17	LEU	2.4
23	W	100	LEU	2.4
2	B	182	VAL	2.4
3	C	13	ASP	2.4
8	H	42	ASP	2.4
8	H	140	TYR	2.4
30	0	969	G	2.4
3	C	131	PHE	2.4
12	L	149	ARG	2.4
26	Z	48	ARG	2.4
3	C	204	ALA	2.4
2	B	183	GLU	2.4
30	0	1168	C	2.4
12	L	145	LEU	2.4
22	V	20	LEU	2.4
20	T	83	ASP	2.4
2	B	168	GLY	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
20	T	59	GLU	2.4
6	F	118	LEU	2.4
14	N	150	TYR	2.4
30	O	1195	G	2.4
26	Z	44	ARG	2.4
6	F	109	GLU	2.4
30	O	1279	U	2.4
2	B	128	ILE	2.4
3	C	61	PHE	2.4
10	J	47	THR	2.4
4	D	50	VAL	2.3
9	I	93	ALA	2.3
10	J	96	GLU	2.3
25	Y	103	THR	2.3
2	B	54	VAL	2.3
4	D	22	VAL	2.3
26	Z	66	CYS	2.3
5	E	45	ASP	2.3
30	O	1164	U	2.3
7	G	25	GLU	2.3
19	S	44	GLN	2.3
22	V	59	ILE	2.3
30	O	2911	C	2.3
14	N	1	ALA	2.3
9	I	117	THR	2.3
21	U	53	ASP	2.3
2	B	245	SER	2.3
22	V	52	ALA	2.3
4	D	42	GLY	2.3
4	D	19	GLU	2.3
2	B	319	ASP	2.3
20	T	40	VAL	2.3
4	D	48	MET	2.3
10	J	70	PHE	2.3
11	K	21	ALA	2.3
11	K	23	ASN	2.3
2	B	64	GLY	2.3
7	G	69	ARG	2.3
26	Z	49	ARG	2.3
28	2	47	THR	2.3
30	O	2254	G	2.3
14	N	164	ASP	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
25	Y	97	LEU	2.3
9	I	124	VAL	2.3
30	O	1966	U	2.3
8	H	83	GLU	2.3
10	J	63	ILE	2.3
8	H	141	CYS	2.3
14	N	156	GLU	2.3
2	B	115	VAL	2.3
2	B	41	PHE	2.3
5	E	80	TRP	2.3
6	F	6	PHE	2.3
6	F	110	ASP	2.3
30	O	285	A	2.2
30	O	1194	A	2.2
2	B	138	GLY	2.2
30	O	1185	U	2.2
8	H	67	ALA	2.2
12	L	89	PHE	2.2
30	O	1176	C	2.2
11	K	1	MET	2.2
16	P	16	VAL	2.2
5	E	6	GLU	2.2
5	E	81	GLU	2.2
10	J	109	TYR	2.2
10	J	113	GLY	2.2
4	D	38	GLU	2.2
8	H	82	GLU	2.2
22	V	26	GLU	2.2
1	A	32	VAL	2.2
1	A	97	ALA	2.2
12	L	90	ARG	2.2
9	I	133	THR	2.2
24	X	59	TRP	2.2
28	2	46	ASP	2.2
2	B	92	TYR	2.2
19	S	47	VAL	2.2
5	E	129	GLU	2.2
6	F	7	ASP	2.2
12	L	139	SER	2.2
12	L	57	VAL	2.2
5	E	94	GLN	2.2
14	N	165	ALA	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	211	THR	2.2
2	B	105	PHE	2.2
28	2	36	ASN	2.2
30	0	128	A	2.2
30	0	514	G	2.2
6	F	22	VAL	2.2
11	K	110	LYS	2.2
1	A	134	ASN	2.2
4	D	151	ILE	2.2
5	E	122	THR	2.2
5	E	152	THR	2.2
5	E	172	PRO	2.2
12	L	147	GLU	2.2
6	F	44	SER	2.2
5	E	42	VAL	2.1
11	K	124	VAL	2.1
17	Q	92	ARG	2.1
29	3	40	ARG	2.1
23	W	98	PHE	2.1
4	D	96	SER	2.1
