



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 05:54 pm BST

PDB ID : 5IB7
Title : Structure of T. thermophilus 70S ribosome complex with mRNA, tRNA^{fMet}, near-cognate tRNA^{Lys} with U-G mismatch in the A-site and antibiotic paromomycin
Authors : Rozov, A.; Demeshkina, N.; Yusupov, M.; Yusupova, G.
Deposited on : 2016-02-22
Resolution : 2.99 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

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:

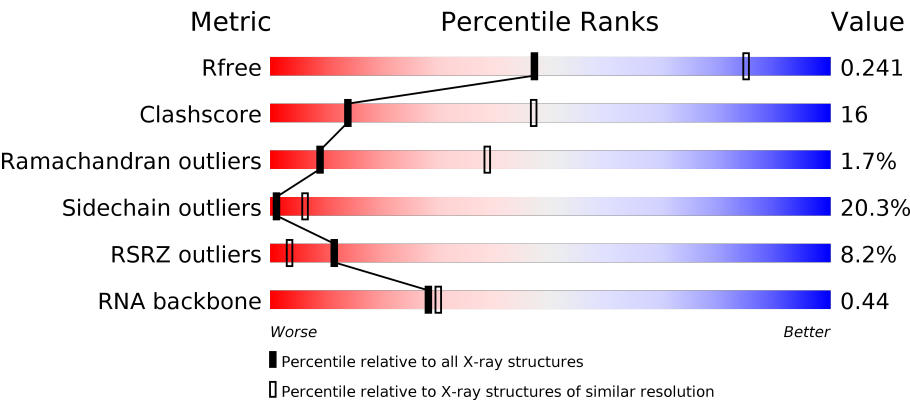
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	13	1522	<div><div></div><div><div>37%</div><div>45%</div><div>15%</div><div>• •</div></div></div>
1	1G	1522	<div><div>10%</div><div><div>39%</div><div>44%</div><div>14%</div><div>• •</div></div></div>
2	12	256	<div><div>10%</div><div><div>34%</div><div>36%</div><div>9%</div><div>•</div><div>19%</div></div></div>
2	1E	256	<div><div>5%</div><div><div>39%</div><div>38%</div><div>12%</div><div>•</div><div>10%</div></div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	22	239	
3	2E	239	
4	32	209	
4	3E	209	
5	42	162	
5	4E	162	
6	52	101	
6	5E	101	
7	62	156	
7	6E	156	
8	72	138	
8	7E	138	
9	82	128	
9	8E	128	
10	1A	105	
10	1I	105	
11	2A	129	
11	2I	129	
12	3A	132	
12	3I	132	
13	4A	126	
13	4I	126	
14	5A	61	
14	5I	61	
15	6A	89	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	6I	89	
16	7A	88	
16	7I	88	
17	8A	105	
17	8I	105	
18	9A	88	
18	9I	88	
19	AA	93	
19	AI	93	
20	BA	106	
20	BI	106	
21	1B	27	
21	1F	27	
22	1K	76	
23	2K	77	
23	2L	77	
24	1L	76	
24	3K	76	
24	3L	76	
25	4K	30	
25	4L	30	
26	14	2917	
26	1H	2917	
27	16	122	
27	1J	122	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	71	229	
29	11	276	
29	19	276	
30	21	206	
30	29	206	
31	31	210	
31	39	210	
32	41	182	
32	49	182	
33	51	180	
33	59	180	
34	61	148	
34	69	148	
35	15	140	
35	58	140	
36	25	122	
36	68	122	
37	35	150	
37	78	150	
38	45	141	
38	88	141	
39	55	118	
39	98	118	
40	65	112	
40	A8	112	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
41	75	146	
41	B8	146	
42	85	118	
42	C8	118	
43	95	101	
43	D8	101	
44	A5	113	
44	E8	113	
45	B5	96	
45	F8	96	
46	C5	110	
46	G8	110	
47	D5	206	
47	H8	206	
48	E5	85	
48	I8	85	
49	F5	98	
49	J8	98	
50	G5	72	
50	K8	72	
51	H5	60	
51	L8	60	
52	M8	71	
53	J5	60	
53	N8	60	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
54	O8	54	
55	L5	49	
55	P8	49	
56	M5	65	
56	Q8	65	

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
57	MG	13	1647	-	-	-	X
57	MG	13	1662	-	-	-	X
57	MG	13	1664	-	-	-	X
57	MG	13	1669	-	-	-	X
57	MG	13	1671	-	-	-	X
57	MG	13	1673	-	-	-	X
57	MG	13	1676	-	-	-	X
57	MG	14	3064	-	-	-	X
57	MG	14	3069	-	-	-	X
57	MG	14	3103	-	-	-	X
57	MG	14	3109	-	-	-	X
57	MG	14	3115	-	-	-	X
57	MG	14	3118	-	-	-	X
57	MG	14	3127	-	-	-	X
57	MG	14	3128	-	-	-	X
57	MG	14	3132	-	-	-	X
57	MG	14	3138	-	-	-	X
57	MG	14	3161	-	-	-	X
57	MG	14	3166	-	-	-	X
57	MG	14	3173	-	-	-	X
57	MG	14	3185	-	-	-	X
57	MG	14	3197	-	-	-	X
57	MG	14	3208	-	-	-	X
57	MG	19	301	-	-	-	X
57	MG	1G	1609	-	-	-	X
57	MG	1G	1618	-	-	-	X
57	MG	1G	1634	-	-	-	X
57	MG	1H	3004	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	1H	3053	-	-	-	X
57	MG	1H	3065	-	-	-	X
57	MG	1H	3081	-	-	-	X
57	MG	1H	3111	-	-	-	X
57	MG	1H	3130	-	-	-	X
57	MG	1H	3135	-	-	-	X
57	MG	1H	3144	-	-	-	X
57	MG	1H	3145	-	-	-	X
57	MG	1H	3150	-	-	-	X
57	MG	1H	3153	-	-	-	X
57	MG	1H	3163	-	-	-	X
57	MG	1H	3168	-	-	-	X
57	MG	1H	3177	-	-	-	X
57	MG	1H	3180	-	-	-	X
57	MG	1H	3205	-	-	-	X
57	MG	1H	3206	-	-	-	X
57	MG	1H	3211	-	-	-	X
57	MG	1H	3217	-	-	-	X
57	MG	1H	3225	-	-	-	X
57	MG	1H	3237	-	-	-	X
57	MG	E5	101	-	-	-	X
57	MG	P8	101	-	-	-	X
59	SF4	32	302	-	-	X	-

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 297444 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	13	1499	Total	C	N	O	P	0	0	0
			32223	14342	5973	10409	1499			
1	1G	1508	Total	C	N	O	P	0	0	0
			32414	14427	6005	10474	1508			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
13	1542	G	-	expression tag	GB 55771382
13	1543	C	-	expression tag	GB 55771382
13	1544	U	-	expression tag	GB 55771382
1G	1542	G	-	expression tag	GB 55771382
1G	1543	C	-	expression tag	GB 55771382
1G	1544	U	-	expression tag	GB 55771382

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1E	231	Total	C	N	O	S	0	0	0
			1874	1199	334	336	5			
2	12	207	Total	C	N	O	S	0	0	0
			1696	1083	306	303	4			

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	2E	205	Total	C	N	O	S	0	0	0
			1605	1011	313	280	1			
3	22	195	Total	C	N	O	S	0	0	0
			1537	973	297	266	1			

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	3E	207	Total	C	N	O	S	0	0	0
			1698	1064	338	289	7			
4	32	208	Total	C	N	O	S	0	0	0
			1702	1066	339	290	7			

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	4E	149	Total	C	N	O	S	0	0	0
			1142	722	216	200	4			
5	42	150	Total	C	N	O	S	0	0	0
			1141	719	217	201	4			

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	5E	100	Total	C	N	O	S	0	0	0
			837	528	154	152	3			
6	52	101	Total	C	N	O	S	0	0	0
			842	531	155	153	3			

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	6E	154	Total	C	N	O	S	0	0	0
			1242	770	250	216	6			
7	62	138	Total	C	N	O	S	0	0	0
			1110	689	221	194	6			

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	7E	138	Total	C	N	O	S	0	0	0
			1115	705	215	192	3			
8	72	137	Total	C	N	O	S	0	0	0
			1107	700	214	191	2			

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	8E	126	Total	C	N	O		0	0	0
			1000	634	196	170				

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	82	121	Total	C	N	O	0	0	0
			953	605	186	162			

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	1I	94	Total	C	N	O	S	0	0	0
			749	468	147	133	1			
10	1A	80	Total	C	N	O		0	0	0
			646	403	129	114				

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	2I	111	Total	C	N	O	S	0	0	0
			823	512	154	154	3			
11	2A	113	Total	C	N	O	S	0	0	0
			835	520	156	156	3			

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	3I	122	Total	C	N	O	S	0	0	0
			956	603	193	159	1			
12	3A	121	Total	C	N	O	S	0	0	0
			947	597	191	158	1			

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	4I	117	Total	C	N	O	S	0	0	0
			933	577	192	162	2			
13	4A	109	Total	C	N	O	S	0	0	0
			879	544	181	152	2			

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	5I	59	Total	C	N	O	S	0	0	0
			486	309	103	70	4			
14	5A	59	Total	C	N	O	S	0	0	0
			486	309	103	70	4			

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	6I	87	Total	C	N	O	S	0	0	0
			729	457	146	124	2			
15	6A	87	Total	C	N	O	S	0	0	0
			729	457	146	124	2			

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	7I	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			
16	7A	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	8I	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
17	8A	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	9I	68	Total	C	N	O	0	0	0
			549	352	105	92			
18	9A	67	Total	C	N	O	0	0	0
			544	349	104	91			

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AI	82	Total	C	N	O	S	0	0	0
			661	422	123	114	2			
19	AA	65	Total	C	N	O	S	0	0	0
			510	324	92	92	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	BI	97	Total	C	N	O	S	0	0	0
			746	461	157	126	2			
20	BA	99	Total	C	N	O	S	0	0	0
			762	470	162	128	2			

- Molecule 21 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	1F	23	Total	C	N	O	0	0	0
			199	122	48	29			
21	1B	22	Total	C	N	O	0	0	0
			188	116	44	28			

- Molecule 22 is a RNA chain called tRNA^{Lys}.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	1K	72	Total	C	N	O	P	S	0	0
			1542	691	269	509	72	1		

- Molecule 23 is a RNA chain called tRNA^{fMet}.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	2K	77	Total	C	N	O	P	S	0	0
			1646	735	298	535	77	1		
23	2L	77	Total	C	N	O	P	S	0	0
			1646	735	298	535	77	1		

- Molecule 24 is a RNA chain called tRNA^{Lys}.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	3K	70	Total	C	N	O	P	0	0	0
			1483	664	260	490	69			
24	1L	66	Total	C	N	O	P	0	0	0
			1401	626	244	465	66			
24	3L	72	Total	C	N	O	P	0	0	0
			1528	684	270	503	71			

- Molecule 25 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	4K	19	Total	C	N	O	P	0	0	0
			420	188	89	124	19			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	4L	19	Total	C	N	O	P	0	0	0
			419	188	89	123	19			

- Molecule 26 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	1H	2860	Total	C	N	O	P	0	0	0
			61609	27418	11525	19806	2860			
26	14	2826	Total	C	N	O	P	0	0	0
			60877	27092	11393	19566	2826			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1H	161	U	UNK	conflict	GB 55771382
1H	654A	A	G	conflict	GB 55771382
1H	654E	C	G	conflict	GB 55771382
1H	654P	G	C	conflict	GB 55771382
1H	654T	A	C	conflict	GB 55771382
1H	1059B	U	G	conflict	GB 55771382
1H	1080	A	C	conflict	GB 55771382
14	158	U	UNK	conflict	GB 55771382
14	654A	A	G	conflict	GB 55771382
14	654E	C	G	conflict	GB 55771382
14	654P	G	C	conflict	GB 55771382
14	654T	A	C	conflict	GB 55771382
14	1058	U	G	conflict	GB 55771382
14	1080	A	C	conflict	GB 55771382

- Molecule 27 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	16	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			
27	1J	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			

- Molecule 28 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	71	132	Total	C	N	O	S	0	0	0
			1027	648	193	185	1			

- Molecule 29 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	11	273	Total	C	N	O	S	0	0	0
			2120	1338	421	358	3			
29	19	274	Total	C	N	O	S	0	0	0
			2125	1341	422	359	3			

- Molecule 30 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	21	203	Total	C	N	O	S	0	0	0
			1546	978	295	267	6			
30	29	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			

- Molecule 31 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	31	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			
31	39	204	Total	C	N	O	S	0	0	0
			1602	1022	299	279	2			

- Molecule 32 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	41	179	Total	C	N	O	S	0	0	0
			1457	931	265	257	4			
32	49	180	Total	C	N	O	S	0	0	0
			1459	931	266	258	4			

- Molecule 33 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	51	174	Total	C	N	O	S	0	0	0
			1328	842	249	236	1			
33	59	169	Total	C	N	O	S	0	0	0
			1295	823	241	230	1			

- Molecule 34 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	61	145	Total	C	N	O	S	0	0	0
			1131	723	200	207	1			
34	69	145	Total	C	N	O	S	0	0	0
			1131	723	200	207	1			

- Molecule 35 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	58	137	Total	C	N	O	S	0	0	0
			1096	706	205	181	4			
35	15	137	Total	C	N	O	S	0	0	0
			1096	707	205	181	3			

- Molecule 36 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	68	122	Total	C	N	O	S	0	0	0
			932	588	171	169	4			
36	25	122	Total	C	N	O	S	0	0	0
			932	588	171	169	4			

- Molecule 37 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	78	147	Total	C	N	O	S	0	0	0
			1122	698	229	192	3			
37	35	147	Total	C	N	O	S	0	0	0
			1122	698	229	192	3			

- Molecule 38 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	88	141	Total	C	N	O	S	0	0	0
			1117	712	211	187	7			
38	45	138	Total	C	N	O	S	0	0	0
			1099	702	208	183	6			

- Molecule 39 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	98	118	Total	C	N	O	S	0	0	0
			967	604	203	159	1			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	55	118	Total	C	N	O	S	0	0	0
			967	604	203	159	1			

- Molecule 40 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	A8	111	Total	C	N	O		0	0	0
			881	556	176	149				
40	65	110	Total	C	N	O		0	0	0
			876	553	175	148				

- Molecule 41 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	B8	135	Total	C	N	O	S	0	0	0
			1119	697	230	191	1			
41	75	133	Total	C	N	O	S	0	0	0
			1109	691	228	189	1			

- Molecule 42 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	C8	115	Total	C	N	O	S	0	0	0
			950	603	199	147	1			
42	85	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			

- Molecule 43 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	D8	100	Total	C	N	O	S	0	0	0
			774	499	141	133	1			
43	95	100	Total	C	N	O	S	0	0	0
			770	496	140	133	1			

- Molecule 44 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	E8	110	Total	C	N	O	S	0	0	0
			876	552	171	151	2			
44	A5	111	Total	C	N	O	S	0	0	0
			886	558	174	152	2			

- Molecule 45 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	F8	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			
45	B5	94	Total	C	N	O		0	0	0
			735	477	133	125				

- Molecule 46 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	G8	103	Total	C	N	O	S	0	0	0
			783	504	148	126	5			
46	C5	104	Total	C	N	O	S	0	0	0
			794	510	152	127	5			

- Molecule 47 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	H8	170	Total	C	N	O	S	0	0	0
			1365	870	246	246	3			
47	D5	177	Total	C	N	O	S	0	0	0
			1411	901	253	255	2			

- Molecule 48 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	I8	77	Total	C	N	O	S	0	0	0
			611	378	129	103	1			
48	E5	76	Total	C	N	O	S	0	0	0
			603	372	128	102	1			

- Molecule 49 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	J8	96	Total	C	N	O	S	0	0	0
			747	469	148	129	1			
49	F5	94	Total	C	N	O	S	0	0	0
			737	463	146	127	1			

- Molecule 50 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	K8	68	Total	C	N	O	S	0	0	0
			575	358	116	100	1			
50	G5	69	Total	C	N	O	S	0	0	0
			576	358	116	101	1			

- Molecule 51 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	L8	58	Total	C	N	O	S	0	0	0
			459	293	89	77				
51	H5	58	Total	C	N	O	S	0	0	0
			459	293	89	77				

- Molecule 52 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	M8	60	Total	C	N	O	S	0	0	0
			475	300	84	86	5			

- Molecule 53 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	N8	48	Total	C	N	O	S	0	0	0
			369	229	75	60	5			
53	J5	56	Total	C	N	O	S	0	0	0
			434	272	87	70	5			

- Molecule 54 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	O8	45	Total	C	N	O	S	0	0	0
			389	241	79	65	4			

- Molecule 55 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	P8	47	Total	C	N	O	S	0	0	0
			401	246	99	54	2			
55	L5	47	Total	C	N	O	S	0	0	0
			401	246	99	54	2			

- Molecule 56 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	Q8	64	Total	C	N	O	S	0	0	0
			516	331	102	81	2			
56	M5	64	Total	C	N	O	S	0	0	0
			516	331	102	81	2			

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

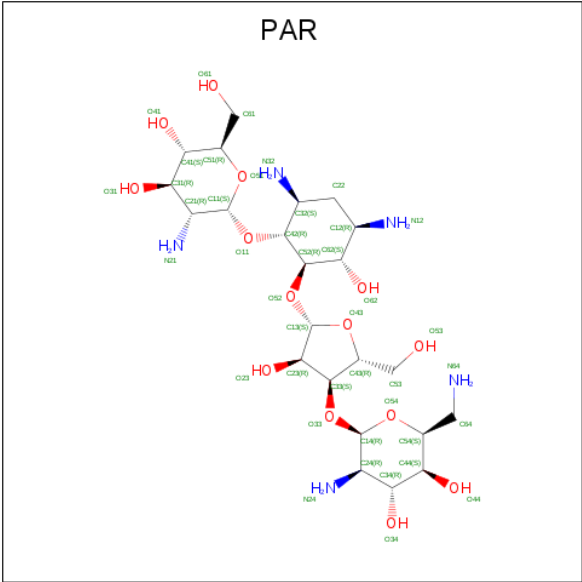
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	45	2	Total	Mg	0	0
			2	2		
57	P8	1	Total	Mg	0	0
			1	1		
57	32	1	Total	Mg	0	0
			1	1		
57	C5	1	Total	Mg	0	0
			1	1		
57	13	140	Total	Mg	0	0
			140	140		
57	1J	8	Total	Mg	0	0
			8	8		
57	5I	1	Total	Mg	0	0
			1	1		
57	35	1	Total	Mg	0	0
			1	1		
57	4L	1	Total	Mg	0	0
			1	1		
57	16	11	Total	Mg	0	0
			11	11		
57	42	1	Total	Mg	0	0
			1	1		
57	25	1	Total	Mg	0	0
			1	1		
57	M5	1	Total	Mg	0	0
			1	1		
57	21	3	Total	Mg	0	0
			3	3		
57	31	2	Total	Mg	0	0
			2	2		
57	Q8	1	Total	Mg	0	0
			1	1		
57	4I	1	Total	Mg	0	0
			1	1		
57	3I	1	Total	Mg	0	0
			1	1		

Continued on next page...

Continued from previous page...

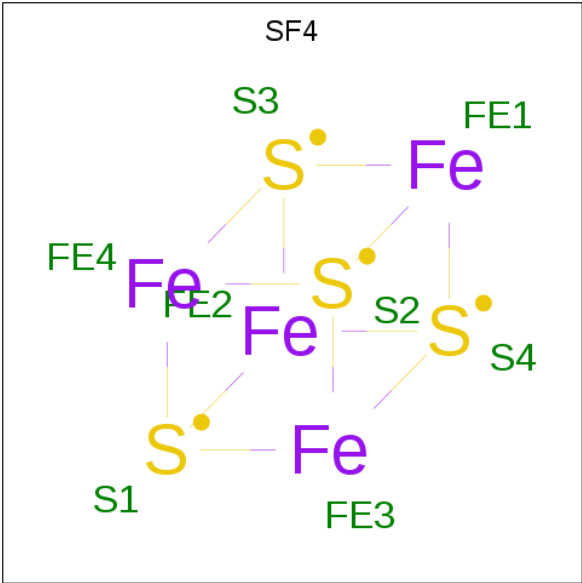
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	I8	2	Total 2	Mg 2	0	0
57	52	1	Total 1	Mg 1	0	0
57	29	1	Total 1	Mg 1	0	0
57	7A	1	Total 1	Mg 1	0	0
57	2K	2	Total 2	Mg 2	0	0
57	39	2	Total 2	Mg 2	0	0
57	1G	102	Total 102	Mg 102	0	0
57	1H	525	Total 525	Mg 525	0	0
57	E5	1	Total 1	Mg 1	0	0
57	88	3	Total 3	Mg 3	0	0
57	14	435	Total 435	Mg 435	0	0
57	78	1	Total 1	Mg 1	0	0
57	19	1	Total 1	Mg 1	0	0
57	41	1	Total 1	Mg 1	0	0
57	2L	2	Total 2	Mg 2	0	0

- Molecule 58 is PAROMOMYCIN (three-letter code: PAR) (formula: C₂₃H₄₅N₅O₁₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
58	13	1	Total	C	N	O	0	0
			42	23	5	14		
58	1G	1	Total	C	N	O	0	0
			42	23	5	14		

- Molecule 59 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).

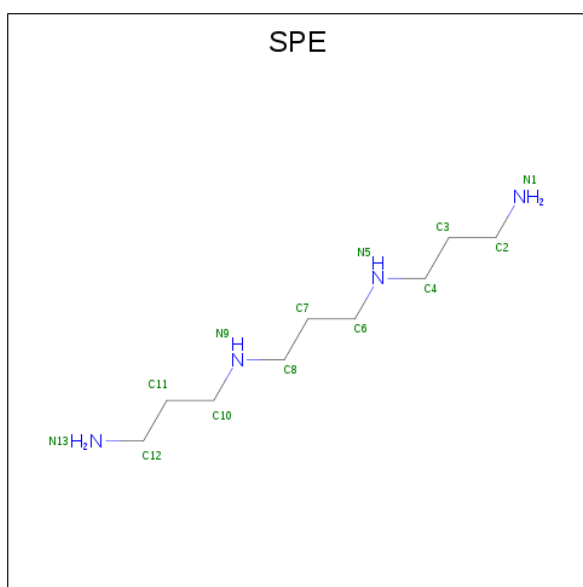


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
59	3E	1	Total	Fe	S	0	0
			8	4	4		
59	32	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	C5	1	Total Zn 1 1	0	0
60	5A	1	Total Zn 1 1	0	0
60	G8	1	Total Zn 1 1	0	0
60	5I	1	Total Zn 1 1	0	0

- Molecule 61 is THERMINE (three-letter code: SPE) (formula: C₉H₂₄N₄).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1G	1	Total C N 13 9 4	0	0
61	14	1	Total C N 13 9 4	0	0
61	14	1	Total C N 13 9 4	0	0

- Molecule 62 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	13	320	Total O 320 320	0	0
62	4E	3	Total O 3 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	8E	2	Total 2	O 2	0	0
62	1I	2	Total 2	O 2	0	0
62	3I	2	Total 2	O 2	0	0
62	5I	2	Total 2	O 2	0	0
62	6I	3	Total 3	O 3	0	0
62	7I	1	Total 1	O 1	0	0
62	BI	2	Total 2	O 2	0	0
62	1F	1	Total 1	O 1	0	0
62	1K	2	Total 2	O 2	0	0
62	2K	8	Total 8	O 8	0	0
62	4K	5	Total 5	O 5	0	0
62	1H	1470	Total 1470	O 1470	0	0
62	16	12	Total 12	O 12	0	0
62	11	17	Total 17	O 17	0	0
62	21	7	Total 7	O 7	0	0
62	31	5	Total 5	O 5	0	0
62	41	1	Total 1	O 1	0	0
62	58	2	Total 2	O 2	0	0
62	78	10	Total 10	O 10	0	0
62	B8	1	Total 1	O 1	0	0
62	C8	3	Total 3	O 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	F8	2	Total 2	O 2	0	0
62	G8	2	Total 2	O 2	0	0
62	I8	6	Total 6	O 6	0	0
62	J8	4	Total 4	O 4	0	0
62	L8	3	Total 3	O 3	0	0
62	P8	1	Total 1	O 1	0	0
62	Q8	5	Total 5	O 5	0	0
62	1G	317	Total 317	O 317	0	0
62	32	1	Total 1	O 1	0	0
62	52	4	Total 4	O 4	0	0
62	1A	1	Total 1	O 1	0	0
62	6A	2	Total 2	O 2	0	0
62	7A	5	Total 5	O 5	0	0
62	9A	2	Total 2	O 2	0	0
62	BA	2	Total 2	O 2	0	0
62	2L	6	Total 6	O 6	0	0
62	4L	6	Total 6	O 6	0	0
62	14	1144	Total 1144	O 1144	0	0
62	1J	12	Total 12	O 12	0	0
62	19	15	Total 15	O 15	0	0
62	29	4	Total 4	O 4	0	0

Continued on next page...

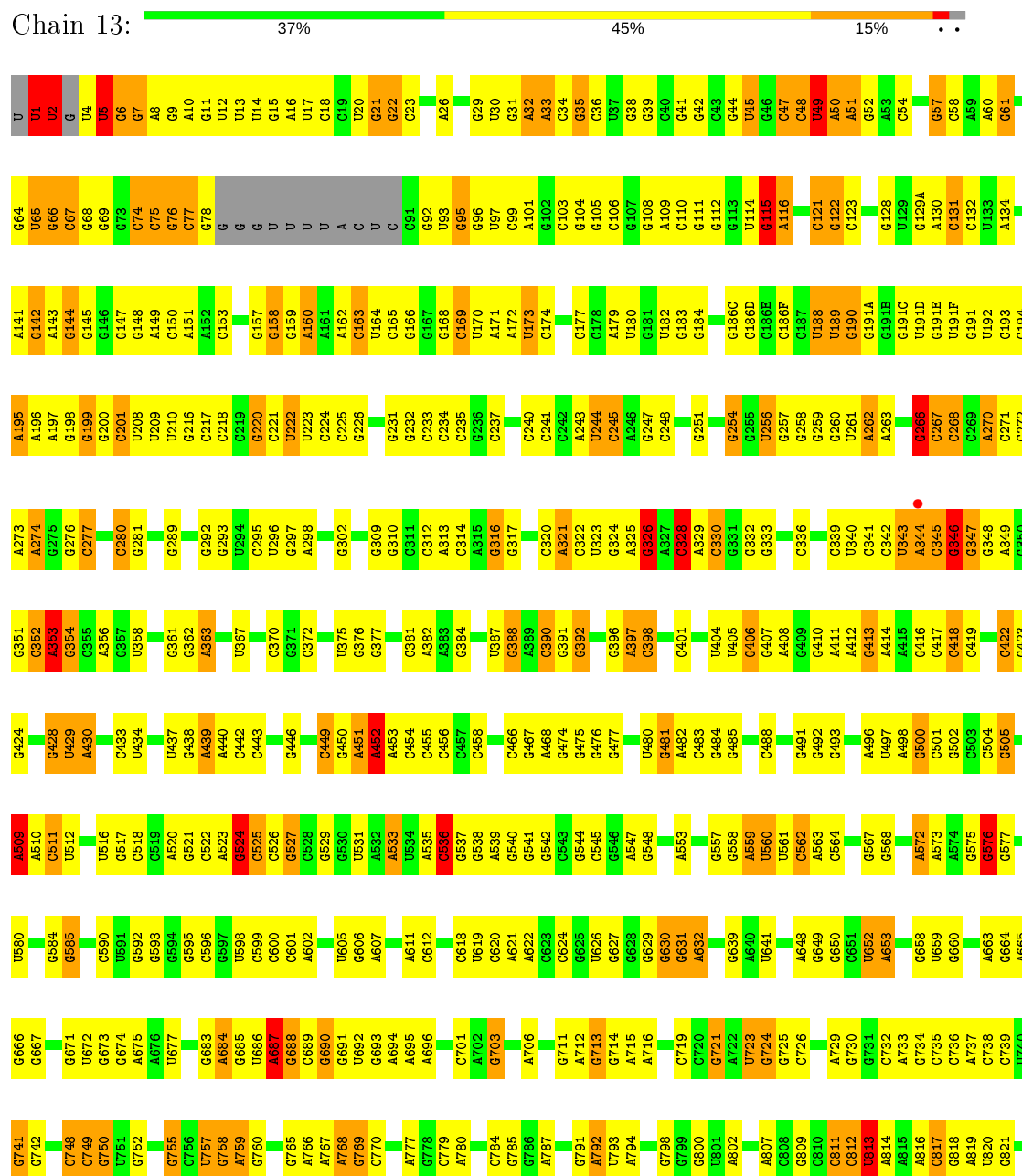
Continued from previous page...

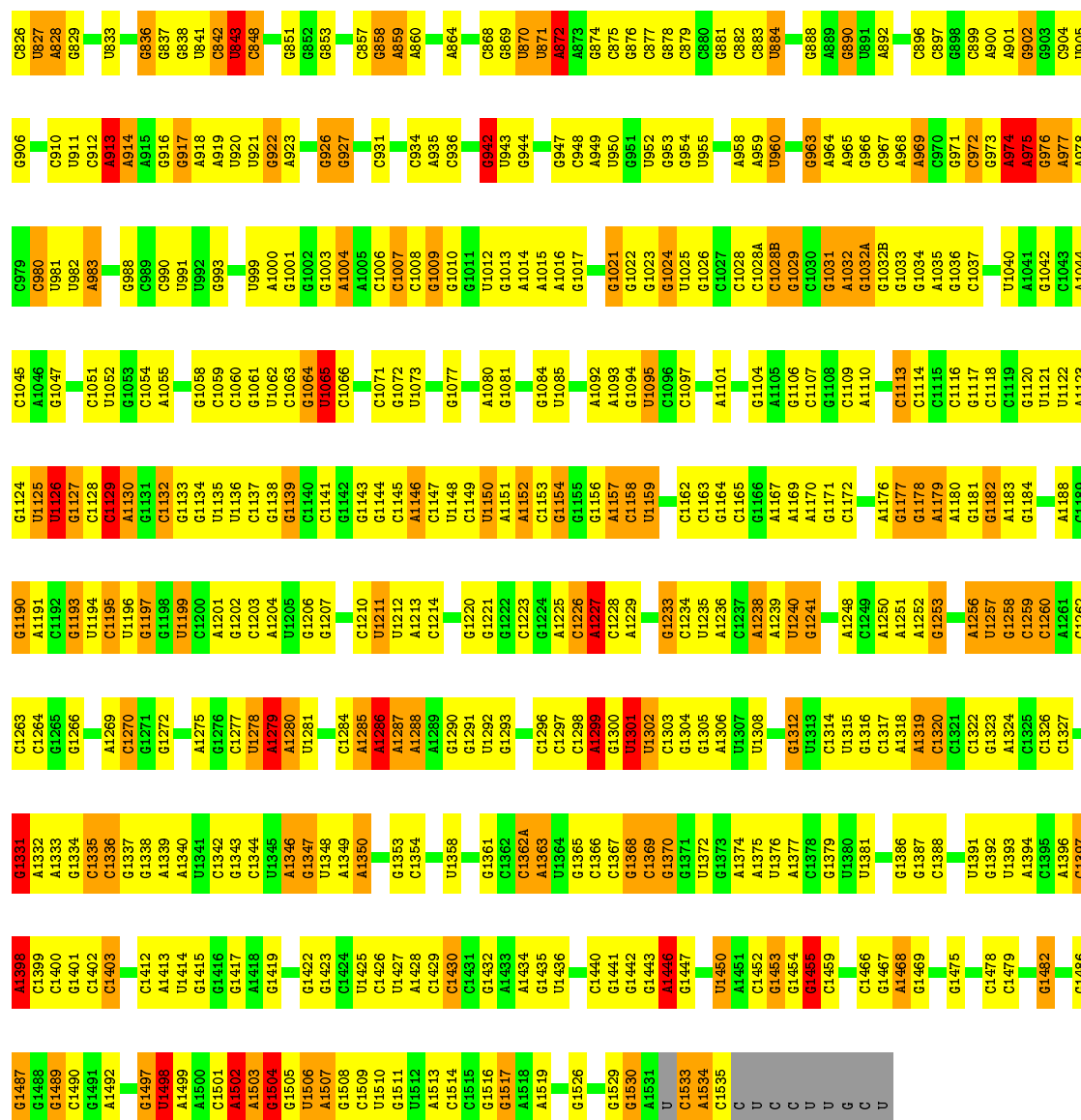
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	39	5	Total	O	0	0
			5	5		
62	15	1	Total	O	0	0
			1	1		
62	25	6	Total	O	0	0
			6	6		
62	35	8	Total	O	0	0
			8	8		
62	55	3	Total	O	0	0
			3	3		
62	85	2	Total	O	0	0
			2	2		
62	A5	1	Total	O	0	0
			1	1		
62	B5	1	Total	O	0	0
			1	1		
62	C5	3	Total	O	0	0
			3	3		
62	F5	1	Total	O	0	0
			1	1		
62	H5	2	Total	O	0	0
			2	2		
62	M5	9	Total	O	0	0
			9	9		

3 Residue-property plots

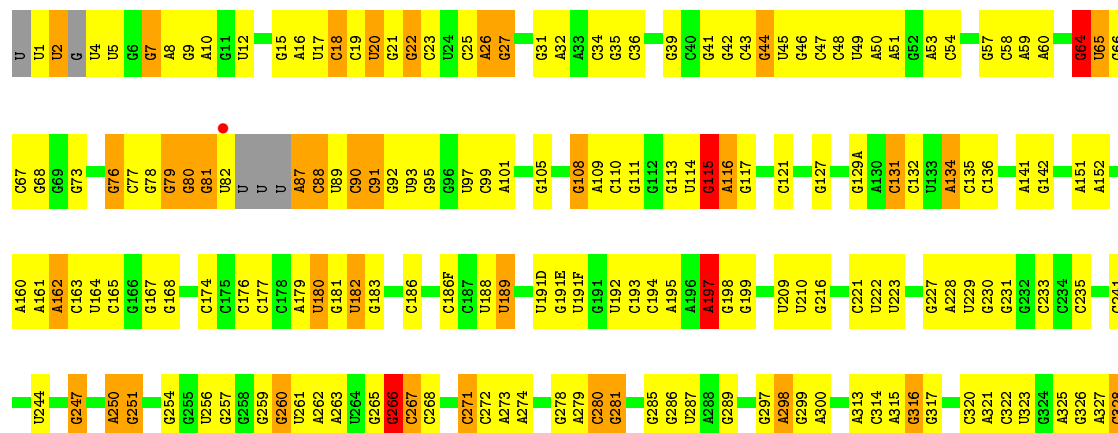
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: 16S ribosomal RNA

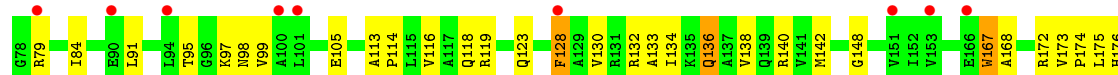


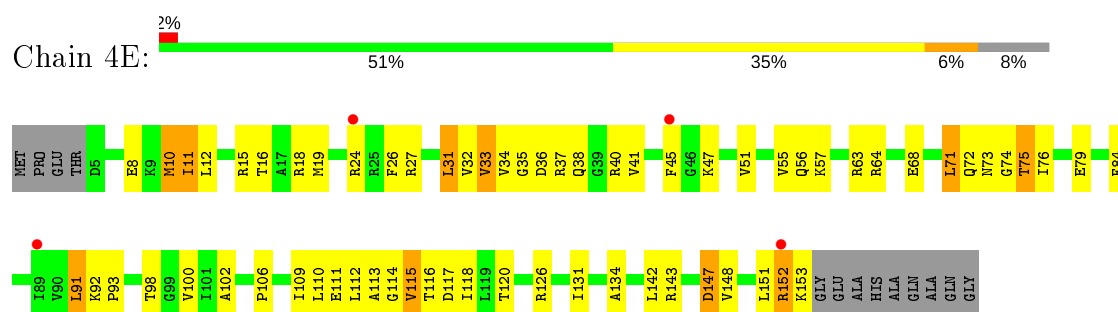


• Molecule 1: 16S ribosomal RNA

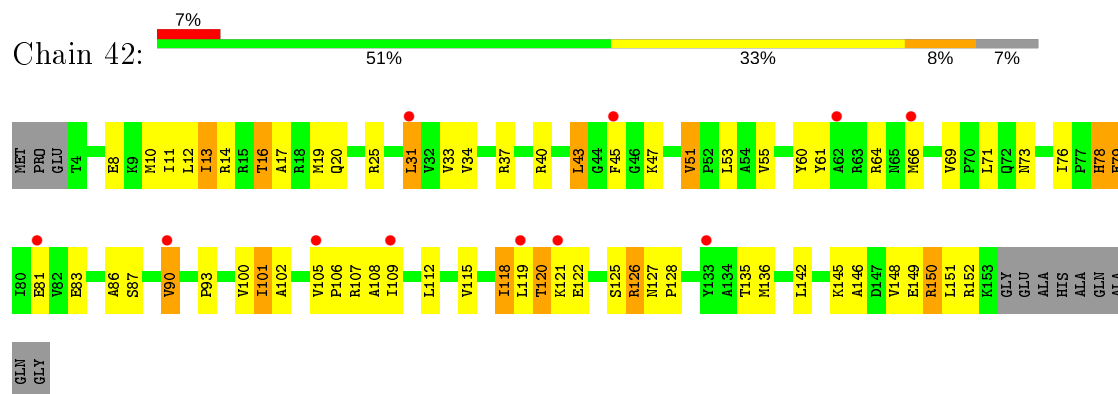


C1397	C1327	G1255	A1183	G1117	U040	U982	A914	G825	G735	G633	U560	C489	G410	A329
A1398	C1328	A1256	G1184	G1117	U1040	A983	A915	C826	C736	A640	U561	G490	A411	C330
C1399	A1329	U1257	G1185	C1119	A1041	C984	A1041	U827	A737	U641	C562		A412	G331
C1400	U1330	G1258	C1102	C1119	C985	C985	G917	A828		A642	A563	A495	G413	G332
G1401	G1331	C1259	A1188	A1123	C1043	A986	U920	G829	G741		C564	A496	A414	
C1402	A1332	G1260	C1189	A1123	A1046	G988	U921	U833	U743	C647	G567	U497	C419	C337
A1403	A1333	A1261	G1190	U1125		C989	G922	C834	C744		G568	A498	C438	A338
C1404	G1334	C1262	A1191	U1126	G1050	C990	A923	U835	C745	G650	C569	G500	U420	C339
C1405	C1335	G1263	U1192	C1127	U1051	U991	C924	G836	A746	C651	C501	C501	U421	U340
U1406	C1336	C1264	U1194	C1128	U1052	U992	G925	G837	C747	U652	A572	C503	C423	
	G1337		C1129	C1129	G1053	G993	G926	G838	C748	A653	A573	C504	G424	A344
G1410	A1338	A1268	U1195	G1054	G1054	A994	G927	U841	C749		A574	G505	G425	C345
C1411	U1196	U1196	A1055	A1055	A1055	C995	C931	C842	G750	U659	G575		G426	C346
G1412	G1197	G1197	U1056	U1056	U1056	C996	C932	U843	G751	G660	G576	A509	G427	G350
A1413	C1200	G1273	G1133	G1133	G1057	A997	C932	U843	U751	G661	G577	A510	U427	G351
U1414	A1201	G1273	G1134	G1134	U1057	U997	G933	C848			C578	A511	G428	C352
U1415	A1201	C1200	U1135	U1135	G1058	C998	G933	G851	G754	G664	G579	U512	U429	A353
A1416	A1346	A1275	U1136	U1136	C1059	C998A	C934	G852	C756	A665	U580	C513	A430	G354
	G1347	G1276	C1137	C1137	G1060	U999	A935	G853	U757	G666	G581		C433	C355
U1419	U1348	C1277	G1138	G1138	G1061	A1000	C936	G854	G758		U582	U516	U434	
A1349	A1349	U1278	U1205	U1205	U1062	A1001	A937	G854	A766	U672	G583	G517	C435	U358
		C1278	G1206	G1206	C1063	G1002	A938	G855	U677	G673	A583	G518	C436	U359
G1422	C1352	A1279	C1140	C1140	G1064	G1003	A938	C856	U677	G674	G584	C519	C437	A360
G1423	G1353	U1280	C1141	C1141	U1065	G1004	G942	C857	A676	G675	G586	A520	G438	G361
C1424	U1281	C1208	G1142	G1142	U1065	A1004	U943	G858	U677	G676	G587	G521	A439	G362
	C1354	C1209	G1143	G1143	C1066	A1005	U943	A859	G769		G588	A522	A440	A363
G1431	G1283	G1283	G1144	G1144	C1069	C1006	G944		G770	G679	C590	A523	C442	
U1432	C1284	U1211	C1145	C1145	U1070	C1007	G947	C862	G776		U591		C442	U367
U1435	A1285	U1212	C1146	C1146	G1071	C1008	G947	C862	G776		C592	C526	U445	U368
G1436	C1359	A1213	C1147	C1147	U1072	G1009	C948	A865	G778	A687	G527	G528	G446	C369
	A1360	A1287	U1148	U1148	U1073	G1010	A949	C867	C784	G688	G529	G528	G447	C370
G1441	G1361	G1215	C1149	C1149	G1074	G1011	U950	C868	G785	G689	G530	G528	G448	G371
C1362	A1288	G1216	U1150	U1150	G1077	G1012	C951	C869	G786	G690	U531	G530	C449	C372
G1362A	G1290	C1217	A1151	A1151	G1077	G1013	U952	C870	G786	G691	U531	G531	G450	A373
A1363	U1291	C1218	C1152	C1152	A1080	A1015	G953	U870	A787	U692	A532	A532	A451	A374
	U1292		C1153	C1153	G1081	A1016	U956	A872		G693	G604	A533	A452	U375
G1293	G1293	G1221	G1154	G1154	G1081	A1017	U957	A873	G791	A694	U605		A452	G376
		G1222	G1155	G1155	G1084	C1018	A958	A873	A792		G606	C536	C466	G377
C1297	C1297	C1223	G1156	G1156	U1085	C1019	A959	A874	U793	U697	A607	G537	C467	
C1298	A1299	G1224	C1157	C1157	U1085	U1020	U960		A794			G538	C468	G380
G1371	C1299	C1225	C1158	C1158	G1088	G1021	U961	G878	G799	G700	A614	A539	G464	C381
U1372	G1300	C1226	U1159	U1159	G1088	G1022	U961	C879		C701	C615	G540	A465	A382
G1373	U1301	C1227	G1160	G1160	U1095	G1024	A965	U884	A702	A702	G616	G541	C466	A383
A1374	C1228	A1227	C1161	C1161	C1096	U1025	A965	G885			G617	G542	C467	
G1454	A1228	A1229	C1162	C1162	U1095	G1024	A965				C618	C543	A468	U387
G1455	C1303		A1167	A1167	C1096	G1026	C967				U619	G544	G474	G388
A1306	U1307	U1232	A1169	A1169	A1101	C1027	A968	A889			A621	G546	G475	A389
U1308	C1308	U1235	A1170	A1170	A1102	C1028	A969	U891	G809	G713	A622	A547	G476	C390
G1309	G1309	U1235	G1171	G1171	G1103	C1028A	A970	U891	C810	C719	G623	G548	G477	G396
		A1238	C1172	C1172	G1104	C1028B	G971	A892	C811	C720	C624		A478	
G1316	G1316	A1239	G1173	G1173	A1105	G1029	C972	C893	C812	G721				G397
C1317	C1317	U1240	G1174	G1174	G1106	C1030	G973			A722	C624			A398
A1318	A1318	G1241	G1175	G1175	C1107	G1031	A974	G898	A815	U723	G625	U552	G481	
A1319	C1320	G1241	A1176	A1176	G1108	A1032	A975	U891	A816	G724	U626	A553	A482	C398
C1321	C1321	A1248	G1177	G1177	C1109	G1032A	A976	G906	C817		G627	C554	C483	C401
	G1322	C1249	G1178	G1178	C1110	G1032B	A977		G818	G727	G628	C555	C484	
G1323	A1250	A1250	A1179	A1179	A1111	G1033	A978	A909	A819		G629	C556	G485	G406
A1324	C1324	A1251	A1180	A1180	C1112	G1034	C979	C910	U820	G730	G630	G557	U486	G407
C1325	A1252		C1113	C1113	G1034	G1034	C980		G821	G731	G631	G558	A487	A408
G1326	C1326		C1114	C1114	C1037	C1037	U981	A913			A632	A559	C488	G409

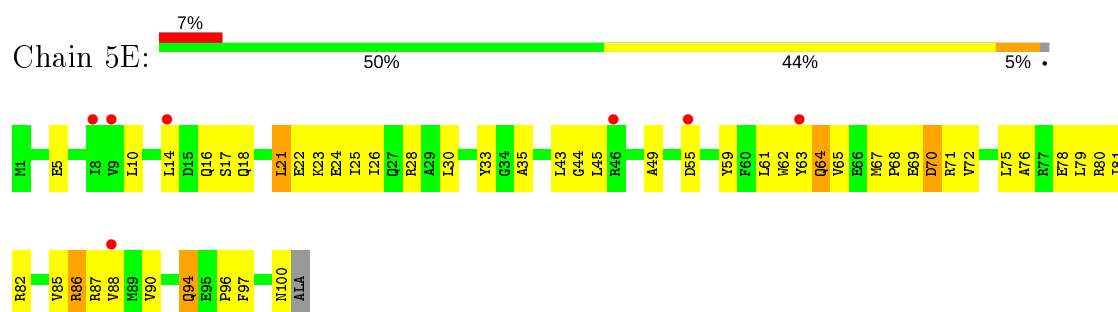




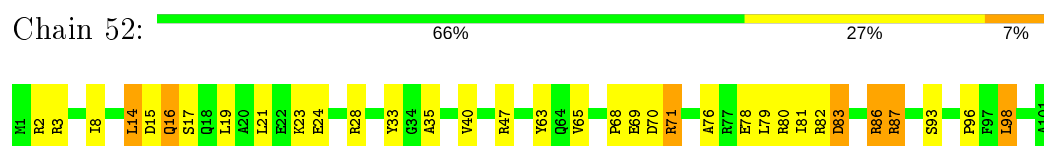
- Molecule 5: 30S ribosomal protein S5



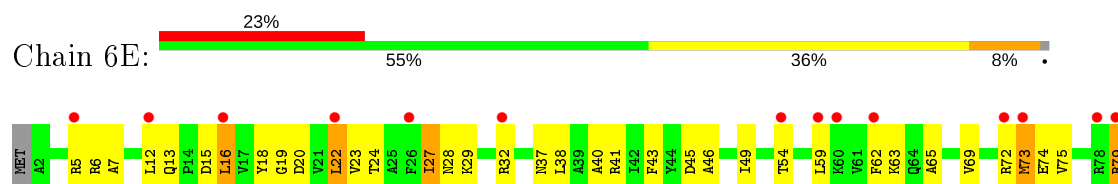
- Molecule 6: 30S ribosomal protein S6

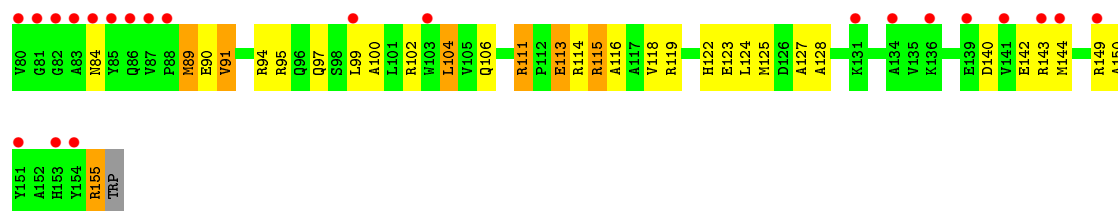


- Molecule 6: 30S ribosomal protein S6

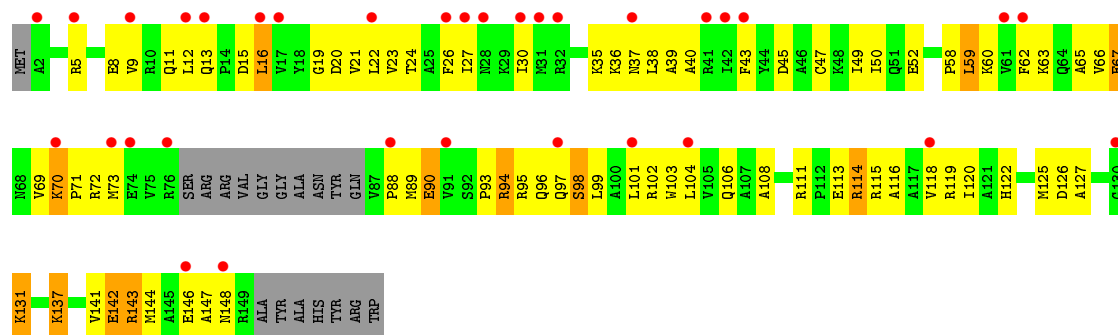


- Molecule 7: 30S ribosomal protein S7

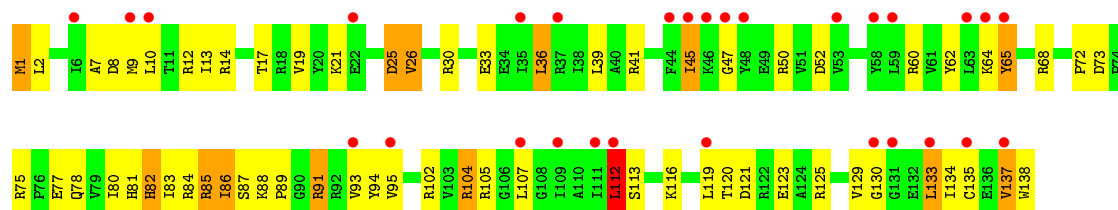




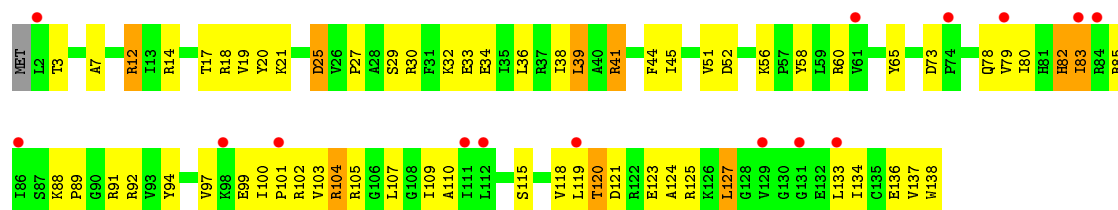
• Molecule 7: 30S ribosomal protein S7



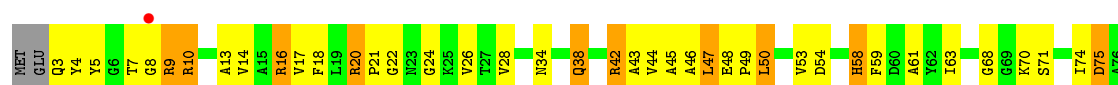
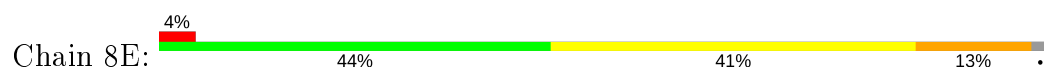
• Molecule 8: 30S ribosomal protein S8

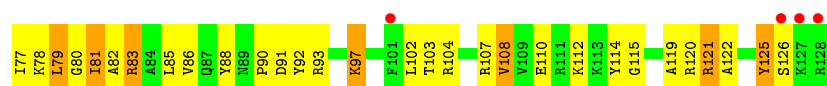


• Molecule 8: 30S ribosomal protein S8

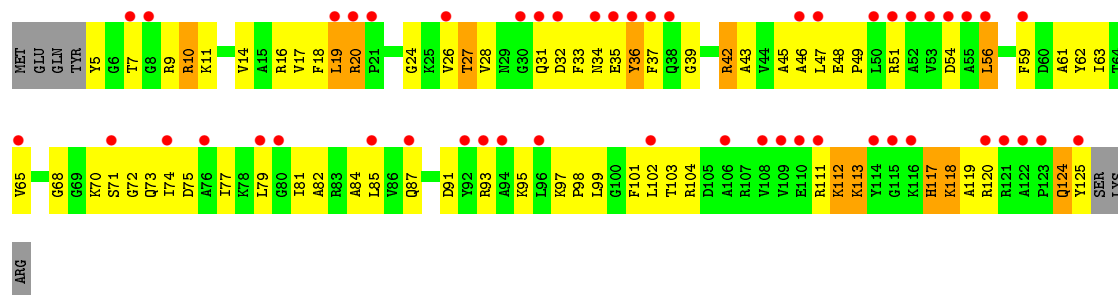


• Molecule 9: 30S ribosomal protein S9

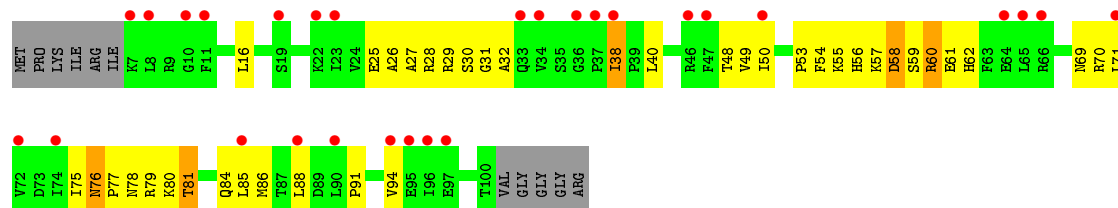




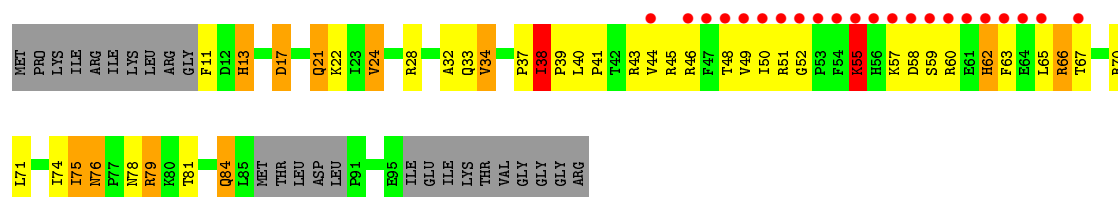
• Molecule 9: 30S ribosomal protein S9



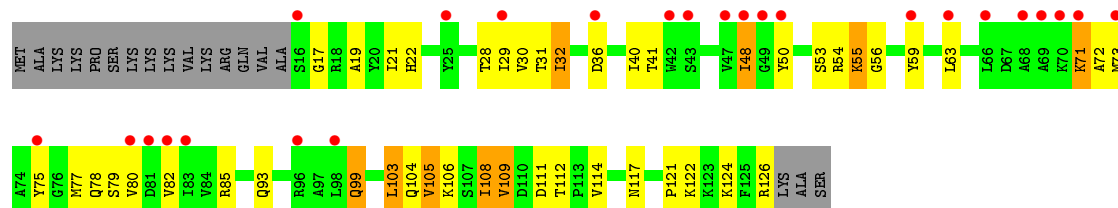
• Molecule 10: 30S ribosomal protein S10



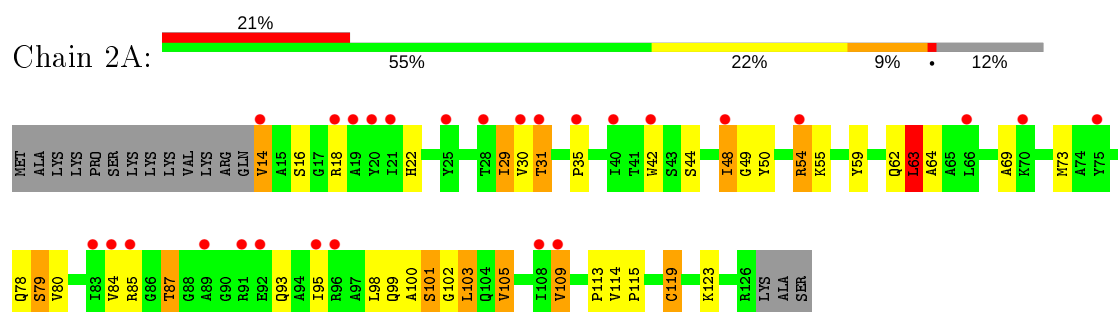
• Molecule 10: 30S ribosomal protein S10



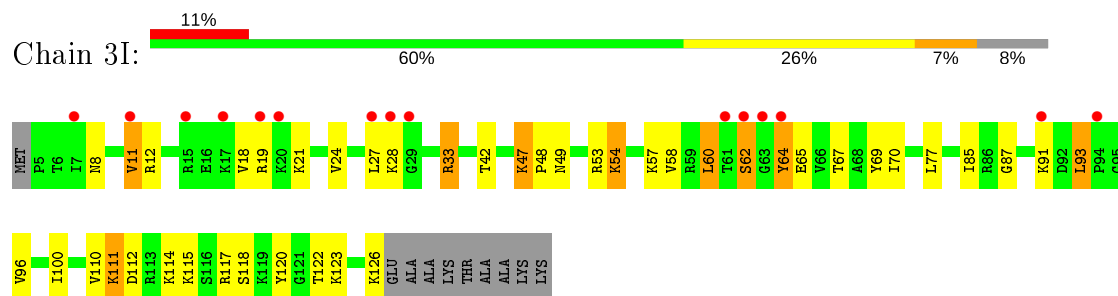
• Molecule 11: 30S ribosomal protein S11



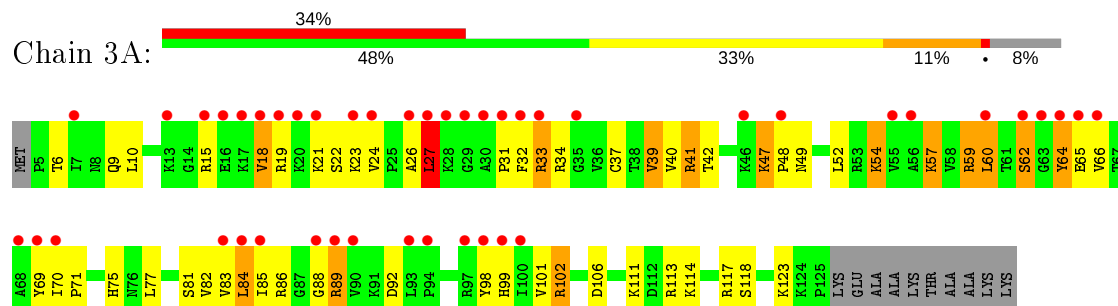
• Molecule 11: 30S ribosomal protein S11



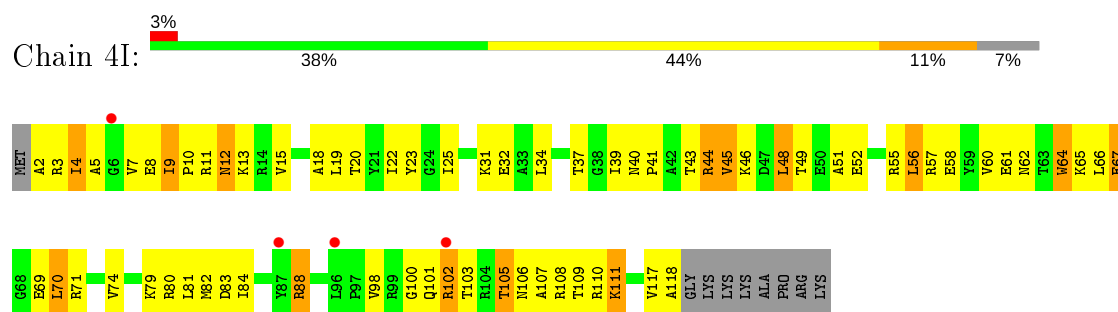
- Molecule 12: 30S ribosomal protein S12



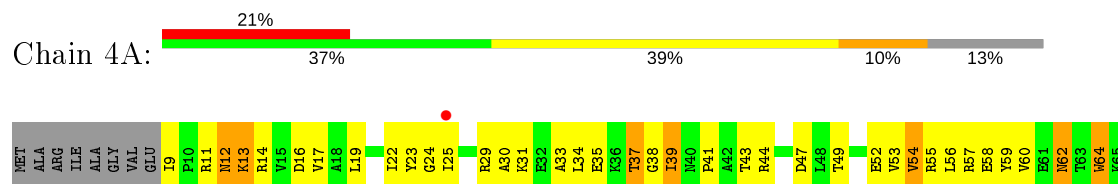
- Molecule 12: 30S ribosomal protein S12

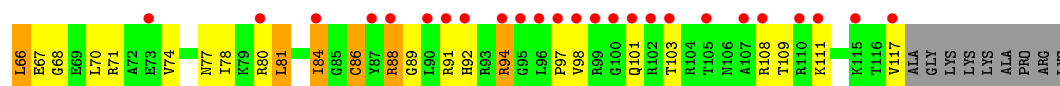


- Molecule 13: 30S ribosomal protein S13

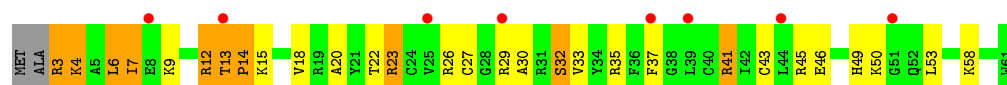


- Molecule 13: 30S ribosomal protein S13

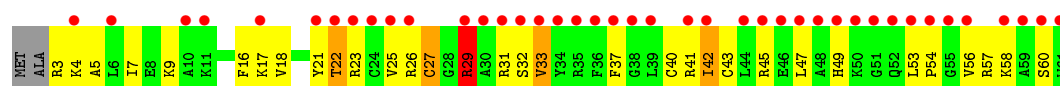




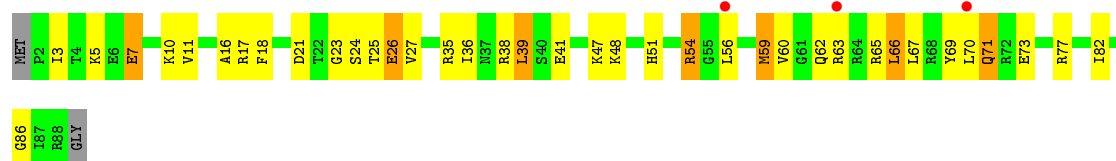
- Molecule 14: 30S ribosomal protein S14 type Z



- Molecule 14: 30S ribosomal protein S14 type Z



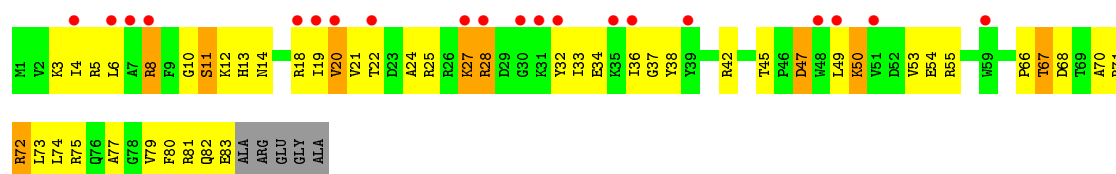
- Molecule 15: 30S ribosomal protein S15



- Molecule 15: 30S ribosomal protein S15

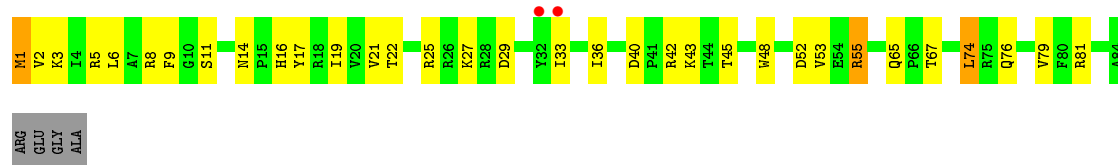


- Molecule 16: 30S ribosomal protein S16

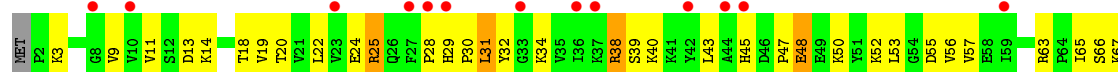


- Molecule 16: 30S ribosomal protein S16

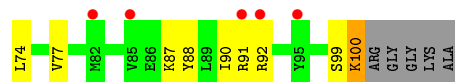
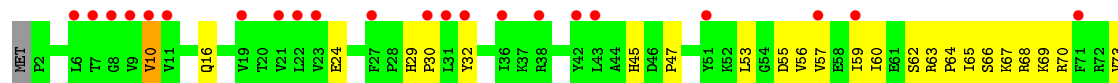




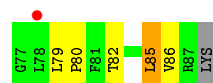
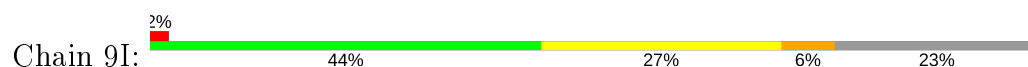
- Molecule 17: 30S ribosomal protein S17



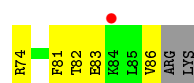
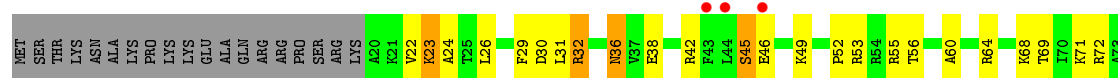
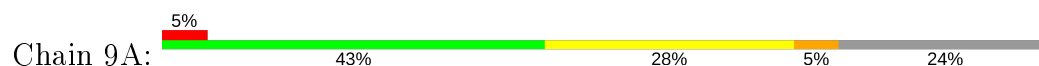
- Molecule 17: 30S ribosomal protein S17



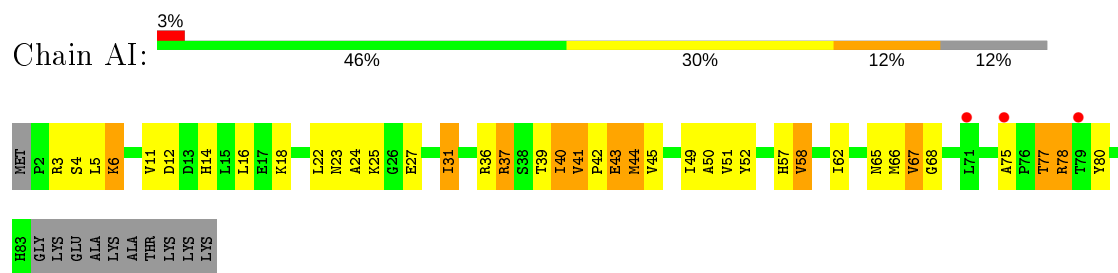
- Molecule 18: 30S ribosomal protein S18



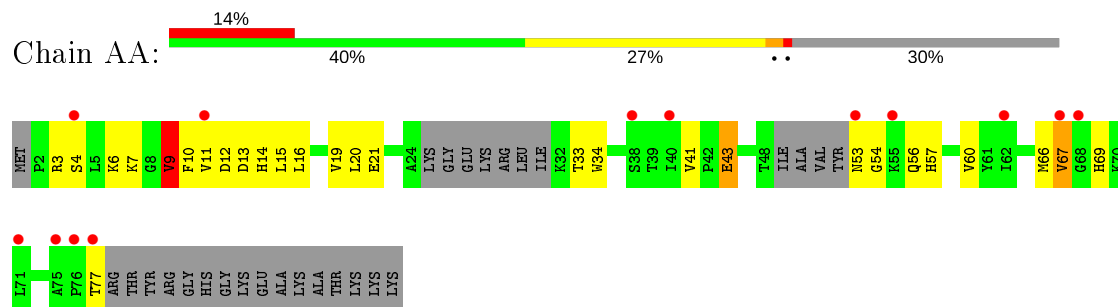
- Molecule 18: 30S ribosomal protein S18



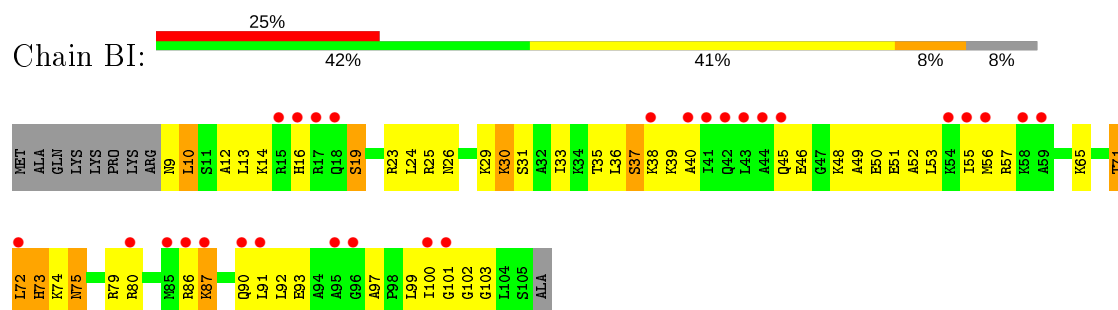
- Molecule 19: 30S ribosomal protein S19



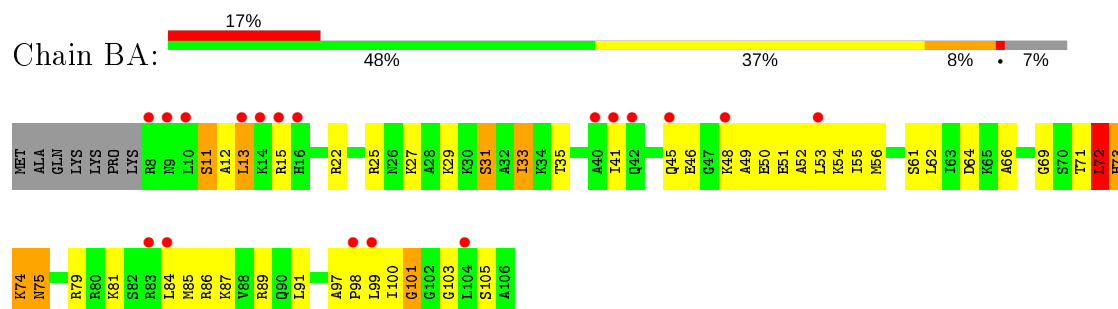
- Molecule 19: 30S ribosomal protein S19



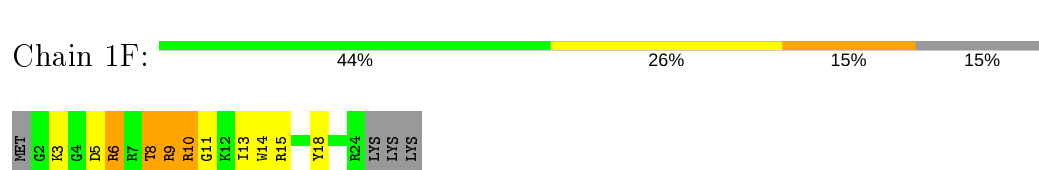
- Molecule 20: 30S ribosomal protein S20



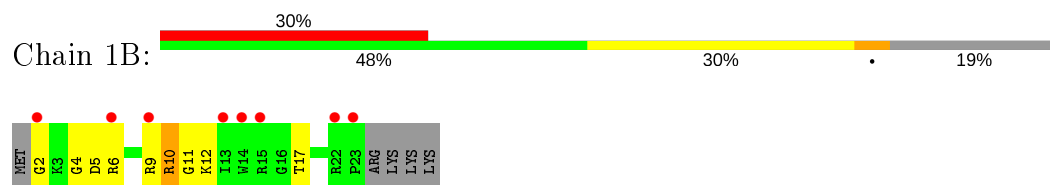
- Molecule 20: 30S ribosomal protein S20



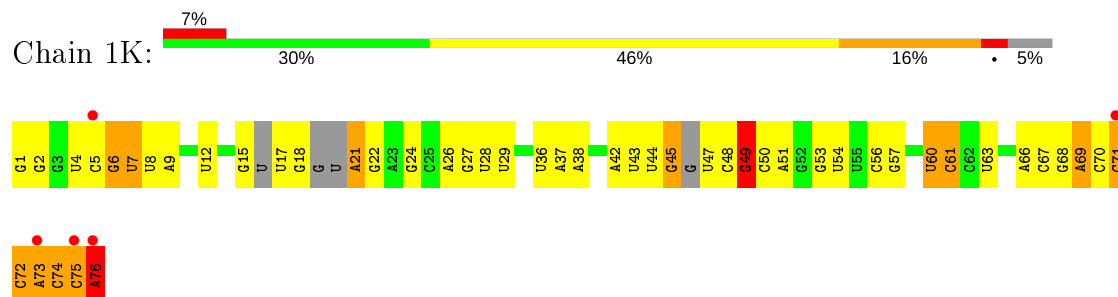
- Molecule 21: 30S ribosomal protein Thx



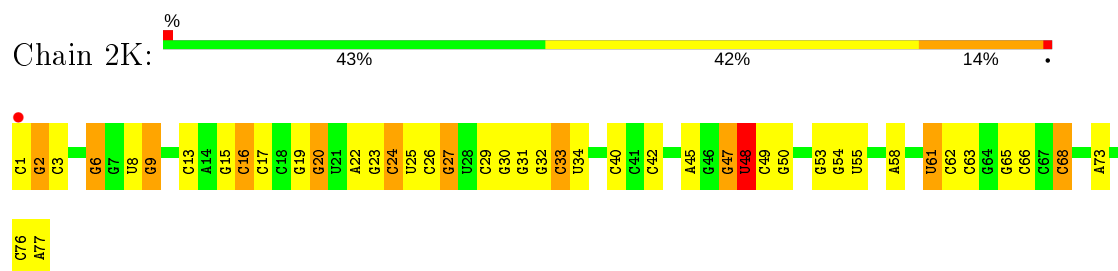
- Molecule 21: 30S ribosomal protein Thx



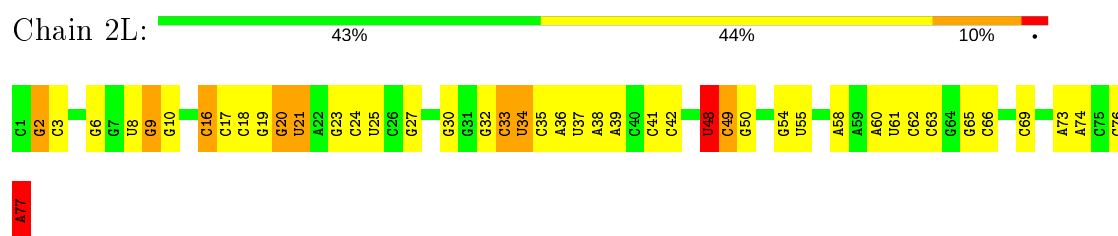
- Molecule 22: tRNA^{Lys}



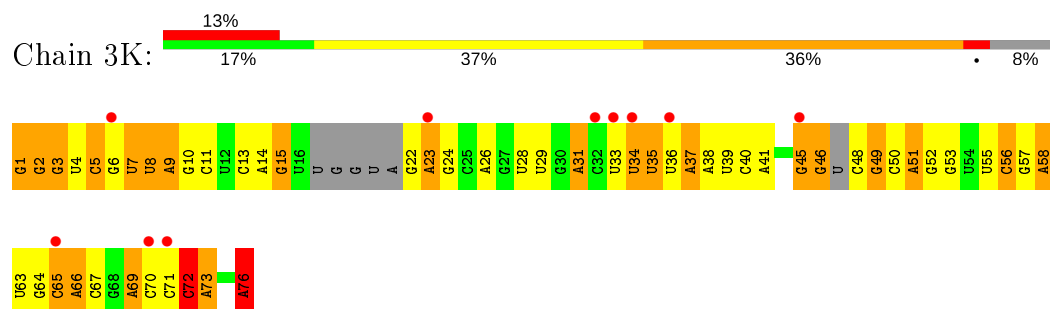
- Molecule 23: tRNA^{fMet}



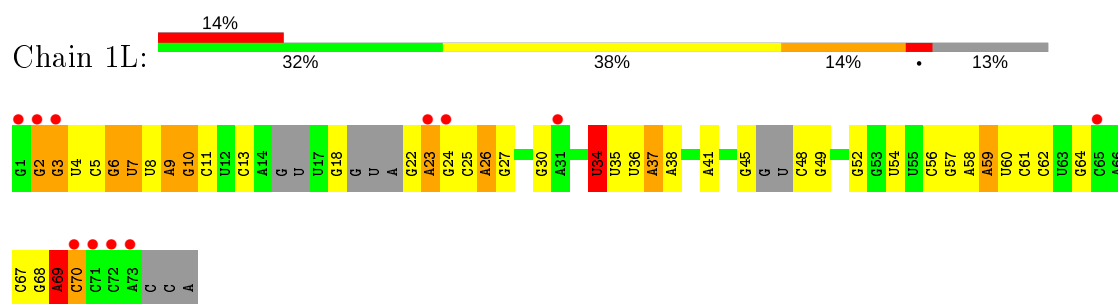
- Molecule 23: tRNA^{fMet}



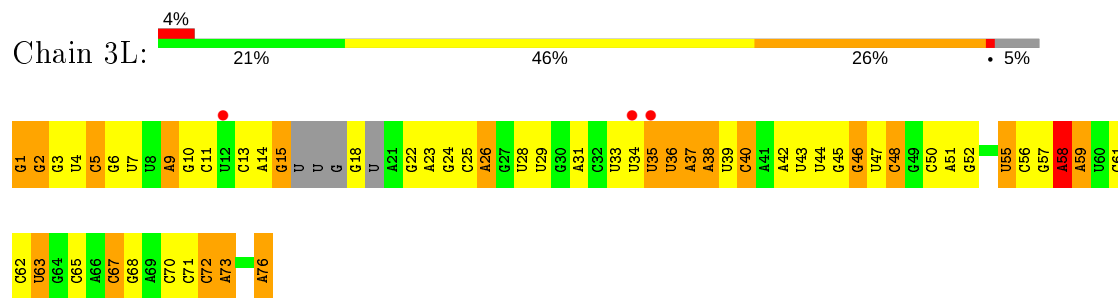
- Molecule 24: tRNA^{Lys}



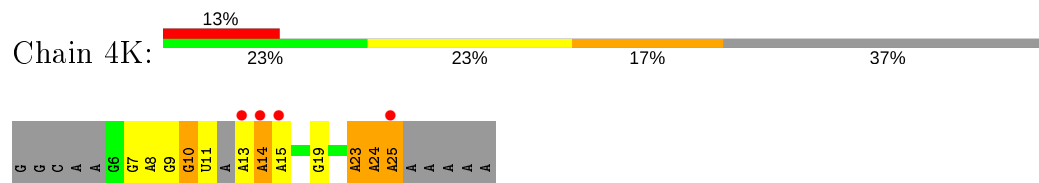
- Molecule 24: tRNA^{Lys}



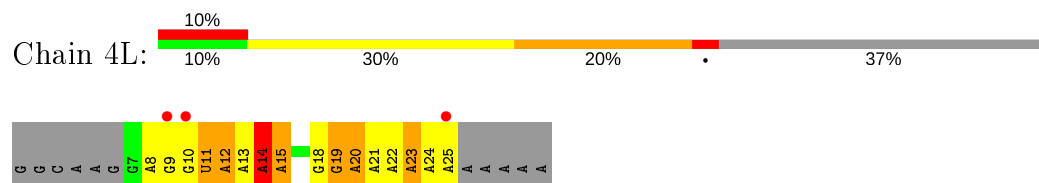
• Molecule 24: tRNA^{Lys}



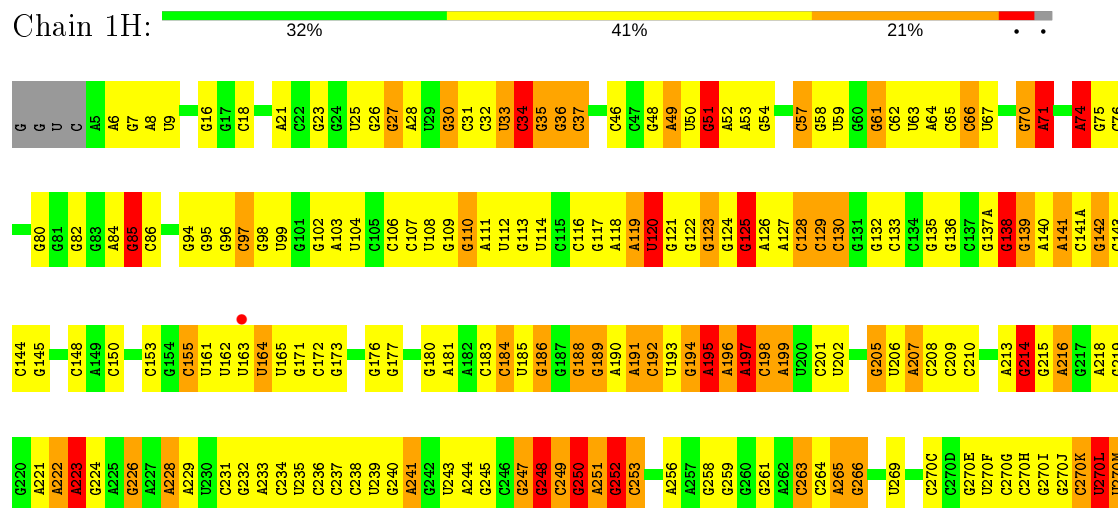
• Molecule 25: mRNA



• Molecule 25: mRNA

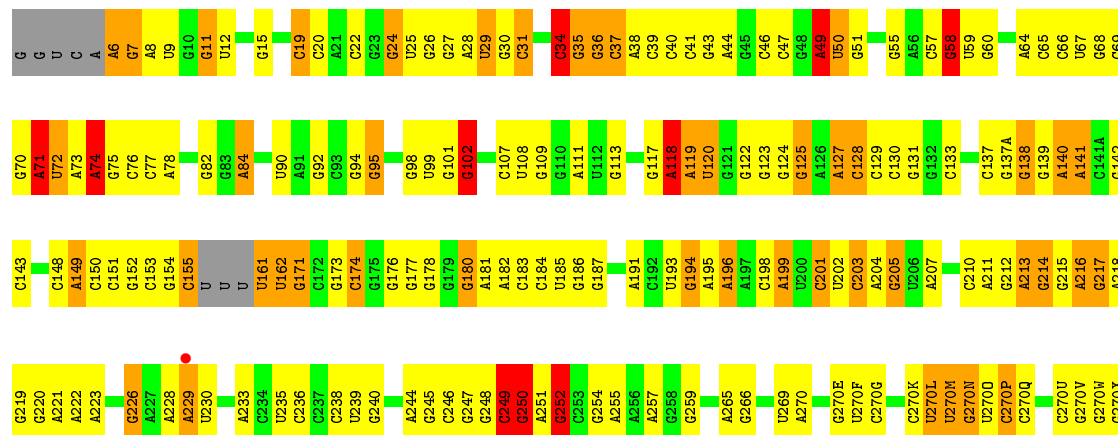


• Molecule 26: 23S ribosomal RNA



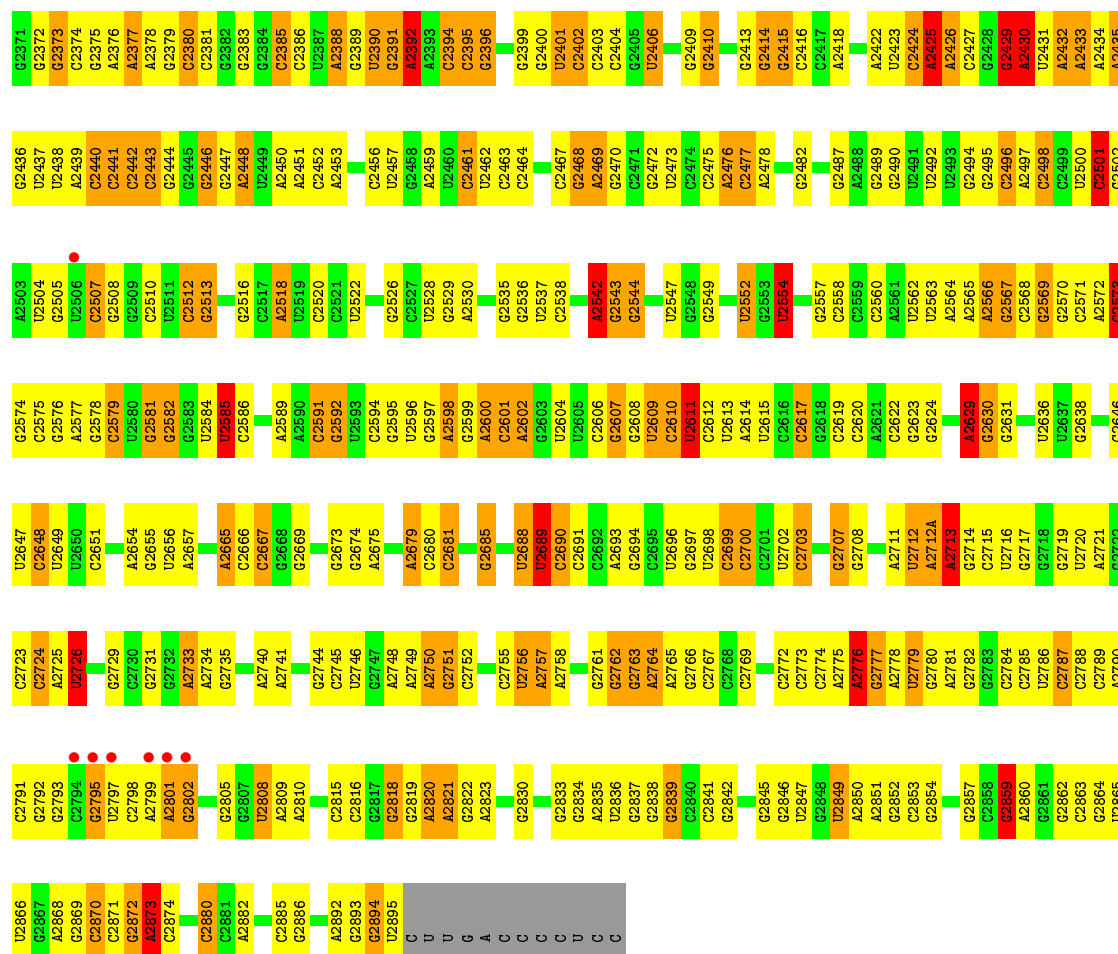
G1203	G1137	G	A1001	A833	A861	C736	U667	G625	U557	A477	G403	G270N
A1204	G1138	A	G1002	G934	G862	C737	A670	U626	G558	A478	U403	U2700
U1205	G1139	A	G1003	C935	A863	G738	C671	A627	G559	A479	C404	C270P
G1206	C1140	G	G1004	C936	A864	G739	C672	G575	C560	A480	U405	C270Q
C1207	U1141	C	G1005	U937	C865	U740	C673	G629	G563	G481	G406	G270R
C1208	U1142	C	G1006	G938	A866	G741	C674	G630	G564	A482	G407	
G1209	A1143	A1070	G1009	G939	G867	G744	G675	A631	C565	A483	G408	C270U
A1210	G1144	C1071	A1010	G940	U868	G745	A676	A632	C566	A484	C409	G270V
U1211	G1145	C	A1011	A941	G869	U746	A677	G633	U567	G485	G410	G270W
G1212	G1146	A	G1012	U942	A870	U747	C678	C634	A568	G491	A411	G270X
A1213	G1149	U1078	C1013	G944	G879	U750	C679	C635	G570	A492	A412	U270Z
C1217	G1152	C1079	G1016	G945	G880	A751	G682	A637		A493	U415	C271A
C1218	C1153	U1081		G946	G881	A752	G683	G638		A494	C416	G271B
G1219	U1154	U1082	U1019	G947	G882	C753	G684	U639		G495	G417	G271C
A1220	A1155	A1085	U1020	G950	C	C754	A685	C640		A501	C418	
C1221	G1157	A1086	A1021	G951	C	C755	G686	A644		A502	C419	G273A
C1222	C1158	G1087	G1022	G952	C	C756	G687	C645		A503	G421	
C1223		A1088	U1023	G953	C	U757	U688	A646		A504	A423	C273D
G1224		A1089	G1024	A954	A	C758	A689	G647		U504	A422	U273E
C1225	G1162	G1089	G1025	G954	C	G759	G690	U648		A505	G425	C273F
G1226	G1163	U1090	U1026	C955	C	G760	G691	G649		G506	G425	G274
A1227	G1164	G1091	U1027	G956	C	G761	C692	C650		A507	C426	G275
G1228	U1165	C1092	A1028	A957	A	A762	G693	G651		G508	U427	A276
	C1166	G1093	U1029	U958	G	U763	U694			C509	A428	C277
G1230	U1167	U	A1030	A959	G893	G764	U695	A654		C510		A278
G1231	G1168	A	G1031	A960	C894	A765	G696	A654A		U511	C433	C279
G1235	G1169	A	U1032	C961	U895	G766	C697			G512	U434	G280
G1236	G1170	U	A1033	G962	A	U767	C698	G654D		A513	G435	G281
A1237	G1171	A		U963	C897	G768	A699	C		A514	G442	A282
G1238	G1172	G	G1038	G966	C898	G769	G700	C		A515	A443	A283
U1240	A1173	U1107	G1039	C967	A900	G770	G701	C		C516	C444	
G1241	G1174	C1102	C1040	G968	A901	G771	G702	G		G517	C445	A289
A1242	A1175	A1103	G1041	U969	C902	C772	U703	C		G518	C446	G290
G1243	G1176	C1104	G1042		C903	G773	G704	A		U519	A447	
G1244	C1177	U1105		G974		A774	A705	C		G520	U448	G295
	C1179	G1106	A1045	C974A	G906	G775		C				G296
	C1180	U1107	A1046		U907	G776	G712	C		U524	C451	C297
	A1181	U1108	G1047	G978	C908	A777	G713	G654N		U525	G452	G298
G1250	G1182	C1109	A1048		A909	G778	U714	G654O			A371	A299
G1251	G1183	A1110	C1049	A981	A910	G779	G715	G654P		A528	C455	A300
G1252	G1184	A1111	U1050	A982	A911	U780	A716	C654Q		A529	C456	G301
A1253	G1185	G1112	G1051	A983	C912	G781	G717	C654R		G530	A457	C302
G1254	G1186	U1113	C1052	A984	U913	A782		G654S		C531	G458	
U1255	G1187		C1053	G985	C914	A783	G721	G654T		A532	U459	U306
G1256	U1188	C1118	A1054	C986	C915	A784	A722	A654U		G533	A460	G307
C1257	G1189	C1119	G1055	G987	U916	G785	G723	A654V		U534	C461	G308
G1191	G1190		G1059		A917	G786	U724	A655		C535	C462	G309
G1192	G1192		A	A990	A918	U787	G725	G656		A536	G463	A310
G1193	G1193	G1122	U	C991	G919	A788	G726	U657		C537	U464	A311
A1194	A1194	A1126	G	C992	G920	A789	A727	C658		C546	C467	G315
G1195	G1195	A1127	U	G993	G921	C790	G728	C659		A547	A470	G316
C1196	C1196	A1128	U	C994	G924	C791	G729	G660		A548	A471	G317
G1197	G1197	A1129	G1062	A926	C925	G792	G730	C661		G549	A472	G318
A1265	U1198	U1130	G1063	A928	C926	A793	G731	G662		G550		C319
G1266	G1131	C		G929	C927	G794	C732	G663		A621		A320
U1267	C1135	U		G930	C928	C795	G733	C664		G622		G321
A1268	G1136	U	A	U999	C931	G796	A734	G665		U554	U475	G322
					G932	C797	A735	G666		G556	G476	A322



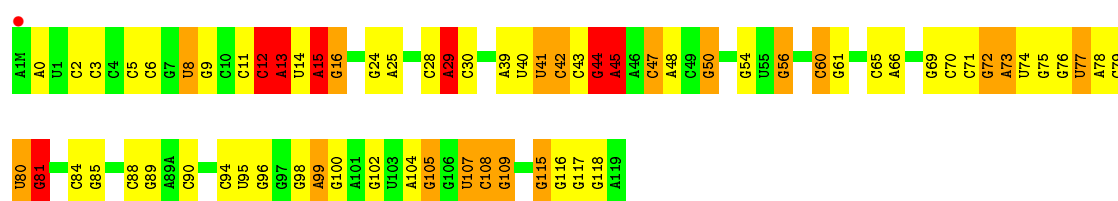
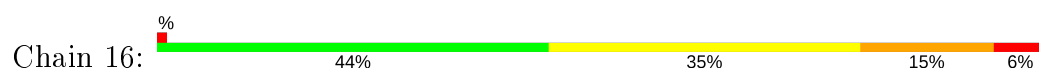




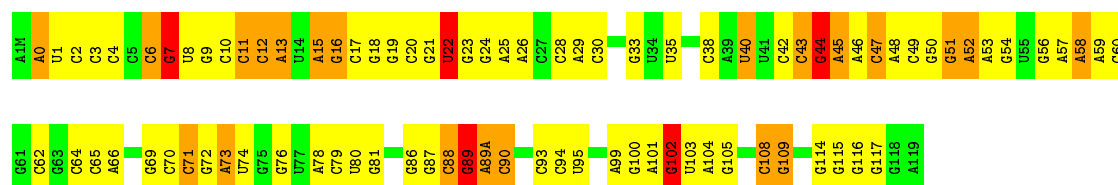
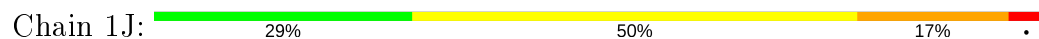
C2306	G2307	U2244	G2156	U2092	G2023	G1947	U1864	A1789	G1699	G1627	C1548	G1465	U1397	C1330
G2308	A2158	U2245	G2157	G2093	G2024	G1948	U1864	C1790	A1700	G1628	C1548	G1466	U1397	A1331
A2309	G2159	G2246	G2160	G2093	G2027	G1950	A1871	G1791	A1701	U1629	C1552	C1468	G1400	G1332
A2310	G2161	A2247	G2162	U2099	U2028	U1951	A1872	G1792	G1704	G1635	C1556	G1470	U1405	G1338
A2311	G2163	A2248	G2164	G2100	G2029	U1952	A1878	U1794	U1709	C1638	C1557	G1471	U1406	G1339
U2312	G2165	U2249	G2166	G2101	A2030	A1953	A1885	C1795	C1710	C1639	C1558	A1471	U1407	U1340
G2313	G2167	G2250	U2102	G2103	A2031	G1954	A1886	C1797	U1716	C1640	G1560	A1472	C1408	U1341
G2314	G2168	G2251	G2104	G2105	G2032	U1955	A1887	G1798	U1717	C1641	C1561	G1476	G1411	G1343
G2315	U2107	G2252	G2106	G2107	U2034	A1960	C1888	U1799	G1718	A1641	C1562	A1477	A1412	G1344
G2316	G2169	G2253	G2108	G2109	G2035	C1961	A1889	C1800	G1719	G1642	C1563	G1478	G1413	A1342
G2317	G2170	G2254	G2110	G2111	G2036	C1962	A1890	G1801	G1726	G1643	C1564			C1345
G2318	G2171	G2255	G2112	G2113	G2037	U1963	A1891	G1802	G1727	G1644	C1565			
G2319	G2172	G2256	G2114	G2115	G2038	G1964	A1892	U1805	U1728	C1646	A1566			G1348
A2320	G2173	U2257	G2116	G2117	G2039	G1965	A1893	C1806	G1729	C1647	A1567			A1349
A2321	G2174	G2258	G2118	G2119	G2040	C1966	A1894	G1807	A1571	C1648	C1574			C1350
A2322	G2175	G2259	G2120	G2121	U2041	G1967	G1899	U1900	U1730	G1651	C1577			C1351
G2323	G2176	G2260	G2122	G2123	A2042	G1968	A1901	G1811	G1731	A1652	C1577			U1352
G2324	G2177	G2261	G2124	G2125	G2043	A1969	A1902	G1812	A1732	G1653	C1577			A1354
G2325	G2178	G2262	G2126	G2127	G2046	A1970	G1903	G1813	U1733	A1654	C1577			G1355
A2326	G2179	G2263	G2128	G2129	G2049	U1971	G1904	G1814	C1742	A1655	U1578			G1356
A2327	G2180	G2264	G2130	G2131	G2050	A1972	G1905	G1815	G1743	C1656	A1580			U1357
A2328	G2181	G2265	G2132	G2133	G2051	C1973	G1906	G1816		C1657	G1581			G1358
G2329	G2182	G2266	G2134	G2135	A2051	G1974	G1907	G1817	C1751	G1658	C1582			A1359
G2330	G2183	G2267	G2136	G2137	G2052	G1975	G1908	U1818	C1752	U1659	C1583			A1360
G2331	G2184	G2268	G2138	G2139	G2053	G1976	G1909	G1819	G1753	C1660	C1585			G1364
G2332	G2185	G2269	G2140	G2141	G2054	G1977	A1912	U1820	A1755	G1661	A1507			A1365
A2333	G2186	G2270	G2142	G2143	G2055	U1978	A1913	G1821	G1756	C1662	A1587			G1366
G2334	G2187	G2271	G2144	G2145	G2056	U1979	A1914	G1822	U1757	A1663	C1588			A1367
A2335	G2188	G2272	G2146	G2147	G2057	U1980	A1915	G1823	G1758	A1664	C1589			G1368
G2336	G2189	G2273	G2148	G2149	A2058	U1981	A1916	G1824	C1759	G1666	C1590			A1369
A2337	G2190	G2274	G2150	G2151	G2059	U1982	A1917	G1825	A1760	G1667	A1510			G1370
G2338	G2191	G2275	G2152	G2153	G2060	U1983	A1918	G1826	G1761	A1668	G1594			G1371
G2339	G2192	G2276	G2154	G2155	A2061	G1984	A1919	G1827	A1762	A1669	G1595			U1372
G2340	G2193	G2277	G2156	G2157	G2062	G1985	A1920	G1828	C1763	A1670	A1596			A1373
G2341	G2194	G2278	G2158	G2159	G2063	U1986	A1921	A1829	G1764	C1670	A1597			G1374
G2342	G2195	G2279	G2160	G2161	G2064	U1987	A1922	C1830		U1671	C1598			C1375
G2343	G2196	G2280	G2162	G2163	G2065	G1988	A1923	G1831	C1767	G1674	C1600			C1376
G2344	G2197	G2281	G2164	G2165	G2066	G1989	A1924	U1832	G1771	C1675	G1601			A1379
A2345	G2198	G2282	G2166	G2167	G2067	G1990	A1925	U1833	G1772	A1676	U1602			G1380
G2346	G2199	G2283	G2168	G2169	G2068	G1991	A1926	U1834	G1773	G1677	U1603			G1381
G2347	G2200	G2284	G2170	G2171	G2069	G1992	A1927	G1835	G1774	U1679	A1609			G1382
G2348	G2201	G2285	G2172	G2173	G2070	G1993	A1928	G1836	U1775	G1680	A1610			C1383
G2349	G2202	G2286	G2174	G2175	G2071	G1994	A1929	G1837	U1776	G1681	C1450			A1384
G2350	G2203	G2287	G2176	G2177	G2072	G1995	A1930	G1838	U1777	G1682	C1451			G1385
A2351	G2204	G2288	G2178	G2179	G2073	G1996	A1931	G1839	U1778	C1685	U1453			C1386
A2352	G2205	G2289	G2180	G2181	G2074	G1997	A1932	G1840	U1779	C1686	A1536			C1387
G2353	G2206	G2290	G2182	G2183	U2075	G1998	A1933	G1841	U1780	C1687	C1537			G1388
G2354	G2207	G2291	G2184	G2185	U2076	G1999	A1934	G1842	A1781	U1688	G1538			A1389
G2355	G2208	G2292	G2186	G2187	U2077	G2000	A1935	G1843	G1772	G1689	G1539			U1390
G2356	G2209	G2293	G2188	G2189	U2078	G2001	A1936	G1844	G1773	C1690	G1540			G1391
G2357	G2210	G2294	G2190	G2191	U2079	G2002	A1937	G1845	G1774	C1691	G1541			A1392
G2358	G2211	G2295	G2192	G2193	U2080	G2003	A1938	G1846	U1775	C1692	G1542			G1393
G2359	G2212	G2296	G2194	G2195	U2081	G2004	A1939	G1847	U1776	C1693	G1543			U1394
A2360	G2213	G2297	G2196	G2197	U2082	G2005	A1940	G1848	G1777	C1694	G1544			A1395
G2361	G2214	G2298	G2198	G2199	U2083	G2006	A1941	G1849	U1778	C1695	G1545			U1396
G2362	G2215	G2299	G2200	G2201	G2084	G2007	A1942	G1850	G1779	C1696	C1547			
G2363	G2216	G2300	G2202	G2203	G2085	G2008	A1943	U1851	G1780	C1697				
A2369	G2217	G2301	G2204	G2205	G2086	G2009	A1944	U1852	G1781	C1698				
G2370	G2218	G2302	G2206	G2207	G2087	G2010	A1945	G1853	G1782	U1689				
	G2219	G2303	G2208	G2209	G2088	G2011	A1946	G1854	G1783	A1690				
	G2220	G2304	G2210	G2211	G2089	G2012	A1947	G1855	G1784	U1621				
	G2221	G2305	G2212	G2213	G2090	G2013	A1948	G1856	G1785	G1622				
	G2222	G2306	G2214	G2215	G2091	G2014	A1949	G1857	A1786	C1625				
	G2223	G2307	G2216	G2217	G2092	G2015	A1950	G1858	A1787	C1626				
	G2224	G2308	G2218	G2219	G2093	G2016	A1951	G1859	C1788					
	G2225	G2309	G2220	G2221	G2094	G2017	A1952	G1860						
	G2226	G2310	G2222	G2223	G2095	G2018	A1953	G1861						
	G2227	G2311	G2224	G2225	G2096	G2019	A1954	G1862						
	G2228	G2312	G2226	G2227	G2097	G2020	A1955	G1863						
	G2229	G2313	G2228	G2229	G2098	G2021	A1956	G1864						
	G2230	G2314	G2230	G2231	G2099	G2022	A1957	G1865						
	G2231	G2315	G2232	G2233	G2100	G2023	A1958	G1866						
	G2232	G2316	G2234	G2235	U2075	G2024	A1959	G1867						
	G2233	G2317	G2236	G2237	U2076	G2025	A1960	G1868						
	G2234	G2318	G2238	G2239	U2077	G2026	A1961	G1869						
	G2235	G2319	G2240	G2241	U2078	G2027	A1962	G1870						
	G2236	G2320	G2242	G2243	U2079	G2028	A1963	G1871						
	G2237	G2321	G2244	G2245	U2080	G2029	A1964	G1872						
	G2238	G2322	G2246	G2247	U2081	G2030	A1965	G1873						
	G2239	G2323	G2248	G2249	U2082	G2031	A1966	G1874						
	G2240	G2324	G2250	G2251	U2083	G2032	A1967	G1875						
	G2241	G2325	G2252	G2253	U2084	G2033	A1968	G1876						
	G2242	G2326	G2254	G2255	U2085	G2034	A1969	G1877						
	G2243	G2327	G2256	G2257	U2086	G2035	A1970	G1878						
	G2244	G2328	G2258	G2259	U2087	G2036	A1971	G1879						
	G2245	G2329	G2260	G2261	U2088	G2037	A1972	G1880						
	G2246	G2330	G2262	G2263	U2089	G2038	A1973	G1881						
	G2247	G2331	G2264	G2265	U2090	G2039	A1974	G1882						
	G2248	G2332	G2266	G2267	U2091	G2040	A1975	G1883						
	G2249	G2333	G2268	G2269	U2092	G2041	A1976	G1884						
	G2250	G2334	G2270	G2271	U2093	G2042	A1977	G1885						
	G2251	G2335	G2272	G2273	U2094	G2043	A1978	G1886						
	G2252	G2336	G2274	G2275	U2095	G2044	A1979	G1887						
	G2253	G2337	G2276	G2277	U2096	G2045	A1980	G1888						
	G2254	G2338	G2278	G2279	U2097	G2046	A1981	G1889						
	G2255	G2339	G2280	G2281	U2098	G2047	A1982	G1890						
	G2256	G2340	G2282	G2283	U2099	G2048	A1983	G1891						
	G2257	G2341	G2284	G2285	U2100	G2049	A1984	G1892						
	G2258	G2342	G2286	G2287	U2101	G2050	A1985	G1893						
	G2259	G2343	G2288	G2289	U2102	G2051	A1986	G1894						
	G2260	G2344	G2290	G2291	U2103	G2052	A1987	G1895						
	G2261	G2345	G2292	G2293	U2104	G20								



• Molecule 27: 5S ribosomal RNA

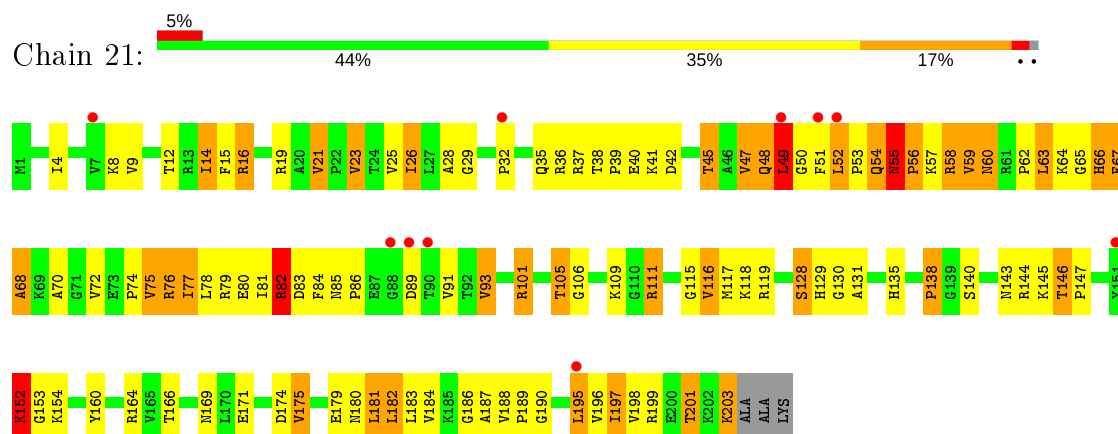


• Molecule 27: 5S ribosomal RNA

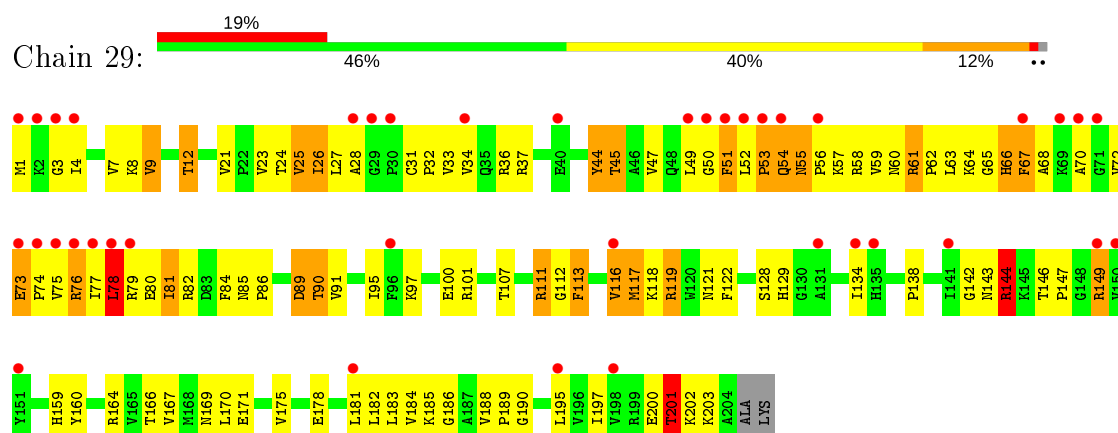


• Molecule 28: 50S ribosomal protein L1

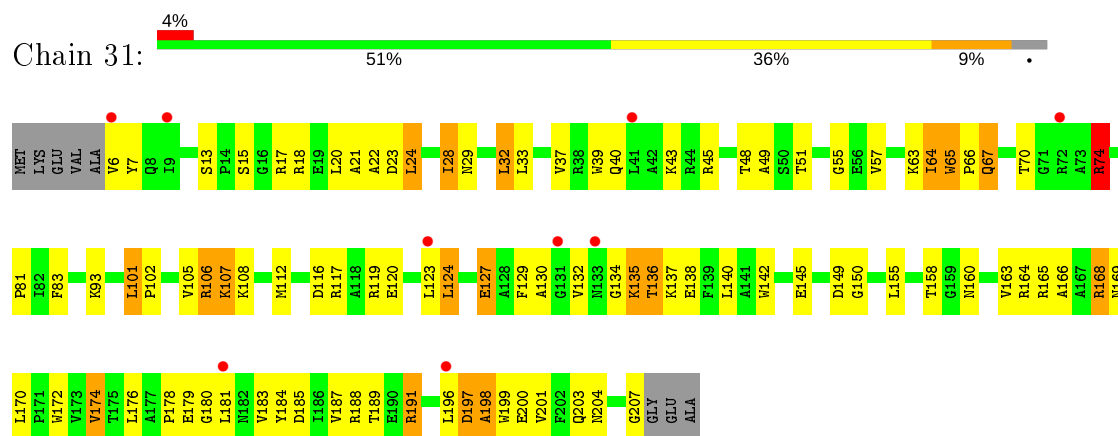
- Molecule 30: 50S ribosomal protein L3



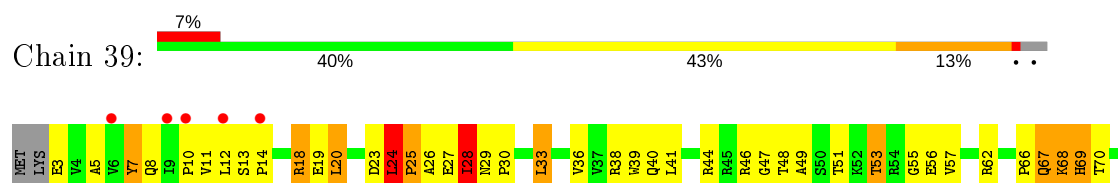
- Molecule 30: 50S ribosomal protein L3

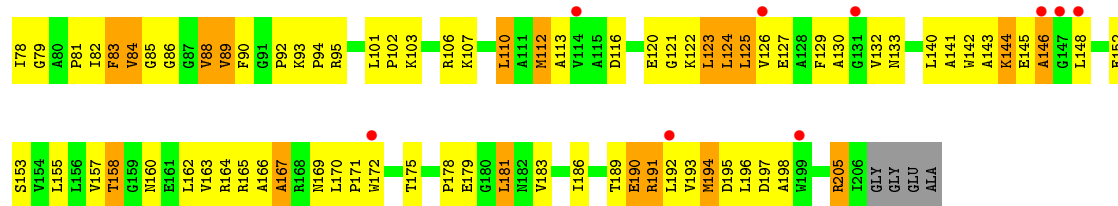


- Molecule 31: 50S ribosomal protein L4

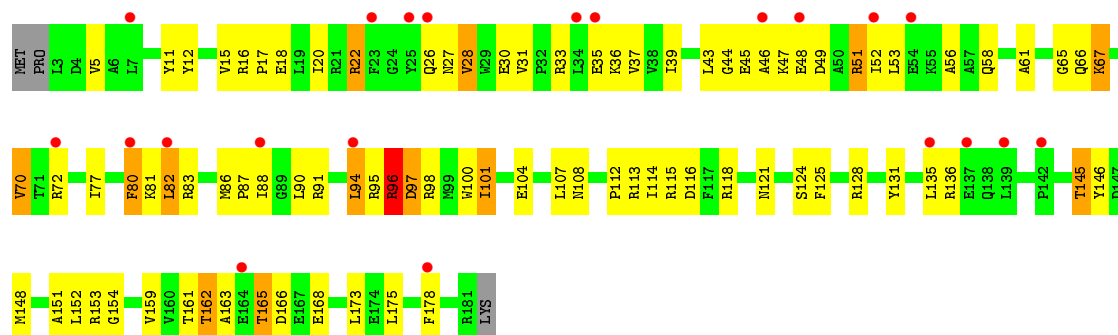


- Molecule 31: 50S ribosomal protein L4

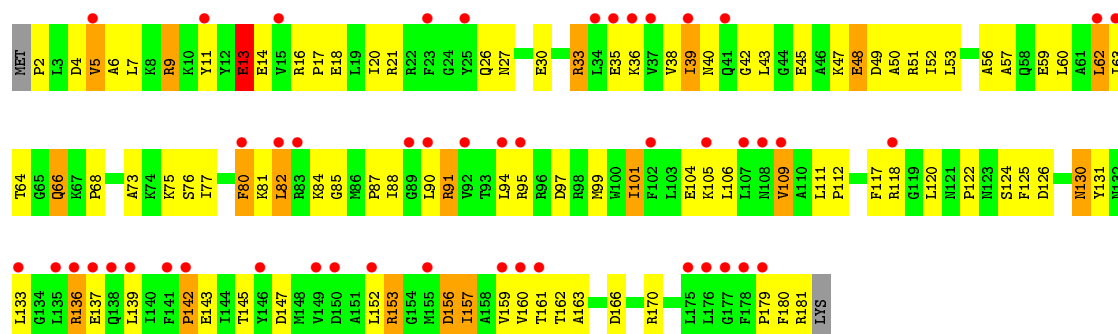




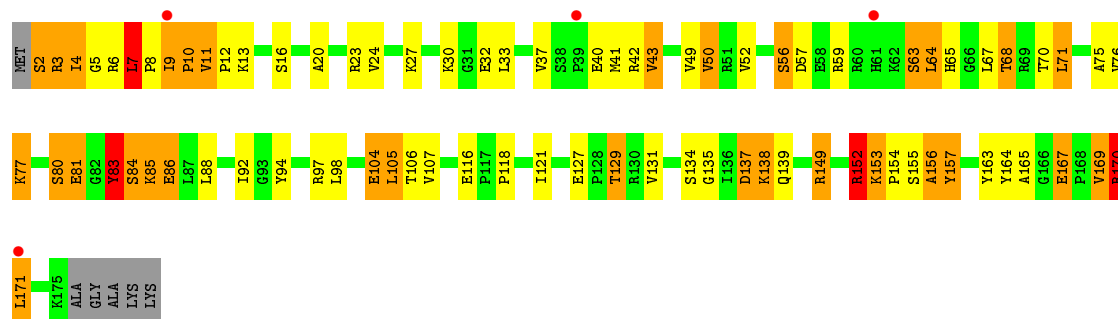
• Molecule 32: 50S ribosomal protein L5



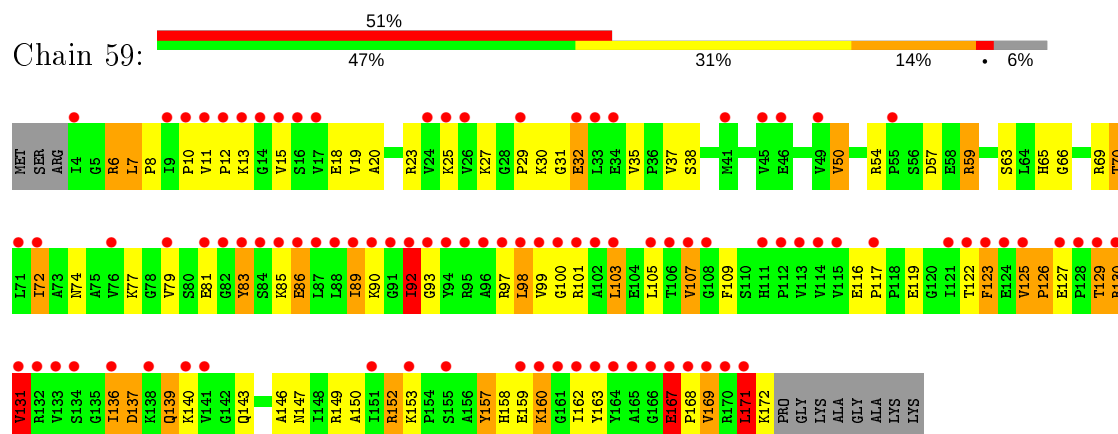
• Molecule 32: 50S ribosomal protein L5



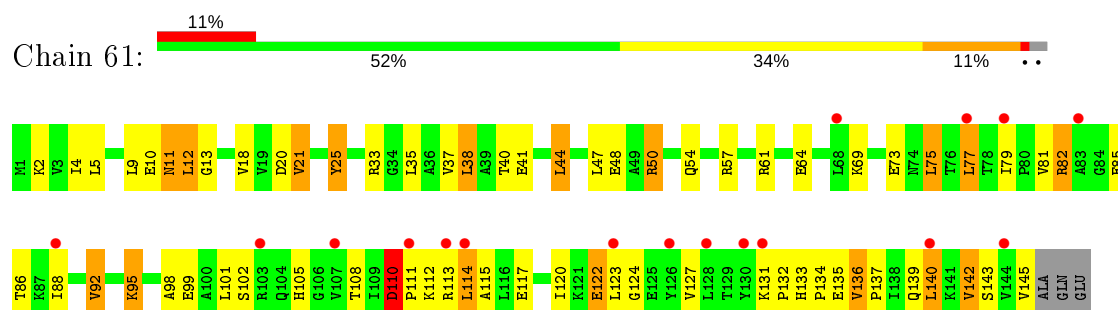
• Molecule 33: 50S ribosomal protein L6



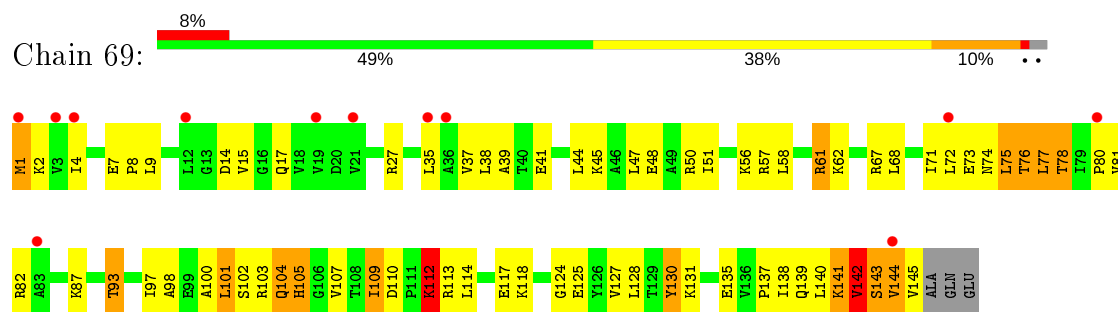
- Molecule 33: 50S ribosomal protein L6



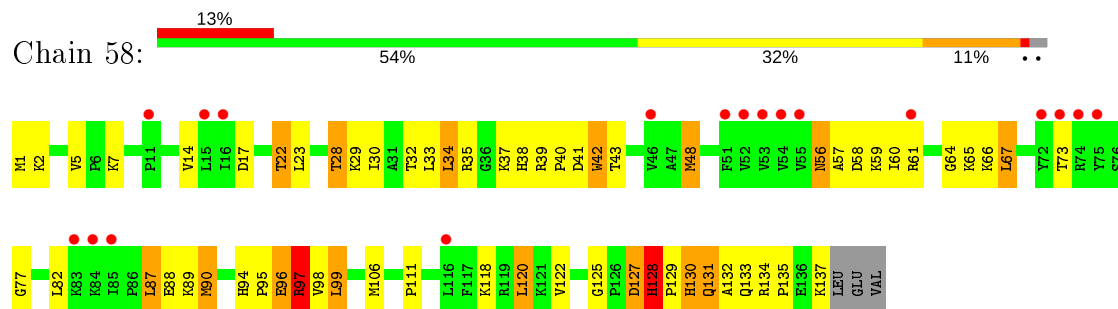
- Molecule 34: 50S ribosomal protein L9



- Molecule 34: 50S ribosomal protein L9

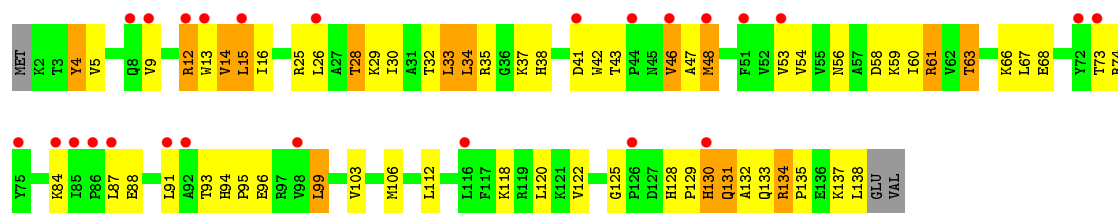


- Molecule 35: 50S ribosomal protein L13

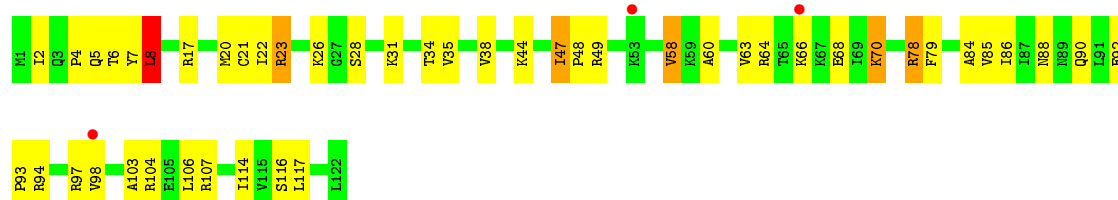


- Molecule 35: 50S ribosomal protein L13

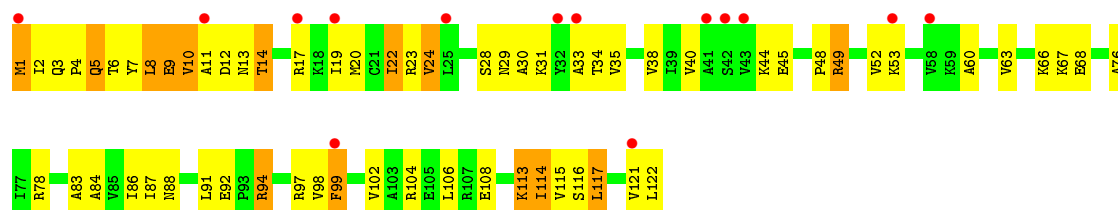




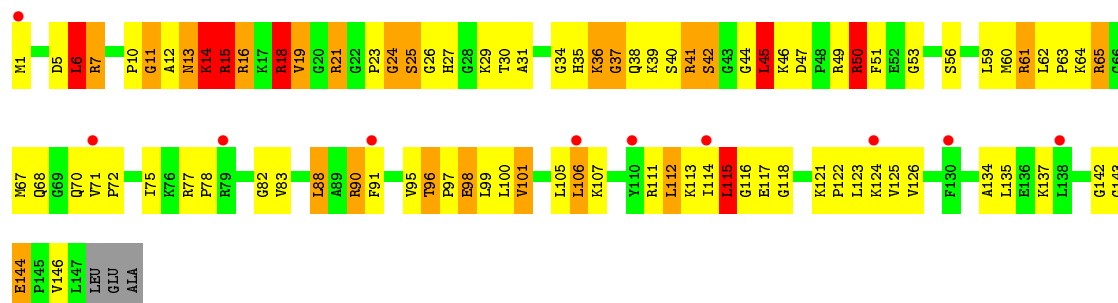
- Molecule 36: 50S ribosomal protein L14



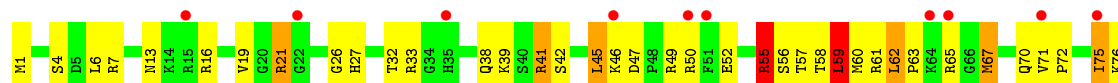
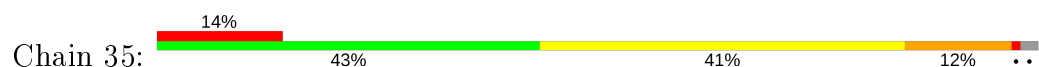
- Molecule 36: 50S ribosomal protein L14

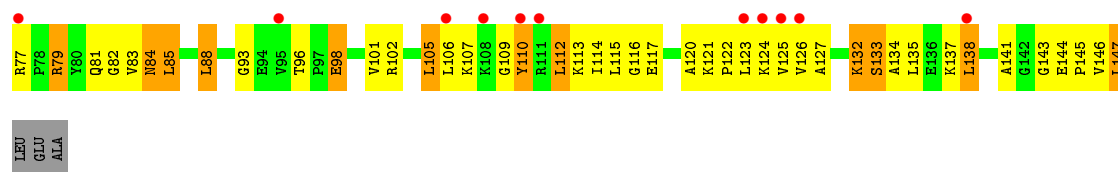


- Molecule 37: 50S ribosomal protein L15

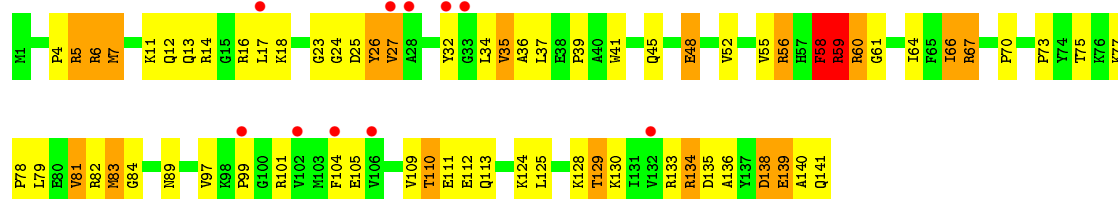


- Molecule 37: 50S ribosomal protein L15

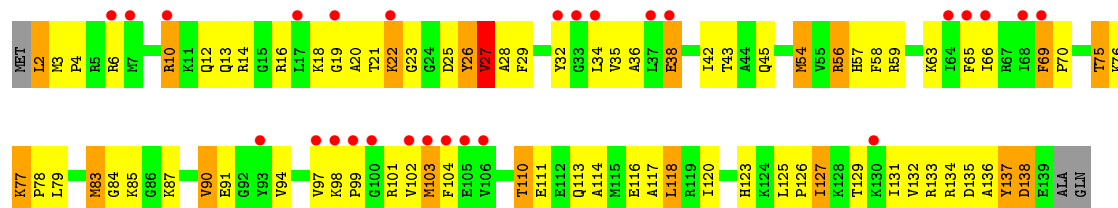
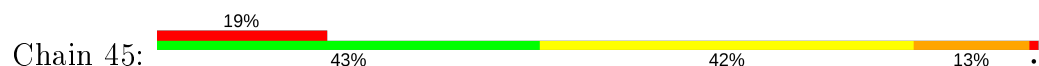




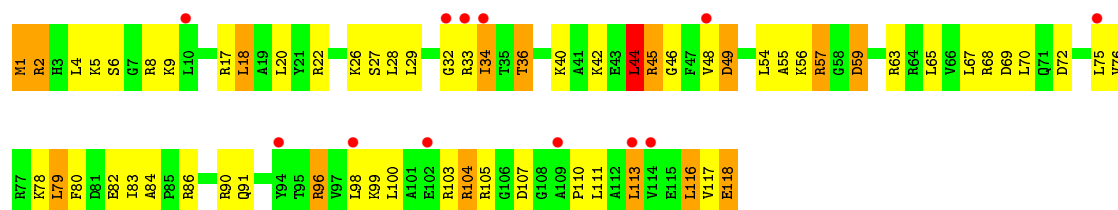
- Molecule 38: 50S ribosomal protein L16



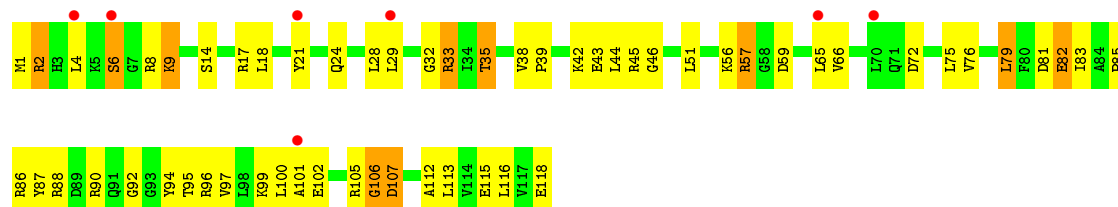
- Molecule 38: 50S ribosomal protein L16



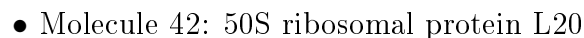
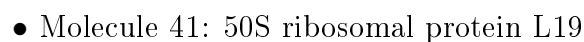
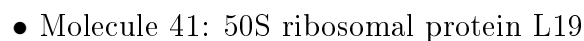
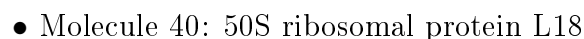
- Molecule 39: 50S ribosomal protein L17

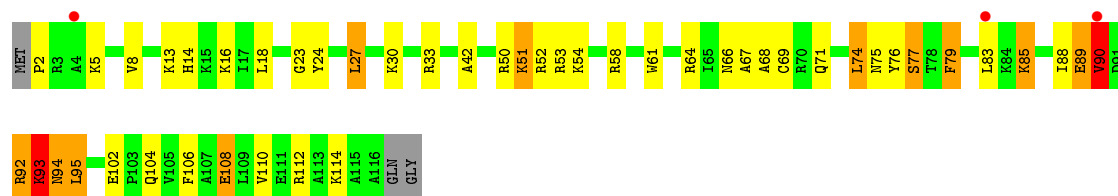


- Molecule 39: 50S ribosomal protein L17

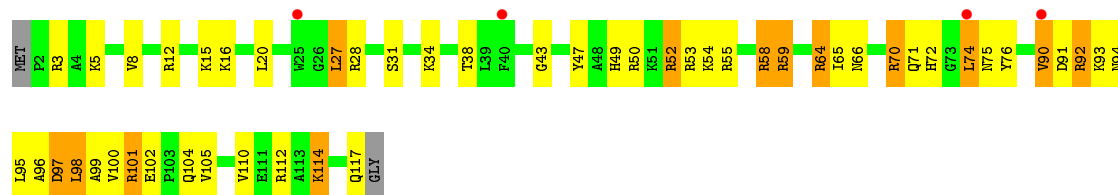


- Chain A8:

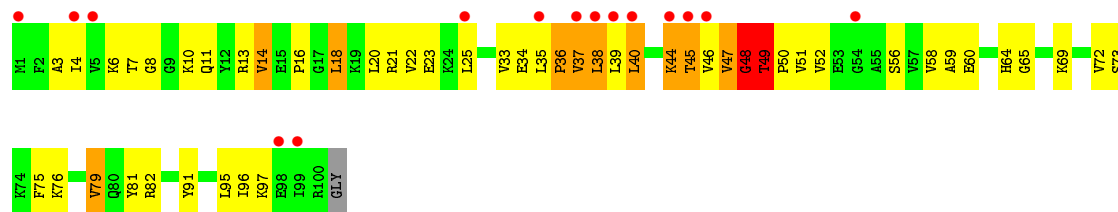




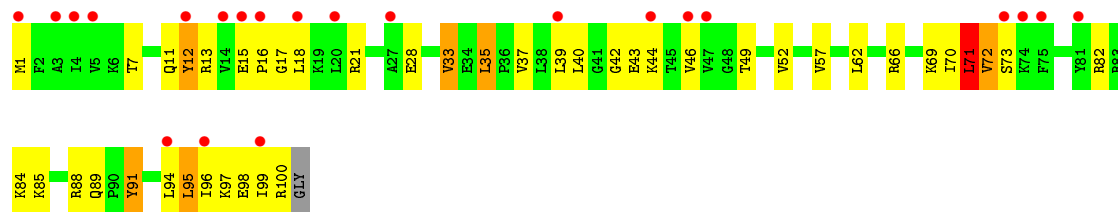
- Molecule 42: 50S ribosomal protein L20



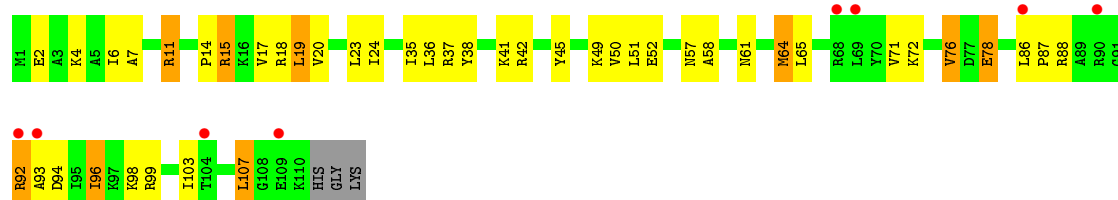
- Molecule 43: 50S ribosomal protein L21



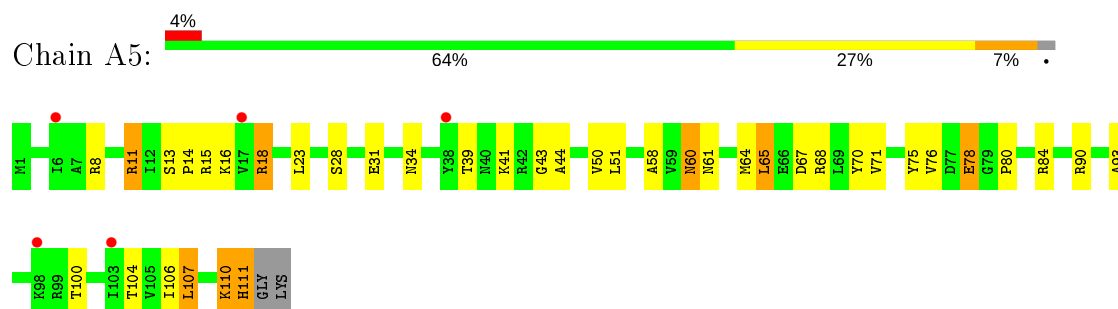
- Molecule 43: 50S ribosomal protein L21



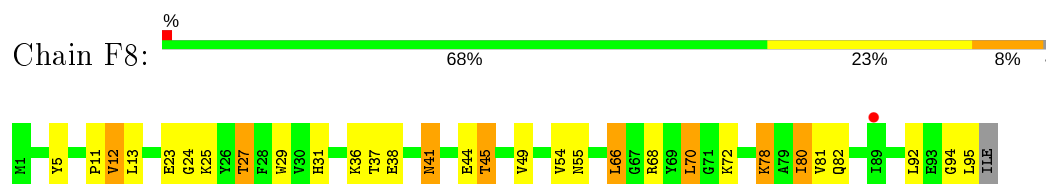
- Molecule 44: 50S ribosomal protein L22



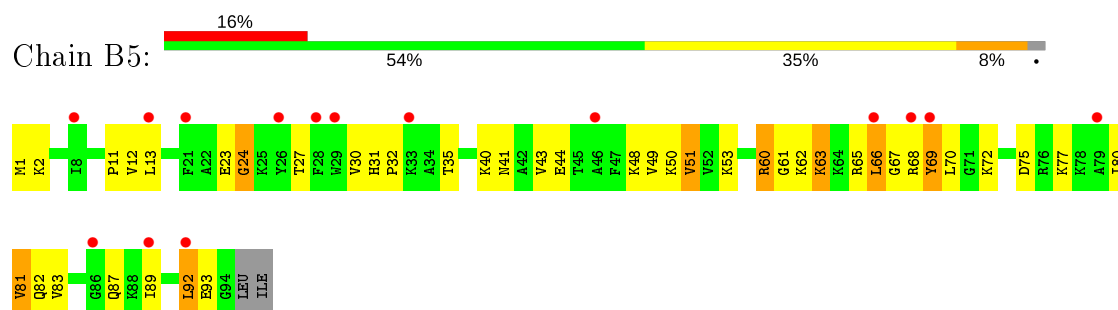
- Molecule 44: 50S ribosomal protein L22



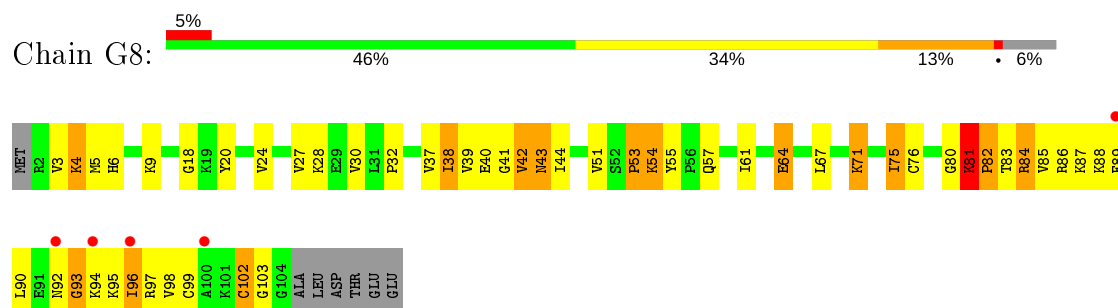
- Molecule 45: 50S ribosomal protein L23



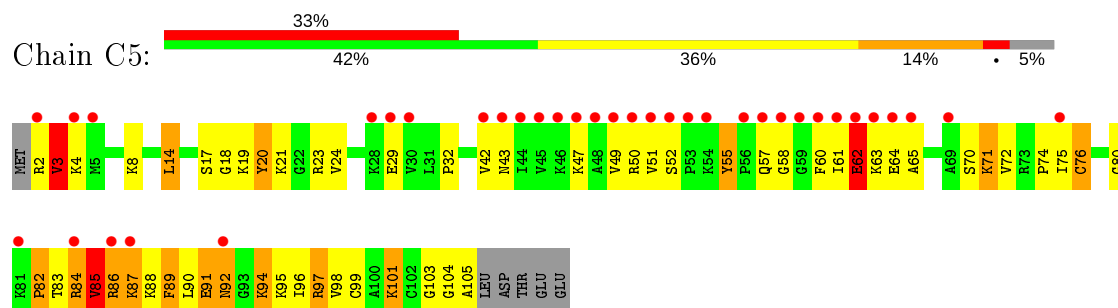
- Molecule 45: 50S ribosomal protein L23



- Molecule 46: 50S ribosomal protein L24

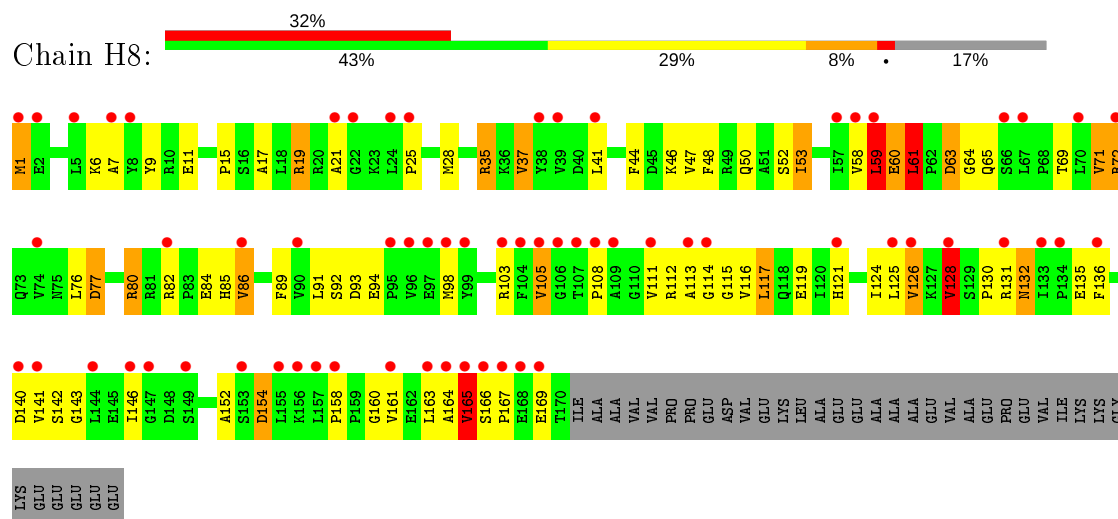


- Molecule 46: 50S ribosomal protein L24



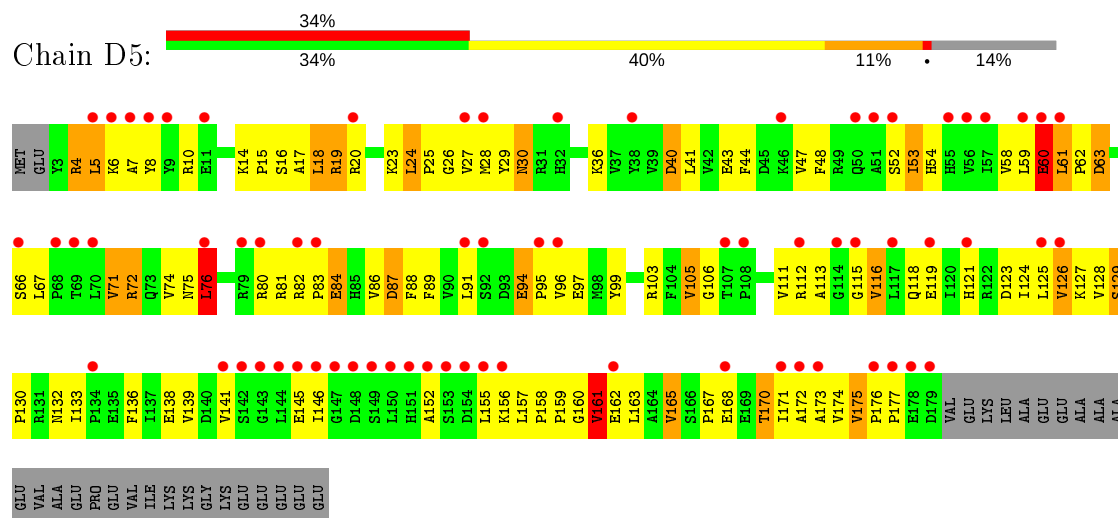
- Molecule 47: 50S ribosomal protein L25

Chain H8:



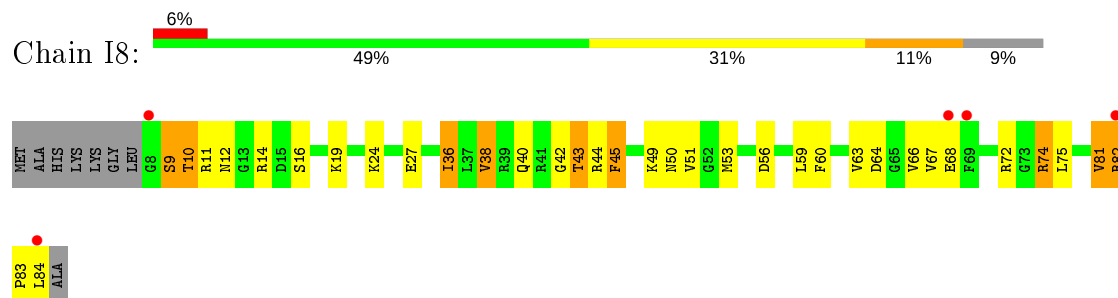
- Molecule 47: 50S ribosomal protein L25

Chain D5:



- Molecule 48: 50S ribosomal protein L27

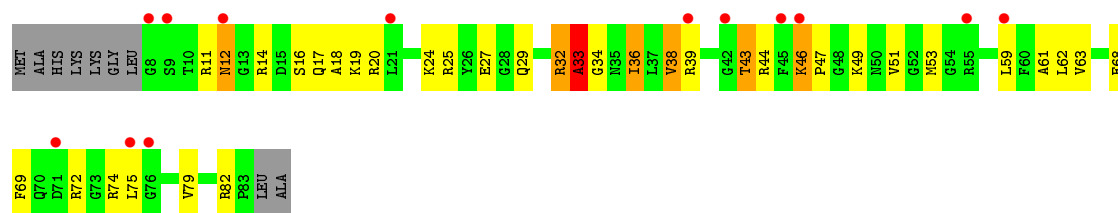
Chain I8:



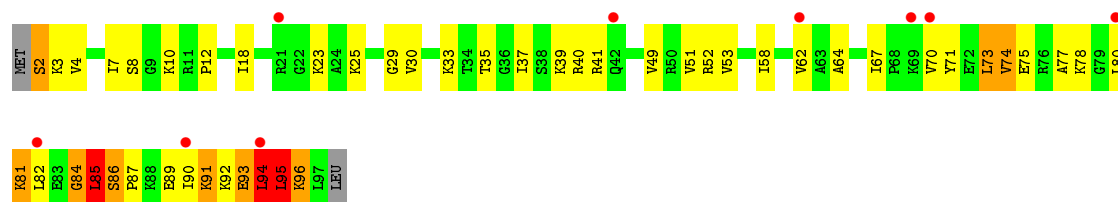
- Molecule 48: 50S ribosomal protein L27

Chain E5:

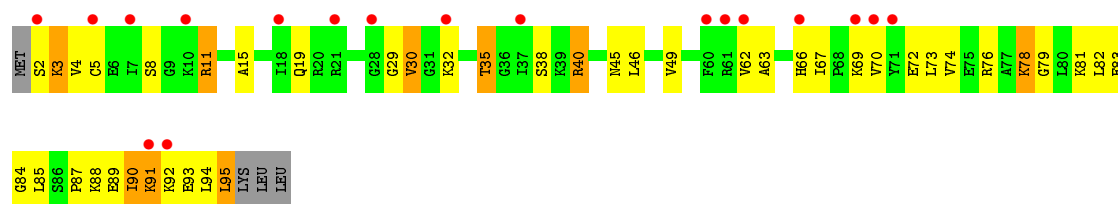




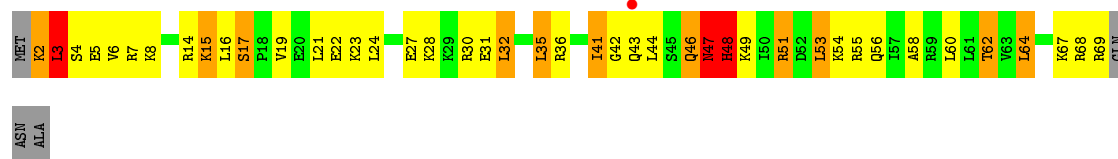
- Molecule 49: 50S ribosomal protein L28



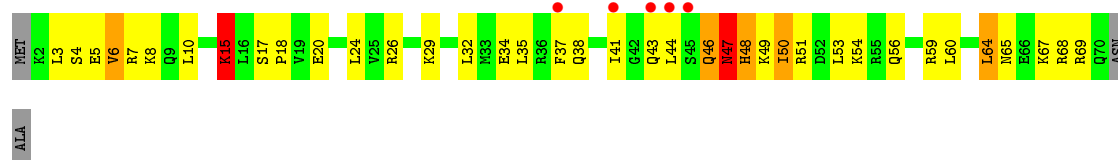
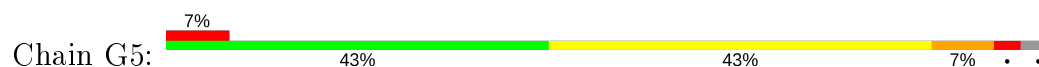
- Molecule 49: 50S ribosomal protein L28



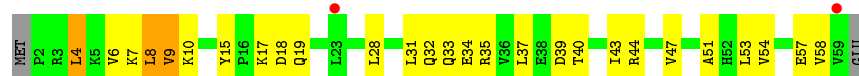
- Molecule 50: 50S ribosomal protein L29



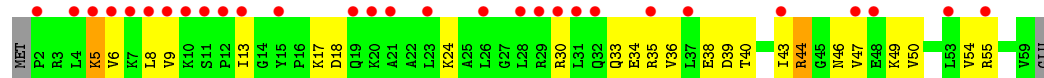
- Molecule 50: 50S ribosomal protein L29



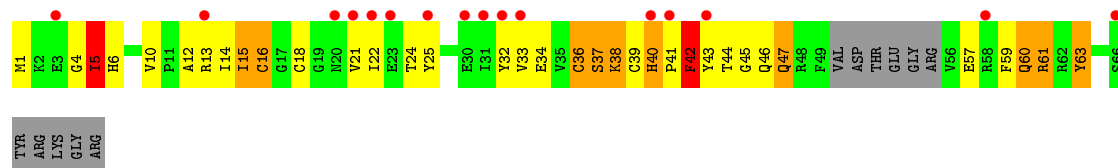
- Molecule 51: 50S ribosomal protein L30



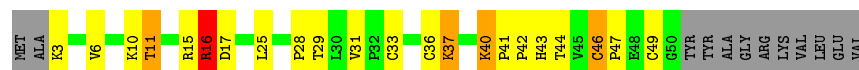
- Molecule 51: 50S ribosomal protein L30



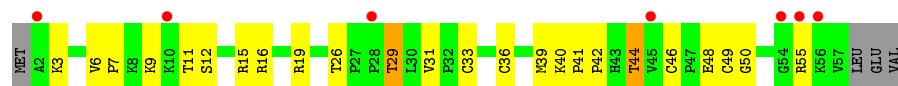
- Molecule 52: 50S ribosomal protein L31



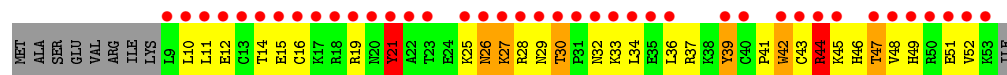
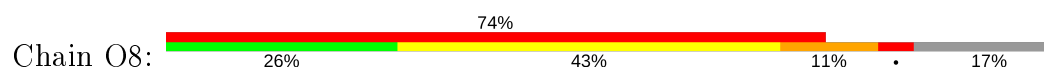
- Molecule 53: 50S ribosomal protein L32



- Molecule 53: 50S ribosomal protein L32



- Molecule 54: 50S ribosomal protein L33



- Molecule 55: 50S ribosomal protein L34

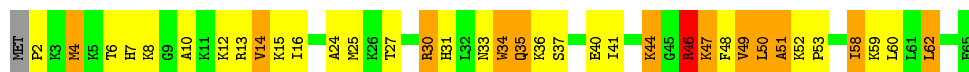




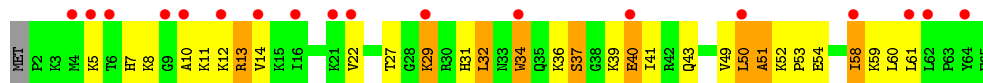
- Molecule 55: 50S ribosomal protein L34



- Molecule 56: 50S ribosomal protein L35



- Molecule 56: 50S ribosomal protein L35



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.30 Å 448.80 Å 620.20 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	147.08 – 2.99 161.81 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.9 (147.08-2.99) 90.8 (161.81-2.99)	Depositor EDS
R_{merge}	0.34	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.92 (at 3.01 Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.202 , 0.241 0.202 , 0.241	Depositor DCC
R_{free} test set	2000 reflections (0.17%)	wwPDB-VP
Wilson B-factor (Å ²)	81.3	Xtriage
Anisotropy	0.342	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 75.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	297444	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

