



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2018 – 12:47 pm GMT

PDB ID : 1VQK  
Title : The structure of CCDA-PHE-CAP-BIO bound to the a site of the ribosomal subunit of haloarcula marismortui  
Authors : Schmeing, T.M.; Steitz, T.A.  
Deposited on : 2004-12-16  
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk31020  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk31020

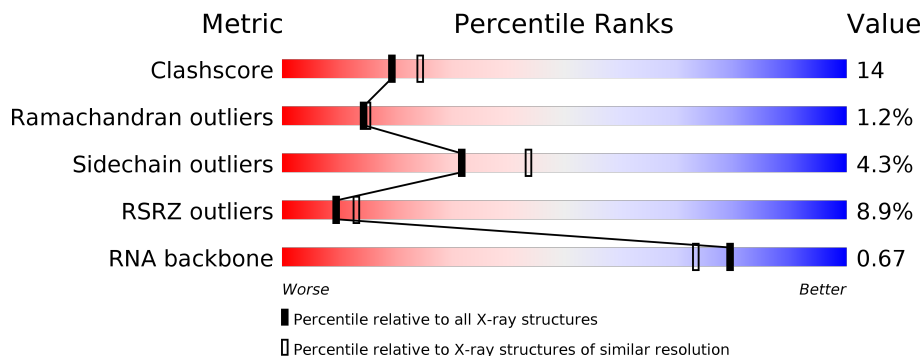
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	122126	5072 (2.30-2.30)
Ramachandran outliers	120053	5022 (2.30-2.30)
Sidechain outliers	120020	5021 (2.30-2.30)
RSRZ outliers	108989	4374 (2.30-2.30)
RNA backbone	2636	1004 (2.76-1.84)

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

Mol	Chain	Length	Quality of chain
1	0	2922	<div> <div>3%</div> <div>65%</div> <div>24%</div> <div>5%</div> <div>6%</div> </div>
2	9	122	<div> <div>5%</div> <div>57%</div> <div>34%</div> <div>8%</div> <div>.</div> </div>
3	4	5	<div> <div>20%</div> <div>40%</div> <div>60%</div> </div>
4	A	240	<div> <div>8%</div> <div>63%</div> <div>32%</div> <div>.</div> <div>.</div> </div>
5	B	338	<div> <div>4%</div> <div>59%</div> <div>35%</div> <div>6%</div> </div>
6	C	246	<div> <div>2%</div> <div>63%</div> <div>32%</div> <div>.</div> </div>

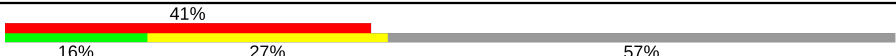
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
7	D	177	
8	E	178	
9	F	120	
10	G	348	
11	H	171	
12	J	145	
13	K	132	
14	L	165	
15	M	195	
16	N	187	
17	O	116	
18	P	149	
19	Q	96	
20	R	155	
21	S	85	
22	T	120	
23	U	66	
24	V	71	
25	W	154	
26	X	92	
27	Y	241	
28	Z	83	
29	1	57	
30	2	50	
31	3	92	

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
32	I	162	

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
3	ACA	4	78	-	-	-	X
33	MG	0	8022	-	-	-	X
33	MG	0	8047	-	-	-	X
33	MG	0	8082	-	-	-	X
33	MG	0	8092	-	-	-	X
35	NA	0	9122	-	-	-	X
35	NA	0	9129	-	-	-	X
35	NA	0	9164	-	-	-	X
37	SR	0	9500	-	-	-	X
37	SR	0	9547	-	-	-	X
37	SR	0	9601	-	-	-	X
37	SR	B	9521	-	-	-	X

## 2 Entry composition [i](#)

There are 39 unique types of molecules in this entry. The entry contains 99036 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S ribosomal rna.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	2754	Total	C	N	O	P	0	0	0
			59021	26350	10878	19048	2745			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	9	122	Total	C	N	O	P	0	0	0
			2600	1160	472	847	121			

- Molecule 3 is a RNA chain called 5'-R(\*CP\*CP\*(DA)\*(PHE)\*(ACA))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	4	5	Total	C	N	O	P	0	0	0
			73	40	12	19	2			

- Molecule 4 is a protein called 50S ribosomal protein L2P.

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

- Molecule 5 is a protein called 50S ribosomal protein L3P.

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

- Molecule 6 is a protein called 50S ribosomal protein L4E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	C	246	Total	C	N	O	S	0	0	0
			1859	1131	344	383	1			

- Molecule 7 is a protein called 50S ribosomal protein L5P.

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

- Molecule 8 is a protein called 50S ribosomal protein L6P.

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

- Molecule 9 is a protein called 50S ribosomal protein L7AE.

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

- Molecule 10 is a protein called ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG.

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

- Molecule 11 is a protein called 50S RIBOSOMAL PROTEIN L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	H	160	Total	C	N	O	S	0	0	0
			1266	785	237	238	6			

- Molecule 12 is a protein called 50S ribosomal protein L13P.

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

- Molecule 13 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	K	132	Total	C	N	O	S	0	0	0
			992	609	187	192	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	44	LEU	HIS	CONFLICT	UNP P22450

- Molecule 14 is a protein called 50S ribosomal protein L15P.

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

- Molecule 15 is a protein called 50S Ribosomal Protein L15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	M	194	Total	C	N	O	S	0	0	0
			1560	943	332	284	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	13	GLU	LYS	CONFLICT	GB 55231501
M	194	ALA	GLY	CONFLICT	GB 55231501

- Molecule 16 is a protein called 50S ribosomal protein L18P.

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

- Molecule 17 is a protein called 50S ribosomal protein L18e.

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

- Molecule 18 is a protein called 50S ribosomal protein L19E.

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

- Molecule 19 is a protein called 50S ribosomal protein L21e.

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

- Molecule 20 is a protein called 50S ribosomal protein L22P.

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

- Molecule 21 is a protein called 50S ribosomal protein L23P.

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

- Molecule 22 is a protein called 50S ribosomal protein L24P.

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

- Molecule 23 is a protein called 50S ribosomal protein L24E.

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

- Molecule 24 is a protein called 50S ribosomal protein L29P.

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

- Molecule 25 is a protein called 50S ribosomal protein L30P.

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

- Molecule 26 is a protein called 50S ribosomal protein L31e.

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

- Molecule 27 is a protein called 50S ribosomal protein L32E.

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

- Molecule 28 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	Z	73	Total	C	N	O	S	0	0	0
			578	346	116	111	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	10	ARG	SER	CONFLICT	GB 55231162

- Molecule 29 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 30 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 31 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L11P.

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

- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	87	Total	Mg	0	0
			87	87		
33	Y	1	Total	Mg	0	0
			1	1		
33	K	1	Total	Mg	0	0
			1	1		
33	B	1	Total	Mg	0	0
			1	1		
33	A	1	Total	Mg	0	0
			1	1		
33	T	1	Total	Mg	0	0
			1	1		
33	9	1	Total	Mg	0	0
			1	1		

- Molecule 34 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	2	Total	K	0	0
			2	2		

- Molecule 35 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	64	Total	Na	0	0
			64	64		
35	J	1	Total	Na	0	0
			1	1		
35	Q	1	Total	Na	0	0
			1	1		
35	D	1	Total	Na	0	0
			1	1		
35	C	1	Total	Na	0	0
			1	1		
35	3	1	Total	Na	0	0
			1	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	R	3	Total 3	Na 3	0	0
35	9	1	Total 1	Na 1	0	0
35	S	1	Total 1	Na 1	0	0
35	M	1	Total 1	Na 1	0	0

- Molecule 36 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	10	Total 10	Cl 10	0	0
36	J	3	Total 3	Cl 3	0	0
36	B	1	Total 1	Cl 1	0	0
36	A	1	Total 1	Cl 1	0	0
36	N	1	Total 1	Cl 1	0	0
36	O	1	Total 1	Cl 1	0	0
36	R	1	Total 1	Cl 1	0	0
36	Y	1	Total 1	Cl 1	0	0
36	L	1	Total 1	Cl 1	0	0
36	3	1	Total 1	Cl 1	0	0
36	M	1	Total 1	Cl 1	0	0

- Molecule 37 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	0	98	Total 98	Sr 98	0	0
37	1	2	Total 2	Sr 2	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	H	1	Total 1	Sr 1	0	0
37	B	2	Total 2	Sr 2	0	0
37	3	1	Total 1	Sr 1	0	0
37	A	3	Total 3	Sr 3	0	0
37	R	1	Total 1	Sr 1	0	0
37	9	3	Total 3	Sr 3	0	0
37	L	1	Total 1	Sr 1	0	0
37	S	1	Total 1	Sr 1	0	0
37	F	1	Total 1	Sr 1	0	0

- Molecule 38 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	O	1	Total 1	Cd 1	0	0
38	Z	1	Total 1	Cd 1	0	0
38	1	1	Total 1	Cd 1	0	0
38	3	1	Total 1	Cd 1	0	0
38	U	1	Total 1	Cd 1	0	0

- Molecule 39 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	0	5769	Total 5769	O 5769	0	0
39	9	140	Total 140	O 140	0	0
39	A	121	Total 121	O 121	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	B	144	Total 144	O 144	0	0
39	C	177	Total 177	O 177	0	0
39	D	48	Total 48	O 48	0	0
39	E	44	Total 44	O 44	0	0
39	F	27	Total 27	O 27	0	0
39	G	17	Total 17	O 17	0	0
39	H	69	Total 69	O 69	0	0
39	J	52	Total 52	O 52	0	0
39	K	57	Total 57	O 57	0	0
39	L	81	Total 81	O 81	0	0
39	M	130	Total 130	O 130	0	0
39	N	61	Total 61	O 61	0	0
39	O	40	Total 40	O 40	0	0
39	P	64	Total 64	O 64	0	0
39	Q	49	Total 49	O 49	0	0
39	R	82	Total 82	O 82	0	0
39	S	32	Total 32	O 32	0	0
39	T	37	Total 37	O 37	0	0
39	U	29	Total 29	O 29	0	0
39	V	14	Total 14	O 14	0	0
39	W	69	Total 69	O 69	0	0

*Continued on next page...*

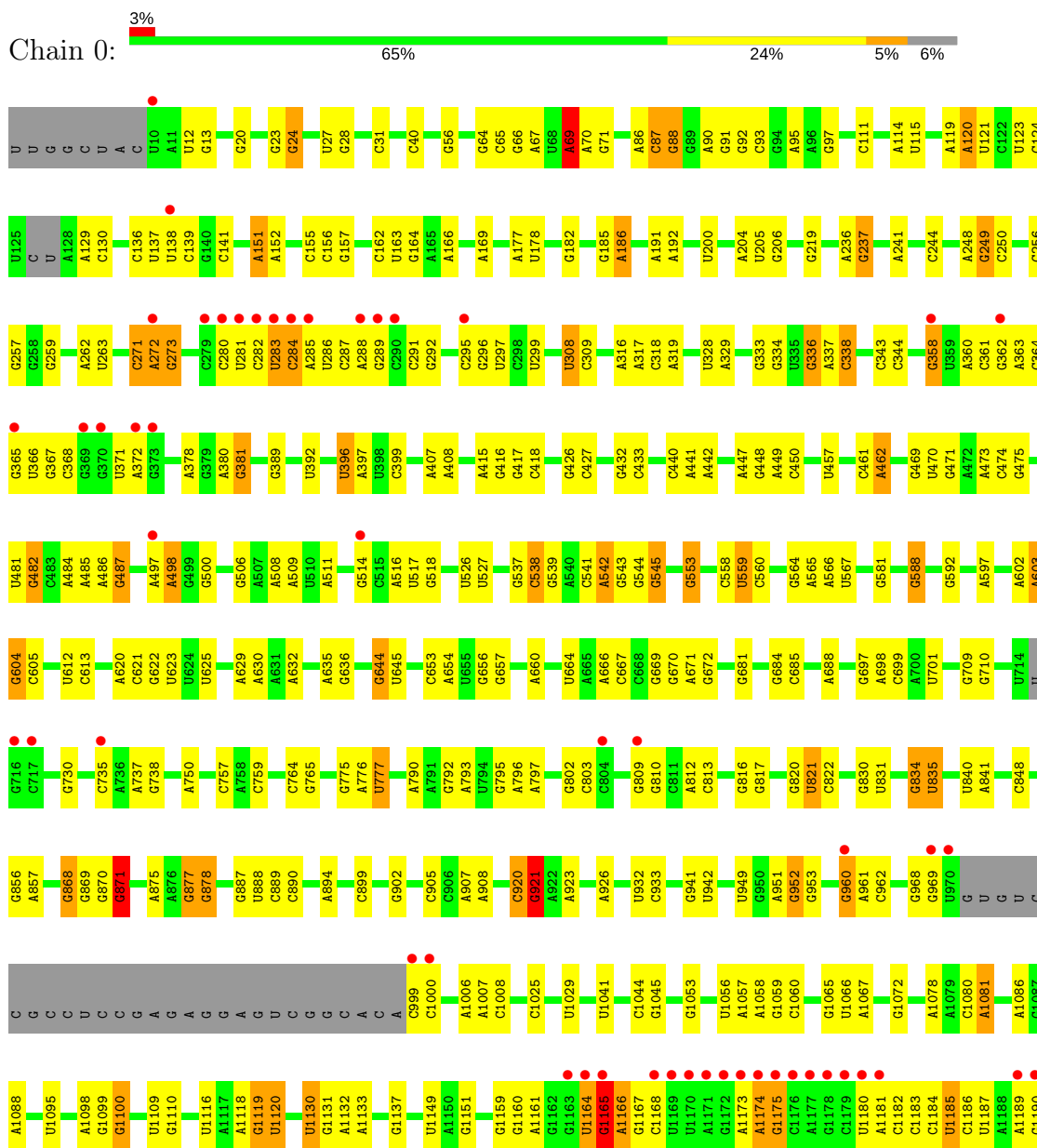
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	X	24	Total 24	O 24	0	0
39	Y	96	Total 96	O 96	0	0
39	Z	31	Total 31	O 31	0	0
39	1	50	Total 50	O 50	0	0
39	2	40	Total 40	O 40	0	0
39	3	67	Total 67	O 67	0	0
39	I	7	Total 7	O 7	0	0

### 3 Residue-property plots

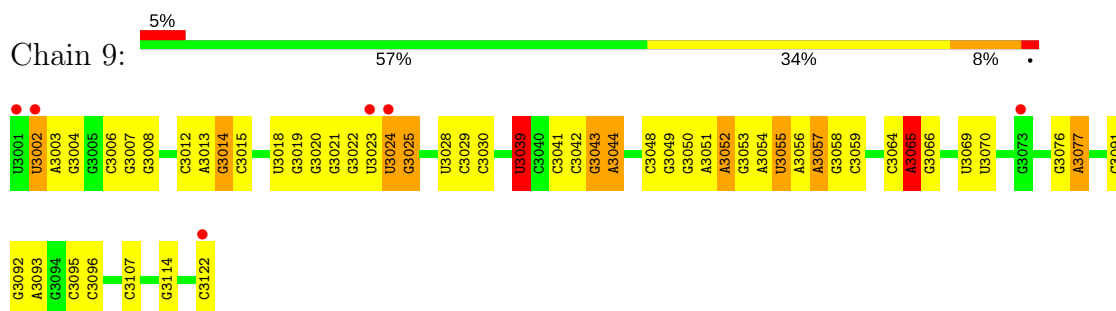
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

- Molecule 1: 23S ribosomal rna

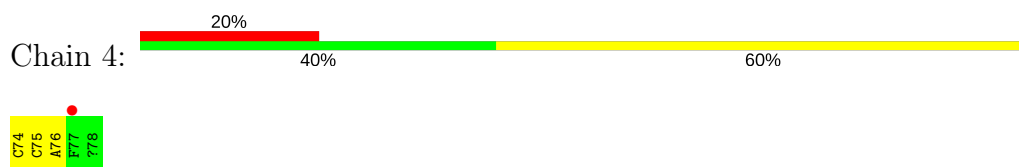


G2842	G2764	A2635	A2521	A2414	A2391	G2136	U2003	C1882	A1767	G1855	U1478	G1311	A1191
G2851	G2755	C2636	G2524	A2416	A2302	A	G2005	G1902	C1768	A1856	C1495	G1314	A1192
U2853	U2756	A2637	G2525	G2417	C2309	C	C2006	U1903	C1769	A1659	G1496	U1314	A1193
A2856	A2761	C2644	C2526	G2418	C2313	U	A2007	A1919	A1778	G1660	A1501	A1328	G1196
C2857	C2762	U2645	U2531	G2419	G2314	G	U2008	C1920	A1779	C1666	A1502	G1197	G1197
U2858	U2765	A2649	A2532	G2420	C2315	U	A2011	A1921	C1786	A1667	U1503	A1331	A1199
U2866	A2768	U2652	C2533	G2421	C2316	C	U2012	A1922	C1787	U1668	A1504	C1332	A1199
C2867	C2769	A2653	G2534	G2422	G2317	U	G2013	G1926	U1788	U1681	U1505	U1333	A1200
G2868	G2770	U2654	C2535	G2426	C2317	C	G2014	G1927	G1789	G1681	U1506	C1334	C1201
G2869	U2771	U2655	A2536	C2427	U2320	C	A2015	A1927	G1794	A1682	U1524	C1335	A1202
G2876	G2779	G2656	U2537	U2435	A2321	A	U2016	G1928	G1795	A1683	G1525	C1203	G1203
U2877	C2780	U2663	U2541	C2443	U2326	C	U2032	G1929	G1796	A1684	A1526	G1204	C1204
U2878	U2781	A	U2542	G2443	U2327	U	G2033	U1937	A1796	A1685	A1527	A1342	U1205
A2879	A2782	U	U2545	G2452	C2329	G	U2034	G1938	A1797	C1686	A1528	C1343	U1206
A2883	C2785	G2667	C2548	G2453	U2330	U	C2035	U1939	C1798	C1687	G1529	U1350	A1207
G2884	G2786	G2670	U2552	A2456	G2338	A	C2036	A1941	G1809	C1692	G1552	U1351	C1208
A2890	U2791	U2671	A2553	U2457	A	G	U2042	A1942	C1818	C1700	G1555	A1352	G1210
C2894	U2792	U2672	U2563	G2462	C	U	G2044	C1943	C1819	U1701	C1556	C1353	G1211
C2895	A2793	G2676	A	A2465	A	A	G2053	C1946	G1820	A1710	U	C1360	G1212
A2896	C2794	U2677	G	G2466	G2344	U	A2054	G1947	A1821	G1821	G1559	G1216	G1216
C2897	G2795	G2678	C	A2467	G2345	G	C	G1948	A1822	A1822	U1561	G1217	U1218
G2898	U2796	U2679	C	A2468	G2346	U	C2061	G1949	A1829	C1714	C1562	U1219	U1219
A2899	A2800	C2682	U	C2472	C2347	C	U2062	G1950	U1835	C1715	C1563	G1226	G1226
G2900	U2807	A2694	U2578	C2476	C2348	A	U2064	U	A1836	A1717	C1564	C1377	G1229
C2901	U2808	U2697	U2586	G2476	A2353	G	A2067	A	U1837	G1722	A1573	G1378	A1230
C2903	G2809	A2697	U2587	G2480	A2354	U	G2068	C	G1837	U1723	C1574	C1384	A1231
A2906	A2810	C2698	G2588	G2481	G2355	C	U2072	U	U1838	G1724	G1592	A1406	A1232
C2907	U2811	U2699	U2589	G2482	A2356	A	G2073	G	A1839	U1725	C1594	A1233	C1593
A2908	A2812	C2700	U2590	A2483	A2361	U	A2074	A	A1845	G1730	C1595	U1408	G1234
G2909	A2813	G2701	C2591	C2487	A2362	C	A2081	C	U1846	C1731	U1596	G1409	A1235
A2910	G2815	U2711	A2599	A2490	A2363	A	A2089	U1964	G1848	A1732	A1597	U1237	C1238
C2911	A2816	G2712	A2601	G2491	A2364	C	G2090	C1965	G1849	A1736	A1603	C1239	G1239
A2912	C2817	U2713	G2602	U2492	A2365	U	C2091	U1966	C1853	G1739	G1604	A1242	A1242
A2914	C2819	G2715	U2603	C2493	A2369	G	A2096	U1967	C1856	U1740	G1605	U1243	C1243
A	G	G2716	U2604	U2499	A2372	U	A2096	G1971	U1856	U1741	A1615	C1245	U1244
C	C2820	C2717	A2504	C2500	U2373	A	A2100	U1972	C1861	G1744	U1825	A1246	A1246
C	C2824	C2718	G2501	G2501	A2379	C	A2101	A1973	G1862	G1745	A1626	U1435	A1252
A	G2825	U2720	A2502	C2502	G2379	C	G2102	G1979	G1863	U1748	G1627	C1451	C1253
U	C2826	G2721	A2503	G2503	C2388	G	A2103	U1980	G1867	U1748	A1630	C1461	C1268
C	A2827	G2722	A2504	A2504	A2398	C	G2110	A1981	G1868	G1752	A1630	A1462	A1278
A	G2828	U2723	G2505	U2505	G2400	U	G2111	U1981	G1873	A1755	C1633	A1470	U1279
U	C2831	U2726	G2506	A2506	G2401	C	G2112	U1992	G1877	G1756	G1634	A1470	C1289
U	U2837	C2747	G2507	A2507	A2402	G	G2113	U1994	G1877	A1759	A1641	C1474	U1298
A	A2840	U2748	G2508	A2508	A2402	C	U2133	G1995	G1878	U1766	A1642	C1477	U1299
A2841	A2841	G2750	G2510	A2511	G2412	G	A2135	U1996	U1879				

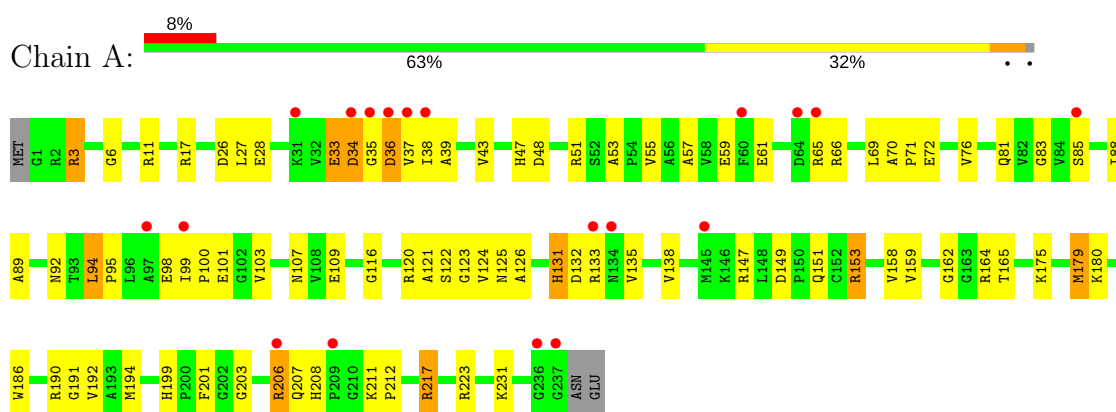
- Molecule 2: 5S ribosomal RNA



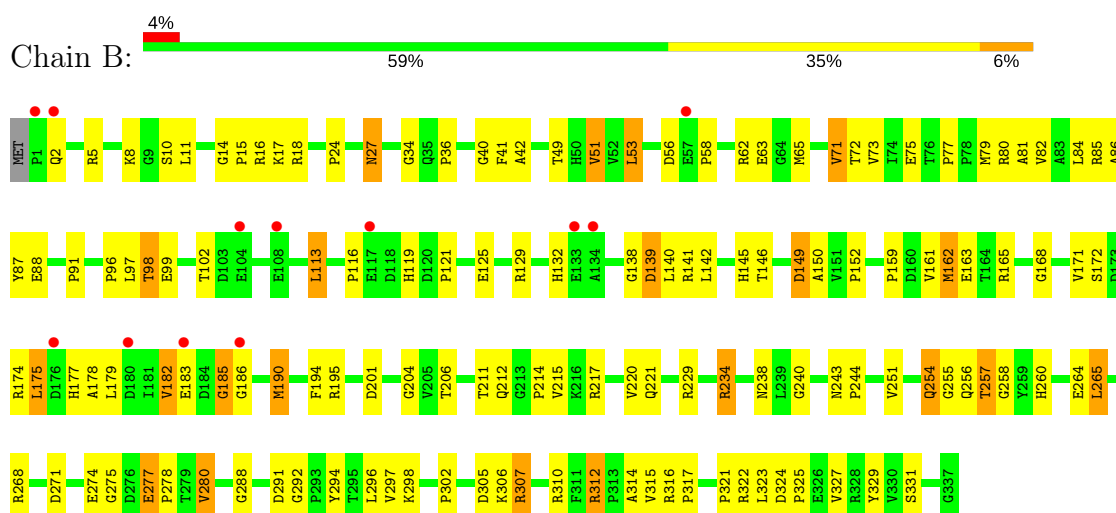
- Molecule 3: 5'-R(\*CP\*CP\*(DA)\*(PHE)\*(ACA))-3'



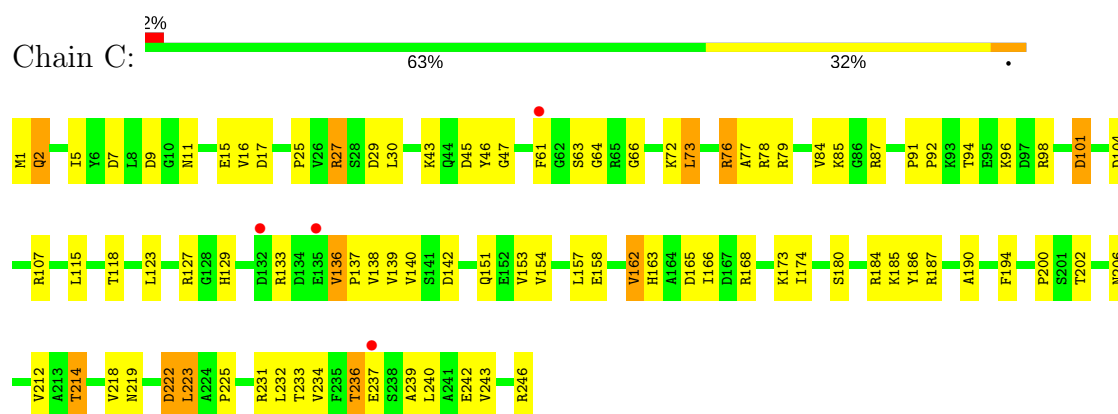
- Molecule 4: 50S ribosomal protein L2P



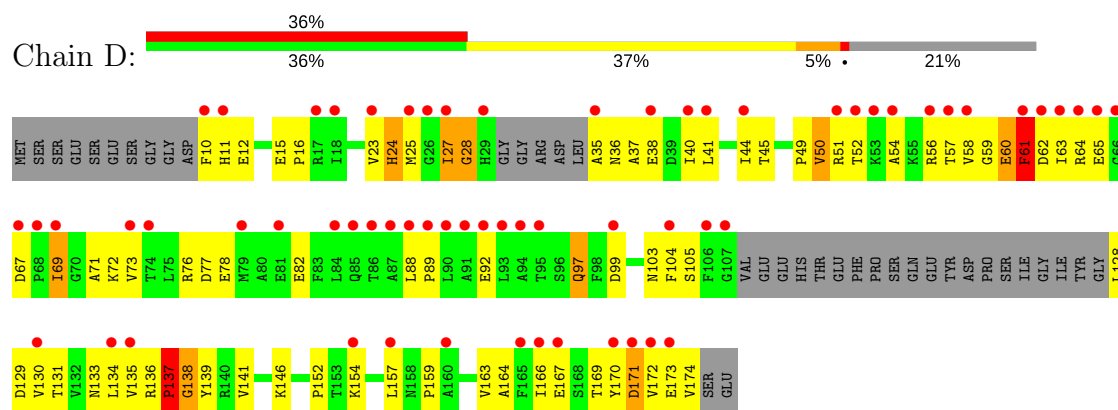
- Molecule 5: 50S ribosomal protein L3P



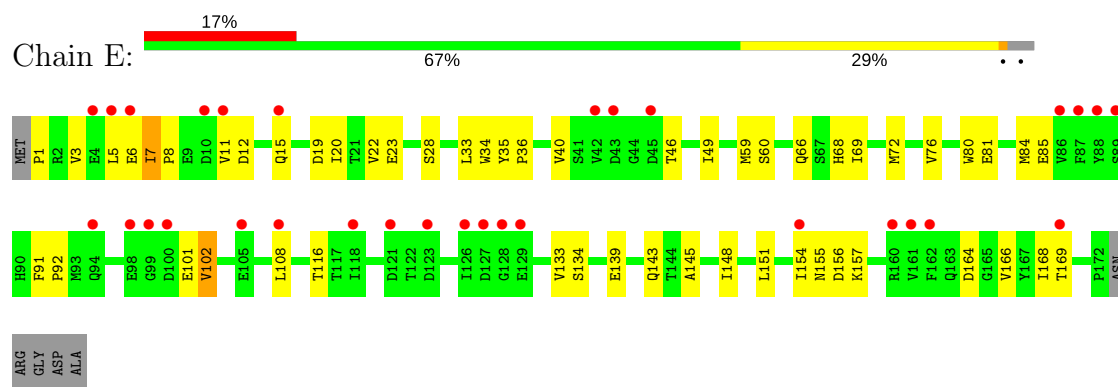
- Molecule 6: 50S ribosomal protein L4E



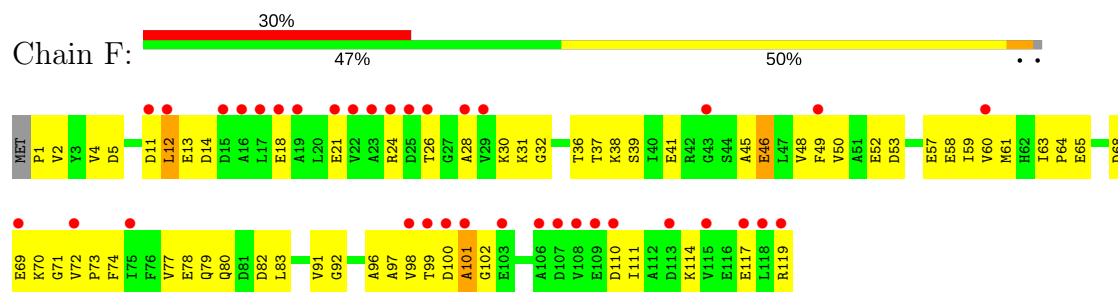
• Molecule 7: 50S ribosomal protein L5P



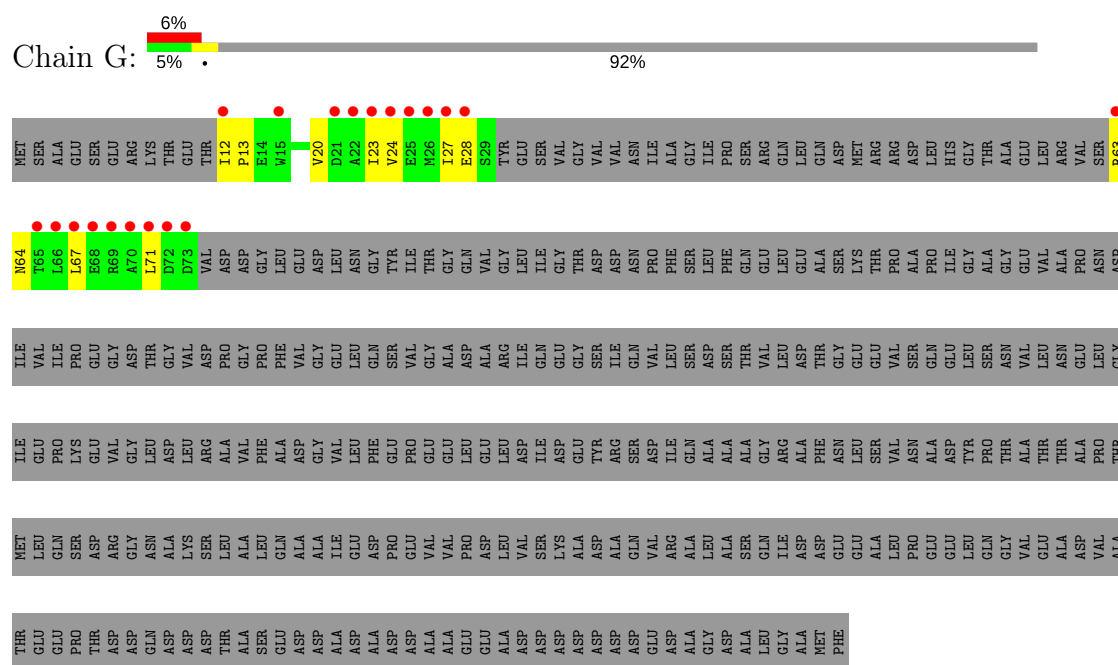
• Molecule 8: 50S ribosomal protein L6P



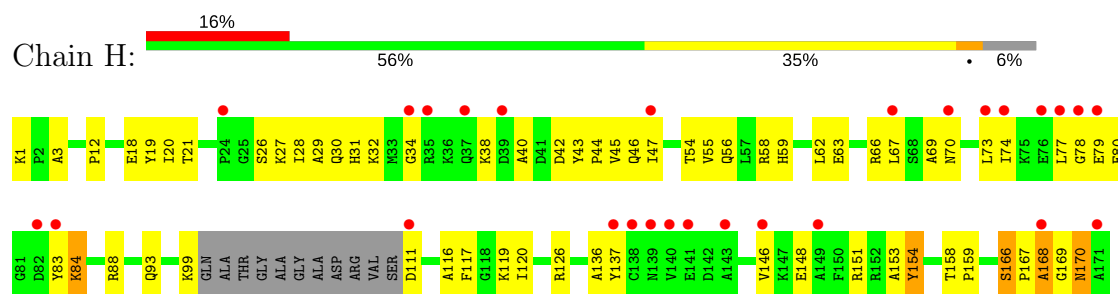
• Molecule 9: 50S ribosomal protein L7AE



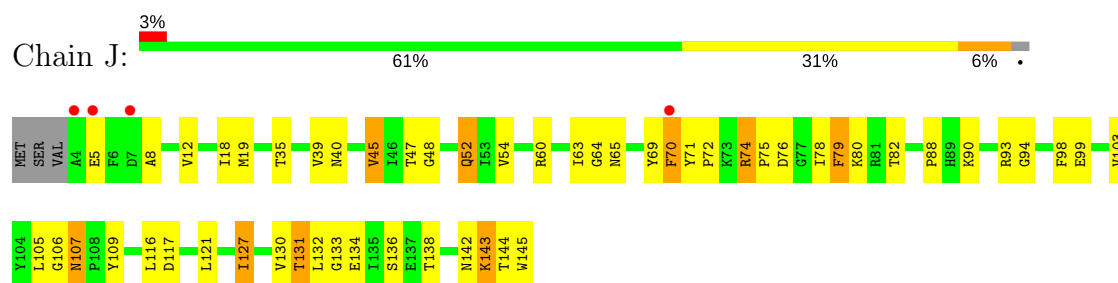
• Molecule 10: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG



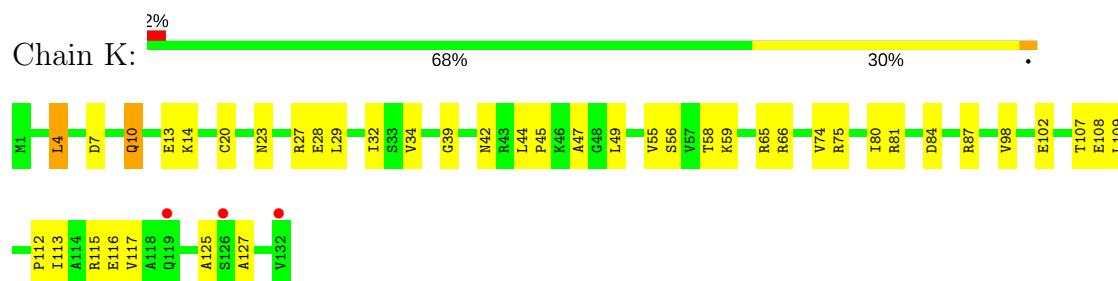
- Molecule 11: 50S RIBOSOMAL PROTEIN L10E



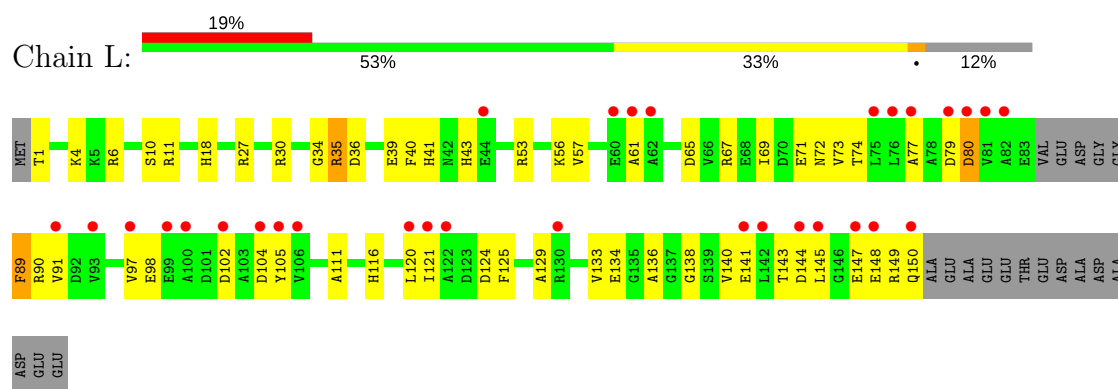
- Molecule 12: 50S ribosomal protein L13P