3	C	143	ASP	2.1
18	R	66	VAL	2.1
6	F	99	THR	2.1
21	U	52	THR	2.1
4	D	159	PRO	2.1
30	0	1190	G	2.1
5	E	131	LEU	2.1
10	J	105	LEU	2.1
2	B	33	ASP	2.1
12	L	99	GLU	2.1
10	J	68	GLY	2.1
30	0	2004	U	2.1
6	F	39	SER	2.1
3	C	146	ASP	2.1
5	E	121	ASP	2.1
12	L	130	ARG	2.1
11	K	106	GLY	2.1
5	E	76	VAL	2.1
20	T	44	ALA	2.1
2	B	27	ASN	2.1
2	B	185	GLY	2.1
30	0	809	G	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
18	R	16	ALA	2.1
5	E	92	PRO	2.1
24	X	43	VAL	2.1
25	Y	200	THR	2.1
30	0	2885	A	2.1
2	B	134	ALA	2.1
29	3	29	ARG	2.1
30	0	289	G	2.1
23	W	35	VAL	2.1
31	9	2	U	2.1
2	B	180	ASP	2.1
2	B	294	TYR	2.1
11	K	131	ILE	2.1
30	0	2255	A	2.1
2	B	109	LEU	2.1
1	A	61	GLU	2.1
6	F	24	ARG	2.1
3	C	58	ALA	2.0
12	L	104	ASP	2.0
24	X	64	ALA	2.0
25	Y	234	VAL	2.0
26	Z	45	VAL	2.0
30	0	1130	U	2.0
30	0	2253	G	2.0
14	N	147	ILE	2.0
14	N	160	SER	2.0
14	N	172	PHE	2.0
14	N	179	LEU	2.0
20	T	112	LEU	2.0
30	0	806	A	2.0
30	0	1193	A	2.0
1	A	89	ALA	2.0
6	F	28	ALA	2.0
3	C	59	GLU	2.0
28	2	37	HIS	2.0
1	A	94	LEU	2.0
8	H	165	ARG	2.0
22	V	27	LEU	2.0
30	0	2250	G	2.0
2	B	176	ASP	2.0
16	P	143	ALA	2.0
22	V	36	ALA	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	275	GLY	2.0
2	B	193	ILE	2.0
6	F	75	ILE	2.0
10	J	11	ILE	2.0
5	E	98	GLU	2.0
30	0	288	A	2.0
30	0	808	A	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
30	OMU	0	2587	21/22	0.90	0.17	-	22,25,27,28	0
30	UR3	0	2619	21/22	0.91	0.20	-	24,27,31,36	0
30	1MA	0	628	23/24	0.93	0.20	-	20,22,23,25	0
30	PSU	0	2621	20/21	0.92	0.22	-	20,23,27,27	0
30	OMG	0	2588	24/25	0.91	0.18	-	22,25,27,28	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
34	NA	0	8374	1/1	0.94	0.61	38.29	47,47,47,47	0
34	NA	0	8372	1/1	0.95	0.59	29.03	60,60,60,60	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
34	NA	R	8386	1/1	0.59	0.68	23.84	80,80,80,80	0
34	NA	0	8368	1/1	0.47	0.41	17.56	48,48,48,48	0
34	NA	0	8371	1/1	0.55	0.36	16.25	48,48,48,48	0
34	NA	0	8376	1/1	0.84	0.43	15.96	42,42,42,42	0
34	NA	0	8379	1/1	0.80	0.57	14.90	46,46,46,46	0
32	MG	0	8060	1/1	0.96	0.28	11.87	33,33,33,33	0
32	MG	0	8066	1/1	0.95	0.59	11.38	88,88,88,88	0