²Theoretical 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: 5MU, OMC, PAR, U8U, MG, SF4, ZN, 7MG, 4SU, T6A, SPE, 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	13	0.70	1/36068 (0.0%)	1.35	292/56287 (0.5%)
1	1G	0.61	0/36282	1.22	170/56623 (0.3%)
2	12	0.37	0/1727	0.61	1/2326 (0.0%)
2	1E	0.40	0/1908	0.63	2/2573 (0.1%)
3	22	0.43	1/1560 (0.1%)	0.56	0/2104
3	2E	0.47	1/1629 (0.1%)	0.62	1/2195 (0.0%)
4	32	0.45	1/1732 (0.1%)	0.64	0/2318
4	3E	0.48	1/1728 (0.1%)	0.62	1/2313 (0.0%)
5	42	0.38	0/1156	0.60	0/1557
5	4E	0.45	0/1158	0.63	0/1559
6	52	0.49	0/855	0.66	1/1154 (0.1%)
6	5E	0.46	0/850	0.61	0/1147
7	62	0.39	0/1122	0.61	0/1500
7	6E	0.39	0/1259	0.54	0/1686
8	72	0.37	0/1127	0.57	0/1517
8	7E	0.41	0/1135	0.64	1/1527 (0.1%)
9	82	0.36	0/971	0.62	0/1304
9	8E	0.39	0/1019	0.61	0/1367
10	1A	1.00	2/658 (0.3%)	0.56	0/885
10	1I	0.40	0/762	0.62	0/1027
11	2A	0.40	0/850	0.61	1/1150 (0.1%)
11	2I	0.47	0/838	0.65	0/1133
12	3A	0.44	0/963	0.66	1/1290 (0.1%)
12	3I	0.63	0/972	0.80	1/1301 (0.1%)
13	4A	0.35	0/889	0.59	0/1192
13	4I	0.50	0/943	0.67	0/1265
14	5A	0.34	0/495	0.65	0/657
14	5I	0.47	0/495	0.69	1/657 (0.2%)
15	6A	0.40	0/740	0.58	0/987
15	6I	0.44	0/740	0.61	0/987
16	7A	0.43	0/721	0.65	0/970
16	7I	0.43	0/716	0.68	0/963

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	8A	0.45	0/836	0.59	0/1117
17	8I	0.51	0/836	0.65	0/1117
18	9A	0.46	0/549	0.67	0/732
18	9I	0.42	0/554	0.63	0/739
19	AA	0.38	0/520	0.67	0/700
19	AI	0.42	0/676	0.72	0/910
20	BA	0.35	0/764	0.67	1/1007 (0.1%)
20	BI	0.50	1/748 (0.1%)	0.63	0/986
21	1B	0.40	0/192	0.61	0/252
21	1F	0.42	0/203	0.71	0/266
22	1K	0.56	0/1589	1.11	6/2464 (0.2%)
23	2K	0.77	0/1721	1.42	16/2682 (0.6%)
23	2L	0.66	1/1721 (0.1%)	1.22	7/2682 (0.3%)
24	1L	0.39	0/1560	0.96	3/2418 (0.1%)
24	3K	0.52	0/1654	1.19	13/2570 (0.5%)
24	3L	0.52	0/1705	1.12	9/2650 (0.3%)
25	4K	0.74	0/473	1.15	0/735
25	4L	0.69	0/473	1.29	3/737 (0.4%)
26	14	0.84	45/68181 (0.1%)	1.54	1291/106432 (1.2%)
26	1H	1.01	117/68997 (0.2%)	1.75	2061/107696 (1.9%)
27	16	0.83	0/2928	1.57	59/4568 (1.3%)
27	1J	0.70	0/2928	1.37	32/4568 (0.7%)
28	7I	0.29	0/1049	0.54	0/1417
29	11	0.66	1/2170 (0.0%)	0.90	4/2926 (0.1%)
29	19	0.64	1/2175 (0.0%)	0.85	2/2933 (0.1%)
30	21	0.57	0/1579	0.92	3/2131 (0.1%)
30	29	0.53	0/1596	0.80	3/2153 (0.1%)
31	31	0.63	1/1620 (0.1%)	0.90	3/2194 (0.1%)
31	39	0.51	0/1637	0.80	1/2218 (0.0%)
32	41	0.47	0/1481	0.68	0/1994
32	49	0.38	0/1483	0.63	1/1997 (0.1%)
33	51	0.53	0/1354	0.86	4/1833 (0.2%)
33	59	0.35	0/1320	0.69	3/1787 (0.2%)
34	61	0.41	0/1146	0.71	1/1551 (0.1%)
34	69	0.41	0/1146	0.70	1/1551 (0.1%)
35	15	0.41	0/1123	0.61	0/1515
35	58	0.52	0/1123	0.75	0/1514
36	25	0.48	0/942	0.71	1/1269 (0.1%)
36	68	0.55	0/942	0.76	2/1269 (0.2%)
37	35	0.53	0/1139	0.83	2/1514 (0.1%)
37	78	0.61	0/1139	1.04	8/1514 (0.5%)
38	45	0.61	2/1120 (0.2%)	0.81	0/1498
38	88	0.69	0/1138	0.92	1/1523 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	55	0.51	0/981	0.83	0/1312
39	98	0.49	0/981	0.81	1/1312 (0.1%)
40	65	0.47	0/886	0.83	3/1180 (0.3%)
40	A8	0.59	0/891	0.83	2/1187 (0.2%)
41	75	0.51	0/1123	0.74	2/1500 (0.1%)
41	B8	0.58	0/1133	0.83	2/1514 (0.1%)
42	85	0.50	0/977	0.67	0/1301
42	C8	0.61	0/968	0.82	2/1289 (0.2%)
43	95	0.47	0/781	0.76	0/1048
43	D8	0.53	0/785	0.74	1/1052 (0.1%)
44	A5	0.55	0/897	0.77	1/1204 (0.1%)
44	E8	0.57	0/886	0.81	0/1189
45	B5	0.57	0/749	0.71	0/1007
45	F8	0.64	0/764	0.80	1/1025 (0.1%)
46	C5	0.52	0/807	0.81	1/1076 (0.1%)
46	G8	0.65	0/796	0.95	2/1062 (0.2%)
47	D5	0.54	1/1443 (0.1%)	0.64	1/1960 (0.1%)
47	H8	0.44	0/1395	0.73	1/1890 (0.1%)
48	E5	0.52	0/611	0.77	0/814
48	I8	0.76	1/619 (0.2%)	0.94	1/825 (0.1%)
49	F5	0.52	0/744	0.90	1/989 (0.1%)
49	J8	0.69	0/754	0.96	4/1003 (0.4%)
50	G5	0.53	0/578	0.73	0/766
50	K8	0.69	0/577	1.02	3/763 (0.4%)
51	H5	0.46	0/464	0.64	0/623
51	L8	0.50	0/464	0.73	0/623
52	M8	0.47	0/485	0.83	0/652
53	J5	0.58	0/448	0.76	0/606
53	N8	0.61	0/381	0.83	1/516 (0.2%)
54	O8	0.63	1/396 (0.3%)	0.90	1/529 (0.2%)
55	L5	0.57	0/409	0.78	0/540
55	P8	0.75	0/409	0.98	2/540 (0.4%)
56	M5	0.65	0/524	0.87	1/691 (0.1%)
56	Q8	0.69	0/524	1.02	3/691 (0.4%)
All	All	0.76	179/317928 (0.1%)	1.36	4051/476129 (0.9%)

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
2	12	0	5

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
2	1E	0	4
4	32	0	2
9	82	0	1
9	8E	0	2
10	1A	0	1
11	2A	0	1
12	3A	0	1
12	3I	0	2
13	4A	0	1
13	4I	0	1
14	5A	0	1
19	AA	0	2
19	AI	0	1
20	BA	0	2
29	11	0	5
29	19	0	3
30	21	0	8
30	29	0	5
31	39	0	7
32	41	0	1
32	49	0	2
33	51	0	5
33	59	0	1
34	61	0	3
34	69	0	4
35	58	0	1
37	35	0	2
37	78	0	6
38	45	0	2
38	88	0	4
39	55	0	1
39	98	0	2
40	65	0	1
40	A8	0	2
41	75	0	3
41	B8	0	3
42	85	0	4
42	C8	0	2
43	D8	0	3
44	A5	0	1
45	B5	0	2
46	C5	0	2

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
46	G8	0	5
47	D5	0	3
47	H8	0	6
48	E5	0	2
48	I8	0	1
49	F5	0	1
49	J8	0	1
50	G5	0	2
50	K8	0	2
52	M8	0	3
54	O8	0	1
55	P8	0	1
56	M5	0	2
56	Q8	0	3
All	All	0	145

All (179) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	1A	38	ILE	C-N	19.47	1.71	1.34
47	D5	94	GLU	C-N	14.46	1.61	1.34
10	1A	76	ASN	C-N	14.15	1.61	1.34
26	1H	774	A	N9-C4	-13.65	1.29	1.37
26	14	783	A	N9-C4	-12.02	1.30	1.37
26	1H	2430	A	N9-C4	-11.31	1.31	1.37
3	22	173	VAL	C-N	11.03	1.55	1.34
26	1H	783	A	N9-C4	-10.93	1.31	1.37
26	1H	2287	A	N9-C4	-10.75	1.31	1.37
26	1H	783	A	N3-C4	-10.14	1.28	1.34
26	1H	1899	G	N9-C4	-9.96	1.29	1.38
26	1H	676	A	N9-C4	-9.78	1.31	1.37
26	1H	1698	A	N9-C4	-9.63	1.32	1.37
26	1H	945	A	N7-C5	-9.55	1.33	1.39
26	1H	1698	A	N3-C4	-9.36	1.29	1.34
26	14	783	A	N3-C4	-9.25	1.29	1.34
26	1H	2346	A	N3-C4	-9.10	1.29	1.34
20	BI	97	ALA	C-N	9.06	1.51	1.34
26	1H	783	A	C5-C6	-8.99	1.32	1.41
26	1H	1332	G	N9-C4	-8.81	1.30	1.38
26	14	74	A	N9-C4	-8.65	1.32	1.37
26	14	1786	A	N9-C4	-8.52	1.32	1.37
3	2E	173	VAL	C-N	8.40	1.50	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	14	528	A	N9-C4	-8.40	1.32	1.37
26	1H	1678	G	N9-C8	8.34	1.43	1.37
26	1H	1786	A	N9-C4	-8.23	1.32	1.37
26	1H	528	A	N9-C4	-8.18	1.32	1.37
26	1H	676	A	N9-C8	8.12	1.44	1.37
26	1H	1899	G	N9-C8	8.06	1.43	1.37
26	1H	192	C	C2-N3	8.02	1.42	1.35
4	3E	36	ARG	C-N	-8.01	1.19	1.34
26	1H	1616	A	C5-C6	-7.95	1.33	1.41
26	1H	2062	A	N9-C4	7.92	1.42	1.37
26	1H	1950	G	N9-C8	7.88	1.43	1.37
26	14	2287	A	N9-C4	-7.86	1.33	1.37
26	1H	2062	A	N7-C5	7.84	1.44	1.39
26	1H	2062	A	N3-C4	7.69	1.39	1.34
26	14	783	A	N7-C5	-7.67	1.34	1.39
26	1H	621	A	N9-C4	-7.61	1.33	1.37
26	1H	1142(A)	A	N9-C4	-7.59	1.33	1.37
26	14	774	A	N9-C4	-7.56	1.33	1.37
26	1H	140	A	N9-C4	-7.47	1.33	1.37
26	1H	945	A	C5-C6	-7.31	1.34	1.41
26	1H	698	C	N1-C6	-7.31	1.32	1.37
26	1H	192	C	N3-C4	7.23	1.39	1.33
26	14	1772	G	N3-C4	7.21	1.40	1.35
26	14	1616	A	N9-C4	-7.17	1.33	1.37
38	45	77	LYS	C-N	-7.17	1.20	1.34
26	1H	71	A	N9-C4	-7.12	1.33	1.37
26	1H	71	A	C5-C6	-7.09	1.34	1.41
26	1H	71	A	C5-C4	7.05	1.43	1.38
26	1H	778	G	P-OP2	7.03	1.60	1.49
26	1H	1966	A	N9-C4	-6.99	1.33	1.37
26	1H	1786	A	C5-C4	6.96	1.43	1.38
26	1H	2392	A	N9-C8	6.88	1.43	1.37
26	1H	2062	A	C5-C6	6.78	1.47	1.41
26	14	783	A	C5-C6	-6.74	1.34	1.41
26	14	2685	G	C6-O6	6.74	1.30	1.24
26	1H	1786	A	N3-C4	-6.73	1.30	1.34
26	1H	138	G	N9-C8	6.72	1.42	1.37
26	1H	676	A	C5-C4	6.70	1.43	1.38
4	32	196	LEU	C-N	6.67	1.47	1.34
26	1H	774	A	N9-C8	6.66	1.43	1.37
26	1H	1786	A	C5-C6	-6.66	1.35	1.41
26	1H	829	A	N9-C4	-6.63	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	1H	2490	G	N9-C8	6.60	1.42	1.37
26	1H	1021	A	N9-C4	-6.52	1.33	1.37
26	1H	2713	A	C5-C4	6.52	1.43	1.38
26	1H	74	A	N9-C4	-6.44	1.33	1.37
26	1H	752	A	N9-C4	-6.43	1.33	1.37
26	1H	2051	A	N7-C5	-6.39	1.35	1.39
26	1H	1678	G	N9-C4	-6.36	1.32	1.38
26	1H	1614	A	N9-C4	-6.33	1.34	1.37
26	1H	1332	G	N9-C8	6.30	1.42	1.37
26	14	2346	A	N3-C4	-6.28	1.31	1.34
31	31	65	TRP	CB-CG	-6.21	1.39	1.50
38	45	69	PHE	C-N	6.20	1.46	1.34
26	1H	1332	G	N3-C4	-6.19	1.31	1.35
26	14	945	A	C5-C6	-6.18	1.35	1.41
26	14	2451	A	N9-C4	-6.16	1.34	1.37
26	14	676	A	N9-C4	-6.15	1.34	1.37
26	14	676	A	N9-C8	6.13	1.42	1.37
26	1H	1899	G	C2-N3	-6.09	1.27	1.32
26	1H	71	A	N9-C8	6.07	1.42	1.37
26	1H	1966	A	N3-C4	-6.06	1.31	1.34
26	14	945	A	N7-C5	-6.05	1.35	1.39
26	14	1903	G	N9-C8	-6.04	1.33	1.37
26	14	1786	A	N3-C4	-6.04	1.31	1.34
26	14	774	A	N9-C8	6.03	1.42	1.37
26	14	2062	A	N7-C5	6.01	1.42	1.39
26	14	786	C	N1-C6	5.99	1.40	1.37
26	1H	1776	G	C8-N7	-5.96	1.27	1.30
26	14	1698	A	N9-C4	-5.95	1.34	1.37
26	1H	825	C	N1-C6	-5.92	1.33	1.37
26	1H	2392	A	C5-C4	5.88	1.42	1.38
26	1H	1824	G	N7-C5	-5.87	1.35	1.39
26	1H	141	A	N9-C8	5.85	1.42	1.37
26	1H	530	G	N9-C8	5.83	1.42	1.37
26	1H	1775	U	C2-O2	-5.82	1.17	1.22
26	1H	573	G	P-OP1	5.79	1.58	1.49
26	1H	2518	A	N9-C4	-5.78	1.34	1.37
26	1H	2506	U	N1-C2	5.76	1.43	1.38
26	14	2873	A	N7-C5	-5.74	1.35	1.39
26	1H	2072	G	C8-N7	-5.72	1.27	1.30
26	1H	1204	A	N9-C4	-5.71	1.34	1.37
26	14	71	A	N9-C4	-5.70	1.34	1.37
26	1H	2689	U	C5-C6	-5.69	1.29	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	14	1786	A	C5-C6	-5.68	1.35	1.41
26	1H	57	C	N3-C4	-5.68	1.29	1.33
26	1H	471	A	N9-C4	-5.66	1.34	1.37
26	1H	1241	A	N9-C4	-5.65	1.34	1.37
26	14	2430	A	N9-C4	-5.65	1.34	1.37
26	1H	1349	A	C5-C4	5.64	1.42	1.38
26	14	2629	A	N9-C4	5.62	1.41	1.37
26	1H	576	U	N3-C4	-5.61	1.33	1.38
26	1H	621	A	C5-C4	5.58	1.42	1.38
23	2L	77	A	N9-C4	-5.58	1.34	1.37
26	1H	945	A	N3-C4	-5.58	1.31	1.34
26	14	1678	G	N9-C4	-5.57	1.33	1.38
26	1H	774	A	N3-C4	-5.56	1.31	1.34
26	1H	783	A	N7-C5	-5.53	1.35	1.39
26	14	1785	A	N7-C5	-5.52	1.35	1.39
26	1H	1786	A	N7-C5	-5.52	1.35	1.39
26	1H	621	A	C5-C6	-5.50	1.36	1.41
26	1H	1899	G	N3-C4	-5.50	1.31	1.35
26	1H	452	G	N1-C2	-5.47	1.33	1.37
26	14	974(A)	C	N1-C2	5.46	1.45	1.40
26	1H	2062	A	C6-N1	5.46	1.39	1.35
26	14	1899	G	C2-N3	5.46	1.37	1.32
26	14	1678	G	N3-C4	-5.45	1.31	1.35
26	1H	860	U	N1-C2	5.43	1.43	1.38
26	1H	945	A	N1-C2	5.43	1.39	1.34
26	14	788	A	N7-C5	-5.42	1.35	1.39
26	1H	917	A	C5-C6	-5.40	1.36	1.41
26	1H	253	C	N1-C6	5.40	1.40	1.37
26	14	1566	A	C5-C6	-5.40	1.36	1.41
26	1H	2688	U	N3-C4	-5.37	1.33	1.38
1	13	963	G	C6-N1	-5.34	1.35	1.39
26	1H	1616	A	N7-C5	-5.34	1.36	1.39
26	14	1021	A	N9-C4	-5.34	1.34	1.37
26	1H	74	A	N3-C4	-5.34	1.31	1.34
26	1H	2448	A	N7-C5	-5.32	1.36	1.39
26	14	774	A	N1-C2	5.31	1.39	1.34
26	1H	2589	A	C5-C4	-5.29	1.35	1.38
26	1H	472	A	N3-C4	-5.28	1.31	1.34
26	1H	1356	G	C6-O6	5.26	1.28	1.24
26	1H	188	G	C2-N3	5.26	1.36	1.32
26	1H	1349	A	N9-C8	5.25	1.42	1.37
26	14	2581	G	N1-C2	-5.25	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	14	2873	A	N3-C4	-5.25	1.31	1.34
26	1H	945	A	C2-N3	5.25	1.38	1.33
26	1H	761	A	N3-C4	-5.24	1.31	1.34
26	1H	1966	A	C5-C4	-5.23	1.35	1.38
26	1H	2430	A	N7-C5	-5.21	1.36	1.39
26	1H	1950	G	N3-C4	-5.21	1.31	1.35
26	14	1899	G	C5-C4	5.19	1.42	1.38
26	14	1786	A	C5-C4	5.18	1.42	1.38
26	1H	1950	G	C5-C4	5.18	1.42	1.38
26	14	2873	A	C5-C6	-5.17	1.36	1.41
26	1H	1678	G	C5-C4	5.17	1.42	1.38
26	1H	1032	A	C6-N1	5.17	1.39	1.35
26	1H	2707	G	N7-C5	5.16	1.42	1.39
26	1H	1313	U	C4-C5	-5.14	1.39	1.43
29	11	122	ASP	CB-CG	5.13	1.62	1.51
26	1H	1889	A	N9-C4	-5.12	1.34	1.37
26	1H	2497	A	N3-C4	-5.12	1.31	1.34
48	I8	45	PHE	C-N	5.11	1.45	1.34
54	O8	42	TRP	CB-CG	5.11	1.59	1.50
26	1H	774	A	C6-N1	5.09	1.39	1.35
26	1H	2392	A	N9-C4	-5.09	1.34	1.37
26	1H	2518	A	C5-C6	-5.09	1.36	1.41
26	1H	1621	U	N1-C6	-5.09	1.33	1.38
26	1H	1676	A	N9-C4	-5.08	1.34	1.37
26	14	2392	A	C5-C4	5.07	1.42	1.38
29	19	30	GLU	CG-CD	5.07	1.59	1.51
26	1H	452	G	C6-N1	-5.04	1.36	1.39
26	1H	2287	A	C5-C6	-5.01	1.36	1.41
26	14	2332	U	N1-C2	5.00	1.43	1.38
26	1H	463	G	N1-C2	-5.00	1.33	1.37