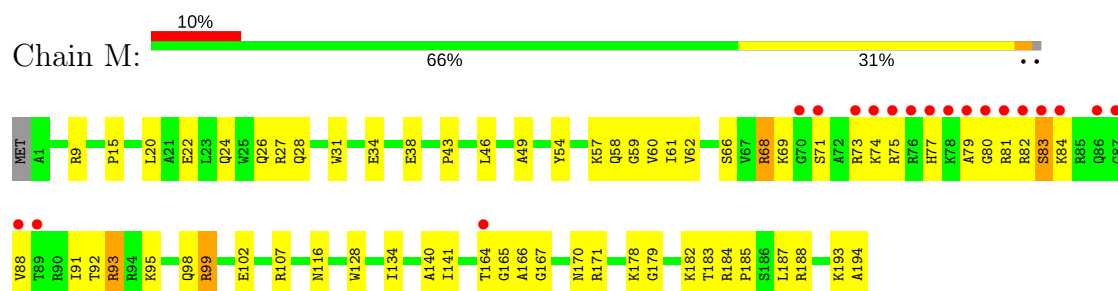
- Molecule 13: 50S ribosomal protein L14P



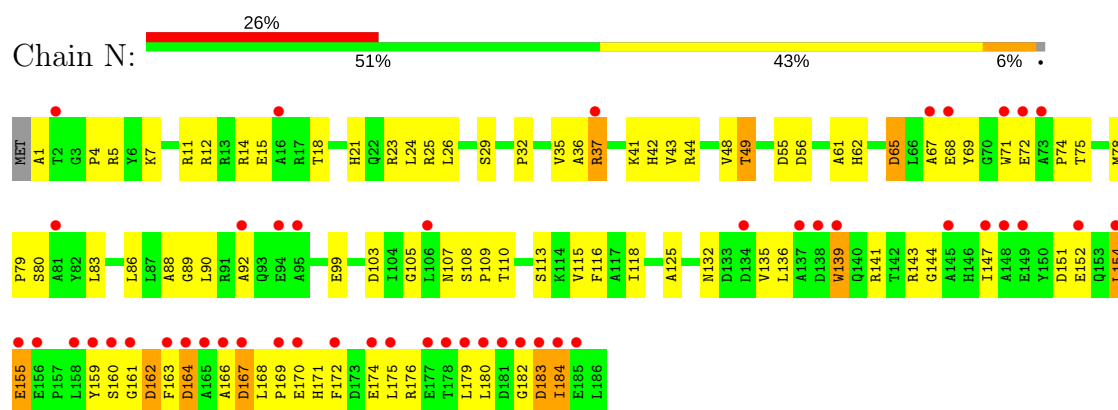
- Molecule 14: 50S ribosomal protein L15P



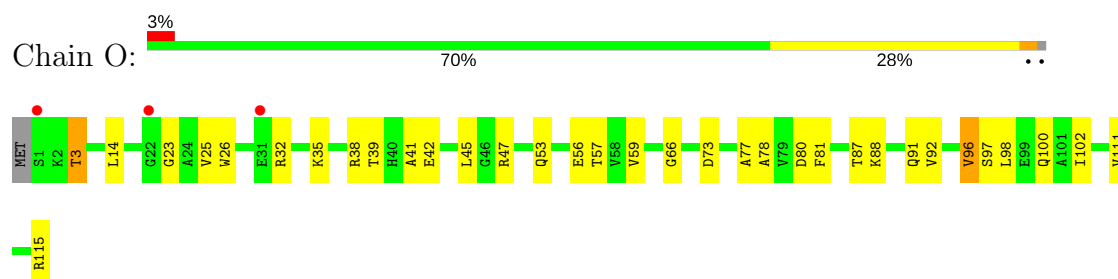
• Molecule 15: 50S Ribosomal Protein L15E



• Molecule 16: 50S ribosomal protein L18P

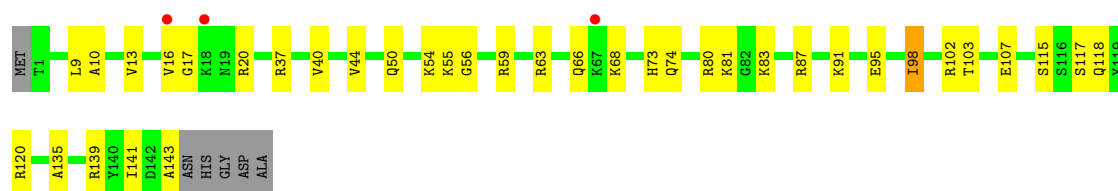


• Molecule 17: 50S ribosomal protein L18e

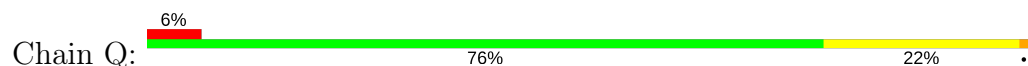


• Molecule 18: 50S ribosomal protein L19E





- Molecule 19: 50S ribosomal protein L21e



- Molecule 20: 50S ribosomal protein L22P



- Molecule 21: 50S ribosomal protein L23P



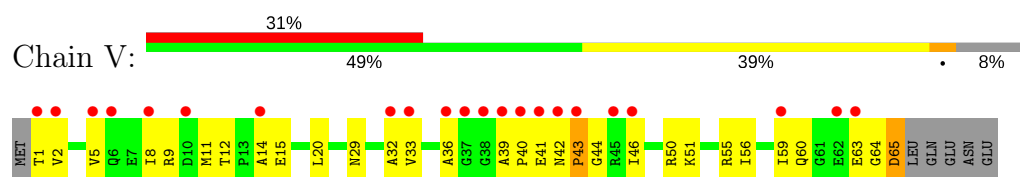
- Molecule 22: 50S ribosomal protein L24P



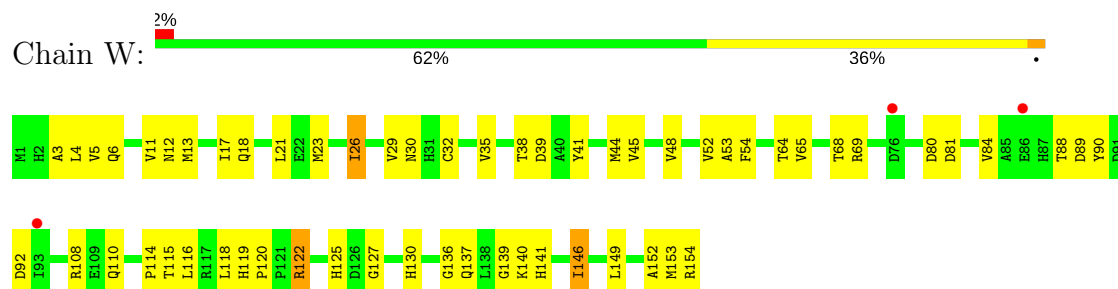
- Molecule 23: 50S ribosomal protein L24E



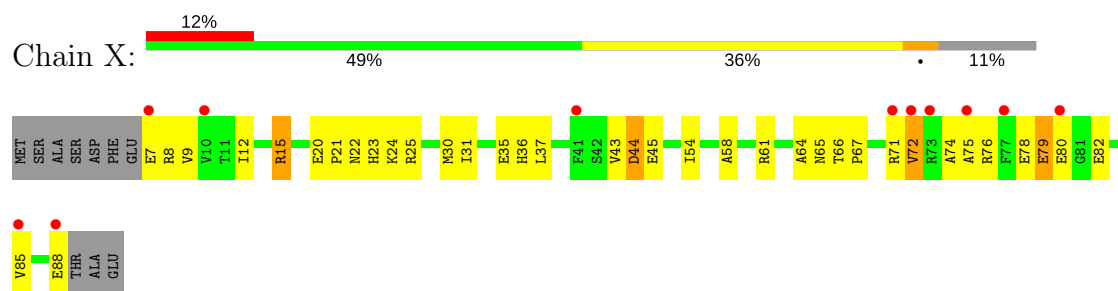
- Molecule 24: 50S ribosomal protein L29P



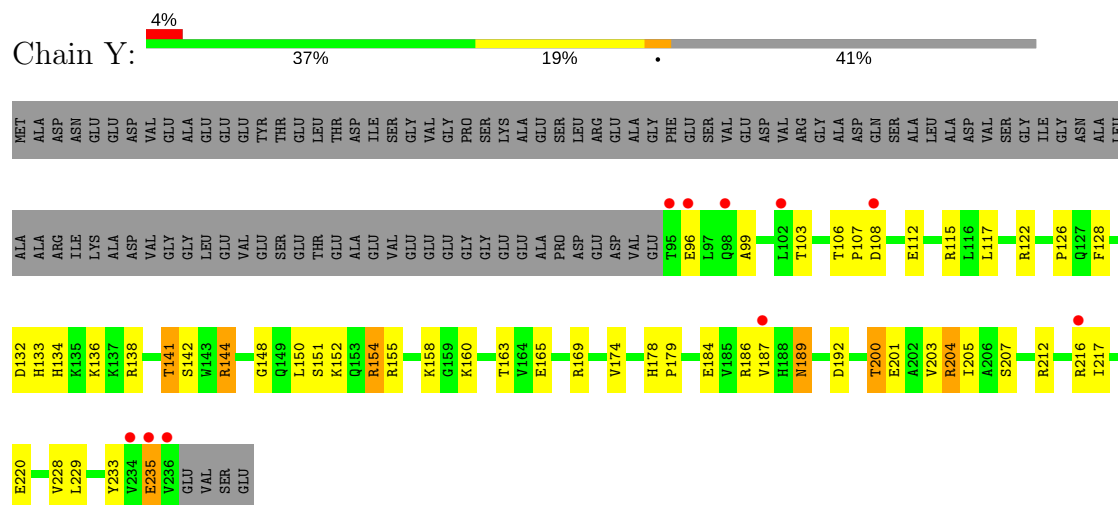
• Molecule 25: 50S ribosomal protein L30P



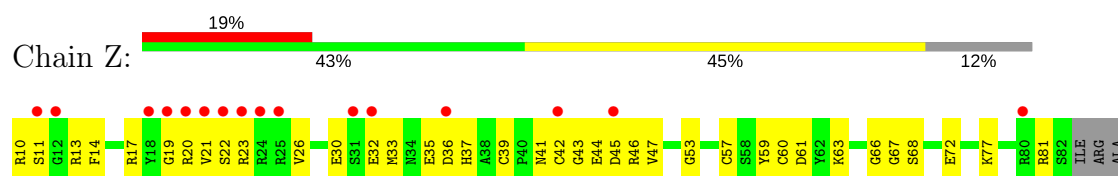
• Molecule 26: 50S ribosomal protein L31e



• Molecule 27: 50S ribosomal protein L32E



• Molecule 28: 50S ribosomal protein L37Ae



ALA  
LEU  
SER  
GLU  
ASP  
GLU  
GLU

- Molecule 29: 50S ribosomal protein L37e



MET  
T1  
Q8  
G9  
K10  
K11  
H16  
T17  
K18  
C19  
R20  
R21  
K25  
H28  
K31  
C37  
D47  
E56

- Molecule 30: 50S ribosomal protein L39e



MET  
G1  
K5  
K9  
R10  
N18  
S19  
R20  
V21  
P22  
V25  
K28  
T29  
D30  
R31  
GLU  
VAL  
GLN  
R35  
R39  
R40  
H41  
R44  
N45  
D48  
E49

- Molecule 31: 50S ribosomal protein L44E



H1  
Q2  
M3  
R6  
H17  
Q18  
E19  
H20  
E21  
V25  
W35  
R38  
E41  
R42  
N48  
P56  
K60  
P61  
T62  
T65  
P66  
L67  
K68  
Y69  
R70  
E73  
A77  
R80  
K84  
L88  
E89  
F90  
Q91  
E92

- Molecule 32: 50S RIBOSOMAL PROTEIN L11P



MET  
ALA  
GLY  
THR  
ILE  
GLU  
VAL  
LEU  
VAL  
PRO  
GLY  
GLY  
ALA  
ASN  
PRO  
GLY  
PRO  
PRO  
LEU  
GLY  
PRO  
GLY  
LEU  
GLY  
PRO  
THR  
VAL  
ASP  
VAL  
GLN  
ALA  
VAL  
GLN  
ILE  
ASN  
ASP  
GLN  
THR  
ALA  
ALA  
PHE  
ASP  
GLY  
THR  
VAL  
VAL  
VAL  
LYS  
TYR  
ASP  
ASP  
GLY

SER  
PHE  
GLU  
ILE  
GLU  
VAL  
G71  
V72  
P73  
T74  
T75  
A76  
E77  
L78  
I79  
K80  
D81  
E82  
A83  
G84  
F85  
E86  
T87  
G88  
S89  
G90  
E91  
P92  
Q93  
E94  
D95  
F96  
V97  
A98  
D99  
L100  
S101  
V102  
D103  
Q104  
V105  
K106  
Q107  
I108  
A109  
E110  
Q111  
K112  
H113  
P114  
D115  
L116  
L117  
S118  
Y119  
D120  
L121  
T122  
A124

A125  
K126  
E127  
V128  
V129  
G130  
T131  
C132  
T133  
S134  
L135  
G136  
V137  
T138  
I139  
E140  
GLY  
GLU  
ASN  
PRO  
ARG  
GLU  
PHE  
LYS  
GLU  
ARG  
ILE  
ASP  
ALA  
GLY  
GLU  
TYR  
ASP  
VAL  
PHE  
ALA  
ALA  
GLU  
ALA  
GLN  
ALA

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	211.87Å 298.57Å 575.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 49.73 – 2.30	Depositor EDS
% Data completeness (in resolution range)	89.5 (50.00-2.30) 89.6 (49.73-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.69 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.218 , 0.250 0.205 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.0	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 61.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	99036	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.60% 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, SR, NA, K, ACA, 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	0	0.37	0/65959	0.70	26/102870 (0.0%)
2	9	0.33	0/2905	0.71	1/4528 (0.0%)
3	4	0.52	0/75	0.73	0/110
4	A	0.34	0/1786	0.66	0/2408
5	B	0.33	0/2690	0.66	0/3652
6	C	0.38	0/1884	0.64	1/2551 (0.0%)
7	D	0.29	0/1111	0.54	0/1498
8	E	0.32	0/1382	0.57	0/1880
9	F	0.31	0/901	0.54	0/1224
10	G	0.27	0/241	0.47	0/324
11	H	0.33	0/1287	0.64	0/1725
12	J	0.35	0/1136	0.61	0/1530
13	K	0.35	0/1001	0.67	0/1347
14	L	0.33	0/1130	0.64	0/1509
15	M	0.34	0/1584	0.60	0/2119
16	N	0.28	0/1474	0.60	0/1999
17	O	0.33	0/874	0.59	1/1181 (0.1%)
18	P	0.34	0/1147	0.56	0/1528
19	Q	0.35	0/749	0.69	0/1005
20	R	0.35	0/1172	0.67	0/1578
21	S	0.32	0/648	0.58	1/875 (0.1%)
22	T	0.31	0/958	0.63	0/1289
23	U	0.35	0/417	0.58	0/562
24	V	0.27	0/502	0.53	0/675
25	W	0.34	0/1219	0.60	0/1655
26	X	0.33	0/664	0.60	0/895
27	Y	0.36	0/1146	0.65	0/1536
28	Z	0.34	0/589	0.61	0/787
29	1	0.43	0/438	0.66	0/578
30	2	0.35	0/401	0.60	0/529
31	3	0.38	0/771	0.58	0/1024
32	I	0.28	0/526	0.50	0/716

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	0.36	0/98767	0.67	30/147687 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	1	39
2	9	0	2
All	All	1	41

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1563	G	C2'-C3'-O3'	9.69	130.83	109.50
2	9	3039	U	N1-C1'-C2'	7.45	123.68	114.00
1	0	1942	A	C5'-C4'-C3'	7.27	127.63	116.00
1	0	1819	G	C5'-C4'-C3'	6.86	126.98	116.00
1	0	1592	G	N9-C1'-C2'	6.67	122.67	114.00
1	0	871	G	C5'-C4'-O4'	-6.63	101.14	109.10
1	0	1819	G	C1'-O4'-C4'	-6.35	104.82	109.90
1	0	1979	G	C2'-C3'-O3'	6.29	123.77	113.70
1	0	777	U	O4'-C1'-N1	6.26	113.21	108.20
1	0	2313	C	C5'-C4'-O4'	5.93	116.22	109.10
1	0	1504	A	C1'-O4'-C4'	-5.91	105.17	109.90
1	0	206	G	C5'-C4'-C3'	-5.84	106.66	116.00
1	0	1819	G	C4'-C3'-C2'	-5.79	96.81	102.60
1	0	1615	A	C5'-C4'-C3'	5.69	125.10	116.00
1	0	1352	A	OP1-P-O3'	5.62	117.57	105.20
1	0	2291	A	N9-C1'-C2'	5.46	121.11	114.00
1	0	2467	A	C1'-O4'-C4'	-5.43	105.56	109.90
1	0	841	A	C1'-O4'-C4'	-5.37	105.61	109.90
1	0	1504	A	N9-C1'-C2'	5.30	120.89	114.00
1	0	1942	A	C1'-O4'-C4'	-5.28	105.68	109.90
1	0	1352	A	C2'-C3'-O3'	5.26	122.12	113.70
1	0	1120	U	C5'-C4'-C3'	-5.23	107.63	116.00
1	0	2313	C	C5'-C4'-C3'	5.21	124.33	116.00
17	O	66	GLY	N-CA-C	5.19	126.08	113.10
21	S	27	ALA	N-CA-C	-5.19	96.99	111.00
6	C	73	LEU	CA-CB-CG	-5.12	103.52	115.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1165	G	C1'-O4'-C4'	-5.11	105.81	109.90
1	0	921	G	N9-C1'-C2'	5.07	120.58	114.00
1	0	389	G	C5'-C4'-C3'	-5.03	107.95	116.00
1	0	69	A	C5'-C4'-O4'	-5.01	103.09	109.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	1563	G	C3'

All (41) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1078	A	Sidechain
1	0	1080	C	Sidechain
1	0	1340	G	Sidechain
1	0	1430	G	Sidechain
1	0	1718	G	Sidechain
1	0	1744	G	Sidechain
1	0	1794	G	Sidechain
1	0	1809	G	Sidechain
1	0	1819	G	Sidechain
1	0	182	G	Sidechain
1	0	1829	A	Sidechain
1	0	1845	A	Sidechain
1	0	1861	C	Sidechain
1	0	1863	G	Sidechain
1	0	1867	G	Sidechain
1	0	1877	G	Sidechain
1	0	1878	G	Sidechain
1	0	2316	G	Sidechain
1	0	24	G	Sidechain
1	0	2465	A	Sidechain
1	0	2493	C	Sidechain
1	0	2503	A	Sidechain
1	0	2506	A	Sidechain
1	0	2552	C	Sidechain
1	0	2599	A	Sidechain
1	0	2632	G	Sidechain
1	0	2793	A	Sidechain
1	0	2842	G	Sidechain
1	0	396	U	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
1	0	462	A	Sidechain
1	0	469	G	Sidechain
1	0	471	G	Sidechain
1	0	482	G	Sidechain
1	0	518	G	Sidechain
1	0	792	G	Sidechain
1	0	795	G	Sidechain
1	0	817	G	Sidechain
1	0	868	G	Sidechain
1	0	952	G	Sidechain
2	9	3039	U	Sidechain
2	9	3065	A	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	0	59021	0	29813	722	0
2	9	2600	0	1326	50	0
3	4	73	0	44	2	0
4	A	1753	0	1766	101	0
5	B	2625	0	2532	145	0
6	C	1859	0	1816	106	0
7	D	1094	0	1085	79	0
8	E	1357	0	1266	45	0
9	F	890	0	843	57	0
10	G	240	0	231	11	0
11	H	1266	0	1268	68	0
12	J	1120	0	1098	68	0
13	K	992	0	1031	53	0
14	L	1118	0	1076	61	0
15	M	1560	0	1568	63	0
16	N	1445	0	1401	97	0
17	O	865	0	873	40	0
18	P	1136	0	1123	35	0
19	Q	735	0	729	18	0
20	R	1149	0	1122	37	0
21	S	641	0	605	16	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	T	950	0	923	47	0
23	U	410	0	364	26	0
24	V	499	0	511	38	0
25	W	1196	0	1137	82	0
26	X	654	0	653	35	0
27	Y	1130	0	1133	57	0
28	Z	578	0	539	28	0
29	1	431	0	426	22	0
30	2	396	0	413	26	0
31	3	755	0	728	26	0
32	I	519	0	500	51	0
33	0	87	0	0	0	0
33	9	1	0	0	0	0
33	A	1	0	0	0	0
33	B	1	0	0	0	0
33	K	1	0	0	0	0
33	T	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	2	0	0	0	0
35	0	64	0	0	0	0
35	3	1	0	0	0	0
35	9	1	0	0	0	0
35	C	1	0	0	0	0
35	D	1	0	0	0	0
35	J	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	3	0	0	0	0
35	S	1	0	0	0	0
36	0	10	0	0	0	0
36	3	1	0	0	0	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	J	3	0	0	1	0
36	L	1	0	0	0	0
36	M	1	0	0	0	0
36	N	1	0	0	1	0
36	O	1	0	0	0	0
36	R	1	0	0	0	0
36	Y	1	0	0	0	0
37	0	98	0	0	0	0
37	1	2	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	3	1	0	0	0	0
37	9	3	0	0	0	0
37	A	3	0	0	0	0
37	B	2	0	0	0	0
37	F	1	0	0	0	0
37	H	1	0	0	0	0
37	L	1	0	0	0	0
37	R	1	0	0	0	0
37	S	1	0	0	0	0
38	1	1	0	0	0	0
38	3	1	0	0	0	0
38	O	1	0	0	0	0
38	U	1	0	0	0	0
38	Z	1	0	0	0	0
39	0	5769	0	0	106	0
39	1	50	0	0	2	0
39	2	40	0	0	3	0
39	3	67	0	0	4	0
39	9	140	0	0	6	0
39	A	121	0	0	11	0
39	B	144	0	0	18	0
39	C	177	0	0	18	0
39	D	48	0	0	10	0
39	E	44	0	0	1	0
39	F	27	0	0	4	0
39	G	17	0	0	1	0
39	H	69	0	0	7	0
39	I	7	0	0	1	0
39	J	52	0	0	4	0
39	K	57	0	0	6	0
39	L	81	0	0	14	0
39	M	130	0	0	3	0
39	N	61	0	0	9	0
39	O	40	0	0	5	0
39	P	64	0	0	2	0
39	Q	49	0	0	5	0
39	R	82	0	0	3	0
39	S	32	0	0	1	0
39	T	37	0	0	3	0
39	U	29	0	0	3	0
39	V	14	0	0	2	0
39	W	69	0	0	5	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	X	24	0	0	6	0
39	Y	96	0	0	9	0
39	Z	31	0	0	2	0
All	All	99036	0	59943	2083	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 14.

All (2083) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:21:LEU:HD21	25:W:48:VAL:HG11	1.29	1.14
26:X:37:LEU:HD13	26:X:85:VAL:HG21	1.29	1.10
6:C:236:THR:HG22	6:C:239:ALA:H	1.19	1.07
1:O:656:G:H5'	17:O:3:THR:HG22	1.38	1.05
1:O:1160:G:H5'	1:O:1161:A:H5'	1.40	1.04
22:T:9:LYS:HE3	22:T:13:ARG:NH1	1.72	1.03
2:9:3076:G:H3'	2:9:3077:A:H5''	1.41	1.02
9:F:91:VAL:HG12	9:F:92:GLY:H	1.25	1.00
28:Z:46:ARG:HD2	28:Z:59:TYR:HB2	1.42	0.99
22:T:71:VAL:HG11	22:T:90:PRO:HB3	1.38	0.99
20:R:99:ALA:HB1	20:R:109:MET:HE1	1.45	0.98
6:C:127:ARG:NH2	6:C:225:PRO:HG2	1.78	0.97
18:P:115:SER:H	18:P:118:GLN:HE21	1.12	0.96
1:O:156:C:H5''	15:M:171:ARG:HD3	1.47	0.95
13:K:81:ARG:HB2	13:K:87:ARG:HH11	1.32	0.94
13:K:39:GLY:HA2	39:K:4183:HOH:O	1.68	0.94
12:J:93:ARG:HH11	12:J:93:ARG:HB3	1.29	0.93
7:D:57:THR:HG23	7:D:63:ILE:HA	1.51	0.93
25:W:137:GLN:HE21	25:W:141:HIS:HE1	1.15	0.93
13:K:29:LEU:HB3	13:K:55:VAL:HG11	1.51	0.93
5:B:307:ARG:HH11	5:B:307:ARG:HG3	1.34	0.92
21:S:57:THR:HG22	21:S:59:ASP:H	1.34	0.92
24:V:12:THR:HG22	24:V:15:GLU:HG3	1.50	0.92
25:W:6:GLN:HB2	25:W:26:ILE:HD12	1.52	0.91
2:9:3056:A:H2'	2:9:3057:A:H5''	1.52	0.89
1:O:2506:A:HO2'	1:O:2507:G:H8	0.92	0.89
8:E:20:ILE:HD11	8:E:40:VAL:HG11	1.54	0.89
5:B:212:GLN:HB2	5:B:257:THR:HG21	1.53	0.89
21:S:51:GLN:HE21	21:S:53:ASN:HD21	1.21	0.89
13:K:74:VAL:HG13	13:K:113:ILE:HG23	1.55	0.89

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2717:C:H2'	1:0:2718:C:H5''	1.54	0.89
8:E:36:PRO:HD3	12:J:127:ILE:HD12	1.53	0.88
13:K:10:GLN:H	13:K:10:GLN:HE21	0.89	0.88
1:0:1593:C:OP1	18:P:117:SER:HB3	1.74	0.88
8:E:15:GLN:HG3	8:E:20:ILE:HG12	1.56	0.88
13:K:10:GLN:N	13:K:10:GLN:HE21	1.71	0.88
1:0:542:A:H5'	1:0:542:A:H8	1.40	0.87
6:C:104:ASP:HA	6:C:107:ARG:HH12	1.37	0.87
1:0:2717:C:C2'	1:0:2718:C:H5''	2.04	0.87
13:K:10:GLN:H	13:K:10:GLN:NE2	1.73	0.87
4:A:81:GLN:HB2	4:A:92:ASN:ND2	1.89	0.87
5:B:238:ASN:HD22	5:B:240:GLY:H	1.17	0.87
1:0:1603:A:H5'	1:0:1605:G:O4'	1.74	0.87
6:C:1:MET:HG2	6:C:2:GLN:H	1.40	0.87
28:Z:11:SER:HB3	28:Z:23:ARG:HB2	1.57	0.87
1:0:1242:A:H5'	12:J:82:THR:HG23	1.55	0.86
1:0:1372:A:H3'	39:0:7681:HOH:O	1.75	0.86
13:K:74:VAL:HG11	13:K:113:ILE:HG12	1.57	0.86
1:0:288:A:H61	1:0:364:C:H42	1.21	0.86
5:B:162:MET:HE2	5:B:310:ARG:HD3	1.57	0.86
25:W:122:ARG:HH11	25:W:122:ARG:HG2	1.40	0.86
16:N:144:GLY:O	16:N:147:ILE:HG22	1.76	0.86
6:C:115:LEU:HD13	6:C:223:LEU:HD21	1.58	0.85
1:0:2812:A:H2	1:0:2814:A:H62	1.21	0.85
7:D:25:MET:HE2	7:D:41:LEU:HG	1.58	0.84
1:0:1835:U:H5	1:0:1840:A:N7	1.75	0.84
7:D:58:VAL:HB	7:D:62:ASP:HB3	1.58	0.84
7:D:28:GLY:HA2	7:D:69:ILE:HG23	1.59	0.84
1:0:2541:U:H3	1:0:2618:G:H1	1.24	0.84
18:P:115:SER:OG	18:P:118:GLN:HG3	1.77	0.83
1:0:2073:G:H5''	39:0:4410:HOH:O	1.77	0.83
1:0:289:G:H22	1:0:363:A:H2	1.22	0.83
25:W:122:ARG:NH2	25:W:154:ARG:HG2	1.93	0.83
27:Y:235:GLU:H	27:Y:235:GLU:CD	1.80	0.83
2:9:3039:U:H1'	2:9:3044:A:H61	1.43	0.83
15:M:164:THR:HG22	15:M:166:ALA:H	1.43	0.83
16:N:113:SER:HB2	39:N:9356:HOH:O	1.77	0.83
1:0:2840:A:OP1	5:B:211:THR:HG23	1.78	0.82
15:M:99:ARG:HH21	15:M:170:ASN:HD22	1.26	0.82
6:C:5:ILE:HD11	6:C:16:VAL:HG23	1.61	0.82
16:N:83:LEU:HD13	16:N:175:LEU:HD23	1.61	0.82

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:V:1:THR:HG23	24:V:2:VAL:H	1.44	0.82
25:W:88:THR:HB	39:W:6679:HOH:O	1.80	0.82
4:A:206:ARG:HD3	4:A:206:ARG:H	1.44	0.81
1:0:560:C:H42	1:0:597:A:H61	1.25	0.81
39:0:5402:HOH:O	12:J:47:THR:HB	1.80	0.81
15:M:134:ILE:HG23	15:M:141:ILE:HD13	1.62	0.81
1:0:2506:A:O2'	1:0:2507:G:H8	1.62	0.81
1:0:1116:U:HO2'	1:0:1118:A:H2	0.82	0.81
4:A:192:VAL:HB	39:A:9578:HOH:O	1.79	0.81
13:K:81:ARG:HB2	13:K:87:ARG:NH1	1.95	0.81
4:A:211:LYS:HG2	4:A:212:PRO:HD2	1.60	0.81
5:B:162:MET:CE	5:B:310:ARG:HD3	2.09	0.81
13:K:4:LEU:HD22	13:K:116:GLU:HB3	1.60	0.81
25:W:6:GLN:HB2	25:W:26:ILE:CD1	2.11	0.80
1:0:1377:C:H6	1:0:1377:C:H5'	1.44	0.80
20:R:8:ALA:HB1	20:R:13:THR:HG21	1.63	0.80
1:0:1041:U:H5'	39:L:9489:HOH:O	1.80	0.80
4:A:192:VAL:HG22	39:A:9618:HOH:O	1.81	0.80
11:H:46:GLN:HB3	11:H:167:PRO:HD2	1.64	0.80
25:W:125:HIS:HD2	25:W:127:GLY:H	1.30	0.80
1:0:1474:C:H6	1:0:1474:C:H5'	1.46	0.79
31:3:65:THR:HG22	31:3:67:LEU:HG	1.64	0.79
25:W:13:MET:HE1	25:W:18:GLN:HA	1.63	0.79
5:B:36:PRO:HA	5:B:168:GLY:HA3	1.64	0.79
1:0:1116:U:O2'	1:0:1118:A:H2	1.64	0.79
26:X:30:MET:HE1	26:X:58:ALA:HB3	1.65	0.79
1:0:2005:G:H3'	1:0:2005:G:OP2	1.83	0.78
6:C:5:ILE:HD11	6:C:16:VAL:CG2	2.14	0.78
1:0:1165:G:H4'	1:0:1174:A:O2'	1.84	0.78
7:D:25:MET:HE1	7:D:37:ALA:HB1	1.66	0.78
22:T:71:VAL:HG11	22:T:90:PRO:CB	2.13	0.78
30:2:41:HIS:H	30:2:45:ASN:HD22	1.32	0.78
5:B:58:PRO:HA	5:B:63:GLU:OE1	1.83	0.78
1:0:2054:A:N3	20:R:128:ARG:NH2	2.32	0.78
1:0:381:G:H5''	39:M:9376:HOH:O	1.85	0.78
18:P:115:SER:H	18:P:118:GLN:NE2	1.82	0.78
6:C:236:THR:HG22	6:C:239:ALA:N	1.97	0.77
9:F:91:VAL:HG12	9:F:92:GLY:N	1.99	0.77
18:P:115:SER:N	18:P:118:GLN:HE21	1.82	0.77
13:K:14:LYS:HB2	13:K:45:PRO:HG2	1.66	0.77
1:0:1701:A:H4'	1:0:1702:U:H5''	1.66	0.77

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1205:U:H2'	1:0:1206:U:H5''	1.67	0.77
1:0:2635:A:O2'	1:0:2636:C:H5'	1.85	0.76
22:T:41:ARG:HG2	22:T:41:ARG:HH11	1.50	0.76
31:3:70:ARG:HG2	31:3:77:ALA:HB2	1.66	0.76
1:0:1166:A:H61	1:0:1180:U:H3	1.31	0.76
5:B:53:LEU:HD11	5:B:327:VAL:HG22	1.65	0.76
25:W:21:LEU:CD2	25:W:48:VAL:HG11	2.13	0.76
20:R:25:PHE:CE2	20:R:29:LYS:HE2	2.20	0.76
1:0:545:G:H8	1:0:545:G:H5'	1.49	0.76
1:0:962:C:H1'	16:N:5:ARG:NH1	2.00	0.76
32:I:132:CYS:HB3	32:I:137:VAL:HB	1.68	0.76
1:0:559:U:H5'	1:0:559:U:H6	1.51	0.76
7:D:135:VAL:HG21	7:D:139:TYR:CD1	2.20	0.76
12:J:19:MET:HE3	12:J:132:LEU:HD11	1.68	0.76
16:N:37:ARG:HG3	36:N:9307:CL:CL	2.23	0.76
1:0:2534:C:H1'	39:0:4089:HOH:O	1.86	0.75
13:K:107:THR:HG22	13:K:108:GLU:HG3	1.68	0.75
15:M:102:GLU:OE1	15:M:164:THR:HG21	1.86	0.75
1:0:1119:G:N2	1:0:1246:A:C2	2.53	0.75
1:0:1206:U:H6	1:0:1206:U:H5'	1.51	0.75
1:0:871:G:H8	1:0:871:G:H5''	1.49	0.75
1:0:1175:G:H1'	1:0:1193:A:H2'	1.67	0.75
4:A:199:HIS:HD2	4:A:201:PHE:H	1.33	0.75
4:A:191:GLY:HA2	4:A:194:MET:CE	2.17	0.75
4:A:33:GLU:CD	4:A:33:GLU:H	1.89	0.75
6:C:236:THR:CG2	6:C:239:ALA:H	1.99	0.75
1:0:544:G:H2'	1:0:545:G:H5''	1.69	0.75
4:A:153:ARG:HH11	4:A:153:ARG:HB2	1.52	0.75
39:0:6067:HOH:O	5:B:298:LYS:HG2	1.86	0.75
8:E:15:GLN:HG2	8:E:19:ASP:O	1.85	0.75
1:0:871:G:C8	1:0:871:G:C5'	2.69	0.75
5:B:179:LEU:O	5:B:183:GLU:HG2	1.86	0.74
16:N:110:THR:HB	16:N:113:SER:OG	1.87	0.74
16:N:49:THR:HG22	16:N:56:ASP:HB2	1.69	0.74
32:I:99:ASP:OD1	32:I:138:THR:HB	1.88	0.74
9:F:96:ALA:HA	39:F:3111:HOH:O	1.88	0.74
13:K:32:ILE:HD11	13:K:56:SER:HB2	1.69	0.74
14:L:73:VAL:HG23	14:L:74:THR:H	1.52	0.74
27:Y:154:ARG:HH12	27:Y:155:ARG:HG3	1.53	0.74
18:P:59:ARG:NH2	18:P:66:GLN:HE22	1.85	0.74
1:0:1973:A:H5'	1:0:1973:A:H8	1.52	0.74