34	NA	0	8331	1/1	0.90	0.32	10.97	35,35,35,35	0
34	NA	0	8340	1/1	0.59	0.47	10.91	49,49,49,49	0
34	NA	0	8350	1/1	0.95	0.42	10.69	41,41,41,41	0
34	NA	0	8335	1/1	0.53	0.38	9.27	31,31,31,31	0
34	NA	0	8320	1/1	0.84	0.35	7.90	37,37,37,37	0
34	NA	0	8362	1/1	0.84	0.39	7.40	46,46,46,46	0
34	NA	0	8326	1/1	0.42	0.25	6.50	37,37,37,37	0
34	NA	0	8323	1/1	0.72	0.28	6.30	31,31,31,31	0
34	NA	0	8302	1/1	0.91	0.23	5.73	44,44,44,44	0
34	NA	0	8364	1/1	0.95	0.31	5.25	40,40,40,40	0
34	NA	0	8359	1/1	0.85	0.27	5.17	39,39,39,39	0
34	NA	0	8366	1/1	0.82	0.22	4.04	63,63,63,63	0
34	NA	0	8305	1/1	0.86	0.28	3.98	33,33,33,33	0
34	NA	0	8325	1/1	0.92	0.25	3.30	50,50,50,50	0
34	NA	0	8378	1/1	0.73	0.38	3.10	40,40,40,40	0
32	MG	0	8064	1/1	0.85	0.22	2.76	26,26,26,26	0
34	NA	0	8327	1/1	0.71	0.25	2.62	36,36,36,36	0
34	NA	0	8356	1/1	0.86	0.22	2.35	35,35,35,35	0
34	NA	0	8303	1/1	0.93	0.24	2.34	32,32,32,32	0
34	NA	0	8321	1/1	0.87	0.28	1.86	42,42,42,42	0
34	NA	0	8373	1/1	0.67	0.18	1.75	44,44,44,44	0
34	NA	0	8324	1/1	0.77	0.21	1.59	48,48,48,48	0
32	MG	0	8080	1/1	0.76	0.24	1.54	40,40,40,40	0
35	CL	M	8518	1/1	0.95	0.20	0.99	32,32,32,32	0
32	MG	0	8015	1/1	0.93	0.25	0.97	25,25,25,25	0
34	NA	0	8369	1/1	0.96	0.23	0.95	42,42,42,42	0
32	MG	0	8057	1/1	0.83	0.19	0.88	34,34,34,34	0
34	NA	0	8365	1/1	0.81	0.23	0.58	31,31,31,31	0
34	NA	0	8361	1/1	0.68	0.24	0.47	41,41,41,41	0
34	NA	0	8339	1/1	0.80	0.21	0.40	19,19,19,19	0
34	NA	9	8383	1/1	0.75	0.17	0.03	46,46,46,46	0
34	NA	M	8347	1/1	0.85	0.17	-0.02	19,19,19,19	0
34	NA	0	8333	1/1	0.63	0.17	-0.04	23,23,23,23	0
32	MG	0	8109	1/1	0.84	0.19	-0.26	25,25,25,25	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	0	8012	1/1	0.90	0.16	-0.33	30,30,30,30	0
35	CL	J	8521	1/1	0.61	0.23	-0.34	47,47,47,47	0
34	NA	0	8353	1/1	0.95	0.18	-0.68	17,17,17,17	0
34	NA	C	8304	1/1	0.85	0.17	-0.71	29,29,29,29	0
35	CL	0	8515	1/1	0.92	0.16	-0.73	53,53,53,53	0
32	MG	0	8086	1/1	0.86	0.14	-0.77	37,37,37,37	0
34	NA	0	8314	1/1	0.93	0.20	-0.77	38,38,38,38	0
34	NA	0	8382	1/1	0.58	0.17	-0.79	67,67,67,67	0
32	MG	0	8038	1/1	0.81	0.16	-0.84	21,21,21,21	0
34	NA	Q	8348	1/1	0.83	0.16	-0.85	30,30,30,30	0