All (4051) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	1899	G	N3-C4-N9	-23.89	111.67	126.00
26	1H	945	A	C6-C5-N7	-20.89	117.67	132.30
26	1H	945	A	N1-C6-N6	20.76	131.05	118.60
26	1H	1899	G	N3-C4-C5	20.42	138.81	128.60
26	1H	2430	A	C2-N3-C4	-20.30	100.45	110.60
26	1H	1786	A	C2-N3-C4	-17.93	101.64	110.60
26	1H	71	A	C5-N7-C8	-17.86	94.97	103.90
26	1H	1786	A	C5-N7-C8	-17.71	95.05	103.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	2430	A	O5'-P-OP2	-17.54	89.65	110.70
26	1H	1786	A	N7-C8-N9	17.36	122.48	113.80
26	1H	71	A	N1-C6-N6	17.13	128.88	118.60
26	1H	2287	A	C2-N3-C4	-17.11	102.05	110.60
26	1H	1332	G	C5-N7-C8	-16.98	95.81	104.30
26	1H	1698	A	C2-N3-C4	-16.87	102.17	110.60
26	1H	1678	G	C2-N3-C4	-16.66	103.57	111.90
26	1H	1332	G	C2-N3-C4	-16.29	103.75	111.90
26	1H	945	A	C4-C5-C6	16.19	125.10	117.00
26	1H	576	U	N3-C2-O2	-16.13	110.91	122.20
26	1H	621	A	C2-N3-C4	-16.09	102.55	110.60
26	1H	74	A	C2-N3-C4	-15.98	102.61	110.60
26	1H	2346	A	N1-C2-N3	15.85	137.22	129.30
26	14	74	A	C2-N3-C4	-15.52	102.84	110.60
26	1H	774	A	N3-C4-C5	15.47	137.63	126.80
26	1H	71	A	C4-C5-N7	15.40	118.40	110.70
26	14	1786	A	C5-N7-C8	-15.24	96.28	103.90
26	1H	140	A	C5-N7-C8	-15.22	96.29	103.90
26	1H	774	A	N3-C4-N9	-15.19	115.25	127.40
26	1H	783	A	C5-N7-C8	-15.18	96.31	103.90
26	1H	783	A	C2-N3-C4	-14.98	103.11	110.60
26	1H	676	A	C2-N3-C4	-14.96	103.12	110.60
26	14	963	U	O5'-P-OP1	-14.82	92.36	105.70
26	1H	2689	U	C2-N1-C1'	14.73	135.37	117.70
26	14	1786	A	C2-N3-C4	-14.68	103.26	110.60
26	1H	917	A	C2-N3-C4	-14.56	103.32	110.60
26	1H	2490	G	C4-C5-N7	14.52	116.61	110.80
26	14	945	A	N1-C6-N6	14.51	127.31	118.60
26	14	945	A	C6-C5-N7	-14.49	122.16	132.30
26	14	510	C	O5'-P-OP2	-14.47	92.68	105.70
26	1H	2490	G	C5-N7-C8	-14.46	97.07	104.30
26	1H	945	A	C5-N7-C8	-14.40	96.70	103.90
26	14	783	A	N1-C6-N6	14.30	127.18	118.60
26	1H	1899	G	C2-N3-C4	-14.26	104.77	111.90
26	1H	1678	G	C5-N7-C8	-14.18	97.21	104.30
26	1H	860	U	C4-C5-C6	14.14	128.18	119.70
26	14	1786	A	N7-C8-N9	14.14	120.87	113.80
26	1H	576	U	C5-C4-O4	14.13	134.38	125.90
26	1H	1332	G	N3-C4-C5	14.05	135.62	128.60
26	1H	774	A	C2-N3-C4	-13.97	103.61	110.60
26	1H	1678	G	N3-C4-C5	13.92	135.56	128.60
26	1H	71	A	C6-C5-N7	-13.79	122.64	132.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	14	1899	G	N1-C2-N2	-13.74	103.83	116.20
26	14	783	A	C2-N3-C4	-13.70	103.75	110.60
26	1H	1616	A	C5-N7-C8	-13.67	97.07	103.90
26	1H	621	A	C5-N7-C8	-13.54	97.13	103.90
26	1H	1678	G	N3-C4-N9	-13.51	117.90	126.00
26	1H	71	A	C5-C6-N6	-13.49	112.91	123.70
26	14	2430	A	C2-N3-C4	-13.43	103.88	110.60
26	1H	71	A	N7-C8-N9	13.37	120.48	113.80
26	1H	676	A	C5-N7-C8	-13.33	97.23	103.90
26	1H	945	A	N7-C8-N9	13.32	120.46	113.80
26	14	1602	U	O5'-P-OP2	13.29	126.64	110.70
26	14	774	A	C2-N3-C4	-13.15	104.03	110.60
26	1H	192	C	C2-N3-C4	-13.08	113.36	119.90
26	1H	987	G	O5'-P-OP2	13.07	126.38	110.70
26	1H	945	A	C4-C5-N7	13.06	117.23	110.70
26	1H	1698	A	N1-C2-N3	12.90	135.75	129.30
26	1H	1332	G	N7-C8-N9	12.90	119.55	113.10
26	1H	1950	G	C5-N7-C8	-12.74	97.93	104.30
26	14	945	A	C2-N3-C4	-12.68	104.26	110.60
26	1H	1786	A	N1-C2-N3	12.68	135.64	129.30
26	1H	71	A	C2-N3-C4	-12.67	104.27	110.60
26	1H	624	C	O5'-P-OP1	-12.66	94.30	105.70
26	1H	140	A	N7-C8-N9	12.65	120.13	113.80
26	1H	1332	G	N3-C4-N9	-12.64	118.42	126.00
26	1H	1616	A	C4-C5-N7	12.59	117.00	110.70
26	1H	1786	A	C6-C5-N7	-12.55	123.52	132.30
26	1H	2582	G	O5'-P-OP2	-12.53	94.42	105.70
26	1H	783	A	N1-C6-N6	12.50	126.10	118.60
26	1H	1786	A	C8-N9-C4	-12.46	100.81	105.80
26	1H	2430	A	N3-C4-C5	12.41	135.49	126.80
26	1H	2430	A	N1-C6-N6	12.38	126.03	118.60
26	1H	2689	U	N3-C4-O4	12.35	128.04	119.40
26	1H	1332	G	C4-C5-N7	12.33	115.73	110.80
26	14	2873	A	C2-N3-C4	-12.32	104.44	110.60
26	1H	2346	A	O4'-C1'-N9	12.28	118.03	108.20
26	1H	49	A	O5'-P-OP2	-12.28	94.65	105.70
26	14	2873	A	C6-C5-N7	-12.27	123.71	132.30
26	1H	1678	G	N7-C8-N9	12.10	119.15	113.10
26	14	528	A	C2-N3-C4	-12.08	104.56	110.60
26	1H	929	G	N1-C6-O6	12.07	127.14	119.90
26	14	783	A	C5-N7-C8	-12.04	97.88	103.90
26	1H	1382	G	C5-C6-O6	-11.91	121.45	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	860	U	C5-C6-N1	-11.90	116.75	122.70
26	1H	1204	A	C2-N3-C4	-11.87	104.66	110.60
26	14	2287	A	C2-N3-C4	-11.87	104.67	110.60
26	14	1816	G	O5'-P-OP1	-11.85	95.04	105.70
26	1H	945	A	O4'-C1'-N9	11.78	117.62	108.20
27	16	13	A	O5'-P-OP2	-11.73	95.15	105.70
26	14	2873	A	N1-C2-N3	11.71	135.15	129.30
26	14	1616	A	C5-N7-C8	-11.70	98.05	103.90
26	14	1678	G	N7-C8-N9	11.70	118.95	113.10
26	14	1899	G	N3-C2-N2	11.67	128.07	119.90
26	1H	74	A	N1-C2-N3	11.62	135.11	129.30
26	14	1678	G	C8-N9-C4	-11.59	101.76	106.40
26	1H	1899	G	N3-C2-N2	-11.57	111.80	119.90
26	14	2873	A	N7-C8-N9	11.52	119.56	113.80
26	14	774	A	N3-C4-C5	11.49	134.84	126.80
26	1H	2406	U	O5'-P-OP1	-11.49	95.36	105.70
26	1H	917	A	C5-N7-C8	-11.48	98.16	103.90
26	1H	1382	G	N1-C6-O6	11.46	126.78	119.90
24	3K	76	A	C5-N7-C8	-11.45	98.17	103.90
26	1H	31	C	O5'-P-OP1	-11.43	95.41	105.70
26	1H	240	G	C5-C6-O6	-11.36	121.79	128.60
1	1G	766	A	O5'-P-OP2	-11.35	95.48	105.70
26	14	676	A	C2-N3-C4	-11.33	104.94	110.60
26	1H	793	A	O5'-P-OP2	-11.32	95.52	105.70
26	1H	783	A	C4-C5-N7	11.31	116.36	110.70
26	1H	2430	A	C5-C6-N1	-11.31	112.05	117.70
26	1H	2430	A	O5'-P-OP1	11.29	124.25	110.70
1	13	690	G	C6-C5-N7	-11.27	123.64	130.40
26	1H	676	A	N3-C4-C5	11.26	134.68	126.80
26	14	1763	G	O5'-P-OP2	-11.23	95.59	105.70
26	1H	1786	A	C4-C5-N7	11.22	116.31	110.70
26	1H	528	A	C6-N1-C2	11.21	125.33	118.60
26	1H	1950	G	N7-C8-N9	11.21	118.70	113.10
26	1H	2688	U	C5-C4-O4	11.19	132.61	125.90
26	14	1496	A	N7-C8-N9	11.19	119.39	113.80
26	1H	2714	G	O5'-P-OP2	-11.17	95.64	105.70
26	1H	2591	C	N1-C2-O2	-11.17	112.20	118.90
26	1H	528	A	N3-C4-C5	11.12	134.59	126.80
26	14	1678	G	C5-N7-C8	-11.06	98.77	104.30
1	13	974	A	N1-C6-N6	11.05	125.23	118.60
26	1H	1624	G	N1-C6-O6	-11.05	113.27	119.90
26	14	945	A	C4-C5-C6	11.04	122.52	117.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	1616	A	N1-C6-N6	11.03	125.22	118.60
26	1H	945	A	C5-C6-N6	-10.99	114.90	123.70
26	14	783	A	C6-C5-N7	-10.99	124.61	132.30
26	1H	2688	U	N3-C2-O2	-10.97	114.52	122.20
26	1H	945	A	C2-N3-C4	-10.93	105.14	110.60
26	1H	1496	A	N7-C8-N9	10.91	119.25	113.80
26	14	676	A	C5-N7-C8	-10.91	98.45	103.90
26	14	2873	A	N1-C6-N6	10.89	125.13	118.60
26	1H	140	A	C4-C5-N7	10.88	116.14	110.70
26	14	330	A	C2-N3-C4	-10.88	105.16	110.60
26	1H	576	U	N1-C2-N3	10.88	121.42	114.90
26	1H	2490	G	N7-C8-N9	10.80	118.50	113.10
26	1H	929	G	C5-C6-O6	-10.79	122.12	128.60
26	1H	783	A	N7-C8-N9	10.78	119.19	113.80
26	1H	1021	A	C2-N3-C4	-10.74	105.23	110.60
26	1H	1610	A	N9-C4-C5	-10.71	101.51	105.80
26	1H	1142(A)	A	C2-N3-C4	-10.71	105.25	110.60
1	13	690	G	C4-N9-C1'	10.70	140.41	126.50
24	3K	76	A	N7-C8-N9	10.68	119.14	113.80
26	1H	2346	A	C2-N3-C4	-10.68	105.26	110.60
26	1H	1639	U	O5'-P-OP2	-10.67	96.10	105.70
1	13	690	G	O4'-C1'-N9	10.66	116.73	108.20
26	1H	1604	C	O5'-P-OP1	-10.65	96.11	105.70
26	14	1772	G	C2-N3-C4	-10.64	106.58	111.90
26	1H	786	C	N3-C4-N4	-10.58	110.59	118.00
26	14	774	A	N1-C6-N6	10.58	124.95	118.60
26	14	2600	A	O5'-P-OP2	-10.57	96.19	105.70
26	1H	2448	A	N1-C6-N6	10.56	124.94	118.60
26	14	2873	A	C5-N7-C8	-10.54	98.63	103.90
26	1H	621	A	N7-C8-N9	10.51	119.05	113.80
26	14	788	A	N1-C6-N6	10.49	124.89	118.60
26	1H	945	A	C4-N9-C1'	10.48	145.16	126.30
26	1H	2287	A	N3-C4-C5	10.47	134.13	126.80
26	14	71	A	C5-N7-C8	-10.46	98.67	103.90
26	1H	2248	C	O5'-P-OP2	-10.43	96.31	105.70
26	1H	2392	A	C5-N7-C8	-10.43	98.69	103.90
26	14	621	A	C2-N3-C4	-10.42	105.39	110.60
26	1H	621	A	C4-C5-N7	10.42	115.91	110.70
26	14	1698	A	C5-N7-C8	-10.40	98.70	103.90
26	14	31	C	O5'-P-OP1	-10.40	96.34	105.70
26	1H	2331	G	N1-C6-O6	10.39	126.14	119.90
1	13	121	C	N1-C2-O2	10.38	125.13	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	2713	A	N7-C8-N9	10.37	118.98	113.80
26	1H	1204	A	O4'-C1'-N9	10.36	116.49	108.20
26	14	778	G	N1-C6-O6	-10.36	113.68	119.90
26	1H	138	G	C4-C5-N7	10.32	114.93	110.80
26	1H	917	A	N1-C6-N6	10.30	124.78	118.60
26	14	2092	U	C5-C4-O4	10.30	132.08	125.90
26	1H	1616	A	N7-C8-N9	10.29	118.94	113.80
26	1H	1698	A	C5-N7-C8	-10.28	98.76	103.90
26	14	2464	C	C6-N1-C2	10.28	124.41	120.30
26	1H	1899	G	N9-C4-C5	10.27	109.51	105.40
26	1H	459	U	O5'-P-OP2	-10.25	96.47	105.70
26	1H	945	A	N1-C2-N3	10.25	134.42	129.30
26	1H	1642	G	O5'-P-OP1	-10.25	96.48	105.70
26	1H	1565	C	C6-N1-C2	10.24	124.39	120.30
26	1H	1678	G	C8-N9-C4	-10.23	102.31	106.40
26	14	2273	A	O5'-P-OP2	-10.22	96.50	105.70
26	1H	1022	G	N9-C4-C5	10.21	109.48	105.40
26	1H	2287	A	C5-C6-N1	-10.21	112.59	117.70
26	1H	1313	U	C5-C6-N1	10.21	127.81	122.70
26	1H	2429	G	OP1-P-OP2	-10.20	104.30	119.60
26	1H	2265	U	O5'-P-OP1	-10.20	96.53	105.70
26	1H	2438	U	C5-C6-N1	-10.17	117.62	122.70
26	1H	1899	G	C8-N9-C1'	10.16	140.21	127.00
26	1H	1950	G	C8-N9-C4	-10.11	102.36	106.40
26	1H	736	C	O5'-P-OP1	-10.10	96.61	105.70
26	14	216	A	O5'-P-OP1	-10.09	96.62	105.70
26	1H	1955	U	C5-C6-N1	-10.09	117.66	122.70
26	14	945	A	N1-C2-N3	10.09	134.34	129.30
26	14	945	A	C5-N7-C8	-10.08	98.86	103.90
26	14	2357	U	O5'-P-OP2	-10.07	96.63	105.70
26	1H	2713	A	C5-N7-C8	-10.06	98.87	103.90
26	14	74	A	N3-C4-C5	10.06	133.84	126.80
26	14	974(A)	C	N1-C2-O2	10.05	124.93	118.90
26	1H	1129	A	O5'-P-OP2	-10.04	96.66	105.70
26	1H	774	A	C5-C6-N1	-10.03	112.69	117.70
31	31	74	ARG	NE-CZ-NH1	10.00	125.30	120.30
26	1H	774	A	C5-N7-C8	-9.99	98.91	103.90
26	1H	2518	A	N1-C6-N6	9.98	124.59	118.60
26	1H	1678	G	C4-C5-N7	9.98	114.79	110.80
26	1H	2700	C	C6-N1-C2	9.96	124.28	120.30
1	13	330	C	N1-C2-O2	9.96	124.88	118.90
26	1H	783	A	C6-C5-N7	-9.94	125.34	132.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	2609	U	C5-C6-N1	-9.92	117.74	122.70
26	1H	34	C	O5'-P-OP1	-9.92	96.78	105.70
26	1H	2689	U	C6-N1-C1'	-9.92	107.31	121.20
26	14	1619	G	O5'-P-OP2	-9.90	96.79	105.70
26	1H	917	A	N1-C2-N3	9.90	134.25	129.30
26	14	1204	A	C2-N3-C4	-9.90	105.65	110.60
26	1H	392	C	O5'-P-OP1	-9.85	96.83	105.70
26	1H	1616	A	C6-C5-N7	-9.85	125.41	132.30
26	14	140	A	N7-C8-N9	9.85	118.72	113.80
26	1H	2688	U	C4-C5-C6	9.84	125.60	119.70
26	1H	787	U	O5'-P-OP1	-9.84	96.85	105.70
26	1H	2584	U	N3-C2-O2	-9.83	115.32	122.20
26	1H	1255	U	N3-C4-O4	9.82	126.27	119.40
26	14	1772	G	N9-C4-C5	-9.82	101.47	105.40
26	14	2346	A	O4'-C1'-N9	9.81	116.05	108.20
26	14	2713	A	C5-N7-C8	-9.81	99.00	103.90
26	14	672	C	O5'-P-OP2	-9.80	96.88	105.70
26	1H	676	A	N3-C4-N9	-9.80	119.56	127.40
26	1H	71	A	N1-C2-N3	9.79	134.20	129.30
26	14	694	U	O5'-P-OP2	-9.79	96.89	105.70
26	14	1332	G	C5-N7-C8	-9.78	99.41	104.30
26	1H	1610	A	N1-C6-N6	9.78	124.47	118.60
26	14	140	A	C5-N7-C8	-9.77	99.02	103.90
26	1H	140	A	N1-C6-N6	9.76	124.46	118.60
26	1H	2432	A	O5'-P-OP2	-9.74	96.93	105.70
26	14	1786	A	C4-C5-N7	9.74	115.57	110.70
26	1H	1496	A	C5-N7-C8	-9.74	99.03	103.90
26	14	2430	A	N1-C6-N6	9.73	124.44	118.60
26	1H	2287	A	N1-C6-N6	9.73	124.44	118.60
26	14	1325	G	O5'-P-OP2	9.72	122.37	110.70
26	1H	528	A	C5-C6-N1	-9.72	112.84	117.70
26	1H	2032	G	C2-N3-C4	-9.71	107.05	111.90
26	14	621	A	C5-C6-N1	-9.69	112.85	117.70
1	13	1195	C	C6-N1-C2	-9.69	116.42	120.30
26	1H	2352	A	O5'-P-OP1	-9.69	96.98	105.70
26	1H	2503	A	N1-C2-N3	-9.69	124.45	129.30
26	1H	2036	C	O5'-P-OP1	-9.69	96.98	105.70
26	1H	210	C	C6-N1-C2	9.68	124.17	120.30
26	1H	1589	C	O5'-P-OP2	9.68	122.32	110.70
26	1H	2688	U	C5-C6-N1	-9.68	117.86	122.70
26	14	1616	A	C4-C5-N7	9.68	115.54	110.70
26	1H	621	A	N1-C6-N6	9.67	124.40	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	125	G	C5-C6-O6	-9.67	122.80	128.60
26	1H	1698	A	C6-C5-N7	-9.66	125.53	132.30
26	1H	1950	G	C4-C5-N7	9.65	114.66	110.80
26	1H	192	C	C5-C4-N4	-9.63	113.46	120.20
26	1H	917	A	C4-C5-N7	9.62	115.51	110.70
26	1H	930	U	C5-C4-O4	9.62	131.67	125.90
26	1H	2062	A	C2-N3-C4	9.62	115.41	110.60
26	1H	1021	A	C5-N7-C8	-9.61	99.10	103.90
26	1H	913	U	O5'-P-OP2	-9.60	97.06	105.70
26	1H	2689	U	N1-C2-O2	9.60	129.52	122.80
26	14	530	G	C4-C5-N7	9.60	114.64	110.80
26	14	963	U	O5'-P-OP2	9.59	122.21	110.70
26	14	1914	C	C6-N1-C2	-9.59	116.47	120.30
26	14	2873	A	C4-C5-C6	9.58	121.79	117.00
26	1H	2689	U	N3-C2-O2	-9.58	115.50	122.20
26	14	2518	A	N1-C6-N6	9.57	124.34	118.60
26	1H	329	G	O5'-P-OP2	-9.57	97.09	105.70
26	1H	752	A	C8-N9-C4	9.56	109.62	105.80
26	1H	141	A	C5-N7-C8	-9.56	99.12	103.90
26	1H	1698	A	N1-C6-N6	9.55	124.33	118.60
26	14	1678	G	N3-C4-N9	-9.55	120.27	126.00
26	1H	2507	C	C6-N1-C2	-9.54	116.48	120.30
26	14	462	C	O5'-P-OP2	-9.54	97.12	105.70
26	1H	676	A	N7-C8-N9	9.52	118.56	113.80
26	1H	224	G	O5'-P-OP2	-9.51	97.14	105.70
26	1H	138	G	C5-N7-C8	-9.50	99.55	104.30
26	1H	1324	G	N1-C6-O6	9.49	125.60	119.90
26	1H	783	A	N3-C4-C5	9.48	133.44	126.80
26	14	1396	U	O5'-P-OP1	-9.47	97.18	105.70
33	59	171	LEU	CA-CB-CG	9.46	137.05	115.30
26	1H	1616	A	C5-C6-N6	-9.45	116.14	123.70
26	1H	207	A	N1-C6-N6	9.44	124.27	118.60
26	14	1496	A	C5-N7-C8	-9.44	99.18	103.90
26	1H	1900	A	O5'-P-OP1	9.44	122.02	110.70
26	14	1678	G	C2-N3-C4	-9.42	107.19	111.90
26	1H	2311	A	C2-N3-C4	-9.41	105.89	110.60
26	14	1332	G	N7-C8-N9	9.41	117.80	113.10
1	13	971	G	O5'-P-OP2	-9.39	97.25	105.70
26	14	205	G	N9-C4-C5	-9.38	101.65	105.40
26	1H	518	G	O5'-P-OP2	-9.38	97.26	105.70
26	14	746	A	O5'-P-OP2	9.38	121.95	110.70
26	14	1496	A	C8-N9-C4	-9.38	102.05	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	14	1342	A	C2-N3-C4	-9.37	105.92	110.60
26	14	2282	G	O5'-P-OP1	-9.36	97.27	105.70
26	14	783	A	C4-C5-N7	9.36	115.38	110.70
26	1H	528	A	N3-C4-N9	-9.35	119.92	127.40
30	21	152	LYS	C-N-CA	-9.32	102.73	122.30
26	1H	2425	A	O5'-P-OP2	-9.30	97.33	105.70
26	1H	2448	A	C5-C6-N6	-9.30	116.26	123.70
26	1H	1899	G	C6-C5-N7	9.30	135.98	130.40
26	1H	2402	C	C6-N1-C2	-9.29	116.58	120.30
26	14	2490	G	N7-C8-N9	9.29	117.75	113.10
26	1H	216	A	O5'-P-OP1	-9.29	97.34	105.70
26	1H	2518	A	C5-N7-C8	-9.28	99.26	103.90
26	14	778	G	C5-C6-O6	9.27	134.16	128.60
26	14	746	A	O5'-P-OP1	-9.27	97.36	105.70
26	1H	16	G	O5'-P-OP2	-9.26	97.36	105.70
26	14	2297	C	O5'-P-OP1	-9.26	97.37	105.70
26	14	945	A	C4-C5-N7	9.24	115.32	110.70
26	1H	528	A	C2-N3-C4	-9.24	105.98	110.60
26	14	672	C	O5'-P-OP1	9.24	121.79	110.70
26	1H	1297	C	OP2-P-O3'	-9.22	84.91	105.20
26	1H	2430	A	N3-C4-N9	-9.22	120.03	127.40
26	14	2346	A	N1-C2-N3	9.20	133.90	129.30
26	1H	1784	A	O5'-P-OP1	-9.20	97.42	105.70
26	14	929	G	N1-C6-O6	9.20	125.42	119.90
26	14	1786	A	C6-C5-N7	-9.19	125.87	132.30
26	1H	137(A)	G	N1-C6-O6	9.19	125.41	119.90
26	14	1342	A	N1-C2-N3	9.19	133.89	129.30
26	1H	676	A	C4-C5-N7	9.18	115.29	110.70
26	1H	1786	A	N1-C6-N6	9.17	124.10	118.60
26	14	1332	G	C6-C5-N7	-9.17	124.90	130.40
26	1H	399	G	O5'-P-OP2	-9.16	97.45	105.70
26	14	786	C	N3-C4-N4	-9.15	111.59	118.00
1	1G	690	G	C5-N7-C8	-9.14	99.73	104.30
24	3K	76	A	N1-C6-N6	9.14	124.08	118.60
26	1H	1639	U	O5'-P-OP1	9.13	121.66	110.70
26	1H	2689	U	C5-C4-O4	-9.12	120.43	125.90
26	1H	828	U	C5-C4-O4	9.12	131.37	125.90
26	14	1249	U	O5'-P-OP1	-9.12	97.50	105.70
26	1H	1021	A	N7-C8-N9	9.09	118.34	113.80
26	1H	2503	A	C5-C6-N6	-9.09	116.43	123.70
26	1H	1022	G	C8-N9-C4	-9.08	102.77	106.40
26	1H	1950	G	C2-N3-C4	-9.07	107.36	111.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	2331	G	C2-N3-C4	-9.06	107.37	111.90
26	1H	1829	A	O5'-P-OP1	-9.06	97.55	105.70
26	1H	1394	U	O5'-P-OP2	9.06	121.57	110.70
26	1H	252	G	O5'-P-OP2	-9.04	97.56	105.70
26	1H	1931	U	C5-C4-O4	9.04	131.33	125.90
26	1H	51	G	O5'-P-OP1	-9.03	97.57	105.70
26	1H	1394	U	O5'-P-OP1	-9.03	97.58	105.70
1	13	974	A	O4'-C1'-N9	9.02	115.42	108.20
26	1H	2712	U	N3-C4-O4	-9.01	113.09	119.40
26	14	1332	G	C2-N3-C4	-9.00	107.40	111.90
31	31	74	ARG	NE-CZ-NH2	-8.99	115.80	120.30
26	1H	945	A	C8-N9-C4	-8.99	102.20	105.80
26	14	1964	G	O5'-P-OP2	-8.97	97.62	105.70
26	1H	624	C	O5'-P-OP2	8.92	121.41	110.70
26	1H	140	A	C8-N9-C4	-8.92	102.23	105.80
1	13	974	A	C6-C5-N7	-8.91	126.06	132.30
26	14	2296	U	C2-N1-C1'	8.90	128.38	117.70
26	1H	2374	C	C5-C6-N1	-8.89	116.56	121.00
26	14	205	G	C8-N9-C4	8.88	109.95	106.40
26	1H	1210	A	C8-N9-C4	-8.87	102.25	105.80
26	1H	933	A	O5'-P-OP2	-8.87	97.72	105.70
26	1H	1982	C	C6-N1-C2	-8.85	116.76	120.30
26	14	1284	A	O5'-P-OP2	-8.84	97.74	105.70
26	1H	788	A	N1-C6-N6	8.84	123.90	118.60
26	14	2713	A	N7-C8-N9	8.84	118.22	113.80
26	14	687	C	O5'-P-OP1	-8.84	97.75	105.70
26	14	2688	U	N3-C2-O2	-8.83	116.02	122.20
26	14	2430	A	N1-C2-N3	8.82	133.71	129.30
26	1H	2394	C	O5'-P-OP2	-8.80	97.78	105.70
26	1H	955	C	O5'-P-OP2	-8.79	97.79	105.70
26	14	1899	G	C2-N3-C4	-8.79	107.51	111.90
26	1H	2598	A	O5'-P-OP1	-8.77	97.81	105.70
26	1H	783	A	C8-N9-C4	-8.77	102.29	105.80
26	14	676	A	O4'-C1'-N9	8.77	115.21	108.20
26	1H	464	U	C5-C6-N1	-8.76	118.32	122.70
26	14	1899	G	C6-C5-N7	-8.75	125.15	130.40
26	1H	915	C	N1-C2-O2	8.75	124.15	118.90
26	1H	576	U	N3-C4-O4	-8.75	113.28	119.40
26	14	1021	A	C2-N3-C4	-8.75	106.23	110.60
26	14	2296	U	O5'-P-OP1	-8.74	97.83	105.70
26	1H	1899	G	C4-C5-C6	-8.74	113.56	118.80
26	14	1989	G	N3-C2-N2	-8.73	113.79	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	14	1566	A	N1-C6-N6	8.72	123.83	118.60
26	1H	1822	G	O5'-P-OP2	8.72	121.16	110.70
26	14	2073	C	O5'-P-OP2	8.71	121.16	110.70
26	1H	446	G	N1-C6-O6	8.71	125.12	119.90
26	1H	1931	U	N3-C2-O2	-8.70	116.11	122.20
26	1H	2427	C	O5'-P-OP2	8.69	121.13	110.70
26	1H	1806	C	O5'-P-OP2	-8.69	97.88	105.70
26	1H	829	A	OP1-P-OP2	8.67	132.60	119.60
26	1H	2346	A	O5'-P-OP1	-8.66	97.91	105.70
26	1H	1332	G	C8-N9-C4	-8.65	102.94	106.40
1	13	576	G	N1-C6-O6	8.63	125.08	119.90
26	1H	446	G	O5'-P-OP2	8.63	121.06	110.70
26	14	1842	G	N1-C6-O6	-8.63	114.72	119.90
26	14	1772	G	C8-N9-C4	8.60	109.84	106.40
26	1H	917	A	N7-C8-N9	8.59	118.09	113.80
26	1H	2441	C	N3-C2-O2	-8.59	115.89	121.90
26	14	1783	A	O5'-P-OP1	-8.59	97.97	105.70
1	13	690	G	C8-N9-C1'	-8.59	115.84	127.00
26	1H	1210	A	N7-C8-N9	8.59	118.09	113.80
26	1H	1361	G	N1-C6-O6	-8.58	114.75	119.90
26	1H	2598	A	O5'-P-OP2	8.58	120.99	110.70
26	14	1616	A	C2-N3-C4	-8.57	106.31	110.60
26	14	1265	A	N1-C6-N6	8.56	123.74	118.60
26	1H	679	C	C5-C6-N1	-8.56	116.72	121.00
26	1H	698	C	C4-C5-C6	8.56	121.68	117.40
26	14	774	A	C4-C5-N7	8.55	114.98	110.70
26	14	2360	A	O5'-P-OP2	-8.55	98.00	105.70
26	1H	251	A	O5'-P-OP1	-8.55	98.01	105.70
26	1H	137(A)	G	C5-C6-O6	-8.54	123.48	128.60
26	1H	1528	A	N7-C8-N9	8.52	118.06	113.80
1	1G	690	G	N7-C8-N9	8.52	117.36	113.10
26	1H	1204	A	C5-C6-N1	-8.52	113.44	117.70
26	1H	2623	G	C8-N9-C4	-8.52	102.99	106.40
1	13	963	G	N1-C2-N2	-8.51	108.54	116.20
26	1H	508	G	C8-N9-C4	-8.51	103.00	106.40
26	1H	1950	G	N3-C4-N9	-8.51	120.89	126.00
26	14	1975	G	O5'-P-OP2	-8.51	98.04	105.70
26	1H	945	A	C8-N9-C1'	-8.51	112.39	127.70
26	1H	71	A	N9-C4-C5	-8.50	102.40	105.80
26	1H	120	U	C5-C6-N1	-8.50	118.45	122.70
26	1H	1784	A	O5'-P-OP2	8.50	120.90	110.70
26	1H	917	A	C6-C5-N7	-8.49	126.36	132.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	14	1698	A	C4-C5-N7	8.49	114.94	110.70
26	14	1963	U	C2-N1-C1'	8.49	127.89	117.70
26	14	2490	G	C5-N7-C8	-8.49	100.06	104.30
26	14	1807	G	C8-N9-C4	8.48	109.79	106.40
26	1H	740	U	O5'-P-OP2	-8.48	98.07	105.70
26	1H	774	A	C8-N9-C1'	8.47	142.95	127.70
1	13	328	C	C2-N1-C1'	8.47	128.12	118.80
26	1H	2392	A	C4-C5-N7	8.46	114.93	110.70
26	14	2429	G	O5'-P-OP1	8.45	120.84	110.70
26	1H	1528	A	C8-N9-C4	-8.45	102.42	105.80
26	1H	2572	A	C8-N9-C4	8.45	109.18	105.80
26	1H	1676	A	C2-N3-C4	-8.45	106.38	110.60
26	1H	1950	G	O4'-C1'-N9	8.45	114.96	108.20
26	1H	1752	C	C6-N1-C2	8.44	123.67	120.30
26	14	1963	U	N1-C2-O2	8.44	128.71	122.80
26	1H	1203	G	O5'-P-OP2	-8.43	98.11	105.70
26	1H	2311	A	N1-C2-N3	8.43	133.51	129.30
26	14	1785	A	OP2-P-O3'	8.43	123.73	105.20
26	14	74	A	C5-C6-N1	-8.42	113.49	117.70
26	1H	1404	C	O5'-P-OP2	-8.40	98.14	105.70
1	13	5	U	N1-C2-O2	8.40	128.68	122.80
26	14	1948	G	O5'-P-OP1	-8.40	98.14	105.70
26	1H	1310	G	N1-C6-O6	8.39	124.93	119.90
26	14	2712	U	C5-C6-N1	-8.39	118.51	122.70
26	1H	778	G	N1-C6-O6	-8.38	114.87	119.90
26	1H	1899	G	C4-N9-C1'	-8.38	115.61	126.50
26	1H	774	A	C6-N1-C2	8.38	123.62	118.60
1	1G	690	G	O4'-C1'-N9	8.37	114.90	108.20
26	1H	124	G	C5-C6-O6	-8.37	123.58	128.60
1	13	1504	G	O5'-P-OP1	-8.36	98.17	105.70
24	3K	76	A	C4-C5-N7	8.35	114.88	110.70
26	1H	125	G	N1-C6-O6	8.34	124.90	119.90
26	14	929	G	C5-C6-O6	-8.34	123.60	128.60
26	14	34	C	N1-C2-O2	8.33	123.90	118.90
26	1H	786	C	C5-C4-N4	8.33	126.03	120.20
26	1H	1379	A	N1-C6-N6	8.32	123.59	118.60
1	13	5	U	N3-C2-O2	-8.32	116.38	122.20
26	14	1614	A	C2-N3-C4	-8.32	106.44	110.60
26	1H	1950	G	N3-C4-C5	8.31	132.76	128.60
26	1H	2346	A	C8-N9-C4	-8.30	102.48	105.80
1	13	980	C	O5'-P-OP1	-8.30	98.23	105.70
26	14	2058	A	O5'-P-OP2	-8.30	98.23	105.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	14	530	G	C6-C5-N7	-8.29	125.42	130.40
26	1H	2360	A	O5'-P-OP2	-8.29	98.24	105.70
26	14	2023	G	O5'-P-OP2	-8.29	98.24	105.70
26	1H	966	G	N1-C6-O6	-8.28	114.93	119.90
26	14	676	A	C4-C5-N7	8.29	114.84	110.70
26	1H	783	A	N3-C4-N9	-8.28	120.78	127.40
26	1H	2506	U	N1-C2-O2	8.28	128.60	122.80
26	14	74	A	N1-C6-N6	8.28	123.57	118.60
26	1H	1496	A	C8-N9-C4	-8.28	102.49	105.80
26	1H	2713	A	C8-N9-C4	-8.28	102.49	105.80
26	1H	731	C	O5'-P-OP2	-8.27	98.25	105.70
26	14	991	C	O5'-P-OP1	-8.27	98.26	105.70
26	1H	2380	C	C5-C6-N1	-8.27	116.87	121.00
26	14	2435	A	C8-N9-C4	-8.27	102.49	105.80
1	13	770	C	O5'-P-OP2	8.25	120.60	110.70
26	1H	821	A	OP1-P-OP2	8.25	131.98	119.60
26	1H	140	A	C6-C5-N7	-8.25	126.53	132.30
26	1H	1365	A	C5-C6-N1	-8.25	113.58	117.70
26	1H	766	C	C2-N3-C4	-8.25	115.78	119.90
26	1H	1888	G	N3-C4-N9	8.25	130.95	126.00
27	16	115	G	C5-C6-O6	-8.24	123.66	128.60
1	13	690	G	N7-C8-N9	8.23	117.22	113.10
26	1H	1781	C	C6-N1-C2	8.23	123.59	120.30
26	1H	2331	G	C4-C5-N7	8.22	114.09	110.80
26	14	621	A	N7-C8-N9	8.22	117.91	113.80
26	1H	2688	U	N1-C2-N3	8.22	119.83	114.90
26	14	2685	G	C5-C6-N1	-8.21	107.39	111.50
26	14	1616	A	N7-C8-N9	8.21	117.90	113.80
26	1H	733	G	O5'-P-OP2	-8.21	98.31	105.70
26	1H	74	A	C5-C6-N1	-8.20	113.60	117.70
26	1H	2503	A	C2-N3-C4	8.20	114.70	110.60
26	1H	751	A	O5'-P-OP1	-8.19	98.33	105.70
29	11	56	GLY	C-N-CA	-8.19	105.11	122.30
26	1H	2244	U	N3-C2-O2	-8.19	116.47	122.20
26	1H	2503	A	N1-C6-N6	8.19	123.51	118.60
26	1H	120	U	C4-C5-C6	8.18	124.61	119.70
26	1H	1301	A	N1-C6-N6	8.18	123.51	118.60
26	1H	467	G	O5'-P-OP2	-8.17	98.34	105.70
26	1H	2085	C	O5'-P-OP2	-8.17	98.35	105.70
26	1H	1271	G	O5'-P-OP2	-8.16	98.35	105.70
26	14	2326	C	C6-N1-C2	-8.16	117.03	120.30
26	1H	451	C	N1-C2-O2	-8.15	114.01	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	1265	A	O5'-P-OP2	-8.14	98.37	105.70
26	1H	2699	C	C6-N1-C2	8.14	123.56	120.30
26	1H	825	C	N3-C4-N4	8.14	123.70	118.00
1	1G	1281	U	N3-C2-O2	-8.14	116.50	122.20
26	1H	2518	A	C4-C5-N7	8.13	114.77	110.70
26	1H	1616	A	O4'-C1'-N9	8.13	114.70	108.20
26	1H	2380	C	C2-N3-C4	-8.13	115.84	119.90
26	1H	915	C	N3-C2-O2	-8.12	116.21	121.90
26	1H	2424	C	OP1-P-OP2	8.12	131.78	119.60
26	14	1786	A	C8-N9-C4	-8.12	102.55	105.80
26	1H	2623	G	N3-C4-C5	-8.12	124.54	128.60
26	1H	1602	U	N3-C4-O4	-8.12	113.72	119.40
23	2K	61	U	O5'-P-OP2	-8.11	98.40	105.70
26	1H	812	C	N1-C2-O2	-8.11	114.03	118.90
26	1H	205	G	C8-N9-C4	8.11	109.64	106.40
26	1H	2258	C	C4-C5-C6	8.10	121.45	117.40
26	14	774	A	C5-N7-C8	-8.10	99.85	103.90
26	1H	621	A	N3-C4-C5	8.10	132.47	126.80
26	1H	778	G	C5-C6-O6	8.10	133.46	128.60
26	14	2067	G	O5'-P-OP1	-8.10	98.41	105.70
26	14	1388	G	O5'-P-OP2	-8.09	98.42	105.70
26	14	1314	C	N1-C2-O2	8.09	123.75	118.90
26	14	1786	A	C5-C6-N1	-8.09	113.66	117.70
27	16	6	C	N1-C2-O2	-8.09	114.05	118.90
26	14	120	U	O5'-P-OP2	-8.08	98.43	105.70
26	1H	2392	A	N7-C8-N9	8.08	117.84	113.80
46	G8	81	LYS	C-N-CD	-8.08	102.83	120.60
26	14	2452	C	O5'-P-OP2	-8.07	98.44	105.70
1	13	422	C	C6-N1-C2	-8.07	117.07	120.30
1	1G	117	G	N1-C6-O6	8.06	124.74	119.90
26	14	2430	A	C5-C6-N1	-8.06	113.67	117.70
26	1H	2346	A	N7-C8-N9	8.06	117.83	113.80
1	13	1260	C	C6-N1-C2	-8.05	117.08	120.30
26	1H	930	U	N3-C4-O4	-8.05	113.76	119.40
26	1H	2402	C	N3-C2-O2	-8.05	116.26	121.90
26	14	140	A	C4-C5-N7	8.05	114.73	110.70
26	1H	2490	G	N3-C4-C5	8.05	132.63	128.60
26	1H	2446	G	C5-C6-O6	-8.05	123.77	128.60
26	1H	621	A	C6-C5-N7	-8.05	126.67	132.30
26	1H	2712	U	N3-C2-O2	-8.05	116.57	122.20
26	14	1602	U	O5'-P-OP1	-8.04	98.46	105.70
26	14	1785	A	C8-N9-C4	-8.04	102.58	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	2272	U	O5'-P-OP1	8.04	120.34	110.70
26	1H	917	A	O5'-P-OP1	-8.03	98.47	105.70
1	1G	690	G	C2-N3-C4	-8.04	107.88	111.90
26	1H	1899	G	C5-C6-O6	8.03	133.41	128.60
1	13	974	A	C4-C5-N7	8.02	114.71	110.70
23	2K	6	G	C8-N9-C4	8.02	109.61	106.40
26	1H	184	C	C6-N1-C2	8.01	123.50	120.30
26	1H	2495	G	N1-C6-O6	8.01	124.70	119.90
26	14	1396	U	N3-C2-O2	-8.01	116.60	122.20
26	14	2258	C	C4-C5-C6	8.00	121.40	117.40
26	14	1698	A	N1-C6-N6	8.00	123.40	118.60
26	1H	71	A	O4'-C1'-N9	-7.99	101.81	108.20
26	14	2609	U	O5'-P-OP2	-7.98	98.52	105.70
1	1G	1128	C	C6-N1-C2	-7.96	117.11	120.30
26	14	2566	A	O5'-P-OP2	-7.96	98.54	105.70
26	14	252	G	O5'-P-OP2	-7.96	98.54	105.70
26	14	945	A	N7-C8-N9	7.96	117.78	113.80
1	13	800	G	N1-C6-O6	7.96	124.67	119.90
26	14	1950	G	N7-C8-N9	7.96	117.08	113.10
26	1H	1660	C	N3-C2-O2	-7.95	116.33	121.90
26	1H	2715	C	N3-C4-C5	7.95	125.08	121.90
26	1H	560	C	O5'-P-OP1	-7.95	98.54	105.70
26	1H	1764	G	C5-C6-O6	7.95	133.37	128.60
26	14	783	A	N7-C8-N9	7.95	117.77	113.80
26	1H	2331	G	C6-C5-N7	-7.94	125.64	130.40
26	1H	1408	C	N1-C2-O2	-7.94	114.14	118.90
26	1H	2346	A	C6-C5-N7	-7.94	126.75	132.30
26	1H	2346	A	C4-N9-C1'	7.94	140.59	126.30
26	1H	837	C	C6-N1-C2	-7.93	117.13	120.30
26	1H	2741	A	C8-N9-C4	7.93	108.97	105.80
26	1H	856	C	O5'-P-OP1	-7.93	98.56	105.70
26	1H	755	C	C6-N1-C2	-7.93	117.13	120.30
26	1H	1835	G	O5'-P-OP1	-7.93	98.57	105.70
26	1H	1624	G	C5-C6-O6	7.92	133.35	128.60
26	1H	1626	G	N3-C2-N2	-7.92	114.36	119.90
26	14	2241	A	O5'-P-OP2	7.92	120.20	110.70
26	14	37	C	O5'-P-OP2	-7.91	98.58	105.70
26	1H	34	C	O5'-P-OP2	7.91	120.19	110.70
26	1H	210	C	N3-C4-C5	7.91	125.06	121.90
26	1H	676	A	O4'-C1'-N9	7.91	114.53	108.20
26	14	1807	G	N1-C6-O6	7.90	124.64	119.90
26	1H	1698	A	C5-C6-N1	-7.90	113.75	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	14	2436	G	N1-C6-O6	7.90	124.64	119.90
26	14	71	A	N7-C8-N9	7.90	117.75	113.80
26	1H	2235	G	C5-C6-O6	-7.90	123.86	128.60
26	1H	730	C	OP2-P-O3'	7.90	122.57	105.20
26	1H	132	G	N1-C6-O6	-7.89	115.16	119.90
26	1H	576	U	C4-C5-C6	7.89	124.44	119.70
26	14	1382	G	C4-C5-N7	7.89	113.96	110.80
26	14	2062	A	C8-N9-C4	7.89	108.96	105.80
26	14	1185	C	O5'-P-OP2	-7.88	98.60	105.70
26	1H	446	G	N9-C4-C5	-7.88	102.25	105.40
26	14	620	G	O5'-P-OP2	-7.88	98.61	105.70
26	1H	739	G	O5'-P-OP2	-7.88	98.61	105.70
26	1H	410	G	C5-C6-O6	-7.87	123.88	128.60
26	1H	2253	G	C5-C6-O6	-7.87	123.88	128.60
26	1H	2346	A	C4-C5-C6	7.87	120.93	117.00
26	14	1332	G	C4-C5-N7	7.86	113.94	110.80
26	14	1904	G	O5'-P-OP2	-7.86	98.63	105.70
26	14	917	A	O5'-P-OP1	-7.86	98.63	105.70
26	1H	192	C	N3-C4-C5	7.85	125.04	121.90
26	1H	265	A	C2-N3-C4	-7.85	106.67	110.60
26	1H	1253	A	C8-N9-C4	7.85	108.94	105.80
26	14	2424	C	O5'-P-OP1	-7.85	98.64	105.70
26	14	985	C	OP2-P-O3'	7.84	122.45	105.20
26	1H	2006	C	C6-N1-C2	7.83	123.43	120.30
26	1H	1255	U	C5-C4-O4	-7.83	121.20	125.90
26	1H	2430	A	N1-C2-N3	7.83	133.21	129.30
26	1H	797	C	C4-C5-C6	7.82	121.31	117.40
26	1H	2525	G	N9-C4-C5	-7.82	102.27	105.40
26	1H	2258	C	C2-N3-C4	-7.82	115.99	119.90
26	1H	1203	G	C5-C6-O6	7.82	133.29	128.60
26	1H	2622	C	O5'-P-OP2	-7.81	98.67	105.70
26	14	676	A	N7-C8-N9	7.81	117.70	113.80
26	14	2392	A	C8-N9-C4	-7.81	102.68	105.80
26	1H	140	A	C2-N3-C4	-7.81	106.70	110.60
26	1H	192	C	N1-C2-O2	-7.81	114.22	118.90
26	1H	1382	G	C4-C5-N7	7.80	113.92	110.80
26	1H	821	A	O5'-P-OP2	-7.80	98.68	105.70
26	1H	2490	G	C2-N3-C4	-7.80	108.00	111.90
26	1H	686	G	N9-C4-C5	-7.79	102.28	105.40
26	14	801	G	O5'-P-OP2	-7.79	98.69	105.70
26	1H	1324	G	N3-C2-N2	-7.79	114.45	119.90
26	14	1780	A	C8-N9-C4	-7.79	102.69	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	13	1369	C	O5'-P-OP2	-7.78	98.70	105.70
26	14	1812	A	O5'-P-OP2	-7.78	98.70	105.70
26	14	2776	A	C8-N9-C4	-7.77	102.69	105.80
26	14	71	A	C4-C5-N7	7.77	114.58	110.70
26	1H	2331	G	C5-C6-O6	-7.76	123.94	128.60
26	14	2324	C	N3-C4-C5	7.76	125.01	121.90
26	1H	1604	C	N1-C2-O2	-7.76	114.24	118.90
26	1H	1610	A	C4-C5-N7	7.76	114.58	110.70
26	14	569	U	C5-C6-N1	-7.75	118.82	122.70
26	1H	1376	C	C6-N1-C2	-7.75	117.20	120.30
26	14	1585	C	N1-C2-O2	7.75	123.55	118.90
26	1H	1970	A	O5'-P-OP1	-7.75	98.73	105.70
26	14	1786	A	N1-C6-N6	7.74	123.25	118.60
26	1H	1352	U	O5'-P-OP2	-7.74	98.73	105.70
26	14	1970	A	O5'-P-OP1	7.74	119.99	110.70
26	1H	2751	G	C8-N9-C4	7.74	109.50	106.40
26	14	1950	G	C5-N7-C8	-7.74	100.43	104.30
26	14	2238	G	O4'-C1'-N9	-7.73	102.01	108.20
26	14	2446	G	N1-C6-O6	-7.73	115.26	119.90
1	13	1446	A	O4'-C1'-N9	7.72	114.38	108.20
26	1H	2318	G	O4'-C1'-N9	7.72	114.38	108.20
26	14	2249	U	C6-N1-C2	-7.72	116.37	121.00
26	1H	852	G	O5'-P-OP2	-7.71	98.76	105.70
27	1J	30	C	C6-N1-C2	-7.71	117.22	120.30
26	1H	1357	U	C4-C5-C6	7.71	124.32	119.70
26	1H	256	A	N1-C6-N6	7.70	123.22	118.60
26	14	49	A	P-O3'-C3'	7.70	128.94	119.70
26	1H	2821	A	N1-C6-N6	7.70	123.22	118.60
26	14	2073	C	OP1-P-OP2	-7.70	108.05	119.60
26	1H	2518	A	C6-C5-N7	-7.70	126.91	132.30
26	14	1302	A	OP1-P-OP2	7.70	131.14	119.60
26	14	74	A	N3-C4-N9	-7.69	121.25	127.40
26	14	2518	A	C6-C5-N7	-7.69	126.92	132.30
26	1H	1763	G	O5'-P-OP2	-7.68	98.78	105.70
26	14	1776	G	N3-C4-N9	7.68	130.61	126.00
27	16	30	C	C6-N1-C2	-7.68	117.23	120.30
26	1H	747	U	O5'-P-OP1	-7.67	98.79	105.70
26	1H	1332	G	N1-C6-O6	7.67	124.50	119.90
26	1H	113	G	N3-C4-N9	-7.67	121.40	126.00
27	16	81	G	C4-C5-N7	7.67	113.87	110.80
1	1G	690	G	N3-C4-C5	7.67	132.43	128.60
26	1H	1778	U	O5'-P-OP1	-7.66	98.80	105.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	795	C	C5-C6-N1	-7.66	117.17	121.00
26	1H	797	C	C5-C6-N1	-7.66	117.17	121.00
26	1H	512	G	O4'-C1'-N9	7.66	114.33	108.20
26	14	2324	C	C6-N1-C2	7.65	123.36	120.30
26	14	1142	U	C2-N1-C1'	7.65	126.88	117.70
26	1H	841	A	O5'-P-OP2	-7.65	98.81	105.70
26	1H	1437	C	N3-C2-O2	-7.65	116.55	121.90
26	14	2436	G	C5-C6-O6	-7.64	124.02	128.60
26	1H	1349	A	O5'-P-OP1	-7.64	98.82	105.70
26	14	676	A	N3-C4-C5	7.64	132.15	126.80
26	1H	869	G	N1-C6-O6	-7.64	115.32	119.90
26	1H	848	G	O5'-P-OP2	-7.64	98.83	105.70
26	14	1162	G	O5'-P-OP1	-7.63	98.83	105.70
26	1H	508	G	N7-C8-N9	7.63	116.92	113.10
26	14	530	G	C5-N7-C8	-7.63	100.48	104.30
26	1H	330	A	C2-N3-C4	-7.63	106.78	110.60
26	1H	774	A	N1-C6-N6	7.63	123.18	118.60
1	13	330	C	N3-C2-O2	-7.63	116.56	121.90
26	14	929	G	C6-C5-N7	-7.62	125.83	130.40
26	14	752	A	P-O3'-C3'	7.62	128.84	119.70
26	1H	1673	U	C5-C6-N1	-7.62	118.89	122.70
26	1H	138	G	N7-C8-N9	7.62	116.91	113.10
1	1G	1286	A	N7-C8-N9	7.62	117.61	113.80
26	14	1616	A	N1-C6-N6	7.62	123.17	118.60
26	14	2066	C	OP1-P-O3'	7.61	121.94	105.20
26	1H	2837	G	C5-N7-C8	-7.61	100.50	104.30
26	14	2490	G	C8-N9-C4	-7.61	103.36	106.40
26	14	1762	A	C5-C6-N1	-7.61	113.90	117.70
26	14	2079	U	O5'-P-OP1	-7.60	98.86	105.70
26	14	2565	A	O5'-P-OP2	7.60	119.82	110.70
26	1H	1314	C	C2-N1-C1'	7.60	127.16	118.80
26	1H	966	G	C5-C6-O6	7.60	133.16	128.60
1	1G	449	C	C6-N1-C2	-7.60	117.26	120.30
26	14	2873	A	C4-C5-N7	7.60	114.50	110.70
27	1J	89	G	O5'-P-OP2	-7.60	98.86	105.70
26	1H	130	C	C5-C4-N4	-7.58	114.89	120.20
26	1H	410	G	N1-C6-O6	7.58	124.45	119.90
26	14	2401	U	C5-C6-N1	7.58	126.49	122.70
26	14	1303	G	C5-C6-O6	7.58	133.15	128.60
26	1H	36	G	O5'-P-OP2	-7.57	98.89	105.70
26	14	1826	G	C4-C5-N7	-7.57	107.77	110.80
26	1H	774	A	C4-N9-C1'	-7.57	112.68	126.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	1998	G	C8-N9-C4	7.57	109.43	106.40
26	1H	2390	U	O5'-P-OP1	-7.56	98.89	105.70
26	1H	1602	U	O5'-P-OP2	7.56	119.77	110.70
26	14	1786	A	N1-C2-N3	7.56	133.08	129.30
24	3K	76	A	C6-C5-N7	-7.55	127.01	132.30
26	1H	2498	C	N3-C4-C5	7.54	124.92	121.90
26	14	71	A	C2-N3-C4	-7.54	106.83	110.60
26	14	1559	G	C6-C5-N7	-7.54	125.88	130.40
1	13	802	A	N1-C6-N6	7.54	123.12	118.60
26	14	1616	A	O4'-C1'-N9	7.53	114.23	108.20
26	14	788	A	C6-C5-N7	-7.53	127.03	132.30
1	13	328	C	N1-C2-O2	7.53	123.42	118.90
26	1H	951	C	N3-C4-N4	-7.53	112.73	118.00
26	1H	2275	C	OP1-P-O3'	7.53	121.76	105.20
26	1H	2287	A	C5-N7-C8	-7.52	100.14	103.90
26	1H	1698	A	O4'-C1'-N9	7.52	114.22	108.20
27	1J	6	C	C6-N1-C2	7.52	123.31	120.30
1	13	509	A	P-O3'-C3'	7.51	128.72	119.70
1	13	853	G	N1-C6-O6	7.51	124.41	119.90
26	14	2287	A	N3-C4-C5	7.51	132.06	126.80
1	13	1279	A	N7-C8-N9	7.50	117.55	113.80
26	14	1304	C	N3-C4-N4	-7.50	112.75	118.00
1	13	108	G	C4-C5-N7	7.50	113.80	110.80
22	1K	76	A	O4'-C1'-N9	7.50	114.20	108.20
26	1H	371	A	O5'-P-OP2	-7.49	98.96	105.70
26	1H	1695	G	OP1-P-OP2	7.49	130.83	119.60
26	1H	451	C	N3-C2-O2	7.49	127.14	121.90
26	14	1993	U	O5'-P-OP1	-7.49	98.96	105.70
26	14	252	G	O5'-P-OP1	7.48	119.68	110.70
26	14	2598	A	C8-N9-C4	7.48	108.79	105.80
26	1H	140	A	O4'-C1'-N9	7.48	114.18	108.20
24	3L	76	A	O4'-C1'-N9	7.47	114.18	108.20
26	14	2838	G	N1-C6-O6	7.47	124.38	119.90
26	1H	929	G	C6-C5-N7	-7.47	125.92	130.40
26	1H	2298	A	O5'-P-OP2	-7.47	98.98	105.70
27	16	81	G	C5-N7-C8	-7.47	100.56	104.30
26	1H	1430	C	OP1-P-O3'	7.46	121.62	105.20
26	14	71	A	N1-C6-N6	7.46	123.08	118.60
26	14	1762	A	C2-N3-C4	-7.46	106.87	110.60
26	1H	451	C	O5'-P-OP2	-7.46	98.99	105.70
26	1H	621	A	N1-C2-N3	7.46	133.03	129.30
26	1H	1142(A)	A	N3-C4-C5	7.46	132.02	126.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	14	2211	G	C4-N9-C1'	7.46	136.20	126.50
26	1H	2713	A	C2-N3-C4	-7.46	106.87	110.60
26	14	613	U	C5-C4-O4	7.46	130.37	125.90
26	14	140	A	N1-C6-N6	7.45	123.07	118.60
26	14	2873	A	C8-N9-C4	-7.45	102.82	105.80
26	1H	1678	G	C5-C6-N1	-7.45	107.78	111.50
24	3L	5	C	C6-N1-C2	-7.45	117.32	120.30
26	1H	2507	C	N3-C2-O2	-7.44	116.69	121.90
26	1H	226	G	O4'-C1'-N9	7.44	114.15	108.20
26	1H	2689	U	C5-C6-N1	7.44	126.42	122.70
26	14	2244	U	N1-C2-N3	7.43	119.36	114.90
26	14	2591	C	N1-C2-O2	-7.43	114.44	118.90
26	14	2490	G	C4-C5-N7	7.43	113.77	110.80
26	14	2873	A	C5-C6-N1	-7.43	113.99	117.70
26	14	528	A	N3-C4-C5	7.43	132.00	126.80
26	1H	783	A	C5-C6-N1	-7.42	113.99	117.70
26	1H	2264	C	OP1-P-O3'	7.42	121.54	105.20
26	14	786	C	N3-C4-C5	7.42	124.87	121.90
26	1H	2439	A	O5'-P-OP2	-7.42	99.02	105.70
26	1H	1784	A	O4'-C1'-N9	-7.42	102.26	108.20
26	1H	1295	C	N1-C2-O2	-7.42	114.45	118.90
37	78	61	ARG	NE-CZ-NH1	7.42	124.01	120.30
26	1H	673	C	N3-C4-N4	7.42	123.19	118.00
26	1H	1930	G	O5'-P-OP1	-7.42	99.03	105.70
26	1H	1544	C	N1-C2-O2	7.41	123.34	118.90
26	1H	195	A	P-O3'-C3'	7.40	128.58	119.70
26	1H	2700	C	C5-C4-N4	-7.40	115.02	120.20
26	14	2448	A	O5'-P-OP1	-7.39	99.05	105.70
26	14	1348	G	O5'-P-OP2	7.39	119.57	110.70
26	14	1899	G	N7-C8-N9	7.39	116.79	113.10
26	1H	951	C	N1-C2-O2	7.38	123.33	118.90
26	1H	1496	A	C4-C5-N7	7.38	114.39	110.70
26	1H	2441	C	N3-C4-N4	-7.38	112.83	118.00
26	1H	2387	U	OP2-P-O3'	7.38	121.44	105.20
26	14	624	C	O5'-P-OP1	-7.38	99.06	105.70
26	14	1796	U	O5'-P-OP2	7.38	119.56	110.70
26	1H	1790	C	N3-C4-C5	7.38	124.85	121.90
26	1H	2623	G	N1-C6-O6	-7.38	115.47	119.90
26	14	140	A	C8-N9-C4	-7.38	102.85	105.80
26	1H	1261	C	C2-N3-C4	-7.38	116.21	119.90
1	13	892	A	N1-C6-N6	7.37	123.02	118.60
26	14	2335	A	O4'-C1'-N9	7.37	114.09	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	14	2688	U	C5-C4-O4	7.37	130.32	125.90
1	1G	909	A	N1-C6-N6	7.36	123.02	118.60
26	14	330	A	N1-C6-N6	7.36	123.02	118.60
26	14	621	A	C8-N9-C4	-7.36	102.86	105.80
26	14	102	G	O4'-C1'-N9	7.35	114.08	108.20
26	14	205	G	OP1-P-OP2	7.35	130.62	119.60
26	14	707	G	C5-C6-N1	-7.34	107.83	111.50
26	1H	1681	G	N3-C4-C5	7.34	132.27	128.60
26	1H	1698	A	N7-C8-N9	7.34	117.47	113.80
26	14	569	U	C2-N3-C4	-7.34	122.60	127.00
26	1H	1321	A	C8-N9-C4	7.33	108.73	105.80
26	1H	1559	G	N1-C6-O6	7.33	124.30	119.90
27	16	13	A	OP1-P-OP2	7.33	130.59	119.60
26	1H	945	A	C5-C6-N1	-7.32	114.04	117.70
26	1H	1239	G	C8-N9-C4	7.32	109.33	106.40
26	14	463	G	O5'-P-OP2	-7.32	99.11	105.70
26	1H	2040	C	C6-N1-C2	7.32	123.23	120.30
1	1G	690	G	N3-C4-N9	-7.32	121.61	126.00
26	14	2335	A	N1-C6-N6	-7.32	114.21	118.60
1	13	562	C	O5'-P-OP2	-7.31	99.12	105.70
26	14	1307	A	C2-N3-C4	-7.31	106.94	110.60
1	13	896	C	C5-C6-N1	-7.31	117.35	121.00
1	1G	1502	A	O5'-P-OP2	-7.31	99.12	105.70
26	14	774	A	N3-C4-N9	-7.30	121.56	127.40
26	14	1777	U	OP2-P-O3'	7.30	121.27	105.20
26	1H	733	G	N1-C6-O6	7.30	124.28	119.90
26	1H	796	C	N3-C4-N4	-7.30	112.89	118.00
26	14	1341	U	O5'-P-OP1	-7.30	99.13	105.70
22	1K	76	A	C8-N9-C4	-7.29	102.88	105.80
26	14	1253	A	C8-N9-C4	7.29	108.72	105.80
26	1H	508	G	C4-N9-C1'	7.29	135.97	126.50
26	1H	839	U	O5'-P-OP2	-7.29	99.14	105.70
26	14	1786	A	N9-C1'-C2'	7.29	123.47	114.00
26	1H	324	A	O5'-P-OP1	-7.28	99.15	105.70
1	1G	1286	A	C8-N9-C4	-7.28	102.89	105.80
26	1H	2446	G	C4-C5-N7	7.28	113.71	110.80
26	1H	797	C	N1-C2-O2	-7.28	114.53	118.90
26	1H	864	G	C2-N3-C4	7.27	115.54	111.90
26	1H	1789	A	O5'-P-OP2	-7.26	99.16	105.70
27	16	85	G	O5'-P-OP2	-7.26	99.16	105.70
26	14	2009	G	O5'-P-OP2	-7.26	99.16	105.70
49	J8	95	LEU	CA-CB-CG	7.26	132.00	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	14	1826	G	C5-N7-C8	7.26	107.93	104.30
26	1H	838	C	N1-C2-O2	-7.26	114.55	118.90
26	14	801	G	N1-C6-O6	-7.26	115.55	119.90
26	14	2032	G	N7-C8-N9	-7.25	109.47	113.10
26	1H	462	C	O5'-P-OP2	-7.25	99.18	105.70
26	1H	576	U	OP2-P-O3'	7.25	121.14	105.20
26	1H	594	U	C5-C6-N1	-7.25	119.08	122.70
26	1H	860	U	N3-C2-O2	-7.25	117.13	122.20
26	14	2352	A	O5'-P-OP1	-7.24	99.18	105.70
26	1H	141	A	C4-C5-N7	7.24	114.32	110.70
26	1H	2513	G	C8-N9-C4	-7.24	103.50	106.40
26	14	1566	A	N9-C4-C5	-7.24	102.90	105.80
26	14	2452	C	OP1-P-OP2	7.24	130.46	119.60
26	1H	1021	A	N1-C2-N3	7.24	132.92	129.30
26	14	613	U	N3-C2-O2	-7.24	117.14	122.20
26	1H	844	C	N1-C2-O2	-7.23	114.56	118.90
26	1H	2700	C	N3-C4-C5	7.23	124.79	121.90
26	14	2210	G	C4-N9-C1'	7.23	135.90	126.50
22	1K	76	A	N7-C8-N9	7.23	117.42	113.80
26	14	797	C	N1-C2-O2	-7.23	114.56	118.90
26	1H	2277	G	C4-C5-N7	-7.22	107.91	110.80
26	14	1807	G	C5-C6-O6	-7.22	124.27	128.60
26	1H	1698	A	C4-C5-N7	7.22	114.31	110.70
26	1H	2211	G	O5'-P-OP2	-7.22	99.20	105.70
26	1H	774	A	C4-C5-C6	-7.21	113.39	117.00
26	14	1902	C	N3-C4-C5	7.21	124.79	121.90
26	14	1559	G	N1-C6-O6	7.21	124.23	119.90
26	1H	1614	A	O5'-P-OP1	-7.20	99.22	105.70
26	1H	2438	U	C2-N3-C4	-7.20	122.68	127.00
26	1H	1517	G	OP1-P-O3'	7.20	121.04	105.20
26	1H	2402	C	N1-C2-O2	7.20	123.22	118.90
26	1H	189	G	C4-C5-N7	7.20	113.68	110.80
26	14	2473	U	C2-N1-C1'	7.20	126.33	117.70
26	1H	2001	A	C2-N3-C4	7.19	114.20	110.60
1	1G	519	C	C6-N1-C2	7.19	123.17	120.30
1	1G	690	G	C8-N9-C4	-7.18	103.53	106.40
26	14	1566	A	C5-C6-N6	-7.18	117.95	123.70
26	14	2873	A	C4-N9-C1'	7.18	139.23	126.30
26	1H	74	A	C5-N7-C8	-7.18	100.31	103.90
1	13	1279	A	C8-N9-C4	-7.18	102.93	105.80
26	1H	733	G	C6-C5-N7	-7.18	126.09	130.40
26	14	2392	A	C5-C6-N1	-7.17	114.11	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	3K	76	A	C8-N9-C4	-7.17	102.93	105.80
24	3L	76	A	N7-C8-N9	7.17	117.38	113.80
26	1H	2430	A	C5-N7-C8	-7.16	100.32	103.90
26	14	621	A	C5-N7-C8	-7.16	100.32	103.90
26	1H	794	G	N3-C4-C5	-7.16	125.02	128.60
26	1H	2232	U	C5-C4-O4	7.15	130.19	125.90
26	14	2596	U	O5'-P-OP2	-7.15	99.26	105.70
26	14	1950	G	C4-C5-N7	7.15	113.66	110.80
26	14	2498	C	C6-N1-C2	7.15	123.16	120.30
26	14	2681	C	N3-C4-N4	-7.15	113.00	118.00
26	1H	967	C	C5-C6-N1	-7.15	117.42	121.00
26	14	1313	U	C6-N1-C2	-7.15	116.71	121.00
26	1H	750	A	OP2-P-O3'	7.15	120.93	105.20
26	1H	1574	C	C6-N1-C2	7.14	123.16	120.30
26	14	783	A	N3-C4-C5	7.14	131.80	126.80
26	1H	245	G	N1-C6-O6	7.14	124.19	119.90
26	1H	1557	C	O5'-P-OP2	-7.14	99.27	105.70
26	14	330	A	N1-C2-N3	7.13	132.87	129.30
26	14	642	G	N7-C8-N9	7.13	116.67	113.10
26	1H	1324	G	C5-C6-O6	-7.13	124.32	128.60
26	1H	1616	A	C8-N9-C4	-7.13	102.95	105.80
26	14	1394	U	O5'-P-OP2	7.13	119.26	110.70
26	14	2575	C	N3-C4-C5	-7.13	119.05	121.90
26	14	783	A	N1-C2-N3	7.12	132.86	129.30
26	1H	2509	G	N1-C6-O6	-7.12	115.63	119.90
26	14	945	A	C5-C6-N1	-7.12	114.14	117.70
26	14	2330	G	N1-C6-O6	7.11	124.17	119.90
26	14	2267	A	OP1-P-OP2	7.11	130.27	119.60
26	14	783	A	C5-C6-N6	-7.11	118.01	123.70
26	1H	845	G	P-O3'-C3'	7.11	128.23	119.70
26	1H	121	G	C5-C6-N1	7.10	115.05	111.50
26	1H	2245	U	OP1-P-OP2	-7.10	108.95	119.60
26	14	2838	G	C5-C6-O6	-7.10	124.34	128.60
26	1H	728	G	C8-N9-C4	7.10	109.24	106.40
27	16	41	U	C5-C6-N1	-7.10	119.15	122.70
26	1H	2688	U	N3-C4-O4	-7.09	114.43	119.40
26	14	1965	C	N3-C4-C5	7.09	124.74	121.90
26	14	1408	C	N1-C2-O2	-7.09	114.64	118.90
26	1H	1395	A	O5'-P-OP2	-7.09	99.32	105.70
26	14	946	G	N1-C6-O6	7.09	124.16	119.90
26	14	2392	A	N7-C8-N9	7.09	117.35	113.80
26	14	808	G	N1-C2-N2	-7.09	109.82	116.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	13	523	A	N1-C6-N6	7.08	122.85	118.60
26	14	703	U	C5-C4-O4	7.08	130.15	125.90
26	1H	124	G	N1-C2-N2	7.08	122.57	116.20
26	14	2425	A	O4'-C1'-N9	7.08	113.87	108.20
26	14	74	A	C5-N7-C8	-7.08	100.36	103.90
1	13	529	G	N1-C6-O6	7.08	124.15	119.90
26	1H	2254	C	N1-C2-O2	-7.08	114.65	118.90
26	14	34	C	C2-N1-C1'	7.07	126.58	118.80
26	14	2426	A	N9-C4-C5	-7.07	102.97	105.80
1	13	1502	A	C2-N3-C4	-7.07	107.06	110.60
48	I8	81	VAL	C-N-CA	-7.07	104.03	121.70
26	1H	74	A	N7-C8-N9	7.06	117.33	113.80
26	1H	744	G	O5'-P-OP2	-7.06	99.34	105.70
26	1H	865	C	O5'-P-OP2	7.06	119.17	110.70
26	1H	2490	G	O4'-C1'-N9	7.06	113.85	108.20
1	13	974	A	C5-C6-N6	-7.06	118.05	123.70
1	13	1354	C	C6-N1-C2	-7.06	117.48	120.30
26	1H	788	A	N9-C4-C5	-7.06	102.98	105.80
26	1H	2070	G	N1-C2-N2	-7.05	109.85	116.20
26	1H	2270	G	C8-N9-C4	7.05	109.22	106.40
26	1H	2713	A	C6-C5-N7	-7.05	127.37	132.30
26	14	1907	G	O5'-P-OP1	-7.05	99.36	105.70
26	14	632	A	O5'-P-OP2	7.05	119.16	110.70
26	1H	755	C	N3-C4-C5	-7.04	119.08	121.90
1	1G	1322	C	N1-C2-O2	7.04	123.12	118.90
26	14	1315	C	N3-C4-N4	-7.04	113.07	118.00
1	13	975	A	N1-C6-N6	7.04	122.82	118.60
26	1H	860	U	C2-N1-C1'	7.04	126.15	117.70
26	1H	2318	G	N7-C8-N9	7.04	116.62	113.10
26	14	1566	A	C4-C5-N7	7.04	114.22	110.70
26	1H	1786	A	N9-C1'-C2'	7.04	123.15	114.00
27	16	115	G	C4-C5-N7	7.04	113.61	110.80
26	1H	999	U	O5'-P-OP2	7.03	119.14	110.70
26	1H	1241	A	C5-C6-N1	-7.03	114.18	117.70
26	1H	125	G	C4-C5-N7	7.03	113.61	110.80
26	14	1698	A	N7-C8-N9	7.03	117.31	113.80
26	1H	1332	G	C6-C5-N7	-7.03	126.18	130.40
26	1H	825	C	N1-C2-O2	-7.02	114.69	118.90
1	13	422	C	P-O3'-C3'	7.02	128.12	119.70
1	13	892	A	C2-N3-C4	-7.02	107.09	110.60
26	14	843	G	N1-C6-O6	7.02	124.11	119.90
26	1H	1365	A	N9-C4-C5	7.02	108.61	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	853	G	O5'-P-OP2	-7.01	99.39	105.70
26	1H	2256	G	O5'-P-OP1	7.01	119.12	110.70
26	14	2092	U	N3-C4-O4	-7.01	114.49	119.40
26	14	2270	G	C5-C6-O6	-7.01	124.39	128.60
26	1H	2550	G	C8-N9-C4	-7.01	103.60	106.40
26	14	1404	C	O5'-P-OP2	-7.01	99.39	105.70
26	14	312	G	O5'-P-OP1	-7.01	99.39	105.70
26	14	2779	U	N3-C2-O2	-7.00	117.30	122.20
26	1H	1996	C	C6-N1-C2	7.00	123.10	120.30
26	14	137	C	C6-N1-C2	-7.00	117.50	120.30
26	14	1899	G	N1-C2-N3	7.00	128.10	123.90
26	14	1653	G	O5'-P-OP2	-7.00	99.40	105.70
26	1H	1297	C	OP1-P-O3'	7.00	120.60	105.20
26	1H	2708	G	C8-N9-C4	7.00	109.20	106.40
50	K8	35	LEU	CA-CB-CG	7.00	131.39	115.30
26	1H	2712	U	N1-C2-N3	6.99	119.10	114.90
1	1G	1401	G	C4-N9-C1'	6.99	135.59	126.50
26	14	827	U	N3-C2-O2	6.99	127.09	122.20
26	14	1644	C	N3-C2-O2	-6.99	117.01	121.90
26	1H	686	G	C8-N9-C4	6.99	109.19	106.40
26	1H	738	G	C5-C6-O6	-6.99	124.41	128.60
1	1G	784	C	C6-N1-C2	6.99	123.09	120.30
26	14	2281	C	C6-N1-C2	-6.99	117.51	120.30
26	1H	1249	U	O5'-P-OP1	-6.98	99.42	105.70
26	1H	2331	G	N3-C4-C5	6.98	132.09	128.60
26	1H	2712	U	C5-C4-O4	6.98	130.09	125.90
26	1H	1352	U	O5'-P-OP1	6.98	119.07	110.70
1	1G	136	C	O5'-P-OP2	-6.98	99.42	105.70
26	1H	795	C	C2-N3-C4	-6.98	116.41	119.90
26	14	2296	U	C5-C6-N1	6.98	126.19	122.70
1	13	353	A	C8-N9-C4	-6.97	103.01	105.80
26	1H	1257	C	C4-C5-C6	6.97	120.89	117.40
26	14	1762	A	N1-C2-N3	6.97	132.78	129.30
26	14	1678	G	N3-C4-C5	6.97	132.08	128.60
26	1H	1955	U	C2-N3-C4	-6.96	122.82	127.00
26	14	802	A	C5-C6-N1	6.96	121.18	117.70
26	14	1698	A	C2-N3-C4	-6.96	107.12	110.60
26	14	2501	C	C2-N1-C1'	-6.96	111.14	118.80
26	14	2575	C	C5-C4-N4	6.96	125.07	120.20
26	1H	1817	G	N1-C6-O6	-6.96	115.72	119.90
27	16	115	G	C5-C6-N1	6.96	114.98	111.50
26	1H	124	G	N3-C4-C5	6.96	132.08	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	1559	G	N3-C4-C5	6.96	132.08	128.60
26	1H	239	U	C5-C6-N1	-6.96	119.22	122.70
33	51	153	LYS	C-N-CD	-6.96	105.30	120.60
1	1G	413	G	C4-N9-C1'	-6.96	117.46	126.50
26	1H	193	U	N1-C2-O2	-6.95	117.93	122.80
26	14	970	C	N1-C2-O2	-6.95	114.73	118.90
1	13	974	A	C5-N7-C8	-6.95	100.42	103.90
26	1H	400	G	N1-C6-O6	6.95	124.07	119.90
26	14	1824	G	C8-N9-C4	-6.95	103.62	106.40
26	1H	917	A	C5-C6-N1	-6.95	114.22	117.70
26	1H	2084	C	C2-N3-C4	-6.95	116.42	119.90
26	1H	1817	G	C5-C6-O6	6.95	132.77	128.60
1	1G	413	G	O4'-C1'-N9	6.95	113.76	108.20
27	1J	60	C	C6-N1-C2	-6.95	117.52	120.30
1	13	346	G	N7-C8-N9	6.95	116.57	113.10
26	1H	1379	A	C5-N7-C8	-6.95	100.43	103.90
1	1G	380	G	N3-C4-N9	-6.95	121.83	126.00
1	1G	950	U	O5'-P-OP2	6.95	119.04	110.70
26	14	2331	G	C5-C6-O6	-6.95	124.43	128.60
1	13	963	G	N1-C6-O6	-6.94	115.73	119.90
26	1H	207	A	C2-N3-C4	-6.94	107.13	110.60
1	1G	27	G	N1-C6-O6	6.94	124.06	119.90
1	1G	576	G	C4-N9-C1'	6.94	135.52	126.50
1	13	254	G	O5'-P-OP1	-6.94	99.46	105.70
26	1H	576	U	N1-C2-O2	6.94	127.66	122.80
26	1H	2311	A	C5-N7-C8	-6.94	100.43	103.90
1	13	585	G	O5'-P-OP2	-6.93	99.46	105.70
1	13	690	G	C4-C5-N7	6.93	113.57	110.80
26	14	2003	G	C5-C6-O6	-6.93	124.44	128.60
26	14	2443	C	O5'-P-OP2	6.93	119.02	110.70
26	14	2573	C	C2-N1-C1'	6.93	126.43	118.80
26	1H	794	G	C4-C5-N7	-6.93	108.03	110.80
26	1H	1310	G	O5'-P-OP2	6.93	119.02	110.70
26	1H	1621	U	N3-C4-O4	6.93	124.25	119.40
26	14	1332	G	N1-C6-O6	6.93	124.06	119.90
26	14	1968	G	C5-N7-C8	-6.93	100.84	104.30
1	13	843	U	C2-N1-C1'	6.93	126.01	117.70
26	1H	263	C	O5'-P-OP2	-6.93	99.46	105.70
26	1H	955	C	OP1-P-OP2	6.92	129.99	119.60
26	14	207	A	C8-N9-C4	6.92	108.57	105.80
26	1H	1574	C	OP2-P-O3'	6.92	120.43	105.20
26	1H	202	U	N3-C4-C5	6.92	118.75	114.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	860	U	C2-N3-C4	-6.92	122.85	127.00
26	1H	1610	A	C5-C6-N6	-6.92	118.17	123.70
26	1H	1827	C	C4-C5-C6	6.91	120.86	117.40
26	1H	1313	U	C6-N1-C2	-6.91	116.86	121.00
26	14	575	A	O5'-P-OP1	-6.91	99.48	105.70
26	1H	132	G	C5-C6-O6	6.91	132.74	128.60
26	1H	739	G	N1-C6-O6	6.91	124.04	119.90
26	14	528	A	N3-C4-N9	-6.91	121.88	127.40
26	1H	2503	A	N9-C4-C5	-6.90	103.04	105.80
26	14	74	A	N1-C2-N3	6.90	132.75	129.30
26	1H	1543	A	C2-N3-C4	-6.90	107.15	110.60
26	14	2685	G	N3-C2-N2	-6.90	115.07	119.90
26	1H	1021	A	C8-N9-C4	-6.89	103.04	105.80
25	4L	23	A	OP1-P-O3'	6.89	120.37	105.20
26	14	2346	A	C2-N3-C4	-6.89	107.15	110.60
26	1H	1790	C	C2-N3-C4	-6.89	116.45	119.90
26	1H	1241	A	C2-N3-C4	-6.89	107.16	110.60
26	1H	2287	A	N3-C4-N9	-6.89	121.89	127.40
26	1H	2370	G	N1-C6-O6	-6.89	115.77	119.90
26	14	2433	A	N1-C6-N6	6.89	122.73	118.60
26	1H	954	G	N3-C2-N2	-6.88	115.08	119.90
26	1H	946	G	C8-N9-C4	6.88	109.15	106.40
26	1H	2598	A	N9-C4-C5	-6.88	103.05	105.80
26	1H	2609	U	C6-N1-C2	6.88	125.13	121.00
26	14	510	C	OP1-P-OP2	6.88	129.92	119.60
26	1H	1395	A	OP1-P-OP2	6.88	129.91	119.60
26	14	2275	C	P-O3'-C3'	6.87	127.94	119.70
1	1G	547	A	C8-N9-C4	6.87	108.55	105.80
40	65	110	LEU	CA-CB-CG	6.87	131.10	115.30
1	13	49	U	P-O3'-C3'	6.87	127.94	119.70
26	1H	631	A	N7-C8-N9	-6.87	110.37	113.80
26	1H	2618	G	N9-C4-C5	6.86	108.14	105.40
26	14	856	C	C6-N1-C2	-6.86	117.55	120.30
26	14	2066	C	C5-C4-N4	-6.86	115.39	120.20
37	78	50	ARG	NE-CZ-NH2	6.86	123.73	120.30
26	14	148	C	C6-N1-C2	6.86	123.04	120.30
26	1H	148	C	C2-N3-C4	-6.86	116.47	119.90
26	14	1989	G	C5-C6-O6	-6.86	124.48	128.60
26	1H	37	C	C5-C4-N4	6.86	125.00	120.20
26	1H	1185	C	O5'-P-OP2	-6.86	99.53	105.70
26	1H	1842	G	N1-C6-O6	-6.86	115.78	119.90
26	14	2211	G	C8-N9-C1'	-6.86	118.08	127.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	1373	A	O5'-P-OP1	6.86	118.93	110.70
26	14	750	A	C8-N9-C4	-6.85	103.06	105.80
26	1H	792	G	O4'-C1'-N9	-6.85	102.72	108.20
1	13	703	G	C6-C5-N7	-6.85	126.29	130.40
26	1H	825	C	C5-C4-N4	-6.84	115.41	120.20
26	1H	1428	C	O5'-P-OP1	-6.84	99.54	105.70
26	14	2092	U	N3-C2-O2	-6.84	117.41	122.20
26	14	509	C	C4-C5-C6	6.84	120.82	117.40
26	1H	2713	A	N1-C6-N6	6.84	122.70	118.60
26	14	1342	A	O4'-C1'-N9	6.84	113.67	108.20
1	13	1502	A	C4-C5-N7	6.84	114.12	110.70
26	1H	508	G	N3-C4-C5	-6.84	125.18	128.60
26	1H	1325	G	C5-C6-O6	-6.84	124.50	128.60
26	1H	2586	C	C2-N3-C4	-6.84	116.48	119.90
26	14	1303	G	N1-C6-O6	-6.84	115.80	119.90
26	1H	2598	A	N1-C6-N6	6.83	122.70	118.60
26	1H	2346	A	C5-N7-C8	-6.83	100.48	103.90
26	14	1600	C	O5'-P-OP2	-6.83	99.55	105.70
26	1H	1528	A	O4'-C1'-N9	6.83	113.66	108.20
26	1H	838	C	C2-N3-C4	-6.83	116.49	119.90
26	1H	1574	C	C5-C6-N1	-6.83	117.59	121.00
26	1H	1798	U	N3-C4-C5	6.82	118.69	114.60
26	1H	2648	C	C6-N1-C2	6.82	123.03	120.30
26	1H	862	G	C5-C6-O6	6.82	132.69	128.60
1	1G	413	G	C6-C5-N7	6.82	134.49	130.40
1	1G	481	G	C6-C5-N7	-6.82	126.31	130.40
26	14	2429	G	O5'-P-OP2	-6.82	99.56	105.70
26	1H	1298	C	OP1-P-O3'	6.82	120.20	105.20
26	1H	1300	U	N1-C2-N3	6.82	118.99	114.90
26	1H	1767	C	O5'-P-OP1	-6.82	99.56	105.70
26	1H	695	G	N3-C2-N2	6.82	124.67	119.90
26	1H	1142(A)	A	C5-C6-N1	-6.81	114.29	117.70
27	16	44	G	C8-N9-C1'	6.81	135.86	127.00
26	14	1939	U	OP2-P-O3'	6.81	120.19	105.20
26	14	2032	G	C5-N7-C8	6.81	107.71	104.30
26	14	2352	A	N1-C2-N3	6.81	132.71	129.30
26	1H	576	U	C5-C6-N1	-6.81	119.30	122.70
26	14	855	G	C8-N9-C4	-6.81	103.68	106.40
26	14	2542	A	C8-N9-C4	6.81	108.52	105.80
26	1H	2593	U	N3-C2-O2	-6.80	117.44	122.20
26	1H	240	G	C5-C6-N1	6.80	114.90	111.50
26	1H	672	C	OP2-P-O3'	6.80	120.16	105.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	1022	G	N3-C2-N2	-6.80	115.14	119.90
26	1H	190	A	N1-C2-N3	-6.80	125.90	129.30
1	13	703	G	N1-C6-O6	6.80	123.98	119.90
26	1H	2507	C	N1-C2-O2	6.80	122.98	118.90
26	1H	2037	G	N1-C6-O6	-6.79	115.82	119.90
26	14	2313	C	C6-N1-C2	-6.79	117.58	120.30
1	13	1434	A	C8-N9-C4	6.79	108.52	105.80
26	14	732	C	N1-C2-O2	-6.79	114.83	118.90
1	1G	990	C	C6-N1-C2	-6.78	117.59	120.30
27	16	44	G	P-O3'-C3'	6.78	127.83	119.70
26	1H	1565	C	N3-C4-C5	6.78	124.61	121.90
26	1H	2712	U	C5-C6-N1	-6.78	119.31	122.70
26	1H	1429	G	C5-C6-O6	6.77	132.66	128.60
26	1H	733	G	C4-C5-C6	6.77	122.86	118.80
26	1H	752	A	N9-C4-C5	-6.77	103.09	105.80
26	1H	1404	C	OP1-P-OP2	6.77	129.76	119.60
26	14	694	U	O5'-P-OP1	6.77	118.82	110.70
26	1H	2235	G	N1-C6-O6	6.77	123.96	119.90
26	14	2249	U	N3-C4-C5	-6.77	110.54	114.60
1	13	449	C	C2-N1-C1'	6.77	126.24	118.80
26	14	571	A	N1-C6-N6	6.76	122.66	118.60
26	14	751	A	O5'-P-OP1	-6.76	99.61	105.70
26	1H	2441	C	N1-C2-O2	6.76	122.96	118.90
26	1H	1558	A	N1-C2-N3	6.76	132.68	129.30
46	G8	81	LYS	C-N-CA	6.76	150.37	122.00
26	1H	1598	C	OP1-P-O3'	6.75	120.06	105.20
26	1H	265	A	N7-C8-N9	6.75	117.17	113.80
26	1H	698	C	C5-C6-N1	-6.75	117.62	121.00
26	1H	1023	U	O5'-P-OP1	-6.75	99.63	105.70
26	14	1313	U	C2-N1-C1'	6.75	125.80	117.70
26	1H	1300	U	C2-N3-C4	-6.74	122.95	127.00
26	1H	2544	G	N1-C6-O6	6.74	123.94	119.90
26	14	2453	A	N1-C6-N6	6.74	122.64	118.60
26	1H	140	A	OP2-P-O3'	6.74	120.02	105.20
26	14	1440	G	O5'-P-OP2	-6.74	99.64	105.70
26	14	2688	U	C5-C6-N1	-6.74	119.33	122.70
26	1H	756	C	C6-N1-C2	-6.74	117.61	120.30
23	2K	6	G	N9-C4-C5	-6.73	102.71	105.40
26	1H	1363	C	N3-C4-N4	-6.73	113.29	118.00
26	1H	621	A	C5-C6-N1	-6.73	114.34	117.70
1	1G	266	G	P-O3'-C3'	6.73	127.78	119.70
26	1H	831	G	C8-N9-C4	6.73	109.09	106.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	13	798	G	N1-C6-O6	6.72	123.94	119.90
26	1H	696	G	C5-C6-N1	6.72	114.86	111.50
27	16	99	A	C8-N9-C4	-6.72	103.11	105.80
26	14	1762	A	C6-C5-N7	-6.72	127.59	132.30
26	14	2248	C	N1-C2-O2	6.72	122.93	118.90
26	1H	1621	U	N1-C2-O2	-6.72	118.09	122.80
26	14	2681	C	C5-C4-N4	6.72	124.91	120.20
37	78	15	ARG	C-N-CA	6.72	138.50	121.70
26	14	933	A	C5-N7-C8	-6.72	100.54	103.90
26	14	2510	C	C5-C6-N1	-6.72	117.64	121.00
26	14	1328	G	C5-C6-O6	-6.72	124.57	128.60
26	1H	2070	G	N3-C2-N2	6.72	124.60	119.90
26	14	1973	G	N3-C2-N2	6.72	124.60	119.90
26	1H	245	G	C6-C5-N7	-6.71	126.37	130.40
26	1H	1558	A	C2-N3-C4	-6.71	107.25	110.60
26	1H	1817	G	N3-C2-N2	6.71	124.60	119.90
26	14	1279	G	O5'-P-OP2	-6.71	99.66	105.70
26	1H	783	A	N9-C1'-C2'	-6.71	104.62	112.00
26	14	467	G	O5'-P-OP2	-6.71	99.67	105.70
26	1H	906	G	N3-C4-N9	-6.70	121.98	126.00
26	1H	1253	A	N7-C8-N9	-6.70	110.45	113.80
26	1H	2540	C	N3-C4-N4	-6.70	113.31	118.00
26	1H	1022	G	N3-C4-N9	-6.70	121.98	126.00
26	1H	593	G	O5'-P-OP2	-6.70	99.67	105.70
1	1G	1054	C	OP1-P-OP2	-6.70	109.56	119.60
26	14	1376	C	O5'-P-OP1	-6.69	99.68	105.70
26	1H	2513	G	N7-C8-N9	6.69	116.45	113.10
26	14	2296	U	C6-N1-C1'	-6.69	111.83	121.20
26	1H	2593	U	N3-C4-O4	-6.69	114.72	119.40
26	1H	2682	U	O5'-P-OP2	-6.69	99.68	105.70
27	16	115	G	C5-N7-C8	-6.69	100.95	104.30
26	14	2286	A	N7-C8-N9	6.69	117.14	113.80
26	1H	386	G	C5-C6-O6	-6.69	124.59	128.60
26	1H	1261	C	C5-C6-N1	-6.69	117.66	121.00
26	1H	2244	U	C4-C5-C6	6.69	123.71	119.70
1	13	328	C	C6-N1-C1'	-6.68	112.78	120.80
26	1H	1914	C	N3-C2-O2	-6.68	117.22	121.90
1	1G	254	G	O5'-P-OP1	-6.68	99.69	105.70
1	13	811	C	O5'-P-OP2	-6.68	99.69	105.70
1	13	1502	A	C5-N7-C8	-6.68	100.56	103.90
26	1H	144	C	C5-C6-N1	-6.68	117.66	121.00
26	1H	481	G	O5'-P-OP2	-6.67	99.69	105.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	14	2712	U	C2-N3-C4	-6.67	123.00	127.00
1	13	5	U	C2-N1-C1'	6.67	125.70	117.70
26	1H	1204	A	C5-N7-C8	-6.67	100.56	103.90
26	1H	2609	U	C2-N3-C4	-6.67	123.00	127.00
26	1H	673	C	C5-C4-N4	-6.67	115.53	120.20
26	1H	863	A	O5'-P-OP2	-6.66	99.70	105.70
26	14	2712	U	O4'-C1'-N1	6.66	113.53	108.20
26	1H	197	A	C5-N7-C8	-6.66	100.57	103.90
26	1H	2032	G	N1-C2-N3	6.66	127.89	123.90
26	14	1812	A	OP1-P-OP2	6.66	129.58	119.60
26	14	1992	G	C8-N9-C4	-6.66	103.74	106.40
1	13	990	C	C6-N1-C2	-6.65	117.64	120.30
2	1E	187	LEU	CA-CB-CG	6.65	130.60	115.30
1	13	690	G	C4-C5-C6	6.65	122.79	118.80
26	1H	696	G	C5-C6-O6	-6.65	124.61	128.60
26	1H	141	A	N7-C8-N9	6.65	117.12	113.80
26	14	1762	A	N1-C6-N6	6.65	122.59	118.60
26	1H	1382	G	C6-C5-N7	-6.64	126.41	130.40
26	1H	626	U	N1-C2-N3	6.64	118.89	114.90
26	1H	138	G	C5-C6-O6	-6.64	124.62	128.60
26	14	668	G	C8-N9-C4	6.64	109.06	106.40
26	1H	1310	G	N3-C2-N2	-6.64	115.25	119.90
26	1H	1496	A	N1-C6-N6	6.64	122.58	118.60
26	1H	1940	U	N1-C2-O2	-6.64	118.15	122.80
26	1H	1986	A	C8-N9-C4	-6.64	103.14	105.80
26	1H	2392	A	C2-N3-C4	-6.64	107.28	110.60
26	1H	1528	A	C5-N7-C8	-6.64	100.58	103.90
26	14	140	A	C6-C5-N7	-6.64	127.66	132.30
26	14	1326	U	OP2-P-O3'	6.64	119.80	105.20
1	13	1129	C	C2-N1-C1'	6.63	126.10	118.80
26	1H	1241	A	C6-N1-C2	6.63	122.58	118.60
26	1H	679	C	C4-C5-C6	6.63	120.72	117.40
26	1H	2256	G	N3-C2-N2	6.63	124.54	119.90
26	1H	809	G	C5-C6-N1	6.63	114.81	111.50
26	1H	746	A	O5'-P-OP2	6.63	118.66	110.70
26	1H	1440	G	O5'-P-OP2	-6.63	99.73	105.70
26	1H	1694	C	C6-N1-C2	6.63	122.95	120.30
26	14	249	C	O5'-P-OP1	-6.63	99.73	105.70
1	13	813	U	N3-C4-O4	-6.63	114.76	119.40
26	1H	270(O)	U	C2-N1-C1'	6.63	125.65	117.70
23	2K	9	G	N1-C6-O6	6.62	123.88	119.90
1	13	690	G	C8-N9-C4	-6.62	103.75	106.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1G	1502	A	N1-C2-N3	6.62	132.61	129.30
26	1H	207	A	C5-C6-N6	-6.62	118.40	123.70
26	1H	631	A	C8-N9-C4	6.62	108.45	105.80
26	1H	2577	A	O5'-P-OP1	-6.62	99.74	105.70
49	J8	85	LEU	CA-CB-CG	6.62	130.53	115.30
1	13	966	G	C5-C6-O6	-6.62	124.63	128.60
26	1H	150	C	N3-C4-N4	-6.62	113.37	118.00
26	1H	2506	U	C2-N1-C1'	6.62	125.64	117.70
26	14	1779	U	C5-C4-O4	-6.62	121.93	125.90
33	51	105	LEU	CA-CB-CG	6.61	130.51	115.30
26	1H	847	U	C5-C6-N1	-6.61	119.39	122.70
1	13	974	A	N9-C4-C5	-6.61	103.16	105.80
26	14	2053	G	C8-N9-C4	6.61	109.04	106.40
26	1H	676	A	C8-N9-C4	-6.61	103.16	105.80
26	14	783	A	C8-N9-C4	-6.61	103.16	105.80
26	1H	1321	A	N7-C8-N9	-6.60	110.50	113.80
1	13	758	G	N1-C6-O6	6.60	123.86	119.90
26	1H	1313	U	C2-N1-C1'	6.60	125.62	117.70
26	1H	2329	G	OP1-P-OP2	6.60	129.50	119.60
26	1H	2441	C	C5-C4-N4	6.60	124.82	120.20
26	1H	530	G	N1-C6-O6	-6.60	115.94	119.90
26	1H	768	G	O5'-P-OP2	-6.60	99.76	105.70
1	13	963	G	N3-C2-N2	6.60	124.52	119.90
26	1H	773	U	C5-C6-N1	-6.60	119.40	122.70
26	1H	1572	A	C2-N3-C4	-6.60	107.30	110.60
26	1H	947	G	C8-N9-C4	-6.60	103.76	106.40
26	1H	1319	G	O5'-P-OP1	-6.60	99.76	105.70
1	1G	1502	A	C6-C5-N7	-6.60	127.68	132.30
26	14	1204	A	C5-C6-N1	-6.60	114.40	117.70
26	1H	1203	G	N1-C6-O6	-6.59	115.94	119.90
26	1H	2591	C	N3-C2-O2	6.59	126.52	121.90
1	13	687	A	P-O3'-C3'	6.59	127.61	119.70
1	1G	1473	A	C8-N9-C4	6.59	108.44	105.80
26	1H	2401	U	C5-C6-N1	6.59	126.00	122.70
26	14	584	C	C6-N1-C2	6.59	122.94	120.30
26	1H	144	C	C6-N1-C2	6.59	122.94	120.30
26	1H	74	A	C6-C5-N7	-6.59	127.69	132.30
26	1H	2346	A	C6-N1-C2	-6.59	114.65	118.60
26	1H	2490	G	C8-N9-C4	-6.59	103.77	106.40
26	14	1999	C	OP2-P-O3'	6.59	119.69	105.20
26	1H	2272	U	O5'-P-OP2	-6.58	99.77	105.70
26	1H	2249	U	N3-C4-O4	-6.58	114.79	119.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1G	449	C	N3-C2-O2	-6.58	117.29	121.90
24	3L	76	A	C5-N7-C8	-6.58	100.61	103.90
26	14	2607	G	N9-C4-C5	-6.58	102.77	105.40
26	1H	202	U	N1-C2-N3	-6.58	110.95	114.90
26	1H	222	A	P-O3'-C3'	6.58	127.59	119.70
26	1H	599	G	N3-C4-N9	6.58	129.95	126.00
26	1H	1367	A	N1-C6-N6	6.58	122.55	118.60
26	1H	1617	C	O5'-P-OP2	6.58	118.59	110.70
26	1H	2318	G	C8-N9-C4	-6.58	103.77	106.40
30	29	78	LEU	CA-CB-CG	6.58	130.43	115.30
26	14	2700	C	C6-N1-C2	6.58	122.93	120.30
1	1G	690	G	C4-C5-N7	6.57	113.43	110.80
1	13	576	G	C6-C5-N7	-6.57	126.46	130.40
1	13	1301	U	P-O3'-C3'	6.57	127.58	119.70
1	13	1450	U	N3-C2-O2	-6.57	117.60	122.20
26	1H	85	G	O5'-P-OP1	6.57	118.58	110.70
26	14	2392	A	C5-N7-C8	-6.57	100.62	103.90
1	1G	60	A	C8-N9-C4	6.56	108.42	105.80
26	1H	1355	G	N1-C6-O6	-6.56	115.97	119.90
26	14	642	G	C8-N9-C4	-6.56	103.78	106.40
26	14	2053	G	C5-C6-O6	-6.56	124.67	128.60
26	1H	236	C	C4-C5-C6	6.56	120.68	117.40
26	14	1156	A	O5'-P-OP2	-6.55	99.80	105.70
26	14	2713	A	N1-C6-N6	6.55	122.53	118.60
1	13	827	U	C2-N1-C1'	6.55	125.56	117.70
26	1H	265	A	C8-N9-C4	-6.55	103.18	105.80
26	1H	774	A	C4-C5-N7	6.55	113.97	110.70
26	1H	809	G	C5-C6-O6	-6.55	124.67	128.60
26	14	199	A	C2-N3-C4	6.55	113.88	110.60
26	1H	728	G	N1-C6-O6	6.55	123.83	119.90
26	14	2713	A	C4-C5-N7	6.55	113.97	110.70
26	1H	834	C	N1-C2-O2	-6.54	114.97	118.90
26	14	1332	G	N1-C2-N3	6.54	127.83	123.90
26	1H	1669	A	C5-C6-N6	-6.54	118.46	123.70
26	14	1614	A	N1-C2-N3	6.54	132.57	129.30
26	1H	1939	U	C4-C5-C6	-6.54	115.78	119.70
26	14	2592	G	N3-C4-N9	6.54	129.93	126.00
26	14	1585	C	C6-N1-C2	-6.54	117.69	120.30
26	14	2239	G	N1-C2-N2	-6.54	110.31	116.20
1	13	1233	G	N1-C6-O6	-6.54	115.98	119.90
26	1H	614	U	C5-C6-N1	6.53	125.97	122.70
26	1H	400	G	C5-C6-O6	-6.53	124.68	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	491	G	O5'-P-OP1	-6.53	99.83	105.70
26	1H	728	G	N9-C4-C5	-6.53	102.79	105.40
26	1H	1617	C	O5'-P-OP1	-6.53	99.82	105.70
26	14	2067	G	C6-N1-C2	-6.53	121.18	125.10
26	14	2446	G	N1-C2-N2	-6.53	110.33	116.20
1	13	1344	C	OP1-P-O3'	6.53	119.56	105.20
26	1H	1259	G	OP2-P-O3'	6.53	119.56	105.20
26	14	2498	C	O5'-P-OP2	-6.53	99.83	105.70
26	14	2542	A	N7-C8-N9	-6.52	110.54	113.80
26	14	2248	C	N3-C2-O2	-6.52	117.33	121.90
26	1H	216	A	O5'-P-OP2	6.52	118.53	110.70
26	1H	1571	A	N1-C6-N6	6.52	122.51	118.60
26	1H	699	A	N1-C6-N6	6.52	122.51	118.60
27	16	115	G	C6-N1-C2	-6.52	121.19	125.10
26	1H	2490	G	C6-C5-N7	-6.51	126.49	130.40
1	1G	315	A	N1-C6-N6	6.51	122.51	118.60
26	14	395	U	O4'-C1'-N1	6.51	113.41	108.20
26	1H	2544	G	C5-C6-O6	-6.51	124.69	128.60
1	1G	576	G	C8-N9-C1'	-6.51	118.53	127.00
1	1G	777	A	O5'-P-OP2	-6.51	99.84	105.70
26	14	1786	A	N3-C4-C5	6.51	131.36	126.80
26	1H	683	C	N3-C4-C5	6.51	124.50	121.90
26	14	1964	G	N3-C2-N2	6.51	124.45	119.90
26	14	2057	A	N1-C6-N6	6.51	122.50	118.60
26	1H	528	A	C5-N7-C8	-6.50	100.65	103.90
26	1H	1444	G	N1-C6-O6	-6.50	116.00	119.90
26	1H	2245	U	C5-C4-O4	-6.50	122.00	125.90
26	14	1342	A	C6-C5-N7	-6.50	127.75	132.30
26	1H	1318	C	O5'-P-OP1	-6.50	99.85	105.70
26	14	774	A	C5-C6-N1	-6.50	114.45	117.70
26	1H	209	C	C2-N3-C4	-6.50	116.65	119.90
1	13	1199	U	C5-C4-O4	6.50	129.80	125.90
26	1H	528	A	C8-N9-C1'	6.50	139.40	127.70
26	1H	1786	A	C5-C6-N1	-6.50	114.45	117.70
26	14	1950	G	O4'-C1'-N9	6.50	113.40	108.20
26	14	2821	A	C2-N3-C4	-6.50	107.35	110.60
26	1H	1370	C	N1-C2-O2	-6.50	115.00	118.90
26	14	1391	U	O5'-P-OP1	-6.50	99.85	105.70
26	14	1831	G	C6-C5-N7	-6.50	126.50	130.40
1	13	33	A	O5'-P-OP2	-6.49	99.86	105.70
26	1H	2710	C	C6-N1-C2	6.49	122.90	120.30
26	14	1396	U	C2-N1-C1'	6.49	125.49	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	1591	G	N1-C6-O6	-6.49	116.01	119.90
26	1H	120	U	N3-C2-O2	-6.49	117.66	122.20
26	14	113	G	C5-C6-O6	-6.49	124.71	128.60
26	14	1852	C	C6-N1-C2	-6.49	117.71	120.30
26	14	2818	G	C8-N9-C4	6.49	109.00	106.40
26	14	2726	U	N3-C2-O2	-6.48	117.66	122.20
26	1H	1392	A	O5'-P-OP1	-6.48	99.87	105.70
26	1H	2392	A	N3-C4-C5	6.48	131.34	126.80
26	1H	1761	C	C5-C4-N4	-6.48	115.66	120.20
26	1H	1657	C	OP1-P-O3'	6.48	119.45	105.20
1	1G	503	C	C6-N1-C2	-6.48	117.71	120.30
1	13	1489	G	C8-N9-C4	6.47	108.99	106.40
26	14	1992	G	P-O3'-C3'	6.47	127.47	119.70
26	1H	1974	C	C6-N1-C2	-6.47	117.71	120.30
26	1H	130	C	C6-N1-C2	6.47	122.89	120.30
26	1H	1357	U	N3-C4-C5	-6.47	110.72	114.60
26	1H	929	G	C8-N9-C4	6.47	108.99	106.40
1	1G	337	C	C6-N1-C2	-6.47	117.71	120.30
26	14	1313	U	N3-C4-O4	6.47	123.93	119.40
26	14	1973	G	C5-C6-O6	6.47	132.48	128.60
26	1H	1202	C	N1-C2-O2	-6.47	115.02	118.90
26	1H	23	G	N3-C2-N2	-6.46	115.38	119.90
26	1H	109	G	N1-C6-O6	-6.46	116.02	119.90
26	1H	202	U	C6-N1-C2	6.46	124.88	121.00
26	1H	1306	C	C2-N3-C4	-6.46	116.67	119.90
26	14	704	G	N3-C2-N2	-6.46	115.38	119.90
14	5I	12	ARG	C-N-CA	6.46	137.84	121.70
26	1H	1327	C	N1-C2-O2	-6.46	115.03	118.90
26	1H	1630	G	O5'-P-OP1	-6.46	99.89	105.70
26	14	511	U	C6-N1-C2	-6.46	117.12	121.00
1	13	2	U	O5'-P-OP1	-6.45	99.89	105.70
26	14	646	A	C8-N9-C4	-6.45	103.22	105.80
26	1H	535	C	O5'-P-OP2	-6.45	99.89	105.70
1	1G	1305	G	N3-C2-N2	-6.45	115.38	119.90
1	1G	1401	G	N1-C6-O6	6.45	123.77	119.90
26	14	2430	A	C6-C5-N7	-6.45	127.79	132.30
26	14	2610	C	O5'-P-OP2	6.45	118.44	110.70
26	14	1781	C	C2-N1-C1'	6.45	125.89	118.80
26	1H	2713	A	N1-C2-N3	6.44	132.52	129.30
26	14	1654	A	N1-C6-N6	-6.44	114.73	118.60
26	1H	739	G	C5-C6-O6	-6.44	124.73	128.60
26	1H	1678	G	N1-C2-N3	6.44	127.76	123.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	14	945	A	C5-C6-N6	-6.44	118.55	123.70
26	14	1209	G	O5'-P-OP2	-6.44	99.91	105.70
26	14	2581	G	C5-C6-O6	6.44	132.46	128.60
26	1H	1969	A	OP1-P-O3'	6.44	119.36	105.20
26	1H	112	U	N3-C2-O2	6.43	126.70	122.20
26	14	2057	A	OP1-P-OP2	6.43	129.25	119.60
26	14	2226	C	N1-C2-O2	6.43	122.76	118.90
26	1H	704	G	N3-C2-N2	-6.42	115.40	119.90
26	1H	2003	G	O5'-P-OP1	-6.42	99.92	105.70
26	14	1807	G	N9-C4-C5	-6.42	102.83	105.40
1	13	1502	A	O5'-P-OP2	-6.42	99.92	105.70
26	14	2386	C	C6-N1-C2	6.42	122.87	120.30
1	13	328	C	N3-C2-O2	-6.42	117.41	121.90
1	13	584	G	C5-C6-O6	6.42	132.45	128.60
27	16	98	G	C4-C5-N7	6.42	113.37	110.80
26	1H	754	C	C2-N3-C4	-6.41	116.69	119.90
26	14	1936	A	O4'-C1'-N9	6.41	113.33	108.20
26	1H	788	A	OP2-P-O3'	6.41	119.30	105.20
26	1H	793	A	OP1-P-OP2	6.41	129.21	119.60
26	1H	1782	C	C4-C5-C6	6.41	120.60	117.40
26	1H	2697	G	OP1-P-OP2	6.41	129.21	119.60
26	1H	1955	U	C4-C5-C6	6.41	123.54	119.70
26	14	199	A	N9-C4-C5	6.41	108.36	105.80
1	13	811	C	C5-C6-N1	-6.40	117.80	121.00
26	14	2592	G	N3-C4-C5	-6.40	125.40	128.60
26	1H	188	G	C6-C5-N7	-6.40	126.56	130.40
26	1H	609	A	N1-C6-N6	6.40	122.44	118.60
26	1H	196	A	O4'-C1'-N9	6.40	113.32	108.20
6	52	14	LEU	CA-CB-CG	6.39	130.01	115.30
26	14	1845	G	N1-C6-O6	6.39	123.74	119.90
26	1H	162	U	C2-N1-C1'	6.39	125.37	117.70
26	1H	580	C	C6-N1-C2	-6.39	117.74	120.30
26	14	2339	G	O5'-P-OP2	-6.39	99.95	105.70
26	14	211	A	N1-C6-N6	6.38	122.43	118.60
26	14	664	C	C5-C6-N1	-6.38	117.81	121.00
26	14	808	G	N3-C4-N9	6.38	129.83	126.00
26	14	1781	C	O4'-C1'-N1	6.38	113.31	108.20
26	1H	412	A	C8-N9-C4	6.38	108.35	105.80
26	1H	686	G	OP1-P-OP2	6.38	129.17	119.60
26	1H	2458	G	N3-C2-N2	-6.38	115.43	119.90
26	1H	194	G	C5-C6-O6	-6.38	124.77	128.60
24	1L	34	U	C5-C6-N1	6.38	125.89	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	1950	G	C6-C5-N7	-6.38	126.57	130.40
26	1H	2430	A	C4-C5-N7	6.38	113.89	110.70
26	1H	835	A	O5'-P-OP2	-6.38	99.96	105.70
26	1H	99	U	N3-C2-O2	-6.38	117.74	122.20
26	1H	1800	C	C4-C5-C6	6.37	120.59	117.40
26	1H	1816	G	O5'-P-OP1	-6.37	99.96	105.70
26	1H	2311	A	N7-C8-N9	6.37	116.99	113.80
26	1H	2445	G	N3-C2-N2	6.37	124.36	119.90
1	1G	1469	G	N1-C6-O6	6.37	123.72	119.90
26	1H	2503	A	C4-C5-N7	6.37	113.89	110.70
1	1G	1446	A	O4'-C1'-N9	6.37	113.30	108.20
26	14	528	A	N1-C2-N3	6.37	132.49	129.30
26	1H	528	A	C4-N9-C1'	-6.37	114.83	126.30
26	1H	1225	C	C6-N1-C2	6.37	122.85	120.30
26	1H	150	C	C5-C4-N4	6.37	124.66	120.20
26	1H	1888	G	C8-N9-C1'	-6.37	118.72	127.00
26	1H	2434	A	C2-N3-C4	-6.37	107.42	110.60
26	1H	750	A	OP1-P-O3'	-6.37	91.19	105.20
26	1H	1142(A)	A	C5-N7-C8	-6.37	100.72	103.90
26	1H	192	C	C6-N1-C2	6.36	122.84	120.30
26	1H	2665	A	N1-C2-N3	6.36	132.48	129.30
1	1G	1487	G	N3-C2-N2	-6.36	115.45	119.90
26	14	667	U	N1-C2-O2	-6.36	118.35	122.80
26	14	1382	G	C5-C6-O6	-6.36	124.78	128.60
26	1H	2256	G	N1-C2-N2	-6.36	110.47	116.20
1	1G	108	G	C4-C5-N7	6.36	113.34	110.80
26	14	1265	A	C5-C6-N6	-6.36	118.61	123.70
26	14	2700	C	C5-C4-N4	-6.36	115.75	120.20
26	1H	858	U	O5'-P-OP2	-6.36	99.98	105.70
26	1H	987	G	OP1-P-OP2	-6.36	110.06	119.60
26	1H	2331	G	N9-C4-C5	-6.36	102.86	105.40
26	1H	2518	A	N7-C8-N9	6.36	116.98	113.80
26	1H	416	C	N3-C4-N4	-6.35	113.55	118.00
26	1H	770	G	C5-C6-O6	-6.35	124.79	128.60
26	14	1559	G	C4-C5-N7	6.35	113.34	110.80
26	1H	1210	A	C6-C5-N7	-6.35	127.85	132.30
26	1H	1437	C	C6-N1-C2	-6.35	117.76	120.30
26	14	1776	G	O5'-P-OP2	-6.35	99.99	105.70
26	14	2496	C	C6-N1-C2	-6.35	117.76	120.30
26	1H	94	G	N1-C6-O6	6.34	123.71	119.90
26	1H	2275	C	O4'-C1'-N1	-6.34	103.12	108.20
26	1H	2437	U	C5-C4-O4	6.34	129.71	125.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	1614	A	OP1-P-OP2	6.34	129.11	119.60
26	14	1760	A	O5'-P-OP2	-6.34	99.99	105.70
27	16	81	G	O4'-C1'-N9	6.34	113.27	108.20
26	14	2463	C	C6-N1-C2	6.34	122.84	120.30
24	3L	1	G	C2-N3-C4	6.34	115.07	111.90
26	1H	1210	A	C5-N7-C8	-6.34	100.73	103.90
1	13	899	C	N1-C2-O2	-6.33	115.10	118.90
26	14	1914	C	C2-N1-C1'	6.33	125.77	118.80
26	1H	917	A	N3-C4-C5	6.33	131.23	126.80
26	1H	2267	A	OP1-P-O3'	6.33	119.13	105.20
26	1H	2562	U	C5-C6-N1	-6.33	119.53	122.70
26	1H	94	G	C5-C6-O6	-6.33	124.80	128.60
26	1H	2081	C	N3-C2-O2	-6.33	117.47	121.90
26	14	629	G	O5'-P-OP2	-6.33	100.00	105.70
26	1H	729	G	C8-N9-C4	-6.33	103.87	106.40
26	14	1939	U	C5-C4-O4	6.33	129.70	125.90
26	1H	481	G	N3-C2-N2	-6.33	115.47	119.90
26	14	2056	G	C5-C6-O6	-6.33	124.81	128.60
1	13	1227	A	O5'-P-OP2	-6.32	100.01	105.70
26	14	2838	G	N3-C2-N2	-6.32	115.47	119.90
26	1H	1782	C	P-O3'-C3'	6.32	127.29	119.70
26	14	1639	U	N3-C2-O2	-6.32	117.78	122.20
26	14	1960	A	O5'-P-OP2	-6.32	100.01	105.70
27	16	6	C	N3-C2-O2	6.32	126.32	121.90
27	16	77	U	C5-C6-N1	-6.32	119.54	122.70
26	14	793	A	O5'-P-OP2	-6.32	100.01	105.70
26	1H	409	C	C6-N1-C2	6.31	122.83	120.30
26	1H	2713	A	C4-C5-N7	6.31	113.86	110.70
1	1G	481	G	C4-N9-C1'	6.31	134.71	126.50
26	14	2595	G	O5'-P-OP1	-6.31	100.02	105.70
1	13	892	A	C6-C5-N7	-6.31	127.88	132.30
26	1H	930	U	N3-C2-O2	-6.31	117.78	122.20
26	1H	1786	A	C4-C5-C6	6.31	120.15	117.00
26	1H	781	A	C8-N9-C4	6.31	108.32	105.80
26	1H	103	A	C8-N9-C4	6.30	108.32	105.80
26	1H	129	C	N3-C4-N4	6.30	122.41	118.00
26	1H	703	U	C5-C4-O4	6.30	129.68	125.90
26	1H	816	C	O5'-P-OP1	6.30	118.27	110.70
26	1H	1558	A	P-O3'-C3'	6.30	127.27	119.70
26	1H	1698	A	C4-C5-C6	6.30	120.15	117.00
26	14	199	A	N1-C6-N6	-6.30	114.82	118.60
26	1H	928	G	N1-C6-O6	6.30	123.68	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	14	732	C	N3-C4-N4	6.30	122.41	118.00
26	14	2355	C	C2-N1-C1'	6.30	125.73	118.80
26	14	2447	G	N1-C6-O6	6.30	123.68	119.90
26	14	2249	U	C5-C6-N1	6.30	125.85	122.70
26	14	2330	G	C5-C6-O6	-6.30	124.82	128.60
26	14	2518	A	C2-N3-C4	-6.30	107.45	110.60
26	14	1142	U	N1-C2-O2	6.30	127.21	122.80
1	13	121	C	N3-C2-O2	-6.30	117.49	121.90
26	1H	1258	C	OP2-P-O3'	6.30	119.05	105.20
26	1H	825	C	C4-C5-C6	6.29	120.55	117.40
26	1H	2513	G	O5'-P-OP2	-6.29	100.04	105.70
26	14	1784	A	C5-N7-C8	-6.29	100.75	103.90
1	13	792	A	O4'-C1'-N9	6.29	113.23	108.20
26	1H	133	C	C6-N1-C2	6.29	122.82	120.30
26	1H	265	A	N1-C2-N3	6.29	132.45	129.30
26	1H	967	C	O5'-P-OP2	-6.29	100.04	105.70
1	1G	413	G	N3-C4-N9	-6.29	122.22	126.00
26	14	912	C	C6-N1-C2	-6.29	117.78	120.30
26	1H	691	C	N1-C2-O2	-6.29	115.13	118.90
26	1H	730	C	N3-C2-O2	-6.29	117.50	121.90
26	1H	2419	U	O5'-P-OP2	6.29	118.24	110.70
26	1H	2712	U	C2-N3-C4	-6.29	123.23	127.00
1	13	346	G	C8-N9-C4	-6.28	103.89	106.40
26	1H	1416	G	O4'-C1'-N9	6.28	113.23	108.20
26	1H	1984	G	O5'-P-OP2	-6.28	100.04	105.70
26	14	2444	G	N3-C2-N2	-6.28	115.50	119.90
27	16	6	C	C5-C4-N4	-6.28	115.80	120.20
1	13	684	A	C8-N9-C4	-6.28	103.29	105.80
26	1H	138	G	C8-N9-C4	-6.28	103.89	106.40
26	14	330	A	C4-C5-N7	6.28	113.84	110.70
26	14	778	G	N1-C2-N2	-6.27	110.56	116.20
26	1H	135	G	N7-C8-N9	-6.27	109.96	113.10
1	13	1519	A	C5-C6-N1	-6.27	114.56	117.70
26	1H	1142(A)	A	N3-C4-N9	-6.27	122.38	127.40
26	1H	1379	A	C5-C6-N6	-6.27	118.69	123.70
26	1H	2442	C	C5-C6-N1	-6.27	117.86	121.00
26	1H	745	G	N3-C4-C5	-6.27	125.47	128.60
26	1H	767	U	C5-C4-O4	6.27	129.66	125.90
26	1H	2287	A	C4-C5-N7	6.26	113.83	110.70
26	1H	311	A	O5'-P-OP2	6.26	118.22	110.70
26	1H	1777	U	OP1-P-O3'	6.26	118.98	105.20
27	16	44	G	C4-N9-C1'	-6.26	118.36	126.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	14	732	C	N3-C2-O2	6.26	126.28	121.90
26	1H	906	G	N9-C4-C5	6.26	107.91	105.40
26	1H	1602	U	C5-C6-N1	-6.26	119.57	122.70
26	1H	1888	G	C4-N9-C1'	6.26	134.64	126.50
26	14	2392	A	C2-N3-C4	-6.26	107.47	110.60
26	1H	862	G	N1-C6-O6	-6.26	116.14	119.90
26	1H	1700	A	O5'-P-OP2	-6.26	100.07	105.70
26	1H	788	A	C6-N1-C2	6.26	122.35	118.60
26	14	2610	C	O5'-P-OP1	-6.26	100.07	105.70
26	14	1258	C	C5-C4-N4	-6.25	115.82	120.20
26	1H	1401	G	C8-N9-C4	-6.25	103.90	106.40
26	14	1339	G	O5'-P-OP2	6.25	118.20	110.70
26	1H	2596	U	OP1-P-OP2	6.25	128.97	119.60
26	1H	664	C	C5-C6-N1	-6.25	117.88	121.00
26	1H	1782	C	C2'-C3'-O3'	6.25	123.70	113.70
26	1H	2269	A	C8-N9-C4	6.25	108.30	105.80
26	14	1796	U	O5'-P-OP1	-6.25	100.08	105.70
26	1H	1775	U	O5'-P-OP2	-6.25	100.08	105.70
26	14	584	C	N3-C2-O2	6.25	126.27	121.90
1	13	525	C	C5-C6-N1	6.25	124.12	121.00
26	1H	1773	A	C2-N3-C4	-6.25	107.48	110.60
26	1H	1838	C	C6-N1-C2	6.24	122.80	120.30
26	1H	2500	U	N3-C4-O4	6.24	123.77	119.40
26	14	2326	C	N3-C4-C5	-6.24	119.40	121.90
26	1H	198	C	N3-C4-C5	6.24	124.40	121.90
26	1H	2665	A	O4'-C1'-N9	6.24	113.19	108.20
26	14	783	A	N3-C4-N9	-6.24	122.41	127.40
26	14	1845	G	N3-C2-N2	-6.24	115.53	119.90
26	14	2581	G	N1-C6-O6	-6.24	116.16	119.90
27	1J	7	G	N1-C6-O6	6.24	123.64	119.90
26	1H	205	G	N9-C4-C5	-6.24	102.90	105.40
26	1H	1339	G	O5'-P-OP2	6.24	118.19	110.70
1	1G	1401	G	C8-N9-C1'	-6.24	118.89	127.00
26	14	1616	A	N3-C4-C5	6.24	131.17	126.80
26	14	2003	G	C4-C5-N7	6.24	113.29	110.80
26	1H	201	C	C2-N3-C4	-6.23	116.78	119.90
24	3K	76	A	O4'-C1'-N9	6.23	113.18	108.20
26	1H	1379	A	N7-C8-N9	6.23	116.92	113.80
26	1H	1771	C	C2-N3-C4	-6.23	116.78	119.90
1	1G	1259	C	C6-N1-C2	-6.23	117.81	120.30
1	13	1502	A	C6-C5-N7	-6.23	127.94	132.30
27	16	44	G	N9-C4-C5	6.23	107.89	105.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	14	830	G	C8-N9-C4	6.23	108.89	106.40
26	14	1963	U	C6-N1-C1'	-6.22	112.49	121.20
26	14	2581	G	OP1-P-OP2	6.22	128.94	119.60
26	14	2239	G	N3-C2-N2	6.22	124.26	119.90
26	14	2518	A	C5-N7-C8	-6.22	100.79	103.90
23	2K	45	A	N1-C6-N6	6.22	122.33	118.60
26	1H	1984	G	N3-C2-N2	6.22	124.25	119.90
26	14	1678	G	C5-C6-N1	-6.22	108.39	111.50
24	3K	76	A	C2-N3-C4	-6.22	107.49	110.60
26	14	133	C	C6-N1-C2	6.22	122.79	120.30
26	14	488	G	N3-C4-N9	6.22	129.73	126.00
26	14	1989	G	N1-C6-O6	6.22	123.63	119.90
27	16	100	G	C8-N9-C4	6.21	108.89	106.40
26	14	2210	G	C8-N9-C1'	-6.21	118.92	127.00
26	1H	930	U	N1-C2-N3	6.21	118.63	114.90
26	1H	1241	A	C5-N7-C8	-6.21	100.80	103.90
26	1H	2053	G	C5-C6-O6	-6.21	124.87	128.60
26	1H	2604	U	N3-C2-O2	-6.21	117.85	122.20
26	14	1698	A	C6-C5-N7	-6.21	127.95	132.30
1	13	817	C	C5-C4-N4	-6.21	115.86	120.20
26	1H	2424	C	N1-C2-O2	6.21	122.62	118.90
27	16	15	A	O4'-C1'-N9	6.21	113.17	108.20
26	1H	1429	G	O5'-P-OP2	-6.20	100.12	105.70
26	1H	1957	C	N3-C2-O2	-6.20	117.56	121.90
26	1H	945	A	N9-C4-C5	-6.20	103.32	105.80
26	1H	1333	C	C5-C4-N4	-6.20	115.86	120.20
26	14	71	A	N1-C2-N3	6.20	132.40	129.30
26	1H	917	A	C8-N9-C4	-6.20	103.32	105.80
26	1H	2346	A	N9-C1'-C2'	6.20	122.05	114.00
26	14	1686	C	C6-N1-C2	6.20	122.78	120.30
26	14	2301	C	C6-N1-C2	-6.20	117.82	120.30
26	1H	752	A	C2-N3-C4	-6.19	107.50	110.60
26	1H	1626	G	O5'-P-OP2	6.19	118.13	110.70
26	1H	2510	C	N3-C4-N4	-6.19	113.67	118.00
26	14	1379	A	C5-N7-C8	-6.19	100.81	103.90
26	14	2473	U	N1-C2-O2	6.19	127.13	122.80
26	1H	96	G	N1-C6-O6	6.19	123.61	119.90
26	1H	1786	A	C4-N9-C1'	6.19	137.44	126.30
26	1H	2397	G	O5'-P-OP2	6.19	118.13	110.70
26	14	676	A	N1-C6-N6	6.19	122.31	118.60
26	1H	845	G	OP1-P-O3'	6.19	118.81	105.20
26	14	845	G	C6-C5-N7	-6.18	126.69	130.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	2417	C	O5'-P-OP2	-6.18	100.14	105.70
26	14	530	G	N1-C6-O6	6.18	123.61	119.90
26	14	1142(A)	A	C2-N3-C4	-6.18	107.51	110.60
26	14	2446	G	N3-C2-N2	6.18	124.22	119.90
1	13	800	G	C5-C6-O6	-6.18	124.89	128.60
26	1H	2035	G	O5'-P-OP1	-6.18	100.14	105.70
26	1H	2593	U	C5-C4-O4	6.18	129.61	125.90
1	13	1398	A	N1-C6-N6	6.18	122.31	118.60
26	1H	1995	U	C5-C6-N1	-6.18	119.61	122.70
1	1G	700	G	C6-C5-N7	6.18	134.11	130.40
26	14	2062	A	C4-C5-C6	-6.18	113.91	117.00
26	14	2427	C	O5'-P-OP2	6.18	118.11	110.70
26	1H	1394	U	C5-C6-N1	6.17	125.79	122.70
26	1H	1611	C	C5-C4-N4	-6.17	115.88	120.20
26	1H	621	A	C8-N9-C4	-6.17	103.33	105.80
27	1J	89	G	C4-N9-C1'	6.17	134.52	126.50
26	1H	1955	U	N1-C2-N3	6.17	118.60	114.90
26	14	933	A	N1-C6-N6	6.17	122.30	118.60
26	14	1241	A	C5-C6-N1	-6.17	114.61	117.70
26	14	2464	C	N3-C4-C5	6.17	124.37	121.90
26	1H	736	C	O5'-P-OP2	6.17	118.10	110.70
23	2L	21	U	N3-C2-O2	-6.17	117.88	122.20
26	14	1797	C	C6-N1-C2	6.17	122.77	120.30
26	1H	760	G	N1-C6-O6	6.17	123.60	119.90
26	14	2245	U	C4-C5-C6	-6.17	116.00	119.70
1	13	326	G	C4-C5-N7	-6.16	108.33	110.80
26	1H	599	G	N3-C4-C5	-6.16	125.52	128.60
26	14	2426	A	N1-C6-N6	6.16	122.30	118.60
26	14	1725	G	C4-N9-C1'	6.16	134.51	126.50
1	13	1220	G	N1-C6-O6	-6.16	116.20	119.90
1	1G	1487	G	N1-C6-O6	6.16	123.59	119.90
1	1G	817	C	C6-N1-C2	6.16	122.76	120.30
26	14	577	G	N1-C6-O6	6.16	123.59	119.90
8	7E	112	LEU	CA-CB-CG	6.16	129.46	115.30
26	14	1314	C	C2-N1-C1'	6.16	125.57	118.80
26	1H	1332	G	N1-C2-N3	6.15	127.59	123.90
26	1H	2572	A	N9-C4-C5	-6.15	103.34	105.80
27	16	69	G	OP2-P-O3'	6.15	118.73	105.20
1	1G	1397	C	C2-N1-C1'	6.15	125.57	118.80
1	1G	1500	A	O5'-P-OP1	-6.15	100.16	105.70
26	14	1241	A	C2-N3-C4	-6.15	107.52	110.60
26	14	2251	G	N1-C6-O6	-6.15	116.21	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	13	266	G	C5-N7-C8	-6.15	101.22	104.30
26	1H	728	G	C5-C6-O6	-6.15	124.91	128.60
26	1H	1611	C	C2-N3-C4	-6.15	116.82	119.90
26	14	1968	G	N7-C8-N9	6.15	116.18	113.10
26	14	2435	A	N7-C8-N9	6.15	116.88	113.80
26	1H	456	C	OP1-P-O3'	6.15	118.73	105.20
26	14	681	G	N1-C2-N2	-6.15	110.67	116.20
26	14	1496	A	C4-C5-N7	6.15	113.78	110.70
26	14	113	G	N3-C4-C5	6.15	131.67	128.60
26	1H	2328	A	N1-C2-N3	6.15	132.37	129.30
26	14	945	A	C4-N9-C1'	6.15	137.36	126.30
26	14	1390	U	OP1-P-O3'	6.15	118.72	105.20
1	13	1158	C	C2-N1-C1'	6.14	125.56	118.80
26	1H	2258	C	C5-C6-N1	-6.14	117.93	121.00
26	1H	2689	U	C6-N1-C2	-6.14	117.31	121.00
26	14	1416	G	C4-N9-C1'	-6.14	118.51	126.50
26	14	2496	C	C5-C6-N1	6.14	124.07	121.00
26	1H	746	A	O4'-C1'-N9	6.14	113.11	108.20
26	1H	2752	C	C6-N1-C2	-6.14	117.84	120.30
26	14	140	A	O4'-C1'-N9	6.14	113.11	108.20
26	14	71	A	P-O3'-C3'	6.14	127.07	119.70
26	1H	651	G	C8-N9-C4	-6.14	103.94	106.40
26	14	1299	G	O5'-P-OP1	-6.13	100.18	105.70
27	16	81	G	N7-C8-N9	6.13	116.17	113.10
26	1H	1599	C	N3-C4-N4	-6.13	113.71	118.00
24	3K	71	C	C6-N1-C2	-6.13	117.85	120.30
26	1H	655	A	N7-C8-N9	6.13	116.86	113.80
26	1H	1797	C	C5-C4-N4	-6.13	115.91	120.20
26	1H	2353	G	OP1-P-OP2	6.13	128.80	119.60
26	14	778	G	N3-C2-N2	6.13	124.19	119.90
26	1H	1365	A	C8-N9-C4	-6.13	103.35	105.80
26	14	72	U	C5-C6-N1	-6.13	119.64	122.70
26	14	2607	G	C6-C5-N7	-6.13	126.72	130.40
26	1H	1396	U	C5-C4-O4	6.12	129.57	125.90
26	1H	1796	U	O5'-P-OP2	6.12	118.05	110.70
26	1H	2377	A	C8-N9-C4	6.12	108.25	105.80
26	14	1333	C	N3-C4-C5	6.12	124.35	121.90
1	13	767	A	C2-N3-C4	-6.12	107.54	110.60
26	1H	983	A	C8-N9-C4	6.12	108.25	105.80
26	1H	1284	A	OP1-P-OP2	6.12	128.78	119.60
26	1H	2518	A	O5'-P-OP2	6.12	118.05	110.70
26	14	1259	G	OP2-P-O3'	6.12	118.67	105.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	25	8	LEU	CA-CB-CG	6.12	129.38	115.30
26	1H	2500	U	OP2-P-O3'	6.12	118.66	105.20
26	1H	2578	G	C5-C6-N1	6.12	114.56	111.50
26	1H	632	A	O5'-P-OP2	6.12	118.04	110.70
26	1H	1899	G	N1-C2-N2	6.12	121.70	116.20
26	1H	2500	U	C5-C4-O4	-6.12	122.23	125.90
1	13	690	G	C5-N7-C8	-6.11	101.24	104.30
23	2L	21	U	C6-N1-C2	-6.11	117.33	121.00
26	1H	932	G	C8-N9-C4	-6.11	103.95	106.40
1	1G	536	C	C6-N1-C2	-6.11	117.86	120.30
26	14	330	A	C5-N7-C8	-6.11	100.84	103.90
26	1H	180	G	N9-C4-C5	-6.11	102.96	105.40
26	1H	213	A	C5-N7-C8	-6.11	100.85	103.90
26	1H	777	A	N1-C2-N3	6.11	132.35	129.30
26	1H	189	G	C6-C5-N7	-6.11	126.74	130.40
26	1H	1663	C	C5-C4-N4	-6.11	115.93	120.20
26	14	2270	G	N1-C6-O6	6.11	123.56	119.90
1	13	57	G	N3-C4-C5	-6.10	125.55	128.60
26	1H	1790	C	P-O3'-C3'	6.10	127.02	119.70
26	14	1475	G	N7-C8-N9	6.10	116.15	113.10
26	14	1638	C	OP2-P-O3'	6.10	118.63	105.20
26	14	2594	C	C5-C4-N4	-6.10	115.93	120.20
1	13	963	G	N3-C4-N9	6.10	129.66	126.00
26	1H	520	G	N1-C6-O6	-6.10	116.24	119.90
26	1H	1184	G	OP2-P-O3'	6.10	118.62	105.20
27	1J	47	C	C6-N1-C2	6.10	122.74	120.30
26	1H	1678	G	C6-C5-N7	-6.10	126.74	130.40
1	13	481	G	N1-C6-O6	6.10	123.56	119.90
26	1H	219	G	C5-C6-N1	6.10	114.55	111.50
26	14	2065	C	N3-C2-O2	-6.10	117.63	121.90
1	13	115	G	P-O3'-C3'	6.09	127.01	119.70
26	14	1308	A	C8-N9-C4	-6.09	103.36	105.80
26	14	2069	G	N9-C4-C5	-6.09	102.96	105.40
26	14	2842	G	N1-C6-O6	6.09	123.55	119.90
26	1H	967	C	N3-C4-C5	6.09	124.33	121.90
27	16	28	C	C6-N1-C2	-6.09	117.86	120.30
1	13	813	U	C5-C4-O4	6.09	129.55	125.90
26	1H	2604	U	N1-C2-O2	6.09	127.06	122.80
26	14	1122	G	C5-C6-O6	-6.09	124.95	128.60
26	14	808	G	N3-C2-N2	6.08	124.16	119.90
26	14	2592	G	O5'-P-OP2	-6.08	100.22	105.70
26	1H	2052	G	N1-C6-O6	-6.08	116.25	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	2830	G	C8-N9-C4	-6.08	103.97	106.40
26	14	2307	G	C4-N9-C1'	6.08	134.41	126.50
26	1H	999	U	OP1-P-OP2	-6.08	110.48	119.60
26	1H	1431	U	C5-C6-N1	6.08	125.74	122.70
26	1H	270(L)	U	O4'-C1'-N1	6.08	113.06	108.20
26	1H	1197	G	C8-N9-C4	6.08	108.83	106.40
26	1H	1611	C	N3-C4-C5	6.08	124.33	121.90
26	1H	1764	G	N1-C6-O6	-6.08	116.25	119.90
26	14	396	G	C4-N9-C1'	6.08	134.40	126.50
1	13	1450	U	N1-C2-O2	6.08	127.05	122.80
1	13	576	G	C5-C6-O6	-6.07	124.96	128.60
26	1H	2837	G	C8-N9-C4	-6.07	103.97	106.40
26	14	1391	U	O5'-P-OP2	6.07	117.99	110.70
26	1H	2706	G	C5-N7-C8	6.07	107.34	104.30
1	1G	197	A	N7-C8-N9	6.07	116.84	113.80
26	14	1932	A	O5'-P-OP1	-6.07	100.23	105.70
26	14	2358	G	N3-C2-N2	-6.07	115.65	119.90
26	1H	1157	G	N3-C4-C5	-6.07	125.56	128.60
26	1H	1191	G	C8-N9-C4	6.07	108.83	106.40
26	1H	2082	A	N1-C2-N3	6.07	132.34	129.30
26	14	827	U	N1-C2-O2	-6.07	118.55	122.80
1	13	703	G	C4-C5-N7	6.07	113.23	110.80
26	1H	189	G	N9-C4-C5	-6.07	102.97	105.40
26	1H	944	G	C4-N9-C1'	6.07	134.38	126.50
26	1H	1555	G	O5'-P-OP1	-6.07	100.24	105.70
26	1H	1970	A	O5'-P-OP2	-6.07	100.24	105.70
26	14	729	G	OP2-P-O3'	6.07	118.54	105.20
26	14	1950	G	C6-C5-N7	-6.07	126.76	130.40
26	1H	1496	A	C6-C5-N7	-6.06	128.06	132.30
26	1H	2512	C	C6-N1-C2	6.06	122.72	120.30
26	1H	1142(A)	A	N1-C6-N6	6.06	122.24	118.60
26	1H	1198	U	N3-C2-O2	-6.06	117.96	122.20
27	1J	30	C	N3-C4-C5	-6.06	119.48	121.90
26	1H	1591	G	C5-C6-O6	6.06	132.23	128.60
26	1H	1858	G	C4-N9-C1'	6.06	134.38	126.50
1	1G	906	G	N1-C6-O6	6.06	123.53	119.90
26	14	331	A	C2-N3-C4	-6.06	107.57	110.60
26	1H	820	A	C5-C6-N6	6.06	128.54	123.70
27	16	12	C	C6-N1-C2	-6.06	117.88	120.30
26	1H	2706	G	N7-C8-N9	-6.05	110.07	113.10
1	13	975	A	O4'-C1'-N9	-6.05	103.36	108.20
26	1H	808	G	N1-C2-N2	-6.05	110.75	116.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1G	1498	U	P-O3'-C3'	6.05	126.96	119.70
26	1H	921	G	C8-N9-C4	-6.05	103.98	106.40
26	1H	121	G	C5-C6-O6	-6.05	124.97	128.60
26	1H	141	A	N3-C4-C5	6.05	131.03	126.80
26	1H	616	A	OP2-P-O3'	6.05	118.51	105.20
26	1H	834	C	OP2-P-O3'	6.05	118.51	105.20
26	1H	2039	C	C6-N1-C2	-6.05	117.88	120.30
26	1H	576	U	C6-N1-C2	-6.05	117.37	121.00
26	14	1934	C	N1-C2-O2	6.05	122.53	118.90
26	14	2842	G	C5-C6-O6	-6.05	124.97	128.60
26	1H	946	G	N7-C8-N9	-6.04	110.08	113.10
26	14	47	C	OP2-P-O3'	6.04	118.50	105.20
26	14	1323	U	OP1-P-O3'	6.04	118.49	105.20
26	14	2068	U	OP1-P-O3'	6.04	118.50	105.20
26	1H	508	G	C6-C5-N7	-6.04	126.78	130.40
26	14	1914	C	N3-C4-C5	-6.04	119.48	121.90
26	1H	2408	U	OP2-P-O3'	6.04	118.49	105.20
1	1G	1401	G	C6-C5-N7	-6.04	126.78	130.40
26	14	2560	C	O5'-P-OP1	-6.04	100.26	105.70
1	13	536	C	N1-C2-O2	-6.04	115.28	118.90
26	1H	2572	A	N1-C6-N6	6.04	122.22	118.60
26	14	1992	G	C2-N3-C4	6.04	114.92	111.90
26	1H	2057	A	OP1-P-O3'	6.03	118.47	105.20
26	14	565	C	C6-N1-C2	6.03	122.71	120.30
26	14	1367	A	N1-C6-N6	6.03	122.22	118.60
26	14	1258	C	OP2-P-O3'	6.03	118.47	105.20
26	1H	824	A	N1-C6-N6	-6.03	114.98	118.60
26	1H	1645	G	OP1-P-O3'	6.03	118.47	105.20
26	14	642	G	C6-C5-N7	-6.03	126.78	130.40
26	14	1671	U	O5'-P-OP1	-6.03	100.27	105.70
26	14	503	A	N1-C6-N6	-6.03	114.98	118.60
26	14	783	A	C4-C5-C6	6.03	120.02	117.00
26	1H	845	G	N3-C4-C5	6.03	131.61	128.60
26	1H	2616	C	N3-C4-C5	6.03	124.31	121.90
1	1G	1128	C	N1-C2-O2	6.03	122.52	118.90
26	1H	590	A	C6-N1-C2	-6.03	114.98	118.60
27	16	98	G	N9-C4-C5	-6.03	102.99	105.40
26	1H	330	A	C5-N7-C8	-6.02	100.89	103.90
26	1H	821	A	OP1-P-O3'	6.02	118.45	105.20
26	1H	860	U	C6-N1-C1'	-6.02	112.77	121.20
26	14	837	C	C6-N1-C2	-6.02	117.89	120.30
26	1H	797	C	C2-N3-C4	-6.02	116.89	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	2706	G	N1-C6-O6	-6.02	116.29	119.90
26	1H	679	C	C2-N3-C4	-6.02	116.89	119.90
26	1H	1776	G	N3-C4-N9	6.02	129.61	126.00
26	14	2304	G	C8-N9-C4	-6.02	103.99	106.40
26	1H	2251	G	C4-C5-N7	-6.02	108.39	110.80
26	14	2708	G	N1-C2-N2	-6.02	110.79	116.20
26	14	252	G	N1-C6-O6	-6.01	116.29	119.90
26	14	1965	C	C6-N1-C2	6.01	122.70	120.30
26	1H	113	G	N3-C4-C5	6.01	131.60	128.60
26	14	2346	A	C4-N9-C1'	6.01	137.12	126.30
26	1H	738	G	C4-C5-N7	6.01	113.20	110.80
26	1H	1445	C	C6-N1-C2	-6.01	117.90	120.30
26	1H	1432	C	N1-C2-O2	-6.01	115.30	118.90
26	1H	2270	G	N9-C4-C5	-6.01	103.00	105.40
26	1H	2485	G	C8-N9-C4	6.01	108.80	106.40
26	14	596	G	N1-C2-N2	6.01	121.61	116.20
26	1H	1858	G	P-O3'-C3'	6.00	126.91	119.70
22	1K	75	C	C5-C6-N1	6.00	124.00	121.00
26	1H	23	G	N1-C2-N2	6.00	121.60	116.20
27	16	47	C	C6-N1-C2	6.00	122.70	120.30
26	1H	585	G	O5'-P-OP2	6.00	117.90	110.70
26	14	2394	C	O5'-P-OP2	-6.00	100.30	105.70
26	1H	245	G	C5-C6-O6	-6.00	125.00	128.60
26	14	1643	G	OP2-P-O3'	6.00	118.40	105.20
26	1H	74	A	N1-C6-N6	6.00	122.20	118.60
26	1H	516	C	C6-N1-C2	-6.00	117.90	120.30
26	1H	2609	U	O5'-P-OP2	-6.00	100.30	105.70
26	1H	142	G	C2-N3-C4	-6.00	108.90	111.90
26	14	1255	U	N1-C2-O2	6.00	127.00	122.80
26	14	2473	U	N3-C2-O2	-6.00	118.00	122.20
26	1H	2084	C	C5-C6-N1	-5.99	118.00	121.00
26	1H	2430	A	C6-C5-N7	-5.99	128.10	132.30
26	1H	832	G	C8-N9-C4	-5.99	104.00	106.40
26	1H	1193	G	C8-N9-C4	5.99	108.80	106.40
26	14	1762	A	C4-N9-C1'	5.99	137.09	126.30
26	1H	113	G	N3-C2-N2	-5.99	115.71	119.90
26	1H	392	C	O5'-P-OP2	5.99	117.89	110.70
26	14	944	G	N3-C4-N9	5.99	129.59	126.00
26	14	621	A	N1-C2-N3	5.99	132.29	129.30
26	14	675	A	N9-C4-C5	-5.99	103.41	105.80
1	1G	687	A	P-O3'-C3'	5.99	126.88	119.70
1	1G	1200	C	C2-N1-C1'	5.99	125.39	118.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	14	1905	C	O5'-P-OP2	-5.99	100.31	105.70
26	1H	2507	C	C2-N1-C1'	5.98	125.38	118.80
26	14	1496	A	C6-C5-N7	-5.98	128.11	132.30
26	1H	2346	A	C8-N9-C1'	-5.98	116.93	127.70
26	14	704	G	N1-C6-O6	5.98	123.49	119.90
26	1H	655	A	C5-N7-C8	-5.98	100.91	103.90
26	1H	1893	C	O5'-P-OP2	-5.98	100.32	105.70
26	1H	124	G	N3-C4-N9	-5.98	122.41	126.00
26	1H	240	G	N9-C4-C5	-5.98	103.01	105.40
26	14	2238	G	OP1-P-O3'	5.98	118.35	105.20
26	1H	1399	C	OP2-P-O3'	5.98	118.35	105.20
26	14	1251	C	N3-C4-N4	5.98	122.18	118.00
26	1H	1022	G	C4-C5-N7	-5.97	108.41	110.80
26	1H	1027	A	C2-N3-C4	-5.97	107.61	110.60
26	1H	1314	C	C6-N1-C1'	-5.97	113.63	120.80
45	F8	70	LEU	CA-CB-CG	5.97	129.04	115.30
1	13	505	G	C4-C5-N7	5.97	113.19	110.80
26	1H	917	A	O5'-P-OP2	5.97	117.87	110.70
26	14	459	U	O5'-P-OP2	-5.97	100.33	105.70
26	14	2213	U	C2-N1-C1'	5.97	124.86	117.70
1	13	1158	C	N1-C2-O2	5.97	122.48	118.90
26	14	530	G	N9-C4-C5	-5.97	103.01	105.40
26	14	1657	C	C6-N1-C2	-5.97	117.91	120.30
26	14	2713	A	C8-N9-C4	-5.97	103.41	105.80
26	1H	2235	G	C4-C5-N7	5.96	113.19	110.80
26	1H	2277	G	C5-N7-C8	5.96	107.28	104.30
26	1H	789	A	O5'-P-OP1	-5.96	100.33	105.70
26	1H	1785	A	OP2-P-O3'	5.96	118.31	105.20
27	16	60	C	C6-N1-C2	-5.96	117.92	120.30
26	14	1767	C	N3-C4-N4	-5.96	113.83	118.00
27	1J	7	G	N9-C4-C5	-5.96	103.02	105.40
26	14	829	A	OP1-P-OP2	5.96	128.54	119.60
26	14	944	G	C8-N9-C1'	-5.96	119.25	127.00
26	14	1617	C	C4-C5-C6	5.96	120.38	117.40
26	14	960	A	OP1-P-O3'	5.96	118.31	105.20
1	13	911	U	N3-C2-O2	-5.95	118.03	122.20
26	1H	141(A)	C	OP1-P-O3'	-5.95	92.10	105.20
26	1H	209	C	N3-C4-C5	5.95	124.28	121.90
26	1H	247	G	C5-C6-O6	-5.95	125.03	128.60
26	1H	807	U	OP1-P-OP2	5.95	128.53	119.60
26	1H	2611	U	N3-C4-O4	-5.95	115.23	119.40
1	1G	449	C	C5-C4-N4	5.95	124.37	120.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	14	445	C	O5'-P-OP1	-5.95	100.34	105.70
26	14	2599	G	OP2-P-O3'	5.95	118.30	105.20
26	1H	337	C	N1-C2-O2	-5.95	115.33	118.90
26	1H	1757	U	OP1-P-O3'	5.95	118.29	105.20
1	13	897	C	C5-C6-N1	-5.95	118.03	121.00
26	1H	1773	A	C5-C6-N1	-5.95	114.72	117.70
26	1H	2031	A	C2-N3-C4	5.95	113.57	110.60
26	14	1616	A	C6-C5-N7	-5.95	128.14	132.30
26	14	2085	C	O5'-P-OP2	-5.95	100.35	105.70
26	14	2256	G	N1-C2-N2	-5.95	110.85	116.20
1	13	1498	U	P-O3'-C3'	5.95	126.83	119.70
23	2K	9	G	C5-C6-O6	-5.95	125.03	128.60
26	14	380	U	O5'-P-OP2	-5.95	100.35	105.70
26	14	2440	C	O5'-P-OP1	-5.95	100.35	105.70
26	1H	247	G	C8-N9-C4	5.94	108.78	106.40
26	1H	273(A)	G	C8-N9-C4	5.94	108.78	106.40
26	1H	1437	C	C2-N1-C1'	5.94	125.34	118.80
26	1H	2554	U	C5-C4-O4	-5.94	122.33	125.90
1	1G	27	G	N3-C2-N2	-5.94	115.74	119.90
1	13	1199	U	N1-C2-N3	5.94	118.46	114.90
26	1H	128	C	N1-C2-O2	5.94	122.47	118.90
26	1H	1625	C	N3-C4-N4	-5.94	113.84	118.00
1	1G	917	G	O5'-P-OP1	-5.94	100.35	105.70
26	14	1639	U	N3-C4-O4	-5.94	115.24	119.40
26	14	1807	G	N9-C1'-C2'	-5.94	105.47	112.00
26	1H	1699	G	O5'-P-OP1	-5.94	100.36	105.70
1	1G	413	G	C8-N9-C1'	5.94	134.72	127.00
26	1H	263	C	O5'-P-OP1	5.94	117.83	110.70
26	1H	815	C	N3-C4-C5	5.94	124.28	121.90
26	1H	2610	C	O5'-P-OP1	-5.94	100.36	105.70
26	14	577	G	C8-N9-C4	5.94	108.78	106.40
26	1H	2754	U	C5-C4-O4	-5.93	122.34	125.90
1	13	917	G	OP1-P-O3'	5.93	118.25	105.20
26	1H	1685	C	O5'-P-OP2	5.93	117.82	110.70
1	1G	422	C	O4'-C1'-N1	5.93	112.94	108.20
1	1G	1157	A	P-O3'-C3'	5.93	126.82	119.70
26	14	2069	G	C8-N9-C4	5.93	108.77	106.40
1	13	827	U	N3-C2-O2	-5.93	118.05	122.20
26	1H	861	A	N9-C4-C5	-5.93	103.43	105.80
26	1H	1604	C	O5'-P-OP2	5.93	117.81	110.70
26	1H	741	G	C5-C6-O6	-5.93	125.04	128.60
26	1H	120	U	O5'-P-OP2	5.93	117.81	110.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	383	U	O5'-P-OP2	5.93	117.81	110.70
26	1H	1931	U	N1-C2-N3	5.93	118.46	114.90
26	1H	376	C	N3-C2-O2	-5.92	117.75	121.90
26	1H	463	G	N3-C2-N2	5.92	124.05	119.90
26	1H	795	C	O5'-P-OP2	-5.92	100.37	105.70
1	13	1199	U	N3-C2-O2	-5.92	118.06	122.20
26	14	2518	A	O4'-C1'-N9	-5.92	103.46	108.20
26	14	1992	G	N3-C4-C5	-5.92	125.64	128.60
26	14	2244	U	C4-C5-C6	5.92	123.25	119.70
26	14	2592	G	N1-C2-N2	-5.92	110.87	116.20
1	13	1129	C	C5-C6-N1	5.92	123.96	121.00
26	1H	1957	C	N3-C4-N4	-5.92	113.86	118.00
26	1H	2388	A	O4'-C1'-N9	5.92	112.93	108.20
23	2L	48	U	P-O3'-C3'	5.92	126.80	119.70
26	14	988	A	N1-C6-N6	5.92	122.15	118.60
26	14	2596	U	OP1-P-OP2	5.92	128.47	119.60
26	1H	859	G	N3-C4-C5	5.91	131.56	128.60
26	1H	2072	G	OP1-P-O3'	5.91	118.21	105.20
27	16	79	C	N3-C2-O2	-5.91	117.76	121.90
41	B8	13	ARG	N-CA-C	5.91	126.97	111.00
26	14	1963	U	C5-C6-N1	5.91	125.66	122.70
27	1J	47	C	OP1-P-O3'	5.91	118.21	105.20
26	1H	816	C	N3-C4-N4	5.91	122.14	118.00
26	1H	1137	G	OP1-P-O3'	5.91	118.20	105.20
26	1H	2837	G	N7-C8-N9	5.91	116.06	113.10
26	14	1496	A	O4'-C1'-N9	5.91	112.93	108.20
4	3E	11	LEU	CA-CB-CG	5.91	128.89	115.30
1	1G	1281	U	N1-C2-O2	5.91	126.94	122.80
26	14	2598	A	OP2-P-O3'	5.91	118.20	105.20
26	14	2607	G	N3-C4-N9	5.91	129.54	126.00
26	1H	2699	C	C5-C4-N4	-5.91	116.06	120.20
26	1H	1825	A	N1-C6-N6	-5.91	115.06	118.60
25	4L	23	A	P-O3'-C3'	5.91	126.79	119.70
26	14	1786	A	C4-N9-C1'	5.91	136.93	126.30
26	14	1815	A	OP1-P-O3'	5.91	118.19	105.20
26	1H	1315	C	N1-C2-O2	5.90	122.44	118.90
26	1H	1520	U	N3-C2-O2	-5.90	118.07	122.20
26	1H	189	G	C5-C6-O6	-5.90	125.06	128.60
1	1G	1301	U	C2-N1-C1'	5.90	124.78	117.70
26	14	1506	C	C6-N1-C2	-5.90	117.94	120.30
26	14	1762	A	N9-C1'-C2'	5.90	121.67	114.00
26	14	512	G	O4'-C1'-N9	5.90	112.92	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	857	C	O5'-P-OP2	-5.90	100.39	105.70
26	1H	1674	G	O4'-C1'-N9	-5.90	103.48	108.20
26	14	1304	C	C5-C4-N4	5.90	124.33	120.20
26	1H	929	G	N9-C4-C5	-5.90	103.04	105.40
26	1H	1376	C	N3-C4-C5	-5.90	119.54	121.90
26	1H	1649	G	N3-C4-C5	-5.90	125.65	128.60
26	14	1304	C	N3-C2-O2	-5.90	117.77	121.90
26	1H	1534	G	C4-N9-C1'	5.89	134.16	126.50
26	1H	2848	G	O5'-P-OP2	-5.89	100.40	105.70
26	1H	835	A	O5'-P-OP1	5.89	117.77	110.70
26	1H	1432	C	N3-C4-N4	5.89	122.12	118.00
1	1G	481	G	N3-C4-N9	5.89	129.53	126.00
26	14	946	G	N9-C4-C5	-5.89	103.04	105.40
26	1H	2450	A	N7-C8-N9	5.89	116.75	113.80
26	1H	2507	C	C5-C6-N1	5.89	123.94	121.00
26	14	750	A	N7-C8-N9	5.89	116.75	113.80
26	1H	598	G	O5'-P-OP2	-5.89	100.40	105.70
26	1H	2518	A	C5-C6-N6	-5.89	118.99	123.70
26	1H	952	G	N3-C2-N2	5.89	124.02	119.90
26	1H	1618	A	C8-N9-C4	-5.89	103.44	105.80
26	1H	1776	G	N9-C4-C5	-5.89	103.05	105.40
26	1H	1899	G	C8-N9-C4	-5.89	104.05	106.40
26	14	2597	G	C6-C5-N7	-5.89	126.87	130.40
26	1H	1585	C	C4-C5-C6	5.88	120.34	117.40
26	14	693	C	OP2-P-O3'	5.88	118.15	105.20
26	14	2413	G	N1-C6-O6	5.88	123.43	119.90
26	1H	112	U	C5-C4-O4	-5.88	122.37	125.90
26	1H	455	C	C6-N1-C2	5.88	122.65	120.30
26	1H	2374	C	C6-N1-C2	5.88	122.65	120.30
26	14	1350	C	O5'-P-OP1	-5.88	100.41	105.70
26	14	2573	C	N1-C2-O2	5.88	122.43	118.90
27	1J	89	G	N3-C4-N9	5.88	129.53	126.00
26	1H	138	G	O4'-C1'-N9	5.88	112.90	108.20
26	14	2724	C	OP2-P-O3'	5.88	118.13	105.20
1	13	905	U	O5'-P-OP2	5.88	117.75	110.70
26	1H	1301	A	C5-C6-N6	-5.87	119.00	123.70
26	1H	1915	U	N3-C2-O2	-5.87	118.09	122.20
1	13	872	A	C6-N1-C2	5.87	122.12	118.60
26	1H	136	G	N1-C6-O6	-5.87	116.38	119.90
26	14	1899	G	C5-C6-O6	5.87	132.12	128.60
27	1J	54	G	C8-N9-C4	-5.87	104.05	106.40
26	1H	99	U	C2-N1-C1'	5.87	124.74	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	378	C	C6-N1-C2	5.87	122.65	120.30
26	1H	1396	U	OP1-P-OP2	5.87	128.40	119.60
26	1H	1672	C	O5'-P-OP2	5.87	117.74	110.70
26	1H	2618	G	C8-N9-C4	-5.87	104.05	106.40
26	14	1939	U	N3-C4-O4	-5.87	115.29	119.40
26	1H	2297	C	OP1-P-OP2	5.87	128.40	119.60
1	1G	817	C	C5-C6-N1	-5.87	118.07	121.00
26	14	953	A	OP1-P-O3'	5.87	118.11	105.20
26	1H	2270	G	C5-C6-O6	-5.87	125.08	128.60
1	13	57	G	N1-C6-O6	-5.86	116.38	119.90
26	1H	66	C	C6-N1-C2	-5.86	117.95	120.30
26	1H	1379	A	C4-C5-N7	5.86	113.63	110.70
26	14	1022	G	C8-N9-C4	-5.86	104.05	106.40
26	14	1902	C	O5'-P-OP2	5.86	117.74	110.70
26	14	2055	C	C2-N1-C1'	-5.86	112.35	118.80
26	1H	226	G	C5-C6-O6	-5.86	125.08	128.60
26	1H	906	G	C8-N9-C1'	5.86	134.62	127.00
26	1H	1940	U	O5'-P-OP2	-5.86	100.42	105.70
26	1H	2574	G	C5-C6-N1	5.86	114.43	111.50
26	14	2270	G	C4-C5-N7	5.86	113.14	110.80
26	1H	2589	A	N7-C8-N9	-5.86	110.87	113.80
26	1H	2752	C	C5-C6-N1	5.86	123.93	121.00
26	1H	674	G	C8-N9-C4	5.86	108.74	106.40
26	1H	2324	C	C5-C4-N4	-5.86	116.10	120.20
26	14	1342	A	N1-C6-N6	5.86	122.11	118.60
47	D5	76	LEU	CA-CB-CG	5.86	128.78	115.30
1	13	703	G	C4-N9-C1'	5.86	134.12	126.50
1	13	1335	C	C6-N1-C2	5.86	122.64	120.30
26	1H	48	G	OP2-P-O3'	5.86	118.09	105.20
26	1H	74	A	O4'-C1'-N9	-5.86	103.51	108.20
26	14	2841	C	C6-N1-C2	5.86	122.64	120.30
26	1H	2582	G	O5'-P-OP1	5.85	117.72	110.70
26	1H	383	U	C5-C6-N1	-5.85	119.78	122.70
26	14	676	A	N3-C4-N9	-5.85	122.72	127.40
26	14	1973	G	N1-C2-N2	-5.85	110.94	116.20
1	13	22	G	N3-C2-N2	-5.85	115.81	119.90
26	14	1520	U	C5-C4-O4	5.85	129.41	125.90
26	14	2415	G	N3-C2-N2	-5.85	115.81	119.90
26	1H	2374	C	C2-N3-C4	-5.85	116.98	119.90
26	1H	2392	A	C6-N1-C2	5.84	122.11	118.60
27	16	98	G	OP1-P-OP2	5.84	128.37	119.60
26	1H	265	A	C5-N7-C8	-5.84	100.98	103.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	14	808	G	N3-C4-C5	-5.84	125.68	128.60
26	1H	786	C	N3-C2-O2	-5.84	117.81	121.90
26	1H	836	G	C2-N3-C4	5.84	114.82	111.90
26	1H	1601	G	OP1-P-O3'	5.84	118.05	105.20
1	13	942	G	OP1-P-O3'	5.84	118.05	105.20
26	14	1819	A	P-O3'-C3'	5.84	126.71	119.70
26	14	2347	C	N3-C2-O2	-5.84	117.81	121.90
26	14	2464	C	C5-C6-N1	-5.84	118.08	121.00
26	1H	1204	A	C4-C5-N7	5.84	113.62	110.70
27	1J	60	C	C5-C6-N1	5.84	123.92	121.00
26	1H	667	U	N3-C4-O4	5.84	123.48	119.40
26	1H	820	A	N1-C6-N6	-5.84	115.10	118.60
26	1H	1752	C	N3-C2-O2	5.84	125.98	121.90
26	1H	2449	U	OP2-P-O3'	5.84	118.04	105.20
26	14	2755	C	C2-N1-C1'	5.84	125.22	118.80
32	49	2	PRO	N-CA-CB	5.84	110.30	103.30
26	1H	1315	C	N3-C2-O2	-5.83	117.82	121.90
26	1H	1763	G	O5'-P-OP1	5.83	117.70	110.70
26	1H	2086	U	C5-C4-O4	5.83	129.40	125.90
26	1H	860	U	O5'-P-OP1	5.83	117.70	110.70
26	1H	1698	A	N3-C4-C5	5.83	130.88	126.80
1	13	802	A	N9-C4-C5	-5.83	103.47	105.80
1	13	1455	G	C8-N9-C4	5.83	108.73	106.40
26	1H	2069	G	C8-N9-C4	5.83	108.73	106.40
26	1H	2392	A	O4'-C1'-N9	5.83	112.86	108.20
12	3A	27	LEU	CA-CB-CG	5.83	128.71	115.30
26	14	1253	A	N9-C4-C5	-5.83	103.47	105.80
26	14	2067	G	N3-C4-C5	-5.83	125.69	128.60
26	1H	2510	C	C5-C4-N4	5.83	124.28	120.20
1	1G	495	A	N1-C6-N6	-5.83	115.10	118.60
1	1G	1338	G	N3-C4-C5	-5.83	125.69	128.60
26	14	793	A	N1-C6-N6	5.83	122.10	118.60
26	1H	1662	C	C2-N3-C4	-5.82	116.99	119.90
26	1H	1799	G	N1-C6-O6	-5.82	116.41	119.90
26	1H	2352	A	C8-N9-C4	5.82	108.13	105.80
26	1H	702	G	O5'-P-OP2	-5.82	100.46	105.70
26	14	1394	U	O5'-P-OP1	-5.82	100.46	105.70
24	3K	76	A	C5-C6-N6	-5.82	119.04	123.70
26	1H	863	A	O5'-P-OP1	5.82	117.68	110.70
27	16	77	U	C2-N3-C4	-5.82	123.51	127.00
26	14	428	A	C8-N9-C4	-5.82	103.47	105.80
26	1H	186	G	C2-N3-C4	5.82	114.81	111.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	761	A	O5'-P-OP2	5.82	117.68	110.70
26	1H	784	A	N9-C4-C5	5.82	108.13	105.80
26	1H	2377	A	C2-N3-C4	-5.82	107.69	110.60
26	14	330	A	C6-C5-N7	-5.82	128.23	132.30
26	14	2070	G	N1-C6-O6	-5.82	116.41	119.90
26	1H	716	A	C8-N9-C4	-5.82	103.47	105.80
26	1H	906	G	C6-C5-N7	5.82	133.89	130.40
26	1H	1396	U	N3-C2-O2	-5.82	118.13	122.20
55	P8	28	ARG	NE-CZ-NH1	5.82	123.21	120.30
26	1H	1660	C	C2-N3-C4	-5.81	116.99	119.90
31	31	32	LEU	CA-CB-CG	5.81	128.67	115.30
26	14	768	G	OP1-P-OP2	5.81	128.32	119.60
26	14	1266	G	C8-N9-C4	5.81	108.72	106.40
26	1H	62	C	C6-N1-C2	5.81	122.62	120.30
26	1H	1136	G	C5-C6-O6	-5.81	125.11	128.60
26	1H	1954	G	C5-C6-N1	-5.81	108.59	111.50
25	4L	14	A	O4'-C1'-N9	5.81	112.85	108.20
26	14	1762	A	N7-C8-N9	5.81	116.70	113.80
1	13	1065	U	P-O3'-C3'	5.81	126.67	119.70
26	14	213	A	C8-N9-C4	5.81	108.12	105.80
26	1H	687	C	C2-N3-C4	5.81	122.80	119.90
26	14	2685	G	N3-C4-N9	-5.81	122.52	126.00
26	1H	634	C	N3-C4-N4	-5.81	113.94	118.00
26	1H	2060	A	P-O3'-C3'	5.80	126.67	119.70
26	14	470	A	O5'-P-OP1	-5.80	100.48	105.70
26	14	1772	G	C6-C5-N7	-5.80	126.92	130.40
26	14	1970	A	O5'-P-OP2	-5.80	100.48	105.70
26	1H	969	U	N3-C4-O4	5.80	123.46	119.40
26	14	2741	A	C8-N9-C4	5.80	108.12	105.80
1	13	309	G	N3-C2-N2	-5.80	115.84	119.90
26	1H	1668	A	C2-N3-C4	5.80	113.50	110.60
26	1H	1957	C	C5-C4-N4	5.80	124.26	120.20
26	1H	2506	U	C5-C6-N1	5.80	125.60	122.70
1	13	509	A	C2'-C3'-O3'	5.80	122.97	113.70
26	1H	35	G	O5'-P-OP2	-5.80	100.48	105.70
26	1H	518	G	N1-C6-O6	-5.80	116.42	119.90
26	1H	762	U	C2-N1-C1'	5.80	124.66	117.70
1	1G	20	U	O5'-P-OP2	-5.80	100.48	105.70
1	1G	337	C	C5-C6-N1	5.80	123.90	121.00
26	14	1789	A	C6-N1-C2	-5.80	115.12	118.60
3	2E	188	LEU	CA-CB-CG	5.79	128.63	115.30
26	1H	210	C	C2-N3-C4	-5.79	117.00	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	14	2038	G	O5'-P-OP1	5.79	117.66	110.70
26	1H	1342	A	N1-C6-N6	5.79	122.08	118.60
26	1H	1396	U	O5'-P-OP1	-5.79	100.49	105.70
26	1H	1979	C	C6-N1-C2	-5.79	117.98	120.30
26	1H	2578	G	OP2-P-O3'	5.79	117.95	105.20
26	14	2258	C	C5-C6-N1	-5.79	118.10	121.00
26	1H	1272	A	O4'-C1'-N9	5.79	112.83	108.20
26	1H	1752	C	C2-N1-C1'	-5.79	112.43	118.80
26	14	1655	A	N7-C8-N9	-5.79	110.91	113.80
26	1H	812	C	C6-N1-C2	-5.79	117.98	120.30
26	1H	1379	A	C6-C5-N7	-5.79	128.25	132.30
26	1H	1803	A	C8-N9-C4	-5.79	103.48	105.80
26	1H	2351	G	N1-C6-O6	-5.79	116.43	119.90
26	14	783	A	C5-C6-N1	-5.79	114.81	117.70
27	1J	74	U	C5-C4-O4	5.79	129.37	125.90
26	1H	2041	U	O5'-P-OP1	-5.79	100.49	105.70
26	14	2623	G	C8-N9-C4	-5.79	104.09	106.40
26	1H	2260	C	N3-C4-C5	5.78	124.21	121.90
26	1H	2611	U	C5-C4-O4	5.78	129.37	125.90
1	13	792	A	C8-N9-C4	5.78	108.11	105.80
26	1H	766	C	C5-C6-N1	-5.78	118.11	121.00
26	14	187	G	N1-C6-O6	-5.78	116.43	119.90
26	14	571	A	C5-C6-N6	-5.78	119.08	123.70
26	1H	994	C	N1-C2-O2	-5.78	115.43	118.90
26	1H	1594	G	OP1-P-O3'	5.78	117.92	105.20
26	1H	683	C	C2-N3-C4	-5.78	117.01	119.90
26	14	180	G	C8-N9-C4	5.78	108.71	106.40
26	1H	137(A)	G	N3-C2-N2	-5.78	115.86	119.90
26	1H	1306	C	C5-C6-N1	-5.78	118.11	121.00
37	78	42	SER	C-N-CA	-5.77	110.17	122.30
26	14	769	G	N7-C8-N9	-5.77	110.21	113.10
1	13	437	U	C6-N1-C2	-5.77	117.54	121.00
26	1H	837	C	N3-C4-N4	5.77	122.04	118.00
1	1G	576	G	C4-C5-C6	5.77	122.26	118.80
26	14	1161	C	C5-C6-N1	5.77	123.89	121.00
26	1H	1377	G	O5'-P-OP2	-5.77	100.51	105.70
26	14	1899	G	C8-N9-C4	-5.77	104.09	106.40
26	1H	1660	C	N3-C4-N4	-5.77	113.96	118.00
26	14	444	C	OP2-P-O3'	5.77	117.89	105.20
26	1H	944	G	N7-C8-N9	5.77	115.98	113.10
26	1H	138	G	N9-C1'-C2'	5.76	121.50	114.00
26	1H	631	A	C5-N7-C8	5.76	106.78	103.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	1622	G	N3-C2-N2	-5.76	115.86	119.90
26	14	1694	C	O5'-P-OP1	-5.76	100.51	105.70
23	2K	1	C	C6-N1-C2	-5.76	118.00	120.30
26	1H	2249	U	C4-C5-C6	-5.76	116.24	119.70
26	1H	2287	A	N1-C2-N3	5.76	132.18	129.30
1	1G	18	C	O5'-P-OP1	-5.76	100.51	105.70
26	1H	180	G	C8-N9-C4	5.76	108.70	106.40
26	1H	1021	A	C5-C6-N1	-5.76	114.82	117.70
26	1H	2392	A	C8-N9-C4	-5.76	103.50	105.80
26	1H	2741	A	N1-C6-N6	5.76	122.06	118.60
24	3L	76	A	N1-C6-N6	5.76	122.06	118.60
26	14	2075	U	OP2-P-O3'	5.76	117.88	105.20
26	1H	482	A	C8-N9-C4	-5.76	103.50	105.80
26	14	207	A	N7-C8-N9	-5.76	110.92	113.80
26	1H	1936	A	N7-C8-N9	5.76	116.68	113.80
26	1H	2586	C	N1-C2-O2	-5.76	115.44	118.90
26	1H	2761	G	N1-C2-N3	5.76	127.36	123.90
26	14	740	U	O5'-P-OP1	5.76	117.61	110.70
26	14	2513	G	C8-N9-C4	-5.76	104.10	106.40
26	1H	768	G	OP1-P-OP2	5.76	128.24	119.60
26	1H	865	C	C6-N1-C2	5.76	122.60	120.30
26	1H	1189	A	N1-C6-N6	5.76	122.05	118.60
26	1H	1623	G	N1-C6-O6	-5.76	116.45	119.90
1	1G	1128	C	C5-C6-N1	5.76	123.88	121.00
26	14	752	A	OP2-P-O3'	5.76	117.87	105.20
26	14	2581	G	O4'-C1'-N9	5.75	112.80	108.20
26	1H	189	G	C2-N3-C4	-5.75	109.02	111.90
26	1H	1300	U	N1-C2-O2	-5.75	118.77	122.80
26	1H	2766	G	C8-N9-C4	-5.75	104.10	106.40
29	11	260	ARG	NE-CZ-NH1	5.75	123.18	120.30
26	14	1372	U	N1-C2-N3	5.75	118.35	114.90
26	1H	2253	G	N1-C6-O6	5.75	123.35	119.90
26	14	773	U	C5-C6-N1	-5.75	119.83	122.70
26	14	974(A)	C	N3-C2-O2	-5.75	117.88	121.90
26	14	1241	A	O4'-C1'-N9	5.75	112.80	108.20
26	14	1315	C	C5-C4-N4	5.75	124.23	120.20
26	1H	659	C	C6-N1-C2	5.75	122.60	120.30
26	14	2776	A	P-O3'-C3'	5.75	126.60	119.70
26	1H	127	A	C5-C6-N6	-5.75	119.10	123.70
26	14	511	U	N3-C4-C5	-5.75	111.15	114.60
26	1H	664	C	C2-N3-C4	-5.75	117.03	119.90
26	1H	1382	G	N9-C4-C5	-5.75	103.10	105.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	14	1930	G	C4-C5-N7	-5.75	108.50	110.80
26	14	2688	U	N3-C4-O4	-5.75	115.38	119.40
26	14	1785	A	N7-C8-N9	5.75	116.67	113.80
26	14	2597	G	O5'-P-OP1	5.75	117.59	110.70
26	1H	145	G	C6-C5-N7	-5.74	126.95	130.40
26	1H	1310	G	N1-C2-N2	5.74	121.37	116.20
26	1H	1681	G	C4-C5-N7	5.74	113.10	110.80
37	78	61	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	1G	1397	C	C6-N1-C1'	-5.74	113.91	120.80
1	1G	1519	A	C8-N9-C4	-5.74	103.50	105.80
26	14	265	A	C2-N3-C4	-5.74	107.73	110.60
26	14	792	G	N1-C6-O6	-5.74	116.45	119.90
26	14	786	C	C2-N3-C4	-5.74	117.03	119.90
26	1H	1561	G	C8-N9-C4	-5.74	104.10	106.40
26	1H	2052	G	C5-C6-O6	5.74	132.04	128.60
26	1H	2497	A	C4-C5-C6	5.74	119.87	117.00
26	14	1142(A)	A	N1-C2-N3	5.74	132.17	129.30
26	1H	1204	A	N3-C4-C5	5.74	130.82	126.80
26	1H	2244	U	N1-C2-N3	5.74	118.34	114.90
26	1H	2550	G	N3-C4-C5	-5.74	125.73	128.60
27	16	80	U	N3-C2-O2	-5.74	118.18	122.20
26	14	2870	C	C6-N1-C2	-5.74	118.00	120.30
1	13	760	G	N1-C6-O6	5.74	123.34	119.90
1	13	1468	A	C5-C6-N1	5.74	120.57	117.70
26	1H	839	U	C5-C4-O4	5.74	129.34	125.90
26	1H	2743	C	N1-C2-O2	-5.74	115.46	118.90
26	1H	2821	A	C5-C6-N6	-5.74	119.11	123.70
26	14	743	G	C8-N9-C4	5.74	108.69	106.40
26	1H	1191	G	O5'-P-OP1	-5.73	100.54	105.70
26	14	1779	U	O4'-C1'-N1	5.73	112.79	108.20
26	14	2287	A	C8-N9-C4	5.73	108.09	105.80
26	1H	463	G	C8-N9-C4	5.73	108.69	106.40
26	1H	1673	U	C2-N3-C4	-5.73	123.56	127.00
1	1G	1200	C	N1-C2-O2	5.73	122.34	118.90
26	14	1558	A	P-O3'-C3'	5.73	126.58	119.70
26	1H	1310	G	C5-C6-O6	-5.73	125.16	128.60
26	14	2323	G	C8-N9-C4	5.73	108.69	106.40
26	1H	1204	A	N1-C6-N6	5.73	122.04	118.60
26	14	1209	G	OP1-P-OP2	5.73	128.19	119.60
26	1H	130	C	N3-C4-C5	5.72	124.19	121.90
26	1H	244	A	N1-C6-N6	5.72	122.03	118.60
26	1H	1357	U	O5'-P-OP2	-5.72	100.55	105.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	14	2688	U	C4-C5-C6	5.72	123.14	119.70
26	1H	59	U	N3-C4-C5	-5.72	111.17	114.60
26	1H	1365	A	C5-C6-N6	5.72	128.28	123.70
26	1H	1665	A	O5'-P-OP1	-5.72	100.55	105.70
26	1H	1777	U	C4-C5-C6	5.72	123.13	119.70
26	14	828	U	N3-C4-C5	-5.72	111.17	114.60
26	14	2582	G	C6-C5-N7	-5.72	126.97	130.40
1	13	505	G	C5-N7-C8	-5.72	101.44	104.30
26	1H	399	G	N1-C6-O6	-5.72	116.47	119.90
26	1H	966	G	N3-C2-N2	5.72	123.90	119.90
26	1H	270(L)	U	C5-C6-N1	5.72	125.56	122.70
26	14	2413	G	C5-C6-O6	-5.72	125.17	128.60
1	13	1486	G	O5'-P-OP2	-5.71	100.56	105.70
26	1H	117	G	N3-C4-N9	5.71	129.43	126.00
26	1H	859	G	C4-N9-C1'	-5.71	119.07	126.50
26	14	1790	C	OP1-P-O3'	5.71	117.77	105.20
26	1H	2067	G	N3-C4-N9	-5.71	122.57	126.00
26	1H	2073	C	C4-C5-C6	5.71	120.26	117.40
1	13	560	U	P-O3'-C3'	5.71	126.55	119.70
26	1H	1307	A	N1-C6-N6	5.71	122.03	118.60
26	14	1527	G	N3-C2-N2	-5.71	115.90	119.90
26	14	1351	C	C5-C6-N1	-5.71	118.15	121.00
26	14	1585	C	N3-C2-O2	-5.71	117.90	121.90
26	14	577	G	C5-C6-O6	-5.71	125.18	128.60
26	14	1427	A	C6-N1-C2	-5.71	115.18	118.60
26	14	503	A	N9-C4-C5	5.70	108.08	105.80
26	14	788	A	C5-C6-N6	-5.70	119.14	123.70
26	14	954	G	N1-C6-O6	-5.70	116.48	119.90
26	14	1297	C	OP2-P-O3'	-5.70	92.65	105.20
26	1H	1888	G	N3-C4-C5	-5.70	125.75	128.60
1	13	169	C	C6-N1-C2	-5.70	118.02	120.30
1	13	703	G	C5-C6-O6	-5.70	125.18	128.60
26	1H	2367	G	N7-C8-N9	5.70	115.95	113.10
1	1G	503	C	N3-C4-C5	-5.70	119.62	121.90
26	14	137	C	N3-C4-C5	-5.70	119.62	121.90
26	14	2544	G	C5-C6-O6	-5.70	125.18	128.60
26	14	2767	C	C6-N1-C2	-5.70	118.02	120.30
26	1H	1324	G	N1-C2-N2	5.69	121.33	116.20
26	1H	758	C	N3-C4-C5	5.69	124.18	121.90
26	1H	1253	A	C5-N7-C8	5.69	106.75	103.90
27	1J	114	G	C8-N9-C4	5.69	108.68	106.40
26	1H	961	C	O4'-C1'-N1	5.69	112.75	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	2572	A	N7-C8-N9	-5.69	110.95	113.80
26	14	1937	A	O4'-C1'-N9	5.69	112.75	108.20
26	14	1985	G	O5'-P-OP2	-5.69	100.58	105.70
1	13	108	G	N9-C4-C5	-5.69	103.12	105.40
26	1H	452	G	N1-C6-O6	-5.69	116.49	119.90
31	39	125	LEU	CA-CB-CG	5.69	128.38	115.30
1	1G	1528	U	C6-N1-C2	5.69	124.41	121.00
26	14	774	A	O5'-P-OP2	-5.69	100.58	105.70
26	14	2057	A	C5-C6-N6	-5.69	119.15	123.70
37	78	45	LEU	CA-CB-CG	5.69	128.38	115.30
26	14	1349	A	C5-N7-C8	-5.69	101.06	103.90
26	14	2063	C	OP2-P-O3'	5.69	117.71	105.20
26	14	2325	G	N3-C2-N2	-5.69	115.92	119.90
26	1H	80	G	C8-N9-C4	-5.68	104.13	106.40
26	1H	110	G	OP1-P-OP2	5.68	128.13	119.60
26	1H	240	G	N1-C6-O6	5.68	123.31	119.90
26	14	1728	G	N3-C4-N9	5.68	129.41	126.00
26	14	1762	A	C4-C5-C6	5.68	119.84	117.00
26	14	1764	G	O5'-P-OP2	-5.68	100.58	105.70
26	1H	513	A	C8-N9-C4	-5.68	103.53	105.80
26	1H	2434	A	OP2-P-O3'	5.68	117.70	105.20
53	N8	16	ARG	NE-CZ-NH1	5.68	123.14	120.30
26	1H	573	G	C2-N3-C4	5.68	114.74	111.90
26	14	769	G	C8-N9-C4	5.68	108.67	106.40
26	14	1313	U	N1-C2-O2	-5.68	118.82	122.80
26	1H	2622	C	OP2-P-O3'	5.68	117.69	105.20
26	1H	2697	G	C5-C6-O6	5.68	132.01	128.60
26	14	2238	G	P-O3'-C3'	5.68	126.52	119.70
26	1H	116	C	OP2-P-O3'	5.68	117.69	105.20
26	1H	1996	C	C5-C6-N1	-5.68	118.16	121.00
26	1H	958	U	C6-N1-C2	-5.68	117.59	121.00
26	14	1781	C	C6-N1-C1'	-5.68	113.99	120.80
26	1H	621	A	O4'-C1'-N9	5.67	112.74	108.20
26	14	1964	G	N1-C6-O6	-5.67	116.50	119.90
26	1H	614	U	C6-N1-C2	-5.67	117.60	121.00
26	1H	937	U	O5'-P-OP1	5.67	117.51	110.70
26	1H	1776	G	OP1-P-O3'	5.67	117.68	105.20
39	98	75	LEU	CA-CB-CG	5.67	128.34	115.30
26	14	581	C	N3-C4-N4	-5.67	114.03	118.00
26	1H	207	A	C4-C5-N7	5.67	113.53	110.70
26	1H	664	C	N3-C4-N4	-5.67	114.03	118.00
26	1H	2458	G	N1-C6-O6	5.67	123.30	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	2367	G	C8-N9-C4	-5.67	104.13	106.40
26	1H	2442	C	C2-N3-C4	-5.67	117.07	119.90
26	14	824	A	C8-N9-C4	5.67	108.07	105.80
26	14	1824	G	O5'-P-OP2	-5.67	100.60	105.70
26	14	2032	G	C8-N9-C4	5.67	108.67	106.40
26	14	2256	G	O5'-P-OP2	-5.67	100.60	105.70
26	14	2598	A	N9-C4-C5	-5.67	103.53	105.80
26	14	2763	G	N3-C4-C5	-5.67	125.77	128.60
26	1H	144	C	C2-N3-C4	-5.67	117.07	119.90
26	1H	399	G	C5-C6-N1	5.67	114.33	111.50
26	1H	953	A	O5'-P-OP1	-5.67	100.60	105.70
26	1H	2392	A	C5-C6-N1	-5.67	114.87	117.70
26	1H	2493	U	C5-C6-N1	-5.67	119.87	122.70
26	14	933	A	N7-C8-N9	5.67	116.63	113.80
26	14	1204	A	O4'-C1'-N9	5.67	112.73	108.20
26	14	675	A	C8-N9-C4	5.67	108.07	105.80
26	14	2629	A	C2-N3-C4	5.67	113.43	110.60
26	1H	2392	A	OP1-P-OP2	-5.66	111.11	119.60
29	19	272	ALA	C-N-CA	5.66	135.86	121.70
26	1H	2266	A	N1-C2-N3	5.66	132.13	129.30
26	1H	560	C	O5'-P-OP2	5.66	117.49	110.70
26	1H	866	A	C4-N9-C1'	5.66	136.49	126.30
26	1H	1936	A	O4'-C1'-N9	5.66	112.73	108.20
27	1J	22	U	C6-N1-C2	-5.66	117.60	121.00
26	1H	180	G	N3-C2-N2	5.66	123.86	119.90
26	1H	770	G	N1-C6-O6	5.66	123.30	119.90
26	1H	1415	U	C5-C4-O4	5.66	129.30	125.90
26	1H	753	C	N1-C2-O2	5.66	122.29	118.90
26	1H	2016	U	C5-C6-N1	-5.66	119.87	122.70
26	14	2030	A	OP1-P-OP2	5.66	128.09	119.60
26	14	2067	G	C4-C5-N7	-5.66	108.54	110.80
26	14	740	U	O5'-P-OP2	-5.66	100.61	105.70
26	14	1271	G	C8-N9-C4	5.66	108.66	106.40
26	1H	1899	G	OP2-P-O3'	5.65	117.64	105.20
40	65	101	LEU	CA-CB-CG	5.65	128.30	115.30
26	1H	1437	C	N1-C2-O2	5.65	122.29	118.90
26	1H	1761	C	N1-C2-O2	-5.65	115.51	118.90
26	1H	1804	C	N3-C4-N4	-5.65	114.04	118.00
26	1H	963	U	O5'-P-OP2	5.65	117.48	110.70
26	1H	2519	U	N1-C2-O2	-5.65	118.84	122.80
26	14	678	C	N3-C4-C5	5.65	124.16	121.90
26	1H	1081	U	P-O3'-C3'	5.65	126.48	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	2572	A	C5-C6-N6	-5.65	119.18	123.70
26	14	1661	G	C8-N9-C4	5.65	108.66	106.40
26	14	1780	A	O5'-P-OP1	5.65	117.48	110.70
26	1H	1564	C	N3-C4-N4	-5.65	114.05	118.00
26	1H	1752	C	N1-C2-O2	-5.65	115.51	118.90
26	1H	2258	C	C5-C4-N4	-5.64	116.25	120.20
26	1H	2497	A	C6-N1-C2	-5.64	115.21	118.60
38	88	24	GLY	N-CA-C	-5.64	98.99	113.10
1	13	527	G	N1-C6-O6	-5.64	116.52	119.90
26	1H	1446	C	C6-N1-C2	-5.64	118.04	120.30
26	1H	2848	G	O4'-C1'-N9	5.64	112.72	108.20
1	1G	115	G	P-O3'-C3'	5.64	126.47	119.70
26	1H	2712	U	P-O3'-C3'	5.64	126.47	119.70
26	1H	1241	A	N3-C4-C5	5.64	130.75	126.80
26	14	2436	G	N3-C2-N2	-5.64	115.95	119.90
26	1H	944	G	C5-C6-N1	-5.64	108.68	111.50
26	14	1142	U	C6-N1-C1'	-5.64	113.31	121.20
1	13	1506	U	C5-C4-O4	-5.64	122.52	125.90
26	1H	2584	U	N1-C2-O2	5.64	126.75	122.80
41	75	13	ARG	N-CA-C	-5.64	95.78	111.00
1	13	11	G	OP1-P-O3'	5.63	117.59	105.20
1	13	326	G	C5-C6-O6	5.63	131.98	128.60
1	13	1319	A	O5'-P-OP2	-5.63	100.63	105.70
26	1H	508	G	N3-C2-N2	5.63	123.84	119.90
26	1H	622	G	C8-N9-C4	5.63	108.65	106.40
26	1H	1636	C	N1-C2-O2	-5.63	115.52	118.90
26	1H	2665	A	C2-N3-C4	-5.63	107.78	110.60
27	16	50	G	OP2-P-O3'	5.63	117.59	105.20
26	14	2779	U	N3-C4-O4	-5.63	115.45	119.40
26	1H	2555	U	O5'-P-OP1	-5.63	100.63	105.70
26	14	1332	G	C4-N9-C1'	5.63	133.82	126.50
1	1G	244	U	C5-C4-O4	-5.63	122.52	125.90
26	1H	1993	U	N1-C2-O2	-5.63	118.86	122.80
26	1H	1804	C	N3-C2-O2	-5.63	117.96	121.90
26	14	74	A	C4-C5-N7	5.63	113.51	110.70
26	14	621	A	N1-C6-N6	5.63	121.98	118.60
26	14	2056	G	OP1-P-O3'	5.63	117.58	105.20
1	13	1286	A	N7-C8-N9	5.62	116.61	113.80
26	1H	951	C	N3-C2-O2	-5.62	117.96	121.90
26	1H	1204	A	C6-C5-N7	-5.62	128.36	132.30
36	68	70	LYS	C-N-CA	5.62	135.76	121.70
1	13	913	A	P-O3'-C3'	5.62	126.45	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	14	913	U	O5'-P-OP2	-5.62	100.64	105.70
26	1H	141(A)	C	C6-N1-C2	5.62	122.55	120.30
26	1H	537	C	O5'-P-OP1	5.62	117.45	110.70
26	1H	2065	C	O5'-P-OP1	-5.62	100.64	105.70
26	1H	2380	C	C6-N1-C2	5.62	122.55	120.30
1	1G	180	U	C5-C6-N1	5.62	125.51	122.70
26	1H	258	G	O5'-P-OP2	-5.62	100.64	105.70
26	1H	1428	C	C6-N1-C2	5.62	122.55	120.30
26	14	574	C	N3-C4-N4	-5.62	114.07	118.00
26	1H	1367	A	C2-N3-C4	-5.62	107.79	110.60
26	14	2401	U	C6-N1-C2	-5.62	117.63	121.00
26	14	2065	C	N1-C2-O2	5.61	122.27	118.90
26	14	2589	A	N9-C4-C5	-5.61	103.56	105.80
26	1H	1375	C	OP1-P-O3'	5.61	117.55	105.20
26	14	2685	G	C4-C5-N7	-5.61	108.56	110.80
26	14	2707	G	C5-C6-N1	5.61	114.31	111.50
26	1H	240	G	C8-N9-C4	5.61	108.64	106.40
26	1H	330	A	N1-C2-N3	5.61	132.10	129.30
26	1H	1196	C	C6-N1-C2	5.61	122.54	120.30
26	1H	2578	G	C8-N9-C4	5.61	108.64	106.40
26	14	194	G	N1-C6-O6	5.61	123.27	119.90
26	14	1313	U	C5-C6-N1	5.61	125.51	122.70
26	14	1678	G	N9-C4-C5	5.61	107.64	105.40
1	13	652	U	O5'-P-OP1	-5.61	100.65	105.70
26	14	2554	U	O5'-P-OP2	5.61	117.43	110.70
1	13	328	C	O5'-P-OP1	-5.61	100.66	105.70
1	13	759	A	O5'-P-OP2	-5.61	100.66	105.70
26	1H	1800	C	N1-C2-N3	5.61	123.12	119.20
26	1H	2711	A	OP1-P-O3'	5.61	117.53	105.20
56	Q8	47	LYS	N-CA-C	-5.61	95.87	111.00
1	1G	576	G	N3-C4-N9	5.61	129.36	126.00
1	1G	700	G	N1-C6-O6	-5.61	116.54	119.90
26	1H	122	G	C8-N9-C4	5.60	108.64	106.40
26	1H	734	A	C2-N3-C4	-5.60	107.80	110.60
26	1H	1351	C	OP1-P-O3'	5.60	117.53	105.20
26	1H	2623	G	N7-C8-N9	5.60	115.90	113.10
44	A5	8	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	13	1517	G	O5'-P-OP2	-5.60	100.66	105.70
26	1H	688	U	C5-C6-N1	-5.60	119.90	122.70
26	1H	860	U	N1-C2-N3	5.60	118.26	114.90
26	1H	2303	G	OP1-P-O3'	5.60	117.52	105.20
26	14	528	A	C5-N7-C8	-5.60	101.10	103.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	14	1574	C	OP2-P-O3'	5.60	117.53	105.20
1	13	1158	C	N3-C2-O2	-5.60	117.98	121.90
26	1H	694	U	O5'-P-OP1	5.60	117.42	110.70
26	1H	1825	A	C2-N3-C4	5.60	113.40	110.60
26	1H	2329	G	C8-N9-C4	5.60	108.64	106.40
26	1H	2741	A	N9-C4-C5	-5.60	103.56	105.80
26	14	680	G	O5'-P-OP1	-5.60	100.66	105.70
26	14	2082	A	C5-C6-N6	-5.60	119.22	123.70
26	14	2415	G	OP1-P-O3'	5.60	117.52	105.20
26	1H	1993	U	C5-C6-N1	-5.60	119.90	122.70
26	1H	2438	U	C4-C5-C6	5.60	123.06	119.70
26	1H	2620	C	N3-C4-N4	-5.60	114.08	118.00
1	1G	271	C	C6-N1-C2	-5.60	118.06	120.30
26	1H	599	G	N3-C2-N2	5.59	123.81	119.90
26	1H	1984	G	N1-C6-O6	-5.59	116.54	119.90
26	1H	1997	G	O5'-P-OP2	-5.59	100.67	105.70
26	14	1930	G	C4-N9-C1'	-5.59	119.23	126.50
26	1H	405	U	C2-N1-C1'	5.59	124.41	117.70
26	1H	969	U	C5-C4-O4	-5.59	122.55	125.90
26	1H	1325	G	OP1-P-OP2	-5.59	111.21	119.60
26	1H	1379	A	C8-N9-C4	-5.59	103.56	105.80
26	14	2053	G	N1-C6-O6	5.59	123.25	119.90
26	1H	302	C	N3-C2-O2	-5.59	117.99	121.90
26	1H	335	C	C2-N3-C4	5.59	122.69	119.90
26	1H	1261	C	C6-N1-C2	5.59	122.54	120.30
26	1H	1574	C	C2-N3-C4	-5.59	117.11	119.90
26	1H	2321	G	O5'-P-OP1	5.59	117.41	110.70
26	14	2554	U	O5'-P-OP1	-5.59	100.67	105.70
26	1H	982	C	C6-N1-C2	-5.59	118.06	120.30
26	1H	2645	G	N3-C4-C5	5.59	131.39	128.60
26	14	1941	C	O5'-P-OP1	-5.59	100.67	105.70
26	1H	936	C	C5-C6-N1	-5.59	118.21	121.00
46	C5	103	GLY	N-CA-C	5.59	127.07	113.10
2	1E	158	LEU	CA-CB-CG	5.58	128.15	115.30
26	1H	1605	C	O5'-P-OP1	-5.58	100.67	105.70
26	1H	124	G	N1-C6-O6	5.58	123.25	119.90
26	1H	135	G	C5-N7-C8	5.58	107.09	104.30
26	1H	236	C	C5-C6-N1	-5.58	118.21	121.00
26	1H	687	C	C6-N1-C2	-5.58	118.07	120.30
26	14	2689	U	P-O3'-C3'	5.58	126.40	119.70
26	1H	929	G	C8-N9-C1'	-5.58	119.75	127.00
26	1H	1021	A	C6-C5-N7	-5.58	128.39	132.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	1141	U	O4'-C1'-N1	5.58	112.67	108.20
26	14	2373	G	OP1-P-OP2	5.58	127.97	119.60
1	1G	898	G	N3-C4-C5	5.58	131.39	128.60
27	1J	11	C	N1-C2-O2	5.58	122.25	118.90
1	13	35	G	C5-C6-N1	-5.58	108.71	111.50
1	13	974	A	C4-N9-C1'	5.58	136.34	126.30
26	1H	141	A	O4'-C1'-N9	5.58	112.66	108.20
26	1H	2257	U	C2-N3-C4	-5.58	123.65	127.00
26	1H	238	C	C5-C6-N1	-5.58	118.21	121.00
26	1H	673	C	OP1-P-OP2	-5.58	111.23	119.60
26	14	71	A	C6-C5-N7	-5.58	128.40	132.30
1	13	1299	A	C2-N3-C4	-5.58	107.81	110.60
26	1H	238	C	C4-C5-C6	5.58	120.19	117.40
26	1H	2031	A	C5-C6-N6	-5.58	119.24	123.70
26	14	2581	G	N1-C2-N2	-5.58	111.18	116.20
26	14	2607	G	O5'-P-OP1	5.58	117.39	110.70
1	13	481	G	C6-C5-N7	-5.57	127.06	130.40
26	14	130	C	N3-C4-C5	5.57	124.13	121.90
26	14	797	C	N3-C2-O2	5.57	125.80	121.90
26	1H	1332	G	O4'-C1'-N9	-5.57	103.74	108.20
26	1H	1669	A	C5-C6-N1	5.57	120.49	117.70
26	14	2565	A	C8-N9-C4	5.57	108.03	105.80
1	13	768	A	C6-N1-C2	-5.57	115.26	118.60
26	1H	335	C	C5-C6-N1	5.57	123.79	121.00
26	1H	1610	A	C6-C5-N7	-5.57	128.40	132.30
26	1H	2276	G	N3-C2-N2	-5.57	116.00	119.90
26	1H	2819	G	N1-C6-O6	5.57	123.24	119.90
27	16	6	C	N3-C4-N4	5.57	121.90	118.00
26	14	127	A	C5-C6-N6	-5.57	119.24	123.70
26	14	2003	G	N1-C6-O6	5.57	123.24	119.90
26	1H	621	A	N3-C4-N9	-5.57	122.94	127.40
26	1H	2064	C	N3-C2-O2	-5.57	118.00	121.90
1	13	690	G	N1-C6-O6	5.57	123.24	119.90
26	1H	127	A	N1-C6-N6	5.57	121.94	118.60
26	1H	1413	G	C8-N9-C4	-5.57	104.17	106.40
26	14	1351	C	C2-N3-C4	-5.57	117.12	119.90
26	14	2512	C	N3-C4-C5	5.57	124.13	121.90
26	1H	1573	G	OP2-P-O3'	5.57	117.44	105.20
26	1H	2064	C	OP1-P-O3'	5.57	117.44	105.20
1	1G	481	G	C8-N9-C1'	-5.57	119.77	127.00
26	14	668	G	N3-C4-C5	5.57	131.38	128.60
26	1H	1261	C	N3-C4-C5	5.56	124.12	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	420	C	C6-N1-C2	5.56	122.53	120.30
26	1H	1761	C	N3-C4-N4	5.56	121.89	118.00
26	1H	2469	A	N1-C6-N6	5.56	121.94	118.60
26	14	2281	C	O5'-P-OP2	5.56	117.38	110.70
1	13	802	A	C4-C5-N7	5.56	113.48	110.70
26	1H	2743	C	C2-N3-C4	-5.56	117.12	119.90
1	1G	413	G	C4-C5-N7	-5.56	108.58	110.80
26	14	1210	A	C5-N7-C8	-5.56	101.12	103.90
1	13	1279	A	C6-C5-N7	-5.56	128.41	132.30
26	1H	52	A	N1-C2-N3	-5.56	126.52	129.30
26	1H	500	G	O5'-P-OP1	-5.56	100.70	105.70
26	1H	2869	G	C8-N9-C4	-5.56	104.18	106.40
1	1G	906	G	C5-C6-O6	-5.56	125.26	128.60
26	14	2490	G	O4'-C1'-N9	5.56	112.65	108.20
26	1H	223	A	O5'-P-OP2	-5.56	100.70	105.70
27	16	98	G	C8-N9-C4	5.56	108.62	106.40
26	14	2276	G	O5'-P-OP1	-5.56	100.70	105.70
26	1H	1489	U	C5-C4-O4	5.56	129.23	125.90
26	14	214	G	C8-N9-C4	-5.55	104.18	106.40
26	14	1614	A	C5-C6-N1	-5.55	114.92	117.70
26	1H	1840	G	N3-C2-N2	-5.55	116.01	119.90
26	1H	2355	C	N3-C4-C5	5.55	124.12	121.90
26	14	1166	C	C6-N1-C2	-5.55	118.08	120.30
26	1H	463	G	N7-C8-N9	-5.55	110.32	113.10
26	1H	508	G	N3-C4-N9	5.55	129.33	126.00
26	1H	918	A	O5'-P-OP2	5.55	117.36	110.70
26	1H	2234	G	C8-N9-C4	5.55	108.62	106.40
26	1H	2544	G	C8-N9-C4	5.55	108.62	106.40
26	1H	915	C	OP1-P-OP2	-5.55	111.28	119.60
26	1H	1899	G	C5-N7-C8	-5.55	101.53	104.30
26	1H	2412	A	O5'-P-OP2	-5.55	100.70	105.70
26	14	945	A	N9-C1'-C2'	5.55	121.21	114.00
1	13	1158	C	C6-N1-C2	-5.55	118.08	120.30
26	1H	1939	U	N3-C4-C5	5.55	117.93	114.60
26	14	945	A	O4'-C1'-N9	5.55	112.64	108.20
26	1H	674	G	N9-C4-C5	-5.55	103.18	105.40
26	1H	1799	G	P-O3'-C3'	5.55	126.36	119.70
26	14	1918	A	N9-C4-C5	-5.55	103.58	105.80
26	1H	109	G	C5-C6-O6	5.54	131.93	128.60
26	1H	2469	A	C2-N3-C4	-5.54	107.83	110.60
26	14	1644	C	N1-C2-O2	5.54	122.22	118.90
26	14	2688	U	N1-C2-N3	5.54	118.22	114.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	14	2518	A	N7-C8-N9	5.54	116.57	113.80
26	1H	122	G	N7-C8-N9	-5.54	110.33	113.10
26	1H	129	C	C4-C5-C6	5.54	120.17	117.40
26	1H	683	C	C5-C4-N4	-5.54	116.32	120.20
26	1H	1032	A	N1-C2-N3	-5.54	126.53	129.30
26	1H	2276	G	C4-C5-N7	-5.54	108.58	110.80
37	78	18	ARG	NE-CZ-NH2	5.54	123.07	120.30
26	14	929	G	C4-C5-N7	5.54	113.02	110.80
1	13	1336	C	C5-C6-N1	5.54	123.77	121.00
26	1H	697	C	C5-C4-N4	-5.54	116.32	120.20
26	1H	2210	G	OP2-P-O3'	5.54	117.38	105.20
26	1H	1678	G	N3-C2-N2	-5.54	116.03	119.90
26	14	680	G	C6-C5-N7	-5.54	127.08	130.40
26	14	226	G	O4'-C1'-N9	5.53	112.63	108.20
1	13	67	C	C6-N1-C2	-5.53	118.09	120.30
26	1H	1900	A	OP1-P-OP2	-5.53	111.31	119.60
43	D8	18	LEU	CA-CB-CG	5.53	128.02	115.30
50	K8	3	LEU	C-N-CA	5.53	135.53	121.70
26	14	2576	G	OP1-P-OP2	-5.53	111.31	119.60
26	1H	1520	U	C5-C4-O4	5.53	129.22	125.90
26	14	1007	C	C6-N1-C2	-5.53	118.09	120.30
1	13	47	C	C4-C5-C6	5.53	120.16	117.40
1	13	336	C	N3-C2-O2	5.53	125.77	121.90
26	1H	74	A	N3-C4-C5	5.53	130.67	126.80
26	1H	2331	G	C8-N9-C4	5.53	108.61	106.40
1	1G	1405	G	C8-N9-C4	5.53	108.61	106.40
26	14	2307	G	O4'-C1'-N9	5.53	112.62	108.20
26	1H	1426	G	C5-C6-O6	-5.53	125.28	128.60
26	14	1444(A)	A	N1-C6-N6	-5.53	115.28	118.60
26	1H	209	C	C5-C6-N1	-5.52	118.24	121.00
26	1H	579	G	N3-C2-N2	-5.52	116.03	119.90
26	1H	1299	G	O5'-P-OP2	5.52	117.33	110.70
26	1H	1700	A	OP1-P-OP2	5.52	127.89	119.60
26	1H	1773	A	N9-C1'-C2'	-5.52	105.93	112.00
26	1H	2094	G	O5'-P-OP2	-5.52	100.73	105.70
26	14	774	A	C6-N1-C2	5.52	121.91	118.60
26	1H	2338	G	O5'-P-OP1	-5.52	100.73	105.70
26	14	726	G	O4'-C1'-N9	5.52	112.62	108.20
26	14	2699	C	C6-N1-C2	5.52	122.51	120.30
26	14	2871	C	O5'-P-OP2	-5.52	100.73	105.70
41	75	6	LEU	N-CA-C	-5.52	96.09	111.00
26	1H	716	A	N7-C8-N9	5.52	116.56	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	2574	G	C5-C6-O6	-5.52	125.29	128.60
26	14	779	U	N3-C4-O4	5.52	123.26	119.40
26	14	2700	C	N3-C4-C5	5.52	124.11	121.90
26	1H	194	G	N1-C6-O6	5.52	123.21	119.90
26	1H	816	C	N3-C4-C5	-5.52	119.69	121.90
26	1H	1571	A	C5-C6-N6	-5.52	119.28	123.70
26	1H	2376	A	C8-N9-C4	5.52	108.01	105.80
26	14	1780	A	N9-C4-C5	5.52	108.01	105.80
23	2K	24	C	C2-N3-C4	-5.51	117.14	119.90
26	1H	629	G	N1-C6-O6	-5.51	116.59	119.90
26	1H	1616	A	OP1-P-O3'	5.51	117.33	105.20
1	1G	913	A	P-O3'-C3'	5.51	126.31	119.70
1	13	121	C	C2-N1-C1'	5.51	124.86	118.80
26	1H	2269	A	C2-N3-C4	-5.51	107.84	110.60
26	1H	2590	A	C2-N3-C4	-5.51	107.84	110.60
26	14	2328	A	C6-N1-C2	-5.51	115.29	118.60
26	14	2427	C	C5-C4-N4	-5.51	116.34	120.20
26	1H	760	G	N9-C4-C5	-5.51	103.20	105.40
26	14	774	A	N9-C4-C5	-5.51	103.60	105.80
26	1H	1363	C	C5-C6-N1	-5.51	118.25	121.00
26	1H	2262	U	O5'-P-OP1	5.51	117.31	110.70
26	1H	2592	G	OP2-P-O3'	5.51	117.32	105.20
26	1H	226	G	N1-C6-O6	5.51	123.20	119.90
26	1H	698	C	O5'-P-OP2	-5.51	100.74	105.70
26	1H	813	U	OP1-P-OP2	5.51	127.86	119.60
26	1H	1407	C	OP1-P-O3'	5.51	117.31	105.20
26	14	1166	C	N3-C4-C5	-5.51	119.70	121.90
26	14	1365	A	C8-N9-C4	-5.51	103.60	105.80
26	14	2082	A	N1-C6-N6	5.51	121.90	118.60
26	1H	2024	G	O5'-P-OP1	-5.50	100.75	105.70
33	51	153	LYS	C-N-CA	5.50	145.12	122.00
26	14	1245	G	C5-C6-O6	-5.50	125.30	128.60
26	14	2385	C	C2-N3-C4	-5.50	117.15	119.90
26	1H	205	G	N3-C2-N2	5.50	123.75	119.90
26	1H	2308	G	C6-N1-C2	5.50	128.40	125.10
1	1G	320	C	C6-N1-C2	5.50	122.50	120.30
26	14	1475	G	C8-N9-C4	-5.50	104.20	106.40
27	1J	114	G	N3-C4-C5	5.50	131.35	128.60
26	14	479	A	N1-C6-N6	-5.50	115.30	118.60
26	14	1585	C	C5-C6-N1	5.50	123.75	121.00
26	14	2448	A	C6-N1-C2	-5.50	115.30	118.60
1	13	108	G	C4-N9-C1'	5.50	133.65	126.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	1786	A	OP1-P-O3'	5.50	117.30	105.20
26	1H	2446	G	C5-N7-C8	-5.50	101.55	104.30
26	14	2227	A	C5-N7-C8	-5.50	101.15	103.90
1	1G	59	A	N1-C6-N6	5.50	121.90	118.60
1	1G	567	G	N3-C4-N9	-5.50	122.70	126.00
26	14	308	G	C4-C5-N7	5.50	113.00	110.80
26	14	2429	G	OP2-P-O3'	5.50	117.29	105.20
26	14	2516	G	OP2-P-O3'	5.50	117.29	105.20
26	14	36	G	OP2-P-O3'	5.50	117.29	105.20
26	1H	21	A	OP2-P-O3'	5.49	117.28	105.20
34	69	131	LYS	C-N-CD	-5.49	108.51	120.60
23	2K	6	G	N1-C6-O6	5.49	123.19	119.90
26	1H	2525	G	C8-N9-C4	5.49	108.60	106.40
40	65	26	LEU	CA-CB-CG	5.49	127.93	115.30
26	1H	1779	U	O5'-P-OP2	-5.49	100.76	105.70
1	1G	812	C	N1-C2-O2	-5.49	115.61	118.90
26	14	470	A	C4-C5-N7	5.49	113.45	110.70
1	13	703	G	C8-N9-C1'	-5.49	119.86	127.00
26	1H	682	G	C8-N9-C1'	-5.49	119.87	127.00
26	1H	703	U	N3-C4-O4	-5.49	115.56	119.40
26	1H	1835	G	C8-N9-C4	-5.49	104.20	106.40
26	1H	1136	G	N1-C2-N2	5.49	121.14	116.20
26	1H	1900	A	C5'-C4'-O4'	-5.49	102.52	109.10
26	1H	2419	U	OP1-P-OP2	-5.49	111.37	119.60
26	1H	2751	G	N3-C4-C5	5.49	131.34	128.60
27	16	29	A	C8-N9-C4	-5.49	103.61	105.80
26	1H	1210	A	C2-N3-C4	-5.48	107.86	110.60
1	13	943	U	N3-C2-O2	5.48	126.04	122.20
26	1H	2585	U	N1-C2-O2	5.48	126.64	122.80
1	1G	810	C	N1-C2-O2	5.48	122.19	118.90
1	1G	893	C	C6-N1-C2	5.48	122.49	120.30
26	14	2256	G	N3-C2-N2	5.48	123.74	119.90
1	13	1455	G	N3-C4-C5	5.48	131.34	128.60
26	1H	250	G	N7-C8-N9	5.48	115.84	113.10
26	1H	1801	G	C5-C6-O6	-5.48	125.31	128.60
27	16	44	G	C4-C5-N7	-5.48	108.61	110.80
26	14	118	A	N1-C6-N6	-5.48	115.31	118.60
26	14	563	G	N1-C6-O6	-5.48	116.61	119.90
26	14	2457	U	OP2-P-O3'	5.48	117.26	105.20
1	13	1446	A	O5'-P-OP1	5.48	117.27	110.70
27	16	98	G	C5-C6-O6	-5.48	125.31	128.60
1	1G	108	G	N3-C2-N2	5.48	123.73	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	1986	A	N7-C8-N9	5.48	116.54	113.80
26	14	707	G	N1-C6-O6	5.48	123.19	119.90
26	14	2437	U	C5-C4-O4	5.48	129.19	125.90
26	14	2776	A	N7-C8-N9	5.48	116.54	113.80
26	1H	1568	G	OP1-P-OP2	-5.48	111.39	119.60
26	14	1780	A	O5'-P-OP2	-5.48	100.77	105.70
26	14	1933	G	OP1-P-OP2	5.48	127.81	119.60
26	1H	1624	G	N3-C2-N2	5.47	123.73	119.90
26	14	835	A	O5'-P-OP1	5.47	117.27	110.70
26	14	855	G	N7-C8-N9	5.47	115.84	113.10
1	13	800	G	C6-C5-N7	-5.47	127.12	130.40
2	12	17	PHE	C-N-CA	5.47	133.79	122.30
26	14	742	G	C5-C6-O6	5.47	131.88	128.60
26	14	822	U	N1-C2-N3	5.47	118.18	114.90
26	14	2008	C	OP2-P-O3'	5.47	117.24	105.20
26	14	2607	G	N3-C2-N2	5.47	123.73	119.90
26	14	1556	C	O5'-P-OP1	-5.47	100.78	105.70
26	1H	795	C	C4-C5-C6	5.47	120.14	117.40
26	1H	1322	A	OP2-P-O3'	5.47	117.23	105.20
26	14	758	C	O5'-P-OP2	-5.47	100.78	105.70
26	14	773	U	C2-N3-C4	-5.47	123.72	127.00
1	1G	579	G	C4-N9-C1'	5.47	133.61	126.50
1	1G	1401	G	C4-C5-C6	5.47	122.08	118.80
26	1H	667	U	C5-C4-O4	-5.47	122.62	125.90
26	14	58	G	C6-C5-N7	-5.47	127.12	130.40
26	14	668	G	N7-C8-N9	-5.47	110.37	113.10
26	14	2490	G	C6-C5-N7	-5.47	127.12	130.40
26	1H	755	C	C4-C5-C6	5.46	120.13	117.40
26	1H	1210	A	C4-C5-C6	5.46	119.73	117.00
26	1H	1280	G	OP1-P-OP2	-5.46	111.41	119.60
26	14	1914	C	N3-C2-O2	-5.46	118.08	121.90
50	K8	3	LEU	CA-C-N	5.46	129.22	117.20
1	13	798	G	C5-C6-N1	-5.46	108.77	111.50
26	1H	195	A	OP1-P-O3'	-5.46	93.19	105.20
26	1H	633	A	N1-C6-N6	5.46	121.88	118.60
26	1H	1971	A	O5'-P-OP2	-5.46	100.78	105.70
26	14	1314	C	C6-N1-C1'	-5.46	114.25	120.80
26	14	1385	G	O4'-C1'-N9	5.46	112.57	108.20
26	14	1899	G	C5-C6-N1	-5.46	108.77	111.50
26	14	2582	G	N1-C6-O6	5.46	123.18	119.90
1	1G	890	G	O4'-C1'-N9	5.46	112.57	108.20
24	3L	76	A	C4-C5-N7	5.46	113.43	110.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	14	1349	A	N1-C6-N6	5.46	121.88	118.60
26	14	681	G	N1-C2-N3	5.46	127.17	123.90
27	1J	102	G	C4-C5-N7	-5.46	108.62	110.80
26	1H	697	C	N3-C4-C5	5.46	124.08	121.90
26	1H	1761	C	C6-N1-C2	5.46	122.48	120.30
26	1H	1796	U	C5-C6-N1	-5.46	119.97	122.70
26	1H	2081	C	N1-C2-O2	5.46	122.17	118.90
26	14	801	G	C6-C5-N7	5.46	133.67	130.40
26	1H	796	C	N3-C2-O2	-5.46	118.08	121.90
27	16	100	G	N3-C4-N9	5.46	129.27	126.00
1	1G	1502	A	C4-N9-C1'	5.46	136.12	126.30
26	1H	141(A)	C	OP2-P-O3'	5.45	117.20	105.20
26	1H	210	C	OP2-P-O3'	5.45	117.20	105.20
26	1H	1432	C	N3-C2-O2	5.45	125.72	121.90
26	14	1558	A	C2-N3-C4	-5.45	107.87	110.60
26	1H	2871	C	O5'-P-OP2	-5.45	100.79	105.70
26	14	672	C	C6-N1-C2	-5.45	118.12	120.30
26	1H	30	G	OP1-P-O3'	5.45	117.19	105.20
26	1H	1356	G	C5-C6-N1	-5.45	108.77	111.50
26	14	2510	C	C4-C5-C6	5.45	120.12	117.40
26	1H	1429	G	OP1-P-OP2	5.45	127.77	119.60
26	1H	2427	C	O5'-P-OP1	-5.45	100.80	105.70
26	1H	2510	C	O5'-P-OP2	-5.45	100.80	105.70
1	13	896	C	C4-C5-C6	5.45	120.12	117.40
24	1L	34	U	C2-N1-C1'	5.45	124.24	117.70
26	1H	97	C	O5'-P-OP1	-5.45	100.80	105.70
26	1H	657	U	N3-C4-O4	-5.45	115.59	119.40
26	14	1407	C	N3-C2-O2	5.45	125.71	121.90
26	14	2592	G	O5'-P-OP1	5.45	117.23	110.70
26	14	1806	C	O5'-P-OP1	-5.44	100.80	105.70
24	3K	71	C	O4'-C1'-N1	5.44	112.55	108.20
1	1G	697	U	C5-C6-N1	-5.44	119.98	122.70
26	14	385	C	OP1-P-OP2	5.44	127.77	119.60
26	14	2873	A	C8-N9-C1'	-5.44	117.90	127.70
26	1H	724	U	C5-C4-O4	5.44	129.16	125.90
26	1H	730	C	N1-C2-O2	5.44	122.16	118.90
26	1H	855	G	C8-N9-C4	-5.44	104.22	106.40
26	14	1396	U	N1-C2-O2	5.44	126.61	122.80
26	14	1585	C	C2-N1-C1'	5.44	124.78	118.80
26	14	1950	G	C8-N9-C4	-5.44	104.22	106.40
1	1G	721	G	C6-C5-N7	-5.44	127.14	130.40
26	14	1680	U	C6-N1-C2	5.44	124.26	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	13	346	G	C4-N9-C1'	5.44	133.57	126.50
1	13	523	A	C2-N3-C4	-5.44	107.88	110.60
26	1H	120	U	C5-C4-O4	5.44	129.16	125.90
26	1H	2373	G	C6-N1-C2	-5.44	121.84	125.10
36	68	8	LEU	CA-CB-CG	5.44	127.81	115.30
1	13	150	C	C6-N1-C2	-5.43	118.13	120.30
26	1H	1571	A	C8-N9-C4	5.43	107.97	105.80
26	1H	2070	G	O5'-P-OP2	-5.43	100.81	105.70
26	1H	2294	C	C6-N1-C2	-5.43	118.13	120.30
1	1G	197	A	C8-N9-C4	-5.43	103.63	105.80
26	14	1674	G	N3-C4-N9	5.43	129.26	126.00
26	1H	2208	U	C5-C6-N1	-5.43	119.98	122.70
49	J8	2	SER	N-CA-C	5.43	125.67	111.00
1	13	15	G	C8-N9-C1'	-5.43	119.94	127.00
26	1H	1970	A	O4'-C1'-N9	-5.43	103.86	108.20
26	14	1304	C	N1-C2-O2	5.43	122.16	118.90
26	14	2518	A	C4-C5-N7	5.43	113.41	110.70
1	13	1498	U	C6-N1-C2	-5.43	117.75	121.00
26	1H	250	G	C8-N9-C4	-5.43	104.23	106.40
27	16	44	G	OP2-P-O3'	5.43	117.14	105.20
26	14	50	U	C6-N1-C2	5.43	124.26	121.00
26	1H	1252	G	N7-C8-N9	-5.42	110.39	113.10
26	1H	1608	A	C8-N9-C4	5.42	107.97	105.80
26	1H	1800	C	C2-N3-C4	-5.42	117.19	119.90
1	13	346	G	C5-N7-C8	-5.42	101.59	104.30
26	1H	956	G	N1-C6-O6	5.42	123.15	119.90
26	1H	1256	G	C8-N9-C4	5.42	108.57	106.40
27	16	45	A	O5'-P-OP1	-5.42	100.82	105.70
1	1G	380	G	N9-C4-C5	5.42	107.57	105.40
26	14	1516	U	N1-C2-O2	5.42	126.60	122.80
1	13	500	G	OP2-P-O3'	5.42	117.13	105.20
26	1H	1026	U	OP1-P-O3'	5.42	117.13	105.20
26	1H	2826	A	C8-N9-C4	5.42	107.97	105.80
26	14	1969	A	OP1-P-OP2	-5.42	111.47	119.60
26	14	2763	G	N3-C4-N9	5.42	129.25	126.00
26	14	2226	C	N3-C2-O2	-5.42	118.11	121.90
26	1H	1982	C	O5'-P-OP2	-5.42	100.82	105.70
26	1H	2838	G	N1-C6-O6	-5.42	116.65	119.90
26	14	1313	U	N1-C2-N3	5.42	118.15	114.90
26	14	1342	A	C5-N7-C8	-5.42	101.19	103.90
26	1H	838	C	N1-C2-N3	5.42	122.99	119.20
26	1H	196	A	C2-N3-C4	-5.42	107.89	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	14	1663	C	C6-N1-C2	5.42	122.47	120.30
26	1H	99	U	N1-C2-O2	5.41	126.59	122.80
1	1G	64	G	P-O3'-C3'	5.41	126.20	119.70
26	14	837	C	C5-C6-N1	5.41	123.71	121.00
49	F5	35	THR	C-N-CA	-5.41	110.93	122.30
1	13	726	C	OP1-P-O3'	5.41	117.11	105.20
26	1H	205	G	N7-C8-N9	-5.41	110.39	113.10
26	1H	1796	U	O5'-P-OP1	-5.41	100.83	105.70
26	1H	2626	C	N3-C4-C5	5.41	124.06	121.90
26	1H	120	U	O5'-P-OP1	-5.41	100.83	105.70
26	1H	270(O)	U	C5-C6-N1	5.41	125.41	122.70
26	1H	686	G	C6-C5-N7	-5.41	127.15	130.40
26	1H	944	G	C6-C5-N7	-5.41	127.15	130.40
26	1H	954	G	N9-C4-C5	5.41	107.56	105.40
26	1H	2286	A	C8-N9-C4	-5.41	103.64	105.80
26	1H	2416	C	C6-N1-C2	-5.41	118.14	120.30
55	P8	23	ARG	C-N-CA	5.41	135.23	121.70
26	14	130	C	C2-N3-C4	-5.41	117.19	119.90
26	14	203	C	N3-C4-N4	-5.41	114.21	118.00
26	1H	2392	A	N1-C6-N6	5.41	121.84	118.60
26	14	2282	G	O5'-P-OP2	5.41	117.19	110.70
26	1H	1365	A	C4-C5-C6	5.41	119.70	117.00
26	1H	2346	A	C1'-O4'-C4'	-5.41	105.58	109.90
26	14	1820	U	C5-C6-N1	-5.41	120.00	122.70
26	1H	2325	G	O5'-P-OP1	-5.40	100.84	105.70
26	14	2304	G	N3-C2-N2	-5.40	116.12	119.90
1	13	1113	C	C6-N1-C2	-5.40	118.14	120.30
1	13	1279	A	C5-N7-C8	-5.40	101.20	103.90
26	1H	606	U	O5'-P-OP2	-5.40	100.84	105.70
56	Q8	50	LEU	CB-CG-CD1	5.40	120.19	111.00
26	14	2334	G	N9-C4-C5	-5.40	103.24	105.40
1	13	858	G	C8-N9-C4	-5.40	104.24	106.40
26	14	1908	C	OP2-P-O3'	5.40	117.08	105.20
1	13	50	A	C2-N3-C4	5.40	113.30	110.60
26	1H	1129	A	OP1-P-OP2	5.40	127.69	119.60
26	14	1906	G	C8-N9-C4	-5.40	104.24	106.40
1	13	354	G	O5'-P-OP2	-5.39	100.85	105.70
26	14	155	C	N1-C2-O2	5.39	122.14	118.90
26	14	1973	G	N1-C6-O6	-5.39	116.66	119.90
26	1H	124	G	N1-C2-N3	-5.39	120.66	123.90
26	1H	1122	G	C5-C6-O6	-5.39	125.36	128.60
26	14	2072	G	OP1-P-OP2	-5.39	111.51	119.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	14	2430	A	C4-C5-C6	5.39	119.70	117.00
1	13	442	C	C6-N1-C2	-5.39	118.14	120.30
1	13	1498	U	N3-C4-O4	5.39	123.17	119.40
26	14	270(Y)	G	C5-C6-O6	5.39	131.84	128.60
26	1H	127	A	N9-C4-C5	-5.39	103.64	105.80
26	14	223	A	C8-N9-C4	-5.39	103.64	105.80
26	14	646	A	N7-C8-N9	5.39	116.49	113.80
1	13	974	A	C8-N9-C1'	-5.39	118.00	127.70
26	1H	2286	A	N1-C6-N6	5.39	121.83	118.60
27	16	12	C	N3-C2-O2	-5.39	118.13	121.90
26	1H	71	A	C6-N1-C2	-5.39	115.37	118.60
26	1H	382	G	OP1-P-O3'	5.39	117.05	105.20
26	1H	1786	A	N3-C4-C5	5.39	130.57	126.80
26	1H	1992	G	P-O3'-C3'	5.39	126.17	119.70
26	1H	311	A	O5'-P-OP1	-5.38	100.85	105.70
1	1G	117	G	C5-C6-O6	-5.38	125.37	128.60
1	1G	345	C	P-O3'-C3'	5.38	126.16	119.70
26	14	1404	C	OP1-P-OP2	5.38	127.68	119.60
26	14	1597	A	O5'-P-OP2	-5.38	100.86	105.70
26	14	1825	A	O5'-P-OP2	-5.38	100.86	105.70
56	Q8	46	ARG	C-N-CA	5.38	135.16	121.70
26	1H	1302	A	C5-C6-N1	5.38	120.39	117.70
1	13	1354	C	N3-C2-O2	-5.38	118.13	121.90
26	1H	2741	A	N7-C8-N9	-5.38	111.11	113.80
26	14	1779	U	O5'-P-OP2	-5.38	100.86	105.70
26	1H	210	C	C5-C6-N1	-5.38	118.31	121.00
26	1H	1367	A	C8-N9-C4	5.38	107.95	105.80
26	1H	2318	G	C5-N7-C8	-5.38	101.61	104.30
26	1H	2665	A	C8-N9-C4	-5.38	103.65	105.80
26	14	1248	G	OP1-P-OP2	-5.38	111.53	119.60
26	1H	1026	U	C2-N1-C1'	5.38	124.15	117.70
26	1H	1882	C	C2-N1-C1'	5.38	124.72	118.80
26	1H	2040	C	C5-C4-N4	-5.38	116.44	120.20
26	14	2067	G	N9-C4-C5	5.38	107.55	105.40
26	14	2346	A	C5-C6-N1	-5.38	115.01	117.70
26	1H	195	A	OP2-P-O3'	5.38	117.02	105.20
26	1H	2591	C	C5-C4-N4	-5.38	116.44	120.20
26	14	2073	C	N1-C2-O2	-5.38	115.67	118.90
26	1H	861	A	O5'-P-OP2	5.37	117.15	110.70
23	2L	76	C	N3-C4-C5	-5.37	119.75	121.90
26	14	596	G	N3-C2-N2	-5.37	116.14	119.90
26	1H	214	G	C8-N9-C4	-5.37	104.25	106.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	1253	A	N9-C4-C5	-5.37	103.65	105.80
26	14	409	C	C6-N1-C2	5.37	122.45	120.30
26	14	639	U	C5-C4-O4	5.37	129.12	125.90
37	35	59	LEU	CA-CB-CG	5.37	127.65	115.30
1	13	888	G	C5-C6-O6	-5.37	125.38	128.60
26	1H	2489	G	OP2-P-O3'	5.37	117.01	105.20
27	16	30	C	O5'-P-OP1	-5.37	100.87	105.70
26	14	1138	G	C8-N9-C4	-5.37	104.25	106.40
26	14	1406	U	OP1-P-O3'	5.37	117.01	105.20
26	14	465	G	O5'-P-OP2	5.37	117.14	110.70
26	14	2712	U	N1-C2-N3	5.37	118.12	114.90
1	13	800	G	N9-C4-C5	-5.37	103.25	105.40
26	1H	1752	C	C5-C6-N1	-5.37	118.32	121.00
26	14	250	G	C5-C6-O6	-5.37	125.38	128.60
1	13	190	G	P-O3'-C3'	5.36	126.14	119.70
26	1H	380	U	N3-C2-O2	-5.36	118.44	122.20
26	14	624	C	N1-C2-O2	-5.36	115.68	118.90
26	14	2056	G	N9-C4-C5	-5.36	103.25	105.40
26	1H	579	G	N1-C2-N2	5.36	121.03	116.20
26	1H	686	G	C8-N9-C1'	-5.36	120.03	127.00
26	1H	2040	C	N3-C2-O2	5.36	125.65	121.90
26	14	1253	A	O4'-C1'-N9	-5.36	103.91	108.20
26	14	1789	A	O5'-P-OP2	-5.36	100.88	105.70
26	1H	967	C	C2-N3-C4	-5.36	117.22	119.90
26	1H	2464	C	C6-N1-C2	5.36	122.44	120.30
1	1G	561	U	O5'-P-OP1	-5.36	100.88	105.70
26	14	988	A	N7-C8-N9	5.36	116.48	113.80
26	14	1022	G	P-O3'-C3'	5.36	126.13	119.70
26	14	1254	A	N1-C2-N3	5.36	131.98	129.30
26	14	2024	G	C5-C6-O6	-5.36	125.38	128.60
26	14	2245	U	OP1-P-O3'	5.36	116.99	105.20
26	1H	788	A	C5-C6-N1	-5.36	115.02	117.70
26	1H	1301	A	C6-C5-N7	-5.36	128.55	132.30
26	1H	1982	C	N3-C4-C5	-5.36	119.76	121.90
1	1G	1195	C	C6-N1-C2	-5.36	118.16	120.30
26	14	204	A	N1-C6-N6	5.36	121.81	118.60
26	14	2076	U	N1-C2-O2	-5.36	119.05	122.80
26	14	2461	C	O5'-P-OP1	-5.36	100.88	105.70
26	1H	978	G	C2-N3-C4	-5.36	109.22	111.90
26	1H	1798	U	N3-C4-O4	-5.36	115.65	119.40
26	14	1963	U	N3-C2-O2	-5.36	118.45	122.20
26	14	2501	C	C6-N1-C1'	5.36	127.23	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	193	U	N1-C2-N3	5.35	118.11	114.90
26	1H	665	C	C6-N1-C2	5.35	122.44	120.30
26	1H	1543	A	C5-C6-N1	-5.35	115.02	117.70
26	1H	1595	G	C5-C6-O6	-5.35	125.39	128.60
1	1G	1523	G	N1-C6-O6	-5.35	116.69	119.90
26	14	1925	C	N1-C2-O2	-5.35	115.69	118.90
24	3K	1	G	O4'-C1'-N9	5.35	112.48	108.20
24	3K	72	C	C6-N1-C2	-5.35	118.16	120.30
26	1H	1284	A	C5-N7-C8	-5.35	101.22	103.90
26	14	2296	U	N3-C4-O4	5.35	123.15	119.40
26	14	2346	A	N9-C1'-C2'	5.35	120.96	114.00
26	14	2592	G	C4-N9-C1'	5.35	133.46	126.50
26	1H	796	C	C5-C4-N4	5.35	123.94	120.20
26	1H	944	G	C8-N9-C1'	-5.35	120.05	127.00
26	1H	1305	C	C5-C6-N1	-5.35	118.33	121.00
26	1H	1346	G	N1-C6-O6	-5.35	116.69	119.90
26	1H	1374	G	C5-C6-N1	-5.35	108.83	111.50
26	1H	1811	G	N3-C2-N2	-5.35	116.16	119.90
1	1G	1301	U	N1-C2-O2	5.35	126.54	122.80
26	1H	752	A	N3-C4-C5	5.35	130.54	126.80
26	1H	2586	C	OP1-P-O3'	5.35	116.96	105.20
26	1H	2745	C	O5'-P-OP1	-5.35	100.89	105.70
26	14	1831	G	C8-N9-C1'	-5.35	120.05	127.00
26	14	137(A)	G	C5-C6-O6	-5.35	125.39	128.60
26	1H	2056	G	OP1-P-O3'	5.34	116.96	105.20
26	1H	2231	C	N1-C2-O2	-5.34	115.69	118.90
26	14	830	G	N9-C4-C5	-5.34	103.26	105.40
26	1H	698	C	OP1-P-OP2	5.34	127.61	119.60
1	1G	1502	A	N7-C8-N9	5.34	116.47	113.80
26	1H	74	A	C8-N9-C4	-5.34	103.66	105.80
26	1H	1417	C	C4-C5-C6	5.34	120.07	117.40
26	1H	1520	U	OP2-P-O3'	5.34	116.95	105.20
26	1H	2023	G	O5'-P-OP1	-5.34	100.89	105.70
26	1H	2030	A	C5-C6-N6	-5.34	119.43	123.70
26	14	2496	C	OP1-P-O3'	5.34	116.95	105.20
26	14	34	C	C6-N1-C1'	-5.34	114.39	120.80
26	14	2424	C	OP1-P-OP2	5.34	127.61	119.60
26	1H	2703	C	C6-N1-C2	-5.34	118.17	120.30
27	16	79	C	OP2-P-O3'	5.34	116.94	105.20
26	1H	733	G	C5-C6-N1	-5.34	108.83	111.50
26	1H	787	U	N3-C4-O4	-5.34	115.66	119.40
26	1H	2611	U	N3-C2-O2	-5.34	118.47	122.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	14	2334	G	N3-C4-N9	5.33	129.20	126.00
26	1H	848	G	O5'-P-OP1	5.33	117.10	110.70
26	1H	2666	C	C6-N1-C2	-5.33	118.17	120.30
26	14	1299	G	O5'-P-OP2	5.33	117.10	110.70
26	14	2287	A	N1-C6-N6	5.33	121.80	118.60
1	13	15	G	N3-C4-N9	5.33	129.20	126.00
1	13	904	C	C6-N1-C2	5.33	122.43	120.30
26	1H	2518	A	C2-N3-C4	-5.33	107.93	110.60
26	14	832	G	OP1-P-O3'	5.33	116.93	105.20
26	14	946	G	C8-N9-C4	5.33	108.53	106.40
26	14	2518	A	C4-C5-C6	5.33	119.67	117.00
1	13	972	C	N3-C2-O2	-5.33	118.17	121.90
26	1H	186	G	C5-C6-N1	5.33	114.17	111.50
1	13	703	G	OP1-P-O3'	5.33	116.92	105.20
26	1H	632	A	OP1-P-OP2	-5.33	111.61	119.60
26	1H	791	C	P-O3'-C3'	5.33	126.09	119.70
26	1H	2555	U	N1-C2-O2	-5.33	119.07	122.80
42	C8	74	LEU	CA-CB-CG	5.33	127.56	115.30
1	1G	576	G	C6-C5-N7	-5.33	127.20	130.40
1	1G	1322	C	N3-C2-O2	-5.33	118.17	121.90
26	14	1836	C	O5'-P-OP1	5.33	117.09	110.70
26	14	2609	U	C5-C6-N1	-5.33	120.04	122.70
29	11	272	ALA	C-N-CA	5.33	135.02	121.70
1	1G	811	C	C6-N1-C2	5.33	122.43	120.30
26	1H	2567	G	O5'-P-OP2	5.33	117.09	110.70
26	14	249	C	O5'-P-OP2	5.33	117.09	110.70
26	1H	2507	C	N3-C4-C5	-5.32	119.77	121.90
26	14	1585	C	C2-N3-C4	5.32	122.56	119.90
26	14	1831	G	N1-C2-N3	5.32	127.09	123.90
26	14	1836	C	OP1-P-O3'	5.32	116.91	105.20
26	1H	835	A	C2-N3-C4	5.32	113.26	110.60
26	1H	1291	C	N1-C2-O2	-5.32	115.71	118.90
26	1H	1610	A	C5-N7-C8	-5.32	101.24	103.90
26	1H	1776	G	C5-C6-O6	-5.32	125.41	128.60
26	14	2700	C	C6-N1-C1'	-5.32	114.41	120.80
26	1H	33	U	OP1-P-O3'	5.32	116.91	105.20
26	1H	2440	C	C5-C4-N4	5.32	123.92	120.20
26	1H	2761	G	C2-N3-C4	-5.32	109.24	111.90
26	14	677	A	O5'-P-OP2	-5.32	100.91	105.70
26	14	819	A	OP2-P-O3'	5.32	116.91	105.20
26	14	864	G	N3-C4-C5	-5.32	125.94	128.60
1	13	1301	U	OP1-P-O3'	5.32	116.90	105.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	869	G	C5-C6-O6	5.32	131.79	128.60
26	1H	938	G	O5'-P-OP1	5.32	117.08	110.70
1	1G	909	A	N9-C4-C5	-5.32	103.67	105.80
1	1G	950	U	O5'-P-OP1	-5.32	100.91	105.70
26	14	205	G	C4-C5-N7	5.32	112.93	110.80
26	1H	1941	C	C6-N1-C2	-5.32	118.17	120.30
26	14	205	G	N3-C2-N2	5.32	123.62	119.90
26	1H	201	C	N3-C4-C5	5.32	124.03	121.90
26	1H	534	U	C5-C6-N1	-5.32	120.04	122.70
26	1H	974(A)	C	C5-C6-N1	-5.32	118.34	121.00
26	1H	1669	A	C6-N1-C2	-5.32	115.41	118.60
1	1G	1260	C	C6-N1-C2	-5.32	118.17	120.30
26	14	124	G	N1-C6-O6	5.32	123.09	119.90
26	14	1899	G	C4-C5-C6	5.32	121.99	118.80
26	1H	446	G	C8-N9-C4	5.31	108.53	106.40
26	1H	508	G	P-O3'-C3'	5.31	126.08	119.70
26	1H	1593	G	C8-N9-C4	-5.31	104.28	106.40
26	1H	2032	G	C8-N9-C4	5.31	108.53	106.40
26	1H	2316	C	O5'-P-OP2	5.31	117.08	110.70
26	14	640	C	OP1-P-O3'	5.31	116.89	105.20
26	14	669	G	N3-C2-N2	-5.31	116.18	119.90
26	14	1204	A	N3-C4-C5	5.31	130.52	126.80
26	14	1382	G	N9-C4-C5	-5.31	103.28	105.40
26	14	1950	G	O5'-P-OP2	-5.31	100.92	105.70
26	1H	479	A	C8-N9-C4	5.31	107.92	105.80
1	13	45	U	OP2-P-O3'	5.31	116.88	105.20
26	1H	139	G	N3-C4-C5	-5.31	125.95	128.60
26	1H	726	G	C8-N9-C4	5.31	108.52	106.40
26	1H	1521	G	N3-C4-C5	-5.31	125.94	128.60
26	1H	1610	A	C8-N9-C4	5.31	107.92	105.80
1	1G	799	G	OP2-P-O3'	5.31	116.88	105.20
26	14	922	U	O5'-P-OP1	-5.31	100.92	105.70
26	1H	2239	G	N3-C2-N2	5.31	123.62	119.90
26	1H	2257	U	OP1-P-OP2	-5.31	111.64	119.60
1	1G	770	C	O5'-P-OP2	-5.31	100.92	105.70
26	14	2055	C	OP1-P-O3'	5.31	116.88	105.20
26	14	2334	G	C8-N9-C4	5.31	108.52	106.40
1	13	108	G	C6-C5-N7	-5.31	127.22	130.40
26	1H	1499	C	O5'-P-OP1	-5.31	100.92	105.70
26	1H	1731	G	N1-C6-O6	-5.31	116.72	119.90
26	1H	2357	U	O5'-P-OP2	-5.31	100.92	105.70
26	14	1659	U	O5'-P-OP1	-5.31	100.92	105.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	14	1793	C	C6-N1-C2	-5.31	118.18	120.30
27	1J	114	G	C4-N9-C1'	-5.31	119.60	126.50
26	1H	509	C	O5'-P-OP2	-5.30	100.92	105.70
26	1H	673	C	N1-C2-O2	-5.30	115.72	118.90
26	14	788	A	C4-C5-N7	5.30	113.35	110.70
26	14	2681	C	C5-C6-N1	-5.30	118.35	121.00
26	1H	831	G	N7-C8-N9	-5.30	110.45	113.10
26	1H	1502	C	C6-N1-C2	-5.30	118.18	120.30
26	1H	1611	C	C6-N1-C2	5.30	122.42	120.30
26	1H	2318	G	C4-N9-C1'	5.30	133.39	126.50
26	14	2390	U	C6-N1-C2	-5.30	117.82	121.00
27	1J	54	G	N7-C8-N9	5.30	115.75	113.10
1	13	690	G	N3-C4-N9	5.30	129.18	126.00
1	13	1516	G	N3-C4-N9	-5.30	122.82	126.00
26	1H	1136	G	N3-C2-N2	-5.30	116.19	119.90
26	1H	1609	A	C6-N1-C2	-5.30	115.42	118.60
26	1H	2062	A	N3-C4-N9	5.30	131.64	127.40
26	1H	2447	G	C6-N1-C2	-5.30	121.92	125.10
26	1H	501	A	O5'-P-OP2	-5.30	100.93	105.70
26	1H	2005	A	N1-C6-N6	5.30	121.78	118.60
26	14	2425	A	C5'-C4'-O4'	5.30	115.46	109.10
1	13	47	C	C5-C6-N1	-5.30	118.35	121.00
26	1H	628	G	C8-N9-C4	5.30	108.52	106.40
26	1H	84	A	N1-C2-N3	-5.30	126.65	129.30
26	1H	2272	U	OP2-P-O3'	5.30	116.85	105.20
26	14	571	A	N9-C4-C5	-5.30	103.68	105.80
26	14	2374	C	C2-N3-C4	-5.30	117.25	119.90
26	14	2377	A	C8-N9-C4	5.30	107.92	105.80
26	1H	2286	A	N7-C8-N9	5.29	116.45	113.80
26	14	2622	C	O5'-P-OP2	-5.29	100.93	105.70
26	1H	1990	C	C2-N3-C4	-5.29	117.25	119.90
26	14	141	A	OP2-P-O3'	5.29	116.84	105.20
26	14	832	G	N1-C2-N2	5.29	120.96	116.20
26	14	1725	G	C8-N9-C1'	-5.29	120.12	127.00
26	1H	817	C	C6-N1-C2	-5.29	118.18	120.30
26	1H	1254	A	N1-C6-N6	5.29	121.78	118.60
1	13	827	U	C4-C5-C6	5.29	122.87	119.70
26	1H	2586	C	C4-C5-C6	5.29	120.05	117.40
26	14	2595	G	C5-C6-N1	5.29	114.14	111.50
26	1H	1594	G	O5'-P-OP1	-5.29	100.94	105.70
23	2L	17	C	N1-C2-O2	5.29	122.07	118.90
26	14	2610	C	N1-C2-O2	5.29	122.07	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	13	721	G	N3-C4-N9	5.29	129.17	126.00
29	11	272	ALA	N-CA-C	5.29	125.27	111.00
26	1H	528	A	O4'-C1'-N9	-5.29	103.97	108.20
1	13	50	A	P-O3'-C3'	5.28	126.04	119.70
26	1H	789	A	C2-N3-C4	-5.28	107.96	110.60
26	1H	2032	G	OP1-P-O3'	5.28	116.82	105.20
1	13	768	A	N7-C8-N9	-5.28	111.16	113.80
26	1H	145	G	C5-C6-O6	-5.28	125.43	128.60
26	1H	1021	A	C4-C5-N7	5.28	113.34	110.70
26	14	1801	G	O5'-P-OP1	-5.28	100.95	105.70
26	1H	1565	C	C5-C6-N1	-5.28	118.36	121.00
26	1H	1957	C	C5-C6-N1	-5.28	118.36	121.00
26	14	779	U	C4-C5-C6	5.28	122.87	119.70
1	13	529	G	C5-C6-O6	-5.28	125.43	128.60
1	13	791	G	OP2-P-O3'	5.28	116.81	105.20
26	1H	231	C	N1-C2-O2	-5.28	115.73	118.90
26	1H	1914	C	C6-N1-C2	-5.28	118.19	120.30
26	14	2307	G	N7-C8-N9	5.28	115.74	113.10
33	59	98	LEU	CA-CB-CG	5.28	127.44	115.30
1	13	452	A	O5'-P-OP1	-5.28	100.95	105.70
26	1H	740	U	O5'-P-OP1	5.28	117.03	110.70
26	14	456	C	N1-C2-O2	-5.28	115.73	118.90
26	1H	2239	G	N1-C6-O6	-5.27	116.74	119.90
26	14	1826	G	N7-C8-N9	-5.27	110.46	113.10
1	13	904	C	N3-C4-C5	5.27	124.01	121.90
12	3I	93	LEU	CA-CB-CG	5.27	127.43	115.30
1	1G	1260	C	C5-C6-N1	5.27	123.64	121.00
26	14	1312	U	O5'-P-OP1	-5.27	100.95	105.70
26	1H	1835	G	N3-C4-C5	-5.27	125.96	128.60
26	1H	2374	C	C4-C5-C6	5.27	120.03	117.40
26	1H	256	A	N9-C4-C5	-5.27	103.69	105.80
1	13	1061	G	N1-C6-O6	5.27	123.06	119.90
1	1G	1259	C	C5-C6-N1	5.27	123.63	121.00
26	14	509	C	C5-C6-N1	-5.27	118.37	121.00
26	14	715	G	C4-C5-N7	5.27	112.91	110.80
26	14	945	A	C8-N9-C1'	-5.27	118.22	127.70
22	1K	49	G	C4-N9-C1'	-5.27	119.65	126.50
26	1H	800	A	C5-N7-C8	5.27	106.53	103.90
26	14	621	A	O4'-C1'-N9	5.27	112.41	108.20
26	14	1842	G	C5-C6-N1	5.27	114.13	111.50
1	13	15	G	C4-N9-C1'	5.26	133.34	126.50
26	1H	213	A	C4-C5-N7	5.26	113.33	110.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	446	G	C6-C5-N7	-5.26	127.24	130.40
26	1H	745	G	N3-C2-N2	-5.26	116.22	119.90
26	1H	1210	A	N1-C6-N6	5.26	121.76	118.60
26	1H	1647	G	O5'-P-OP1	-5.26	100.96	105.70
26	1H	2011	U	C2-N1-C1'	-5.26	111.38	117.70
26	1H	2709	G	C8-N9-C4	-5.26	104.29	106.40
26	14	1216	G	OP1-P-O3'	5.26	116.78	105.20
1	13	388	G	C8-N9-C4	5.26	108.50	106.40
56	M5	50	LEU	CA-CB-CG	-5.26	103.19	115.30
26	1H	1888	G	N9-C4-C5	-5.26	103.30	105.40
26	14	1681	G	N7-C8-N9	5.26	115.73	113.10
26	14	1831	G	C4-N9-C1'	5.26	133.34	126.50
26	14	2056	G	N3-C4-N9	5.26	129.16	126.00
26	14	2598	A	N7-C8-N9	-5.26	111.17	113.80
26	1H	737	C	N1-C2-O2	-5.26	115.75	118.90
26	1H	1224	G	C4-N9-C1'	-5.26	119.66	126.50
26	1H	2505	G	C2-N3-C4	-5.26	109.27	111.90
26	1H	2558	C	N1-C2-O2	-5.26	115.74	118.90
26	1H	2718	G	C4-C5-N7	5.26	112.90	110.80
1	13	807	A	C8-N9-C4	-5.26	103.70	105.80
26	1H	140	A	C5-C6-N6	-5.26	119.49	123.70
1	1G	481	G	C4-C5-C6	5.26	121.95	118.80
26	14	2258	C	OP1-P-O3'	5.26	116.77	105.20
1	13	1403	C	O5'-P-OP2	-5.26	100.97	105.70
26	1H	199	A	N1-C2-N3	-5.26	126.67	129.30
26	1H	481	G	N1-C6-O6	5.26	123.05	119.90
26	1H	2517	C	O4'-C1'-N1	5.26	112.41	108.20
34	61	110	ASP	C-N-CD	-5.26	109.04	120.60
1	13	108	G	C8-N9-C1'	-5.25	120.17	127.00
26	1H	698	C	N3-C4-N4	5.25	121.68	118.00
26	1H	1770	G	N1-C6-O6	-5.25	116.75	119.90
26	1H	2469	A	C4-C5-N7	5.25	113.33	110.70
26	14	774	A	OP1-P-O3'	-5.25	93.64	105.20
26	1H	141	A	C4-C5-C6	-5.25	114.37	117.00
26	1H	2438	U	C6-N1-C2	5.25	124.15	121.00
26	14	22	C	N3-C4-C5	5.25	124.00	121.90
26	14	773	U	N3-C2-O2	-5.25	118.52	122.20
26	14	1635	G	OP1-P-O3'	5.25	116.76	105.20
26	14	1950	G	C4-N9-C1'	5.25	133.33	126.50
1	13	899	C	OP2-P-O3'	5.25	116.75	105.20
26	1H	110	G	N7-C8-N9	-5.25	110.47	113.10
26	1H	512	G	N7-C8-N9	-5.25	110.47	113.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1G	1128	C	N3-C2-O2	-5.25	118.22	121.90
26	14	29	U	C2-N1-C1'	5.25	124.00	117.70
26	14	621	A	C6-C5-N7	-5.25	128.62	132.30
1	13	703	G	N9-C4-C5	-5.25	103.30	105.40
26	1H	1878	G	N9-C4-C5	5.25	107.50	105.40
26	1H	2552	U	N1-C2-O2	-5.25	119.12	122.80
40	A8	101	LEU	CA-CB-CG	5.25	127.38	115.30
26	14	2731	G	C6-C5-N7	-5.25	127.25	130.40
26	1H	1678	G	N1-C6-O6	5.25	123.05	119.90
26	1H	2375	G	OP2-P-O3'	5.25	116.75	105.20
27	16	105	G	N3-C4-C5	-5.25	125.98	128.60
26	14	1819	A	N9-C4-C5	5.25	107.90	105.80
26	14	2873	A	N9-C1'-C2'	5.25	120.82	114.00
29	19	257	LEU	CA-CB-CG	5.25	127.37	115.30
1	13	817	C	N3-C4-N4	5.25	121.67	118.00
26	1H	141(A)	C	C2-N3-C4	-5.25	117.28	119.90
26	14	1757	U	C5-C4-O4	5.25	129.05	125.90
26	14	2329	G	C5-C6-N1	5.25	114.12	111.50
26	1H	248	G	C6-N1-C2	-5.24	121.95	125.10
26	1H	664	C	N3-C2-O2	-5.24	118.23	121.90
26	1H	2040	C	N1-C2-O2	-5.24	115.75	118.90
23	2K	73	A	C8-N9-C4	5.24	107.90	105.80
26	1H	815	C	C6-N1-C2	5.24	122.40	120.30
26	1H	2603	G	O5'-P-OP1	-5.24	100.98	105.70
1	1G	1496	C	O5'-P-OP2	-5.24	100.98	105.70
11	2A	63	LEU	CA-CB-CG	5.24	127.35	115.30
26	14	137(A)	G	N1-C6-O6	5.24	123.05	119.90
26	14	2332	U	C5-C4-O4	5.24	129.04	125.90
1	13	910	C	O5'-P-OP2	-5.24	100.99	105.70
1	13	963	G	N3-C4-C5	-5.24	125.98	128.60
26	1H	835	A	N9-C4-C5	5.24	107.90	105.80
37	78	23	PRO	C-N-CA	-5.24	111.30	122.30
1	1G	924	C	OP1-P-OP2	5.24	127.46	119.60
26	14	1781	C	C5-C4-N4	-5.24	116.53	120.20
26	1H	2458	G	C5-C6-O6	-5.24	125.46	128.60
1	13	1	U	N1-C1'-C2'	5.24	120.81	114.00
1	13	1126	U	C6-N1-C2	-5.24	117.86	121.00
26	1H	1432	C	C5-C4-N4	-5.24	116.53	120.20
26	1H	1496	A	O4'-C1'-N9	5.24	112.39	108.20
26	1H	2347	C	OP2-P-O3'	5.24	116.72	105.20
26	14	552	G	C8-N9-C4	5.24	108.49	106.40
26	14	2013	A	C2-N3-C4	-5.24	107.98	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1G	1502	A	C5-N7-C8	-5.23	101.28	103.90
26	14	773	U	N1-C2-N3	5.23	118.04	114.90
26	14	827	U	O5'-P-OP1	5.23	116.98	110.70
26	14	916	G	O5'-P-OP1	-5.23	100.99	105.70
26	14	1772	G	C4-C5-N7	5.23	112.89	110.80
26	1H	123	G	C5-C6-N1	5.23	114.12	111.50
26	14	2729	G	C4-C5-N7	5.23	112.89	110.80
26	1H	1361	G	C6-C5-N7	5.23	133.54	130.40
26	14	788	A	C4-C5-C6	5.23	119.61	117.00
26	14	972	G	OP1-P-O3'	5.23	116.70	105.20
1	13	952	U	N1-C2-N3	5.23	118.04	114.90
26	1H	350	U	C5-C4-O4	5.23	129.04	125.90
26	1H	655	A	C8-N9-C4	-5.23	103.71	105.80
26	14	133	C	N3-C4-C5	5.23	123.99	121.90
26	14	764	A	N1-C2-N3	-5.23	126.69	129.30
26	1H	36	G	OP2-P-O3'	5.23	116.70	105.20
26	1H	121	G	C6-N1-C2	-5.23	121.97	125.10
26	14	608	A	C4-C5-C6	5.23	119.61	117.00
26	1H	1157	G	C4-N9-C1'	5.22	133.29	126.50
26	14	2438	U	O5'-P-OP2	-5.22	101.00	105.70
1	13	800	G	N3-C4-N9	5.22	129.13	126.00
26	1H	125	G	N9-C4-C5	-5.22	103.31	105.40
26	1H	591	C	C4-C5-C6	5.22	120.01	117.40
26	14	1571	A	C5-C6-N6	-5.22	119.52	123.70
26	14	1762	A	C8-N9-C1'	-5.22	118.30	127.70
26	14	2346	A	C8-N9-C1'	-5.22	118.30	127.70
23	2K	40	C	C5-C6-N1	5.22	123.61	121.00
26	14	845	G	C4-C5-N7	5.22	112.89	110.80
26	14	944	G	C4-N9-C1'	5.22	133.29	126.50
26	14	1767	C	C5-C4-N4	5.22	123.86	120.20
26	1H	428	A	OP1-P-O3'	5.22	116.68	105.20
26	1H	717	G	C6-C5-N7	-5.22	127.27	130.40
26	14	203	C	N3-C4-C5	5.22	123.99	121.90
26	1H	1302	A	C2-N3-C4	5.22	113.21	110.60
26	1H	2286	A	C6-C5-N7	-5.22	128.65	132.30
26	14	2388	A	O5'-P-OP1	5.22	116.96	110.70
26	14	2565	A	N9-C4-C5	-5.22	103.71	105.80
26	1H	1448	G	O5'-P-OP1	-5.22	101.01	105.70
27	1J	22	U	C5-C6-N1	5.22	125.31	122.70
26	1H	1598	C	C5-C6-N1	-5.21	118.39	121.00
26	14	2573	C	C6-N1-C1'	-5.21	114.54	120.80
26	1H	2062	A	C8-N9-C4	5.21	107.89	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	2891	G	C5-C6-O6	-5.21	125.47	128.60
27	16	80	U	N1-C2-O2	5.21	126.45	122.80
26	14	946	G	C2-N3-C4	-5.21	109.30	111.90
26	14	1379	A	C4-C5-N7	5.21	113.31	110.70
37	35	55	ARG	NE-CZ-NH1	-5.21	117.69	120.30
26	14	2287	A	N1-C2-N3	5.21	131.91	129.30
26	1H	1544	C	C2-N1-C1'	5.21	124.53	118.80
26	1H	2699	C	N3-C4-C5	5.21	123.98	121.90
26	1H	2765	A	OP1-P-OP2	5.21	127.41	119.60
49	J8	2	SER	CB-CA-C	-5.21	100.20	110.10
26	14	246	C	C6-N1-C2	5.21	122.38	120.30
26	14	2275	C	C5'-C4'-O4'	-5.21	102.85	109.10
30	29	44	TYR	CA-CB-CG	5.21	123.30	113.40
26	1H	462	C	OP1-P-OP2	5.21	127.41	119.60
26	1H	2281	C	C5-C4-N4	-5.21	116.56	120.20
26	14	679	C	N1-C2-O2	-5.21	115.78	118.90
26	1H	124	G	C4-N9-C1'	-5.21	119.73	126.50
26	1H	1602	U	C5-C4-O4	5.20	129.02	125.90
40	A8	9	ARG	NE-CZ-NH1	-5.20	117.70	120.30
1	1G	810	C	N3-C2-O2	-5.20	118.26	121.90
26	14	970	C	C6-N1-C1'	5.20	127.04	120.80
26	1H	1252	G	C5-N7-C8	5.20	106.90	104.30
26	14	1799	G	C5-C6-O6	5.20	131.72	128.60
26	1H	207	A	N9-C4-C5	-5.20	103.72	105.80
26	1H	1882	C	C6-N1-C2	-5.20	118.22	120.30
26	1H	1934	C	N3-C4-C5	-5.20	119.82	121.90
26	1H	2370	G	N1-C2-N2	-5.20	111.52	116.20
1	13	853	G	C5-C6-N1	-5.20	108.90	111.50
26	1H	1497	U	OP1-P-O3'	5.20	116.64	105.20
1	1G	1305	G	N3-C4-N9	-5.20	122.88	126.00
26	14	641	C	C6-N1-C2	5.20	122.38	120.30
27	16	100	G	N9-C4-C5	-5.20	103.32	105.40
1	13	963	G	C5-C6-O6	5.20	131.72	128.60
1	13	1502	A	N7-C8-N9	5.20	116.40	113.80
26	1H	1275	A	C2-N3-C4	-5.20	108.00	110.60
26	1H	2375	G	N9-C1'-C2'	-5.20	106.28	112.00
26	1H	2623	G	N9-C4-C5	5.20	107.48	105.40
1	1G	1499	A	C8-N9-C4	5.20	107.88	105.80
26	14	141	A	C5-N7-C8	-5.20	101.30	103.90
26	14	933	A	C4-C5-N7	5.20	113.30	110.70
26	14	998	C	N1-C2-O2	5.20	122.02	118.90
26	14	2211	G	O5'-P-OP2	-5.20	101.02	105.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	14	2297	C	OP1-P-OP2	5.20	127.39	119.60
1	13	741	G	O5'-P-OP2	-5.19	101.03	105.70
26	14	2446	G	OP2-P-O3'	5.19	116.63	105.20
26	1H	245	G	C4-C5-N7	5.19	112.88	110.80
26	1H	478	A	N1-C6-N6	-5.19	115.48	118.60
26	1H	695	G	N1-C6-O6	-5.19	116.78	119.90
26	1H	2282	G	C5-C6-O6	5.19	131.72	128.60
26	1H	2390	U	C2-N1-C1'	5.19	123.93	117.70
26	14	2331	G	C4-C5-N7	5.19	112.88	110.80
26	14	2581	G	N3-C4-C5	-5.19	126.00	128.60
1	13	533	A	C2-N3-C4	-5.19	108.00	110.60
26	1H	136	G	C5-C6-N1	5.19	114.09	111.50
26	1H	1410	G	N3-C4-C5	5.19	131.20	128.60
26	1H	627	A	OP1-P-O3'	5.19	116.62	105.20
1	13	413	G	O4'-C1'-N9	5.19	112.35	108.20
1	13	522	C	O5'-P-OP2	-5.19	101.03	105.70
26	1H	766	C	N3-C4-C5	5.19	123.97	121.90
26	1H	1777	U	N1-C2-N3	5.19	118.01	114.90
26	1H	2007	C	O5'-P-OP2	-5.19	101.03	105.70
26	1H	2502	G	C8-N9-C4	-5.19	104.33	106.40
26	1H	2872	G	O5'-P-OP2	-5.19	101.03	105.70
26	1H	1344	G	C8-N9-C4	-5.19	104.33	106.40
26	1H	1470	G	N1-C6-O6	5.19	123.01	119.90
26	1H	1799	G	N3-C4-C5	-5.19	126.01	128.60
26	14	201	C	C6-N1-C2	5.19	122.38	120.30
26	14	393	C	C5-C4-N4	5.19	123.83	120.20
26	14	2681	C	N3-C2-O2	-5.19	118.27	121.90
26	1H	1842	G	C5-C6-O6	5.18	131.71	128.60
26	1H	2033	A	C5-C6-N6	-5.18	119.55	123.70
23	2L	6	G	C8-N9-C4	5.18	108.47	106.40
26	14	1678	G	C4-C5-N7	5.18	112.87	110.80
26	14	2304	G	N9-C4-C5	5.18	107.47	105.40
27	1J	71	C	C2-N1-C1'	5.18	124.50	118.80
26	1H	840	C	O5'-P-OP2	-5.18	101.04	105.70
26	1H	1997	G	C2-N3-C4	-5.18	109.31	111.90
26	1H	2821	A	N9-C4-C5	-5.18	103.73	105.80
26	1H	2280	G	OP1-P-OP2	-5.18	111.83	119.60
26	14	1742	C	C6-N1-C2	-5.18	118.23	120.30
26	1H	829	A	O5'-P-OP1	-5.18	101.04	105.70
26	1H	2328	A	C2-N3-C4	-5.18	108.01	110.60
1	1G	25	C	O5'-P-OP2	-5.18	101.04	105.70
26	14	2699	C	C5-C6-N1	-5.18	118.41	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	471	A	C6-N1-C2	5.18	121.71	118.60
26	1H	772	C	C6-N1-C2	5.18	122.37	120.30
26	14	2281	C	C5-C6-N1	5.18	123.59	121.00
1	13	1227	A	C2-N3-C4	-5.18	108.01	110.60
26	1H	630	G	C4-N9-C1'	-5.18	119.77	126.50
26	1H	848	G	C4-N9-C1'	5.18	133.23	126.50
26	1H	1307	A	N9-C4-C5	-5.18	103.73	105.80
26	1H	1357	U	OP1-P-OP2	5.18	127.36	119.60
26	1H	1669	A	N3-C4-N9	5.18	131.54	127.40
26	1H	1858	G	C8-N9-C1'	-5.18	120.27	127.00
26	1H	2519	U	N3-C2-O2	5.18	125.82	122.20
26	14	852	G	O5'-P-OP2	-5.18	101.04	105.70
26	14	1667	G	N1-C6-O6	5.18	123.01	119.90
26	1H	733	G	N3-C4-N9	5.17	129.10	126.00
26	1H	1674	G	N1-C6-O6	5.17	123.00	119.90
26	14	1785	A	C4-C5-C6	5.17	119.59	117.00
26	1H	126	A	OP2-P-O3'	5.17	116.58	105.20
26	1H	726	G	OP1-P-OP2	5.17	127.36	119.60
26	14	566	U	O5'-P-OP2	-5.17	101.04	105.70
26	1H	74	A	C4-C5-C6	5.17	119.59	117.00
26	1H	952	G	O5'-P-OP2	5.17	116.91	110.70
26	1H	2509	G	C8-N9-C4	5.17	108.47	106.40
26	14	250	G	C8-N9-C4	-5.17	104.33	106.40
26	14	744	G	O5'-P-OP2	-5.17	101.05	105.70
26	1H	71	A	C8-N9-C4	-5.17	103.73	105.80
26	14	973	A	OP1-P-OP2	-5.17	111.84	119.60
1	13	827	U	C6-N1-C1'	-5.17	113.97	121.20
26	1H	745	G	OP1-P-OP2	-5.17	111.85	119.60
26	1H	2713	A	O4'-C1'-N9	-5.17	104.06	108.20
24	3L	76	A	C6-C5-N7	-5.17	128.68	132.30
26	14	2029	G	O5'-P-OP1	-5.17	101.05	105.70
1	13	757	U	C5-C6-N1	-5.17	120.12	122.70
1	13	1530	G	N1-C6-O6	5.17	123.00	119.90
26	1H	123	G	O5'-P-OP2	-5.17	101.05	105.70
26	1H	1315	C	N3-C4-N4	-5.17	114.38	118.00
26	1H	2446	G	N1-C6-O6	5.17	123.00	119.90
26	1H	2581	G	N3-C2-N2	5.17	123.52	119.90
1	13	966	G	C8-N9-C4	5.17	108.47	106.40
26	1H	1978	A	N1-C6-N6	-5.17	115.50	118.60
26	1H	103	A	N9-C4-C5	-5.16	103.73	105.80
26	1H	140	A	N3-C4-C5	5.16	130.41	126.80
26	1H	528	A	N1-C6-N6	5.16	121.70	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	1210	A	C5-C6-N1	-5.16	115.12	117.70
26	1H	1973	G	N1-C6-O6	-5.16	116.80	119.90
26	1H	1978	A	N9-C4-C5	5.16	107.87	105.80
1	1G	1370	G	C5-C6-N1	-5.16	108.92	111.50
26	14	149	A	C4-C5-C6	5.16	119.58	117.00
26	14	530	G	N7-C8-N9	5.16	115.68	113.10
26	14	2042	A	C8-N9-C4	5.16	107.87	105.80
26	14	2057	A	O5'-P-OP2	-5.16	101.06	105.70
26	14	2703	C	N3-C2-O2	-5.16	118.29	121.90
26	1H	451	C	C6-N1-C2	5.16	122.36	120.30
26	1H	602	G	C6-C5-N7	-5.16	127.30	130.40
26	1H	1473	G	OP1-P-O3'	5.16	116.55	105.20
26	1H	2249	U	N3-C4-C5	5.16	117.69	114.60
26	1H	2706	G	C5-C6-N1	5.16	114.08	111.50
30	21	49	LEU	CA-CB-CG	-5.16	103.44	115.30
26	14	372	G	O4'-C1'-N9	5.16	112.33	108.20
26	14	1831	G	N1-C2-N2	-5.16	111.56	116.20
26	14	2030	A	O5'-P-OP2	-5.16	101.06	105.70
1	13	813	U	N3-C2-O2	-5.16	118.59	122.20
1	13	1516	G	C5-C6-O6	5.16	131.69	128.60
26	14	1899	G	C4-C5-N7	5.16	112.86	110.80
26	1H	139	G	C2-N3-C4	5.16	114.48	111.90
26	1H	1573	G	C4-C5-N7	5.16	112.86	110.80
26	14	678	C	C6-N1-C2	5.16	122.36	120.30
26	14	2263	C	C6-N1-C2	-5.16	118.24	120.30
26	14	2380	C	N1-C2-O2	-5.16	115.81	118.90
26	14	2607	G	N1-C2-N2	-5.16	111.56	116.20
27	1J	44	G	N7-C8-N9	-5.16	110.52	113.10
26	1H	2623	G	N1-C2-N2	-5.15	111.56	116.20
26	1H	2697	G	N1-C6-O6	-5.15	116.81	119.90
27	16	44	G	C6-C5-N7	5.15	133.49	130.40
27	16	108	C	O4'-C1'-N1	5.15	112.32	108.20
26	14	783	A	N9-C1'-C2'	-5.15	106.33	112.00
26	14	1776	G	N9-C4-C5	-5.15	103.34	105.40
26	1H	1888	G	O4'-C1'-N9	5.15	112.32	108.20
26	1H	2623	G	C5-C6-O6	5.15	131.69	128.60
26	14	1610	A	C8-N9-C4	5.15	107.86	105.80
26	14	1975	G	O5'-P-OP1	5.15	116.88	110.70
27	1J	71	C	C6-N1-C2	-5.15	118.24	120.30
1	13	108	G	C5-N7-C8	-5.15	101.72	104.30
1	13	1197	G	OP1-P-O3'	5.15	116.53	105.20
26	1H	1604	C	C2-N3-C4	-5.15	117.33	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1G	932	C	N1-C2-O2	5.15	121.99	118.90
1	1G	1071	C	C6-N1-C2	-5.15	118.24	120.30
1	1G	898	G	O5'-P-OP2	-5.15	101.07	105.70
26	14	2430	A	N3-C4-C5	5.15	130.40	126.80
26	14	2589	A	C8-N9-C4	5.15	107.86	105.80
1	13	988	G	C8-N9-C4	-5.15	104.34	106.40
1	13	1489	G	N9-C4-C5	-5.15	103.34	105.40
26	1H	241	A	C2-N3-C4	-5.15	108.03	110.60
26	1H	1393	A	O5'-P-OP2	-5.15	101.07	105.70
26	14	2542	A	O5'-P-OP2	-5.15	101.07	105.70
1	13	1519	A	C5-C6-N6	5.15	127.82	123.70
26	1H	591	C	C2-N3-C4	-5.15	117.33	119.90
26	1H	463	G	N1-C2-N2	-5.14	111.57	116.20
26	1H	803	U	O4'-C1'-N1	5.14	112.31	108.20
26	1H	2537	U	N3-C4-O4	-5.14	115.80	119.40
26	14	161	U	C5-C6-N1	5.14	125.27	122.70
26	14	681	G	C8-N9-C4	5.14	108.46	106.40
26	14	772	C	O5'-P-OP1	-5.14	101.07	105.70
26	14	1642	G	OP2-P-O3'	5.14	116.52	105.20
26	14	1799	G	C4-C5-N7	-5.14	108.74	110.80
26	1H	481	G	C5-C6-O6	-5.14	125.51	128.60
26	1H	1308	A	N1-C2-N3	5.14	131.87	129.30
26	1H	1996	C	N3-C4-N4	-5.14	114.40	118.00
26	14	746	A	O4'-C1'-N9	5.14	112.31	108.20
26	14	775	G	N3-C4-N9	5.14	129.09	126.00
26	14	1681	G	C8-N9-C4	-5.14	104.34	106.40
27	1J	35	U	N3-C4-O4	-5.14	115.80	119.40
26	14	2359	C	O5'-P-OP1	-5.14	101.07	105.70
26	1H	265	A	N9-C1'-C2'	5.14	120.68	114.00
26	1H	777	A	OP2-P-O3'	5.14	116.50	105.20
26	1H	1022	G	P-O3'-C3'	5.14	125.87	119.70
26	14	1379	A	N7-C8-N9	5.14	116.37	113.80
1	13	896	C	C6-N1-C2	5.14	122.36	120.30
26	1H	1401	G	C5-C6-O6	5.14	131.68	128.60
26	1H	1673	U	C6-N1-C2	5.14	124.08	121.00
26	1H	2257	U	N1-C2-N3	5.14	117.98	114.90
26	1H	126	A	OP1-P-OP2	5.14	127.31	119.60
26	1H	1778	U	OP2-P-O3'	5.14	116.50	105.20
26	1H	2078	C	N3-C4-N4	5.14	121.59	118.00
1	1G	509	A	P-O3'-C3'	5.14	125.86	119.70
1	1G	576	G	N3-C4-C5	-5.14	126.03	128.60
26	14	514	A	OP1-P-OP2	5.14	127.31	119.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	14	804	A	O4'-C1'-N9	5.14	112.31	108.20
26	14	1680	U	C5-C4-O4	-5.14	122.82	125.90
26	1H	411	G	OP1-P-OP2	5.13	127.30	119.60
26	1H	868	U	N3-C2-O2	-5.13	118.61	122.20
26	1H	906	G	C5-C6-O6	5.13	131.68	128.60
26	1H	2415	G	N3-C2-N2	-5.13	116.31	119.90
26	14	1300	U	O5'-P-OP1	5.13	116.86	110.70
26	14	1807	G	O5'-P-OP2	-5.13	101.08	105.70
26	1H	963	U	N3-C4-O4	5.13	122.99	119.40
1	1G	1228	C	O5'-P-OP2	-5.13	101.08	105.70
26	14	784	A	P-O3'-C3'	5.13	125.86	119.70
26	14	1349	A	C4-C5-N7	5.13	113.27	110.70
26	14	1379	A	P-O3'-C3'	5.13	125.86	119.70
26	14	1482	U	C6-N1-C1'	5.13	128.38	121.20
26	14	2392	A	N3-C4-N9	-5.13	123.30	127.40
26	14	2518	A	O5'-P-OP2	-5.13	101.08	105.70
26	1H	2261	C	OP2-P-O3'	5.13	116.48	105.20
26	1H	2604	U	C2-N1-C1'	5.13	123.86	117.70
24	1L	69	A	P-O3'-C3'	5.13	125.86	119.70
1	13	266	G	N7-C8-N9	5.13	115.66	113.10
26	1H	1683	C	C2-N3-C4	-5.13	117.34	119.90
26	1H	1801	G	N3-C4-N9	5.13	129.08	126.00
26	1H	2380	C	N1-C2-O2	-5.13	115.82	118.90
1	1G	1518	A	O5'-P-OP1	-5.13	101.08	105.70
1	13	268	C	O5'-P-OP2	5.13	116.85	110.70
26	1H	252	G	C6-C5-N7	-5.13	127.33	130.40
26	1H	535	C	C2-N1-C1'	-5.13	113.16	118.80
26	1H	829	A	C2-N3-C4	-5.13	108.04	110.60
26	1H	2377	A	N3-C4-C5	5.13	130.39	126.80
26	1H	2599	G	N1-C6-O6	-5.13	116.82	119.90
26	1H	2689	U	N3-C4-C5	-5.13	111.52	114.60
26	14	1463	C	C6-N1-C2	-5.13	118.25	120.30
26	1H	1804	C	N3-C4-C5	5.12	123.95	121.90
26	14	1251	C	C5-C4-N4	-5.12	116.61	120.20
26	14	1482	U	C2-N1-C1'	-5.12	111.55	117.70
26	1H	139	G	O5'-P-OP1	-5.12	101.09	105.70
26	1H	767	U	N1-C2-N3	5.12	117.97	114.90
26	14	2251	G	C4-C5-N7	-5.12	108.75	110.80
26	14	2430	A	O4'-C1'-N9	-5.12	104.10	108.20
1	13	572	A	N1-C6-N6	-5.12	115.53	118.60
1	1G	134	A	N1-C6-N6	5.12	121.67	118.60
23	2K	27	G	N1-C6-O6	5.12	122.97	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	625	G	N9-C4-C5	5.12	107.45	105.40
26	1H	1032	A	N1-C6-N6	5.12	121.67	118.60
26	1H	1818	U	N3-C4-C5	5.12	117.67	114.60
26	1H	2716	U	OP2-P-O3'	5.12	116.47	105.20
26	1H	602	G	N1-C2-N2	-5.12	111.59	116.20
26	1H	766	C	N1-C2-O2	-5.12	115.83	118.90
26	1H	1162	G	O5'-P-OP1	-5.12	101.09	105.70
26	1H	2070	G	N1-C6-O6	-5.12	116.83	119.90
26	14	238	C	N1-C2-O2	-5.12	115.83	118.90
1	13	524	G	O5'-P-OP1	-5.12	101.09	105.70
26	1H	737	C	OP1-P-O3'	-5.12	93.94	105.20
26	1H	1021	A	N1-C6-N6	5.12	121.67	118.60
26	1H	1535	U	OP1-P-O3'	5.12	116.45	105.20
26	1H	1555	G	O5'-P-OP2	5.12	116.84	110.70
1	1G	541	G	N1-C6-O6	5.12	122.97	119.90
27	1J	89	G	C8-N9-C1'	-5.12	120.35	127.00
26	1H	732	C	C4-C5-C6	5.11	119.96	117.40
26	14	1588	C	C6-N1-C2	-5.11	118.25	120.30
26	14	608	A	C8-N9-C4	-5.11	103.76	105.80
26	14	1372	U	C2-N3-C4	-5.11	123.93	127.00
26	14	2490	G	C4-N9-C1'	5.11	133.14	126.50
1	13	302	G	N1-C6-O6	-5.11	116.83	119.90
26	1H	958	U	N1-C2-N3	5.11	117.97	114.90
1	1G	331	G	N1-C6-O6	5.11	122.97	119.90
26	14	1998	G	C2-N3-C4	-5.11	109.35	111.90
23	2K	68	C	C6-N1-C2	-5.11	118.26	120.30
26	1H	191	A	O5'-P-OP1	5.11	116.83	110.70
26	1H	2566	A	P-O3'-C3'	5.11	125.83	119.70
26	14	113	G	N1-C6-O6	5.11	122.96	119.90
26	14	1682	G	O5'-P-OP2	-5.11	101.10	105.70
1	13	843	U	C5-C6-N1	5.11	125.25	122.70
26	1H	1574	C	N3-C4-C5	5.11	123.94	121.90
1	13	1503	A	C8-N9-C4	5.10	107.84	105.80
26	1H	1423	G	O5'-P-OP2	-5.10	101.11	105.70
47	H8	128	VAL	C-N-CA	-5.10	108.94	121.70
26	1H	682	G	C4-N9-C1'	5.10	133.13	126.50
26	1H	2330	G	C6-C5-N7	-5.10	127.34	130.40
33	51	156	ALA	C-N-CA	5.10	134.46	121.70
26	14	1379	A	C8-N9-C4	-5.10	103.76	105.80
26	1H	754	C	C5-C6-N1	-5.10	118.45	121.00
26	1H	821	A	C8-N9-C4	-5.10	103.76	105.80
42	C8	27	LEU	CA-CB-CG	5.10	127.03	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	2279	G	C5-C6-O6	5.10	131.66	128.60
26	14	842	G	N1-C6-O6	-5.10	116.84	119.90
26	14	2286	A	C8-N9-C4	-5.10	103.76	105.80
26	1H	590	A	C5-C6-N6	-5.10	119.62	123.70
26	1H	686	G	N3-C2-N2	5.10	123.47	119.90
26	1H	1603	A	P-O3'-C3'	5.10	125.82	119.70
27	16	54	G	N7-C8-N9	5.10	115.65	113.10
26	1H	909	A	C2-N3-C4	5.10	113.15	110.60
26	1H	1348	G	N9-C1'-C2'	-5.10	106.39	112.00
26	1H	1401	G	N7-C8-N9	5.10	115.65	113.10
26	14	1930	G	C8-N9-C1'	5.10	133.62	127.00
1	13	833	U	C2-N1-C1'	-5.09	111.59	117.70
26	1H	1931	U	C4-C5-C6	5.09	122.76	119.70
26	1H	2336	A	O5'-P-OP1	-5.09	101.12	105.70
26	14	863	A	O5'-P-OP2	-5.09	101.12	105.70
26	14	866	A	N9-C4-C5	-5.09	103.76	105.80
26	14	1617	C	C5-C6-N1	-5.09	118.45	121.00
26	14	2726	U	C5-C4-O4	5.09	128.96	125.90
1	13	978	A	N1-C6-N6	5.09	121.66	118.60
26	1H	2266	A	C6-N1-C2	-5.09	115.54	118.60
26	1H	2326	C	C6-N1-C2	-5.09	118.26	120.30
26	1H	2506	U	N3-C2-O2	-5.09	118.64	122.20
26	14	308	G	O5'-P-OP2	-5.09	101.12	105.70
26	14	1776	G	N3-C4-C5	-5.09	126.05	128.60
26	1H	1298	C	OP2-P-O3'	-5.09	94.00	105.20
26	1H	1634	A	OP1-P-OP2	5.09	127.24	119.60
26	1H	2827	C	C5-C4-N4	-5.09	116.64	120.20
26	14	186	G	C8-N9-C4	5.09	108.44	106.40
26	14	871	U	OP1-P-O3'	5.09	116.40	105.20
1	13	356	A	O4'-C1'-N9	5.09	112.27	108.20
26	1H	838	C	OP2-P-O3'	5.09	116.40	105.20
26	14	90	U	N3-C2-O2	-5.09	118.64	122.20
26	14	1215	G	C8-N9-C4	-5.09	104.36	106.40
26	14	2442	C	C2-N3-C4	-5.09	117.36	119.90
26	14	2552	U	N3-C4-O4	5.09	122.96	119.40
1	13	703	G	N3-C4-N9	5.09	129.05	126.00
26	14	2390	U	N1-C2-N3	5.09	117.95	114.90
26	14	2433	A	N9-C4-C5	-5.09	103.77	105.80
26	14	2733	A	C8-N9-C4	-5.09	103.77	105.80
27	1J	7	G	C6-C5-N7	-5.09	127.35	130.40
26	1H	330	A	O5'-P-OP2	-5.09	101.12	105.70
26	1H	513	A	N1-C6-N6	-5.09	115.55	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	733	G	C2-N3-C4	-5.09	109.36	111.90
26	1H	1496	A	C5-C6-N6	-5.09	119.63	123.70
26	1H	2440	C	OP1-P-O3'	5.09	116.39	105.20
1	1G	1374	A	O4'-C1'-N9	5.09	112.27	108.20
26	1H	2244	U	C6-N1-C2	-5.08	117.95	121.00
1	13	713	G	C8-N9-C4	5.08	108.43	106.40
26	1H	1626	G	N1-C2-N2	5.08	120.78	116.20
26	1H	1993	U	C2-N3-C4	-5.08	123.95	127.00
26	1H	2311	A	N1-C6-N6	5.08	121.65	118.60
26	1H	2586	C	C5-C4-N4	-5.08	116.64	120.20
26	1H	2618	G	O5'-P-OP2	-5.08	101.12	105.70
26	14	1424	G	N1-C6-O6	5.08	122.95	119.90
27	1J	102	G	C5-C6-O6	5.08	131.65	128.60
26	1H	532	A	C5-N7-C8	-5.08	101.36	103.90
26	1H	832	G	C5-C6-N1	-5.08	108.96	111.50
26	1H	983	A	OP2-P-O3'	5.08	116.38	105.20
26	1H	1025	G	C4-C5-N7	-5.08	108.77	110.80
26	1H	1951	U	O5'-P-OP2	5.08	116.80	110.70
26	1H	1998	G	N7-C8-N9	-5.08	110.56	113.10
26	1H	2023	G	C8-N9-C4	-5.08	104.37	106.40
26	1H	2726	U	C5-C6-N1	-5.08	120.16	122.70
26	14	503	A	C5-C6-N6	5.08	127.77	123.70
26	14	521	G	OP1-P-OP2	-5.08	111.98	119.60
1	13	1468	A	C6-N1-C2	-5.08	115.55	118.60
26	1H	837	C	N3-C4-C5	-5.08	119.87	121.90
26	1H	2047	U	N3-C4-O4	-5.08	115.84	119.40
26	1H	2287	A	C6-N1-C2	5.08	121.65	118.60
41	B8	105	LEU	CA-CB-CG	5.08	126.98	115.30
26	14	19	C	C6-N1-C2	5.08	122.33	120.30
26	14	2724	C	N1-C2-O2	-5.08	115.85	118.90
30	29	144	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	13	723	U	C5-C6-N1	5.08	125.24	122.70
23	2K	6	G	C2-N3-C4	-5.08	109.36	111.90
26	1H	634	C	O5'-P-OP2	-5.08	101.13	105.70
26	1H	712	G	N1-C6-O6	5.08	122.95	119.90
26	1H	1609	A	C5-C6-N6	-5.08	119.64	123.70
26	1H	1936	A	C5-N7-C8	-5.08	101.36	103.90
26	1H	2618	G	C4-C5-N7	-5.08	108.77	110.80
26	1H	141(A)	C	N3-C4-C5	5.08	123.93	121.90
26	1H	410	G	N3-C2-N2	-5.08	116.35	119.90
26	1H	114	U	OP1-P-O3'	5.08	116.36	105.20
26	1H	747	U	OP1-P-OP2	5.08	127.21	119.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	1630	G	O5'-P-OP2	5.08	116.79	110.70
26	1H	2350	C	N3-C2-O2	-5.08	118.35	121.90
26	1H	2387	U	OP1-P-O3'	-5.08	94.03	105.20
54	O8	21	TYR	C-N-CA	5.08	134.39	121.70
26	14	24	G	N3-C4-N9	-5.08	122.95	126.00
26	14	1758	G	O5'-P-OP1	-5.08	101.13	105.70
26	14	940	G	O5'-P-OP2	-5.07	101.13	105.70
26	1H	808	G	N1-C6-O6	-5.07	116.86	119.90
26	1H	2870	C	OP2-P-O3'	5.07	116.36	105.20
1	1G	909	A	C5-C6-N6	-5.07	119.64	123.70
26	14	1675	C	OP1-P-O3'	5.07	116.36	105.20
26	1H	49	A	N9-C4-C5	-5.07	103.77	105.80
26	1H	98	G	OP1-P-OP2	5.07	127.20	119.60
26	1H	1770	G	OP1-P-O3'	5.07	116.36	105.20
1	1G	1397	C	N1-C2-O2	5.07	121.94	118.90
26	14	470	A	N9-C4-C5	-5.07	103.77	105.80
26	14	2489	G	OP2-P-O3'	5.07	116.36	105.20
26	14	2729	G	N9-C4-C5	-5.07	103.37	105.40
26	1H	762	U	C6-N1-C1'	-5.07	114.10	121.20
26	14	396	G	C8-N9-C1'	-5.07	120.41	127.00
26	1H	237	C	C4-C5-C6	5.07	119.93	117.40
26	1H	1797	C	C2-N3-C4	-5.07	117.37	119.90
26	1H	1964	G	O4'-C1'-N9	-5.07	104.15	108.20
1	1G	1145	C	P-O3'-C3'	5.07	125.78	119.70
1	1G	1508	G	O5'-P-OP1	-5.07	101.14	105.70
26	14	1258	C	C5-C6-N1	5.07	123.53	121.00
26	14	1806	C	O5'-P-OP2	-5.07	101.14	105.70
1	13	963	G	N1-C2-N3	5.07	126.94	123.90
23	2L	35	C	C2-N1-C1'	5.07	124.37	118.80
26	14	130	C	C6-N1-C2	5.07	122.33	120.30
26	14	1446	C	N1-C2-O2	5.07	121.94	118.90
26	14	2576	G	C2-N3-C4	5.07	114.43	111.90
26	14	140	A	C2-N3-C4	-5.06	108.07	110.60
26	14	1432	C	N1-C2-O2	-5.06	115.86	118.90
26	14	2062	A	N9-C4-C5	-5.06	103.77	105.80
26	14	2281	C	OP1-P-O3'	5.06	116.34	105.20
26	1H	192	C	N3-C2-O2	5.06	125.44	121.90
26	1H	377	C	C6-N1-C2	5.06	122.33	120.30
26	1H	1678	G	O4'-C1'-N9	-5.06	104.15	108.20
26	1H	2227	A	N1-C6-N6	-5.06	115.56	118.60
26	14	782	A	C8-N9-C4	5.06	107.83	105.80
26	14	1283	G	N3-C4-C5	-5.06	126.07	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	14	1400	G	O5'-P-OP1	5.06	116.78	110.70
26	14	2032	G	O4'-C1'-N9	-5.06	104.15	108.20
26	14	2211	G	C6-C5-N7	-5.06	127.36	130.40
23	2K	42	C	O5'-P-OP2	-5.06	101.14	105.70
20	BA	11	SER	C-N-CA	5.06	134.35	121.70
26	1H	695	G	N1-C2-N2	-5.06	111.65	116.20
1	1G	518	C	O5'-P-OP2	-5.06	101.15	105.70
26	14	858	U	C6-N1-C2	-5.06	117.96	121.00
26	1H	692	C	C5-C6-N1	-5.06	118.47	121.00
26	1H	1325	G	N1-C6-O6	5.06	122.94	119.90
26	1H	2584	U	N1-C2-N3	5.06	117.93	114.90
26	14	24	G	N3-C4-C5	5.06	131.13	128.60
26	14	472	A	N9-C4-C5	5.06	107.82	105.80
26	14	639	U	N3-C2-O2	-5.06	118.66	122.20
26	14	1395	A	O4'-C1'-N9	5.06	112.25	108.20
26	14	1462	C	C6-N1-C2	-5.06	118.28	120.30
26	14	1777	U	P-O3'-C3'	5.06	125.77	119.70
26	14	691	C	C4-C5-C6	5.06	119.93	117.40
26	14	2250	G	O5'-P-OP1	-5.06	101.15	105.70
1	13	1475	G	N7-C8-N9	5.05	115.63	113.10
26	1H	984	A	OP1-P-O3'	5.05	116.32	105.20
1	1G	700	G	C8-N9-C1'	5.05	133.57	127.00
26	14	929	G	N7-C8-N9	5.05	115.63	113.10
1	13	353	A	OP2-P-O3'	5.05	116.32	105.20
23	2K	48	U	P-O3'-C3'	5.05	125.76	119.70
26	1H	698	C	C5-C4-N4	-5.05	116.66	120.20
26	1H	2101	G	C5-C6-N1	-5.05	108.97	111.50
1	13	346	G	C4-C5-N7	5.05	112.82	110.80
26	1H	987	G	O5'-P-OP1	-5.05	101.15	105.70
26	1H	1594	G	N3-C2-N2	-5.05	116.36	119.90
26	14	229	A	O4'-C1'-N9	5.05	112.24	108.20
26	14	1660	C	N3-C4-C5	5.05	123.92	121.90
26	14	2329	G	O5'-P-OP1	5.05	116.76	110.70
26	1H	804	A	O4'-C1'-N9	5.05	112.24	108.20
26	1H	2826	A	N7-C8-N9	-5.05	111.28	113.80
26	14	2307	G	C8-N9-C4	-5.05	104.38	106.40
26	14	2859	G	P-O3'-C3'	5.05	125.76	119.70
26	1H	688	U	C2-N3-C4	-5.05	123.97	127.00
30	21	195	LEU	CA-CB-CG	5.05	126.91	115.30
26	14	1674	G	N3-C4-C5	-5.05	126.08	128.60
26	14	2248	C	C5-C4-N4	5.05	123.73	120.20
33	59	92	ILE	CG1-CB-CG2	-5.05	100.29	111.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	13	890	G	O4'-C1'-N9	5.05	112.24	108.20
1	13	1259	C	N1-C2-O2	5.05	121.93	118.90
26	1H	74	A	N3-C4-N9	-5.05	123.36	127.40
26	1H	241	A	N1-C2-N3	5.05	131.82	129.30
26	1H	528	A	C4-C5-C6	-5.05	114.48	117.00
26	1H	866	A	C8-N9-C1'	-5.05	118.62	127.70
26	1H	2257	U	C5-C6-N1	-5.05	120.18	122.70
26	14	468	G	OP1-P-OP2	-5.05	112.03	119.60
26	1H	25	U	C5-C4-O4	-5.04	122.87	125.90
26	1H	1626	G	N3-C4-N9	-5.04	122.97	126.00
26	1H	2422	A	C8-N9-C4	-5.04	103.78	105.80
26	14	2437	U	OP1-P-OP2	5.04	127.17	119.60
1	13	320	C	C6-N1-C2	5.04	122.32	120.30
26	1H	51	G	N1-C6-O6	-5.04	116.87	119.90
26	1H	566	U	OP1-P-O3'	5.04	116.30	105.20
26	1H	684	G	C5-C6-N1	5.04	114.02	111.50
26	1H	732	C	C2-N3-C4	-5.04	117.38	119.90
26	1H	1235	G	C8-N9-C4	-5.04	104.38	106.40
26	1H	2598	A	C5-C6-N6	-5.04	119.67	123.70
1	1G	1514	C	N1-C2-O2	-5.04	115.87	118.90
26	14	961	C	N1-C2-O2	-5.04	115.87	118.90
26	14	2355	C	C6-N1-C1'	-5.04	114.75	120.80
26	14	2685	G	N1-C2-N2	5.04	120.74	116.20
1	13	1430	C	O5'-P-OP1	-5.04	101.16	105.70
1	13	1482	G	O5'-P-OP2	-5.04	101.16	105.70
26	1H	684	G	N3-C4-C5	-5.04	126.08	128.60
26	1H	1153	C	N1-C2-O2	-5.04	115.88	118.90
26	1H	1644	C	N3-C2-O2	-5.04	118.37	121.90
26	1H	2047	U	N1-C2-O2	5.04	126.33	122.80
26	1H	2287	A	C6-C5-N7	-5.04	128.77	132.30
27	16	81	G	C2-N3-C4	-5.04	109.38	111.90
26	14	1827	C	C5-C6-N1	-5.04	118.48	121.00
26	14	1953	A	O5'-P-OP2	5.04	116.75	110.70
26	14	2426	A	C5-N7-C8	-5.04	101.38	103.90
26	1H	586	A	OP1-P-O3'	5.04	116.29	105.20
26	1H	764	A	OP1-P-O3'	5.04	116.29	105.20
26	14	49	A	OP2-P-O3'	5.04	116.29	105.20
26	14	1496	A	N1-C6-N6	5.04	121.62	118.60
26	14	1831	G	C2-N3-C4	-5.04	109.38	111.90
1	13	1434	A	N7-C8-N9	-5.04	111.28	113.80
26	1H	446	G	O5'-P-OP1	-5.04	101.17	105.70
26	1H	476	G	O5'-P-OP2	-5.04	101.17	105.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	829	A	N1-C6-N6	5.04	121.62	118.60
26	14	1601	G	OP1-P-O3'	5.04	116.28	105.20
26	14	1638	C	OP1-P-O3'	-5.04	94.11	105.20
27	1J	7	G	C4-C5-N7	5.04	112.81	110.80
26	1H	82	G	C5-C6-O6	5.04	131.62	128.60
26	1H	1204	A	N1-C2-N3	5.04	131.82	129.30
26	1H	1616	A	C2-N3-C4	-5.04	108.08	110.60
26	1H	2639	A	C2-N3-C4	-5.04	108.08	110.60
26	14	2277	G	C4-C5-N7	-5.04	108.78	110.80
1	13	405	U	C5-C6-N1	5.04	125.22	122.70
26	1H	244	A	C5-C6-N6	-5.04	119.67	123.70
26	1H	1029	A	N1-C6-N6	5.04	121.62	118.60
26	1H	1198	U	C5-C6-N1	-5.04	120.18	122.70
26	1H	1268	A	C2-N3-C4	-5.04	108.08	110.60
27	16	9	G	OP2-P-O3'	5.04	116.28	105.20
26	14	828	U	C6-N1-C2	-5.04	117.98	121.00
1	13	277	C	OP2-P-O3'	5.03	116.27	105.20
26	1H	757	U	C5-C6-N1	-5.03	120.18	122.70
26	1H	1306	C	C6-N1-C2	5.03	122.31	120.30
26	1H	1761	C	N3-C2-O2	5.03	125.42	121.90
26	1H	2600	A	C6-N1-C2	-5.03	115.58	118.60
1	1G	1512	U	O5'-P-OP2	-5.03	101.17	105.70
26	14	2611	U	OP2-P-O3'	5.03	116.27	105.20
1	13	1331	G	O5'-P-OP2	-5.03	101.17	105.70
27	16	5	C	C5-C4-N4	-5.03	116.68	120.20
26	14	1992	G	N1-C6-O6	-5.03	116.88	119.90
1	13	280	C	C6-N1-C2	5.03	122.31	120.30
26	1H	746	A	O5'-P-OP1	-5.03	101.17	105.70
26	1H	2240	C	OP1-P-O3'	5.03	116.27	105.20
26	14	1344	G	N1-C6-O6	5.03	122.92	119.90
26	14	2037	G	N1-C6-O6	-5.03	116.88	119.90
27	1J	43	C	C6-N1-C2	-5.03	118.29	120.30
26	1H	113	G	C4-N9-C1'	-5.03	119.96	126.50
26	1H	528	A	N1-C2-N3	-5.03	126.79	129.30
26	1H	651	G	OP1-P-OP2	-5.03	112.06	119.60
26	1H	945	A	C6-N1-C2	-5.03	115.58	118.60
26	14	1969	A	O5'-P-OP2	5.03	116.73	110.70
27	1J	6	C	C5-C6-N1	-5.03	118.48	121.00
1	13	1498	U	C2-N1-C1'	5.03	123.73	117.70
26	1H	1156	A	O4'-C1'-N9	-5.03	104.18	108.20
24	3L	58	A	OP1-P-O3'	5.03	116.26	105.20
26	14	786	C	OP2-P-O3'	5.03	116.26	105.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	14	1571	A	N1-C6-N6	5.03	121.62	118.60
26	14	1615	C	N1-C2-O2	5.03	121.92	118.90
1	13	317	G	N3-C4-N9	5.03	129.02	126.00
1	13	960	U	C6-N1-C2	-5.03	117.98	121.00
26	1H	2301	C	C6-N1-C2	-5.03	118.29	120.30
26	14	278	A	OP1-P-O3'	5.03	116.26	105.20
26	14	1968	G	C4-C5-N7	5.03	112.81	110.80
26	1H	2067	G	C5-C6-O6	5.02	131.61	128.60
1	1G	1502	A	C2-N3-C4	-5.02	108.09	110.60
26	14	960	A	N1-C6-N6	5.02	121.61	118.60
26	14	1255	U	N3-C2-O2	-5.02	118.68	122.20
26	1H	599	G	OP1-P-OP2	5.02	127.13	119.60
27	16	6	C	C6-N1-C2	5.02	122.31	120.30
26	14	671	C	C2-N3-C4	-5.02	117.39	119.90
26	14	768	G	O5'-P-OP2	-5.02	101.18	105.70
26	14	1598	C	OP1-P-OP2	-5.02	112.07	119.60
26	14	2211	G	N3-C4-N9	5.02	129.01	126.00
26	1H	781	A	N7-C8-N9	-5.02	111.29	113.80
26	14	801	G	C5-C6-O6	5.02	131.61	128.60
26	14	2595	G	C8-N9-C4	5.02	108.41	106.40
26	1H	113	G	C6-C5-N7	5.02	133.41	130.40
26	1H	205	G	O5'-P-OP2	-5.02	101.18	105.70
26	1H	1605	C	C2-N3-C4	-5.02	117.39	119.90
26	1H	1835	G	C4-N9-C1'	5.02	133.03	126.50
26	1H	2197	U	OP2-P-O3'	5.02	116.24	105.20
1	1G	449	C	N3-C4-N4	-5.02	114.49	118.00
1	1G	889	A	N1-C6-N6	5.02	121.61	118.60
26	14	725	G	N1-C6-O6	5.02	122.91	119.90
26	14	1646	C	OP1-P-O3'	5.02	116.24	105.20
26	14	1918	A	C8-N9-C4	5.02	107.81	105.80
1	13	1214	C	C6-N1-C2	5.02	122.31	120.30
26	1H	66	C	C5-C6-N1	5.02	123.51	121.00
26	1H	648	G	O5'-P-OP2	-5.02	101.18	105.70
26	1H	649	G	C8-N9-C4	-5.02	104.39	106.40
26	1H	1608	A	C2-N3-C4	-5.02	108.09	110.60
26	14	1655	A	C8-N9-C4	5.02	107.81	105.80
26	14	2003	G	C6-C5-N7	-5.02	127.39	130.40
26	1H	247	G	N9-C4-C5	-5.02	103.39	105.40
26	1H	508	G	C8-N9-C1'	-5.02	120.48	127.00
26	1H	1905	C	C2-N3-C4	5.02	122.41	119.90
26	14	1021	A	C5-C6-N1	-5.02	115.19	117.70
1	13	871	U	P-O3'-C3'	5.01	125.72	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	80	G	N7-C8-N9	5.01	115.61	113.10
26	1H	2819	G	C5-C6-O6	-5.01	125.59	128.60
26	1H	2827	C	C2-N3-C4	-5.01	117.39	119.90
26	14	1274	A	N1-C6-N6	5.01	121.61	118.60
1	1G	700	G	N9-C4-C5	5.01	107.41	105.40
26	14	1569	A	C8-N9-C4	-5.01	103.80	105.80
26	1H	1831	G	C8-N9-C4	-5.01	104.39	106.40
26	1H	2265	U	O5'-P-OP2	5.01	116.71	110.70
26	1H	2501	C	OP2-P-O3'	5.01	116.22	105.20
1	1G	197	A	C5-N7-C8	-5.01	101.39	103.90
26	14	102	G	C4-N9-C1'	-5.01	119.98	126.50
26	14	210	C	C6-N1-C2	5.01	122.31	120.30
26	14	733	G	C6-C5-N7	-5.01	127.39	130.40
26	14	747	U	OP1-P-O3'	5.01	116.23	105.20
26	14	2585	U	N1-C2-O2	5.01	126.31	122.80
1	13	346	G	C6-C5-N7	-5.01	127.39	130.40
26	1H	197	A	C2-N3-C4	-5.01	108.09	110.60
26	1H	994	C	O5'-P-OP1	-5.01	101.19	105.70
26	1H	1930	G	C6-N1-C2	5.01	128.10	125.10
26	1H	2269	A	N9-C4-C5	-5.01	103.80	105.80
26	14	801	G	C4-N9-C1'	-5.01	119.99	126.50
26	1H	232	G	N9-C4-C5	-5.01	103.40	105.40
1	1G	317	G	N1-C6-O6	5.01	122.91	119.90
26	14	446	G	N1-C6-O6	5.01	122.91	119.90
26	14	2447	G	C5-C6-O6	-5.01	125.59	128.60
26	1H	575	A	O5'-P-OP2	5.01	116.71	110.70
26	1H	1303	G	N3-C2-N2	5.01	123.41	119.90
26	1H	1772	G	N9-C1'-C2'	-5.01	106.49	112.00
26	1H	2302	G	N1-C6-O6	-5.01	116.90	119.90
26	14	2346	A	C1'-O4'-C4'	-5.01	105.90	109.90
26	1H	1625	C	N1-C2-O2	5.00	121.90	118.90
26	1H	1914	C	N1-C2-O2	5.00	121.90	118.90
1	13	809	G	N1-C6-O6	-5.00	116.90	119.90
22	1K	69	A	P-O3'-C3'	5.00	125.70	119.70
26	1H	1644	C	N3-C4-C5	5.00	123.90	121.90
26	1H	1824	G	C5-C6-O6	-5.00	125.60	128.60
26	1H	2033	A	C5-C6-N1	5.00	120.20	117.70
26	1H	2268	A	N9-C4-C5	-5.00	103.80	105.80
27	16	85	G	C5-C6-O6	-5.00	125.60	128.60
26	14	1131	G	O4'-C1'-N9	5.00	112.20	108.20
26	14	2679	A	C8-N9-C4	5.00	107.80	105.80
1	13	274	A	N1-C6-N6	-5.00	115.60	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1H	202	U	C6-N1-C1'	-5.00	114.20	121.20
26	1H	577	G	OP1-P-OP2	-5.00	112.10	119.60
26	1H	1257	C	N1-C2-N3	5.00	122.70	119.20
26	1H	1797	C	C5-C6-N1	-5.00	118.50	121.00
26	1H	2018	G	N1-C6-O6	5.00	122.90	119.90
26	1H	2448	A	N9-C4-C5	-5.00	103.80	105.80
26	14	211	A	C4-C5-N7	5.00	113.20	110.70
26	14	308	G	C5-C6-O6	-5.00	125.60	128.60
26	14	800	A	O5'-P-OP1	-5.00	101.20	105.70
26	14	2038	G	C8-N9-C4	5.00	108.40	106.40
26	14	2433	A	N7-C8-N9	5.00	116.30	113.80

There are no chirality outliers.