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:871:G:H8	1:0:871:G:C5'	2.01	0.74
15:M:107:ARG:HH11	15:M:107:ARG:HG3	1.51	0.74
1:0:1159:G:H21	1:0:1189:A:H8	1.36	0.73
25:W:88:THR:HG23	25:W:110:GLN:NE2	2.02	0.73
9:F:46:GLU:OE1	9:F:100:ASP:HA	1.89	0.73
1:0:656:G:C5'	17:O:3:THR:HG22	2.17	0.73
1:0:1667:A:H8	1:0:1667:A:H5'	1.54	0.73
11:H:27:LYS:H	11:H:59:HIS:HD2	1.35	0.73
6:C:107:ARG:NH1	6:C:107:ARG:HB3	2.03	0.73
1:0:2491:G:H1'	39:O:7375:HOH:O	1.88	0.73
1:0:656:G:H5'	17:O:3:THR:CG2	2.17	0.73
25:W:68:THR:HG23	25:W:69:ARG:HG2	1.70	0.73
1:0:2851:G:C2'	1:0:2852:A:H5'	2.18	0.73
1:0:506:G:H22	1:0:509:A:C5'	2.02	0.73
25:W:4:LEU:HD22	25:W:52:VAL:HG21	1.70	0.73
1:0:1299:G:O6	14:L:6:ARG:HD3	1.89	0.72
16:N:80:SER:HB2	39:N:9335:HOH:O	1.89	0.72
21:S:57:THR:HG22	21:S:59:ASP:N	2.02	0.72
22:T:49:GLU:HB3	22:T:59:GLU:HG2	1.70	0.72
1:0:2749:U:H5'	39:O:8471:HOH:O	1.89	0.72
7:D:58:VAL:HG12	7:D:60:GLU:HG2	1.71	0.72
13:K:58:THR:HG22	13:K:59:LYS:HG3	1.70	0.72
1:0:1160:G:C5'	1:0:1161:A:H5'	2.15	0.72
1:0:481:U:H5''	39:O:6188:HOH:O	1.89	0.72
4:A:192:VAL:HG12	4:A:207:GLN:HB3	1.71	0.72
1:0:1118:A:H3'	1:0:1118:A:H8	1.55	0.72
7:D:23:VAL:HG22	7:D:73:VAL:HB	1.70	0.72
1:0:1116:U:O2'	1:0:1118:A:C2	2.41	0.72
5:B:141:ARG:HD2	5:B:163:GLU:OE2	1.90	0.72
2:9:3014:G:H8	2:9:3014:G:H5'	1.55	0.71
4:A:94:LEU:HD12	4:A:98:GLU:HB2	1.71	0.71
27:Y:165:GLU:HB3	39:Y:9394:HOH:O	1.90	0.71
1:0:541:C:H2'	1:0:542:A:H5''	1.72	0.71
11:H:30:GLN:H	11:H:66:ARG:NH1	1.87	0.71
25:W:137:GLN:HE21	25:W:141:HIS:CE1	2.04	0.71
4:A:35:GLY:O	4:A:36:ASP:HB3	1.89	0.71
10:G:12:ILE:N	10:G:13:PRO:HD3	2.06	0.71
1:0:1700:C:H5''	1:0:1701:A:OP2	1.91	0.71
1:0:506:G:H22	1:0:509:A:H5''	1.54	0.71
32:I:110:GLU:HA	32:I:113:HIS:CE1	2.25	0.71
9:F:50:VAL:HG13	9:F:60:VAL:HG11	1.73	0.71