34	NA	0	8309	1/1	0.69	0.15	-1.15	25,25,25,25	0
34	NA	L	8380	1/1	0.92	0.20	-1.34	44,44,44,44	0
34	NA	J	8346	1/1	0.74	0.18	-1.36	37,37,37,37	0
35	CL	0	8512	1/1	0.92	0.16	-1.38	35,35,35,35	0
35	CL	B	8519	1/1	0.76	0.19	-1.38	34,34,34,34	0
32	MG	0	8054	1/1	0.89	0.18	-1.42	16,16,16,16	0
32	MG	0	8008	1/1	0.90	0.14	-1.61	26,26,26,26	0
34	NA	0	8317	1/1	0.84	0.15	-1.70	28,28,28,28	0
34	NA	A	8345	1/1	0.80	0.13	-1.89	43,43,43,43	0
32	MG	0	8044	1/1	0.85	0.14	-2.00	33,33,33,33	0
32	MG	0	8013	1/1	0.93	0.17	-2.04	22,22,22,22	0
32	MG	0	8020	1/1	0.91	0.14	-2.04	22,22,22,22	0
32	MG	0	8007	1/1	0.90	0.16	-2.09	21,21,21,21	0
32	MG	0	8074	1/1	0.97	0.07	-2.16	35,35,35,35	0
32	MG	0	8010	1/1	0.75	0.18	-2.17	24,24,24,24	0
32	MG	Y	8108	1/1	0.67	0.14	-2.23	25,25,25,25	0
34	NA	0	8332	1/1	0.93	0.12	-2.25	31,31,31,31	0
36	CD	Z	8403	1/1	0.95	0.11	-2.27	43,43,43,43	0
34	NA	0	8344	1/1	0.83	0.12	-2.30	24,24,24,24	0
35	CL	0	8505	1/1	0.91	0.12	-2.38	41,41,41,41	0
32	MG	3	8078	1/1	0.86	0.12	-2.53	37,37,37,37	0
32	MG	0	8056	1/1	0.72	0.13	-2.55	34,34,34,34	0
35	CL	0	8516	1/1	0.90	0.14	-2.67	41,41,41,41	0
36	CD	U	8401	1/1	0.90	0.09	-2.75	48,48,48,48	0
32	MG	0	8053	1/1	0.92	0.15	-2.76	33,33,33,33	0
35	CL	O	8508	1/1	0.93	0.08	-2.84	51,51,51,51	0
34	NA	0	8343	1/1	0.86	0.11	-2.92	28,28,28,28	0
32	MG	0	8107	1/1	0.86	0.13	-2.93	68,68,68,68	0
32	MG	0	8003	1/1	0.88	0.16	-2.97	21,21,21,21	0
36	CD	3	8404	1/1	0.94	0.07	-3.05	45,45,45,45	0
32	MG	0	8033	1/1	0.58	0.14	-3.11	19,19,19,19	0
32	MG	0	8077	1/1	0.72	0.17	-3.13	22,22,22,22	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	T	8073	1/1	0.75	0.13	-3.16	40,40,40,40	0
36	CD	1	8402	1/1	0.96	0.09	-3.17	45,45,45,45	0
33	K	0	8201	1/1	0.82	0.17	-3.32	60,60,60,60	0
32	MG	0	8058	1/1	0.82	0.09	-3.34	29,29,29,29	0
32	MG	0	8111	1/1	0.87	0.08	-3.37	23,23,23,23	0
34	NA	0	8334	1/1	0.97	0.09	-3.65	36,36,36,36	0
32	MG	0	8067	1/1	0.90	0.11	-3.73	28,28,28,28	0
32	MG	B	8055	1/1	0.37	0.12	-3.97	42,42,42,42	0
32	MG	0	8084	1/1	0.83	0.16	-3.97	38,38,38,38	0
34	NA	0	8338	1/1	0.83	0.10	-4.17	41,41,41,41	0