All (145) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
29	11	113	VAL	Peptide
29	11	114	GLY	Peptide
29	11	122	ASP	Peptide
29	11	197	GLY	Peptide
29	11	237	GLU	Peptide
2	12	15	VAL	Peptide
2	12	19	HIS	Peptide
2	12	199	TYR	Peptide
2	12	219	VAL	Peptide
2	12	22	LYS	Peptide
29	19	197	GLY	Peptide
29	19	27	THR	Peptide
29	19	28	GLU	Peptide
10	1A	55	LYS	Peptide
2	1E	15	VAL	Peptide
2	1E	194	PRO	Peptide
2	1E	234	PRO	Peptide
2	1E	236	TYR	Peptide
30	21	153	GLY	Peptide
30	21	186	GLY	Peptide
30	21	187	ALA	Peptide
30	21	56	PRO	Peptide
30	21	58	ARG	Peptide
30	21	66	HIS	Peptide
30	21	68	ALA	Peptide
30	21	82	ARG	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
30	29	117	MET	Peptide
30	29	186	GLY	Peptide
30	29	201	THR	Peptide
30	29	53	PRO	Peptide
30	29	61	ARG	Peptide
11	2A	49	GLY	Peptide
4	32	152	SER	Peptide
4	32	179	GLU	Peptide
37	35	110	TYR	Peptide
37	35	70	GLN	Peptide
31	39	127	GLU	Peptide
31	39	146	ALA	Peptide
31	39	166	ALA	Peptide
31	39	20	LEU	Peptide
31	39	24	LEU	Peptide
31	39	26	ALA	Peptide
31	39	89	VAL	Peptide
12	3A	18	VAL	Peptide
12	3I	47	LYS	Peptide
12	3I	87	GLY	Peptide
32	41	95	ARG	Peptide
38	45	58	PHE	Peptide
38	45	78	PRO	Peptide
32	49	13	GLU	Peptide
32	49	142	PRO	Peptide
13	4A	94	ARG	Peptide
13	4I	105	THR	Peptide
33	51	137	ASP	Peptide
33	51	152	ARG	Peptide
33	51	156	ALA	Peptide
33	51	170	ARG	Peptide
33	51	7	LEU	Peptide
39	55	106	GLY	Peptide
35	58	56	ASN	Peptide
33	59	90	LYS	Peptide
14	5A	27	CYS	Peptide
34	61	11	ASN	Peptide
34	61	134	PRO	Peptide
34	61	82	ARG	Peptide
40	65	53	SER	Peptide
34	69	101	LEU	Peptide
34	69	112	LYS	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
34	69	142	VAL	Peptide
34	69	143	SER	Peptide
41	75	10	VAL	Peptide
41	75	12	SER	Peptide
41	75	5	ALA	Peptide
37	78	11	GLY	Peptide
37	78	115	LEU	Peptide
37	78	15	ARG	Peptide
37	78	24	GLY	Peptide
37	78	36	LYS	Peptide
37	78	70	GLN	Peptide
9	82	117	HIS	Peptide
42	85	72	HIS	Peptide
42	85	90	VAL	Peptide
42	85	98	LEU	Peptide
42	85	99	ALA	Peptide
38	88	139	GLU	Peptide
38	88	23	GLY	Peptide
38	88	58	PHE	Peptide
38	88	59	ARG	Peptide
9	8E	110	GLU	Peptide
9	8E	4	TYR	Peptide
39	98	44	LEU	Peptide
39	98	8	ARG	Peptide
44	A5	43	GLY	Peptide
40	A8	107	GLU	Peptide
40	A8	108	GLY	Peptide
19	AA	4	SER	Peptide
19	AA	9	VAL	Peptide
19	AI	24	ALA	Peptide
45	B5	24	GLY	Peptide
45	B5	61	GLY	Peptide
41	B8	12	SER	Peptide
41	B8	4	GLY	Peptide
41	B8	58	ASN	Peptide
20	BA	101	GLY	Peptide
20	BA	72	LEU	Peptide
46	C5	82	PRO	Peptide
46	C5	91	GLU	Peptide
42	C8	90	VAL	Peptide
42	C8	95	LEU	Peptide
47	D5	175	VAL	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
47	D5	60	GLU	Peptide
47	D5	61	LEU	Peptide
43	D8	36	PRO	Peptide
43	D8	44	LYS	Peptide
43	D8	48	GLY	Peptide
48	E5	32	ARG	Peptide
48	E5	33	ALA	Peptide
49	F5	81	LYS	Peptide
50	G5	15	LYS	Peptide
50	G5	43	GLN	Peptide
46	G8	53	PRO	Peptide
46	G8	54	LYS	Peptide
46	G8	80	GLY	Peptide
46	G8	84	ARG	Peptide
46	G8	93	GLY	Peptide
47	H8	117	LEU	Peptide
47	H8	143	GLY	Peptide
47	H8	158	PRO	Peptide
47	H8	165	VAL	Peptide
47	H8	59	LEU	Peptide
47	H8	63	ASP	Peptide
48	I8	44	ARG	Peptide
49	J8	84	GLY	Peptide
50	K8	17	SER	Peptide
50	K8	46	GLN	Peptide
56	M5	40	GLU	Peptide
56	M5	51	ALA	Peptide
52	M8	37	SER	Peptide
52	M8	40	HIS	Peptide
52	M8	42	PHE	Peptide
54	O8	44	ARG	Peptide
55	P8	45	ALA	Peptide
56	Q8	30	ARG	Peptide
56	Q8	49	VAL	Peptide
56	Q8	51	ALA	Peptide

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	13	32223	0	16267	692	0
1	1G	32414	0	16360	752	0
2	12	1696	0	1730	89	0
2	1E	1874	0	1926	95	0
3	22	1537	0	1603	84	0
3	2E	1605	0	1668	54	0
4	32	1702	0	1765	93	0
4	3E	1698	0	1759	84	0
5	42	1141	0	1199	40	0
5	4E	1142	0	1204	40	0
6	52	842	0	857	19	0
6	5E	837	0	852	34	0
7	62	1110	0	1163	53	0
7	6E	1242	0	1286	51	0
8	72	1107	0	1165	49	0
8	7E	1115	0	1177	46	0
9	82	953	0	983	62	0
9	8E	1000	0	1031	63	0
10	1A	646	0	662	45	0
10	1I	749	0	767	42	0
11	2A	835	0	847	25	0
11	2I	823	0	833	29	0
12	3A	947	0	1033	45	0
12	3I	956	0	1046	35	0
13	4A	879	0	935	46	0
13	4I	933	0	992	57	0
14	5A	486	0	525	35	0
14	5I	486	0	524	29	0
15	6A	729	0	768	26	0
15	6I	729	0	768	23	0
16	7A	705	0	725	23	0
16	7I	700	0	720	45	0
17	8A	823	0	891	22	0
17	8I	823	0	891	34	0
18	9A	544	0	605	19	0
18	9I	549	0	607	21	0
19	AA	510	0	507	21	0
19	AI	661	0	683	43	0
20	BA	762	0	861	43	0
20	BI	746	0	843	44	0
21	1B	188	0	195	8	0
21	1F	199	0	208	9	0
22	1K	1542	0	790	25	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	2K	1646	0	845	18	0
23	2L	1646	0	845	25	0
24	1L	1401	0	713	22	0
24	3K	1483	0	756	50	0
24	3L	1528	0	778	42	0
25	4K	420	0	209	7	0
25	4L	419	0	208	17	0
26	14	60877	0	30690	1171	0
26	1H	61609	0	31058	1189	0
27	16	2617	0	1328	50	0
27	1J	2617	0	1328	76	0
28	71	1027	0	1043	57	0
29	11	2120	0	2197	100	0
29	19	2125	0	2199	105	0
30	21	1546	0	1602	86	0
30	29	1563	0	1629	93	0
31	31	1585	0	1632	70	0
31	39	1602	0	1649	88	0
32	41	1457	0	1514	68	0
32	49	1459	0	1507	65	0
33	51	1328	0	1396	64	0
33	59	1295	0	1366	58	0
34	61	1131	0	1218	36	0
34	69	1131	0	1218	49	0
35	15	1096	0	1168	47	0
35	58	1096	0	1169	48	0
36	25	932	0	996	46	0
36	68	932	0	996	41	0
37	35	1122	0	1206	75	0
37	78	1122	0	1206	80	0
38	45	1099	0	1154	73	0
38	88	1117	0	1168	58	0
39	55	967	0	1033	42	0
39	98	967	0	1033	45	0
40	65	876	0	938	63	0
40	A8	881	0	943	54	0
41	75	1109	0	1170	61	0
41	B8	1119	0	1177	72	0
42	85	959	0	1019	40	0
42	C8	950	0	1011	58	0
43	95	770	0	838	32	0
43	D8	774	0	849	40	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	A5	886	0	948	23	0
44	E8	876	0	941	30	0
45	B5	735	0	785	30	0
45	F8	750	0	814	19	0
46	C5	794	0	885	52	0
46	G8	783	0	869	49	0
47	D5	1411	0	1436	82	0
47	H8	1365	0	1391	57	0
48	E5	603	0	620	33	0
48	I8	611	0	631	34	0
49	F5	737	0	813	32	0
49	J8	747	0	817	42	0
50	G5	576	0	625	27	0
50	K8	575	0	634	42	0
51	H5	459	0	512	11	0
51	L8	459	0	512	13	0
52	M8	475	0	465	34	0
53	J5	434	0	454	22	0
53	N8	369	0	388	21	0
54	O8	389	0	404	26	0
55	L5	401	0	436	10	0
55	P8	401	0	436	11	0
56	M5	516	0	582	25	0
56	Q8	516	0	582	37	0
57	13	140	0	0	0	0
57	14	435	0	0	0	0
57	16	11	0	0	0	0
57	19	1	0	0	0	0
57	1G	102	0	0	0	0
57	1H	525	0	0	0	0
57	1J	8	0	0	0	0
57	21	3	0	0	0	0
57	25	1	0	0	0	0
57	29	1	0	0	0	0
57	2K	2	0	0	0	0
57	2L	2	0	0	0	0
57	31	2	0	0	0	0
57	32	1	0	0	0	0
57	35	1	0	0	0	0
57	39	2	0	0	0	0
57	3I	1	0	0	0	0
57	41	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	42	1	0	0	0	0
57	45	2	0	0	0	0
57	4I	1	0	0	0	0
57	4L	1	0	0	0	0
57	52	1	0	0	0	0
57	5I	1	0	0	0	0
57	78	1	0	0	0	0
57	7A	1	0	0	0	0
57	88	3	0	0	0	0
57	C5	1	0	0	0	0
57	E5	1	0	0	0	0
57	I8	2	0	0	0	0
57	M5	1	0	0	0	0
57	P8	1	0	0	0	0
57	Q8	1	0	0	0	0
58	13	42	0	43	0	0
58	1G	42	0	45	1	0
59	32	8	0	0	3	0
59	3E	8	0	0	1	0
60	5A	1	0	0	0	0
60	5I	1	0	0	0	0
60	C5	1	0	0	0	0
60	G8	1	0	0	0	0
61	14	26	0	45	8	0
61	1G	13	0	24	0	0
62	11	17	0	0	4	0
62	13	320	0	0	12	0
62	14	1144	0	0	65	0
62	15	1	0	0	0	0
62	16	12	0	0	1	0
62	19	15	0	0	3	0
62	1A	1	0	0	0	0
62	1F	1	0	0	0	0
62	1G	317	0	0	21	0
62	1H	1470	0	0	90	0
62	1I	2	0	0	0	0
62	1J	12	0	0	1	0
62	1K	2	0	0	0	0
62	21	7	0	0	1	0
62	25	6	0	0	0	0
62	29	4	0	0	0	0
62	2K	8	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	2L	6	0	0	0	0
62	31	5	0	0	0	0
62	32	1	0	0	0	0
62	35	8	0	0	1	0
62	39	5	0	0	1	0
62	3I	2	0	0	0	0
62	41	1	0	0	0	0
62	4E	3	0	0	0	0
62	4K	5	0	0	0	0
62	4L	6	0	0	0	0
62	52	4	0	0	0	0
62	55	3	0	0	0	0
62	58	2	0	0	0	0
62	5I	2	0	0	0	0
62	6A	2	0	0	0	0
62	6I	3	0	0	0	0
62	78	10	0	0	0	0
62	7A	5	0	0	0	0
62	7I	1	0	0	0	0
62	85	2	0	0	0	0
62	8E	2	0	0	0	0
62	9A	2	0	0	0	0
62	A5	1	0	0	0	0
62	B5	1	0	0	0	0
62	B8	1	0	0	0	0
62	BA	2	0	0	0	0
62	BI	2	0	0	1	0
62	C5	3	0	0	0	0
62	C8	3	0	0	0	0
62	F5	1	0	0	1	0
62	F8	2	0	0	0	0
62	G8	2	0	0	0	0
62	H5	2	0	0	1	0
62	I8	6	0	0	1	0
62	J8	4	0	0	0	0
62	L8	3	0	0	1	0
62	M5	9	0	0	1	0
62	P8	1	0	0	0	0
62	Q8	5	0	0	2	0
All	All	297444	0	197360	7486	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 16.