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:74:ARG:NH1	12:J:76:ASP:HB2	2.05	0.71
1:0:541:C:C2'	1:0:542:A:H5''	2.20	0.71
4:A:191:GLY:HA2	4:A:194:MET:HE2	1.71	0.71
9:F:13:GLU:OE2	9:F:78:GLU:HG2	1.90	0.71
20:R:99:ALA:HB1	20:R:109:MET:CE	2.19	0.71
14:L:80:ASP:HB2	14:L:90:ARG:O	1.91	0.71
23:U:17:THR:HG22	23:U:18:GLY:N	2.06	0.71
1:0:1166:A:H1'	1:0:1192:A:C2	2.26	0.70
9:F:53:ASP:OD1	9:F:80:GLN:HB2	1.91	0.70
12:J:45:VAL:HG11	12:J:121:LEU:HD22	1.73	0.70
26:X:71:ARG:HD3	39:X:2171:HOH:O	1.90	0.70
1:0:2716:G:H5''	5:B:206:THR:HG21	1.73	0.70
2:9:3039:U:H1'	2:9:3044:A:N6	2.06	0.70
5:B:268:ARG:NH2	5:B:325:PRO:HG3	2.06	0.70
1:0:2765:C:H4'	39:0:6067:HOH:O	1.92	0.70
18:P:91:LYS:O	18:P:95:GLU:HG3	1.91	0.70
20:R:18:LEU:HB2	20:R:143:VAL:CG1	2.21	0.70
27:Y:189:ASN:HA	27:Y:217:ILE:HD11	1.72	0.70
1:0:2042:U:H1'	39:0:7798:HOH:O	1.90	0.70
1:0:2586:U:H3	1:0:2592:G:H22	1.39	0.70
1:0:949:U:H4'	19:Q:95:GLU:HA	1.72	0.70
4:A:48:ASP:HB3	39:A:9587:HOH:O	1.91	0.70
7:D:23:VAL:HG21	7:D:45:THR:HG21	1.73	0.70
16:N:12:ARG:HD3	16:N:18:THR:OG1	1.92	0.70
1:0:1838:U:O2'	1:0:2644:C:H5'	1.91	0.70
1:0:1979:G:H2'	39:0:3890:HOH:O	1.90	0.70
4:A:192:VAL:CG1	4:A:207:GLN:HB3	2.22	0.70
27:Y:200:THR:HG22	27:Y:201:GLU:HG3	1.72	0.70
1:0:1878:G:H1'	39:0:6649:HOH:O	1.90	0.70
1:0:796:A:HO2'	28:Z:10:ARG:N	1.89	0.70
1:0:470:U:O2'	29:1:16:HIS:HD2	1.75	0.70
6:C:2:GLN:HB3	39:C:9191:HOH:O	1.90	0.70
6:C:194:PHE:CD2	6:C:234:VAL:HG11	2.26	0.70
13:K:109:LEU:HD13	13:K:113:ILE:HD11	1.73	0.70
15:M:69:LYS:O	15:M:73:ARG:NH2	2.25	0.70
1:0:1183:C:N4	1:0:1184:C:H41	1.90	0.70
1:0:2073:G:OP2	1:0:2490:A:H5'	1.92	0.70
12:J:19:MET:HE1	12:J:132:LEU:HD21	1.74	0.70
28:Z:22:SER:O	28:Z:26:VAL:HG23	1.92	0.70
39:0:7927:HOH:O	5:B:211:THR:HG21	1.92	0.69
8:E:20:ILE:CD1	8:E:40:VAL:HG11	2.21	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:141:THR:HG23	39:Y:9389:HOH:O	1.92	0.69
1:0:1118:A:C8	1:0:1118:A:H3'	2.27	0.69
1:0:1206:U:H2'	1:0:1207:A:O4'	1.92	0.69
24:V:39:ALA:N	24:V:40:PRO:HD2	2.08	0.69
5:B:307:ARG:NH1	5:B:307:ARG:HG3	2.02	0.69
6:C:104:ASP:HA	6:C:107:ARG:NH1	2.07	0.69
14:L:148:GLU:HB2	39:L:9485:HOH:O	1.91	0.69
25:W:125:HIS:CD2	25:W:127:GLY:H	2.11	0.69
2:9:3029:C:O3'	7:D:138:GLY:HA2	1.92	0.69
39:0:8484:HOH:O	5:B:2:GLN:HG3	1.91	0.69
16:N:48:VAL:CG1	16:N:55:ASP:HB3	2.23	0.69
1:0:280:C:H2'	1:0:281:U:O4'	1.93	0.69
4:A:51:ARG:HB2	39:A:9587:HOH:O	1.90	0.69
6:C:1:MET:HG2	6:C:2:GLN:N	2.08	0.69
15:M:134:ILE:CG2	15:M:141:ILE:HD13	2.23	0.69
1:0:282:C:H1'	1:0:368:C:N4	2.07	0.69
20:R:18:LEU:HD12	20:R:143:VAL:HG11	1.75	0.69
1:0:2578:G:H5'	1:0:2578:G:H8	1.57	0.69
2:9:3056:A:C2'	2:9:3057:A:H5''	2.23	0.69
5:B:5:ARG:NH1	5:B:8:LYS:HE2	2.08	0.69
8:E:35:TYR:HA	12:J:127:ILE:HD12	1.75	0.69
18:P:9:LEU:O	18:P:13:VAL:HG12	1.93	0.69
1:0:1666:C:H2'	1:0:1667:A:H5'	1.75	0.68
1:0:2468:A:H61	31:3:48:ASN:HD21	1.38	0.68
5:B:201:ASP:HB2	5:B:312:ARG:HD2	1.75	0.68
22:T:9:LYS:HE3	22:T:13:ARG:CZ	2.22	0.68
1:0:2533:C:H5'	1:0:2533:C:H6	1.57	0.68
29:1:18:LYS:HB2	30:2:49:GLU:HG2	1.76	0.68
9:F:37:THR:O	9:F:41:GLU:HG3	1.94	0.68
25:W:81:ASP:OD1	25:W:92:ASP:HB2	1.94	0.68
1:0:1160:G:H5'	1:0:1161:A:C5'	2.19	0.68
5:B:140:LEU:HA	39:B:9576:HOH:O	1.91	0.68
5:B:190:MET:HE2	5:B:194:PHE:HD1	1.57	0.68
26:X:9:VAL:HG22	26:X:88:GLU:OE2	1.94	0.68
17:O:32:ARG:HD3	17:O:32:ARG:O	1.93	0.68
1:0:541:C:H2'	1:0:542:A:C5'	2.23	0.68
1:0:2890:A:H1'	23:U:56:ARG:NH2	2.08	0.68
1:0:93:C:H5''	24:V:1:THR:HB	1.76	0.68
5:B:125:GLU:O	5:B:129:ARG:HG3	1.94	0.68
11:H:166:SER:HB3	11:H:167:PRO:HD3	1.74	0.68
1:0:111:C:O2'	29:1:20:ARG:HG2	1.94	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:81:GLN:HB2	4:A:92:ASN:HD21	1.57	0.68
20:R:39:THR:HB	20:R:42:GLU:HG3	1.74	0.68
25:W:88:THR:HG22	25:W:89:ASP:N	2.09	0.67
4:A:95:PRO:HG2	4:A:98:GLU:HG2	1.75	0.67
9:F:63:ILE:HB	9:F:64:PRO:HD3	1.75	0.67
17:O:32:ARG:NE	17:O:35:LYS:HD2	2.08	0.67
1:0:1474:C:C6	1:0:1474:C:H5'	2.28	0.67
1:0:281:U:H2'	1:0:282:C:O4'	1.94	0.67
6:C:78:ARG:HG3	6:C:78:ARG:HH11	1.59	0.67
32:I:89:SER:HB2	32:I:95:ASP:HB2	1.76	0.67
27:Y:144:ARG:CZ	39:Y:9412:HOH:O	2.42	0.67
1:0:2346:C:O2'	7:D:52:THR:HG21	1.94	0.67
25:W:122:ARG:HH11	25:W:122:ARG:CG	2.08	0.67
6:C:27:ARG:HG3	6:C:29:ASP:OD1	1.95	0.67
8:E:116:THR:HG22	8:E:151:LEU:HD22	1.77	0.67
21:S:10:VAL:HG11	24:V:36:ALA:HA	1.77	0.67
14:L:143:THR:HG22	14:L:144:ASP:N	2.09	0.67
1:0:1209:C:H2'	1:0:1210:G:H8	1.60	0.67
32:I:102:VAL:HG12	32:I:106:LYS:HE3	1.76	0.67
1:0:1184:C:H4'	32:I:126:LYS:HB3	1.77	0.67
9:F:2:VAL:HG22	9:F:57:GLU:OE1	1.95	0.66
1:0:553:G:P	27:Y:204:ARG:HH22	2.18	0.66
11:H:166:SER:CB	11:H:167:PRO:CD	2.73	0.66
12:J:75:PRO:HG2	12:J:105:LEU:HD21	1.76	0.66
1:0:1189:A:H3'	39:O:8231:HOH:O	1.95	0.66
16:N:7:LYS:HE3	19:Q:21:ARG:O	1.94	0.66
28:Z:11:SER:CB	28:Z:23:ARG:HB2	2.25	0.66
13:K:98:VAL:HG13	13:K:102:GLU:HA	1.76	0.66
5:B:102:THR:HG23	5:B:182:VAL:HG12	1.78	0.66
4:A:69:LEU:HD23	4:A:107:ASN:HB2	1.76	0.66
5:B:275:GLY:O	5:B:291:ASP:HA	1.95	0.66
24:V:12:THR:HG22	24:V:15:GLU:CG	2.24	0.66
25:W:21:LEU:HD22	25:W:26:ILE:CD1	2.25	0.66
25:W:80:ASP:O	25:W:84:VAL:HG23	1.94	0.66
1:0:2779:G:H21	8:E:143:GLN:NE2	1.94	0.66
1:0:380:A:OP2	15:M:9:ARG:HD2	1.96	0.66
1:0:657:G:OP1	6:C:27:ARG:NH2	2.26	0.66
29:I:25:LYS:HD2	30:2:49:GLU:N	2.11	0.66
5:B:102:THR:HG21	5:B:182:VAL:O	1.96	0.66
1:0:797:A:C4'	28:Z:10:ARG:N	2.59	0.66
1:0:544:G:C2'	1:0:545:G:H5''	2.25	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3013:A:O2'	2:9:3014:G:H5''	1.95	0.66
8:E:68:HIS:O	8:E:72:MET:HG3	1.94	0.66
15:M:80:GLY:O	15:M:81:ARG:HD2	1.95	0.66
4:A:100:PRO:HG2	4:A:103:VAL:HG21	1.77	0.65
5:B:8:LYS:HG3	5:B:220:VAL:HG12	1.78	0.65
11:H:170:ASN:N	11:H:170:ASN:HD22	1.95	0.65
1:0:871:G:C8	1:0:871:G:H5'	2.30	0.65
1:0:338:C:H4'	6:C:174:ILE:CD1	2.26	0.65
7:D:154:LYS:HD2	7:D:154:LYS:H	1.61	0.65
11:H:3:ALA:HA	11:H:58:ARG:NH1	2.10	0.65
1:0:2363:G:O2'	19:Q:11:ARG:HG3	1.97	0.65
11:H:46:GLN:HE21	11:H:137:TYR:HE2	1.45	0.65
14:L:91:VAL:HG13	14:L:120:LEU:HD23	1.78	0.65
19:Q:25:PRO:HB2	39:Q:4350:HOH:O	1.96	0.65
27:Y:154:ARG:NH1	27:Y:155:ARG:HG3	2.11	0.65
7:D:65:GLU:HA	39:D:6752:HOH:O	1.97	0.65
12:J:93:ARG:NH1	12:J:93:ARG:HB3	2.08	0.65
15:M:183:THR:HG22	15:M:194:ALA:HB1	1.78	0.65
4:A:125:ASN:HB3	4:A:158:VAL:HG12	1.78	0.65
1:0:1244:U:OP1	12:J:18:ILE:HD13	1.97	0.65
16:N:164:ASP:CG	16:N:167:ASP:HA	2.15	0.65
1:0:709:G:O2'	17:O:25:VAL:HG12	1.96	0.65
12:J:19:MET:CE	12:J:132:LEU:HD11	2.26	0.65
1:0:1426:C:H2'	39:O:3209:HOH:O	1.96	0.65
1:0:1641:A:H2'	1:0:1642:A:H5'	1.78	0.65
9:F:58:GLU:OE1	15:M:27:ARG:NH2	2.25	0.65
11:H:56:GLN:HE21	11:H:126:ARG:HE	1.43	0.65
13:K:29:LEU:HB3	13:K:55:VAL:CG1	2.26	0.65
1:0:447:A:P	22:T:1:SER:HB2	2.37	0.65
29:1:25:LYS:HD2	30:2:49:GLU:H	1.60	0.65
5:B:51:VAL:CG2	5:B:327:VAL:HG13	2.26	0.65
9:F:77:VAL:HG21	9:F:83:LEU:HD13	1.77	0.65
22:T:26:THR:HA	22:T:39:ASN:HB3	1.79	0.65
4:A:199:HIS:CD2	4:A:201:PHE:H	2.13	0.64
4:A:66:ARG:HH11	4:A:66:ARG:HB2	1.62	0.64
15:M:107:ARG:NH1	15:M:107:ARG:HG3	2.11	0.64
21:S:51:GLN:NE2	21:S:53:ASN:HD21	1.94	0.64
1:0:1184:C:H1'	39:O:7937:HOH:O	1.95	0.64
7:D:159:PRO:O	7:D:163:VAL:HG23	1.96	0.64
23:U:47:ARG:HG3	39:U:4381:HOH:O	1.97	0.64
24:V:56:ILE:O	24:V:60:GLN:HG3	1.96	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1201:C:H2'	1:0:1202:A:H5'	1.79	0.64
1:0:2718:C:H6	1:0:2718:C:H5'	1.63	0.64
1:0:2661:U:H3	1:0:2812:A:H62	1.44	0.64
23:U:52:THR:HG22	23:U:54:THR:N	2.13	0.64
25:W:13:MET:HE3	25:W:17:ILE:HG22	1.79	0.64
18:P:80:ARG:HG2	18:P:87:ARG:CZ	2.27	0.64
1:0:1205:U:H2'	1:0:1206:U:C5'	2.27	0.64
1:0:2420:G:O2'	1:0:2421:G:H5'	1.97	0.64
1:0:2780:C:H1'	8:E:143:GLN:HE21	1.62	0.64
32:I:105:VAL:HG11	32:I:129:VAL:HG22	1.80	0.64
15:M:187:LEU:CD2	15:M:194:ALA:HB3	2.27	0.64
26:X:37:LEU:CD1	26:X:85:VAL:HG21	2.19	0.64
27:Y:126:PRO:HG2	27:Y:128:PHE:CE1	2.33	0.64
28:Z:17:ARG:HD3	39:Z:9219:HOH:O	1.97	0.64
5:B:62:ARG:HA	5:B:65:MET:CE	2.28	0.64
1:0:962:C:H1'	16:N:5:ARG:HH12	1.63	0.64
16:N:163:PHE:HZ	16:N:171:HIS:HD1	1.44	0.64
22:T:38:ARG:NH1	39:T:6217:HOH:O	2.31	0.64
22:T:71:VAL:HG12	22:T:72:ILE:N	2.13	0.64
25:W:48:VAL:HG12	25:W:48:VAL:O	1.98	0.64
26:X:25:ARG:HD3	26:X:64:ALA:O	1.98	0.64
1:0:1205:U:C2'	1:0:1206:U:H5''	2.27	0.64
8:E:8:PRO:HB2	8:E:11:VAL:HG23	1.80	0.64
25:W:13:MET:CE	25:W:17:ILE:HG22	2.28	0.64
1:0:1119:G:H22	1:0:1246:A:H2	1.40	0.63
11:H:20:ILE:HG23	11:H:120:ILE:HD11	1.80	0.63
11:H:56:GLN:NE2	11:H:126:ARG:HE	1.96	0.63
1:0:2507:G:H2'	1:0:2510:C:H42	1.62	0.63
1:0:1666:C:O2'	1:0:1667:A:H5''	1.98	0.63
1:0:2896:A:N3	1:0:2896:A:H2'	2.14	0.63
6:C:129:HIS:CE1	6:C:231:ARG:HA	2.34	0.63
6:C:139:VAL:HG13	39:C:9254:HOH:O	1.98	0.63
9:F:12:LEU:HD21	9:F:111:ILE:HG23	1.79	0.63
13:K:74:VAL:CG1	13:K:113:ILE:HG12	2.26	0.63
16:N:132:ASN:O	16:N:135:VAL:HG12	1.97	0.63
15:M:164:THR:HG22	15:M:166:ALA:N	2.11	0.63
1:0:1687:C:O2	29:I:9:GLY:HA2	1.99	0.63
1:0:2748:G:H2'	39:O:8049:HOH:O	1.99	0.63
32:I:125:ALA:O	32:I:129:VAL:HG23	1.99	0.63
1:0:1168:C:H5''	32:I:87:THR:HG23	1.81	0.63
16:N:23:ARG:HH11	16:N:23:ARG:HG2	1.63	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:59:HIS:HA	11:H:62:LEU:HD23	1.79	0.63
1:O:1182:C:H1'	1:O:1192:A:H8	1.63	0.63
1:O:1563:G:H4'	39:O:4808:HOH:O	1.98	0.63
14:L:40:PHE:HB3	39:L:9458:HOH:O	1.99	0.63
27:Y:144:ARG:HH11	27:Y:144:ARG:HG3	1.63	0.63
30:2:22:PRO:HG2	30:2:25:VAL:CG2	2.29	0.63
4:A:88:ILE:HD13	4:A:100:PRO:HD3	1.81	0.63
17:O:32:ARG:HE	17:O:35:LYS:HD2	1.62	0.63
1:O:1766:U:O2	1:O:1778:A:H5'	1.99	0.63
5:B:254:GLN:HG2	5:B:255:GLY:N	2.13	0.63
20:R:106:GLY:HA2	20:R:109:MET:HE3	1.80	0.63
5:B:102:THR:CG2	5:B:182:VAL:HG12	2.29	0.62
16:N:164:ASP:OD1	16:N:167:ASP:HA	1.99	0.62
1:O:1377:C:H5'	1:O:1377:C:C6	2.30	0.62
7:D:138:GLY:N	39:D:7597:HOH:O	2.32	0.62
15:M:79:ALA:HB3	15:M:81:ARG:NH1	2.14	0.62
6:C:236:THR:HG21	39:C:9180:HOH:O	1.98	0.62
18:P:10:ALA:HA	18:P:13:VAL:CG1	2.29	0.62
1:O:2878:U:H2'	1:O:2879:A:O4'	1.99	0.62
31:3:25:VAL:HG22	31:3:68:LYS:HG3	1.82	0.62
11:H:27:LYS:N	11:H:59:HIS:HD2	1.98	0.62
24:V:56:ILE:HG22	24:V:60:GLN:HE21	1.63	0.62
5:B:212:GLN:HB2	5:B:257:THR:CG2	2.26	0.62
1:O:1116:U:H3	1:O:1246:A:H62	1.47	0.62
5:B:18:ARG:HG3	5:B:256:GLN:HG3	1.80	0.62
7:D:58:VAL:CG1	7:D:60:GLU:HG2	2.29	0.62
12:J:74:ARG:NH1	12:J:105:LEU:HD11	2.14	0.62
11:H:154:TYR:HB2	39:H:9555:HOH:O	1.99	0.62
11:H:166:SER:CB	11:H:167:PRO:HD3	2.30	0.62
7:D:170:TYR:O	7:D:171:ASP:HB3	1.99	0.62
26:X:76:ARG:HH11	26:X:76:ARG:HG3	1.63	0.62
2:9:3020:G:O2'	2:9:3021:G:H5'	1.99	0.62
18:P:59:ARG:HH22	18:P:66:GLN:HE22	1.48	0.61
27:Y:144:ARG:HH11	27:Y:144:ARG:CG	2.11	0.61
1:O:282:C:O2'	1:O:283:U:H5'	2.00	0.61
5:B:215:VAL:HB	5:B:234:ARG:HH12	1.65	0.61
32:I:92:PRO:C	32:I:94:GLU:H	2.02	0.61
16:N:143:ARG:HH21	16:N:169:PRO:HB2	1.65	0.61
16:N:179:LEU:HD23	16:N:184:ILE:HD12	1.82	0.61
24:V:43:PRO:O	24:V:46:ILE:HG22	2.00	0.61
1:O:396:U:O2'	1:O:418:C:H4'	2.00	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:121:ALA:O	4:A:124:VAL:HG22	2.01	0.61
9:F:50:VAL:CG1	9:F:60:VAL:HG11	2.29	0.61
1:O:902:G:N7	14:L:18:HIS:HD2	1.98	0.61
20:R:18:LEU:HB2	20:R:143:VAL:HG12	1.81	0.61
1:O:2502:C:H2'	1:O:2503:A:H5'	1.82	0.61
32:I:110:GLU:HA	32:I:113:HIS:NE2	2.16	0.61
13:K:81:ARG:HD3	13:K:87:ARG:NH1	2.15	0.61
16:N:86:LEU:HD21	16:N:180:LEU:CD1	2.31	0.61
22:T:115:GLU:HG3	22:T:116:ASP:N	2.16	0.61
23:U:17:THR:CG2	23:U:18:GLY:N	2.64	0.61
24:V:64:GLY:O	24:V:65:ASP:HB2	2.00	0.61
25:W:84:VAL:HG12	39:W:6679:HOH:O	2.00	0.61
1:O:1118:A:H62	1:O:1244:U:H3	1.47	0.61
1:O:156:C:H5''	15:M:171:ARG:CD	2.27	0.61
1:O:1701:A:H4'	1:O:1702:U:C5'	2.31	0.61
11:H:3:ALA:HA	11:H:58:ARG:HH12	1.65	0.61
32:I:102:VAL:O	32:I:106:LYS:HG3	2.00	0.61
24:V:39:ALA:C	24:V:41:GLU:H	2.03	0.61
25:W:52:VAL:HG22	25:W:53:ALA:H	1.64	0.61
6:C:107:ARG:NE	39:C:9264:HOH:O	2.31	0.61
14:L:133:VAL:HA	39:L:9470:HOH:O	2.01	0.61
1:O:164:G:H4'	14:L:30:ARG:HD3	1.82	0.61
22:T:71:VAL:CG1	22:T:90:PRO:HB3	2.24	0.61
1:O:2769:C:H2'	1:O:2770:G:O4'	1.99	0.60
12:J:74:ARG:HB3	12:J:74:ARG:HH11	1.64	0.60
22:T:48:VAL:HG22	22:T:96:VAL:HG22	1.82	0.60
1:O:2064:U:H5'	1:O:2652:U:H4'	1.82	0.60
5:B:5:ARG:HH11	5:B:8:LYS:HE2	1.65	0.60
25:W:130:HIS:O	25:W:136:GLY:HA3	2.01	0.60
1:O:1528:A:H2'	1:O:1529:G:O4'	2.02	0.60
1:O:2851:G:H2'	1:O:2852:A:H5'	1.82	0.60
1:O:621:C:H5'	27:Y:132:ASP:OD2	2.02	0.60
5:B:71:VAL:HG11	5:B:296:LEU:HD22	1.82	0.60
6:C:16:VAL:HG12	6:C:17:ASP:H	1.65	0.60
32:I:138:THR:HG22	32:I:139:ILE:H	1.65	0.60
15:M:31:TRP:HA	15:M:34:GLU:HG3	1.83	0.60
16:N:110:THR:HB	16:N:113:SER:HG	1.64	0.60
29:1:10:LYS:HG3	39:1:9488:HOH:O	2.00	0.60
6:C:118:THR:O	6:C:136:VAL:HG13	2.00	0.60
27:Y:189:ASN:HD22	27:Y:189:ASN:C	2.04	0.60
6:C:236:THR:HA	39:C:9257:HOH:O	2.00	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:681:G:N3	1:0:681:G:H5'	2.17	0.60
4:A:125:ASN:CB	4:A:158:VAL:HG12	2.31	0.60
5:B:16:ARG:NH1	39:B:9615:HOH:O	2.33	0.60
7:D:25:MET:SD	7:D:40:ILE:HD11	2.42	0.60
12:J:74:ARG:HH12	12:J:76:ASP:HB2	1.65	0.60
25:W:88:THR:HG22	25:W:90:TYR:HD1	1.66	0.60
1:0:1201:C:H5''	39:0:6761:HOH:O	2.02	0.60
2:9:3029:C:H2'	2:9:3030:C:H5'	1.83	0.60
12:J:131:THR:HG22	12:J:134:GLU:H	1.65	0.60
1:0:2748:G:H5'	39:0:8049:HOH:O	2.00	0.60
30:2:22:PRO:HG2	30:2:25:VAL:HG23	1.84	0.60
11:H:166:SER:HB2	11:H:167:PRO:CD	2.32	0.60
12:J:93:ARG:HH11	12:J:93:ARG:CB	2.07	0.60
16:N:61:ALA:HB3	16:N:88:ALA:HB2	1.84	0.60
27:Y:187:VAL:HG12	27:Y:205:ILE:HA	1.83	0.60
31:3:18:GLN:OE1	31:3:73:GLU:HB3	2.02	0.60
2:9:3014:G:C8	2:9:3014:G:H5'	2.35	0.60
18:P:40:VAL:O	18:P:44:VAL:HG23	2.01	0.60
1:0:1555:G:H4'	1:0:1630:A:H2	1.67	0.60
1:0:2291:A:C8	1:0:2309:C:H5'	2.37	0.60
1:0:960:G:H4'	39:0:7904:HOH:O	2.00	0.60
32:I:134:SER:O	32:I:135:LEU:HD23	2.02	0.60
1:0:2502:C:C2'	1:0:2503:A:H5'	2.32	0.59
1:0:272:A:H5'	1:0:273:G:OP2	2.02	0.59
1:0:380:A:H2'	39:0:7718:HOH:O	2.01	0.59
6:C:140:VAL:HB	39:C:9257:HOH:O	2.01	0.59
17:O:32:ARG:HH21	17:O:35:LYS:HZ1	1.50	0.59
1:0:263:U:O4'	9:F:59:ILE:HD13	2.02	0.59
32:I:78:LEU:HD12	32:I:112:LYS:NZ	2.16	0.59
12:J:74:ARG:O	12:J:78:ILE:HG12	2.02	0.59
14:L:35:ARG:HB2	14:L:35:ARG:HH11	1.67	0.59
16:N:139:TRP:HA	16:N:139:TRP:CE3	2.37	0.59
20:R:111:ILE:HG23	20:R:145:LEU:HD11	1.84	0.59
28:Z:37:HIS:HB2	28:Z:47:VAL:HB	1.83	0.59
5:B:297:VAL:HB	39:B:9604:HOH:O	2.01	0.59
5:B:85:ARG:NH1	39:B:9633:HOH:O	2.35	0.59
9:F:91:VAL:CG1	9:F:92:GLY:H	2.08	0.59
17:O:42:GLU:HB2	39:O:2176:HOH:O	2.02	0.59
1:0:834:G:H4'	1:0:835:U:OP2	2.03	0.59
15:M:77:HIS:HD2	15:M:79:ALA:O	1.85	0.59
16:N:62:HIS:HB3	16:N:65:ASP:OD1	2.02	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:542:A:H5'	1:0:542:A:C8	2.28	0.59
5:B:96:PRO:HG3	39:B:9633:HOH:O	2.00	0.59
7:D:136:ARG:HH12	7:D:157:LEU:HA	1.65	0.59
14:L:73:VAL:HG23	14:L:74:THR:N	2.17	0.59
16:N:176:ARG:HG3	16:N:180:LEU:HD13	1.84	0.59
1:0:2100:A:H4'	6:C:64:GLY:O	2.02	0.59
16:N:154:LEU:O	16:N:155:GLU:HB3	2.03	0.59
24:V:1:THR:HG23	24:V:2:VAL:N	2.16	0.59
1:0:2003:U:H4'	1:0:2004:U:H5	1.68	0.59
1:0:2795:C:O2'	1:0:2796:U:H5'	2.03	0.59
32:I:113:HIS:N	32:I:114:PRO:HD2	2.18	0.59
13:K:98:VAL:CG1	13:K:102:GLU:HA	2.33	0.59
25:W:88:THR:HG23	25:W:110:GLN:HE21	1.68	0.59
1:0:516:A:H5'	39:0:6188:HOH:O	2.03	0.59
20:R:111:ILE:HG23	20:R:145:LEU:CD1	2.33	0.59
1:0:316:A:N3	1:0:336:G:O2'	2.35	0.59
1:0:870:G:H2'	1:0:871:G:H5''	1.85	0.59
39:0:9698:HOH:O	5:B:214:PRO:HD2	2.03	0.59
1:0:2721:U:H4'	13:K:87:ARG:HG3	1.84	0.59
1:0:1328:A:OP1	27:Y:169:ARG:HD2	2.02	0.59
1:0:1819:G:H2'	1:0:1820:G:H4'	1.84	0.59
1:0:2851:G:O2'	1:0:2852:A:H5'	2.03	0.59
1:0:2676:C:H4'	12:J:70:PHE:CD1	2.38	0.59
14:L:35:ARG:HB2	14:L:35:ARG:NH1	2.18	0.59
21:S:51:GLN:HE21	21:S:53:ASN:ND2	1.95	0.59
23:U:14:GLU:OE1	23:U:15:PRO:HD2	2.03	0.59
39:0:9972:HOH:O	29:1:1:THR:HA	2.03	0.58
5:B:88:GLU:HB3	5:B:97:LEU:HD12	1.84	0.58
9:F:46:GLU:O	9:F:73:PRO:HD2	2.03	0.58
13:K:23:ASN:HD21	13:K:107:THR:HB	1.68	0.58
9:F:58:GLU:CD	15:M:27:ARG:HH22	2.05	0.58
1:0:2505:G:O2'	1:0:2506:A:H5'	2.04	0.58
4:A:33:GLU:O	4:A:34:ASP:HB2	2.03	0.58
16:N:69:TYR:HE2	16:N:184:ILE:HG13	1.67	0.58
1:0:545:G:C8	1:0:545:G:H5'	2.35	0.58
7:D:59:GLY:O	7:D:61:PHE:N	2.36	0.58
17:O:53:GLN:HG2	17:O:56:GLU:OE1	2.03	0.58
15:M:68:ARG:NH2	15:M:73:ARG:HD3	2.18	0.58
39:0:3154:HOH:O	18:P:81:LYS:HG2	2.03	0.58
1:0:20:G:H21	20:R:117:HIS:HD2	1.48	0.58
24:V:39:ALA:N	24:V:40:PRO:CD	2.66	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:X:12:ILE:HD12	26:X:36:HIS:ND1	2.19	0.58
1:0:2676:C:H4'	12:J:70:PHE:CE1	2.39	0.58
1:0:289:G:N2	1:0:363:A:H2	1.96	0.58
1:0:877:G:H5'	1:0:878:G:OP1	2.03	0.58
1:0:969:G:H1	1:0:999:C:H42	1.49	0.58
11:H:63:GLU:HA	39:H:9544:HOH:O	2.03	0.58
14:L:143:THR:HG22	14:L:144:ASP:H	1.68	0.58
20:R:18:LEU:HD12	20:R:143:VAL:CG1	2.32	0.58
1:0:2426:G:H1'	39:0:6621:HOH:O	2.03	0.58
1:0:625:U:H5'	39:0:3784:HOH:O	2.04	0.58
4:A:57:ALA:HB1	4:A:65:ARG:HE	1.69	0.58
11:H:111:ASP:HA	39:H:9510:HOH:O	2.02	0.58
1:0:2081:A:H4'	12:J:69:TYR:CE1	2.39	0.58
16:N:169:PRO:O	16:N:172:PHE:HB3	2.03	0.58
22:T:112:LEU:CD2	22:T:119:ALA:HB3	2.33	0.58
1:0:2726:U:O2'	26:X:22:ASN:ND2	2.37	0.58
1:0:558:C:C2'	1:0:559:U:H5''	2.34	0.58
26:X:71:ARG:HB3	26:X:88:GLU:OE1	2.03	0.58
5:B:238:ASN:ND2	5:B:240:GLY:H	1.95	0.58
6:C:236:THR:H	6:C:239:ALA:HB3	1.68	0.58
8:E:20:ILE:HD12	8:E:33:LEU:HD12	1.86	0.58
10:G:20:VAL:O	10:G:24:VAL:HG23	2.03	0.58
20:R:96:VAL:HG13	20:R:106:GLY:HA3	1.86	0.58
21:S:73:ASP:OD1	21:S:76:GLU:HG3	2.04	0.58
14:L:104:ASP:HB2	39:L:9460:HOH:O	2.03	0.58
25:W:21:LEU:HB3	25:W:26:ILE:HG12	1.85	0.58
1:0:1352:A:O2'	1:0:1353:C:OP1	2.20	0.58
5:B:238:ASN:HD22	5:B:240:GLY:N	1.95	0.58
1:0:1181:A:H5'	32:I:94:GLU:OE2	2.04	0.58
1:0:1384:C:H5'	26:X:30:MET:HG2	1.85	0.57
4:A:26:ASP:O	4:A:28:GLU:N	2.36	0.57
5:B:221:GLN:HE22	13:K:42:ASN:HD22	1.51	0.57
1:0:1268:C:O2'	27:Y:169:ARG:HB2	2.04	0.57
1:0:447:A:OP2	22:T:1:SER:HB2	2.04	0.57
1:0:558:C:O2'	1:0:559:U:H5''	2.04	0.57
17:O:57:THR:O	17:O:111:VAL:HG23	2.03	0.57
22:T:49:GLU:OE2	22:T:97:ARG:HD2	2.04	0.57
24:V:20:LEU:HD22	24:V:60:GLN:HE22	1.69	0.57
24:V:55:ARG:O	24:V:59:ILE:HG12	2.04	0.57
39:0:9983:HOH:O	4:A:180:LYS:HG2	2.04	0.57
5:B:190:MET:HE2	5:B:194:PHE:CD1	2.39	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:195:ARG:HG2	5:B:323:LEU:HD22	1.86	0.57
32:I:78:LEU:HD12	32:I:112:LYS:HZ2	1.68	0.57
16:N:170:GLU:O	16:N:174:GLU:HG3	2.04	0.57
22:T:112:LEU:HD23	22:T:119:ALA:HB3	1.86	0.57
26:X:31:ILE:O	26:X:35:GLU:HG3	2.05	0.57
27:Y:112:GLU:OE2	27:Y:115:ARG:NH1	2.37	0.57
1:O:1552:G:N2	1:O:1634:G:H1'	2.19	0.57
1:O:2726:U:O2	1:O:2749:U:O5'	2.22	0.57
5:B:185:GLY:HA2	39:B:9632:HOH:O	2.04	0.57
7:D:172:VAL:HG12	7:D:173:GLU:N	2.18	0.57
9:F:21:GLU:O	9:F:24:ARG:HG3	2.05	0.57
14:L:67:ARG:O	14:L:71:GLU:HG3	2.04	0.57
27:Y:203:VAL:CG1	27:Y:228:VAL:HG22	2.35	0.57
1:O:1066:U:H2'	1:O:1067:A:C8	2.40	0.57
1:O:2421:G:H1'	39:O:4289:HOH:O	2.03	0.57
1:O:558:C:H2'	1:O:559:U:C5'	2.34	0.57
31:3:3:MET:HB2	31:3:88:LEU:HD11	1.85	0.57
31:3:62:THR:HB	39:3:9482:HOH:O	2.04	0.57
1:O:1943:C:H4'	4:A:211:LYS:O	2.05	0.57
6:C:236:THR:HG22	6:C:239:ALA:CB	2.34	0.57
14:L:136:ALA:HB3	39:L:9470:HOH:O	2.03	0.57
1:O:1189:A:O2'	1:O:1208:C:H2'	2.04	0.57
1:O:538:C:OP2	27:Y:134:HIS:HE1	1.88	0.57
2:9:3069:U:OP1	16:N:4:PRO:HG3	2.05	0.57
15:M:164:THR:CG2	15:M:165:GLY:N	2.68	0.57
16:N:139:TRP:HA	16:N:139:TRP:HE3	1.70	0.57
1:O:308:U:H5'	22:T:97:ARG:NH2	2.19	0.57
1:O:1218:U:H2'	1:O:1219:U:C6	2.40	0.57
1:O:871:G:C8	1:O:871:G:H5''	2.34	0.57
10:G:12:ILE:N	10:G:13:PRO:CD	2.68	0.57
14:L:36:ASP:HB2	39:L:9433:HOH:O	2.05	0.57
1:O:256:C:H2'	1:O:257:G:O4'	2.05	0.57
12:J:39:VAL:HG13	12:J:106:GLY:O	2.05	0.57
7:D:146:LYS:NZ	16:N:107:ASN:HD21	2.02	0.57
39:9:4707:HOH:O	16:N:147:ILE:HD12	2.05	0.57
17:O:39:THR:O	17:O:115:ARG:NH2	2.37	0.57
1:O:138:U:H5''	1:O:139:C:OP2	2.04	0.56
1:O:2270:G:H4'	4:A:223:ARG:HH12	1.70	0.56
4:A:107:ASN:OD1	4:A:120:ARG:HD2	2.04	0.56
4:A:33:GLU:CD	4:A:33:GLU:N	2.57	0.56
6:C:214:THR:HG23	39:C:9242:HOH:O	2.03	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:244:C:OP2	9:F:38:LYS:HE3	2.05	0.56
9:F:39:SER:HB3	9:F:45:ALA:HB2	1.85	0.56
18:P:16:VAL:HG12	18:P:17:GLY:N	2.20	0.56
21:S:77:VAL:O	21:S:80:ARG:HG2	2.05	0.56
2:9:3002:U:OP2	2:9:3003:A:H5'	2.06	0.56
7:D:54:ALA:HB2	7:D:69:ILE:HD12	1.87	0.56
8:E:34:TRP:O	12:J:127:ILE:HD11	2.05	0.56
26:X:21:PRO:HG2	26:X:24:LYS:HD3	1.85	0.56
1:O:1634:G:H3'	39:O:4478:HOH:O	2.05	0.56
1:O:2563:U:H2'	1:O:2565:C:O5'	2.05	0.56
6:C:194:PHE:HA	6:C:234:VAL:HG13	1.86	0.56
13:K:55:VAL:HG12	13:K:56:SER:N	2.19	0.56
15:M:182:LYS:O	15:M:194:ALA:HB2	2.06	0.56
1:O:775:G:OP1	29:I:16:HIS:HE1	1.89	0.56
5:B:145:HIS:HD2	5:B:146:THR:O	1.89	0.56
15:M:60:VAL:C	15:M:61:ILE:HD12	2.25	0.56
9:F:1:PRO:H3	9:F:4:VAL:HG23	1.71	0.56
11:H:148:GLU:HA	11:H:148:GLU:OE1	2.05	0.56
11:H:56:GLN:HE22	11:H:93:GLN:HG2	1.70	0.56
25:W:65:VAL:HA	25:W:68:THR:HG22	1.87	0.56
1:O:2064:U:H5'	1:O:2652:U:O3'	2.05	0.56
5:B:51:VAL:HG23	5:B:329:TYR:O	2.06	0.56
2:9:3014:G:O2'	16:N:1:ALA:HB2	2.05	0.56
25:W:88:THR:HG22	25:W:89:ASP:H	1.69	0.56
1:O:151:A:H2'	1:O:152:A:O4'	2.05	0.56
1:O:2032:U:H2'	1:O:2033:G:C5'	2.35	0.56
1:O:432:G:O2'	1:O:433:C:H5'	2.06	0.56
23:U:5:GLU:HG2	23:U:10:GLY:O	2.05	0.56
5:B:264:GLU:OE2	5:B:302:PRO:HD3	2.05	0.56
6:C:154:VAL:O	6:C:158:GLU:HG3	2.06	0.56
11:H:38:LYS:HE2	11:H:42:ASP:HB2	1.88	0.56
1:O:185:G:H4'	1:O:186:A:H4'	1.87	0.56
12:J:107:ASN:HD22	12:J:109:TYR:H	1.53	0.56
22:T:49:GLU:CB	22:T:59:GLU:HG2	2.34	0.56
25:W:4:LEU:HD11	25:W:45:VAL:HG12	1.87	0.56
26:X:25:ARG:HG2	39:X:5356:HOH:O	2.06	0.56
1:O:1118:A:H8	1:O:1119:G:H5''	1.71	0.56
1:O:1187:U:O2'	1:O:1189:A:H2	1.89	0.56
1:O:316:A:H5'	22:T:54:ASP:OD2	2.03	0.56
7:D:54:ALA:CB	7:D:69:ILE:HD12	2.35	0.56
1:O:2694:A:H4'	8:E:91:PHE:HE1	1.70	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:24:VAL:O	10:G:28:GLU:HB2	2.05	0.56
32:I:138:THR:HG22	32:I:139:ILE:N	2.20	0.56
12:J:75:PRO:HG2	12:J:105:LEU:CD2	2.35	0.56
23:U:39:ASN:ND2	23:U:44:ARG:HH11	2.03	0.56
1:O:558:C:H2'	1:O:559:U:H5'	1.88	0.56
6:C:162:VAL:HG22	6:C:232:LEU:HD21	1.88	0.56
39:O:9738:HOH:O	15:M:82:ARG:HD2	2.06	0.56
39:9:1361:HOH:O	16:N:41:LYS:HE3	2.05	0.56
4:A:135:VAL:HG11	4:A:147:ARG:NH1	2.21	0.55
10:G:67:LEU:O	10:G:71:LEU:HG	2.05	0.55
12:J:107:ASN:ND2	12:J:109:TYR:H	2.04	0.55
25:W:108:ARG:HG3	25:W:114:PRO:HG3	1.88	0.55
28:Z:30:GLU:HA	28:Z:33:MET:HE3	1.88	0.55
1:O:1736:A:H1'	39:O:8143:HOH:O	2.07	0.55
2:9:3076:G:C3'	2:9:3077:A:H5''	2.27	0.55
5:B:53:LEU:CD1	5:B:327:VAL:HG22	2.36	0.55
9:F:58:GLU:HA	9:F:61:MET:HE2	1.88	0.55
26:X:61:ARG:HB2	26:X:65:ASN:HB2	1.87	0.55
1:O:1926:G:H2'	1:O:1927:A:C8	2.41	0.55
4:A:36:ASP:OD2	4:A:85:SER:HB2	2.06	0.55
30:2:49:GLU:HB2	39:2:131:HOH:O	2.06	0.55
4:A:89:ALA:HB3	39:A:9608:HOH:O	2.05	0.55
9:F:48:VAL:HG23	9:F:74:PHE:CB	2.36	0.55
1:O:1778:A:H2'	1:O:1779:A:H5'	1.88	0.55
1:O:2456:A:H2'	1:O:2457:U:C6	2.42	0.55
1:O:291:C:H2'	1:O:292:G:O4'	2.06	0.55
5:B:305:ASP:O	5:B:306:LYS:HB2	2.07	0.55
13:K:4:LEU:CD2	13:K:116:GLU:HB3	2.35	0.55
1:O:475:G:H5'	6:C:73:LEU:HD23	1.87	0.55
15:M:71:SER:HB2	15:M:92:THR:HG22	1.89	0.55
5:B:329:TYR:CE2	23:U:15:PRO:HG2	2.41	0.55
4:A:123:GLY:HA3	4:A:162:GLY:HA2	1.87	0.55
10:G:12:ILE:HD12	39:G:692:HOH:O	2.06	0.55
12:J:75:PRO:HD3	12:J:136:SER:OG	2.05	0.55
14:L:57:VAL:HG12	14:L:57:VAL:O	2.07	0.55
16:N:11:ARG:HG3	16:N:14:ARG:NH1	2.21	0.55
25:W:21:LEU:HD22	25:W:26:ILE:HD11	1.88	0.55
1:O:1789:G:O6	18:P:73:HIS:HE1	1.89	0.55
1:O:1973:A:H5'	1:O:1973:A:C8	2.39	0.55
1:O:960:G:H2'	1:O:960:G:N3	2.21	0.55
6:C:246:ARG:NH1	6:C:246:ARG:HB3	2.22	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:106:THR:HG23	27:Y:107:PRO:HD2	1.88	0.55
27:Y:154:ARG:HH12	27:Y:155:ARG:CG	2.17	0.55
1:0:625:U:H5''	1:0:1044:C:N4	2.21	0.55
1:0:441:A:H1'	1:0:442:A:N7	2.21	0.55
4:A:194:MET:HE1	4:A:199:HIS:HB2	1.88	0.55
8:E:20:ILE:CD1	8:E:33:LEU:HD12	2.37	0.55
17:O:14:LEU:CD2	17:O:102:ILE:HD11	2.37	0.55
22:T:32:ARG:NH1	22:T:38:ARG:HH12	2.05	0.55
27:Y:189:ASN:ND2	27:Y:192:ASP:H	2.05	0.55
39:O:8105:HOH:O	31:3:60:LYS:HG3	2.06	0.55
2:9:3051:A:H5'	16:N:160:SER:HB3	1.89	0.55
4:A:191:GLY:HA2	4:A:194:MET:HE3	1.89	0.55
7:D:135:VAL:HG22	7:D:136:ARG:H	1.72	0.55
1:0:1882:C:OP1	4:A:192:VAL:HG23	2.07	0.54
5:B:307:ARG:HB3	39:B:9650:HOH:O	2.06	0.54
1:0:1183:C:H2'	39:O:6772:HOH:O	2.07	0.54
5:B:258:GLY:H	5:B:260:HIS:CE1	2.25	0.54
15:M:68:ARG:HD3	15:M:68:ARG:O	2.08	0.54
1:0:2769:C:O2'	1:0:2770:G:H5'	2.07	0.54
1:0:2827:A:H2'	1:0:2828:G:O4'	2.06	0.54
1:0:2866:U:H4'	1:0:2867:G:H5'	1.89	0.54
31:3:42:ARG:HH11	31:3:42:ARG:HG3	1.72	0.54
9:F:60:VAL:HG12	9:F:60:VAL:O	2.06	0.54
16:N:11:ARG:O	16:N:15:GLU:HG3	2.07	0.54
2:9:3051:A:H5'	16:N:160:SER:CB	2.37	0.54
22:T:78:THR:HB	22:T:87:VAL:O	2.08	0.54
1:0:1189:A:H1'	1:0:1209:C:O4'	2.07	0.54
7:D:24:HIS:HB2	7:D:72:LYS:CB	2.37	0.54
32:I:139:ILE:HG22	32:I:140:GLU:N	2.23	0.54
16:N:115:VAL:HG22	39:N:9356:HOH:O	2.07	0.54
1:0:2591:C:H2'	1:0:2592:G:O4'	2.07	0.54
12:J:107:ASN:HD22	12:J:107:ASN:C	2.11	0.54
1:0:2533:C:C6	1:0:2533:C:H5'	2.42	0.54
4:A:153:ARG:CB	4:A:153:ARG:HH11	2.21	0.54
11:H:21:THR:O	11:H:120:ILE:HD12	2.08	0.54
16:N:154:LEU:HG	16:N:155:GLU:H	1.71	0.54
1:0:1626:A:H2'	1:0:1627:G:O4'	2.08	0.54
1:0:1681:G:H5''	1:0:1682:A:H5'	1.89	0.54
1:0:1878:G:O2'	1:0:1879:U:OP2	2.25	0.54
1:0:797:A:H4'	28:Z:10:ARG:N	2.22	0.54
5:B:40:GLY:HA3	39:B:9645:HOH:O	2.08	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:72:THR:HB	39:B:9604:HOH:O	2.07	0.54
1:O:474:C:O3'	6:C:73:LEU:HD21	2.07	0.54
23:U:14:GLU:O	23:U:17:THR:HB	2.08	0.54
26:X:43:VAL:HG12	26:X:44:ASP:N	2.23	0.54
1:O:1350:U:H2'	1:O:1351:G:O4'	2.07	0.54
1:O:1666:C:H2'	1:O:1667:A:C5'	2.36	0.54
1:O:2670:G:O2'	1:O:2671:U:H5'	2.08	0.54
1:O:2717:C:O2'	1:O:2718:C:H5''	2.07	0.54
1:O:2769:C:C2'	1:O:2770:G:H5'	2.38	0.54
7:D:50:VAL:O	7:D:71:ALA:HA	2.07	0.54
28:Z:72:GLU:OE1	28:Z:77:LYS:HE2	2.07	0.54
1:O:1209:C:H2'	1:O:1210:G:C8	2.42	0.54
4:A:190:ARG:NH2	4:A:207:GLN:OE1	2.40	0.54
11:H:46:GLN:NE2	11:H:137:TYR:HE2	2.05	0.54
1:O:1595:G:O2'	1:O:1596:U:H5'	2.08	0.54
31:3:60:LYS:HG3	31:3:61:PRO:HD2	1.88	0.54
5:B:254:GLN:HG3	39:B:9530:HOH:O	2.08	0.54
5:B:62:ARG:HA	5:B:65:MET:HE2	1.90	0.54
12:J:8:ALA:HA	12:J:35:THR:HG22	1.90	0.54
17:O:59:VAL:HG23	17:O:111:VAL:CG2	2.37	0.54
22:T:12:ARG:NH1	39:T:3035:HOH:O	2.40	0.54
25:W:4:LEU:O	25:W:32:CYS:HA	2.08	0.54
27:Y:99:ALA:HB2	27:Y:233:TYR:CE2	2.42	0.54
1:O:1406:A:H4'	1:O:1407:A:H5''	1.90	0.53
1:O:1625:U:H4'	39:O:5232:HOH:O	2.08	0.53
1:O:2817:G:P	39:O:8476:HOH:O	2.66	0.53
5:B:17:LYS:O	5:B:260:HIS:HD2	1.91	0.53
5:B:56:ASP:OD1	5:B:322:ARG:HB3	2.08	0.53
15:M:59:GLY:HA3	15:M:141:ILE:HD12	1.89	0.53
25:W:21:LEU:HD13	25:W:26:ILE:HD11	1.90	0.53
1:O:949:U:O2'	19:Q:40:HIS:HE1	1.91	0.53
1:O:1594:C:OP2	18:P:120:ARG:HD2	2.08	0.53
23:U:49:LEU:HG	39:U:3805:HOH:O	2.07	0.53
1:O:2265:U:H2'	1:O:2266:A:C8	2.43	0.53
5:B:195:ARG:HD2	5:B:324:ASP:OD1	2.07	0.53
6:C:107:ARG:HH11	6:C:107:ARG:HB3	1.71	0.53
39:O:7381:HOH:O	15:M:178:LYS:HB2	2.07	0.53
1:O:2645:U:OP2	1:O:2645:U:C6	2.61	0.53
1:O:2894:C:O2'	1:O:2895:C:H5'	2.08	0.53
31:3:3:MET:O	31:3:90:PHE:HA	2.09	0.53
5:B:51:VAL:HG23	5:B:327:VAL:HG13	1.90	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:78:ARG:HG3	6:C:78:ARG:NH1	2.21	0.53
1:O:2694:A:H4'	8:E:91:PHE:CE1	2.44	0.53
30:2:18:ASN:ND2	30:2:40:ARG:H	2.06	0.53
7:D:172:VAL:HG12	7:D:173:GLU:H	1.74	0.53
7:D:92:GLU:HB2	39:D:3862:HOH:O	2.07	0.53
12:J:47:THR:HG22	12:J:48:GLY:N	2.23	0.53
24:V:42:ASN:HB3	39:V:7247:HOH:O	2.08	0.53
1:O:1419:U:H2'	1:O:1685:A:C2	2.43	0.53
31:3:65:THR:HG23	31:3:88:LEU:HD22	1.91	0.53
5:B:51:VAL:HG22	5:B:53:LEU:HD13	1.90	0.53
6:C:25:PRO:HG2	39:C:9126:HOH:O	2.08	0.53
1:O:1168:C:H5''	32:I:87:THR:CG2	2.38	0.53
27:Y:187:VAL:HG23	27:Y:192:ASP:CB	2.38	0.53
1:O:2456:A:H2'	1:O:2457:U:H6	1.73	0.53
1:O:2676:C:H6	1:O:2676:C:H5''	1.73	0.53
5:B:86:ALA:HA	39:B:9576:HOH:O	2.09	0.53
11:H:136:ALA:HB3	11:H:146:VAL:HG21	1.90	0.53
26:X:7:GLU:HA	26:X:74:ALA:O	2.09	0.53
1:O:951:A:C2'	1:O:952:G:H5'	2.38	0.53
4:A:203:GLY:HA2	39:A:9531:HOH:O	2.08	0.53
5:B:18:ARG:HE	5:B:256:GLN:NE2	2.06	0.53
12:J:103:VAL:HG12	39:J:5907:HOH:O	2.09	0.53
1:O:2320:U:H4'	1:O:2321:A:O4'	2.08	0.53
1:O:2912:C:H2'	1:O:2913:A:O4'	2.09	0.53
5:B:51:VAL:HG21	5:B:327:VAL:HG13	1.90	0.53
6:C:233:THR:HG22	6:C:234:VAL:N	2.23	0.53
14:L:80:ASP:CB	14:L:90:ARG:HB3	2.38	0.53
1:O:1501:A:OP2	18:P:37:ARG:HD2	2.08	0.53
22:T:89:ARG:HG3	22:T:89:ARG:O	2.09	0.53
22:T:92:ASP:OD1	22:T:94:SER:HB3	2.08	0.53
1:O:1724:U:H5''	39:O:4320:HOH:O	2.08	0.53
29:1:21:ARG:HD2	29:1:37:CYS:SG	2.48	0.53
5:B:141:ARG:HG2	5:B:165:ARG:HA	1.90	0.53
5:B:62:ARG:HA	5:B:65:MET:HE3	1.90	0.53
6:C:246:ARG:NH1	39:C:9176:HOH:O	2.40	0.53
11:H:45:VAL:HA	11:H:167:PRO:O	2.09	0.53
13:K:55:VAL:CG1	13:K:56:SER:N	2.72	0.53
18:P:103:THR:O	18:P:107:GLU:HG3	2.08	0.53
23:U:4:ARG:HH11	23:U:4:ARG:HG2	1.74	0.53
1:O:2419:U:H5''	1:O:2420:G:H5'	1.91	0.52
5:B:321:PRO:HA	39:B:9655:HOH:O	2.09	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2548:C:OP2	5:B:5:ARG:NH2	2.41	0.52
24:V:56:ILE:HG22	24:V:60:GLN:NE2	2.24	0.52
1:0:564:G:H1'	39:0:6837:HOH:O	2.09	0.52
9:F:50:VAL:HG21	9:F:63:ILE:HG21	1.91	0.52
15:M:107:ARG:NH1	39:M:9383:HOH:O	2.42	0.52
1:0:248:A:H5'	1:0:249:G:OP2	2.10	0.52
6:C:47:GLY:HA2	6:C:92:PRO:HB2	1.90	0.52
10:G:64:ASN:N	10:G:64:ASN:HD22	2.05	0.52
32:I:93:GLN:HA	32:I:96:PHE:HE2	1.74	0.52
22:T:41:ARG:NH1	22:T:41:ARG:HG2	2.22	0.52
1:0:2508:C:H2'	39:0:7264:HOH:O	2.09	0.52
4:A:69:LEU:HD23	4:A:107:ASN:CB	2.40	0.52
7:D:136:ARG:HB3	7:D:137:PRO:HD2	1.90	0.52
19:Q:32:GLU:HA	19:Q:71:TYR:OH	2.09	0.52
20:R:18:LEU:HB2	20:R:143:VAL:HG13	1.91	0.52
25:W:122:ARG:CG	25:W:122:ARG:NH1	2.70	0.52
25:W:6:GLN:CB	25:W:26:ILE:HD12	2.33	0.52
1:0:121:U:OP2	30:2:10:ARG:NH2	2.38	0.52
1:0:848:C:H5'	39:0:7760:HOH:O	2.10	0.52
4:A:109:GLU:HG2	4:A:116:GLY:N	2.25	0.52
6:C:127:ARG:CZ	6:C:225:PRO:HG2	2.39	0.52
9:F:48:VAL:HG12	9:F:97:ALA:HB2	1.91	0.52
32:I:129:VAL:O	32:I:129:VAL:HG12	2.10	0.52
14:L:145:LEU:O	14:L:148:GLU:HG3	2.08	0.52
17:O:59:VAL:CG2	17:O:111:VAL:HG21	2.39	0.52
1:0:119:A:H2'	1:0:120:A:H5''	1.92	0.52
1:0:1234:U:N3	5:B:244:PRO:HB3	2.25	0.52
1:0:2541:U:O2	1:0:2618:G:N2	2.43	0.52
1:0:2816:A:H2'	39:0:8476:HOH:O	2.10	0.52
4:A:88:ILE:HG22	4:A:88:ILE:O	2.09	0.52
32:I:106:LYS:O	32:I:110:GLU:HG3	2.09	0.52
14:L:97:VAL:HG12	14:L:98:GLU:O	2.09	0.52
16:N:154:LEU:O	16:N:155:GLU:CB	2.58	0.52
16:N:162:ASP:HA	39:N:9331:HOH:O	2.10	0.52
1:0:1462:C:H2'	1:0:1463:A:C8	2.45	0.52
1:0:1527:A:H1'	1:0:1528:A:C8	2.45	0.52
4:A:179:MET:HA	4:A:179:MET:CE	2.39	0.52
14:L:91:VAL:CG1	14:L:120:LEU:HD23	2.39	0.52
22:T:69:LYS:O	22:T:71:VAL:HG23	2.10	0.52
1:0:1218:U:H2'	1:0:1219:U:H6	1.74	0.52
1:0:2896:A:H5''	39:X:5399:HOH:O	2.09	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:737:A:H2'	1:0:738:G:O4'	2.09	0.52
4:A:94:LEU:HB2	4:A:95:PRO:HD2	1.90	0.52
5:B:41:PHE:CD1	5:B:79:MET:HE2	2.45	0.52
12:J:80:LYS:NZ	39:J:7377:HOH:O	2.42	0.52
15:M:98:GLN:O	15:M:102:GLU:HG3	2.10	0.52
15:M:164:THR:HG22	15:M:165:GLY:N	2.23	0.52
15:M:24:GLN:NE2	15:M:27:ARG:HH11	2.08	0.52
21:S:33:SER:OG	21:S:36:GLU:HG3	2.10	0.52
24:V:8:ILE:HG21	24:V:59:ILE:HG13	1.91	0.52
25:W:38:THR:HG22	25:W:39:ASP:N	2.24	0.52
1:0:1211:G:O2'	1:0:1212:C:H5'	2.10	0.52
5:B:41:PHE:CD2	5:B:190:MET:HE3	2.45	0.52
1:0:2101:A:H2'	6:C:63:SER:OG	2.10	0.52
8:E:23:GLU:HG2	8:E:28:SER:HB3	1.91	0.52
1:0:1946:C:H2'	1:0:1971:G:C8	2.45	0.52
13:K:28:GLU:HB3	13:K:59:LYS:HB2	1.91	0.52
14:L:53:ARG:NH2	14:L:57:VAL:HG12	2.25	0.52
16:N:152:GLU:C	16:N:154:LEU:H	2.13	0.52
16:N:42:HIS:CE1	16:N:75:THR:HG1	2.28	0.52
17:O:97:SER:OG	17:O:100:GLN:HG3	2.10	0.52
18:P:10:ALA:HA	18:P:13:VAL:HG12	1.92	0.52
28:Z:53:GLY:HA2	28:Z:67:GLY:O	2.10	0.52
1:0:1741:U:H3'	39:0:3369:HOH:O	2.09	0.51
15:M:99:ARG:NH2	15:M:170:ASN:HD22	2.00	0.51
6:C:163:HIS:HD2	39:C:9243:HOH:O	1.92	0.51
6:C:142:ASP:OD1	6:C:237:GLU:HB3	2.10	0.51
15:M:24:GLN:O	15:M:28:GLN:HG3	2.11	0.51
16:N:18:THR:HG21	39:N:9346:HOH:O	2.08	0.51
16:N:49:THR:HG22	16:N:56:ASP:CB	2.40	0.51
20:R:44:VAL:O	20:R:48:GLU:HG3	2.10	0.51
1:0:1477:C:H5'	1:0:1868:G:C5'	2.40	0.51
1:0:1835:U:C5	1:0:1840:A:N7	2.67	0.51
7:D:57:THR:HG23	7:D:63:ILE:CA	2.31	0.51
9:F:48:VAL:HG23	9:F:74:PHE:HB3	1.92	0.51
12:J:90:LYS:HB2	36:J:9302:CL:CL	2.46	0.51
15:M:15:PRO:HA	15:M:20:LEU:HD23	1.92	0.51
15:M:79:ALA:HB3	15:M:81:ARG:HH12	1.72	0.51
1:0:284:C:H4'	1:0:285:A:H8	1.74	0.51
1:0:776:A:OP1	29:1:28:HIS:HE1	1.92	0.51
4:A:36:ASP:O	4:A:38:ILE:N	2.42	0.51
7:D:23:VAL:CG2	7:D:73:VAL:HB	2.41	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:110:GLN:HE21	25:W:110:GLN:HA	1.76	0.51
1:O:2032:U:H2'	1:O:2033:G:H5''	1.92	0.51
1:O:407:A:H5'	39:O:6556:HOH:O	2.10	0.51
39:O:8484:HOH:O	5:B:2:GLN:CG	2.53	0.51
6:C:115:LEU:O	6:C:118:THR:HB	2.10	0.51
1:O:1363:G:OP1	6:C:76:ARG:NH2	2.43	0.51
12:J:39:VAL:HG11	12:J:107:ASN:CG	2.30	0.51
13:K:20:CYS:HB2	13:K:29:LEU:HG	1.92	0.51
6:C:118:THR:HG22	6:C:137:PRO:HB3	1.92	0.51
18:P:55:LYS:HG2	18:P:56:GLY:N	2.25	0.51
20:R:18:LEU:HG	20:R:91:LEU:HD13	1.92	0.51
1:O:2883:A:H2'	1:O:2884:G:O4'	2.11	0.51
5:B:62:ARG:HG2	5:B:65:MET:HE3	1.92	0.51
14:L:120:LEU:HD12	14:L:133:VAL:HG21	1.92	0.51
14:L:90:ARG:NH2	14:L:121:ILE:HD11	2.25	0.51
20:R:29:LYS:NZ	39:R:9449:HOH:O	2.44	0.51
1:O:1067:A:H5'	39:O:4922:HOH:O	2.10	0.51
1:O:1919:A:H4'	39:O:5416:HOH:O	2.10	0.51
1:O:2270:G:H4'	4:A:223:ARG:NH1	2.25	0.51
1:O:2443:C:H5'	14:L:57:VAL:HG21	1.93	0.51
1:O:2626:C:H2'	1:O:2627:G:C8	2.46	0.51
1:O:2717:C:H2'	1:O:2718:C:C5'	2.35	0.51
4:A:36:ASP:C	4:A:38:ILE:H	2.14	0.51
9:F:49:PHE:HE1	9:F:98:VAL:HG23	1.76	0.51
11:H:54:THR:O	11:H:55:VAL:HG13	2.11	0.51
16:N:86:LEU:HD21	16:N:180:LEU:HD12	1.92	0.51
1:O:1278:A:H4'	1:O:1279:U:C4	2.46	0.51
1:O:1966:U:H2'	1:O:1967:U:H2'	1.93	0.51
1:O:2524:G:H21	1:O:2526:C:N4	2.08	0.51
1:O:2711:U:H1'	39:O:4035:HOH:O	2.09	0.51
1:O:559:U:H2'	1:O:560:C:O4'	2.11	0.51
1:O:69:A:H5'	1:O:69:A:C8	2.45	0.51
8:E:11:VAL:HG12	8:E:12:ASP:N	2.26	0.51
19:Q:3:SER:HB3	39:Q:5998:HOH:O	2.11	0.51
22:T:40:VAL:HG22	22:T:41:ARG:N	2.26	0.51
1:O:1333:U:H2'	1:O:1334:C:C6	2.46	0.51
6:C:142:ASP:CG	6:C:237:GLU:HB3	2.31	0.51
9:F:58:GLU:HA	9:F:61:MET:HG3	1.93	0.51
13:K:7:ASP:OD2	13:K:81:ARG:NH2	2.44	0.51
1:O:2821:C:H4'	5:B:116:PRO:HG3	1.92	0.50
1:O:1853:C:OP1	4:A:231:LYS:HG3	2.12	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:41:PHE:CG	5:B:79:MET:HE2	2.46	0.50
8:E:7:ILE:HD11	8:E:11:VAL:C	2.32	0.50
12:J:54:VAL:HG11	12:J:138:THR:HG21	1.93	0.50
12:J:99:GLU:HA	39:J:7377:HOH:O	2.09	0.50
21:S:57:THR:CG2	21:S:58:MET:N	2.74	0.50
1:0:1165:G:H1'	1:0:1174:A:H1'	1.94	0.50
1:0:90:A:H2'	1:0:91:G:O4'	2.11	0.50
2:9:3008:G:O6	16:N:11:ARG:NH1	2.39	0.50
5:B:175:LEU:O	5:B:175:LEU:HD23	2.11	0.50
1:0:1363:G:P	6:C:76:ARG:HH22	2.35	0.50
9:F:26:THR:HG21	9:F:102:GLY:C	2.32	0.50
11:H:116:ALA:O	11:H:117:PHE:C	2.50	0.50
32:I:72:VAL:CG1	32:I:73:PRO:HD2	2.41	0.50
15:M:167:GLY:O	15:M:171:ARG:HG3	2.11	0.50
25:W:110:GLN:NE2	25:W:110:GLN:HA	2.26	0.50
26:X:78:GLU:HG2	26:X:79:GLU:OE2	2.11	0.50
26:X:7:GLU:HA	26:X:75:ALA:HA	1.92	0.50
1:0:1198:U:H2'	1:0:1200:A:OP2	2.11	0.50
6:C:16:VAL:HG12	6:C:17:ASP:N	2.25	0.50
7:D:104:PHE:CE2	7:D:166:ILE:HD13	2.46	0.50
1:0:1120:U:H5''	1:0:1120:U:C6	2.46	0.50
1:0:926:A:O2'	14:L:41:HIS:HD2	1.94	0.50
31:3:35:TRP:HB2	39:3:9488:HOH:O	2.09	0.50
1:0:475:G:C5'	6:C:73:LEU:HD23	2.42	0.50
11:H:58:ARG:HG3	11:H:58:ARG:HH11	1.75	0.50
26:X:72:VAL:HG22	26:X:85:VAL:HG12	1.92	0.50
1:0:1118:A:C8	1:0:1118:A:C3'	2.89	0.50
1:0:2812:A:C2	1:0:2814:A:N6	2.68	0.50
1:0:362:G:H2'	1:0:363:A:C8	2.46	0.50
1:0:474:C:O3'	6:C:73:LEU:CD2	2.60	0.50
1:0:485:A:N3	1:0:487:G:H5''	2.26	0.50
5:B:310:ARG:HD2	39:B:9588:HOH:O	2.10	0.50
7:D:51:ARG:HD3	39:D:7636:HOH:O	2.11	0.50
23:U:9:CYS:O	23:U:52:THR:HG23	2.10	0.50
1:0:1592:G:O2'	1:0:1593:C:O4'	2.29	0.50
6:C:162:VAL:CG2	6:C:232:LEU:HD21	2.42	0.50
32:I:100:LEU:O	32:I:139:ILE:HG23	2.11	0.50
12:J:107:ASN:HD21	12:J:109:TYR:HB2	1.77	0.50
28:Z:19:GLY:O	28:Z:23:ARG:HG2	2.11	0.50
28:Z:42:CYS:SG	28:Z:43:GLY:N	2.85	0.50
1:0:1119:G:H8	12:J:52:GLN:NE2	2.10	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1167:G:H2'	1:0:1168:C:O4'	2.11	0.50
1:0:1252:A:H2'	1:0:1253:C:O4'	2.12	0.50
1:0:1979:G:O2'	1:0:1980:U:OP1	2.30	0.50
1:0:482:G:H4'	1:0:508:A:N1	2.27	0.50
7:D:10:PHE:CE1	7:D:11:HIS:HB3	2.47	0.50
25:W:119:HIS:HD2	25:W:120:PRO:O	1.94	0.50
1:0:1972:U:H2'	1:0:1973:A:H5'	1.94	0.50
1:0:447:A:O2'	1:0:448:G:H5'	2.12	0.50
6:C:118:THR:CG2	6:C:137:PRO:HB3	2.41	0.50
8:E:154:ILE:HD11	8:E:157:LYS:HB2	1.92	0.50
12:J:76:ASP:HA	39:J:5907:HOH:O	2.11	0.50
39:K:7438:HOH:O	23:U:20:MET:HE1	2.11	0.50
1:0:1189:A:H1'	1:0:1209:C:C1'	2.41	0.50
1:0:2815:G:OP2	12:J:99:GLU:HG2	2.12	0.50
1:0:87:C:H2'	30:2:28:LYS:O	2.12	0.50
1:0:920:C:H5''	1:0:921:G:O5'	2.12	0.50
4:A:153:ARG:NH1	4:A:153:ARG:HB2	2.24	0.50
7:D:167:GLU:C	7:D:169:THR:H	2.14	0.50
11:H:3:ALA:CA	11:H:58:ARG:HH12	2.24	0.50
24:V:59:ILE:O	24:V:63:GLU:HG2	2.11	0.50
1:0:1132:A:N6	1:0:1229:C:H2'	2.27	0.49
1:0:1477:C:O2'	1:0:1478:U:H5'	2.12	0.49
1:0:1942:A:H3'	39:0:7828:HOH:O	2.12	0.49
2:9:3044:A:O4'	7:D:76:ARG:NE	2.44	0.49
4:A:65:ARG:C	4:A:66:ARG:HG3	2.32	0.49
5:B:314:ALA:HB3	5:B:317:PRO:HG3	1.93	0.49
7:D:41:LEU:HA	7:D:44:ILE:HG22	1.94	0.49
1:0:155:C:OP2	15:M:188:ARG:HD3	2.11	0.49
17:O:78:ALA:C	17:O:98:LEU:HD13	2.32	0.49
25:W:88:THR:HG22	25:W:90:TYR:CD1	2.47	0.49
1:0:1119:G:N2	1:0:1246:A:N1	2.60	0.49
1:0:1159:G:H1	1:0:1208:C:H42	1.60	0.49
1:0:1921:A:O2'	1:0:1922:A:H5'	2.12	0.49
1:0:449:A:N7	6:C:43:LYS:HG2	2.26	0.49
2:9:3054:A:H2	39:9:3535:HOH:O	1.94	0.49
11:H:40:ALA:HB1	11:H:137:TYR:CE2	2.47	0.49
16:N:164:ASP:OD2	16:N:167:ASP:HA	2.11	0.49
4:A:132:ASP:OD1	4:A:133:ARG:N	2.42	0.49
1:0:894:A:N1	6:C:87:ARG:NH2	2.61	0.49
11:H:73:LEU:HD21	11:H:146:VAL:HA	1.95	0.49
11:H:27:LYS:H	11:H:59:HIS:CD2	2.23	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1119:G:H8	12:J:52:GLN:HE22	1.59	0.49
16:N:183:ASP:O	16:N:184:ILE:O	2.30	0.49
1:0:317:A:OP1	22:T:52:ARG:O	2.30	0.49
1:0:1666:C:C2'	1:0:1667:A:C5'	2.91	0.49
1:0:292:G:H2'	1:0:358:G:N2	2.27	0.49
1:0:821:U:H2'	1:0:822:C:H6	1.77	0.49
5:B:49:THR:CG2	5:B:280:VAL:HG23	2.43	0.49
6:C:219:ASN:O	6:C:222:ASP:OD1	2.30	0.49
11:H:169:GLY:HA3	39:H:9553:HOH:O	2.11	0.49
27:Y:187:VAL:HG23	27:Y:192:ASP:HB3	1.93	0.49
1:0:2786:G:H2'	39:0:7679:HOH:O	2.12	0.49
4:A:131:HIS:O	4:A:132:ASP:HB2	2.11	0.49
32:I:74:PRO:C	32:I:112:LYS:HZ1	2.15	0.49
26:X:30:MET:HE1	26:X:58:ALA:CB	2.40	0.49
1:0:2453:G:H5''	39:L:9438:HOH:O	2.11	0.49
1:0:820:G:O2'	1:0:856:G:H4'	2.13	0.49
16:N:167:ASP:C	16:N:168:LEU:HG	2.33	0.49
25:W:108:ARG:HE	25:W:114:PRO:HG3	1.77	0.49
1:0:1667:A:H2'	1:0:1668:U:C6	2.48	0.49
1:0:204:A:C2'	1:0:205:U:H5'	2.43	0.49
1:0:470:U:O2'	29:1:16:HIS:CD2	2.62	0.49
1:0:951:A:O2'	1:0:952:G:H5'	2.13	0.49
31:3:70:ARG:HB3	39:3:9504:HOH:O	2.13	0.49
4:A:223:ARG:CZ	39:A:9556:HOH:O	2.60	0.49
4:A:33:GLU:OE1	4:A:33:GLU:N	2.45	0.49
39:0:9730:HOH:O	5:B:229:ARG:HD2	2.13	0.49
8:E:49:ILE:HD11	8:E:69:ILE:HD12	1.94	0.49
32:I:116:LEU:HD22	32:I:127:GLU:OE1	2.12	0.49
25:W:115:THR:HB	39:W:6871:HOH:O	2.12	0.49
1:0:2090:G:H2'	1:0:2091:G:C8	2.47	0.49
5:B:113:LEU:HD21	5:B:161:VAL:HG21	1.95	0.49
6:C:107:ARG:HH11	6:C:107:ARG:CB	2.25	0.49
6:C:200:PRO:HB3	6:C:212:VAL:HG23	1.95	0.49
7:D:128:LEU:HB2	39:D:6007:HOH:O	2.13	0.49
20:R:39:THR:HB	20:R:42:GLU:CG	2.42	0.49
24:V:39:ALA:O	24:V:41:GLU:N	2.41	0.49
25:W:88:THR:CG2	25:W:90:TYR:HD1	2.24	0.49
1:0:1878:G:O2'	1:0:1879:U:C6	2.62	0.49
1:0:2895:C:H4'	39:X:4132:HOH:O	2.13	0.49
1:0:299:U:H5'	39:0:7818:HOH:O	2.12	0.49
12:J:142:ASN:O	12:J:144:THR:N	2.45	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:34:VAL:HG22	13:K:47:ALA:HB2	1.94	0.49
23:U:17:THR:CG2	23:U:18:GLY:H	2.25	0.49
23:U:52:THR:HG22	23:U:54:THR:H	1.76	0.49
1:O:2365:G:H5''	39:Q:6597:HOH:O	2.11	0.49
2:9:3028:U:H2'	2:9:3029:C:C6	2.47	0.49
5:B:81:ALA:O	5:B:186:GLY:HA3	2.12	0.49
9:F:14:ASP:O	9:F:18:GLU:HG3	2.12	0.49
1:O:2521:A:OP2	11:H:3:ALA:HB3	2.13	0.49
12:J:45:VAL:HG11	12:J:121:LEU:CD2	2.42	0.49
2:9:3004:G:H21	16:N:44:ARG:NH1	2.10	0.49
28:Z:36:ASP:HB3	28:Z:45:ASP:HB3	1.95	0.49
1:O:399:C:H5'	15:M:179:GLY:O	2.13	0.48
1:O:1654:U:H2'	4:A:47:HIS:HD2	1.76	0.48
7:D:35:ALA:O	7:D:38:GLU:HG3	2.13	0.48
13:K:125:ALA:C	13:K:127:ALA:H	2.15	0.48
1:O:392:U:H5''	15:M:193:LYS:HB3	1.95	0.48
7:D:146:LYS:NZ	16:N:107:ASN:ND2	2.61	0.48
16:N:37:ARG:NH2	16:N:105:GLY:HA3	2.27	0.48
17:O:41:ALA:HA	39:O:5104:HOH:O	2.12	0.48
18:P:16:VAL:HG13	18:P:20:ARG:NH1	2.28	0.48
24:V:29:ASN:O	24:V:33:VAL:HG23	2.13	0.48
25:W:52:VAL:HG22	25:W:53:ALA:N	2.27	0.48
1:O:1180:U:H2'	1:O:1181:A:C8	2.47	0.48
31:3:20:HIS:HA	31:3:70:ARG:O	2.13	0.48
7:D:57:THR:HA	39:D:5728:HOH:O	2.13	0.48
11:H:169:GLY:C	11:H:170:ASN:HD22	2.15	0.48
11:H:170:ASN:N	11:H:170:ASN:ND2	2.57	0.48
12:J:131:THR:HB	12:J:134:GLU:OE1	2.13	0.48
12:J:70:PHE:CG	12:J:70:PHE:O	2.65	0.48
24:V:64:GLY:O	24:V:65:ASP:CB	2.59	0.48
25:W:4:LEU:HD23	25:W:54:PHE:HB3	1.95	0.48
1:O:1056:U:H2'	1:O:1057:A:O4'	2.12	0.48
1:O:2507:G:H2'	1:O:2510:C:N4	2.28	0.48
1:O:541:C:H2'	1:O:542:A:H5'	1.94	0.48
1:O:1654:U:H2'	4:A:47:HIS:CD2	2.48	0.48
5:B:217:ARG:HG3	5:B:257:THR:HG22	1.94	0.48
15:M:187:LEU:HD23	15:M:194:ALA:HB3	1.94	0.48
16:N:1:ALA:HB3	39:N:9368:HOH:O	2.13	0.48
18:P:98:ILE:HD12	18:P:102:ARG:NE	2.29	0.48
16:N:24:LEU:HD13	19:Q:26:PRO:HB3	1.94	0.48
27:Y:203:VAL:HG12	27:Y:228:VAL:HG22	1.94	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1299:G:H5'	39:0:4654:HOH:O	2.13	0.48
1:0:1745:G:H22	1:0:2033:G:H5'	1.78	0.48
1:0:2253:G:O2'	1:0:2254:G:H5'	2.14	0.48
1:0:2414:A:H2'	1:0:2415:A:C8	2.49	0.48
1:0:2649:A:H5'	1:0:2649:A:H8	1.78	0.48
1:0:2748:G:H4'	1:0:2749:U:C5'	2.43	0.48
1:0:475:G:OP1	6:C:73:LEU:HD22	2.13	0.48
21:S:33:SER:O	21:S:37:VAL:HG23	2.13	0.48
39:0:5842:HOH:O	25:W:122:ARG:NH2	2.47	0.48
27:Y:126:PRO:HG2	27:Y:128:PHE:CZ	2.48	0.48
1:0:1902:G:H2'	1:0:1903:U:O4'	2.14	0.48
1:0:603:A:H5''	1:0:604:G:OP1	2.12	0.48
4:A:179:MET:HG2	4:A:186:TRP:CB	2.44	0.48
9:F:11:ASP:O	9:F:14:ASP:HB2	2.14	0.48
32:I:131:THR:O	32:I:135:LEU:HG	2.13	0.48