32	MG	0	8004	1/1	0.91	0.13	-4.20	19,19,19,19	0
34	NA	0	8310	1/1	0.97	0.12	-4.28	30,30,30,30	0
32	MG	0	8021	1/1	0.95	0.10	-4.42	25,25,25,25	0
32	MG	0	8017	1/1	0.90	0.12	-4.64	11,11,11,11	0
32	MG	0	8096	1/1	0.76	0.10	-5.31	34,34,34,34	0
32	MG	0	8027	1/1	0.83	0.09	-5.52	36,36,36,36	0
35	CL	3	8504	1/1	0.95	0.09	-5.81	43,43,43,43	0
32	MG	0	8113	1/1	0.97	0.07	-6.02	31,31,31,31	0
32	MG	0	8106	1/1	0.91	0.04	-6.07	31,31,31,31	0
32	MG	0	8006	1/1	0.86	0.08	-6.49	29,29,29,29	0
32	MG	0	8032	1/1	0.93	0.08	-6.65	26,26,26,26	0
32	MG	0	8028	1/1	0.94	0.07	-6.69	27,27,27,27	0
32	MG	0	8052	1/1	0.39	0.14	-7.54	48,48,48,48	0
32	MG	0	8019	1/1	0.81	0.07	-7.59	23,23,23,23	0
32	MG	0	8091	1/1	0.86	0.08	-8.36	41,41,41,41	0
32	MG	0	8035	1/1	0.81	0.10	-9.60	34,34,34,34	0
33	K	0	8202	1/1	0.95	0.11	-10.18	37,37,37,37	0
32	MG	A	8065	1/1	0.94	0.05	-10.92	23,23,23,23	0
32	MG	0	8001	1/1	0.96	0.10	-12.13	24,24,24,24	0
32	MG	0	8039	1/1	0.94	0.06	-13.27	33,33,33,33	0
32	MG	0	8018	1/1	0.67	0.09	-15.81	30,30,30,30	0
32	MG	0	8002	1/1	0.86	0.12	-16.00	25,25,25,25	0
32	MG	0	8048	1/1	0.94	0.28	-	41,41,41,41	0
32	MG	0	8005	1/1	0.94	0.13	-	25,25,25,25	0
32	MG	0	8079	1/1	0.85	0.15	-	20,20,20,20	0
34	NA	R	8337	1/1	0.89	0.15	-	33,33,33,33	0
32	MG	0	8009	1/1	0.82	0.21	-	25,25,25,25	0
32	MG	0	8114	1/1	0.90	0.13	-	38,38,38,38	0
32	MG	0	8031	1/1	0.95	0.14	-	24,24,24,24	0
32	MG	0	8089	1/1	0.79	0.16	-	43,43,43,43	0
34	NA	0	8375	1/1	0.86	0.33	-	38,38,38,38	0
32	MG	0	8112	1/1	0.53	0.28	-	39,39,39,39	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	0	8029	1/1	0.85	0.10	-	34,34,34,34	0
32	MG	0	8034	1/1	0.88	0.12	-	30,30,30,30	0
32	MG	0	8047	1/1	0.78	0.26	-	59,59,59,59	0
32	MG	0	8071	1/1	0.73	0.12	-	61,61,61,61	0
34	NA	H	8322	1/1	0.78	0.33	-	54,54,54,54	0
34	NA	0	8363	1/1	0.84	0.52	-	50,50,50,50	0
32	MG	0	8093	1/1	0.84	0.21	-	37,37,37,37	0
32	MG	0	8042	1/1	0.93	0.17	-	31,31,31,31	0
34	NA	0	8306	1/1	0.96	0.18	-	29,29,29,29	0
35	CL	0	8522	1/1	0.83	0.21	-	44,44,44,44	0
34	NA	0	8384	1/1	0.60	0.15	-	53,53,53,53	0
34	NA	0	8313	1/1	0.90	0.10	-	55,55,55,55	0
32	MG	0	8099	1/1	0.84	0.33	-	40,40,40,40	0