All (7486) 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)
10:1A:38:ILE:C	10:1A:39:PRO:N	1.71	1.44
38:45:27:VAL:HB	38:45:28:ALA:HA	1.19	1.13
29:11:182:LEU:H	29:11:272:ALA:HB3	1.23	1.02
37:78:63:PRO:HB2	56:Q8:30:ARG:HH21	1.23	1.01
26:1H:1496:A:H8	26:1H:1577:C:HO2'	1.00	0.99
26:14:330:A:H2	26:14:1210:A:HO2'	1.05	0.98
8:7E:87:SER:HB2	8:7E:93:VAL:HB	1.47	0.97
29:19:39:LYS:HG3	29:19:40:THR:H	1.31	0.96
29:19:44:ASN:HA	29:19:47:GLY:H	1.30	0.95
29:19:44:ASN:HB3	29:19:45:ASN:HA	1.48	0.94
1:13:1502:A:H2	1:13:1505:G:H1	1.14	0.94
19:AI:40:ILE:HG12	19:AI:41:VAL:HG13	1.49	0.94
26:1H:1689:A:H62	26:1H:1698:A:H2	1.08	0.94
31:31:101:LEU:HD23	31:31:102:PRO:HD2	1.51	0.93
26:1H:1359:A:N1	26:1H:1372:U:N3	2.17	0.93
26:1H:1771:C:HO2'	26:1H:1786:A:H8	0.95	0.92
26:14:2032:G:H21	30:29:146:THR:HG23	1.32	0.92
27:1J:80:U:H2'	27:1J:81:G:H21	1.36	0.91
26:1H:1055:G:N2	26:1H:1104:C:N3	2.18	0.91
26:1H:620:G:H4'	26:1H:621:A:H5''	1.54	0.90
26:14:67:U:H3	26:14:74:A:H2	1.19	0.90
30:29:60:ASN:HB2	30:29:62:PRO:HD2	1.53	0.90
47:D5:115:GLY:HA2	47:D5:177:PRO:HG2	1.52	0.90
26:1H:1456:G:OP2	62:1H:3742:HOH:O	1.89	0.90
26:1H:2308:G:H1	26:1H:2311:A:H2	1.11	0.89
4:3E:107:ARG:HH22	4:3E:194:LEU:HD22	1.37	0.89
1:1G:1368:G:H5'	9:82:112:LYS:HB3	1.56	0.88
30:29:54:GLN:HA	30:29:74:PRO:HA	1.55	0.88
26:1H:1653:G:H3'	39:98:2:ARG:HG3	1.52	0.88
47:H8:108:PRO:HB2	47:H8:112:ARG:HA	1.55	0.88
38:45:21:THR:HG22	38:45:23:GLY:HA3	1.56	0.88
13:4I:3:ARG:HB3	13:4I:9:ILE:HG12	1.55	0.88
26:14:676:A:H8	26:14:2069:G:H21	1.18	0.87
26:1H:442:G:H1'	31:31:48:THR:HG21	1.55	0.87
26:14:2873:A:H8	39:55:6:SER:H	1.17	0.87
26:1H:138:G:N2	45:F8:44:GLU:OE2	2.07	0.87
26:1H:607:U:H3	26:1H:621:A:H2	1.19	0.87
9:82:28:VAL:HG22	9:82:63:ILE:HB	1.56	0.87
41:B8:57:PHE:O	41:B8:58:ASN:ND2	2.08	0.87
26:1H:674:G:H1'	31:31:74:ARG:HD3	1.57	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:3K:7:U:H2'	24:3K:49:G:H5'	1.56	0.86
26:14:2624:G:N7	62:14:3631:HOH:O	2.09	0.86
1:13:975:A:H4'	1:13:976:G:H5''	1.57	0.86
31:39:25:PRO:HB2	31:39:27:GLU:H	1.38	0.86
26:14:123:G:N7	62:14:3630:HOH:O	2.08	0.86
26:1H:780:G:H21	26:1H:783:A:H62	1.18	0.86
1:13:1348:U:H3	1:13:1374:A:H2	1.24	0.86
1:1G:1028:C:N3	1:1G:1033:G:N2	2.22	0.86
31:39:122:LYS:HD2	31:39:191:ARG:HE	1.41	0.86
26:14:607:U:H3	26:14:621:A:H2	1.20	0.85
1:13:601:C:H2'	1:13:602:A:H8	1.42	0.85
1:1G:1502:A:H2	1:1G:1505:G:H1	1.23	0.85
38:45:27:VAL:CB	38:45:28:ALA:HA	2.06	0.85
26:14:1899:G:H21	26:14:1902:C:N4	1.75	0.85
26:1H:2032:G:H21	30:21:146:THR:HG23	1.40	0.84
48:E5:27:GLU:HG3	48:E5:68:GLU:HA	1.58	0.84
2:12:75:LYS:HA	2:12:78:GLN:HB2	1.59	0.84
26:1H:49:A:N7	26:1H:120:U:H5	1.75	0.84
38:45:26:TYR:CD1	38:45:27:VAL:HG23	2.13	0.84
26:14:1689:A:H62	26:14:1698:A:H2	1.24	0.84
26:1H:1678:G:H22	26:1H:1989:G:H22	1.24	0.84
26:14:483:A:H4'	46:C5:49:VAL:HA	1.60	0.84
26:1H:270(K):C:O2'	26:1H:270(N):G:N2	2.09	0.84
26:1H:1210:A:H8	26:1H:1210:A:H5'	1.42	0.84
13:4I:23:TYR:HD2	13:4I:67:GLU:HA	1.42	0.84
40:A8:78:LEU:HD12	40:A8:108:GLY:HA2	1.58	0.84
7:62:93:PRO:HD2	7:62:94:ARG:HH21	1.42	0.84
27:16:80:U:H2'	27:16:81:G:H21	1.43	0.83
26:1H:1049:C:N3	33:51:3:ARG:NH1	2.26	0.83
29:19:182:LEU:H	29:19:272:ALA:HB3	1.43	0.83
1:13:153:C:H42	1:13:168:G:H1	1.24	0.83
26:14:1757:U:H3	26:14:1762:A:H2	1.25	0.83
26:1H:2867:G:OP2	41:B8:119:LYS:NZ	2.09	0.83
3:22:135:LYS:NZ	3:22:135:LYS:O	2.11	0.83
24:3K:76:A:H8	26:1H:2394:C:H42	1.22	0.83
26:1H:2749:A:H5''	33:51:4:ILE:HD11	1.59	0.83
13:4I:10:PRO:HB2	13:4I:18:ALA:HB1	1.60	0.83
26:1H:67:U:H3	26:1H:74:A:H2	1.26	0.83
31:39:53:THR:HG22	31:39:56:GLU:HG3	1.58	0.83
2:12:91:PRO:HG2	2:12:155:LEU:HG	1.57	0.83
34:61:98:ALA:HB2	34:61:111:PRO:HB3	1.57	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:82:112:LYS:HA	9:82:119:ALA:HB2	1.58	0.82
26:14:84:A:N6	26:14:102:G:O2'	2.11	0.82
47:D5:27:VAL:HG12	47:D5:87:ASP:HB3	1.61	0.82
26:1H:2781:A:H5''	26:1H:2782:G:H5'	1.60	0.82
26:1H:847:U:OP2	62:1H:3743:HOH:O	1.96	0.82
10:1I:61:GLU:OE2	14:5I:45:ARG:NH1	2.13	0.82
26:14:2287:A:N6	26:14:2344:U:H3	1.77	0.82
1:13:1104:G:OP1	2:1E:144:ARG:NH2	2.11	0.82
4:32:23:GLY:N	4:32:26:CYS:SG	2.51	0.82
26:1H:1332:G:N2	26:1H:1609:A:O2'	2.13	0.81
34:69:81:VAL:H	34:69:143:SER:HB3	1.42	0.81
39:98:86:ARG:HH21	39:98:118:GLU:HG2	1.42	0.81
32:49:125:PHE:HB3	32:49:166:ASP:HB2	1.60	0.81
1:13:1305:G:H22	1:13:1331:G:H2'	1.43	0.81
26:14:1496:A:H8	26:14:1577:C:HO2'	1.28	0.81
26:14:2292:C:OP1	40:65:17:ARG:NH2	2.13	0.81
3:2E:16:ARG:HD2	3:2E:54:ARG:HH21	1.45	0.81
1:1G:1352:C:H42	1:1G:1370:G:H1	1.24	0.81
47:D5:157:LEU:HA	47:D5:161:VAL:HG11	1.59	0.81
26:1H:860:U:H5	26:1H:917:A:C2	1.97	0.81
26:14:958:U:OP2	38:45:14:ARG:NH1	2.11	0.81
26:14:152:G:H1	26:14:174:C:H42	1.28	0.81
4:3E:167:GLY:HA2	29:19:135:PHE:HE1	1.44	0.81
49:J8:92:LYS:HA	49:J8:95:LEU:HG	1.62	0.81
26:14:780:G:H21	26:14:783:A:H62	1.28	0.81
26:1H:1670:C:OP1	62:1H:3744:HOH:O	1.98	0.81
33:59:15:VAL:HG12	33:59:29:PRO:HD2	1.62	0.81
1:13:659:U:H2'	1:13:660:G:H8	1.45	0.81
26:1H:2418:A:N7	62:1H:3763:HOH:O	2.12	0.81
26:1H:270(I):G:H1	26:1H:270(Q):C:H42	1.29	0.81
30:29:81:ILE:HG22	30:29:82:ARG:H	1.46	0.81
1:13:1178:G:OP2	9:8E:93:ARG:NH2	2.14	0.81
47:H8:9:TYR:HE1	47:H8:35:ARG:HG2	1.45	0.81
48:I8:38:VAL:HG23	48:I8:59:LEU:HB2	1.63	0.81
54:O8:15:GLU:OE2	54:O8:44:ARG:NH2	2.14	0.80
29:11:84:TYR:HE1	29:11:86:PRO:HB3	1.46	0.80
26:14:1814:G:OP1	29:19:40:THR:HG21	1.81	0.80
38:88:138:ASP:N	38:88:138:ASP:OD1	2.13	0.80
26:1H:958:U:OP2	38:88:14:ARG:NH1	2.14	0.80
26:1H:1604:C:OP2	62:1H:3611:HOH:O	1.99	0.80
31:39:123:LEU:O	31:39:125:LEU:N	2.14	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1H:1434:A:H61	26:1H:1558:A:N6	1.80	0.80
4:32:157:LEU:O	4:32:161:ASN:ND2	2.14	0.80
33:51:7:LEU:HD12	33:51:7:LEU:H	1.44	0.80
20:BI:71:THR:HG22	20:BI:72:LEU:H	1.47	0.80
26:14:1138:G:H21	35:15:106:MET:HE3	1.47	0.80
11:2A:29:ILE:HG22	11:2A:44:SER:HB2	1.64	0.80
51:L8:8:LEU:HB2	51:L8:28:LEU:HD22	1.64	0.80
26:1H:1899:G:H22	26:1H:1902:C:H5	1.30	0.80
1:13:812:C:N3	62:13:1840:HOH:O	2.13	0.79
1:1G:976:G:N2	1:1G:1362(A):C:OP2	2.15	0.79
17:8I:67:LYS:HA	17:8I:70:ARG:HH12	1.46	0.79
26:1H:1021:A:H62	26:1H:1141:U:H3	1.30	0.79
2:1E:208:ILE:HG22	2:1E:211:ILE:HD11	1.62	0.79
26:1H:2111:C:N4	26:1H:2147:G:O6	2.14	0.79
26:1H:2176:A:H1'	28:71:215:THR:HG21	1.65	0.79
50:K8:15:LYS:HZ2	50:K8:15:LYS:H	1.28	0.79
26:14:2681:C:H5	26:14:2725:A:H62	1.29	0.79
26:14:275:G:N2	26:14:276:A:N7	2.31	0.79
37:78:71:VAL:HG13	37:78:72:PRO:HD3	1.65	0.79
1:1G:1288:A:O2'	21:1B:10:ARG:NH2	2.15	0.79
26:1H:1138:G:H21	35:58:106:MET:HE3	1.45	0.79
26:1H:1900:A:H5'	26:1H:1900:A:H8	1.47	0.79
37:35:79:ARG:HG2	37:35:110:TYR:HB2	1.64	0.79
11:2I:54:ARG:O	11:2I:56:GLY:N	2.15	0.79
16:7A:53:VAL:HG13	16:7A:79:VAL:HG22	1.65	0.79
26:1H:1778:U:H2'	26:1H:1784:A:N6	1.97	0.78
11:2I:22:HIS:HB3	11:2I:29:ILE:HG23	1.64	0.78
38:45:27:VAL:HG22	38:45:137:TYR:O	1.83	0.78
48:I8:11:ARG:O	48:I8:14:ARG:NH2	2.16	0.78
51:L8:10:LYS:NZ	51:L8:15:TYR:OH	2.16	0.78
26:1H:676:A:H8	26:1H:2069:G:H21	1.30	0.78
13:4I:39:ILE:HD12	13:4I:56:LEU:HD23	1.65	0.78
25:4L:21:A:H2'	25:4L:22:A:H5''	1.63	0.78
24:3L:6:G:N1	24:3L:67:C:O2	2.15	0.78
29:19:69:ARG:NH2	29:19:128:GLY:O	2.17	0.78
20:BI:26:ASN:HB2	20:BI:71:THR:HG23	1.63	0.78
1:1G:1324:A:H4'	1:1G:1362:C:H4'	1.63	0.78
26:1H:1022:G:N2	26:1H:1023:U:O4	2.16	0.78
26:1H:2392:A:H2	26:1H:2424:C:H42	1.30	0.78
9:82:5:TYR:N	9:82:87:GLN:OE1	2.16	0.78
43:D8:44:LYS:O	43:D8:46:VAL:N	2.17	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:14:2720:U:H3	26:14:2873:A:H2	1.30	0.78
26:1H:1382:G:O6	62:1H:3746:HOH:O	2.02	0.78
37:35:26:GLY:O	62:35:301:HOH:O	2.02	0.78
47:D5:74:VAL:HG13	47:D5:86:VAL:HG22	1.64	0.78
47:H8:116:VAL:HG22	47:H8:146:ILE:HG12	1.65	0.78
26:1H:2061:G:H5'	62:1H:4045:HOH:O	1.82	0.78
38:45:138:ASP:N	38:45:138:ASP:OD1	2.16	0.78
26:14:1678:G:N2	26:14:1989:G:H22	1.80	0.78
1:1G:1248:A:N3	9:82:70:LYS:NZ	2.29	0.78
26:1H:607:U:OP1	31:31:102:PRO:HA	1.83	0.78
30:29:91:VAL:HB	30:29:95:ILE:HD11	1.66	0.78
23:2K:76:C:OP1	62:2K:202:HOH:O	2.01	0.77
1:1G:523:A:H61	12:3A:92:ASP:HB2	1.48	0.77
13:4A:16:ASP:HB3	13:4A:34:LEU:HD11	1.66	0.77
1:1G:975:A:H4'	1:1G:976:G:H5''	1.66	0.77
1:13:1422:G:H5''	36:68:48:PRO:HB3	1.66	0.77
26:14:71:A:H2	45:B5:31:HIS:HE2	1.30	0.77
47:H8:165:VAL:HB	47:H8:167:PRO:HD3	1.65	0.77
29:11:235:GLY:O	62:11:301:HOH:O	2.01	0.77
1:13:143:A:H2	1:13:220:G:H1	1.33	0.77
26:1H:2447:G:O5'	62:1H:3745:HOH:O	2.01	0.77
7:62:148:ASN:ND2	7:62:148:ASN:O	2.16	0.77
1:13:1256:A:N6	1:13:1278:U:OP2	2.17	0.77
26:14:2357:U:OP1	48:E5:20:ARG:NH1	2.17	0.77
26:1H:2656:U:H3	26:1H:2665:A:H2	1.29	0.77
1:13:974:A:OP2	14:5I:41:ARG:NH1	2.17	0.77
26:14:2719:G:OP2	62:14:3625:HOH:O	2.01	0.77
10:1A:51:ARG:HB2	10:1A:60:ARG:HA	1.66	0.77
26:1H:1728:G:H8	26:1H:1732:A:H62	1.33	0.77
10:1A:28:ARG:HH21	10:1A:34:VAL:H	1.30	0.77
1:13:1305:G:N2	1:13:1331:G:H2'	1.99	0.77
12:3A:52:LEU:O	12:3A:54:LYS:NZ	2.17	0.77
5:42:43:LEU:HD22	5:42:136:MET:HG3	1.66	0.77
20:BA:53:LEU:HD12	20:BA:100:ILE:HG22	1.66	0.77
26:14:259:G:H21	26:14:621:A:H8	1.31	0.77
26:1H:1009:A:OP2	35:58:37:LYS:NZ	2.17	0.77
3:22:70:VAL:HG12	3:22:72:LYS:H	1.50	0.77
31:31:185:ASP:OD1	31:31:188:ARG:NH1	2.18	0.77
1:1G:1281:U:OP2	1:1G:1282:C:N4	2.17	0.77
42:85:49:HIS:HA	42:85:52:ARG:HB3	1.67	0.77
38:88:109:VAL:HG13	38:88:113:GLN:HB3	1.67	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:14:2456:C:N4	62:14:3643:HOH:O	2.17	0.76
36:68:88:ASN:HD21	36:68:92:GLU:HB2	1.50	0.76
26:1H:993:G:OP1	42:C8:50:ARG:NH2	2.16	0.76
1:13:780:A:OP2	62:13:1837:HOH:O	2.02	0.76
26:1H:2469:A:H2	26:1H:2481:G:H21	1.33	0.76
22:1K:36:U:H3	25:4K:19:G:H1	1.33	0.76
12:3A:60:LEU:HB2	12:3A:64:TYR:HB2	1.67	0.76
24:3K:33:U:H2'	24:3K:34:U:H2'	1.67	0.76
41:B8:56:GLY:O	41:B8:59:THR:HG22	1.84	0.76
2:1E:16:HIS:HE1	2:1E:213:LEU:HD12	1.49	0.76
41:75:56:GLY:O	41:75:59:THR:HG23	1.85	0.76
43:95:98:GLU:OE1	43:95:100:ARG:NH1	2.16	0.76
53:N8:33:CYS:SG	53:N8:40:LYS:NZ	2.54	0.76
26:14:2392:A:H2	26:14:2424:C:H42	1.31	0.76
30:21:38:THR:HG22	30:21:40:GLU:H	1.51	0.76
7:6E:122:HIS:HA	7:6E:125:MET:HE2	1.68	0.76
26:14:761:A:N7	61:14:3437:SPE:H112	2.01	0.76
3:22:106:VAL:HB	3:22:109:PRO:HB3	1.68	0.76
30:29:50:GLY:HA2	30:29:78:LEU:HB3	1.68	0.76
46:G8:30:VAL:HG22	46:G8:37:VAL:HG12	1.67	0.76
31:39:157:VAL:HB	31:39:194:MET:HG3	1.67	0.76
24:3L:3:G:N2	24:3L:70:C:N3	2.32	0.76
6:52:76:ALA:HB1	6:52:80:ARG:HH21	1.49	0.76
46:G8:102:CYS:SG	46:G8:103:GLY:N	2.59	0.76
47:H8:19:ARG:NH1	47:H8:84:GLU:O	2.19	0.76
26:1H:2334:G:O6	48:I8:74:ARG:NH2	2.18	0.76
2:12:40:HIS:HD2	2:12:190:THR:HG21	1.50	0.76
26:14:1141:U:OP2	35:15:63:THR:OG1	2.03	0.76
26:1H:2580:U:H4'	30:21:130:GLY:HA3	1.68	0.76
26:14:1019:U:OP1	26:14:1035:U:O2'	2.02	0.76
26:1H:780:G:H21	26:1H:783:A:N6	1.83	0.76
26:14:907:U:O2'	38:45:101:ARG:NH2	2.17	0.76
41:75:50:ILE:HD11	41:75:102:ILE:HD11	1.68	0.76
46:C5:88:LYS:HG3	46:C5:89:PHE:H	1.48	0.76
1:13:524:G:H2'	1:13:525:C:C6	2.21	0.75
26:1H:2312:U:H5'	32:41:88:ILE:HD11	1.68	0.75
33:51:2:SER:HB2	33:51:3:ARG:HD3	1.67	0.75
26:14:889:C:H2'	26:14:890:A:H4'	1.69	0.75
1:1G:999:U:H3	1:1G:1041:A:H61	1.32	0.75
26:1H:2099:U:N3	26:1H:2190:G:O6	2.17	0.75
27:1J:80:U:H2'	27:1J:81:G:N2	2.01	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4E:102:ALA:HB1	5:4E:106:PRO:HG2	1.68	0.75
42:C8:92:ARG:O	42:C8:94:ASN:N	2.19	0.75
1:1G:827:U:H3	1:1G:872:A:H62	1.32	0.75
26:1H:1332:G:OP1	62:1H:3747:HOH:O	2.04	0.75
30:21:53:PRO:HA	30:21:75:VAL:H	1.50	0.75
16:7I:47:ASP:N	16:7I:47:ASP:OD1	2.20	0.75
44:A5:13:SER:HB3	44:A5:16:LYS:HD2	1.67	0.75
10:1A:28:ARG:NH2	10:1A:34:VAL:O	2.18	0.75
24:3L:3:G:H1	24:3L:70:C:H42	1.31	0.75
26:14:6:A:H3'	26:14:7:G:H5'	1.69	0.75
29:19:228:PRO:O	62:19:401:HOH:O	2.04	0.75
30:21:197:ILE:HD11	30:21:199:ARG:HE	1.52	0.75
19:AI:41:VAL:O	52:M8:63:TYR:OH	2.05	0.75
2:1E:80:ILE:HG12	2:1E:212:GLN:HB2	1.69	0.75
1:1G:176:C:OP1	20:BA:29:LYS:NZ	2.17	0.75
26:1H:70:G:H21	26:1H:71:A:N6	1.85	0.75
30:21:74:PRO:HA	30:21:75:VAL:HB	1.67	0.75
48:I8:27:GLU:HG3	48:I8:68:GLU:HA	1.69	0.75
1:13:1007:C:H42	1:13:1022:G:H1	1.34	0.75
1:13:141:A:O2'	1:13:182:U:O2	2.04	0.75
26:14:2789:C:O2	26:14:2894:G:N2	2.20	0.75
26:1H:259:G:O2'	26:1H:621:A:O2'	2.05	0.75
31:39:25:PRO:HB3	31:39:28:ILE:HG23	1.68	0.75
43:D8:65:GLY:HA3	43:D8:91:TYR:CZ	2.21	0.75
26:14:270(W):G:N7	62:14:3651:HOH:O	2.20	0.75
1:1G:576:G:N2	1:1G:759:A:OP1	2.20	0.75
1:1G:542:G:OP1	4:32:10:ARG:NH2	2.19	0.75
8:7E:21:LYS:O	8:7E:65:TYR:OH	2.05	0.75
52:M8:13:ARG:HH12	52:M8:22:ILE:HG23	1.52	0.75
26:14:2226:C:OP2	62:14:3627:HOH:O	2.05	0.74
29:19:30:GLU:HG3	29:19:63:ARG:CZ	2.17	0.74
31:39:181:LEU:HD21	31:39:186:ILE:HD11	1.67	0.74
26:1H:1604:C:OP2	62:1H:3748:HOH:O	2.05	0.74
36:25:14:THR:HG21	36:25:86:ILE:HG13	1.69	0.74
24:3K:49:G:H1'	24:3K:66:A:C6	2.22	0.74
35:58:96:GLU:O	35:58:98:VAL:N	2.19	0.74
1:1G:793:U:OP1	62:1G:1854:HOH:O	2.04	0.74
26:1H:1016:G:N7	62:1H:3777:HOH:O	2.20	0.74
15:6I:26:GLU:OE2	15:6I:77:ARG:NH1	2.20	0.74
56:M5:40:GLU:HA	56:M5:43:GLN:HB2	1.67	0.74
1:1G:54:C:N4	1:1G:353:A:OP2	2.20	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:8E:121:ARG:NH1	9:8E:122:ALA:O	2.19	0.74
50:K8:4:SER:H	50:K8:7:ARG:H	1.34	0.74
40:A8:48:LEU:HD23	40:A8:82:ILE:HD11	1.68	0.74
2:12:184:VAL:HG23	2:12:198:ASP:H	1.53	0.74
26:14:1864:U:OP1	26:14:2410:G:O2'	2.06	0.74
28:71:7:TYR:HA	28:71:10:LEU:HB2	1.68	0.74
53:N8:40:LYS:HE2	53:N8:47:PRO:HD2	1.68	0.74
33:51:10:PRO:HD2	33:51:50:VAL:O	1.87	0.74
28:71:57:ASN:HA	28:71:165:ASN:HD21	1.50	0.74
50:G5:50:ILE:HD12	50:G5:51:ARG:H	1.52	0.74
50:K8:42:GLY:O	50:K8:44:LEU:N	2.20	0.74
26:14:2255:G:OP2	62:14:3626:HOH:O	2.04	0.74
26:1H:1021:A:H8	26:1H:1022:G:H5''	1.50	0.74
47:D5:76:LEU:HA	47:D5:83:PRO:HA	1.69	0.74
2:1E:80:ILE:HG21	2:1E:212:GLN:HA	1.70	0.74
1:13:346:G:OP1	41:B8:41:ARG:NH2	2.20	0.74
49:J8:89:GLU:OE2	49:J8:89:GLU:N	2.20	0.74
1:1G:1028(B):C:O2	1:1G:1030:C:N4	2.20	0.74
42:C8:69:CYS:HG	42:C8:79:PHE:HD2	1.34	0.74
30:29:36:ARG:HH21	30:29:89:ASP:HB3	1.53	0.73
29:19:39:LYS:HG3	29:19:40:THR:N	2.03	0.73
1:1G:1305:G:HO2'	1:1G:1306:A:H8	1.34	0.73
1:1G:558:G:OP1	62:1G:1855:HOH:O	2.05	0.73
26:1H:1597:A:N7	62:1H:3778:HOH:O	2.20	0.73
26:1H:2849:U:O2'	62:1H:3749:HOH:O	2.05	0.73
28:71:23:ASP:HB2	28:71:190:ARG:HH22	1.54	0.73
45:B5:11:PRO:HB3	45:B5:92:LEU:HD11	1.70	0.73
26:14:1022:G:O2'	26:14:1023:U:OP2	2.06	0.73
1:1G:235:C:H5'	17:8A:70:ARG:HG2	1.69	0.73
26:14:815:C:OP1	43:95:85:LYS:NZ	2.21	0.73
32:49:161:THR:HG22	32:49:163:ALA:H	1.54	0.73
1:13:76:G:N1	1:13:93:U:O2	2.19	0.73
26:14:1537:C:H2'	26:14:1538:G:C8	2.23	0.73
26:14:1729:A:H2'	26:14:1731:G:N2	2.04	0.73
26:14:2404:C:OP2	62:14:3628:HOH:O	2.07	0.73
1:1G:1435:G:H2'	1:1G:1436:U:C6	2.23	0.73
1:1G:617:G:N7	62:1G:1865:HOH:O	2.21	0.73
26:1H:568:U:O4	62:1H:3683:HOH:O	2.06	0.73
39:98:100:LEU:HD11	39:98:113:LEU:HD13	1.71	0.73
37:35:122:PRO:HB3	37:35:141:ALA:HB1	1.70	0.73
1:13:455:C:N3	1:13:477:G:N2	2.37	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1H:2329:G:N7	62:1H:3782:HOH:O	2.21	0.73
26:1H:617:G:OP1	31:31:40:GLN:NE2	2.22	0.73
1:13:692:U:O4	11:2I:53:SER:HB2	1.88	0.73
31:39:192:LEU:HD13	31:39:194:MET:HE1	1.70	0.73
31:39:53:THR:HG23	31:39:55:GLY:H	1.52	0.73
12:3A:41:ARG:HB3	12:3A:41:ARG:HH11	1.53	0.73
32:41:67:LYS:HE2	52:M8:6:HIS:CE1	2.23	0.73
26:14:1022:G:H22	26:14:1142(A):A:H2	1.37	0.73
26:1H:1174:A:H1'	26:1H:1178:C:H41	1.54	0.73
24:3L:9:A:H2'	24:3L:11:C:H41	1.54	0.73
1:1G:377:G:OP1	16:7A:3:LYS:NZ	2.22	0.73
1:13:1348:U:H4'	9:8E:120:ARG:HD2	1.70	0.72
27:1J:86:G:N2	27:1J:90:C:O2	2.17	0.72
34:69:78:THR:HG21	34:69:104:GLN:HG3	1.70	0.72
41:B8:26:ASP:HB3	41:B8:92:GLY:H	1.54	0.72
26:14:141:A:H8	26:14:1595:G:H21	1.37	0.72
3:22:138:VAL:HG23	3:22:151:VAL:HG23	1.70	0.72
13:4I:7:VAL:HB	32:41:115:ARG:HH22	1.54	0.72
1:1G:1204:A:OP1	14:5A:3:ARG:NH1	2.23	0.72
19:AA:3:ARG:HD2	19:AA:7:LYS:HG2	1.71	0.72
47:H8:9:TYR:CE1	47:H8:35:ARG:HG2	2.24	0.72
2:12:22:LYS:HB3	2:12:40:HIS:CE1	2.23	0.72
26:14:761:A:C8	61:14:3437:SPE:H112	2.25	0.72
14:5I:6:LEU:HD13	14:5I:23:ARG:HH22	1.55	0.72
41:75:45:PHE:CE2	41:75:74:ARG:HG3	2.24	0.72
46:C5:74:PRO:HG2	46:C5:82:PRO:HG2	1.71	0.72
50:G5:47:ASN:O	50:G5:49:LYS:N	2.19	0.72
50:K8:32:LEU:HA	50:K8:35:LEU:HD23	1.72	0.72
29:11:38:LYS:HG2	29:11:40:THR:HG23	1.70	0.72
26:14:848:G:H2'	26:14:849:A:C8	2.25	0.72
26:1H:763:G:OP1	62:1H:3751:HOH:O	2.07	0.72
35:58:56:ASN:N	35:58:125:GLY:O	2.15	0.72
26:14:1678:G:H22	26:14:1989:G:H22	1.35	0.72
26:14:6:A:H62	35:15:131:GLN:H	1.35	0.72
24:3K:53:G:N2	24:3K:61:C:N3	2.36	0.72
1:13:449:C:H5	16:7I:42:ARG:HH11	1.38	0.72
1:13:501:C:H2'	1:13:502:G:H8	1.53	0.72
1:13:563:A:N6	62:13:1843:HOH:O	2.23	0.72
26:14:2655:G:N2	26:14:2665:A:OP2	2.23	0.72
22:1K:12:U:O2	22:1K:24:G:N2	2.22	0.72
3:22:84:ILE:HG23	3:22:85:ARG:HD2	1.71	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:71:35:ALA:HB2	28:71:218:MET:HG2	1.72	0.72
26:1H:2882:A:OP1	39:98:96:ARG:NH1	2.22	0.72
1:13:501:C:H2'	1:13:502:G:C8	2.24	0.72
26:14:1342:A:H2	26:14:1602:U:H3	1.36	0.72
26:14:1762:A:H2'	62:14:4247:HOH:O	1.89	0.72
1:1G:448:A:OP2	1:1G:485:G:N2	2.19	0.72
26:1H:1055:G:H1	26:1H:1104:C:H42	1.36	0.72
22:1K:6:G:N2	22:1K:67:C:O2'	2.23	0.72
29:19:30:GLU:HG3	29:19:63:ARG:NH2	2.05	0.72
1:1G:1162:C:H42	1:1G:1174:G:H1	1.35	0.72
26:1H:1364:G:N7	49:J8:2:SER:HB3	2.04	0.72
42:C8:69:CYS:SG	42:C8:79:PHE:HD2	2.13	0.72
47:D5:30:ASN:HA	47:D5:89:PHE:HE1	1.54	0.72
26:14:1899:G:H21	26:14:1902:C:H42	1.38	0.72
1:1G:1535:C:H41	25:4L:10:G:H21	1.38	0.72
22:1K:17:U:HO2'	22:1K:57:G:H1	1.36	0.72
26:1H:2313:C:H4'	32:41:91:ARG:HG3	1.70	0.72
26:1H:1903:G:OP1	29:11:241:PRO:HB2	1.90	0.72
1:13:1291:G:OP1	7:6E:37:ASN:ND2	2.23	0.72
26:14:2293:C:H5''	40:65:89:ARG:HH21	1.54	0.72
10:1A:48:THR:HA	10:1A:62:HIS:HB3	1.71	0.72
31:31:6:VAL:N	31:31:24:LEU:O	2.22	0.72
5:4E:110:LEU:HD13	5:4E:118:ILE:HD13	1.72	0.72
40:65:88:ASP:O	40:65:89:ARG:HB3	1.90	0.72
36:68:2:ILE:HD12	36:68:6:THR:HG21	1.71	0.72
56:M5:14:VAL:HG11	56:M5:58:ILE:HD11	1.70	0.72
26:14:2711:A:OP2	62:14:3508:HOH:O	2.08	0.71
1:1G:1347:G:O2'	1:1G:1373:G:O6	2.08	0.71
26:1H:2711:A:OP2	62:1H:3750:HOH:O	2.06	0.71
39:55:33:ARG:HB2	39:55:115:GLU:HB3	1.71	0.71
38:88:59:ARG:HB3	38:88:61:GLY:H	1.53	0.71
24:1L:5:C:H42	24:1L:68:G:H1	1.38	0.71
31:39:12:LEU:HD23	31:39:14:PRO:HD3	1.72	0.71
8:72:29:SER:HB3	8:72:32:LYS:HG3	1.71	0.71
54:O8:28:ARG:HE	54:O8:30:THR:HG23	1.54	0.71
1:13:659:U:H2'	1:13:660:G:C8	2.25	0.71
1:1G:1305:G:H22	1:1G:1331:G:H2'	1.55	0.71
1:1G:576:G:OP1	62:1G:1856:HOH:O	2.06	0.71
33:51:30:LYS:HD2	33:51:81:GLU:H	1.54	0.71
36:25:115:VAL:HG13	36:25:121:VAL:HG21	1.70	0.71
4:3E:85:LYS:HE2	4:3E:89:THR:HA	1.73	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:B5:43:VAL:HG23	45:B5:51:VAL:HG21	1.72	0.71
1:13:165:C:H2'	1:13:166:G:H8	1.56	0.71
31:31:29:ASN:H	31:31:112:MET:HE1	1.56	0.71
12:3I:117:ARG:HB3	12:3I:122:THR:HB	1.70	0.71
32:49:7:LEU:HD12	32:49:104:GLU:HA	1.72	0.71
38:88:140:ALA:O	38:88:141:GLN:NE2	2.23	0.71
1:13:235:C:H5'	17:8I:70:ARG:HG2	1.72	0.71
51:H5:44:ARG:HB2	51:H5:44:ARG:HH11	1.54	0.71
26:14:323:G:HO2'	26:14:1205:U:H3	1.38	0.71
26:14:2598:A:OP1	62:14:3629:HOH:O	2.08	0.71
4:3E:129:ASN:ND2	4:3E:144:ASP:OD1	2.24	0.71
16:7I:53:VAL:HG13	16:7I:79:VAL:HG22	1.71	0.71
47:H8:7:ALA:HB2	47:H8:59:LEU:HD22	1.73	0.71
26:14:2331:G:H4'	48:E5:43:THR:H	1.54	0.71
29:19:37:LEU:HD12	29:19:37:LEU:H	1.54	0.71
30:21:101:ARG:HG2	30:21:169:ASN:OD1	1.91	0.71
33:59:89:ILE:HG21	33:59:130:ARG:HA	1.73	0.71
39:98:32:GLY:HA2	39:98:116:LEU:HD12	1.72	0.71
52:M8:57:GLU:O	52:M8:61:ARG:NH1	2.23	0.71
1:13:598:U:H4'	8:7E:94:TYR:CD2	2.26	0.71
1:13:664:G:H22	1:13:741:G:H1	1.38	0.71
1:1G:1023:G:C5	1:1G:1024:G:H1'	2.26	0.71
1:1G:1443:G:O2'	41:75:122:ASP:OD2	2.09	0.71
1:1G:987:G:H1	1:1G:1218:C:H42	1.39	0.71
26:1H:2487:G:O6	62:1H:3754:HOH:O	2.09	0.71
26:1H:248:G:OP1	62:1H:3753:HOH:O	2.09	0.71
26:1H:731:C:H5''	62:1H:3885:HOH:O	1.90	0.71
36:25:2:ILE:HD12	36:25:6:THR:HG21	1.70	0.71
26:14:832:G:H5'	37:35:45:LEU:HD11	1.71	0.71
37:78:65:ARG:HB3	62:Q8:404:HOH:O	1.90	0.71
9:82:112:LYS:HE3	9:82:118:LYS:H	1.55	0.71
30:21:9:VAL:HG13	41:B8:3:ARG:HG3	1.73	0.71
44:E8:86:LEU:HD12	44:E8:87:PRO:HD2	1.73	0.71
1:13:1124:G:N7	1:13:1145:C:O2'	2.23	0.71
1:13:1391:U:H2'	1:13:1392:G:C8	2.26	0.71
1:13:963:G:H21	10:1I:55:LYS:NZ	1.89	0.71
1:1G:1345:U:OP2	62:1G:1857:HOH:O	2.09	0.71
37:35:71:VAL:HG13	37:35:72:PRO:HD3	1.71	0.71
34:69:98:ALA:HA	34:69:109:ILE:HD11	1.73	0.71
26:14:2656:U:H3	26:14:2665:A:H2	1.38	0.70
10:1A:40:LEU:HD22	10:1A:71:LEU:HD13	1.73	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1G:1003:G:N2	1:1G:1005:A:OP1	2.24	0.70
3:2E:136:GLN:OE1	3:2E:140:ARG:NH1	2.24	0.70
34:61:110:ASP:OD1	34:61:110:ASP:N	2.21	0.70
41:75:77:PRO:HG2	41:75:80:SER:HB2	1.73	0.70
16:7A:74:LEU:HD12	16:7A:79:VAL:HG21	1.72	0.70
26:14:1154:G:OP2	42:85:58:ARG:NH1	2.23	0.70
26:1H:1228:G:OP2	42:C8:16:LYS:NZ	2.24	0.70
1:13:1306:A:H61	1:13:1331:G:H1'	1.55	0.70
29:19:69:ARG:HD3	29:19:105:ILE:HD11	1.73	0.70
3:22:87:LEU:HD12	3:22:88:ARG:HH21	1.55	0.70
18:9I:59:SER:HB3	18:9I:62:GLU:HB2	1.74	0.70
20:BA:69:GLY:O	20:BA:73:HIS:NE2	2.24	0.70
48:I8:14:ARG:NH1	62:I8:201:HOH:O	2.22	0.70
1:1G:1353:G:OP1	21:1B:10:ARG:NH1	2.23	0.70
26:1H:1899:G:N2	26:1H:1902:C:H5	1.88	0.70
31:31:66:PRO:O	31:31:67:GLN:HB3	1.89	0.70
4:3E:65:ARG:NH1	4:3E:70:ILE:O	2.23	0.70
34:61:92:VAL:HG13	34:61:120:ILE:HG23	1.73	0.70
8:7E:41:ARG:NH2	8:7E:123:GLU:OE1	2.22	0.70
1:13:1062:U:H2'	1:13:1063:C:C6	2.26	0.70
1:1G:1256:A:N6	1:1G:1278:U:OP2	2.24	0.70
26:1H:2135:A:N6	26:1H:2156:G:O2'	2.24	0.70
3:22:152:ILE:HB	3:22:199:LYS:HB2	1.72	0.70
4:3E:89:THR:HG23	4:3E:91:SER:H	1.57	0.70
26:14:2882:A:H5'	39:55:96:ARG:HG3	1.74	0.70
29:11:238:GLY:O	62:11:302:HOH:O	2.10	0.70
1:13:262:A:H2'	1:13:263:A:C8	2.27	0.70
26:14:1418:G:N7	62:14:3668:HOH:O	2.24	0.70
26:1H:2789:C:O2	26:1H:2894:G:N2	2.16	0.70
36:68:104:ARG:HH11	41:B8:36:GLU:HG3	1.55	0.70
47:D5:60:GLU:HA	47:D5:66:SER:HA	1.74	0.70
49:J8:91:LYS:HD3	49:J8:91:LYS:N	2.06	0.70
1:13:944:G:OP1	62:13:1838:HOH:O	2.09	0.70
33:51:149:ARG:NH1	33:51:167:GLU:OE2	2.25	0.70
10:1I:49:VAL:HG23	14:5I:41:ARG:HB2	1.72	0.70
20:BI:33:ILE:O	20:BI:37:SER:OG	2.06	0.70
46:G8:9:LYS:HA	46:G8:27:VAL:HG22	1.72	0.70
29:11:10:THR:OG1	29:11:13:ARG:HB2	1.90	0.70
27:1J:15:A:OP2	27:1J:69:G:N2	2.24	0.70
30:29:101:ARG:HG3	30:29:203:LYS:HD3	1.72	0.70
1:13:601:C:H2'	1:13:602:A:C8	2.26	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:14:816:C:OP2	62:14:3632:HOH:O	2.09	0.70
26:14:932:G:N7	62:14:3670:HOH:O	2.25	0.70
1:1G:1401:G:OP1	62:1G:1858:HOH:O	2.10	0.70
38:45:135:ASP:N	38:45:136:ALA:HA	2.06	0.70
1:1G:1095:U:P	1:1G:1108:G:H1	2.14	0.70
26:1H:1525:G:H2'	26:1H:1526:G:H8	1.55	0.70
26:1H:1607:C:H4'	26:1H:1608:A:O5'	1.92	0.70
8:72:12:ARG:NH2	8:72:27:PRO:HD3	2.07	0.70
26:1H:1156:A:C8	42:C8:51:LYS:HG2	2.27	0.69
27:1J:11:C:OP2	27:1J:12:C:N4	2.20	0.69
3:22:18:TRP:HE3	3:22:18:TRP:H	1.40	0.69
37:78:47:ASP:OD2	37:78:50:ARG:NH2	2.25	0.69
1:1G:1346:A:H5''	9:82:120:ARG:HH12	1.57	0.69
1:13:1240:U:OP2	7:6E:116:ALA:N	2.25	0.69
26:14:2306:C:H3'	26:14:2307:G:H5''	1.74	0.69
1:1G:564:C:O2'	8:72:91:ARG:NH2	2.22	0.69
26:1H:1900:A:C8	26:1H:1900:A:H5'	2.26	0.69
1:13:404:U:H5'	4:3E:122:ARG:HD2	1.73	0.69
15:6I:63:ARG:HG2	15:6I:67:LEU:HD12	1.75	0.69
29:11:8:PRO:HB3	29:11:14:ARG:HB2	1.73	0.69
26:14:2785:C:O2'	30:29:64:LYS:NZ	2.24	0.69
35:15:128:HIS:ND1	35:15:129:PRO:O	2.25	0.69
1:1G:1286:A:C8	1:1G:1287:A:H4'	2.26	0.69
1:1G:501:C:H2'	1:1G:502:G:H8	1.57	0.69
5:42:16:THR:OG1	5:42:17:ALA:N	2.24	0.69
7:62:113:GLU:HB2	7:62:119:ARG:HG2	1.73	0.69
26:1H:270(L):U:C2	34:61:50:ARG:HG2	2.27	0.69
5:4E:45:PHE:CE2	5:4E:47:LYS:HD2	2.28	0.69
2:12:27:LYS:O	2:12:30:ARG:NH1	2.26	0.69
1:1G:1262:C:H42	1:1G:1273:G:H1	1.40	0.69
26:1H:1534:G:N1	26:1H:1539:G:N3	2.40	0.69
26:1H:1843:C:H5'	29:11:253:GLN:OE1	1.92	0.69
26:1H:2503:A:OP2	62:1H:3755:HOH:O	2.10	0.69
26:1H:259:G:H21	26:1H:621:A:H8	1.39	0.69
33:59:8:PRO:HB2	33:59:69:ARG:HH21	1.56	0.69
26:14:94:G:H21	50:G5:47:ASN:HD22	1.40	0.69
1:1G:1226:C:O2'	13:4A:111:LYS:NZ	2.21	0.69
26:1H:1534:G:H21	26:1H:1538:G:N2	1.91	0.69
26:1H:1932:A:OP2	62:1H:3752:HOH:O	2.09	0.69
26:1H:2217:G:O6	62:1H:3757:HOH:O	2.10	0.69
30:21:105:THR:OG1	30:21:199:ARG:NH2	2.25	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:22:150:LYS:HG3	3:22:169:ALA:HB2	1.72	0.69
26:14:1952:A:C6	36:25:22:ILE:HD11	2.27	0.69
36:68:93:PRO:HG3	36:68:114:ILE:HG12	1.74	0.69
26:14:1035:U:H2'	26:14:1036:G:C8	2.27	0.69
26:14:1043:C:H42	26:14:1112:G:H1	1.38	0.69
1:1G:1347:G:N7	9:82:10:ARG:NH2	2.41	0.69
37:78:50:ARG:HH21	37:78:50:ARG:HG3	1.57	0.69
52:M8:45:GLY:O	52:M8:47:GLN:NE2	2.25	0.69
1:1G:1028(A):C:H42	1:1G:1032(B):G:H1	1.40	0.69
26:1H:2124:G:O6	26:1H:2173:A:N6	2.25	0.69
26:1H:2210:G:H4'	26:1H:2211:G:OP2	1.92	0.69
26:1H:635:C:O2'	26:1H:639:U:OP1	2.11	0.69
32:41:77:ILE:HG22	32:41:82:LEU:HD12	1.75	0.69
33:51:153:LYS:HB2	33:51:155:SER:H	1.58	0.69
7:6E:111:ARG:NH1	7:6E:113:GLU:OE2	2.26	0.69
24:3K:63:U:H6	28:71:53:ARG:HH22	1.41	0.69
1:13:468:A:H5''	16:7I:80:PHE:HB3	1.74	0.69
19:AI:11:VAL:HG11	19:AI:16:LEU:HD22	1.75	0.69
44:E8:14:PRO:HG2	44:E8:78:GLU:HB2	1.75	0.69
1:13:1455:G:OP1	20:BI:35:THR:OG1	2.04	0.69
26:14:674:G:OP2	62:14:3634:HOH:O	2.10	0.69
26:14:910:A:H62	38:45:12:GLN:HA	1.57	0.69
10:1A:50:ILE:HG22	10:1A:52:GLY:H	1.58	0.69
1:1G:1218:C:OP2	14:5A:9:LYS:NZ	2.22	0.69
1:1G:1401:G:N7	62:1G:1867:HOH:O	2.24	0.69
1:13:8:A:N7	4:3E:208:SER:HB3	2.06	0.69
1:13:362:G:O2'	12:3I:33:ARG:NH2	2.26	0.69
32:41:112:PRO:HB3	52:M8:37:SER:HB2	1.73	0.69
1:13:735:C:H2'	1:13:736:C:H6	1.58	0.69
26:14:2379:G:O2'	40:65:17:ARG:NH1	2.25	0.69
1:1G:957:U:O2'	1:1G:959:A:N7	2.22	0.69
26:1H:1006:C:OP2	62:1H:3756:HOH:O	2.10	0.69
26:1H:1210:A:C8	26:1H:1210:A:H5'	2.28	0.69
36:25:102:VAL:HB	36:25:106:LEU:HD12	1.74	0.69
44:E8:88:ARG:HB2	44:E8:92:ARG:HB3	1.73	0.69
26:1H:2210:G:H5'	26:1H:2211:G:N7	2.08	0.69
26:1H:2314:C:H2'	26:1H:2315:G:H8	1.56	0.69
30:29:134:ILE:O	30:29:134:ILE:HD12	1.93	0.69
26:1H:2689:U:C6	26:1H:2689:U:H5'	2.28	0.68
62:1H:3693:HOH:O	30:21:135:HIS:NE2	2.25	0.68
24:3L:76:A:H8	26:14:2394:C:H42	1.38	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1H:6:A:H4'	35:58:129:PRO:HB3	1.76	0.68
8:7E:9:MET:HG3	8:7E:26:VAL:HG21	1.74	0.68
45:B5:41:ASN:HA	45:B5:44:GLU:HB2	1.75	0.68
26:14:483:A:H5'	46:C5:49:VAL:HG22	1.76	0.68
44:E8:2:GLU:OE1	44:E8:72:LYS:NZ	2.27	0.68
26:14:1622:G:OP2	62:14:3633:HOH:O	2.09	0.68
29:19:237:GLU:OE2	62:19:402:HOH:O	2.09	0.68
1:1G:1014:A:H2'	1:1G:1015:A:C8	2.29	0.68
1:1G:1154:G:H2'	1:1G:1155:G:H8	1.57	0.68
1:1G:278:G:OP2	17:8A:92:ARG:NH2	2.26	0.68
1:1G:998:G:H22	1:1G:1043:C:H42	1.38	0.68
26:1H:2270:G:OP2	62:1H:3758:HOH:O	2.10	0.68
26:1H:982:C:OP2	62:1H:3759:HOH:O	2.11	0.68
13:4I:80:ARG:NH1	19:AI:65:ASN:O	2.26	0.68
26:14:602:G:HO2'	26:14:604:G:HO2'	1.39	0.68
1:1G:1263:C:N4	1:1G:1272:G:O6	2.20	0.68
1:1G:79:G:H1	1:1G:90:C:H42	1.40	0.68
26:1H:2118:U:O2	26:1H:2148:G:O2'	2.11	0.68
26:1H:2275:C:H5'	26:1H:2275:C:H6	1.57	0.68
41:75:24:PRO:HD3	41:75:52:ILE:HD12	1.76	0.68
1:13:963:G:H1	1:13:972:C:H42	1.38	0.68
26:14:1041:C:H42	26:14:1114:G:H1	1.40	0.68
40:A8:74:ALA:HB1	40:A8:108:GLY:HA3	1.73	0.68
1:13:323:U:H5'	20:BI:23:ARG:HB2	1.75	0.68
26:1H:1165:U:H2'	26:1H:1166:C:C6	2.29	0.68
27:1J:76:G:N7	62:1J:305:HOH:O	2.26	0.68
26:14:1359:A:H62	26:14:1372:U:H3	1.42	0.68
1:1G:1124:G:O2'	1:1G:1145:C:N4	2.27	0.68
1:1G:345:C:OP2	41:75:39:ARG:NH2	2.27	0.68
1:1G:362:G:H4'	12:3A:33:ARG:HH21	1.57	0.68
26:1H:1381:G:N7	62:1H:3795:HOH:O	2.27	0.68
26:1H:1486:A:H2'	26:1H:1487:G:H8	1.59	0.68
26:1H:2352:A:OP2	62:1H:3760:HOH:O	2.12	0.68
27:1J:44:G:H1'	27:1J:47:C:H42	1.58	0.68
11:2I:99:GLN:HB3	11:2I:105:VAL:HG11	1.76	0.68
36:25:68:GLU:OE2	36:25:78:ARG:NH1	2.27	0.68
5:42:102:ALA:HB1	5:42:106:PRO:HG2	1.76	0.68
34:69:77:LEU:HD23	34:69:78:THR:H	1.58	0.68
45:B5:1:MET:H2	50:G5:29:LYS:HE3	1.59	0.68
41:B8:12:SER:HA	41:B8:14:TYR:H	1.58	0.68
26:14:389:G:N1	37:35:71:VAL:HG12	2.09	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:4I:37:THR:O	13:4I:55:ARG:NH1	2.27	0.68
1:1G:1196:U:H5	1:1G:1397:C:H41	1.42	0.68
26:1H:2154:G:H2'	26:1H:2155:G:H8	1.59	0.68
26:1H:860:U:C5	26:1H:917:A:C2	2.81	0.68
3:2E:123:GLN:O	3:2E:128:PHE:HB2	1.94	0.68
32:41:161:THR:HG22	32:41:163:ALA:H	1.57	0.68
39:98:20:LEU:HD21	39:98:40:LYS:HD3	1.75	0.68
26:14:1430:C:H2'	26:14:1431:U:C6	2.29	0.68
26:14:1676:A:N7	62:14:3674:HOH:O	2.26	0.68
8:72:12:ARG:HH21	8:72:27:PRO:HD3	1.59	0.68
18:9I:38:GLU:OE1	18:9I:41:LYS:NZ	2.25	0.68
1:1G:1274:G:H21	1:1G:1275:A:H62	1.41	0.67
33:51:86:GLU:CD	33:51:86:GLU:H	1.97	0.67
35:58:132:ALA:O	35:58:134:ARG:NH2	2.27	0.67
42:C8:68:ALA:O	42:C8:71:GLN:HB2	1.94	0.67
26:1H:2688:U:H5	26:1H:2720:U:OP2	1.77	0.67
32:49:56:ALA:HA	32:49:59:GLU:HB3	1.76	0.67
33:51:6:ARG:HH21	33:51:7:LEU:HD11	1.59	0.67
17:8I:22:LEU:HD11	17:8I:39:SER:HB3	1.76	0.67
19:AA:10:PHE:N	19:AA:11:VAL:HB	2.09	0.67
43:D8:45:THR:O	43:D8:47:VAL:HG23	1.95	0.67
26:14:2331:G:O3'	48:E5:43:THR:HG22	1.94	0.67
1:13:353:A:H5'	1:13:353:A:H8	1.59	0.67
1:13:953:G:OP2	62:13:1839:HOH:O	2.11	0.67
26:14:2247:A:N6	62:14:3676:HOH:O	2.26	0.67
31:31:29:ASN:H	31:31:112:MET:CE	2.05	0.67
32:49:130:ASN:HB3	32:49:160:VAL:HA	1.75	0.67
3:22:6:HIS:HB2	14:5A:49:HIS:HD2	1.59	0.67
45:B5:51:VAL:HG13	45:B5:81:VAL:HG23	1.76	0.67
1:13:1446:A:OP1	1:13:1446:A:H4'	1.95	0.67
1:1G:971:G:N2	1:1G:1363:A:OP2	2.27	0.67
26:1H:2751:G:N7	33:51:3:ARG:CZ	2.57	0.67
5:42:11:ILE:HD12	5:42:31:LEU:HD12	1.77	0.67
38:88:104:PHE:HE2	38:88:125:LEU:HD11	1.57	0.67
1:13:145:G:H1	1:13:177:C:H42	1.40	0.67
26:14:1970:A:H4'	62:14:3695:HOH:O	1.92	0.67
27:16:102:G:N7	62:16:302:HOH:O	2.27	0.67
40:65:50:SER:O	40:65:76:LYS:NZ	2.23	0.67
42:C8:92:ARG:NH1	42:C8:94:ASN:OD1	2.27	0.67
1:13:1015:A:H2'	1:13:1016:A:C8	2.30	0.67
26:14:1364:G:OP2	49:F5:2:SER:N	2.27	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:14:2836:U:H2'	26:14:2837:G:C8	2.29	0.67
1:1G:1452:C:H4'	1:1G:1453:G:H5'	1.75	0.67
26:1H:634:C:H2'	26:1H:635:C:C6	2.30	0.67
27:16:42:C:O2'	32:41:67:LYS:HE3	1.94	0.67
5:4E:8:GLU:OE2	5:4E:63:ARG:NH2	2.28	0.67
35:58:96:GLU:C	35:58:98:VAL:H	1.96	0.67
19:AI:36:ARG:NH1	19:AI:52:TYR:O	2.26	0.67
46:G8:82:PRO:HB3	46:G8:99:CYS:HB2	1.77	0.67
26:1H:191:A:N1	62:1H:3798:HOH:O	2.27	0.67
26:1H:2048:G:N7	62:1H:3802:HOH:O	2.28	0.67
26:1H:2233:U:H2'	26:1H:2234:G:C8	2.29	0.67
26:1H:848:G:H2'	26:1H:849:A:C8	2.30	0.67
12:3A:37:CYS:SG	12:3A:81:SER:OG	2.47	0.67
24:1L:36:U:H3	25:4L:19:G:H1	1.41	0.67
1:13:160:A:N6	1:13:346:G:O6	2.28	0.67
26:14:2520:C:H41	26:14:2542:A:H62	1.42	0.67
26:1H:601:C:N4	62:1H:3799:HOH:O	2.28	0.67
40:A8:27:SER:HA	40:A8:88:ASP:HB2	1.77	0.67
41:B8:24:PRO:HD3	41:B8:52:ILE:HD12	1.77	0.67
53:J5:49:CYS:SG	53:J5:50:GLY:N	2.67	0.67
1:13:410:G:OP1	4:3E:30:LYS:NZ	2.26	0.67
26:14:275:G:O2'	26:14:276:A:O4'	2.10	0.67
2:1E:16:HIS:CE1	2:1E:213:LEU:HD12	2.28	0.67
26:1H:1406:U:H2'	26:1H:1407:C:C6	2.30	0.67
9:8E:10:ARG:HG3	9:8E:75:ASP:HB3	1.77	0.67
41:B8:16:ARG:NH2	41:B8:83:ILE:O	2.28	0.67
20:BA:11:SER:HA	20:BA:13:LEU:HD23	1.77	0.67
26:14:271(B):G:N7	26:14:421:U:H2'	2.09	0.67
26:14:6:A:C8	35:15:129:PRO:HB2	2.30	0.67
10:1A:24:VAL:HG21	10:1A:37:PRO:HD3	1.76	0.67
1:1G:1023:G:H5''	1:1G:1024:G:H21	1.59	0.67
1:1G:1192:C:OP2	3:22:4:LYS:NZ	2.28	0.67
14:5A:27:CYS:O	14:5A:29:ARG:NH2	2.25	0.67
42:85:28:ARG:NH1	42:85:38:THR:OG1	2.26	0.67
7:6E:16:LEU:HG	9:8E:42:ARG:HA	1.77	0.67
46:C5:42:VAL:HG13	46:C5:65:ALA:HB3	1.76	0.67
54:O8:19:ARG:HG3	54:O8:21:TYR:HE1	1.60	0.67
29:19:93:ALA:HB3	29:19:105:ILE:HG22	1.77	0.66
26:1H:1380:G:N7	62:1H:3767:HOH:O	2.28	0.66
26:14:389:G:H1	37:35:71:VAL:HG12	1.59	0.66
13:4A:66:LEU:HA	13:4A:70:LEU:HB2	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:D5:111:VAL:HG12	47:D5:145:GLU:HB2	1.76	0.66
1:13:200:G:N2	1:13:218:C:N3	2.43	0.66
26:14:95:G:H4'	50:G5:46:GLN:HB2	1.76	0.66
1:1G:1235:U:O2'	1:1G:1305:G:O5'	2.12	0.66
26:1H:2287:A:H62	26:1H:2344:U:H3	1.42	0.66
12:3A:47:LYS:HD2	12:3A:48:PRO:HD2	1.75	0.66
32:49:60:LEU:HD22	32:49:68:PRO:HB3	1.77	0.66
42:85:92:ARG:HG3	42:85:94:ASN:HB3	1.76	0.66
35:15:56:ASN:H	35:15:125:GLY:HA3	1.60	0.66
26:1H:862:G:OP2	62:1H:3764:HOH:O	2.13	0.66
10:1I:78:ASN:O	10:1I:81:THR:OG1	2.14	0.66
37:35:39:LYS:HG3	37:35:45:LEU:HD22	1.77	0.66
13:4A:22:ILE:HB	13:4A:25:ILE:HG13	1.77	0.66
14:5A:22:THR:HB	14:5A:33:VAL:HG21	1.77	0.66
14:5I:27:CYS:SG	14:5I:29:ARG:HB2	2.36	0.66
43:D8:37:VAL:HG23	43:D8:51:VAL:HG21	1.78	0.66
1:13:411:A:C4	1:13:413:G:H1'	2.29	0.66
26:14:2400:G:H2'	26:14:2401:U:C6	2.31	0.66
26:1H:1899:G:H1	26:1H:1902:C:H41	1.44	0.66
26:14:1952:A:C5	36:25:22:ILE:HD11	2.31	0.66
3:2E:72:LYS:HD3	3:2E:75:VAL:HG21	1.77	0.66
37:35:93:GLY:H	37:35:123:LEU:HD22	1.59	0.66
17:8A:66:SER:O	17:8A:70:ARG:NH1	2.28	0.66
1:13:8:A:N6	4:3E:205:GLU:O	2.27	0.66
26:14:1997:G:OP2	62:14:3635:HOH:O	2.13	0.66
1:1G:353:A:H8	1:1G:353:A:H5'	1.60	0.66
1:1G:973:G:O3'	14:5A:41:ARG:NH2	2.28	0.66
26:1H:1491:G:O4'	29:11:99:ASP:HB3	1.96	0.66
26:1H:945:A:N3	62:1H:3796:HOH:O	2.27	0.66
12:3I:42:THR:HG22	12:3I:54:LYS:HD2	1.77	0.66
47:D5:5:LEU:HD11	47:D5:44:PHE:HA	1.77	0.66
47:H8:128:VAL:HB	47:H8:161:VAL:HG12	1.76	0.66
26:1H:1292:U:H2'	26:1H:1293:C:C6	2.31	0.66
26:1H:637:A:H2'	37:78:117:GLU:OE1	1.96	0.66
26:1H:969:U:OP1	51:L8:17:LYS:HG2	1.96	0.66
30:21:64:LYS:HA	30:21:67:PHE:O	1.95	0.66
24:3K:15:G:O6	24:3K:48:C:N4	2.29	0.66
26:14:1044:G:O2'	26:14:1047:G:O2'	2.14	0.66
26:14:1727:U:H3	26:14:1733:G:H1	1.44	0.66
26:14:247:G:H4'	26:14:386:G:C5	2.31	0.66
26:14:71:A:OP2	26:14:71:A:H3'	1.96	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1G:1300:G:O2'	1:1G:1301:U:O5'	2.13	0.66
1:1G:1352:C:N4	1:1G:1370:G:H1	1.93	0.66
1:1G:300:A:N1	62:1G:1872:HOH:O	2.29	0.66
26:1H:1412:A:H2'	26:1H:1413:G:C8	2.30	0.66
27:1J:7:G:H4'	40:65:29:PHE:CD2	2.31	0.66
23:2L:24:C:H2'	23:2L:25:U:C6	2.30	0.66
2:12:71:VAL:HB	2:12:165:VAL:HG22	1.77	0.66
26:14:2162:G:O2'	26:14:2173:A:OP1	2.13	0.66
2:1E:166:ASP:HB3	2:1E:169:LYS:HB2	1.77	0.66
4:32:7:PRO:HB2	4:32:10:ARG:HD2	1.78	0.66
37:35:55:ARG:HG2	37:35:56:SER:N	2.11	0.66
41:75:10:VAL:O	41:75:12:SER:N	2.29	0.66
29:11:35:LYS:HD3	29:11:36:PRO:HD2	1.78	0.66
2:1E:178:ARG:NH1	2:1E:196:LEU:O	2.27	0.66
38:88:66:ILE:O	38:88:104:PHE:N	2.28	0.66
1:13:1346:A:H5''	9:8E:120:ARG:NH1	2.11	0.66
26:1H:581:C:OP1	42:C8:33:ARG:HG3	1.96	0.66
47:D5:10:ARG:HH21	47:D5:26:GLY:H	1.40	0.66
2:12:50:GLU:HB2	2:12:199:TYR:HB3	1.77	0.66
1:1G:659:U:OP1	15:6A:9:GLN:NE2	2.29	0.66
1:1G:838:G:N2	1:1G:848:C:N3	2.43	0.66
34:61:110:ASP:HB2	34:61:112:LYS:HG2	1.78	0.66
43:95:1:MET:HA	43:95:42:GLY:H	1.61	0.66
40:A8:59:LYS:HG2	40:A8:60:GLY:H	1.60	0.66
41:B8:26:ASP:O	41:B8:49:VAL:HG13	1.96	0.66
41:B8:26:ASP:HB2	41:B8:91:ARG:HA	1.77	0.66
1:13:1034:G:N2	1:13:1035:A:N7	2.44	0.65
26:14:993:G:OP1	42:85:50:ARG:NH2	2.28	0.65
26:1H:65:C:H2'	26:1H:66:C:H6	1.61	0.65
26:1H:71:A:H2	45:F8:31:HIS:HE2	1.44	0.65
37:35:98:GLU:HA	37:35:101:VAL:HG12	1.77	0.65
1:13:345:C:N4	36:68:116:SER:O	2.24	0.65
56:Q8:33:ASN:HA	56:Q8:36:LYS:HD2	1.78	0.65
1:1G:1274:G:N2	1:1G:1275:A:H62	1.94	0.65
1:1G:474:G:H2'	1:1G:475:G:H8	1.61	0.65
1:1G:548:G:OP1	62:1G:1859:HOH:O	2.12	0.65
30:21:82:ARG:O	30:21:84:PHE:N	2.29	0.65
5:42:31:LEU:HD22	5:42:45:PHE:HB2	1.78	0.65
26:14:1653:G:H3'	39:55:2:ARG:HG2	1.77	0.65
38:88:110:THR:HG23	38:88:113:GLN:OE1	1.96	0.65
17:8A:87:LYS:O	17:8A:91:ARG:HG3	1.95	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:A5:65:LEU:HD13	44:A5:68:ARG:HD3	1.77	0.65
1:1G:261:U:OP2	20:BA:79:ARG:NH2	2.29	0.65
26:14:1015:G:N2	26:14:1147:C:O2	2.26	0.65
26:1H:2324:C:H5''	26:1H:2325:G:H5'	1.79	0.65
26:1H:2409:G:N7	62:1H:3809:HOH:O	2.29	0.65
26:1H:981:A:OP1	62:1H:3765:HOH:O	2.14	0.65
38:45:75:THR:OG1	38:45:87:LYS:NZ	2.30	0.65
1:13:1202:G:N2	14:5I:46:GLU:OE1	2.24	0.65
34:69:104:GLN:OE1	34:69:105:HIS:ND1	2.30	0.65
26:14:1044:G:HO2'	26:14:1047:G:HO2'	1.40	0.65
26:14:945:A:N3	62:14:3683:HOH:O	2.28	0.65
1:1G:1028:C:H42	1:1G:1033:G:H1	1.44	0.65
26:1H:548:A:H2'	26:1H:549:G:H5'	1.79	0.65
4:3E:154:ASN:OD1	4:3E:154:ASN:N	2.30	0.65
4:3E:30:LYS:HA	4:3E:35:ARG:HE	1.62	0.65
1:13:474:G:H5''	16:7I:81:ARG:HE	1.60	0.65
26:1H:881:G:H1	26:1H:895:U:H3	1.44	0.65
42:C8:92:ARG:HD3	42:C8:94:ASN:HB3	1.76	0.65
47:H8:77:ASP:OD1	47:H8:80:ARG:HD2	1.96	0.65
1:13:619:U:H3	4:3E:134:ASP:HB2	1.62	0.65
26:14:1113:U:OP1	26:14:2751:G:N2	2.30	0.65
26:14:1495:A:N7	62:14:3690:HOH:O	2.30	0.65
10:1A:55:LYS:NZ	10:1A:57:LYS:HG2	2.12	0.65
30:29:54:GLN:HB2	30:29:72:VAL:HB	1.78	0.65
26:14:2745:C:O2	33:59:139:GLN:NE2	2.30	0.65
26:1H:910:A:C5	38:88:13:GLN:HG3	2.32	0.65
47:H8:165:VAL:HB	47:H8:166:SER:HA	1.78	0.65
26:14:2148:G:H2'	26:14:2149:G:H8	1.60	0.65
1:1G:1316:G:H4'	14:5A:18:VAL:HG11	1.79	0.65
38:45:27:VAL:HB	38:45:28:ALA:CA	2.10	0.65
5:4E:8:GLU:HG2	5:4E:34:VAL:HG22	1.77	0.65
14:5I:23:ARG:HH11	14:5I:30:ALA:HB2	1.61	0.65
40:65:29:PHE:HD1	40:65:30:ARG:N	1.93	0.65
1:13:719:C:O2'	18:9I:49:LYS:HB3	1.97	0.65
2:12:71:VAL:HG11	2:12:164:VAL:HA	1.77	0.65
1:13:611:A:H61	1:13:629:G:H1	1.44	0.65
1:1G:862:C:H1'	1:1G:874:G:H5''	1.78	0.65
26:1H:860:U:C5	26:1H:917:A:H2	2.15	0.65
31:39:79:GLY:HA2	31:39:86:GLY:HA2	1.77	0.65
38:45:34:LEU:HB2	38:45:118:LEU:HD13	1.78	0.65
2:12:118:LEU:HB3	2:12:142:LEU:HD12	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:14:620:G:H4'	26:14:621:A:H5''	1.79	0.65
1:1G:976:G:P	14:5A:32:SER:H	2.20	0.65
26:1H:573:G:O2'	26:1H:574:C:H3'	1.97	0.65
36:25:49:ARG:HA	36:25:53:LYS:HZ2	1.60	0.65
41:75:18:ASP:N	41:75:18:ASP:OD1	2.30	0.65
38:88:66:ILE:HG13	38:88:67:ARG:H	1.61	0.65
9:8E:13:ALA:HB2	9:8E:68:GLY:HA3	1.77	0.65
9:8E:17:VAL:HG11	9:8E:81:ILE:HD13	1.79	0.65
42:C8:90:VAL:HG22	43:D8:39:LEU:HB3	1.79	0.65
49:J8:84:GLY:HA2	49:J8:85:LEU:HB3	1.78	0.65
10:1A:32:ALA:HA	10:1A:76:ASN:HD21	1.62	0.65
1:1G:587:G:N2	1:1G:754:C:OP2	2.29	0.65
1:1G:620:C:H2'	1:1G:621:A:O4'	1.97	0.65
26:1H:1049:C:H2'	26:1H:1050:A:H5'	1.78	0.65
26:1H:832:G:H5'	37:78:45:LEU:HD11	1.78	0.65
23:2L:24:C:H2'	23:2L:25:U:H6	1.61	0.65
39:55:38:VAL:HG22	39:55:112:ALA:HB2	1.79	0.65
27:1J:9:G:P	40:65:25:ARG:HH22	2.20	0.65
37:78:18:ARG:HG3	37:78:18:ARG:HH21	1.60	0.65
10:1A:75:ILE:HG13	10:1A:76:ASN:N	2.11	0.64
1:1G:664:G:H22	1:1G:741:G:H1	1.45	0.64
26:1H:1430:C:H2'	26:1H:1431:U:C6	2.32	0.64
26:1H:1453:A:OP2	62:1H:3766:HOH:O	2.14	0.64
26:1H:2849:U:H4'	26:1H:2868:A:C2	2.33	0.64
42:85:91:ASP:O	42:85:92:ARG:HG2	1.97	0.64
40:A8:38:GLN:HG2	40:A8:47:THR:HG21	1.79	0.64
47:D5:10:ARG:NH2	47:D5:26:GLY:O	2.30	0.64
26:14:1169:G:N2	26:14:1180:C:N3	2.40	0.64
26:14:1329:U:H5''	26:14:1330:C:H5	1.62	0.64
26:14:2210:G:H3'	26:14:2211:G:C8	2.33	0.64
26:14:6:A:H62	35:15:131:GLN:N	1.95	0.64
26:1H:2105:C:H2'	26:1H:2106:G:H8	1.62	0.64
8:7E:121:ASP:HB2	8:7E:125:ARG:NH2	2.12	0.64
43:95:21:ARG:NH1	43:95:91:TYR:OH	2.29	0.64
41:B8:4:GLY:HA2	41:B8:7:ILE:HG12	1.78	0.64
26:14:498:G:H21	46:C5:47:LYS:NZ	1.93	0.64
1:13:67:C:H2'	1:13:68:G:C8	2.32	0.64
26:14:30:G:H2'	26:14:31:C:C6	2.32	0.64
26:14:900:A:H3'	26:14:901:A:H8	1.60	0.64
1:1G:1319:A:OP2	19:AA:3:ARG:HG3	1.97	0.64
1:1G:1305:G:H22	1:1G:1331:G:C2'	2.09	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1H:1386:C:H2'	26:1H:1387:C:H6	1.61	0.64
26:14:1670:C:O2	30:29:129:HIS:NE2	2.27	0.64
11:2A:48:ILE:HD11	11:2A:64:ALA:HA	1.79	0.64
1:13:1296:C:OP1	13:4I:44:ARG:NH2	2.29	0.64
25:4K:24:A:H2'	25:4K:25:A:C8	2.32	0.64
47:D5:30:ASN:HA	47:D5:89:PHE:CE1	2.32	0.64
37:35:63:PRO:HD3	56:M5:27:THR:HG22	1.79	0.64
52:M8:16:CYS:HB3	52:M8:36:CYS:HB3	1.79	0.64
1:13:737:A:H2'	1:13:738:C:C6	2.32	0.64
26:14:2147:G:H2'	26:14:2148:G:H4'	1.78	0.64
35:15:42:TRP:O	42:85:64:ARG:NH2	2.30	0.64
1:1G:972:C:O2'	10:1A:55:LYS:HG3	1.97	0.64
2:1E:53:ARG:NH2	2:1E:198:ASP:O	2.30	0.64
1:1G:1268:A:H2'	1:1G:1269:A:C8	2.33	0.64
1:1G:1401:G:OP1	25:4L:18:G:O2'	2.13	0.64
30:29:116:VAL:HG11	30:29:138:PRO:HB3	1.78	0.64
34:61:123:LEU:HD23	34:61:143:SER:HA	1.77	0.64
1:1G:1147:C:O2	9:82:16:ARG:NH1	2.30	0.64
9:8E:26:VAL:HG13	9:8E:61:ALA:HB3	1.78	0.64
40:A8:28:VAL:HG11	40:A8:98:VAL:HG13	1.80	0.64
36:68:104:ARG:HD3	41:B8:36:GLU:HG3	1.79	0.64
1:13:1286:A:C8	1:13:1287:A:H4'	2.33	0.64
26:14:1040:C:H2'	26:14:1041:C:C6	2.33	0.64
27:16:66:A:H61	27:16:107:U:H2'	1.62	0.64
26:1H:176:G:O2'	26:1H:177:G:H5'	1.98	0.64
14:5A:41:ARG:HG3	14:5A:42:ILE:HG13	1.80	0.64
17:8I:9:VAL:HG21	17:8I:84:LEU:HD12	1.79	0.64
40:A8:106:ARG:NH1	40:A8:107:GLU:HG2	2.13	0.64
48:E5:12:ASN:HA	48:E5:14:ARG:HH21	1.61	0.64
53:N8:36:CYS:HB2	53:N8:49:CYS:SG	2.37	0.64
33:51:157:TYR:H	33:51:171:LEU:HA	1.61	0.64
37:78:18:ARG:O	37:78:19:VAL:HB	1.97	0.64
9:8E:50:LEU:HA	9:8E:53:VAL:HG22	1.80	0.64
47:H8:132:ASN:OD1	47:H8:132:ASN:N	2.31	0.64
26:14:1169:G:H1	26:14:1180:C:H42	1.44	0.64
26:14:990:A:H8	26:14:990:A:H5'	1.63	0.64
26:1H:1521:G:N7	62:1H:3812:HOH:O	2.30	0.64
30:21:116:VAL:O	30:21:117:MET:HB3	1.97	0.64
26:14:1428:C:N4	26:14:1570:A:OP2	2.27	0.64
26:14:2712:U:O2'	62:14:3636:HOH:O	2.14	0.64
26:1H:1364:G:OP2	49:J8:2:SER:OG	2.14	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:1K:17:U:O2'	22:1K:57:G:N1	2.30	0.64
33:59:70:THR:O	33:59:74:ASN:ND2	2.22	0.64
33:59:7:LEU:HD12	33:59:8:PRO:HD3	1.80	0.64
1:13:974:A:OP2	14:5I:29:ARG:NH1	2.30	0.64
35:15:13:TRP:O	35:15:135:PRO:HD2	1.97	0.64
29:19:108:PRO:HB3	29:19:143:HIS:CE1	2.33	0.64
1:1G:1134:G:C2	1:1G:1135:U:H1'	2.33	0.64
1:1G:1127:G:N2	1:1G:1145:C:N3	2.46	0.64
26:1H:1021:A:C8	26:1H:1022:G:H5''	2.32	0.64
26:1H:1113:U:OP1	33:51:2:SER:N	2.30	0.64
26:1H:2130:U:OP2	28:71:6:ARG:NH1	2.23	0.64
1:1G:8:A:N6	4:32:209:ARG:HB2	2.11	0.64
4:3E:107:ARG:NH2	4:3E:194:LEU:HD22	2.11	0.64
15:6A:16:ALA:HB1	15:6A:21:ASP:HB3	1.78	0.64
8:72:120:THR:HG23	8:72:123:GLU:H	1.62	0.64
41:75:7:ILE:HG13	41:75:8:LYS:H	1.63	0.64
38:88:35:VAL:HG13	38:88:130:LYS:HB3	1.78	0.64
26:1H:2723:C:H5''	39:98:1:MET:HE2	1.80	0.64
48:E5:27:GLU:HB2	48:E5:69:PHE:HD1	1.63	0.64
26:14:34:C:H1'	26:14:35:G:OP1	1.99	0.64
1:1G:448:A:P	1:1G:485:G:H22	2.21	0.64
30:29:97:LYS:N	30:29:100:GLU:OE1	2.28	0.64
26:14:2773:C:OP1	30:29:166:THR:OG1	2.15	0.64
1:1G:36:C:OP1	12:3A:123:LYS:NZ	2.31	0.64
32:49:11:TYR:OH	32:49:16:ARG:NH2	2.30	0.64
34:69:45:LYS:HA	34:69:48:GLU:HB3	1.80	0.64
42:85:66:ASN:O	42:85:70:ARG:HB2	1.97	0.64
19:AI:41:VAL:HG12	19:AI:44:MET:HB2	1.80	0.64
1:13:1223:C:P	19:AI:78:ARG:HH12	2.21	0.64
41:B8:42:ILE:HD12	41:B8:42:ILE:H	1.63	0.64
26:14:1614:A:H2	62:14:4025:HOH:O	1.81	0.63
1:1G:1203:C:H2'	1:1G:1204:A:C8	2.33	0.63
1:1G:1251:A:H2'	1:1G:1252:A:C8	2.33	0.63
26:1H:620:G:H4'	26:1H:621:A:C5'	2.28	0.63
26:1H:631:A:H5'	62:1H:4891:HOH:O	1.98	0.63
26:1H:900:A:H3'	26:1H:901:A:H8	1.61	0.63
27:1J:15:A:H1'	27:1J:109:G:C8	2.33	0.63
13:4I:107:ALA:HB3	13:4I:111:LYS:HD3	1.79	0.63
1:13:1368:G:H5''	9:8E:112:LYS:HB3	1.80	0.63
26:14:1771:C:HO2'	26:14:1786:A:H8	1.46	0.63
26:14:2156:G:N7	26:14:2157:G:N2	2.46	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:14:2296:U:OP2	40:65:9:ARG:NH1	2.26	0.63
1:1G:973:G:OP1	10:1A:57:LYS:NZ	2.32	0.63
2:1E:237:ALA:O	2:1E:239:VAL:N	2.31	0.63
1:1G:1104:G:O2'	2:12:111:ARG:NH2	2.31	0.63
1:1G:560:U:O2'	1:1G:561:U:OP2	2.15	0.63
35:58:57:ALA:C	35:58:59:LYS:H	2.00	0.63
1:13:453:A:H4'	16:7I:72:ARG:HB2	1.78	0.63
9:8E:5:TYR:HE1	9:8E:16:ARG:HG2	1.62	0.63
46:C5:86:ARG:HG3	46:C5:87:LYS:N	2.11	0.63
26:14:451:C:OP2	62:14:3637:HOH:O	2.15	0.63
4:3E:167:GLY:HA2	29:19:135:PHE:CE1	2.31	0.63
26:1H:2336:A:H61	48:I8:43:THR:HB	1.64	0.63
26:1H:320:A:H2'	31:31:136:THR:HG21	1.80	0.63
26:1H:33:U:H4'	26:1H:34:C:OP1	1.97	0.63
31:39:178:PRO:HB3	31:39:198:ALA:HA	1.80	0.63
14:5I:3:ARG:HB2	14:5I:3:ARG:NH1	2.12	0.63
26:14:2432:A:H2'	26:14:2433:A:C8	2.34	0.63
26:14:588:U:H2'	26:14:589:C:C6	2.33	0.63
1:1G:1181:G:N2	1:1G:1182:G:O2'	2.32	0.63
26:1H:273(F):C:H3'	26:1H:274:G:H5''	1.80	0.63
3:2E:8:ILE:HG23	3:2E:16:ARG:HG2	1.81	0.63
4:3E:98:GLU:HG2	4:3E:189:PRO:HG2	1.81	0.63
5:4E:33:VAL:HG11	5:4E:109:ILE:HA	1.80	0.63
5:4E:10:MET:HB3	5:4E:32:VAL:HG22	1.80	0.63
19:AI:41:VAL:HA	19:AI:44:MET:HG3	1.81	0.63
26:14:370:G:N7	62:14:3691:HOH:O	2.31	0.63
30:29:25:VAL:HG12	30:29:26:ILE:H	1.63	0.63
28:7I:185:LEU:O	28:7I:189:ILE:N	2.31	0.63
39:98:55:ALA:HA	39:98:80:PHE:CE1	2.33	0.63
47:D5:23:LYS:HD3	47:D5:40:ASP:HA	1.81	0.63
26:14:1843:C:H5'	29:19:253:GLN:OE1	1.97	0.63
26:14:2520:C:H41	26:14:2542:A:N6	1.97	0.63
26:14:273(C):C:H42	26:14:363(C):G:H1	1.45	0.63
10:1A:44:VAL:HG22	10:1A:66:ARG:HB3	1.80	0.63
1:1G:1127:G:O2'	1:1G:1148:U:O2	2.17	0.63
1:1G:785:G:N7	62:1G:1873:HOH:O	2.30	0.63
26:1H:974(A):C:OP1	62:1H:3768:HOH:O	2.15	0.63
27:1J:103:U:HO2'	47:D5:29:TYR:HH	1.44	0.63
26:14:993:G:N3	43:95:89:GLN:NE2	2.46	0.63
41:B8:84:GLN:HG2	41:B8:85:LYS:HD2	1.81	0.63
2:1E:17:PHE:HD1	2:1E:44:LEU:HD11	1.64	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1G:1127:G:H2'	1:1G:1128:C:H6	1.64	0.63
26:1H:2068:U:H3	26:1H:2430:A:H2	1.44	0.63
26:1H:2347:C:OP1	54:O8:39:TYR:OH	2.10	0.63
26:1H:61:G:OP1	50:K8:51:ARG:NH1	2.32	0.63
12:3I:57:LYS:HD3	12:3I:67:THR:HG22	1.81	0.63
26:14:2839:G:H5'	39:55:46:GLY:HA2	1.81	0.63
33:59:159:GLU:O	33:59:163:TYR:OH	2.15	0.63
26:1H:2124:G:H4'	28:71:174:PRO:HG3	1.80	0.63
1:1G:1349:A:OP2	9:82:118:LYS:NZ	2.32	0.63
39:98:55:ALA:HB2	39:98:79:LEU:HD13	1.80	0.63
1:13:1023:G:H3'	1:13:1024:G:H5''	1.81	0.63
26:1H:1329:U:H5''	26:1H:1330:C:H5	1.63	0.63
26:1H:534:U:H5'	42:C8:42:ALA:HB1	1.81	0.63
11:2I:121:PRO:HG2	11:2I:126:ARG:HG2	1.79	0.63
34:61:10:GLU:OE1	34:61:11:ASN:ND2	2.30	0.63
41:75:54:ARG:HG3	41:75:59:THR:HG21	1.79	0.63
56:Q8:49:VAL:HG12	56:Q8:49:VAL:O	1.98	0.63
1:1G:1028(A):C:N3	1:1G:1032(B):G:N2	2.41	0.63
1:1G:1521:G:N3	62:1G:1874:HOH:O	2.31	0.63
10:1I:26:ALA:O	10:1I:30:SER:OG	2.09	0.63
13:4I:37:THR:HB	13:4I:55:ARG:HD2	1.79	0.63
1:13:280:C:C2	17:8I:38:ARG:HG3	2.34	0.63
20:BI:75:ASN:N	20:BI:75:ASN:OD1	2.27	0.63
50:K8:42:GLY:C	50:K8:44:LEU:H	2.02	0.63
26:1H:2032:G:H21	30:21:146:THR:CG2	2.10	0.62
26:1H:2287:A:C2	26:1H:2346:A:H2	2.17	0.62
22:1K:7:U:H3	22:1K:66:A:H61	1.47	0.62
26:14:587:C:O2	37:35:33:ARG:NH1	2.31	0.62
31:39:157:VAL:HG12	31:39:198:ALA:HB1	1.81	0.62
1:13:590:C:O3'	8:7E:30:ARG:NH1	2.30	0.62
9:82:46:ALA:HB2	9:82:74:ILE:HG23	1.80	0.62
42:C8:92:ARG:HD2	43:D8:11:GLN:HB2	1.80	0.62
52:M8:37:SER:HB3	52:M8:42:PHE:CZ	2.33	0.62
19:AI:42:PRO:HD3	52:M8:63:TYR:OH	1.98	0.62
29:11:2:ALA:HA	29:11:20:ASP:CB	2.29	0.62
1:13:1454:G:OP1	20:BI:39:LYS:NZ	2.29	0.62
26:1H:863:A:H2'	26:1H:864:G:H8	1.63	0.62
1:1G:777:A:H2	11:2A:119:CYS:HB3	1.64	0.62
11:2A:14:VAL:HG11	11:2A:35:PRO:HD3	1.81	0.62
3:2E:15:THR:HG21	3:2E:181:ASN:HA	1.80	0.62
1:1G:363:A:OP1	12:3A:33:ARG:HG3	1.99	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:59:30:LYS:HB3	33:59:79:VAL:O	1.99	0.62
39:98:104:ARG:NH1	39:98:107:ASP:OD2	2.30	0.62
18:9A:22:VAL:HG22	18:9A:23:LYS:H	1.64	0.62
26:14:1198:U:H2'	26:14:1199:U:C6	2.34	0.62
26:14:142:G:H5''	26:14:1598:C:O2'	1.99	0.62
26:14:1794:U:H2'	26:14:1795:C:H6	1.64	0.62
26:14:774:A:H2	26:14:787:U:HO2'	1.46	0.62
1:1G:770:C:OP1	62:1G:1860:HOH:O	2.16	0.62
26:1H:1345:C:OP2	62:1H:3769:HOH:O	2.16	0.62
1:1G:1534:A:N6	25:4L:11:U:O4	2.33	0.62
6:5E:94:GLN:HE21	18:9I:32:ARG:HG2	1.64	0.62
1:1G:584:G:H5'	17:8A:91:ARG:HH12	1.64	0.62
26:1H:1178:C:H4'	26:1H:1179:C:OP1	1.98	0.62
26:1H:1786:A:H2	26:1H:2606:C:H1'	1.64	0.62
26:1H:76:C:O2'	50:K8:62:THR:HG21	2.00	0.62
5:4E:35:GLY:H	5:4E:112:LEU:HD13	1.64	0.62
45:F8:11:PRO:HG2	45:F8:13:LEU:HD21	1.80	0.62
1:13:973:G:H3'	1:13:974:A:H5''	1.82	0.62
26:14:193:U:OP2	62:14:3639:HOH:O	2.16	0.62
26:14:71:A:C8	26:14:71:A:H5'	2.35	0.62
29:19:145:VAL:HG13	29:19:191:ALA:HB2	1.79	0.62
2:1E:84:GLU:HB3	2:1E:219:VAL:HG21	1.80	0.62
1:1G:1513:A:H2'	1:1G:1514:C:C6	2.35	0.62
1:1G:181:G:O2'	1:1G:183:G:O6	2.18	0.62
1:1G:589:C:H42	1:1G:650:G:H1	1.48	0.62
26:1H:226:G:H21	26:1H:228:A:H2	1.46	0.62
13:4A:14:ARG:HA	13:4A:43:THR:O	1.99	0.62
1:13:1149:C:H2'	1:13:1150:U:C6	2.34	0.62
1:13:1301:U:O2'	1:13:1302:U:H3'	2.00	0.62
26:1H:1525:G:H2'	26:1H:1526:G:C8	2.35	0.62
26:1H:2400:G:H2'	26:1H:2401:U:H6	1.64	0.62
26:1H:2784:C:O2'	30:21:37:ARG:NH1	2.32	0.62
40:65:89:ARG:HG3	40:65:92:TYR:O	1.99	0.62
26:1H:2178:C:O2'	28:71:168:THR:OG1	2.12	0.62
41:75:55:ASN:N	41:75:59:THR:HG22	2.15	0.62
1:13:624:C:O3'	16:7I:10:GLY:HA2	1.99	0.62
17:8I:45:HIS:HB2	17:8I:65:ILE:HD13	1.81	0.62
1:13:714:G:H2'	1:13:715:A:C8	2.33	0.62
1:1G:673:G:H2'	1:1G:674:G:C8	2.34	0.62
1:13:256:U:H2'	1:13:257:G:C8	2.34	0.62
26:14:1266:G:O5'	44:A5:15:ARG:NH2	2.33	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:14:270:A:OP2	26:14:270(Y):G:N1	2.32	0.62
26:14:305:U:H2'	26:14:306:U:C6	2.35	0.62
26:1H:639:U:H2'	26:1H:640:C:C6	2.35	0.62
3:22:6:HIS:HB2	14:5A:49:HIS:CD2	2.35	0.62
11:2A:100:ALA:O	11:2A:102:GLY:N	2.33	0.62
12:3A:59:ARG:HA	12:3A:65:GLU:H	1.64	0.62
40:65:67:ARG:CZ	40:65:67:ARG:HB2	2.30	0.62
41:B8:54:ARG:HA	41:B8:59:THR:HB	1.82	0.62
2:12:40:HIS:CD2	2:12:190:THR:HG21	2.35	0.62
1:13:1504:G:OP1	1:13:1507:A:H4'	2.00	0.62
26:14:1048:A:N6	26:14:1111:A:O2'	2.33	0.62
26:14:1771:C:O2'	26:14:1786:A:H8	1.81	0.62
26:14:636:G:N7	37:35:113:LYS:NZ	2.40	0.62
1:1G:1157:A:H61	1:1G:1177:G:H1	1.47	0.62
1:1G:114:U:H2'	1:1G:115:G:C8	2.35	0.62
26:1H:270(E):G:H1	26:1H:270(U):C:H42	1.48	0.62
26:1H:336:C:OP1	46:G8:83:THR:HG23	2.00	0.62
30:29:111:ARG:HD2	30:29:160:TYR:CE2	2.34	0.62
24:3L:50:C:H2'	24:3L:51:A:H8	1.65	0.62
24:3L:72:C:H3'	24:3L:73:A:H5''	1.82	0.62
26:1H:2470:G:H5'	38:88:56:ARG:HH12	1.64	0.62
19:AI:51:VAL:O	19:AI:57:HIS:HA	2.00	0.62
51:H5:13:ILE:O	62:H5:101:HOH:O	2.16	0.62
26:1H:1796:U:H2'	26:1H:1797:C:C6	2.34	0.62
4:3E:64:LEU:HD22	4:3E:198:VAL:HG11	1.82	0.62
53:N8:40:LYS:HG2	53:N8:46:CYS:HA	1.82	0.62
26:14:581:C:H2'	26:14:582:G:H8	1.65	0.61
1:1G:842:C:O2'	1:1G:848:C:N3	2.33	0.61
26:1H:2789:C:H1'	26:1H:2892:A:H2	1.65	0.61
23:2K:54:G:H2'	23:2K:55:5MU:H6	1.65	0.61
34:61:69:LYS:HG3	34:61:136:VAL:HB	1.82	0.61
9:82:27:THR:OG1	9:82:31:GLN:O	2.11	0.61
9:8E:112:LYS:HA	9:8E:119:ALA:HB2	1.81	0.61
20:BI:57:ARG:HH11	20:BI:102:GLY:HA2	1.64	0.61
26:14:987:G:O2'	26:14:1000:A:N3	2.29	0.61
26:14:2537:U:H2'	26:14:2538:C:C6	2.34	0.61
10:1A:11:PHE:HE1	10:1A:67:THR:HG22	1.65	0.61
36:25:10:VAL:HG12	36:25:19:ILE:HG12	1.82	0.61
12:3A:41:ARG:HD2	12:3A:42:THR:H	1.65	0.61
15:6I:82:ILE:O	15:6I:86:GLY:N	2.33	0.61
28:71:212:VAL:HG21	28:71:226:PRO:HG3	1.81	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:82:43:ALA:HA	9:82:74:ILE:HD13	1.82	0.61
26:14:1012:U:OP1	42:85:75:ASN:ND2	2.33	0.61
52:M8:36:CYS:SG	52:M8:37:SER:N	2.72	0.61
26:14:2415:G:H4'	37:35:67:MET:N	2.16	0.61
26:14:38:A:H2'	26:14:39:C:C6	2.36	0.61
26:14:491:G:H2'	26:14:492:A:C8	2.35	0.61
26:14:635:C:O2'	26:14:639:U:OP1	2.18	0.61
26:1H:1729:A:O2'	26:1H:1730:U:O5'	2.18	0.61
26:1H:2101:G:H1	26:1H:2188:C:H42	1.47	0.61
22:1K:53:G:H1	22:1K:61:C:H42	1.48	0.61
7:62:23:VAL:HG13	7:62:43:PHE:HE2	1.66	0.61
1:13:1118:C:H1'	1:13:1179:A:C4	2.35	0.61
1:13:77:C:O2'	1:13:92:G:N2	2.34	0.61
26:14:1021:A:H62	26:14:1141:U:H3	1.48	0.61
26:14:2648:C:H2'	26:14:2649:U:C6	2.36	0.61
33:51:64:LEU:O	33:51:68:THR:OG1	2.18	0.61
34:69:143:SER:OG	34:69:144:VAL:N	2.34	0.61
18:9A:32:ARG:HA	18:9A:69:THR:HG21	1.82	0.61
45:B5:65:ARG:HG3	45:B5:67:GLY:H	1.65	0.61
20:BA:46:GLU:HB2	20:BA:48:LYS:HG2	1.82	0.61
37:35:50:ARG:HD3	56:M5:7:HIS:CD2	2.36	0.61
1:13:153:C:N4	1:13:168:G:H1	1.98	0.61
1:13:595:G:H1	1:13:641:U:HO2'	1.48	0.61
1:13:618:C:H5''	1:13:619:U:H5''	1.83	0.61
1:13:953:G:H5'	1:13:965:A:H61	1.66	0.61
1:1G:920:U:H2'	1:1G:921:U:C6	2.36	0.61
26:1H:2706:G:O6	62:1H:3761:HOH:O	2.12	0.61
4:32:60:GLU:OE2	4:32:199:ASN:N	2.31	0.61
12:3I:53:ARG:HG3	12:3I:53:ARG:HH11	1.66	0.61
1:1G:564:C:HO2'	8:72:91:ARG:HH22	1.47	0.61
38:88:78:PRO:O	38:88:79:LEU:HB3	2.00	0.61
40:A8:34:HIS:CE1	40:A8:54:LEU:HD23	2.35	0.61
1:1G:1460:A:OP2	20:BA:27:LYS:NZ	2.32	0.61
1:13:163:C:O2'	1:13:164:U:O4'	2.19	0.61
1:13:837:G:OP2	1:13:842:C:N4	2.34	0.61
26:14:2611:U:C4	53:J5:3:LYS:HG3	2.36	0.61
26:14:273(F):C:H3'	26:14:274:G:H5''	1.83	0.61
26:14:2788:C:O2'	26:14:2809:A:N3	2.34	0.61
26:14:34:C:O2'	26:14:35:G:O5'	2.14	0.61
26:1H:587:C:OP2	37:78:21:ARG:NH2	2.34	0.61
3:22:50:ALA:HB2	3:22:75:VAL:HB	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:85:92:ARG:NH2	43:95:11:GLN:H	1.98	0.61
46:C5:88:LYS:O	46:C5:89:PHE:HB3	1.98	0.61
50:K8:4:SER:N	50:K8:7:ARG:H	1.98	0.61
26:14:2294:C:P	40:65:89:ARG:HH22	2.24	0.61
35:15:132:ALA:HB1	35:15:133:GLN:HG2	1.83	0.61
29:19:242:ARG:HG2	29:19:246:PRO:HG3	1.82	0.61
2:1E:18:GLY:H	2:1E:42:ILE:HB	1.66	0.61
26:1H:1405:U:H2'	26:1H:1406:U:C6	2.35	0.61
26:1H:2138:C:N3	26:1H:2154:G:N2	2.49	0.61
26:1H:2275:C:H5'	26:1H:2275:C:C6	2.36	0.61
26:1H:71:A:H8	26:1H:71:A:H5'	1.65	0.61
24:3L:5:C:H2'	24:3L:6:G:C8	2.36	0.61
32:49:6:ALA:O	32:49:9:ARG:N	2.34	0.61
35:58:73:THR:HB	35:58:82:LEU:HD11	1.82	0.61
33:59:92:ILE:HG22	33:59:93:GLY:N	2.16	0.61
41:75:26:ASP:O	41:75:49:VAL:HG22	2.00	0.61
2:12:71:VAL:HG11	2:12:164:VAL:HG13	1.82	0.61
26:1H:1449:A:H5'	26:1H:1449(A):G:OP2	2.00	0.61
26:1H:71:A:H5'	26:1H:71:A:C8	2.36	0.61
26:14:872:A:H4'	38:45:66:ILE:HD11	1.83	0.61
41:75:2:ASN:C	41:75:4:GLY:HA3	2.21	0.61
20:BI:49:ALA:HB3	20:BI:99:LEU:HD22	1.81	0.61
49:J8:18:ILE:HG12	49:J8:37:ILE:HG12	1.82	0.61
50:K8:58:ALA:O	50:K8:62:THR:HG22	2.00	0.61
2:12:24:TRP:HE1	2:12:26:PRO:HG3	1.66	0.61
2:12:56:ARG:O	2:12:56:ARG:NH1	2.33	0.61
26:14:1778:U:H2'	26:14:1784:A:N6	2.16	0.61
26:14:1786:A:H2	26:14:2606:C:H1'	1.65	0.61
26:14:2363:C:O2	48:E5:39:ARG:NH2	2.32	0.61
1:1G:1129:C:H5''	1:1G:1139:G:N7	2.16	0.61
1:1G:1273:G:H3'	1:1G:1274:G:H8	1.66	0.61
1:1G:474:G:H2'	1:1G:475:G:C8	2.35	0.61
22:1K:76:A:H8	26:1H:2583:G:H21	1.46	0.61
26:1H:2698:U:H2'	26:1H:2699:C:C6	2.36	0.61
3:22:14:ILE:HG23	3:22:15:THR:HG23	1.81	0.61
30:29:68:ALA:C	30:29:70:ALA:H	2.04	0.61
5:4E:36:ASP:OD2	5:4E:38:GLN:HB2	2.01	0.61
28:71:39:GLU:HG3	28:71:178:ALA:HB2	1.82	0.61
50:K8:2:LYS:HD3	50:K8:6:VAL:HG23	1.83	0.61
52:M8:37:SER:HB3	52:M8:42:PHE:CE2	2.35	0.61
1:13:407:G:OP1	4:3E:115:ARG:NH2	2.34	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:14:1341:U:OP2	26:14:1394:U:O2'	2.16	0.61
26:14:2232:U:P	49:F5:40:ARG:HH22	2.24	0.61
26:14:2273:A:H2'	26:14:2274:A:C8	2.36	0.61
1:1G:1007:C:H1'	1:1G:1023:G:N1	2.16	0.61
26:1H:322:A:P	31:31:168:ARG:HH21	2.24	0.61
26:1H:507:A:H5''	26:1H:508:G:H3'	1.83	0.61
41:75:7:ILE:HG13	41:75:8:LYS:N	2.15	0.61
53:J5:41:PRO:O	53:J5:44:THR:OG1	2.19	0.61
2:12:91:PRO:HG3	2:12:154:LEU:HB2	1.83	0.60
26:14:1149:G:H2'	26:14:1150:C:C6	2.36	0.60
24:3L:71:C:O2'	26:14:1851:U:O2'	2.03	0.60
1:1G:1124:G:HO2'	1:1G:1145:C:N4	1.99	0.60
1:1G:1321:C:N4	1:1G:1322:C:H41	1.99	0.60
26:1H:1639:U:O2'	26:1H:1640:C:H5''	2.01	0.60
26:1H:252:G:OP2	37:78:50:ARG:NH1	2.34	0.60
36:25:49:ARG:HA	36:25:53:LYS:NZ	2.15	0.60
25:4L:14:A:O2'	25:4L:15:A:O5'	2.19	0.60
8:7E:36:LEU:HA	8:7E:39:LEU:HB2	1.83	0.60
20:BA:86:ARG:NH1	20:BA:86:ARG:HB2	2.16	0.60
48:E5:38:VAL:HG13	48:E5:59:LEU:HB2	1.82	0.60
44:E8:38:TYR:OH	53:N8:47:PRO:HG2	2.01	0.60
46:G8:42:VAL:HG23	46:G8:43:ASN:H	1.66	0.60
29:11:2:ALA:HA	29:11:20:ASP:HB2	1.83	0.60
1:13:677:U:H3	1:13:713:G:H22	1.50	0.60
29:19:182:LEU:N	29:19:272:ALA:HB3	2.14	0.60
26:1H:863:A:H2'	26:1H:864:G:C8	2.36	0.60
30:29:60:ASN:ND2	30:29:62:PRO:O	2.34	0.60
23:2L:62:C:H2'	23:2L:63:C:H6	1.66	0.60
1:13:438:G:H4'	4:3E:123:HIS:CD2	2.35	0.60
40:65:106:ARG:HA	40:65:110:LEU:HD11	1.82	0.60
8:7E:87:SER:HB2	8:7E:93:VAL:CB	2.27	0.60
26:14:2016:U:O2	53:J5:7:PRO:HG2	2.01	0.60
26:1H:2591:C:P	29:11:239:ARG:HG3	2.41	0.60
1:13:443:C:H42	1:13:491:G:H1	1.46	0.60
26:14:524:U:H2'	26:14:525:U:C6	2.36	0.60
29:19:264:LYS:HE2	29:19:266:SER:HB3	1.82	0.60
1:1G:1392:G:H21	1:1G:1502:A:H8	1.49	0.60
26:1H:511:U:OP2	62:1H:3770:HOH:O	2.16	0.60
37:35:59:LEU:O	37:35:59:LEU:HD22	2.01	0.60
31:39:24:LEU:HD22	31:39:25:PRO:HD3	1.83	0.60
24:3K:14:A:H2'	24:3K:15:G:C8	2.36	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:F5:90:ILE:HA	49:F5:93:GLU:OE1	2.02	0.60
1:13:1347:G:H5''	9:8E:107:ARG:HB3	1.83	0.60
26:14:498:G:H21	46:C5:47:LYS:HZ2	1.49	0.60
26:14:528:A:C2	26:14:2043:C:H4'	2.37	0.60
2:1E:5:ILE:HB	2:1E:221:LEU:HD23	1.83	0.60
1:1G:41:G:H2'	1:1G:42:G:C8	2.36	0.60
26:1H:1026:U:H4'	26:1H:1027:A:OP1	2.00	0.60
26:1H:1991:U:H2'	26:1H:1992:G:H5''	1.83	0.60
26:1H:2062:A:OP1	62:1H:3771:HOH:O	2.16	0.60
26:1H:451:C:H5'	62:1H:3709:HOH:O	1.94	0.60
30:29:64:LYS:N	30:29:73:GLU:OE2	2.34	0.60
4:32:31:CYS:HB2	4:32:33:MET:O	2.01	0.60
26:14:2467:C:H4'	38:45:123:HIS:CD2	2.35	0.60
7:62:22:LEU:HD23	7:62:62:PHE:HE2	1.66	0.60
20:BI:30:LYS:HE3	20:BI:80:ARG:HH22	1.65	0.60
46:C5:17:SER:HB2	46:C5:71:LYS:HE2	1.83	0.60
1:13:1366:C:H2'	1:13:1367:C:H6	1.66	0.60
26:14:2128:C:H42	26:14:2160:G:H1	1.50	0.60
2:1E:21:ARG:O	2:1E:23:ARG:N	2.33	0.60
1:1G:1021:G:H2'	1:1G:1022:G:C8	2.36	0.60
26:1H:2321:G:H5''	62:1H:3776:HOH:O	2.01	0.60
26:1H:443:A:H1'	26:1H:1201:C:O4'	2.01	0.60
1:13:1367:C:H5'	10:1I:60:ARG:NH1	2.15	0.60
4:3E:31:CYS:SG	4:3E:33:MET:HB2	2.42	0.60
41:B8:58:ASN:C	41:B8:58:ASN:HD22	2.03	0.60
41:B8:26:ASP:CB	41:B8:92:GLY:H	2.14	0.60
26:14:517:C:OP1	53:J5:16:ARG:NH2	2.34	0.60
29:11:37:LEU:HD23	29:11:62:TYR:HB2	1.84	0.60
1:13:1073:U:OP2	5:4E:57:LYS:NZ	2.35	0.60
1:13:1145:C:H4'	1:13:1146:A:H5'	1.83	0.60
26:14:2378:A:H4'	40:65:23:ARG:HH11	1.66	0.60
26:14:38:A:H1'	31:39:48:THR:HB	1.83	0.60
27:16:15:A:H5'	27:16:16:G:C8	2.37	0.60
37:35:85:LEU:HA	37:35:88:LEU:HB2	1.84	0.60
13:4I:58:GLU:O	13:4I:62:ASN:ND2	2.31	0.60
6:52:83:ASP:N	6:52:83:ASP:OD1	2.34	0.60
39:55:38:VAL:HG12	39:55:42:LYS:HD2	1.83	0.60
24:3K:62:C:H2'	28:71:53:ARG:HH21	1.65	0.60
19:AA:10:PHE:H	19:AA:11:VAL:HB	1.65	0.60
26:14:125:G:H5''	55:L5:19:ARG:HD3	1.82	0.60
26:14:1817:G:OP1	29:19:88:ARG:NH2	2.33	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:14:2118:U:O2	26:14:2147:G:N2	2.34	0.60
26:14:2734:A:H2'	26:14:2735:G:O4'	2.01	0.60
26:14:796:C:H2'	26:14:797:C:C6	2.36	0.60
26:1H:910:A:N7	38:88:13:GLN:HG3	2.17	0.60
33:51:153:LYS:CB	33:51:155:SER:H	2.14	0.60
33:59:6:ARG:HB3	33:59:66:GLY:HA2	1.84	0.60
6:5E:80:ARG:NH1	6:5E:88:VAL:O	2.34	0.60
37:78:19:VAL:HG13	37:78:31:ALA:HB1	1.82	0.60
38:88:77:LYS:HE3	38:88:84:GLY:O	2.01	0.60
26:14:582:G:H2'	26:14:583:G:C8	2.37	0.60
26:1H:2315:G:OP1	32:41:36:LYS:NZ	2.33	0.60
26:1H:870:A:OP1	38:88:5:ARG:NH2	2.34	0.60
3:22:70:VAL:HG21	3:22:76:VAL:HG11	1.84	0.60
11:2I:53:SER:HA	11:2I:54:ARG:C	2.22	0.60
31:39:66:PRO:O	31:39:67:GLN:HB3	2.01	0.60
38:45:77:LYS:HE3	38:45:84:GLY:H	1.65	0.60
7:6E:15:ASP:HB3	7:6E:20:ASP:H	1.65	0.60
41:B8:77:PRO:HG2	41:B8:80:SER:HB2	1.83	0.60
35:58:38:HIS:O	42:C8:67:ALA:HB1	2.02	0.60
37:35:50:ARG:HG2	56:M5:61:LEU:HD21	1.83	0.60
29:11:70:TRP:O	29:11:73:VAL:HG23	2.02	0.60
2:12:118:LEU:HD11	2:12:141:GLU:HG2	1.82	0.60
1:13:1226:C:H2'	13:4I:103:THR:HB	1.84	0.60
26:14:1430:C:H2'	26:14:1431:U:H6	1.66	0.60
26:1H:1420:U:O2'	26:1H:1421:G:OP1	2.16	0.60
4:32:127:THR:HG21	4:32:149:ALA:HB2	1.83	0.60
5:42:105:VAL:HG21	5:42:128:PRO:HB3	1.84	0.60
32:49:124:SER:HB2	32:49:131:TYR:CE1	2.36	0.60
34:69:57:ARG:O	34:69:61:ARG:HB2	2.01	0.60
41:B8:64:ARG:HB2	41:B8:73:GLU:HG2	1.84	0.60
45:F8:5:TYR:CE1	50:K8:30:ARG:HG3	2.36	0.60
50:G5:4:SER:HA	50:G5:7:ARG:H	1.67	0.60
49:J8:64:ALA:HA	49:J8:67:ILE:HG13	1.83	0.60
50:K8:4:SER:OG	50:K8:4:SER:O	2.15	0.60
1:13:1129:C:H42	1:13:1143:G:H1	1.49	0.60
26:14:1593:G:H2'	26:14:1594:G:C8	2.37	0.60
26:14:2409:G:N7	62:14:3692:HOH:O	2.31	0.60
26:14:270(X):G:OP2	62:14:3641:HOH:O	2.16	0.60
26:1H:796:C:H2'	26:1H:797:C:C6	2.37	0.60
3:22:180:ALA:HB1	3:22:203:PHE:HE1	1.66	0.60
26:1H:674:G:C1'	31:31:74:ARG:HD3	2.29	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:39:129:PHE:HA	31:39:142:TRP:NE1	2.16	0.60
24:3K:57:G:N2	24:3K:60:U:O4	2.35	0.60
1:13:310:G:OP2	16:7I:27:LYS:NZ	2.33	0.60
41:B8:90:GLN:OE1	41:B8:91:ARG:N	2.32	0.60
20:BA:12:ALA:O	20:BA:15:ARG:N	2.34	0.60
26:14:2577:A:H5'	53:J5:3:LYS:HD3	1.84	0.60
26:1H:1570:A:H2'	26:1H:1571:A:C8	2.36	0.59
10:1I:16:LEU:HD11	10:1I:70:ARG:HB2	1.84	0.59
13:4A:12:ASN:O	13:4A:12:ASN:ND2	2.31	0.59
33:51:107:VAL:HB	33:51:152:ARG:HG2	1.84	0.59
33:59:152:ARG:HG3	33:59:153:LYS:HB2	1.84	0.59
14:5A:26:ARG:HH12	14:5A:47:LEU:HD21	1.65	0.59
9:8E:28:VAL:HA	9:8E:63:ILE:O	2.02	0.59
49:F5:4:VAL:HG12	49:F5:11:ARG:HB3	1.83	0.59
51:L8:9:VAL:HG12	51:L8:53:LEU:O	2.02	0.59
1:13:1129:C:H1'	1:13:1146:A:H61	1.67	0.59
1:1G:1423:G:OP1	36:25:49:ARG:NH2	2.34	0.59
1:1G:979:C:H3'	1:1G:980:C:H5''	1.84	0.59
26:1H:2432:A:C4	49:J8:33:LYS:HG2	2.38	0.59
31:39:116:ASP:OD2	37:35:1:MET:N	2.35	0.59
9:8E:114:TYR:HE2	10:1I:59:SER:HA	1.67	0.59
47:D5:80:ARG:HH11	47:D5:82:ARG:HH21	1.50	0.59
29:11:24:ILE:HG23	29:11:83:GLU:HA	1.84	0.59
26:14:2693:A:H2'	26:14:2694:G:H8	1.67	0.59
26:14:2713:A:OP2	62:14:3636:HOH:O	2.16	0.59
26:14:2745:C:H1'	33:59:143:GLN:HG2	1.83	0.59
29:19:31:LYS:NZ	29:19:33:LEU:HB3	2.17	0.59
26:1H:1332:G:H21	26:1H:1610:A:H8	1.48	0.59
26:1H:243:U:OP1	56:Q8:6:THR:OG1	2.20	0.59
26:1H:270(F):U:H2'	26:1H:270(G):C:C6	2.37	0.59
9:8E:7:THR:O	9:8E:83:ARG:NH1	2.35	0.59
26:14:495:G:N3	44:A5:61:ASN:ND2	2.51	0.59
47:D5:139:VAL:HA	47:D5:156:LYS:HE3	1.84	0.59
26:14:850:C:O3'	51:H5:49:LYS:HE2	2.00	0.59
50:K8:23:LYS:NZ	50:K8:27:GLU:OE2	2.35	0.59
52:M8:13:ARG:HA	52:M8:24:THR:HG21	1.85	0.59
1:13:868:C:H2'	1:13:869:G:O4'	2.03	0.59
26:14:1927:A:H2'	26:14:1928:A:C8	2.37	0.59
29:19:39:LYS:CG	29:19:40:THR:H	2.11	0.59
2:1E:185:ILE:HB	2:1E:199:TYR:HB2	1.85	0.59
1:1G:164:U:H2'	1:1G:165:C:C6	2.38	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1H:1932:A:H2'	26:1H:1933:G:O4'	2.02	0.59
26:1H:577:G:OP2	62:1H:3772:HOH:O	2.17	0.59
30:29:119:ARG:HG2	30:29:160:TYR:HB2	1.84	0.59
3:2E:91:LEU:HB2	3:2E:99:VAL:HG21	1.85	0.59
11:2I:85:ARG:HG2	11:2I:112:THR:H	1.68	0.59
23:2L:41:C:H2'	23:2L:42:C:H6	1.66	0.59
38:45:133:ARG:O	38:45:134:ARG:HG3	2.03	0.59
38:45:35:VAL:HG12	38:45:36:ALA:H	1.67	0.59
15:6I:25:THR:HG21	15:6I:70:LEU:HB2	1.84	0.59
9:8E:47:LEU:HB2	9:8E:50:LEU:HD11	1.83	0.59
44:E8:92:ARG:NH1	44:E8:94:ASP:OD1	2.36	0.59
46:G8:42:VAL:HG23	46:G8:43:ASN:N	2.18	0.59
48:I8:72:ARG:HB3	48:I8:75:LEU:HB2	1.84	0.59
26:14:2577:A:O4'	53:J5:3:LYS:HB2	2.01	0.59
50:K8:3:LEU:H	50:K8:5:GLU:N	2.00	0.59
2:12:114:ARG:NH1	2:12:117:GLU:OE1	2.36	0.59
29:19:37:LEU:H	29:19:37:LEU:CD1	2.06	0.59
2:1E:212:GLN:NE2	2:1E:233:SER:O	2.36	0.59
1:1G:1160:G:H1	1:1G:1176:A:H61	1.49	0.59
26:1H:86:C:H4'	26:1H:104:U:H1'	1.82	0.59
26:1H:2801:A:H5'	26:1H:2895:U:H1'	1.84	0.59
27:1J:89(A):A:H5'	27:1J:90:C:OP2	2.03	0.59
4:3E:84:LYS:HB3	4:3E:86:LYS:HG3	1.84	0.59
7:6E:69:VAL:HG12	7:6E:100:ALA:HA	1.85	0.59
28:71:64:LEU:HD21	28:71:188:ASN:ND2	2.18	0.59
41:75:2:ASN:HB3	41:75:4:GLY:O	2.03	0.59
41:B8:24:PRO:HA	41:B8:49:VAL:HG22	1.83	0.59
1:13:1126:U:H2'	1:13:1127:G:H5'	1.84	0.59
26:14:2062:A:O2'	26:14:2063:C:OP1	2.19	0.59
26:14:570:G:H5''	62:14:4024:HOH:O	2.01	0.59
29:19:37:LEU:N	29:19:37:LEU:HD12	2.18	0.59
1:1G:191(F):U:H3	20:BA:105:SER:HG	1.48	0.59
1:1G:371:G:H1	1:1G:390:C:H42	1.50	0.59
26:1H:860:U:H5	26:1H:917:A:N1	2.00	0.59
10:1I:40:LEU:HB2	10:1I:69:ASN:HB2	1.83	0.59
27:1J:15:A:H3'	27:1J:16:G:H5'	1.83	0.59
30:21:116:VAL:HG11	30:21:138:PRO:HB3	1.84	0.59
3:22:182:ILE:HG23	3:22:203:PHE:HD1	1.66	0.59
31:31:197:ASP:N	31:31:197:ASP:OD1	2.33	0.59
33:51:59:ARG:O	33:51:63:SER:OG	2.20	0.59
6:52:35:ALA:HB1	6:52:65:VAL:HG11	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:59:32:GLU:H	33:59:32:GLU:CD	2.06	0.59
26:1H:2176:A:H5'	28:71:221:SER:HB3	1.83	0.59
38:88:78:PRO:HB2	38:88:81:VAL:HG11	1.83	0.59
9:8E:28:VAL:HG22	9:8E:63:ILE:HB	1.83	0.59
20:BI:73:HIS:HB3	20:BI:74:LYS:HG2	1.85	0.59
47:H8:111:VAL:HG11	47:H8:146:ILE:HG13	1.85	0.59
54:O8:43:CYS:HB3	54:O8:44:ARG:NH1	2.17	0.59
26:14:782:A:H5'	26:14:783:A:C2	2.38	0.59
35:15:130:HIS:HB3	35:15:134:ARG:HH21	1.67	0.59
1:1G:79:G:N2	1:1G:90:C:N3	2.46	0.59
26:1H:49:A:N7	26:1H:120:U:C5	2.66	0.59
8:7E:73:ASP:OD1	8:7E:75:ARG:NE	2.36	0.59
45:B5:32:PRO:HA	45:B5:77:LYS:HB2	1.85	0.59
54:O8:27:LYS:HZ2	54:O8:27:LYS:H	1.50	0.59
1:13:1347:G:C8	9:8E:107:ARG:HB2	2.38	0.59
26:14:1449(A):G:H2'	26:14:1450:C:H6	1.67	0.59
26:14:1568:G:P	29:19:63:ARG:HH12	2.26	0.59
26:1H:827:U:H2'	26:1H:2430:A:C2	2.38	0.59
10:1I:86:MET:SD	10:1I:86:MET:N	2.76	0.59
12:3I:93:LEU:O	12:3I:96:VAL:HG13	2.02	0.59
13:4A:54:VAL:HA	13:4A:57:ARG:HB3	1.83	0.59
6:5E:100:ASN:HB2	18:9I:28:GLU:HA	1.85	0.59
37:78:36:LYS:O	37:78:40:SER:HB3	2.03	0.59
26:1H:2208:U:H4'	29:11:151:LYS:HG2	1.83	0.59
26:14:1019:U:H3	26:14:1142(A):A:H62	1.50	0.59
1:1G:490:G:P	4:32:132:ARG:HH22	2.25	0.59
1:1G:973:G:H5'	10:1A:55:LYS:HZ2	1.68	0.59
26:1H:1230:C:H2'	26:1H:1231:G:C8	2.38	0.59
26:1H:1762:A:N1	62:1H:3823:HOH:O	2.32	0.59
26:1H:1678:G:N2	26:1H:1989:G:H22	1.97	0.59
26:1H:736:C:H42	26:1H:760:G:H1	1.51	0.59
26:1H:994:C:H3'	42:C8:54:LYS:HE3	1.85	0.59
13:4I:12:ASN:OD1	13:4I:46:LYS:NZ	2.30	0.59
8:7E:7:ALA:HB2	8:7E:85:ARG:HH11	1.68	0.59
46:G8:38:ILE:HD11	46:G8:64:GLU:HG3	1.83	0.59
2:12:33:TYR:HB3	2:12:41:ILE:HG23	1.85	0.59
26:14:1198:U:H2'	26:14:1199:U:H6	1.66	0.59
2:1E:231:GLU:OE1	2:1E:231:GLU:N	2.31	0.59
1:1G:1157:A:H2	1:1G:1180:A:C6	2.21	0.59
1:1G:1469:G:H2'	1:1G:1470:G:C8	2.37	0.59
26:1H:1111:A:N3	26:1H:1112:G:H1'	2.18	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1H:1858:G:O2'	26:1H:1859:A:OP2	2.21	0.59
31:39:3:GLU:HA	31:39:24:LEU:HD12	1.85	0.59
34:61:110:ASP:OD2	34:61:113:ARG:HD3	2.03	0.59
34:69:110:ASP:N	34:69:130:TYR:OH	2.26	0.59
15:6I:16:ALA:HB1	15:6I:21:ASP:HB3	1.85	0.59
9:82:36:TYR:OH	9:82:73:GLN:NE2	2.33	0.59
51:H5:39:ASP:O	51:H5:44:ARG:NH1	2.36	0.59
26:1H:593:G:H1'	56:Q8:4:MET:HE1	1.84	0.59
1:13:1435:G:H2'	1:13:1436:U:C6	2.38	0.58
1:13:735:C:H2'	1:13:736:C:C6	2.37	0.58
26:14:1028:A:N6	26:14:1125:G:H2'	2.18	0.58
3:2E:58:GLU:H	3:2E:65:ALA:HB3	1.69	0.58
56:Q8:52:LYS:H	56:Q8:53:PRO:HD2	1.68	0.58
26:14:2819:G:N7	62:14:3699:HOH:O	2.32	0.58
26:14:548:A:C6	26:14:549:G:H1'	2.39	0.58
26:14:824:A:H1'	26:14:2358:G:N7	2.18	0.58
26:1H:2306:C:H3'	26:1H:2307:G:C5'	2.33	0.58
26:1H:85:G:OP2	46:G8:9:LYS:HB2	2.03	0.58
30:21:152:LYS:HD3	35:58:77:GLY:HA3	1.85	0.58
40:65:62:LYS:O	40:65:66:ALA:N	2.35	0.58
1:1G:581:G:OP1	15:6A:61:GLY:HA3	2.03	0.58
26:14:71:A:H2	45:B5:31:HIS:NE2	1.99	0.58
1:13:1259:C:N4	1:13:1260:C:O2	2.36	0.58
1:13:1292:U:H2'	1:13:1293:G:C8	2.37	0.58
26:14:375:C:H2'	26:14:376:C:C6	2.37	0.58
1:1G:1018:C:H2'	1:1G:1019:C:O4'	2.04	0.58
1:1G:838:G:H1	1:1G:848:C:H42	1.52	0.58
26:1H:614:U:H6	26:1H:614:U:OP2	1.86	0.58
4:32:31:CYS:H	4:32:35:ARG:CZ	2.16	0.58
24:3K:57:G:H2'	24:3K:58:A:H5'	1.85	0.58
24:3K:5:C:H2'	24:3K:6:G:H8	1.68	0.58
5:42:69:VAL:O	5:42:71:LEU:N	2.35	0.58
32:49:118:ARG:HB3	32:49:181:ARG:HD3	1.85	0.58
13:4I:60:VAL:HG13	13:4I:64:TRP:HE1	1.67	0.58
39:98:55:ALA:HB1	39:98:84:ALA:HB2	1.86	0.58
43:D8:65:GLY:HA3	43:D8:91:TYR:CE1	2.38	0.58
50:K8:28:LYS:HB3	50:K8:53:LEU:HD21	1.84	0.58
1:13:1000:A:H2'	1:13:1001:G:C8	2.38	0.58
26:14:1420:U:O2'	26:14:1421:G:OP1	2.20	0.58
36:25:24:VAL:HB	36:25:33:ALA:HB2	1.85	0.58
30:29:12:THR:HG22	41:75:58:ASN:OD1	2.02	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:2I:59:TYR:CE2	11:2I:63:LEU:HD11	2.39	0.58
31:31:101:LEU:O	31:31:106:ARG:NH1	2.37	0.58
1:1G:426:G:OP1	4:32:36:ARG:NH2	2.35	0.58
31:39:170:LEU:HD22	31:39:172:TRP:HE1	1.68	0.58
33:59:10:PRO:HD2	33:59:50:VAL:HG13	1.85	0.58
14:5A:45:ARG:O	14:5A:49:HIS:ND1	2.33	0.58
7:62:26:PHE:O	7:62:30:ILE:HG13	2.03	0.58
26:1H:2129:C:OP2	28:71:36:LYS:NZ	2.36	0.58
48:E5:47:PRO:HG3	48:E5:53:MET:HB2	1.84	0.58
1:13:652:U:O2'	1:13:653:A:O5'	2.21	0.58
26:1H:1278:A:OP1	39:98:36:THR:HG22	2.04	0.58
26:1H:2776:A:H4'	26:1H:2777:G:H5''	1.85	0.58
26:1H:671:C:OP1	37:78:42:SER:O	2.20	0.58
36:25:4:PRO:O	36:25:5:GLN:HB2	2.03	0.58
4:3E:173:TRP:CD1	4:3E:174:LEU:HG	2.38	0.58
40:65:107:GLU:H	40:65:110:LEU:HD11	1.69	0.58
37:78:46:LYS:O	37:78:47:ASP:HB3	2.03	0.58
16:7I:71:ARG:O	16:7I:75:ARG:N	2.35	0.58
1:13:1117:G:H5''	9:8E:104:ARG:NH1	2.18	0.58
39:98:72:ASP:O	39:98:76:VAL:HG23	2.04	0.58
2:12:121:LEU:HG	2:12:126:GLU:HG2	1.85	0.58
1:13:7:G:H5'	1:13:298:A:O4'	2.03	0.58
26:14:2287:A:H62	26:14:2344:U:H3	1.48	0.58
26:14:2779:U:OP1	62:14:3640:HOH:O	2.16	0.58
26:14:67:U:N3	26:14:74:A:H2	1.95	0.58
26:14:821:A:O2'	26:14:946:G:OP2	2.21	0.58
26:1H:1512:G:H2'	26:1H:1513:C:C6	2.39	0.58
26:1H:1605:C:O3'	62:1H:3773:HOH:O	2.17	0.58
36:25:13:ASN:HD21	36:25:97:ARG:H	1.51	0.58
31:31:116:ASP:O	31:31:120:GLU:HG3	2.04	0.58
36:68:68:GLU:OE2	36:68:78:ARG:NH1	2.36	0.58
9:82:119:ALA:O	9:82:120:ARG:HB2	2.03	0.58
39:98:27:SER:HB3	39:98:34:ILE:HD11	1.84	0.58
20:BA:49:ALA:HA	20:BA:52:ALA:HB3	1.86	0.58
2:12:73:THR:HG21	2:12:97:TRP:H	1.68	0.58
1:13:1510:U:H2'	1:13:1511:G:C8	2.39	0.58
1:13:667:G:H4'	15:6I:51:HIS:ND1	2.19	0.58
1:13:685:G:O2'	1:13:686:U:H5'	2.04	0.58
1:13:93:U:H5'	1:13:95:G:OP2	2.04	0.58
26:14:1292:U:H2'	26:14:1293:C:C6	2.38	0.58
26:14:1794:U:H2'	26:14:1795:C:C6	2.38	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:14:2572:A:OP1	26:14:2574:G:O2'	2.22	0.58
26:14:2648:C:H2'	26:14:2649:U:H6	1.66	0.58
26:14:2749:A:N1	26:14:2750:A:N6	2.52	0.58
26:14:2830:G:O6	62:14:3642:HOH:O	2.16	0.58
29:19:17:THR:O	29:19:211:ARG:NH2	2.37	0.58
1:1G:1305:G:O2'	1:1G:1306:A:H8	1.87	0.58
30:21:131:ALA:HB1	62:21:403:HOH:O	2.03	0.58
30:29:53:PRO:HA	30:29:74:PRO:HB3	1.86	0.58
31:39:85:GLY:O	62:39:401:HOH:O	2.17	0.58
32:41:16:ARG:O	32:41:20:ILE:HG13	2.03	0.58
33:51:20:ALA:HB3	33:51:23:ARG:HG3	1.86	0.58
35:58:130:HIS:C	35:58:134:ARG:HH12	2.07	0.58
44:A5:71:VAL:HA	44:A5:107:LEU:HD12	1.86	0.58
41:B8:108:ARG:HA	41:B8:111:ARG:NE	2.19	0.58
20:BI:26:ASN:O	20:BI:30:LYS:HB2	2.03	0.58
1:13:1226:C:OP2	13:4I:103:THR:OG1	2.15	0.58
1:13:376:G:H1	1:13:387:U:H3	1.50	0.58
26:14:2391:G:O6	26:14:2425:A:H8	1.87	0.58
2:1E:73:THR:HG22	2:1E:74:LYS:HG2	1.86	0.58
1:1G:247:G:OP2	17:8A:100:LYS:HA	2.04	0.58
1:1G:727:G:N2	1:1G:730:G:OP2	2.29	0.58
26:1H:1331:A:O2'	26:1H:1332:G:H8	1.87	0.58
26:1H:2211:G:O2'	26:1H:2212:A:OP1	2.20	0.58
26:1H:330:A:HO2'	26:1H:331:A:H8	1.52	0.58
26:1H:960:A:H2'	26:1H:962:G:H5'	1.86	0.58
3:22:121:ALA:HB1	3:22:189:ALA:HB2	1.85	0.58
31:31:51:THR:O	31:31:93:LYS:HE2	2.04	0.58
47:D5:132:ASN:HD22	47:D5:159:PRO:HG2	1.68	0.58
26:14:607:U:OP1	31:39:102:PRO:HA	2.04	0.58
1:1G:19:C:OP1	5:42:125:SER:OG	2.18	0.58
1:1G:572:A:H5'	1:1G:573:A:OP2	2.03	0.58
1:1G:972:C:O3'	10:1A:55:LYS:NZ	2.37	0.58
26:1H:2145:C:H5	26:1H:2148:G:H21	1.50	0.58
26:1H:2401:U:H2'	26:1H:2402:C:O4'	2.04	0.58
1:13:963:G:N3	10:1I:55:LYS:NZ	2.52	0.58
31:39:92:PRO:O	31:39:93:LYS:HD2	2.02	0.58
26:1H:2751:G:N7	33:51:3:ARG:NH2	2.52	0.58
33:59:35:VAL:HG11	33:59:72:ILE:HG12	1.84	0.58
28:71:45:ALA:HB2	28:71:212:VAL:HG22	1.86	0.58
49:F5:88:LYS:O	49:F5:91:LYS:HB3	2.04	0.58
46:G8:89:PHE:HD1	46:G8:90:LEU:N	2.02	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:G8:76:CYS:SG	46:G8:97:ARG:HG3	2.43	0.58
2:12:165:VAL:HG23	2:12:166:ASP:H	1.68	0.58
1:13:964:A:N3	1:13:969:A:O2'	2.33	0.58
26:14:2776:A:OP1	26:14:2776:A:H3'	2.04	0.58
1:1G:1:U:H1'	1:1G:2:U:H5'	1.86	0.58
26:1H:1113:U:H5'	33:51:2:SER:OG	2.03	0.58
26:1H:1264:G:H5'	53:N8:11:THR:HG21	1.86	0.58
26:1H:2327:A:H2'	26:1H:2328:A:C8	2.39	0.58
24:1L:8:U:H3'	24:1L:13:C:H42	1.69	0.58
23:2L:48:U:O2'	23:2L:49:C:OP2	2.21	0.58
31:31:160:ASN:OD1	31:31:163:VAL:HG23	2.04	0.58
31:31:66:PRO:HD2	31:31:70:THR:HG21	1.86	0.58
4:32:13:ARG:C	4:32:15:GLU:H	2.07	0.58
32:41:17:PRO:HA	32:41:20:ILE:HD12	1.85	0.58
32:49:106:LEU:O	32:49:111:LEU:HD12	2.04	0.58
25:4L:20:A:H2'	25:4L:21:A:O4'	2.04	0.58
6:52:70:ASP:OD1	6:52:70:ASP:N	2.34	0.58
51:H5:46:ASN:O	51:H5:50:VAL:HG22	2.04	0.58
56:M5:54:GLU:O	56:M5:58:ILE:HG23	2.04	0.58
2:12:78:GLN:O	2:12:94:ASN:ND2	2.36	0.57
1:13:1239:A:H62	1:13:1299:A:H62	1.51	0.57
26:1H:827:U:H2'	26:1H:2430:A:H2	1.69	0.57
26:1H:994:C:OP1	42:C8:53:ARG:NH2	2.37	0.57
31:39:164:ARG:O	31:39:167:ALA:HB3	2.03	0.57
13:4A:34:LEU:HD13	13:4A:41:PRO:HB3	1.86	0.57
38:88:58:PHE:O	38:88:60:ARG:N	2.36	0.57
20:BI:57:ARG:HH22	20:BI:100:ILE:HD13	1.68	0.57
49:J8:73:LEU:HD13	49:J8:93:GLU:HB3	1.86	0.57
26:14:2528:U:O2'	26:14:2530:A:OP1	2.18	0.57
2:1E:189:ASP:CG	2:1E:205:ASP:HB3	2.24	0.57
26:1H:2392:A:H2	26:1H:2424:C:N4	2.02	0.57
30:21:53:PRO:HA	30:21:75:VAL:N	2.16	0.57
13:4A:91:ARG:NH1	13:4A:97:PRO:O	2.37	0.57
1:1G:1346:A:H5''	9:82:120:ARG:NH1	2.18	0.57
42:85:97:ASP:OD1	42:85:98:LEU:N	2.37	0.57
46:C5:17:SER:HB2	46:C5:71:LYS:CE	2.34	0.57
1:1G:1104:G:H4'	2:12:111:ARG:HE	1.69	0.57
26:14:2415:G:H4'	37:35:67:MET:H	1.69	0.57
1:1G:1028:C:N4	1:1G:1033:G:H1	2.02	0.57
3:22:44:GLU:HG3	3:22:52:LEU:HD21	1.86	0.57
31:31:155:LEU:HD11	31:31:176:LEU:HD13	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:3K:9:A:O2'	24:3K:46:G:O4'	2.19	0.57
20:BI:86:ARG:O	20:BI:90:GLN:NE2	2.37	0.57
47:D5:158:PRO:HB2	47:D5:159:PRO:HD2	1.86	0.57
45:F8:29:TRP:CZ3	45:F8:78:LYS:HG2	2.40	0.57
26:1H:309:G:H4'	46:G8:18:GLY:HA2	1.86	0.57
52:M8:12:ALA:HB3	52:M8:24:THR:HB	1.86	0.57
29:11:71:ASP:N	29:11:71:ASP:OD1	2.36	0.57
1:13:313:A:H2'	1:13:314:C:C6	2.40	0.57
1:1G:222:U:H2'	1:1G:223:U:C6	2.40	0.57
1:1G:458:C:H2'	1:1G:464:G:H8	1.70	0.57
26:1H:2128:C:H2'	26:1H:2129:C:C6	2.39	0.57
36:68:63:VAL:HG12	36:68:106:LEU:HD11	1.87	0.57
8:72:36:LEU:HA	8:72:39:LEU:HB2	1.87	0.57
48:E5:36:ILE:HD11	48:E5:39:ARG:HG2	1.85	0.57
1:13:456:C:H42	1:13:476:G:H1	1.50	0.57
26:14:315:G:H2'	26:14:316:C:C6	2.39	0.57
21:1F:5:ASP:HB3	21:1F:8:THR:HG22	1.87	0.57
1:1G:1203:C:H2'	1:1G:1204:A:H8	1.69	0.57
1:1G:297:G:N2	1:1G:300:A:OP2	2.36	0.57
1:1G:44:G:H2'	1:1G:45:U:O4'	2.04	0.57
26:1H:760:G:H5''	62:1H:3668:HOH:O	2.05	0.57
4:32:76:ARG:NH2	4:32:80:GLU:OE1	2.38	0.57
31:39:28:ILE:HA	31:39:112:MET:HG2	1.85	0.57
27:1J:90:C:P	38:45:16:ARG:HH21	2.27	0.57
33:51:77:LYS:HE2	33:51:138:LYS:HD2	1.84	0.57
34:61:113:ARG:HH21	34:61:132:PRO:HB3	1.70	0.57
16:7A:8:ARG:HD3	16:7A:17:TYR:CE1	2.40	0.57
9:82:77:ILE:O	9:82:81:ILE:HG12	2.04	0.57
42:85:91:ASP:OD1	42:85:96:ALA:HB2	2.03	0.57
9:8E:43:ALA:HA	9:8E:74:ILE:HD13	1.84	0.57
40:A8:35:ILE:HD11	40:A8:101:LEU:HD23	1.87	0.57
26:14:138:G:N2	45:B5:44:GLU:OE2	2.25	0.57
47:D5:113:ALA:O	47:D5:116:VAL:N	2.23	0.57
47:D5:115:GLY:HA3	47:D5:174:VAL:HG13	1.86	0.57
51:L8:7:LYS:HE2	51:L8:32:GLN:O	2.05	0.57
1:13:158:G:H2'	1:13:159:G:H8	1.68	0.57
1:1G:376:G:H5''	16:7A:5:ARG:HB2	1.85	0.57
26:1H:1042:G:H1	26:1H:1113:U:H3	1.51	0.57
26:1H:125:G:H5'	26:1H:125:G:C8	2.39	0.57
26:1H:2257:U:O2'	26:1H:2258:C:H5'	2.05	0.57
26:1H:2061:G:OP2	26:1H:2502:G:H5'	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:31:129:PHE:HA	31:31:142:TRP:NE1	2.19	0.57
33:51:164:TYR:O	33:51:167:GLU:HB3	2.05	0.57
1:1G:976:G:OP1	14:5A:32:SER:N	2.36	0.57
26:14:2378:A:O2'	40:65:21:THR:HG21	2.05	0.57
1:13:750:G:N3	15:6I:23:GLY:HA3	2.20	0.57
19:AI:41:VAL:HG12	19:AI:44:MET:CB	2.34	0.57
45:B5:63:LYS:HA	45:B5:72:LYS:HA	1.87	0.57
42:C8:92:ARG:CZ	43:D8:11:GLN:H	2.16	0.57
46:G8:97:ARG:NH2	46:G8:103:GLY:O	2.34	0.57
29:11:182:LEU:N	29:11:272:ALA:HB3	2.06	0.57
26:14:1381:G:OP2	62:14:3645:HOH:O	2.18	0.57
26:14:2425:A:H5'	26:14:2426:A:H3'	1.87	0.57
1:1G:501:C:H2'	1:1G:502:G:C8	2.37	0.57
26:1H:754:C:H2'	26:1H:755:C:H6	1.70	0.57
23:2L:33:OMC:O5'	23:2L:33:OMC:H6	1.88	0.57
24:3K:15:G:H1	24:3K:48:C:H41	1.52	0.57
24:3K:76:A:H8	26:1H:2394:C:N4	1.99	0.57
13:4A:37:THR:HG22	13:4A:55:ARG:HE	1.70	0.57
17:8I:66:SER:O	17:8I:70:ARG:NH1	2.37	0.57
41:B8:1:MET:N	41:B8:2:ASN:OD1	2.33	0.57
42:C8:88:ILE:O	42:C8:90:VAL:N	2.38	0.57
47:D5:157:LEU:HB3	47:D5:161:VAL:HG21	1.86	0.57
2:12:110:GLN:HB3	2:12:111:ARG:HH12	1.70	0.57
1:13:1266:G:N2	1:13:1270:C:N3	2.52	0.57
26:14:1614:A:OP1	26:14:1617:C:N4	2.31	0.57
2:1E:209:ARG:HD2	2:1E:239:VAL:HG13	1.85	0.57
1:1G:1025:U:H5'	1:1G:1026:G:H5'	1.85	0.57
1:1G:1127:G:H2'	1:1G:1128:C:C6	2.40	0.57
1:1G:1154:G:H2'	1:1G:1155:G:C8	2.38	0.57
1:1G:1345:U:OP1	62:1G:1861:HOH:O	2.17	0.57
1:1G:458:C:N3	1:1G:474:G:N2	2.49	0.57
1:1G:87:A:H4'	1:1G:88:C:OP1	2.03	0.57
3:22:58:GLU:HB2	3:22:65:ALA:HB3	1.86	0.57
5:4E:142:LEU:O	5:4E:143:ARG:NH1	2.34	0.57
36:68:107:ARG:NH1	41:B8:36:GLU:HG2	2.20	0.57
34:69:1:MET:HE1	34:69:38:LEU:HD23	1.86	0.57
1:1G:135:C:O2	16:7A:1:MET:HB3	2.05	0.57
16:7A:22:THR:HA	16:7A:33:ILE:HD12	1.84	0.57
38:88:39:PRO:HA	38:88:97:VAL:O	2.05	0.57
26:1H:1188:U:H4'	43:D8:79:VAL:HG22	1.87	0.57
1:13:446:G:H1	1:13:488:C:H42	1.51	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:14:1997:G:OP2	62:14:3644:HOH:O	2.18	0.57
26:14:2275:C:H6	26:14:2275:C:H5'	1.70	0.57
27:16:40:U:H1'	27:16:45:A:N6	2.20	0.57
26:1H:223:A:O4'	26:1H:422:A:H5'	2.05	0.57
30:21:63:LEU:O	30:21:66:HIS:HB3	2.05	0.57
24:3L:4:U:H2'	24:3L:5:C:O4'	2.05	0.57
35:58:96:GLU:O	35:58:98:VAL:HG12	2.04	0.57
6:5E:86:ARG:O	6:5E:87:ARG:HG2	2.05	0.57
7:62:27:ILE:HD12	7:62:40:ALA:HA	1.86	0.57
15:6I:39:LEU:HD13	15:6I:56:LEU:HB2	1.87	0.57
5:42:93:PRO:HG2	8:72:105:ARG:HG3	1.87	0.57
1:13:1130:A:H5'	9:8E:18:PHE:CE2	2.40	0.57
44:A5:14:PRO:HG2	44:A5:78:GLU:HB2	1.85	0.57
1:13:201:C:H42	1:13:216:G:H1	1.53	0.57
26:14:827:U:H2'	26:14:2430:A:H2	1.70	0.57
1:1G:1:U:H4'	1:1G:630:G:N2	2.20	0.57
24:1L:3:G:N2	24:1L:4:U:O4	2.37	0.57
1:13:881:G:OP2	12:3I:12:ARG:NH2	2.37	0.57
7:6E:13:GLN:O	7:6E:24:THR:HG21	2.05	0.57
16:7A:14:ASN:OD1	16:7A:42:ARG:NH2	2.38	0.57
49:J8:86:SER:HB2	49:J8:87:PRO:HD2	1.87	0.57
49:J8:90:ILE:HG22	49:J8:94:LEU:HD22	1.87	0.57
1:13:316:G:OP2	1:13:351:G:O2'	2.22	0.56
1:13:769:G:N7	62:13:1852:HOH:O	2.32	0.56
26:14:2324:C:H5''	26:14:2325:G:H5'	1.85	0.56
26:14:395:U:O2'	26:14:396:G:C8	2.52	0.56
26:1H:1264:G:H5'	53:N8:11:THR:CG2	2.35	0.56
26:1H:2298:A:H62	26:1H:2318:G:H8	1.51	0.56
3:2E:16:ARG:NH2	3:2E:183:ASP:OD1	2.38	0.56
3:2E:40:ARG:O	3:2E:44:GLU:HG2	2.05	0.56
26:1H:1257:C:H4'	31:31:83:PHE:CD1	2.40	0.56
4:3E:122:ARG:HG2	4:3E:122:ARG:HH11	1.68	0.56
32:41:151:ALA:O	32:41:153:ARG:NH1	2.38	0.56
30:29:12:THR:HG21	41:75:11:GLU:OE1	2.04	0.56
1:1G:1342:C:H4'	9:82:125:TYR:HB3	1.86	0.56
41:B8:12:SER:CA	41:B8:14:TYR:H	2.19	0.56
41:B8:35:LYS:HE3	41:B8:38:ASN:HA	1.86	0.56
47:D5:19:ARG:NH1	47:D5:84:GLU:O	2.38	0.56
48:E5:34:GLY:HA2	48:E5:61:ALA:O	2.05	0.56
1:13:1003:G:H1	1:13:1037:C:H42	1.52	0.56
1:13:1071:C:H2'	1:13:1072:G:C8	2.40	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:13:683:G:N7	62:13:1853:HOH:O	2.33	0.56
26:14:2262:U:H4'	26:14:2328:A:C2	2.39	0.56
26:14:71:A:C2	45:B5:31:HIS:NE2	2.73	0.56
1:1G:1238:A:N3	1:1G:1241:G:O2'	2.27	0.56
1:1G:376:G:H1	1:1G:387:U:H3	1.53	0.56
27:16:42:C:O3'	32:41:67:LYS:NZ	2.38	0.56
33:59:6:ARG:HB2	33:59:65:HIS:CD2	2.39	0.56
6:5E:45:LEU:HD12	6:5E:59:TYR:HD2	1.69	0.56
17:8I:67:LYS:O	17:8I:68:ARG:HB3	2.05	0.56
45:F8:11:PRO:HB3	45:F8:92:LEU:HD21	1.87	0.56
48:I8:72:ARG:NH1	48:I8:75:LEU:HD12	2.20	0.56
26:1H:1500:G:O2'	29:11:100:GLY:O	2.18	0.56
26:14:122:G:OP1	26:14:149:A:O2'	2.21	0.56
26:14:1332:G:H21	26:14:1610:A:H8	1.54	0.56
26:14:1786:A:C2	26:14:2606:C:H1'	2.39	0.56
2:1E:60:ASP:O	2:1E:64:ARG:NE	2.38	0.56
1:1G:1478:C:H2'	1:1G:1479:C:H6	1.70	0.56
26:1H:1593:G:H2'	26:1H:1594:G:C8	2.40	0.56
26:1H:880:G:H1	26:1H:897:C:H42	1.53	0.56
26:1H:991:C:H2'	26:1H:992:C:H6	1.70	0.56
26:1H:444:C:H4'	31:31:49:ALA:HB2	1.87	0.56
26:14:637:A:H2'	37:35:117:GLU:OE2	2.05	0.56
37:35:57:THR:HG22	37:35:60:MET:H	1.71	0.56
7:62:70:LYS:HG2	7:62:96:GLN:HB3	1.88	0.56
34:69:77:LEU:HA	34:69:141:LYS:HB3	1.86	0.56
34:69:81:VAL:H	34:69:143:SER:CB	2.15	0.56
15:6A:39:LEU:HD12	15:6A:56:LEU:HB2	1.87	0.56
28:71:64:LEU:HD21	28:71:188:ASN:HD21	1.69	0.56
26:1H:661:C:O2'	37:78:13:ASN:O	2.23	0.56
39:98:86:ARG:NH2	39:98:118:GLU:HG2	2.16	0.56
19:AI:50:ALA:HB1	19:AI:57:HIS:HB3	1.87	0.56
26:14:2331:G:O2'	48:E5:43:THR:HB	2.06	0.56
29:11:33:LEU:O	29:11:64:ILE:HG23	2.04	0.56
2:12:22:LYS:HB3	2:12:40:HIS:HE1	1.70	0.56
27:16:66:A:N6	27:16:107:U:H2'	2.20	0.56
2:1E:12:GLU:HB3	2:1E:44:LEU:HD13	1.86	0.56
1:1G:1213:A:N6	1:1G:1215:G:N3	2.53	0.56
26:1H:1871:A:H2'	26:1H:1872:A:C8	2.40	0.56
26:1H:2584:U:H2'	26:1H:2585:U:H2'	1.87	0.56
11:2I:17:GLY:O	11:2I:80:VAL:HA	2.05	0.56
31:39:192:LEU:O	31:39:193:VAL:HG23	2.04	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:55:97:VAL:HA	39:55:113:LEU:O	2.05	0.56
41:75:108:ARG:HA	41:75:111:ARG:HG2	1.87	0.56
37:78:116:GLY:H	37:78:134:ALA:HB2	1.70	0.56
41:B8:99:LEU:HB3	41:B8:101:PHE:CE1	2.41	0.56
47:D5:29:TYR:CE2	47:D5:87:ASP:HB2	2.41	0.56
50:G5:4:SER:HB3	50:G5:7:ARG:HB2	1.88	0.56
26:1H:189:G:OP2	49:J8:39:LYS:HE3	2.05	0.56
1:13:177:C:OP2	20:BI:65:LYS:NZ	2.36	0.56
26:14:2158:A:H1'	26:14:2159:G:C8	2.40	0.56
26:14:403:U:H4'	26:14:404:C:H5'	1.86	0.56
26:14:491:G:H2'	26:14:492:A:H8	1.70	0.56
1:1G:1052:U:O2'	1:1G:1055:A:OP2	2.13	0.56
1:1G:971:G:OP1	1:1G:972:C:H5''	2.05	0.56
26:1H:370:G:H4'	26:1H:371:A:OP2	2.04	0.56
27:1J:13:A:H5''	27:1J:15:A:C6	2.40	0.56
33:51:94:TYR:HA	33:51:106:THR:O	2.06	0.56
34:61:79:ILE:HB	34:61:142:VAL:HG12	1.88	0.56
1:1G:1291:G:O3'	9:82:39:GLY:HA3	2.06	0.56
9:82:19:LEU:HD11	9:82:84:ALA:HB1	1.86	0.56
18:9A:74:ARG:NH1	18:9A:81:PHE:HA	2.20	0.56
26:1H:1188:U:C4'	43:D8:79:VAL:HG22	2.35	0.56
48:E5:32:ARG:O	48:E5:34:GLY:N	2.36	0.56
49:F5:62:VAL:HG21	49:F5:70:VAL:HG21	1.88	0.56
47:H8:163:LEU:HB3	47:H8:165:VAL:H	1.69	0.56
54:O8:41:PRO:HB2	54:O8:44:ARG:HH12	1.69	0.56
29:11:38:LYS:HG2	29:11:40:THR:CG2	2.36	0.56
2:12:132:LYS:HA	2:12:135:GLN:HB2	1.88	0.56
26:14:270(M):U:H5''	26:14:270(N):G:OP1	2.05	0.56
26:14:29:U:H2'	26:14:30:G:C8	2.39	0.56
10:1A:81:THR:O	10:1A:84:GLN:NE2	2.36	0.56
2:1E:60:ASP:HB3	2:1E:64:ARG:HH21	1.71	0.56
1:1G:991:U:H5	1:1G:1212:U:H1'	1.71	0.56
1:1G:604:G:H2'	1:1G:605:U:O4'	2.05	0.56
26:1H:2473:U:H2'	26:1H:2474:C:H5'	1.87	0.56
26:1H:65:C:H2'	26:1H:66:C:C6	2.41	0.56
11:2A:87:THR:O	11:2A:87:THR:OG1	2.21	0.56
32:41:47:LYS:HD2	32:41:81:LYS:HB2	1.86	0.56
5:42:100:VAL:HG23	5:42:118:ILE:HG22	1.87	0.56
41:75:45:PHE:CZ	41:75:74:ARG:HG3	2.40	0.56
37:78:59:LEU:O	56:Q8:13:ARG:HD2	2.05	0.56
37:78:78:PRO:HB3	37:78:111:ARG:NH2	2.20	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:82:51:ARG:HG2	9:82:56:LEU:HD13	1.87	0.56
39:98:46:GLY:HA2	39:98:49:ASP:HB2	1.88	0.56
40:A8:3:ARG:HG3	40:A8:4:LEU:HB2	1.88	0.56
20:BA:25:ARG:HG3	20:BA:29:LYS:HE3	1.88	0.56
52:M8:14:ILE:HG23	52:M8:21:VAL:HB	1.85	0.56
1:13:838:G:H1	1:13:848:C:H42	1.53	0.56
26:14:198:C:H5'	26:14:2244:U:OP1	2.05	0.56
26:14:2280:G:O2'	26:14:2388:A:N1	2.34	0.56
35:15:58:ASP:N	35:15:58:ASP:OD1	2.37	0.56
2:1E:114:ARG:O	2:1E:118:LEU:HB2	2.05	0.56
2:1E:71:VAL:HG23	2:1E:164:VAL:HA	1.88	0.56
26:1H:1412:A:H2'	26:1H:1413:G:H8	1.71	0.56
26:1H:1508:A:O2'	26:1H:1509:C:O5'	2.23	0.56
26:1H:646:A:H2'	26:1H:647:G:O4'	2.05	0.56
26:1H:663:G:OP1	37:78:16:ARG:HB2	2.04	0.56
26:1H:754:C:H2'	26:1H:755:C:C6	2.41	0.56
26:1H:762:U:H4'	26:1H:763:G:O5'	2.06	0.56
31:31:183:VAL:O	31:31:187:VAL:HG23	2.05	0.56
1:1G:1148:U:O3'	9:82:14:VAL:HG11	2.06	0.56
37:78:63:PRO:CB	56:Q8:30:ARG:HH21	2.09	0.56
26:1H:1800:C:OP2	29:11:183:ARG:NH2	2.38	0.56
2:12:72:GLY:HA3	2:12:81:VAL:HG21	1.87	0.56
1:13:1125:U:HO2'	1:13:1126:U:H6	1.50	0.56
1:13:838:G:O6	1:13:848:C:N4	2.38	0.56
26:14:1018:C:H2'	26:14:1019:U:H6	1.71	0.56
26:14:1693:U:O2'	29:19:14:ARG:NH2	2.39	0.56
26:14:2719:G:O6	62:14:3638:HOH:O	2.15	0.56
35:15:61:ARG:HH11	35:15:61:ARG:HA	1.71	0.56
27:16:2:C:O2	27:16:118:G:N2	2.19	0.56
26:1H:1520:U:H2'	26:1H:1521:G:O4'	2.06	0.56
4:32:108:LEU:HD21	4:32:183:GLY:HA3	1.88	0.56
4:32:18:LYS:HG2	59:32:302:SF4:S1	2.45	0.56
31:39:155:LEU:HD23	31:39:186:ILE:HD13	1.87	0.56
6:5E:78:GLU:O	6:5E:81:ILE:HG22	2.06	0.56
1:1G:376:G:H5''	16:7A:5:ARG:HD2	1.86	0.56
18:9A:71:LYS:HA	18:9A:74:ARG:HD2	1.88	0.56
26:14:1582:C:HO2'	26:14:1586:A:H8	1.51	0.56
26:14:2037:G:H2'	26:14:2038:G:C8	2.40	0.56
26:14:2117:A:H2'	26:14:2118:U:H5	1.71	0.56
26:14:981:A:N1	26:14:2027:G:O2'	2.35	0.56
2:1E:32:ILE:HD13	2:1E:40:HIS:HB3	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1G:1343:G:H2'	1:1G:1344:C:H6	1.71	0.56
1:1G:323:U:O3'	20:BA:22:ARG:HD3	2.06	0.56
1:1G:973:G:H5''	1:1G:974:A:H5''	1.88	0.56
26:1H:2292:C:P	40:A8:17:ARG:HH22	2.29	0.56
22:1K:76:A:H1'	26:1H:2583:G:H21	1.70	0.56
1:13:963:G:H21	10:1I:55:LYS:CE	2.18	0.56
4:32:34:GLU:HB2	4:32:35:ARG:HH22	1.71	0.56
32:41:39:ILE:HD12	32:41:94:LEU:HD21	1.88	0.56
13:4I:23:TYR:HB3	13:4I:67:GLU:HB2	1.88	0.56
6:5E:22:GLU:OE1	6:5E:82:ARG:NH2	2.39	0.56
17:8A:99:SER:OG	17:8A:100:LYS:N	2.37	0.56
9:8E:34:ASN:O	9:8E:38:GLN:HB2	2.06	0.56
47:D5:111:VAL:HG22	47:D5:112:ARG:HG2	1.88	0.56
47:H8:60:GLU:O	47:H8:61:LEU:HB3	2.05	0.56
1:13:1497:G:H2'	1:13:1498:U:H5'	1.87	0.56
26:14:2142:C:H2'	26:14:2143:C:C6	2.41	0.56
26:14:2418:A:OP2	56:M5:29:LYS:NZ	2.27	0.56
26:14:1775:U:O2'	61:14:3437:SPE:N1	2.39	0.56
26:14:646:A:H2'	26:14:647:G:O4'	2.06	0.56
1:1G:1251:A:O2'	1:1G:1369:C:O2'	2.24	0.56
1:1G:811:C:N4	62:1G:1884:HOH:O	2.38	0.56
26:1H:1221:C:H2'	26:1H:1222:C:H6	1.71	0.56
26:1H:1230:C:H2'	26:1H:1231:G:H8	1.70	0.56
26:1H:2688:U:C5	26:1H:2720:U:OP2	2.59	0.56
26:1H:2789:C:H1'	26:1H:2892:A:C2	2.41	0.56
26:1H:926:A:N7	62:1H:3826:HOH:O	2.33	0.56
26:1H:997:G:OP1	42:C8:93:LYS:HD2	2.05	0.56
31:39:89:VAL:HG12	31:39:90:PHE:H	1.71	0.56
32:49:27:ASN:HB3	32:49:30:GLU:HG3	1.86	0.56
26:14:2822:G:O6	39:55:2:ARG:HD3	2.06	0.56
8:72:51:VAL:HG11	8:72:60:ARG:HE	1.71	0.56
26:1H:625:G:N7	37:78:107:LYS:NZ	2.54	0.56
37:78:13:ASN:O	37:78:15:ARG:N	2.39	0.56
16:7I:4:ILE:HG12	16:7I:21:VAL:HG12	1.87	0.56
26:14:486:C:O2'	44:A5:60:ASN:ND2	2.39	0.56
40:A8:30:ARG:O	40:A8:30:ARG:HG3	2.05	0.56
51:L8:43:ILE:O	51:L8:47:VAL:HG23	2.06	0.56
56:M5:8:LYS:HB3	56:M5:12:LYS:HE3	1.88	0.56
54:O8:25:LYS:HB3	56:Q8:34:TRP:CD1	2.41	0.56
1:13:922:G:C6	1:13:923:A:C6	2.94	0.56
26:14:1416:G:HO2'	26:14:1417:C:H6	1.54	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:14:2117:A:H2'	26:14:2118:U:C5	2.41	0.56
26:14:2327:A:H2'	26:14:2328:A:C8	2.41	0.56
1:1G:1259:C:N4	1:1G:1260:C:O2	2.39	0.56
1:1G:1469:G:H2'	1:1G:1470:G:H8	1.71	0.56
3:22:14:ILE:HG12	3:22:15:THR:H	1.71	0.56
3:22:32:LEU:HD22	3:22:59:ARG:HH22	1.71	0.56
38:45:20:ALA:HA	38:45:99:PRO:HG2	1.87	0.56
13:4A:70:LEU:O	13:4A:74:VAL:HG23	2.06	0.56
6:52:76:ALA:HB1	6:52:80:ARG:NH2	2.19	0.56
33:59:149:ARG:HA	33:59:162:ILE:HG21	1.88	0.56
14:5A:32:SER:O	14:5A:40:CYS:HA	2.06	0.56
16:7I:21:VAL:O	16:7I:33:ILE:N	2.36	0.56
44:E8:58:ALA:HB1	44:E8:64:MET:HB2	1.88	0.56
54:O8:43:CYS:HB3	54:O8:44:ARG:HH11	1.71	0.56
1:13:1060:C:HO2'	10:1I:56:HIS:HD1	1.54	0.55
1:13:592:G:H2'	1:13:593:G:H8	1.71	0.55
26:14:1581:G:H2'	26:14:1582:C:O4'	2.04	0.55
26:14:2275:C:H5'	26:14:2275:C:C6	2.41	0.55
27:16:94:C:H2'	27:16:95:U:C6	2.41	0.55
29:19:141:VAL:HG23	29:19:162:SER:HB2	1.88	0.55
29:19:70:TRP:C	29:19:70:TRP:CD1	2.80	0.55
1:1G:692:U:O2'	1:1G:694:A:N7	2.36	0.55
26:1H:1126:A:H4'	26:1H:1127:A:O5'	2.06	0.55
26:1H:2362:G:OP1	56:Q8:44:LYS:NZ	2.29	0.55
26:1H:271(B):G:N7	26:1H:421:U:H2'	2.20	0.55
23:2K:47:7MG:O2'	23:2K:48:U:OP2	2.21	0.55
4:32:163:GLU:HA	4:32:166:LYS:HE3	1.88	0.55
33:59:54:ARG:NH2	33:59:57:ASP:OD1	2.29	0.55
1:1G:878:G:H5'	8:72:89:PRO:HG2	1.87	0.55
1:13:1248:A:N3	9:8E:70:LYS:HE2	2.22	0.55
40:A8:111:GLU:HB2	40:A8:112:PHE:CE2	2.41	0.55
40:A8:27:SER:HA	40:A8:88:ASP:CB	2.36	0.55
47:D5:59:LEU:O	47:D5:60:GLU:HB3	2.05	0.55
43:D8:16:PRO:HA	43:D8:96:ILE:HG22	1.87	0.55
52:M8:24:THR:OG1	52:M8:25:TYR:N	2.38	0.55
2:12:71:VAL:HG21	2:12:164:VAL:HA	1.88	0.55
2:12:166:ASP:OD2	2:12:169:LYS:HB2	2.05	0.55
1:13:148:G:H2'	1:13:149:A:C8	2.41	0.55
1:13:179:A:H2'	1:13:180:U:C6	2.41	0.55
1:13:339:C:OP2	36:68:97:ARG:NH1	2.39	0.55
1:13:673:G:H2'	1:13:674:G:C8	2.41	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:14:1449(A):G:H2'	26:14:1450:C:C6	2.41	0.55
26:14:2113:U:H3'	26:14:2114:A:H4'	1.88	0.55
26:14:2139:C:N3	26:14:2153:G:N2	2.54	0.55
2:1E:17:PHE:HB3	2:1E:44:LEU:HG	1.88	0.55
1:1G:316:G:OP2	1:1G:351:G:O2'	2.22	0.55
26:1H:1315:C:OP2	62:1H:3747:HOH:O	2.17	0.55
26:1H:247:G:H4'	26:1H:386:G:C5	2.41	0.55
27:1J:2:C:H2'	27:1J:3:C:H6	1.69	0.55
30:29:47:VAL:HG21	30:29:86:PRO:HD2	1.87	0.55
37:35:59:LEU:HD21	56:M5:10:ALA:HA	1.88	0.55
1:1G:527:G:O6	12:3A:49:ASN:ND2	2.37	0.55
13:4A:13:LYS:HD3	13:4A:14:ARG:H	1.70	0.55
41:75:91:ARG:NH1	41:75:124:ASP:OD2	2.30	0.55
37:78:82:GLY:HA2	37:78:113:LYS:O	2.06	0.55
41:B8:74:ARG:HD3	41:B8:76:PHE:CZ	2.41	0.55
47:D5:97:GLU:HB3	47:D5:125:LEU:HD11	1.87	0.55
26:1H:1266:G:O5'	44:E8:15:ARG:NH2	2.40	0.55
1:13:1028(B):C:H41	1:13:1032(A):G:H21	1.52	0.55
1:13:1226:C:O3'	13:4I:111:LYS:NZ	2.39	0.55
1:13:1233:G:H2'	1:13:1234:C:C6	2.41	0.55
26:14:1041:C:H42	26:14:1114:G:H22	1.54	0.55
26:14:323:G:O2'	26:14:1205:U:N3	2.31	0.55
1:1G:1177:G:O2'	1:1G:1178:G:O4'	2.24	0.55
1:1G:411:A:H62	1:1G:413:G:H21	1.53	0.55
26:1H:1827:C:C2'	26:1H:1828:G:H5'	2.36	0.55
38:45:110:THR:HG23	38:45:113:GLN:HB2	1.88	0.55
1:13:10:A:OP2	5:4E:126:ARG:HD3	2.06	0.55
1:13:580:U:OP1	15:6I:54:ARG:NH2	2.39	0.55
8:7E:119:LEU:HB3	8:7E:123:GLU:HG3	1.87	0.55
6:5E:94:GLN:NE2	18:9I:33:ASP:OD1	2.30	0.55
47:H8:77:ASP:N	47:H8:84:GLU:HG2	2.21	0.55
2:12:118:LEU:HD22	2:12:142:LEU:HB2	1.87	0.55
26:14:886:C:H1'	26:14:890:A:H2	1.70	0.55
1:1G:998:G:H22	1:1G:1043:C:N4	2.05	0.55
26:1H:142:G:H1'	45:F8:37:THR:HG21	1.88	0.55
26:1H:2208:U:O2'	26:1H:2209:C:H5'	2.05	0.55
26:1H:34:C:O2'	26:1H:35:G:OP2	2.18	0.55
26:1H:7:G:H2'	26:1H:8:A:O4'	2.06	0.55
3:2E:7:PRO:O	3:2E:11:ARG:HG2	2.06	0.55
38:45:57:HIS:NE2	38:45:116:GLU:HG2	2.21	0.55
13:4I:4:ILE:HG23	13:4I:57:ARG:HA	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:59:18:GLU:HB2	33:59:25:LYS:HB2	1.89	0.55
18:9A:31:LEU:H	18:9A:31:LEU:HD23	1.71	0.55
41:B8:94:ALA:HB1	41:B8:99:LEU:HD21	1.89	0.55
29:11:17:THR:CG2	29:11:204:ILE:HA	2.36	0.55
1:13:1286:A:H8	1:13:1287:A:H4'	1.71	0.55
26:14:2308:G:O2'	26:14:2309:A:OP1	2.20	0.55
26:14:802:A:H4'	62:14:4111:HOH:O	2.05	0.55
29:19:237:GLU:OE1	62:19:403:HOH:O	2.17	0.55
1:1G:1352:C:H2'	1:1G:1353:G:C8	2.41	0.55
26:1H:1586:A:H5''	26:1H:1586:A:N3	2.21	0.55
26:1H:2122:U:H2'	26:1H:2123:G:C8	2.41	0.55
26:1H:218:A:H2	26:1H:235:U:H4'	1.72	0.55
26:1H:479:A:N3	26:1H:481:G:H5''	2.22	0.55
3:2E:167:TRP:CD1	3:2E:168:ALA:N	2.75	0.55
4:32:31:CYS:C	4:32:33:MET:H	2.10	0.55
46:C5:20:TYR:CZ	46:C5:42:VAL:HA	2.42	0.55
46:C5:76:CYS:SG	46:C5:97:ARG:HG3	2.45	0.55
29:11:75:ILE:HG21	29:11:99:ASP:OD2	2.07	0.55
2:12:160:ASP:N	2:12:160:ASP:OD1	2.40	0.55
1:13:376:G:H5''	16:7I:5:ARG:HB2	1.89	0.55
1:13:652:U:O4	1:13:752:G:O2'	2.17	0.55
1:13:688:G:H2'	1:13:689:C:H6	1.72	0.55
26:14:1359:A:H5'	26:14:1359:A:H8	1.70	0.55
26:14:1939:U:OP1	26:14:2604:U:O2'	2.20	0.55
26:14:2068:U:H3	26:14:2430:A:H2	1.55	0.55
26:14:2123:G:N2	26:14:2176:A:N1	2.54	0.55
1:1G:1308:U:H5''	13:4A:98:VAL:HG22	1.89	0.55
1:1G:1512:U:H2'	1:1G:1513:A:C8	2.42	0.55
1:1G:540:G:H2'	1:1G:541:G:O4'	2.06	0.55
26:1H:500:G:N7	62:1H:3827:HOH:O	2.33	0.55
11:2I:122:LYS:HE3	11:2I:124:LYS:HE3	1.89	0.55
34:69:109:ILE:HB	34:69:130:TYR:CZ	2.42	0.55
46:C5:83:THR:HG22	46:C5:84:ARG:H	1.70	0.55
52:M8:4:GLY:C	52:M8:5:ILE:HG13	2.27	0.55
26:14:1166:C:O2'	62:14:3646:HOH:O	2.18	0.55
26:14:2646:C:H2'	26:14:2647:U:O4'	2.07	0.55
10:1I:61:GLU:OE1	14:5I:58:LYS:NZ	2.27	0.55
3:22:112:SER:HB3	3:22:115:LEU:HB2	1.88	0.55
4:32:31:CYS:HB2	4:32:33:MET:H	1.72	0.55
37:35:106:LEU:HD13	37:35:112:LEU:HD23	1.89	0.55
4:3E:61:LYS:NZ	4:3E:72:GLU:OE2	2.24	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:41:124:SER:HB2	32:41:131:TYR:CE2	2.42	0.55
35:58:40:PRO:O	42:C8:64:ARG:HG2	2.07	0.55
17:8I:18:THR:OG1	17:8I:69:LYS:NZ	2.26	0.55
42:C8:95:LEU:HD22	43:D8:4:ILE:HD13	1.89	0.55
45:B5:11:PRO:HD3	50:G5:37:PHE:CD2	2.42	0.55
1:13:134:A:H61	16:7I:25:ARG:NH1	2.05	0.55
26:14:127:A:H5''	26:14:128:C:C6	2.42	0.55
26:14:2118:U:O2'	26:14:2145:C:N3	2.39	0.55
26:14:2406:U:H2'	26:14:2406:U:OP2	2.07	0.55
26:14:270(E):G:H2'	26:14:270(F):U:C6	2.42	0.55
26:14:774:A:O2'	26:14:775:G:O5'	2.23	0.55
26:14:848:G:H2'	26:14:849:A:H8	1.68	0.55
1:1G:1065:U:C5	1:1G:1190:G:H1'	2.42	0.55
1:1G:1466:C:H2'	1:1G:1467:G:O4'	2.06	0.55
1:1G:1499:A:H1'	1:1G:1520:G:H5'	1.89	0.55
1:1G:45:U:H2'	1:1G:46:G:C8	2.42	0.55
26:1H:1021:A:H8	26:1H:1021:A:H3'	1.71	0.55
26:1H:1354:A:H2'	26:1H:1355:G:O4'	2.07	0.55
26:1H:919:G:H4'	27:16:81:G:H4'	1.88	0.55
3:2E:15:THR:HG22	3:2E:16:ARG:N	2.22	0.55
31:39:178:PRO:HG2	31:39:179:GLU:OE1	2.07	0.55
5:42:71:LEU:HD21	5:42:115:VAL:HG22	1.89	0.55
36:68:7:TYR:CZ	36:68:44:LYS:HG3	2.42	0.55
45:B5:63:LYS:O	45:B5:63:LYS:NZ	2.29	0.55
20:BA:41:ILE:HD13	20:BA:87:LYS:HD2	1.89	0.55
46:C5:8:LYS:HZ3	46:C5:95:LYS:HD3	1.70	0.55
47:D5:170:THR:O	47:D5:172:ALA:N	2.39	0.55
50:K8:28:LYS:HE3	50:K8:56:GLN:NE2	2.22	0.55
1:13:157:G:H2'	1:13:158:G:H8	1.72	0.55
1:13:535:A:H5''	62:13:1845:HOH:O	2.06	0.55
26:14:1417:C:H42	26:14:1581:G:H1	1.55	0.55
26:14:2542:A:H5''	26:14:2542:A:N3	2.22	0.55
1:1G:1181:G:C2	1:1G:1182:G:H1'	2.42	0.55
1:1G:1396:A:H4'	1:1G:1397:C:H5''	1.88	0.55
26:1H:2228:G:OP2	29:11:263:ARG:NH2	2.40	0.55
26:1H:870:A:OP1	38:88:6:ARG:NH2	2.39	0.55
30:21:128:SER:OG	30:21:129:HIS:N	2.40	0.55
3:22:36:ASP:HA	3:22:39:ILE:HD12	1.88	0.55
3:2E:16:ARG:HH22	3:2E:183:ASP:HA	1.72	0.55
4:3E:127:THR:HG22	4:3E:147:ALA:HB3	1.89	0.55
5:42:78:HIS:CD2	8:72:107:LEU:HD22	2.42	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:49:120:LEU:HB2	32:49:180:PHE:CD1	2.41	0.55
39:55:72:ASP:O	39:55:76:VAL:HG23	2.07	0.55
34:69:76:THR:HG23	34:69:139:GLN:O	2.06	0.55
19:AA:13:ASP:O	19:AA:16:LEU:HB3	2.07	0.55
43:D8:36:PRO:O	43:D8:38:LEU:N	2.40	0.55
29:11:72:LYS:HE2	29:11:101:GLU:OE2	2.06	0.55
26:14:1486:A:H2'	26:14:1487:G:C8	2.42	0.55
26:14:1810:A:H2'	26:14:1811:G:O4'	2.07	0.55
26:14:2270:G:OP2	62:14:3648:HOH:O	2.18	0.55
26:14:2629:A:N3	26:14:2629:A:H2'	2.21	0.55
26:14:2693:A:H2'	26:14:2694:G:C8	2.43	0.55
1:1G:736:C:H2'	1:1G:737:A:C8	2.42	0.55
1:1G:978:A:H5'	1:1G:979:C:OP2	2.07	0.55
26:1H:1021:A:C8	26:1H:1021:A:H3'	2.42	0.55
26:1H:1639:U:C2'	26:1H:1640:C:H5''	2.37	0.55
26:1H:524:U:H2'	26:1H:525:U:C6	2.43	0.55
30:29:68:ALA:O	30:29:70:ALA:N	2.40	0.55
4:32:4:TYR:CE2	4:32:11:LEU:HD11	2.42	0.55
1:1G:619:U:N3	4:32:134:ASP:OD1	2.38	0.55
25:4L:21:A:C2'	25:4L:22:A:H5''	2.35	0.55
39:98:56:LYS:NZ	39:98:90:ARG:O	2.38	0.55
1:13:1182:G:H4'	1:13:1183:A:H5''	1.89	0.54
26:14:2849:U:H4'	26:14:2868:A:C2	2.42	0.54
2:1E:115:LEU:HD13	2:1E:145:LEU:HB3	1.89	0.54
1:1G:1413:A:H2'	1:1G:1414:U:O4'	2.07	0.54
26:1H:1165:U:H2'	26:1H:1166:C:H6	1.72	0.54
26:1H:1339:G:H21	26:1H:1603:A:H1'	1.72	0.54
22:1K:72:C:H2'	22:1K:73:A:H5''	1.89	0.54
23:2L:54:G:H2'	23:2L:55:5MU:H6	1.71	0.54
12:3A:6:THR:OG1	12:3A:9:GLN:HG3	2.07	0.54
26:14:873:G:O3'	38:45:63:LYS:NZ	2.39	0.54
35:58:17:ASP:O	35:58:56:ASN:HB2	2.07	0.54
14:5A:29:ARG:NH2	14:5A:40:CYS:SG	2.80	0.54
7:6E:22:LEU:HD23	7:6E:62:PHE:CE2	2.42	0.54
42:85:98:LEU:HB2	42:85:102:GLU:HB2	1.89	0.54
43:D8:14:VAL:HB	43:D8:96:ILE:HG13	1.89	0.54
45:F8:41:ASN:O	45:F8:45:THR:HG23	2.07	0.54
26:14:528:A:C2	26:14:2042:A:H2'	2.42	0.54
26:14:586:A:N1	26:14:809:G:O2'	2.32	0.54
26:14:843:G:H1	26:14:935:C:H42	1.54	0.54
2:1E:234:PRO:HB2	2:1E:236:TYR:H	1.71	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1G:942:G:C2	1:1G:1342:C:C2	2.95	0.54
1:1G:596:C:H3'	62:1G:1801:HOH:O	2.07	0.54
26:1H:1179:C:H2'	26:1H:1180:C:C6	2.41	0.54
26:1H:1590:U:H2'	26:1H:1591:G:C8	2.42	0.54
26:1H:300:A:N6	62:1H:3860:HOH:O	2.39	0.54
3:22:8:ILE:O	3:22:11:ARG:N	2.39	0.54
30:29:60:ASN:OD1	30:29:63:LEU:HD22	2.06	0.54
3:2E:18:TRP:H	3:2E:18:TRP:HE3	1.55	0.54
4:3E:155:LEU:O	4:3E:157:LEU:N	2.40	0.54
36:68:2:ILE:HG13	36:68:8:LEU:HD11	1.90	0.54
41:75:3:ARG:HA	41:75:6:LEU:HB2	1.88	0.54
8:7E:85:ARG:HD3	8:7E:88:LYS:HG2	1.89	0.54
20:BI:10:LEU:HD11	20:BI:12:ALA:HB3	1.88	0.54
47:D5:60:GLU:HG2	47:D5:60:GLU:O	2.06	0.54
50:G5:32:LEU:HD21	50:G5:54:LYS:HG2	1.90	0.54
46:G8:94:LYS:HZ2	46:G8:95:LYS:H	1.53	0.54
1:13:396:G:O2'	1:13:398:C:OP1	2.08	0.54
26:14:2295:C:OP1	40:65:10:ARG:NH1	2.40	0.54
26:14:754:C:H2'	26:14:755:C:C6	2.42	0.54
1:1G:1028(A):C:N4	1:1G:1032(B):G:H1	2.05	0.54
26:1H:1062:G:H1'	26:1H:1088:A:C5	2.42	0.54
26:1H:1441:G:H2'	26:1H:1442:G:C8	2.42	0.54
10:1I:85:LEU:HB2	10:1I:86:MET:SD	2.47	0.54
27:1J:3:C:H2'	27:1J:4:C:C6	2.42	0.54
26:1H:2572:A:C8	30:21:144:ARG:HD3	2.42	0.54
3:2E:119:ARG:O	3:2E:123:GLN:HG3	2.07	0.54
4:32:28:SER:HB3	4:32:29:PRO:HA	1.89	0.54
31:39:122:LYS:HB3	31:39:191:ARG:HB2	1.89	0.54
13:4I:40:ASN:HB3	13:4I:43:THR:HG23	1.88	0.54
33:51:10:PRO:O	33:51:11:VAL:HG13	2.08	0.54
34:61:4:ILE:HD11	34:61:44:LEU:HD13	1.89	0.54
7:62:113:GLU:O	7:62:119:ARG:HD3	2.07	0.54
37:78:63:PRO:HG2	56:Q8:25:MET:HB2	1.89	0.54
17:8I:81:ARG:HB3	17:8I:83:ASP:OD1	2.08	0.54
47:D5:87:ASP:N	47:D5:87:ASP:OD1	2.41	0.54
48:I8:36:ILE:HD13	48:I8:36:ILE:O	2.07	0.54
49:J8:95:LEU:HD12	49:J8:96:LYS:HD2	1.89	0.54
1:13:1414:U:H2'	1:13:1415:G:H8	1.73	0.54
1:13:165:C:H2'	1:13:166:G:C8	2.38	0.54
1:13:224:C:H2'	1:13:225:C:C6	2.42	0.54
1:13:540:G:H2'	1:13:541:G:O4'	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1G:588:G:H1	1:1G:651:C:H42	1.56	0.54
26:1H:1050:A:H2'	26:1H:1051:G:O4'	2.07	0.54
26:1H:1697:G:OP2	26:1H:1698:A:O2'	2.18	0.54
26:1H:2000:G:HO2'	26:1H:2689:U:H5	1.52	0.54
26:1H:2256:G:H4'	48:I8:9:SER:HB2	1.90	0.54
26:1H:2817:G:OP1	39:98:99:LYS:NZ	2.32	0.54
26:14:2724:C:OP1	30:29:118:LYS:HE3	2.07	0.54
38:45:38:GLU:HG3	38:45:127:ILE:HG22	1.88	0.54
33:51:56:SER:OG	33:51:57:ASP:N	2.39	0.54
7:6E:89:MET:HE1	7:6E:155:ARG:HD2	1.89	0.54
55:L5:5:TRP:NE1	55:L5:7:PRO:HG3	2.22	0.54
1:13:31:G:O2'	1:13:48:C:N4	2.41	0.54
26:14:2162:G:H2'	26:14:2163:C:H5'	1.90	0.54
26:14:2726:U:H4'	36:25:1:MET:HE3	1.90	0.54
26:1H:918:A:O2'	27:16:96:G:N2	2.41	0.54
1:1G:115:G:H1'	1:1G:116:A:N7	2.23	0.54
1:1G:421:U:O2'	1:1G:423:G:N7	2.39	0.54
1:1G:555:C:H2'	1:1G:556:C:C6	2.42	0.54
1:1G:628:G:H2'	1:1G:629:G:C8	2.43	0.54
26:1H:1332:G:N2	26:1H:1610:A:C8	2.76	0.54
26:1H:768:G:O2'	26:1H:1379:A:N6	2.40	0.54
30:29:12:THR:O	30:29:23:VAL:HG22	2.08	0.54
31:39:3:GLU:O	31:39:19:GLU:HB2	2.07	0.54
4:3E:156:GLU:O	4:3E:160:GLN:HB3	2.08	0.54
24:3K:22:G:N7	24:3K:46:G:N1	2.55	0.54
38:45:19:GLY:O	38:45:98:LYS:HB3	2.08	0.54
15:6A:39:LEU:HD12	15:6A:56:LEU:HD13	1.88	0.54
28:71:7:TYR:CE1	28:71:220:PRO:HB3	2.43	0.54
28:71:214:VAL:HG23	28:71:224:ILE:HG12	1.89	0.54
8:7E:8:ASP:O	8:7E:12:ARG:HG3	2.07	0.54
9:8E:5:TYR:CE1	9:8E:16:ARG:HG2	2.43	0.54
48:E5:18:ALA:HB3	48:E5:20:ARG:HH21	1.73	0.54
48:E5:25:ARG:HD2	48:E5:29:GLN:NE2	2.22	0.54
44:E8:37:ARG:HD3	44:E8:38:TYR:CE2	2.42	0.54
29:11:70:TRP:CD1	29:11:70:TRP:C	2.81	0.54
1:13:1133:G:N2	1:13:1141:C:O2	2.41	0.54
1:13:182:U:H5	1:13:183:G:C4	2.26	0.54
26:14:2318:G:H5'	26:14:2319:G:OP2	2.08	0.54
26:14:252:G:OP2	37:35:50:ARG:NH2	2.41	0.54
26:14:270(L):U:O2	34:69:50:ARG:HD3	2.07	0.54
26:14:531:C:H4'	26:14:532:A:H5''	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1G:192:U:H2'	1:1G:193:C:H6	1.72	0.54
1:1G:983:A:H2	1:1G:984:C:C6	2.25	0.54
26:1H:2315:G:H2'	26:1H:2316:C:C6	2.42	0.54
26:1H:533:G:H5'	42:C8:24:TYR:CD1	2.43	0.54
3:22:113:ALA:HA	3:22:202:ILE:HD11	1.88	0.54
1:13:35:G:O2'	12:3I:118:SER:O	2.18	0.54
13:4I:5:ALA:HB2	13:4I:61:GLU:HG2	1.90	0.54
39:55:106:GLY:O	39:55:107:ASP:HB3	2.07	0.54
35:58:96:GLU:HB2	35:58:122:VAL:HG12	1.90	0.54
35:58:22:THR:OG1	35:58:23:LEU:N	2.41	0.54
47:H8:93:ASP:HB3	47:H8:131:ARG:HH21	1.73	0.54
1:13:401:C:OP2	4:3E:73:ARG:HD3	2.08	0.54
1:13:686:U:O4	1:13:703:G:H1'	2.07	0.54
26:14:673:C:H5''	31:39:81:PRO:HD2	1.90	0.54
1:1G:1024:G:OP1	1:1G:1024:G:H4'	2.08	0.54
1:1G:1431:C:H42	1:1G:1469:G:H1	1.55	0.54
1:1G:250:A:H4'	1:1G:251:G:O5'	2.08	0.54
26:1H:2518:A:H8	26:1H:2518:A:H5'	1.73	0.54
26:1H:536:A:H2'	26:1H:537:C:C6	2.43	0.54
27:1J:4:C:H42	27:1J:116:G:H1	1.55	0.54
30:21:105:THR:HG21	30:21:164:ARG:NH1	2.22	0.54
43:95:17:GLY:H	43:95:96:ILE:HB	1.71	0.54
20:BA:86:ARG:HH11	20:BA:86:ARG:HB2	1.72	0.54
46:C5:75:ILE:HG13	46:C5:80:GLY:HA2	1.89	0.54
26:1H:2017:U:O2	53:N8:10:LYS:HB2	2.07	0.54
26:14:1434:A:H61	26:14:1558:A:H62	1.56	0.54
26:14:2233:U:H2'	26:14:2234:G:C8	2.42	0.54
26:14:278:A:OP2	26:14:278:A:H2'	2.08	0.54
26:14:363(E):U:H5'	26:14:363(F):A:OP2	2.07	0.54
26:14:955:C:OP1	38:45:87:LYS:HE2	2.07	0.54
26:1H:2507:C:OP1	62:1H:3774:HOH:O	2.18	0.54
23:2K:24:C:H2'	23:2K:25:U:C6	2.42	0.54
4:32:104:VAL:O	4:32:108:LEU:HB2	2.08	0.54
4:32:173:TRP:CZ3	4:32:193:ASP:HB3	2.43	0.54
24:3K:72:C:H2'	24:3K:73:A:H5''	1.90	0.54
42:85:92:ARG:C	42:85:94:ASN:H	2.10	0.54
52:M8:14:ILE:HG22	52:M8:24:THR:HG22	1.89	0.54
1:13:631:G:O2'	1:13:632:A:O5'	2.21	0.54
26:14:1946:U:H2'	26:14:1947:C:C6	2.43	0.54
26:14:67:U:H2'	26:14:68:G:C8	2.43	0.54
35:15:47:ALA:HB2	35:15:112:LEU:HD21	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:16:15:A:H3'	27:16:16:G:H5'	1.88	0.54
2:1E:100:GLY:O	2:1E:104:ASN:N	2.36	0.54
26:1H:1290:C:H2'	26:1H:1291:C:C6	2.43	0.54
26:1H:1420:U:HO2'	26:1H:1421:G:P	2.31	0.54
26:1H:2232:U:P	49:J8:40:ARG:HH12	2.31	0.54
26:1H:364:C:H3'	62:1H:3873:HOH:O	2.07	0.54
26:1H:569:U:C4	26:1H:570:G:C6	2.96	0.54
26:1H:593:G:C1'	56:Q8:4:MET:HE1	2.38	0.54
30:29:4:ILE:HD13	30:29:28:ALA:HB1	1.89	0.54
26:14:811:U:O2'	37:35:21:ARG:HG3	2.08	0.54
13:4A:13:LYS:HD3	13:4A:14:ARG:N	2.23	0.54
35:58:42:TRP:HA	35:58:48:MET:SD	2.48	0.54
26:1H:2820:A:O5'	39:98:4:LEU:HD23	2.07	0.54
1:13:244:U:H4'	1:13:245:C:O5'	2.08	0.54
1:13:648:A:N6	1:13:649:G:O6	2.40	0.54
10:1A:11:PHE:CE1	10:1A:67:THR:HG22	2.43	0.54
1:1G:1139:G:H22	1:1G:1143:G:H1	1.55	0.54
1:1G:1178:G:H5''	9:82:93:ARG:NH2	2.23	0.54
26:1H:107:C:H2'	26:1H:108:U:H6	1.73	0.54
26:1H:1259:G:H2'	26:1H:1260:G:C8	2.43	0.54
26:1H:1386:C:H2'	26:1H:1387:C:C6	2.41	0.54
26:1H:1533:C:H3'	26:1H:1534:G:H5''	1.90	0.54
26:1H:259:G:N2	26:1H:621:A:H8	2.05	0.54
10:1I:54:PHE:CZ	10:1I:55:LYS:NZ	2.68	0.54
3:2E:114:PRO:O	3:2E:118:GLN:HG3	2.08	0.54
13:4A:91:ARG:HB2	13:4A:98:VAL:HG12	1.89	0.54
33:59:27:LYS:HD3	33:59:32:GLU:HG3	1.90	0.54
7:62:59:LEU:HD21	7:62:63:LYS:HZ2	1.72	0.54
9:8E:8:GLY:HA3	9:8E:79:LEU:HB3	1.90	0.54
1:1G:719:C:O2'	18:9A:49:LYS:HB3	2.08	0.54
41:B8:58:ASN:O	41:B8:58:ASN:ND2	2.40	0.54
47:D5:128:VAL:HG22	47:D5:129:SER:H	1.73	0.54
26:1H:142:G:H1'	45:F8:37:THR:CG2	2.38	0.54
1:13:1149:C:H2'	1:13:1150:U:H6	1.72	0.53
1:13:271:C:H2'	1:13:272:C:H6	1.73	0.53
1:13:2:U:H5''	1:13:630:G:H21	1.73	0.53
1:13:843:U:H3'	1:13:848:C:C6	2.43	0.53
26:14:579:G:H2'	26:14:580:C:C6	2.43	0.53
26:14:754:C:H2'	26:14:755:C:H6	1.73	0.53
27:16:73:A:C4	27:16:104:A:C2	2.96	0.53
27:16:80:U:H2'	27:16:81:G:N2	2.20	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1H:1019:U:HO2'	26:1H:1021:A:H2	1.56	0.53
26:1H:2518:A:C8	26:1H:2518:A:H5'	2.42	0.53
26:1H:2053:G:H5'	30:21:144:ARG:O	2.08	0.53
26:1H:2572:A:N7	30:21:145:LYS:HB2	2.22	0.53
36:25:63:VAL:HB	36:25:102:VAL:HG12	1.89	0.53
30:29:51:PHE:CG	30:29:52:LEU:N	2.74	0.53
11:2I:72:ALA:HB1	11:2I:77:MET:HE3	1.88	0.53
40:65:23:ARG:HB2	40:65:86:ALA:HB2	1.89	0.53
37:78:63:PRO:HB2	56:Q8:30:ARG:NH2	2.06	0.53
41:B8:50:ILE:HD11	41:B8:102:ILE:HG13	1.88	0.53
49:F5:32:LYS:O	62:F5:101:HOH:O	2.18	0.53
53:N8:41:PRO:O	53:N8:44:THR:OG1	2.24	0.53
37:78:59:LEU:HD11	56:Q8:10:ALA:HA	1.90	0.53
29:11:84:TYR:CE1	29:11:86:PRO:HB3	2.36	0.53
1:13:1126:U:O2	1:13:1280:A:C8	2.62	0.53
26:14:1569:A:O2'	29:19:37:LEU:HD23	2.09	0.53
26:14:1332:G:N2	26:14:1609:A:O2'	2.42	0.53
26:14:273(C):C:N4	26:14:363(C):G:H1	2.07	0.53
26:14:67:U:H2'	26:14:68:G:H8	1.73	0.53
2:1E:11:LEU:HG	2:1E:213:LEU:HD13	1.91	0.53
1:1G:1494:G:N7	58:1G:1702:PAR:N32	2.56	0.53
26:1H:1203:G:H3'	26:1H:1204:A:H5''	1.91	0.53
26:1H:1359:A:C2	26:1H:1372:U:O4	2.61	0.53
26:1H:2788:C:O2'	26:1H:2809:A:N3	2.41	0.53
26:1H:315:G:H2'	26:1H:316:C:C6	2.42	0.53
27:1J:44:G:H1'	27:1J:47:C:N4	2.23	0.53
3:2E:15:THR:CG2	3:2E:181:ASN:HA	2.38	0.53
31:39:146:ALA:HB3	31:39:148:LEU:HG	1.89	0.53
24:3L:35:U:O2	24:3L:36:U:N3	2.41	0.53
32:41:97:ASP:O	32:41:100:TRP:N	2.42	0.53
38:45:57:HIS:ND1	38:45:117:ALA:HB2	2.23	0.53
13:4A:29:ARG:HD3	13:4A:64:TRP:CE2	2.44	0.53
7:62:69:VAL:HG12	7:62:103:TRP:HE3	1.72	0.53
34:69:124:GLY:O	34:69:142:VAL:HG23	2.07	0.53
47:D5:10:ARG:HH21	47:D5:26:GLY:N	2.06	0.53
47:H8:98:MET:O	47:H8:125:LEU:HA	2.08	0.53
50:K8:15:LYS:HZ2	50:K8:15:LYS:N	2.03	0.53
55:P8:12:ARG:NH2	55:P8:44:PRO:HB3	2.23	0.53
2:12:103:THR:HG23	2:12:176:GLU:HB3	1.90	0.53
1:13:1157:A:H61	1:13:1178:G:H21	1.57	0.53
1:13:157:G:H2'	1:13:158:G:C8	2.44	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:13:536:C:H2'	1:13:537:G:C8	2.42	0.53
1:13:5:U:O2'	1:13:6:G:O5'	2.26	0.53
1:13:920:U:H2'	1:13:921:U:C6	2.42	0.53
26:14:1871:A:H2'	26:14:1872:A:C8	2.42	0.53
26:14:2125:G:H21	26:14:2173:A:N6	2.07	0.53
26:14:235:U:H2'	26:14:236:C:C6	2.44	0.53
26:14:602:G:OP2	26:14:602:G:H8	1.91	0.53
2:1E:178:ARG:HG3	8:7E:72:PRO:HA	1.91	0.53
1:1G:1306:A:N6	1:1G:1331:G:O2'	2.41	0.53
26:1H:1486:A:H2'	26:1H:1487:G:C8	2.42	0.53
26:1H:2125:G:H21	26:1H:2173:A:H62	1.57	0.53
30:29:37:ARG:HD2	30:29:44:TYR:OH	2.08	0.53
31:31:198:ALA:O	31:31:201:VAL:N	2.41	0.53
24:3K:35:U:H2'	24:3K:36:U:C6	2.43	0.53
5:42:51:VAL:O	5:42:55:VAL:HG23	2.07	0.53
13:4A:19:LEU:HB3	13:4A:25:ILE:HG21	1.90	0.53
33:51:4:ILE:HG23	33:51:6:ARG:NH2	2.23	0.53
46:G8:43:ASN:O	46:G8:64:GLU:HA	2.08	0.53
49:J8:77:ALA:HA	49:J8:78:LYS:C	2.28	0.53
29:11:238:GLY:HA2	62:11:311:HOH:O	2.08	0.53
1:13:976:G:N2	1:13:1362(A):C:OP2	2.39	0.53
1:13:345:C:H4'	1:13:346:G:N7	2.23	0.53
26:14:1520:U:H2'	26:14:1521:G:O4'	2.09	0.53
26:14:307:G:N2	26:14:309:G:H3'	2.24	0.53
2:1E:54:THR:HG23	2:1E:185:ILE:HD11	1.90	0.53
1:1G:1228:C:H2'	1:1G:1229:A:H8	1.73	0.53
1:1G:1316:G:H2'	1:1G:1317:C:H5"	1.89	0.53
1:1G:1344:C:H5"	9:82:120:ARG:O	2.09	0.53
26:1H:1088:A:H5'	26:1H:1089:G:H5'	1.90	0.53
26:1H:2235:G:H2'	26:1H:2236:C:C6	2.44	0.53
26:1H:2306:C:H3'	26:1H:2307:G:H5'	1.91	0.53
26:1H:2308:G:N1	26:1H:2311:A:H2	1.94	0.53
26:1H:2573:C:H3'	62:1H:3962:HOH:O	2.07	0.53
26:1H:2756:U:H4'	26:1H:2757:A:OP1	2.07	0.53
30:21:101:ARG:CZ	30:21:171:GLU:HB2	2.39	0.53
26:1H:2786:U:O2'	30:21:62:PRO:O	2.20	0.53
26:14:1665:A:H4'	36:25:67:LYS:HB2	1.91	0.53
30:29:101:ARG:CZ	30:29:171:GLU:HB2	2.38	0.53
30:29:31:CYS:SG	30:29:51:PHE:HB2	2.48	0.53
11:2I:21:ILE:HG12	11:2I:30:VAL:HG12	1.89	0.53
12:3A:60:LEU:HD23	12:3A:64:TYR:HB3	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:3I:8:ASN:O	12:3I:11:VAL:HG23	2.09	0.53
6:5E:96:PRO:HB3	18:9I:30:ASP:OD2	2.08	0.53
14:5I:3:ARG:HB2	14:5I:3:ARG:HH11	1.72	0.53
8:72:103:VAL:HG21	8:72:110:ALA:HB2	1.91	0.53
38:88:32:TYR:OH	38:88:111:GLU:OE1	2.19	0.53
38:88:37:LEU:HD21	38:88:130:LYS:HE3	1.89	0.53
45:B5:50:LYS:HB2	45:B5:87:GLN:NE2	2.24	0.53
1:13:491:G:H2'	1:13:492:G:O4'	2.08	0.53
1:13:703:G:H8	1:13:703:G:O5'	1.90	0.53
26:14:2849:U:OP1	41:75:95:ARG:NH1	2.42	0.53
26:14:94:G:N3	50:G5:47:ASN:ND2	2.56	0.53
1:1G:1167:A:H2'	1:1G:1169:A:O4'	2.09	0.53
1:1G:1169:A:C6	1:1G:1170:A:C6	2.97	0.53
1:1G:1238:A:H62	1:1G:1301:U:H3	1.57	0.53
1:1G:828:A:H2'	1:1G:829:G:O4'	2.08	0.53
1:1G:8:A:C6	4:32:209:ARG:HB2	2.44	0.53
26:1H:2001:A:H2'	26:1H:2002:G:C8	2.44	0.53
3:22:175:LEU:H	3:22:175:LEU:HD12	1.74	0.53
40:65:67:ARG:NH1	40:65:67:ARG:HB2	2.23	0.53
1:1G:750:G:N3	15:6A:23:GLY:HA3	2.23	0.53
8:72:20:TYR:HA	8:72:65:TYR:CZ	2.43	0.53
41:75:88:ILE:HD11	41:75:91:ARG:HG2	1.89	0.53
16:7A:21:VAL:HG22	16:7A:33:ILE:HB	1.91	0.53
2:12:95:GLN:HB2	2:12:148:TYR:HA	1.90	0.53
2:12:97:TRP:HZ3	2:12:99:GLY:HA2	1.74	0.53
1:13:1376:U:H2'	1:13:1377:A:C8	2.43	0.53
1:13:1402:C:H2'	1:13:1403:C:O4'	2.07	0.53
1:13:1478:C:H2'	1:13:1479:C:C6	2.44	0.53
1:13:417:C:H2'	1:13:418:C:H6	1.73	0.53
1:13:542:G:OP1	4:3E:10:ARG:NH2	2.42	0.53
1:13:690:G:H2'	1:13:691:G:O4'	2.08	0.53
26:14:1203:G:H3'	26:14:1204:A:H5''	1.90	0.53
26:14:1321:A:H2'	26:14:1322:A:O4'	2.09	0.53
26:14:2129:C:H3'	26:14:2130:U:C6	2.43	0.53
26:14:39:C:H2'	26:14:40:C:C6	2.44	0.53
26:14:636:G:O2'	26:14:638:G:O2'	2.19	0.53
27:16:8:U:O3'	40:A8:25:ARG:NH2	2.41	0.53
33:51:83:TYR:HB3	33:51:135:GLY:H	1.74	0.53
33:59:167:GLU:HG3	33:59:169:VAL:HG23	1.90	0.53
14:5A:17:LYS:HZ3	14:5A:18:VAL:HG13	1.74	0.53
1:13:976:G:OP1	14:5I:32:SER:N	2.41	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1G:751:U:H4'	15:6A:24:SER:HA	1.89	0.53
9:82:71:SER:HA	9:82:74:ILE:HD12	1.90	0.53
42:85:110:VAL:HG12	42:85:114:LYS:HD3	1.90	0.53
9:8E:21:PRO:HA	9:8E:59:PHE:HD1	1.73	0.53
26:14:2396:G:H4'	49:F5:30:VAL:H	1.74	0.53
27:16:44:G:H1'	27:16:47:C:N4	2.24	0.53
29:19:77:ALA:HB2	29:19:97:TYR:CD2	2.44	0.53
10:1A:40:LEU:HG	10:1A:41:PRO:HD2	1.90	0.53
26:1H:2287:A:N1	26:1H:2346:A:H2	2.07	0.53
26:1H:2780:G:OP1	35:58:118:LYS:HE2	2.09	0.53
10:1I:84:GLN:HB3	10:1I:88:LEU:HD23	1.90	0.53
27:1J:7:G:H4'	40:65:29:PHE:HD2	1.70	0.53
39:55:82:GLU:H	39:55:85:PRO:HG2	1.73	0.53
36:68:34:THR:OG1	36:68:35:VAL:N	2.42	0.53
7:6E:102:ARG:O	7:6E:106:GLN:HG3	2.08	0.53
41:75:132:LYS:HB3	41:75:133:GLU:OE1	2.08	0.53
16:7I:5:ARG:HE	16:7I:22:THR:HG21	1.73	0.53
26:1H:910:A:H62	38:88:12:GLN:HA	1.74	0.53
9:8E:46:ALA:HB2	9:8E:74:ILE:HG23	1.90	0.53
20:BI:71:THR:HG22	20:BI:72:LEU:N	2.21	0.53
47:H8:116:VAL:H	47:H8:146:ILE:HG12	1.74	0.53
1:13:1000:A:H2'	1:13:1001:G:H8	1.74	0.53
35:15:30:ILE:HG22	35:15:34:LEU:HD22	1.90	0.53
1:1G:422:C:HO2'	1:1G:423:G:N2	2.06	0.53
1:1G:438:G:H4'	4:32:123:HIS:ND1	2.24	0.53
26:1H:1899:G:H22	26:1H:1902:C:H41	1.56	0.53
26:1H:1968:G:OP1	62:1H:3775:HOH:O	2.19	0.53
26:1H:528:A:N1	26:1H:2042:A:H2'	2.23	0.53
27:1J:94:C:H2'	27:1J:95:U:C6	2.43	0.53
1:1G:777:A:C2	11:2A:119:CYS:HB3	2.44	0.53
37:35:105:LEU:O	37:35:106:LEU:HB3	2.09	0.53
11:2A:54:ARG:NH2	24:3L:40:C:OP1	2.41	0.53
13:4I:34:LEU:HD13	13:4I:41:PRO:HA	1.90	0.53
16:7A:19:ILE:HB	16:7A:36:ILE:O	2.09	0.53
9:8E:86:VAL:O	9:8E:90:PRO:HB3	2.09	0.53
26:14:495:G:H21	44:A5:61:ASN:HD21	1.57	0.53
41:B8:29:ARG:HB2	41:B8:46:GLU:HG3	1.91	0.53
52:M8:42:PHE:CG	52:M8:42:PHE:O	2.61	0.53
1:13:1256:A:O2'	1:13:1257:U:O5'	2.25	0.53
26:14:363:G:H2'	26:14:363(A):A:H8	1.74	0.53
1:1G:345:C:H5'	1:1G:346:G:C5	2.44	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1G:998(A):C:H2'	1:1G:999:U:C6	2.43	0.53
4:32:12:CYS:SG	4:32:18:LYS:HA	2.49	0.53
37:35:85:LEU:HG	37:35:120:ALA:HA	1.91	0.53
45:B5:89:ILE:O	45:B5:93:GLU:HG2	2.09	0.53
26:14:2291:U:H2'	26:14:2292:C:C6	2.44	0.53
26:14:399:G:OP2	62:14:3647:HOH:O	2.18	0.53
2:1E:54:THR:HG21	2:1E:201:ILE:HD11	1.90	0.53
1:1G:867:G:O2'	1:1G:868:C:H5'	2.09	0.53
26:1H:2108:C:H2'	26:1H:2109:U:O4'	2.09	0.53
26:1H:2314:C:H2'	26:1H:2315:G:C8	2.41	0.53
26:1H:950:G:H2'	26:1H:951:C:C6	2.44	0.53
26:1H:95:G:O2'	50:K8:48:HIS:HB3	2.08	0.53
30:21:143:ASN:HD22	30:21:147:PRO:HD2	1.74	0.53
26:14:2823:A:OP1	30:29:113:PHE:HB2	2.09	0.53
1:13:1190:G:H5''	3:2E:176:HIS:CE1	2.44	0.53
4:3E:161:ASN:O	4:3E:165:MET:HB2	2.09	0.53
14:5A:37:PHE:CE1	14:5A:53:LEU:HD13	2.44	0.53
8:7E:129:VAL:HG23	8:7E:130:GLY:H	1.74	0.53
1:13:376:G:H5''	16:7I:5:ARG:HD2	1.90	0.53
7:62:16:LEU:HD11	9:82:45:ALA:HB2	1.91	0.53
17:8A:88:TYR:CZ	17:8A:92:ARG:HD2	2.44	0.53
44:A5:60:ASN:OD1	44:A5:60:ASN:N	2.41	0.53
29:11:126:GLN:HG2	29:11:127:VAL:N	2.24	0.52
1:13:1396:A:H4'	1:13:1397:C:H5''	1.91	0.52
1:13:411:A:N9	1:13:413:G:H1'	2.24	0.52
26:14:1678:G:N2	26:14:1989:G:N2	2.56	0.52
1:1G:1343:G:H2'	1:1G:1344:C:C6	2.44	0.52
1:1G:629:G:H2'	1:1G:630:G:O4'	2.09	0.52
26:1H:1332:G:N2	26:1H:1609:A:HO2'	2.07	0.52
26:1H:1378:A:O2'	62:1H:3767:HOH:O	2.15	0.52
26:1H:2656:U:N3	26:1H:2665:A:H2	2.04	0.52
31:31:107:LYS:HE2	31:31:207:GLY:N	2.24	0.52
32:41:97:ASP:H	32:41:100:TRP:HD1	1.56	0.52
5:4E:10:MET:HA	5:4E:32:VAL:HA	1.91	0.52
26:14:1652:A:OP1	39:55:8:ARG:NH1	2.42	0.52
33:59:171:LEU:HD13	33:59:172:LYS:H	1.74	0.52
41:75:88:ILE:HG13	41:75:88:ILE:O	2.08	0.52
40:A8:10:ARG:O	40:A8:14:VAL:HG13	2.08	0.52
47:H8:103:ARG:HD3	47:H8:136:PHE:CD1	2.44	0.52
47:H8:61:LEU:O	47:H8:64:GLY:HA2	2.09	0.52
56:Q8:46:ARG:HB2	56:Q8:47:LYS:HB2	1.89	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:13:429:U:H3'	4:3E:9:CYS:SG	2.49	0.52
1:13:757:U:H2'	1:13:758:G:O4'	2.08	0.52
26:14:273(F):C:H3'	26:14:274:G:C5'	2.39	0.52
27:16:60:C:C2	27:16:61:G:C8	2.97	0.52
1:1G:1062:U:H2'	1:1G:1063:C:C6	2.44	0.52
1:1G:1132:C:H2'	1:1G:1133:G:C8	2.43	0.52
1:1G:256:U:H2'	1:1G:257:G:C8	2.45	0.52
1:1G:736:C:OP1	18:9A:72:ARG:NH2	2.43	0.52
26:1H:2689:U:H6	26:1H:2689:U:H5'	1.74	0.52
26:1H:600:G:N2	26:1H:605:C:O3'	2.42	0.52
3:22:11:ARG:NH2	3:22:182:ILE:HD11	2.24	0.52
31:39:133:ASN:HA	31:39:162:LEU:HD23	1.91	0.52
36:68:4:PRO:HA	36:68:21:CYS:O	2.09	0.52
34:69:72:LEU:HD21	34:69:107:VAL:HG11	1.90	0.52
34:69:77:LEU:HG	34:69:141:LYS:HE2	1.91	0.52
34:69:14:ASP:O	34:69:17:GLN:HB2	2.09	0.52
41:75:3:ARG:N	41:75:4:GLY:O	2.42	0.52
42:85:92:ARG:CZ	43:95:11:GLN:H	2.22	0.52
9:8E:45:ALA:O	9:8E:78:LYS:NZ	2.35	0.52
39:98:32:GLY:HA2	39:98:116:LEU:CD1	2.39	0.52
46:G8:55:TYR:CZ	46:G8:61:ILE:HD11	2.44	0.52
56:Q8:52:LYS:N	56:Q8:53:PRO:HD2	2.23	0.52
1:13:313:A:H2'	1:13:314:C:H6	1.75	0.52
26:14:1239:G:H2'	26:14:1240:U:O4'	2.09	0.52
26:14:2689:U:P	26:14:2719:G:H22	2.32	0.52
26:14:2777:G:OP2	26:14:2781:A:O2'	2.20	0.52
26:14:662:G:H5"	37:35:16:ARG:HG2	1.91	0.52
26:14:7:G:H2'	26:14:8:A:C8	2.45	0.52
1:1G:934:C:O2'	1:1G:1344:C:OP2	2.26	0.52
1:1G:41:G:H2'	1:1G:42:G:H8	1.74	0.52
26:1H:389:G:H1	37:78:71:VAL:HG12	1.74	0.52
24:1L:9:A:N6	24:1L:23:A:N7	2.57	0.52
23:2K:16:C:O2'	23:2K:62:C:OP1	2.25	0.52
24:3L:9:A:H2'	24:3L:11:C:N4	2.24	0.52
1:13:1423:G:OP1	36:68:49:ARG:NH2	2.42	0.52
37:78:118:GLY:O	37:78:137:LYS:NZ	2.42	0.52
17:8I:88:TYR:CD1	17:8I:89:LEU:HD23	2.45	0.52
43:D8:65:GLY:HA3	43:D8:91:TYR:CE2	2.45	0.52
47:H8:113:ALA:N	47:H8:114:GLY:HA2	2.24	0.52
29:11:146:GLU:HB2	29:11:189:CYS:HB3	1.91	0.52
26:14:1133:U:O2	26:14:1137:G:H5"	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:14:1416:G:O2'	26:14:1417:C:O5'	2.25	0.52
26:14:2129:C:H5''	26:14:2130:U:C5	2.44	0.52
29:19:133:LEU:HB3	29:19:173:VAL:HG11	1.92	0.52
2:1E:162:ILE:O	2:1E:185:ILE:HG23	2.09	0.52
2:1E:93:VAL:HG11	2:1E:97:TRP:HD1	1.75	0.52
1:1G:1142:G:H3'	1:1G:1143:G:C8	2.45	0.52
26:1H:2065:C:H2'	26:1H:2066:C:C6	2.44	0.52
26:1H:2105:C:H2'	26:1H:2106:G:C8	2.41	0.52
26:1H:2680:C:H5'	30:21:189:PRO:HA	1.92	0.52
26:1H:760:G:H2'	26:1H:761:A:O4'	2.09	0.52
1:13:963:G:N2	10:1I:55:LYS:NZ	2.57	0.52
3:22:43:LEU:HD23	3:22:47:LEU:HB2	1.90	0.52
4:32:31:CYS:H	4:32:35:ARG:NH1	2.06	0.52
9:8E:17:VAL:HA	9:8E:63:ILE:HG12	1.90	0.52
47:D5:99:TYR:HD2	47:D5:123:ASP:HB3	1.74	0.52
29:11:79:VAL:O	29:11:113:VAL:HG23	2.09	0.52
1:13:1190:G:H5''	3:2E:176:HIS:NE2	2.23	0.52
1:13:130:A:O2'	1:13:131:C:O5'	2.24	0.52
26:14:450:G:N7	62:14:3706:HOH:O	2.34	0.52
26:14:823:G:H2'	26:14:824:A:C8	2.44	0.52
1:1G:1289:A:OP1	21:1B:9:ARG:NH2	2.43	0.52
21:1F:10:ARG:HH11	21:1F:10:ARG:HB3	1.74	0.52
1:1G:134:A:H61	16:7A:25:ARG:NH1	2.07	0.52
1:1G:67:C:H2'	1:1G:68:G:C8	2.45	0.52
1:1G:892:A:O2'	1:1G:1415:G:H4'	2.09	0.52
26:1H:1449(A):G:H2'	26:1H:1450:C:H6	1.74	0.52
4:32:70:ILE:HD11	4:32:75:PHE:HD1	1.75	0.52
13:4A:31:LYS:O	13:4A:35:GLU:HG2	2.09	0.52
5:4E:148:VAL:HG21	8:7E:107:LEU:HG	1.91	0.52
25:4K:13:A:N6	25:4K:14:A:N7	2.57	0.52
28:71:27:HIS:HA	28:71:182:PRO:HB3	1.90	0.52
16:7I:3:LYS:HG2	16:7I:24:ALA:HB2	1.90	0.52
42:85:98:LEU:HA	42:85:100:VAL:O	2.10	0.52
17:8I:45:HIS:HB3	17:8I:72:ARG:HG2	1.89	0.52
40:A8:99:LYS:O	40:A8:103:GLU:HG2	2.09	0.52
42:C8:102:GLU:OE1	43:D8:13:ARG:NH2	2.42	0.52
47:D5:5:LEU:HG	47:D5:47:VAL:HG21	1.92	0.52
44:E8:24:ILE:HD12	44:E8:24:ILE:O	2.10	0.52
26:14:2018:G:P	53:J5:9:LYS:HZ1	2.32	0.52
49:J8:53:VAL:HB	49:J8:58:ILE:HD13	1.92	0.52
52:M8:15:ILE:HB	52:M8:32:TYR:CD1	2.45	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:13:1015:A:H2'	1:13:1016:A:H8	1.74	0.52
1:13:1126:U:H2'	1:13:1127:G:C5'	2.40	0.52
1:13:539:A:H2'	1:13:540:G:C8	2.44	0.52
1:13:827:U:C5	1:13:872:A:N1	2.77	0.52
26:14:1190:G:H2'	26:14:1191:G:H8	1.75	0.52
26:14:1568:G:OP1	29:19:63:ARG:NH1	2.38	0.52
26:14:1757:U:N3	26:14:1762:A:H2	2.02	0.52
26:14:2282:G:H4'	26:14:2389:G:O2'	2.09	0.52
29:19:35:LYS:HG2	29:19:35:LYS:O	2.10	0.52
29:19:44:ASN:CB	29:19:45:ASN:HA	2.31	0.52
1:1G:411:A:OP1	4:32:30:LYS:NZ	2.43	0.52
1:1G:411:A:H62	1:1G:413:G:N2	2.07	0.52
1:1G:429:U:H3'	4:32:9:CYS:SG	2.50	0.52
1:1G:815:A:N7	1:1G:1509:C:O2'	2.36	0.52
26:1H:1107:G:H2'	26:1H:1108:U:C6	2.45	0.52
26:1H:1314:C:OP1	62:1H:3747:HOH:O	2.19	0.52
26:1H:2068:U:N3	26:1H:2430:A:H2	2.08	0.52
26:1H:2836:U:H2'	26:1H:2837:G:C8	2.45	0.52
26:1H:515:A:H1'	26:1H:581:C:H1'	1.92	0.52
26:1H:945:A:H4'	62:1H:3603:HOH:O	2.09	0.52
3:22:150:LYS:HE3	3:22:152:ILE:HG13	1.91	0.52
26:1H:443:A:N7	31:31:45:ARG:HG2	2.24	0.52
31:39:124:LEU:HG	31:39:126:VAL:HG12	1.91	0.52
31:39:129:PHE:HA	31:39:142:TRP:CD1	2.45	0.52
32:41:114:ILE:HG22	32:41:115:ARG:O	2.10	0.52
38:45:137:TYR:HD1	38:45:137:TYR:C	2.13	0.52
26:14:2820:A:P	39:55:2:ARG:HH12	2.33	0.52
1:1G:1059:C:O3'	14:5A:45:ARG:NH2	2.43	0.52
37:78:121:LYS:O	37:78:123:LEU:N	2.42	0.52
56:M5:22:VAL:O	56:M5:50:LEU:HB3	2.10	0.52
52:M8:42:PHE:CD2	52:M8:42:PHE:O	2.63	0.52
1:13:1315:U:H2'	1:13:1316:G:O4'	2.10	0.52
1:13:1533:C:O2'	1:13:1534:A:OP1	2.23	0.52
26:14:1641:A:H2'	26:14:1642:G:O4'	2.10	0.52
26:14:2105:C:H2'	26:14:2106:G:O4'	2.09	0.52
26:14:691:C:O4'	29:19:43:ARG:NH2	2.43	0.52
1:1G:554:C:H2'	1:1G:555:C:H6	1.75	0.52
1:1G:583:A:H2'	1:1G:584:G:O4'	2.10	0.52
26:1H:1794:U:H2'	26:1H:1795:C:H6	1.75	0.52
26:1H:2131:G:H5'	26:1H:2132:U:H3'	1.92	0.52
26:1H:2389:G:H5''	26:1H:2390:U:O4'	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1H:589:C:H2'	26:1H:590:A:C8	2.45	0.52
26:1H:658:C:H2'	26:1H:659:C:C6	2.45	0.52
26:1H:729:G:O5'	29:11:208:LYS:NZ	2.42	0.52
30:21:59:VAL:HG13	30:21:60:ASN:H	1.75	0.52
3:2E:175:LEU:HD21	3:2E:201:TYR:CE2	2.45	0.52
11:2I:79:SER:HB2	11:2I:106:LYS:HD2	1.90	0.52
4:32:61:LYS:NZ	4:32:72:GLU:OE2	2.31	0.52
31:39:130:ALA:H	31:39:142:TRP:HD1	1.58	0.52
33:51:33:LEU:HD12	33:51:75:ALA:HA	1.91	0.52
33:51:43:VAL:HB	33:51:52:VAL:HG22	1.91	0.52
28:71:218:MET:N	28:71:218:MET:SD	2.82	0.52
16:7I:4:ILE:HB	16:7I:66:PRO:HB3	1.91	0.52
39:98:117:VAL:O	39:98:118:GLU:HB2	2.09	0.52
18:9I:52:PRO:O	18:9I:56:THR:HG23	2.09	0.52
40:A8:106:ARG:HA	40:A8:110:LEU:H	1.75	0.52
20:BI:46:GLU:HB2	20:BI:48:LYS:HG3	1.91	0.52
47:D5:53:ILE:HG22	47:D5:71:VAL:HG13	1.90	0.52
50:K8:47:ASN:O	50:K8:49:LYS:HG3	2.10	0.52
50:K8:3:LEU:H	50:K8:4:SER:C	2.13	0.52
2:12:127:ILE:HA	2:12:130:ARG:CZ	2.39	0.52
1:13:1194:U:H2'	1:13:1195:C:C6	2.45	0.52
1:13:17:U:H2'	1:13:18:C:C6	2.45	0.52
1:13:129(A):G:C2	1:13:188:U:O2'	2.63	0.52
26:14:1108:U:H5''	26:14:1109:C:OP2	2.09	0.52
26:14:2329:G:H2'	26:14:2330:G:C8	2.44	0.52
1:1G:113:G:O4'	1:1G:354:G:H4'	2.10	0.52
1:1G:26:A:N6	1:1G:558:G:O2'	2.41	0.52
1:1G:973:G:H1'	10:1A:55:LYS:HG2	1.92	0.52
26:1H:1050:A:C8	26:1H:2751:G:N7	2.78	0.52
26:1H:1359:A:H2'	26:1H:1360:A:H5'	1.92	0.52
27:1J:17:C:H2'	27:1J:18:G:O4'	2.09	0.52
24:3K:8:U:H5'	24:3K:48:C:O2'	2.09	0.52
7:62:115:ARG:O	7:62:118:VAL:HG22	2.09	0.52
1:13:1240:U:OP1	7:6E:119:ARG:NH2	2.41	0.52
1:1G:192:U:C4'	20:BA:103:GLY:HA2	2.40	0.52
47:D5:94:GLU:HB3	47:D5:96:VAL:HG23	1.91	0.52
43:D8:59:ALA:HB2	43:D8:96:ILE:HD13	1.92	0.52
56:M5:14:VAL:CG1	56:M5:22:VAL:HG13	2.39	0.52
54:O8:15:GLU:HA	54:O8:49:HIS:HA	1.92	0.52
26:14:185:U:H4'	26:14:218:A:H4'	1.92	0.52
26:14:2689:U:OP2	26:14:2719:G:N2	2.42	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:14:395:U:O2'	26:14:396:G:N7	2.32	0.52
26:14:827:U:H2'	26:14:2430:A:C2	2.44	0.52
1:1G:1008:C:H42	1:1G:1021:G:H22	1.57	0.52
1:1G:1324:A:H2'	1:1G:1325:C:H6	1.75	0.52
1:1G:1423:G:H2'	1:1G:1424:C:H6	1.75	0.52
1:1G:198:G:H2'	1:1G:199:G:H8	1.75	0.52
1:1G:1:U:O5'	1:1G:630:G:N2	2.42	0.52
1:1G:690:G:H2'	1:1G:691:G:O4'	2.10	0.52
1:1G:742:G:OP2	15:6A:35:ARG:NH2	2.34	0.52
26:1H:2389:G:H5''	26:1H:2390:U:H5'	1.91	0.52
26:1H:2563:U:H1'	26:1H:2566:A:N6	2.25	0.52
30:21:51:PHE:CE2	30:21:52:LEU:HD23	2.44	0.52
36:25:22:ILE:HG22	36:25:40:VAL:HB	1.92	0.52
31:31:130:ALA:H	31:31:132:VAL:HG13	1.73	0.52
32:41:56:ALA:HB2	32:41:153:ARG:HE	1.75	0.52
5:42:33:VAL:HG21	5:42:109:ILE:HG12	1.92	0.52
5:4E:75:THR:OG1	5:4E:76:ILE:N	2.42	0.52
7:62:126:ASP:HB3	7:62:131:LYS:O	2.09	0.52
41:75:23:ARG:HG3	41:75:120:ARG:NH1	2.25	0.52
40:A8:106:ARG:CZ	40:A8:107:GLU:HG2	2.39	0.52
47:D5:15:PRO:HA	47:D5:18:LEU:HB2	1.92	0.52
46:G8:39:VAL:O	46:G8:42:VAL:HG22	2.09	0.52
46:G8:28:LYS:NZ	46:G8:64:GLU:OE2	2.30	0.52
53:N8:31:VAL:HG23	53:N8:42:PRO:HG3	1.92	0.52
26:1H:1797:C:O2'	29:11:259:THR:OG1	2.23	0.52
1:13:1258:G:H2'	1:13:1259:C:C6	2.45	0.52
1:1G:1055:A:N7	1:1G:1200:C:N4	2.58	0.52
1:1G:652:U:H1'	1:1G:653:A:H2	1.74	0.52
26:1H:1025:G:C4	26:1H:1135:C:H1'	2.45	0.52
26:1H:1636:C:H2'	26:1H:1637:A:C8	2.45	0.52
26:1H:1675:C:N3	30:21:128:SER:OG	2.42	0.52
26:1H:459:U:H2'	26:1H:460:A:H8	1.75	0.52
12:3I:53:ARG:HB3	12:3I:69:TYR:HE1	1.75	0.52
38:45:90:VAL:O	38:45:91:GLU:HB2	2.10	0.52
33:51:164:TYR:HB2	33:51:167:GLU:HB2	1.92	0.52
7:6E:45:ASP:O	7:6E:49:ILE:HG13	2.10	0.52
40:A8:105:ALA:O	40:A8:109:GLY:HA3	2.10	0.52
50:K8:28:LYS:HB3	50:K8:53:LEU:CD2	2.40	0.52
52:M8:39:CYS:SG	52:M8:41:PRO:HD2	2.50	0.52
1:13:1298:C:P	7:6E:114:ARG:HH22	2.33	0.51
1:13:191(C):G:H2'	1:13:191(D):U:O4'	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:13:191(D):U:H2'	1:13:191(E):G:C8	2.44	0.51
26:14:1154:G:OP1	42:85:58:ARG:HD3	2.11	0.51
26:14:528:A:O2'	26:14:529:A:H5'	2.09	0.51
29:19:72:LYS:HB3	29:19:75:ILE:HD12	1.92	0.51
1:1G:1105:A:H2'	1:1G:1106:G:H8	1.75	0.51
1:1G:1512:U:H2'	1:1G:1513:A:H8	1.75	0.51
26:1H:155:C:H5'	26:1H:161:U:OP2	2.10	0.51
24:3K:56:C:H1'	26:1H:2169:A:H62	1.73	0.51
26:1H:2747:G:O6	26:1H:2755:C:H5''	2.10	0.51
24:1L:59:A:H5''	24:1L:60:U:C5	2.45	0.51
36:25:10:VAL:HG13	36:25:17:ARG:O	2.10	0.51
3:2E:64:VAL:HG12	3:2E:66:VAL:HG23	1.91	0.51
31:31:191:ARG:HB3	31:31:191:ARG:HH11	1.74	0.51
13:4I:8:GLU:O	13:4I:10:PRO:HD3	2.09	0.51
33:59:107:VAL:HG11	33:59:152:ARG:HG2	1.93	0.51
7:62:26:PHE:CE2	7:62:30:ILE:HD11	2.45	0.51
8:7E:86:ILE:HG13	8:7E:133:LEU:HD22	1.92	0.51
38:88:52:VAL:O	38:88:56:ARG:HB2	2.10	0.51
40:A8:36:TYR:HB3	40:A8:52:SER:HB3	1.92	0.51
56:Q8:51:ALA:HB1	56:Q8:52:LYS:HA	1.92	0.51
1:13:827:U:H5	1:13:872:A:N1	2.07	0.51
1:13:890:G:O2'	1:13:906:G:O6	2.24	0.51
26:14:2010:G:O6	62:14:3650:HOH:O	2.19	0.51
24:3L:76:A:O2'	26:14:2394:C:N3	2.40	0.51
26:14:1758:G:C2	26:14:2696:U:H5'	2.45	0.51
2:1E:28:PHE:CE2	2:1E:190:THR:HA	2.44	0.51
1:1G:108:G:H5'	1:1G:109:A:H5''	1.92	0.51
1:1G:998(A):C:O2	1:1G:1042:G:N2	2.33	0.51
26:1H:1174:A:H1'	26:1H:1178:C:N4	2.23	0.51
26:1H:1658:C:H2'	26:1H:1659:U:C6	2.44	0.51
26:1H:1728:G:O6	26:1H:1730:U:H5''	2.10	0.51
26:1H:306:U:H2'	26:1H:307:G:O4'	2.10	0.51
26:1H:35:G:H2'	26:1H:36:G:O4'	2.10	0.51
26:1H:50:U:H3'	26:1H:51:G:H5'	1.90	0.51
24:1L:52:G:N2	24:1L:62:C:O2	2.31	0.51
4:3E:112:VAL:HG12	4:3E:116:GLN:OE1	2.10	0.51
32:49:66:GLN:HE21	32:49:94:LEU:HD23	1.74	0.51
1:1G:1535:C:H41	25:4L:10:G:N2	2.05	0.51
14:5I:6:LEU:HB3	14:5I:23:ARG:NH2	2.25	0.51
15:6I:18:PHE:CZ	15:6I:21:ASP:HB2	2.45	0.51
1:1G:1371:G:OP1	9:82:11:LYS:HG2	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:8A:67:LYS:HA	17:8A:70:ARG:HH12	1.75	0.51
46:G8:87:LYS:HD2	46:G8:89:PHE:HD2	1.75	0.51
26:14:1012:U:C5	35:15:28:THR:HG21	2.44	0.51
26:14:1028:A:H2'	26:14:1029:A:C8	2.46	0.51
26:14:1759:A:H4'	26:14:2715:C:O4'	2.11	0.51
26:14:2238:G:N7	62:14:3707:HOH:O	2.34	0.51
26:1H:1259:G:H2'	26:1H:1260:G:H8	1.74	0.51
26:1H:1678:G:H22	26:1H:1989:G:N2	2.00	0.51
26:1H:2111:C:N3	26:1H:2118:U:O2'	2.39	0.51
26:1H:2321:G:H5''	26:1H:2322:A:OP2	2.09	0.51
26:1H:270(K):C:H1'	26:1H:270(N):G:H1	1.75	0.51
26:1H:818:G:H4'	26:1H:838:C:O3'	2.11	0.51
27:1J:93:C:H2'	27:1J:94:C:H6	1.75	0.51
30:21:68:ALA:HB1	30:21:70:ALA:O	2.11	0.51
30:29:52:LEU:O	30:29:74:PRO:HB2	2.10	0.51
3:2E:142:MET:SD	3:2E:148:GLY:HA2	2.51	0.51
4:3E:50:ARG:HD3	4:3E:51:PRO:HD2	1.91	0.51
6:5E:70:ASP:N	6:5E:70:ASP:OD1	2.41	0.51
9:82:112:LYS:HA	9:82:119:ALA:CB	2.34	0.51
9:82:26:VAL:HG13	9:82:61:ALA:O	2.10	0.51
1:13:128:G:O2'	17:8I:3:LYS:NZ	2.40	0.51
20:BI:50:GLU:HG2	20:BI:100:ILE:HB	1.92	0.51
26:14:111:A:H4'	50:G5:69:ARG:HH22	1.76	0.51
48:I8:63:VAL:HG23	48:I8:64:ASP:O	2.10	0.51
51:L8:4:LEU:HD11	51:L8:39:ASP:HA	1.92	0.51
1:13:1331:G:OP2	13:4I:23:TYR:HD1	1.92	0.51
1:13:51:A:OP2	1:13:52:G:H8	1.94	0.51
26:14:1442:G:H2'	26:14:1443:G:C8	2.45	0.51
26:14:2152:G:N3	26:14:2152:G:H2'	2.25	0.51
26:14:2542:A:H4'	26:14:2542:A:OP1	2.09	0.51
26:14:2651:C:H42	26:14:2669:G:H1	1.57	0.51
26:14:307:G:H21	26:14:330:A:H62	1.59	0.51
26:14:443:A:H1'	26:14:1201:C:O4'	2.10	0.51
26:14:768:G:O2'	26:14:1379:A:N6	2.43	0.51
29:19:35:LYS:HB2	29:19:62:TYR:O	2.10	0.51
2:1E:163:PHE:HA	2:1E:185:ILE:O	2.11	0.51
26:1H:1614:A:H8	26:1H:1614:A:P	2.33	0.51
26:1H:2052:G:H4'	30:21:143:ASN:O	2.11	0.51
26:1H:97:C:H5''	50:K8:2:LYS:HB2	1.92	0.51
27:1J:13:A:H5''	27:1J:15:A:N6	2.26	0.51
26:14:2572:A:C8	30:29:144:ARG:HD2	2.45	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2E:113:ALA:N	3:2E:183:ASP:OD2	2.41	0.51
31:39:3:GLU:N	31:39:3:GLU:OE1	2.44	0.51
33:51:83:TYR:HB2	33:51:134:SER:HA	1.93	0.51
6:52:96:PRO:HB3	18:9A:30:ASP:CG	2.31	0.51
33:59:109:PHE:CZ	33:59:152:ARG:HD3	2.45	0.51
40:65:14:VAL:HG21	40:65:89:ARG:HD3	1.92	0.51
15:6I:67:LEU:O	15:6I:71:GLN:HB2	2.11	0.51
26:1H:2132:U:H3	28:7I:5:LYS:HB2	1.76	0.51
37:78:64:LYS:HD2	56:Q8:12:LYS:HB3	1.92	0.51
9:8E:53:VAL:HG21	9:8E:85:LEU:HD22	1.92	0.51
45:B5:1:MET:N	50:G5:29:LYS:HE3	2.24	0.51
55:P8:15:THR:HG22	55:P8:16:HIS:CE1	2.46	0.51
1:13:1412:C:H2'	1:13:1413:A:C8	2.46	0.51
1:13:266:G:H5''	1:13:267:C:C5	2.46	0.51
1:13:77:C:H2'	1:13:78:G:H8	1.74	0.51
1:13:8:A:H62	4:3E:208:SER:HB2	1.75	0.51
26:14:1425:G:H2'	26:14:1426:G:C8	2.46	0.51
26:14:2513:G:N2	30:29:143:ASN:HD21	2.08	0.51
26:14:2579:C:H4'	30:29:134:ILE:HG12	1.93	0.51
26:14:2711:A:OP2	62:14:3507:HOH:O	2.19	0.51
26:14:994:C:OP2	42:85:54:LYS:NZ	2.34	0.51
27:16:88:C:H2'	27:16:89:G:O4'	2.10	0.51
26:1H:1568:G:H5''	29:11:61:LEU:CD2	2.41	0.51
26:1H:1799:G:O2'	26:1H:1800:C:OP2	2.19	0.51
26:1H:1919:A:H5''	26:1H:1920:C:OP2	2.10	0.51
30:29:54:GLN:HG2	30:29:55:ASN:N	2.25	0.51
24:3L:76:A:H8	26:14:2394:C:N4	2.08	0.51
6:52:33:TYR:CE1	6:52:78:GLU:HG3	2.46	0.51
6:5E:97:PHE:HD1	18:9I:31:LEU:HD11	1.75	0.51
7:6E:15:ASP:HB3	7:6E:19:GLY:N	2.26	0.51
41:75:24:PRO:HA	41:75:49:VAL:HG23	1.91	0.51
38:88:4:PRO:HD3	38:88:70:PRO:O	2.10	0.51
9:8E:3:GLN:HB3	9:8E:20:ARG:HD3	1.92	0.51
17:8I:88:TYR:HD1	17:8I:89:LEU:HD23	1.76	0.51
18:9I:34:TYR:HB3	18:9I:69:THR:HG23	1.92	0.51
47:D5:126:VAL:HG12	47:D5:163:LEU:HA	1.92	0.51
47:H8:128:VAL:HG12	47:H8:161:VAL:HB	1.91	0.51
55:P8:5:TRP:HA	55:P8:5:TRP:CE3	2.44	0.51
1:13:1346:A:H5''	9:8E:120:ARG:HH12	1.73	0.51
1:13:1478:C:H2'	1:13:1479:C:H6	1.76	0.51
1:13:963:G:N2	1:13:972:C:N3	2.43	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:14:1003:G:N2	26:14:1153:C:C2	2.79	0.51
26:14:1007:C:OP1	35:15:37:LYS:NZ	2.37	0.51
26:14:1342:A:H2	26:14:1602:U:N3	2.05	0.51
26:14:1464:C:HO2'	26:14:1528:A:H8	1.58	0.51
26:14:270(E):G:N2	26:14:270(U):C:O2	2.35	0.51
26:14:2839:G:H5'	39:55:46:GLY:CA	2.40	0.51
35:15:96:GLU:H	35:15:96:GLU:CD	2.13	0.51
29:19:73:VAL:HG13	29:19:120:GLY:HA3	1.92	0.51
1:1G:1133:G:N2	1:1G:1141:C:O2	2.43	0.51
1:1G:1160:G:H2'	1:1G:1161:C:C6	2.45	0.51
1:1G:1216:G:H2'	1:1G:1217:C:C6	2.45	0.51
1:1G:827:U:H3	1:1G:872:A:N6	2.06	0.51
26:1H:1494:A:C2'	26:1H:1495:A:H5'	2.41	0.51
26:1H:234:C:H2'	26:1H:235:U:H6	1.74	0.51
26:1H:984:A:H5''	26:1H:985:C:H5	1.75	0.51
22:1K:76:A:H1'	26:1H:2583:G:N2	2.25	0.51
23:2L:60:A:H2'	23:2L:61:U:H5'	1.93	0.51
4:32:24:GLU:HG2	4:32:25:ARG:H	1.74	0.51
12:3A:70:ILE:HD13	12:3A:77:LEU:HD12	1.92	0.51
5:42:76:ILE:HG23	5:42:142:LEU:HD13	1.93	0.51
33:59:125:VAL:HG22	33:59:126:PRO:HA	1.91	0.51
33:59:92:ILE:HD13	33:59:160:LYS:HD3	1.92	0.51
36:68:58:VAL:HG21	36:68:86:ILE:HG12	1.93	0.51
8:7E:120:THR:H	8:7E:123:GLU:CG	2.23	0.51
8:7E:33:GLU:HA	8:7E:36:LEU:HD12	1.92	0.51
40:A8:32:LEU:O	40:A8:62:LYS:NZ	2.35	0.51
41:B8:12:SER:CB	41:B8:15:VAL:H	2.23	0.51
47:H8:126:VAL:HG12	47:H8:163:LEU:HA	1.91	0.51
1:13:953:G:H2'	1:13:954:G:O4'	2.11	0.51
26:14:1530:G:O6	26:14:1542:G:N2	2.43	0.51
26:14:2468:G:H3'	26:14:2476:A:N1	2.25	0.51
35:15:73:THR:HG22	35:15:84:LYS:HB3	1.93	0.51
27:16:40:U:H1'	27:16:45:A:H61	1.76	0.51
27:16:78:A:C2	27:16:99:A:C4	2.99	0.51
1:1G:134:A:H61	16:7A:25:ARG:HH12	1.59	0.51
26:1H:111:A:H4'	50:K8:69:ARG:NH2	2.26	0.51
26:1H:1432:C:H2'	26:1H:1433:U:O4'	2.11	0.51
26:1H:1942:C:OP2	26:1H:1943:U:O2'	2.18	0.51
26:1H:7:G:H1	26:1H:2896:C:H42	1.58	0.51
26:1H:581:C:H2'	26:1H:582:G:C8	2.45	0.51
22:1K:43:U:H2'	22:1K:44:U:C6	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:29:171:GLU:OE1	30:29:185:LYS:HE2	2.11	0.51
11:2I:53:SER:HA	11:2I:55:LYS:HB2	1.93	0.51
4:3E:164:ALA:O	4:3E:168:ARG:NE	2.43	0.51
5:42:101:ILE:HD11	5:42:119:LEU:HD23	1.93	0.51
38:45:137:TYR:CD1	38:45:137:TYR:C	2.84	0.51
5:4E:91:LEU:HD12	5:4E:120:THR:HG22	1.92	0.51
13:4I:46:LYS:HZ2	13:4I:46:LYS:HB2	1.75	0.51
13:4I:60:VAL:HG12	13:4I:66:LEU:HD11	1.92	0.51
35:58:96:GLU:HB2	35:58:122:VAL:CG1	2.40	0.51
33:59:6:ARG:HG2	33:59:7:LEU:H	1.74	0.51
6:5E:44:GLY:HA2	6:5E:59:TYR:CZ	2.46	0.51
40:65:67:ARG:HH21	40:65:103:GLU:HB2	1.75	0.51
5:42:78:HIS:HD2	8:72:107:LEU:HD22	1.75	0.51
42:85:66:ASN:HB2	42:85:76:TYR:HB2	1.93	0.51
39:98:78:LYS:HE2	39:98:83:ILE:HD11	1.91	0.51
40:A8:37:ALA:HB2	40:A8:101:LEU:HD21	1.93	0.51
46:C5:17:SER:O	46:C5:21:LYS:HB2	2.11	0.51
46:C5:62:GLU:CD	46:C5:63:LYS:H	2.14	0.51
1:13:1007:C:N4	1:13:1022:G:H1	2.05	0.51
1:13:1348:U:H2'	1:13:1349:A:H8	1.76	0.51
1:13:626:U:C2	1:13:627:G:C8	2.99	0.51
1:13:748:C:O5'	1:13:748:C:H6	1.94	0.51
26:14:1533:C:H5'	26:14:1534:G:OP2	2.11	0.51
26:14:2107:C:N3	26:14:2182:G:N2	2.56	0.51
26:14:495:G:N2	44:A5:61:ASN:HD21	2.09	0.51
26:14:733:G:N7	61:14:3437:SPE:H121	2.26	0.51
26:14:882:G:H22	26:14:894:C:H42	1.59	0.51
1:1G:108:G:H5'	1:1G:109:A:C5'	2.41	0.51
1:1G:1369:C:OP2	9:82:112:LYS:N	2.44	0.51
1:1G:626:U:C2	1:1G:627:G:C8	2.99	0.51
26:1H:1210:A:H5''	26:1H:1212:G:O4'	2.11	0.51
26:1H:2564:A:C2	26:1H:2647:U:H4'	2.46	0.51
26:1H:443:A:OP2	26:1H:615:G:N2	2.33	0.51
37:35:107:LYS:O	37:35:109:GLY:N	2.40	0.51
26:14:1247:A:OP1	31:39:95:ARG:NH2	2.44	0.51
4:3E:149:ALA:O	4:3E:153:ARG:HG2	2.11	0.51
4:3E:85:LYS:HG3	4:3E:88:VAL:O	2.11	0.51
33:51:169:VAL:HG13	33:51:170:ARG:HG3	1.93	0.51
28:71:163:PHE:HB3	28:71:192:PHE:HZ	1.76	0.51
8:72:110:ALA:O	8:72:121:ASP:N	2.44	0.51
49:F5:84:GLY:HA3	49:F5:87:PRO:HD2	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:M5:51:ALA:HB1	56:M5:52:LYS:HA	1.91	0.51
1:13:1133:G:H2'	1:13:1134:G:H8	1.75	0.51
1:13:144:G:H2'	1:13:145:G:O4'	2.10	0.51
1:13:649:G:H2'	1:13:650:G:H8	1.74	0.51
1:13:674:G:H2'	1:13:675:A:C8	2.46	0.51
26:14:1291:C:H2'	26:14:1292:U:C6	2.46	0.51
26:14:1357:U:H2'	26:14:1358:G:O4'	2.11	0.51
26:14:1486:A:H2'	26:14:1487:G:H8	1.76	0.51
26:14:2287:A:C2	26:14:2346:A:H2	2.28	0.51
26:14:2461:C:H2'	26:14:2462:U:C6	2.46	0.51
26:14:34:C:HO2'	26:14:35:G:P	2.34	0.51
26:14:890:A:H2'	26:14:892:G:C8	2.46	0.51
1:1G:1423:G:H2'	1:1G:1424:C:C6	2.45	0.51
1:1G:407:G:P	4:32:115:ARG:HH21	2.33	0.51
1:1G:967:C:H3'	1:1G:968:A:H2'	1.93	0.51
26:1H:125:G:H5'	26:1H:125:G:H8	1.76	0.51
26:1H:274:G:H2'	26:1H:275:G:O4'	2.10	0.51
26:1H:353:G:H2'	26:1H:354:G:H8	1.76	0.51
26:1H:721:C:H2'	26:1H:722:A:H8	1.75	0.51
30:21:36:ARG:NH1	30:21:85:ASN:OD1	2.43	0.51
30:29:171:GLU:O	30:29:184:VAL:HA	2.10	0.51
31:31:29:ASN:HB3	31:31:112:MET:HE1	1.92	0.51
4:3E:108:LEU:HD12	4:3E:170:VAL:HG11	1.93	0.51
4:3E:9:CYS:O	4:3E:13:ARG:HG3	2.11	0.51
12:3I:58:VAL:O	12:3I:65:GLU:HA	2.11	0.51
5:42:37:ARG:HG2	5:42:112:LEU:HA	1.92	0.51
1:1G:1080:A:OP1	5:42:14:ARG:NH2	2.44	0.51
39:55:57:ARG:HE	39:55:59:ASP:CG	2.15	0.51
34:61:5:LEU:HD13	34:61:13:GLY:O	2.11	0.51
28:71:64:LEU:HG	28:71:65:PRO:HD2	1.92	0.51
38:88:48:GLU:O	38:88:48:GLU:HG3	2.11	0.51
2:12:16:HIS:CE1	2:12:213:LEU:HD22	2.47	0.51
1:13:292:G:N7	1:13:293:G:H1'	2.26	0.51
1:13:765:G:H5''	1:13:766:A:OP1	2.11	0.51
26:14:180:G:P	55:L5:32:LYS:HD2	2.51	0.51
26:14:308:G:H5''	26:14:309:G:OP2	2.11	0.51
1:1G:1329:A:H2'	1:1G:1330:U:O4'	2.11	0.51
1:1G:757:U:H2'	1:1G:758:G:O4'	2.11	0.51
22:1K:2:G:N2	22:1K:71:C:O2	2.40	0.51
30:21:29:GLY:H	30:21:51:PHE:HE1	1.58	0.51
12:3A:71:PRO:O	12:3A:102:ARG:NH1	2.42	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:32:57:ARG:HH22	5:42:107:ARG:HD2	1.76	0.51
28:71:11:LEU:HD13	28:71:220:PRO:HB2	1.93	0.51
8:72:38:ILE:HD11	8:72:118:VAL:O	2.11	0.51
43:95:62:LEU:HD21	43:95:95:LEU:HB2	1.92	0.51
41:B8:11:GLU:HG2	41:B8:57:PHE:HB3	1.93	0.51
47:D5:130:PRO:HA	47:D5:133:ILE:HD11	1.93	0.51
49:J8:3:LYS:O	49:J8:12:PRO:HD3	2.11	0.51
54:O8:11:LEU:HD11	54:O8:51:GLU:HG3	1.91	0.51
1:13:57:G:C5	1:13:58:C:C4	2.99	0.50
26:14:2314:C:H5'	32:49:38:VAL:HG11	1.94	0.50
26:14:2441:C:OP2	26:14:2586:C:O2'	2.25	0.50
29:19:108:PRO:HB3	29:19:143:HIS:HE1	1.71	0.50
1:1G:1224:G:O2'	1:1G:1322:C:OP2	2.29	0.50
26:1H:1406:U:H2'	26:1H:1407:C:H6	1.76	0.50
26:1H:274:G:N2	26:1H:276:A:H61	2.09	0.50
26:1H:582:G:H2'	26:1H:583:G:C8	2.46	0.50
27:1J:70:C:H2'	27:1J:71:C:H6	1.76	0.50
3:22:155:GLY:HA3	3:22:196:LEU:HD13	1.92	0.50
3:2E:47:LEU:HG	3:2E:76:VAL:HG12	1.93	0.50
1:1G:552:U:O2'	12:3A:86:ARG:O	2.26	0.50
12:3I:54:LYS:N	12:3I:54:LYS:HD3	2.25	0.50
24:3K:1:G:N3	24:3K:1:G:H2'	2.26	0.50
32:49:75:LYS:HA	32:49:84:LYS:HG3	1.93	0.50
7:62:111:ARG:NH2	7:62:122:HIS:HB3	2.26	0.50
8:72:123:GLU:O	8:72:127:LEU:HB2	2.11	0.50
43:95:72:VAL:HG13	43:95:72:VAL:O	2.11	0.50
39:55:101:ALA:HA	53:J5:44:THR:HG21	1.92	0.50
54:O8:44:ARG:H	54:O8:44:ARG:HH11	1.58	0.50
29:11:17:THR:HG22	29:11:204:ILE:HA	1.93	0.50
2:12:48:MET:HA	2:12:51:LEU:HD11	1.93	0.50
26:14:1034:G:H2'	26:14:1035:U:O4'	2.11	0.50
26:14:1533:C:H3'	26:14:1534:G:H4'	1.93	0.50
26:14:1666:G:OP1	36:25:66:LYS:HD3	2.12	0.50
26:14:2185:C:H2'	26:14:2186:G:C8	2.46	0.50
26:14:2655:G:H1'	26:14:2656:U:H5	1.76	0.50
26:14:997:G:O2'	26:14:998:C:H5'	2.12	0.50
29:19:146:GLU:HB2	29:19:189:CYS:HB3	1.93	0.50
29:19:68:LYS:HB3	29:19:70:TRP:CH2	2.47	0.50
1:1G:10:A:OP2	5:42:126:ARG:HG2	2.11	0.50
1:1G:1134:G:N2	1:1G:1140:C:O2	2.40	0.50
1:1G:1162:C:N4	1:1G:1174:G:H1	2.07	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1G:562:C:H1'	12:3A:15:ARG:HD2	1.92	0.50
26:1H:1914:C:H2'	26:1H:1915:U:O4'	2.11	0.50
26:1H:2127:G:H2'	26:1H:2128:C:O4'	2.10	0.50
26:1H:2895:U:H2'	26:1H:2896:C:C6	2.46	0.50
27:1J:88:C:H5''	27:1J:89:G:C5	2.46	0.50
1:1G:537:G:H5''	12:3A:113:ARG:NH1	2.27	0.50
13:4A:53:VAL:O	13:4A:57:ARG:N	2.25	0.50
4:3E:197:PRO:HD3	6:52:16:GLN:HG3	1.94	0.50
3:22:13:GLY:HA2	14:5A:57:ARG:HD2	1.93	0.50
34:61:21:VAL:HG21	34:61:25:TYR:HD2	1.76	0.50
7:6E:5:ARG:CZ	7:6E:7:ALA:HA	2.41	0.50
1:1G:1179:A:H4'	9:82:103:THR:HA	1.94	0.50
43:D8:60:GLU:HB2	43:D8:97:LYS:HE2	1.93	0.50
46:G8:82:PRO:HG3	46:G8:97:ARG:HB3	1.92	0.50
53:J5:33:CYS:SG	53:J5:46:CYS:SG	3.04	0.50
52:M8:13:ARG:NH1	52:M8:22:ILE:HG23	2.23	0.50
2:12:15:VAL:HB	2:12:16:HIS:CE1	2.46	0.50
1:13:57:G:H2'	1:13:58:C:C6	2.46	0.50
1:13:736:C:H2'	1:13:737:A:C8	2.46	0.50
1:1G:1132:C:H2'	1:1G:1133:G:H8	1.77	0.50
1:1G:1151:A:O2'	1:1G:1152:A:O5'	2.30	0.50
1:1G:1348:U:H4'	9:82:120:ARG:HD2	1.93	0.50
1:1G:661:G:H1	1:1G:744:C:H42	1.59	0.50
26:1H:2282:G:H4'	26:1H:2389:G:O2'	2.12	0.50
26:1H:2377:A:H2'	26:1H:2378:A:C8	2.46	0.50
10:1I:38:ILE:HG12	10:1I:71:LEU:O	2.11	0.50
30:21:105:THR:HG1	30:21:199:ARG:NH2	2.09	0.50
31:31:63:LYS:NZ	31:31:67:GLN:HB2	2.27	0.50
37:35:126:VAL:HA	37:35:145:PRO:HD2	1.93	0.50
12:3I:8:ASN:OD1	17:8I:34:LYS:NZ	2.42	0.50
32:41:35:GLU:OE1	32:41:36:LYS:N	2.44	0.50
39:98:2:ARG:CZ	39:98:2:ARG:HB3	2.41	0.50
20:BA:89:ARG:NH1	20:BA:105:SER:O	2.44	0.50
45:F8:27:THR:HB	45:F8:80:ILE:HB	1.93	0.50
47:H8:111:VAL:HB	47:H8:115:GLY:HA3	1.93	0.50
49:J8:93:GLU:O	49:J8:96:LYS:N	2.35	0.50
26:1H:102:G:OP1	50:K8:7:ARG:NH2	2.44	0.50
53:N8:33:CYS:SG	53:N8:40:LYS:HD3	2.52	0.50
1:13:160:A:N6	1:13:343:U:O2'	2.40	0.50
1:13:950:U:OP2	13:4I:102:ARG:HD2	2.10	0.50
26:14:577:G:O2'	26:14:1254:A:OP1	2.27	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:14:1525:G:H2'	26:14:1526:G:H8	1.76	0.50
26:14:2584:U:H2'	26:14:2585:U:H2'	1.93	0.50
35:15:133:GLN:O	35:15:134:ARG:HG3	2.11	0.50
29:19:24:ILE:HG13	29:19:83:GLU:HA	1.94	0.50
29:19:35:LYS:HA	29:19:64:ILE:HG22	1.92	0.50
1:1G:1004:A:C2	1:1G:1006:C:H1'	2.46	0.50
1:1G:1288:A:H2'	1:1G:1289:A:H8	1.76	0.50
1:1G:192:U:H2'	1:1G:193:C:C6	2.45	0.50
1:1G:408:A:H2'	1:1G:409:G:O4'	2.11	0.50
26:1H:1055:G:O2'	26:1H:1086:A:N6	2.43	0.50
26:1H:1204:A:C2	26:1H:1241:A:N1	2.79	0.50
26:1H:1221:C:H2'	26:1H:1222:C:C6	2.47	0.50
26:1H:1478:G:O6	26:1H:1510:A:N6	2.44	0.50
26:1H:1530:G:O6	26:1H:1542:G:N2	2.44	0.50
26:1H:2170:A:OP2	26:1H:2170:A:H3'	2.11	0.50
26:1H:2400:G:H2'	26:1H:2401:U:C6	2.44	0.50
26:1H:2031:A:C6	26:1H:2498:C:H1'	2.46	0.50
26:1H:860:U:H5	26:1H:917:A:H2	1.46	0.50
26:1H:962:G:H2'	26:1H:963:U:C6	2.46	0.50
27:1J:51:G:C6	27:1J:52:A:C2	2.99	0.50
4:32:33:MET:C	4:32:35:ARG:HH12	2.13	0.50
4:3E:153:ARG:HB3	4:3E:181:MET:SD	2.51	0.50
24:3K:2:G:H2'	24:3K:3:G:C8	2.46	0.50
32:49:53:LEU:HD13	32:49:90:LEU:HD21	1.93	0.50
26:14:2820:A:C6	39:55:4:LEU:HD11	2.47	0.50
41:75:4:GLY:N	41:75:5:ALA:C	2.65	0.50
46:C5:14:LEU:HB2	46:C5:75:ILE:HD11	1.93	0.50
37:78:65:ARG:HD3	56:Q8:25:MET:SD	2.52	0.50
1:13:145:G:H1	1:13:177:C:N4	2.09	0.50
26:14:1412:A:H2'	26:14:1413:G:C8	2.47	0.50
26:14:1729:A:H2'	26:14:1731:G:H22	1.74	0.50
26:14:372:G:OP2	49:F5:69:LYS:NZ	2.45	0.50
10:1A:78:ASN:O	10:1A:81:THR:OG1	2.27	0.50
2:1E:19:HIS:NE2	2:1E:206:ASP:HB2	2.25	0.50
1:1G:1206:G:OP1	3:22:190:ARG:NH2	2.38	0.50
1:1G:1224:G:C6	1:1G:1322:C:H1'	2.46	0.50
1:1G:328:C:H4'	1:1G:329:A:H5"	1.94	0.50
1:1G:539:A:H2'	1:1G:540:G:C8	2.47	0.50
26:1H:1731:G:H2'	26:1H:1732:A:H8	1.76	0.50
26:1H:2845:G:H2'	26:1H:2846:G:C8	2.47	0.50
27:1J:13:A:H2'	27:1J:70:C:O2'	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:1J:52:A:N6	40:65:33:LYS:HG3	2.27	0.50
27:1J:90:C:OP2	38:45:16:ARG:NH2	2.45	0.50
3:22:9:GLY:HA3	14:5A:49:HIS:HA	1.93	0.50
32:41:28:VAL:O	32:41:31:VAL:HG13	2.12	0.50
32:49:56:ALA:HB2	32:49:153:ARG:CZ	2.41	0.50
13:4I:49:THR:HB	13:4I:52:GLU:HG2	1.94	0.50
13:4I:81:LEU:HD22	13:4I:88:ARG:HB3	1.92	0.50
1:13:667:G:H4'	15:6I:51:HIS:CE1	2.46	0.50
17:8A:45:HIS:HB2	17:8A:65:ILE:HD13	1.92	0.50
39:98:67:LEU:HD22	39:98:76:VAL:HG21	1.93	0.50
1:1G:664:G:P	18:9A:64:ARG:HH21	2.34	0.50
18:9I:59:SER:H	18:9I:62:GLU:HB2	1.75	0.50
40:A8:89:ARG:HG3	40:A8:92:TYR:O	2.12	0.50
27:1J:103:U:O2'	47:D5:72:ARG:HG3	2.10	0.50
26:1H:728:G:H4'	29:11:13:ARG:HD3	1.94	0.50
1:13:1003:G:H2'	1:13:1004:A:H4'	1.93	0.50
1:13:1226:C:H4'	19:AI:80:TYR:OH	2.12	0.50
1:13:134:A:H1'	1:13:325:A:C5	2.47	0.50
1:13:1459:C:OP1	20:BI:31:SER:OG	2.25	0.50
1:13:259:G:C6	1:13:260:G:C5	2.99	0.50
1:13:323:U:H2'	1:13:324:G:O4'	2.12	0.50
26:14:1338:G:N3	26:14:1393:A:H2	2.10	0.50
26:14:1366:A:H2'	26:14:1367:A:O4'	2.11	0.50
26:14:2147:G:C5	26:14:2148:G:H1'	2.46	0.50
26:14:900:A:N3	26:14:900:A:H2'	2.27	0.50
29:19:44:ASN:HA	29:19:47:GLY:N	2.13	0.50
1:1G:1007:C:H2'	1:1G:1008:C:C6	2.47	0.50
1:1G:458:C:H2'	1:1G:464:G:C8	2.45	0.50
26:1H:2756:U:H1'	26:1H:2757:A:H5''	1.93	0.50
27:1J:2:C:H2'	27:1J:3:C:C6	2.46	0.50
37:35:120:ALA:O	37:35:121:LYS:HD2	2.12	0.50
26:14:2429:G:O6	37:35:61:ARG:NH2	2.44	0.50
5:42:61:TYR:HA	5:42:64:ARG:HG3	1.92	0.50
33:51:169:VAL:HG13	33:51:170:ARG:N	2.25	0.50
40:65:36:TYR:HA	40:65:52:SER:HB3	1.93	0.50
7:6E:20:ASP:HB3	7:6E:23:VAL:H	1.76	0.50
16:7I:4:ILE:HA	16:7I:20:VAL:O	2.12	0.50
26:14:2012:G:OP1	44:A5:11:ARG:NH2	2.43	0.50
40:A8:89:ARG:HG2	40:A8:89:ARG:O	2.12	0.50
48:E5:68:GLU:OE1	48:E5:82:ARG:HG3	2.12	0.50
26:1H:1614:A:C2	44:E8:93:ALA:HB2	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:13:170:U:H2'	1:13:171:A:H8	1.77	0.50
26:14:1204:A:C2	26:14:1241:A:N1	2.80	0.50
26:14:2674:G:H2'	26:14:2675:A:C8	2.46	0.50
26:14:597:U:H2'	26:14:598:G:C8	2.47	0.50
26:14:1012:U:H5	35:15:28:THR:HG21	1.76	0.50
1:1G:1129:C:H1'	1:1G:1132:C:H41	1.77	0.50
1:1G:1273:G:H3'	1:1G:1274:G:C8	2.45	0.50
1:1G:1375:A:H2'	1:1G:1376:U:O4'	2.11	0.50
26:1H:2331:G:O3'	48:18:43:THR:HG22	2.11	0.50
26:1H:2335:A:C8	26:1H:2337:G:C5	3.00	0.50
26:1H:459:U:H2'	26:1H:460:A:C8	2.46	0.50
26:1H:581:C:H2'	26:1H:582:G:H8	1.76	0.50
27:1J:78:A:H2'	27:1J:79:C:O4'	2.12	0.50
27:1J:7:G:O5'	40:65:29:PHE:HE2	1.94	0.50
30:21:55:ASN:HB3	30:21:58:ARG:H	1.76	0.50
4:3E:60:GLU:OE2	4:3E:199:ASN:N	2.42	0.50
26:14:910:A:C5	38:45:13:GLN:HG3	2.46	0.50
1:1G:974:A:P	14:5A:41:ARG:HH22	2.35	0.50
6:5E:82:ARG:HB2	6:5E:85:VAL:HG23	1.94	0.50
15:6I:17:ARG:CZ	15:6I:77:ARG:HD2	2.42	0.50
40:A8:111:GLU:HB2	40:A8:112:PHE:CD2	2.46	0.50
42:C8:88:ILE:C	42:C8:90:VAL:H	2.13	0.50
47:D5:105:VAL:HG13	47:D5:106:GLY:H	1.77	0.50
38:45:132:VAL:HG21	47:D5:81:ARG:HE	1.77	0.50
49:F5:45:ASN:O	49:F5:63:ALA:HA	2.11	0.50
1:13:1256:A:OP2	3:2E:26:LYS:NZ	2.45	0.50
1:13:191(F):U:H2'	1:13:191:G:C8	2.46	0.50
1:13:345:C:H4'	1:13:346:G:C5	2.46	0.50
1:13:407:G:H2'	1:13:408:A:C8	2.46	0.50
26:14:2615:U:C2	53:J5:7:PRO:HA	2.47	0.50
29:19:34:VAL:O	29:19:35:LYS:HE2	2.12	0.50
26:1H:1434:A:H61	26:1H:1558:A:H61	1.55	0.50
26:1H:2261:C:H1'	26:1H:2388:A:N3	2.27	0.50
26:1H:26:G:C6	26:1H:27:G:N1	2.80	0.50
26:1H:607:U:N3	26:1H:621:A:C2	2.73	0.50
3:22:40:ARG:HG3	3:22:55:VAL:HG11	1.93	0.50
12:3A:62:SER:OG	12:3A:62:SER:O	2.29	0.50
33:59:37:VAL:HG13	33:59:38:SER:O	2.12	0.50
34:69:8:PRO:N	34:69:15:VAL:HG22	2.26	0.50
15:6A:76:GLU:HA	15:6A:79:ARG:HD2	1.94	0.50
1:13:1291:G:P	7:6E:37:ASN:HD22	2.34	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6E:95:ARG:NH2	7:6E:99:LEU:HD11	2.27	0.50
41:75:55:ASN:H	41:75:59:THR:HG22	1.75	0.50
19:AI:40:ILE:HG12	19:AI:41:VAL:H	1.76	0.50
47:D5:170:THR:C	47:D5:172:ALA:H	2.15	0.50
29:11:96:HIS:CE1	29:11:102:LYS:HE2	2.47	0.50
1:13:1287:A:H2'	1:13:1288:A:C8	2.46	0.50
1:13:141:A:H2'	1:13:142:G:H8	1.77	0.50
1:13:429:U:H1'	1:13:430:A:H5''	1.94	0.50
26:14:1165:U:H2'	26:14:1166:C:C6	2.47	0.50
26:14:1434:A:H2'	26:14:1435:G:C8	2.47	0.50
26:14:1686:C:H2'	26:14:1687:G:O4'	2.12	0.50
26:14:395:U:H2'	62:14:4364:HOH:O	2.11	0.50
26:14:729:G:C6	29:19:208:LYS:HB2	2.46	0.50
26:14:6:A:C3'	26:14:7:G:H5'	2.41	0.50
29:19:137:PRO:O	29:19:140:THR:OG1	2.23	0.50
10:1A:49:VAL:O	10:1A:60:ARG:HB2	2.12	0.50
1:1G:538:G:H2'	1:1G:539:A:C8	2.47	0.50
1:1G:756:C:H2'	1:1G:757:U:O4'	2.11	0.50
26:1H:1509:C:O2'	26:1H:1510:A:OP1	2.23	0.50
26:1H:2593:U:H2'	26:1H:2594:C:C6	2.47	0.50
26:1H:2652:C:H2'	26:1H:2653:U:O4'	2.12	0.50
26:1H:831:G:N7	62:1H:3831:HOH:O	2.34	0.50
22:1K:37:T6A:H2'	22:1K:38:A:O4'	2.12	0.50
30:29:47:VAL:HG21	30:29:85:ASN:HA	1.94	0.50
30:29:3:GLY:HA3	30:29:81:ILE:HD12	1.93	0.50
31:31:134:GLY:CA	31:31:166:ALA:HB2	2.42	0.50
31:39:83:PHE:O	31:39:84:VAL:HB	2.10	0.50
13:4A:78:ILE:HG23	13:4A:92:HIS:ND1	2.27	0.50
8:72:44:PHE:HD1	8:72:80:ILE:HG13	1.76	0.50
37:78:71:VAL:CG1	37:78:72:PRO:HD3	2.39	0.50
42:85:110:VAL:O	42:85:114:LYS:HG2	2.11	0.50
18:9A:36:ASN:N	18:9A:36:ASN:HD22	2.08	0.50
26:14:64:A:C4	45:B5:66:LEU:HD12	2.47	0.50
50:G5:47:ASN:N	50:G5:47:ASN:OD1	2.45	0.50
50:G5:15:LYS:H	50:G5:67:LYS:NZ	2.10	0.50
46:G8:89:PHE:CD1	46:G8:90:LEU:N	2.80	0.50
47:H8:152:ALA:HB3	47:H8:167:PRO:O	2.12	0.50
51:L8:35:ARG:HB3	51:L8:37:LEU:HD21	1.94	0.50
2:12:219:VAL:CG2	2:12:221:LEU:H	2.25	0.49
1:13:105:G:H2'	1:13:106:C:C6	2.47	0.49
1:13:297:G:H4'	1:13:557:G:H4'	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:14:1704:G:O6	61:14:3436:SPE:H82	2.11	0.49
26:14:270(F):U:H2'	26:14:270(G):C:C6	2.47	0.49
26:14:329:G:P	46:C5:71:LYS:HE3	2.52	0.49
26:14:877:U:H4'	26:14:878:A:OP1	2.10	0.49
29:19:273:ARG:O	29:19:273:ARG:HG2	2.12	0.49
29:19:30:GLU:HG3	29:19:63:ARG:NE	2.26	0.49
2:1E:18:GLY:HA2	2:1E:42:ILE:HG13	1.93	0.49
1:1G:983:A:N1	1:1G:1222:G:N2	2.60	0.49
1:1G:1432:G:OP1	41:75:107:ASP:HB2	2.12	0.49
1:1G:554:C:H2'	1:1G:555:C:C6	2.46	0.49
26:1H:1446:C:H2'	26:1H:1447:G:H8	1.77	0.49
26:1H:1980:G:O2'	26:1H:1982:C:OP2	2.23	0.49
26:1H:2154:G:H2'	26:1H:2155:G:C8	2.43	0.49
26:1H:2175:C:H1'	28:71:217:THR:O	2.12	0.49
26:1H:270(W):G:N7	62:1H:3838:HOH:O	2.35	0.49
26:14:2787:C:O2'	30:29:61:ARG:O	2.16	0.49
26:1H:321:G:O3'	31:31:168:ARG:NH2	2.45	0.49
12:3A:114:LYS:O	12:3A:117:ARG:HG3	2.12	0.49
32:41:33:ARG:O	32:41:162:THR:HG23	2.12	0.49
6:52:2:ARG:NH2	6:52:69:GLU:HG3	2.27	0.49
35:58:133:GLN:C	35:58:134:ARG:HE	2.14	0.49
33:59:86:GLU:H	33:59:86:GLU:CD	2.15	0.49
7:6E:115:ARG:O	7:6E:118:VAL:HG12	2.12	0.49
19:AA:66:MET:HA	19:AA:67:VAL:C	2.32	0.49
1:13:1314:C:OP2	19:AI:4:SER:OG	2.29	0.49
26:14:309:G:H4'	46:C5:18:GLY:HA3	1.92	0.49
47:D5:152:ALA:HB3	47:D5:167:PRO:HA	1.94	0.49
43:D8:3:ALA:HB3	43:D8:14:VAL:HG22	1.93	0.49
50:G5:64:LEU:HD22	50:G5:64:LEU:O	2.12	0.49
50:K8:4:SER:N	50:K8:7:ARG:HG2	2.27	0.49
1:13:112:G:P	16:7I:27:LYS:HD2	2.53	0.49
26:14:1109:C:H2'	26:14:1110:G:H1'	1.93	0.49
26:14:1268:A:H2'	26:14:1269:A:O4'	2.12	0.49
26:14:1274:A:N3	26:14:1297:C:H1'	2.27	0.49
26:14:1828:G:H8	26:14:1828:G:OP2	1.95	0.49
26:14:2103:C:H2'	26:14:2104:G:C8	2.47	0.49
27:16:116:G:H2'	27:16:117:G:O4'	2.11	0.49
1:1G:1117:G:O2'	9:82:104:ARG:HG2	2.12	0.49
1:1G:1324:A:H2'	1:1G:1325:C:C6	2.47	0.49
1:1G:1422:G:H5''	36:25:48:PRO:HB3	1.93	0.49
1:1G:520:A:N1	1:1G:536:C:H1'	2.27	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1H:1170:G:N2	26:1H:1180:C:C2	2.80	0.49
26:1H:1864:U:H2'	26:1H:1869:G:H5''	1.93	0.49
26:1H:2134:A:HO2'	26:1H:2159:G:N2	2.10	0.49
26:1H:330:A:O2'	26:1H:331:A:H8	1.95	0.49
26:1H:375:C:H5''	62:1H:4278:HOH:O	2.12	0.49
26:1H:724:U:H2'	26:1H:725:G:O4'	2.12	0.49
26:1H:840:C:H2'	26:1H:841:A:C8	2.48	0.49
4:32:35:ARG:HH11	4:32:35:ARG:HB2	1.76	0.49
12:3A:86:ARG:HB2	12:3A:101:VAL:HG23	1.94	0.49
4:3E:12:CYS:SG	4:3E:19:LEU:N	2.69	0.49
13:4I:4:ILE:HG22	13:4I:5:ALA:H	1.76	0.49
39:55:56:LYS:NZ	39:55:90:ARG:O	2.44	0.49
43:95:46:VAL:HG22	43:95:52:VAL:HG22	1.92	0.49
18:9A:38:GLU:OE2	18:9A:38:GLU:N	2.42	0.49
41:B8:125:ARG:O	41:B8:129:ARG:N	2.37	0.49
46:G8:89:PHE:HD1	46:G8:90:LEU:H	1.61	0.49
29:11:92:ILE:HD12	29:11:104:TYR:CD1	2.47	0.49
2:12:61:LEU:HG	2:12:160:ASP:CG	2.32	0.49
1:13:1167:A:OP1	1:13:1167:A:H8	1.95	0.49
1:13:1333:A:H2'	1:13:1334:G:O4'	2.12	0.49
1:13:826:C:H2'	1:13:827:U:O2	2.12	0.49
26:14:2119:A:H61	26:14:2170:A:H62	1.60	0.49
26:14:706:A:H2'	26:14:707:G:O4'	2.12	0.49
26:14:958:U:O2	27:1J:89(A):A:O2'	2.24	0.49
26:14:997:G:H2'	26:14:998:C:H6	1.78	0.49
1:1G:397:A:N3	1:1G:397:A:H3'	2.28	0.49
1:1G:957:U:H2'	1:1G:959:A:OP2	2.11	0.49
26:1H:1170:G:N2	26:1H:1180:C:O2	2.45	0.49
3:22:91:LEU:HD21	3:22:101:LEU:HD21	1.93	0.49
30:29:101:ARG:O	30:29:201:THR:OG1	2.30	0.49
1:1G:362:G:H4'	12:3A:33:ARG:NH2	2.23	0.49
12:3A:88:GLY:O	12:3A:99:HIS:HD2	1.94	0.49
5:42:145:LYS:O	5:42:149:GLU:HG3	2.11	0.49
32:49:42:GLY:O	32:49:43:LEU:HD13	2.12	0.49
7:62:122:HIS:HA	7:62:125:MET:HE2	1.94	0.49
40:65:95:HIS:HA	40:65:99:LYS:HD2	1.94	0.49
15:6I:7:GLU:O	15:6I:11:VAL:HG23	2.13	0.49
9:82:99:LEU:HB3	9:82:101:PHE:CE1	2.47	0.49
17:8A:66:SER:OG	17:8A:69:LYS:HB2	2.13	0.49
26:1H:1754:C:OP1	41:B8:96:ARG:NH1	2.44	0.49
20:BA:72:LEU:O	20:BA:73:HIS:HB2	2.11	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:F5:29:GLY:O	49:F5:30:VAL:HG22	2.11	0.49
46:G8:87:LYS:HD3	46:G8:88:LYS:N	2.28	0.49
53:N8:40:LYS:NZ	53:N8:46:CYS:HB3	2.26	0.49
26:1H:243:U:OP2	56:Q8:8:LYS:NZ	2.45	0.49
26:1H:1798:U:H5'	29:11:259:THR:OG1	2.12	0.49
1:13:1413:A:H2	1:13:1487:G:H22	1.60	0.49
1:13:1399:C:C2	1:13:1502:A:N6	2.81	0.49
26:14:1126:A:OP1	26:14:1126:A:H8	1.96	0.49
26:14:1444(A):A:N3	26:14:1444(A):A:H2'	2.28	0.49
26:14:239:U:H2'	26:14:240:G:O4'	2.12	0.49
26:14:2734:A:C8	26:14:2735:G:C8	2.99	0.49
1:1G:1152:A:H5'	10:1A:13:HIS:HD2	1.77	0.49
1:1G:1316:G:N2	1:1G:1318:A:H3'	2.28	0.49
1:1G:313:A:H2'	1:1G:314:C:C6	2.47	0.49
1:1G:910:C:OP2	12:3A:21:LYS:NZ	2.40	0.49
26:1H:1339:G:N2	26:1H:1603:A:H1'	2.28	0.49
26:1H:141:A:C8	26:1H:1408:C:H1'	2.47	0.49
26:1H:1791:A:C8	26:1H:1792:G:C8	3.00	0.49
26:1H:198:C:H5'	26:1H:2244:U:OP1	2.12	0.49
26:1H:2243:U:H2'	26:1H:2244:U:C6	2.47	0.49
30:21:14:ILE:HB	30:21:21:VAL:HG22	1.92	0.49
30:21:15:PHE:HA	30:21:19:ARG:O	2.13	0.49
36:25:98:VAL:HG12	36:25:117:LEU:HB3	1.94	0.49
4:3E:81:GLU:CD	4:3E:139:ARG:HH22	2.16	0.49
13:4I:69:GLU:HG3	32:41:118:ARG:NH2	2.26	0.49
35:58:96:GLU:C	35:58:98:VAL:N	2.64	0.49
26:14:2864:G:OP1	41:75:119:LYS:HD3	2.13	0.49
20:BA:50:GLU:HA	20:BA:100:ILE:HG21	1.93	0.49
42:C8:66:ASN:HB2	42:C8:76:TYR:HB2	1.95	0.49
1:13:963:G:H1	1:13:972:C:N4	2.08	0.49
26:14:2062:A:HO2'	26:14:2063:C:P	2.34	0.49
26:14:2292:C:H4'	26:14:2375:G:H4'	1.93	0.49
26:14:244:A:C2	26:14:255:A:C4	3.00	0.49
26:14:2689:U:H5''	26:14:2713:A:C2	2.47	0.49
26:14:868:U:C4	26:14:869:G:N7	2.80	0.49
35:15:46:VAL:HG12	35:15:48:MET:HG3	1.94	0.49
10:1A:55:LYS:HZ1	10:1A:57:LYS:HG2	1.76	0.49
1:1G:78:G:H1	1:1G:91:C:H42	1.59	0.49
26:1H:107:C:H2'	26:1H:108:U:C6	2.48	0.49
26:1H:2287:A:C2	26:1H:2346:A:C2	2.98	0.49
26:1H:2298:A:H2'	26:1H:2299:G:O4'	2.11	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1L:34:U:H6	24:1L:34:U:H5''	1.77	0.49
36:25:20:MET:HE3	36:25:44:LYS:HE3	1.94	0.49
32:41:125:PHE:HB3	32:41:166:ASP:OD2	2.13	0.49
33:59:136:ILE:H	33:59:136:ILE:HD12	1.78	0.49
33:59:157:TYR:CD1	33:59:171:LEU:HD23	2.47	0.49
40:65:34:HIS:CE1	40:65:54:LEU:HD12	2.47	0.49
41:75:2:ASN:OD1	41:75:4:GLY:HA3	2.13	0.49
16:7A:9:PHE:HB2	16:7A:16:HIS:O	2.13	0.49
9:82:99:LEU:HB3	9:82:101:PHE:HE1	1.77	0.49
42:85:92:ARG:HD3	42:85:95:LEU:HG	1.94	0.49
48:18:72:ARG:HH11	48:18:75:LEU:HD12	1.77	0.49
2:12:219:VAL:HA	2:12:220:ASP:HB3	1.93	0.49
1:13:276:G:O3'	17:8I:68:ARG:NH1	2.45	0.49
1:13:784:C:H2'	1:13:785:G:O4'	2.12	0.49
26:14:1041:C:N4	26:14:1114:G:H22	2.10	0.49
26:14:2784:C:O2	30:29:37:ARG:NH2	2.46	0.49
35:15:15:LEU:HB2	35:15:134:ARG:HB2	1.94	0.49
29:19:70:TRP:CH2	29:19:150:LYS:HA	2.47	0.49
1:1G:1320:C:H2'	1:1G:1321:C:C6	2.47	0.49
26:1H:814:C:O2'	26:1H:1225:C:N3	2.46	0.49
26:1H:2393:A:H2'	26:1H:2394:C:H6	1.76	0.49
31:39:39:TRP:CH2	31:39:106:ARG:HD3	2.46	0.49
31:39:11:VAL:HG22	31:39:13:SER:CB	2.42	0.49
4:3E:102:ASP:OD1	4:3E:103:ASN:N	2.46	0.49
4:3E:141:ARG:HB2	4:3E:141:ARG:NH1	2.28	0.49
26:1H:558:G:OP1	35:58:111:PRO:HD2	2.11	0.49
1:1G:1240:U:OP2	7:62:116:ALA:N	2.45	0.49
34:69:75:LEU:HG	34:69:76:THR:H	1.78	0.49
40:A8:78:LEU:CD1	40:A8:108:GLY:HA2	2.37	0.49
46:G8:20:TYR:CE2	46:G8:43:ASN:HA	2.47	0.49
49:J8:93:GLU:HA	49:J8:96:LYS:HD3	1.92	0.49
2:12:185:ILE:HG23	2:12:199:TYR:HB2	1.95	0.49
1:13:1009:G:C2	1:13:1010:G:C8	3.01	0.49
1:13:1113:C:H2'	1:13:1114:C:H6	1.77	0.49
1:13:1129:C:H3'	1:13:1139:G:N7	2.27	0.49
1:13:671:G:H2'	1:13:672:U:H6	1.76	0.49
26:14:1443:G:H1	26:14:1548:C:H42	1.60	0.49
26:14:2110:G:O2'	26:14:2120:G:H5'	2.13	0.49
26:14:218:A:H2	26:14:235:U:H4'	1.78	0.49
26:14:2520:C:N4	26:14:2542:A:H62	2.08	0.49
26:14:634:C:H2'	26:14:635:C:C6	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:14:850:C:O5'	26:14:850:C:H6	1.96	0.49
1:1G:1261:A:H5'	1:1G:1283:G:O3'	2.12	0.49
1:1G:371:G:O2'	1:1G:373:A:N7	2.45	0.49
1:1G:986:A:H1'	19:AA:54:GLY:O	2.12	0.49
26:1H:1103:A:H3'	26:1H:1104:C:C6	2.48	0.49
26:1H:1359:A:N1	26:1H:1372:U:C4	2.79	0.49
26:1H:265:A:H1'	26:1H:266:G:O4'	2.12	0.49
26:1H:2000:G:O2'	26:1H:2689:U:C5	2.60	0.49
26:1H:415:A:H2'	26:1H:416:C:O4'	2.13	0.49
26:1H:606:U:H4'	26:1H:658:C:H4'	1.95	0.49
26:1H:192:C:O2'	26:1H:802:A:N3	2.39	0.49
10:1I:32:ALA:HB3	10:1I:76:ASN:O	2.12	0.49
30:29:112:GLY:O	30:29:159:HIS:HA	2.13	0.49
4:32:105:VAL:HG13	4:32:110:PHE:HB2	1.94	0.49
12:3A:27:LEU:HD23	12:3A:60:LEU:HG	1.93	0.49
33:51:163:TYR:HB3	33:51:167:GLU:HG2	1.94	0.49
37:78:90:ARG:HD3	37:78:91:PHE:CE2	2.47	0.49
48:E5:53:MET:HG3	48:E5:59:LEU:HD23	1.94	0.49
49:J8:85:LEU:O	49:J8:86:SER:OG	2.27	0.49
29:11:132:PRO:HG3	29:11:190:TYR:CE1	2.48	0.49
2:12:180:LEU:HB2	2:12:182:ILE:HD12	1.93	0.49
1:13:1031:G:H2'	1:13:1032:A:H5'	1.95	0.49
1:13:955:U:H1'	1:13:1227:A:N6	2.28	0.49
1:13:1369:C:H2'	1:13:1370:G:C8	2.48	0.49
1:13:381:C:H2'	1:13:382:A:O4'	2.13	0.49
1:13:60:A:H4'	1:13:61:G:H5'	1.93	0.49
1:13:67:C:H2'	1:13:68:G:H8	1.75	0.49
26:14:2557:G:H2'	26:14:2558:C:C6	2.48	0.49
26:14:2816:C:O3'	39:55:99:LYS:NZ	2.44	0.49
26:14:481:G:OP2	46:C5:47:LYS:HB2	2.13	0.49
26:14:853:G:C2'	26:14:854:G:H5'	2.42	0.49
1:1G:179:A:H2'	1:1G:180:U:C6	2.48	0.49
1:1G:428:G:C5	1:1G:430:A:C6	3.00	0.49
26:1H:197:A:N6	26:1H:2430:A:H2'	2.27	0.49
26:1H:2544:G:H2'	26:1H:2545:G:H8	1.77	0.49
26:1H:2592:G:C6	26:1H:2593:U:C4	3.01	0.49
26:1H:459:U:H5''	55:P8:40:TRP:CD2	2.48	0.49
3:22:195:VAL:O	3:22:196:LEU:HD22	2.13	0.49
3:22:35:GLU:OE1	3:22:59:ARG:NH2	2.46	0.49
4:32:26:CYS:HB3	59:32:302:SF4:S1	2.53	0.49
31:39:181:LEU:CD2	31:39:186:ILE:HD11	2.41	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:41:165:THR:OG1	32:41:168:GLU:HG3	2.13	0.49
32:41:67:LYS:HE2	32:41:67:LYS:H	1.78	0.49
32:49:50:ALA:HA	32:49:53:LEU:HD23	1.93	0.49
13:4A:23:TYR:HB3	13:4A:67:GLU:HA	1.94	0.49
13:4I:23:TYR:CE2	13:4I:71:ARG:HG3	2.48	0.49
33:51:170:ARG:HA	33:51:171:LEU:HB2	1.95	0.49
26:1H:1022:G:N7	35:58:66:LYS:NZ	2.61	0.49
34:61:37:VAL:HG12	34:61:38:LEU:HD12	1.93	0.49
26:14:2685:G:P	41:75:51:ARG:HH22	2.36	0.49
37:78:114:ILE:HD13	37:78:125:VAL:HG11	1.93	0.49
26:1H:598:G:H5'	37:78:11:GLY:HA3	1.94	0.49
17:8I:56:VAL:HB	17:8I:78:GLU:HB2	1.93	0.49
11:2I:109:VAL:HA	18:9I:85:LEU:O	2.12	0.49
20:BI:100:ILE:HG12	20:BI:101:GLY:H	1.77	0.49
46:C5:88:LYS:CG	46:C5:89:PHE:H	2.21	0.49
42:C8:92:ARG:NH1	43:D8:11:GLN:O	2.46	0.49
47:D5:158:PRO:O	47:D5:161:VAL:HG22	2.13	0.49
48:I8:51:VAL:HG23	48:I8:81:VAL:HG23	1.95	0.49
55:P8:10:ARG:O	55:P8:14:LYS:HB2	2.13	0.49
2:12:98:LEU:O	2:12:101:MET:HG2	2.13	0.49
1:13:1159:U:O4'	1:13:1182:G:N2	2.46	0.49
1:13:345:C:O2'	1:13:346:G:N3	2.40	0.49
1:13:450:G:N7	1:13:481:G:C6	2.80	0.49
1:13:4:U:O4	8:7E:105:ARG:HG3	2.13	0.49
26:14:1204:A:H2	26:14:1241:A:N1	2.10	0.49
26:14:2115:G:N1	26:14:2117:A:N7	2.61	0.49
26:14:2394:C:H1'	62:14:3815:HOH:O	2.12	0.49
26:14:249:C:H4'	26:14:250:G:O5'	2.13	0.49
26:14:2869:G:H2'	26:14:2870:C:O4'	2.13	0.49
26:14:581:C:H2'	26:14:582:G:C8	2.45	0.49
1:1G:1353:G:P	21:1B:10:ARG:HH12	2.35	0.49
1:1G:110:C:H2'	1:1G:111:G:O4'	2.12	0.49
1:1G:1300:G:HO2'	1:1G:1301:U:P	2.36	0.49
1:1G:1459:C:OP1	20:BA:31:SER:OG	2.20	0.49
1:1G:20:U:H2'	1:1G:21:G:O4'	2.13	0.49
1:1G:973:G:H5'	10:1A:55:LYS:NZ	2.26	0.49
26:1H:1140:C:OP1	35:58:23:LEU:HB3	2.13	0.49
26:1H:1206:G:C6	26:1H:1207:C:C4	3.01	0.49
26:1H:1434:A:H61	26:1H:1558:A:H62	1.57	0.49
26:1H:2505:G:O6	26:1H:2576:G:H2'	2.12	0.49
27:1J:103:U:O2'	47:D5:29:TYR:OH	2.18	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:1J:18:G:H1	27:1J:65:C:H42	1.61	0.49
3:22:119:ARG:NH2	3:22:140:ARG:HD2	2.28	0.49
37:35:127:ALA:O	37:35:147:LEU:HB2	2.13	0.49
24:3L:10:G:H22	24:3L:26:A:H1'	1.78	0.49
24:3L:48:C:C6	24:3L:59:A:H1'	2.48	0.49
40:65:101:LEU:O	40:65:105:ALA:N	2.43	0.49
9:82:24:GLY:HA2	9:82:59:PHE:O	2.13	0.49
26:14:2012:G:OP2	44:A5:16:LYS:NZ	2.45	0.49
44:A5:75:TYR:CZ	44:A5:104:THR:HG21	2.48	0.49
29:11:142:VAL:HG23	29:11:193:VAL:HA	1.94	0.49
2:12:178:ARG:HD2	2:12:196:LEU:O	2.12	0.49
1:13:1126:U:C4	1:13:1127:G:C4	3.01	0.49
1:13:1469:G:O6	62:13:1841:HOH:O	2.20	0.49
1:13:2:U:H5''	1:13:630:G:N2	2.28	0.49
1:13:813:U:OP2	1:13:816:A:N6	2.42	0.49
26:14:1204:A:O2'	26:14:1205:U:OP2	2.29	0.49
26:14:304:G:H2'	26:14:305:U:C6	2.48	0.49
26:14:311:A:C6	26:14:328:U:C4	3.01	0.49
26:14:77:C:OP1	50:G5:59:ARG:HD3	2.13	0.49
2:1E:158:LEU:HD22	2:1E:182:ILE:HD11	1.95	0.49
1:1G:1011:G:N2	1:1G:1019:C:H1'	2.28	0.49
1:1G:426:G:OP1	4:32:38:TYR:OH	2.26	0.49
1:1G:730:G:C5	1:1G:731:G:H1'	2.48	0.49
1:1G:979:C:H3'	1:1G:980:C:C5'	2.42	0.49
26:1H:2308:G:N3	26:1H:2308:G:H2'	2.28	0.49
26:1H:493:G:H2'	26:1H:494:G:O4'	2.12	0.49
26:1H:721:C:H2'	26:1H:722:A:C8	2.47	0.49
27:1J:44:G:H5''	27:1J:45:A:OP1	2.13	0.49
30:29:147:PRO:HB2	30:29:149:ARG:HD3	1.95	0.49
30:29:81:ILE:HG22	30:29:82:ARG:N	2.23	0.49
24:3L:22:G:C8	24:3L:46:G:N2	2.79	0.49
38:45:66:ILE:HG22	38:45:104:PHE:HE1	1.78	0.49
33:59:149:ARG:NH1	33:59:162:ILE:O	2.46	0.49
7:62:116:ALA:O	7:62:120:ILE:HG12	2.13	0.49
34:69:102:SER:OG	34:69:103:ARG:N	2.45	0.49
15:6A:11:VAL:HG21	15:6A:34:LEU:HD12	1.94	0.49
39:98:78:LYS:O	39:98:83:ILE:HG13	2.12	0.49
40:A8:70:GLY:HA2	40:A8:101:LEU:HD13	1.95	0.49
47:D5:40:ASP:OD1	47:D5:43:GLU:N	2.33	0.49
47:D5:6:LYS:HG3	47:D5:7:ALA:H	1.77	0.49
47:H8:52:SER:O	47:H8:53:ILE:HG12	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:O8:41:PRO:HB2	54:O8:44:ARG:NH1	2.27	0.49
56:Q8:15:LYS:HG3	56:Q8:16:ILE:N	2.28	0.49
1:13:1071:C:H2'	1:13:1072:G:H8	1.77	0.48
1:13:35:G:H2'	1:13:36:C:C6	2.48	0.48
1:13:411:A:C8	1:13:413:G:H1'	2.48	0.48
1:13:953:G:C2	1:13:954:G:H1'	2.48	0.48
26:14:1181:C:H2'	26:14:1182:A:H8	1.78	0.48
26:14:2280:G:C2'	26:14:2281:C:H5'	2.43	0.48
26:14:959:A:N6	26:14:960:A:N1	2.61	0.48
26:14:975:G:H1'	26:14:990:A:C2	2.47	0.48
1:1G:1143:G:H2'	1:1G:1144:G:C8	2.48	0.48
1:1G:976:G:N7	1:1G:1358:U:C5	2.80	0.48
1:1G:227:G:H2'	1:1G:228:A:C8	2.48	0.48
1:1G:266:G:H5'	1:1G:268:C:H41	1.78	0.48
1:1G:433:C:H2'	1:1G:434:U:H6	1.78	0.48
1:1G:592:G:H1	1:1G:647:C:H42	1.61	0.48
1:1G:828:A:H5''	1:1G:859:A:C2	2.48	0.48
26:1H:1358:G:N2	26:1H:1372:U:C5	2.81	0.48
26:1H:1491:G:O2'	29:11:101:GLU:HB2	2.13	0.48
26:1H:1705:G:C6	26:1H:1706:U:C4	3.00	0.48
26:1H:2056:G:C2	26:1H:2057:A:C8	3.01	0.48
26:1H:2287:A:N6	26:1H:2344:U:H3	2.10	0.48
26:1H:234:C:H2'	26:1H:235:U:C6	2.47	0.48
26:1H:2854:G:H2'	26:1H:2855:C:C6	2.48	0.48
26:1H:847:U:C5	26:1H:933:A:N1	2.81	0.48
31:39:68:LYS:HB3	31:39:69:HIS:CD2	2.48	0.48
38:45:32:TYR:CE1	38:45:133:ARG:HG3	2.48	0.48
13:4I:79:LYS:O	13:4I:83:ASP:HB2	2.13	0.48
1:13:1308:U:OP1	13:4I:98:VAL:HG22	2.14	0.48
34:61:110:ASP:OD1	34:61:111:PRO:HA	2.12	0.48
26:1H:1243:G:O2'	37:78:7:ARG:NH2	2.46	0.48
44:A5:110:LYS:HG3	44:A5:111:HIS:ND1	2.27	0.48
20:BA:33:ILE:HD11	20:BA:62:LEU:O	2.13	0.48
43:D8:37:VAL:O	43:D8:38:LEU:HG	2.13	0.48
51:H5:6:VAL:O	51:H5:34:GLU:HA	2.13	0.48
26:1H:2261:C:C5	48:I8:16:SER:HB3	2.48	0.48
1:13:1016:A:H2'	1:13:1017:G:O4'	2.13	0.48
1:13:347:G:H2'	1:13:348:G:O4'	2.12	0.48
1:13:814:A:N7	1:13:816:A:C4	2.81	0.48
26:14:152:G:H1	26:14:174:C:N4	2.04	0.48
26:14:1585:C:H2'	26:14:1585:C:O2	2.12	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:14:1973:G:H2'	26:14:1974:C:C6	2.47	0.48
26:14:1999:C:H4'	26:14:2723:C:O2	2.13	0.48
26:14:2315:G:H2'	26:14:2316:C:C6	2.48	0.48
26:14:569:U:C4	26:14:570:G:C6	3.01	0.48
1:1G:1316:G:HO2'	1:1G:1318:A:H62	1.60	0.48
1:1G:141:A:H1'	1:1G:182:U:O2	2.13	0.48
1:1G:995:C:O2'	1:1G:996:A:H5'	2.13	0.48
26:1H:141:A:H8	26:1H:1595:G:H21	1.60	0.48
26:1H:2320:A:N3	26:1H:2320:A:H2'	2.29	0.48
26:1H:2462:U:H1'	26:1H:2491:U:O4	2.13	0.48
9:8E:114:TYR:CE2	10:1I:59:SER:HA	2.48	0.48
11:2I:41:THR:HG21	11:2I:71:LYS:HD2	1.95	0.48
31:31:134:GLY:HA2	31:31:166:ALA:HB2	1.95	0.48
1:1G:407:G:O2'	4:32:116:GLN:HG3	2.13	0.48
26:14:627:A:H62	37:35:84:ASN:ND2	2.11	0.48
26:14:322:A:OP2	31:39:169:ASN:HB2	2.13	0.48
5:42:107:ARG:NH2	5:42:108:ALA:HB2	2.28	0.48
32:49:120:LEU:HG	32:49:179:PRO:O	2.12	0.48
6:52:68:PRO:HG2	6:52:71:ARG:HG3	1.94	0.48
26:1H:558:G:P	35:58:111:PRO:HD2	2.53	0.48
34:61:81:VAL:HG11	34:61:88:ILE:HD13	1.94	0.48
16:7A:45:THR:O	16:7A:48:TRP:HD1	1.97	0.48
8:7E:10:LEU:HD22	8:7E:83:ILE:HD11	1.95	0.48
1:1G:1372:U:OP1	9:82:72:GLY:N	2.46	0.48
30:21:111:ARG:HA	39:98:1:MET:HE3	1.95	0.48
42:C8:75:ASN:HB3	42:C8:77:SER:H	1.78	0.48
42:C8:90:VAL:O	42:C8:92:ARG:N	2.46	0.48
50:G5:4:SER:N	50:G5:5:GLU:HB2	2.28	0.48
54:O8:47:THR:HG22	54:O8:48:VAL:HG23	1.95	0.48
54:O8:47:THR:HG22	54:O8:48:VAL:H	1.77	0.48
2:12:95:GLN:HB3	2:12:148:TYR:HD1	1.78	0.48
1:13:1210:C:H2'	1:13:1211:U:H5'	1.94	0.48
1:13:1342:C:H4'	9:8E:125:TYR:HB3	1.94	0.48
1:13:1417:G:N2	1:13:1482:G:H2'	2.28	0.48
1:13:148:G:H2'	1:13:149:A:H8	1.76	0.48
26:14:1332:G:H5'	26:14:1332:G:C8	2.47	0.48
26:14:141:A:C8	26:14:1408:C:H1'	2.48	0.48
26:14:1622:G:OP1	62:14:3652:HOH:O	2.20	0.48
26:14:2126:A:H2	26:14:2162:G:H22	1.60	0.48
26:14:376:C:H2'	26:14:377:C:C6	2.48	0.48
2:1E:25:ASN:ND2	2:1E:193:ASP:HB3	2.28	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1G:1084:G:H5'	1:1G:1102:A:OP2	2.13	0.48
1:1G:956:U:H1'	1:1G:1225:A:H2	1.76	0.48
1:1G:407:G:H2'	1:1G:408:A:C8	2.48	0.48
1:1G:457:C:H2'	1:1G:458:C:C6	2.48	0.48
26:1H:1441:G:H2'	26:1H:1442:G:H8	1.78	0.48
26:1H:2259:G:H1'	26:1H:2427:C:H2'	1.95	0.48
26:1H:2502:G:N7	62:1H:3840:HOH:O	2.35	0.48
26:1H:2895:U:H2'	26:1H:2896:C:H6	1.78	0.48
26:1H:723:G:H2'	26:1H:724:U:O4'	2.13	0.48
26:1H:991:C:H2'	26:1H:992:C:C6	2.48	0.48
3:22:70:VAL:HG12	3:22:72:LYS:N	2.25	0.48
23:2L:2:G:H2'	23:2L:3:C:C6	2.48	0.48
31:31:197:ASP:O	31:31:199:TRP:N	2.46	0.48
5:42:146:ALA:HB1	5:42:150:ARG:HH21	1.78	0.48
32:49:101:ILE:HD12	32:49:105:LYS:HD2	1.95	0.48
32:49:97:ASP:O	32:49:101:ILE:HG23	2.14	0.48
13:4I:11:ARG:HG2	13:4I:12:ASN:H	1.79	0.48
1:1G:1535:C:N4	25:4L:10:G:H21	2.08	0.48
33:51:118:PRO:HD2	33:51:121:ILE:HG21	1.95	0.48
34:61:86:THR:HA	34:61:123:LEU:HD13	1.94	0.48
26:1H:811:U:H2'	37:78:21:ARG:HA	1.94	0.48
26:1H:2469:A:O2'	38:88:56:ARG:NH1	2.46	0.48
17:8I:29:HIS:CD2	17:8I:30:PRO:HD2	2.48	0.48
44:A5:34:ASN:ND2	53:J5:39:MET:HG3	2.28	0.48
19:AI:23:ASN:HD21	19:AI:43:GLU:HB2	1.79	0.48
41:B8:60:THR:HG22	41:B8:77:PRO:HA	1.95	0.48
42:C8:88:ILE:C	42:C8:90:VAL:N	2.67	0.48
51:H5:6:VAL:HB	51:H5:54:VAL:HG21	1.93	0.48
45:F8:5:TYR:O	50:K8:36:ARG:NH2	2.46	0.48
51:L8:18:ASP:HB3	62:L8:102:HOH:O	2.13	0.48
1:13:198:G:N7	1:13:220:G:N2	2.61	0.48
1:13:260:G:H2'	1:13:261:U:C6	2.48	0.48
26:14:1019:U:H2'	26:14:1020:A:C8	2.48	0.48
26:14:1181:C:H2'	26:14:1182:A:C8	2.49	0.48
26:14:1224:G:N2	26:14:1227:A:OP2	2.34	0.48
26:14:1270:C:H5''	26:14:1271:G:O5'	2.12	0.48
26:14:140:A:C8	26:14:1408:C:O2'	2.61	0.48
26:14:2238:G:N3	26:14:2238:G:H2'	2.28	0.48
26:14:774:A:H2	26:14:787:U:O2'	1.96	0.48
26:14:881:G:H3'	26:14:882:G:C8	2.48	0.48
1:1G:1054:C:H4'	1:1G:1055:A:H5''	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1G:1255:G:OP1	10:1A:45:ARG:NH1	2.47	0.48
1:1G:142:G:H1	1:1G:221:C:H42	1.60	0.48
1:1G:622:A:C8	1:1G:623:C:C6	3.01	0.48
1:1G:922:G:N3	1:1G:1398:A:H2	2.10	0.48
26:1H:2630:G:H2'	26:1H:2631:G:O4'	2.13	0.48
26:1H:265:A:C8	26:1H:266:G:H1'	2.48	0.48
26:1H:2772:C:H2'	26:1H:2773:C:C6	2.48	0.48
26:1H:500:G:N2	26:1H:502:A:H3'	2.28	0.48
3:2E:113:ALA:HB2	3:2E:202:ILE:HG13	1.94	0.48
4:32:61:LYS:HB2	4:32:203:VAL:HG13	1.95	0.48
4:32:89:THR:HG21	4:32:204:ILE:HD11	1.95	0.48
24:3K:3:G:H1	24:3K:70:C:H42	1.61	0.48
28:71:53:ARG:HA	28:71:53:ARG:HD3	1.54	0.48
16:7A:40:ASP:HB3	16:7A:48:TRP:HB2	1.95	0.48
16:7A:43:LYS:HG2	16:7A:48:TRP:CD2	2.47	0.48
42:85:90:VAL:O	42:85:92:ARG:N	2.47	0.48
27:16:90:C:H5'	38:88:18:LYS:HA	1.95	0.48
43:95:39:LEU:HD23	43:95:40:LEU:N	2.28	0.48
18:9A:22:VAL:HG12	18:9A:55:ARG:O	2.14	0.48
20:BI:87:LYS:HA	20:BI:87:LYS:HD2	1.53	0.48
46:C5:8:LYS:NZ	46:C5:95:LYS:HD3	2.28	0.48
42:C8:79:PHE:O	42:C8:79:PHE:HD1	1.96	0.48
47:D5:174:VAL:O	47:D5:175:VAL:HB	2.12	0.48
46:G8:88:LYS:HD2	46:G8:92:ASN:OD1	2.13	0.48
50:K8:64:LEU:HD11	50:K8:68:ARG:HH11	1.79	0.48
2:12:210:SER:O	2:12:214:ILE:HG12	2.13	0.48
1:13:872:A:C4	1:13:874:G:N7	2.81	0.48
26:14:1375:C:H2'	26:14:1376:C:H6	1.77	0.48
26:14:483:A:H1'	46:C5:60:PHE:HE1	1.77	0.48
26:14:780:G:H21	26:14:783:A:N6	2.03	0.48
26:14:994:C:OP1	42:85:53:ARG:NH2	2.46	0.48
1:1G:1006:C:H2'	1:1G:1007:C:C6	2.48	0.48
1:1G:640:A:N3	8:72:115:SER:HB2	2.28	0.48
1:1G:938:A:N3	1:1G:1376:U:O2'	2.33	0.48
26:1H:1001:A:H2'	26:1H:1002:G:O4'	2.13	0.48
26:1H:1126:A:H8	26:1H:1126:A:O5'	1.96	0.48
26:1H:2159:G:H2'	26:1H:2160:G:H8	1.78	0.48
26:1H:2172:U:H5'	26:1H:2173:A:OP2	2.13	0.48
26:1H:2186:G:H2'	26:1H:2187:G:H8	1.78	0.48
26:1H:2414:G:H21	37:78:67:MET:HE1	1.78	0.48
26:1H:2846:G:H2'	26:1H:2847:U:O4'	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1H:698:C:O2'	26:1H:734:A:N6	2.47	0.48
26:1H:916:G:C2'	26:1H:917:A:H5''	2.43	0.48
1:13:963:G:H21	10:1I:55:LYS:HZ3	1.60	0.48
27:1J:44:G:O2'	27:1J:47:C:N4	2.46	0.48
30:29:60:ASN:OD1	30:29:61:ARG:N	2.47	0.48
23:2L:41:C:H2'	23:2L:42:C:C6	2.48	0.48
37:35:132:LYS:HD2	37:35:132:LYS:HA	1.61	0.48
12:3I:24:VAL:HB	12:3I:27:LEU:HD12	1.96	0.48
32:49:73:ALA:HB3	32:49:85:GLY:H	1.78	0.48
13:4A:13:LYS:HA	13:4A:44:ARG:HH11	1.79	0.48
34:61:10:GLU:O	34:61:10:GLU:HG3	2.12	0.48
36:68:64:ARG:HD3	36:68:79:PHE:CD2	2.49	0.48
15:6A:87:ILE:HG22	15:6A:88:ARG:N	2.29	0.48
8:72:14:ARG:O	8:72:18:ARG:HG2	2.13	0.48
1:1G:1342:C:H1'	9:82:124:GLN:NE2	2.29	0.48
26:1H:1614:A:N1	44:E8:93:ALA:HB2	2.28	0.48
45:F8:12:VAL:HG13	45:F8:27:THR:O	2.13	0.48
51:L8:7:LYS:HB2	51:L8:34:GLU:HG2	1.94	0.48
1:13:1171:G:H2'	1:13:1172:C:C6	2.49	0.48
1:13:1297:C:OP1	13:4I:13:LYS:NZ	2.39	0.48
1:13:666:G:H5''	1:13:732:C:O2	2.14	0.48
1:13:901:A:C5	1:13:902:G:H1'	2.48	0.48
26:14:1432:C:H2'	26:14:1433:U:O4'	2.13	0.48
26:14:1639:U:O2'	26:14:1640:C:H5'	2.14	0.48
26:14:2138:C:N4	26:14:2153:G:H22	2.12	0.48
26:14:2232:U:OP1	49:F5:40:ARG:NH2	2.47	0.48
26:14:2286:A:H4'	26:14:2287:A:O4'	2.12	0.48
26:14:528:A:N1	26:14:2042:A:H2'	2.28	0.48
26:14:618:G:H2'	26:14:618(A):C:O4'	2.12	0.48
26:14:71:A:H5'	26:14:71:A:H8	1.76	0.48
26:14:755:C:H2'	26:14:756:C:C6	2.48	0.48
29:19:228:PRO:HD3	29:19:235:GLY:N	2.28	0.48
1:1G:1223:C:H5''	1:1G:1224:G:H5''	1.94	0.48
1:1G:1327:C:H2'	1:1G:1328:C:C6	2.47	0.48
26:1H:1464:C:HO2'	26:1H:1528:A:H8	1.59	0.48
26:1H:1683:C:H2'	26:1H:1684:C:H6	1.78	0.48
26:1H:1683:C:H2'	26:1H:1684:C:C6	2.48	0.48
26:1H:2383:G:O2'	26:1H:2384:G:H5'	2.13	0.48
26:1H:2483:C:N3	38:88:124:LYS:HE3	2.28	0.48
26:1H:2801:A:H5'	26:1H:2895:U:O2'	2.13	0.48
26:1H:783:A:C8	26:1H:783:A:H3'	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:1I:50:ILE:HA	10:1I:60:ARG:HB3	1.96	0.48
30:21:181:LEU:HD21	41:B8:6:LEU:HG	1.95	0.48
23:2L:24:C:C2	23:2L:25:U:C5	3.01	0.48
12:3A:47:LYS:CD	12:3A:48:PRO:HD2	2.43	0.48
1:1G:1329:A:H4'	13:4A:24:GLY:HA2	1.95	0.48
5:4E:71:LEU:HD22	5:4E:114:GLY:HA3	1.96	0.48
14:5I:9:LYS:HA	14:5I:12:ARG:HG2	1.95	0.48
40:65:87:PHE:CZ	40:65:102:ALA:HB2	2.49	0.48
43:95:33:VAL:HG22	43:95:35:LEU:HD23	1.96	0.48
19:AI:40:ILE:HD11	19:AI:62:ILE:HG23	1.95	0.48
1:1G:192:U:O4'	20:BA:103:GLY:HA2	2.13	0.48
44:E8:19:LEU:HB3	53:N8:25:LEU:HD11	1.96	0.48
1:13:674:G:H2'	1:13:675:A:H8	1.79	0.48
26:14:251:A:C5	26:14:252:G:H1'	2.49	0.48
26:14:2820:A:C5	39:55:4:LEU:HD11	2.48	0.48
2:1E:155:LEU:HA	2:1E:155:LEU:HD23	1.72	0.48
1:1G:1287:A:H2'	1:1G:1288:A:C8	2.48	0.48
1:1G:197:A:C6	1:1G:221:C:H4'	2.48	0.48
1:1G:23:C:OP2	1:1G:561:U:N3	2.44	0.48
1:1G:407:G:OP1	4:32:115:ARG:NE	2.43	0.48
26:1H:1142(A):A:C4	26:1H:1144:G:C8	3.00	0.48
26:1H:1164:G:H2'	26:1H:1165:U:C6	2.48	0.48
26:1H:2291:U:H2'	26:1H:2292:C:C6	2.48	0.48
26:1H:2292:C:OP2	40:A8:17:ARG:NH2	2.47	0.48
27:1J:116:G:H5''	40:65:55:ALA:HB2	1.95	0.48
1:13:1190:G:OP1	3:2E:5:ILE:HG23	2.13	0.48
11:2I:19:ALA:HA	11:2I:32:ILE:HG22	1.95	0.48
4:32:12:CYS:SG	4:32:19:LEU:N	2.70	0.48
4:3E:10:ARG:HB2	4:3E:10:ARG:NH1	2.29	0.48
24:3K:5:C:H2'	24:3K:6:G:C8	2.47	0.48
5:4E:15:ARG:HE	5:4E:26:PHE:HE2	1.59	0.48
6:5E:69:GLU:O	6:5E:72:VAL:HG12	2.14	0.48
14:5I:13:THR:HG23	14:5I:20:ALA:HB2	1.96	0.48
41:75:5:ALA:HB3	41:75:9:LEU:HB2	1.94	0.48
26:1H:389:G:N1	37:78:71:VAL:HG12	2.28	0.48
45:B5:67:GLY:C	45:B5:69:TYR:H	2.17	0.48
41:B8:20:PRO:HG2	41:B8:86:ILE:O	2.13	0.48
1:13:1453:G:H2'	20:BI:39:LYS:HE2	1.96	0.48
48:E5:51:VAL:N	48:E5:62:LEU:HD12	2.29	0.48
47:H8:98:MET:O	47:H8:125:LEU:HD12	2.13	0.48
1:13:1122:U:O4	1:13:1123:A:N6	2.47	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:14:857:C:H2'	26:14:858:U:C6	2.49	0.48
29:19:133:LEU:HD13	29:19:173:VAL:HG11	1.95	0.48
29:19:31:LYS:HZ1	29:19:33:LEU:HB3	1.77	0.48
1:1G:972:C:C2'	10:1A:55:LYS:HG3	2.44	0.48
2:1E:111:ARG:HD2	2:1E:145:LEU:HD21	1.94	0.48
1:1G:1104:G:H4'	2:12:111:ARG:NE	2.29	0.48
1:1G:1151:A:HO2'	1:1G:1152:A:C5'	2.26	0.48
1:1G:164:U:H2'	1:1G:165:C:H6	1.79	0.48
1:1G:322:C:H5	1:1G:328:C:C5	2.32	0.48
1:1G:952:U:H4'	1:1G:964:A:N1	2.29	0.48
26:1H:1108:U:C2'	26:1H:1109:C:H5'	2.44	0.48
26:1H:1171:G:N2	26:1H:1178:C:N3	2.55	0.48
26:1H:1791:A:H5'	29:11:206:LEU:HD12	1.96	0.48
26:1H:2118:U:O4'	26:1H:2147:G:N1	2.43	0.48
26:1H:2126:A:H8	26:1H:2163:C:H1'	1.79	0.48
26:1H:2740:A:H2'	26:1H:2741:A:C8	2.48	0.48
26:1H:518:G:H2'	26:1H:519:U:C6	2.49	0.48
27:1J:88:C:H5''	27:1J:89:G:C6	2.49	0.48
3:2E:57:ILE:HG12	3:2E:66:VAL:HG22	1.96	0.48
11:2I:73:MET:HG2	11:2I:103:LEU:HD13	1.96	0.48
23:2L:54:G:H2'	23:2L:55:5MU:C6	2.49	0.48
31:31:101:LEU:HD23	31:31:102:PRO:CD	2.33	0.48
37:35:101:VAL:HA	37:35:105:LEU:O	2.14	0.48
24:3L:2:G:H1	24:3L:71:C:H42	1.62	0.48
32:41:81:LYS:HZ2	32:41:81:LYS:H	1.61	0.48
13:4A:81:LEU:CD2	13:4A:88:ARG:HH21	2.26	0.48
5:4E:33:VAL:HB	5:4E:112:LEU:HD12	1.95	0.48
33:59:77:LYS:HA	33:59:77:LYS:HD2	1.60	0.48
34:69:39:ALA:O	34:69:44:LEU:HG	2.14	0.48
28:71:45:ALA:H	28:71:171:ILE:HG22	1.79	0.48
8:72:101:PRO:HG2	8:72:133:LEU:HD11	1.95	0.48
19:AI:41:VAL:HB	19:AI:42:PRO:C	2.34	0.48
44:E8:18:ARG:HD3	44:E8:76:VAL:HG13	1.96	0.48
49:J8:51:VAL:HG21	49:J8:74:VAL:HG11	1.95	0.48
50:K8:2:LYS:O	50:K8:3:LEU:HD23	2.14	0.48
2:12:73:THR:HG21	2:12:97:TRP:N	2.29	0.48
1:13:1151:A:O2'	1:13:1152:A:H8	1.96	0.48
1:13:1179:A:H2'	1:13:1180:A:O4'	2.14	0.48
26:14:228:A:H2'	26:14:230:U:O4'	2.14	0.48
26:14:2680:C:H5'	30:29:189:PRO:HA	1.95	0.48
26:14:642:G:H3'	26:14:642:G:C8	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:15:33:LEU:HD12	35:15:38:HIS:CE1	2.49	0.48
29:19:27:THR:HG22	29:19:29:PRO:O	2.13	0.48
29:19:49:ILE:HD11	29:19:52:ARG:HA	1.96	0.48
1:1G:1008:C:N4	1:1G:1021:G:H22	2.11	0.48
1:1G:921:U:O2	5:42:19:MET:HB3	2.14	0.48
26:1H:1021:A:H3'	26:1H:1022:G:H5''	1.95	0.48
26:1H:1899:G:H1	26:1H:1902:C:N4	2.10	0.48
26:1H:2062:A:H2'	26:1H:2062:A:N3	2.29	0.48
26:1H:2322:A:OP2	62:1H:3776:HOH:O	2.20	0.48
26:1H:275:G:N2	26:1H:278:A:H61	2.11	0.48
26:1H:297:C:H2'	26:1H:298:G:O4'	2.14	0.48
30:21:8:LYS:NZ	30:21:190:GLY:O	2.39	0.48
30:29:169:ASN:OD1	30:29:201:THR:HG21	2.14	0.48
30:29:76:ARG:HG2	30:29:195:LEU:HD13	1.95	0.48
37:35:82:GLY:HA2	37:35:113:LYS:O	2.12	0.48
4:3E:122:ARG:HG2	4:3E:122:ARG:NH1	2.29	0.48
32:41:96:ARG:HB2	32:41:96:ARG:HH11	1.79	0.48
38:45:136:ALA:N	38:45:137:TYR:HA	2.29	0.48
5:4E:11:ILE:HG12	5:4E:31:LEU:HB3	1.96	0.48
33:51:2:SER:C	33:51:3:ARG:HE	2.16	0.48
1:13:974:A:P	14:5I:41:ARG:HH12	2.37	0.48
17:8I:45:HIS:O	17:8I:73:VAL:HG23	2.14	0.48
18:9I:73:ALA:HB3	18:9I:79:LEU:HD12	1.95	0.48
20:BI:90:GLN:HA	20:BI:93:GLU:HB2	1.94	0.48
47:D5:157:LEU:CB	47:D5:161:VAL:HG21	2.43	0.48
47:D5:75:ASN:O	47:D5:84:GLU:HG3	2.13	0.48
45:B5:11:PRO:HD3	50:G5:37:PHE:CE2	2.49	0.48
48:I8:82:ARG:NH2	48:I8:83:PRO:O	2.47	0.48
1:1G:1104:G:H4'	2:12:111:ARG:HH21	1.79	0.48
1:13:1022:G:H2'	1:13:1023:G:H8	1.79	0.48
1:13:1156:G:H2'	1:13:1157:A:H5''	1.96	0.48
1:13:1193:G:P	3:2E:167:TRP:HZ3	2.37	0.48
1:13:1306:A:N6	1:13:1331:G:H1'	2.26	0.48
1:13:346:G:H21	1:13:347:G:H1'	1.79	0.48
1:13:351:G:H4'	1:13:352:C:OP1	2.13	0.48
1:13:688:G:H2'	1:13:689:C:C6	2.49	0.48
26:14:1048:A:OP2	26:14:1110:G:N2	2.46	0.48
26:14:194:G:H2'	26:14:195:A:O4'	2.14	0.48
27:16:70:C:H2'	27:16:71:C:H6	1.79	0.48
2:1E:70:PHE:HE1	2:1E:90:MET:HB3	1.79	0.48
1:1G:1273:G:C4	1:1G:1274:G:C8	3.02	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1G:45:U:H2'	1:1G:46:G:H8	1.79	0.48
1:1G:689:C:C2'	1:1G:690:G:H5'	2.44	0.48
1:1G:980:C:H3'	1:1G:981:U:C6	2.49	0.48
26:1H:1794:U:H2'	26:1H:1795:C:C6	2.49	0.48
26:1H:2210:G:H3'	26:1H:2211:G:C4	2.48	0.48
26:1H:2352:A:C4	26:1H:2366:A:C2	3.02	0.48
26:1H:2443:C:O2'	26:1H:2444:G:H5'	2.14	0.48
26:1H:2543:G:H2'	26:1H:2544:G:C8	2.48	0.48
26:1H:322:A:OP2	31:31:169:ASN:HB2	2.12	0.48
27:1J:49:C:H2'	27:1J:50:G:C8	2.49	0.48
30:21:16:ARG:O	30:21:16:ARG:HG3	2.14	0.48
3:22:135:LYS:HZ1	3:22:139:GLN:HB2	1.79	0.48
23:2K:26:C:H2'	23:2K:27:G:O4'	2.14	0.48
23:2L:32:G:C6	23:2L:33:OMC:N4	2.82	0.48
4:32:173:TRP:CD1	4:32:174:LEU:HG	2.49	0.48
31:39:27:GLU:O	31:39:28:ILE:HG12	2.13	0.48
24:3K:6:G:N2	24:3K:67:C:O2	2.47	0.48
38:45:29:PHE:HB3	38:45:65:PHE:CE2	2.48	0.48
40:65:27:SER:HA	40:65:88:ASP:HB2	1.96	0.48
36:68:7:TYR:HE1	36:68:20:MET:HE3	1.79	0.48
8:7E:88:LYS:HB3	8:7E:89:PRO:HD2	1.95	0.48
18:9I:31:LEU:HD21	18:9I:62:GLU:HG2	1.96	0.48
26:14:1323:U:OP1	44:A5:84:ARG:HD2	2.13	0.48
41:B8:16:ARG:HB2	41:B8:18:ASP:OD1	2.14	0.48
42:C8:79:PHE:HE2	42:C8:106:PHE:CZ	2.32	0.48
49:J8:71:TYR:HA	49:J8:74:VAL:HG13	1.96	0.48
56:M5:52:LYS:N	56:M5:53:PRO:HD2	2.29	0.48
1:13:221:C:H2'	1:13:222:U:H6	1.79	0.47
1:13:256:U:H3	1:13:270:A:H61	1.62	0.47
1:13:321:A:H62	1:13:328:C:H1'	1.79	0.47
1:13:981:U:H5	1:13:982:U:HO2'	1.60	0.47
26:14:1827:C:C2'	26:14:1828:G:H5'	2.43	0.47
26:14:1889:A:N1	26:14:2234:G:H1'	2.29	0.47
29:19:12:SER:HB2	29:19:208:LYS:HB3	1.95	0.47
2:1E:46:LYS:HA	2:1E:49:GLU:OE1	2.13	0.47
1:1G:1288:A:H2'	1:1G:1289:A:C8	2.49	0.47
26:1H:1171:G:C5	26:1H:1174:A:N6	2.82	0.47
26:1H:1332:G:C8	26:1H:1332:G:H5'	2.49	0.47
26:1H:2840:C:H2'	26:1H:2841:C:C6	2.48	0.47
26:1H:699:A:H2'	26:1H:700:G:O4'	2.13	0.47
26:1H:722:A:H2'	26:1H:723:G:C8	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1H:963:U:H5'	62:1H:4635:HOH:O	2.13	0.47
30:21:105:THR:HG21	30:21:164:ARG:CZ	2.44	0.47
30:29:117:MET:HA	30:29:122:PHE:N	2.28	0.47
7:6E:150:ALA:HB2	11:2I:50:TYR:HE2	1.77	0.47
4:32:126:ILE:HG22	4:32:127:THR:N	2.29	0.47
31:39:51:THR:HG23	31:39:92:PRO:HG2	1.95	0.47
12:3A:41:ARG:NH1	12:3A:41:ARG:HB3	2.25	0.47
24:3L:15:G:H22	24:3L:48:C:H41	1.61	0.47
32:41:11:TYR:OH	32:41:16:ARG:NH1	2.46	0.47
32:41:161:THR:CG2	32:41:163:ALA:H	2.24	0.47
32:49:63:ILE:HG22	32:49:143:GLU:HB2	1.96	0.47
32:49:49:ASP:O	32:49:52:ILE:HG22	2.14	0.47
6:52:81:ILE:HG23	6:52:82:ARG:HG3	1.95	0.47
6:5E:5:GLU:HA	6:5E:63:TYR:O	2.14	0.47
7:62:23:VAL:HG13	7:62:43:PHE:CE2	2.48	0.47
27:1J:52:A:H62	40:65:33:LYS:HG3	1.78	0.47
8:72:7:ALA:HB2	8:72:85:ARG:HD3	1.95	0.47
41:75:26:ASP:OD1	41:75:120:ARG:NH2	2.41	0.47
18:9A:22:VAL:C	18:9A:24:ALA:H	2.17	0.47
20:BI:49:ALA:O	20:BI:52:ALA:N	2.47	0.47
46:C5:75:ILE:HG22	46:C5:76:CYS:N	2.28	0.47
26:14:76:C:O3'	50:G5:59:ARG:HG3	2.13	0.47
47:H8:58:VAL:O	47:H8:60:GLU:N	2.47	0.47
54:O8:44:ARG:O	54:O8:45:LYS:HG2	2.14	0.47
26:1H:764:A:H2	29:11:219:PRO:HG3	1.79	0.47
26:1H:1826:G:H4'	29:11:242:ARG:CZ	2.45	0.47
1:13:157:G:N2	1:13:165:C:O2	2.47	0.47
1:13:295:C:H2'	1:13:296:U:O4'	2.14	0.47
26:14:1022:G:C6	26:14:1140:C:C4	3.03	0.47
26:14:1147:C:H2'	26:14:1148:A:C8	2.50	0.47
26:14:1188:U:O2'	26:14:1189:A:H5'	2.14	0.47
26:14:1235:G:C6	26:14:1236:G:N1	2.82	0.47
26:14:1342:A:C2	26:14:1397:U:C2	3.02	0.47
26:14:1494:A:C2	26:14:1495:A:C4	3.02	0.47
26:14:1651:G:H5'	39:55:39:PRO:HG2	1.96	0.47
26:14:1889:A:H2'	26:14:1890:A:O4'	2.14	0.47
26:14:702:G:C2	26:14:731:C:C2	3.02	0.47
26:14:882:G:H22	26:14:894:C:N4	2.12	0.47
21:1F:3:LYS:HB3	21:1F:14:TRP:CD1	2.49	0.47
1:1G:485:G:O2'	1:1G:486:U:O5'	2.33	0.47
1:1G:978:A:H1'	1:1G:1322:C:C2	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1H:1535:U:O4	26:1H:1538:G:O2'	2.15	0.47
26:1H:2837:G:H2'	26:1H:2838:G:H8	1.80	0.47
26:1H:320:A:OP1	31:31:135:LYS:NZ	2.47	0.47
26:1H:456:C:O2'	26:1H:457:A:OP2	2.31	0.47
3:22:141:VAL:HA	3:22:144:SER:HB3	1.96	0.47
1:1G:1422:G:OP1	36:25:48:PRO:HA	2.14	0.47
36:25:60:ALA:HB1	36:25:84:ALA:HB1	1.96	0.47
31:39:101:LEU:O	31:39:106:ARG:NH1	2.46	0.47
31:39:107:LYS:HZ1	31:39:205:ARG:HD2	1.78	0.47
32:41:107:LEU:HD21	32:41:178:PHE:CE1	2.50	0.47
13:4I:49:THR:HG22	13:4I:51:ALA:H	1.79	0.47
7:6E:94:ARG:O	7:6E:97:GLN:HB3	2.14	0.47
37:78:15:ARG:HA	37:78:15:ARG:HD2	1.62	0.47
37:78:29:LYS:HG2	37:78:30:THR:N	2.29	0.47
37:78:97:PRO:HB3	37:78:112:LEU:HB2	1.96	0.47
37:78:98:GLU:O	37:78:101:VAL:HG13	2.13	0.47
1:13:375:U:O3'	16:7I:6:LEU:HB2	2.13	0.47
9:8E:77:ILE:O	9:8E:81:ILE:HG12	2.14	0.47
37:78:50:ARG:HD3	56:Q8:7:HIS:CD2	2.49	0.47
2:12:77:ALA:O	2:12:81:VAL:HG23	2.14	0.47
1:13:1125:U:C2	1:13:1126:U:C5	3.02	0.47
26:14:1239:G:H5''	62:14:4324:HOH:O	2.14	0.47
26:14:1331:A:O2'	26:14:1332:G:H8	1.96	0.47
26:14:1351:C:H2'	26:14:1352:U:C6	2.50	0.47
26:14:2115:G:O2'	26:14:2171:A:N6	2.47	0.47
26:14:2592:G:N7	62:14:3715:HOH:O	2.35	0.47
26:14:43:G:H2'	26:14:44:A:O4'	2.13	0.47
26:14:529:A:H4'	26:14:530:G:H5'	1.96	0.47
26:14:774:A:HO2'	26:14:775:G:P	2.37	0.47
2:1E:84:GLU:OE2	2:1E:216:SER:HA	2.14	0.47
1:1G:976:G:H5'	1:1G:1358:U:O2'	2.14	0.47
1:1G:451:A:OP1	1:1G:481:G:N2	2.36	0.47
1:1G:660:G:H1	1:1G:745:C:H42	1.60	0.47
26:1H:1541:U:H2'	26:1H:1542:G:O4'	2.14	0.47
26:1H:1639:U:H4'	26:1H:2699:C:H4'	1.96	0.47
26:1H:1686:C:H2'	26:1H:1687:G:O4'	2.15	0.47
31:31:184:TYR:CE2	31:31:188:ARG:HD2	2.49	0.47
26:14:805:G:OP2	37:35:41:ARG:HG2	2.14	0.47
31:39:7:TYR:HD1	31:39:18:ARG:H	1.61	0.47
5:42:8:GLU:HA	5:42:34:VAL:HA	1.96	0.47
13:4I:15:VAL:O	13:4I:19:LEU:HD23	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:62:20:ASP:HB3	7:62:23:VAL:HB	1.95	0.47
7:62:88:PRO:O	7:62:89:MET:HG2	2.14	0.47
7:62:97:GLN:O	7:62:101:LEU:HG	2.14	0.47
36:68:47:ILE:HG13	36:68:48:PRO:HD2	1.97	0.47
7:6E:140:ASP:O	7:6E:144:MET:HG2	2.14	0.47
7:6E:150:ALA:HB2	11:2I:50:TYR:CE2	2.49	0.47
15:6I:56:LEU:O	15:6I:60:VAL:HG23	2.14	0.47
1:1G:826:C:H5'	8:72:12:ARG:NH1	2.28	0.47
41:75:91:ARG:HD2	41:75:124:ASP:OD2	2.14	0.47
26:1H:1187:G:H5''	43:D8:81:TYR:CE1	2.49	0.47
1:13:345:C:H4'	1:13:346:G:C8	2.50	0.47
1:13:963:G:N7	62:13:1854:HOH:O	2.35	0.47
26:14:1199:U:O2'	62:14:3649:HOH:O	2.19	0.47
26:14:1536:A:H8	26:14:1537:C:H1'	1.78	0.47
26:14:1784:A:H4'	26:14:1785:A:O5'	2.15	0.47
26:14:2328:A:H2'	26:14:2329:G:O4'	2.15	0.47
26:14:2402:C:H5	26:14:2415:G:H22	1.63	0.47
26:14:49:A:H5''	26:14:51:G:O4'	2.14	0.47
26:14:819:A:H2'	26:14:820:A:H5'	1.95	0.47
26:14:959:A:C6	26:14:960:A:N1	2.82	0.47
29:19:8:PRO:HB3	29:19:14:ARG:HB2	1.96	0.47
1:1G:382:A:H2'	1:1G:383:A:C8	2.50	0.47
1:1G:487:A:H2'	1:1G:488:C:O4'	2.15	0.47
1:1G:858:G:H8	1:1G:858:G:OP2	1.97	0.47
1:1G:999:U:H2'	1:1G:1000:A:C8	2.50	0.47
26:1H:2330:G:H2'	26:1H:2331:G:O4'	2.14	0.47
26:1H:782:A:H5'	26:1H:783:A:C2	2.49	0.47
22:1K:7:U:O2'	22:1K:8:U:H5'	2.15	0.47
3:22:113:ALA:HB3	3:22:114:PRO:HD3	1.96	0.47
26:1H:444:C:C4'	31:31:49:ALA:HB2	2.44	0.47
31:39:121:GLY:O	31:39:122:LYS:HD3	2.15	0.47
24:3L:18:G:O2'	24:3L:57:G:H2'	2.14	0.47
32:49:95:ARG:O	32:49:99:MET:HG2	2.14	0.47
33:59:59:ARG:O	33:59:63:SER:OG	2.20	0.47
15:6A:39:LEU:CD1	15:6A:56:LEU:HB2	2.43	0.47
28:71:6:ARG:CZ	28:71:6:ARG:HB3	2.43	0.47
8:7E:104:ARG:HG3	8:7E:138:TRP:CD1	2.50	0.47
9:8E:97:LYS:HB2	9:8E:102:LEU:HD12	1.97	0.47
39:98:26:LYS:HE2	39:98:70:LEU:O	2.14	0.47
41:B8:88:ILE:O	41:B8:88:ILE:HG13	2.13	0.47
47:D5:4:ARG:NH1	47:D5:60:GLU:OE2	2.46	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:E5:72:ARG:HH21	48:E5:75:LEU:CD1	2.28	0.47
45:F8:41:ASN:OD1	45:F8:41:ASN:N	2.47	0.47
50:G5:17:SER:HB2	50:G5:20:GLU:HG3	1.95	0.47
2:12:188:ALA:O	2:12:203:GLY:N	2.48	0.47
1:13:131:C:H2'	1:13:132:C:C6	2.49	0.47
1:13:1466:C:H2'	1:13:1467:G:O4'	2.15	0.47
1:13:392:G:H5''	16:7I:12:LYS:HE3	1.96	0.47
1:13:475:G:H2'	1:13:476:G:O4'	2.14	0.47
26:14:1033:U:H3'	26:14:1033:U:H6	1.79	0.47
26:14:2865:U:C4	26:14:2866:U:C4	3.02	0.47
26:14:332:A:O2'	26:14:334:C:OP2	2.23	0.47
26:14:853:G:O2'	26:14:854:G:H5'	2.15	0.47
27:16:29:A:OP2	40:A8:31:SER:HB2	2.13	0.47
21:1B:2:GLY:O	21:1B:4:GLY:N	2.47	0.47
1:1G:991:U:C5	1:1G:1212:U:H1'	2.48	0.47
1:1G:1281:U:H3'	1:1G:1282:C:C5	2.49	0.47
1:1G:281:G:H8	1:1G:281:G:OP2	1.96	0.47
26:1H:941:A:H4'	62:1H:4465:HOH:O	2.13	0.47
3:22:5:ILE:HG21	10:1A:51:ARG:HH21	1.80	0.47
30:29:23:VAL:HG11	30:29:183:LEU:HD23	1.95	0.47
4:32:65:ARG:HD2	4:32:72:GLU:HA	1.96	0.47
24:3K:9:A:H1'	24:3K:46:G:C8	2.49	0.47
5:4E:27:ARG:HE	5:4E:27:ARG:HB2	1.39	0.47
1:13:947:G:O3'	13:4I:109:THR:OG1	2.32	0.47
33:59:19:VAL:HG12	33:59:20:ALA:H	1.79	0.47
34:69:128:LEU:O	34:69:137:PRO:HA	2.14	0.47
1:13:1375:A:H4'	7:6E:29:LYS:HD3	1.97	0.47
8:72:119:LEU:HD12	8:72:124:ALA:HA	1.95	0.47
26:1H:1250:G:OP2	37:78:21:ARG:HD3	2.15	0.47
37:78:59:LEU:HB2	56:Q8:58:ILE:CD1	2.44	0.47
8:7E:83:ILE:HB	8:7E:137:VAL:HG13	1.96	0.47
9:8E:9:ARG:HE	9:8E:14:VAL:HG13	1.79	0.47
9:8E:17:VAL:HG21	9:8E:80:GLY:HA3	1.96	0.47
17:8I:28:PRO:HA	17:8I:34:LYS:O	2.14	0.47
40:A8:26:LEU:HD22	40:A8:87:PHE:CD1	2.50	0.47
46:C5:97:ARG:NH1	46:C5:104:GLY:O	2.47	0.47
47:D5:105:VAL:HG13	47:D5:106:GLY:N	2.30	0.47
37:78:59:LEU:HB2	56:Q8:58:ILE:HD11	1.96	0.47
1:13:1028(A):C:N4	1:13:1029:G:N7	2.62	0.47
1:13:1162:C:H2'	1:13:1163:C:C6	2.49	0.47
1:13:1322:C:H5''	13:4I:100:GLY:HA2	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:14:142:G:H2'	26:14:143:C:C6	2.50	0.47
26:14:2124:G:H2'	26:14:2124:G:N3	2.29	0.47
26:14:2688:U:H5	26:14:2720:U:OP2	1.97	0.47
1:1G:411:A:C5	1:1G:413:G:H1'	2.49	0.47
1:1G:804:U:H5''	1:1G:805:C:OP2	2.15	0.47
26:1H:185:U:H4'	26:1H:218:A:H4'	1.97	0.47
26:1H:1678:G:N2	26:1H:1989:G:N2	2.60	0.47
26:1H:2436:G:C5	26:1H:2437:U:C5	3.03	0.47
26:1H:2775:A:N6	62:1H:3724:HOH:O	2.48	0.47
26:1H:2877:G:H2'	26:1H:2878:U:O4'	2.14	0.47
26:1H:775:G:O5'	26:1H:777:A:H1'	2.14	0.47
26:1H:847:U:H5'	62:1H:3743:HOH:O	2.15	0.47
27:1J:21:G:H2'	27:1J:22:U:O4'	2.15	0.47
23:2K:65:G:C2	23:2K:66:C:C2	3.03	0.47
4:32:24:GLU:OE2	4:32:24:GLU:N	2.48	0.47
37:35:6:LEU:HA	37:35:6:LEU:HD12	1.52	0.47
1:13:881:G:P	12:3I:12:ARG:HH22	2.37	0.47
24:3L:44:U:H2'	24:3L:45:G:O4'	2.14	0.47
13:4I:70:LEU:O	13:4I:74:VAL:HG23	2.15	0.47
33:59:137:ASP:CB	33:59:140:LYS:HB2	2.45	0.47
6:5E:96:PRO:HB3	18:9I:30:ASP:CG	2.35	0.47
36:68:64:ARG:HB2	36:68:79:PHE:CG	2.49	0.47
7:6E:111:ARG:HE	7:6E:123:GLU:HB2	1.79	0.47
9:8E:112:LYS:CA	9:8E:119:ALA:HB2	2.43	0.47
40:A8:58:LEU:HD12	40:A8:68:GLN:OE1	2.15	0.47
19:AA:53:ASN:HB2	19:AA:77:THR:HG22	1.97	0.47
29:11:79:VAL:HG21	29:11:111:LEU:HD11	1.97	0.47
29:11:77:ALA:HB2	29:11:97:TYR:CD2	2.49	0.47
1:13:1164:G:C6	1:13:1165:C:C4	3.03	0.47
1:13:1427:U:H2'	1:13:1428:A:C8	2.48	0.47
1:13:41:G:H2'	1:13:42:G:C8	2.49	0.47
1:13:452:A:H2'	1:13:453:A:C8	2.50	0.47
1:13:631:G:HO2'	1:13:632:A:P	2.37	0.47
26:14:1621:U:OP1	62:14:3652:HOH:O	2.20	0.47
26:14:2261:C:C6	48:E5:16:SER:HB3	2.49	0.47
26:14:631:A:H2'	26:14:632:A:O4'	2.15	0.47
27:16:15:A:H5'	27:16:16:G:H8	1.80	0.47
1:1G:855:G:C2	1:1G:856:C:C2	3.02	0.47
26:1H:1053:C:N4	26:1H:1106:G:H1	2.13	0.47
26:1H:1688:U:O2	26:1H:1700:A:H5''	2.14	0.47
26:1H:1971:A:C4	29:11:241:PRO:HD3	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1H:2061:G:H5''	26:1H:2503:A:C2	2.50	0.47
26:1H:2648:C:H2'	26:1H:2649:U:C6	2.49	0.47
26:1H:32:C:O2'	26:1H:33:U:H5'	2.15	0.47
1:1G:1112:C:C4	3:22:178:LEU:HD23	2.49	0.47
30:29:76:ARG:HD3	30:29:76:ARG:HA	1.59	0.47
31:39:30:PRO:O	31:39:33:LEU:N	2.47	0.47
5:4E:98:THR:HB	5:4E:117:ASP:HB3	1.97	0.47
25:4L:19:G:N3	25:4L:20:A:C8	2.83	0.47
33:51:97:ARG:NH2	33:51:104:GLU:OE2	2.42	0.47
33:51:5:GLY:HA2	33:51:8:PRO:HD3	1.97	0.47
26:14:1653:G:H3'	39:55:2:ARG:CG	2.43	0.47
34:61:33:ARG:HB3	34:61:35:LEU:HD13	1.97	0.47
34:69:143:SER:O	34:69:144:VAL:HG22	2.14	0.47
28:71:23:ASP:HB2	28:71:190:ARG:NH2	2.26	0.47
30:29:9:VAL:HA	41:75:3:ARG:HD2	1.97	0.47
16:7A:52:ASP:OD2	16:7A:55:ARG:HG3	2.15	0.47
16:7I:20:VAL:HG21	16:7I:32:TYR:CD2	2.50	0.47
9:82:81:ILE:HG22	9:82:85:LEU:HD23	1.96	0.47
40:A8:58:LEU:HD23	40:A8:58:LEU:H	1.80	0.47
20:BA:87:LYS:O	20:BA:91:LEU:HG	2.15	0.47
20:BI:40:ALA:HB2	20:BI:55:ILE:HG22	1.97	0.47
46:G8:96:ILE:HA	46:G8:102:CYS:O	2.14	0.47
47:H8:116:VAL:HG13	47:H8:146:ILE:HD13	1.97	0.47
27:16:43:C:H5''	52:M8:1:MET:HG2	1.96	0.47
29:11:92:ILE:HD12	29:11:104:TYR:CE1	2.49	0.47
1:13:1120:G:H2'	1:13:1121:U:C6	2.50	0.47
1:13:1391:U:H2'	1:13:1392:G:H8	1.72	0.47
1:13:737:A:H2'	1:13:738:C:H6	1.74	0.47
26:14:1445:C:H2'	26:14:1446:C:C6	2.49	0.47
26:14:1551:C:H2'	26:14:1552:G:O4'	2.15	0.47
26:14:1579:A:H2'	26:14:1580:A:C8	2.49	0.47
26:14:1833:U:O2'	26:14:1969:A:N1	2.38	0.47
26:14:202:U:H2'	26:14:203:C:O4'	2.14	0.47
26:14:2182:G:H2'	26:14:2183:C:C6	2.50	0.47
26:14:2104:G:C2	26:14:2186:G:C2	3.03	0.47
26:14:2400:G:H2'	26:14:2401:U:H6	1.79	0.47
26:14:2591:C:H2'	26:14:2592:G:C8	2.50	0.47
26:14:2839:G:H21	39:55:92:GLY:CA	2.28	0.47
26:14:582:G:H2'	26:14:583:G:H8	1.79	0.47
35:15:61:ARG:NH1	35:15:61:ARG:HA	2.29	0.47
26:14:1826:G:H4'	29:19:242:ARG:CZ	2.45	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1G:1152:A:H2'	1:1G:1153:C:C6	2.49	0.47
1:1G:843:U:H3'	1:1G:848:C:O4'	2.13	0.47
26:1H:139:G:N3	26:1H:141:A:N1	2.63	0.47
26:1H:1771:C:H1'	26:1H:1786:A:C8	2.50	0.47
26:1H:1799:G:H5'	26:1H:1819:A:N6	2.29	0.47
26:1H:2439:A:C8	26:1H:2439:A:H5'	2.49	0.47
26:1H:270(J):G:N2	26:1H:270(P):C:O2	2.30	0.47
26:1H:482:A:H5''	26:1H:483:A:OP1	2.15	0.47
3:22:18:TRP:HE1	14:5A:56:VAL:H	1.62	0.47
1:1G:690:G:H22	11:2A:55:LYS:HE2	1.79	0.47
4:32:112:VAL:HG12	4:32:116:GLN:OE1	2.14	0.47
37:35:113:LYS:HD3	37:35:115:LEU:HD21	1.96	0.47
37:35:27:HIS:HB3	37:35:32:THR:HG23	1.96	0.47
4:3E:108:LEU:HB3	4:3E:110:PHE:CD1	2.50	0.47
1:13:553:A:H5''	12:3I:24:VAL:HG21	1.97	0.47
6:52:33:TYR:HE1	6:52:78:GLU:HG3	1.80	0.47
39:55:51:LEU:HD22	39:55:66:VAL:HG13	1.97	0.47
8:72:121:ASP:OD1	8:72:125:ARG:NH2	2.47	0.47
26:1H:806:C:OP2	37:78:41:ARG:HD3	2.15	0.47
26:1H:249:C:O2'	37:78:64:LYS:HE2	2.15	0.47
37:78:96:THR:C	37:78:98:GLU:H	2.18	0.47
9:82:37:PHE:HB3	9:82:43:ALA:CB	2.44	0.47
38:88:34:LEU:HD11	38:88:129:THR:OG1	2.14	0.47
39:98:2:ARG:O	39:98:5:LYS:HB2	2.15	0.47
41:B8:12:SER:HA	41:B8:14:TYR:N	2.26	0.47
29:11:69:ARG:NH2	29:11:128:GLY:O	2.28	0.47
1:13:1210:C:C2'	1:13:1211:U:H5'	2.44	0.47
1:13:1422:G:H5''	36:68:48:PRO:CB	2.41	0.47
1:13:1:U:C6	1:13:630:G:H2'	2.48	0.47
26:14:1570:A:H2'	26:14:1571:A:C8	2.49	0.47
26:14:2019:A:OP2	53:J5:9:LYS:NZ	2.44	0.47
26:14:276:A:H2'	26:14:277:C:C5	2.50	0.47
26:14:278:A:HO2'	26:14:279:C:H5	1.63	0.47
26:14:384:U:H2'	26:14:385:C:H6	1.79	0.47
1:1G:1001:G:N2	1:1G:1040:U:O2	2.48	0.47
1:1G:1028:C:N4	1:1G:1034:G:H21	2.12	0.47
1:1G:1095:U:OP1	1:1G:1108:G:N1	2.47	0.47
26:1H:106:C:H2'	26:1H:107:C:C6	2.50	0.47
26:1H:1534:G:N2	26:1H:1535:U:H5	2.13	0.47
26:1H:214:G:OP1	26:1H:214:G:H4'	2.14	0.47
26:1H:2285:C:H5	54:O8:27:LYS:HD2	1.80	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1H:2453:A:H2'	26:1H:2454:G:O4'	2.15	0.47
26:1H:2728:U:H2'	26:1H:2729:G:C8	2.49	0.47
26:1H:818:G:H5'	26:1H:839:U:OP1	2.15	0.47
22:1K:7:U:O2'	22:1K:49:G:N2	2.48	0.47
31:31:155:LEU:HB2	31:31:189:THR:HG21	1.97	0.47
4:32:96:LEU:HD22	4:32:139:ARG:NH1	2.30	0.47
37:35:59:LEU:HD22	56:M5:13:ARG:HD2	1.96	0.47
32:41:11:TYR:HA	32:41:15:VAL:HB	1.97	0.47
32:41:18:GLU:O	32:41:22:ARG:HB2	2.14	0.47
32:49:99:MET:HE2	32:49:99:MET:HB2	1.66	0.47
13:4I:67:GLU:HG2	13:4I:71:ARG:NH2	2.30	0.47
7:62:47:CYS:O	7:62:50:ILE:HB	2.15	0.47
28:71:171:ILE:HA	28:71:171:ILE:HD12	1.81	0.47
37:78:68:GLN:HG3	56:Q8:12:LYS:HD3	1.95	0.47
37:78:83:VAL:O	37:78:114:ILE:HA	2.15	0.47
8:7E:113:SER:HB3	8:7E:134:ILE:HD11	1.96	0.47
17:8A:56:VAL:O	17:8A:77:VAL:N	2.43	0.47
19:AI:5:LEU:HA	19:AI:5:LEU:HD12	1.80	0.47
20:BI:38:LYS:HE2	20:BI:38:LYS:HB3	1.73	0.47
44:E8:71:VAL:HA	44:E8:107:LEU:HD12	1.95	0.47
44:E8:96:ILE:HD13	44:E8:96:ILE:H	1.79	0.47
49:J8:7:ILE:HG13	49:J8:62:VAL:HG12	1.97	0.47
52:M8:16:CYS:HB3	52:M8:36:CYS:H	1.80	0.47
1:13:342:C:C2	1:13:348:G:C2	3.03	0.47
1:13:439:A:H3'	1:13:440:A:H8	1.79	0.47
26:14:1259:G:H2'	26:14:1260:G:C8	2.50	0.47
26:14:2074:U:H2'	26:14:2075:U:C6	2.50	0.47
26:14:2352:A:C2	48:E5:33:ALA:HB1	2.50	0.47
26:14:276:A:N3	26:14:277:C:N4	2.63	0.47
26:14:2795:G:N3	26:14:2795:G:H2'	2.30	0.47
26:14:2850:A:C2	26:14:2851:A:C4	3.03	0.47
26:14:68:G:H2'	26:14:69:C:O4'	2.15	0.47
2:1E:100:GLY:N	2:1E:176:GLU:OE2	2.47	0.47
2:1E:68:ILE:O	2:1E:91:PRO:HD2	2.14	0.47
1:1G:134:A:H1'	1:1G:325:A:C5	2.50	0.47
1:1G:1410:G:H2'	1:1G:1411:C:C6	2.50	0.47
1:1G:1482:G:O6	62:1G:1863:HOH:O	2.20	0.47
1:1G:298:A:H5''	1:1G:299:G:OP2	2.14	0.47
26:1H:1668:A:C8	26:1H:1674:G:C6	3.03	0.47
26:1H:1268:A:C2	26:1H:2013:A:C4	3.03	0.47
26:1H:2130:U:H2'	26:1H:2131:G:N7	2.30	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1H:2210:G:H3'	26:1H:2211:G:C5	2.50	0.47
26:1H:2436:G:C6	26:1H:2437:U:C4	3.03	0.47
26:1H:275:G:N2	26:1H:276:A:N7	2.42	0.47
26:1H:602:G:N2	26:1H:655:A:C8	2.70	0.47
22:1K:45:G:O2'	22:1K:47:U:H5'	2.15	0.47
36:25:10:VAL:HG23	36:25:12:ASP:OD1	2.15	0.47
30:29:9:VAL:HG23	30:29:26:ILE:O	2.15	0.47
12:3I:70:ILE:HD13	12:3I:77:LEU:HD12	1.97	0.47
26:14:870:A:H5''	38:45:6:ARG:HB3	1.97	0.47
32:49:33:ARG:NH2	32:49:162:THR:HG21	2.30	0.47
13:4A:39:ILE:HG23	13:4A:52:GLU:HG2	1.97	0.47
13:4A:59:TYR:CD2	13:4A:60:VAL:HG22	2.50	0.47
26:14:2690:C:OP2	39:55:14:SER:HB2	2.14	0.47
39:55:79:LEU:HA	39:55:83:ILE:HB	1.95	0.47
35:58:35:ARG:O	35:58:42:TRP:HZ3	1.97	0.47
33:59:107:VAL:CG1	33:59:152:ARG:HG2	2.45	0.47
33:59:152:ARG:HD2	33:59:153:LYS:HG3	1.96	0.47
7:62:22:LEU:HD23	7:62:62:PHE:CE2	2.48	0.47
42:85:92:ARG:O	42:85:94:ASN:N	2.48	0.47
9:8E:86:VAL:HG11	9:8E:93:ARG:HG3	1.97	0.47
17:8I:31:LEU:HD22	17:8I:32:TYR:CE1	2.50	0.47
49:F5:92:LYS:O	49:F5:94:LEU:N	2.48	0.47
2:12:42:ILE:HG21	2:12:202:PRO:HB2	1.97	0.47
1:13:1318:A:H1'	19:AI:37:ARG:HH21	1.79	0.47
26:14:1639:U:C2'	26:14:1640:C:H5'	2.45	0.47
26:14:1665:A:H2'	26:14:1666:G:O4'	2.14	0.47
26:14:195:A:H4'	26:14:251:A:O2'	2.15	0.47
26:14:2846:G:H2'	26:14:2847:U:O4'	2.14	0.47
26:14:480:A:N3	26:14:480:A:H2'	2.30	0.47
26:14:57:C:H2'	26:14:58:G:O4'	2.15	0.47
35:15:35:ARG:HB3	35:15:42:TRP:CZ3	2.50	0.47
1:1G:1069:C:O2'	1:1G:1192:C:H1'	2.15	0.47
1:1G:1072:G:H2'	1:1G:1073:U:O4'	2.15	0.47
1:1G:1352:C:N3	1:1G:1370:G:N2	2.51	0.47
1:1G:577:G:H2'	1:1G:578:C:H6	1.80	0.47
1:1G:922:G:O5'	5:42:20:GLN:NE2	2.43	0.47
26:1H:270(H):C:H2'	26:1H:270(I):G:C8	2.50	0.47
26:1H:627:A:H4'	26:1H:628:G:OP1	2.15	0.47
26:1H:739:G:H8	26:1H:739:G:OP2	1.97	0.47
4:3E:101:LEU:HD11	4:3E:126:ILE:HG21	1.97	0.47
24:3L:72:C:C3'	24:3L:73:A:H5''	2.45	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:59:97:ARG:HG2	33:59:98:LEU:H	1.79	0.47
26:1H:1952:A:C2	36:68:22:ILE:HG23	2.50	0.47
36:68:35:VAL:HG21	36:68:103:ALA:HB3	1.97	0.47
1:1G:750:G:N2	15:6A:23:GLY:HA3	2.30	0.47
28:71:64:LEU:HD22	28:71:175:VAL:O	2.15	0.47
1:13:377:G:H5'	16:7I:5:ARG:HH12	1.80	0.47
16:7I:73:LEU:O	16:7I:77:ALA:HB2	2.15	0.47
38:88:27:VAL:HA	38:88:105:GLU:OE1	2.15	0.47
19:AA:56:GLN:HG2	19:AA:57:HIS:H	1.79	0.47
1:13:1432:G:OP1	41:B8:107:ASP:HB2	2.14	0.47
20:BA:51:GLU:HA	20:BA:54:LYS:HE3	1.96	0.47
26:1H:1816:G:H8	29:11:62:TYR:CZ	2.34	0.46
1:13:44:G:C2	1:13:45:U:H1'	2.50	0.46
1:13:520:A:N1	1:13:536:C:H1'	2.30	0.46
26:14:1379:A:H1'	26:14:1380:G:OP1	2.15	0.46
26:14:1790:C:H2'	26:14:1791:A:C5	2.50	0.46
26:14:2859:G:H3'	26:14:2859:G:C8	2.51	0.46
26:14:817:C:H3'	26:14:818:G:H8	1.80	0.46
29:19:173:VAL:HG12	29:19:185:VAL:O	2.15	0.46
1:1G:973:G:C5'	10:1A:55:LYS:HZ2	2.27	0.46
2:1E:59:GLU:HB2	2:1E:221:LEU:HD11	1.97	0.46
1:1G:1286:A:H3'	1:1G:1286:A:C8	2.50	0.46
1:1G:529:G:O6	12:3A:49:ASN:HA	2.15	0.46
1:1G:750:G:C2	15:6A:23:GLY:HA3	2.50	0.46
26:1H:1379:A:H1'	26:1H:1380:G:OP1	2.14	0.46
26:1H:353:G:H2'	26:1H:354:G:C8	2.49	0.46
1:13:963:G:N2	10:1I:55:LYS:HZ3	2.13	0.46
27:1J:117:G:H8	27:1J:117:G:O5'	1.97	0.46
27:1J:21:G:H1	27:1J:62:C:H42	1.63	0.46
24:1L:8:U:H3'	24:1L:13:C:N4	2.30	0.46
23:2L:9:G:O2'	23:2L:10:G:N7	2.40	0.46
31:31:150:GLY:HA2	31:31:172:TRP:CD2	2.50	0.46
31:31:20:LEU:HD12	31:31:21:ALA:H	1.79	0.46
4:32:162:LEU:HD23	4:32:162:LEU:HA	1.57	0.46
26:14:588:U:H1'	31:39:90:PHE:CG	2.49	0.46
13:4I:117:VAL:HG13	13:4I:118:ALA:H	1.79	0.46
8:7E:77:GLU:HG2	8:7E:78:GLN:H	1.79	0.46
16:7I:68:ASP:O	16:7I:71:ARG:HG2	2.15	0.46
38:88:16:ARG:HB3	38:88:16:ARG:HE	1.46	0.46
19:AA:9:VAL:CB	19:AA:10:PHE:HA	2.45	0.46
19:AI:40:ILE:HG21	19:AI:66:MET:O	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:D8:48:GLY:O	43:D8:49:THR:O	2.33	0.46
48:E5:49:LYS:HB2	48:E5:82:ARG:HH21	1.79	0.46
49:F5:3:LYS:HA	49:F5:46:LEU:HD22	1.96	0.46
48:I8:84:LEU:HD12	48:I8:84:LEU:HA	1.79	0.46
56:Q8:6:THR:HG22	56:Q8:62:LEU:HA	1.97	0.46
1:13:1316:G:N2	1:13:1318:A:H3'	2.30	0.46
1:13:1349:A:H2'	1:13:1350:A:C8	2.49	0.46
1:13:232:G:H1'	1:13:262:A:N1	2.29	0.46
1:13:729:A:H2'	1:13:730:G:H8	1.79	0.46
26:14:1771:C:H1'	26:14:1786:A:C8	2.51	0.46
26:14:2745:C:H2'	26:14:2746:U:O4'	2.16	0.46
26:14:329:G:OP2	46:C5:71:LYS:HE3	2.16	0.46
26:14:854:G:H2'	26:14:855:G:H8	1.81	0.46
27:16:41:U:C5	32:41:70:VAL:HG13	2.50	0.46
29:19:49:ILE:CD1	29:19:52:ARG:HA	2.45	0.46
1:1G:1023:G:H3'	1:1G:1024:G:O4'	2.15	0.46
1:1G:1095:U:OP1	1:1G:1108:G:N2	2.48	0.46
1:1G:1145:C:H5''	1:1G:1146:A:OP1	2.15	0.46
1:1G:131:C:H2'	1:1G:132:C:C6	2.51	0.46
1:1G:401:C:N4	62:1G:1898:HOH:O	2.48	0.46
1:1G:420:U:O2'	1:1G:423:G:O6	2.26	0.46
1:1G:538:G:H2'	1:1G:539:A:H8	1.80	0.46
1:1G:560:U:OP2	62:1G:1864:HOH:O	2.20	0.46
26:1H:1899:G:H22	26:1H:1902:C:N4	2.12	0.46
26:1H:2273:A:H2'	26:1H:2274:A:C8	2.49	0.46
26:1H:2402:C:H1'	26:1H:2403:C:H5	1.80	0.46
26:1H:662:G:O2'	26:1H:663:G:H5'	2.16	0.46
30:21:111:ARG:HG3	30:21:160:TYR:CD2	2.51	0.46
31:31:23:ASP:CG	31:31:24:LEU:H	2.18	0.46
24:3K:65:C:H2'	24:3K:66:A:H5''	1.97	0.46
38:45:42:ILE:HD13	38:45:97:VAL:CG2	2.45	0.46
32:49:47:LYS:HG2	32:49:48:GLU:H	1.80	0.46
32:49:66:GLN:NE2	32:49:94:LEU:HD23	2.31	0.46
35:58:134:ARG:HB2	35:58:134:ARG:HE	1.49	0.46
33:59:137:ASP:HB3	33:59:140:LYS:HB2	1.96	0.46
34:61:18:VAL:HG21	34:61:44:LEU:HD11	1.96	0.46
7:62:95:ARG:HH21	7:62:99:LEU:HD11	1.80	0.46
40:65:15:ARG:HD2	40:65:25:ARG:HH21	1.80	0.46
15:6A:12:ILE:HG12	15:6A:31:LEU:HD11	1.97	0.46
37:78:14:LYS:O	37:78:15:ARG:HB2	2.15	0.46
8:7E:116:LYS:HG3	8:7E:129:VAL:HG11	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:13:112:G:OP2	16:7I:27:LYS:HD2	2.15	0.46
9:8E:93:ARG:NH2	9:8E:97:LYS:HD2	2.30	0.46
46:G8:94:LYS:HZ2	46:G8:95:LYS:N	2.12	0.46
47:H8:132:ASN:ND2	47:H8:160:GLY:HA3	2.31	0.46
54:O8:27:LYS:NZ	54:O8:27:LYS:H	2.12	0.46
2:12:75:LYS:H	2:12:78:GLN:HG3	1.81	0.46
2:12:82:ARG:HB2	2:12:94:ASN:OD1	2.15	0.46
1:13:1058:G:C6	1:13:1059:C:N3	2.84	0.46
1:13:1092:A:C6	1:13:1093:A:C6	3.03	0.46
1:13:1203:C:H2'	1:13:1204:A:O4'	2.14	0.46
1:13:237:C:H5''	17:8I:25:ARG:CZ	2.46	0.46
1:13:575:G:H4'	1:13:576:G:O5'	2.15	0.46
1:13:948:C:O2'	1:13:949:A:H5'	2.15	0.46
26:14:1485:G:H2'	26:14:1486:A:C8	2.51	0.46
26:14:1754:C:H2'	26:14:1755:A:C8	2.49	0.46
26:14:196:A:H2'	26:14:196:A:N3	2.31	0.46
26:14:270(P):C:H2'	26:14:270(Q):C:C6	2.50	0.46
27:16:13:A:O2'	27:16:14:U:H3'	2.16	0.46
1:1G:1348:U:H3	1:1G:1374:A:H2	1.56	0.46
1:1G:735:C:H2'	1:1G:736:C:H6	1.79	0.46
26:1H:1453:A:O2'	26:1H:1454:U:H2'	2.14	0.46
26:1H:1478:G:H2'	26:1H:1479:G:H8	1.80	0.46
26:1H:1680:U:H2'	26:1H:1681:G:O4'	2.15	0.46
26:1H:2343:C:HO2'	26:1H:2373:G:HO2'	1.57	0.46
26:1H:2414:G:H21	37:78:67:MET:CE	2.29	0.46
26:1H:2503:A:OP2	26:1H:2503:A:H3'	2.15	0.46
26:1H:445:C:O2'	26:1H:446:G:H5'	2.15	0.46
26:1H:533:G:H5'	42:C8:24:TYR:CE1	2.50	0.46
27:1J:73:A:C4	27:1J:104:A:C2	3.04	0.46
26:1H:2575:C:H5'	30:21:144:ARG:HB2	1.97	0.46
31:39:146:ALA:CB	31:39:148:LEU:HG	2.44	0.46
31:39:78:ILE:HA	31:39:83:PHE:CD2	2.50	0.46
31:39:49:ALA:O	31:39:92:PRO:HB2	2.15	0.46
4:3E:15:GLU:HG3	4:3E:63:LYS:HB2	1.97	0.46
40:65:110:LEU:HD13	40:65:112:PHE:CE1	2.50	0.46
40:65:27:SER:HA	40:65:88:ASP:CB	2.45	0.46
15:6A:84:LYS:HA	15:6A:84:LYS:HD3	1.63	0.46
7:6E:79:ARG:HE	7:6E:84:ASN:HD22	1.64	0.46
8:7E:25:ASP:OD2	8:7E:60:ARG:HG3	2.15	0.46
16:7I:12:LYS:O	16:7I:13:HIS:HB2	2.14	0.46
42:85:50:ARG:NH1	43:95:72:VAL:HG23	2.31	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:B5:1:MET:HA	45:B5:2:LYS:HA	1.50	0.46
46:C5:52:SER:HA	46:C5:55:TYR:O	2.16	0.46
42:C8:88:ILE:O	42:C8:88:ILE:HG22	2.15	0.46
26:14:180:G:OP2	55:L5:32:LYS:HD2	2.15	0.46
52:M8:42:PHE:CD1	52:M8:43:TYR:HB3	2.50	0.46
56:Q8:4:MET:HB2	56:Q8:4:MET:HE2	1.59	0.46
29:11:85:ASP:OD2	29:11:88:ARG:NH1	2.39	0.46
2:12:92:TYR:HH	2:12:150:SER:HG	1.64	0.46
1:13:1044:A:C5	1:13:1045:C:H1'	2.51	0.46
1:13:1113:C:H2'	1:13:1114:C:C6	2.51	0.46
1:13:1132:C:H2'	1:13:1133:G:C8	2.50	0.46
1:13:1263:C:H2'	1:13:1264:C:H6	1.80	0.46
1:13:1292:U:H2'	1:13:1293:G:H8	1.77	0.46
1:13:258:G:H2'	1:13:259:G:H8	1.79	0.46
1:13:443:C:N4	1:13:491:G:H1	2.12	0.46
26:14:2046:G:H5'	53:J5:19:ARG:HG3	1.98	0.46
26:14:2212:A:O2'	26:14:2213:U:O5'	2.34	0.46
26:14:2557:G:H2'	26:14:2558:C:H6	1.81	0.46
26:14:2562:U:H1'	36:25:23:ARG:NE	2.31	0.46
26:14:2720:U:N3	26:14:2873:A:H2	2.08	0.46
27:16:11:C:H3'	27:16:12:C:H6	1.80	0.46
1:1G:1502:A:H2	1:1G:1505:G:N1	2.02	0.46
1:1G:337:C:H2'	1:1G:338:A:C8	2.51	0.46
26:1H:1991:U:C2'	26:1H:1992:G:H5''	2.46	0.46
26:1H:530:G:C5	26:1H:2022:U:H5''	2.50	0.46
26:1H:2126:A:OP1	28:71:38:ASP:HB3	2.14	0.46
26:1H:2150:U:H2'	26:1H:2151:G:C8	2.50	0.46
26:1H:2171:A:O2'	26:1H:2172:U:O4'	2.23	0.46
26:1H:2186:G:H2'	26:1H:2187:G:C8	2.50	0.46
26:1H:2400:G:O2'	26:1H:2401:U:H5'	2.16	0.46
26:1H:270(I):G:H1	26:1H:270(Q):C:N4	2.05	0.46
26:1H:403:U:H3'	62:1H:4080:HOH:O	2.15	0.46
3:2E:16:ARG:HD2	3:2E:54:ARG:NH2	2.23	0.46
4:3E:104:VAL:HG21	4:3E:140:VAL:HG21	1.97	0.46
5:42:148:VAL:O	5:42:152:ARG:HG3	2.15	0.46
32:49:111:LEU:HB2	32:49:112:PRO:HD3	1.98	0.46
5:4E:76:ILE:HG13	5:4E:93:PRO:HG3	1.98	0.46
7:62:102:ARG:HG2	7:62:106:GLN:NE2	2.30	0.46
1:13:1292:U:P	7:6E:41:ARG:HH22	2.38	0.46
37:78:124:LYS:HA	37:78:143:GLY:O	2.14	0.46
1:13:878:G:H5'	8:7E:89:PRO:HG2	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:82:18:PHE:HD2	9:82:62:TYR:HD2	1.63	0.46
26:1H:2250:G:C5	38:88:83:MET:HB3	2.51	0.46
19:AA:66:MET:N	19:AA:67:VAL:HB	2.29	0.46
41:B8:107:ASP:O	41:B8:110:ILE:HG23	2.16	0.46
46:G8:5:MET:HE1	46:G8:32:PRO:HA	1.98	0.46
51:H5:5:LYS:HG2	51:H5:36:VAL:HG22	1.96	0.46
50:K8:3:LEU:O	50:K8:6:VAL:HB	2.15	0.46
53:N8:16:ARG:HG3	53:N8:17:ASP:N	2.30	0.46
54:O8:27:LYS:HB2	54:O8:27:LYS:HZ2	1.80	0.46
1:13:1238:A:N3	1:13:1241:G:O2'	2.39	0.46
1:13:1262:C:H2'	1:13:1263:C:C6	2.49	0.46
1:13:1386:G:O2'	1:13:1387:G:H5'	2.16	0.46
26:14:2104:G:H2'	26:14:2105:C:C6	2.51	0.46
26:14:2168:G:H3'	26:14:2168:G:N3	2.31	0.46
26:14:2761:G:H1'	33:59:143:GLN:HE22	1.80	0.46
35:15:15:LEU:HD22	35:15:53:VAL:HB	1.96	0.46
27:16:44:G:C2	27:16:48:A:C2	3.04	0.46
26:14:1901:A:OP2	29:19:255:LYS:HE2	2.14	0.46
2:1E:174:VAL:HG13	2:1E:184:VAL:HG11	1.97	0.46
1:1G:1305:G:N2	1:1G:1331:G:O2'	2.48	0.46
1:1G:21:G:H2'	1:1G:22:G:C8	2.51	0.46
26:1H:1727:U:H2'	26:1H:1728:G:O4'	2.16	0.46
26:1H:2146:C:H4'	26:1H:2147:G:N7	2.30	0.46
26:1H:2629:A:OP1	26:1H:2629:A:H4'	2.16	0.46
26:1H:492:A:H2'	26:1H:493:G:O4'	2.15	0.46
24:3K:37:A:H3'	24:3K:38:A:C8	2.50	0.46
38:45:134:ARG:HG2	38:45:136:ALA:CB	2.46	0.46
38:45:69:PHE:CD1	38:45:70:PRO:HD2	2.51	0.46
5:4E:74:GLY:O	5:4E:115:VAL:HA	2.16	0.46
1:1G:974:A:P	14:5A:41:ARG:HH12	2.39	0.46
10:1A:63:PHE:CD1	14:5A:58:LYS:HA	2.50	0.46
28:71:30:LYS:HG3	28:71:182:PRO:HD3	1.96	0.46
28:71:45:ALA:HA	28:71:211:SER:O	2.15	0.46
17:8I:22:LEU:HD12	17:8I:40:LYS:O	2.16	0.46
45:B5:67:GLY:O	45:B5:69:TYR:N	2.47	0.46
20:BA:12:ALA:O	20:BA:15:ARG:HB2	2.15	0.46
47:H8:52:SER:O	47:H8:52:SER:OG	2.21	0.46
47:H8:92:SER:O	47:H8:130:PRO:HG2	2.15	0.46
29:11:38:LYS:HB3	29:11:39:LYS:HA	1.97	0.46
1:13:1278:U:H5'	1:13:1279:A:C5'	2.45	0.46
1:13:1260:C:O5'	1:13:1284:C:H4'	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:13:1298:C:C5	7:6E:114:ARG:HD3	2.50	0.46
1:13:280:C:H4'	1:13:281:G:OP2	2.16	0.46
1:13:353:A:C8	1:13:353:A:H5'	2.47	0.46
26:14:1826:G:H2'	26:14:1827:C:O4'	2.16	0.46
26:14:1839:G:C8	26:14:1927:A:H1'	2.50	0.46
26:14:384:U:H2'	26:14:385:C:C6	2.51	0.46
2:1E:166:ASP:C	2:1E:168:THR:H	2.19	0.46
1:1G:509:A:C8	1:1G:509:A:H3'	2.50	0.46
1:1G:757:U:O2'	1:1G:879:C:O2	2.31	0.46
26:1H:1105:U:H2'	26:1H:1106:G:C8	2.51	0.46
26:1H:1163:G:C2	26:1H:1164:G:C8	3.03	0.46
26:1H:1396:U:H2'	26:1H:1396:U:O2	2.15	0.46
26:1H:780:G:N2	26:1H:783:A:N6	2.59	0.46
3:22:73:PRO:O	3:22:76:VAL:HG22	2.16	0.46
30:29:8:LYS:HE2	30:29:188:VAL:HG22	1.98	0.46
3:2E:77:ILE:O	3:2E:84:ILE:HG22	2.15	0.46
4:32:139:ARG:HG3	4:32:139:ARG:HH11	1.81	0.46
31:39:66:PRO:O	31:39:67:GLN:CB	2.64	0.46
38:45:43:THR:HG22	38:45:94:VAL:HG12	1.98	0.46
25:4K:9:G:H3'	25:4K:10:G:O4'	2.16	0.46
39:55:33:ARG:NH2	39:55:115:GLU:OE2	2.41	0.46
26:14:2839:G:H21	39:55:92:GLY:HA2	1.81	0.46
1:13:1047:G:O3'	14:5I:4:LYS:HB2	2.15	0.46
34:61:124:GLY:H	34:61:142:VAL:HG23	1.80	0.46
7:62:65:ALA:HB1	7:62:127:ALA:HB3	1.96	0.46
7:6E:143:ARG:NH1	24:3K:41:A:O2'	2.49	0.46
28:71:180:PHE:HA	28:71:181:PRO:HD3	1.80	0.46
1:13:377:G:H5'	16:7I:5:ARG:NH1	2.30	0.46
38:88:32:TYR:O	38:88:105:GLU:HA	2.16	0.46
39:98:59:ASP:OD1	39:98:59:ASP:N	2.37	0.46
19:AI:40:ILE:HG23	19:AI:41:VAL:N	2.31	0.46
41:B8:7:ILE:O	41:B8:11:GLU:HB2	2.15	0.46
20:BA:87:LYS:HG2	20:BA:91:LEU:HD11	1.98	0.46
47:D5:132:ASN:N	47:D5:132:ASN:OD1	2.47	0.46
43:D8:36:PRO:C	43:D8:38:LEU:H	2.19	0.46
45:F8:94:GLY:O	45:F8:95:LEU:HB2	2.15	0.46
46:G8:95:LYS:HE2	46:G8:97:ARG:HH12	1.80	0.46
48:I8:53:MET:HB2	48:I8:59:LEU:CD2	2.45	0.46
26:1H:705:A:O3'	29:11:7:LYS:HD2	2.16	0.46
2:12:71:VAL:HG23	2:12:165:VAL:HG13	1.98	0.46
1:13:1240:U:P	7:6E:116:ALA:HB2	2.55	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:14:1036:G:H1	26:14:1119:C:H42	1.62	0.46
26:14:991:C:O2	26:14:1164:G:C2	2.69	0.46
26:14:2291:U:H5''	26:14:2380:C:O2'	2.15	0.46
26:14:451:C:H41	26:14:454:A:H5'	1.81	0.46
26:14:521:G:H2'	26:14:522:G:H8	1.80	0.46
26:14:533:G:H2'	26:14:534:U:O4'	2.16	0.46
26:14:65:C:H2'	26:14:66:C:H6	1.80	0.46
26:14:588:U:O4	26:14:670:A:H1'	2.15	0.46
35:15:67:LEU:HG	35:15:88:GLU:HG2	1.97	0.46
10:1A:79:ARG:HH11	10:1A:79:ARG:HB3	1.80	0.46
1:1G:1142:G:H3'	1:1G:1143:G:H8	1.79	0.46
1:1G:1206:G:O2'	3:22:193:TYR:HA	2.16	0.46
1:1G:501:C:OP1	12:3A:117:ARG:NH2	2.48	0.46
26:1H:1869:G:H5''	26:1H:1869:G:H8	1.80	0.46
26:1H:207:A:H2'	26:1H:208:C:O4'	2.16	0.46
26:1H:2262:U:H4'	26:1H:2328:A:C2	2.51	0.46
26:1H:2492:U:H2'	26:1H:2493:U:C6	2.50	0.46
26:1H:2544:G:H2'	26:1H:2545:G:C8	2.51	0.46
27:1J:104:A:H2'	27:1J:105:G:O4'	2.16	0.46
27:1J:116:G:C5'	40:65:55:ALA:HB2	2.46	0.46
30:21:4:ILE:HD13	30:21:28:ALA:HB1	1.98	0.46
23:2K:20:G:C2	23:2K:58:A:N3	2.84	0.46
37:35:126:VAL:HG12	37:35:147:LEU:HD22	1.97	0.46
37:35:59:LEU:HA	37:35:62:LEU:HD22	1.97	0.46
13:4I:12:ASN:HD22	13:4I:13:LYS:N	2.13	0.46
7:62:141:VAL:HA	7:62:142:GLU:HB2	1.97	0.46
7:62:94:ARG:HA	7:62:97:GLN:HB3	1.97	0.46
40:65:101:LEU:HD12	40:65:105:ALA:HB2	1.97	0.46
41:75:61:PHE:CE1	41:75:76:PHE:HB2	2.51	0.46
17:8A:59:ILE:HD13	17:8A:73:VAL:HA	1.98	0.46
20:BI:45:GLN:HA	20:BI:91:LEU:HB3	1.98	0.46
42:C8:50:ARG:NH2	43:D8:72:VAL:HG22	2.30	0.46
26:14:459:U:H5''	55:L5:40:TRP:CD2	2.51	0.46
2:12:24:TRP:NE1	2:12:26:PRO:HG3	2.31	0.46
1:13:1129:C:H4'	1:13:1130:A:OP1	2.15	0.46
1:13:1468:A:P	62:13:1850:HOH:O	2.73	0.46
1:13:342:C:C2'	1:13:343:U:H5'	2.46	0.46
1:13:724:G:C2	1:13:725:G:C8	3.03	0.46
26:14:1178:C:H2'	26:14:1179:C:C6	2.51	0.46
26:14:1364:G:OP1	49:F5:3:LYS:HD2	2.15	0.46
26:14:1921:G:H2'	26:14:1922:G:H8	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:14:2360:A:H2'	26:14:2361:A:O4'	2.15	0.46
26:14:734:A:O2'	26:14:1635:G:H5'	2.16	0.46
2:1E:16:HIS:CE1	2:1E:213:LEU:HB2	2.51	0.46
1:1G:1256:A:N6	1:1G:1277:C:H3'	2.31	0.46
1:1G:631:G:H1'	1:1G:632:A:H5'	1.98	0.46
1:1G:953:G:H5''	1:1G:965:A:H61	1.80	0.46
26:1H:1470:G:N7	62:1H:3844:HOH:O	2.36	0.46
26:1H:194:G:H2'	26:1H:195:A:O4'	2.15	0.46
26:1H:2109:U:H1'	26:1H:2181:G:N2	2.31	0.46
26:1H:270(M):U:OP2	34:61:57:ARG:NH2	2.49	0.46
26:1H:2711:A:P	62:1H:3750:HOH:O	2.74	0.46
26:1H:2766:G:H2'	26:1H:2766:G:N3	2.31	0.46
26:1H:674:G:O2'	31:31:74:ARG:HG3	2.16	0.46
26:1H:910:A:N1	26:1H:2277:G:H1'	2.31	0.46
26:1H:934:G:H2'	26:1H:935:C:C6	2.51	0.46
10:1I:80:LYS:O	10:1I:84:GLN:HG2	2.15	0.46
22:1K:27:G:H1	22:1K:43:U:H3	1.62	0.46
30:29:128:SER:OG	30:29:129:HIS:N	2.49	0.46
23:2K:54:G:H2'	23:2K:55:5MU:C6	2.49	0.46
31:31:108:LYS:O	31:31:112:MET:HG3	2.15	0.46
37:35:50:ARG:HD3	56:M5:7:HIS:HD2	1.79	0.46
12:3A:32:PHE:HB3	12:3A:84:LEU:HD22	1.97	0.46
13:4I:57:ARG:O	13:4I:61:GLU:HG3	2.15	0.46
43:95:71:LEU:O	43:95:85:LYS:O	2.33	0.46
39:98:42:LYS:O	39:98:45:ARG:HD3	2.16	0.46
45:B5:63:LYS:H	45:B5:63:LYS:CE	2.29	0.46
47:D5:48:PHE:O	47:D5:52:SER:HB3	2.16	0.46
26:14:94:G:N2	50:G5:47:ASN:HD22	2.11	0.46
47:H8:59:LEU:HD23	47:H8:59:LEU:HA	1.82	0.46
52:M8:38:LYS:HE2	52:M8:44:THR:HG21	1.98	0.46
1:13:1171:G:O2'	1:13:1172:C:H5'	2.16	0.46
1:13:1:U:H6	1:13:630:G:H2'	1.80	0.46
26:14:1109:C:H2'	26:14:1110:G:C1'	2.46	0.46
26:14:1111:A:O3'	26:14:1112:G:H4'	2.15	0.46
26:14:1114:G:H2'	26:14:1115:G:C8	2.51	0.46
26:14:1448:G:H1'	26:14:1528:A:H62	1.81	0.46
26:14:2542:A:O2'	26:14:2543:G:OP2	2.24	0.46
26:14:640:C:H42	26:14:648:G:H1	1.64	0.46
26:14:886:C:H1'	26:14:890:A:C2	2.49	0.46
1:1G:433:C:H2'	1:1G:434:U:C6	2.51	0.46
1:1G:437:U:C4	1:1G:438:G:C6	3.04	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1H:1329:U:H5'	26:1H:1330:C:C5	2.48	0.46
26:1H:1878:G:H2'	26:1H:1879:C:C6	2.51	0.46
26:1H:2126:A:C8	26:1H:2163:C:H1'	2.51	0.46
26:1H:2164:C:OP2	26:1H:2166:G:N2	2.48	0.46
26:1H:638:G:C5	26:1H:651:G:C2	3.03	0.46
3:22:61:ALA:C	3:22:63:ASN:H	2.19	0.46
3:22:94:LEU:H	3:22:94:LEU:HG	1.36	0.46
30:29:81:ILE:O	30:29:82:ARG:HB2	2.15	0.46
23:2L:73:A:C6	23:2L:74:A:C6	3.04	0.46
23:2L:77:A:O2'	26:14:2602:A:N7	2.49	0.46
31:31:37:VAL:HG21	37:78:6:LEU:HD21	1.97	0.46
4:32:57:ARG:NH2	5:42:107:ARG:HD2	2.31	0.46
13:4A:92:HIS:CD2	13:4A:98:VAL:HG11	2.51	0.46
33:59:103:LEU:HD22	33:59:123:PHE:CZ	2.51	0.46
8:72:88:LYS:O	8:72:92:ARG:HD3	2.16	0.46
26:1H:2251:G:OP1	38:88:82:ARG:NH1	2.48	0.46
40:A8:25:ARG:NH1	40:A8:42:ASP:OD1	2.47	0.46
49:J8:23:LYS:HB3	49:J8:29:GLY:HA3	1.97	0.46
50:K8:4:SER:H	50:K8:7:ARG:HG2	1.79	0.46
55:L5:12:ARG:NH2	55:L5:44:PRO:HB3	2.31	0.46
1:13:1171:G:H2'	1:13:1172:C:H6	1.81	0.46
1:13:223:U:H2'	1:13:224:C:H6	1.81	0.46
1:13:272:C:H2'	1:13:273:A:C8	2.51	0.46
1:13:458:C:H42	1:13:474:G:H1	1.64	0.46
1:13:652:U:H1'	1:13:653:A:C2	2.51	0.46
26:14:1141:U:OP1	35:15:25:ARG:NE	2.39	0.46
26:14:2152:G:C6	26:14:2153:G:H1'	2.51	0.46
26:14:2186:G:H2'	26:14:2187:G:H8	1.81	0.46
26:14:2772:C:H2'	26:14:2773:C:C6	2.51	0.46
26:14:2815:C:H5'	53:J5:29:THR:HG21	1.98	0.46
35:15:133:GLN:C	35:15:134:ARG:HG3	2.37	0.46
2:1E:11:LEU:HD11	2:1E:209:ARG:NH2	2.31	0.46
1:1G:1148:U:H2'	1:1G:1149:C:O4'	2.16	0.46
1:1G:1211:U:O2	1:1G:1213:A:H2	1.99	0.46
1:1G:1258:G:H8	1:1G:1258:G:OP2	1.99	0.46
1:1G:80:G:O2'	1:1G:81:G:OP1	2.32	0.46
26:1H:1049:C:C2'	26:1H:1050:A:H5'	2.44	0.46
26:1H:1337:G:H2'	26:1H:1338:G:H8	1.81	0.46
26:1H:1731:G:H2'	26:1H:1732:A:C8	2.50	0.46
26:1H:2074:U:H2'	26:1H:2075:U:C6	2.51	0.46
26:1H:2126:A:H1'	26:1H:2162:G:H21	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1H:6:A:H1'	35:58:131:GLN:HG3	1.98	0.46
26:1H:817:C:H4'	26:1H:932:G:C5	2.51	0.46
26:1H:847:U:C5'	62:1H:3743:HOH:O	2.64	0.46
26:1H:918:A:H8	26:1H:918:A:O5'	1.99	0.46
30:21:81:ILE:HG22	30:21:81:ILE:O	2.16	0.46
30:29:111:ARG:HD2	30:29:160:TYR:CD2	2.50	0.46
31:31:64:ILE:HG23	31:31:65:TRP:CD1	2.51	0.46
12:3I:85:ILE:HD13	12:3I:85:ILE:HA	1.67	0.46
32:41:81:LYS:NZ	32:41:81:LYS:H	2.14	0.46
38:45:117:ALA:HA	38:45:120:ILE:HB	1.96	0.46
38:45:36:ALA:HB2	38:45:103:MET:SD	2.55	0.46
5:4E:147:ASP:O	5:4E:151:LEU:HB2	2.16	0.46
5:4E:37:ARG:HH12	5:4E:111:GLU:HG2	1.80	0.46
14:5A:29:ARG:HD3	14:5A:31:ARG:O	2.16	0.46
7:62:12:LEU:HB2	7:62:21:VAL:HB	1.98	0.46
37:78:122:PRO:HA	37:78:142:GLY:CA	2.46	0.46
1:1G:235:C:C5'	17:8A:70:ARG:HG2	2.43	0.46
26:14:1614:A:H62	44:A5:93:ALA:HB2	1.81	0.46
20:BI:26:ASN:HB2	20:BI:71:THR:CG2	2.39	0.46
47:H8:53:ILE:HG22	47:H8:71:VAL:HG22	1.97	0.46
50:K8:47:ASN:C	50:K8:49:LYS:H	2.19	0.46
29:11:68:LYS:HB3	29:11:70:TRP:CH2	2.52	0.45
2:12:51:LEU:H	2:12:51:LEU:HG	1.41	0.45
1:13:1084:G:C5	1:13:1085:U:C4	3.03	0.45
1:13:1126:U:C5	1:13:1127:G:N7	2.84	0.45
1:13:1372:U:H5''	9:8E:71:SER:HB3	1.98	0.45
1:13:1425:U:H2'	1:13:1426:C:H6	1.81	0.45
26:14:1047:G:N3	26:14:1047:G:H2'	2.31	0.45
26:14:1442:G:H2'	26:14:1443:G:H8	1.81	0.45
26:14:1496:A:H8	26:14:1577:C:O2'	1.95	0.45
26:14:2006:C:H2'	26:14:2007:C:H6	1.81	0.45
26:14:2099:U:H3	26:14:2190:G:H1	1.65	0.45
26:14:2343:C:O2'	26:14:2373:G:O2'	2.14	0.45
26:14:2773:C:H2'	26:14:2774:C:H6	1.82	0.45
26:14:2801:A:H2'	26:14:2802:G:O4'	2.16	0.45
26:14:289:A:H3'	26:14:290:G:H8	1.80	0.45
26:14:492:A:H2'	26:14:493:G:O4'	2.16	0.45
26:14:603:A:H8	26:14:604:G:H1'	1.81	0.45
26:14:654(C):G:H2'	26:14:654(D):G:H5'	1.99	0.45
21:1F:9:ARG:HD3	21:1F:13:ILE:HD11	1.97	0.45
26:1H:1217:C:H2'	26:1H:1218:C:H5''	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1H:1728:G:H2'	26:1H:1731:G:O6	2.16	0.45
26:1H:1820:U:H4'	26:1H:1821:A:OP2	2.16	0.45
26:1H:18:C:O3'	42:C8:23:GLY:HA2	2.16	0.45
26:1H:2334:G:H5'	40:A8:9:ARG:HG2	1.96	0.45
3:22:90:GLU:H	3:22:90:GLU:CD	2.20	0.45
3:2E:50:ALA:O	3:2E:70:VAL:HG22	2.16	0.45
26:14:2416:C:OP1	37:35:65:ARG:O	2.33	0.45
31:39:7:TYR:HE2	31:39:10:PRO:HG3	1.81	0.45
31:39:155:LEU:HB2	31:39:189:THR:HG21	1.98	0.45
4:3E:90:GLY:O	4:3E:93:PHE:HB3	2.16	0.45
24:3K:2:G:O2'	24:3K:3:G:OP1	2.28	0.45
24:3K:50:C:H2'	24:3K:51:A:O4'	2.17	0.45
38:45:34:LEU:HD11	38:45:129:THR:HB	1.98	0.45
13:4I:45:VAL:HA	13:4I:48:LEU:HD22	1.96	0.45
6:5E:18:GLN:HA	6:5E:21:LEU:HB2	1.97	0.45
7:62:137:LYS:HE2	7:62:137:LYS:HB3	1.81	0.45
7:62:146:GLU:HG3	11:2A:50:TYR:OH	2.16	0.45
7:62:16:LEU:HD21	9:82:45:ALA:HB2	1.98	0.45
38:88:26:TYR:CD2	38:88:141:GLN:HG2	2.51	0.45
1:13:967:C:O2'	9:8E:125:TYR:OH	2.21	0.45
43:95:37:VAL:O	43:95:39:LEU:N	2.45	0.45
40:A8:108:GLY:O	40:A8:110:LEU:HD12	2.16	0.45
41:B8:51:ARG:HG3	41:B8:98:LYS:HD3	1.98	0.45
42:C8:85:LYS:HD2	42:C8:85:LYS:HA	1.50	0.45
44:E8:11:ARG:HH21	44:E8:99:ARG:N	2.14	0.45
52:M8:15:ILE:HB	52:M8:32:TYR:HD1	1.80	0.45
29:11:182:LEU:H	29:11:272:ALA:CB	2.10	0.45
2:12:124:SER:O	2:12:126:GLU:N	2.45	0.45
1:13:1129:C:N4	1:13:1143:G:H1	2.14	0.45
1:13:755:G:OP2	15:6I:65:ARG:HD2	2.16	0.45
26:14:1525:G:H2'	26:14:1526:G:C8	2.51	0.45
26:14:1628:G:H2'	26:14:1629:U:C6	2.50	0.45
26:14:2086:U:H2'	26:14:2087:G:C8	2.51	0.45
26:14:2286:A:H8	26:14:2287:A:N6	2.14	0.45
26:14:2394:C:H2'	26:14:2395:C:H5'	1.98	0.45
26:14:259:G:HO2'	26:14:621:A:HO2'	1.63	0.45
26:14:307:G:H21	26:14:330:A:N6	2.13	0.45
26:14:607:U:N3	26:14:621:A:C2	2.74	0.45
26:14:882:G:H1	26:14:894:C:H42	1.64	0.45
26:14:952:G:C6	26:14:966:G:C6	3.04	0.45
27:16:15:A:H1'	27:16:109:G:C8	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:19:36:PRO:HB2	29:19:37:LEU:HD12	1.99	0.45
2:1E:97:TRP:CZ3	2:1E:172:ILE:HB	2.51	0.45
2:1E:231:GLU:CD	2:1E:231:GLU:H	2.18	0.45
1:1G:1194:U:H2'	1:1G:1195:C:C6	2.52	0.45
1:1G:280:C:H3'	1:1G:281:G:H5'	1.98	0.45
1:1G:430:A:OP2	4:32:8:VAL:HG23	2.16	0.45
26:1H:1019:U:H3	26:1H:1142(A):A:H62	1.64	0.45
26:1H:1316:U:H2'	26:1H:1317:A:C8	2.51	0.45
26:1H:2210:G:H3'	26:1H:2211:G:C8	2.51	0.45
26:1H:2689:U:H5'	26:1H:2713:A:C2	2.51	0.45
26:1H:433:C:H2'	26:1H:434:U:C6	2.50	0.45
26:1H:900:A:H5'	26:1H:901:A:OP2	2.17	0.45
26:1H:940:G:H2'	26:1H:941:A:O4'	2.16	0.45
10:1I:91:PRO:HB3	10:1I:94:VAL:HB	1.98	0.45
22:1K:28:U:H3	22:1K:42:A:H2	1.62	0.45
36:25:113:LYS:O	36:25:117:LEU:HD22	2.16	0.45
30:29:34:VAL:HG12	30:29:64:LYS:HE3	1.98	0.45
31:31:28:ILE:HG12	31:31:119:ARG:HH21	1.82	0.45
1:13:881:G:P	12:3I:12:ARG:NH2	2.89	0.45
24:3K:1:G:C2	24:3K:73:A:C6	3.04	0.45
13:4I:66:LEU:O	13:4I:70:LEU:HB2	2.17	0.45
10:1I:61:GLU:OE1	14:5I:49:HIS:HE1	1.99	0.45
40:65:10:ARG:O	40:65:14:VAL:HG12	2.16	0.45
34:69:102:SER:HA	34:69:107:VAL:O	2.16	0.45
15:6A:17:ARG:HD3	15:6A:26:GLU:HG3	1.98	0.45
41:75:123:GLN:HA	41:75:126:ALA:HB3	1.96	0.45
9:82:32:ASP:HB3	9:82:35:GLU:HB3	1.98	0.45
39:98:117:VAL:HG22	39:98:118:GLU:H	1.81	0.45
44:A5:28:SER:OG	44:A5:31:GLU:HB2	2.16	0.45
47:D5:99:TYR:CD2	47:D5:123:ASP:HB3	2.51	0.45
49:F5:32:LYS:HB3	49:F5:32:LYS:HE3	1.82	0.45
46:G8:40:GLU:HA	46:G8:41:GLY:HA2	1.80	0.45
50:K8:21:LEU:HD13	50:K8:64:LEU:HA	1.98	0.45
26:1H:729:G:C6	29:11:208:LYS:HB2	2.51	0.45
2:12:141:GLU:O	2:12:145:LEU:HB2	2.17	0.45
1:13:1013:G:N2	1:13:1016:A:OP2	2.48	0.45
1:13:1399:C:C2	1:13:1401:G:C5	3.05	0.45
1:13:397:A:C6	1:13:548:G:N7	2.84	0.45
1:13:663:A:H5'	1:13:836:G:OP1	2.16	0.45
1:13:74:C:H2'	1:13:75:C:C5	2.51	0.45
26:14:28:A:C2	26:14:513:A:C8	3.05	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:1A:32:ALA:HA	10:1A:76:ASN:ND2	2.31	0.45
2:1E:156:LYS:HA	2:1E:156:LYS:HD2	1.68	0.45
21:1F:5:ASP:O	21:1F:11:GLY:HA3	2.15	0.45
1:1G:1171:G:H2'	1:1G:1172:C:C6	2.52	0.45
1:1G:129(A):G:C6	1:1G:188:U:H4'	2.51	0.45
1:1G:1446:A:N3	41:75:118:ARG:HD2	2.30	0.45
1:1G:688:G:H2'	1:1G:689:C:H6	1.81	0.45
1:1G:872:A:C4	1:1G:874:G:N7	2.84	0.45
26:1H:1049:C:C4	26:1H:1050:A:C2	3.04	0.45
26:1H:2022:U:O2'	26:1H:2617:C:H5'	2.16	0.45
26:1H:2051:A:H5'	26:1H:2578:G:O4'	2.17	0.45
26:1H:2461:C:H2'	26:1H:2462:U:C6	2.51	0.45
26:1H:942:G:H5'	62:1H:3621:HOH:O	2.16	0.45
27:1J:46:A:H2'	27:1J:47:C:C6	2.51	0.45
30:21:60:ASN:OD1	30:21:63:LEU:HB2	2.16	0.45
3:22:76:VAL:O	3:22:84:ILE:HA	2.15	0.45
36:25:114:ILE:H	36:25:114:ILE:HG12	1.50	0.45
4:32:149:ALA:O	4:32:153:ARG:NE	2.49	0.45
4:3E:108:LEU:HB3	4:3E:110:PHE:CE1	2.50	0.45
4:3E:18:LYS:HG2	59:3E:301:SF4:S1	2.57	0.45
32:49:125:PHE:HB3	32:49:166:ASP:CB	2.38	0.45
5:4E:19:MET:HE1	5:4E:24:ARG:HH21	1.82	0.45
13:4I:2:ALA:O	13:4I:10:PRO:HD2	2.17	0.45
33:51:97:ARG:HH21	33:51:104:GLU:CD	2.19	0.45
35:58:96:GLU:HG2	35:58:97:ARG:N	2.31	0.45
40:65:36:TYR:HE2	40:65:54:LEU:HD22	1.81	0.45
8:72:30:ARG:O	8:72:34:GLU:HG2	2.17	0.45
36:25:104:ARG:HD3	41:75:36:GLU:HB2	1.99	0.45
16:7I:21:VAL:HG23	16:7I:34:GLU:H	1.82	0.45
38:88:14:ARG:HG2	38:88:41:TRP:HH2	1.81	0.45
17:8A:29:HIS:CG	17:8A:30:PRO:HD2	2.51	0.45
6:5E:97:PHE:CD1	18:9I:31:LEU:HD11	2.51	0.45
1:13:1014:A:H4'	19:AI:14:HIS:NE2	2.31	0.45
45:B5:62:LYS:HB3	45:B5:63:LYS:HZ1	1.81	0.45
41:B8:120:ARG:HA	41:B8:123:GLN:HG2	1.98	0.45
45:F8:25:LYS:HA	45:F8:81:VAL:O	2.16	0.45
47:H8:53:ILE:HA	47:H8:71:VAL:HG13	1.97	0.45
26:1H:2364:C:H4'	48:I8:56:ASP:OD1	2.17	0.45
29:11:145:VAL:HG12	29:11:146:GLU:O	2.16	0.45
29:11:59:LYS:HG2	29:11:60:ARG:N	2.31	0.45
1:13:188:U:H2'	1:13:189:U:H5''	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:13:695:A:H2'	1:13:696:A:C8	2.51	0.45
26:14:2014:A:H2'	26:14:2015:A:C8	2.51	0.45
26:14:1701:A:OP2	61:14:3436:SPE:N1	2.49	0.45
26:14:639:U:H2'	26:14:640:C:C6	2.51	0.45
27:16:94:C:H2'	27:16:95:U:H6	1.82	0.45
2:1E:6:THR:OG1	2:1E:7:VAL:N	2.49	0.45
2:1E:97:TRP:HZ3	2:1E:172:ILE:HB	1.81	0.45
1:1G:1058:G:H2'	1:1G:1059:C:O4'	2.16	0.45
1:1G:1277:C:O2'	1:1G:1279:A:H8	1.99	0.45
1:1G:49:U:C2	1:1G:361:G:N2	2.85	0.45
1:1G:959:A:HO2'	1:1G:984:C:HO2'	1.64	0.45
26:1H:1030:G:OP2	38:88:128:LYS:NZ	2.43	0.45
26:1H:1425:G:N2	26:1H:1573:G:N7	2.65	0.45
10:1I:31:GLY:HA2	10:1I:78:ASN:HB2	1.98	0.45
3:22:37:GLN:O	3:22:40:ARG:N	2.48	0.45
23:2K:62:C:H2'	23:2K:63:C:H6	1.81	0.45
26:14:627:A:H62	37:35:84:ASN:HD21	1.63	0.45
31:39:11:VAL:HG23	31:39:12:LEU:N	2.31	0.45
31:39:141:ALA:O	31:39:144:LYS:HB3	2.17	0.45
31:39:89:VAL:HG12	31:39:90:PHE:N	2.32	0.45
24:3K:48:C:C5	24:3K:59:A:H1'	2.51	0.45
32:41:80:PHE:O	32:41:82:LEU:HB2	2.17	0.45
5:42:60:TYR:HB3	5:42:64:ARG:CZ	2.46	0.45
38:45:38:GLU:HG3	38:45:127:ILE:CG2	2.47	0.45
35:58:57:ALA:C	35:58:59:LYS:N	2.68	0.45
1:1G:1241:G:OP1	7:62:35:LYS:NZ	2.48	0.45
40:65:106:ARG:NH1	40:65:107:GLU:OE2	2.49	0.45
34:69:74:ASN:O	34:69:75:LEU:HB2	2.16	0.45
1:13:1374:A:O2'	7:6E:28:ASN:HB3	2.17	0.45
1:13:277:C:P	17:8I:68:ARG:HH12	2.39	0.45
46:C5:52:SER:H	46:C5:57:GLN:N	2.15	0.45
46:G8:95:LYS:O	46:G8:103:GLY:HA2	2.15	0.45
49:J8:81:LYS:HG3	49:J8:82:LEU:H	1.81	0.45
54:O8:41:PRO:HD2	54:O8:46:HIS:N	2.31	0.45
2:12:57:PHE:HZ	2:12:199:TYR:CZ	2.35	0.45
1:13:1125:U:O2'	1:13:1126:U:H6	1.97	0.45
26:14:1754:C:N3	26:14:2716:U:O2'	2.48	0.45
26:14:2027:G:H2'	26:14:2028:U:O4'	2.16	0.45
26:14:336:C:OP1	46:C5:83:THR:HG23	2.16	0.45
26:14:573:G:O2'	26:14:574:C:H3'	2.16	0.45
26:14:730:C:O2'	26:14:731:C:H5'	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:14:910:A:N3	26:14:2264:C:O2'	2.43	0.45
26:14:922:U:H2'	26:14:923:C:C6	2.51	0.45
26:14:999:U:H5''	26:14:1154:G:O6	2.16	0.45
29:19:13:ARG:HD2	29:19:13:ARG:HA	1.75	0.45
1:1G:1286:A:H3'	1:1G:1286:A:H8	1.81	0.45
1:1G:422:C:O2'	1:1G:423:G:N2	2.50	0.45
1:1G:407:G:C2	1:1G:436:C:C2	3.05	0.45
26:1H:142:G:H2'	26:1H:143:C:C6	2.50	0.45
26:1H:1828:G:H8	26:1H:1828:G:OP2	1.99	0.45
26:1H:2356:C:H2'	26:1H:2357:U:O4'	2.17	0.45
26:1H:2557:G:H2'	26:1H:2558:C:C6	2.51	0.45
22:1K:1:G:H2'	22:1K:2:G:O4'	2.16	0.45
26:1H:2619:C:OP1	30:21:152:LYS:HE3	2.17	0.45
36:25:34:THR:OG1	36:25:35:VAL:N	2.50	0.45
11:2A:103:LEU:HD12	11:2A:103:LEU:HA	1.71	0.45
1:1G:1523:G:OP1	11:2A:123:LYS:HD2	2.17	0.45
23:2L:50:G:H1	23:2L:66:C:H42	1.63	0.45
26:1H:801:G:OP2	31:31:55:GLY:HA2	2.17	0.45
31:39:103:LYS:HA	31:39:106:ARG:HG3	1.98	0.45
12:3A:39:VAL:HG23	12:3A:57:LYS:HD3	1.97	0.45
24:3K:3:G:O6	24:3K:69:A:N6	2.49	0.45
32:49:80:PHE:O	32:49:82:LEU:HB2	2.17	0.45
6:52:98:LEU:H	6:52:98:LEU:HD12	1.82	0.45
35:58:67:LEU:O	35:58:88:GLU:HG2	2.17	0.45
6:5E:67:MET:HB2	6:5E:68:PRO:HD2	1.98	0.45
40:65:62:LYS:HA	40:65:65:VAL:HB	1.99	0.45
34:69:109:ILE:HB	34:69:130:TYR:OH	2.17	0.45
7:6E:65:ALA:HB1	7:6E:127:ALA:HB3	1.99	0.45
28:71:225:ASN:HB3	28:71:227:HIS:ND1	2.31	0.45
41:75:2:ASN:HB3	41:75:4:GLY:C	2.37	0.45
16:7I:36:ILE:HG13	16:7I:36:ILE:O	2.16	0.45
9:82:63:ILE:HD11	9:82:81:ILE:HD11	1.98	0.45
38:88:138:ASP:HA	38:88:139:GLU:HA	1.69	0.45
38:88:5:ARG:H	38:88:5:ARG:HG3	1.61	0.45
18:9A:52:PRO:O	18:9A:56:THR:HG23	2.17	0.45
20:BA:50:GLU:CA	20:BA:100:ILE:HG12	2.46	0.45
20:BA:64:ASP:OD2	20:BA:81:LYS:NZ	2.40	0.45
35:58:42:TRP:O	42:C8:64:ARG:HD2	2.16	0.45
47:D5:94:GLU:O	47:D5:129:SER:HA	2.15	0.45
47:H8:63:ASP:OD1	47:H8:65:GLN:NE2	2.36	0.45
2:12:152:PHE:O	2:12:155:LEU:HD12	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:14:1005:C:C2	26:14:1143:A:C5	3.05	0.45
26:14:1131:G:O6	26:14:2040:C:H1'	2.16	0.45
26:14:1248:G:C5	42:85:3:ARG:HB2	2.52	0.45
26:14:1253:A:OP1	62:14:3654:HOH:O	2.21	0.45
26:14:176:G:O2'	26:14:177:G:H5'	2.16	0.45
26:14:2023:G:OP2	26:14:2617:C:H4'	2.17	0.45
26:14:2038:G:H2'	26:14:2039:C:C6	2.52	0.45
26:14:2129:C:H3'	26:14:2130:U:H6	1.80	0.45
26:14:860:U:C2	26:14:2268:A:C8	3.05	0.45
26:14:2262:U:H4'	26:14:2328:A:H2	1.79	0.45
26:14:2472:G:H1	26:14:2477:C:P	2.39	0.45
26:14:2740:A:C6	26:14:2764:A:C8	3.05	0.45
26:14:839:U:H2'	26:14:840:C:C6	2.52	0.45
2:1E:11:LEU:HD12	2:1E:15:VAL:HG23	1.99	0.45
1:1G:109:A:H5'	1:1G:110:C:C5	2.52	0.45
1:1G:17:U:H2'	1:1G:18:C:C6	2.51	0.45
1:1G:500:G:H2'	1:1G:501:C:C6	2.52	0.45
26:1H:1429:G:O2'	26:1H:1430:C:H5'	2.16	0.45
26:1H:2023:G:H5'	26:1H:2617:C:H4'	1.98	0.45
26:1H:2562:U:H1'	36:68:23:ARG:HD3	1.98	0.45
10:1I:27:ALA:HA	10:1I:81:THR:HG22	1.97	0.45
27:1J:72:G:O2'	27:1J:104:A:N6	2.44	0.45
30:21:75:VAL:HG12	30:21:75:VAL:O	2.16	0.45
12:3I:60:LEU:HD12	12:3I:62:SER:OG	2.17	0.45
24:3K:48:C:OP2	24:3K:59:A:O2'	2.31	0.45
5:42:122:GLU:O	5:42:126:ARG:NH1	2.50	0.45
33:51:11:VAL:HG23	33:51:76:VAL:HG11	1.98	0.45
3:22:18:TRP:HD1	14:5A:54:PRO:HA	1.81	0.45
6:5E:16:GLN:HG2	6:5E:17:SER:N	2.31	0.45
40:65:54:LEU:O	40:65:56:LEU:N	2.44	0.45
7:6E:27:ILE:HD13	7:6E:40:ALA:HA	1.99	0.45
7:6E:73:MET:HG3	7:6E:89:MET:O	2.16	0.45
8:72:17:THR:HG23	8:72:65:TYR:HE2	1.80	0.45
17:8A:88:TYR:CE1	17:8A:92:ARG:HD2	2.52	0.45
9:8E:21:PRO:HA	9:8E:59:PHE:HA	1.99	0.45
44:A5:13:SER:O	44:A5:16:LYS:HB2	2.16	0.45
46:C5:89:PHE:O	46:C5:90:LEU:HB3	2.16	0.45
1:13:1153:C:H2'	1:13:1154:G:O4'	2.16	0.45
1:13:347:G:C2	1:13:348:G:H1'	2.52	0.45
1:13:509:A:H5''	4:3E:55:ALA:HB2	1.99	0.45
1:13:648:A:C6	1:13:649:G:C6	3.05	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:14:195:A:H61	26:14:198:C:H3'	1.81	0.45
26:14:2126:A:O2'	26:14:2127:G:H5''	2.17	0.45
26:14:2261:C:H1'	26:14:2388:A:N3	2.31	0.45
2:1E:11:LEU:HG	2:1E:213:LEU:HD22	1.98	0.45
2:1E:187:LEU:HD11	2:1E:204:ASN:O	2.16	0.45
1:1G:1179:A:O3'	9:82:103:THR:HG23	2.17	0.45
1:1G:262:A:C6	1:1G:263:A:C6	3.05	0.45
1:1G:325:A:H2'	1:1G:326:G:O4'	2.16	0.45
1:1G:358:U:H2'	1:1G:359:U:H6	1.81	0.45
26:1H:129:C:H2'	26:1H:130:C:C6	2.52	0.45
26:1H:2136:C:H2'	26:1H:2137:C:O4'	2.17	0.45
26:1H:2607:G:H2'	26:1H:2608:G:O4'	2.17	0.45
26:1H:270(Y):G:C2	26:1H:270(Z):U:O4	2.70	0.45
26:1H:475:U:C4	26:1H:481:G:O6	2.70	0.45
26:1H:638:G:H2'	26:1H:639:U:C6	2.52	0.45
26:1H:755:C:H2'	26:1H:756:C:C6	2.52	0.45
30:29:182:LEU:HA	30:29:182:LEU:HD12	1.63	0.45
30:29:52:LEU:HA	30:29:52:LEU:HD12	1.56	0.45
11:2I:79:SER:HA	11:2I:104:GLN:O	2.16	0.45
11:2I:40:ILE:CG2	11:2I:75:TYR:HD2	2.30	0.45
23:2L:20:G:C4	23:2L:58:A:C2	3.04	0.45
31:31:149:ASP:OD1	31:31:149:ASP:N	2.41	0.45
32:49:18:GLU:OE2	32:49:21:ARG:NH2	2.43	0.45
32:49:50:ALA:HB2	32:49:87:PRO:HG3	1.99	0.45
13:4A:81:LEU:HD11	13:4A:86:CYS:SG	2.57	0.45
7:62:15:ASP:HB3	7:62:19:GLY:N	2.31	0.45
34:69:128:LEU:O	34:69:138:ILE:HG22	2.17	0.45
15:6A:11:VAL:HG21	15:6A:34:LEU:CD1	2.47	0.45
41:75:10:VAL:C	41:75:12:SER:H	2.20	0.45
37:78:97:PRO:HD3	37:78:126:VAL:O	2.16	0.45
37:78:88:LEU:HD12	37:78:88:LEU:HA	1.72	0.45
9:82:42:ARG:NH1	9:82:75:ASP:OD1	2.37	0.45
18:9A:36:ASN:HB2	18:9A:38:GLU:OE1	2.16	0.45
46:C5:104:GLY:HA2	46:C5:105:ALA:HA	1.74	0.45
48:E5:27:GLU:HB2	48:E5:69:PHE:CD1	2.48	0.45
47:H8:105:VAL:HG22	47:H8:140:ASP:HA	1.99	0.45
1:13:1127:G:H2'	1:13:1128:C:O4'	2.16	0.45
1:13:1239:A:C4	1:13:1298:C:N4	2.85	0.45
1:13:1326:C:H2'	1:13:1327:C:C6	2.51	0.45
1:13:1349:A:H2'	1:13:1350:A:H8	1.81	0.45
1:13:272:C:H2'	1:13:273:A:H8	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:14:108:U:H4'	26:14:347:A:H2	1.82	0.45
26:14:1116:C:H2'	26:14:1117:G:C8	2.52	0.45
26:14:1204:A:N1	26:14:1241:A:C2	2.84	0.45
26:14:2261:C:O2'	26:14:2262:U:H5'	2.17	0.45
26:14:2342:C:OP2	26:14:2342:C:H6	1.98	0.45
26:14:2389:G:H5''	26:14:2390:U:O4'	2.15	0.45
26:14:2399:G:H2'	26:14:2400:G:O4'	2.17	0.45
26:14:2591:C:OP1	29:19:239:ARG:HG2	2.16	0.45
26:14:2845:G:H5''	41:75:55:ASN:HA	1.99	0.45
26:14:183:C:H1'	26:14:433:C:H1'	1.98	0.45
26:14:1805:U:O2	29:19:50:THR:HB	2.17	0.45
1:1G:1073:U:H2'	1:1G:1074:G:C8	2.52	0.45
1:1G:1221:G:OP1	1:1G:1321:C:N4	2.47	0.45
26:1H:1553:A:HO2'	26:1H:1554:A:H8	1.62	0.45
26:1H:1931:U:O4'	26:1H:1931:U:O2	2.35	0.45
26:1H:2138:C:H42	26:1H:2153:G:H1	1.64	0.45
26:1H:250:G:C6	26:1H:251:A:C6	3.04	0.45
26:1H:2820:A:C6	39:98:4:LEU:HD11	2.52	0.45
26:1H:2820:A:OP2	26:1H:2821:A:N6	2.45	0.45
26:1H:576:U:OP1	62:1H:3779:HOH:O	2.21	0.45
10:1I:50:ILE:HD11	10:1I:57:LYS:HD2	1.98	0.45
3:22:18:TRP:HE3	3:22:18:TRP:N	2.13	0.45
30:29:23:VAL:HA	30:29:184:VAL:O	2.17	0.45
11:2A:48:ILE:HG21	11:2A:63:LEU:HD12	1.98	0.45
31:31:197:ASP:O	31:31:198:ALA:HB3	2.16	0.45
4:32:34:GLU:HB2	4:32:35:ARG:NH2	2.31	0.45
38:45:79:LEU:HD23	38:45:79:LEU:HA	1.73	0.45
32:49:145:THR:C	32:49:147:ASP:H	2.19	0.45
5:4E:152:ARG:HA	8:7E:64:LYS:HZ3	1.80	0.45
14:5A:17:LYS:NZ	14:5A:18:VAL:HG13	2.31	0.45
14:5I:6:LEU:CD1	14:5I:23:ARG:HH22	2.26	0.45
34:61:86:THR:HG22	34:61:122:GLU:HG2	1.99	0.45
34:61:95:LYS:HB3	34:61:95:LYS:HE3	1.87	0.45
26:1H:2562:U:H1'	36:68:23:ARG:NH1	2.32	0.45
34:69:14:ASP:N	34:69:17:GLN:OE1	2.41	0.45
7:6E:65:ALA:HB2	7:6E:128:ALA:HB2	1.99	0.45
38:88:133:ARG:O	38:88:134:ARG:HB2	2.17	0.45
38:88:36:ALA:O	38:88:99:PRO:HA	2.16	0.45
17:8I:78:GLU:OE2	17:8I:81:ARG:HD2	2.16	0.45
47:H8:15:PRO:HB2	47:H8:19:ARG:NH2	2.32	0.45
49:J8:84:GLY:HA2	49:J8:85:LEU:CB	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:K8:41:ILE:HD13	50:K8:44:LEU:HG	1.99	0.45
56:M5:14:VAL:HG13	56:M5:22:VAL:HG13	1.97	0.45
26:1H:1805:U:O2	29:11:50:THR:HB	2.17	0.45
1:13:1147:C:O2	9:8E:16:ARG:NH1	2.50	0.45
1:13:1234:C:H2'	1:13:1235:U:C6	2.51	0.45
1:13:612:C:O2	1:13:629:G:N2	2.50	0.45
26:14:1796:U:H2'	26:14:1797:C:C6	2.52	0.45
26:14:2212:A:H1'	26:14:2215:G:C5	2.51	0.45
26:14:2512:C:H2'	26:14:2513:G:O4'	2.17	0.45
26:14:524:U:H2'	26:14:525:U:H6	1.80	0.45
26:14:923:C:H2'	26:14:924:C:C6	2.52	0.45
35:15:99:LEU:O	35:15:103:VAL:HG23	2.17	0.45
1:1G:1004:A:H8	1:1G:1026:G:C8	2.35	0.45
1:1G:1224:G:O6	1:1G:1322:C:H1'	2.17	0.45
1:1G:1322:C:O2'	1:1G:1323:G:H5'	2.16	0.45
1:1G:362:G:O2'	12:3A:33:ARG:NH2	2.49	0.45
26:1H:1108:U:H2'	26:1H:1109:C:H5'	1.99	0.45
26:1H:205:G:HO2'	26:1H:206:U:P	2.39	0.45
26:1H:747:U:O2	26:1H:2014:A:H1'	2.17	0.45
26:1H:781:A:C8	29:11:219:PRO:HG2	2.52	0.45
27:1J:38:C:O2'	40:65:93:LYS:NZ	2.50	0.45
30:21:59:VAL:HG22	30:21:60:ASN:N	2.32	0.45
3:2E:134:ILE:HG22	3:2E:168:ALA:HB3	1.98	0.45
31:31:101:LEU:HD22	31:31:105:VAL:HB	1.99	0.45
4:32:33:MET:O	4:32:34:GLU:HB2	2.17	0.45
26:14:1244:G:OP1	37:35:7:ARG:HD3	2.17	0.45
12:3A:60:LEU:HD13	12:3A:60:LEU:HA	1.75	0.45
24:3K:45:G:H4'	24:3K:46:G:OP1	2.16	0.45
1:1G:947:G:O3'	13:4A:109:THR:OG1	2.35	0.45
5:4E:36:ASP:OD2	5:4E:40:ARG:NH1	2.50	0.45
5:4E:51:VAL:O	5:4E:55:VAL:HG23	2.17	0.45
26:1H:270(L):U:O2	34:61:50:ARG:HG2	2.16	0.45
8:72:41:ARG:H	8:72:41:ARG:HG3	1.49	0.45
16:7I:74:LEU:HD22	16:7I:79:VAL:HG21	1.99	0.45
43:95:70:ILE:O	43:95:70:ILE:HG22	2.17	0.45
19:AA:12:ASP:OD1	19:AA:13:ASP:N	2.48	0.45
19:AI:51:VAL:HG12	19:AI:52:TYR:H	1.81	0.45
41:B8:50:ILE:HG13	41:B8:99:LEU:O	2.17	0.45
46:C5:89:PHE:O	46:C5:89:PHE:CG	2.70	0.45
42:C8:58:ARG:HA	42:C8:61:TRP:CE3	2.51	0.45
47:D5:128:VAL:HG23	47:D5:160:GLY:O	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:E8:88:ARG:HB2	44:E8:92:ARG:CB	2.44	0.45
49:F5:84:GLY:HA2	49:F5:85:LEU:HB3	1.99	0.45
46:G8:93:GLY:O	46:G8:94:LYS:HB2	2.17	0.45
52:M8:43:TYR:O	52:M8:46:GLN:HA	2.16	0.45
26:14:1138:G:H21	35:15:106:MET:CE	2.25	0.45
26:14:11:G:H2'	26:14:12:U:H5'	1.98	0.45
26:14:1316:U:H2'	26:14:1317:A:C8	2.51	0.45
26:14:1784:A:H4'	26:14:1785:A:C5'	2.47	0.45
26:14:387:U:H4'	26:14:388:G:O5'	2.17	0.45
26:14:921:G:C6	26:14:922:U:C4	3.06	0.45
29:19:245:PRO:HG2	29:19:253:GLN:NE2	2.32	0.45
2:1E:187:LEU:HA	2:1E:201:ILE:O	2.17	0.45
1:1G:1052:U:H5''	1:1G:1053:G:OP2	2.17	0.45
1:1G:746:A:H2'	1:1G:747:C:C6	2.52	0.45
1:1G:957:U:H1'	1:1G:960:U:C5	2.52	0.45
1:1G:991:U:O2	1:1G:993:G:H8	2.00	0.45
26:1H:1048:A:H5'	26:1H:1049:C:OP2	2.17	0.45
26:1H:1359:A:H2	26:1H:1372:U:O4	1.99	0.45
26:1H:1470:G:H5''	26:1H:1471:A:OP1	2.17	0.45
26:1H:1557:C:OP2	26:1H:1558:A:O2'	2.28	0.45
26:1H:1614:A:H8	26:1H:1614:A:O5'	2.00	0.45
26:1H:2855:C:H2'	26:1H:2856:C:H6	1.81	0.45
26:1H:524:U:H4'	26:1H:554:U:H4'	1.98	0.45
27:1J:101:A:H3'	27:1J:102:G:H8	1.82	0.45
3:22:152:ILE:O	3:22:198:VAL:HA	2.17	0.45
3:2E:17:ASP:O	3:2E:54:ARG:NH2	2.40	0.45
3:2E:72:LYS:HD3	3:2E:75:VAL:CG2	2.47	0.45
26:1H:616:A:C4	31:31:180:GLY:HA3	2.52	0.45
37:35:57:THR:O	37:35:61:ARG:HG3	2.17	0.45
31:39:69:HIS:CD2	31:39:69:HIS:N	2.84	0.45
24:3K:56:C:H2'	24:3K:57:G:O4'	2.16	0.45
24:3L:28:U:H2'	24:3L:29:U:C6	2.52	0.45
38:45:98:LYS:HB3	38:45:99:PRO:HD2	1.99	0.45
13:4A:80:ARG:O	13:4A:84:ILE:HB	2.17	0.45
5:4E:110:LEU:HD13	5:4E:118:ILE:HG21	1.99	0.45
33:51:4:ILE:HG23	33:51:6:ARG:CZ	2.47	0.45
34:69:9:LEU:HD11	34:69:35:LEU:HB3	1.99	0.45
34:69:73:GLU:OE2	34:69:137:PRO:HD2	2.16	0.45
34:69:93:THR:O	34:69:97:ILE:HG13	2.17	0.45
8:72:83:ILE:HB	8:72:137:VAL:HG13	1.98	0.45
9:82:5:TYR:HA	9:82:17:VAL:O	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:85:102:GLU:HB3	42:85:105:VAL:HG13	1.99	0.45
43:95:1:MET:HA	43:95:42:GLY:N	2.30	0.45
40:A8:93:LYS:HG2	40:A8:95:HIS:HB2	1.99	0.45
44:E8:7:ALA:HB2	44:E8:50:VAL:HG22	1.99	0.45
53:J5:11:THR:HG23	53:J5:15:ARG:HB3	1.99	0.45
34:61:38:LEU:HD11	49:J8:75:GLU:HG3	1.99	0.45
52:M8:38:LYS:HE3	52:M8:38:LYS:HA	1.99	0.45
53:N8:33:CYS:SG	53:N8:46:CYS:HB3	2.56	0.45
1:13:828:A:H2'	1:13:829:G:O4'	2.16	0.44
26:14:1283:G:N2	26:14:1285:G:H3'	2.32	0.44
26:14:2062:A:O2'	26:14:2063:C:P	2.75	0.44
26:14:470:A:H8	26:14:470:A:C5'	2.30	0.44
26:14:657:U:H2'	26:14:658:C:C6	2.52	0.44
26:14:65:C:H2'	26:14:66:C:C6	2.52	0.44
2:1E:55:PHE:CD1	2:1E:58:ILE:HD12	2.52	0.44
21:1F:6:ARG:HH11	21:1F:15:ARG:NE	2.16	0.44
1:1G:987:G:N2	1:1G:1218:C:N3	2.46	0.44
1:1G:1497:G:H2'	1:1G:1498:U:H5'	1.99	0.44
1:1G:322:C:H5	1:1G:328:C:H5	1.65	0.44
1:1G:589:C:N3	1:1G:650:G:N2	2.46	0.44
1:1G:947:G:H2'	1:1G:948:C:C6	2.53	0.44
26:1H:141:A:H8	26:1H:1408:C:H1'	1.82	0.44
26:1H:1550:C:H2'	26:1H:1551:C:H6	1.83	0.44
26:1H:2845:G:H2'	26:1H:2846:G:H8	1.82	0.44
26:1H:517:C:OP1	53:N8:16:ARG:NH2	2.39	0.44
27:1J:56:G:H4'	27:1J:57:A:C8	2.51	0.44
30:21:49:LEU:HD12	30:21:49:LEU:HA	1.40	0.44
3:22:51:GLY:O	3:22:70:VAL:HG13	2.17	0.44
37:35:122:PRO:CB	37:35:141:ALA:HB1	2.45	0.44
31:39:25:PRO:C	31:39:27:GLU:N	2.70	0.44
1:13:363:A:OP1	12:3I:33:ARG:HG3	2.17	0.44
24:3L:13:C:H2'	24:3L:14:A:H8	1.82	0.44
24:3L:55:U:H2'	24:3L:57:G:P	2.56	0.44
32:41:145:THR:O	32:41:146:TYR:HB3	2.18	0.44
6:5E:22:GLU:O	6:5E:26:ILE:HG13	2.16	0.44
34:61:73:GLU:OE2	34:61:137:PRO:HD2	2.17	0.44
16:7A:11:SER:H	16:7A:14:ASN:HB3	1.82	0.44
18:9I:44:LEU:HD11	18:9I:70:ILE:HG21	1.99	0.44
47:D5:62:PRO:O	47:D5:63:ASP:HB3	2.17	0.44
43:D8:49:THR:HG23	43:D8:51:VAL:H	1.81	0.44
51:H5:5:LYS:HB3	51:H5:5:LYS:HE3	1.72	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:H8:164:ALA:O	47:H8:165:VAL:HG22	2.18	0.44
32:41:67:LYS:CE	52:M8:6:HIS:CE1	2.98	0.44
54:08:14:THR:OG1	54:08:15:GLU:N	2.50	0.44
6:5E:81:ILE:HD11	29:11:125:ILE:HB	2.00	0.44
1:13:158:G:C4	1:13:159:G:C8	3.05	0.44
26:14:142:G:H2'	26:14:143:C:H6	1.81	0.44
26:14:656:G:H2'	26:14:657:U:O4'	2.16	0.44
26:14:817:C:H2'	26:14:818:G:O4'	2.17	0.44
35:15:26:LEU:HD23	35:15:60:ILE:HD11	1.98	0.44
27:16:75:G:H21	47:H8:85:HIS:CE1	2.34	0.44
1:1G:1441:G:H8	1:1G:1441:G:O5'	2.00	0.44
1:1G:922:G:H2'	1:1G:923:A:C8	2.52	0.44
1:1G:931:C:H2'	1:1G:932:C:H6	1.82	0.44
1:1G:951:G:O4'	1:1G:971:G:H5'	2.17	0.44
26:1H:1019:U:O2'	26:1H:1021:A:H2	1.99	0.44
26:1H:330:A:H2	26:1H:1210:A:O2'	2.01	0.44
26:1H:1484:G:C2	26:1H:1506:C:C2	3.05	0.44
26:1H:184:C:H2'	26:1H:185:U:C6	2.52	0.44
26:1H:2244:U:H2'	26:1H:2245:U:O4'	2.17	0.44
26:1H:2774:C:H2'	26:1H:2775:A:O4'	2.16	0.44
26:1H:495:G:H1'	44:E8:57:ASN:OD1	2.18	0.44
26:1H:761:A:OP1	62:1H:3780:HOH:O	2.21	0.44
26:1H:770:G:C8	62:1H:4083:HOH:O	2.56	0.44
26:1H:813:U:H2'	26:1H:814:C:C6	2.52	0.44
30:21:26:ILE:HD11	30:21:198:VAL:HG21	1.99	0.44
36:25:3:GLN:HB2	36:25:4:PRO:HD2	2.00	0.44
36:25:13:ASN:ND2	36:25:97:ARG:H	2.13	0.44
31:31:155:LEU:HD13	31:31:174:VAL:HG22	1.98	0.44
4:32:81:GLU:OE2	4:32:139:ARG:NH2	2.51	0.44
4:32:173:TRP:HZ3	4:32:193:ASP:HB3	1.82	0.44
26:14:671:C:OP1	37:35:42:SER:O	2.34	0.44
12:3A:47:LYS:HB3	12:3A:48:PRO:HD2	1.99	0.44
4:3E:98:GLU:OE2	4:3E:107:ARG:NH1	2.50	0.44
4:3E:109:GLY:HA3	4:3E:165:MET:SD	2.57	0.44
4:3E:86:LYS:H	4:3E:86:LYS:HD3	1.83	0.44
32:41:49:ASP:OD2	32:41:51:ARG:NH2	2.50	0.44
32:41:46:ALA:HB2	32:41:52:ILE:HB	2.00	0.44
38:45:126:PRO:O	38:45:127:ILE:HG23	2.17	0.44
38:45:29:PHE:HB3	38:45:65:PHE:CZ	2.52	0.44
38:45:4:PRO:HD3	38:45:70:PRO:O	2.18	0.44
6:52:35:ALA:HB1	6:52:65:VAL:CG1	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:69:44:LEU:HD23	34:69:44:LEU:HA	1.74	0.44
9:82:79:LEU:HD22	9:82:82:ALA:HB3	1.99	0.44
42:85:47:TYR:HA	42:85:50:ARG:NH2	2.32	0.44
17:8I:11:VAL:HG23	17:8I:20:THR:HB	1.99	0.44
39:98:18:LEU:HD23	39:98:18:LEU:HA	1.73	0.44
26:1H:2378:A:O2'	40:A8:21:THR:HG21	2.17	0.44
19:AI:5:LEU:O	19:AI:6:LYS:HB3	2.17	0.44
46:C5:101:LYS:HE3	46:C5:101:LYS:H	1.81	0.44
46:C5:63:LYS:HA	46:C5:63:LYS:NZ	2.32	0.44
26:14:297:C:OP1	46:C5:84:ARG:NH2	2.51	0.44
43:D8:34:GLU:HG2	43:D8:56:SER:OG	2.17	0.44
44:E8:11:ARG:CZ	44:E8:98:LYS:HB3	2.46	0.44
46:G8:81:LYS:HD2	46:G8:99:CYS:SG	2.58	0.44
50:K8:3:LEU:HA	50:K8:3:LEU:HD23	1.50	0.44
29:11:17:THR:HG21	29:11:204:ILE:HA	2.00	0.44
2:12:91:PRO:HB3	2:12:151:GLY:O	2.18	0.44
1:13:1226:C:H4'	1:13:1227:A:OP1	2.17	0.44
1:13:321:A:C2	1:13:333:G:C2	3.05	0.44
26:14:1929:G:H4'	26:14:1930:G:OP1	2.17	0.44
26:14:2619:C:H2'	26:14:2620:C:C6	2.53	0.44
26:14:396:G:H8	26:14:396:G:O5'	2.00	0.44
26:14:861:A:N3	27:1J:79:C:O2'	2.51	0.44
26:14:957:A:N6	26:14:2459:A:C8	2.86	0.44
2:1E:155:LEU:HD13	2:1E:157:ARG:O	2.17	0.44
2:1E:237:ALA:O	2:1E:239:VAL:HG23	2.18	0.44
1:1G:545:C:OP1	4:32:61:LYS:NZ	2.50	0.44
26:1H:1011:G:OP1	42:C8:77:SER:OG	2.19	0.44
26:1H:1204:A:N1	26:1H:1241:A:C2	2.85	0.44
26:1H:1317:A:H2'	26:1H:1318:C:C6	2.52	0.44
26:1H:1338:G:O2'	26:1H:1393:A:N1	2.40	0.44
26:1H:2160:G:C5	26:1H:2161:C:H1'	2.52	0.44
26:1H:270(Y):G:H5''	26:1H:273(A):G:OP1	2.17	0.44
26:1H:660:G:H21	37:78:12:ALA:HA	1.82	0.44
3:22:106:VAL:O	3:22:109:PRO:HD3	2.18	0.44
3:22:113:ALA:O	3:22:116:VAL:HG12	2.16	0.44
3:2E:175:LEU:HD11	3:2E:201:TYR:CD2	2.52	0.44
4:32:148:VAL:O	4:32:152:SER:OG	2.28	0.44
31:39:5:ALA:HB1	31:39:125:LEU:HD21	1.98	0.44
31:39:164:ARG:HG2	31:39:175:THR:OG1	2.18	0.44
12:3I:21:LYS:HB3	12:3I:21:LYS:HE2	1.52	0.44
32:41:37:VAL:HG22	32:41:159:VAL:HG13	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:6E:5:ARG:HG3	7:6E:7:ALA:H	1.81	0.44
28:71:59:ARG:HG3	28:71:164:ARG:HD2	1.98	0.44
8:72:44:PHE:HA	8:72:79:VAL:HG11	1.99	0.44
8:7E:82:HIS:HE1	8:7E:84:ARG:HD3	1.81	0.44
9:82:5:TYR:CE1	9:82:16:ARG:HG2	2.51	0.44
18:9I:66:LEU:O	18:9I:70:ILE:HG13	2.17	0.44
19:AA:3:ARG:NH2	19:AA:11:VAL:HG12	2.32	0.44
47:D5:27:VAL:HG23	47:D5:36:LYS:HA	2.00	0.44
47:D5:95:PRO:HA	47:D5:128:VAL:O	2.16	0.44
26:14:2271:G:H5''	48:E5:20:ARG:NE	2.32	0.44
26:1H:2261:C:C6	48:I8:16:SER:HB3	2.52	0.44
53:J5:31:VAL:HG13	53:J5:42:PRO:HG3	2.00	0.44
50:K8:31:GLU:HB3	50:K8:53:LEU:HD11	1.98	0.44
51:L8:18:ASP:OD1	51:L8:19:GLN:N	2.50	0.44
51:L8:51:ALA:HA	51:L8:54:VAL:HG12	1.99	0.44
56:M5:40:GLU:HG3	56:M5:43:GLN:NE2	2.32	0.44
19:AI:68:GLY:HA3	52:M8:59:PHE:HD2	1.83	0.44
1:13:110:C:H2'	1:13:111:G:O4'	2.17	0.44
1:13:1392:G:O2'	1:13:1393:U:H5'	2.18	0.44
1:13:820:U:H4'	1:13:821:G:OP2	2.18	0.44
26:14:2076:U:O5'	26:14:2076:U:H6	1.99	0.44
26:14:2151:G:C2	26:14:2152:G:H1'	2.51	0.44
26:14:235:U:H2'	26:14:236:C:H6	1.80	0.44
26:14:2823:A:OP1	30:29:159:HIS:NE2	2.48	0.44
26:14:2872:G:C4	26:14:2873:A:C2	3.05	0.44
26:14:312:G:H4'	26:14:331:A:N3	2.33	0.44
26:14:41:C:H2'	26:14:43:G:H8	1.82	0.44
26:14:839:U:H2'	26:14:840:C:H6	1.82	0.44
35:15:63:THR:O	35:15:66:LYS:HE2	2.17	0.44
27:16:11:C:H3'	27:16:12:C:C6	2.53	0.44
29:19:268:ARG:HG3	29:19:268:ARG:O	2.17	0.44
10:1A:55:LYS:HZ3	10:1A:57:LYS:HG2	1.81	0.44
1:1G:1519:A:H5''	1:1G:1520:G:OP2	2.17	0.44
1:1G:266:G:H2'	1:1G:266:G:N3	2.32	0.44
26:1H:1510:A:N3	26:1H:1510:A:H2'	2.32	0.44
26:1H:1535:U:OP2	26:1H:1538:G:N2	2.50	0.44
26:1H:2025:C:H2'	26:1H:2026:C:C6	2.52	0.44
26:1H:2310:A:H5''	26:1H:2311:A:OP2	2.17	0.44
26:1H:2542:A:H4'	26:1H:2543:G:C8	2.53	0.44
26:1H:273(E):U:H2'	26:1H:273(F):C:H5'	1.99	0.44
27:1J:66:A:N6	27:1J:108:C:O5'	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:1K:21:A:C5	22:1K:47:U:C4	3.06	0.44
24:1L:22:G:OP1	24:1L:48:C:N4	2.50	0.44
3:22:18:TRP:CE3	3:22:18:TRP:N	2.85	0.44
3:22:151:VAL:HA	3:22:199:LYS:O	2.17	0.44
3:22:44:GLU:HA	3:22:52:LEU:HD11	1.99	0.44
11:2A:69:ALA:O	11:2A:73:MET:HG3	2.18	0.44
11:2A:85:ARG:HD3	11:2A:113:PRO:HD3	1.98	0.44
4:32:177:ASP:O	4:32:180:GLY:N	2.46	0.44
4:32:189:PRO:HB2	4:32:194:LEU:HD21	1.99	0.44
12:3I:110:VAL:CG2	12:3I:120:TYR:HB3	2.47	0.44
38:45:26:TYR:HD1	38:45:27:VAL:HG23	1.73	0.44
13:4A:37:THR:HG22	13:4A:55:ARG:NE	2.33	0.44
5:4E:113:ALA:O	5:4E:115:VAL:HG23	2.18	0.44
13:4I:22:ILE:HB	13:4I:25:ILE:HD12	1.99	0.44
13:4I:82:MET:C	13:4I:84:ILE:H	2.21	0.44
25:4L:21:A:H8	25:4L:21:A:O5'	2.01	0.44
6:52:8:ILE:HD11	6:52:79:LEU:HD13	1.98	0.44
39:55:33:ARG:HB2	39:55:115:GLU:CB	2.45	0.44
35:58:127:ASP:O	35:58:128:HIS:HB3	2.17	0.44
28:71:226:PRO:HD2	28:71:227:HIS:CE1	2.53	0.44
18:9A:22:VAL:CG1	18:9A:56:THR:HA	2.47	0.44
19:AA:66:MET:O	19:AA:69:HIS:HB2	2.18	0.44
41:B8:11:GLU:O	41:B8:12:SER:HB2	2.18	0.44
47:D5:6:LYS:HD2	47:D5:40:ASP:CB	2.47	0.44
47:D5:4:ARG:NH2	47:D5:58:VAL:HG11	2.33	0.44
47:H8:48:PHE:HE1	47:H8:71:VAL:HG11	1.81	0.44
54:O8:26:ASN:ND2	54:O8:28:ARG:O	2.51	0.44
1:13:1394:A:C6	1:13:1501:C:H4'	2.53	0.44
1:13:1513:A:H2'	1:13:1514:C:C6	2.52	0.44
1:13:737:A:H5'	6:5E:90:VAL:O	2.18	0.44
1:13:741:G:H2'	1:13:742:G:O4'	2.17	0.44
26:14:1000:A:C6	26:14:1001:A:N1	2.85	0.44
26:14:1820:U:H4'	26:14:1821:A:OP2	2.17	0.44
26:14:244:A:H2'	26:14:245:G:O4'	2.18	0.44
26:14:924:C:H2'	26:14:925:C:C6	2.52	0.44
29:19:245:PRO:HG2	29:19:253:GLN:HE21	1.83	0.44
2:1E:194:PRO:O	2:1E:196:LEU:N	2.44	0.44
1:1G:1051:C:H2'	1:1G:1052:U:C6	2.53	0.44
1:1G:373:A:C2	1:1G:374:A:C8	3.05	0.44
1:1G:588:G:H1	1:1G:651:C:N4	2.14	0.44
1:1G:659:U:H2'	1:1G:660:G:O4'	2.16	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1G:784:C:H2'	1:1G:785:G:O4'	2.17	0.44
26:1H:2028:U:H2'	26:1H:2029:G:O4'	2.18	0.44
26:1H:270(G):C:H2'	26:1H:270(H):C:O4'	2.18	0.44
26:1H:370:G:H5''	26:1H:423:A:N6	2.33	0.44
26:1H:937:U:H2'	26:1H:938:G:O4'	2.18	0.44
26:1H:992:C:H2'	26:1H:993:G:H8	1.82	0.44
26:1H:2032:G:N2	30:21:146:THR:HG23	2.20	0.44
30:21:67:PHE:HA	30:21:68:ALA:HA	1.71	0.44
30:21:65:GLY:HA2	30:21:67:PHE:O	2.18	0.44
3:2E:3:ASN:OD1	3:2E:3:ASN:N	2.50	0.44
4:32:31:CYS:CB	4:32:33:MET:H	2.29	0.44
4:3E:10:ARG:HB2	4:3E:10:ARG:HH11	1.82	0.44
12:3I:8:ASN:O	12:3I:12:ARG:HG3	2.18	0.44
24:3K:9:A:O2'	24:3K:46:G:O5'	2.36	0.44
24:3L:67:C:H2'	24:3L:68:G:C8	2.52	0.44
32:41:61:ALA:HB2	32:41:67:LYS:HA	1.98	0.44
32:41:83:ARG:H	32:41:86:MET:CE	2.30	0.44
39:55:86:ARG:HB3	39:55:118:GLU:OE1	2.17	0.44
33:59:31:GLY:O	33:59:79:VAL:HB	2.18	0.44
7:62:146:GLU:OE2	11:2A:54:ARG:NE	2.48	0.44
36:68:22:ILE:HG21	36:68:22:ILE:HD13	1.69	0.44
1:1G:755:G:OP2	15:6A:65:ARG:HD3	2.17	0.44
7:6E:74:GLU:HG2	7:6E:91:VAL:HG13	1.99	0.44
28:71:189:ILE:O	28:71:193:ILE:HD13	2.18	0.44
28:71:49:ILE:HG22	28:71:204:ALA:HB1	2.00	0.44
8:72:19:VAL:CG2	8:72:21:LYS:HB3	2.48	0.44
19:AA:3:ARG:HD2	19:AA:7:LYS:CG	2.44	0.44
41:B8:23:ARG:HG3	41:B8:120:ARG:NH1	2.31	0.44
42:C8:79:PHE:C	42:C8:79:PHE:CD1	2.91	0.44
43:D8:50:PRO:HB2	43:D8:51:VAL:HG12	2.00	0.44
48:E5:72:ARG:HB3	48:E5:75:LEU:HB2	1.99	0.44
26:14:459:U:H4'	55:L5:40:TRP:CZ3	2.52	0.44
2:12:111:ARG:HA	2:12:111:ARG:HD3	1.84	0.44
1:13:183:G:H2'	1:13:184:G:H8	1.82	0.44
1:13:599:C:H2'	1:13:600:C:H6	1.82	0.44
1:13:827:U:C5	1:13:870:U:C4	3.06	0.44
1:13:977:A:H1'	1:13:982:U:O4	2.18	0.44
26:14:1287:A:C5	26:14:1288:U:C4	3.06	0.44
26:14:1915:U:H2'	26:14:1916:A:H5'	1.99	0.44
26:14:1996:C:OP1	36:25:31:LYS:HE2	2.17	0.44
26:14:2353:G:N7	62:14:3712:HOH:O	2.36	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:14:2494:G:H2'	26:14:2495:G:H8	1.82	0.44
26:14:868:U:C2	26:14:869:G:C8	3.05	0.44
26:14:1567:A:O2'	29:19:63:ARG:NH2	2.51	0.44
29:19:68:LYS:HB3	29:19:70:TRP:CZ3	2.53	0.44
2:1E:87:ARG:HH11	2:1E:223:ILE:HD11	1.83	0.44
2:1E:63:MET:HB2	2:1E:225:ALA:HB1	1.98	0.44
1:1G:1119:C:H42	1:1G:1154:G:H1	1.65	0.44
1:1G:1309:G:C6	1:1G:1329:A:N1	2.86	0.44
1:1G:1347:G:N2	1:1G:1373:G:H2'	2.33	0.44
1:1G:511:C:H4'	4:32:43:HIS:CD2	2.52	0.44
1:1G:547:A:OP2	4:32:2:GLY:N	2.51	0.44
1:1G:652:U:O2'	1:1G:653:A:N3	2.46	0.44
1:1G:652:U:O2'	1:1G:653:A:O5'	2.35	0.44
1:1G:748:C:O5'	1:1G:748:C:H6	2.01	0.44
1:1G:836:G:C6	1:1G:851:G:C6	3.05	0.44
26:1H:1408:C:C2	26:1H:1595:G:N2	2.86	0.44
26:1H:1900:A:N1	26:1H:1970:A:C6	2.86	0.44
26:1H:2331:G:H4'	48:I8:42:GLY:HA3	1.98	0.44
26:1H:713:G:H2'	26:1H:714:U:C6	2.53	0.44
26:1H:828:U:H4'	26:1H:831:G:N1	2.32	0.44
31:31:29:ASN:N	31:31:112:MET:HE1	2.30	0.44
31:31:119:ARG:HB3	31:31:119:ARG:CZ	2.46	0.44
37:35:55:ARG:HG2	37:35:56:SER:H	1.82	0.44
31:39:41:LEU:O	31:39:44:ARG:HG2	2.16	0.44
24:3K:38:A:H2'	24:3K:39:U:O4'	2.18	0.44
32:41:107:LEU:HD11	32:41:178:PHE:CE1	2.53	0.44
35:58:95:PRO:O	35:58:96:GLU:CD	2.56	0.44
33:59:10:PRO:HD2	33:59:50:VAL:O	2.17	0.44
10:1I:49:VAL:CG2	14:5I:41:ARG:HB2	2.46	0.44
8:72:17:THR:HG23	8:72:65:TYR:CE2	2.52	0.44
9:82:5:TYR:HE1	9:82:16:ARG:HG2	1.83	0.44
41:B8:108:ARG:HA	41:B8:111:ARG:CZ	2.48	0.44
1:1G:1454:G:H5''	20:BA:35:THR:HG21	2.00	0.44
20:BI:25:ARG:O	20:BI:29:LYS:HG3	2.17	0.44
50:K8:42:GLY:C	50:K8:44:LEU:N	2.70	0.44
55:P8:5:TRP:NE1	55:P8:7:PRO:HG3	2.33	0.44
37:78:62:LEU:O	56:Q8:13:ARG:HD3	2.17	0.44
1:13:1064:G:H4'	1:13:1065:U:OP1	2.17	0.44
1:13:20:U:H2'	1:13:21:G:O4'	2.18	0.44
1:13:22:G:H2'	1:13:23:C:C6	2.53	0.44
1:13:624:C:H4'	16:7I:11:SER:N	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:13:857:C:H2'	1:13:858:G:O4'	2.18	0.44
26:14:1536:A:C8	26:14:1537:C:H1'	2.53	0.44
26:14:1669:A:H5''	26:14:1670:C:OP2	2.18	0.44
26:14:19:C:H2'	26:14:20:C:H6	1.83	0.44
26:14:2138:C:H42	26:14:2153:G:H22	1.65	0.44
26:14:2064:C:H1'	26:14:2450:A:C2	2.53	0.44
26:14:24:G:H2'	26:14:25:U:O4'	2.17	0.44
26:14:873:G:C2	26:14:905:U:O2	2.71	0.44
29:19:34:VAL:C	29:19:35:LYS:HE2	2.39	0.44
21:1B:5:ASP:O	21:1B:11:GLY:HA3	2.17	0.44
2:1E:28:PHE:CD2	2:1E:190:THR:HA	2.53	0.44
2:1E:87:ARG:NH1	2:1E:223:ILE:HD11	2.33	0.44
1:1G:1277:C:O2'	1:1G:1279:A:H1'	2.18	0.44
1:1G:1399:C:C2	1:1G:1502:A:N6	2.86	0.44
1:1G:513:C:H42	1:1G:538:G:H1	1.66	0.44
1:1G:713:G:H2'	1:1G:714:G:C8	2.53	0.44
1:1G:722:A:H5''	1:1G:723:U:OP2	2.17	0.44
1:1G:865:A:H8	1:1G:865:A:O5'	1.99	0.44
26:1H:1000:A:H62	26:1H:1154:G:H2'	1.83	0.44
26:1H:1446:C:H2'	26:1H:1447:G:C8	2.53	0.44
26:1H:1729:A:C8	26:1H:1731:G:C8	3.05	0.44
26:1H:1786:A:H1'	26:1H:1938:A:N6	2.33	0.44
26:1H:382:G:H5''	26:1H:383:U:OP2	2.17	0.44
26:1H:978:G:C2	26:1H:986:C:C2	3.06	0.44
10:1I:77:PRO:HG2	10:1I:79:ARG:HH12	1.82	0.44
4:32:19:LEU:HB2	4:32:21:LEU:HD22	2.00	0.44
4:32:31:CYS:HB2	4:32:35:ARG:HH12	1.82	0.44
37:35:46:LYS:HE2	37:35:46:LYS:HB3	1.62	0.44
4:3E:22:LYS:HB2	4:3E:26:CYS:SG	2.57	0.44
12:3I:123:LYS:H	12:3I:123:LYS:HG2	1.65	0.44
24:3K:35:U:H2'	24:3K:36:U:H6	1.82	0.44
32:41:27:ASN:HB3	32:41:30:GLU:HG3	1.99	0.44
32:41:83:ARG:H	32:41:86:MET:HE1	1.82	0.44
33:59:81:GLU:HG3	33:59:83:TYR:HB2	1.98	0.44
36:68:4:PRO:O	36:68:5:GLN:HB2	2.18	0.44
8:72:41:ARG:HE	8:72:41:ARG:HB2	1.27	0.44
41:75:54:ARG:HG3	41:75:59:THR:CG2	2.47	0.44
16:7I:3:LYS:O	16:7I:21:VAL:HA	2.17	0.44
16:7I:74:LEU:HA	16:7I:77:ALA:HB2	1.99	0.44
42:85:43:GLY:HA3	43:95:73:SER:OG	2.18	0.44
42:C8:30:LYS:HD3	42:C8:30:LYS:HA	1.85	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:E8:17:VAL:HG13	44:E8:76:VAL:HG11	1.99	0.44
49:J8:87:PRO:HA	49:J8:90:ILE:HD12	1.99	0.44
29:11:126:GLN:HG2	29:11:127:VAL:H	1.83	0.44
2:12:145:LEU:O	2:12:149:LEU:HB2	2.18	0.44
2:12:36:ARG:N	2:12:38:GLY:O	2.50	0.44
1:13:1342:C:H2'	1:13:1343:G:C8	2.53	0.44
1:13:192:U:C1'	20:BI:103:GLY:HA2	2.47	0.44
1:13:34:C:H2'	1:13:35:G:C8	2.53	0.44
26:14:1115:G:H2'	26:14:1116:C:C6	2.53	0.44
26:14:1163:G:H2'	26:14:1164:G:H8	1.82	0.44
26:14:1260:G:H2'	26:14:1261:C:C6	2.53	0.44
26:14:1659:U:C4	26:14:1660:C:C5	3.05	0.44
26:14:2115:G:H1'	26:14:2171:A:H61	1.82	0.44
26:14:2394:C:C2'	26:14:2395:C:H5'	2.48	0.44
26:14:270(M):U:H4'	26:14:270(N):G:O5'	2.18	0.44
26:14:442:G:C6	26:14:444:C:N4	2.86	0.44
26:14:259:G:N2	26:14:621:A:H8	2.07	0.44
26:14:634:C:H2'	26:14:635:C:H6	1.82	0.44
26:14:736:C:H5''	62:14:3926:HOH:O	2.17	0.44
26:14:868:U:N3	26:14:869:G:N7	2.65	0.44
35:15:120:LEU:HG	35:15:122:VAL:HG23	1.98	0.44
29:19:6:PHE:HE1	29:19:18:VAL:HG23	1.82	0.44
1:1G:1013:G:O2'	1:1G:1014:A:N7	2.35	0.44
1:1G:1109:C:H2'	1:1G:1110:A:O4'	2.18	0.44
1:1G:129(A):G:O2'	1:1G:189:U:OP1	2.24	0.44
1:1G:373:A:N3	1:1G:374:A:C8	2.86	0.44
1:1G:434:U:H2'	1:1G:435:C:C6	2.53	0.44
1:1G:440:A:H3'	1:1G:442:C:C6	2.53	0.44
1:1G:516:U:O2'	1:1G:519:C:N3	2.51	0.44
1:1G:573:A:H5'	1:1G:573:A:H8	1.83	0.44
26:1H:1055:G:H1	26:1H:1104:C:N4	2.10	0.44
26:1H:1425:G:H2'	26:1H:1426:G:O4'	2.17	0.44
26:1H:1482:U:O4	26:1H:1510:A:H1'	2.17	0.44
26:1H:1590:U:H2'	26:1H:1591:G:H8	1.82	0.44
26:1H:1675:C:H2'	26:1H:1676:A:O4'	2.18	0.44
26:1H:1858:G:HO2'	26:1H:1859:A:P	2.41	0.44
26:1H:2111:C:C4	26:1H:2145:C:C2	3.06	0.44
26:1H:2135:A:C6	26:1H:2136:C:C2	3.06	0.44
26:1H:484:C:H2'	26:1H:485:C:C6	2.53	0.44
26:1H:784:A:O4'	29:11:227:ASN:ND2	2.51	0.44
23:2K:20:G:OP1	23:2K:61:U:N3	2.48	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:13:1060:C:OP1	14:5I:45:ARG:NH2	2.50	0.44
34:61:40:THR:O	34:61:44:LEU:HB2	2.17	0.44
40:65:95:HIS:N	40:65:99:LYS:HB2	2.33	0.44
28:71:194:ARG:NH2	28:71:226:PRO:O	2.47	0.44
8:72:19:VAL:HG23	8:72:21:LYS:HB3	2.00	0.44
16:7I:12:LYS:C	16:7I:14:ASN:H	2.21	0.44
40:A8:7:TYR:HA	40:A8:10:ARG:NH2	2.32	0.44
19:AI:37:ARG:HG3	19:AI:37:ARG:H	1.35	0.44
47:D5:139:VAL:HG21	47:D5:155:LEU:HD22	2.00	0.44
47:D5:24:LEU:HD12	47:D5:25:PRO:O	2.18	0.44
42:C8:92:ARG:NE	43:D8:11:GLN:H	2.16	0.44
26:1H:2396:G:H5''	49:J8:25:LYS:NZ	2.33	0.44
26:1H:1693:U:O2'	29:11:14:ARG:NH2	2.51	0.44
2:12:27:LYS:HE3	2:12:194:PRO:HD2	2.00	0.44
1:13:1144:G:H21	1:13:1146:A:H62	1.64	0.44
1:13:141:A:H2'	1:13:142:G:C8	2.51	0.44
1:13:516:U:C4	1:13:517:G:C6	3.06	0.44
26:14:150:C:H2'	26:14:151:C:C6	2.53	0.44
26:14:196:A:OP2	37:35:46:LYS:NZ	2.50	0.44
26:14:2165:G:H3'	26:14:2166:G:H5'	2.00	0.44
26:14:2354:G:O2'	48:E5:36:ILE:HG23	2.18	0.44
26:14:2543:G:H2'	26:14:2544:G:C8	2.53	0.44
26:14:747:U:O2	26:14:2014:A:H1'	2.17	0.44
26:14:877:U:O4	26:14:899:A:N6	2.51	0.44
26:14:947:G:H2'	26:14:948:G:C8	2.52	0.44
29:19:245:PRO:HA	29:19:246:PRO:HD3	1.92	0.44
26:14:1797:C:O2'	29:19:259:THR:OG1	2.28	0.44
2:1E:125:PRO:HA	2:1E:127:ILE:HG12	2.00	0.44
1:1G:135:C:C2	16:7A:1:MET:HB3	2.52	0.44
1:1G:1251:A:HO2'	1:1G:1369:C:HO2'	1.63	0.44
1:1G:1378:C:H3'	1:1G:1379:G:H5''	2.00	0.44
1:1G:1404:C:H2'	1:1G:1405:G:C8	2.53	0.44
1:1G:561:U:O2'	1:1G:562:C:OP2	2.35	0.44
1:1G:567:G:H1'	62:1G:1897:HOH:O	2.18	0.44
1:1G:580:U:H2'	1:1G:581:G:O4'	2.17	0.44
1:1G:964:A:N3	1:1G:969:A:O2'	2.41	0.44
26:1H:1639:U:H5''	62:1H:4619:HOH:O	2.17	0.44
26:1H:2134:A:O2'	26:1H:2159:G:N2	2.50	0.44
10:1I:57:LYS:O	10:1I:60:ARG:NH2	2.48	0.44
27:1J:87:G:N2	27:1J:89:G:H3'	2.33	0.44
3:22:180:ALA:O	3:22:181:ASN:HB3	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:22:88:ARG:HA	3:22:91:LEU:HD13	1.98	0.44
24:3L:13:C:H2'	24:3L:14:A:C8	2.53	0.44
38:45:97:VAL:HG21	38:45:103:MET:HE2	2.00	0.44
38:45:114:ALA:O	38:45:118:LEU:HB2	2.18	0.44
38:45:25:ASP:HA	38:45:102:VAL:HG23	2.00	0.44
26:14:2469:A:O2'	38:45:56:ARG:HG2	2.18	0.44
33:51:10:PRO:C	33:51:11:VAL:HG22	2.39	0.44
7:62:15:ASP:OD1	7:62:16:LEU:N	2.51	0.44
7:62:45:ASP:O	7:62:49:ILE:HG13	2.18	0.44
40:65:102:ALA:HA	40:65:105:ALA:HB3	1.99	0.44
28:71:196:LEU:HD12	28:71:196:LEU:HA	1.66	0.44
16:7A:1:MET:HE3	16:7A:1:MET:HB2	1.51	0.44
9:82:111:ARG:HB2	9:82:113:LYS:HE2	1.99	0.44
19:AA:41:VAL:HG23	19:AA:43:GLU:H	1.82	0.44
20:BA:73:HIS:CB	20:BA:74:LYS:HZ2	2.31	0.44
48:E5:43:THR:HG23	48:E5:46:LYS:HE2	2.00	0.44
45:F8:66:LEU:HD22	45:F8:66:LEU:HA	1.80	0.44
47:H8:44:PHE:CE2	47:H8:86:VAL:HG11	2.53	0.44
32:41:101:ILE:HG13	52:M8:25:TYR:O	2.17	0.44
1:13:1095:U:H5'	1:13:1109:C:O2	2.17	0.43
1:13:1256:A:HO2'	1:13:1257:U:P	2.40	0.43
1:13:1505:G:OP1	62:13:1842:HOH:O	2.21	0.43
1:13:67:C:O2'	1:13:171:A:N3	2.45	0.43
1:13:605:U:H2'	1:13:606:G:O4'	2.18	0.43
1:13:652:U:C4	1:13:752:G:N3	2.86	0.43
26:14:108:U:H2'	26:14:109:G:C8	2.53	0.43
26:14:1154:G:P	42:85:58:ARG:HH11	2.41	0.43
26:14:51:G:N3	26:14:119:A:C2	2.86	0.43
26:14:350:U:H2'	26:14:351:G:O4'	2.18	0.43
26:14:452:G:N3	26:14:457:A:H2	2.15	0.43
26:14:493:G:H2'	26:14:494:G:O4'	2.18	0.43
26:14:70:G:H21	26:14:71:A:H62	1.66	0.43
29:19:71:ASP:OD2	29:19:103:ARG:NH2	2.49	0.43
1:1G:1503:A:H1'	25:4L:12:A:H61	1.83	0.43
1:1G:42:G:H2'	1:1G:43:C:O4'	2.17	0.43
26:1H:129:C:H2'	26:1H:130:C:H6	1.83	0.43
26:1H:1515:C:H2'	26:1H:1516:U:H6	1.82	0.43
26:1H:164:U:H5'	26:1H:165:U:OP2	2.18	0.43
26:1H:2058:A:H5''	26:1H:2059:A:OP2	2.18	0.43
26:1H:2211:G:O2'	26:1H:2212:A:P	2.76	0.43
26:1H:2704:C:H2'	26:1H:2705:A:C8	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1H:2771:C:H2'	26:1H:2772:C:C6	2.53	0.43
26:1H:2810:A:H2'	26:1H:2811:G:O4'	2.18	0.43
26:1H:317:G:C2	26:1H:318:C:C2	3.06	0.43
26:1H:53:A:H2'	26:1H:54:G:O4'	2.18	0.43
26:1H:805:G:O5'	37:78:41:ARG:HG2	2.18	0.43
27:1J:48:A:O2'	40:65:95:HIS:HE1	2.01	0.43
27:1J:65:C:H41	27:1J:108:C:C2'	2.31	0.43
30:21:111:ARG:HG2	30:21:111:ARG:H	1.58	0.43
30:21:32:PRO:HD2	30:21:50:GLY:O	2.17	0.43
3:22:181:ASN:ND2	3:22:204:LEU:HB2	2.33	0.43
4:32:13:ARG:HG2	4:32:13:ARG:H	1.53	0.43
4:3E:85:LYS:CE	4:3E:89:THR:HA	2.46	0.43
5:42:118:ILE:HG12	5:42:119:LEU:H	1.82	0.43
5:42:60:TYR:HB3	5:42:64:ARG:NH2	2.33	0.43
38:45:57:HIS:CG	38:45:117:ALA:HB2	2.52	0.43
5:4E:100:VAL:HG22	5:4E:115:VAL:HG12	2.00	0.43
6:52:15:ASP:O	6:52:19:LEU:HB2	2.17	0.43
33:59:11:VAL:HB	33:59:13:LYS:HD2	2.00	0.43
8:72:82:HIS:HE1	8:72:136:GLU:HG3	1.83	0.43
41:75:54:ARG:HA	41:75:59:THR:HB	2.00	0.43
37:78:39:LYS:HB2	37:78:45:LEU:HD21	1.99	0.43
9:8E:22:GLY:N	9:8E:58:HIS:O	2.37	0.43
40:A8:110:LEU:O	40:A8:111:GLU:HB2	2.17	0.43
40:A8:88:ASP:O	40:A8:89:ARG:HB3	2.17	0.43
19:AI:65:ASN:OD1	19:AI:65:ASN:N	2.51	0.43
20:BI:16:HIS:O	20:BI:19:SER:HB2	2.18	0.43
44:E8:64:MET:HE3	44:E8:64:MET:HB3	1.83	0.43
1:13:1022:G:H2'	1:13:1023:G:C8	2.54	0.43
1:13:1132:C:H2'	1:13:1133:G:H8	1.82	0.43
1:13:706:A:N3	11:2I:31:THR:HG21	2.33	0.43
1:13:721:G:C6	1:13:733:A:C2	3.07	0.43
26:14:151:C:H2'	26:14:152:G:C8	2.54	0.43
26:14:1839:G:N3	26:14:1839:G:H2'	2.33	0.43
26:14:2299:G:N1	26:14:2318:G:C8	2.86	0.43
26:14:2657:A:O3'	33:59:160:LYS:NZ	2.48	0.43
26:14:2862:G:H2'	26:14:2863:C:C6	2.53	0.43
1:1G:1391:U:H2'	1:1G:1392:G:C8	2.54	0.43
1:1G:1478:C:H2'	1:1G:1479:C:C6	2.52	0.43
1:1G:265:G:H5'	17:8A:64:PRO:O	2.18	0.43
1:1G:536:C:H2'	1:1G:537:G:C8	2.54	0.43
1:1G:980:C:H5'	1:1G:981:U:C5	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1H:1131:G:O6	26:1H:2040:C:H1'	2.18	0.43
26:1H:1226:G:OP1	43:D8:69:LYS:NZ	2.31	0.43
26:1H:1296:G:OP1	26:1H:2709:G:O2'	2.30	0.43
26:1H:1337:G:C4	26:1H:1338:G:C8	3.07	0.43
26:1H:1538:G:H2'	26:1H:1539:G:C8	2.52	0.43
26:1H:2062:A:C2'	26:1H:2062:A:N3	2.80	0.43
1:1G:1191:A:H5''	3:22:4:LYS:NZ	2.33	0.43
1:1G:676:A:H1'	11:2A:115:PRO:HB3	1.99	0.43
4:32:15:GLU:HG2	4:32:66:ARG:HH11	1.83	0.43
4:3E:165:MET:O	4:3E:168:ARG:HD2	2.18	0.43
4:3E:93:PHE:HA	4:3E:96:LEU:HD22	2.00	0.43
24:3L:15:G:H1	24:3L:48:C:N4	2.16	0.43
32:41:145:THR:HG1	32:41:148:MET:CG	2.31	0.43
32:49:39:ILE:HG23	32:49:157:ILE:HG23	2.00	0.43
13:4A:81:LEU:HD13	13:4A:81:LEU:HA	1.69	0.43
3:2E:6:HIS:CD2	14:5I:49:HIS:HB3	2.52	0.43
7:62:116:ALA:HA	7:62:119:ARG:NE	2.33	0.43
40:65:29:PHE:CD1	40:65:30:ARG:N	2.81	0.43
40:65:49:VAL:HG22	40:65:80:LEU:HD12	2.01	0.43
36:68:98:VAL:HG11	36:68:114:ILE:HG23	2.00	0.43
8:72:29:SER:HB3	8:72:32:LYS:CG	2.45	0.43
41:75:5:ALA:N	41:75:6:LEU:CA	2.81	0.43
41:75:62:THR:HG22	41:75:75:ILE:HG12	1.99	0.43
37:78:18:ARG:HA	37:78:18:ARG:HD2	1.71	0.43
20:BA:74:LYS:HG3	20:BA:75:ASN:H	1.83	0.43
46:G8:4:LYS:HD3	46:G8:4:LYS:HA	1.71	0.43
46:G8:41:GLY:HA2	46:G8:64:GLU:OE1	2.18	0.43
27:16:75:G:H21	47:H8:85:HIS:HE1	1.64	0.43
26:1H:2336:A:N6	48:I8:43:THR:HB	2.29	0.43
56:M5:37:SER:OG	56:M5:39:LYS:O	2.32	0.43
1:13:192:U:H1'	20:BI:103:GLY:HA2	1.99	0.43
1:13:343:U:H2'	1:13:344:A:H5''	2.01	0.43
26:14:1176:G:H8	26:14:1177:A:H2	1.66	0.43
26:14:1259:G:H2'	26:14:1260:G:H8	1.83	0.43
26:14:2146:C:H4'	26:14:2147:G:C8	2.53	0.43
26:14:322:A:H3'	31:39:169:ASN:OD1	2.18	0.43
26:14:606:U:H4'	26:14:658:C:H4'	2.00	0.43
26:14:685:A:H1'	26:14:688:U:O4	2.18	0.43
26:14:740:U:H2'	26:14:741:G:C8	2.53	0.43
29:19:70:TRP:O	29:19:73:VAL:HG23	2.18	0.43
2:1E:16:HIS:CE1	2:1E:210:SER:O	2.71	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1E:7:VAL:HG21	2:1E:217:ARG:HH11	1.84	0.43
1:1G:34:C:H2'	1:1G:35:G:C8	2.53	0.43
1:1G:64:G:H4'	1:1G:65:U:O5'	2.17	0.43
1:1G:66:G:C2	1:1G:67:C:C6	3.06	0.43
1:1G:965:A:C2	1:1G:969:A:C2	3.06	0.43
26:1H:1266:G:O2'	26:1H:2012:G:O6	2.28	0.43
26:1H:2345:G:H4'	26:1H:2346:A:O5'	2.17	0.43
26:1H:2663:G:C6	26:1H:2664:G:C4	3.07	0.43
26:1H:654(A):A:C2	26:1H:654(T):A:N1	2.85	0.43
9:8E:115:GLY:HA2	10:1I:58:ASP:OD2	2.17	0.43
22:1K:17:U:H4'	22:1K:60:U:C4	2.53	0.43
30:21:50:GLY:HA2	30:21:77:ILE:O	2.18	0.43
3:22:32:LEU:HB3	3:22:59:ARG:HH12	1.83	0.43
3:2E:16:ARG:HB2	3:2E:16:ARG:HH11	1.84	0.43
11:2I:78:GLN:O	11:2I:103:LEU:HA	2.18	0.43
32:49:109:VAL:HG12	32:49:142:PRO:HG3	2.01	0.43
35:58:94:HIS:C	35:58:95:PRO:O	2.56	0.43
14:5A:21:TYR:HE1	14:5A:23:ARG:HB2	1.83	0.43
1:1G:994:A:C2	14:5A:5:ALA:HB2	2.53	0.43
34:61:50:ARG:HA	34:61:50:ARG:HD3	1.40	0.43
16:7I:49:LEU:HD22	16:7I:73:LEU:HD22	2.01	0.43
38:88:75:THR:HG22	38:88:89:ASN:C	2.38	0.43
17:8I:48:GLU:O	17:8I:50:LYS:HG2	2.18	0.43
43:95:43:GLU:HA	43:95:44:LYS:HA	1.81	0.43
40:A8:110:LEU:HB3	40:A8:111:GLU:H	1.66	0.43
1:13:1320:C:N4	19:AI:36:ARG:HG3	2.33	0.43
47:D5:43:GLU:O	47:D5:47:VAL:HG23	2.18	0.43
44:E8:6:ILE:HA	44:E8:103:ILE:O	2.18	0.43
46:G8:81:LYS:HB2	46:G8:99:CYS:SG	2.58	0.43
26:1H:2361:A:O5'	56:Q8:27:THR:OG1	2.36	0.43
29:11:11:PRO:O	29:11:12:SER:OG	2.33	0.43
29:11:67:PHE:HB3	29:11:153:ALA:H	1.83	0.43
29:11:232:PRO:HB3	29:11:244:ARG:CZ	2.48	0.43
2:12:171:ALA:HA	2:12:174:VAL:HG23	2.01	0.43
2:12:19:HIS:CE1	2:12:206:ASP:HB2	2.54	0.43
1:13:103:C:C2	1:13:104:G:C8	3.07	0.43
1:13:875:C:O2'	8:7E:14:ARG:NH1	2.50	0.43
26:14:1025:G:C4	26:14:1135:C:H1'	2.54	0.43
26:14:1142:U:O2	26:14:1142:U:H2'	2.18	0.43
26:14:565:C:H4'	26:14:1253:A:C6	2.53	0.43
26:14:2290:G:O2'	26:14:2381:C:H1'	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:14:2494:G:C4	26:14:2495:G:C8	3.06	0.43
1:1G:973:G:C1'	10:1A:55:LYS:HG2	2.48	0.43
1:1G:1007:C:H1'	1:1G:1023:G:H1	1.81	0.43
1:1G:1017:G:H2'	1:1G:1018:C:O4'	2.19	0.43
1:1G:1149:C:H2'	1:1G:1150:U:O4'	2.19	0.43
1:1G:429:U:H1'	1:1G:430:A:H5''	2.01	0.43
1:1G:560:U:H4'	1:1G:561:U:O5'	2.17	0.43
1:1G:744:C:O2'	1:1G:851:G:N2	2.50	0.43
1:1G:825:G:O2'	8:72:12:ARG:NH1	2.51	0.43
1:1G:927:G:N2	1:1G:1391:U:H1'	2.33	0.43
26:1H:1062:G:H2'	26:1H:1063:G:O4'	2.19	0.43
26:1H:2078:C:H2'	26:1H:2079:U:O4'	2.19	0.43
26:1H:2164:C:H41	26:1H:2165:G:N2	2.15	0.43
26:1H:273(D):C:H2'	26:1H:273(E):U:C6	2.53	0.43
26:1H:389:G:H8	26:1H:389:G:O5'	2.01	0.43
26:1H:644:A:H4'	26:1H:645:C:C5	2.53	0.43
27:1J:19:G:H2'	27:1J:20:C:O4'	2.18	0.43
22:1K:66:A:H5''	22:1K:67:C:C5	2.54	0.43
30:21:64:LYS:HD2	30:21:65:GLY:HA2	2.00	0.43
30:29:81:ILE:HG21	30:29:84:PHE:HD2	1.84	0.43
3:2E:175:LEU:HD21	3:2E:201:TYR:HE2	1.82	0.43
23:2K:33:OMC:HM22	23:2K:34:U:H5'	2.00	0.43
31:31:123:LEU:HD12	31:31:124:LEU:H	1.83	0.43
12:3A:32:PHE:HD1	12:3A:86:ARG:HA	1.84	0.43
1:1G:19:C:H5''	5:42:86:ALA:HB3	2.00	0.43
32:49:33:ARG:HE	32:49:33:ARG:HB2	1.54	0.43
13:4A:62:ASN:N	13:4A:62:ASN:OD1	2.52	0.43
13:4A:77:ASN:O	13:4A:81:LEU:HD23	2.18	0.43
26:14:2880:C:H1'	39:55:92:GLY:HA3	2.00	0.43
14:5I:3:ARG:HD3	14:5I:3:ARG:O	2.19	0.43
40:65:46:VAL:HG12	40:65:48:LEU:HD12	1.99	0.43
40:65:18:ILE:HD13	40:65:87:PHE:O	2.19	0.43
34:69:76:THR:HA	34:69:105:HIS:NE2	2.34	0.43
15:6I:26:GLU:H	15:6I:26:GLU:HG2	1.44	0.43
1:13:660:G:OP1	15:6I:5:LYS:HD3	2.18	0.43
8:7E:121:ASP:OD1	8:7E:121:ASP:N	2.48	0.43
1:13:1130:A:O2'	9:8E:3:GLN:OE1	2.22	0.43
47:D5:8:TYR:HA	47:D5:62:PRO:CD	2.48	0.43
45:F8:36:LYS:HE2	45:F8:54:VAL:O	2.18	0.43
50:K8:64:LEU:O	50:K8:68:ARG:HG3	2.18	0.43
26:1H:1158:C:H4'	51:L8:32:GLN:HB2	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:M5:50:LEU:HA	56:M5:50:LEU:HD12	1.52	0.43
2:12:49:GLU:O	2:12:52:GLU:HG3	2.18	0.43
2:12:98:LEU:HD23	2:12:98:LEU:HA	1.66	0.43
1:13:1228:C:H2'	1:13:1229:A:H8	1.83	0.43
1:13:38:G:C2	1:13:397:A:C2	3.06	0.43
1:13:433:C:H2'	1:13:434:U:C6	2.53	0.43
1:13:926:G:H5'	1:13:927:G:O5'	2.17	0.43
26:14:125:G:H1'	55:L5:13:ALA:HB1	2.01	0.43
26:14:1460:A:H3'	26:14:1461:G:H5'	2.00	0.43
26:14:162:U:H4'	26:14:171:G:C4	2.52	0.43
26:14:1653:G:C6	39:55:9:LYS:HB3	2.53	0.43
26:14:1894:C:O2'	26:14:1895:C:H5'	2.19	0.43
26:14:2175:C:N4	26:14:2176:A:N7	2.66	0.43
26:14:648:G:O2'	26:14:2351:G:OP1	2.30	0.43
26:14:738:G:H3'	26:14:739:G:C8	2.53	0.43
26:14:818:G:C2	26:14:1190:G:O6	2.70	0.43
26:14:932:G:H4'	26:14:933:A:O5'	2.19	0.43
35:15:96:GLU:OE1	35:15:96:GLU:N	2.37	0.43
21:1B:12:LYS:HB3	21:1B:17:THR:O	2.18	0.43
1:1G:1372:U:H2'	1:1G:1373:G:O4'	2.19	0.43
1:1G:1497:G:C2'	1:1G:1498:U:H5'	2.49	0.43
1:1G:562:C:H4'	1:1G:563:A:O5'	2.18	0.43
26:1H:1059:G:H1	26:1H:1088:A:H8	1.67	0.43
26:1H:1498:C:O4'	26:1H:1577:C:H4'	2.18	0.43
26:1H:2259:G:C2	26:1H:2282:G:N1	2.87	0.43
26:1H:2272:U:H5''	26:1H:2273:A:OP1	2.17	0.43
26:1H:2287:A:N1	26:1H:2346:A:C2	2.87	0.43
26:1H:528:A:C2	26:1H:2043:C:H4'	2.53	0.43
26:1H:600:G:H2'	26:1H:601:C:C6	2.54	0.43
26:1H:757:U:H2'	26:1H:758:C:O4'	2.18	0.43
30:21:47:VAL:O	30:21:80:GLU:HA	2.18	0.43
3:22:9:GLY:HA2	3:22:12:LEU:HG	2.00	0.43
36:25:1:MET:O	36:25:2:ILE:HD13	2.19	0.43
11:2A:109:VAL:HG13	18:9A:86:VAL:HG22	2.00	0.43
3:2E:178:LEU:HD13	3:2E:178:LEU:HA	1.78	0.43
24:3K:13:C:H42	24:3K:22:G:N2	2.17	0.43
38:45:102:VAL:O	38:45:102:VAL:HG12	2.19	0.43
32:49:136:ARG:H	32:49:136:ARG:HG3	1.57	0.43
5:4E:35:GLY:HA3	5:4E:112:LEU:HB3	1.99	0.43
1:1G:1202:G:O2'	14:5A:27:CYS:HB2	2.18	0.43
7:62:63:LYS:O	7:62:67:GLU:N	2.47	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:68:60:ALA:HB1	36:68:84:ALA:HB1	2.01	0.43
7:6E:15:ASP:OD2	7:6E:18:TYR:N	2.48	0.43
15:6I:69:TYR:CE1	15:6I:73:GLU:HG3	2.53	0.43
9:82:118:LYS:HG2	9:82:118:LYS:O	2.19	0.43
42:85:100:VAL:O	42:85:101:ARG:HG2	2.18	0.43
41:B8:4:GLY:HA2	41:B8:7:ILE:CG1	2.46	0.43
20:BA:84:LEU:HD23	20:BA:84:LEU:HA	1.85	0.43
20:BI:57:ARG:NH2	20:BI:100:ILE:HD13	2.33	0.43
20:BI:36:LEU:HD12	20:BI:55:ILE:HD12	2.01	0.43
42:C8:50:ARG:HH22	43:D8:72:VAL:HG22	1.83	0.43
47:D5:99:TYR:HA	47:D5:124:ILE:O	2.18	0.43
44:E8:57:ASN:O	44:E8:61:ASN:HB2	2.17	0.43
49:F5:84:GLY:CA	49:F5:85:LEU:HB3	2.49	0.43
50:G5:18:PRO:HB2	50:G5:68:ARG:NH2	2.34	0.43
26:1H:2079:U:O3'	49:J8:35:THR:HB	2.18	0.43
52:M8:60:GLN:HG3	52:M8:61:ARG:NH1	2.33	0.43
53:N8:42:PRO:HB2	53:N8:43:HIS:ND1	2.33	0.43
2:12:54:THR:HA	2:12:57:PHE:CD2	2.53	0.43
1:13:1320:C:H42	19:AI:36:ARG:HG3	1.83	0.43
1:13:942:G:C2	1:13:1342:C:C2	3.06	0.43
1:13:256:U:H2'	1:13:257:G:H8	1.81	0.43
1:13:49:U:C2	1:13:361:G:N2	2.87	0.43
26:14:1716:U:H2'	26:14:1717:G:H8	1.82	0.43
26:14:1885:A:H3'	26:14:1886:C:C6	2.54	0.43
26:14:2129:C:H5''	26:14:2130:U:H5	1.84	0.43
26:14:2129:C:H5'	26:14:2130:U:OP2	2.19	0.43
26:14:2197:U:H1'	26:14:2198:A:C8	2.53	0.43
26:14:2255:G:C6	26:14:2256:G:C5	3.06	0.43
26:14:2461:C:H2'	26:14:2462:U:H6	1.84	0.43
26:14:2552:U:H2'	26:14:2554:U:H5''	2.00	0.43
26:14:2781:A:H5''	26:14:2782:G:H5'	1.99	0.43
26:14:433:C:C4	26:14:434:U:O4	2.72	0.43
35:15:91:LEU:O	35:15:95:PRO:HB3	2.19	0.43
29:19:134:ARG:NH1	29:19:188:GLU:OE2	2.46	0.43
2:1E:187:LEU:HD23	2:1E:201:ILE:HG22	2.01	0.43
1:1G:241:C:H42	1:1G:285:G:H1	1.67	0.43
1:1G:973:G:H5''	1:1G:974:A:C5'	2.48	0.43
26:1H:130:C:O3'	26:1H:1349:A:H1'	2.19	0.43
26:1H:1465:G:C4	26:1H:1466:G:C8	3.05	0.43
26:1H:1825:A:H2'	26:1H:1826:G:C8	2.53	0.43
26:1H:189:G:H2'	26:1H:205:G:N2	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1H:2171:A:O2'	26:1H:2172:U:O5'	2.36	0.43
26:1H:654(O):G:H5''	26:1H:654(P):G:C2	2.54	0.43
26:1H:900:A:H3'	26:1H:901:A:C8	2.49	0.43
24:1L:68:G:N3	24:1L:69:A:N6	2.66	0.43
30:21:101:ARG:HB3	30:21:201:THR:OG1	2.18	0.43
30:21:37:ARG:HD2	30:21:42:ASP:CG	2.39	0.43
30:29:202:LYS:N	30:29:202:LYS:HD2	2.34	0.43
11:2A:59:TYR:O	11:2A:62:GLN:HB3	2.18	0.43
3:2E:43:LEU:O	3:2E:47:LEU:HB2	2.18	0.43
3:2E:50:ALA:HB2	3:2E:75:VAL:HB	2.01	0.43
23:2K:65:G:H2'	23:2K:66:C:O4'	2.18	0.43
4:32:57:ARG:NH2	4:32:205:GLU:OE1	2.51	0.43
32:41:173:LEU:HD13	32:41:173:LEU:HA	1.82	0.43
32:41:66:GLN:OE1	32:41:98:ARG:NH1	2.51	0.43
32:49:88:ILE:HD12	32:49:88:ILE:HA	1.82	0.43
13:4A:67:GLU:HG3	13:4A:68:GLY:H	1.83	0.43
6:52:23:LYS:HB3	6:52:23:LYS:HE2	1.76	0.43
35:58:67:LEU:HA	35:58:87:LEU:HD13	2.01	0.43
40:65:89:ARG:O	40:65:90:GLY:C	2.57	0.43
34:69:51:ILE:HD13	34:69:51:ILE:HA	1.90	0.43
1:1G:742:G:P	15:6A:35:ARG:HH22	2.41	0.43
7:6E:104:LEU:HD13	7:6E:104:LEU:HA	1.80	0.43
8:7E:86:ILE:HG12	8:7E:135:CYS:HA	2.00	0.43
8:7E:45:ILE:HD12	8:7E:47:GLY:HA2	1.99	0.43
42:85:74:LEU:HD11	42:85:110:VAL:HG13	1.99	0.43
42:C8:14:HIS:O	42:C8:18:LEU:HD12	2.18	0.43
42:C8:58:ARG:HH11	42:C8:93:LYS:HE2	1.84	0.43
47:D5:15:PRO:HB2	47:D5:19:ARG:NH2	2.33	0.43
47:D5:52:SER:O	47:D5:54:HIS:N	2.51	0.43
48:E5:11:ARG:HB2	48:E5:11:ARG:HE	1.68	0.43
48:I8:45:PHE:O	48:I8:59:LEU:HD11	2.18	0.43
40:A8:20:ARG:NH2	48:I8:51:VAL:O	2.52	0.43
49:J8:87:PRO:HB2	49:J8:91:LYS:HZ3	1.83	0.43
54:O8:19:ARG:HG3	54:O8:21:TYR:CE1	2.47	0.43
29:11:120:GLY:O	29:11:123:ALA:HB3	2.19	0.43
2:12:220:ASP:H	2:12:222:ILE:HG13	1.83	0.43
1:13:1120:G:H2'	1:13:1121:U:H6	1.83	0.43
1:13:1124:G:O2'	1:13:1145:C:C4	2.71	0.43
1:13:198:G:C2	1:13:199:G:C8	3.07	0.43
1:13:266:G:H5''	1:13:267:C:H5	1.83	0.43
1:13:428:G:O4'	1:13:430:A:C8	2.72	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:13:600:C:H2'	1:13:601:C:C6	2.54	0.43
1:13:859:A:H2'	1:13:860:A:O4'	2.19	0.43
1:13:947:G:H2'	1:13:948:C:C6	2.53	0.43
26:14:1420:U:HO2'	26:14:1421:G:P	2.41	0.43
26:14:1677:A:H2'	26:14:1678:G:C8	2.54	0.43
26:14:1885:A:H3'	26:14:1886:C:H6	1.84	0.43
26:14:191:A:N1	62:14:3718:HOH:O	2.36	0.43
26:14:2056:G:C2	26:14:2057:A:C8	3.06	0.43
26:14:2067:G:O2'	26:14:2069:G:H5''	2.19	0.43
26:14:2629:A:H4'	26:14:2630:G:H5'	2.01	0.43
26:14:479:A:N3	26:14:481:G:H5''	2.34	0.43
26:14:630:G:N2	26:14:633:A:OP2	2.45	0.43
26:14:675:A:C4	26:14:804:A:C2	3.07	0.43
26:14:751:A:H5'	44:A5:90:ARG:HA	1.99	0.43
26:14:962:G:H2'	26:14:963:U:C6	2.54	0.43
27:16:24:G:N7	27:16:56:G:H2'	2.33	0.43
29:19:74:GLY:O	29:19:76:PRO:HD3	2.18	0.43
1:1G:109:A:H2'	1:1G:326:G:N2	2.33	0.43
1:1G:1324:A:C4'	1:1G:1362:C:H4'	2.40	0.43
1:1G:1402:C:H2'	1:1G:1403:C:O4'	2.18	0.43
1:1G:1:U:H4'	1:1G:630:G:H21	1.84	0.43
1:1G:519:C:H2'	1:1G:520:A:O4'	2.18	0.43
1:1G:756:C:N4	62:1G:1906:HOH:O	2.52	0.43
26:1H:1101:U:H2'	26:1H:1102:C:C6	2.54	0.43
26:1H:1728:G:C6	26:1H:1730:U:H5''	2.53	0.43
26:1H:2301:C:H2'	26:1H:2302:G:H8	1.84	0.43
26:1H:241:A:H5'	26:1H:243:U:O4'	2.18	0.43
26:1H:2468:G:N3	26:1H:2468:G:O4'	2.51	0.43
26:1H:2801:A:H2'	26:1H:2802:G:H8	1.84	0.43
26:1H:280:C:C2	26:1H:361:G:C2	3.07	0.43
26:1H:500:G:N1	26:1H:503:A:OP2	2.48	0.43
26:1H:906:G:OP1	38:88:26:TYR:OH	2.27	0.43
26:1H:999:U:H5''	26:1H:1154:G:O6	2.19	0.43
27:1J:7:G:H4'	40:65:29:PHE:CE2	2.54	0.43
30:21:38:THR:O	30:21:42:ASP:N	2.52	0.43
30:21:59:VAL:HG22	30:21:60:ASN:H	1.83	0.43
36:25:88:ASN:HB3	36:25:94:ARG:HD3	2.00	0.43
30:29:65:GLY:O	30:29:68:ALA:HB2	2.17	0.43
23:2L:16:C:O2'	23:2L:62:C:OP1	2.29	0.43
31:39:113:ALA:HB1	31:39:186:ILE:HG21	2.01	0.43
1:13:509:A:H5'	4:3E:54:TYR:CD2	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:3L:50:C:H2'	24:3L:51:A:C8	2.51	0.43
24:3L:59:A:N3	24:3L:59:A:H2'	2.32	0.43
32:41:173:LEU:HD12	32:41:178:PHE:CE2	2.54	0.43
39:55:35:THR:HG21	39:55:100:LEU:HD11	1.99	0.43
7:6E:15:ASP:OD1	7:6E:16:LEU:N	2.51	0.43
7:6E:79:ARG:NH2	24:3K:33:U:O2'	2.51	0.43
41:75:51:ARG:HD3	41:75:100:TYR:OH	2.19	0.43
16:7I:37:GLY:HA3	16:7I:50:LYS:O	2.19	0.43
43:95:15:GLU:HG3	43:95:16:PRO:HD2	2.00	0.43
43:95:21:ARG:HB3	43:95:91:TYR:HD2	1.84	0.43
45:B5:24:GLY:O	45:B5:83:VAL:HG12	2.19	0.43
20:BI:55:ILE:HD13	20:BI:55:ILE:HA	1.91	0.43
47:D5:59:LEU:HB2	47:D5:67:LEU:O	2.19	0.43
49:F5:78:LYS:HG2	49:F5:79:GLY:N	2.32	0.43
46:G8:87:LYS:HE3	46:G8:89:PHE:HB3	1.99	0.43
47:H8:69:THR:HA	47:H8:89:PHE:O	2.18	0.43
56:M5:34:TRP:CE3	56:M5:34:TRP:HA	2.54	0.43
1:13:1004:A:H5''	1:13:1024:G:H2'	2.01	0.43
1:13:1117:G:H5''	9:8E:104:ARG:CZ	2.49	0.43
1:13:1126:U:C4	1:13:1127:G:C5	3.07	0.43
1:13:345:C:H41	36:68:116:SER:C	2.17	0.43
1:13:468:A:O2'	16:7I:82:GLN:HG2	2.18	0.43
1:13:64:G:H4'	1:13:65:U:H5'	2.00	0.43
1:13:958:A:C6	1:13:959:A:N1	2.87	0.43
26:14:128:C:H3'	26:14:128:C:C6	2.54	0.43
26:14:1471:A:C2	26:14:1472:A:C4	3.07	0.43
26:14:1753:G:N1	26:14:1756:G:C2	2.86	0.43
26:14:118:A:N3	26:14:178:G:H1'	2.33	0.43
26:14:184:C:H2'	26:14:185:U:C6	2.53	0.43
26:14:629:G:H5''	26:14:650:C:O2'	2.19	0.43
26:14:828:U:C5	26:14:2247:A:H4'	2.54	0.43
1:1G:1016:A:O2'	1:1G:1217:C:O2'	2.34	0.43
1:1G:1084:G:H2'	1:1G:1085:U:C6	2.54	0.43
1:1G:983:A:N3	1:1G:983:A:H3'	2.33	0.43
26:1H:2064:C:H1'	26:1H:2450:A:C2	2.53	0.43
26:1H:2086:U:H2'	26:1H:2087:G:C8	2.54	0.43
26:1H:2309:A:N6	26:1H:2310:A:N6	2.67	0.43
26:1H:2327:A:H2'	26:1H:2328:A:H8	1.81	0.43
26:1H:270(I):G:C2	26:1H:270(R):G:C2	3.06	0.43
26:1H:2820:A:O2'	26:1H:2821:A:OP1	2.31	0.43
26:1H:442:G:C4	26:1H:444:C:C5	3.06	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:22:135:LYS:NZ	3:22:139:GLN:HB2	2.34	0.43
3:2E:15:THR:HG22	3:2E:16:ARG:H	1.84	0.43
31:39:160:ASN:HB3	31:39:163:VAL:HB	2.00	0.43
1:13:542:G:H5'	4:3E:41:GLY:HA3	2.01	0.43
32:41:11:TYR:O	32:41:15:VAL:HB	2.18	0.43
13:4I:11:ARG:HG2	13:4I:12:ASN:N	2.34	0.43
13:4I:65:LYS:HD2	13:4I:69:GLU:CD	2.39	0.43
24:1L:37:A:C6	25:4L:19:G:C6	3.07	0.43
33:51:129:THR:OG1	33:51:129:THR:O	2.37	0.43
40:65:24:LEU:O	40:65:86:ALA:N	2.51	0.43
28:71:64:LEU:HD11	28:71:188:ASN:HD21	1.84	0.43
8:7E:81:HIS:HB2	8:7E:138:TRP:CE3	2.54	0.43
8:7E:13:ILE:O	8:7E:17:THR:HG23	2.19	0.43
43:95:37:VAL:C	43:95:39:LEU:H	2.22	0.43
40:A8:11:LYS:HD3	40:A8:91:PRO:HD3	1.99	0.43
40:A8:32:LEU:N	40:A8:32:LEU:HD23	2.34	0.43
19:AA:66:MET:HA	19:AA:67:VAL:O	2.19	0.43
45:B5:40:LYS:HA	45:B5:51:VAL:HG11	2.01	0.43
41:B8:16:ARG:NH2	41:B8:19:LEU:HD21	2.34	0.43
46:C5:91:GLU:HG3	46:C5:92:ASN:N	2.34	0.43
47:D5:118:GLN:HB2	47:D5:173:ALA:O	2.19	0.43
47:H8:1:MET:CE	47:H8:135:GLU:HG2	2.49	0.43
26:1H:2213:U:O4'	49:J8:52:ARG:NH2	2.52	0.43
55:P8:24:THR:HG23	55:P8:27:GLY:H	1.83	0.43
29:11:105:ILE:HA	29:11:105:ILE:HD12	1.78	0.43
1:13:1051:C:H2'	1:13:1052:U:C6	2.54	0.43
1:13:116:A:H61	1:13:313:A:H1'	1.84	0.43
1:13:122:G:O5'	1:13:122:G:H8	2.00	0.43
1:13:411:A:C5	1:13:413:G:H1'	2.54	0.43
35:15:137:LYS:O	35:15:138:LEU:HD23	2.18	0.43
35:15:28:THR:HG22	35:15:29:LYS:N	2.34	0.43
2:1E:150:SER:OG	2:1E:151:GLY:N	2.50	0.43
1:1G:12:U:H4'	1:1G:526:C:H4'	2.00	0.43
1:1G:1333:A:H2'	1:1G:1334:G:O4'	2.18	0.43
1:1G:1369:C:H2'	1:1G:1370:G:O4'	2.19	0.43
1:1G:616:G:H1'	1:1G:625:G:N2	2.33	0.43
1:1G:678:U:H2'	1:1G:679:C:C6	2.54	0.43
26:1H:1181:C:O2'	26:1H:1182:A:H5'	2.18	0.43
26:1H:1405:U:H2'	26:1H:1406:U:H6	1.81	0.43
26:1H:1818:U:O4	29:11:154:LYS:HE3	2.19	0.43
26:1H:2241:A:H2'	26:1H:2242:G:C8	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1H:2341:G:H2'	26:1H:2342:C:C6	2.54	0.43
26:1H:2712(A):A:OP2	62:1H:3750:HOH:O	2.21	0.43
26:1H:2728:U:H2'	26:1H:2729:G:H8	1.82	0.43
26:1H:183:C:H1'	26:1H:433:C:H1'	2.00	0.43
26:1H:633:A:H2'	26:1H:634:C:H5'	2.01	0.43
24:1L:6:G:O2'	24:1L:7:U:OP1	2.33	0.43
3:22:172:ARG:HH21	3:22:174:PRO:HG2	1.84	0.43
30:29:167:VAL:HG11	30:29:189:PRO:HD3	2.01	0.43
37:35:82:GLY:HA3	37:35:115:LEU:HD11	2.01	0.43
12:3A:27:LEU:HG	12:3A:33:ARG:HG2	2.01	0.43
1:1G:362:G:C4'	12:3A:33:ARG:HH21	2.29	0.43
24:3K:69:A:H2'	24:3K:70:C:C6	2.53	0.43
6:5E:24:GLU:HG2	6:5E:28:ARG:NH2	2.33	0.43
34:69:77:LEU:CD2	34:69:78:THR:H	2.30	0.43
28:71:10:LEU:HA	28:71:10:LEU:HD12	1.74	0.43
28:71:46:LYS:HB3	28:71:210:ARG:HB2	2.01	0.43
1:1G:1250:A:H4'	9:82:68:GLY:N	2.33	0.43
17:8I:14:LYS:HD2	17:8I:14:LYS:N	2.33	0.43
19:AI:41:VAL:HG21	19:AI:45:VAL:HG23	2.01	0.43
41:B8:16:ARG:NH1	41:B8:18:ASP:OD2	2.52	0.43
1:1G:192:U:H4'	20:BA:103:GLY:HA2	1.99	0.43
20:BA:29:LYS:O	20:BA:33:ILE:HD12	2.18	0.43
42:C8:92:ARG:HD3	42:C8:94:ASN:CB	2.45	0.43
46:G8:71:LYS:HE3	46:G8:71:LYS:HB3	1.71	0.43
47:H8:161:VAL:HG23	47:H8:161:VAL:O	2.19	0.43
49:J8:49:VAL:HG11	49:J8:70:VAL:HG11	2.00	0.43
26:1H:686:G:H8	55:P8:6:GLN:O	2.01	0.43
56:Q8:24:ALA:O	56:Q8:48:PHE:N	2.50	0.43
56:Q8:49:VAL:CG1	56:Q8:49:VAL:O	2.65	0.43
29:11:238:GLY:CA	62:11:311:HOH:O	2.66	0.43
1:13:1126:U:C5	1:13:1127:G:C8	3.07	0.43
1:13:1427:U:H2'	1:13:1428:A:H8	1.84	0.43
1:13:141:A:C2	1:13:142:G:C5	3.07	0.43
1:13:390:C:H2'	1:13:391:G:C8	2.54	0.43
26:14:1156:A:O5'	26:14:1156:A:H8	2.02	0.43
26:14:1199:U:H2'	26:14:1200:C:C6	2.54	0.43
26:14:1223:C:OP2	43:95:88:ARG:NH2	2.52	0.43
26:14:1475:G:H5'	26:14:1476:C:OP2	2.19	0.43
26:14:1515:C:H2'	26:14:1516:U:H6	1.83	0.43
26:14:1582:C:O2'	26:14:1586:A:C8	2.72	0.43
26:14:2057:A:H2'	26:14:2058:A:C8	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:14:2287:A:C2	26:14:2346:A:C2	3.06	0.43
26:14:2401:U:H2'	26:14:2402:C:H5''	2.00	0.43
26:14:2068:U:N3	26:14:2430:A:H2	2.17	0.43
26:14:2600:A:H2'	26:14:2601:C:C6	2.54	0.43
26:14:2749:A:O4'	33:59:63:SER:HA	2.19	0.43
26:14:675:A:N6	26:14:676:A:N6	2.67	0.43
26:14:753:C:O2'	26:14:754:C:H5'	2.19	0.43
27:16:44:G:H1'	27:16:47:C:H42	1.84	0.43
2:1E:135:GLN:HG3	2:1E:135:GLN:H	1.65	0.43
2:1E:91:PRO:HB3	2:1E:154:LEU:HB2	2.00	0.43
1:1G:151:A:H2'	1:1G:152:A:O4'	2.18	0.43
1:1G:853:G:H2'	1:1G:854:G:H8	1.83	0.43
1:1G:92:G:H2'	1:1G:93:U:O4'	2.18	0.43
26:1H:1514:U:H2'	26:1H:1515:C:C6	2.53	0.43
26:1H:1800:C:OP1	29:11:266:SER:OG	2.33	0.43
26:1H:2137:C:O2	26:1H:2155:G:N1	2.52	0.43
26:1H:218:A:C2	26:1H:235:U:H4'	2.53	0.43
26:1H:2577:A:H5''	26:1H:2578:G:H5'	2.01	0.43
26:1H:841:A:H2'	26:1H:842:G:C8	2.54	0.43
26:1H:998:C:OP2	42:C8:58:ARG:NH1	2.52	0.43
1:13:1059:C:O2'	10:1I:53:PRO:HD3	2.19	0.43
1:13:973:G:H4'	10:1I:54:PHE:O	2.19	0.43
27:1J:40:U:O2	27:1J:43:C:H5''	2.19	0.43
24:1L:59:A:H5''	24:1L:60:U:H5	1.83	0.43
24:1L:69:A:H1'	24:1L:70:C:O5'	2.18	0.43
3:22:135:LYS:HA	3:22:135:LYS:HD2	1.73	0.43
3:22:7:PRO:O	3:22:11:ARG:HB2	2.19	0.43
30:29:33:VAL:HG13	30:29:47:VAL:HG13	2.00	0.43
30:29:54:GLN:O	30:29:55:ASN:ND2	2.52	0.43
3:2E:32:LEU:HD13	3:2E:59:ARG:HD3	2.01	0.43
23:2L:10:G:N2	23:2L:27:G:H1'	2.34	0.43
24:3L:37:A:H2'	24:3L:38:A:O4'	2.18	0.43
38:45:19:GLY:O	38:45:99:PRO:HD2	2.19	0.43
32:49:56:ALA:HB2	32:49:153:ARG:NE	2.34	0.43
13:4A:68:GLY:HA2	13:4A:71:ARG:NE	2.33	0.43
13:4I:3:ARG:HB2	13:4I:7:VAL:O	2.18	0.43
14:5A:53:LEU:HD23	14:5A:53:LEU:HA	1.67	0.43
15:6I:24:SER:HB3	15:6I:27:VAL:HG23	2.00	0.43
17:8I:13:ASP:HA	17:8I:19:VAL:HG12	2.01	0.43
17:8I:43:LEU:HD12	17:8I:68:ARG:HG2	2.00	0.43
40:A8:36:TYR:N	40:A8:36:TYR:CD1	2.87	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:AI:41:VAL:HG13	19:AI:41:VAL:H	1.55	0.43
20:BI:57:ARG:NH1	20:BI:102:GLY:HA2	2.32	0.43
46:C5:50:ARG:HB2	46:C5:58:GLY:O	2.19	0.43
47:D5:10:ARG:HD2	47:D5:36:LYS:HD2	2.00	0.43
38:45:137:TYR:CE2	47:D5:76:LEU:HD22	2.53	0.43
49:F5:88:LYS:HA	49:F5:90:ILE:HG22	2.00	0.43
50:G5:4:SER:H	50:G5:6:VAL:HG13	1.84	0.43
49:J8:25:LYS:HB3	49:J8:25:LYS:HE3	1.72	0.43
1:13:390:C:O3'	16:7I:28:ARG:NH2	2.52	0.42
1:13:416:G:C5	1:13:417:C:C4	3.06	0.42
1:13:430:A:OP2	4:3E:8:VAL:HG23	2.19	0.42
1:13:715:A:H2'	1:13:716:A:C8	2.54	0.42
26:14:1647:G:P	26:14:1647:G:H3'	2.59	0.42
26:14:2128:C:N3	26:14:2160:G:N2	2.66	0.42
26:14:226:G:H21	26:14:228:A:H62	1.67	0.42
26:14:2508:G:HO2'	26:14:2554:U:HO2'	1.66	0.42
26:14:587:C:C2	37:35:33:ARG:NH1	2.86	0.42
26:14:733:G:O6	26:14:761:A:C8	2.72	0.42
26:14:792:G:H5''	26:14:793:A:H5'	1.99	0.42
29:19:228:PRO:HD3	29:19:235:GLY:CA	2.49	0.42
2:1E:74:LYS:C	2:1E:208:ILE:HG21	2.40	0.42
1:1G:265:G:O3'	17:8A:66:SER:HA	2.18	0.42
1:1G:27:G:H8	1:1G:27:G:O5'	2.02	0.42
1:1G:498:A:H4'	1:1G:500:G:OP1	2.19	0.42
1:1G:591:U:H2'	1:1G:592:G:C8	2.54	0.42
1:1G:890:G:O2'	1:1G:906:G:O6	2.32	0.42
26:1H:1448:G:O2'	26:1H:1529:A:N1	2.42	0.42
26:1H:1581:G:H2'	26:1H:1582:C:C6	2.54	0.42
26:1H:1655:A:H3'	26:1H:1656:C:H6	1.84	0.42
26:1H:1899:G:N2	26:1H:1902:C:H41	2.17	0.42
26:1H:2159:G:H2'	26:1H:2160:G:C8	2.54	0.42
26:1H:2701:C:H2'	26:1H:2702:U:H2'	2.00	0.42
26:1H:2751:G:C6	33:51:3:ARG:CG	3.02	0.42
26:1H:322:A:H5'	26:1H:340:A:H1'	2.00	0.42
26:1H:839:U:H2'	26:1H:840:C:C6	2.54	0.42
30:21:105:THR:HG22	30:21:106:GLY:H	1.83	0.42
26:1H:2820:A:C8	30:21:109:LYS:HE2	2.54	0.42
30:21:169:ASN:OD1	30:21:201:THR:HG21	2.19	0.42
30:21:38:THR:HB	30:21:41:LYS:H	1.83	0.42
30:21:79:ARG:HD3	30:21:79:ARG:HA	1.73	0.42
1:1G:1256:A:H3'	3:22:27:LYS:NZ	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:29:56:PRO:HD2	30:29:58:ARG:NH2	2.34	0.42
23:2K:47:7MG:O2'	23:2K:48:U:C6	2.72	0.42
31:31:28:ILE:HA	31:31:112:MET:HE3	2.00	0.42
31:31:127:GLU:OE2	31:31:127:GLU:HA	2.18	0.42
4:32:126:ILE:HG22	4:32:127:THR:H	1.84	0.42
4:32:98:GLU:OE2	4:32:103:ASN:ND2	2.50	0.42
31:39:46:ARG:O	31:39:48:THR:HG23	2.19	0.42
1:13:406:G:H21	4:3E:119:GLN:HE22	1.67	0.42
4:3E:25:ARG:NH1	4:3E:30:LYS:O	2.52	0.42
24:3L:1:G:N3	24:3L:1:G:H2'	2.34	0.42
32:41:113:ARG:HD2	52:M8:33:VAL:HG13	2.01	0.42
32:49:122:PRO:O	32:49:125:PHE:HD2	2.02	0.42
33:51:9:ILE:HB	33:51:49:VAL:HB	2.00	0.42
34:61:75:LEU:HG	34:61:105:HIS:HD1	1.82	0.42
7:62:114:ARG:H	7:62:114:ARG:HG2	1.30	0.42
34:69:112:LYS:HE2	34:69:112:LYS:HB3	1.87	0.42
7:6E:72:ARG:HG3	7:6E:142:GLU:OE1	2.19	0.42
28:71:19:ILE:HG12	28:71:223:ARG:HD3	2.01	0.42
41:75:64:ARG:HB2	41:75:73:GLU:HG2	2.01	0.42
9:82:97:LYS:HB3	9:82:98:PRO:HD3	2.00	0.42
38:88:37:LEU:HA	38:88:37:LEU:HD23	1.64	0.42
1:13:1116:C:O2'	9:8E:108:VAL:HG21	2.19	0.42
44:A5:58:ALA:HB1	44:A5:64:MET:HB2	2.01	0.42
45:B5:11:PRO:HG2	45:B5:13:LEU:HD21	2.01	0.42
46:C5:19:LYS:HB3	46:C5:20:TYR:H	1.61	0.42
46:C5:17:SER:HB3	46:C5:71:LYS:HB3	2.00	0.42
49:J8:87:PRO:HB2	49:J8:91:LYS:NZ	2.34	0.42
56:Q8:41:ILE:HG13	56:Q8:41:ILE:H	1.62	0.42
29:11:148:GLU:HB2	29:11:151:LYS:HD2	2.01	0.42
1:13:1199:U:H4'	10:1I:54:PHE:CE2	2.54	0.42
1:13:1510:U:H1'	1:13:1526:G:N2	2.34	0.42
1:13:199:G:O6	1:13:218:C:N4	2.52	0.42
1:13:29:G:O2'	1:13:30:U:H5'	2.19	0.42
1:13:658:G:C6	1:13:659:U:C4	3.07	0.42
1:13:687:A:H2'	1:13:701:C:H41	1.85	0.42
1:13:836:G:C6	1:13:851:G:C6	3.07	0.42
1:13:883:C:C2'	1:13:884:U:H5'	2.49	0.42
26:14:1048:A:N6	26:14:1112:G:O2'	2.36	0.42
26:14:1198:U:C2	26:14:1199:U:C5	3.07	0.42
26:14:1354:A:H2'	26:14:1355:G:O4'	2.19	0.42
26:14:1404:C:O2'	26:14:1405:U:H5'	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:14:1912:A:C8	26:14:1918:A:C2	3.07	0.42
26:14:2345:G:N3	26:14:2381:C:H2'	2.35	0.42
26:14:2611:U:OP2	26:14:2611:U:H3'	2.18	0.42
26:14:221:A:C4	26:14:266:G:N7	2.87	0.42
26:14:2697:G:H2'	26:14:2698:U:O4'	2.18	0.42
26:14:2756:U:H1'	26:14:2757:A:H5''	2.01	0.42
26:14:35:G:H2'	26:14:36:G:O4'	2.20	0.42
26:14:483:A:H5''	46:C5:49:VAL:HG13	2.01	0.42
26:14:596:G:H2'	26:14:597:U:O4'	2.19	0.42
26:14:914:C:N4	26:14:915:C:C2	2.88	0.42
26:14:2780:G:OP2	35:15:118:LYS:HD3	2.19	0.42
29:19:124:PRO:HG2	29:19:129:ASN:ND2	2.34	0.42
2:1E:79:ASP:N	2:1E:81:VAL:HG22	2.34	0.42
1:1G:1022:G:C6	1:1G:1023:G:C8	3.07	0.42
1:1G:1206:G:H2'	1:1G:1207:G:C8	2.54	0.42
1:1G:1510:U:H2'	1:1G:1511:G:C8	2.55	0.42
1:1G:229:U:H2'	1:1G:230:G:O4'	2.18	0.42
1:1G:539:A:H2'	1:1G:540:G:H8	1.84	0.42
1:1G:854:G:C2	1:1G:855:G:C8	3.07	0.42
26:1H:1316:U:H2'	26:1H:1317:A:H8	1.83	0.42
26:1H:1430:C:H2'	26:1H:1431:U:H6	1.83	0.42
26:1H:1475:G:C4	26:1H:1519:G:N2	2.86	0.42
26:1H:2093:G:C6	26:1H:2225:A:C8	3.08	0.42
26:1H:2302:G:C4	26:1H:2303:G:C8	3.07	0.42
26:1H:273(E):U:C2'	26:1H:273(F):C:H5'	2.49	0.42
26:1H:2845:G:H5''	41:B8:54:ARG:O	2.19	0.42
26:1H:36:G:C5	26:1H:37:C:C5	3.07	0.42
26:1H:455:C:N3	26:1H:472:A:H2'	2.34	0.42
26:1H:590:A:H2'	26:1H:591:C:C6	2.54	0.42
26:1H:760:G:H4'	26:1H:1776:G:OP1	2.19	0.42
26:1H:840:C:H2'	26:1H:841:A:H8	1.84	0.42
27:1J:0:A:H2'	27:1J:1:U:C6	2.54	0.42
3:22:63:ASN:HA	3:22:98:ASN:HB2	2.01	0.42
11:2A:84:VAL:HG11	11:2A:95:ILE:HD11	2.00	0.42
4:32:150:GLU:C	4:32:152:SER:H	2.21	0.42
4:32:61:LYS:HD2	4:32:206:PHE:CE2	2.54	0.42
26:14:805:G:O4'	37:35:38:GLN:NE2	2.52	0.42
31:39:186:ILE:HD12	31:39:192:LEU:HD11	2.01	0.42
5:4E:84:PHE:HB3	5:4E:134:ALA:HB2	2.01	0.42
33:51:27:LYS:HD2	33:51:32:GLU:OE1	2.19	0.42
33:51:84:SER:O	33:51:85:LYS:HB2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:55:32:GLY:HA2	39:55:116:LEU:HD12	2.01	0.42
39:55:45:ARG:HA	39:55:95:THR:HG21	2.00	0.42
34:61:75:LEU:HG	34:61:105:HIS:ND1	2.34	0.42
28:71:14:VAL:HG11	28:71:222:VAL:HG22	2.02	0.42
28:71:44:HIS:O	28:71:212:VAL:HA	2.20	0.42
8:72:39:LEU:HB3	8:72:45:ILE:HG12	2.00	0.42
9:82:63:ILE:HD13	9:82:77:ILE:HG23	2.01	0.42
43:95:21:ARG:HB3	43:95:91:TYR:CD2	2.54	0.42
40:A8:56:LEU:CB	40:A8:58:LEU:HD22	2.49	0.42
41:B8:1:MET:HA	41:B8:3:ARG:H	1.83	0.42
41:B8:2:ASN:HD21	41:B8:6:LEU:HD13	1.84	0.42
41:B8:2:ASN:O	41:B8:6:LEU:N	2.48	0.42
41:B8:81:PRO:HG2	41:B8:82:LEU:HD12	2.00	0.42
46:C5:82:PRO:HB3	46:C5:97:ARG:HB3	2.01	0.42
44:E8:107:LEU:HA	44:E8:107:LEU:HD12	1.82	0.42
46:G8:75:ILE:HD12	46:G8:75:ILE:HA	1.61	0.42
49:J8:87:PRO:O	49:J8:91:LYS:HE2	2.19	0.42
2:12:222:ILE:H	2:12:222:ILE:HG13	1.52	0.42
1:13:1221:G:O3'	19:AI:77:THR:HG21	2.19	0.42
1:13:1366:C:H2'	1:13:1367:C:C6	2.52	0.42
1:13:342:C:N4	1:13:343:U:O4	2.52	0.42
1:13:418:C:H2'	1:13:419:C:C6	2.54	0.42
1:13:509:A:H5'	4:3E:54:TYR:HD2	1.83	0.42
1:13:963:G:H21	10:II:55:LYS:HE2	1.84	0.42
26:14:1022:G:N2	26:14:1142(A):A:H2	2.11	0.42
26:14:1543:A:H1'	26:14:1545:A:H1'	2.00	0.42
26:14:2392:A:H2	26:14:2424:C:N4	2.06	0.42
26:14:2853:C:H2'	26:14:2854:G:C8	2.53	0.42
26:14:2862:G:H2'	26:14:2863:C:H6	1.84	0.42
26:14:601:C:O2	26:14:605:C:H4'	2.19	0.42
26:14:901:A:H2'	26:14:901:A:N3	2.34	0.42
26:14:975:G:C2	26:14:990:A:C8	3.06	0.42
26:14:1007:C:P	35:15:37:LYS:HZ2	2.41	0.42
27:16:90:C:P	38:88:16:ARG:HH21	2.42	0.42
1:1G:1104:G:C2	1:1G:1105:A:C4	3.07	0.42
26:1H:1062:G:H1'	26:1H:1088:A:C4	2.54	0.42
26:1H:110:G:N7	62:1H:3849:HOH:O	2.37	0.42
26:1H:1213:A:H1'	26:1H:1238:G:N3	2.33	0.42
26:1H:172:C:H2'	26:1H:173:G:H8	1.84	0.42
26:1H:1788:C:H2'	26:1H:1789:A:H8	1.83	0.42
26:1H:1826:G:H2'	26:1H:1827:C:O4'	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1H:1857:G:C6	26:1H:1858:G:N1	2.88	0.42
26:1H:2394:C:H2'	26:1H:2395:C:H6	1.84	0.42
26:1H:252:G:O2'	26:1H:253:C:H5'	2.19	0.42
26:1H:263:C:H2'	26:1H:264:C:O4'	2.19	0.42
26:1H:1637:A:H4'	26:1H:2711:A:O2'	2.19	0.42
26:1H:319:C:OP1	31:31:137:LYS:NZ	2.36	0.42
26:1H:902:C:O2'	26:1H:903:C:H5'	2.19	0.42
22:1K:74:C:N4	26:1H:2507:C:O3'	2.53	0.42
3:22:152:ILE:HD12	3:22:199:LYS:HD2	2.00	0.42
36:25:122:LEU:HD13	41:75:72:VAL:HG11	2.00	0.42
30:29:52:LEU:O	30:29:75:VAL:N	2.50	0.42
4:32:148:VAL:HG12	4:32:152:SER:CB	2.49	0.42
4:32:172:PRO:HB2	4:32:187:ARG:NH1	2.34	0.42
37:35:133:SER:O	37:35:137:LYS:HG3	2.19	0.42
12:3A:102:ARG:HB3	12:3A:102:ARG:HE	1.63	0.42
12:3I:42:THR:HA	12:3I:53:ARG:O	2.19	0.42
32:41:35:GLU:HG3	32:41:36:LYS:HB2	2.00	0.42
38:45:57:HIS:CE1	38:45:116:GLU:HG2	2.55	0.42
38:45:2:LEU:O	38:45:70:PRO:HG2	2.20	0.42
13:4A:30:ALA:O	13:4A:34:LEU:N	2.39	0.42
13:4A:92:HIS:HD2	13:4A:98:VAL:HG11	1.84	0.42
5:4E:131:ILE:HA	5:4E:131:ILE:HD13	1.89	0.42
33:51:4:ILE:O	33:51:6:ARG:NE	2.51	0.42
14:5I:37:PHE:CE1	14:5I:53:LEU:HD13	2.54	0.42
34:61:114:LEU:HB2	34:61:115:ALA:H	1.73	0.42
34:69:71:ILE:HG22	34:69:72:LEU:HD23	2.00	0.42
15:6A:54:ARG:O	15:6A:58:MET:HG3	2.20	0.42
1:13:1240:U:C4	7:6E:32:ARG:HD2	2.54	0.42
41:75:12:SER:HA	41:75:15:VAL:HG22	2.00	0.42
8:7E:1:MET:HB3	8:7E:2:LEU:H	1.46	0.42
19:AI:41:VAL:HG11	19:AI:45:VAL:HG23	2.01	0.42
41:B8:2:ASN:O	41:B8:5:ALA:HB3	2.18	0.42
46:C5:3:VAL:HG11	46:C5:32:PRO:O	2.19	0.42
26:1H:18:C:H4'	42:C8:23:GLY:O	2.20	0.42
47:D5:127:LYS:O	47:D5:162:GLU:HB2	2.19	0.42
47:D5:72:ARG:HD2	47:D5:72:ARG:HA	1.31	0.42
26:14:2352:A:H2	48:E5:33:ALA:O	2.02	0.42
50:G5:38:GLN:O	50:G5:41:ILE:HG12	2.19	0.42
29:11:102:LYS:C	29:11:103:ARG:HG2	2.39	0.42
29:11:119:ALA:CB	29:11:130:ALA:HB3	2.49	0.42
1:13:1121:U:H2'	1:13:1122:U:C6	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:13:1397:C:H4'	1:13:1398:A:O5'	2.18	0.42
1:13:1401:G:C2	1:13:1402:C:H1'	2.53	0.42
1:13:439:A:OP2	1:13:493:G:N2	2.46	0.42
1:13:711:G:H2'	1:13:712:A:H8	1.84	0.42
26:14:1268:A:OP1	62:14:3656:HOH:O	2.21	0.42
26:14:1441:G:H2'	26:14:1442:G:H8	1.84	0.42
26:14:1515:C:H2'	26:14:1516:U:C6	2.54	0.42
26:14:2056:G:H1	53:J5:3:LYS:HB3	1.83	0.42
26:14:2607:G:O3'	62:14:3658:HOH:O	2.22	0.42
26:14:2543:G:H21	26:14:2646:C:H5''	1.84	0.42
26:14:1999:C:H5''	26:14:2723:C:O2'	2.20	0.42
26:14:813:U:C2	26:14:1195:G:N2	2.87	0.42
29:19:71:ASP:OD1	29:19:71:ASP:N	2.52	0.42
10:1A:66:ARG:HE	10:1A:66:ARG:HB3	1.63	0.42
2:1E:67:THR:HG21	2:1E:155:LEU:HG	2.01	0.42
1:1G:1173:G:OP1	7:62:5:ARG:NH2	2.47	0.42
1:1G:1279:A:H5''	1:1G:1280:A:OP2	2.20	0.42
1:1G:1367:C:H5'	10:1A:60:ARG:NH2	2.34	0.42
1:1G:1442:G:C6	1:1G:1446:A:N6	2.87	0.42
1:1G:834:C:H2'	1:1G:835:U:C6	2.54	0.42
26:1H:1086:A:H1'	26:1H:1103:A:C2	2.54	0.42
26:1H:1386:C:OP2	26:1H:1396:U:H5	2.03	0.42
26:1H:1799:G:H5'	26:1H:1819:A:H61	1.83	0.42
26:1H:2431:U:P	62:1H:3605:HOH:O	2.77	0.42
26:1H:2646:C:H2'	26:1H:2647:U:O4'	2.19	0.42
26:1H:289:A:H2'	26:1H:290:G:O4'	2.20	0.42
1:13:963:G:C2	10:1I:55:LYS:NZ	2.88	0.42
3:2E:130:VAL:HG12	3:2E:134:ILE:HD11	2.02	0.42
3:2E:95:THR:HB	3:2E:97:LYS:HG3	2.01	0.42
26:14:1244:G:P	37:35:7:ARG:HD3	2.60	0.42
1:13:538:G:O3'	12:3I:114:LYS:HD3	2.20	0.42
12:3I:28:LYS:HD3	12:3I:28:LYS:HA	1.72	0.42
12:3I:47:LYS:HA	12:3I:49:ASN:H	1.84	0.42
32:49:48:GLU:H	32:49:48:GLU:HG2	1.40	0.42
13:4I:15:VAL:HG23	13:4I:43:THR:O	2.19	0.42
33:51:80:SER:O	33:51:81:GLU:HG3	2.19	0.42
35:58:131:GLN:HG2	35:58:131:GLN:H	1.59	0.42
7:62:71:PRO:HG3	7:62:103:TRP:CH2	2.55	0.42
36:68:117:LEU:HA	36:68:117:LEU:HD23	1.84	0.42
34:69:128:LEU:O	34:69:138:ILE:N	2.41	0.42
15:6A:32:LEU:O	15:6A:36:ILE:HG13	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:88:12:GLN:HG2	38:88:73:PRO:HD2	2.01	0.42
38:88:135:ASP:N	38:88:135:ASP:OD1	2.52	0.42
1:13:967:C:H4'	9:8E:125:TYR:HE1	1.84	0.42
26:1H:996:A:H4'	42:C8:92:ARG:NE	2.34	0.42
26:14:98:G:OP1	50:G5:3:LEU:HB3	2.20	0.42
29:11:123:ALA:HB3	29:11:131:LEU:HG	2.02	0.42
1:13:1162:C:O5'	1:13:1162:C:H6	2.02	0.42
1:13:1399:C:H4'	1:13:1400:C:O5'	2.19	0.42
1:13:222:U:H2'	1:13:223:U:C6	2.54	0.42
1:13:376:G:O3'	16:7I:5:ARG:NH1	2.45	0.42
1:13:872:A:C5	1:13:874:G:C8	3.06	0.42
26:14:1121:C:H2'	26:14:1122:G:O4'	2.20	0.42
26:14:1131:G:C2	26:14:1132:A:C4	3.08	0.42
26:14:201:C:H4'	26:14:386:G:C2	2.53	0.42
26:14:2552:U:C2	26:14:2554:U:H5'	2.54	0.42
26:14:2674:G:H4'	36:25:30:ALA:HB2	2.01	0.42
26:14:26:G:C6	26:14:27:G:N1	2.87	0.42
26:14:270(V):G:H2'	26:14:270(W):G:H8	1.83	0.42
26:14:2857:G:N2	26:14:2859:G:H3'	2.35	0.42
26:14:785:G:OP2	62:14:3657:HOH:O	2.22	0.42
26:14:895:U:H4'	26:14:896:A:C2	2.55	0.42
26:14:987:G:OP2	62:14:3655:HOH:O	2.21	0.42
21:1F:9:ARG:O	21:1F:13:ILE:HG13	2.19	0.42
1:1G:1279:A:H5''	1:1G:1280:A:P	2.58	0.42
1:1G:160:A:H1'	1:1G:344:A:N7	2.35	0.42
1:1G:191(E):G:H2'	1:1G:191(F):U:C6	2.55	0.42
1:1G:456:C:H42	1:1G:476:G:H1	1.67	0.42
1:1G:79:G:H1	1:1G:90:C:N4	2.10	0.42
26:1H:1449(A):G:H2'	26:1H:1450:C:C6	2.53	0.42
26:1H:1478:G:H2'	26:1H:1479:G:C8	2.55	0.42
26:1H:2376:A:H2'	26:1H:2377:A:O4'	2.19	0.42
26:1H:2378:A:H4'	40:A8:23:ARG:NH1	2.35	0.42
26:1H:2740:A:C6	26:1H:2764:A:C8	3.07	0.42
27:1J:15:A:H1'	27:1J:109:G:C5	2.54	0.42
27:1J:18:G:H2'	27:1J:19:G:C8	2.54	0.42
27:1J:6:C:H2'	27:1J:7:G:O4'	2.19	0.42
11:2A:31:THR:HA	11:2A:42:TRP:HA	2.02	0.42
24:3L:3:G:H2'	24:3L:4:U:O4'	2.18	0.42
38:45:54:MET:O	38:45:57:HIS:N	2.52	0.42
32:49:4:ASP:OD2	32:49:9:ARG:NH1	2.52	0.42
39:55:35:THR:HG23	39:55:113:LEU:HD12	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:5E:10:LEU:HD13	6:5E:61:LEU:HD13	2.00	0.42
7:62:15:ASP:HB3	7:62:20:ASP:H	1.83	0.42
7:62:97:GLN:HG3	7:62:98:SER:N	2.35	0.42
40:65:102:ALA:O	40:65:105:ALA:N	2.53	0.42
7:6E:15:ASP:CB	7:6E:20:ASP:H	2.32	0.42
41:75:33:LYS:HA	41:75:42:ILE:HD12	2.01	0.42
37:78:113:LYS:HG2	37:78:115:LEU:HD23	2.02	0.42
18:9A:60:ALA:O	18:9A:64:ARG:HG3	2.20	0.42
18:9I:55:ARG:HD2	18:9I:55:ARG:HA	1.91	0.42
19:AI:25:LYS:HG2	19:AI:27:GLU:OE1	2.20	0.42
20:BA:56:MET:HG3	20:BA:84:LEU:HD13	2.02	0.42
42:C8:83:LEU:HG	42:C8:88:ILE:HB	2.01	0.42
47:D5:17:ALA:O	47:D5:20:ARG:HB2	2.19	0.42
48:E5:69:PHE:CE2	48:E5:79:VAL:HG22	2.55	0.42
49:F5:85:LEU:O	49:F5:88:LYS:N	2.32	0.42
48:I8:36:ILE:C	48:I8:36:ILE:HD13	2.40	0.42
53:J5:40:LYS:HE3	53:J5:44:THR:O	2.19	0.42
56:M5:32:LEU:HA	56:M5:32:LEU:HD12	1.82	0.42
56:M5:32:LEU:O	56:M5:36:LYS:HE3	2.20	0.42
1:13:112:G:OP1	16:7I:27:LYS:HD2	2.20	0.42
1:13:1284:C:H2'	1:13:1285:A:N7	2.34	0.42
1:13:129(A):G:H4'	1:13:130:A:H5''	2.01	0.42
1:13:1304:G:N2	1:13:1332:A:OP2	2.49	0.42
1:13:186(C):G:H2'	1:13:186(D):C:C6	2.55	0.42
1:13:585:G:O2'	1:13:879:C:H5''	2.19	0.42
1:13:980:C:H2'	1:13:981:U:O4'	2.19	0.42
26:14:1041:C:H42	26:14:1114:G:N2	2.17	0.42
26:14:1385:G:C4	26:14:1386:C:C5	3.08	0.42
26:14:1441:G:H2'	26:14:1442:G:C8	2.55	0.42
26:14:1990:C:H2'	26:14:1991:U:C6	2.55	0.42
26:14:270(Q):C:H5''	34:69:45:LYS:HE3	2.01	0.42
26:14:459:U:H2'	26:14:460:A:H8	1.84	0.42
26:14:59:U:O2'	26:14:73:A:H2'	2.20	0.42
26:14:637:A:OP2	37:35:116:GLY:N	2.50	0.42
1:1G:64:G:OP1	1:1G:64:G:H3'	2.19	0.42
26:1H:1207:C:H2'	26:1H:1208:C:H6	1.84	0.42
26:1H:1604:C:P	62:1H:3611:HOH:O	2.72	0.42
26:1H:165:U:H2'	26:1H:165:U:H6	1.62	0.42
26:1H:1916:A:H2'	26:1H:1917:U:O4'	2.20	0.42
26:1H:858:U:O2	26:1H:2268:A:H2'	2.19	0.42
26:1H:2529:G:OP2	26:1H:2530:A:H5''	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1H:508:G:N3	26:1H:508:G:H5''	2.35	0.42
26:1H:588:U:O4	26:1H:670:A:H1'	2.19	0.42
22:1K:53:G:O2'	22:1K:54:5MU:H5''	2.20	0.42
30:29:107:THR:O	30:29:190:GLY:HA2	2.19	0.42
30:29:117:MET:HA	30:29:122:PHE:H	1.84	0.42
3:2E:34:LEU:HD22	3:2E:38:ARG:NH1	2.34	0.42
23:2L:62:C:H2'	23:2L:63:C:C6	2.50	0.42
4:32:162:LEU:HD12	4:32:181:MET:HG2	2.02	0.42
4:32:58:LEU:HA	4:32:58:LEU:HD23	1.89	0.42
4:3E:196:LEU:H	4:3E:196:LEU:HD12	1.85	0.42
12:3I:70:ILE:HG12	12:3I:100:ILE:HD12	2.01	0.42
24:3L:22:G:N2	24:3L:23:A:C5	2.87	0.42
24:3L:28:U:H3	24:3L:43:U:H3	1.68	0.42
32:49:106:LEU:HG	32:49:111:LEU:HD12	2.01	0.42
35:58:128:HIS:HB2	35:58:129:PRO:HD2	2.01	0.42
33:59:146:ALA:O	33:59:150:ALA:N	2.49	0.42
14:5I:4:LYS:O	14:5I:7:ILE:HG23	2.19	0.42
40:65:83:LYS:HE3	40:65:83:LYS:HB3	1.96	0.42
40:65:89:ARG:O	40:65:92:TYR:N	2.45	0.42
1:1G:750:G:H21	15:6A:23:GLY:HA3	1.84	0.42
37:78:106:LEU:O	37:78:107:LYS:C	2.58	0.42
37:78:38:GLN:O	37:78:41:ARG:HB2	2.20	0.42
42:85:8:VAL:HB	42:85:12:ARG:HE	1.85	0.42
38:88:112:GLU:CD	38:88:112:GLU:H	2.22	0.42
38:88:35:VAL:HA	38:88:101:ARG:O	2.18	0.42
40:A8:15:ARG:O	40:A8:19:LYS:HD2	2.20	0.42
41:B8:29:ARG:HD3	41:B8:46:GLU:OE2	2.20	0.42
20:BA:66:ALA:HB1	20:BA:71:THR:HB	2.02	0.42
46:C5:2:ARG:HD2	46:C5:2:ARG:HA	1.90	0.42
46:G8:87:LYS:HD2	46:G8:89:PHE:CD2	2.54	0.42
50:K8:22:GLU:OE2	50:K8:68:ARG:NH1	2.51	0.42
53:N8:36:CYS:SG	53:N8:37:LYS:N	2.92	0.42
29:11:68:LYS:HB3	29:11:70:TRP:CZ3	2.55	0.42
29:11:70:TRP:CD1	29:11:71:ASP:N	2.87	0.42
1:13:1126:U:O4	1:13:1127:G:C4	2.72	0.42
1:13:1319:A:O2'	1:13:1323:G:N7	2.47	0.42
1:13:14:U:H2'	1:13:16:A:OP2	2.20	0.42
1:13:233:C:H2'	1:13:234:C:H6	1.84	0.42
1:13:652:U:HO2'	1:13:653:A:P	2.42	0.42
26:14:111:A:H4'	50:G5:69:ARG:NH2	2.33	0.42
26:14:1477:A:H2'	26:14:1478:G:O4'	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:14:2257:U:O2'	26:14:2258:C:H5'	2.19	0.42
26:14:330:A:H2	26:14:1210:A:O2'	1.83	0.42
26:14:717:G:H2'	26:14:718:A:O4'	2.18	0.42
26:14:818:G:O2'	26:14:838:C:O2'	2.28	0.42
1:1G:1181:G:N1	1:1G:1182:G:H1'	2.34	0.42
1:1G:1255:G:H5'	1:1G:1256:A:OP2	2.18	0.42
1:1G:1509:C:H2'	1:1G:1510:U:O4'	2.20	0.42
1:1G:18:C:H6	1:1G:18:C:O5'	2.03	0.42
1:1G:979:C:H5''	1:1G:980:C:OP2	2.18	0.42
26:1H:1021:A:C3'	26:1H:1021:A:C8	3.02	0.42
26:1H:1655:A:H4'	30:21:115:GLY:N	2.34	0.42
26:1H:1988:C:H2'	26:1H:1989:G:O4'	2.19	0.42
26:1H:270(E):G:H1	26:1H:270(U):C:N4	2.16	0.42
26:1H:300:A:H2'	26:1H:334:C:O2'	2.19	0.42
26:1H:28:A:O2'	26:1H:583:G:H5'	2.20	0.42
26:1H:675:A:C8	26:1H:804:A:C6	3.07	0.42
26:1H:960:A:C8	26:1H:962:G:C8	3.07	0.42
10:1I:26:ALA:HA	10:1I:29:ARG:CZ	2.49	0.42
24:1L:35:U:H2'	24:1L:36:U:O4'	2.20	0.42
3:22:7:PRO:O	3:22:11:ARG:NH1	2.53	0.42
36:25:22:ILE:HD13	36:25:22:ILE:HA	1.41	0.42
23:2L:38:A:H2'	23:2L:39:A:O4'	2.18	0.42
37:35:75:ILE:HG13	37:35:77:ARG:NH2	2.35	0.42
31:39:158:THR:HA	31:39:195:ASP:HB2	2.01	0.42
4:3E:196:LEU:HB3	4:3E:197:PRO:HD2	2.02	0.42
32:49:170:ARG:HA	32:49:170:ARG:HD2	1.80	0.42
32:49:36:LYS:HD2	32:49:95:ARG:HH22	1.85	0.42
32:49:62:LEU:HD12	32:49:63:ILE:HG23	2.02	0.42
33:51:169:VAL:HG22	33:51:170:ARG:H	1.84	0.42
6:5E:26:ILE:O	6:5E:30:LEU:HD12	2.20	0.42
36:68:85:VAL:HG11	36:68:114:ILE:HD13	2.02	0.42
28:71:185:LEU:HD23	28:71:185:LEU:HA	1.87	0.42
8:7E:112:LEU:HD12	8:7E:113:SER:N	2.35	0.42
16:7I:8:ARG:HB3	16:7I:28:ARG:NH1	2.34	0.42
26:1H:2483:C:O2	38:88:124:LYS:HE3	2.19	0.42
39:98:113:LEU:HD12	39:98:113:LEU:HA	1.84	0.42
19:AA:3:ARG:HB3	19:AA:7:LYS:CB	2.49	0.42
41:B8:105:LEU:O	41:B8:107:ASP:OD1	2.38	0.42
48:E5:24:LYS:O	48:E5:25:ARG:HD3	2.20	0.42
26:1H:484:C:OP1	46:G8:51:VAL:HG22	2.19	0.42
46:G8:88:LYS:HA	46:G8:88:LYS:HD3	1.78	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:J8:90:ILE:O	49:J8:94:LEU:HB2	2.18	0.42
56:M5:14:VAL:HG11	56:M5:22:VAL:HG13	2.02	0.42
29:11:101:GLU:OE1	29:11:103:ARG:HD3	2.20	0.42
2:12:52:GLU:O	2:12:55:PHE:HB2	2.19	0.42
2:12:55:PHE:CD1	2:12:221:LEU:HG	2.55	0.42
1:13:1009:G:C2	1:13:1021:G:C6	3.08	0.42
1:13:114:U:O2'	1:13:115:G:H5'	2.20	0.42
1:13:1170:A:H2'	1:13:1171:G:O4'	2.20	0.42
1:13:13:U:O2	1:13:914:A:H3'	2.19	0.42
1:13:1425:U:H2'	1:13:1426:C:C6	2.55	0.42
1:13:123:C:OP1	1:13:312:C:H5'	2.20	0.42
1:13:345:C:O2'	1:13:346:G:C4	2.69	0.42
1:13:734:G:C6	1:13:735:C:C4	3.08	0.42
26:14:1024:G:C8	26:14:1025:G:H2'	2.55	0.42
26:14:1022:G:N2	26:14:1142(A):A:C2	2.86	0.42
26:14:1542:G:H3'	26:14:1543:A:H5''	2.01	0.42
26:14:579:G:C8	26:14:2017:U:C4	3.08	0.42
26:14:219:G:C6	26:14:220:G:C6	3.08	0.42
26:14:2228:G:OP2	29:19:263:ARG:NH2	2.53	0.42
26:14:240:G:O2'	26:14:257:A:N6	2.41	0.42
26:14:2414:G:H21	37:35:67:MET:HE1	1.85	0.42
26:14:2577:A:H2'	26:14:2614:A:N6	2.35	0.42
26:14:2051:A:H5'	26:14:2578:G:O4'	2.19	0.42
26:14:2638:G:OP2	30:29:82:ARG:NH2	2.50	0.42
29:19:260:ARG:HH12	29:19:267:SER:HB3	1.84	0.42
29:19:96:HIS:CD2	29:19:102:LYS:HE2	2.55	0.42
21:1B:6:ARG:O	21:1B:12:LYS:HE2	2.20	0.42
1:1G:1208:C:H2'	1:1G:1209:C:H6	1.84	0.42
1:1G:1224:G:C2	1:1G:1322:C:H4'	2.55	0.42
1:1G:1228:C:H2'	1:1G:1229:A:C8	2.54	0.42
1:1G:176:C:H2'	1:1G:177:C:C6	2.54	0.42
1:1G:259:G:H2'	1:1G:260:G:O4'	2.19	0.42
1:1G:689:C:H2'	1:1G:690:G:H5'	2.02	0.42
1:1G:943:U:H1'	9:82:124:GLN:OE1	2.20	0.42
26:1H:1038:C:H2'	26:1H:1039:G:O4'	2.19	0.42
26:1H:1260:G:C6	26:1H:1261:C:C4	3.08	0.42
26:1H:1263:U:O2'	53:N8:11:THR:HG23	2.20	0.42
26:1H:1299:G:H3'	26:1H:1639:U:O4	2.20	0.42
26:1H:1543:A:C8	26:1H:1545:A:H5''	2.55	0.42
26:1H:270(E):G:C5	26:1H:270(F):U:C4	3.08	0.42
26:1H:852:G:O2'	26:1H:853:G:H5'	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:2A:98:LEU:O	11:2A:101:SER:OG	2.24	0.42
4:32:25:ARG:HG2	4:32:30:LYS:O	2.20	0.42
37:35:65:ARG:HB2	62:M5:204:HOH:O	2.20	0.42
4:3E:62:GLN:O	4:3E:66:ARG:HB2	2.20	0.42
38:45:103:MET:HE1	38:45:125:LEU:HD13	2.02	0.42
32:49:13:GLU:H	32:49:13:GLU:HG3	1.76	0.42
32:49:5:VAL:O	32:49:5:VAL:HG12	2.20	0.42
5:4E:147:ASP:OD1	5:4E:147:ASP:N	2.43	0.42
35:58:57:ALA:O	35:58:59:LYS:N	2.52	0.42
33:59:37:VAL:HG22	33:59:38:SER:H	1.84	0.42
6:5E:76:ALA:HA	6:5E:79:LEU:HD12	2.00	0.42
14:5I:13:THR:N	14:5I:14:PRO:HD2	2.35	0.42
7:6E:124:LEU:HD23	7:6E:124:LEU:HA	1.72	0.42
41:75:8:LYS:O	41:75:11:GLU:HB3	2.20	0.42
19:AI:31:ILE:HG23	19:AI:49:ILE:HG12	2.02	0.42
41:B8:27:THR:HG23	41:B8:90:GLN:HB3	2.02	0.42
46:G8:94:LYS:NZ	46:G8:95:LYS:H	2.18	0.42
53:N8:49:CYS:O	53:N8:49:CYS:SG	2.78	0.42
26:1H:1569:A:O5'	29:11:61:LEU:HD21	2.19	0.42
29:11:75:ILE:HD13	29:11:99:ASP:OD2	2.20	0.42
1:13:1023:G:C3'	1:13:1024:G:H5''	2.49	0.42
1:13:1106:G:C6	1:13:1107:C:C4	3.07	0.42
1:13:363:A:N7	12:3I:33:ARG:CZ	2.83	0.42
1:13:779:C:H2'	1:13:780:A:O4'	2.20	0.42
1:13:811:C:H4'	1:13:900:A:N6	2.35	0.42
26:14:1625:C:H2'	26:14:1626:G:O4'	2.20	0.42
26:14:1820:U:O2	29:19:201:HIS:HB3	2.20	0.42
26:14:2196:C:O2'	26:14:2197:U:H5'	2.19	0.42
26:14:690:G:H2'	26:14:691:C:C6	2.54	0.42
26:14:819:A:C2'	26:14:820:A:H5'	2.50	0.42
27:16:15:A:H1'	27:16:109:G:C4	2.55	0.42
29:19:206:LEU:HD23	29:19:206:LEU:HA	1.80	0.42
2:1E:192:SER:OG	2:1E:193:ASP:N	2.51	0.42
2:1E:223:ILE:HG12	2:1E:223:ILE:H	1.52	0.42
1:1G:994:A:N7	1:1G:1216:G:H4'	2.35	0.42
1:1G:677:U:H3	1:1G:713:G:H22	1.68	0.42
26:1H:1168:G:C2	26:1H:1182:A:C2	3.08	0.42
26:1H:2159:G:C4	26:1H:2160:G:C8	3.08	0.42
26:1H:2262:U:C2'	26:1H:2263:C:H5'	2.49	0.42
26:1H:2517:C:C2	26:1H:2542:A:N6	2.87	0.42
26:1H:2552:U:O5'	26:1H:2552:U:H6	2.03	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1H:2881:C:C2	26:1H:2882:A:C8	3.07	0.42
26:1H:589:C:H2'	26:1H:590:A:H8	1.85	0.42
26:1H:58:G:N2	26:1H:70:G:C4	2.88	0.42
26:1H:825:C:H5''	62:1H:4527:HOH:O	2.19	0.42
27:1J:23:G:C2	27:1J:24:G:O6	2.73	0.42
30:21:182:LEU:HD12	30:21:183:LEU:N	2.34	0.42
31:31:165:ARG:HA	31:31:168:ARG:HD3	2.02	0.42
4:32:162:LEU:HD22	4:32:178:VAL:HG13	2.02	0.42
37:35:81:GLN:OE1	37:35:107:LYS:HB2	2.20	0.42
4:3E:74:GLN:O	4:3E:78:LEU:HG	2.20	0.42
12:3I:111:LYS:HD3	12:3I:112:ASP:N	2.35	0.42
25:4L:21:A:H61	25:4L:22:A:N6	2.18	0.42
33:59:6:ARG:HG2	33:59:7:LEU:HG	2.02	0.42
14:5A:3:ARG:HA	14:5A:4:LYS:HA	1.76	0.42
26:1H:2562:U:H1'	36:68:23:ARG:HH11	1.85	0.42
34:69:144:VAL:O	34:69:144:VAL:HG23	2.19	0.42
15:6A:75:PRO:HB2	15:6A:79:ARG:NH2	2.35	0.42
37:78:50:ARG:NH2	37:78:50:ARG:HG3	2.24	0.42
8:7E:39:LEU:HB3	8:7E:45:ILE:HG12	2.00	0.42
8:7E:60:ARG:HD3	8:7E:62:TYR:OH	2.20	0.42
9:8E:26:VAL:HA	9:8E:61:ALA:HB3	2.01	0.42
26:14:456:C:C2	45:B5:69:TYR:CE2	3.08	0.42
41:B8:105:LEU:O	41:B8:107:ASP:N	2.52	0.42
41:B8:1:MET:H2	41:B8:2:ASN:HB3	1.85	0.42
46:C5:85:VAL:HG23	46:C5:96:ILE:O	2.19	0.42
42:C8:110:VAL:O	42:C8:114:LYS:HG3	2.20	0.42
47:D5:146:ILE:HD12	47:D5:146:ILE:HA	1.88	0.42
50:G5:5:GLU:O	50:G5:8:LYS:N	2.51	0.42
46:G8:9:LYS:HA	46:G8:27:VAL:CG2	2.47	0.42
29:11:108:PRO:HG3	29:11:143:HIS:CE1	2.54	0.42
29:11:176:ARG:HH11	29:11:176:ARG:HG2	1.85	0.42
1:13:1036:G:N7	1:13:1037:C:C4	2.88	0.42
1:13:406:G:H2'	1:13:407:G:H8	1.83	0.42
1:13:417:C:H2'	1:13:418:C:C6	2.52	0.42
1:13:451:A:N6	1:13:480:U:H2'	2.35	0.42
1:13:454:C:H3'	1:13:455:C:C6	2.55	0.42
1:13:954:G:C2	1:13:955:U:C2	3.08	0.42
26:14:1384:A:N3	26:14:1405:U:H1'	2.35	0.42
26:14:1709:U:H2'	26:14:1710:C:C6	2.55	0.42
26:14:1899:G:N2	26:14:1902:C:N4	2.56	0.42
26:14:2119:A:C6	26:14:2171:A:H2	2.38	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:14:2250:G:OP2	26:14:2275:C:H2'	2.19	0.42
26:14:2467:C:H4'	38:45:123:HIS:CG	2.55	0.42
26:14:2697:G:C6	26:14:2698:U:C4	3.08	0.42
26:14:304:G:H2'	26:14:305:U:H6	1.85	0.42
27:16:77:U:OP1	47:H8:19:ARG:NH2	2.53	0.42
29:19:71:ASP:CG	29:19:103:ARG:HH22	2.23	0.42
1:1G:559:A:H4'	1:1G:560:U:H5''	2.02	0.42
26:1H:51:G:N3	26:1H:119:A:C2	2.88	0.42
26:1H:1834:U:H4'	26:1H:1969:A:C6	2.55	0.42
26:1H:1836:C:H2'	26:1H:1837:C:H6	1.84	0.42
26:1H:185:U:H2'	26:1H:186:G:H8	1.85	0.42
26:1H:1917:U:H2'	26:1H:1918:A:O4'	2.19	0.42
26:1H:2119:A:C2	26:1H:2171:A:H2	2.38	0.42
26:1H:2248:C:H2'	26:1H:2249:U:O4'	2.20	0.42
26:1H:282:A:C4	26:1H:359:A:C2	3.08	0.42
24:1L:37:A:N6	24:1L:38:A:C2	2.88	0.42
30:21:54:GLN:HB3	30:21:76:ARG:HH21	1.84	0.42
3:22:6:HIS:CE1	3:22:184:TYR:CE2	3.08	0.42
30:29:68:ALA:C	30:29:70:ALA:N	2.71	0.42
3:2E:60:ALA:N	3:2E:63:ASN:OD1	2.53	0.42
11:2I:48:ILE:HA	11:2I:48:ILE:HD12	1.73	0.42
23:2K:17:C:H5'	23:2K:62:C:OP1	2.20	0.42
31:31:178:PRO:HG2	31:31:179:GLU:CD	2.40	0.42
31:39:116:ASP:O	31:39:120:GLU:HG2	2.20	0.42
31:39:3:GLU:CA	31:39:24:LEU:HD12	2.50	0.42
31:39:51:THR:HB	31:39:88:VAL:HG11	2.02	0.42
4:3E:162:LEU:HA	4:3E:162:LEU:HD23	1.80	0.42
4:3E:18:LYS:HD3	4:3E:31:CYS:SG	2.60	0.42
4:3E:82:ALA:O	4:3E:85:LYS:HE3	2.20	0.42
24:3K:31:A:OP2	24:3K:31:A:H8	2.02	0.42
24:3L:48:C:H6	24:3L:59:A:H1'	1.84	0.42
13:4A:35:GLU:O	13:4A:38:GLY:N	2.52	0.42
13:4A:56:LEU:O	13:4A:60:VAL:HG23	2.20	0.42
13:4A:88:ARG:HG3	13:4A:88:ARG:H	1.41	0.42
33:51:71:LEU:HD12	33:51:71:LEU:HA	1.77	0.42
1:1G:673:G:H5''	6:52:87:ARG:NH1	2.35	0.42
35:58:34:LEU:HD21	35:58:120:LEU:HB2	2.02	0.42
6:5E:44:GLY:HA2	6:5E:59:TYR:CE2	2.55	0.42
7:62:36:LYS:O	7:62:39:ALA:N	2.53	0.42
15:6I:66:LEU:HA	15:6I:66:LEU:HD12	1.78	0.42
8:72:120:THR:OG1	8:72:121:ASP:N	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:85:65:ILE:HD11	42:85:96:ALA:HB3	2.02	0.42
42:85:92:ARG:HD2	43:95:11:GLN:HB2	2.01	0.42
38:88:17:LEU:HA	38:88:17:LEU:HD23	1.66	0.42
9:8E:125:TYR:HD1	9:8E:126:SER:H	1.67	0.42
39:98:44:LEU:HA	39:98:44:LEU:HD23	1.87	0.42
19:AI:39:THR:HG22	19:AI:40:ILE:H	1.84	0.42
45:B5:60:ARG:HB2	45:B5:60:ARG:HE	1.56	0.42
26:1H:2864:G:OP1	41:B8:119:LYS:HD2	2.20	0.42
20:BA:73:HIS:C	20:BA:74:LYS:HG2	2.40	0.42
46:C5:87:LYS:H	46:C5:94:LYS:HG2	1.85	0.42
47:D5:52:SER:C	47:D5:54:HIS:H	2.23	0.42
49:F5:15:ALA:O	49:F5:40:ARG:HG3	2.20	0.42
48:I8:60:PHE:CD1	48:I8:60:PHE:N	2.88	0.42
1:13:1036:G:H5'	1:13:1037:C:OP2	2.20	0.41
1:13:1176:A:H2'	1:13:1177:G:O4'	2.20	0.41
1:13:1277:C:O2'	1:13:1279:A:H8	2.03	0.41
1:13:1323:G:H2'	1:13:1324:A:C8	2.54	0.41
1:13:1338:G:C6	1:13:1339:A:C6	3.08	0.41
1:13:1508:G:H2'	1:13:1509:C:O4'	2.19	0.41
1:13:339:C:H2'	1:13:340:U:H6	1.85	0.41
1:13:502:G:OP1	12:3I:118:SER:HB2	2.19	0.41
1:13:917:G:H2'	1:13:918:A:C8	2.55	0.41
26:14:1180:C:H2'	26:14:1181:C:C6	2.54	0.41
26:14:973:A:O4'	26:14:1188:U:C6	2.73	0.41
26:14:1448:G:H2'	26:14:1449:A:C8	2.55	0.41
26:14:1582:C:O2'	26:14:1586:A:H8	2.01	0.41
26:14:1615:C:C5	26:14:1617:C:C4	3.08	0.41
26:14:1689:A:N6	26:14:1698:A:H2	2.03	0.41
26:14:1716:U:H2'	26:14:1717:G:C8	2.54	0.41
26:14:1742:C:H5'	26:14:1743:G:OP2	2.19	0.41
26:14:296:C:OP2	46:C5:4:LYS:NZ	2.44	0.41
26:14:483:A:H1'	46:C5:60:PHE:CE1	2.54	0.41
26:14:620:G:H8	26:14:622:G:O6	2.03	0.41
26:14:811:U:H2'	37:35:21:ARG:HA	2.01	0.41
26:14:825:C:H2'	26:14:826:U:O4'	2.20	0.41
10:1A:44:VAL:HG21	10:1A:66:ARG:HH21	1.85	0.41
1:1G:1063:C:H3'	1:1G:1064:G:H2'	2.02	0.41
1:1G:1258:G:H2'	1:1G:1259:C:H6	1.85	0.41
1:1G:743:U:H2'	1:1G:744:C:C6	2.55	0.41
1:1G:791:G:C6	1:1G:792:A:N7	2.87	0.41
1:1G:834:C:H2'	1:1G:835:U:H6	1.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1G:97:U:H2'	1:1G:99:C:C6	2.55	0.41
26:1H:1110:G:O2'	26:1H:1111:A:O5'	2.34	0.41
26:1H:1118:C:H2'	26:1H:1119:C:C6	2.55	0.41
26:1H:1280:G:N2	26:1H:1291:C:C2	2.88	0.41
26:1H:1628:G:H2'	26:1H:1629:U:C6	2.55	0.41
26:1H:1692:U:H2'	26:1H:1694:C:C5	2.54	0.41
26:1H:249:C:H4'	26:1H:250:G:O5'	2.20	0.41
26:1H:2649:U:H2'	26:1H:2650:U:C6	2.54	0.41
26:1H:448:U:C4	26:1H:583:G:H1'	2.55	0.41
26:1H:909:A:H2'	26:1H:912:C:C5	2.55	0.41
4:32:13:ARG:C	4:32:15:GLU:N	2.73	0.41
4:32:86:LYS:HD2	4:32:86:LYS:HA	1.75	0.41
37:35:122:PRO:O	37:35:123:LEU:HD23	2.20	0.41
26:14:805:G:C8	37:35:38:GLN:NE2	2.88	0.41
12:3A:69:TYR:CE2	12:3A:71:PRO:HA	2.55	0.41
12:3A:89:ARG:HE	12:3A:89:ARG:HB3	1.51	0.41
4:3E:107:ARG:HH22	4:3E:194:LEU:CD2	2.19	0.41
32:41:115:ARG:HB3	32:41:115:ARG:NH1	2.35	0.41
32:41:12:TYR:HA	32:41:16:ARG:HG3	2.02	0.41
32:41:125:PHE:CD1	32:41:131:TYR:HB2	2.55	0.41
5:4E:100:VAL:HA	5:4E:118:ILE:HG22	2.02	0.41
33:51:86:GLU:CD	33:51:165:ALA:HB3	2.40	0.41
33:59:99:VAL:HG13	33:59:100:GLY:H	1.84	0.41
33:59:130:ARG:O	33:59:131:VAL:HB	2.20	0.41
1:1G:4:U:O4	8:72:105:ARG:HD3	2.20	0.41
9:8E:46:ALA:O	9:8E:78:LYS:HA	2.20	0.41
43:95:97:LYS:HD3	43:95:97:LYS:HA	1.81	0.41
49:F5:49:VAL:HG21	49:F5:67:ILE:HD12	2.02	0.41
47:H8:154:ASP:OD1	47:H8:154:ASP:N	2.43	0.41
48:I8:10:THR:C	48:I8:12:ASN:H	2.24	0.41
55:P8:37:LYS:HG2	55:P8:37:LYS:O	2.20	0.41
26:1H:2422:A:N7	56:Q8:31:HIS:HE1	2.16	0.41
2:12:149:LEU:HA	2:12:149:LEU:HD23	1.78	0.41
1:13:1151:A:C2	1:13:1152:A:C5	3.08	0.41
1:13:1206:G:C6	1:13:1207:G:C5	3.08	0.41
1:13:1440:C:H2'	1:13:1441:G:O4'	2.20	0.41
1:13:492:G:C6	1:13:493:G:C4	3.07	0.41
1:13:598:U:H4'	8:7E:94:TYR:CG	2.55	0.41
1:13:621:A:H2'	1:13:622:A:O4'	2.20	0.41
1:13:693:G:H2'	1:13:694:A:C8	2.55	0.41
1:13:953:G:O5'	1:13:953:G:H8	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:14:1288:U:H4'	26:14:1289:C:OP2	2.20	0.41
26:14:1996:C:P	36:25:31:LYS:HE2	2.60	0.41
26:14:2065:C:H2'	26:14:2066:C:C6	2.55	0.41
26:14:2070:G:H2'	26:14:2071:A:C8	2.55	0.41
26:14:2130:U:O2'	26:14:2134:A:H1'	2.20	0.41
35:15:12:ARG:HG2	35:15:14:VAL:HG22	2.02	0.41
1:1G:1262:C:N4	1:1G:1273:G:H1	2.13	0.41
1:1G:183:G:O5'	1:1G:183:G:H8	2.03	0.41
1:1G:641:U:O3'	1:1G:642:A:H8	2.03	0.41
1:1G:973:G:H4'	10:1A:55:LYS:HD3	2.02	0.41
26:1H:1222:C:H2'	26:1H:1223:C:C6	2.55	0.41
26:1H:1321:A:H2'	26:1H:1322:A:O4'	2.21	0.41
26:1H:1424:G:H2'	26:1H:1425:G:O4'	2.21	0.41
26:1H:1591:G:H2'	26:1H:1592:C:C6	2.55	0.41
26:1H:2188:C:N4	26:1H:2189:U:O2	2.53	0.41
26:1H:2360:A:H2'	26:1H:2361:A:O4'	2.20	0.41
26:1H:2563:U:O2'	36:68:28:SER:HB3	2.20	0.41
26:1H:30:G:OP2	42:C8:5:LYS:NZ	2.52	0.41
26:1H:771:G:OP1	55:P8:10:ARG:NH1	2.54	0.41
27:1J:16:G:H2'	27:1J:17:C:C6	2.54	0.41
30:21:14:ILE:O	30:21:15:PHE:HB2	2.20	0.41
23:2L:30:G:N2	23:2L:42:C:O2	2.49	0.41
31:31:39:TRP:O	31:31:43:LYS:HG2	2.20	0.41
4:32:20:TYR:HD1	4:32:26:CYS:HB2	1.84	0.41
31:39:36:VAL:HG11	31:39:183:VAL:HG21	2.01	0.41
4:3E:111:ALA:HB2	4:3E:120:LEU:HD12	2.01	0.41
38:45:22:LYS:N	38:45:23:GLY:HA3	2.35	0.41
26:1H:2748:A:P	33:51:70:THR:HG21	2.60	0.41
33:59:10:PRO:O	33:59:12:PRO:HD3	2.20	0.41
33:59:97:ARG:O	33:59:99:VAL:HG12	2.20	0.41
6:5E:63:TYR:HB3	6:5E:65:VAL:HG12	2.01	0.41
14:5I:23:ARG:NH1	14:5I:30:ALA:HB2	2.31	0.41
40:65:86:ALA:O	40:65:87:PHE:HB2	2.20	0.41
26:1H:2132:U:N3	28:71:5:LYS:HD2	2.35	0.41
39:98:103:ARG:NH2	39:98:110:PRO:HD3	2.34	0.41
39:98:2:ARG:NH1	39:98:2:ARG:HB3	2.35	0.41
20:BI:35:THR:HG23	62:BI:202:HOH:O	2.20	0.41
48:E5:17:GLN:O	48:E5:19:LYS:NZ	2.46	0.41
44:E8:86:LEU:HD12	44:E8:87:PRO:CD	2.46	0.41
47:H8:17:ALA:O	47:H8:21:ALA:N	2.50	0.41
47:H8:28:MET:HE2	47:H8:37:VAL:CG1	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:14:254:G:O6	56:M5:5:LYS:HG2	2.20	0.41
2:12:164:VAL:HB	2:12:186:ALA:HB2	2.02	0.41
1:13:1021:G:H2'	1:13:1022:G:O4'	2.21	0.41
1:13:1363:A:H1'	1:13:1365:G:N7	2.35	0.41
1:13:567:G:H2'	1:13:568:G:O4'	2.20	0.41
1:13:749:C:H2'	1:13:750:G:H8	1.85	0.41
1:13:843:U:H5''	1:13:848:C:C5	2.55	0.41
1:13:912:C:O2'	1:13:913:A:H5'	2.20	0.41
26:14:1171:G:O2'	26:14:1173:G:OP2	2.37	0.41
26:14:1174:A:H2'	26:14:1176:G:OP1	2.19	0.41
26:14:1429:G:H2'	26:14:1430:C:C6	2.55	0.41
26:14:2001:A:H2'	26:14:2002:G:C8	2.55	0.41
26:14:2008:C:H2'	26:14:2009:G:H8	1.84	0.41
26:14:2070:G:C2	26:14:2442:C:C2	3.08	0.41
26:14:2228:G:C5	26:14:2229:C:C4	3.08	0.41
26:14:288:C:H2'	26:14:289:A:C8	2.55	0.41
26:14:870:A:H2'	26:14:871:U:O4'	2.19	0.41
26:14:986:C:C2'	26:14:987:G:H5'	2.50	0.41
26:14:6:A:N9	35:15:129:PRO:HB2	2.34	0.41
27:16:50:G:OP1	40:A8:63:THR:OG1	2.29	0.41
29:19:218:ARG:HB3	29:19:219:PRO:HD2	2.02	0.41
29:19:36:PRO:O	29:19:61:LEU:HD12	2.20	0.41
29:19:44:ASN:HB3	29:19:45:ASN:CA	2.34	0.41
10:1A:40:LEU:HD13	10:1A:71:LEU:HD22	2.00	0.41
10:1A:75:ILE:HG13	10:1A:76:ASN:H	1.82	0.41
2:1E:212:GLN:OE1	2:1E:216:SER:OG	2.35	0.41
1:1G:1073:U:H2'	1:1G:1074:G:H8	1.84	0.41
1:1G:1357:A:C5	1:1G:1358:U:N3	2.83	0.41
1:1G:1368:G:H4'	10:1A:46:ARG:HH22	1.85	0.41
1:1G:407:G:OP1	4:32:115:ARG:NH2	2.51	0.41
1:1G:409:G:H2'	1:1G:410:G:O4'	2.20	0.41
26:1H:1086:A:H1'	26:1H:1103:A:N1	2.35	0.41
26:1H:1198:U:H2'	26:1H:1199:U:C6	2.55	0.41
26:1H:1533:C:C6	26:1H:1534:G:H5''	2.54	0.41
26:1H:1539:G:C2	26:1H:1540:G:C5	3.08	0.41
26:1H:1591:G:H2'	26:1H:1592:C:H6	1.86	0.41
26:1H:2712:U:H1'	26:1H:2712(A):A:C8	2.55	0.41
26:1H:685:A:H1'	26:1H:688:U:O4	2.20	0.41
26:1H:881:G:H3'	26:1H:881:G:N3	2.35	0.41
30:21:93:VAL:HG21	30:21:180:ASN:HA	2.01	0.41
30:21:26:ILE:O	30:21:26:ILE:HG12	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:21:39:PRO:HD3	30:21:45:THR:HG22	2.03	0.41
1:1G:1191:A:H5''	3:22:4:LYS:HZ2	1.84	0.41
36:25:7:TYR:CE1	36:25:20:MET:HB2	2.56	0.41
30:29:37:ARG:NH1	30:29:80:GLU:OE2	2.50	0.41
23:2L:33:OMC:O2'	23:2L:34:U:H6	2.03	0.41
31:39:11:VAL:CG2	31:39:12:LEU:N	2.83	0.41
4:3E:4:TYR:CG	4:3E:5:ILE:N	2.88	0.41
12:3I:64:TYR:O	12:3I:65:GLU:HB3	2.20	0.41
32:41:44:GLY:O	32:41:47:LYS:HB2	2.20	0.41
27:16:42:C:H4'	32:41:67:LYS:HD2	2.02	0.41
5:42:13:ILE:HG13	5:42:13:ILE:O	2.20	0.41
38:45:10:ARG:CZ	38:45:10:ARG:HA	2.50	0.41
32:49:161:THR:CG2	32:49:163:ALA:H	2.30	0.41
35:58:90:MET:O	35:58:94:HIS:N	2.53	0.41
33:59:129:THR:C	33:59:130:ARG:HG3	2.39	0.41
6:5E:14:LEU:HD22	6:5E:18:GLN:HB3	2.01	0.41
14:5I:26:ARG:HB3	14:5I:43:CYS:SG	2.60	0.41
26:1H:2674:G:H5'	36:68:26:LYS:HE2	2.02	0.41
36:68:2:ILE:N	36:68:2:ILE:HD13	2.35	0.41
36:68:88:ASN:OD1	36:68:90:GLN:HB2	2.21	0.41
34:69:97:ILE:O	34:69:100:ALA:HB3	2.20	0.41
7:6E:90:GLU:H	7:6E:90:GLU:HG2	1.64	0.41
15:6I:36:ILE:HG12	15:6I:59:MET:HE3	2.02	0.41
41:75:55:ASN:ND2	41:75:55:ASN:O	2.51	0.41
62:1H:4624:HOH:O	37:78:26:GLY:HA3	2.20	0.41
8:7E:75:ARG:HE	8:7E:75:ARG:HB2	1.73	0.41
39:98:44:LEU:O	39:98:45:ARG:C	2.58	0.41
27:16:48:A:P	40:A8:30:ARG:HH22	2.43	0.41
41:B8:110:ILE:HG13	41:B8:111:ARG:N	2.35	0.41
26:1H:445:C:OP1	42:C8:2:PRO:HA	2.20	0.41
43:D8:38:LEU:HD12	43:D8:40:LEU:H	1.86	0.41
49:F5:91:LYS:HB2	49:F5:91:LYS:HE2	1.67	0.41
49:F5:95:LEU:HA	49:F5:95:LEU:HD13	1.76	0.41
47:H8:124:ILE:HD12	47:H8:125:LEU:H	1.84	0.41
47:H8:132:ASN:HD22	47:H8:160:GLY:HA3	1.85	0.41
47:H8:53:ILE:HG13	47:H8:53:ILE:O	2.21	0.41
56:M5:40:GLU:HG3	56:M5:43:GLN:HB2	2.03	0.41
1:13:1180:A:OP1	9:8E:103:THR:OG1	2.34	0.41
1:13:1223:C:P	19:AI:78:ARG:NH1	2.92	0.41
1:13:738:C:H2'	1:13:739:C:C6	2.55	0.41
26:14:107:C:H2'	26:14:108:U:C6	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:14:1204:A:N1	26:14:1241:A:H2	2.18	0.41
26:14:1849:G:H2'	26:14:1850:G:H8	1.86	0.41
26:14:2238:G:H4'	26:14:2239:G:N7	2.35	0.41
26:14:2273:A:O2'	26:14:2274:A:H5'	2.20	0.41
26:14:2298:A:N6	26:14:2318:G:C8	2.86	0.41
26:14:2570:G:H2'	26:14:2571:C:O4'	2.21	0.41
26:14:2775:A:N7	62:14:3613:HOH:O	2.52	0.41
26:14:362:U:H5'	26:14:363:G:OP2	2.21	0.41
26:14:577:G:H8	26:14:577:G:O5'	2.04	0.41
26:14:589:C:H5''	31:39:95:ARG:HH12	1.85	0.41
26:14:753:C:H2'	26:14:754:C:H6	1.84	0.41
35:15:4:TYR:O	42:85:64:ARG:NH1	2.53	0.41
29:19:130:ALA:HA	29:19:192:THR:HA	2.01	0.41
1:1G:1207:G:H2'	1:1G:1208:C:C6	2.55	0.41
1:1G:598:U:H4'	8:72:94:TYR:CG	2.55	0.41
1:1G:947:G:H2'	1:1G:948:C:H6	1.85	0.41
26:1H:1182:A:H2'	26:1H:1183:G:O4'	2.21	0.41
26:1H:1191:G:P	62:1H:3785:HOH:O	2.79	0.41
26:1H:1401:G:H2'	26:1H:1402:C:C6	2.56	0.41
26:1H:2692:C:OP1	26:1H:2871:C:H5'	2.20	0.41
26:1H:270(E):G:C6	26:1H:270(F):U:C4	3.09	0.41
26:1H:2849:U:H1'	26:1H:2866:U:O2	2.20	0.41
26:1H:2883:A:H5'	26:1H:2884:U:H5'	2.02	0.41
26:1H:320:A:H2'	31:31:136:THR:CG2	2.49	0.41
26:1H:259:G:N2	26:1H:621:A:C8	2.86	0.41
26:1H:657:U:H2'	26:1H:658:C:C6	2.56	0.41
26:1H:725:G:C6	26:1H:726:G:N1	2.88	0.41
27:1J:10:C:C4	27:1J:11:C:C5	3.08	0.41
27:1J:88:C:H4'	27:1J:89:G:OP2	2.21	0.41
30:21:201:THR:HB	30:21:203:LYS:HA	2.02	0.41
36:25:9:GLU:O	36:25:83:ALA:HA	2.20	0.41
30:29:101:ARG:NH2	30:29:171:GLU:HB2	2.34	0.41
11:2I:79:SER:HB2	11:2I:106:LYS:CD	2.50	0.41
23:2L:36:A:H2'	23:2L:37:U:C6	2.55	0.41
31:31:196:LEU:C	31:31:197:ASP:O	2.58	0.41
1:13:407:G:O2'	4:3E:116:GLN:HG3	2.21	0.41
24:3K:53:G:H1	24:3K:61:C:N4	2.18	0.41
26:14:960:A:H61	38:45:83:MET:HE2	1.86	0.41
39:55:35:THR:CG2	39:55:100:LEU:HD11	2.51	0.41
35:58:30:ILE:HG22	35:58:34:LEU:HD22	2.02	0.41
34:61:77:LEU:H	34:61:77:LEU:HD12	1.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:62:141:VAL:O	7:62:143:ARG:HG3	2.20	0.41
36:68:106:LEU:HD23	36:68:106:LEU:HA	1.84	0.41
15:6I:3:ILE:HA	15:6I:7:GLU:OE1	2.19	0.41
28:71:39:GLU:O	28:71:178:ALA:HB2	2.19	0.41
37:78:114:ILE:HD13	37:78:114:ILE:HG21	1.87	0.41
17:8I:25:ARG:O	17:8I:25:ARG:HG2	2.19	0.41
19:AI:18:LYS:O	19:AI:22:LEU:HD13	2.19	0.41
41:B8:12:SER:CB	41:B8:14:TYR:H	2.33	0.41
43:D8:22:VAL:HG12	43:D8:23:GLU:O	2.20	0.41
43:D8:76:LYS:O	43:D8:79:VAL:HG12	2.20	0.41
51:H5:18:ASP:OD1	51:H5:18:ASP:N	2.53	0.41
47:H8:47:VAL:O	47:H8:50:GLN:HB2	2.21	0.41
48:I8:19:LYS:HD3	48:I8:19:LYS:HA	1.67	0.41
50:K8:4:SER:H	50:K8:7:ARG:N	2.10	0.41
50:K8:64:LEU:HD21	50:K8:68:ARG:NH1	2.35	0.41
26:1H:2347:C:P	54:O8:39:TYR:HH	2.36	0.41
2:12:16:HIS:ND1	2:12:213:LEU:HD22	2.35	0.41
1:13:109:A:N7	1:13:326:G:H2'	2.35	0.41
1:13:192:U:O4'	20:BI:103:GLY:HA2	2.21	0.41
1:13:254:G:O3'	17:8I:69:LYS:NZ	2.43	0.41
1:13:498:A:H4'	1:13:500:G:OP1	2.21	0.41
1:13:66:G:O4'	1:13:173:U:C4	2.74	0.41
1:13:77:C:H2'	1:13:78:G:C8	2.54	0.41
26:14:1392:A:N6	26:14:1393:A:N6	2.68	0.41
26:14:1505:C:H2'	26:14:1506:C:H6	1.85	0.41
26:14:1568:G:OP2	29:19:63:ARG:NH2	2.53	0.41
26:14:1751:C:H2'	26:14:1752:C:C6	2.56	0.41
26:14:1963:U:H4'	26:14:1964:G:OP2	2.20	0.41
26:14:571:A:H5'	26:14:2030:A:N7	2.35	0.41
26:14:212:G:H2'	26:14:213:A:O4'	2.21	0.41
26:14:2569:G:C2	26:14:2570:G:C8	3.09	0.41
26:14:2607:G:H2'	26:14:2608:G:O4'	2.20	0.41
26:14:2749:A:O5'	26:14:2749:A:H8	2.04	0.41
26:14:696:G:H2'	26:14:697:C:H6	1.84	0.41
26:14:864:G:C2'	26:14:865:C:H5'	2.50	0.41
27:16:40:U:C1'	27:16:45:A:H61	2.33	0.41
1:1G:1123:A:H4'	10:1A:37:PRO:HD2	2.01	0.41
2:1E:131:PRO:O	2:1E:135:GLN:HG3	2.21	0.41
2:1E:178:ARG:HD3	2:1E:178:ARG:HA	1.82	0.41
2:1E:213:LEU:HG	2:1E:213:LEU:H	1.58	0.41
1:1G:1077:G:N2	1:1G:1080:A:OP2	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1G:1216:G:H2'	1:1G:1217:C:H6	1.85	0.41
1:1G:1277:C:H1'	1:1G:1282:C:O2	2.21	0.41
1:1G:1321:C:N4	1:1G:1322:C:N4	2.66	0.41
1:1G:161:A:C6	1:1G:162:A:C6	3.08	0.41
1:1G:631:G:OP2	1:1G:631:G:H8	2.03	0.41
1:1G:833:U:O2'	1:1G:834:C:H5'	2.21	0.41
26:1H:991:C:C4	26:1H:1185:C:N4	2.89	0.41
26:1H:1222:C:H2'	26:1H:1223:C:H6	1.86	0.41
26:1H:1475:G:H2'	26:1H:1476:C:C6	2.56	0.41
26:1H:1380:G:N2	26:1H:1570:A:C2	2.88	0.41
26:1H:729:G:C4	26:1H:1775:U:O2	2.74	0.41
26:1H:2707:G:O3'	39:98:68:ARG:HG2	2.21	0.41
26:1H:311:A:C6	26:1H:328:U:C4	3.09	0.41
26:1H:639:U:O2'	26:1H:640:C:H5'	2.21	0.41
26:1H:910:A:H2'	26:1H:911:A:C8	2.55	0.41
30:21:47:VAL:HG11	30:21:86:PRO:HD2	2.01	0.41
26:14:2572:A:N7	30:29:144:ARG:HD2	2.36	0.41
3:2E:27:LYS:HA	3:2E:27:LYS:HD2	1.77	0.41
31:39:11:VAL:HG22	31:39:13:SER:HB2	2.01	0.41
4:3E:119:GLN:HG2	4:3E:119:GLN:O	2.21	0.41
4:3E:188:LEU:HA	4:3E:188:LEU:HD22	1.81	0.41
32:41:173:LEU:HD12	32:41:178:PHE:CD2	2.56	0.41
5:42:101:ILE:HG12	5:42:101:ILE:H	1.74	0.41
5:42:90:VAL:HG23	5:42:121:LYS:HB3	2.02	0.41
32:49:106:LEU:HG	32:49:111:LEU:CD1	2.50	0.41
32:49:64:THR:HB	32:49:94:LEU:HD21	2.02	0.41
13:4I:12:ASN:HD22	13:4I:13:LYS:H	1.69	0.41
13:4I:13:LYS:HZ3	13:4I:13:LYS:HA	1.85	0.41
33:59:117:PRO:HB3	33:59:123:PHE:HZ	1.84	0.41
26:1H:2128:C:H3'	28:71:36:LYS:NZ	2.35	0.41
41:75:16:ARG:NH2	41:75:19:LEU:HD21	2.35	0.41
41:75:27:THR:OG1	41:75:89:VAL:HG22	2.20	0.41
37:78:116:GLY:N	37:78:134:ALA:HB2	2.35	0.41
37:78:38:GLN:O	37:78:44:GLY:HA2	2.19	0.41
16:7A:43:LYS:HG2	16:7A:48:TRP:CG	2.55	0.41
9:8E:48:GLU:N	9:8E:49:PRO:HD2	2.35	0.41
19:AA:41:VAL:HG23	19:AA:43:GLU:N	2.36	0.41
41:B8:33:LYS:HG2	41:B8:82:LEU:O	2.20	0.41
20:BA:100:ILE:HG23	20:BA:101:GLY:N	2.35	0.41
20:BI:35:THR:O	20:BI:38:LYS:HB2	2.21	0.41
42:C8:92:ARG:HB2	43:D8:11:GLN:NE2	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:D8:75:PHE:HD1	43:D8:82:ARG:HG3	1.86	0.41
47:H8:72:ARG:HA	47:H8:72:ARG:HD3	1.90	0.41
48:I8:24:LYS:HG3	48:I8:36:ILE:HD11	2.02	0.41
54:O8:29:ASN:O	54:O8:32:ASN:HB3	2.21	0.41
2:12:187:LEU:HA	2:12:201:ILE:O	2.20	0.41
2:12:219:VAL:HG23	2:12:221:LEU:H	1.86	0.41
1:13:1252:A:H2'	1:13:1253:G:O4'	2.20	0.41
1:13:263:A:OP2	20:BI:79:ARG:NH1	2.54	0.41
1:13:322:C:OP2	1:13:328:C:N4	2.53	0.41
1:13:358:U:OP1	34:69:87:LYS:NZ	2.50	0.41
1:13:26:A:N6	1:13:558:G:O2'	2.46	0.41
1:13:768:A:H2'	1:13:769:G:O4'	2.21	0.41
26:14:1952:A:C6	26:14:1953:A:C6	3.09	0.41
26:14:2077:A:O2'	26:14:2078:C:H5'	2.21	0.41
26:14:2303:G:C2'	26:14:2304:G:H5'	2.50	0.41
27:16:60:C:N3	27:16:61:G:N7	2.68	0.41
1:1G:114:U:O2'	1:1G:115:G:H5'	2.20	0.41
1:1G:1386:G:C2	1:1G:1387:G:C8	3.09	0.41
1:1G:517:G:N2	1:1G:530:G:OP1	2.44	0.41
26:1H:1176:G:H5'	26:1H:1177:A:P	2.61	0.41
26:1H:2070:G:C2	26:1H:2442:C:C2	3.08	0.41
26:1H:2154:G:O5'	26:1H:2154:G:H8	2.03	0.41
26:1H:2666:C:H3'	26:1H:2667:C:H6	1.86	0.41
26:1H:2688:U:H1'	26:1H:2721:A:N6	2.35	0.41
26:1H:2807:G:H3'	26:1H:2808:U:H5''	2.02	0.41
26:1H:330:A:O2'	26:1H:331:A:C8	2.72	0.41
26:1H:70:G:H21	26:1H:71:A:H62	1.59	0.41
26:1H:803:U:C4	26:1H:804:A:N7	2.88	0.41
24:1L:2:G:N3	24:1L:2:G:H2'	2.36	0.41
3:22:156:ARG:NH2	3:22:159:GLY:O	2.40	0.41
11:2I:59:TYR:O	11:2I:63:LEU:HD12	2.21	0.41
23:2K:29:C:H2'	23:2K:30:G:H8	1.86	0.41
37:35:134:ALA:O	37:35:138:LEU:HB2	2.20	0.41
24:3K:28:U:H2'	24:3K:29:U:C6	2.56	0.41
32:41:135:LEU:O	32:41:154:GLY:HA3	2.20	0.41
13:4A:33:ALA:HA	13:4A:59:TYR:CE2	2.55	0.41
33:51:13:LYS:HD3	33:51:13:LYS:HA	1.83	0.41
39:55:87:TYR:HD1	39:55:90:ARG:HE	1.68	0.41
35:58:99:LEU:HD23	35:58:99:LEU:HA	1.77	0.41
28:7I:41:VAL:HA	28:7I:216:THR:HG23	2.02	0.41
16:7I:45:THR:HB	16:7I:47:ASP:OD1	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:7I:67:THR:H	16:7I:70:ALA:HB3	1.85	0.41
17:8A:45:HIS:CD2	17:8A:47:PRO:HD3	2.55	0.41
43:95:84:LYS:O	43:95:85:LYS:HG3	2.20	0.41
39:98:118:GLU:OE1	39:98:118:GLU:HA	2.21	0.41
26:14:26:G:OP1	44:A5:80:PRO:HB3	2.21	0.41
20:BA:50:GLU:HA	20:BA:100:ILE:CG2	2.50	0.41
1:13:103:C:OP2	20:BI:14:LYS:HD2	2.20	0.41
26:14:329:G:H1	46:C5:19:LYS:NZ	2.18	0.41
46:C5:64:GLU:HG3	46:C5:64:GLU:H	1.70	0.41
44:E8:24:ILE:HG12	44:E8:36:LEU:HD21	2.02	0.41
49:F5:73:LEU:HA	49:F5:73:LEU:HD23	1.87	0.41
47:H8:25:PRO:O	47:H8:85:HIS:HA	2.20	0.41
55:L5:34:ARG:NH1	55:L5:41:ARG:O	2.54	0.41
1:13:1223:C:OP1	19:AI:78:ARG:NH1	2.54	0.41
1:13:1256:A:O2'	1:13:1257:U:P	2.79	0.41
1:13:658:G:H2'	1:13:659:U:C6	2.56	0.41
26:14:117:G:C6	26:14:119:A:C6	3.08	0.41
26:14:1322:A:N1	26:14:1333:C:O2'	2.35	0.41
26:14:1542:G:O5'	26:14:1543:A:H5''	2.20	0.41
26:14:1966:A:H4'	26:14:1967:C:OP1	2.20	0.41
26:14:2535:G:N3	26:14:2536:G:C8	2.89	0.41
26:14:2591:C:H2'	26:14:2592:G:H8	1.85	0.41
26:14:2522:U:H4'	26:14:2648:C:OP1	2.21	0.41
26:14:2698:U:H2'	26:14:2699:C:C6	2.56	0.41
26:14:2852:G:H2'	26:14:2853:C:C6	2.56	0.41
26:14:732:C:C5	61:14:3437:SPE:H102	2.56	0.41
27:16:66:A:C5	27:16:108:C:C5	3.09	0.41
27:16:71:C:C2	27:16:72:G:C8	3.08	0.41
2:1E:149:LEU:HD23	2:1E:149:LEU:HA	1.71	0.41
1:1G:1328:C:O2'	13:4A:29:ARG:NH2	2.47	0.41
1:1G:167:G:O2'	1:1G:168:G:H5'	2.20	0.41
1:1G:271:C:H2'	1:1G:272:C:H6	1.86	0.41
1:1G:345:C:H4'	1:1G:346:G:O5'	2.20	0.41
1:1G:427:U:H4'	1:1G:541:G:H5''	2.02	0.41
1:1G:672:U:H2'	1:1G:673:G:C8	2.55	0.41
1:1G:741:G:H2'	1:1G:742:G:O4'	2.21	0.41
26:1H:1087:G:N7	26:1H:1089:G:H1'	2.35	0.41
26:1H:1091:G:C6	26:1H:1101:U:C2	3.09	0.41
26:1H:1164:G:C6	26:1H:1165:U:C4	3.09	0.41
26:1H:1389:G:C2	26:1H:1390:U:C2	3.09	0.41
26:1H:1677:A:H2'	26:1H:1678:G:C8	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1H:1894:C:C2'	26:1H:1895:C:H5'	2.51	0.41
26:1H:1931:U:H5	26:1H:1969:A:N7	2.18	0.41
26:1H:2000:G:OP1	39:98:5:LYS:NZ	2.51	0.41
26:1H:2347:C:H4'	54:O8:39:TYR:HE1	1.86	0.41
26:1H:2359:C:H2'	26:1H:2360:A:O4'	2.21	0.41
26:1H:2395:C:H5''	26:1H:2396:G:OP2	2.20	0.41
26:1H:2688:U:H1'	26:1H:2721:A:H61	1.86	0.41
26:1H:654:A:N3	26:1H:654(A):A:H5''	2.35	0.41
26:1H:934:G:H2'	26:1H:935:C:H6	1.86	0.41
26:1H:956:G:H5''	26:1H:957:A:OP2	2.21	0.41
4:32:132:ARG:HB3	4:32:132:ARG:HE	1.41	0.41
4:32:15:GLU:OE1	4:32:59:ARG:NH2	2.43	0.41
4:32:31:CYS:HA	59:32:302:SF4:S2	2.60	0.41
4:32:39:PRO:O	4:32:44:GLY:HA3	2.21	0.41
26:14:661:C:H4'	37:35:13:ASN:OD1	2.20	0.41
31:39:110:LEU:HD21	31:39:181:LEU:HD22	2.03	0.41
12:3A:10:LEU:HB3	17:8A:32:TYR:CE2	2.56	0.41
1:1G:363:A:C5	12:3A:31:PRO:HD2	2.55	0.41
12:3A:40:VAL:HG11	12:3A:75:HIS:HE1	1.86	0.41
32:49:53:LEU:O	32:49:57:ALA:N	2.53	0.41
32:49:81:LYS:HB3	32:49:82:LEU:H	1.52	0.41
13:4I:117:VAL:O	13:4I:118:ALA:HB2	2.21	0.41
25:4K:23:A:O2'	25:4K:24:A:N7	2.37	0.41
33:51:80:SER:C	33:51:81:GLU:HG3	2.40	0.41
39:55:21:TYR:OH	39:55:43:GLU:HG2	2.21	0.41
6:5E:35:ALA:HA	6:5E:67:MET:HB3	2.02	0.41
6:5E:33:TYR:HD1	6:5E:71:ARG:HB3	1.86	0.41
40:65:80:LEU:HD23	40:65:80:LEU:HA	1.86	0.41
15:6A:87:ILE:HG22	15:6A:88:ARG:H	1.85	0.41
8:7E:77:GLU:HG2	8:7E:78:GLN:N	2.36	0.41
42:85:16:LYS:HE3	42:85:16:LYS:HB3	1.91	0.41
38:88:32:TYR:CE2	38:88:133:ARG:HG3	2.56	0.41
18:9I:22:VAL:HA	18:9I:25:THR:OG1	2.21	0.41
44:A5:18:ARG:HA	44:A5:76:VAL:HG11	2.03	0.41
24:3K:76:A:H5''	49:J8:30:VAL:HG11	2.02	0.41
29:11:108:PRO:HD2	29:11:111:LEU:HG	2.02	0.41
29:11:118:VAL:HG22	29:11:119:ALA:N	2.36	0.41
29:11:127:VAL:HA	29:11:193:VAL:HG22	2.02	0.41
26:1H:1568:G:P	29:11:63:ARG:HH12	2.44	0.41
29:11:80:ALA:HB2	29:11:96:HIS:CD2	2.56	0.41
2:12:168:THR:HG21	2:12:191:ASP:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:13:339:C:H2'	1:13:340:U:C6	2.56	0.41
1:13:664:G:N2	1:13:741:G:H1	2.11	0.41
26:14:1681:G:N2	62:14:3653:HOH:O	2.20	0.41
26:14:1829:A:N3	29:19:15:PHE:HE2	2.19	0.41
26:14:2134:A:H2'	26:14:2134:A:N3	2.36	0.41
26:14:807:U:H4'	26:14:2446:G:OP1	2.20	0.41
26:14:2500:U:H5''	26:14:2501:C:OP2	2.21	0.41
26:14:2688:U:H1'	26:14:2721:A:N6	2.35	0.41
26:14:547:A:H2'	26:14:548:A:C8	2.56	0.41
26:14:670:A:H4'	26:14:671:C:O5'	2.20	0.41
26:14:807:U:C2	26:14:808:G:C8	3.08	0.41
29:19:132:PRO:HA	29:19:189:CYS:O	2.20	0.41
1:1G:1152:A:H5'	10:1A:13:HIS:CD2	2.55	0.41
1:1G:1264:C:H1'	1:1G:1272:G:N2	2.36	0.41
1:1G:1300:G:O2'	1:1G:1301:U:P	2.78	0.41
1:1G:1465:C:H2'	1:1G:1466:C:O4'	2.21	0.41
1:1G:339:C:H2'	1:1G:340:U:C6	2.55	0.41
1:1G:909:A:H2'	1:1G:910:C:O4'	2.20	0.41
26:1H:1176:G:H5'	26:1H:1177:A:OP2	2.20	0.41
26:1H:2129:C:P	28:71:6:ARG:HH11	2.44	0.41
26:1H:2131:G:H1'	26:1H:2158:A:C6	2.55	0.41
26:1H:1889:A:N1	26:1H:2234:G:H1'	2.35	0.41
26:1H:2820:A:HO2'	26:1H:2821:A:P	2.43	0.41
26:1H:957:A:N1	26:1H:2458:G:H4'	2.35	0.41
27:1J:15:A:H1'	27:1J:109:G:C4	2.56	0.41
30:21:181:LEU:HD12	30:21:181:LEU:HA	1.85	0.41
30:21:23:VAL:HA	30:21:184:VAL:O	2.20	0.41
30:29:32:PRO:HA	30:29:90:THR:HA	2.03	0.41
37:35:71:VAL:CG1	37:35:72:PRO:HD3	2.46	0.41
31:39:143:ALA:O	31:39:148:LEU:HB2	2.20	0.41
4:3E:207:TYR:O	4:3E:209:ARG:HG3	2.21	0.41
24:3K:1:G:N2	24:3K:2:G:N7	2.69	0.41
13:4A:81:LEU:HD12	13:4A:89:GLY:HA3	2.03	0.41
6:52:86:ARG:O	6:52:87:ARG:HG2	2.20	0.41
35:58:127:ASP:OD1	35:58:127:ASP:N	2.53	0.41
33:59:20:ALA:HB3	33:59:23:ARG:O	2.21	0.41
40:65:3:ARG:HD2	40:65:4:LEU:N	2.36	0.41
7:6E:15:ASP:O	7:6E:19:GLY:HA2	2.20	0.41
37:78:60:MET:HE3	37:78:60:MET:HB2	1.94	0.41
9:82:20:ARG:O	9:82:20:ARG:HG3	2.21	0.41
9:82:48:GLU:N	9:82:49:PRO:HD2	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:88:17:LEU:HB3	38:88:39:PRO:HB2	2.03	0.41
9:8E:82:ALA:O	9:8E:86:VAL:HG23	2.21	0.41
43:95:12:TYR:CD1	43:95:12:TYR:N	2.88	0.41
19:AI:51:VAL:HB	19:AI:75:ALA:HB2	2.03	0.41
45:B5:66:LEU:HD23	45:B5:66:LEU:HA	1.82	0.41
41:B8:1:MET:HA	41:B8:3:ARG:N	2.35	0.41
20:BI:49:ALA:HA	20:BI:92:LEU:HD11	2.03	0.41
29:11:33:LEU:HD12	29:11:33:LEU:HA	1.73	0.41
2:12:167:PRO:O	2:12:171:ALA:N	2.54	0.41
2:12:218:ALA:O	2:12:219:VAL:HG22	2.21	0.41
1:13:1134:G:N1	1:13:1135:U:H1'	2.35	0.41
1:13:1277:C:O2'	1:13:1279:A:H1'	2.20	0.41
1:13:1286:A:C2	21:1F:18:TYR:OH	2.74	0.41
1:13:1326:C:H2'	1:13:1327:C:H6	1.86	0.41
1:13:200:G:N2	1:13:218:C:C2	2.88	0.41
1:13:199:G:H2'	1:13:200:G:O4'	2.21	0.41
1:13:416:G:C6	1:13:417:C:C4	3.08	0.41
26:14:597:U:H2'	26:14:598:G:H8	1.83	0.41
26:14:863:A:H2'	26:14:864:G:C8	2.55	0.41
26:14:861:A:C2	26:14:917:A:C4	3.09	0.41
26:14:933:A:C5	26:14:934:G:C8	3.09	0.41
26:14:950:G:C2	26:14:968:G:C2	3.09	0.41
29:19:126:GLN:O	29:19:193:VAL:HG22	2.21	0.41
29:19:16:MET:HG3	29:19:206:LEU:O	2.21	0.41
2:1E:130:ARG:HA	2:1E:131:PRO:HD3	1.92	0.41
2:1E:68:ILE:HG13	2:1E:161:ALA:HB3	2.02	0.41
1:1G:1104:G:H4'	2:12:111:ARG:NH2	2.35	0.41
1:1G:1385:G:C6	1:1G:1386:G:N7	2.88	0.41
1:1G:1517:G:C6	1:1G:1518:A:C5	3.08	0.41
1:1G:15:G:H2'	1:1G:16:A:C8	2.55	0.41
1:1G:690:G:H2'	1:1G:691:G:C8	2.56	0.41
26:1H:1047:G:H2'	26:1H:1110:G:N1	2.35	0.41
26:1H:1152:C:H4'	42:C8:77:SER:HA	2.03	0.41
26:1H:1583:A:O5'	26:1H:1585:C:H5	2.04	0.41
26:1H:1657:C:H2'	26:1H:1658:C:C6	2.56	0.41
26:1H:2331:G:C4'	48:I8:42:GLY:HA3	2.51	0.41
26:1H:2346:A:H5'	26:1H:2383:G:O4'	2.21	0.41
26:1H:2507:C:H5'	26:1H:2573:C:N4	2.36	0.41
27:1J:13:A:N1	27:1J:69:G:O2'	2.43	0.41
27:1J:51:G:C6	27:1J:52:A:H2	2.38	0.41
30:21:35:GLN:HB3	30:21:48:GLN:HB2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:22:172:ARG:HE	3:22:172:ARG:HB3	1.68	0.41
36:25:11:ALA:HB1	36:25:99:PHE:O	2.21	0.41
31:31:135:LYS:HB3	31:31:138:GLU:HG3	2.03	0.41
31:39:170:LEU:HA	31:39:171:PRO:HD3	1.90	0.41
31:39:194:MET:HB2	31:39:194:MET:HE3	1.83	0.41
24:3K:72:C:N3	24:3K:73:A:C8	2.89	0.41
24:3L:55:U:H2'	24:3L:57:G:OP1	2.21	0.41
5:42:90:VAL:O	5:42:120:THR:HA	2.20	0.41
32:49:136:ARG:HD3	32:49:137:GLU:HG3	2.03	0.41
32:49:14:GLU:O	32:49:17:PRO:HG2	2.21	0.41
32:49:84:LYS:HE2	32:49:84:LYS:HB3	1.92	0.41
33:51:92:ILE:HD12	33:51:92:ILE:N	2.36	0.41
35:58:39:ARG:NH2	35:58:41:ASP:OD2	2.54	0.41
26:1H:1141:U:C5	35:58:64:GLY:HA3	2.56	0.41
14:5I:3:ARG:HG3	14:5I:4:LYS:N	2.35	0.41
7:62:108:ALA:O	7:62:111:ARG:HG3	2.21	0.41
34:69:140:LEU:HD12	34:69:140:LEU:HA	1.74	0.41
34:69:41:GLU:HA	34:69:44:LEU:HB2	2.03	0.41
15:6A:48:LYS:HB2	15:6A:48:LYS:HE3	1.87	0.41
1:1G:878:G:H1'	8:72:3:THR:HG21	2.03	0.41
9:8E:70:LYS:O	9:8E:74:ILE:HG13	2.20	0.41
39:98:57:ARG:HB3	39:98:59:ASP:OD1	2.20	0.41
39:98:22:ARG:HG2	39:98:69:ASP:HB3	2.03	0.41
39:98:98:LEU:HA	39:98:98:LEU:HD23	1.86	0.41
42:C8:95:LEU:HD22	43:D8:4:ILE:CD1	2.49	0.41
26:1H:302:C:OP1	46:G8:81:LYS:HD3	2.21	0.41
48:I8:66:VAL:O	48:I8:82:ARG:N	2.53	0.41
27:16:12:C:O2'	48:I8:74:ARG:HG2	2.20	0.41
53:J5:12:SER:OG	53:J5:15:ARG:HB2	2.20	0.41
29:11:16:MET:HG3	29:11:207:GLY:HA3	2.03	0.41
1:13:1157:A:C6	1:13:1180:A:C5	3.09	0.41
1:13:1179:A:H4'	9:8E:103:THR:HA	2.03	0.41
1:13:1260:C:H6	1:13:1260:C:H3'	1.86	0.41
1:13:160:A:H2'	1:13:160:A:N3	2.35	0.41
1:13:240:C:H2'	1:13:241:C:H6	1.85	0.41
1:13:564:C:O2'	8:7E:91:ARG:NH2	2.53	0.41
1:13:703:G:O5'	1:13:703:G:C8	2.71	0.41
26:14:1019:U:H2'	26:14:1020:A:H8	1.86	0.41
26:14:1628:G:H2'	26:14:1629:U:H6	1.85	0.41
26:14:2287:A:H61	26:14:2344:U:H3	1.60	0.41
26:14:2579:C:C4'	30:29:134:ILE:HG12	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:14:2716:U:O2'	26:14:2717:G:H5'	2.21	0.41
26:14:271:G:H2'	26:14:272:G:C8	2.56	0.41
26:14:488:G:N2	26:14:492:A:OP2	2.54	0.41
2:1E:55:PHE:HD1	2:1E:58:ILE:HD12	1.83	0.41
1:1G:1285:A:OP1	1:1G:1285:A:H8	2.03	0.41
1:1G:1343:G:O2'	1:1G:1344:C:H5'	2.21	0.41
1:1G:1415:G:C6	1:1G:1486:G:C6	3.08	0.41
1:1G:109:A:C6	1:1G:326:G:C6	3.08	0.41
1:1G:445:G:H2'	1:1G:446:G:H8	1.86	0.41
1:1G:629:G:H3'	1:1G:630:G:H5''	2.02	0.41
1:1G:693:G:H2'	1:1G:694:A:C8	2.56	0.41
26:1H:1970:A:H4'	26:1H:1971:A:OP1	2.21	0.41
26:1H:2145:C:H5	26:1H:2148:G:N2	2.17	0.41
26:1H:2783:G:H2'	26:1H:2784:C:C6	2.55	0.41
26:1H:2791:C:N4	26:1H:2807:G:H1	2.19	0.41
30:21:174:ASP:OD1	30:21:175:VAL:N	2.54	0.41
26:14:2052:G:O4'	30:29:142:GLY:HA3	2.21	0.41
11:2I:59:TYR:CZ	11:2I:63:LEU:HD11	2.56	0.41
4:32:162:LEU:HD12	4:32:181:MET:CE	2.50	0.41
31:39:152:GLU:HA	31:39:190:GLU:OE2	2.20	0.41
31:39:47:GLY:O	31:39:94:PRO:HA	2.21	0.41
24:3K:22:G:N2	24:3K:23:A:N7	2.68	0.41
24:3L:55:U:N3	24:3L:58:A:OP1	2.36	0.41
13:4I:7:VAL:H	32:41:115:ARG:HH12	1.69	0.41
5:4E:126:ARG:HH11	5:4E:126:ARG:HG3	1.85	0.41
26:1H:2758:A:C4	33:51:67:LEU:HD21	2.56	0.41
1:1G:1114:C:O2'	14:5A:60:SER:O	2.33	0.41
7:6E:113:GLU:HG2	7:6E:119:ARG:HG2	2.03	0.41
8:72:85:ARG:NH1	8:72:134:ILE:HG23	2.35	0.41
16:7A:11:SER:HB2	16:7A:14:ASN:HB3	2.03	0.41
20:BA:48:LYS:O	20:BA:50:GLU:N	2.54	0.41
26:14:2432:A:C2	49:F5:35:THR:HG22	2.56	0.41
46:G8:28:LYS:NZ	46:G8:40:GLU:HG3	2.36	0.41
56:Q8:14:VAL:HG11	56:Q8:58:ILE:HG21	2.02	0.41
1:13:1023:G:H3'	1:13:1024:G:C5'	2.48	0.41
1:13:439:A:C8	1:13:440:A:C8	3.09	0.41
1:13:12:U:O2'	1:13:526:C:H4'	2.21	0.41
26:14:1328:G:H2'	26:14:1330:C:C4	2.56	0.41
26:14:1685:C:H2'	26:14:1686:C:C6	2.56	0.41
26:14:1827:C:O2'	26:14:1828:G:H5'	2.21	0.41
26:14:2273:A:H2'	26:14:2274:A:H8	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:14:2305:A:H8	32:49:156:ASP:OD1	2.03	0.41
26:14:2369:A:H2'	26:14:2370:G:H8	1.86	0.41
26:14:2430:A:OP1	62:14:3659:HOH:O	2.22	0.41
26:14:2711:A:P	62:14:3507:HOH:O	2.78	0.41
26:14:442:G:HO2'	26:14:444:C:H6	1.67	0.41
26:14:522:G:H2'	26:14:523:C:C6	2.56	0.41
26:14:564:C:H2'	26:14:565:C:O4'	2.21	0.41
35:15:56:ASN:N	35:15:125:GLY:HA3	2.32	0.41
1:1G:1128:C:H4'	9:82:16:ARG:HH22	1.85	0.41
1:1G:1292:U:H2'	1:1G:1293:G:C8	2.56	0.41
1:1G:1410:G:H2'	1:1G:1411:C:H6	1.86	0.41
1:1G:1414:U:H2'	1:1G:1415:G:C8	2.56	0.41
1:1G:448:A:H2'	1:1G:449:C:O2	2.21	0.41
1:1G:7:G:H5'	1:1G:298:A:O4'	2.20	0.41
1:1G:926:G:C6	1:1G:1505:G:C6	3.08	0.41
1:1G:984:C:H2'	1:1G:985:C:C6	2.56	0.41
26:1H:1204:A:H2	26:1H:1241:A:N1	2.18	0.41
26:1H:125:G:C6	55:P8:10:ARG:HG3	2.56	0.41
26:1H:1533:C:H2'	26:1H:1534:G:C8	2.56	0.41
26:1H:1580:A:OP2	26:1H:1580:A:H8	2.04	0.41
26:1H:2430:A:H8	26:1H:2431:U:C5	2.38	0.41
26:1H:2483:C:C2	38:88:124:LYS:HE3	2.56	0.41
26:1H:654(R):C:C2'	26:1H:654(S):G:H5'	2.51	0.41
27:1J:57:A:C2'	27:1J:58:A:H5'	2.51	0.41
3:2E:58:GLU:N	3:2E:65:ALA:HB3	2.35	0.41
23:2K:2:G:H2'	23:2K:3:C:C6	2.56	0.41
4:32:117:ALA:O	4:32:121:VAL:HG23	2.20	0.41
24:3L:22:G:H8	24:3L:46:G:N2	2.19	0.41
25:4K:13:A:N3	25:4K:13:A:H2'	2.36	0.41
1:1G:1400:C:H4'	25:4L:18:G:C5	2.56	0.41
33:51:137:ASP:OD1	33:51:138:LYS:N	2.44	0.41
26:1H:2748:A:C2	33:51:63:SER:HB3	2.56	0.41
33:51:92:ILE:C	33:51:94:TYR:H	2.24	0.41
6:5E:62:TRP:HH2	6:5E:64:GLN:HG3	1.86	0.41
7:62:36:LYS:O	7:62:40:ALA:N	2.54	0.41
40:65:21:THR:HG22	40:65:21:THR:H	1.56	0.41
34:69:80:PRO:HA	34:69:143:SER:HB2	2.03	0.41
1:13:626:U:H5''	16:7I:38:TYR:CD2	2.56	0.41
38:88:136:ALA:CB	47:H8:52:SER:HB2	2.51	0.41
38:88:37:LEU:HD21	38:88:130:LYS:CE	2.50	0.41
26:14:565:C:OP1	43:95:82:ARG:NH2	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:AA:3:ARG:HH22	19:AA:9:VAL:C	2.24	0.41
42:C8:79:PHE:C	42:C8:79:PHE:HD1	2.24	0.41
49:F5:8:SER:HB3	49:F5:66:HIS:CD2	2.56	0.41
49:F5:73:LEU:HB3	49:F5:90:ILE:HD11	2.02	0.41
46:G8:30:VAL:HG12	46:G8:32:PRO:HD3	2.03	0.41
51:H5:43:ILE:O	51:H5:47:VAL:HG23	2.21	0.41
53:J5:41:PRO:HG2	53:J5:44:THR:OG1	2.21	0.41
26:1H:2432:A:C5	49:J8:33:LYS:HG2	2.56	0.41
50:K8:15:LYS:HD3	50:K8:15:LYS:HA	1.76	0.41
44:E8:35:ILE:HG23	53:N8:28:PRO:HD2	2.02	0.41
29:11:61:LEU:HA	29:11:61:LEU:HD13	1.95	0.40
2:12:85:ALA:HB1	2:12:92:TYR:HB3	2.02	0.40
1:13:1097:C:O2'	1:13:1169:A:N3	2.40	0.40
1:13:1429:C:H2'	1:13:1430:C:H6	1.86	0.40
1:13:1489:G:H2'	1:13:1490:C:O4'	2.20	0.40
1:13:21:G:H2'	1:13:22:G:C8	2.56	0.40
1:13:544:G:C6	1:13:545:C:C4	3.09	0.40
26:14:1132:A:H2'	26:14:1133:U:C6	2.56	0.40
26:14:1788:C:C2	26:14:1789:A:C8	3.09	0.40
26:14:2335:A:C8	26:14:2337:G:C5	3.09	0.40
26:14:2340:G:O2'	26:14:2341:G:H5'	2.21	0.40
26:14:2567:G:H2'	26:14:2568:C:C6	2.56	0.40
26:14:26:G:H1'	26:14:515:A:H61	1.86	0.40
26:14:2808:U:O2'	26:14:2809:A:H5'	2.21	0.40
26:14:761:A:OP2	61:14:3437:SPE:H111	2.21	0.40
26:14:445:C:O2'	26:14:446:G:H5'	2.21	0.40
26:14:996:A:C2	26:14:997:G:C8	3.09	0.40
35:15:16:ILE:HB	35:15:54:VAL:HG22	2.01	0.40
29:19:40:THR:OG1	29:19:41:GLY:N	2.53	0.40
10:1A:17:ASP:O	10:1A:21:GLN:HB2	2.21	0.40
1:1G:1248:A:C6	1:1G:1249:C:N4	2.89	0.40
1:1G:1387:G:H2'	1:1G:1388:C:C6	2.57	0.40
1:1G:1471:G:H2'	1:1G:1472:U:C6	2.56	0.40
26:1H:1049:C:H1'	26:1H:1113:U:O2'	2.21	0.40
26:1H:1593:G:H2'	26:1H:1594:G:H8	1.83	0.40
26:1H:2248:C:C5	26:1H:2249:U:C4	3.09	0.40
26:1H:2684:U:H1'	36:68:70:LYS:HD2	2.03	0.40
26:1H:2772:C:H2'	26:1H:2773:C:H6	1.85	0.40
26:1H:667:U:O2	56:Q8:2:PRO:HD2	2.21	0.40
26:1H:696:G:O2'	26:1H:697:C:H5'	2.21	0.40
10:1I:48:THR:OG1	10:1I:62:HIS:CE1	2.74	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:29:143:ASN:HB2	30:29:147:PRO:HD2	2.03	0.40
30:29:70:ALA:O	30:29:72:VAL:N	2.53	0.40
11:2A:105:VAL:HG22	11:2A:105:VAL:O	2.20	0.40
11:2A:22:HIS:HB3	11:2A:29:ILE:HG12	2.03	0.40
11:2A:16:SER:OG	11:2A:79:SER:HB3	2.22	0.40
23:2K:54:G:O2'	23:2K:55:5MU:H5''	2.21	0.40
37:35:124:LYS:HE2	37:35:143:GLY:O	2.22	0.40
37:35:47:ASP:HB3	37:35:49:ARG:N	2.37	0.40
24:3L:15:G:C4	24:3L:59:A:C2	3.09	0.40
32:41:72:ARG:NH1	32:41:87:PRO:HD3	2.35	0.40
32:49:76:SER:O	32:49:77:ILE:HG13	2.21	0.40
33:51:2:SER:HB2	33:51:3:ARG:CD	2.43	0.40
33:51:6:ARG:HB3	33:51:65:HIS:CG	2.56	0.40
39:55:107:ASP:C	39:55:107:ASP:OD1	2.60	0.40
35:58:28:THR:HG22	35:58:29:LYS:N	2.36	0.40
34:61:77:LEU:HD13	34:61:140:LEU:HB3	2.03	0.40
8:72:25:ASP:OD1	8:72:25:ASP:N	2.53	0.40
26:1H:637:A:O5'	37:78:116:GLY:HA3	2.21	0.40
37:78:39:LYS:HB2	37:78:45:LEU:CD2	2.50	0.40
42:85:27:LEU:O	42:85:31:SER:HB3	2.22	0.40
43:95:94:LEU:HA	43:95:94:LEU:HD23	1.81	0.40
43:95:18:LEU:O	43:95:96:ILE:HG12	2.22	0.40
40:A8:23:ARG:NH1	40:A8:111:GLU:HG2	2.36	0.40
43:D8:8:GLY:O	43:D8:10:LYS:HE3	2.21	0.40
43:D8:96:ILE:HD13	43:D8:96:ILE:HA	1.86	0.40
44:E8:45:TYR:CE2	44:E8:49:LYS:HD2	2.57	0.40
45:F8:24:GLY:CA	45:F8:82:GLN:HE22	2.33	0.40
56:Q8:14:VAL:C	62:Q8:401:HOH:O	2.59	0.40
1:13:1269:A:H2	1:13:1312:G:N3	2.20	0.40
1:13:1347:G:H22	1:13:1374:A:P	2.44	0.40
1:13:32:A:H2'	1:13:33:A:C8	2.56	0.40
1:13:511:C:C2	1:13:512:U:C5	3.09	0.40
1:13:982:U:H4'	1:13:983:A:O5'	2.21	0.40
26:14:1034:G:H8	26:14:1034:G:OP1	2.03	0.40
26:14:819:A:C4	26:14:1189:A:C2	3.09	0.40
26:14:1372:U:H2'	26:14:1373:A:O4'	2.21	0.40
26:14:1992:G:C8	26:14:1992:G:O5'	2.74	0.40
26:14:217:G:H2'	26:14:218:A:O4'	2.22	0.40
26:14:2075:U:H2'	26:14:2238:G:N2	2.36	0.40
26:14:2666:C:H3'	26:14:2667:C:H6	1.85	0.40
26:14:270(L):U:H1'	34:69:50:ARG:HD3	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:14:2762:G:H5'	26:14:2763:G:OP2	2.22	0.40
26:14:565:C:H2'	26:14:566:U:O4'	2.21	0.40
26:14:671:C:H2'	26:14:672:C:C6	2.56	0.40
26:14:836:G:C5	26:14:837:C:C4	3.09	0.40
35:15:137:LYS:HE3	35:15:137:LYS:HB3	1.97	0.40
1:1G:266:G:H5''	1:1G:267:C:C5	2.56	0.40
1:1G:272:C:H2'	1:1G:273:A:C8	2.56	0.40
1:1G:522:C:H2'	1:1G:523:A:O4'	2.21	0.40
1:1G:57:G:C6	1:1G:58:C:C4	3.09	0.40
1:1G:652:U:H1'	1:1G:653:A:C2	2.55	0.40
1:1G:852:G:C6	1:1G:853:G:N7	2.90	0.40
26:1H:2189:U:H2'	26:1H:2190:G:C8	2.56	0.40
26:1H:2542:A:H4'	26:1H:2543:G:H8	1.86	0.40
26:1H:2710:C:P	62:1H:4023:HOH:O	2.79	0.40
26:1H:2766:G:H5''	26:1H:2767:C:OP2	2.22	0.40
26:1H:301:G:C4	26:1H:302:C:C5	3.09	0.40
26:1H:425:G:H2'	26:1H:426:C:H6	1.86	0.40
26:1H:57:C:H2'	26:1H:58:G:O4'	2.21	0.40
24:1L:57:G:H2'	24:1L:58:A:H5'	2.03	0.40
3:22:173:VAL:HG12	3:22:175:LEU:HG	2.02	0.40
26:14:1665:A:C4'	36:25:67:LYS:HB2	2.50	0.40
3:2E:133:ALA:O	3:2E:136:GLN:HG3	2.21	0.40
26:14:389:G:H22	37:35:72:PRO:HD3	1.86	0.40
32:41:61:ALA:O	32:41:65:GLY:N	2.52	0.40
32:41:82:LEU:HD22	32:41:82:LEU:HA	1.97	0.40
38:45:132:VAL:HG21	47:D5:81:ARG:NE	2.35	0.40
6:5E:49:ALA:HB1	18:9I:80:PRO:HB3	2.03	0.40
40:65:72:ALA:O	40:65:76:LYS:HG3	2.21	0.40
7:6E:15:ASP:HB3	7:6E:19:GLY:H	1.86	0.40
28:71:59:ARG:HG2	28:71:163:PHE:O	2.21	0.40
9:82:18:PHE:HD2	9:82:62:TYR:CD2	2.38	0.40
40:A8:25:ARG:O	40:A8:39:ILE:HA	2.21	0.40
20:BI:26:ASN:HD22	20:BI:71:THR:HA	1.86	0.40
46:G8:94:LYS:CE	46:G8:95:LYS:H	2.34	0.40
48:I8:50:ASN:ND2	48:I8:83:PRO:HD3	2.36	0.40
48:I8:38:VAL:HG21	48:I8:59:LEU:HD12	2.04	0.40
1:13:1125:U:C4	1:13:1126:U:C4	3.09	0.40
1:13:1468:A:H8	1:13:1468:A:O5'	2.04	0.40
1:13:406:G:H2'	1:13:407:G:C8	2.56	0.40
1:13:684:A:N6	1:13:685:G:C6	2.89	0.40
26:14:1392:A:C6	26:14:1393:A:C6	3.09	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:14:1827:C:H2'	26:14:1828:G:O4'	2.21	0.40
26:14:19:C:H2'	26:14:20:C:C6	2.56	0.40
26:14:2321:G:H2'	26:14:2321:G:N3	2.37	0.40
26:14:2376:A:H2'	26:14:2377:A:O4'	2.21	0.40
26:14:2688:U:C5	26:14:2720:U:OP2	2.75	0.40
26:14:2786:U:H5''	30:29:66:HIS:HB3	2.02	0.40
26:14:37:C:H4'	26:14:451:C:OP1	2.21	0.40
26:14:608:A:H2'	26:14:609:A:C8	2.57	0.40
26:14:675:A:N3	26:14:2443:C:O2'	2.48	0.40
26:14:838:C:O2'	26:14:839:U:H5'	2.22	0.40
27:16:24:G:C2	27:16:56:G:C2	3.09	0.40
29:19:121:PRO:HB3	29:19:135:PHE:CD2	2.56	0.40
1:1G:1095:U:H2'	1:1G:1096:C:O4'	2.21	0.40
1:1G:1149:C:OP2	9:82:9:ARG:NH1	2.55	0.40
1:1G:1286:A:C8	1:1G:1286:A:C3'	3.05	0.40
1:1G:194:C:H3'	62:1G:1806:HOH:O	2.18	0.40
1:1G:197:A:N1	1:1G:221:C:H4'	2.37	0.40
26:1H:123:G:O6	26:1H:128:C:N3	2.55	0.40
26:1H:1568:G:H5'	29:11:60:ARG:HA	2.02	0.40
26:1H:2663:G:H3'	26:1H:2664:G:H8	1.86	0.40
26:1H:2820:A:OP1	39:98:2:ARG:NH2	2.45	0.40
26:1H:2852:G:H2'	26:1H:2853:C:O4'	2.21	0.40
26:1H:365:C:H2'	26:1H:366:C:O4'	2.22	0.40
26:1H:773:U:H5'	29:11:47:GLY:HA3	2.03	0.40
26:1H:990:A:H5''	26:1H:991:C:OP1	2.21	0.40
26:1H:990:A:N6	26:1H:1186:G:H1'	2.37	0.40
27:1J:64:C:H2'	27:1J:65:C:C6	2.57	0.40
30:29:66:HIS:CG	30:29:67:PHE:N	2.89	0.40
30:29:54:GLN:HG3	30:29:72:VAL:O	2.21	0.40
4:32:13:ARG:O	4:32:14:ARG:HB3	2.21	0.40
12:3I:111:LYS:HD3	12:3I:112:ASP:H	1.86	0.40
32:41:11:TYR:O	32:41:16:ARG:HG3	2.21	0.40
32:41:15:VAL:HG13	32:41:175:LEU:HB2	2.03	0.40
38:45:84:GLY:HA2	38:45:85:LYS:HB2	2.03	0.40
13:4A:89:GLY:HA2	13:4A:92:HIS:HB2	2.03	0.40
5:4E:35:GLY:HA3	5:4E:112:LEU:O	2.22	0.40
39:55:90:ARG:HD2	39:55:94:TYR:HD1	1.86	0.40
3:22:6:HIS:CG	14:5A:49:HIS:HB3	2.57	0.40
34:61:61:ARG:HA	34:61:61:ARG:HD3	1.74	0.40
7:62:47:CYS:HB3	7:62:58:PRO:CB	2.51	0.40
7:62:59:LEU:HD21	7:62:63:LYS:NZ	2.36	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:62:90:GLU:HG2	7:62:90:GLU:H	1.61	0.40
40:65:66:ALA:O	40:65:69:VAL:HG13	2.21	0.40
36:68:64:ARG:HB2	36:68:79:PHE:CD1	2.56	0.40
34:69:130:TYR:HD1	34:69:130:TYR:HA	1.74	0.40
5:42:79:GLU:OE1	8:72:104:ARG:HA	2.21	0.40
36:25:76:ALA:HB3	41:75:75:ILE:HB	2.04	0.40
37:78:122:PRO:HA	37:78:142:GLY:HA3	2.03	0.40
37:78:37:GLY:HA2	37:78:41:ARG:NH2	2.36	0.40
37:78:51:PHE:CE2	37:78:53:GLY:HA2	2.56	0.40
20:BA:50:GLU:HA	20:BA:100:ILE:HG12	2.03	0.40
47:D5:60:GLU:HB2	47:D5:66:SER:OG	2.22	0.40
49:J8:58:ILE:HG23	49:J8:90:ILE:HG13	2.03	0.40
29:11:158:ALA:O	29:11:159:ALA:C	2.59	0.40
1:13:1148:U:H2'	1:13:1149:C:O4'	2.21	0.40
1:13:1366:C:O2'	10:1L:60:ARG:NH1	2.36	0.40
1:13:1064:G:OP1	1:13:1386:G:H4'	2.21	0.40
1:13:183:G:H2'	1:13:184:G:C8	2.56	0.40
1:13:193:C:O2'	1:13:194:C:H5'	2.21	0.40
1:13:195:A:C5	1:13:196:A:N1	2.89	0.40
1:13:818:G:O2'	1:13:819:A:H5'	2.21	0.40
1:13:848:C:H6	1:13:848:C:O5'	2.05	0.40
26:14:1176:G:H5'	26:14:1177:A:OP1	2.22	0.40
26:14:1288:U:C2	26:14:1327:C:O2	2.75	0.40
26:14:1407:C:C2	26:14:1596:A:C2	3.09	0.40
26:14:1434:A:H61	26:14:1558:A:N6	2.18	0.40
26:14:2303:G:O4'	32:49:126:ASP:HB3	2.21	0.40
26:14:2526:G:C2	26:14:2538:C:O2	2.75	0.40
26:14:2547:U:O2	36:25:23:ARG:NH2	2.54	0.40
26:14:2699:C:H2'	26:14:2700:C:O4'	2.21	0.40
26:14:527:C:H5''	62:14:3502:HOH:O	2.21	0.40
26:14:602:G:N2	26:14:655:A:C8	2.89	0.40
29:19:30:GLU:HB2	29:19:35:LYS:NZ	2.37	0.40
2:1E:189:ASP:CG	2:1E:191:ASP:HB2	2.41	0.40
2:1E:21:ARG:C	2:1E:23:ARG:H	2.20	0.40
2:1E:82:ARG:HG3	2:1E:92:TYR:CE2	2.56	0.40
1:1G:1101:A:C8	2:12:172:ILE:HD11	2.56	0.40
1:1G:1112:C:N3	3:22:178:LEU:HD23	2.37	0.40
1:1G:1154:G:N3	1:1G:1155:G:C8	2.89	0.40
1:1G:1331:G:OP1	1:1G:1331:G:H4'	2.22	0.40
1:1G:1489:G:H2'	1:1G:1490:C:O4'	2.21	0.40
1:1G:247:G:OP1	1:1G:247:G:H4'	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1G:359:U:H2'	1:1G:360:A:C8	2.56	0.40
1:1G:569:C:H1'	1:1G:574:A:C4	2.57	0.40
1:1G:617:G:H1	1:1G:623:C:H42	1.70	0.40
1:1G:76:G:C6	1:1G:77:C:C4	3.10	0.40
26:1H:1368:G:C2	26:1H:1369:G:C8	3.09	0.40
26:1H:1516:U:H2'	26:1H:1517:G:H8	1.86	0.40
26:1H:1568:G:H5''	29:11:61:LEU:HD22	2.02	0.40
26:1H:1578:U:H5	62:1H:4883:HOH:O	2.03	0.40
26:1H:1668:A:N6	26:1H:1676:A:H61	2.19	0.40
26:1H:1669:A:H5''	26:1H:2550:G:OP1	2.21	0.40
26:1H:172:C:H2'	26:1H:173:G:C8	2.57	0.40
26:1H:2228:G:H2'	26:1H:2229:C:C6	2.56	0.40
26:1H:2593:U:O2'	26:1H:2594:C:H5'	2.21	0.40
26:1H:419:C:H2'	26:1H:420:C:O4'	2.22	0.40
26:1H:443:A:H5''	26:1H:444:C:OP1	2.21	0.40
26:1H:617:G:OP2	31:31:43:LYS:HE2	2.22	0.40
26:1H:962:G:H2'	26:1H:963:U:H6	1.85	0.40
3:2E:172:ARG:HH21	3:2E:174:PRO:HG2	1.86	0.40
31:31:22:ALA:HB1	31:31:24:LEU:HD13	2.02	0.40
31:39:107:LYS:HA	31:39:107:LYS:HD3	1.61	0.40
12:3A:82:VAL:N	12:3A:106:ASP:OD2	2.33	0.40
24:3L:52:G:C6	24:3L:63:U:C4	3.10	0.40
38:45:32:TYR:OH	38:45:111:GLU:HB2	2.21	0.40
38:45:77:LYS:HE3	38:45:84:GLY:N	2.34	0.40
32:49:117:PHE:CG	32:49:117:PHE:O	2.74	0.40
13:4A:88:ARG:HB2	13:4A:88:ARG:CZ	2.51	0.40
25:4K:14:A:OP2	25:4K:14:A:H3'	2.21	0.40
1:1G:1216:G:H5''	14:5A:5:ALA:HB3	2.02	0.40
8:72:109:ILE:HG22	8:72:137:VAL:HB	2.02	0.40
26:14:1008:C:H4'	42:85:59:ARG:HH12	1.87	0.40
38:88:135:ASP:O	38:88:138:ASP:N	2.44	0.40
17:8A:10:VAL:HG12	17:8A:55:ASP:O	2.22	0.40
17:8I:45:HIS:NE2	17:8I:47:PRO:HG3	2.37	0.40
17:8I:55:ASP:HB3	17:8I:57:VAL:CG1	2.51	0.40
19:AI:41:VAL:CA	19:AI:44:MET:HG3	2.50	0.40
19:AI:50:ALA:HA	19:AI:58:VAL:O	2.21	0.40
46:C5:19:LYS:C	46:C5:21:LYS:H	2.24	0.40
47:D5:127:LYS:HB3	47:D5:127:LYS:HE2	1.81	0.40
47:D5:19:ARG:NH1	47:D5:84:GLU:HB2	2.37	0.40
49:F5:91:LYS:HZ2	49:F5:92:LYS:H	1.69	0.40
26:1H:298:G:OP2	46:G8:84:ARG:HD2	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:J8:8:SER:OG	49:J8:10:LYS:HG3	2.22	0.40
1:13:1077:G:N2	1:13:1080:A:OP2	2.53	0.40
1:13:1250:A:H2'	1:13:1251:A:C8	2.57	0.40
1:13:267:C:H2'	1:13:268:C:C6	2.57	0.40
1:13:370:C:C2	1:13:392:G:N2	2.90	0.40
1:13:559:A:H2'	1:13:559:A:N3	2.37	0.40
1:13:881:G:H2'	1:13:882:C:O4'	2.22	0.40
1:13:919:A:O2'	1:13:920:U:H5'	2.20	0.40
1:13:955:U:H1'	1:13:1227:A:H61	1.86	0.40
26:14:1329:U:H5''	26:14:1330:C:C5	2.49	0.40
26:14:1359:A:N7	26:14:1372:U:O4	2.54	0.40
26:14:1386:C:H2'	26:14:1387:C:C6	2.56	0.40
26:14:1421:G:C2	26:14:1422:G:C8	3.10	0.40
26:14:1620:G:O4'	55:L5:1:MET:N	2.50	0.40
26:14:1688:U:H2'	26:14:1698:A:N6	2.36	0.40
26:14:1945:G:H2'	26:14:1946:U:H6	1.87	0.40
26:14:1961:C:O2'	26:14:1962:C:H5'	2.21	0.40
26:14:1268:A:C2	26:14:2013:A:C4	3.10	0.40
26:14:2507:C:H5''	26:14:2573:C:N4	2.36	0.40
26:14:2712:U:H1'	26:14:2712(A):A:C8	2.56	0.40
26:14:521:G:H2'	26:14:522:G:C8	2.56	0.40
26:14:635:C:H2'	26:14:636:G:O4'	2.22	0.40
29:19:206:LEU:HD22	29:19:211:ARG:HG2	2.02	0.40
21:1F:8:THR:OG1	21:1F:9:ARG:N	2.54	0.40
1:1G:1072:G:C5	1:1G:1073:U:C4	3.10	0.40
1:1G:1275:A:H2'	1:1G:1276:G:O4'	2.21	0.40
1:1G:198:G:H2'	1:1G:199:G:C8	2.54	0.40
1:1G:286:G:C6	1:1G:287:U:C4	3.10	0.40
26:1H:1728:G:C2	26:1H:1730:U:OP2	2.75	0.40
26:1H:1915:U:H2'	26:1H:1916:A:O4'	2.21	0.40
26:1H:2123:G:H2'	26:1H:2124:G:O4'	2.21	0.40
26:1H:2503:A:P	62:1H:3755:HOH:O	2.78	0.40
26:1H:34:C:C6	26:1H:34:C:OP2	2.75	0.40
26:1H:812:C:H5''	26:1H:1250:G:O2'	2.22	0.40
27:1J:12:C:O2'	48:E5:74:ARG:HG2	2.21	0.40
24:1L:25:C:C2	24:1L:26:A:H1'	2.57	0.40
24:1L:59:A:C8	24:1L:60:U:C4	3.10	0.40
24:1L:9:A:H3'	24:1L:10:G:C8	2.56	0.40
30:21:37:ARG:O	30:21:45:THR:HA	2.21	0.40
3:22:182:ILE:HG22	3:22:203:PHE:HA	2.03	0.40
30:29:24:THR:HG21	30:29:188:VAL:HG22	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:14:2786:U:H5''	30:29:66:HIS:CB	2.52	0.40
11:2I:32:ILE:HG12	11:2I:41:THR:O	2.21	0.40
26:1H:673:C:H5''	31:31:81:PRO:HD2	2.04	0.40
38:45:118:LEU:HD12	38:45:131:ILE:HG23	2.02	0.40
32:49:91:ARG:HB3	32:49:91:ARG:HE	1.43	0.40
25:4L:19:G:O2'	25:4L:20:A:OP2	2.38	0.40
33:51:4:ILE:HD13	33:51:4:ILE:HG21	1.88	0.40
7:6E:43:PHE:O	7:6E:46:ALA:HB3	2.21	0.40
8:72:82:HIS:CE1	8:72:136:GLU:HG3	2.56	0.40
8:72:51:VAL:HG22	8:72:58:TYR:O	2.22	0.40
41:75:86:ILE:HG21	41:75:86:ILE:HD13	1.87	0.40
37:78:125:VAL:O	37:78:144:GLU:HB2	2.22	0.40
9:82:14:VAL:O	9:82:65:VAL:HG23	2.22	0.40
17:8A:45:HIS:HB2	17:8A:65:ILE:CD1	2.51	0.40
9:8E:24:GLY:HA2	9:8E:59:PHE:O	2.21	0.40
18:9A:45:SER:OG	18:9A:46:GLU:N	2.55	0.40
19:AA:16:LEU:HD12	19:AA:19:VAL:HB	2.03	0.40
20:BA:55:ILE:HD13	20:BA:55:ILE:HA	1.97	0.40
20:BA:97:ALA:HA	20:BA:98:PRO:HD3	1.92	0.40
42:C8:108:GLU:HG3	43:D8:44:LYS:CE	2.52	0.40
49:F5:92:LYS:HA	49:F5:95:LEU:HB2	2.03	0.40
45:F8:55:ASN:HB2	45:F8:80:ILE:HG23	2.03	0.40
26:14:2019:A:N7	53:J5:9:LYS:HD2	2.36	0.40
50:K8:60:LEU:HA	50:K8:60:LEU:HD23	1.90	0.40
56:Q8:37:SER:O	56:Q8:40:GLU:N	2.54	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
2	12	203/256 (79%)	173 (85%)	25 (12%)	5 (2%)	5 28