22:T:71:VAL:CG1	22:T:72:ILE:N	2.76	0.48
25:W:122:ARG:NH2	39:W:5817:HOH:O	2.46	0.48
11:H:34:GLY:HA3	11:H:84:LYS:HA	1.94	0.48
15:M:57:LYS:HE2	15:M:140:ALA:O	2.13	0.48
15:M:99:ARG:HH21	15:M:170:ASN:ND2	2.02	0.48
17:O:59:VAL:HG21	17:O:111:VAL:HG21	1.95	0.48
1:0:2831:C:O3'	20:R:71:LYS:HE2	2.14	0.48
1:0:558:C:C2'	1:0:559:U:C5'	2.92	0.48
31:3:6:ARG:NH1	31:3:21:GLU:HB2	2.28	0.48
2:9:3039:U:O2'	2:9:3042:C:C5	2.65	0.48
7:D:136:ARG:NH1	7:D:157:LEU:HA	2.27	0.48
8:E:84:MET:HE1	8:E:148:ILE:HD12	1.96	0.48
39:0:4952:HOH:O	15:M:83:SER:HB3	2.14	0.48
25:W:54:PHE:CZ	25:W:140:LYS:HB2	2.48	0.48
1:0:1203:G:O2'	1:0:1204:C:H5'	2.13	0.48
30:2:10:ARG:HD2	30:2:49:GLU:OE2	2.13	0.48
4:A:53:ALA:HB3	39:A:9587:HOH:O	2.14	0.48
11:H:146:VAL:HG22	39:H:9541:HOH:O	2.14	0.48
32:I:105:VAL:HG11	32:I:129:VAL:CG2	2.44	0.48
12:J:19:MET:HE2	12:J:79:PHE:HA	1.94	0.48
16:N:78:MET:HB2	16:N:79:PRO:HD3	1.96	0.48
25:W:29:VAL:O	25:W:30:ASN:HB2	2.14	0.48
1:0:137:U:H2'	1:0:139:C:C5	2.48	0.48
1:0:2781:U:H1'	8:E:139:GLU:OE2	2.14	0.48
1:0:343:C:O2'	1:0:344:C:H5'	2.12	0.48
1:0:500:G:H21	20:R:98:ASN:HD21	1.60	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:932:U:H2'	1:0:933:C:C6	2.49	0.48
2:9:3057:A:C8	7:D:141:VAL:HG21	2.48	0.48
4:A:26:ASP:CG	4:A:26:ASP:O	2.53	0.48
16:N:36:ALA:HB1	16:N:118:ILE:HD12	1.95	0.48
16:N:43:VAL:HG13	16:N:118:ILE:HD11	1.94	0.48
22:T:71:VAL:HG13	22:T:91:LEU:O	2.13	0.48
25:W:149:LEU:HG	25:W:153:MET:CE	2.44	0.48
28:Z:32:GLU:HA	28:Z:35:GLU:HG3	1.95	0.48
1:0:1130:U:H2'	1:0:1131:G:O4'	2.14	0.48
1:0:2443:C:O3'	14:L:56:LYS:HE3	2.14	0.48
1:0:2681:A:H4'	1:0:2682:C:H5'	1.96	0.48
1:0:329:A:OP2	6:C:206:ASN:HB2	2.14	0.48
6:C:153:VAL:O	6:C:157:LEU:HG	2.14	0.48
6:C:61:PHE:HB3	39:C:9250:HOH:O	2.12	0.48
7:D:49:PRO:HA	7:D:73:VAL:HG22	1.96	0.48
32:I:113:HIS:N	32:I:114:PRO:CD	2.77	0.48
12:J:75:PRO:HB3	12:J:132:LEU:HB3	1.95	0.48
17:O:80:ASP:OD1	17:O:81:PHE:N	2.46	0.48
22:T:48:VAL:HG23	22:T:98:VAL:HA	1.96	0.48
25:W:139:GLY:O	25:W:141:HIS:HD2	1.95	0.48
25:W:88:THR:CG2	25:W:89:ASP:N	2.75	0.48
27:Y:117:LEU:HA	27:Y:174:VAL:HG11	1.96	0.48
1:0:2003:U:H4'	1:0:2004:U:C5	2.46	0.47
1:0:2748:G:C5'	39:0:8049:HOH:O	2.59	0.47
6:C:157:LEU:HD13	6:C:166:ILE:HD11	1.95	0.47
8:E:7:ILE:HD11	8:E:11:VAL:O	2.14	0.47
15:M:43:PRO:HG3	15:M:62:VAL:HG21	1.96	0.47
39:9:5851:HOH:O	16:N:115:VAL:HG13	2.13	0.47
27:Y:150:LEU:HB3	39:Y:9358:HOH:O	2.13	0.47
27:Y:178:HIS:CG	27:Y:179:PRO:HD2	2.49	0.47
1:0:1118:A:C8	1:0:1119:G:H5''	2.48	0.47
1:0:1506:U:H6	1:0:1506:U:H5'	1.79	0.47
1:0:1717:A:H5''	18:P:54:LYS:HB2	1.95	0.47
1:0:486:A:H1'	39:0:7288:HOH:O	2.13	0.47
1:0:757:C:OP1	14:L:27:ARG:HD2	2.13	0.47
2:9:3049:G:H5''	39:9:4707:HOH:O	2.14	0.47
4:A:70:ALA:HA	4:A:71:PRO:HD3	1.77	0.47
11:H:79:GLU:C	11:H:80:GLU:HG3	2.35	0.47
27:Y:122:ARG:NH2	39:Y:9335:HOH:O	2.48	0.47
1:0:1451:C:H5'	1:0:1505:U:C5	2.49	0.47
1:0:2072:G:H3'	1:0:2073:G:C5'	2.44	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2825:C:H4'	1:0:2826:G:O5'	2.14	0.47
2:9:3092:G:H2'	2:9:3093:A:C8	2.50	0.47
5:B:36:PRO:HB3	5:B:174:ARG:CB	2.44	0.47
6:C:127:ARG:HD3	6:C:129:HIS:HE1	1.80	0.47
10:G:27:ILE:HD13	10:G:71:LEU:HD23	1.97	0.47
17:O:14:LEU:HG	17:O:102:ILE:HD11	1.97	0.47
24:V:5:VAL:HG23	39:V:2271:HOH:O	2.13	0.47
1:0:1755:A:H2'	1:0:1756:G:O4'	2.14	0.47
1:0:830:G:O2'	1:0:831:U:H5'	2.14	0.47
5:B:254:GLN:NE2	39:B:9589:HOH:O	2.46	0.47
8:E:101:GLU:HB2	8:E:116:THR:O	2.14	0.47
9:F:117:GLU:C	9:F:119:ARG:H	2.18	0.47
10:G:23:ILE:HD13	10:G:67:LEU:HD23	1.95	0.47
17:O:32:ARG:HB2	39:O:4656:HOH:O	2.13	0.47
27:Y:235:GLU:CD	27:Y:235:GLU:N	2.52	0.47
1:0:1406:A:H4'	1:0:1407:A:C5'	2.44	0.47
1:0:2102:G:H5''	1:0:2538:A:C2	2.50	0.47
1:0:2908:A:H2'	1:0:2909:G:O4'	2.13	0.47
1:0:952:G:N3	1:0:2302:A:H2'	2.29	0.47
2:9:3058:G:H1'	39:D:3839:HOH:O	2.14	0.47
8:E:22:VAL:HG12	8:E:76:VAL:HG11	1.97	0.47
9:F:5:ASP:O	9:F:119:ARG:NH1	2.47	0.47
11:H:20:ILE:HG23	11:H:120:ILE:CD1	2.43	0.47
11:H:167:PRO:O	11:H:168:ALA:HB2	2.14	0.47
32:I:89:SER:CB	32:I:95:ASP:HB2	2.44	0.47
1:0:1525:G:H5'	1:0:1526:A:OP2	2.15	0.47
1:0:2032:U:C2'	1:0:2033:G:H5''	2.44	0.47
1:0:2852:A:H5''	39:O:5787:HOH:O	2.14	0.47
1:0:542:A:H2'	1:0:543:G:O4'	2.15	0.47
1:0:588:G:O6	25:W:154:ARG:NH1	2.48	0.47
5:B:24:PRO:HG3	5:B:204:GLY:HA2	1.95	0.47
5:B:162:MET:HE3	5:B:310:ARG:HD3	1.90	0.47
6:C:129:HIS:HE1	6:C:231:ARG:HA	1.78	0.47
6:C:242:GLU:HB2	39:C:9188:HOH:O	2.14	0.47
6:C:46:TYR:CE2	6:C:98:ARG:NH1	2.82	0.47
9:F:68:ASP:C	9:F:70:LYS:H	2.18	0.47
13:K:28:GLU:OE2	13:K:58:THR:HG21	2.15	0.47
18:P:13:VAL:HG11	18:P:40:VAL:CG1	2.45	0.47
25:W:21:LEU:HD21	25:W:48:VAL:CG1	2.21	0.47
1:0:1120:U:H6	1:0:1120:U:H5''	1.80	0.47
1:0:2509:A:H2'	1:0:2510:C:O4'	2.15	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:603:A:H4'	1:0:604:G:O5'	2.14	0.47
2:9:3042:C:H5'	2:9:3043:G:OP2	2.14	0.47
4:A:94:LEU:N	4:A:94:LEU:HD23	2.30	0.47
5:B:41:PHE:CG	5:B:190:MET:HE3	2.49	0.47
7:D:134:LEU:HD11	7:D:166:ILE:HD11	1.97	0.47
8:E:102:VAL:HG13	8:E:116:THR:HG23	1.95	0.47
8:E:1:PRO:HG2	8:E:59:MET:SD	2.54	0.47
9:F:101:ALA:HA	39:F:5413:HOH:O	2.15	0.47
9:F:36:THR:HG23	9:F:97:ALA:HB2	1.96	0.47
12:J:39:VAL:HG11	12:J:107:ASN:CB	2.44	0.47
12:J:130:VAL:HG12	12:J:131:THR:H	1.80	0.47
13:K:13:GLU:OE1	13:K:44:LEU:HD12	2.14	0.47
16:N:74:PRO:HG2	16:N:159:TYR:CE1	2.49	0.47
1:0:1007:A:H2'	11:H:19:TYR:CZ	2.49	0.47
1:0:1878:G:O2'	1:0:1879:U:P	2.72	0.47
1:0:2649:A:C8	1:0:2649:A:H5'	2.49	0.47
1:0:2819:C:O4'	5:B:96:PRO:HB2	2.14	0.47
1:0:87:C:C2	30:2:30:ASP:OD2	2.68	0.47
8:E:69:ILE:HA	8:E:72:MET:CE	2.44	0.47
1:0:645:U:OP2	14:L:4:LYS:HE2	2.13	0.47
15:M:34:GLU:HB3	15:M:38:GLU:HG3	1.96	0.47
20:R:9:ASP:O	20:R:13:THR:HB	2.14	0.47
1:0:1422:U:H2'	1:0:1423:C:C6	2.50	0.47
1:0:1603:A:H5''	1:0:1605:G:H5'	1.96	0.47
1:0:2644:C:O2'	1:0:2645:U:H5'	2.14	0.47
1:0:2837:U:H2'	39:0:7345:HOH:O	2.14	0.47
1:0:380:A:H4'	1:0:381:G:OP1	2.15	0.47
1:0:506:G:H22	1:0:509:A:H5'	1.75	0.47
1:0:870:G:OP2	4:A:3:ARG:HD3	2.15	0.47
1:0:894:A:C2	6:C:87:ARG:NH2	2.83	0.47
8:E:80:TRP:O	8:E:134:SER:HA	2.14	0.47
11:H:158:THR:HB	11:H:159:PRO:HD3	1.97	0.47
1:0:1181:A:N1	1:0:1192:A:O2'	2.46	0.47
1:0:1972:U:H2'	1:0:1973:A:C5'	2.45	0.47
1:0:2346:C:O5'	1:0:2346:C:H6	1.96	0.47
1:0:2712:G:H5'	39:K:4183:HOH:O	2.14	0.47
1:0:241:A:C2	1:0:378:A:H4'	2.50	0.47
1:0:1836:A:H1'	29:1:1:THR:O	2.14	0.47
5:B:190:MET:CE	5:B:194:PHE:CD1	2.98	0.47
9:F:28:ALA:CB	9:F:99:THR:HG23	2.45	0.47
14:L:35:ARG:HD3	14:L:35:ARG:C	2.36	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:69:TYR:CE2	16:N:184:ILE:HG13	2.48	0.47
1:0:1352:A:HO2'	1:0:1353:C:P	2.36	0.47
2:9:3091:C:H2'	2:9:3092:G:O4'	2.15	0.47
4:A:126:ALA:HB1	4:A:138:VAL:CG1	2.45	0.47
5:B:265:LEU:HD21	5:B:316:ARG:HD3	1.97	0.47
6:C:133:ARG:NE	6:C:138:VAL:HG22	2.30	0.47
7:D:99:ASP:O	7:D:159:PRO:HG3	2.14	0.47
12:J:80:LYS:HE2	12:J:98:PHE:CZ	2.50	0.47
14:L:61:ALA:HB2	14:L:105:TYR:CZ	2.50	0.47
15:M:66:SER:HB3	15:M:128:TRP:CD1	2.50	0.47
1:0:2364:A:H5''	19:Q:15:LYS:HD3	1.96	0.47
1:0:1201:C:C2'	1:0:1202:A:H5'	2.45	0.46
1:0:2252:A:H2'	1:0:2253:G:O4'	2.16	0.46
29:1:28:HIS:CE1	29:1:31:LYS:HE2	2.49	0.46
30:2:22:PRO:HG2	30:2:25:VAL:HG21	1.97	0.46
2:9:3039:U:HO2'	2:9:3042:C:H5	1.55	0.46
2:9:3048:C:H4'	16:N:141:ARG:HH21	1.80	0.46
5:B:14:GLY:HA2	5:B:15:PRO:C	2.35	0.46
9:F:99:THR:O	9:F:100:ASP:HB2	2.15	0.46
16:N:67:ALA:HA	16:N:71:TRP:HB3	1.97	0.46
17:O:73:ASP:HA	17:O:92:VAL:O	2.14	0.46
1:0:1242:A:OP2	12:J:60:ARG:NH2	2.45	0.46
1:0:1331:A:OP2	27:Y:142:SER:OG	2.32	0.46
1:0:2338:G:H2'	7:D:129:ASP:OD1	2.15	0.46
31:3:70:ARG:CG	31:3:77:ALA:HB2	2.42	0.46
2:9:3049:G:O2'	2:9:3050:G:H5'	2.14	0.46
4:A:72:GLU:HG3	28:Z:66:GLY:HA2	1.96	0.46
5:B:132:HIS:CE1	5:B:171:VAL:HG21	2.51	0.46
14:L:145:LEU:O	14:L:145:LEU:HD23	2.15	0.46
39:0:5295:HOH:O	16:N:21:HIS:HD2	1.97	0.46
39:0:4570:HOH:O	22:T:82:THR:HA	2.15	0.46
27:Y:151:SER:HB3	27:Y:154:ARG:HB3	1.98	0.46
1:0:1095:U:O2	25:W:120:PRO:HG2	2.16	0.46
1:0:2748:G:H4'	1:0:2749:U:H5'	1.95	0.46
4:A:194:MET:CE	4:A:199:HIS:HB2	2.45	0.46
5:B:277:GLU:N	5:B:278:PRO:HD2	2.30	0.46
7:D:135:VAL:HG22	7:D:136:ARG:N	2.29	0.46
1:0:2346:C:H4'	7:D:52:THR:CG2	2.46	0.46
11:H:66:ARG:HD3	39:H:9544:HOH:O	2.14	0.46
17:O:38:ARG:NH1	39:O:7674:HOH:O	2.47	0.46
23:U:6:CYS:HB2	23:U:32:CYS:HB3	1.97	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1053:G:OP1	11:H:12:PRO:HG3	2.15	0.46
1:0:1098:A:H2'	1:0:1099:G:O4'	2.15	0.46
1:0:1435:U:H5'	39:0:3209:HOH:O	2.14	0.46
1:0:1748:U:H4'	39:0:7993:HOH:O	2.14	0.46
1:0:2635:A:C2'	1:0:2636:C:H5'	2.45	0.46
1:0:407:A:H2'	1:0:408:A:C8	2.51	0.46
1:0:920:C:H4'	1:0:921:G:C2	2.51	0.46
39:0:6852:HOH:O	8:E:35:TYR:HB2	2.16	0.46
11:H:47:ILE:HD12	11:H:146:VAL:CG1	2.45	0.46
13:K:14:LYS:HG3	13:K:32:ILE:O	2.15	0.46
14:L:143:THR:CG2	14:L:144:ASP:N	2.76	0.46
1:0:709:G:O2'	17:O:25:VAL:CG1	2.61	0.46
17:O:47:ARG:HG3	17:O:47:ARG:HH11	1.80	0.46
19:Q:25:PRO:HA	19:Q:26:PRO:HD3	1.81	0.46
27:Y:133:HIS:HD2	39:Y:9382:HOH:O	1.97	0.46
28:Z:26:VAL:O	28:Z:30:GLU:HG3	2.16	0.46
1:0:2906:A:H5'	1:0:2907:C:O4'	2.15	0.46
1:0:333:G:O2'	1:0:334:G:H5'	2.16	0.46
1:0:653:C:H2'	1:0:654:A:C8	2.51	0.46
2:9:3024:U:H3'	2:9:3025:G:H5'	1.97	0.46
5:B:81:ALA:HB1	5:B:142:LEU:HD13	1.97	0.46
7:D:36:ASN:HB3	39:D:1655:HOH:O	2.16	0.46
14:L:134:GLU:HG3	39:L:9453:HOH:O	2.15	0.46
14:L:89:PHE:CD1	14:L:89:PHE:N	2.83	0.46
25:W:88:THR:CG2	25:W:89:ASP:H	2.28	0.46
1:0:2044:G:OP1	26:X:23:HIS:HE1	1.98	0.46
1:0:2362:A:H2'	1:0:2363:G:C8	2.51	0.46
1:0:2415:A:O2'	16:N:29:SER:HB3	2.15	0.46
1:0:684:G:H2'	1:0:685:C:C6	2.51	0.46
7:D:173:GLU:HG3	7:D:174:VAL:N	2.30	0.46
8:E:35:TYR:HA	12:J:127:ILE:CD1	2.44	0.46
32:I:89:SER:HB3	32:I:97:VAL:CG2	2.46	0.46
13:K:87:ARG:NH1	39:K:4066:HOH:O	2.49	0.46
20:R:114:VAL:HA	20:R:144:GLU:O	2.15	0.46
26:X:25:ARG:HD2	39:X:3861:HOH:O	2.16	0.46
27:Y:136:LYS:HE3	27:Y:138:ARG:NH1	2.30	0.46
1:0:1173:A:H4'	1:0:1174:A:C8	2.51	0.46
1:0:271:C:H41	1:0:378:A:H2	1.64	0.46
1:0:2784:A:H1'	8:E:60:SER:OG	2.15	0.46
1:0:2824:C:H5''	1:0:2825:C:H5'	1.98	0.46
1:0:40:C:H6	1:0:40:C:O5'	1.99	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:129:HIS:HD2	6:C:165:ASP:OD2	1.98	0.46
14:L:121:ILE:HG12	14:L:141:GLU:HB2	1.98	0.46
16:N:32:PRO:HD2	16:N:99:GLU:O	2.16	0.46
1:O:1342:C:O2'	1:O:1343:C:H5'	2.15	0.46
1:O:136:C:H2'	1:O:137:U:O4'	2.15	0.46
1:O:1786:C:OP1	18:P:74:GLN:HG2	2.16	0.46
1:O:2472:C:O2'	1:O:2634:G:H4'	2.15	0.46
1:O:2911:C:O2'	1:O:2912:C:H5'	2.16	0.46
1:O:899:C:H5'	39:O:3799:HOH:O	2.16	0.46
4:A:94:LEU:HD12	4:A:98:GLU:CB	2.43	0.46
5:B:80:ARG:HB2	5:B:145:HIS:CE1	2.51	0.46
39:O:6254:HOH:O	13:K:87:ARG:CZ	2.64	0.46
19:Q:64:GLU:HG3	19:Q:74:ASP:OD2	2.16	0.46
1:O:602:A:O2'	1:O:605:C:H4'	2.15	0.46
29:1:28:HIS:CD2	29:1:31:LYS:HG3	2.50	0.46
5:B:75:GLU:C	5:B:77:PRO:HD3	2.36	0.46
5:B:41:PHE:HA	5:B:79:MET:HE1	1.96	0.46
6:C:27:ARG:HG2	6:C:30:LEU:HG	1.97	0.46
1:O:2348:C:H1'	7:D:131:THR:HG21	1.98	0.46
8:E:85:GLU:HG3	8:E:169:THR:OG1	2.16	0.46
11:H:63:GLU:O	11:H:67:LEU:HB2	2.16	0.46
13:K:34:VAL:CG2	13:K:47:ALA:HB2	2.46	0.46
15:M:49:ALA:C	15:M:54:TYR:HB3	2.36	0.46
16:N:151:ASP:OD1	16:N:166:ALA:HA	2.16	0.46
16:N:86:LEU:O	16:N:90:LEU:HG	2.15	0.46
1:O:710:G:H5'	17:O:25:VAL:CG1	2.46	0.46
17:O:96:VAL:HG13	17:O:100:GLN:HB2	1.98	0.46
24:V:12:THR:HG23	24:V:14:ALA:N	2.31	0.46
24:V:1:THR:CG2	24:V:2:VAL:H	2.15	0.46
1:O:123:U:H1'	39:O:7856:HOH:O	2.16	0.46
1:O:834:G:H3'	1:O:835:U:H4'	1.98	0.46
29:1:56:GLU:HG2	29:1:56:GLU:OXT	2.16	0.46
4:A:217:ARG:CG	4:A:217:ARG:HH11	2.29	0.46
4:A:39:ALA:HB3	4:A:61:GLU:OE2	2.16	0.46
5:B:312:ARG:HD3	5:B:315:VAL:HG13	1.97	0.46
8:E:81:GLU:HA	8:E:133:VAL:O	2.15	0.46
32:I:113:HIS:HE1	32:I:121:LEU:HD22	1.81	0.46
12:J:71:TYR:CD1	12:J:72:PRO:HD2	2.51	0.46
14:L:1:THR:HB	14:L:6:ARG:NH1	2.31	0.46
25:W:21:LEU:HD22	25:W:26:ILE:HD13	1.96	0.46
1:O:1183:C:H5	1:O:1192:A:OP1	2.00	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1200:A:H3'	39:0:6295:HOH:O	2.16	0.45
1:0:1847:A:OP1	4:A:175:LYS:HG3	2.16	0.45
1:0:2064:U:H4'	1:0:2653:A:OP1	2.15	0.45
1:0:2679:G:H2'	1:0:2681:A:OP2	2.15	0.45
5:B:294:TYR:HE2	39:B:9647:HOH:O	1.99	0.45
5:B:265:LEU:CD2	5:B:316:ARG:HD3	2.46	0.45
11:H:78:GLY:C	11:H:80:GLU:H	2.20	0.45
14:L:129:ALA:O	14:L:133:VAL:HG23	2.16	0.45
1:0:392:U:C5'	15:M:193:LYS:HB3	2.46	0.45
16:N:23:ARG:NH1	16:N:23:ARG:HG2	2.31	0.45
16:N:86:LEU:HD12	16:N:125:ALA:HB2	1.98	0.45
22:T:38:ARG:HG3	22:T:38:ARG:HH11	1.81	0.45
1:0:121:U:O4	29:1:18:LYS:HG2	2.15	0.45
1:0:1503:U:H2'	1:0:1504:A:O4'	2.16	0.45
1:0:236:A:H8	1:0:236:A:OP1	1.99	0.45
1:0:288:A:H2'	1:0:289:G:C8	2.50	0.45
2:9:3050:G:H5''	16:N:159:TYR:HE1	1.81	0.45
9:F:48:VAL:CG2	9:F:74:PHE:HB3	2.46	0.45
14:L:73:VAL:HG21	14:L:116:HIS:CD2	2.51	0.45
17:O:59:VAL:CG2	17:O:111:VAL:CG2	2.94	0.45
20:R:132:ARG:CZ	39:R:9492:HOH:O	2.63	0.45
20:R:84:ALA:O	20:R:88:PHE:HD1	1.99	0.45
1:0:1025:C:H5'	25:W:23:MET:O	2.16	0.45
1:0:2356:A:H5'	39:0:6178:HOH:O	2.16	0.45
1:0:622:G:P	27:Y:148:GLY:HA3	2.56	0.45
1:0:968:G:H1'	11:H:32:LYS:HD2	1.98	0.45
7:D:64:ARG:NE	7:D:67:ASP:HB3	2.32	0.45
9:F:52:GLU:OE1	9:F:78:GLU:OE1	2.34	0.45
32:I:118:SER:HB2	32:I:123:ASN:HB2	1.98	0.45
32:I:72:VAL:HG13	32:I:73:PRO:HD2	1.98	0.45
12:J:63:ILE:HG22	12:J:64:GLY:N	2.30	0.45
15:M:74:LYS:HG3	15:M:75:ARG:N	2.31	0.45
22:T:32:ARG:NH1	22:T:38:ARG:NH1	2.63	0.45
25:W:11:VAL:O	25:W:12:ASN:HB2	2.16	0.45
1:0:259:G:H21	15:M:58:GLN:NE2	2.15	0.45
1:0:2748:G:H8	39:0:8049:HOH:O	2.00	0.45
1:0:2779:G:H21	8:E:143:GLN:HE22	1.64	0.45
6:C:84:VAL:HG12	6:C:85:LYS:HG2	1.97	0.45
7:D:10:PHE:CG	7:D:11:HIS:N	2.85	0.45
8:E:6:GLU:HA	8:E:46:THR:HG22	1.97	0.45
1:0:56:G:H5''	24:V:50:ARG:NH1	2.32	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:X:76:ARG:NH1	26:X:76:ARG:HG3	2.31	0.45
1:O:1335:C:OP2	27:Y:207:SER:HB3	2.16	0.45
1:O:157:G:H4'	15:M:95:LYS:HE2	1.98	0.45
1:O:1603:A:H5'	1:O:1605:G:C4'	2.46	0.45
1:O:2015:A:H2'	1:O:2016:U:O4'	2.17	0.45
1:O:810:G:H1'	39:O:7740:HOH:O	2.17	0.45
30:2:35:ARG:HB2	39:2:2691:HOH:O	2.16	0.45
2:9:3042:C:O2	7:D:76:ARG:NH1	2.48	0.45
2:9:3107:C:H5	39:9:3167:HOH:O	1.99	0.45
4:A:94:LEU:HG	4:A:99:ILE:HD11	1.97	0.45
11:H:28:ILE:HG23	39:H:9544:HOH:O	2.16	0.45
13:K:49:LEU:HD12	13:K:80:ILE:HD13	1.97	0.45
16:N:108:SER:HA	16:N:109:PRO:HD3	1.81	0.45
26:X:66:THR:HG23	26:X:67:PRO:HD2	1.99	0.45
1:O:2421:G:H2'	39:O:4659:HOH:O	2.16	0.45
5:B:178:ALA:O	5:B:182:VAL:HG23	2.16	0.45
5:B:84:LEU:HB2	5:B:182:VAL:HG21	1.99	0.45
5:B:87:TYR:O	5:B:138:GLY:N	2.35	0.45
12:J:88:PRO:O	12:J:94:GLY:HA3	2.17	0.45
18:P:50:GLN:HG2	39:P:204:HOH:O	2.16	0.45
27:Y:212:ARG:HD2	39:Y:9402:HOH:O	2.16	0.45
1:O:2398:A:H2'	1:O:2399:G:O4'	2.16	0.45
1:O:88:G:N7	30:2:28:LYS:HD2	2.31	0.45
1:O:999:C:H2'	1:O:1000:C:O4'	2.17	0.45
4:A:123:GLY:HA2	4:A:159:VAL:O	2.17	0.45
5:B:243:ASN:HA	5:B:244:PRO:C	2.37	0.45
7:D:40:ILE:HG13	7:D:41:LEU:N	2.32	0.45
8:E:15:GLN:NE2	8:E:40:VAL:O	2.50	0.45
16:N:143:ARG:HE	16:N:143:ARG:HB3	1.56	0.45
21:S:11:THR:H	21:S:14:ALA:HB3	1.81	0.45
23:U:4:ARG:NH1	23:U:4:ARG:HG2	2.31	0.45
1:O:1151:G:OP1	10:G:63:ARG:NH1	2.50	0.45
1:O:1192:A:H3'	1:O:1193:A:H5'	1.99	0.45
1:O:1592:G:H2'	1:O:1593:C:C6	2.52	0.45
1:O:2809:G:H2'	1:O:2810:G:O4'	2.17	0.45
1:O:2857:C:H2'	1:O:2858:U:C6	2.52	0.45
1:O:328:U:O4'	6:C:202:THR:HG22	2.16	0.45
1:O:812:A:H2'	1:O:813:C:C6	2.51	0.45
29:1:18:LYS:HB2	30:2:49:GLU:CG	2.45	0.45
31:3:6:ARG:NH1	31:3:21:GLU:HG3	2.32	0.45
7:D:103:ASN:ND2	7:D:134:LEU:H	2.14	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:10:SER:O	14:L:11:ARG:HB3	2.17	0.45
14:L:144:ASP:O	14:L:147:GLU:HB2	2.17	0.45
14:L:72:ASN:HB2	39:L:9478:HOH:O	2.16	0.45
25:W:139:GLY:O	25:W:141:HIS:CD2	2.70	0.45
27:Y:148:GLY:O	27:Y:154:ARG:HD3	2.17	0.45
1:0:371:U:H2'	1:0:372:A:H8	1.82	0.45
1:0:95:A:H5''	1:0:97:G:O4'	2.17	0.45
39:O:7282:HOH:O	16:N:4:PRO:HD2	2.17	0.45
1:0:793:A:H5''	18:P:83:LYS:HG2	1.99	0.45
20:R:114:VAL:HG13	20:R:114:VAL:O	2.17	0.45
22:T:20:HIS:HB3	22:T:41:ARG:HD2	1.98	0.45
22:T:3:GLN:HA	22:T:4:PRO:HD3	1.82	0.45
1:0:1555:G:H4'	1:0:1630:A:C2	2.51	0.45
1:0:1667:A:C8	1:0:1667:A:H5'	2.42	0.45
1:0:1994:A:P	13:K:66:ARG:HH22	2.40	0.45
1:0:2699:A:H2'	1:0:2700:G:O4'	2.15	0.45
2:9:3054:A:O2'	2:9:3055:U:H5'	2.16	0.45
7:D:170:TYR:O	7:D:171:ASP:CB	2.65	0.45
32:I:99:ASP:O	32:I:100:LEU:HD23	2.17	0.45
24:V:51:LYS:O	24:V:55:ARG:HG3	2.17	0.45
27:Y:115:ARG:NE	39:Y:9356:HOH:O	2.50	0.45
1:0:1787:C:OP1	18:P:68:LYS:HE2	2.18	0.44
1:0:1834:C:H2'	1:0:1840:A:N6	2.32	0.44
1:0:2568:A:H5''	1:0:2702:A:O2'	2.17	0.44
1:0:497:A:H2'	1:0:498:A:C5'	2.47	0.44
6:C:180:SER:HB2	39:C:9251:HOH:O	2.17	0.44
6:C:218:VAL:N	39:C:9229:HOH:O	2.50	0.44
6:C:142:ASP:OD1	6:C:236:THR:HG23	2.18	0.44
7:D:60:GLU:O	7:D:60:GLU:HG3	2.17	0.44
14:L:124:ASP:OD1	14:L:149:ARG:NH2	2.50	0.44
16:N:49:THR:CG2	16:N:56:ASP:HB2	2.45	0.44
21:S:81:ILE:HG23	39:S:9494:HOH:O	2.17	0.44
1:0:2866:U:C4	23:U:50:GLU:HB3	2.52	0.44
25:W:122:ARG:HH22	25:W:154:ARG:HG2	1.79	0.44
1:0:2890:A:H1'	23:U:56:ARG:CZ	2.46	0.44
4:A:65:ARG:HH11	4:A:65:ARG:HG2	1.82	0.44
1:0:2545:U:OP2	5:B:2:GLN:NE2	2.50	0.44
11:H:29:ALA:C	11:H:30:GLN:HG3	2.37	0.44
15:M:22:GLU:HG2	15:M:26:GLN:NE2	2.32	0.44
18:P:16:VAL:HG13	18:P:20:ARG:CZ	2.47	0.44
22:T:49:GLU:OE2	22:T:51:LEU:HD21	2.17	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:U:52:THR:CG2	23:U:54:THR:HB	2.47	0.44
25:W:88:THR:HG23	25:W:110:GLN:HB3	1.99	0.44
1:0:366:U:H2'	1:0:367:G:O4'	2.17	0.44
1:0:415:A:O2'	1:0:416:G:H5'	2.18	0.44
1:0:629:A:H2'	1:0:630:A:O4'	2.17	0.44
6:C:168:ARG:NH2	6:C:190:ALA:O	2.50	0.44
9:F:60:VAL:O	9:F:60:VAL:CG1	2.64	0.44
14:L:134:GLU:HA	14:L:138:GLY:O	2.17	0.44
18:P:135:ALA:HB1	18:P:139:ARG:HH12	1.82	0.44
20:R:39:THR:HG22	20:R:41:GLY:H	1.83	0.44
24:V:5:VAL:CG1	24:V:9:ARG:NH1	2.81	0.44
39:0:6811:HOH:O	27:Y:158:LYS:HD3	2.18	0.44
4:A:101:GLU:OE2	4:A:131:HIS:HB2	2.18	0.44
4:A:69:LEU:HD23	4:A:107:ASN:CG	2.37	0.44
5:B:71:VAL:CG1	5:B:296:LEU:HD22	2.48	0.44
32:I:87:THR:HG22	32:I:88:GLY:N	2.32	0.44
13:K:65:ARG:NE	39:K:5358:HOH:O	2.46	0.44
1:0:1666:C:C2'	1:0:1667:A:H5''	2.47	0.44
1:0:1878:G:C1'	39:0:6649:HOH:O	2.60	0.44
1:0:2480:G:H3'	39:0:4764:HOH:O	2.16	0.44
1:0:338:C:H4'	6:C:174:ILE:HD11	1.99	0.44
1:0:40:C:H4'	39:0:7503:HOH:O	2.17	0.44
1:0:2101:A:OP2	6:C:66:GLY:HA2	2.18	0.44
15:M:187:LEU:HD22	15:M:194:ALA:HB3	1.99	0.44
22:T:52:ARG:O	22:T:53:GLY:O	2.35	0.44
1:0:1641:A:C2'	1:0:1642:A:H5'	2.46	0.44
1:0:236:A:H4'	1:0:237:G:H5'	2.00	0.44
1:0:2505:G:C2'	1:0:2506:A:H5'	2.48	0.44
1:0:2907:C:H2'	1:0:2908:A:O4'	2.17	0.44
30:2:20:ARG:HG3	30:2:21:VAL:N	2.33	0.44
2:9:3049:G:H2'	2:9:3050:G:O4'	2.18	0.44
4:A:207:GLN:O	4:A:208:HIS:HB3	2.17	0.44
5:B:5:ARG:HD2	5:B:8:LYS:NZ	2.33	0.44
13:K:109:LEU:HD13	13:K:113:ILE:CD1	2.45	0.44
14:L:65:ASP:CG	14:L:111:ALA:HB3	2.37	0.44
16:N:152:GLU:HA	16:N:152:GLU:OE1	2.18	0.44
22:T:48:VAL:CG1	22:T:96:VAL:HG21	2.47	0.44
1:0:1086:A:C6	25:W:11:VAL:HG11	2.53	0.44
25:W:5:VAL:O	25:W:52:VAL:CG2	2.65	0.44
1:0:12:U:H2'	1:0:13:G:H5'	2.00	0.44
1:0:2506:A:O2'	1:0:2507:G:O5'	2.35	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:3:69:TYR:CZ	31:3:80:ARG:HD2	2.53	0.44
7:D:154:LYS:HD2	7:D:154:LYS:N	2.28	0.44
9:F:70:LYS:C	9:F:72:VAL:H	2.21	0.44
14:L:149:ARG:O	14:L:150:GLN:HB2	2.17	0.44
22:T:24:ARG:HH21	22:T:39:ASN:HD22	1.65	0.44
25:W:118:LEU:HD12	25:W:153:MET:HE3	1.99	0.44
1:0:2718:C:H5'	1:0:2718:C:C6	2.48	0.44
1:0:120:A:H5'	29:1:20:ARG:HH21	1.82	0.44
4:A:36:ASP:HA	4:A:83:GLY:HA3	1.99	0.44
8:E:23:GLU:HG2	8:E:28:SER:CB	2.47	0.44
11:H:3:ALA:CB	11:H:58:ARG:HH12	2.30	0.44
1:0:566:A:H2'	1:0:567:U:O4'	2.17	0.44
4:A:3:ARG:H	4:A:3:ARG:HG2	1.66	0.44
5:B:171:VAL:HG23	5:B:172:SER:N	2.33	0.44
5:B:56:ASP:HB3	5:B:322:ARG:HH21	1.83	0.44
6:C:107:ARG:NH1	39:C:9236:HOH:O	2.51	0.44
7:D:37:ALA:O	7:D:40:ILE:HG12	2.18	0.44
7:D:78:GLU:O	7:D:82:GLU:HG3	2.17	0.44
9:F:50:VAL:CG2	9:F:63:ILE:HG21	2.47	0.44
10:G:64:ASN:N	10:G:64:ASN:ND2	2.66	0.44
32:I:124:ALA:O	32:I:128:VAL:HG23	2.18	0.44
16:N:23:ARG:NH1	39:N:9346:HOH:O	2.51	0.44
16:N:72:GLU:HG2	16:N:72:GLU:O	2.17	0.44
1:0:1298:U:H2'	1:0:1299:G:C8	2.52	0.43
1:0:1314:U:H2'	39:0:6410:HOH:O	2.18	0.43
1:0:2541:U:O2'	3:4:76:DA:H4'	2.17	0.43
5:B:138:GLY:O	5:B:139:ASP:O	2.36	0.43
8:E:145:ALA:HB1	8:E:168:ILE:CD1	2.48	0.43
9:F:65:GLU:O	9:F:69:GLU:HG2	2.18	0.43
32:I:102:VAL:HG23	32:I:140:GLU:O	2.18	0.43
16:N:89:GLY:O	16:N:92:ALA:HB3	2.18	0.43
22:T:47:THR:HB	22:T:100:ASP:HB3	1.99	0.43
27:Y:189:ASN:HD22	27:Y:192:ASP:H	1.64	0.43
28:Z:13:ARG:NH1	39:Z:9218:HOH:O	2.51	0.43
1:0:2531:U:O2'	1:0:2532:A:H5'	2.17	0.43
5:B:234:ARG:HH11	5:B:234:ARG:HB3	1.83	0.43
12:J:132:LEU:HA	12:J:132:LEU:HD23	1.85	0.43
14:L:125:PHE:CE1	14:L:140:VAL:HG13	2.53	0.43
16:N:167:ASP:O	16:N:168:LEU:HG	2.17	0.43
23:U:20:MET:CG	23:U:28:THR:HG23	2.48	0.43
25:W:122:ARG:NH1	25:W:152:ALA:O	2.51	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:26:ILE:HG13	25:W:26:ILE:O	2.18	0.43
27:Y:187:VAL:CG2	27:Y:192:ASP:HB2	2.48	0.43
1:0:1180:U:H1'	39:0:3831:HOH:O	2.18	0.43
1:0:2372:A:H2'	1:0:2373:U:C6	2.53	0.43
1:0:2415:A:H2'	1:0:2416:G:H5'	2.00	0.43
1:0:2720:C:O2	13:K:87:ARG:NH2	2.51	0.43
1:0:2807:U:P	5:B:27:ASN:HD21	2.40	0.43
5:B:139:ASP:HB3	39:B:9547:HOH:O	2.17	0.43
5:B:149:ASP:HB2	39:B:9577:HOH:O	2.18	0.43
5:B:41:PHE:HA	5:B:79:MET:CE	2.49	0.43
6:C:79:ARG:O	6:C:87:ARG:HG2	2.18	0.43
9:F:110:ASP:O	9:F:114:LYS:HG3	2.18	0.43
39:0:5535:HOH:O	11:H:58:ARG:HG3	2.18	0.43
1:0:2036:C:O4'	13:K:44:LEU:HG	2.18	0.43
14:L:145:LEU:C	14:L:145:LEU:HD23	2.38	0.43
16:N:116:PHE:HB3	16:N:136:LEU:HD23	2.00	0.43
20:R:34:GLU:HG2	20:R:46:TYR:OH	2.17	0.43
22:T:79:LEU:HG	22:T:89:ARG:HB2	2.00	0.43
28:Z:72:GLU:HB3	28:Z:77:LYS:HE3	2.00	0.43
1:0:360:A:H2'	1:0:361:C:O4'	2.18	0.43
1:0:450:C:OP1	6:C:184:ARG:NH2	2.38	0.43
1:0:462:A:H2'	39:0:5450:HOH:O	2.17	0.43
1:0:635:A:H2'	1:0:636:G:H5''	2.00	0.43
7:D:25:MET:CE	7:D:41:LEU:HG	2.39	0.43
7:D:49:PRO:HB3	39:D:5828:HOH:O	2.19	0.43
1:0:2338:G:OP1	7:D:97:GLN:HG2	2.19	0.43
32:I:88:GLY:C	32:I:97:VAL:HG21	2.38	0.43
25:W:122:ARG:HG2	25:W:152:ALA:O	2.17	0.43
27:Y:184:GLU:HG2	27:Y:229:LEU:HD11	2.00	0.43
1:0:1741:U:O2'	1:0:2723:G:H4'	2.19	0.43
1:0:2589:U:H2'	1:0:2590:U:C6	2.53	0.43
1:0:2698:G:H2'	1:0:2699:A:C8	2.53	0.43
5:B:24:PRO:CG	5:B:204:GLY:HA2	2.48	0.43
1:0:2898:G:H4'	5:B:288:GLY:HA2	1.99	0.43
5:B:305:ASP:O	5:B:306:LYS:CB	2.66	0.43
5:B:73:VAL:HG22	5:B:296:LEU:CD2	2.48	0.43
7:D:25:MET:HE1	7:D:37:ALA:O	2.18	0.43
7:D:25:MET:CE	7:D:40:ILE:HD11	2.49	0.43
11:H:28:ILE:HA	11:H:63:GLU:OE1	2.18	0.43
13:K:115:ARG:HG3	13:K:116:GLU:N	2.32	0.43
14:L:143:THR:CG2	14:L:144:ASP:H	2.31	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:48:VAL:HG11	16:N:55:ASP:HB3	2.00	0.43
1:0:2663:U:O2	39:0:8476:HOH:O	2.20	0.43
1:0:2820:A:H2'	1:0:2821:C:C6	2.53	0.43
1:0:558:C:H2'	1:0:559:U:H5''	1.98	0.43
31:3:38:ARG:CB	31:3:42:ARG:HH12	2.31	0.43
31:3:38:ARG:HB3	31:3:42:ARG:HH12	1.84	0.43
2:9:3014:G:H2'	2:9:3015:C:H5'	2.01	0.43
2:9:3029:C:C2'	2:9:3030:C:H5'	2.48	0.43
4:A:17:ARG:HD2	39:A:9527:HOH:O	2.18	0.43
5:B:91:PRO:O	12:J:144:THR:HG21	2.18	0.43
14:L:133:VAL:HB	39:L:9453:HOH:O	2.19	0.43
14:L:150:GLN:HB3	39:L:9466:HOH:O	2.19	0.43
25:W:48:VAL:CG1	25:W:48:VAL:O	2.66	0.43
26:X:66:THR:HG22	26:X:67:PRO:O	2.18	0.43
1:0:2011:A:H4'	1:0:2012:U:O5'	2.19	0.43
1:0:2237:G:H1'	1:0:2238:A:C8	2.54	0.43
1:0:2353:A:H4'	1:0:2354:A:O5'	2.17	0.43
1:0:249:G:O2'	1:0:250:C:H5'	2.19	0.43
1:0:969:G:H1	1:0:999:C:N4	2.16	0.43
30:2:48:ASP:O	30:2:49:GLU:HB2	2.18	0.43
7:D:146:LYS:HZ3	16:N:107:ASN:HD21	1.66	0.43
8:E:20:ILE:HD11	8:E:40:VAL:CG1	2.39	0.43
9:F:48:VAL:HG12	9:F:97:ALA:CB	2.47	0.43
32:I:139:ILE:CG2	32:I:140:GLU:N	2.82	0.43
13:K:49:LEU:HD12	13:K:80:ILE:HG21	2.00	0.43
18:P:37:ARG:HG2	18:P:37:ARG:HH11	1.84	0.43
24:V:8:ILE:CG2	24:V:59:ILE:HG13	2.48	0.43
1:0:2499:U:H2'	1:0:2500:C:H6	1.84	0.43
1:0:2587:OMU:H2'	1:0:2589:U:H5''	2.00	0.43
1:0:40:C:N3	1:0:441:A:H2	2.16	0.43
1:0:644:G:N3	1:0:644:G:H5'	2.34	0.43
1:0:681:G:N7	39:0:7461:HOH:O	2.36	0.43
1:0:941:G:C5	1:0:942:U:C4	3.07	0.43
4:A:164:ARG:CZ	39:A:9571:HOH:O	2.66	0.43
6:C:45:ASP:OD2	6:C:98:ARG:HD2	2.19	0.43
7:D:60:GLU:O	7:D:61:PHE:C	2.56	0.43
1:0:1992:U:OP2	13:K:66:ARG:HD2	2.18	0.43
17:O:14:LEU:HD23	17:O:102:ILE:HD11	1.99	0.43
24:V:8:ILE:HA	24:V:11:MET:HE2	2.00	0.43
25:W:5:VAL:O	25:W:52:VAL:HG23	2.19	0.43
1:0:1057:A:H2'	1:0:1058:A:C8	2.54	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1174:A:C5	1:0:1201:C:H4'	2.54	0.43
1:0:1470:A:OP1	15:M:93:ARG:HD2	2.18	0.43
1:0:204:A:H2'	1:0:205:U:H5'	1.99	0.43
1:0:802:G:H2'	1:0:803:C:C6	2.54	0.43
3:4:74:C:H2'	3:4:75:C:H5'	2.01	0.43
4:A:26:ASP:OD2	4:A:28:GLU:HG3	2.18	0.43
5:B:119:HIS:O	5:B:121:PRO:HD3	2.19	0.43
6:C:151:GLN:O	6:C:154:VAL:HB	2.18	0.43
11:H:154:TYR:C	11:H:154:TYR:CD1	2.92	0.43
11:H:83:TYR:C	11:H:83:TYR:CD1	2.91	0.43
12:J:63:ILE:CG2	12:J:64:GLY:N	2.82	0.43
39:0:5842:HOH:O	25:W:119:HIS:CG	2.72	0.43
25:W:3:ALA:O	25:W:54:PHE:HA	2.19	0.43
1:0:1160:G:HO2'	1:0:1190:G:H8	1.63	0.43
1:0:1236:A:C8	12:J:63:ILE:HD11	2.54	0.43
1:0:1477:C:H5'	1:0:1868:G:H5''	2.00	0.43
1:0:2697:A:H2'	1:0:2698:G:O4'	2.19	0.43
1:0:286:U:H2'	1:0:287:C:C6	2.54	0.43
2:9:3050:G:H5''	16:N:159:TYR:CE1	2.54	0.43
12:J:131:THR:HG22	12:J:133:GLY:N	2.34	0.43
16:N:71:TRP:HB2	39:N:9338:HOH:O	2.18	0.43
17:O:25:VAL:HG23	17:O:26:TRP:N	2.33	0.43
26:X:45:GLU:HG3	39:X:6178:HOH:O	2.19	0.43
1:0:1299:G:N2	39:0:5248:HOH:O	2.51	0.42
1:0:2416:G:O2'	16:N:25:ARG:HG2	2.19	0.42
1:0:2452:G:H5'	39:3:9488:HOH:O	2.17	0.42
1:0:364:C:H2'	1:0:365:G:O4'	2.19	0.42
6:C:185:LYS:HD3	6:C:186:TYR:CE1	2.54	0.42
13:K:49:LEU:HD22	13:K:117:VAL:CG2	2.49	0.42
15:M:61:ILE:N	15:M:61:ILE:HD12	2.33	0.42
20:R:132:ARG:NH2	39:R:9492:HOH:O	2.52	0.42
22:T:38:ARG:HG3	22:T:38:ARG:NH1	2.34	0.42
23:U:11:THR:HG22	23:U:53:ASP:OD2	2.19	0.42
26:X:80:GLU:O	26:X:80:GLU:HG2	2.19	0.42
27:Y:186:ARG:HG2	27:Y:186:ARG:HH11	1.84	0.42
1:0:1351:G:OP1	6:C:96:LYS:NZ	2.41	0.42
1:0:396:U:OP2	31:3:38:ARG:HD2	2.18	0.42
1:0:526:U:H2'	1:0:527:U:C6	2.54	0.42
1:0:669:G:O2'	1:0:670:G:H5'	2.19	0.42
1:0:92:G:H4'	24:V:44:GLY:HA3	2.01	0.42
30:2:18:ASN:HD21	30:2:40:ARG:H	1.66	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3059:C:O5'	2:9:3059:C:H6	2.02	0.42
7:D:27:ILE:HG22	7:D:28:GLY:N	2.32	0.42
11:H:119:LYS:HB2	11:H:119:LYS:HE3	1.81	0.42
32:I:75:THR:HA	32:I:112:LYS:NZ	2.34	0.42
14:L:80:ASP:HB2	14:L:90:ARG:HB3	2.01	0.42
16:N:103:ASP:OD1	16:N:103:ASP:C	2.58	0.42
1:0:1200:A:H4'	39:0:7822:HOH:O	2.19	0.42
1:0:200:U:H2'	39:0:4038:HOH:O	2.18	0.42
1:0:2238:A:O2'	1:0:2239:C:H5'	2.18	0.42
1:0:2769:C:H2'	1:0:2770:G:C5'	2.48	0.42
30:2:20:ARG:HD2	30:2:39:ARG:NH2	2.34	0.42
5:B:42:ALA:H	5:B:79:MET:HE2	1.85	0.42
6:C:157:LEU:CD1	6:C:166:ILE:HD11	2.49	0.42
32:I:129:VAL:HG13	32:I:139:ILE:HD11	2.01	0.42
16:N:152:GLU:C	16:N:154:LEU:N	2.72	0.42
19:Q:11:ARG:HD3	39:Q:5620:HOH:O	2.18	0.42
19:Q:77:ASP:HB3	19:Q:82:LYS:HE3	2.01	0.42
24:V:42:ASN:O	24:V:44:GLY:N	2.52	0.42
1:0:2421:G:H4'	39:0:5345:HOH:O	2.18	0.42
1:0:2487:C:H5	39:0:5455:HOH:O	2.02	0.42
2:9:3064:C:C2'	2:9:3065:A:H5'	2.49	0.42
4:A:51:ARG:HH21	4:A:55:VAL:HG23	1.84	0.42
5:B:36:PRO:CA	5:B:168:GLY:HA3	2.44	0.42
6:C:218:VAL:HG12	39:C:9229:HOH:O	2.18	0.42
8:E:166:VAL:HG12	39:E:3134:HOH:O	2.18	0.42
12:J:39:VAL:CG1	12:J:40:ASN:N	2.82	0.42
1:0:2036:C:C1'	13:K:44:LEU:HG	2.50	0.42
14:L:77:ALA:C	14:L:79:ASP:H	2.23	0.42
26:X:74:ALA:CB	26:X:85:VAL:HG22	2.49	0.42
27:Y:187:VAL:HB	27:Y:203:VAL:CG2	2.50	0.42
28:Z:57:CYS:SG	28:Z:59:TYR:HB3	2.59	0.42
1:0:1821:A:O2'	1:0:1822:A:H5'	2.20	0.42
1:0:1477:C:C5'	1:0:1868:G:H5''	2.50	0.42
1:0:185:G:C4'	1:0:186:A:H4'	2.50	0.42
1:0:2900:G:H2'	1:0:2901:C:O4'	2.19	0.42
1:0:426:G:H2'	1:0:427:C:O4'	2.19	0.42
1:0:666:A:H2'	1:0:667:C:O4'	2.20	0.42
1:0:69:A:H5'	1:0:69:A:H8	1.85	0.42
1:0:889:C:H2'	1:0:890:C:C6	2.55	0.42
6:C:98:ARG:NH1	39:C:9163:HOH:O	2.51	0.42
9:F:79:GLN:HG3	9:F:82:ASP:OD2	2.18	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:I:92:PRO:C	32:I:94:GLU:N	2.70	0.42
14:L:79:ASP:O	14:L:80:ASP:O	2.37	0.42
20:R:69:LYS:HB2	20:R:72:VAL:HG23	2.00	0.42
24:V:8:ILE:HA	24:V:11:MET:CE	2.50	0.42
25:W:64:THR:O	25:W:68:THR:HG22	2.20	0.42
1:O:1044:C:H5''	39:O:9648:HOH:O	2.19	0.42
1:O:1099:G:H2'	1:O:1100:G:O4'	2.20	0.42
1:O:120:A:H2'	1:O:120:A:N3	2.35	0.42
1:O:23:G:C6	1:O:24:G:N1	2.88	0.42
1:O:2568:A:H2'	1:O:2569:A:O4'	2.20	0.42
30:2:35:ARG:HG2	39:2:6391:HOH:O	2.19	0.42
9:F:30:LYS:HE2	9:F:99:THR:HG21	2.01	0.42
13:K:115:ARG:HG2	13:K:116:GLU:OE1	2.19	0.42
13:K:27:ARG:HD2	39:K:4747:HOH:O	2.18	0.42
17:O:77:ALA:HA	17:O:96:VAL:O	2.20	0.42
27:Y:108:ASP:N	27:Y:108:ASP:OD1	2.49	0.42
1:O:1236:A:H2'	1:O:1237:U:O4'	2.19	0.42
1:O:1328:A:C8	27:Y:169:ARG:HD3	2.54	0.42
1:O:27:U:H2'	1:O:28:G:O4'	2.20	0.42
1:O:319:A:H4'	1:O:338:C:C5	2.54	0.42
1:O:371:U:H2'	1:O:372:A:C8	2.55	0.42
1:O:440:C:H2'	1:O:441:A:C8	2.55	0.42
1:O:697:G:H4'	1:O:730:G:O3'	2.19	0.42
1:O:960:G:N3	1:O:960:G:C2'	2.82	0.42
6:C:236:THR:HG22	6:C:239:ALA:HB2	2.01	0.42
32:I:80:LYS:HD3	32:I:86:GLU:O	2.20	0.42
15:M:82:ARG:O	15:M:84:LYS:N	2.52	0.42
16:N:24:LEU:HD22	39:Q:2847:HOH:O	2.19	0.42
25:W:125:HIS:HE1	39:W:3071:HOH:O	2.02	0.42
1:O:1168:C:H4'	39:I:5128:HOH:O	2.19	0.42
1:O:1289:C:H3'	39:O:6930:HOH:O	2.20	0.42
31:3:17:HIS:O	31:3:18:GLN:HG3	2.20	0.42
39:O:4983:HOH:O	4:A:11:ARG:CZ	2.68	0.42
6:C:136:VAL:HG22	6:C:137:PRO:HA	2.01	0.42
6:C:7:ASP:OD1	6:C:11:ASN:HB2	2.20	0.42
7:D:76:ARG:O	7:D:77:ASP:HB2	2.20	0.42
11:H:28:ILE:HG21	11:H:31:HIS:CE1	2.54	0.42
12:J:143:LYS:HG3	12:J:145:TRP:CE2	2.55	0.42
39:O:3171:HOH:O	25:W:119:HIS:HE1	2.03	0.42
26:X:54:ILE:HD11	26:X:85:VAL:HG12	2.02	0.42
27:Y:96:GLU:O	27:Y:235:GLU:HA	2.20	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1081:A:H5''	39:0:3751:HOH:O	2.19	0.42
1:0:1131:G:C6	1:0:1230:A:C4	3.08	0.42
1:0:1878:G:O2'	1:0:1879:U:C5	2.66	0.42
1:0:2072:G:C6	1:0:2533:C:H1'	2.55	0.42
1:0:2133:U:H4'	1:0:2134:G:H5'	2.01	0.42
1:0:65:C:O2'	1:0:66:G:H5'	2.19	0.42
31:3:91:GLN:O	31:3:92:GLU:HB2	2.19	0.42
1:0:2820:A:OP1	5:B:98:THR:HG22	2.20	0.42
2:9:3014:G:C2'	16:N:1:ALA:HB2	2.50	0.42
19:Q:64:GLU:HG3	19:Q:74:ASP:CG	2.40	0.42
27:Y:99:ALA:HB2	27:Y:233:TYR:CZ	2.55	0.42
1:0:1181:A:H2'	1:0:1182:C:H5'	2.02	0.42
1:0:1714:C:O2'	1:0:1715:C:H5'	2.20	0.42
1:0:2329:C:O2'	1:0:2330:U:H5'	2.20	0.42
4:A:34:ASP:OD1	4:A:35:GLY:N	2.38	0.42
4:A:36:ASP:HB2	4:A:83:GLY:HA3	2.02	0.42
6:C:123:LEU:HD23	6:C:123:LEU:HA	1.83	0.42
6:C:165:ASP:O	6:C:168:ARG:HB3	2.20	0.42
12:J:19:MET:CE	12:J:132:LEU:HD21	2.48	0.42
14:L:69:ILE:HA	39:L:9478:HOH:O	2.20	0.42
2:9:3006:C:H4'	16:N:35:VAL:HG11	2.02	0.42
39:0:4845:HOH:O	19:Q:55:ARG:HD2	2.19	0.42
24:V:11:MET:HB3	24:V:15:GLU:HB2	2.00	0.42
25:W:41:TYR:CD2	25:W:44:MET:HE3	2.55	0.42
1:0:1495:C:H2'	1:0:1496:G:C8	2.54	0.41
1:0:2112:A:H2'	1:0:2113:G:C8	2.55	0.41
1:0:2587:OMU:H6	1:0:2587:OMU:O5'	2.20	0.41
1:0:2672:C:O2'	1:0:2673:U:H5'	2.20	0.41
1:0:2908:A:C2'	1:0:2909:G:H5'	2.49	0.41
29:1:10:LYS:N	39:1:9488:HOH:O	2.42	0.41
1:0:1311:G:O6	6:C:173:LYS:HE3	2.20	0.41
6:C:7:ASP:OD2	6:C:9:ASP:HB2	2.21	0.41
7:D:173:GLU:O	7:D:174:VAL:C	2.59	0.41
11:H:43:TYR:HA	11:H:44:PRO:HD3	1.78	0.41
1:0:1180:U:O2'	32:I:92:PRO:HD2	2.20	0.41
12:J:130:VAL:HG12	12:J:131:THR:N	2.35	0.41
17:O:45:LEU:CD1	17:O:88:LYS:HD2	2.50	0.41
19:Q:30:VAL:O	19:Q:30:VAL:HG12	2.19	0.41
19:Q:53:HIS:HA	19:Q:54:PRO:HD3	1.95	0.41
24:V:12:THR:HG23	24:V:14:ALA:H	1.84	0.41
25:W:122:ARG:CG	25:W:152:ALA:O	2.68	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:76:VAL:HG23	28:Z:63:LYS:HB3	2.01	0.41
1:0:1202:A:H2'	1:0:1203:G:O4'	2.20	0.41
2:9:3018:U:H2'	2:9:3019:G:H8	1.85	0.41
5:B:254:GLN:HG2	5:B:255:GLY:H	1.81	0.41
6:C:184:ARG:HB3	39:C:9169:HOH:O	2.19	0.41
8:E:91:PHE:HA	8:E:92:PRO:HD3	1.87	0.41
9:F:72:VAL:HA	9:F:73:PRO:HD3	1.90	0.41
11:H:40:ALA:HB1	11:H:137:TYR:CD2	2.55	0.41
11:H:26:SER:HA	11:H:59:HIS:CD2	2.55	0.41
11:H:70:ASN:O	11:H:74:ILE:HG13	2.20	0.41
13:K:75:ARG:HD3	13:K:112:PRO:O	2.21	0.41
22:T:21:LYS:HA	22:T:24:ARG:HG3	2.02	0.41
26:X:20:GLU:CD	26:X:21:PRO:HD2	2.40	0.41
1:0:2089:A:O2'	1:0:2090:G:H5'	2.19	0.41
1:0:517:U:H1'	39:0:8135:HOH:O	2.20	0.41
1:0:664:U:O4	1:0:681:G:H5''	2.20	0.41
1:0:764:C:H2'	1:0:765:G:O4'	2.20	0.41
30:2:5:LYS:O	30:2:9:LYS:HG3	2.20	0.41
1:0:2427:C:OP2	31:3:84:ARG:HD2	2.18	0.41
9:F:49:PHE:CD1	9:F:49:PHE:N	2.88	0.41
11:H:99:LYS:HD3	11:H:119:LYS:HD3	2.01	0.41
12:J:71:TYR:CG	12:J:72:PRO:HD2	2.55	0.41
15:M:59:GLY:HA3	15:M:141:ILE:CD1	2.49	0.41
17:O:87:THR:O	17:O:91:GLN:HG3	2.19	0.41
1:0:2388:C:H5'	19:Q:83:THR:O	2.20	0.41
25:W:65:VAL:CG1	25:W:116:LEU:HD13	2.50	0.41
1:0:2067:A:H2'	1:0:2068:G:O4'	2.20	0.41
1:0:2326:U:H4'	1:0:2412:G:C4'	2.50	0.41
1:0:1838:U:H1'	1:0:2644:C:O4'	2.21	0.41
1:0:559:U:H5'	1:0:559:U:C6	2.41	0.41
1:0:907:A:H2'	1:0:908:A:C8	2.55	0.41
1:0:2715:G:N2	5:B:264:GLU:OE1	2.53	0.41
2:9:3057:A:O2'	7:D:152:PRO:HD2	2.20	0.41
32:I:139:ILE:C	32:I:140:GLU:HG3	2.40	0.41
1:0:1164:U:OP1	32:I:74:PRO:HA	2.20	0.41
14:L:80:ASP:HB3	14:L:90:ARG:HB3	2.02	0.41
18:P:141:ILE:C	18:P:143:ALA:H	2.22	0.41
20:R:25:PHE:CE2	20:R:29:LYS:CE	2.99	0.41
21:S:10:VAL:HG11	24:V:36:ALA:CA	2.48	0.41
1:0:1342:C:C2'	1:0:1343:C:H5'	2.50	0.41
1:0:1759:A:N3	1:0:1818:C:H2'	2.35	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2032:U:H2'	1:0:2033:G:H5'	2.01	0.41
1:0:612:U:H2'	1:0:613:C:C6	2.56	0.41
2:9:3052:A:O2'	2:9:3053:G:H5'	2.20	0.41
5:B:62:ARG:CB	5:B:65:MET:HE3	2.50	0.41
6:C:30:LEU:HA	6:C:30:LEU:HD23	1.90	0.41
32:I:75:THR:HA	32:I:112:LYS:HZ3	1.86	0.41
1:0:1119:G:H2'	12:J:52:GLN:NE2	2.35	0.41
13:K:80:ILE:O	13:K:87:ARG:HA	2.20	0.41
1:0:926:A:H5'	14:L:39:GLU:OE2	2.20	0.41
16:N:37:ARG:CZ	16:N:105:GLY:HA3	2.51	0.41
1:0:1189:A:H1'	1:0:1209:C:H1'	2.02	0.41
1:0:710:G:H5'	17:O:25:VAL:HG13	2.03	0.41
1:0:821:U:H2'	1:0:822:C:C6	2.56	0.41
29:1:18:LYS:CB	30:2:49:GLU:HG2	2.47	0.41
4:A:135:VAL:HG21	4:A:147:ARG:HG2	2.02	0.41
4:A:66:ARG:CB	4:A:66:ARG:HH11	2.30	0.41
9:F:31:LYS:HE3	39:F:2623:HOH:O	2.20	0.41
32:I:132:CYS:C	32:I:134:SER:N	2.74	0.41
16:N:61:ALA:CB	16:N:88:ALA:HB2	2.48	0.41
17:O:97:SER:H	17:O:100:GLN:NE2	2.18	0.41
20:R:106:GLY:HA2	20:R:109:MET:CE	2.46	0.41
26:X:9:VAL:HG13	26:X:88:GLU:OE1	2.21	0.41
1:0:2326:U:H4'	1:0:2412:G:H4'	2.03	0.41
1:0:816:G:H5'	1:0:1598:A:H4'	2.02	0.41
30:2:44:ARG:HA	30:2:44:ARG:HD3	1.78	0.41
5:B:146:THR:O	5:B:159:PRO:HB3	2.21	0.41
5:B:294:TYR:C	5:B:294:TYR:CD1	2.93	0.41
1:0:500:G:O2'	20:R:94:ASN:ND2	2.54	0.41
25:W:146:ILE:HA	25:W:146:ILE:HD13	1.88	0.41
1:0:1226:G:H5'	39:0:5101:HOH:O	2.20	0.41
1:0:1573:A:H2'	1:0:1574:C:O4'	2.21	0.41
1:0:1603:A:C5'	1:0:1605:G:H5'	2.50	0.41
1:0:2314:G:C2'	1:0:2315:C:H5'	2.51	0.41
1:0:565:A:OP2	1:0:592:G:N1	2.48	0.41
1:0:671:A:O2'	1:0:672:G:H2'	2.21	0.41
4:A:66:ARG:NH1	4:A:66:ARG:CB	2.84	0.41
5:B:150:ALA:O	5:B:152:PRO:HD3	2.21	0.41
9:F:28:ALA:HB3	9:F:99:THR:O	2.20	0.41
13:K:107:THR:HG22	13:K:108:GLU:CG	2.43	0.41
18:P:63:ARG:NH2	39:P:191:HOH:O	2.54	0.41
20:R:39:THR:CG2	20:R:107:GLU:O	2.68	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:75:GLU:O	22:T:76:ASP:HB2	2.21	0.41
27:Y:187:VAL:HB	27:Y:203:VAL:HG22	2.02	0.41
1:0:1132:A:H2'	1:0:1133:A:C8	2.56	0.41
1:0:123:U:O2'	1:0:124:C:H5'	2.20	0.41
1:0:1659:A:H2'	1:0:1660:G:O4'	2.19	0.41
1:0:1768:C:H2'	1:0:1769:C:O4'	2.20	0.41
1:0:177:A:H2'	1:0:178:U:O4'	2.21	0.41
1:0:1940:C:H4'	39:0:7828:HOH:O	2.19	0.41
1:0:2103:A:N3	1:0:2103:A:H2'	2.35	0.41
1:0:2481:G:H5''	39:0:5116:HOH:O	2.20	0.41
1:0:2578:G:H5'	1:0:2578:G:C8	2.45	0.41
1:0:1739:G:H1'	1:0:2726:U:O4	2.20	0.41
4:A:43:VAL:HG21	4:A:59:GLU:HG3	2.03	0.41
5:B:260:HIS:HE1	39:B:9585:HOH:O	2.03	0.41
5:B:271:ASP:HB3	5:B:296:LEU:HD12	2.03	0.41
5:B:277:GLU:N	5:B:278:PRO:CD	2.84	0.41
1:0:2717:C:H5'	5:B:302:PRO:HA	2.02	0.41
7:D:44:ILE:HG23	7:D:45:THR:HG23	2.03	0.41
1:0:1119:G:N2	1:0:1246:A:H2	2.09	0.41
1:0:1849:G:H1'	1:0:2011:A:N1	2.35	0.41
1:0:2053:G:H4'	20:R:136:TRP:CE2	2.56	0.41
1:0:2361:A:H2'	1:0:2362:A:C8	2.55	0.41
1:0:2435:U:H1'	39:0:5981:HOH:O	2.21	0.41
1:0:2503:A:OP1	11:H:151:ARG:NH2	2.49	0.41
1:0:750:A:O3'	6:C:101:ASP:HB2	2.21	0.41
1:0:887:G:H2'	1:0:888:U:C6	2.55	0.41
4:A:206:ARG:N	4:A:206:ARG:HD3	2.23	0.41
4:A:6:GLY:HA3	39:A:9550:HOH:O	2.20	0.41
5:B:49:THR:HG21	5:B:280:VAL:HG23	2.03	0.41
14:L:89:PHE:N	39:L:9468:HOH:O	2.54	0.41
39:0:8066:HOH:O	15:M:91:ILE:HG12	2.21	0.41
17:O:45:LEU:HD12	17:O:88:LYS:HD2	2.02	0.41
18:P:16:VAL:CG1	18:P:20:ARG:CZ	2.99	0.41
20:R:4:TYR:CZ	20:R:15:LYS:HB3	2.55	0.41
22:T:88:PRO:HB3	39:T:6320:HOH:O	2.20	0.41
23:U:44:ARG:HB3	39:U:3805:HOH:O	2.20	0.41
1:0:797:A:O4'	28:Z:10:ARG:N	2.54	0.41
28:Z:39:CYS:SG	28:Z:41:ASN:HB3	2.60	0.41
1:0:1065:G:H5'	39:0:4141:HOH:O	2.20	0.41
1:0:1166:A:H1'	1:0:1192:A:N3	2.36	0.41
1:0:162:C:H2'	1:0:163:U:H5'	2.02	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2061:C:C2'	1:0:2062:A:H5'	2.51	0.41
1:0:2506:A:O2'	1:0:2507:G:P	2.78	0.41
1:0:289:G:N1	1:0:363:A:C2	2.83	0.41
29:1:8:GLN:HE22	29:1:11:LYS:NZ	2.19	0.41
2:9:3095:C:O2'	2:9:3096:C:H5'	2.21	0.41
4:A:122:SER:O	4:A:124:VAL:HG13	2.21	0.41
7:D:105:SER:HA	7:D:130:VAL:O	2.21	0.41
7:D:12:GLU:O	7:D:15:GLU:HG2	2.21	0.41
8:E:5:LEU:HD21	8:E:66:GLN:HG3	2.03	0.41
15:M:73:ARG:HG3	39:M:9411:HOH:O	2.21	0.41
17:O:23:GLY:C	39:O:3062:HOH:O	2.59	0.41
17:O:26:TRP:HA	17:O:26:TRP:CE3	2.56	0.41
21:S:29:ASP:OD1	21:S:31:ARG:NH1	2.54	0.41
21:S:8:PRO:HD2	24:V:32:ALA:HA	2.04	0.41
26:X:9:VAL:HG13	26:X:88:GLU:OE2	2.21	0.41
27:Y:189:ASN:ND2	27:Y:189:ASN:C	2.73	0.41
1:0:1149:U:H5''	1:0:1151:G:O4'	2.21	0.40
1:0:2791:U:H1'	1:0:2792:A:H5''	2.03	0.40
1:0:2856:A:OP1	26:X:15:ARG:NH2	2.52	0.40
4:A:123:GLY:HA3	4:A:162:GLY:CA	2.49	0.40
5:B:217:ARG:HG3	5:B:257:THR:CG2	2.51	0.40
7:D:88:LEU:N	7:D:89:PRO:CD	2.84	0.40
9:F:32:GLY:N	39:F:3111:HOH:O	2.54	0.40
1:0:262:A:OP2	9:F:91:VAL:HG11	2.21	0.40
39:O:5961:HOH:O	14:L:34:GLY:HA2	2.20	0.40
17:O:98:LEU:O	17:O:102:ILE:HG13	2.21	0.40
24:V:39:ALA:C	24:V:41:GLU:N	2.71	0.40
28:Z:60:CYS:O	28:Z:61:ASP:HB2	2.21	0.40
4:A:164:ARG:HB2	28:Z:68:SER:OG	2.21	0.40
1:0:2793:A:H2'	1:0:2794:G:H5'	2.03	0.40
1:0:64:G:H2'	1:0:65:C:O4'	2.21	0.40
1:0:790:A:H1'	1:0:1710:A:H2'	2.03	0.40
1:0:920:C:H5'	1:0:921:G:C4	2.56	0.40
30:2:41:HIS:HD2	30:2:44:ARG:H	1.69	0.40
4:A:65:ARG:NH1	4:A:65:ARG:HG2	2.36	0.40
5:B:174:ARG:HA	5:B:177:HIS:HB3	2.02	0.40
5:B:85:ARG:HB2	5:B:99:GLU:HG2	2.03	0.40
6:C:5:ILE:HG13	6:C:15:GLU:HA	2.03	0.40
11:H:47:ILE:HD12	11:H:146:VAL:HG13	2.03	0.40
12:J:12:VAL:HG21	12:J:116:LEU:HD11	2.03	0.40
18:P:16:VAL:CG1	18:P:17:GLY:N	2.83	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:112:GLU:OE1	27:Y:112:GLU:HA	2.21	0.40
27:Y:216:ARG:HD2	39:Y:9370:HOH:O	2.20	0.40
28:Z:11:SER:O	28:Z:14:PHE:HB2	2.21	0.40
1:0:1937:U:O2'	1:0:1938:G:H5'	2.21	0.40
1:0:2361:A:H8	1:0:2361:A:H5'	1.86	0.40
1:0:2401:A:H2'	1:0:2402:A:C8	2.57	0.40
1:0:2379:G:N3	1:0:2418:G:H2'	2.36	0.40
1:0:2868:C:H2'	1:0:2869:G:O4'	2.22	0.40
1:0:484:A:N1	1:0:506:G:H4'	2.36	0.40
1:0:797:A:H5'	28:Z:10:ARG:N	2.36	0.40
31:3:70:ARG:HG2	31:3:70:ARG:HH11	1.86	0.40
6:C:194:PHE:CD2	6:C:234:VAL:CG1	3.01	0.40
6:C:234:VAL:HG13	6:C:234:VAL:O	2.21	0.40
15:M:184:ARG:HG3	15:M:185:PRO:HA	2.03	0.40
15:M:183:THR:CG2	15:M:194:ALA:HB1	2.50	0.40
16:N:182:GLY:O	16:N:183:ASP:C	2.60	0.40
5:B:331:SER:OG	23:U:14:GLU:OE2	2.33	0.40
26:X:12:ILE:HD12	26:X:36:HIS:CG	2.56	0.40
1:0:2568:A:C2'	1:0:2569:A:H5'	2.51	0.40
1:0:2611:G:H5'	1:0:2613:G:C8	2.57	0.40
1:0:2754:G:H2'	1:0:2755:G:O4'	2.22	0.40
1:0:2780:C:H1'	8:E:143:GLN:NE2	2.33	0.40
1:0:295:C:H2'	1:0:296:G:O4'	2.21	0.40
1:0:297:U:H1'	39:0:4518:HOH:O	2.21	0.40
30:2:20:ARG:HD2	30:2:39:ARG:HH21	1.85	0.40
2:9:3012:C:H5'	2:9:3070:U:O4'	2.22	0.40
5:B:274:GLU:HA	5:B:292:GLY:O	2.21	0.40
7:D:36:ASN:HA	39:D:7500:HOH:O	2.22	0.40
9:F:79:GLN:HB2	9:F:82:ASP:OD2	2.22	0.40
11:H:69:ALA:HB2	11:H:153:ALA:HB2	2.04	0.40
11:H:77:LEU:HD12	11:H:83:TYR:CD2	2.57	0.40
23:U:52:THR:HG21	23:U:54:THR:HB	2.03	0.40
27:Y:152:LYS:HB3	27:Y:160:LYS:HG3	2.03	0.40
1:0:1185:U:H2'	1:0:1186:C:C6	2.56	0.40
1:0:1795:G:H2'	1:0:1796:A:O4'	2.22	0.40
1:0:1797:A:H2'	1:0:1799:G:O5'	2.21	0.40
1:0:1819:G:H2'	1:0:1820:G:C4'	2.51	0.40
1:0:1838:U:H1'	1:0:2644:C:H5'	2.04	0.40
1:0:2756:U:O2	1:0:2896:A:H2	2.05	0.40
1:0:622:G:O2'	1:0:623:U:H5'	2.20	0.40
4:A:149:ASP:OD1	4:A:151:GLN:HB2	2.22	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:10:SER:O	5:B:16:ARG:NH1	2.52	0.40
6:C:72:LYS:HG2	6:C:77:ALA:HA	2.03	0.40
16:N:23:ARG:HD2	39:N:9357:HOH:O	2.20	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	
4	A	235/240 (98%)	209 (89%)	23 (10%)	3 (1%)	13	13
5	B	335/338 (99%)	314 (94%)	17 (5%)	4 (1%)	14	15
6	C	244/246 (99%)	229 (94%)	15 (6%)	0	100	100
7	D	134/177 (76%)	105 (78%)	17 (13%)	12 (9%)	1	0
8	E	170/178 (96%)	165 (97%)	5 (3%)	0	100	100
9	F	117/120 (98%)	100 (86%)	15 (13%)	2 (2%)	10	9
10	G	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
11	H	156/171 (91%)	140 (90%)	14 (9%)	2 (1%)	13	13
12	J	140/145 (97%)	131 (94%)	6 (4%)	3 (2%)	8	6
13	K	130/132 (98%)	123 (95%)	7 (5%)	0	100	100
14	L	141/165 (86%)	118 (84%)	22 (16%)	1 (1%)	24	29
15	M	192/195 (98%)	182 (95%)	8 (4%)	2 (1%)	17	19
16	N	184/187 (98%)	163 (89%)	12 (6%)	9 (5%)	2	1
17	O	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
18	P	141/149 (95%)	139 (99%)	2 (1%)	0	100	100
19	Q	93/96 (97%)	90 (97%)	3 (3%)	0	100	100
20	R	148/155 (96%)	141 (95%)	7 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	S	79/85 (93%)	76 (96%)	2 (2%)	1 (1%)	13	13
22	T	117/120 (98%)	109 (93%)	7 (6%)	1 (1%)	19	22
23	U	51/66 (77%)	48 (94%)	3 (6%)	0	100	100
24	V	63/71 (89%)	59 (94%)	3 (5%)	1 (2%)	11	10
25	W	152/154 (99%)	148 (97%)	4 (3%)	0	100	100
26	X	80/92 (87%)	73 (91%)	7 (9%)	0	100	100
27	Y	140/241 (58%)	138 (99%)	2 (1%)	0	100	100
28	Z	71/83 (86%)	61 (86%)	7 (10%)	3 (4%)	3	1
29	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
30	2	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
31	3	90/92 (98%)	88 (98%)	1 (1%)	1 (1%)	16	17
32	I	68/162 (42%)	55 (81%)	12 (18%)	1 (2%)	11	11
All	All	3705/4431 (84%)	3430 (93%)	229 (6%)	46 (1%)	14	15