34	NA	0	8316	1/1	0.72	0.28	-	38,38,38,38	0
35	CL	A	8509	1/1	0.94	0.18	-	49,49,49,49	0
32	MG	0	8036	1/1	0.86	0.11	-	31,31,31,31	0
32	MG	0	8097	1/1	0.74	0.11	-	30,30,30,30	0
35	CL	N	8507	1/1	0.96	0.10	-	44,44,44,44	0
32	MG	0	8083	1/1	0.74	0.15	-	33,33,33,33	0
32	MG	9	8095	1/1	0.86	0.23	-	64,64,64,64	0
34	NA	0	8311	1/1	0.83	0.28	-	52,52,52,52	0
32	MG	K	8069	1/1	0.81	0.19	-	47,47,47,47	0
32	MG	0	8025	1/1	0.78	0.13	-	32,32,32,32	0
32	MG	0	8043	1/1	0.90	0.07	-	32,32,32,32	0
32	MG	0	8024	1/1	0.92	0.25	-	22,22,22,22	0
34	NA	0	8328	1/1	0.95	0.13	-	31,31,31,31	0
32	MG	0	8110	1/1	0.89	0.11	-	29,29,29,29	0
32	MG	0	8040	1/1	0.91	0.18	-	38,38,38,38	0
32	MG	0	8046	1/1	0.61	0.14	-	39,39,39,39	0
36	CD	O	8405	1/1	0.95	0.07	-	71,71,71,71	0
34	NA	9	8351	1/1	0.91	0.07	-	45,45,45,45	0
32	MG	0	8081	1/1	0.94	0.09	-	39,39,39,39	0
32	MG	0	8022	1/1	0.94	0.17	-	31,31,31,31	0
32	MG	0	8041	1/1	0.94	0.15	-	34,34,34,34	0
32	MG	0	8062	1/1	0.63	0.21	-	42,42,42,42	0
35	CL	0	8514	1/1	0.85	0.23	-	39,39,39,39	0
32	MG	0	8045	1/1	0.63	0.18	-	55,55,55,55	0
32	MG	0	8011	1/1	0.88	0.20	-	21,21,21,21	0
32	MG	0	8051	1/1	0.90	0.15	-	54,54,54,54	0
34	NA	0	8329	1/1	0.73	0.17	-	55,55,55,55	0
34	NA	0	8315	1/1	0.96	0.23	-	30,30,30,30	0
32	MG	0	8049	1/1	0.77	0.22	-	54,54,54,54	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
34	NA	0	8377	1/1	0.76	0.33	-	50,50,50,50	0
35	CL	J	8502	1/1	0.88	0.18	-	55,55,55,55	0
32	MG	0	8030	1/1	0.42	0.15	-	21,21,21,21	0
34	NA	0	8381	1/1	0.80	0.20	-	43,43,43,43	0
32	MG	0	8085	1/1	0.90	0.13	-	37,37,37,37	0
32	MG	0	8087	1/1	0.92	0.16	-	57,57,57,57	0
32	MG	0	8103	1/1	0.76	0.18	-	55,55,55,55	0
35	CL	J	8501	1/1	0.79	0.10	-	46,46,46,46	0
35	CL	0	8503	1/1	0.94	0.19	-	38,38,38,38	0
32	MG	0	8088	1/1	0.85	0.17	-	24,24,24,24	0
32	MG	0	8102	1/1	0.87	0.16	-	48,48,48,48	0
32	MG	0	8050	1/1	0.66	0.14	-	66,66,66,66	0
34	NA	9	8352	1/1	0.92	0.20	-	41,41,41,41	0
34	NA	0	8385	1/1	0.85	0.37	-	44,44,44,44	0
35	CL	0	8517	1/1	0.87	0.12	-	47,47,47,47	0
32	MG	0	8014	1/1	0.23	0.17	-	25,25,25,25	0
32	MG	0	8092	1/1	0.68	0.15	-	66,66,66,66	0