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	1E	227/256 (89%)	185 (82%)	39 (17%)	3 (1%)	12	45
3	22	191/239 (80%)	171 (90%)	20 (10%)	0	100	100
3	2E	203/239 (85%)	186 (92%)	17 (8%)	0	100	100
4	32	206/209 (99%)	184 (89%)	21 (10%)	1 (0%)	29	68
4	3E	205/209 (98%)	192 (94%)	12 (6%)	1 (0%)	29	68
5	42	148/162 (91%)	141 (95%)	7 (5%)	0	100	100
5	4E	147/162 (91%)	141 (96%)	5 (3%)	1 (1%)	22	60
6	52	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
6	5E	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
7	62	134/156 (86%)	123 (92%)	10 (8%)	1 (1%)	22	60
7	6E	152/156 (97%)	144 (95%)	8 (5%)	0	100	100
8	72	135/138 (98%)	125 (93%)	8 (6%)	2 (2%)	10	42
8	7E	136/138 (99%)	125 (92%)	10 (7%)	1 (1%)	22	60
9	82	119/128 (93%)	109 (92%)	9 (8%)	1 (1%)	19	57
9	8E	124/128 (97%)	108 (87%)	16 (13%)	0	100	100
10	1A	76/105 (72%)	71 (93%)	5 (7%)	0	100	100
10	1I	92/105 (88%)	85 (92%)	7 (8%)	0	100	100
11	2A	111/129 (86%)	101 (91%)	8 (7%)	2 (2%)	8	37
11	2I	109/129 (84%)	94 (86%)	12 (11%)	3 (3%)	5	25
12	3A	119/132 (90%)	100 (84%)	15 (13%)	4 (3%)	3	20
12	3I	120/132 (91%)	107 (89%)	12 (10%)	1 (1%)	19	57
13	4A	107/126 (85%)	88 (82%)	18 (17%)	1 (1%)	17	55
13	4I	115/126 (91%)	96 (84%)	18 (16%)	1 (1%)	17	55
14	5A	57/61 (93%)	48 (84%)	8 (14%)	1 (2%)	8	37
14	5I	57/61 (93%)	48 (84%)	7 (12%)	2 (4%)	3	20
15	6A	85/89 (96%)	81 (95%)	4 (5%)	0	100	100
15	6I	85/89 (96%)	77 (91%)	8 (9%)	0	100	100
16	7A	82/88 (93%)	76 (93%)	6 (7%)	0	100	100
16	7I	81/88 (92%)	77 (95%)	4 (5%)	0	100	100
17	8A	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
17	8I	97/105 (92%)	92 (95%)	4 (4%)	1 (1%)	15	53