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	27	LEU
4	A	37	VAL
5	B	139	ASP
7	D	137	PRO
9	F	101	ALA
11	H	166	SER
11	H	168	ALA
14	L	80	ASP
16	N	154	LEU
16	N	184	ILE
28	Z	81	ARG
4	A	34	ASP
7	D	27	ILE
7	D	60	GLU
7	D	171	ASP
12	J	143	LYS
15	M	83	SER
16	N	162	ASP
16	N	183	ASP
22	T	53	GLY
24	V	43	PRO

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
7	D	28	GLY
7	D	56	ARG
7	D	61	PHE
12	J	5	GLU
16	N	155	GLU
16	N	164	ASP
28	Z	20	ARG
31	3	56	PRO
5	B	185	GLY
7	D	97	GLN
7	D	164	ALA
9	F	71	GLY
12	J	65	ASN
16	N	68	GLU
16	N	167	ASP
32	I	76	ALA
5	B	34	GLY
7	D	138	GLY
21	S	46	ASP
5	B	182	VAL
7	D	69	ILE
28	Z	21	VAL
16	N	161	GLY
7	D	16	PRO
15	M	88	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	179/182 (98%)	169 (94%)	10 (6%)	23	32
5	B	282/283 (100%)	261 (93%)	21 (7%)	15	19
6	C	193/193 (100%)	178 (92%)	15 (8%)	14	17
7	D	117/148 (79%)	112 (96%)	5 (4%)	32	43
8	E	152/156 (97%)	145 (95%)	7 (5%)	29	41