32	MG	0	8105	1/1	0.90	0.10	-	45,45,45,45	0
32	MG	0	8115	1/1	0.93	0.08	-	41,41,41,41	0
32	MG	0	8059	1/1	0.89	0.14	-	22,22,22,22	0
32	MG	0	8070	1/1	0.76	0.20	-	44,44,44,44	0
32	MG	0	8075	1/1	0.90	0.11	-	27,27,27,27	0
34	NA	0	8342	1/1	0.84	0.24	-	35,35,35,35	0
32	MG	0	8094	1/1	0.68	0.17	-	59,59,59,59	0
34	NA	0	8355	1/1	0.82	0.44	-	53,53,53,53	0
34	NA	0	8360	1/1	0.65	0.37	-	41,41,41,41	0
34	NA	0	8336	1/1	0.82	0.10	-	37,37,37,37	0
32	MG	0	8116	1/1	0.91	0.08	-	35,35,35,35	0
34	NA	0	8367	1/1	0.88	0.34	-	46,46,46,46	0
34	NA	0	8358	1/1	0.88	0.30	-	73,73,73,73	0
32	MG	0	8026	1/1	0.95	0.15	-	23,23,23,23	0
34	NA	0	8330	1/1	0.92	0.10	-	37,37,37,37	0
32	MG	0	8104	1/1	0.88	0.30	-	50,50,50,50	0
32	MG	0	8100	1/1	0.78	0.22	-	63,63,63,63	0
32	MG	0	8098	1/1	0.85	0.23	-	25,25,25,25	0
34	NA	0	8357	1/1	0.94	0.07	-	39,39,39,39	0
34	NA	0	8341	1/1	0.84	0.19	-	41,41,41,41	0
35	CL	0	8511	1/1	0.92	0.12	-	37,37,37,37	0
32	MG	0	8072	1/1	0.88	0.13	-	47,47,47,47	0
32	MG	0	8076	1/1	0.45	0.14	-	44,44,44,44	0
34	NA	0	8307	1/1	0.81	0.34	-	42,42,42,42	0
32	MG	0	8037	1/1	0.94	0.06	-	35,35,35,35	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
34	NA	0	8354	1/1	0.85	0.20	-	23,23,23,23	0
34	NA	0	8319	1/1	0.80	0.19	-	31,31,31,31	0
32	MG	0	8101	1/1	0.72	0.24	-	44,44,44,44	0
35	CL	0	8513	1/1	0.86	0.16	-	44,44,44,44	0
34	NA	S	8312	1/1	0.95	0.11	-	28,28,28,28	0
34	NA	0	8308	1/1	0.89	0.12	-	45,45,45,45	0
32	MG	0	8082	1/1	0.87	0.12	-	62,62,62,62	0
35	CL	Y	8520	1/1	0.89	0.12	-	35,35,35,35	0
32	MG	0	8023	1/1	0.87	0.25	-	28,28,28,28	0
32	MG	0	8061	1/1	0.84	0.17	-	30,30,30,30	0
35	CL	R	8506	1/1	0.77	0.22	-	40,40,40,40	0
32	MG	0	8068	1/1	0.47	0.17	-	46,46,46,46	0
32	MG	0	8090	1/1	0.36	0.38	-	56,56,56,56	0
35	CL	L	8510	1/1	0.90	0.14	-	40,40,40,40	0
34	NA	0	8318	1/1	0.69	0.32	-	47,47,47,47	0
32	MG	0	8016	1/1	0.95	0.14	-	30,30,30,30	0
32	MG	0	8063	1/1	0.68	0.13	-	60,60,60,60	0
34	NA	0	8301	1/1	0.97	0.20	-	34,34,34,34	0
34	NA	0	8370	1/1	0.83	0.68	-	70,70,70,70	0
34	NA	0	8349	1/1	0.90	0.18	-	32,32,32,32	0

## 6.5 Other polymers

There are no such residues in this entry.