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	9A	65/88 (74%)	62 (95%)	3 (5%)	0	100	100
18	9I	66/88 (75%)	64 (97%)	1 (2%)	1 (2%)	10	42
19	AA	59/93 (63%)	49 (83%)	8 (14%)	2 (3%)	3	20
19	AI	80/93 (86%)	68 (85%)	9 (11%)	3 (4%)	3	18
20	BA	97/106 (92%)	83 (86%)	13 (13%)	1 (1%)	15	53
20	BI	95/106 (90%)	84 (88%)	10 (10%)	1 (1%)	14	50
21	1B	20/27 (74%)	19 (95%)	1 (5%)	0	100	100
21	1F	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
28	7I	128/229 (56%)	120 (94%)	8 (6%)	0	100	100
29	11	271/276 (98%)	249 (92%)	17 (6%)	5 (2%)	8	37
29	19	272/276 (99%)	246 (90%)	23 (8%)	3 (1%)	14	50
30	21	201/206 (98%)	158 (79%)	33 (16%)	10 (5%)	2	12
30	29	202/206 (98%)	149 (74%)	42 (21%)	11 (5%)	2	11
31	31	200/210 (95%)	181 (90%)	17 (8%)	2 (1%)	15	53
31	39	202/210 (96%)	162 (80%)	34 (17%)	6 (3%)	4	24
32	41	177/182 (97%)	156 (88%)	18 (10%)	3 (2%)	9	39
32	49	178/182 (98%)	155 (87%)	22 (12%)	1 (1%)	25	64
33	51	172/180 (96%)	141 (82%)	20 (12%)	11 (6%)	1	7
33	59	167/180 (93%)	129 (77%)	32 (19%)	6 (4%)	3	19
34	61	143/148 (97%)	122 (85%)	19 (13%)	2 (1%)	11	43
34	69	143/148 (97%)	111 (78%)	29 (20%)	3 (2%)	7	33
35	15	135/140 (96%)	122 (90%)	13 (10%)	0	100	100
35	58	135/140 (96%)	114 (84%)	17 (13%)	4 (3%)	4	24
36	25	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
36	68	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
37	35	145/150 (97%)	119 (82%)	26 (18%)	0	100	100
37	78	145/150 (97%)	114 (79%)	22 (15%)	9 (6%)	1	8
38	45	136/141 (96%)	115 (85%)	19 (14%)	2 (2%)	10	42
38	88	139/141 (99%)	116 (84%)	18 (13%)	5 (4%)	3	19
39	55	116/118 (98%)	110 (95%)	5 (4%)	1 (1%)	17	55
39	98	116/118 (98%)	104 (90%)	11 (10%)	1 (1%)	17	55