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	F	93/94 (99%)	91 (98%)	2 (2%)	55	72
10	G	27/283 (10%)	27 (100%)	0	100	100
11	H	132/138 (96%)	126 (96%)	6 (4%)	30	42
12	J	118/121 (98%)	109 (92%)	9 (8%)	14	18
13	K	106/106 (100%)	103 (97%)	3 (3%)	47	63
14	L	113/127 (89%)	109 (96%)	4 (4%)	39	53
15	M	158/159 (99%)	153 (97%)	5 (3%)	42	58
16	N	149/150 (99%)	144 (97%)	5 (3%)	40	55
17	O	93/94 (99%)	91 (98%)	2 (2%)	55	72
18	P	113/117 (97%)	112 (99%)	1 (1%)	81	90
19	Q	79/80 (99%)	75 (95%)	4 (5%)	26	36
20	R	117/122 (96%)	114 (97%)	3 (3%)	49	66
21	S	71/74 (96%)	69 (97%)	2 (3%)	47	63
22	T	105/106 (99%)	101 (96%)	4 (4%)	36	50
23	U	44/52 (85%)	44 (100%)	0	100	100
24	V	51/57 (90%)	50 (98%)	1 (2%)	58	75
25	W	130/130 (100%)	126 (97%)	4 (3%)	43	59
26	X	66/74 (89%)	60 (91%)	6 (9%)	10	12
27	Y	120/196 (61%)	110 (92%)	10 (8%)	12	15
28	Z	60/68 (88%)	59 (98%)	1 (2%)	63	79
29	1	46/47 (98%)	45 (98%)	1 (2%)	55	72
30	2	42/46 (91%)	41 (98%)	1 (2%)	52	69
31	3	79/79 (100%)	78 (99%)	1 (1%)	71	84
32	I	58/130 (45%)	58 (100%)	0	100	100
All	All	3093/3612 (86%)	2960 (96%)	133 (4%)	32	43

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	3	ARG
4	A	33	GLU
4	A	36	ASP
4	A	94	LEU
4	A	131	HIS

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
4	A	153	ARG
4	A	165	THR
4	A	179	MET
4	A	206	ARG
4	A	217	ARG
5	B	11	LEU
5	B	27	ASN
5	B	51	VAL
5	B	53	LEU
5	B	71	VAL
5	B	82	VAL
5	B	98	THR
5	B	113	LEU
5	B	149	ASP
5	B	162	MET
5	B	175	LEU
5	B	190	MET
5	B	234	ARG
5	B	251	VAL
5	B	254	GLN
5	B	257	THR
5	B	265	LEU
5	B	277	GLU
5	B	280	VAL
5	B	307	ARG
5	B	312	ARG
6	C	2	GLN
6	C	27	ARG
6	C	76	ARG
6	C	91	PRO
6	C	94	THR
6	C	101	ASP
6	C	136	VAL
6	C	162	VAL
6	C	187	ARG
6	C	214	THR
6	C	222	ASP
6	C	223	LEU
6	C	236	THR
6	C	240	LEU
6	C	243	VAL
7	D	24	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
7	D	50	VAL
7	D	61	PHE
7	D	133	ASN
7	D	137	PRO
8	E	3	VAL
8	E	7	ILE
8	E	102	VAL
8	E	108	LEU
8	E	155	ASN
8	E	156	ASP
8	E	164	ASP
9	F	12	LEU
9	F	46	GLU
11	H	1	LYS
11	H	18	GLU
11	H	84	LYS
11	H	88	ARG
11	H	154	TYR
11	H	170	ASN
12	J	45	VAL
12	J	52	GLN
12	J	70	PHE
12	J	74	ARG
12	J	79	PHE
12	J	107	ASN
12	J	117	ASP
12	J	127	ILE
12	J	131	THR
13	K	4	LEU
13	K	10	GLN
13	K	84	ASP
14	L	35	ARG
14	L	43	HIS
14	L	89	PHE
14	L	102	ASP
15	M	46	LEU
15	M	68	ARG
15	M	93	ARG
15	M	99	ARG
15	M	116	ASN
16	N	26	LEU
16	N	37	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
16	N	49	THR
16	N	65	ASP
16	N	139	TRP
17	O	3	THR
17	O	96	VAL
18	P	98	ILE
19	Q	16	ASN
19	Q	18	PRO
19	Q	57	ASP
19	Q	95	GLU
20	R	13	THR
20	R	82	GLU
20	R	132	ARG
21	S	3	ASP
21	S	71	ASP
22	T	39	ASN
22	T	48	VAL
22	T	89	ARG
22	T	96	VAL
24	V	65	ASP
25	W	26	ILE
25	W	35	VAL
25	W	122	ARG
25	W	146	ILE
26	X	8	ARG
26	X	15	ARG
26	X	44	ASP
26	X	72	VAL
26	X	79	GLU
26	X	82	GLU
27	Y	103	THR
27	Y	141	THR
27	Y	144	ARG
27	Y	154	ARG
27	Y	163	THR
27	Y	189	ASN
27	Y	200	THR
27	Y	204	ARG
27	Y	220	GLU
27	Y	235	GLU
28	Z	44	GLU
29	1	47	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
30	2	18	ASN
31	3	56	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (90) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	199	HIS
5	B	2	GLN
5	B	27	ASN
5	B	145	HIS
5	B	191	ASN
5	B	221	GLN
5	B	238	ASN
5	B	256	GLN
5	B	260	HIS
5	B	320	GLN
5	B	332	ASN
6	C	2	GLN
6	C	39	GLN
6	C	129	HIS
7	D	103	ASN
7	D	133	ASN
8	E	90	HIS
8	E	106	ASN
8	E	119	HIS
8	E	143	GLN
10	G	64	ASN
11	H	31	HIS
11	H	56	GLN
11	H	59	HIS
11	H	170	ASN
12	J	25	GLN
12	J	52	GLN
12	J	107	ASN
12	J	126	ASN
13	K	10	GLN
14	L	18	HIS
14	L	41	HIS
14	L	42	ASN
14	L	43	HIS
15	M	24	GLN
15	M	26	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
15	M	58	GLN
15	M	77	HIS
15	M	137	ASN
15	M	143	ASN
15	M	170	ASN
16	N	93	GLN
16	N	107	ASN
16	N	153	GLN
17	O	53	GLN
17	O	100	GLN
18	P	50	GLN
18	P	66	GLN
18	P	73	HIS
18	P	88	GLN
18	P	89	ASN
18	P	118	GLN
19	Q	16	ASN
19	Q	40	HIS
20	R	61	GLN
20	R	94	ASN
20	R	98	ASN
20	R	113	HIS
20	R	117	HIS
21	S	53	ASN
22	T	37	GLN
22	T	39	ASN
22	T	73	HIS
23	U	39	ASN
23	U	48	ASN
24	V	60	GLN
25	W	12	ASN
25	W	28	HIS
25	W	110	GLN
25	W	119	HIS
25	W	125	HIS
25	W	141	HIS
26	X	22	ASN
26	X	23	HIS
27	Y	133	HIS
27	Y	134	HIS
27	Y	149	GLN
27	Y	189	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
29	1	8	GLN
29	1	16	HIS
29	1	28	HIS
30	2	16	ASN
30	2	18	ASN
30	2	41	HIS
30	2	45	ASN
31	3	30	GLN
31	3	48	ASN
32	I	93	GLN
32	I	104	GLN
32	I	113	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	238 (8%)	33 (1%)
2	9	121/122 (99%)	16 (13%)	2 (1%)
3	4	1/5 (20%)	0	0
All	All	2867/3049 (94%)	254 (8%)	35 (1%)

All (254) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	67	A
1	0	69	A
1	0	70	A
1	0	71	G
1	0	86	A
1	0	87	C
1	0	88	G
1	0	114	A
1	0	115	U
1	0	120	A
1	0	130	C
1	0	141	C
1	0	151	A
1	0	166	A
1	0	186	A
1	0	191	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	0	192	A
1	0	219	G
1	0	237	G
1	0	249	G
1	0	271	C
1	0	272	A
1	0	273	G
1	0	283	U
1	0	284	C
1	0	308	U
1	0	309	C
1	0	318	C
1	0	336	G
1	0	337	A
1	0	358	G
1	0	381	G
1	0	397	A
1	0	417	G
1	0	457	U
1	0	461	C
1	0	473	A
1	0	487	G
1	0	498	A
1	0	511	A
1	0	514	G
1	0	537	G
1	0	538	C
1	0	539	G
1	0	542	A
1	0	545	G
1	0	553	G
1	0	559	U
1	0	581	G
1	0	588	G
1	0	604	G
1	0	620	A
1	0	632	A
1	0	644	G
1	0	660	A
1	0	688	A
1	0	698	A
1	0	701	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	0	735	C
1	0	759	C
1	0	777	U
1	0	809	G
1	0	821	U
1	0	835	U
1	0	840	U
1	0	868	G
1	0	869	G
1	0	871	G
1	0	875	A
1	0	877	G
1	0	878	G
1	0	905	C
1	0	920	C
1	0	921	G
1	0	923	A
1	0	953	G
1	0	960	G
1	0	961	A
1	0	1006	A
1	0	1008	C
1	0	1029	U
1	0	1045	G
1	0	1059	G
1	0	1060	C
1	0	1072	G
1	0	1081	A
1	0	1088	A
1	0	1100	G
1	0	1109	U
1	0	1110	G
1	0	1119	G
1	0	1130	U
1	0	1137	G
1	0	1164	U
1	0	1165	G
1	0	1166	A
1	0	1174	A
1	0	1175	G
1	0	1185	U
1	0	1192	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	0	1193	A
1	0	1206	U
1	0	1208	C
1	0	1216	G
1	0	1237	U
1	0	1238	C
1	0	1239	G
1	0	1279	U
1	0	1289	C
1	0	1342	C
1	0	1353	C
1	0	1360	C
1	0	1377	C
1	0	1378	G
1	0	1407	A
1	0	1409	G
1	0	1474	C
1	0	1505	U
1	0	1506	U
1	0	1524	U
1	0	1525	G
1	0	1526	A
1	0	1528	A
1	0	1562	C
1	0	1564	C
1	0	1592	G
1	0	1625	U
1	0	1626	A
1	0	1633	C
1	0	1634	G
1	0	1656	A
1	0	1667	A
1	0	1682	A
1	0	1684	A
1	0	1685	A
1	0	1692	C
1	0	1701	A
1	0	1722	U
1	0	1723	G
1	0	1725	C
1	0	1730	G
1	0	1731	C

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	0	1732	A
1	0	1752	G
1	0	1778	A
1	0	1798	C
1	0	1819	G
1	0	1820	G
1	0	1829	A
1	0	1856	C
1	0	1873	G
1	0	1879	U
1	0	1919	A
1	0	1942	A
1	0	1967	U
1	0	1971	G
1	0	1973	A
1	0	1979	G
1	0	1980	U
1	0	1996	U
1	0	2004	U
1	0	2006	C
1	0	2008	U
1	0	2011	A
1	0	2012	U
1	0	2013	G
1	0	2033	G
1	0	2034	U
1	0	2064	U
1	0	2072	G
1	0	2073	G
1	0	2074	A
1	0	2096	A
1	0	2101	A
1	0	2102	G
1	0	2110	G
1	0	2238	A
1	0	2243	C
1	0	2258	A
1	0	2271	G
1	0	2272	G
1	0	2291	A
1	0	2317	C
1	0	2321	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	0	2354	A
1	0	2361	A
1	0	2369	A
1	0	2379	G
1	0	2422	U
1	0	2462	G
1	0	2476	C
1	0	2480	G
1	0	2483	A
1	0	2507	G
1	0	2509	A
1	0	2511	A
1	0	2533	C
1	0	2536	C
1	0	2537	G
1	0	2541	U
1	0	2553	A
1	0	2564	G
1	0	2589	U
1	0	2601	A
1	0	2602	G
1	0	2608	C
1	0	2611	G
1	0	2613	G
1	0	2634	G
1	0	2644	C
1	0	2645	U
1	0	2649	A
1	0	2664	A
1	0	2681	A
1	0	2682	C
1	0	2726	U
1	0	2747	C
1	0	2748	G
1	0	2749	U
1	0	2750	G
1	0	2762	C
1	0	2768	A
1	0	2783	A
1	0	2786	G
1	0	2792	A
1	0	2800	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	0	2811	A
1	0	2812	A
1	0	2825	C
1	0	2852	A
1	0	2853	U
1	0	2867	G
1	0	2876	G
1	0	2890	A
1	0	2896	A
1	0	2903	C
1	0	2914	A
2	9	3002	U
2	9	3007	G
2	9	3014	G
2	9	3022	G
2	9	3023	U
2	9	3024	U
2	9	3025	G
2	9	3041	C
2	9	3043	G
2	9	3044	A
2	9	3052	A
2	9	3057	A
2	9	3066	G
2	9	3077	A
2	9	3114	G
2	9	3122	C

All (35) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	69	A
1	0	129	A
1	0	169	A
1	0	338	C
1	0	603	A
1	0	644	G
1	0	699	C
1	0	834	G
1	0	857	A
1	0	871	G
1	0	877	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	0	1232	A
1	0	1237	U
1	0	1246	A
1	0	1352	A
1	0	1506	U
1	0	1563	G
1	0	1684	A
1	0	1685	A
1	0	1692	C
1	0	1856	C
1	0	1942	A
1	0	1979	G
1	0	2011	A
1	0	2313	C
1	0	2467	A
1	0	2526	C
1	0	2536	C
1	0	2649	A
1	0	2718	C
1	0	2761	A
1	0	2791	U
1	0	2852	A
2	9	3055	U
2	9	3065	A

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

6 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	$\# Z  > 2$
1	OMU	0	2587	1	14,22,23	0.96	1 (7%)	18,31,34	3.70	2 (11%)
1	OMG	0	2588	1,3	19,26,27	1.05	2 (10%)	22,38,41	2.47	4 (18%)
1	UR3	0	2619	1	13,22,23	0.83	1 (7%)	15,32,35	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	PSU	0	2621	1	16,21,22	1.68	3 (18%)	20,30,33	5.36	4 (20%)
1	1MA	0	628	1,35	16,25,26	0.99	1 (6%)	12,37,40	1.22	1 (8%)
3	ACA	4	78	3	3,3,8	0.59	0	2,2,8	0.77	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	0	2587	1	-	0/5/27/28	0/2/2/2
1	OMG	0	2588	1,3	-	0/5/27/28	0/3/3/3
1	UR3	0	2619	1	-	0/3/25/26	0/2/2/2
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	1MA	0	628	1,35	-	0/3/25/26	0/3/3/3
3	ACA	4	78	3	-	0/0/1/6	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C5-C1'	-4.99	1.47	1.52
1	0	2619	UR3	C6-C5	-2.11	1.33	1.38
1	0	2588	OMG	C8-N7	-2.05	1.30	1.34
1	0	2587	OMU	C4-N3	2.55	1.37	1.33
1	0	2621	PSU	C2-N1	2.74	1.43	1.38
1	0	628	1MA	C6-N6	2.84	1.33	1.27
1	0	2621	PSU	C4-N3	2.92	1.38	1.33
1	0	2588	OMG	C6-N1	3.39	1.39	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	N1-C2-N3	-16.93	114.80	128.41
1	0	2588	OMG	C5-C6-N1	-8.39	111.54	123.47
1	0	2621	PSU	C5-C4-N3	-8.31	114.65	125.36
1	0	628	1MA	C2-N3-C4	-3.72	110.83	116.51
1	0	2587	OMU	C5-C4-N3	-3.67	114.66	123.17
1	0	2588	OMG	C2-N3-C4	-2.73	111.98	115.16
1	0	2588	OMG	N3-C2-N1	-2.28	124.06	127.41
1	0	2621	PSU	C6-N1-C2	2.66	119.62	115.36
1	0	2588	OMG	C6-N1-C2	6.27	125.08	116.06
1	0	2621	PSU	C4-N3-C2	14.09	127.14	115.14

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2587	OMU	C4-N3-C2	15.08	127.12	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2587	OMU	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 311 ligands modelled in this entry, 311 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	0	2749/2922 (94%)	-0.06	95 (3%) 44 51	22, 45, 89, 149	0
2	9	122/122 (100%)	0.18	6 (4%) 29 37	38, 63, 87, 149	0
3	4	4/5 (80%)	1.57	1 (25%) 0 0	61, 64, 71, 74	0
4	A	237/240 (98%)	0.57	19 (8%) 12 16	28, 50, 82, 104	0
5	B	337/338 (99%)	0.29	12 (3%) 42 49	28, 50, 75, 86	0
6	C	246/246 (100%)	0.12	4 (1%) 72 77	25, 46, 68, 80	0
7	D	140/177 (79%)	2.16	63 (45%) 0 0	58, 88, 120, 130	0
8	E	172/178 (96%)	0.93	31 (18%) 1 1	40, 62, 80, 86	0
9	F	119/120 (99%)	1.37	36 (30%) 0 0	44, 71, 100, 110	0
10	G	29/348 (8%)	2.90	20 (68%) 0 0	71, 89, 99, 100	0
11	H	160/171 (93%)	0.85	27 (16%) 1 2	43, 61, 93, 101	0
12	J	142/145 (97%)	0.12	4 (2%) 53 60	36, 47, 67, 89	0
13	K	132/132 (100%)	0.01	3 (2%) 60 67	33, 46, 67, 72	0
14	L	145/165 (87%)	0.95	31 (21%) 1 1	27, 64, 110, 120	0
15	M	194/195 (99%)	0.63	19 (9%) 7 10	31, 44, 77, 87	0
16	N	186/187 (99%)	1.20	48 (25%) 0 0	43, 63, 108, 113	0
17	O	115/116 (99%)	0.17	3 (2%) 56 63	39, 53, 67, 75	0
18	P	143/149 (95%)	0.22	3 (2%) 63 70	38, 51, 65, 76	0
19	Q	95/96 (98%)	0.26	6 (6%) 20 26	38, 47, 61, 76	0
20	R	150/155 (96%)	0.03	3 (2%) 65 71	29, 43, 61, 71	0
21	S	81/85 (95%)	0.49	7 (8%) 10 14	42, 58, 80, 95	0
22	T	119/120 (99%)	0.71	10 (8%) 11 15	40, 54, 81, 110	0
23	U	53/66 (80%)	0.31	2 (3%) 40 47	40, 50, 68, 79	0
24	V	65/71 (91%)	1.96	22 (33%) 0 0	52, 76, 110, 116	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	W	154/154 (100%)	0.17	3 (1%) 66 73	37, 49, 69, 78	0
26	X	82/92 (89%)	0.89	11 (13%) 3 4	40, 53, 82, 101	0
27	Y	142/241 (58%)	0.30	10 (7%) 16 22	29, 42, 63, 85	0
28	Z	73/83 (87%)	0.93	16 (21%) 0 1	48, 70, 85, 92	0
29	1	56/57 (98%)	-0.30	0 100 100	26, 32, 39, 49	0
30	2	46/50 (92%)	0.63	5 (10%) 5 8	33, 51, 67, 80	0
31	3	92/92 (100%)	0.37	4 (4%) 35 42	33, 55, 70, 83	0
32	I	70/162 (43%)	6.28	66 (94%) 0 0	111, 123, 141, 143	0
All	All	6650/7480 (88%)	0.38	590 (8%) 9 13	22, 50, 95, 149	0

All (590) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	I	71	GLY	17.6
7	D	63	ILE	15.2
24	V	1	THR	14.6
32	I	133	THR	13.9
32	I	79	ILE	12.9
16	N	166	ALA	11.7
32	I	96	PHE	11.4
24	V	39	ALA	11.3
32	I	88	GLY	11.2
32	I	76	ALA	11.0
32	I	116	LEU	10.7
24	V	40	PRO	10.7
7	D	57	THR	10.5
32	I	85	PHE	10.5
32	I	118	SER	10.4
22	T	119	ALA	10.3
32	I	105	VAL	10.2
32	I	113	HIS	10.0
32	I	87	THR	9.8
32	I	75	THR	9.3
7	D	61	PHE	9.3
32	I	121	LEU	9.2
32	I	137	VAL	9.2
32	I	102	VAL	9.1
26	X	88	GLU	8.5
4	A	237	GLY	8.5

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
32	I	109	ALA	8.1
32	I	93	GLN	8.0
32	I	81	ASP	7.9
32	I	132	CYS	7.9
32	I	108	ILE	7.8
2	9	3001	U	7.7
4	A	37	VAL	7.7
32	I	129	VAL	7.7
15	M	70	GLY	7.5
32	I	125	ALA	7.4
30	2	49	GLU	7.3
32	I	104	GLN	7.3
7	D	90	LEU	7.2
32	I	77	GLU	7.1
1	0	1951	G	7.1
32	I	107	GLN	7.0
24	V	38	GLY	6.9
1	0	282	C	6.9
32	I	91	GLU	6.8
32	I	89	SER	6.8
32	I	111	GLN	6.8
32	I	78	LEU	6.7
10	G	23	ILE	6.4
28	Z	11	SER	6.4
32	I	97	VAL	6.3
32	I	117	LEU	6.3
1	0	1177	A	6.2
15	M	79	ALA	6.2
32	I	114	PRO	6.2
10	G	26	MET	6.1
32	I	74	PRO	6.1
1	0	1199	A	6.0
22	T	118	SER	6.0
7	D	170	TYR	6.0
15	M	74	LYS	5.9
32	I	86	GLU	5.8
32	I	103	ASP	5.7
2	9	3024	U	5.6
10	G	27	ILE	5.5
1	0	2637	A	5.4
16	N	68	GLU	5.4
26	X	80	GLU	5.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
32	I	98	ALA	5.4
14	L	106	VAL	5.4
14	L	75	LEU	5.3
7	D	44	ILE	5.2
32	I	126	LYS	5.2
21	S	81	ILE	5.2
1	0	1172	G	5.2
7	D	69	ILE	5.2
9	F	16	ALA	5.2
30	2	35	ARG	5.1
1	0	285	A	5.1
9	F	110	ASP	5.1
1	0	999	C	5.1
1	0	1173	A	5.1
1	0	10	U	5.1
8	E	45	ASP	5.1
16	N	163	PHE	5.1
1	0	960	G	5.0
1	0	1948	G	5.0
32	I	122	THR	5.0
1	0	2238	A	5.0
1	0	280	C	5.0
7	D	10	PHE	4.9
2	9	3023	U	4.9
24	V	37	GLY	4.8
16	N	175	LEU	4.8
9	F	119	ARG	4.8
4	A	35	GLY	4.8
7	D	64	ARG	4.8
32	I	123	ASN	4.8
28	Z	20	ARG	4.8
32	I	83	ALA	4.8
8	E	87	PHE	4.7
32	I	120	ASP	4.7
1	0	2748	G	4.7
12	J	70	PHE	4.7
28	Z	24	ARG	4.7
1	0	272	A	4.7
1	0	1965	C	4.7
32	I	138	THR	4.7
1	0	2004	U	4.7
32	I	115	ASP	4.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
32	I	106	LYS	4.6
7	D	92	GLU	4.6
1	0	2769	C	4.6
7	D	62	ASP	4.6
1	0	514	G	4.6
14	L	97	VAL	4.6
32	I	124	ALA	4.5
2	9	3002	U	4.5
1	0	1200	A	4.5
7	D	73	VAL	4.5
10	G	71	LEU	4.5
1	0	497	A	4.5
12	J	4	ALA	4.4
9	F	106	ALA	4.4
10	G	22	ALA	4.4
9	F	117	GLU	4.4
1	0	2237	G	4.4
10	G	24	VAL	4.4
14	L	76	LEU	4.4
1	0	970	U	4.3
1	0	288	A	4.3
32	I	136	GLY	4.3
1	0	1202	A	4.3
27	Y	235	GLU	4.3
16	N	161	GLY	4.3
7	D	11	HIS	4.2
11	H	111	ASP	4.2
24	V	41	GLU	4.2
16	N	147	ILE	4.2
1	0	1198	U	4.2
28	Z	22	SER	4.2
9	F	22	VAL	4.2
26	X	85	VAL	4.2
1	0	1525	G	4.1
9	F	28	ALA	4.1
6	C	61	PHE	4.1
14	L	91	VAL	4.1
24	V	36	ALA	4.1
32	I	119	TYR	4.1
8	E	6	GLU	4.1
14	L	145	LEU	4.1
7	D	51	ARG	4.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
7	D	166	ILE	4.0
1	0	1171	A	4.0
7	D	66	GLY	4.0
7	D	173	GLU	4.0
7	D	18	ILE	4.0
1	0	1950	G	4.0
11	H	171	ALA	4.0
19	Q	95	GLU	4.0
7	D	93	LEU	4.0
32	I	135	LEU	4.0
22	T	116	ASP	4.0
4	A	133	ARG	4.0
31	3	92	GLU	4.0
23	U	47	ARG	3.9
7	D	172	VAL	3.9
32	I	112	LYS	3.9
1	0	2508	C	3.9
1	0	2511	A	3.9
10	G	66	LEU	3.9
16	N	165	ALA	3.9
8	E	86	VAL	3.9
16	N	184	ILE	3.9
11	H	146	VAL	3.8
11	H	34	GLY	3.8
3	4	77	PHE	3.8
28	Z	21	VAL	3.8
10	G	69	ARG	3.8
32	I	72	VAL	3.8
4	A	99	ILE	3.8
32	I	80	LYS	3.8
11	H	73	LEU	3.7
16	N	154	LEU	3.7
15	M	78	LYS	3.7
8	E	100	ASP	3.7
11	H	35	ARG	3.7
26	X	10	VAL	3.7
22	T	112	LEU	3.7
7	D	26	GLY	3.7
7	D	40	ILE	3.7
7	D	107	GLY	3.7
7	D	171	ASP	3.7
8	E	154	ILE	3.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
16	N	155	GLU	3.7
32	I	95	ASP	3.7
7	D	134	LEU	3.7
10	G	21	ASP	3.7
27	Y	95	THR	3.7
27	Y	108	ASP	3.6
11	H	74	ILE	3.6
11	H	37	GLN	3.6
32	I	110	GLU	3.6
11	H	143	ALA	3.6
16	N	95	ALA	3.6
14	L	80	ASP	3.6
9	F	15	ASP	3.6
9	F	107	ASP	3.6
22	T	82	THR	3.6
16	N	172	PHE	3.6
32	I	127	GLU	3.6
4	A	31	LYS	3.6
7	D	104	PHE	3.5
16	N	180	LEU	3.5
1	0	2747	C	3.5
4	A	38	ILE	3.5
14	L	60	GLU	3.5
9	F	99	THR	3.5
32	I	90	GLY	3.5
9	F	49	PHE	3.5
7	D	88	LEU	3.5
2	9	3122	C	3.5
17	O	22	GLY	3.5
1	0	1169	U	3.5
9	F	25	ASP	3.5
9	F	118	LEU	3.4
10	G	12	ILE	3.4
10	G	67	LEU	3.4
1	0	281	U	3.4
32	I	99	ASP	3.4
28	Z	25	ARG	3.4
7	D	167	GLU	3.4
24	V	8	ILE	3.4
4	A	36	ASP	3.4
10	G	70	ALA	3.4
7	D	23	VAL	3.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
7	D	85	GLN	3.4
32	I	134	SER	3.4
9	F	108	VAL	3.4
11	H	82	ASP	3.4
1	O	735	C	3.4
4	A	85	SER	3.4
16	N	139	TRP	3.3
10	G	25	GLU	3.3
11	H	83	TYR	3.3
15	M	86	GLN	3.3
24	V	59	ILE	3.3
8	E	10	ASP	3.3
4	A	97	ALA	3.3
7	D	91	ALA	3.3
1	O	283	U	3.3
1	O	1168	C	3.3
8	E	43	ASP	3.3
1	O	1966	U	3.3
26	X	71	ARG	3.3
14	L	99	GLU	3.3
26	X	7	GLU	3.3
1	O	284	C	3.3
14	L	105	TYR	3.3
24	V	43	PRO	3.3
11	H	47	ILE	3.3
16	N	183	ASP	3.3
8	E	160	ARG	3.3
8	E	108	LEU	3.2
1	O	2645	U	3.2
22	T	115	GLU	3.2
1	O	1967	U	3.2
9	F	100	ASP	3.2
16	N	181	ASP	3.2
7	D	81	GLU	3.2
8	E	4	GLU	3.2
32	I	94	GLU	3.2
14	L	130	ARG	3.2
1	O	1000	C	3.2
4	A	236	GLY	3.2
1	O	716	G	3.2
1	O	969	G	3.2
14	L	102	ASP	3.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
32	I	84	GLY	3.2
7	D	27	ILE	3.1
11	H	78	GLY	3.1
32	I	82	GLU	3.1
21	S	20	PHE	3.1
1	0	1163	G	3.1
9	F	98	VAL	3.1
1	0	1170	U	3.1
1	0	1947	G	3.1
8	E	89	SER	3.1
15	M	71	SER	3.1
16	N	185	GLU	3.1
11	H	138	CYS	3.1
13	K	132	VAL	3.0
27	Y	236	VAL	3.0
24	V	63	GLU	3.0
27	Y	234	VAL	3.0
1	0	279	C	3.0
1	0	2103	A	3.0
32	I	92	PRO	3.0
5	B	57	GLU	3.0
16	N	145	ALA	3.0
25	W	86	GLU	3.0
1	0	370	G	3.0
16	N	71	TRP	3.0
28	Z	12	GLY	3.0
31	3	41	GLU	3.0
7	D	56	ARG	3.0
1	0	358	G	3.0
1	0	295	C	3.0
5	B	1	PRO	3.0
6	C	132	ASP	2.9
16	N	178	THR	2.9
32	I	140	GLU	2.9
1	0	362	G	2.9
1	0	1929	G	2.9
19	Q	76	VAL	2.9
28	Z	36	ASP	2.9
15	M	75	ARG	2.9
16	N	72	GLU	2.9
16	N	152	GLU	2.9
24	V	14	ALA	2.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	0	138	U	2.9
8	E	128	GLY	2.9
9	F	17	LEU	2.9
7	D	35	ALA	2.9
28	Z	45	ASP	2.9
9	F	103	GLU	2.9
16	N	37	ARG	2.9
16	N	158	LEU	2.9
27	Y	216	ARG	2.9
1	0	2344	G	2.9
7	D	106	PHE	2.9
7	D	130	VAL	2.9
27	Y	98	GLN	2.9
7	D	38	GLU	2.9
25	W	76	ASP	2.9
31	3	62	THR	2.8
28	Z	42	CYS	2.8
15	M	89	THR	2.8
1	0	1189	A	2.8
8	E	88	TYR	2.8
16	N	159	TYR	2.8
14	L	104	ASP	2.8
7	D	135	VAL	2.8
15	M	84	LYS	2.8
1	0	1178	G	2.8
1	0	1195	G	2.8
7	D	79	MET	2.8
7	D	84	LEU	2.8
14	L	79	ASP	2.8
16	N	149	GLU	2.8
14	L	148	GLU	2.8
21	S	2	TRP	2.8
10	G	73	ASP	2.8
15	M	87	GLY	2.8
7	D	165	PHE	2.7
28	Z	19	GLY	2.7
7	D	68	PRO	2.7
10	G	15	TRP	2.7
14	L	100	ALA	2.7
14	L	121	ILE	2.7
9	F	19	ALA	2.7
8	E	161	VAL	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
14	L	81	VAL	2.7
24	V	2	VAL	2.7
8	E	94	GLN	2.7
1	0	1181	A	2.7
4	A	65	ARG	2.7
9	F	115	VAL	2.7
22	T	117	ASP	2.7
8	E	127	ASP	2.7
7	D	154	LYS	2.7
1	0	1165	G	2.7
1	0	372	A	2.7
8	E	15	GLN	2.7
14	L	93	VAL	2.7
1	0	1196	C	2.7
16	N	177	GLU	2.6
32	I	139	ILE	2.6
14	L	147	GLU	2.6
15	M	83	SER	2.6
1	0	1180	U	2.6
1	0	1625	U	2.6
16	N	137	ALA	2.6
10	G	68	GLU	2.6
10	G	63	ARG	2.6
15	M	88	VAL	2.6
24	V	6	GLN	2.6
1	0	1190	G	2.6
7	D	52	THR	2.6
11	H	70	ASN	2.6
8	E	129	GLU	2.6
16	N	94	GLU	2.6
1	0	2345	A	2.6
15	M	80	GLY	2.6
27	Y	96	GLU	2.6
15	M	76	ARG	2.6
19	Q	18	PRO	2.6
24	V	33	VAL	2.6
26	X	77	PHE	2.6
1	0	1179	C	2.6
22	T	59	GLU	2.6
11	H	24	PRO	2.5
7	D	41	LEU	2.5
1	0	1164	U	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
15	M	77	HIS	2.5
7	D	17	ARG	2.5
26	X	73	ARG	2.5
16	N	160	SER	2.5
1	0	1279	U	2.5
8	E	5	LEU	2.5
9	F	12	LEU	2.5
24	V	10	ASP	2.5
15	M	73	ARG	2.5
15	M	164	THR	2.5
4	A	64	ASP	2.5
14	L	62	ALA	2.5
1	0	289	G	2.5
1	0	1197	G	2.5
7	D	95	THR	2.5
9	F	11	ASP	2.5
10	G	72	ASP	2.5
4	A	145	MET	2.5
8	E	98	GLU	2.5
26	X	41	PHE	2.5
32	I	128	VAL	2.5
8	E	121	ASP	2.5
16	N	138	ASP	2.5
16	N	164	ASP	2.5
1	0	1192	A	2.5
9	F	23	ALA	2.5
14	L	61	ALA	2.5
9	F	24	ARG	2.5
24	V	46	ILE	2.5
1	0	369	G	2.4
5	B	183	GLU	2.4
16	N	179	LEU	2.4
7	D	89	PRO	2.4
30	2	39	ARG	2.4
16	N	134	ASP	2.4
16	N	81	ALA	2.4
11	H	39	ASP	2.4
1	0	717	C	2.4
9	F	109	GLU	2.4
11	H	79	GLU	2.4
11	H	141	GLU	2.4
1	0	1981	A	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
5	B	134	ALA	2.4
7	D	54	ALA	2.4
8	E	123	ASP	2.4
14	L	82	ALA	2.4
16	N	67	ALA	2.4
20	R	104	PHE	2.4
21	S	70	GLU	2.4
28	Z	18	TYR	2.4
9	F	18	GLU	2.4
14	L	150	GLN	2.4
16	N	170	GLU	2.4
8	E	118	ILE	2.3
8	E	99	GLY	2.3
22	T	35	TYR	2.3
7	D	160	ALA	2.3
14	L	120	LEU	2.3
32	I	73	PRO	2.3
1	0	1208	C	2.3
11	H	137	TYR	2.3
11	H	67	LEU	2.3
1	0	1174	A	2.3
11	H	139	ASN	2.3
8	E	42	VAL	2.3
6	C	135	GLU	2.3
20	R	7	GLU	2.3
16	N	169	PRO	2.3
1	0	1964	U	2.3
11	H	168	ALA	2.3
30	2	44	ARG	2.3
1	0	373	G	2.3
1	0	1203	G	2.3
24	V	45	ARG	2.3
7	D	99	ASP	2.3
12	J	5	GLU	2.3
26	X	75	ALA	2.3
10	G	65	THR	2.3
7	D	29	HIS	2.3
9	F	21	GLU	2.3
1	0	2507	G	2.3
7	D	53	LYS	2.3
16	N	156	GLU	2.3
1	0	1527	A	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
18	P	16	VAL	2.3
1	0	2239	C	2.3
1	0	365	G	2.3
9	F	101	ALA	2.3
14	L	141	GLU	2.2
23	U	4	ARG	2.2
28	Z	23	ARG	2.2
9	F	113	ASP	2.2
14	L	144	ASP	2.2
9	F	69	GLU	2.2
19	Q	64	GLU	2.2
28	Z	31	SER	2.2
28	Z	32	GLU	2.2
4	A	206	ARG	2.2
11	H	149	ALA	2.2
16	N	148	ALA	2.2
1	0	1175	G	2.2
8	E	11	VAL	2.2
11	H	140	VAL	2.2
4	A	60	PHE	2.2
5	B	186	GLY	2.2
7	D	74	THR	2.2
7	D	87	ALA	2.2
19	Q	17	LYS	2.2
4	A	34	ASP	2.2
1	0	1949	G	2.2
7	D	25	MET	2.2
26	X	72	VAL	2.2
7	D	157	LEU	2.2
2	9	3073	G	2.2
30	2	20	ARG	2.2
4	A	209	PRO	2.2
9	F	43	GLY	2.2
5	B	117	GLU	2.2
16	N	167	ASP	2.2
1	0	290	C	2.2
13	K	126	SER	2.2
8	E	162	PHE	2.2
16	N	2	THR	2.2
24	V	32	ALA	2.2
5	B	133	GLU	2.2
9	F	60	VAL	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
25	W	93	ILE	2.1
27	Y	102	LEU	2.1
16	N	182	GLY	2.1
1	0	809	G	2.1
5	B	104	GLU	2.1
8	E	105	GLU	2.1
21	S	45	TYR	2.1
20	R	96	VAL	2.1
11	H	77	LEU	2.1
28	Z	80	ARG	2.1
6	C	237	GLU	2.1
8	E	169	THR	2.1
5	B	108	GLU	2.1
8	E	126	ILE	2.1
24	V	42	ASN	2.1
1	0	1176	C	2.1
7	D	67	ASP	2.1
12	J	7	ASP	2.1
7	D	86	THR	2.1
14	L	122	ALA	2.1
21	S	78	ALA	2.1
24	V	5	VAL	2.1
7	D	65	GLU	2.1
17	O	1	SER	2.1
18	P	67	LYS	2.1
15	M	81	ARG	2.1
16	N	174	GLU	2.1
17	O	31	GLU	2.1
31	3	6	ARG	2.1
7	D	94	ALA	2.1
14	L	77	ALA	2.1
16	N	73	ALA	2.1
27	Y	187	VAL	2.1
5	B	2	GLN	2.1
5	B	180	ASP	2.1
21	S	72	ASP	2.1
24	V	62	GLU	2.1
1	0	804	C	2.1
9	F	29	VAL	2.1
14	L	142	LEU	2.0
1	0	1526	A	2.0
16	N	92	ALA	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
10	G	28	GLU	2.0
18	P	18	LYS	2.0
9	F	75	ILE	2.0
1	0	1201	C	2.0
1	0	2506	A	2.0
14	L	44	GLU	2.0
9	F	26	THR	2.0
5	B	176	ASP	2.0
7	D	58	VAL	2.0
9	F	72	VAL	2.0
22	T	77	VAL	2.0
4	A	134	ASN	2.0
11	H	76	GLU	2.0
16	N	106	LEU	2.0
19	Q	84	ILE	2.0
13	K	119	GLN	2.0
15	M	82	ARG	2.0
16	N	16	ALA	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	ACA	4	78	4/9	0.59	0.43	70,71,72,72	0
1	OMG	0	2588	24/25	0.97	0.12	32,34,38,40	0
1	1MA	0	628	23/24	0.98	0.14	31,33,36,39	0
1	UR3	0	2619	21/22	0.98	0.14	42,46,49,51	0
1	PSU	0	2621	20/21	0.98	0.12	33,36,44,45	0
1	OMU	0	2587	21/22	0.98	0.12	35,37,38,39	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
35	NA	0	9129	1/1	-0.06	0.43	88,88,88,88	0
37	SR	0	9601	1/1	0.06	1.47	200,200,200,200	0
37	SR	0	9500	1/1	0.17	1.74	200,200,200,200	0
37	SR	B	9521	1/1	0.21	0.71	200,200,200,200	0
37	SR	0	9484	1/1	0.28	0.16	150,150,150,150	0
35	NA	0	9122	1/1	0.34	0.44	98,98,98,98	0
33	MG	0	8108	1/1	0.40	0.28	115,115,115,115	0
35	NA	S	9112	1/1	0.46	0.16	74,74,74,74	0
37	SR	0	9501	1/1	0.49	0.34	200,200,200,200	0
35	NA	0	9171	1/1	0.52	0.25	63,63,63,63	0
33	MG	0	8094	1/1	0.54	0.39	82,82,82,82	0
35	NA	0	9184	1/1	0.55	0.31	86,86,86,86	0
33	MG	0	8092	1/1	0.56	1.61	83,83,83,83	0
37	SR	0	9537	1/1	0.59	0.17	152,152,152,152	0
33	MG	0	8052	1/1	0.62	0.31	72,72,72,72	0
35	NA	0	9164	1/1	0.63	0.57	67,67,67,67	0
33	MG	0	8061	1/1	0.63	0.13	81,81,81,81	0
33	MG	0	8047	1/1	0.66	0.52	94,94,94,94	0
33	MG	0	8082	1/1	0.68	0.48	103,103,103,103	0
37	SR	0	9468	1/1	0.69	0.05	115,115,115,115	0
33	MG	0	8050	1/1	0.71	0.25	94,94,94,94	0
37	SR	0	9547	1/1	0.71	0.52	200,200,200,200	0
37	SR	0	9590	1/1	0.72	0.09	142,142,142,142	0
37	SR	0	9581	1/1	0.73	0.07	134,134,134,134	0
33	MG	0	8022	1/1	0.73	0.54	113,113,113,113	0
35	NA	0	9111	1/1	0.77	0.21	57,57,57,57	0
33	MG	0	8014	1/1	0.77	0.30	78,78,78,78	0
33	MG	0	8059	1/1	0.78	0.28	60,60,60,60	0
33	MG	0	8114	1/1	0.79	0.17	83,83,83,83	0
33	MG	0	8104	1/1	0.80	0.33	83,83,83,83	0
33	MG	0	8054	1/1	0.80	0.13	58,58,58,58	0
35	NA	0	9185	1/1	0.81	0.56	54,54,54,54	0
35	NA	0	9113	1/1	0.81	0.14	64,64,64,64	0
33	MG	0	8101	1/1	0.81	0.11	51,51,51,51	0
37	SR	0	9539	1/1	0.81	0.38	167,167,167,167	0
35	NA	0	9172	1/1	0.81	0.41	68,68,68,68	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
35	NA	0	9182	1/1	0.82	0.13	84,84,84,84	0
35	NA	0	9181	1/1	0.82	0.12	48,48,48,48	0
35	NA	9	9183	1/1	0.82	0.23	72,72,72,72	0
33	MG	0	8107	1/1	0.82	0.22	68,68,68,68	0
35	NA	0	9126	1/1	0.83	0.14	55,55,55,55	0
35	NA	J	9146	1/1	0.83	0.13	62,62,62,62	0
35	NA	0	9163	1/1	0.83	0.32	77,77,77,77	0
33	MG	B	8055	1/1	0.84	0.27	104,104,104,104	0
35	NA	0	9152	1/1	0.84	0.38	67,67,67,67	0
35	NA	0	9174	1/1	0.84	0.24	67,67,67,67	0
35	NA	0	9168	1/1	0.84	0.28	72,72,72,72	0
35	NA	0	9110	1/1	0.85	0.20	49,49,49,49	0
35	NA	0	9132	1/1	0.85	0.38	61,61,61,61	0
33	MG	0	8013	1/1	0.85	0.38	16,16,16,16	0
35	NA	0	9141	1/1	0.86	0.12	61,61,61,61	0
35	NA	0	9140	1/1	0.86	0.34	61,61,61,61	0
37	SR	9	9588	1/1	0.86	0.14	122,122,122,122	0
33	MG	0	8103	1/1	0.87	0.31	79,79,79,79	0
33	MG	0	8065	1/1	0.87	0.33	92,92,92,92	0
35	NA	0	9150	1/1	0.87	0.33	54,54,54,54	0
33	MG	0	8090	1/1	0.87	0.27	81,81,81,81	0
33	MG	9	8095	1/1	0.87	0.24	44,44,44,44	0
33	MG	0	8021	1/1	0.87	0.24	51,51,51,51	0
34	K	0	9001	1/1	0.87	0.48	95,95,95,95	0
33	MG	0	8040	1/1	0.88	0.34	94,94,94,94	0
33	MG	0	8024	1/1	0.88	0.93	90,90,90,90	0
33	MG	0	8057	1/1	0.88	0.39	79,79,79,79	0
37	SR	0	9452	1/1	0.89	0.20	114,114,114,114	0
33	MG	0	8032	1/1	0.89	0.11	36,36,36,36	0
33	MG	0	8042	1/1	0.90	0.06	53,53,53,53	0
35	NA	0	9125	1/1	0.90	1.07	106,106,106,106	0
35	NA	0	9170	1/1	0.90	0.33	75,75,75,75	0
35	NA	0	9173	1/1	0.90	0.39	66,66,66,66	0
37	SR	0	9529	1/1	0.90	0.09	116,116,116,116	0
33	MG	0	8091	1/1	0.90	0.07	56,56,56,56	0
33	MG	0	8025	1/1	0.90	0.34	23,23,23,23	0
34	K	0	9002	1/1	0.91	0.19	86,86,86,86	0
35	NA	D	9151	1/1	0.91	0.12	63,63,63,63	0
35	NA	0	9179	1/1	0.91	0.81	84,84,84,84	0
37	SR	0	9504	1/1	0.91	0.11	92,92,92,92	0
35	NA	0	9166	1/1	0.91	0.11	65,65,65,65	0
35	NA	0	9178	1/1	0.91	0.17	54,54,54,54	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
35	NA	0	9124	1/1	0.91	0.15	51,51,51,51	0
33	MG	0	8102	1/1	0.91	0.15	70,70,70,70	0
33	MG	0	8098	1/1	0.92	0.08	43,43,43,43	0
35	NA	R	9186	1/1	0.92	0.16	64,64,64,64	0
33	MG	0	8080	1/1	0.92	0.24	48,48,48,48	0
33	MG	0	8083	1/1	0.92	0.07	51,51,51,51	0
35	NA	0	9154	1/1	0.92	0.20	51,51,51,51	0
36	CL	B	9319	1/1	0.92	0.15	59,59,59,59	0
33	MG	0	8058	1/1	0.92	0.47	85,85,85,85	0
33	MG	0	8085	1/1	0.92	0.41	102,102,102,102	0
33	MG	0	8084	1/1	0.92	0.53	109,109,109,109	0
35	NA	0	9135	1/1	0.92	0.14	46,46,46,46	0
33	MG	0	8113	1/1	0.92	0.08	45,45,45,45	0
36	CL	J	9302	1/1	0.92	0.11	55,55,55,55	0
36	CL	0	9316	1/1	0.93	0.17	74,74,74,74	0
35	NA	0	9107	1/1	0.93	0.24	58,58,58,58	0
35	NA	3	9169	1/1	0.93	0.41	102,102,102,102	0
35	NA	0	9159	1/1	0.93	0.17	56,56,56,56	0
37	SR	0	9505	1/1	0.93	0.13	104,104,104,104	0
35	NA	0	9101	1/1	0.93	0.15	43,43,43,43	0
37	SR	0	9522	1/1	0.93	0.06	104,104,104,104	0
33	MG	0	8030	1/1	0.93	0.04	34,34,34,34	0
35	NA	0	9175	1/1	0.93	0.19	52,52,52,52	0
35	NA	0	9157	1/1	0.93	0.16	41,41,41,41	0
33	MG	0	8088	1/1	0.93	0.06	43,43,43,43	0
36	CL	N	9307	1/1	0.93	0.12	54,54,54,54	0
33	MG	0	8075	1/1	0.93	0.06	37,37,37,37	0
33	MG	0	8099	1/1	0.93	0.17	77,77,77,77	0
35	NA	0	9177	1/1	0.93	0.40	70,70,70,70	0
33	MG	0	8045	1/1	0.94	0.21	75,75,75,75	0
35	NA	0	9165	1/1	0.94	0.22	41,41,41,41	0
33	MG	0	8115	1/1	0.94	0.14	53,53,53,53	0
36	CL	0	9322	1/1	0.94	0.10	54,54,54,54	0
37	SR	0	9489	1/1	0.94	0.09	87,87,87,87	0
33	MG	0	8097	1/1	0.94	0.20	55,55,55,55	0
33	MG	0	8089	1/1	0.94	0.12	61,61,61,61	0
33	MG	0	8043	1/1	0.94	0.08	47,47,47,47	0
35	NA	0	9118	1/1	0.94	0.22	41,41,41,41	0
33	MG	0	8027	1/1	0.94	0.19	30,30,30,30	0
35	NA	0	9158	1/1	0.94	0.10	62,62,62,62	0
33	MG	0	8041	1/1	0.94	0.12	47,47,47,47	0
35	NA	0	9127	1/1	0.94	0.20	65,65,65,65	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	T	8073	1/1	0.94	0.14	42,42,42,42	0
35	NA	0	9160	1/1	0.94	0.15	42,42,42,42	0
35	NA	0	9120	1/1	0.94	0.30	61,61,61,61	0
37	SR	0	9482	1/1	0.94	0.19	118,118,118,118	0
33	MG	0	8072	1/1	0.95	0.25	74,74,74,74	0
38	CD	O	9205	1/1	0.95	0.04	85,85,85,85	0
35	NA	0	9134	1/1	0.95	0.07	47,47,47,47	0
35	NA	0	9161	1/1	0.95	0.30	57,57,57,57	0
35	NA	R	9137	1/1	0.95	0.11	32,32,32,32	0
33	MG	0	8009	1/1	0.95	0.07	31,31,31,31	0
35	NA	0	9115	1/1	0.95	0.24	43,43,43,43	0
33	MG	0	8060	1/1	0.95	0.10	81,81,81,81	0
33	MG	0	8093	1/1	0.95	0.14	42,42,42,42	0
37	SR	0	9495	1/1	0.95	0.11	88,88,88,88	0
37	SR	0	9530	1/1	0.95	0.12	94,94,94,94	0
35	NA	0	9130	1/1	0.95	0.08	45,45,45,45	0
33	MG	0	8076	1/1	0.95	0.21	55,55,55,55	0
35	NA	0	9102	1/1	0.95	0.20	58,58,58,58	0
33	MG	0	8051	1/1	0.95	0.29	22,22,22,22	0
36	CL	3	9304	1/1	0.95	0.11	59,59,59,59	0
35	NA	0	9149	1/1	0.95	0.14	41,41,41,41	0
37	SR	0	9626	1/1	0.95	0.30	140,140,140,140	0
37	SR	0	9459	1/1	0.96	0.07	96,96,96,96	0
37	SR	0	9490	1/1	0.96	0.11	105,105,105,105	0
33	MG	0	8046	1/1	0.96	0.08	40,40,40,40	0
35	NA	0	9106	1/1	0.96	0.20	37,37,37,37	0
35	NA	0	9131	1/1	0.96	0.10	47,47,47,47	0
33	MG	0	8063	1/1	0.96	0.07	74,74,74,74	0
33	MG	0	8039	1/1	0.96	0.04	56,56,56,56	0
33	MG	A	8066	1/1	0.96	0.18	53,53,53,53	0
35	NA	0	9108	1/1	0.96	0.12	34,34,34,34	0
37	SR	0	9474	1/1	0.96	0.09	96,96,96,96	0
36	CL	0	9315	1/1	0.96	0.10	54,54,54,54	0
36	CL	J	9301	1/1	0.96	0.09	55,55,55,55	0
33	MG	0	8036	1/1	0.96	0.09	63,63,63,63	0
35	NA	0	9155	1/1	0.96	0.24	54,54,54,54	0
37	SR	0	9447	1/1	0.96	0.10	66,66,66,66	0
36	CL	L	9310	1/1	0.96	0.09	56,56,56,56	0
37	SR	0	9466	1/1	0.96	0.04	87,87,87,87	0
35	NA	0	9156	1/1	0.96	0.21	55,55,55,55	0
37	SR	0	9506	1/1	0.96	0.07	86,86,86,86	0
37	SR	0	9431	1/1	0.96	0.14	55,55,55,55	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
37	SR	0	9534	1/1	0.96	0.11	106,106,106,106	0
35	NA	0	9139	1/1	0.96	0.13	57,57,57,57	0
33	MG	0	8015	1/1	0.96	0.10	29,29,29,29	0
33	MG	0	8003	1/1	0.96	0.19	29,29,29,29	0
37	SR	9	9503	1/1	0.96	0.03	109,109,109,109	0
37	SR	H	9486	1/1	0.96	0.19	121,121,121,121	0
37	SR	0	9467	1/1	0.97	0.10	74,74,74,74	0
33	MG	0	8019	1/1	0.97	0.05	53,53,53,53	0
36	CL	Y	9320	1/1	0.97	0.10	42,42,42,42	0
37	SR	0	9570	1/1	0.97	0.07	96,96,96,96	0
37	SR	0	9421	1/1	0.97	0.10	65,65,65,65	0
37	SR	0	9405	1/1	0.97	0.14	54,54,54,54	0
37	SR	0	9475	1/1	0.97	0.14	77,77,77,77	0
37	SR	0	9585	1/1	0.97	0.08	86,86,86,86	0
36	CL	0	9311	1/1	0.97	0.10	56,56,56,56	0
37	SR	0	9629	1/1	0.97	0.10	69,69,69,69	0
35	NA	0	9167	1/1	0.97	0.07	50,50,50,50	0
37	SR	0	9454	1/1	0.97	0.09	73,73,73,73	0
35	NA	0	9116	1/1	0.97	0.26	45,45,45,45	0
35	NA	0	9143	1/1	0.97	0.07	38,38,38,38	0
37	SR	0	9509	1/1	0.97	0.12	83,83,83,83	0
37	SR	0	9560	1/1	0.97	0.08	97,97,97,97	0
35	NA	0	9114	1/1	0.97	0.19	51,51,51,51	0
35	NA	0	9136	1/1	0.97	0.11	31,31,31,31	0
37	SR	0	9433	1/1	0.97	0.11	73,73,73,73	0
37	SR	F	9595	1/1	0.97	0.14	95,95,95,95	0
33	MG	0	8116	1/1	0.97	0.04	51,51,51,51	0
33	MG	0	8020	1/1	0.97	0.18	30,30,30,30	0
37	SR	0	9477	1/1	0.97	0.10	82,82,82,82	0
37	SR	0	9446	1/1	0.97	0.10	80,80,80,80	0
35	NA	C	9104	1/1	0.97	0.17	27,27,27,27	0
37	SR	0	9465	1/1	0.97	0.08	96,96,96,96	0
33	MG	0	8079	1/1	0.97	0.14	30,30,30,30	0
33	MG	0	8096	1/1	0.97	0.13	44,44,44,44	0
37	SR	A	9437	1/1	0.97	0.13	64,64,64,64	0
37	SR	0	9517	1/1	0.97	0.06	96,96,96,96	0
36	CL	0	9314	1/1	0.97	0.05	47,47,47,47	0
33	MG	0	8001	1/1	0.97	0.22	17,17,17,17	0
37	SR	9	9481	1/1	0.98	0.06	83,83,83,83	0
33	MG	0	8110	1/1	0.98	0.13	46,46,46,46	0
33	MG	0	8031	1/1	0.98	0.13	48,48,48,48	0
37	SR	0	9442	1/1	0.98	0.12	59,59,59,59	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
36	CL	J	9321	1/1	0.98	0.12	58,58,58,58	0
33	MG	0	8017	1/1	0.98	0.18	20,20,20,20	0
37	SR	0	9455	1/1	0.98	0.10	61,61,61,61	0
35	NA	0	9162	1/1	0.98	0.30	51,51,51,51	0
37	SR	0	9568	1/1	0.98	0.08	75,75,75,75	0
36	CL	0	9305	1/1	0.98	0.07	52,52,52,52	0
33	MG	0	8037	1/1	0.98	0.06	40,40,40,40	0
37	SR	0	9407	1/1	0.98	0.14	42,42,42,42	0
35	NA	0	9105	1/1	0.98	0.15	41,41,41,41	0
36	CL	O	9308	1/1	0.98	0.06	67,67,67,67	0
37	SR	0	9508	1/1	0.98	0.08	83,83,83,83	0
33	MG	0	8005	1/1	0.98	0.09	29,29,29,29	0
37	SR	B	9458	1/1	0.98	0.09	73,73,73,73	0
33	MG	0	8029	1/1	0.98	0.22	27,27,27,27	0
37	SR	0	9441	1/1	0.98	0.08	54,54,54,54	0
37	SR	0	9464	1/1	0.98	0.05	80,80,80,80	0
37	SR	0	9438	1/1	0.98	0.09	63,63,63,63	0
37	SR	0	9427	1/1	0.98	0.12	53,53,53,53	0
37	SR	0	9432	1/1	0.98	0.12	63,63,63,63	0
36	CL	0	9313	1/1	0.98	0.11	51,51,51,51	0
35	NA	Q	9148	1/1	0.98	0.13	50,50,50,50	0
33	MG	0	8002	1/1	0.98	0.13	22,22,22,22	0
37	SR	0	9478	1/1	0.98	0.07	70,70,70,70	0
37	SR	0	9426	1/1	0.98	0.08	66,66,66,66	0
37	SR	1	9460	1/1	0.98	0.12	49,49,49,49	0
37	SR	0	9483	1/1	0.98	0.08	67,67,67,67	0
37	SR	0	9566	1/1	0.98	0.07	75,75,75,75	0
33	MG	0	8028	1/1	0.98	0.10	34,34,34,34	0
37	SR	0	9448	1/1	0.98	0.07	62,62,62,62	0
37	SR	0	9453	1/1	0.98	0.09	68,68,68,68	0
33	MG	0	8117	1/1	0.98	0.11	39,39,39,39	0
33	MG	Y	8109	1/1	0.98	0.10	38,38,38,38	0
33	MG	0	8067	1/1	0.98	0.12	36,36,36,36	0
37	SR	0	9488	1/1	0.98	0.13	78,78,78,78	0
33	MG	0	8068	1/1	0.98	0.14	47,47,47,47	0
37	SR	A	9497	1/1	0.98	0.11	85,85,85,85	0
36	CL	0	9303	1/1	0.98	0.17	49,49,49,49	0
35	NA	M	9147	1/1	0.98	0.10	38,38,38,38	0
37	SR	0	9417	1/1	0.98	0.13	53,53,53,53	0
37	SR	0	9412	1/1	0.98	0.12	43,43,43,43	0
33	MG	0	8056	1/1	0.98	0.18	47,47,47,47	0
37	SR	0	9456	1/1	0.98	0.06	67,67,67,67	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
37	SR	0	9469	1/1	0.99	0.04	85,85,85,85	0
35	NA	0	9123	1/1	0.99	0.10	37,37,37,37	0
37	SR	0	9473	1/1	0.99	0.04	69,69,69,69	0
38	CD	Z	9203	1/1	0.99	0.07	75,75,75,75	0
33	MG	0	8004	1/1	0.99	0.12	27,27,27,27	0
37	SR	0	9450	1/1	0.99	0.08	64,64,64,64	0
36	CL	0	9317	1/1	0.99	0.08	49,49,49,49	0
35	NA	R	9138	1/1	0.99	0.08	52,52,52,52	0
37	SR	S	9470	1/1	0.99	0.14	95,95,95,95	0
33	MG	0	8074	1/1	0.99	0.21	20,20,20,20	0
37	SR	0	9425	1/1	0.99	0.09	71,71,71,71	0
37	SR	0	9445	1/1	0.99	0.10	62,62,62,62	0
37	SR	0	9422	1/1	0.99	0.12	53,53,53,53	0
37	SR	0	9461	1/1	0.99	0.04	73,73,73,73	0
37	SR	0	9451	1/1	0.99	0.09	63,63,63,63	0
33	MG	K	8069	1/1	0.99	0.21	23,23,23,23	0
36	CL	R	9306	1/1	0.99	0.17	46,46,46,46	0
38	CD	U	9201	1/1	0.99	0.09	56,56,56,56	0
33	MG	0	8106	1/1	0.99	0.03	37,37,37,37	0
37	SR	0	9498	1/1	0.99	0.06	63,63,63,63	0
37	SR	0	9449	1/1	0.99	0.09	59,59,59,59	0
37	SR	0	9423	1/1	0.99	0.11	51,51,51,51	0
37	SR	0	9457	1/1	0.99	0.10	47,47,47,47	0
37	SR	0	9435	1/1	0.99	0.07	68,68,68,68	0
37	SR	0	9424	1/1	0.99	0.15	43,43,43,43	0
33	MG	0	8112	1/1	0.99	0.04	44,44,44,44	0
37	SR	0	9440	1/1	0.99	0.04	63,63,63,63	0
35	NA	0	9128	1/1	0.99	0.13	40,40,40,40	0
33	MG	0	8026	1/1	0.99	0.18	26,26,26,26	0
37	SR	0	9414	1/1	0.99	0.13	53,53,53,53	0
35	NA	0	9117	1/1	0.99	0.16	32,32,32,32	0
37	SR	0	9532	1/1	0.99	0.05	100,100,100,100	0
37	SR	0	9408	1/1	0.99	0.15	38,38,38,38	0
36	CL	M	9318	1/1	0.99	0.16	37,37,37,37	0
37	SR	R	9418	1/1	0.99	0.15	53,53,53,53	0
33	MG	0	8070	1/1	0.99	0.18	21,21,21,21	0
37	SR	0	9429	1/1	0.99	0.11	63,63,63,63	0
38	CD	3	9204	1/1	0.99	0.06	58,58,58,58	0
37	SR	0	9413	1/1	0.99	0.12	44,44,44,44	0
37	SR	0	9515	1/1	0.99	0.19	100,100,100,100	0
37	SR	1	9419	1/1	0.99	0.12	38,38,38,38	0
36	CL	A	9309	1/1	0.99	0.17	64,64,64,64	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
37	SR	0	9545	1/1	0.99	0.05	67,67,67,67	0
37	SR	0	9480	1/1	0.99	0.06	86,86,86,86	0
33	MG	0	8038	1/1	0.99	0.26	13,13,13,13	0
37	SR	A	9436	1/1	0.99	0.06	57,57,57,57	0
37	SR	0	9434	1/1	0.99	0.15	58,58,58,58	0
37	SR	0	9420	1/1	0.99	0.15	60,60,60,60	0
37	SR	0	9462	1/1	0.99	0.13	66,66,66,66	0
37	SR	0	9443	1/1	0.99	0.10	59,59,59,59	0
33	MG	0	8044	1/1	0.99	0.06	42,42,42,42	0
37	SR	3	9439	1/1	0.99	0.06	63,63,63,63	0
37	SR	0	9411	1/1	0.99	0.16	42,42,42,42	0
33	MG	0	8008	1/1	0.99	0.22	14,14,14,14	0
33	MG	0	8012	1/1	0.99	0.26	37,37,37,37	0
37	SR	L	9409	1/1	1.00	0.12	36,36,36,36	0
37	SR	0	9430	1/1	1.00	0.14	41,41,41,41	0
36	CL	0	9312	1/1	1.00	0.08	45,45,45,45	0
37	SR	0	9428	1/1	1.00	0.07	43,43,43,43	0
37	SR	0	9406	1/1	1.00	0.17	33,33,33,33	0
37	SR	0	9415	1/1	1.00	0.11	50,50,50,50	0
37	SR	0	9416	1/1	1.00	0.09	45,45,45,45	0
38	CD	1	9202	1/1	1.00	0.04	51,51,51,51	0
37	SR	0	9410	1/1	1.00	0.15	34,34,34,34	0
37	SR	0	9444	1/1	1.00	0.09	47,47,47,47	0

## 6.5 Other polymers

There are no such residues in this entry.