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	65	108/112 (96%)	89 (82%)	16 (15%)	3 (3%)	5	25
40	A8	109/112 (97%)	90 (83%)	19 (17%)	0	100	100
41	75	131/146 (90%)	117 (89%)	12 (9%)	2 (2%)	10	42
41	B8	133/146 (91%)	118 (89%)	15 (11%)	0	100	100
42	85	114/118 (97%)	104 (91%)	9 (8%)	1 (1%)	17	55
42	C8	113/118 (96%)	104 (92%)	6 (5%)	3 (3%)	5	26
43	95	98/101 (97%)	80 (82%)	15 (15%)	3 (3%)	4	23
43	D8	98/101 (97%)	88 (90%)	6 (6%)	4 (4%)	3	16
44	A5	109/113 (96%)	101 (93%)	7 (6%)	1 (1%)	17	55
44	E8	108/113 (96%)	100 (93%)	8 (7%)	0	100	100
45	B5	92/96 (96%)	84 (91%)	6 (6%)	2 (2%)	6	31
45	F8	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
46	C5	102/110 (93%)	74 (72%)	21 (21%)	7 (7%)	1	6
46	G8	101/110 (92%)	81 (80%)	16 (16%)	4 (4%)	3	17
47	D5	175/206 (85%)	136 (78%)	31 (18%)	8 (5%)	2	14
47	H8	168/206 (82%)	136 (81%)	25 (15%)	7 (4%)	3	16
48	E5	74/85 (87%)	66 (89%)	6 (8%)	2 (3%)	5	26
48	I8	75/85 (88%)	67 (89%)	7 (9%)	1 (1%)	12	45
49	F5	92/98 (94%)	79 (86%)	12 (13%)	1 (1%)	14	50
49	J8	94/98 (96%)	83 (88%)	9 (10%)	2 (2%)	7	33
50	G5	67/72 (93%)	61 (91%)	4 (6%)	2 (3%)	4	24
50	K8	66/72 (92%)	60 (91%)	3 (4%)	3 (4%)	2	14
51	H5	56/60 (93%)	53 (95%)	3 (5%)	0	100	100
51	L8	56/60 (93%)	54 (96%)	2 (4%)	0	100	100
52	M8	56/71 (79%)	40 (71%)	15 (27%)	1 (2%)	8	37
53	J5	54/60 (90%)	50 (93%)	4 (7%)	0	100	100
53	N8	46/60 (77%)	43 (94%)	3 (6%)	0	100	100
54	O8	43/54 (80%)	30 (70%)	12 (28%)	1 (2%)	6	30
55	L5	45/49 (92%)	42 (93%)	3 (7%)	0	100	100
55	P8	45/49 (92%)	42 (93%)	3 (7%)	0	100	100
56	M5	62/65 (95%)	52 (84%)	9 (14%)	1 (2%)	9	40

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
56	Q8	62/65 (95%)	53 (86%)	7 (11%)	2 (3%)	4	22
All	All	11128/12158 (92%)	9762 (88%)	1180 (11%)	186 (2%)	9	39

All (186) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	2I	55	LYS
12	3I	48	PRO
18	9I	22	VAL
19	AI	41	VAL
30	21	83	ASP
37	78	37	GLY
42	C8	89	GLU
47	H8	165	VAL
2	12	219	VAL
9	82	118	LYS
20	BA	73	HIS
30	29	25	VAL
30	29	54	GLN
31	39	28	ILE
31	39	84	VAL
32	49	5	VAL
39	55	107	ASP
41	75	10	VAL
41	75	11	GLU
47	D5	53	ILE
47	D5	171	ILE
49	F5	30	VAL
8	7E	86	ILE
29	11	239	ARG
30	21	59	VAL
30	21	60	ASN
30	21	77	ILE
30	21	118	LYS
33	51	10	PRO
33	51	157	TYR
33	51	171	LEU
37	78	25	SER
37	78	35	HIS
38	88	6	ARG
38	88	66	ILE
42	C8	93	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
43	D8	45	THR
46	G8	54	LYS
46	G8	81	LYS
47	H8	6	LYS
47	H8	60	GLU
49	J8	94	LEU
56	Q8	50	LEU
11	2A	48	ILE
12	3A	18	VAL
12	3A	26	ALA
14	5A	29	ARG
19	AA	9	VAL
29	19	273	ARG
30	29	59	VAL
30	29	81	ILE
33	59	131	VAL
34	69	113	ARG
40	65	87	PHE
40	65	89	ARG
46	C5	20	TYR
46	C5	92	ASN
47	D5	105	VAL
47	D5	165	VAL
50	G5	48	HIS
14	5I	13	THR
29	11	273	ARG
30	21	72	VAL
33	51	83	TYR
33	51	84	SER
33	51	138	LYS
35	58	97	ARG
35	58	128	HIS
37	78	6	LEU
38	88	7	MET
38	88	134	ARG
50	K8	43	GLN
50	K8	48	HIS
11	2A	101	SER
30	29	9	VAL
30	29	51	PHE
30	29	55	ASN
31	39	25	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	39	124	LEU
31	39	132	VAL
31	39	167	ALA
33	59	92	ILE
38	45	27	VAL
38	45	90	VAL
48	E5	33	ALA
50	G5	47	ASN
2	1E	238	LEU
4	3E	155	LEU
14	5I	14	PRO
17	8I	79	SER
29	11	3	VAL
29	11	122	ASP
30	21	21	VAL
32	41	96	ARG
32	41	97	ASP
33	51	154	PRO
35	58	22	THR
42	C8	90	VAL
43	D8	49	THR
47	H8	59	LEU
49	J8	86	SER
50	K8	47	ASN
56	Q8	35	GLN
2	12	220	ASP
12	3A	19	ARG
30	29	90	THR
33	59	168	PRO
34	69	112	LYS
40	65	111	GLU
43	95	71	LEU
45	B5	68	ARG
46	C5	29	GLU
47	D5	116	VAL
47	D5	176	PRO
56	M5	34	TRP
2	1E	10	LEU
19	AI	67	VAL
20	BI	71	THR
29	11	240	ALA
30	21	56	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	31	198	ALA
32	41	5	VAL
33	51	12	PRO
33	51	169	VAL
34	61	12	LEU
34	61	133	HIS
35	58	135	PRO
37	78	14	LYS
37	78	19	VAL
37	78	95	VAL
46	G8	42	VAL
48	I8	9	SER
7	62	147	ALA
8	72	73	ASP
30	29	26	ILE
30	29	45	THR
42	85	93	LYS
44	A5	44	ALA
46	C5	99	CYS
47	D5	161	VAL
2	1E	127	ILE
11	2I	82	VAL
33	51	85	LYS
33	51	170	ARG
37	78	34	GLY
39	98	45	ARG
46	G8	53	PRO
4	32	28	SER
29	19	239	ARG
33	59	167	GLU
46	C5	62	GLU
48	E5	44	ARG
19	AI	40	ILE
30	21	55	ASN
30	21	75	VAL
47	H8	61	LEU
47	H8	141	VAL
12	3A	47	LYS
29	19	3	VAL
13	4I	4	ILE
43	D8	47	VAL
43	95	72	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
45	B5	51	VAL
46	C5	85	VAL
5	4E	115	VAL
38	88	27	VAL
43	D8	48	GLY
47	H8	53	ILE
54	O8	52	VAL
2	12	39	ILE
33	59	169	VAL
34	69	144	VAL
43	95	99	ILE
46	C5	3	VAL
11	2I	108	ILE
31	31	24	LEU
37	78	24	GLY
52	M8	5	ILE
2	12	32	ILE
2	12	223	ILE
8	72	100	ILE
13	4A	84	ILE
30	29	77	ILE
47	D5	141	VAL
19	AA	67	VAL
33	59	126	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	12	179/220 (81%)	143 (80%)	36 (20%)	1	6
2	1E	200/220 (91%)	154 (77%)	46 (23%)	1	4
3	22	154/188 (82%)	128 (83%)	26 (17%)	2	11
3	2E	159/188 (85%)	131 (82%)	28 (18%)	2	10
4	32	180/181 (99%)	151 (84%)	29 (16%)	2	12

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	3E	180/181 (99%)	146 (81%)	34 (19%)	1	8
5	42	114/123 (93%)	87 (76%)	27 (24%)	1	3
5	4E	115/123 (94%)	93 (81%)	22 (19%)	1	8
6	52	90/90 (100%)	74 (82%)	16 (18%)	2	9
6	5E	90/90 (100%)	80 (89%)	10 (11%)	6	25
7	62	114/127 (90%)	88 (77%)	26 (23%)	1	4
7	6E	125/127 (98%)	105 (84%)	20 (16%)	2	12
8	72	118/119 (99%)	101 (86%)	17 (14%)	3	15
8	7E	119/119 (100%)	99 (83%)	20 (17%)	2	11
9	82	92/99 (93%)	73 (79%)	19 (21%)	1	6
9	8E	97/99 (98%)	75 (77%)	22 (23%)	1	4
10	1A	71/92 (77%)	51 (72%)	20 (28%)	0	2
10	1I	81/92 (88%)	73 (90%)	8 (10%)	8	30
11	2A	85/99 (86%)	67 (79%)	18 (21%)	1	5
11	2I	84/99 (85%)	70 (83%)	14 (17%)	2	11
12	3A	102/109 (94%)	79 (78%)	23 (22%)	1	4
12	3I	103/109 (94%)	91 (88%)	12 (12%)	5	22
13	4A	90/101 (89%)	68 (76%)	22 (24%)	0	3
13	4I	94/101 (93%)	74 (79%)	20 (21%)	1	5
14	5A	49/50 (98%)	41 (84%)	8 (16%)	2	11
14	5I	49/50 (98%)	36 (74%)	13 (26%)	0	2
15	6A	79/80 (99%)	71 (90%)	8 (10%)	7	29
15	6I	79/80 (99%)	65 (82%)	14 (18%)	2	9
16	7A	72/74 (97%)	61 (85%)	11 (15%)	2	13
16	7I	72/74 (97%)	58 (81%)	14 (19%)	1	7
17	8A	94/97 (97%)	82 (87%)	12 (13%)	4	19
17	8I	94/97 (97%)	82 (87%)	12 (13%)	4	19
18	9A	58/77 (75%)	47 (81%)	11 (19%)	1	8
18	9I	58/77 (75%)	49 (84%)	9 (16%)	2	13
19	AA	56/80 (70%)	47 (84%)	9 (16%)	2	12
19	AI	72/80 (90%)	61 (85%)	11 (15%)	2	13

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	BA	76/82 (93%)	66 (87%)	10 (13%)	4	18
20	BI	75/82 (92%)	61 (81%)	14 (19%)	1	8
21	1B	17/22 (77%)	16 (94%)	1 (6%)	19	54
21	1F	18/22 (82%)	14 (78%)	4 (22%)	1	4
28	71	108/181 (60%)	87 (81%)	21 (19%)	1	7
29	11	214/218 (98%)	173 (81%)	41 (19%)	1	8
29	19	214/218 (98%)	171 (80%)	43 (20%)	1	6
30	21	162/166 (98%)	118 (73%)	44 (27%)	0	2
30	29	165/166 (99%)	135 (82%)	30 (18%)	1	9
31	31	161/166 (97%)	128 (80%)	33 (20%)	1	6
31	39	163/166 (98%)	126 (77%)	37 (23%)	1	4
32	41	153/156 (98%)	126 (82%)	27 (18%)	2	10
32	49	152/156 (97%)	125 (82%)	27 (18%)	2	9
33	51	143/148 (97%)	106 (74%)	37 (26%)	0	2
33	59	140/148 (95%)	106 (76%)	34 (24%)	0	3
34	61	122/124 (98%)	86 (70%)	36 (30%)	0	1
34	69	122/124 (98%)	89 (73%)	33 (27%)	0	2
35	15	116/119 (98%)	90 (78%)	26 (22%)	1	4
35	58	116/119 (98%)	87 (75%)	29 (25%)	0	3
36	25	100/100 (100%)	76 (76%)	24 (24%)	0	3
36	68	100/100 (100%)	90 (90%)	10 (10%)	7	29
37	35	114/116 (98%)	82 (72%)	32 (28%)	0	2
37	78	114/116 (98%)	78 (68%)	36 (32%)	0	1
38	45	109/111 (98%)	88 (81%)	21 (19%)	1	8
38	88	110/111 (99%)	90 (82%)	20 (18%)	1	9
39	55	101/101 (100%)	80 (79%)	21 (21%)	1	5
39	98	101/101 (100%)	72 (71%)	29 (29%)	0	2
40	65	87/88 (99%)	61 (70%)	26 (30%)	0	1
40	A8	87/88 (99%)	66 (76%)	21 (24%)	0	3
41	75	117/127 (92%)	95 (81%)	22 (19%)	1	8
41	B8	117/127 (92%)	83 (71%)	34 (29%)	0	2

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	85	93/94 (99%)	73 (78%)	20 (22%)	1	5
42	C8	92/94 (98%)	76 (83%)	16 (17%)	2	10
43	95	81/82 (99%)	68 (84%)	13 (16%)	2	12
43	D8	82/82 (100%)	63 (77%)	19 (23%)	1	4
44	A5	91/92 (99%)	74 (81%)	17 (19%)	1	8
44	E8	90/92 (98%)	73 (81%)	17 (19%)	1	8
45	B5	74/78 (95%)	56 (76%)	18 (24%)	0	3
45	F8	77/78 (99%)	64 (83%)	13 (17%)	2	11
46	C5	85/91 (93%)	63 (74%)	22 (26%)	0	2
46	G8	84/91 (92%)	66 (79%)	18 (21%)	1	5
47	D5	156/179 (87%)	124 (80%)	32 (20%)	1	6
47	H8	151/179 (84%)	124 (82%)	27 (18%)	2	9
48	E5	61/67 (91%)	55 (90%)	6 (10%)	8	30
48	I8	62/67 (92%)	53 (86%)	9 (14%)	3	15
49	F5	79/83 (95%)	63 (80%)	16 (20%)	1	6
49	J8	79/83 (95%)	67 (85%)	12 (15%)	3	14
50	G5	63/67 (94%)	46 (73%)	17 (27%)	0	2
50	K8	64/67 (96%)	43 (67%)	21 (33%)	0	1
51	H5	50/52 (96%)	38 (76%)	12 (24%)	0	3
51	L8	50/52 (96%)	40 (80%)	10 (20%)	1	7
52	M8	52/63 (82%)	38 (73%)	14 (27%)	0	2
53	J5	48/52 (92%)	41 (85%)	7 (15%)	3	15
53	N8	43/52 (83%)	34 (79%)	9 (21%)	1	5
54	O8	44/52 (85%)	29 (66%)	15 (34%)	0	1
55	L5	38/42 (90%)	32 (84%)	6 (16%)	2	12
55	P8	38/42 (90%)	31 (82%)	7 (18%)	1	9
56	M5	54/55 (98%)	43 (80%)	11 (20%)	1	6
56	Q8	54/55 (98%)	44 (82%)	10 (18%)	1	8
All	All	9397/10064 (93%)	7493 (80%)	1904 (20%)	1	6

All (1904) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1E	8	LYS
2	1E	11	LEU
2	1E	21	ARG
2	1E	28	PHE
2	1E	33	TYR
2	1E	55	PHE
2	1E	67	THR
2	1E	69	LEU
2	1E	71	VAL
2	1E	79	ASP
2	1E	83	MET
2	1E	86	GLU
2	1E	87	ARG
2	1E	95	GLN
2	1E	96	ARG
2	1E	108	ILE
2	1E	111	ARG
2	1E	118	LEU
2	1E	122	PHE
2	1E	127	ILE
2	1E	135	GLN
2	1E	144	ARG
2	1E	154	LEU
2	1E	155	LEU
2	1E	158	LEU
2	1E	160	ASP
2	1E	163	PHE
2	1E	169	LYS
2	1E	172	ILE
2	1E	178	ARG
2	1E	184	VAL
2	1E	185	ILE
2	1E	187	LEU
2	1E	190	THR
2	1E	197	VAL
2	1E	200	ILE
2	1E	205	ASP
2	1E	209	ARG
2	1E	210	SER
2	1E	211	ILE
2	1E	214	ILE
2	1E	217	ARG
2	1E	222	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	1E	223	ILE
2	1E	224	GLN
2	1E	230	VAL
3	2E	3	ASN
3	2E	5	ILE
3	2E	8	ILE
3	2E	16	ARG
3	2E	17	ASP
3	2E	21	ARG
3	2E	29	TYR
3	2E	31	HIS
3	2E	32	LEU
3	2E	44	GLU
3	2E	56	ASP
3	2E	58	GLU
3	2E	63	ASN
3	2E	70	VAL
3	2E	72	LYS
3	2E	79	ARG
3	2E	98	ASN
3	2E	105	GLU
3	2E	116	VAL
3	2E	128	PHE
3	2E	132	ARG
3	2E	136	GLN
3	2E	138	VAL
3	2E	167	TRP
3	2E	179	ARG
3	2E	190	ARG
3	2E	202	ILE
3	2E	206	GLU
4	3E	3	ARG
4	3E	5	ILE
4	3E	8	VAL
4	3E	10	ARG
4	3E	12	CYS
4	3E	15	GLU
4	3E	21	LEU
4	3E	31	CYS
4	3E	46	LYS
4	3E	47	ARG
4	3E	58	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	3E	66	ARG
4	3E	84	LYS
4	3E	85	LYS
4	3E	86	LYS
4	3E	96	LEU
4	3E	106	TYR
4	3E	107	ARG
4	3E	108	LEU
4	3E	115	ARG
4	3E	122	ARG
4	3E	127	THR
4	3E	135	LEU
4	3E	145	GLU
4	3E	152	SER
4	3E	154	ASN
4	3E	160	GLN
4	3E	168	ARG
4	3E	184	LYS
4	3E	188	LEU
4	3E	190	ASP
4	3E	193	ASP
4	3E	196	LEU
4	3E	200	GLU
5	4E	10	MET
5	4E	11	ILE
5	4E	12	LEU
5	4E	16	THR
5	4E	18	ARG
5	4E	31	LEU
5	4E	33	VAL
5	4E	41	VAL
5	4E	56	GLN
5	4E	64	ARG
5	4E	68	GLU
5	4E	71	LEU
5	4E	72	GLN
5	4E	73	ASN
5	4E	75	THR
5	4E	79	GLU
5	4E	91	LEU
5	4E	92	LYS
5	4E	116	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	4E	147	ASP
5	4E	152	ARG
5	4E	153	LYS
6	5E	21	LEU
6	5E	23	LYS
6	5E	25	ILE
6	5E	43	LEU
6	5E	55	ASP
6	5E	64	GLN
6	5E	70	ASP
6	5E	75	LEU
6	5E	86	ARG
6	5E	94	GLN
7	6E	6	ARG
7	6E	12	LEU
7	6E	16	LEU
7	6E	22	LEU
7	6E	27	ILE
7	6E	38	LEU
7	6E	54	THR
7	6E	59	LEU
7	6E	63	LYS
7	6E	73	MET
7	6E	75	VAL
7	6E	79	ARG
7	6E	89	MET
7	6E	91	VAL
7	6E	104	LEU
7	6E	111	ARG
7	6E	113	GLU
7	6E	115	ARG
7	6E	149	ARG
7	6E	155	ARG
8	7E	1	MET
8	7E	19	VAL
8	7E	25	ASP
8	7E	26	VAL
8	7E	36	LEU
8	7E	45	ILE
8	7E	50	ARG
8	7E	52	ASP
8	7E	65	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	7E	68	ARG
8	7E	80	ILE
8	7E	82	HIS
8	7E	85	ARG
8	7E	91	ARG
8	7E	95	VAL
8	7E	102	ARG
8	7E	104	ARG
8	7E	112	LEU
8	7E	133	LEU
8	7E	137	VAL
9	8E	9	ARG
9	8E	10	ARG
9	8E	16	ARG
9	8E	20	ARG
9	8E	38	GLN
9	8E	42	ARG
9	8E	44	VAL
9	8E	47	LEU
9	8E	50	LEU
9	8E	54	ASP
9	8E	58	HIS
9	8E	75	ASP
9	8E	79	LEU
9	8E	81	ILE
9	8E	83	ARG
9	8E	88	TYR
9	8E	91	ASP
9	8E	92	TYR
9	8E	97	LYS
9	8E	108	VAL
9	8E	121	ARG
9	8E	125	TYR
10	1I	25	GLU
10	1I	28	ARG
10	1I	38	ILE
10	1I	58	ASP
10	1I	60	ARG
10	1I	75	ILE
10	1I	76	ASN
10	1I	81	THR
11	2I	28	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	2I	32	ILE
11	2I	36	ASP
11	2I	48	ILE
11	2I	71	LYS
11	2I	93	GLN
11	2I	99	GLN
11	2I	103	LEU
11	2I	105	VAL
11	2I	108	ILE
11	2I	109	VAL
11	2I	111	ASP
11	2I	114	VAL
11	2I	117	ASN
12	3I	11	VAL
12	3I	18	VAL
12	3I	19	ARG
12	3I	33	ARG
12	3I	54	LYS
12	3I	60	LEU
12	3I	62	SER
12	3I	64	TYR
12	3I	91	LYS
12	3I	111	LYS
12	3I	115	LYS
12	3I	126	LYS
13	4I	9	ILE
13	4I	12	ASN
13	4I	20	THR
13	4I	31	LYS
13	4I	32	GLU
13	4I	44	ARG
13	4I	45	VAL
13	4I	48	LEU
13	4I	56	LEU
13	4I	64	TRP
13	4I	67	GLU
13	4I	70	LEU
13	4I	88	ARG
13	4I	101	GLN
13	4I	102	ARG
13	4I	105	THR
13	4I	106	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	4I	108	ARG
13	4I	110	ARG
13	4I	111	LYS
14	5I	3	ARG
14	5I	4	LYS
14	5I	6	LEU
14	5I	7	ILE
14	5I	15	LYS
14	5I	18	VAL
14	5I	22	THR
14	5I	23	ARG
14	5I	32	SER
14	5I	33	VAL
14	5I	35	ARG
14	5I	41	ARG
14	5I	50	LYS
15	6I	7	GLU
15	6I	10	LYS
15	6I	26	GLU
15	6I	35	ARG
15	6I	38	ARG
15	6I	39	LEU
15	6I	41	GLU
15	6I	47	LYS
15	6I	48	LYS
15	6I	54	ARG
15	6I	59	MET
15	6I	62	GLN
15	6I	66	LEU
15	6I	71	GLN
16	7I	8	ARG
16	7I	11	SER
16	7I	18	ARG
16	7I	19	ILE
16	7I	20	VAL
16	7I	27	LYS
16	7I	28	ARG
16	7I	47	ASP
16	7I	50	LYS
16	7I	54	GLU
16	7I	55	ARG
16	7I	67	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	7I	72	ARG
16	7I	83	GLU
17	8I	24	GLU
17	8I	25	ARG
17	8I	31	LEU
17	8I	38	ARG
17	8I	48	GLU
17	8I	52	LYS
17	8I	53	LEU
17	8I	63	ARG
17	8I	68	ARG
17	8I	74	LEU
17	8I	97	SER
17	8I	100	LYS
18	9I	31	LEU
18	9I	32	ARG
18	9I	42	ARG
18	9I	45	SER
18	9I	55	ARG
18	9I	76	LEU
18	9I	82	THR
18	9I	85	LEU
18	9I	86	VAL
19	AI	3	ARG
19	AI	6	LYS
19	AI	12	ASP
19	AI	31	ILE
19	AI	37	ARG
19	AI	43	GLU
19	AI	44	MET
19	AI	58	VAL
19	AI	67	VAL
19	AI	77	THR
19	AI	78	ARG
20	BI	9	ASN
20	BI	10	LEU
20	BI	13	LEU
20	BI	19	SER
20	BI	24	LEU
20	BI	30	LYS
20	BI	37	SER
20	BI	51	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	BI	53	LEU
20	BI	56	MET
20	BI	72	LEU
20	BI	73	HIS
20	BI	75	ASN
20	BI	87	LYS
21	1F	6	ARG
21	1F	8	THR
21	1F	9	ARG
21	1F	10	ARG
28	71	3	HIS
28	71	6	ARG
28	71	10	LEU
28	71	14	VAL
28	71	15	ASP
28	71	23	ASP
28	71	34	THR
28	71	36	LYS
28	71	37	PHE
28	71	42	GLU
28	71	53	ARG
28	71	55	ASP
28	71	59	ARG
28	71	166	ASP
28	71	168	THR
28	71	174	PRO
28	71	180	PHE
28	71	211	SER
28	71	216	THR
28	71	218	MET
28	71	224	ILE
29	11	3	VAL
29	11	4	LYS
29	11	13	ARG
29	11	16	MET
29	11	17	THR
29	11	23	GLU
29	11	33	LEU
29	11	35	LYS
29	11	37	LEU
29	11	38	LYS
29	11	39	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
29	11	43	ARG
29	11	64	ILE
29	11	65	ILE
29	11	72	LYS
29	11	78	LYS
29	11	83	GLU
29	11	88	ARG
29	11	94	LEU
29	11	103	ARG
29	11	105	ILE
29	11	113	VAL
29	11	117	VAL
29	11	126	GLN
29	11	142	VAL
29	11	154	LYS
29	11	165	ILE
29	11	183	ARG
29	11	192	THR
29	11	200	ASP
29	11	211	ARG
29	11	212	SER
29	11	217	ARG
29	11	221	VAL
29	11	229	VAL
29	11	242	ARG
29	11	257	LEU
29	11	259	THR
29	11	260	ARG
29	11	271	ILE
29	11	273	ARG
30	21	12	THR
30	21	14	ILE
30	21	16	ARG
30	21	23	VAL
30	21	25	VAL
30	21	26	ILE
30	21	45	THR
30	21	47	VAL
30	21	48	GLN
30	21	49	LEU
30	21	52	LEU
30	21	54	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	21	55	ASN
30	21	57	LYS
30	21	63	LEU
30	21	67	PHE
30	21	76	ARG
30	21	78	LEU
30	21	82	ARG
30	21	89	ASP
30	21	91	VAL
30	21	93	VAL
30	21	101	ARG
30	21	105	THR
30	21	111	ARG
30	21	116	VAL
30	21	119	ARG
30	21	128	SER
30	21	138	PRO
30	21	140	SER
30	21	146	THR
30	21	152	LYS
30	21	154	LYS
30	21	166	THR
30	21	175	VAL
30	21	179	GLU
30	21	181	LEU
30	21	182	LEU
30	21	188	VAL
30	21	195	LEU
30	21	196	VAL
30	21	197	ILE
30	21	201	THR
30	21	203	LYS
31	31	7	TYR
31	31	13	SER
31	31	15	SER
31	31	17	ARG
31	31	18	ARG
31	31	28	ILE
31	31	32	LEU
31	31	33	LEU
31	31	57	VAL
31	31	64	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	31	67	GLN
31	31	74	ARG
31	31	101	LEU
31	31	106	ARG
31	31	107	LYS
31	31	117	ARG
31	31	124	LEU
31	31	127	GLU
31	31	135	LYS
31	31	136	THR
31	31	140	LEU
31	31	145	GLU
31	31	158	THR
31	31	164	ARG
31	31	168	ARG
31	31	170	LEU
31	31	174	VAL
31	31	181	LEU
31	31	191	ARG
31	31	197	ASP
31	31	200	GLU
31	31	203	GLN
31	31	204	ASN
32	41	22	ARG
32	41	26	GLN
32	41	28	VAL
32	41	43	LEU
32	41	45	GLU
32	41	48	GLU
32	41	51	ARG
32	41	53	LEU
32	41	58	GLN
32	41	67	LYS
32	41	70	VAL
32	41	80	PHE
32	41	82	LEU
32	41	90	LEU
32	41	94	LEU
32	41	96	ARG
32	41	101	ILE
32	41	104	GLU
32	41	108	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	41	116	ASP
32	41	121	ASN
32	41	128	ARG
32	41	136	ARG
32	41	145	THR
32	41	152	LEU
32	41	162	THR
32	41	165	THR
33	51	2	SER
33	51	3	ARG
33	51	4	ILE
33	51	7	LEU
33	51	9	ILE
33	51	11	VAL
33	51	16	SER
33	51	24	VAL
33	51	37	VAL
33	51	40	GLU
33	51	41	MET
33	51	42	ARG
33	51	43	VAL
33	51	50	VAL
33	51	56	SER
33	51	63	SER
33	51	64	LEU
33	51	68	THR
33	51	71	LEU
33	51	77	LYS
33	51	80	SER
33	51	81	GLU
33	51	83	TYR
33	51	86	GLU
33	51	88	LEU
33	51	98	LEU
33	51	104	GLU
33	51	105	LEU
33	51	116	GLU
33	51	127	GLU
33	51	129	THR
33	51	131	VAL
33	51	139	GLN
33	51	149	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	51	152	ARG
33	51	167	GLU
33	51	170	ARG
34	61	2	LYS
34	61	9	LEU
34	61	12	LEU
34	61	20	ASP
34	61	21	VAL
34	61	25	TYR
34	61	38	LEU
34	61	41	GLU
34	61	44	LEU
34	61	47	LEU
34	61	48	GLU
34	61	50	ARG
34	61	54	GLN
34	61	64	GLU
34	61	75	LEU
34	61	77	LEU
34	61	82	ARG
34	61	85	GLU
34	61	92	VAL
34	61	95	LYS
34	61	99	GLU
34	61	101	LEU
34	61	102	SER
34	61	108	THR
34	61	110	ASP
34	61	114	LEU
34	61	117	GLU
34	61	122	GLU
34	61	127	VAL
34	61	131	LYS
34	61	135	GLU
34	61	136	VAL
34	61	139	GLN
34	61	140	LEU
34	61	142	VAL
34	61	145	VAL
35	58	1	MET
35	58	2	LYS
35	58	5	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	58	7	LYS
35	58	14	VAL
35	58	28	THR
35	58	32	THR
35	58	33	LEU
35	58	34	LEU
35	58	42	TRP
35	58	43	THR
35	58	48	MET
35	58	58	ASP
35	58	60	ILE
35	58	61	ARG
35	58	65	LYS
35	58	67	LEU
35	58	87	LEU
35	58	89	LYS
35	58	90	MET
35	58	96	GLU
35	58	97	ARG
35	58	99	LEU
35	58	120	LEU
35	58	127	ASP
35	58	128	HIS
35	58	130	HIS
35	58	131	GLN
35	58	137	LYS
36	68	8	LEU
36	68	17	ARG
36	68	23	ARG
36	68	31	LYS
36	68	38	VAL
36	68	47	ILE
36	68	58	VAL
36	68	66	LYS
36	68	78	ARG
36	68	94	ARG
37	78	1	MET
37	78	5	ASP
37	78	6	LEU
37	78	7	ARG
37	78	10	PRO
37	78	13	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	78	14	LYS
37	78	15	ARG
37	78	16	ARG
37	78	18	ARG
37	78	21	ARG
37	78	25	SER
37	78	27	HIS
37	78	41	ARG
37	78	45	LEU
37	78	49	ARG
37	78	50	ARG
37	78	56	SER
37	78	61	ARG
37	78	65	ARG
37	78	75	ILE
37	78	77	ARG
37	78	88	LEU
37	78	90	ARG
37	78	96	THR
37	78	98	GLU
37	78	99	LEU
37	78	100	LEU
37	78	101	VAL
37	78	105	LEU
37	78	106	LEU
37	78	112	LEU
37	78	115	LEU
37	78	135	LEU
37	78	144	GLU
37	78	146	VAL
38	88	5	ARG
38	88	7	MET
38	88	11	LYS
38	88	25	ASP
38	88	26	TYR
38	88	35	VAL
38	88	45	GLN
38	88	48	GLU
38	88	55	VAL
38	88	56	ARG
38	88	58	PHE
38	88	59	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	88	60	ARG
38	88	64	ILE
38	88	67	ARG
38	88	81	VAL
38	88	83	MET
38	88	110	THR
38	88	129	THR
38	88	138	ASP
39	98	1	MET
39	98	2	ARG
39	98	6	SER
39	98	9	LYS
39	98	17	ARG
39	98	18	LEU
39	98	28	LEU
39	98	29	LEU
39	98	33	ARG
39	98	34	ILE
39	98	36	THR
39	98	44	LEU
39	98	48	VAL
39	98	49	ASP
39	98	54	LEU
39	98	57	ARG
39	98	59	ASP
39	98	63	ARG
39	98	65	LEU
39	98	79	LEU
39	98	82	GLU
39	98	91	GLN
39	98	96	ARG
39	98	104	ARG
39	98	105	ARG
39	98	111	LEU
39	98	113	LEU
39	98	116	LEU
39	98	118	GLU
40	A8	3	ARG
40	A8	8	GLU
40	A8	14	VAL
40	A8	24	LEU
40	A8	30	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	A8	32	LEU
40	A8	35	ILE
40	A8	36	TYR
40	A8	43	GLU
40	A8	46	VAL
40	A8	54	LEU
40	A8	56	LEU
40	A8	58	LEU
40	A8	69	VAL
40	A8	73	LEU
40	A8	83	LYS
40	A8	89	ARG
40	A8	97	ARG
40	A8	101	LEU
40	A8	106	ARG
40	A8	110	LEU
41	B8	2	ASN
41	B8	3	ARG
41	B8	10	VAL
41	B8	16	ARG
41	B8	21	GLU
41	B8	27	THR
41	B8	33	LYS
41	B8	38	ASN
41	B8	39	ARG
41	B8	42	ILE
41	B8	50	ILE
41	B8	55	ASN
41	B8	58	ASN
41	B8	59	THR
41	B8	62	THR
41	B8	64	ARG
41	B8	74	ARG
41	B8	85	LYS
41	B8	86	ILE
41	B8	87	ASP
41	B8	88	ILE
41	B8	96	ARG
41	B8	98	LYS
41	B8	99	LEU
41	B8	106	SER
41	B8	108	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	B8	110	ILE
41	B8	111	ARG
41	B8	112	ARG
41	B8	115	ARG
41	B8	118	ARG
41	B8	128	GLU
41	B8	129	ARG
41	B8	133	GLU
42	C8	8	VAL
42	C8	13	LYS
42	C8	27	LEU
42	C8	51	LYS
42	C8	52	ARG
42	C8	74	LEU
42	C8	77	SER
42	C8	79	PHE
42	C8	85	LYS
42	C8	89	GLU
42	C8	92	ARG
42	C8	93	LYS
42	C8	94	ASN
42	C8	104	GLN
42	C8	108	GLU
42	C8	112	ARG
43	D8	6	LYS
43	D8	7	THR
43	D8	14	VAL
43	D8	18	LEU
43	D8	20	LEU
43	D8	21	ARG
43	D8	25	LEU
43	D8	33	VAL
43	D8	35	LEU
43	D8	37	VAL
43	D8	38	LEU
43	D8	40	LEU
43	D8	49	THR
43	D8	52	VAL
43	D8	58	VAL
43	D8	64	HIS
43	D8	73	SER
43	D8	79	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
43	D8	95	LEU
44	E8	4	LYS
44	E8	11	ARG
44	E8	15	ARG
44	E8	19	LEU
44	E8	20	VAL
44	E8	23	LEU
44	E8	41	LYS
44	E8	42	ARG
44	E8	51	LEU
44	E8	52	GLU
44	E8	64	MET
44	E8	65	LEU
44	E8	76	VAL
44	E8	78	GLU
44	E8	92	ARG
44	E8	96	ILE
44	E8	107	LEU
45	F8	12	VAL
45	F8	23	GLU
45	F8	27	THR
45	F8	38	GLU
45	F8	41	ASN
45	F8	45	THR
45	F8	49	VAL
45	F8	66	LEU
45	F8	68	ARG
45	F8	70	LEU
45	F8	72	LYS
45	F8	78	LYS
45	F8	80	ILE
46	G8	3	VAL
46	G8	4	LYS
46	G8	6	HIS
46	G8	24	VAL
46	G8	38	ILE
46	G8	43	ASN
46	G8	44	ILE
46	G8	57	GLN
46	G8	64	GLU
46	G8	67	LEU
46	G8	71	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
46	G8	75	ILE
46	G8	82	PRO
46	G8	85	VAL
46	G8	86	ARG
46	G8	96	ILE
46	G8	98	VAL
46	G8	102	CYS
47	H8	1	MET
47	H8	11	GLU
47	H8	19	ARG
47	H8	35	ARG
47	H8	37	VAL
47	H8	41	LEU
47	H8	46	LYS
47	H8	61	LEU
47	H8	71	VAL
47	H8	72	ARG
47	H8	76	LEU
47	H8	77	ASP
47	H8	80	ARG
47	H8	82	ARG
47	H8	86	VAL
47	H8	91	LEU
47	H8	94	GLU
47	H8	105	VAL
47	H8	117	LEU
47	H8	119	GLU
47	H8	121	HIS
47	H8	126	VAL
47	H8	128	VAL
47	H8	132	ASN
47	H8	142	SER
47	H8	154	ASP
47	H8	169	GLU
48	I8	10	THR
48	I8	36	ILE
48	I8	38	VAL
48	I8	40	GLN
48	I8	43	THR
48	I8	49	LYS
48	I8	67	VAL
48	I8	74	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
48	I8	82	ARG
49	J8	4	VAL
49	J8	41	ARG
49	J8	73	LEU
49	J8	74	VAL
49	J8	80	LEU
49	J8	81	LYS
49	J8	85	LEU
49	J8	91	LYS
49	J8	93	GLU
49	J8	94	LEU
49	J8	95	LEU
49	J8	96	LYS
50	K8	2	LYS
50	K8	3	LEU
50	K8	8	LYS
50	K8	14	ARG
50	K8	15	LYS
50	K8	16	LEU
50	K8	17	SER
50	K8	19	VAL
50	K8	24	LEU
50	K8	32	LEU
50	K8	41	ILE
50	K8	46	GLN
50	K8	47	ASN
50	K8	48	HIS
50	K8	51	ARG
50	K8	53	LEU
50	K8	54	LYS
50	K8	55	ARG
50	K8	62	THR
50	K8	64	LEU
50	K8	67	LYS
51	L8	4	LEU
51	L8	6	VAL
51	L8	8	LEU
51	L8	9	VAL
51	L8	31	LEU
51	L8	33	GLN
51	L8	40	THR
51	L8	44	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	L8	57	GLU
51	L8	58	VAL
52	M8	5	ILE
52	M8	10	VAL
52	M8	15	ILE
52	M8	16	CYS
52	M8	18	CYS
52	M8	34	GLU
52	M8	36	CYS
52	M8	38	LYS
52	M8	40	HIS
52	M8	42	PHE
52	M8	47	GLN
52	M8	60	GLN
52	M8	61	ARG
52	M8	63	TYR
53	N8	3	LYS
53	N8	6	VAL
53	N8	11	THR
53	N8	15	ARG
53	N8	16	ARG
53	N8	29	THR
53	N8	37	LYS
53	N8	40	LYS
53	N8	46	CYS
54	O8	10	LEU
54	O8	12	GLU
54	O8	16	CYS
54	O8	21	TYR
54	O8	26	ASN
54	O8	27	LYS
54	O8	30	THR
54	O8	33	LYS
54	O8	34	LEU
54	O8	36	LEU
54	O8	37	ARG
54	O8	39	TYR
54	O8	42	TRP
54	O8	44	ARG
54	O8	47	THR
55	P8	4	THR
55	P8	8	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
55	P8	14	LYS
55	P8	24	THR
55	P8	29	LYS
55	P8	32	LYS
55	P8	43	THR
56	Q8	4	MET
56	Q8	14	VAL
56	Q8	34	TRP
56	Q8	35	GLN
56	Q8	44	LYS
56	Q8	46	ARG
56	Q8	58	ILE
56	Q8	59	LYS
56	Q8	60	LEU
56	Q8	62	LEU
2	12	19	HIS
2	12	21	ARG
2	12	24	TRP
2	12	32	ILE
2	12	36	ARG
2	12	40	HIS
2	12	41	ILE
2	12	44	LEU
2	12	49	GLU
2	12	51	LEU
2	12	52	GLU
2	12	55	PHE
2	12	58	ILE
2	12	60	ASP
2	12	76	GLN
2	12	80	ILE
2	12	84	GLU
2	12	90	MET
2	12	94	ASN
2	12	96	ARG
2	12	108	ILE
2	12	126	GLU
2	12	129	GLU
2	12	145	LEU
2	12	155	LEU
2	12	160	ASP
2	12	165	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	12	172	ILE
2	12	179	LYS
2	12	185	ILE
2	12	187	LEU
2	12	191	ASP
2	12	193	ASP
2	12	220	ASP
2	12	221	LEU
2	12	224	GLN
3	22	4	LYS
3	22	6	HIS
3	22	11	ARG
3	22	16	ARG
3	22	18	TRP
3	22	22	TRP
3	22	29	TYR
3	22	34	LEU
3	22	47	LEU
3	22	52	LEU
3	22	59	ARG
3	22	76	VAL
3	22	85	ARG
3	22	90	GLU
3	22	94	LEU
3	22	104	GLN
3	22	124	ILE
3	22	128	PHE
3	22	131	ARG
3	22	164	ARG
3	22	167	TRP
3	22	175	LEU
3	22	179	ARG
3	22	182	ILE
3	22	202	ILE
3	22	204	LEU
4	32	3	ARG
4	32	4	TYR
4	32	5	ILE
4	32	8	VAL
4	32	12	CYS
4	32	13	ARG
4	32	17	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	32	21	LEU
4	32	26	CYS
4	32	30	LYS
4	32	35	ARG
4	32	58	LEU
4	32	59	ARG
4	32	73	ARG
4	32	83	SER
4	32	122	ARG
4	32	127	THR
4	32	131	ARG
4	32	134	ASP
4	32	135	LEU
4	32	137	SER
4	32	150	GLU
4	32	152	SER
4	32	170	VAL
4	32	187	ARG
4	32	191	ARG
4	32	196	LEU
4	32	200	GLU
4	32	204	ILE
5	42	10	MET
5	42	12	LEU
5	42	13	ILE
5	42	16	THR
5	42	25	ARG
5	42	31	LEU
5	42	40	ARG
5	42	43	LEU
5	42	47	LYS
5	42	51	VAL
5	42	53	LEU
5	42	66	MET
5	42	73	ASN
5	42	78	HIS
5	42	79	GLU
5	42	81	GLU
5	42	83	GLU
5	42	87	SER
5	42	90	VAL
5	42	101	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	42	118	ILE
5	42	120	THR
5	42	126	ARG
5	42	127	ASN
5	42	135	THR
5	42	150	ARG
5	42	151	LEU
6	52	3	ARG
6	52	14	LEU
6	52	16	GLN
6	52	17	SER
6	52	21	LEU
6	52	24	GLU
6	52	28	ARG
6	52	40	VAL
6	52	47	ARG
6	52	63	TYR
6	52	71	ARG
6	52	83	ASP
6	52	86	ARG
6	52	87	ARG
6	52	93	SER
6	52	98	LEU
7	62	8	GLU
7	62	9	VAL
7	62	11	GLN
7	62	13	GLN
7	62	16	LEU
7	62	24	THR
7	62	37	ASN
7	62	38	LEU
7	62	52	GLU
7	62	59	LEU
7	62	60	LYS
7	62	66	VAL
7	62	67	GLU
7	62	70	LYS
7	62	72	ARG
7	62	73	MET
7	62	90	GLU
7	62	94	ARG
7	62	98	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	62	104	LEU
7	62	114	ARG
7	62	131	LYS
7	62	137	LYS
7	62	142	GLU
7	62	143	ARG
7	62	144	MET
8	72	12	ARG
8	72	25	ASP
8	72	33	GLU
8	72	39	LEU
8	72	41	ARG
8	72	52	ASP
8	72	56	LYS
8	72	78	GLN
8	72	82	HIS
8	72	83	ILE
8	72	97	VAL
8	72	99	GLU
8	72	102	ARG
8	72	104	ARG
8	72	120	THR
8	72	127	LEU
8	72	138	TRP
9	82	7	THR
9	82	10	ARG
9	82	19	LEU
9	82	20	ARG
9	82	27	THR
9	82	33	PHE
9	82	34	ASN
9	82	36	TYR
9	82	42	ARG
9	82	47	LEU
9	82	54	ASP
9	82	56	LEU
9	82	91	ASP
9	82	95	LYS
9	82	102	LEU
9	82	112	LYS
9	82	113	LYS
9	82	117	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	82	124	GLN
10	1A	13	HIS
10	1A	17	ASP
10	1A	21	GLN
10	1A	22	LYS
10	1A	24	VAL
10	1A	33	GLN
10	1A	34	VAL
10	1A	38	ILE
10	1A	43	ARG
10	1A	55	LYS
10	1A	58	ASP
10	1A	59	SER
10	1A	62	HIS
10	1A	65	LEU
10	1A	66	ARG
10	1A	70	ARG
10	1A	74	ILE
10	1A	75	ILE
10	1A	79	ARG
10	1A	84	GLN
11	2A	14	VAL
11	2A	18	ARG
11	2A	29	ILE
11	2A	30	VAL
11	2A	31	THR
11	2A	54	ARG
11	2A	63	LEU
11	2A	78	GLN
11	2A	79	SER
11	2A	80	VAL
11	2A	87	THR
11	2A	93	GLN
11	2A	99	GLN
11	2A	103	LEU
11	2A	105	VAL
11	2A	109	VAL
11	2A	114	VAL
11	2A	119	CYS
12	3A	22	SER
12	3A	23	LYS
12	3A	24	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	3A	27	LEU
12	3A	33	ARG
12	3A	34	ARG
12	3A	39	VAL
12	3A	41	ARG
12	3A	54	LYS
12	3A	57	LYS
12	3A	59	ARG
12	3A	60	LEU
12	3A	62	SER
12	3A	64	TYR
12	3A	66	VAL
12	3A	83	VAL
12	3A	84	LEU
12	3A	85	ILE
12	3A	89	ARG
12	3A	98	TYR
12	3A	102	ARG
12	3A	111	LYS
12	3A	118	SER
13	4A	9	ILE
13	4A	11	ARG
13	4A	12	ASN
13	4A	13	LYS
13	4A	17	VAL
13	4A	37	THR
13	4A	39	ILE
13	4A	47	ASP
13	4A	49	THR
13	4A	54	VAL
13	4A	58	GLU
13	4A	62	ASN
13	4A	64	TRP
13	4A	66	LEU
13	4A	81	LEU
13	4A	86	CYS
13	4A	88	ARG
13	4A	94	ARG
13	4A	101	GLN
13	4A	103	THR
13	4A	108	ARG
13	4A	117	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	5A	7	ILE
14	5A	16	PHE
14	5A	22	THR
14	5A	25	VAL
14	5A	29	ARG
14	5A	33	VAL
14	5A	42	ILE
14	5A	43	CYS
15	6A	3	ILE
15	6A	17	ARG
15	6A	22	THR
15	6A	41	GLU
15	6A	47	LYS
15	6A	68	ARG
15	6A	71	GLN
15	6A	84	LYS
16	7A	1	MET
16	7A	2	VAL
16	7A	6	LEU
16	7A	27	LYS
16	7A	29	ASP
16	7A	55	ARG
16	7A	65	GLN
16	7A	67	THR
16	7A	74	LEU
16	7A	76	GLN
16	7A	81	ARG
17	8A	10	VAL
17	8A	16	GLN
17	8A	24	GLU
17	8A	53	LEU
17	8A	57	VAL
17	8A	60	ILE
17	8A	62	SER
17	8A	63	ARG
17	8A	68	ARG
17	8A	74	LEU
17	8A	90	ILE
17	8A	100	LYS
18	9A	23	LYS
18	9A	26	LEU
18	9A	29	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	9A	32	ARG
18	9A	36	ASN
18	9A	42	ARG
18	9A	45	SER
18	9A	53	ARG
18	9A	68	LYS
18	9A	82	THR
18	9A	83	GLU
19	AA	6	LYS
19	AA	14	HIS
19	AA	15	LEU
19	AA	20	LEU
19	AA	21	GLU
19	AA	33	THR
19	AA	34	TRP
19	AA	43	GLU
19	AA	60	VAL
20	BA	13	LEU
20	BA	31	SER
20	BA	33	ILE
20	BA	45	GLN
20	BA	61	SER
20	BA	72	LEU
20	BA	74	LYS
20	BA	75	ASN
20	BA	85	MET
20	BA	99	LEU
21	1B	10	ARG
29	19	10	THR
29	19	13	ARG
29	19	24	ILE
29	19	27	THR
29	19	28	GLU
29	19	31	LYS
29	19	33	LEU
29	19	34	VAL
29	19	35	LYS
29	19	37	LEU
29	19	38	LYS
29	19	46	GLN
29	19	49	ILE
29	19	54	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
29	19	61	LEU
29	19	64	ILE
29	19	69	ARG
29	19	78	LYS
29	19	82	ILE
29	19	88	ARG
29	19	94	LEU
29	19	99	ASP
29	19	103	ARG
29	19	105	ILE
29	19	111	LEU
29	19	116	GLN
29	19	141	VAL
29	19	147	LEU
29	19	182	LEU
29	19	192	THR
29	19	211	ARG
29	19	217	ARG
29	19	239	ARG
29	19	242	ARG
29	19	244	ARG
29	19	253	GLN
29	19	257	LEU
29	19	260	ARG
29	19	262	ARG
29	19	266	SER
29	19	268	ARG
29	19	271	ILE
29	19	273	ARG
30	29	1	MET
30	29	7	VAL
30	29	12	THR
30	29	21	VAL
30	29	27	LEU
30	29	45	THR
30	29	49	LEU
30	29	57	LYS
30	29	66	HIS
30	29	67	PHE
30	29	73	GLU
30	29	76	ARG
30	29	78	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	29	79	ARG
30	29	89	ASP
30	29	111	ARG
30	29	113	PHE
30	29	116	VAL
30	29	119	ARG
30	29	121	ASN
30	29	144	ARG
30	29	149	ARG
30	29	164	ARG
30	29	170	LEU
30	29	175	VAL
30	29	178	GLU
30	29	181	LEU
30	29	197	ILE
30	29	200	GLU
30	29	201	THR
31	39	7	TYR
31	39	8	GLN
31	39	18	ARG
31	39	20	LEU
31	39	23	ASP
31	39	24	LEU
31	39	28	ILE
31	39	29	ASN
31	39	33	LEU
31	39	38	ARG
31	39	40	GLN
31	39	53	THR
31	39	57	VAL
31	39	62	ARG
31	39	67	GLN
31	39	68	LYS
31	39	69	HIS
31	39	70	THR
31	39	82	ILE
31	39	83	PHE
31	39	88	VAL
31	39	110	LEU
31	39	112	MET
31	39	123	LEU
31	39	140	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	39	144	LYS
31	39	145	GLU
31	39	153	SER
31	39	158	THR
31	39	165	ARG
31	39	181	LEU
31	39	190	GLU
31	39	191	ARG
31	39	194	MET
31	39	196	LEU
31	39	197	ASP
31	39	205	ARG
32	49	9	ARG
32	49	13	GLU
32	49	20	ILE
32	49	26	GLN
32	49	33	ARG
32	49	35	GLU
32	49	39	ILE
32	49	40	ASN
32	49	45	GLU
32	49	48	GLU
32	49	51	ARG
32	49	62	LEU
32	49	66	GLN
32	49	80	PHE
32	49	82	LEU
32	49	91	ARG
32	49	101	ILE
32	49	109	VAL
32	49	130	ASN
32	49	133	LEU
32	49	136	ARG
32	49	139	LEU
32	49	152	LEU
32	49	153	ARG
32	49	156	ASP
32	49	157	ILE
32	49	159	VAL
33	59	6	ARG
33	59	7	LEU
33	59	32	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	59	50	VAL
33	59	59	ARG
33	59	70	THR
33	59	72	ILE
33	59	83	TYR
33	59	85	LYS
33	59	86	GLU
33	59	89	ILE
33	59	101	ARG
33	59	103	LEU
33	59	105	LEU
33	59	107	VAL
33	59	116	GLU
33	59	119	GLU
33	59	122	THR
33	59	123	PHE
33	59	125	VAL
33	59	127	GLU
33	59	129	THR
33	59	130	ARG
33	59	131	VAL
33	59	136	ILE
33	59	137	ASP
33	59	139	GLN
33	59	147	ASN
33	59	152	ARG
33	59	157	TYR
33	59	158	HIS
33	59	160	LYS
33	59	167	GLU
33	59	171	LEU
34	69	1	MET
34	69	2	LYS
34	69	4	ILE
34	69	7	GLU
34	69	27	ARG
34	69	37	VAL
34	69	47	LEU
34	69	56	LYS
34	69	58	LEU
34	69	61	ARG
34	69	62	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	69	67	ARG
34	69	68	LEU
34	69	75	LEU
34	69	76	THR
34	69	77	LEU
34	69	78	THR
34	69	82	ARG
34	69	93	THR
34	69	101	LEU
34	69	104	GLN
34	69	105	HIS
34	69	109	ILE
34	69	114	LEU
34	69	117	GLU
34	69	118	LYS
34	69	125	GLU
34	69	127	VAL
34	69	130	TYR
34	69	135	GLU
34	69	141	LYS
34	69	142	VAL
34	69	145	VAL
35	15	4	TYR
35	15	5	VAL
35	15	9	VAL
35	15	12	ARG
35	15	14	VAL
35	15	15	LEU
35	15	28	THR
35	15	32	THR
35	15	33	LEU
35	15	34	LEU
35	15	41	ASP
35	15	43	THR
35	15	46	VAL
35	15	48	MET
35	15	59	LYS
35	15	61	ARG
35	15	63	THR
35	15	68	GLU
35	15	74	ARG
35	15	87	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	15	93	THR
35	15	94	HIS
35	15	99	LEU
35	15	130	HIS
35	15	131	GLN
35	15	134	ARG
36	25	1	MET
36	25	5	GLN
36	25	8	LEU
36	25	9	GLU
36	25	10	VAL
36	25	14	THR
36	25	22	ILE
36	25	24	VAL
36	25	28	SER
36	25	29	ASN
36	25	38	VAL
36	25	45	GLU
36	25	49	ARG
36	25	52	VAL
36	25	87	ILE
36	25	91	LEU
36	25	92	GLU
36	25	94	ARG
36	25	99	PHE
36	25	108	GLU
36	25	113	LYS
36	25	114	ILE
36	25	116	SER
36	25	117	LEU
37	35	4	SER
37	35	19	VAL
37	35	21	ARG
37	35	41	ARG
37	35	45	LEU
37	35	52	GLU
37	35	55	ARG
37	35	58	THR
37	35	59	LEU
37	35	62	LEU
37	35	67	MET
37	35	75	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	35	76	LYS
37	35	79	ARG
37	35	83	VAL
37	35	84	ASN
37	35	85	LEU
37	35	88	LEU
37	35	96	THR
37	35	98	GLU
37	35	102	ARG
37	35	105	LEU
37	35	112	LEU
37	35	114	ILE
37	35	125	VAL
37	35	132	LYS
37	35	133	SER
37	35	135	LEU
37	35	138	LEU
37	35	144	GLU
37	35	146	VAL
37	35	147	LEU
38	45	2	LEU
38	45	3	MET
38	45	10	ARG
38	45	18	LYS
38	45	22	LYS
38	45	26	TYR
38	45	27	VAL
38	45	38	GLU
38	45	45	GLN
38	45	54	MET
38	45	56	ARG
38	45	59	ARG
38	45	75	THR
38	45	76	LYS
38	45	83	MET
38	45	103	MET
38	45	110	THR
38	45	118	LEU
38	45	127	ILE
38	45	137	TYR
38	45	138	ASP
39	55	1	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
39	55	2	ARG
39	55	6	SER
39	55	9	LYS
39	55	17	ARG
39	55	18	LEU
39	55	24	GLN
39	55	28	LEU
39	55	29	LEU
39	55	33	ARG
39	55	35	THR
39	55	44	LEU
39	55	57	ARG
39	55	65	LEU
39	55	75	LEU
39	55	79	LEU
39	55	81	ASP
39	55	82	GLU
39	55	88	ARG
39	55	102	GLU
39	55	105	ARG
40	65	3	ARG
40	65	8	GLU
40	65	12	PHE
40	65	14	VAL
40	65	17	ARG
40	65	19	LYS
40	65	20	ARG
40	65	21	THR
40	65	27	SER
40	65	29	PHE
40	65	42	ASP
40	65	43	GLU
40	65	50	SER
40	65	62	LYS
40	65	69	VAL
40	65	71	ARG
40	65	73	LEU
40	65	75	GLU
40	65	89	ARG
40	65	98	VAL
40	65	101	LEU
40	65	106	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	65	107	GLU
40	65	110	LEU
40	65	111	GLU
40	65	112	PHE
41	75	13	ARG
41	75	17	THR
41	75	21	GLU
41	75	27	THR
41	75	36	GLU
41	75	42	ILE
41	75	50	ILE
41	75	55	ASN
41	75	57	PHE
41	75	62	THR
41	75	64	ARG
41	75	65	LYS
41	75	67	SER
41	75	86	ILE
41	75	87	ASP
41	75	88	ILE
41	75	91	ARG
41	75	93	ARG
41	75	105	LEU
41	75	112	ARG
41	75	115	ARG
41	75	118	ARG
42	85	5	LYS
42	85	15	LYS
42	85	20	LEU
42	85	27	LEU
42	85	34	LYS
42	85	52	ARG
42	85	55	ARG
42	85	58	ARG
42	85	59	ARG
42	85	64	ARG
42	85	70	ARG
42	85	71	GLN
42	85	74	LEU
42	85	92	ARG
42	85	97	ASP
42	85	101	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
42	85	104	GLN
42	85	112	ARG
42	85	114	LYS
42	85	117	GLN
43	95	7	THR
43	95	12	TYR
43	95	13	ARG
43	95	28	GLU
43	95	33	VAL
43	95	35	LEU
43	95	49	THR
43	95	57	VAL
43	95	66	ARG
43	95	69	LYS
43	95	71	LEU
43	95	91	TYR
43	95	95	LEU
44	A5	11	ARG
44	A5	18	ARG
44	A5	23	LEU
44	A5	39	THR
44	A5	41	LYS
44	A5	50	VAL
44	A5	51	LEU
44	A5	60	ASN
44	A5	65	LEU
44	A5	67	ASP
44	A5	70	TYR
44	A5	78	GLU
44	A5	100	THR
44	A5	106	ILE
44	A5	107	LEU
44	A5	110	LYS
44	A5	111	HIS
45	B5	12	VAL
45	B5	23	GLU
45	B5	27	THR
45	B5	30	VAL
45	B5	35	THR
45	B5	48	LYS
45	B5	49	VAL
45	B5	53	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
45	B5	60	ARG
45	B5	63	LYS
45	B5	66	LEU
45	B5	69	TYR
45	B5	70	LEU
45	B5	75	ASP
45	B5	80	ILE
45	B5	81	VAL
45	B5	82	GLN
45	B5	92	LEU
46	C5	3	VAL
46	C5	14	LEU
46	C5	23	ARG
46	C5	24	VAL
46	C5	43	ASN
46	C5	51	VAL
46	C5	55	TYR
46	C5	61	ILE
46	C5	62	GLU
46	C5	70	SER
46	C5	71	LYS
46	C5	72	VAL
46	C5	76	CYS
46	C5	84	ARG
46	C5	85	VAL
46	C5	86	ARG
46	C5	87	LYS
46	C5	89	PHE
46	C5	94	LYS
46	C5	97	ARG
46	C5	98	VAL
46	C5	101	LYS
47	D5	4	ARG
47	D5	5	LEU
47	D5	14	LYS
47	D5	16	SER
47	D5	18	LEU
47	D5	19	ARG
47	D5	24	LEU
47	D5	28	MET
47	D5	30	ASN
47	D5	40	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
47	D5	41	LEU
47	D5	60	GLU
47	D5	61	LEU
47	D5	63	ASP
47	D5	71	VAL
47	D5	72	ARG
47	D5	76	LEU
47	D5	84	GLU
47	D5	87	ASP
47	D5	88	PHE
47	D5	91	LEU
47	D5	103	ARG
47	D5	119	GLU
47	D5	121	HIS
47	D5	126	VAL
47	D5	129	SER
47	D5	136	PHE
47	D5	138	GLU
47	D5	161	VAL
47	D5	165	VAL
47	D5	168	GLU
47	D5	170	THR
48	E5	12	ASN
48	E5	36	ILE
48	E5	38	VAL
48	E5	43	THR
48	E5	46	LYS
48	E5	63	VAL
49	F5	3	LYS
49	F5	5	CYS
49	F5	11	ARG
49	F5	19	GLN
49	F5	38	SER
49	F5	40	ARG
49	F5	72	GLU
49	F5	74	VAL
49	F5	76	ARG
49	F5	78	LYS
49	F5	82	LEU
49	F5	83	GLU
49	F5	89	GLU
49	F5	90	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	F5	91	LYS
49	F5	95	LEU
50	G5	6	VAL
50	G5	10	LEU
50	G5	15	LYS
50	G5	24	LEU
50	G5	26	ARG
50	G5	34	GLU
50	G5	35	LEU
50	G5	44	LEU
50	G5	46	GLN
50	G5	47	ASN
50	G5	48	HIS
50	G5	50	ILE
50	G5	53	LEU
50	G5	56	GLN
50	G5	60	LEU
50	G5	64	LEU
50	G5	65	ASN
51	H5	5	LYS
51	H5	8	LEU
51	H5	9	VAL
51	H5	17	LYS
51	H5	24	LYS
51	H5	30	ARG
51	H5	33	GLN
51	H5	35	ARG
51	H5	38	GLU
51	H5	40	THR
51	H5	44	ARG
51	H5	55	ARG
53	J5	6	VAL
53	J5	26	THR
53	J5	29	THR
53	J5	36	CYS
53	J5	44	THR
53	J5	48	GLU
53	J5	55	ARG
55	L5	1	MET
55	L5	4	THR
55	L5	8	ASN
55	L5	32	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
55	L5	36	GLN
55	L5	43	THR
56	M5	11	LYS
56	M5	13	ARG
56	M5	29	LYS
56	M5	31	HIS
56	M5	32	LEU
56	M5	37	SER
56	M5	41	ILE
56	M5	49	VAL
56	M5	58	ILE
56	M5	59	LYS
56	M5	60	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
7	6E	84	ASN
19	AI	23	ASN
28	71	188	ASN
2	12	16	HIS
2	12	19	HIS
2	12	40	HIS
5	42	78	HIS
18	9A	36	ASN
29	19	227	ASN
29	19	253	GLN
40	65	95	HIS
50	G5	47	ASN
51	H5	33	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	13	1497/1522 (98%)	331 (22%)	33 (2%)
1	1G	1506/1522 (98%)	352 (23%)	33 (2%)
22	1K	68/76 (89%)	27 (39%)	4 (5%)
23	2K	76/77 (98%)	21 (27%)	2 (2%)
23	2L	76/77 (98%)	15 (19%)	2 (2%)
24	1L	61/76 (80%)	24 (39%)	2 (3%)

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
24	3K	67/76 (88%)	37 (55%)	2 (2%)
24	3L	69/76 (90%)	30 (43%)	2 (2%)
25	4K	17/30 (56%)	9 (52%)	1 (5%)
25	4L	18/30 (60%)	12 (66%)	1 (5%)
26	14	2821/2917 (96%)	675 (23%)	42 (1%)
26	1H	2850/2917 (97%)	630 (22%)	52 (1%)
27	16	121/122 (99%)	24 (19%)	1 (0%)
27	1J	121/122 (99%)	32 (26%)	3 (2%)
All	All	9368/9640 (97%)	2219 (23%)	180 (1%)

All (2219) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	13	2	U
1	13	5	U
1	13	6	G
1	13	7	G
1	13	9	G
1	13	21	G
1	13	32	A
1	13	39	G
1	13	47	C
1	13	48	C
1	13	49	U
1	13	50	A
1	13	51	A
1	13	54	C
1	13	61	G
1	13	65	U
1	13	66	G
1	13	69	G
1	13	74	C
1	13	75	C
1	13	76	G
1	13	77	C
1	13	95	G
1	13	96	G
1	13	97	U
1	13	99	C
1	13	101	A
1	13	116	A
1	13	121	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	13	122	G
1	13	131	C
1	13	142	G
1	13	144	G
1	13	147	G
1	13	151	A
1	13	158	G
1	13	160	A
1	13	162	A
1	13	163	C
1	13	169	C
1	13	172	A
1	13	173	U
1	13	174	C
1	13	186(F)	C
1	13	188	U
1	13	189	U
1	13	191(A)	G
1	13	195	A
1	13	197	A
1	13	199	G
1	13	201	C
1	13	208	U
1	13	209	U
1	13	210	U
1	13	217	C
1	13	220	G
1	13	222	U
1	13	226	G
1	13	231	G
1	13	243	A
1	13	244	U
1	13	245	C
1	13	247	G
1	13	248	C
1	13	251	G
1	13	256	U
1	13	262	A
1	13	266	G
1	13	267	C
1	13	270	A
1	13	274	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	13	289	G
1	13	316	G
1	13	321	A
1	13	326	G
1	13	328	C
1	13	329	A
1	13	330	C
1	13	332	G
1	13	341	C
1	13	343	U
1	13	344	A
1	13	345	C
1	13	346	G
1	13	347	G
1	13	349	A
1	13	352	C
1	13	353	A
1	13	354	G
1	13	363	A
1	13	367	U
1	13	372	C
1	13	384	G
1	13	388	G
1	13	390	C
1	13	392	G
1	13	397	A
1	13	398	C
1	13	406	G
1	13	412	A
1	13	414	A
1	13	418	C
1	13	423	G
1	13	424	G
1	13	429	U
1	13	430	A
1	13	439	A
1	13	451	A
1	13	452	A
1	13	466	C
1	13	467	G
1	13	482	A
1	13	483	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	13	485	G
1	13	496	A
1	13	497	U
1	13	504	C
1	13	505	G
1	13	509	A
1	13	510	A
1	13	511	C
1	13	518	C
1	13	521	G
1	13	524	G
1	13	527	G
1	13	531	U
1	13	533	A
1	13	536	C
1	13	547	A
1	13	559	A
1	13	561	U
1	13	562	C
1	13	572	A
1	13	573	A
1	13	576	G
1	13	577	G
1	13	596	C
1	13	607	A
1	13	620	C
1	13	630	G
1	13	631	G
1	13	632	A
1	13	639	G
1	13	653	A
1	13	665	A
1	13	687	A
1	13	688	G
1	13	723	U
1	13	724	G
1	13	749	C
1	13	750	G
1	13	755	G
1	13	759	A
1	13	769	G
1	13	777	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	13	787	A
1	13	792	A
1	13	793	U
1	13	794	A
1	13	812	C
1	13	813	U
1	13	817	C
1	13	828	A
1	13	836	G
1	13	841	U
1	13	842	C
1	13	843	U
1	13	848	C
1	13	859	A
1	13	864	A
1	13	870	U
1	13	872	A
1	13	876	G
1	13	877	C
1	13	884	U
1	13	902	G
1	13	914	A
1	13	916	G
1	13	922	G
1	13	926	G
1	13	927	G
1	13	931	C
1	13	934	C
1	13	935	A
1	13	936	C
1	13	942	G
1	13	960	U
1	13	968	A
1	13	969	A
1	13	974	A
1	13	975	A
1	13	976	G
1	13	977	A
1	13	983	A
1	13	991	U
1	13	993	G
1	13	999	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	13	1004	A
1	13	1006	C
1	13	1007	C
1	13	1008	C
1	13	1009	G
1	13	1012	U
1	13	1021	G
1	13	1024	G
1	13	1025	U
1	13	1026	G
1	13	1028	C
1	13	1028(B)	C
1	13	1029	G
1	13	1031	G
1	13	1032	A
1	13	1032(A)	G
1	13	1032(B)	G
1	13	1033	G
1	13	1040	U
1	13	1042	G
1	13	1054	C
1	13	1055	A
1	13	1064	G
1	13	1065	U
1	13	1066	C
1	13	1081	G
1	13	1094	G
1	13	1095	U
1	13	1101	A
1	13	1110	A
1	13	1125	U
1	13	1126	U
1	13	1127	G
1	13	1129	C
1	13	1130	A
1	13	1132	C
1	13	1136	U
1	13	1137	C
1	13	1138	G
1	13	1139	G
1	13	1146	A
1	13	1150	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	13	1152	A
1	13	1154	G
1	13	1157	A
1	13	1158	C
1	13	1159	U
1	13	1177	G
1	13	1178	G
1	13	1179	A
1	13	1181	G
1	13	1182	G
1	13	1184	G
1	13	1188	A
1	13	1190	G
1	13	1191	A
1	13	1193	G
1	13	1196	U
1	13	1197	G
1	13	1201	A
1	13	1211	U
1	13	1212	U
1	13	1213	A
1	13	1225	A
1	13	1226	C
1	13	1227	A
1	13	1236	A
1	13	1238	A
1	13	1240	U
1	13	1241	G
1	13	1253	G
1	13	1256	A
1	13	1257	U
1	13	1258	G
1	13	1270	C
1	13	1272	G
1	13	1275	A
1	13	1278	U
1	13	1279	A
1	13	1280	A
1	13	1281	U
1	13	1286	A
1	13	1287	A
1	13	1288	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	13	1290	G
1	13	1299	A
1	13	1300	G
1	13	1301	U
1	13	1302	U
1	13	1303	C
1	13	1312	G
1	13	1317	C
1	13	1320	C
1	13	1331	G
1	13	1335	C
1	13	1336	C
1	13	1337	G
1	13	1340	A
1	13	1346	A
1	13	1347	G
1	13	1350	A
1	13	1353	G
1	13	1358	U
1	13	1361	G
1	13	1362(A)	C
1	13	1363	A
1	13	1368	G
1	13	1370	G
1	13	1379	G
1	13	1381	U
1	13	1388	C
1	13	1398	A
1	13	1419	G
1	13	1442	G
1	13	1443	G
1	13	1446	A
1	13	1447	G
1	13	1450	U
1	13	1452	C
1	13	1453	G
1	13	1455	G
1	13	1487	G
1	13	1492	A
1	13	1497	G
1	13	1499	A
1	13	1502	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	13	1504	G
1	13	1506	U
1	13	1507	A
1	13	1517	G
1	13	1529	G
1	13	1530	G
1	13	1534	A
1	13	1535	C
22	1K	4	U
22	1K	5	C
22	1K	6	G
22	1K	7	U
22	1K	9	A
22	1K	15	G
22	1K	18	G
22	1K	22	G
22	1K	26	A
22	1K	29	U
22	1K	45	G
22	1K	48	C
22	1K	50	C
22	1K	51	A
22	1K	56	C
22	1K	60	U
22	1K	61	C
22	1K	63	U
22	1K	68	G
22	1K	69	A
22	1K	70	C
22	1K	71	C
22	1K	72	C
22	1K	73	A
22	1K	74	C
22	1K	75	C
22	1K	76	A
23	2K	2	G
23	2K	6	G
23	2K	8	4SU
23	2K	9	G
23	2K	13	C
23	2K	15	G
23	2K	16	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
23	2K	19	G
23	2K	20	G
23	2K	22	A
23	2K	23	G
23	2K	31	G
23	2K	32	G
23	2K	33	OMC
23	2K	47	7MG
23	2K	48	U
23	2K	49	C
23	2K	50	G
23	2K	53	G
23	2K	68	C
23	2K	77	A
24	3K	2	G
24	3K	3	G
24	3K	4	U
24	3K	5	C
24	3K	7	U
24	3K	8	U
24	3K	9	A
24	3K	10	G
24	3K	11	C
24	3K	15	G
24	3K	23	A
24	3K	24	G
24	3K	26	A
24	3K	31	A
24	3K	34	U
24	3K	35	U
24	3K	37	A
24	3K	40	C
24	3K	45	G
24	3K	46	G
24	3K	49	G
24	3K	51	A
24	3K	52	G
24	3K	55	U
24	3K	56	C
24	3K	58	A
24	3K	59	A
24	3K	60	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	3K	61	C
24	3K	62	C
24	3K	64	G
24	3K	65	C
24	3K	66	A
24	3K	69	A
24	3K	72	C
24	3K	73	A
24	3K	76	A
25	4K	7	G
25	4K	8	A
25	4K	10	G
25	4K	11	U
25	4K	14	A
25	4K	15	A
25	4K	23	A
25	4K	24	A
25	4K	25	A
26	1H	9	U
26	1H	27	G
26	1H	34	C
26	1H	46	C
26	1H	51	G
26	1H	61	G
26	1H	63	U
26	1H	64	A
26	1H	70	G
26	1H	71	A
26	1H	74	A
26	1H	75	G
26	1H	85	G
26	1H	118	A
26	1H	119	A
26	1H	120	U
26	1H	125	G
26	1H	138	G
26	1H	153	C
26	1H	155	C
26	1H	163	U
26	1H	164	U
26	1H	171	G
26	1H	181	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	1H	188	G
26	1H	196	A
26	1H	197	A
26	1H	199	A
26	1H	214	G
26	1H	215	G
26	1H	216	A
26	1H	221	A
26	1H	222	A
26	1H	223	A
26	1H	228	A
26	1H	229	A
26	1H	233	A
26	1H	248	G
26	1H	250	G
26	1H	252	G
26	1H	261	G
26	1H	266	G
26	1H	269	U
26	1H	270(C)	C
26	1H	270(K)	C
26	1H	270(L)	U
26	1H	270(M)	U
26	1H	270(N)	G
26	1H	270(O)	U
26	1H	270(P)	C
26	1H	270(Y)	G
26	1H	271(C)	U
26	1H	271	G
26	1H	274	G
26	1H	275	G
26	1H	277	C
26	1H	278	A
26	1H	279	C
26	1H	283	A
26	1H	295	G
26	1H	299	A
26	1H	311	A
26	1H	323	G
26	1H	324	A
26	1H	326	G
26	1H	329	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	1H	330	A
26	1H	335	C
26	1H	342	G
26	1H	346	A
26	1H	352	G
26	1H	357	A
26	1H	363	G
26	1H	370	G
26	1H	372	G
26	1H	375	C
26	1H	382	G
26	1H	386	G
26	1H	405	U
26	1H	406	G
26	1H	407	G
26	1H	408	G
26	1H	411	G
26	1H	412	A
26	1H	418	G
26	1H	421	U
26	1H	427	U
26	1H	428	A
26	1H	434	U
26	1H	443	A
26	1H	444	C
26	1H	447	A
26	1H	448	U
26	1H	451	C
26	1H	455	C
26	1H	456	C
26	1H	457	A
26	1H	470	A
26	1H	471	A
26	1H	481	G
26	1H	482	A
26	1H	483	A
26	1H	494	G
26	1H	505	A
26	1H	508	G
26	1H	509	C
26	1H	510	C
26	1H	513	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	1H	528	A
26	1H	529	A
26	1H	531	C
26	1H	532	A
26	1H	533	G
26	1H	546	C
26	1H	548	A
26	1H	549	G
26	1H	550	G
26	1H	556	G
26	1H	563	G
26	1H	564	C
26	1H	573	G
26	1H	575	A
26	1H	584	C
26	1H	586	A
26	1H	588	U
26	1H	603	A
26	1H	607	U
26	1H	614	U
26	1H	615	G
26	1H	617	G
26	1H	621	A
26	1H	622	G
26	1H	626	U
26	1H	627	A
26	1H	637	A
26	1H	645	C
26	1H	646	A
26	1H	647	G
26	1H	654	A
26	1H	654(A)	A
26	1H	654(D)	G
26	1H	654(O)	G
26	1H	654(P)	G
26	1H	654(Q)	C
26	1H	654(S)	G
26	1H	654(T)	A
26	1H	654(V)	A
26	1H	678	C
26	1H	686	G
26	1H	689	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	1H	699	A
26	1H	714	U
26	1H	717	G
26	1H	730	C
26	1H	731	C
26	1H	739	G
26	1H	747	U
26	1H	757	U
26	1H	764	A
26	1H	765	G
26	1H	771	G
26	1H	776	G
26	1H	782	A
26	1H	784	A
26	1H	785	G
26	1H	790	C
26	1H	792	G
26	1H	802	A
26	1H	805	G
26	1H	812	C
26	1H	816	C
26	1H	827	U
26	1H	828	U
26	1H	832	G
26	1H	836	G
26	1H	845	G
26	1H	846	C
26	1H	853	G
26	1H	858	U
26	1H	859	G
26	1H	860	U
26	1H	866	A
26	1H	878	A
26	1H	879	G
26	1H	882	G
26	1H	894	C
26	1H	899	A
26	1H	900	A
26	1H	901	A
26	1H	902	C
26	1H	907	U
26	1H	910	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	1H	914	C
26	1H	917	A
26	1H	926	A
26	1H	932	G
26	1H	938	G
26	1H	941	A
26	1H	946	G
26	1H	947	G
26	1H	953	A
26	1H	959	A
26	1H	961	C
26	1H	962	G
26	1H	968	G
26	1H	974	G
26	1H	974(A)	C
26	1H	983	A
26	1H	990	A
26	1H	995	C
26	1H	996	A
26	1H	1003	G
26	1H	1005	C
26	1H	1011	G
26	1H	1012	U
26	1H	1013	C
26	1H	1020	A
26	1H	1022	G
26	1H	1023	U
26	1H	1025	G
26	1H	1026	U
26	1H	1027	A
26	1H	1031	G
26	1H	1033	U
26	1H	1040	C
26	1H	1045	A
26	1H	1046	A
26	1H	1047	G
26	1H	1054	A
26	1H	1055	G
26	1H	1071	G
26	1H	1072	C
26	1H	1079	C
26	1H	1080	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	1H	1081	U
26	1H	1082	U
26	1H	1085	A
26	1H	1086	A
26	1H	1087	G
26	1H	1088	A
26	1H	1090	U
26	1H	1093	G
26	1H	1101	U
26	1H	1106	G
26	1H	1109	C
26	1H	1110	G
26	1H	1111	A
26	1H	1112	G
26	1H	1126	A
26	1H	1129	A
26	1H	1130	U
26	1H	1135	C
26	1H	1136	G
26	1H	1138	G
26	1H	1139	G
26	1H	1142	U
26	1H	1142(A)	A
26	1H	1144	G
26	1H	1149	G
26	1H	1170	G
26	1H	1177	A
26	1H	1178	C
26	1H	1179	C
26	1H	1194	A
26	1H	1195	G
26	1H	1204	A
26	1H	1205	U
26	1H	1210	A
26	1H	1211	U
26	1H	1218	C
26	1H	1220	A
26	1H	1225	C
26	1H	1237	A
26	1H	1241	A
26	1H	1244	G
26	1H	1250	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	1H	1253	A
26	1H	1256	G
26	1H	1267	U
26	1H	1268	A
26	1H	1271	G
26	1H	1272	A
26	1H	1273	U
26	1H	1275	A
26	1H	1276	A
26	1H	1282	U
26	1H	1300	U
26	1H	1301	A
26	1H	1303	G
26	1H	1306	C
26	1H	1319	G
26	1H	1329	U
26	1H	1332	G
26	1H	1349	A
26	1H	1359	A
26	1H	1360	A
26	1H	1365	A
26	1H	1379	A
26	1H	1380	G
26	1H	1384	A
26	1H	1385	G
26	1H	1386	C
26	1H	1388	G
26	1H	1389	G
26	1H	1395	A
26	1H	1407	C
26	1H	1416	G
26	1H	1417	C
26	1H	1420	U
26	1H	1421	G
26	1H	1428	C
26	1H	1444(A)	A
26	1H	1449	A
26	1H	1449(A)	G
26	1H	1453	A
26	1H	1455	G
26	1H	1458	C
26	1H	1459	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	1H	1460	A
26	1H	1461	G
26	1H	1467	C
26	1H	1471	A
26	1H	1483	G
26	1H	1493	C
26	1H	1494	A
26	1H	1495	A
26	1H	1497	U
26	1H	1500	G
26	1H	1505	C
26	1H	1508	A
26	1H	1509	C
26	1H	1510	A
26	1H	1511	A
26	1H	1517	G
26	1H	1522	G
26	1H	1526	G
26	1H	1534	G
26	1H	1535	U
26	1H	1537	C
26	1H	1538	G
26	1H	1539	G
26	1H	1540	G
26	1H	1543	A
26	1H	1545	A
26	1H	1548	C
26	1H	1554	A
26	1H	1558	A
26	1H	1559	G
26	1H	1560	G
26	1H	1566	A
26	1H	1569	A
26	1H	1578	U
26	1H	1580	A
26	1H	1585	C
26	1H	1586	A
26	1H	1587	A
26	1H	1594	G
26	1H	1604	C
26	1H	1608	A
26	1H	1609	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	1H	1610	A
26	1H	1617	C
26	1H	1619	G
26	1H	1625	C
26	1H	1634	A
26	1H	1640	C
26	1H	1647	G
26	1H	1648	C
26	1H	1653	G
26	1H	1656	C
26	1H	1660	C
26	1H	1661	G
26	1H	1664	A
26	1H	1674	G
26	1H	1695	G
26	1H	1706	U
26	1H	1728	G
26	1H	1730	U
26	1H	1731	G
26	1H	1733	G
26	1H	1750	G
26	1H	1756	G
26	1H	1758	G
26	1H	1762	A
26	1H	1763	G
26	1H	1764	G
26	1H	1773	A
26	1H	1782	C
26	1H	1783	A
26	1H	1791	A
26	1H	1799	G
26	1H	1800	C
26	1H	1801	G
26	1H	1816	G
26	1H	1828	G
26	1H	1829	A
26	1H	1836	C
26	1H	1847	A
26	1H	1859	A
26	1H	1869	G
26	1H	1870	C
26	1H	1878	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	1H	1889	A
26	1H	1895	C
26	1H	1900	A
26	1H	1901	A
26	1H	1906	G
26	1H	1913	A
26	1H	1914	C
26	1H	1919	A
26	1H	1926	U
26	1H	1929	G
26	1H	1930	G
26	1H	1936	A
26	1H	1938	A
26	1H	1945	G
26	1H	1955	U
26	1H	1960	A
26	1H	1963	U
26	1H	1965	C
26	1H	1967	C
26	1H	1969	A
26	1H	1970	A
26	1H	1971	A
26	1H	1972	A
26	1H	1982	C
26	1H	1992	G
26	1H	1993	U
26	1H	1994	C
26	1H	2020	A
26	1H	2021	C
26	1H	2023	G
26	1H	2031	A
26	1H	2033	A
26	1H	2043	C
26	1H	2049	G
26	1H	2055	C
26	1H	2056	G
26	1H	2060	A
26	1H	2061	G
26	1H	2062	A
26	1H	2069	G
26	1H	2072	G
26	1H	2093	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	1H	2096	U
26	1H	2099	U
26	1H	2108	C
26	1H	2111	C
26	1H	2113	U
26	1H	2114	A
26	1H	2115	G
26	1H	2116	G
26	1H	2117	A
26	1H	2119	A
26	1H	2123	G
26	1H	2126	A
26	1H	2127	G
26	1H	2128	C
26	1H	2131	G
26	1H	2132	U
26	1H	2133	G
26	1H	2134	A
26	1H	2135	A
26	1H	2136	C
26	1H	2138	C
26	1H	2139	C
26	1H	2145	C
26	1H	2147	G
26	1H	2148	G
26	1H	2156	G
26	1H	2157	G
26	1H	2158	A
26	1H	2161	C
26	1H	2162	G
26	1H	2165	G
26	1H	2166	G
26	1H	2168	G
26	1H	2170	A
26	1H	2171	A
26	1H	2172	U
26	1H	2173	A
26	1H	2175	C
26	1H	2176	A
26	1H	2177	C
26	1H	2181	G
26	1H	2189	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	1H	2190	G
26	1H	2198	A
26	1H	2210	G
26	1H	2211	G
26	1H	2212	A
26	1H	2215	G
26	1H	2225	A
26	1H	2226	C
26	1H	2238	G
26	1H	2240	C
26	1H	2263	C
26	1H	2267	A
26	1H	2268	A
26	1H	2273	A
26	1H	2275	C
26	1H	2279	G
26	1H	2280	G
26	1H	2283	C
26	1H	2285	C
26	1H	2286	A
26	1H	2287	A
26	1H	2288	A
26	1H	2294	C
26	1H	2298	A
26	1H	2307	G
26	1H	2308	G
26	1H	2310	A
26	1H	2311	A
26	1H	2312	U
26	1H	2314	C
26	1H	2320	A
26	1H	2321	G
26	1H	2322	A
26	1H	2324	C
26	1H	2325	G
26	1H	2326	C
26	1H	2335	A
26	1H	2336	A
26	1H	2343	C
26	1H	2346	A
26	1H	2347	C
26	1H	2350	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	1H	2364	C
26	1H	2376	A
26	1H	2377	A
26	1H	2383	G
26	1H	2385	C
26	1H	2395	C
26	1H	2402	C
26	1H	2403	C
26	1H	2405	G
26	1H	2406	U
26	1H	2408	U
26	1H	2410	G
26	1H	2414	G
26	1H	2422	A
26	1H	2423	U
26	1H	2425	A
26	1H	2428	G
26	1H	2429	G
26	1H	2430	A
26	1H	2431	U
26	1H	2435	A
26	1H	2439	A
26	1H	2440	C
26	1H	2441	C
26	1H	2448	A
26	1H	2468	G
26	1H	2474	C
26	1H	2476	A
26	1H	2477	C
26	1H	2480	C
26	1H	2482	G
26	1H	2484	G
26	1H	2497	A
26	1H	2498	C
26	1H	2502	G
26	1H	2505	G
26	1H	2506	U
26	1H	2507	C
26	1H	2518	A
26	1H	2529	G
26	1H	2549	G
26	1H	2554	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	1H	2566	A
26	1H	2567	G
26	1H	2573	C
26	1H	2582	G
26	1H	2594	C
26	1H	2601	C
26	1H	2602	A
26	1H	2609	U
26	1H	2611	U
26	1H	2612	C
26	1H	2629	A
26	1H	2630	G
26	1H	2632	A
26	1H	2634	G
26	1H	2636	U
26	1H	2643	G
26	1H	2654	A
26	1H	2663	G
26	1H	2665	A
26	1H	2666	C
26	1H	2673	G
26	1H	2689	U
26	1H	2702	U
26	1H	2703	C
26	1H	2707	G
26	1H	2712(A)	A
26	1H	2713	A
26	1H	2714	G
26	1H	2726	U
26	1H	2733	A
26	1H	2749	A
26	1H	2752	C
26	1H	2756	U
26	1H	2757	A
26	1H	2764	A
26	1H	2765	A
26	1H	2766	G
26	1H	2777	G
26	1H	2778	A
26	1H	2781	A
26	1H	2789	C
26	1H	2791	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	1H	2793	G
26	1H	2795	G
26	1H	2803	C
26	1H	2808	U
26	1H	2820	A
26	1H	2821	A
26	1H	2833	G
26	1H	2834	G
26	1H	2835	A
26	1H	2849	U
26	1H	2872	G
26	1H	2875	C
26	1H	2885	C
26	1H	2891	G
26	1H	2892	A
26	1H	2893	G
26	1H	2894	G
26	1H	2895	U
27	16	0	A
27	16	3	C
27	16	8	U
27	16	12	C
27	16	13	A
27	16	15	A
27	16	16	G
27	16	25	A
27	16	29	A
27	16	39	A
27	16	42	C
27	16	45	A
27	16	56	G
27	16	65	C
27	16	72	G
27	16	73	A
27	16	74	U
27	16	76	G
27	16	81	G
27	16	84	C
27	16	105	G
27	16	107	U
27	16	109	G
27	16	115	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1G	2	U
1	1G	5	U
1	1G	7	G
1	1G	9	G
1	1G	22	G
1	1G	26	A
1	1G	31	G
1	1G	32	A
1	1G	39	G
1	1G	44	G
1	1G	47	C
1	1G	48	C
1	1G	50	A
1	1G	51	A
1	1G	53	A
1	1G	65	U
1	1G	73	G
1	1G	76	G
1	1G	79	G
1	1G	81	G
1	1G	82	U
1	1G	88	C
1	1G	90	C
1	1G	91	C
1	1G	95	G
1	1G	101	A
1	1G	105	G
1	1G	115	G
1	1G	116	A
1	1G	121	C
1	1G	127	G
1	1G	131	C
1	1G	162	A
1	1G	163	C
1	1G	174	C
1	1G	182	U
1	1G	186	C
1	1G	186(F)	C
1	1G	189	U
1	1G	191(D)	U
1	1G	195	A
1	1G	197	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1G	209	U
1	1G	210	U
1	1G	216	G
1	1G	231	G
1	1G	233	C
1	1G	247	G
1	1G	251	G
1	1G	260	G
1	1G	266	G
1	1G	267	C
1	1G	274	A
1	1G	279	A
1	1G	280	C
1	1G	281	G
1	1G	289	G
1	1G	298	A
1	1G	316	G
1	1G	321	A
1	1G	328	C
1	1G	329	A
1	1G	332	G
1	1G	346	G
1	1G	350	G
1	1G	351	G
1	1G	352	C
1	1G	353	A
1	1G	354	G
1	1G	355	C
1	1G	367	U
1	1G	369	C
1	1G	372	C
1	1G	388	G
1	1G	396	G
1	1G	397	A
1	1G	398	C
1	1G	406	G
1	1G	412	A
1	1G	413	G
1	1G	414	A
1	1G	419	C
1	1G	421	U
1	1G	422	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1G	423	G
1	1G	424	G
1	1G	429	U
1	1G	430	A
1	1G	439	A
1	1G	442	C
1	1G	452	A
1	1G	465	A
1	1G	466	C
1	1G	467	G
1	1G	475	G
1	1G	478	A
1	1G	482	A
1	1G	484	G
1	1G	485	G
1	1G	486	U
1	1G	496	A
1	1G	497	U
1	1G	498	A
1	1G	500	G
1	1G	505	G
1	1G	509	A
1	1G	510	A
1	1G	511	C
1	1G	517	G
1	1G	518	C
1	1G	521	G
1	1G	527	G
1	1G	531	U
1	1G	532	A
1	1G	533	A
1	1G	544	G
1	1G	547	A
1	1G	553	A
1	1G	559	A
1	1G	561	U
1	1G	562	C
1	1G	564	C
1	1G	572	A
1	1G	573	A
1	1G	576	G
1	1G	586	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1G	607	A
1	1G	614	A
1	1G	615	C
1	1G	617	G
1	1G	620	C
1	1G	621	A
1	1G	630	G
1	1G	631	G
1	1G	632	A
1	1G	633	G
1	1G	651	C
1	1G	653	A
1	1G	661	G
1	1G	665	A
1	1G	666	G
1	1G	687	A
1	1G	688	G
1	1G	702	A
1	1G	723	U
1	1G	724	G
1	1G	731	G
1	1G	749	C
1	1G	755	G
1	1G	769	G
1	1G	770	C
1	1G	776	G
1	1G	777	A
1	1G	778	G
1	1G	787	A
1	1G	792	A
1	1G	793	U
1	1G	794	A
1	1G	809	G
1	1G	816	A
1	1G	817	C
1	1G	819	A
1	1G	820	U
1	1G	821	G
1	1G	827	U
1	1G	828	A
1	1G	842	C
1	1G	843	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1G	848	C
1	1G	859	A
1	1G	870	U
1	1G	873	A
1	1G	874	G
1	1G	885	G
1	1G	914	A
1	1G	915	A
1	1G	916	G
1	1G	926	G
1	1G	927	G
1	1G	934	C
1	1G	935	A
1	1G	936	C
1	1G	944	G
1	1G	953	G
1	1G	960	U
1	1G	961	U
1	1G	968	A
1	1G	969	A
1	1G	971	G
1	1G	972	C
1	1G	974	A
1	1G	975	A
1	1G	976	G
1	1G	977	A
1	1G	978	A
1	1G	979	C
1	1G	980	C
1	1G	982	U
1	1G	983	A
1	1G	989	C
1	1G	991	U
1	1G	992	U
1	1G	993	G
1	1G	995	C
1	1G	996	A
1	1G	1001	G
1	1G	1002	G
1	1G	1004	A
1	1G	1006	C
1	1G	1008	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1G	1009	G
1	1G	1017	G
1	1G	1021	G
1	1G	1023	G
1	1G	1024	G
1	1G	1026	G
1	1G	1028	C
1	1G	1028(A)	C
1	1G	1028(B)	C
1	1G	1029	G
1	1G	1030	C
1	1G	1031	G
1	1G	1032	A
1	1G	1032(A)	G
1	1G	1033	G
1	1G	1037	C
1	1G	1040	U
1	1G	1046	A
1	1G	1050	G
1	1G	1054	C
1	1G	1056	U
1	1G	1064	G
1	1G	1081	G
1	1G	1084	G
1	1G	1088	G
1	1G	1094	G
1	1G	1095	U
1	1G	1101	A
1	1G	1118	C
1	1G	1124	G
1	1G	1125	U
1	1G	1127	G
1	1G	1128	C
1	1G	1129	C
1	1G	1133	G
1	1G	1135	U
1	1G	1136	U
1	1G	1137	C
1	1G	1139	G
1	1G	1140	C
1	1G	1144	G
1	1G	1146	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1G	1147	C
1	1G	1154	G
1	1G	1157	A
1	1G	1158	C
1	1G	1159	U
1	1G	1160	G
1	1G	1169	A
1	1G	1177	G
1	1G	1178	G
1	1G	1181	G
1	1G	1183	A
1	1G	1185	G
1	1G	1188	A
1	1G	1189	C
1	1G	1196	U
1	1G	1197	G
1	1G	1201	A
1	1G	1208	C
1	1G	1211	U
1	1G	1212	U
1	1G	1213	A
1	1G	1225	A
1	1G	1227	A
1	1G	1232	U
1	1G	1238	A
1	1G	1240	U
1	1G	1241	G
1	1G	1248	A
1	1G	1256	A
1	1G	1257	U
1	1G	1258	G
1	1G	1260	C
1	1G	1268	A
1	1G	1273	G
1	1G	1274	G
1	1G	1275	A
1	1G	1278	U
1	1G	1279	A
1	1G	1280	A
1	1G	1286	A
1	1G	1287	A
1	1G	1288	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1G	1297	C
1	1G	1298	C
1	1G	1299	A
1	1G	1301	U
1	1G	1305	G
1	1G	1317	C
1	1G	1320	C
1	1G	1322	C
1	1G	1323	G
1	1G	1324	A
1	1G	1331	G
1	1G	1335	C
1	1G	1336	C
1	1G	1338	G
1	1G	1346	A
1	1G	1347	G
1	1G	1353	G
1	1G	1354	C
1	1G	1358	U
1	1G	1359	C
1	1G	1360	A
1	1G	1362(A)	C
1	1G	1363	A
1	1G	1368	G
1	1G	1370	G
1	1G	1379	G
1	1G	1382	C
1	1G	1387	G
1	1G	1400	C
1	1G	1401	G
1	1G	1406	U
1	1G	1416	G
1	1G	1419	G
1	1G	1442	G
1	1G	1443	G
1	1G	1446	A
1	1G	1447	G
1	1G	1450	U
1	1G	1451	A
1	1G	1452	C
1	1G	1453	G
1	1G	1491	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1G	1492	A
1	1G	1499	A
1	1G	1502	A
1	1G	1503	A
1	1G	1504	G
1	1G	1506	U
1	1G	1507	A
1	1G	1508	G
1	1G	1517	G
1	1G	1519	A
1	1G	1520	G
1	1G	1529	G
1	1G	1530	G
1	1G	1532	U
1	1G	1533	C
1	1G	1534	A
24	1L	2	G
24	1L	3	G
24	1L	7	U
24	1L	9	A
24	1L	10	G
24	1L	11	C
24	1L	18	G
24	1L	23	A
24	1L	24	G
24	1L	26	A
24	1L	27	G
24	1L	30	G
24	1L	34	U
24	1L	37	A
24	1L	41	A
24	1L	45	G
24	1L	49	G
24	1L	54	U
24	1L	56	C
24	1L	59	A
24	1L	61	C
24	1L	64	G
24	1L	67	C
24	1L	70	C
23	2L	2	G
23	2L	8	4SU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
23	2L	9	G
23	2L	16	C
23	2L	18	C
23	2L	19	G
23	2L	20	G
23	2L	21	U
23	2L	23	G
23	2L	34	U
23	2L	48	U
23	2L	49	C
23	2L	65	G
23	2L	69	C
23	2L	77	A
24	3L	2	G
24	3L	7	U
24	3L	9	A
24	3L	15	G
24	3L	24	G
24	3L	25	C
24	3L	26	A
24	3L	31	A
24	3L	33	U
24	3L	34	U
24	3L	35	U
24	3L	37	A
24	3L	38	A
24	3L	39	U
24	3L	40	C
24	3L	42	A
24	3L	46	G
24	3L	47	U
24	3L	48	C
24	3L	55	U
24	3L	56	C
24	3L	58	A
24	3L	59	A
24	3L	61	C
24	3L	62	C
24	3L	63	U
24	3L	65	C
24	3L	67	C
24	3L	72	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	3L	73	A
25	4L	8	A
25	4L	9	G
25	4L	11	U
25	4L	12	A
25	4L	13	A
25	4L	14	A
25	4L	15	A
25	4L	19	G
25	4L	20	A
25	4L	23	A
25	4L	24	A
25	4L	25	A
26	14	7	G
26	14	9	U
26	14	11	G
26	14	15	G
26	14	35	G
26	14	46	C
26	14	49	A
26	14	50	U
26	14	55	G
26	14	58	G
26	14	60	G
26	14	71	A
26	14	72	U
26	14	74	A
26	14	75	G
26	14	78	A
26	14	82	G
26	14	84	A
26	14	92	G
26	14	95	G
26	14	99	U
26	14	101	G
26	14	102	G
26	14	118	A
26	14	119	A
26	14	120	U
26	14	125	G
26	14	129	C
26	14	131	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	14	138	G
26	14	139	G
26	14	153	C
26	14	154	G
26	14	155	C
26	14	161	U
26	14	162	U
26	14	171	G
26	14	173	G
26	14	174	C
26	14	181	A
26	14	182	A
26	14	196	A
26	14	199	A
26	14	205	G
26	14	214	G
26	14	215	G
26	14	216	A
26	14	217	G
26	14	222	A
26	14	229	A
26	14	233	A
26	14	248	G
26	14	249	C
26	14	250	G
26	14	252	G
26	14	269	U
26	14	270(K)	C
26	14	270(L)	U
26	14	270(N)	G
26	14	270(O)	U
26	14	270(P)	C
26	14	271(B)	G
26	14	271(C)	U
26	14	271	G
26	14	273(C)	C
26	14	273(D)	C
26	14	273(F)	C
26	14	274	G
26	14	275	G
26	14	276	A
26	14	277	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	14	278	A
26	14	279	C
26	14	283	A
26	14	289	A
26	14	290	G
26	14	308	G
26	14	311	A
26	14	312	G
26	14	316	C
26	14	324	A
26	14	329	G
26	14	330	A
26	14	331	A
26	14	352	G
26	14	354	G
26	14	362	U
26	14	363	G
26	14	363(E)	U
26	14	366	C
26	14	372	G
26	14	380	U
26	14	386	G
26	14	391	G
26	14	396	G
26	14	405	U
26	14	406	G
26	14	407	G
26	14	411	G
26	14	428	A
26	14	443	A
26	14	444	C
26	14	447	A
26	14	448	U
26	14	451	C
26	14	454	A
26	14	455	C
26	14	456	C
26	14	457	A
26	14	470	A
26	14	471	A
26	14	481	G
26	14	501	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	14	505	A
26	14	509	C
26	14	517	C
26	14	528	A
26	14	531	C
26	14	532	A
26	14	533	G
26	14	537	C
26	14	549	G
26	14	556	G
26	14	563	G
26	14	573	G
26	14	575	A
26	14	587	C
26	14	603	A
26	14	607	U
26	14	617	G
26	14	619	G
26	14	621	A
26	14	622	G
26	14	627	A
26	14	634	C
26	14	637	A
26	14	645	C
26	14	646	A
26	14	650	C
26	14	651	G
26	14	654	A
26	14	654(A)	A
26	14	654(B)	C
26	14	654(C)	G
26	14	654(D)	G
26	14	654(S)	G
26	14	654(T)	A
26	14	677	A
26	14	686	G
26	14	717	G
26	14	722	A
26	14	730	C
26	14	731	C
26	14	734	A
26	14	738	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	14	749	C
26	14	750	A
26	14	752	A
26	14	753	C
26	14	764	A
26	14	765	G
26	14	775	G
26	14	776	G
26	14	779	U
26	14	782	A
26	14	784	A
26	14	785	G
26	14	791	C
26	14	792	G
26	14	805	G
26	14	812	C
26	14	814	C
26	14	816	C
26	14	819	A
26	14	827	U
26	14	828	U
26	14	830	G
26	14	832	G
26	14	840	C
26	14	845	G
26	14	846	C
26	14	847	U
26	14	854	G
26	14	859	G
26	14	860	U
26	14	861	A
26	14	865	C
26	14	866	A
26	14	878	A
26	14	880	G
26	14	881	G
26	14	882	G
26	14	883	G
26	14	884	C
26	14	885	C
26	14	886	C
26	14	887	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	14	888	C
26	14	889	C
26	14	890	A
26	14	892	G
26	14	894	C
26	14	896	A
26	14	897	C
26	14	899	A
26	14	900	A
26	14	901	A
26	14	903	C
26	14	904	C
26	14	907	U
26	14	910	A
26	14	911	A
26	14	917	A
26	14	918	A
26	14	925	C
26	14	926	A
26	14	932	G
26	14	933	A
26	14	935	C
26	14	938	G
26	14	941	A
26	14	945	A
26	14	946	G
26	14	953	A
26	14	958	U
26	14	959	A
26	14	961	C
26	14	967	C
26	14	974	G
26	14	974(A)	C
26	14	980	A
26	14	983	A
26	14	987	G
26	14	989	G
26	14	990	A
26	14	991	C
26	14	996	A
26	14	1004	C
26	14	1012	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	14	1013	C
26	14	1015	G
26	14	1017	G
26	14	1022	G
26	14	1023	U
26	14	1025	G
26	14	1026	U
26	14	1028	A
26	14	1037	G
26	14	1040	C
26	14	1044	G
26	14	1050	A
26	14	1105	U
26	14	1106	G
26	14	1107	G
26	14	1108	U
26	14	1110	G
26	14	1111	A
26	14	1112	G
26	14	1113	U
26	14	1117	G
26	14	1122	G
26	14	1128	A
26	14	1129	A
26	14	1130	U
26	14	1131	G
26	14	1135	C
26	14	1136	G
26	14	1138	G
26	14	1139	G
26	14	1142(A)	A
26	14	1143	A
26	14	1157	G
26	14	1170	G
26	14	1173	G
26	14	1174	A
26	14	1175	U
26	14	1176	G
26	14	1177	A
26	14	1178	C
26	14	1188	U
26	14	1194	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	14	1204	A
26	14	1205	U
26	14	1206	G
26	14	1220	A
26	14	1221	C
26	14	1237	A
26	14	1250	G
26	14	1253	A
26	14	1256	G
26	14	1268	A
26	14	1271	G
26	14	1272	A
26	14	1300	U
26	14	1301	A
26	14	1303	G
26	14	1325	G
26	14	1329	U
26	14	1332	G
26	14	1345	C
26	14	1349	A
26	14	1352	U
26	14	1359	A
26	14	1360	A
26	14	1365	A
26	14	1368	G
26	14	1370	C
26	14	1379	A
26	14	1380	G
26	14	1385	G
26	14	1386	C
26	14	1406	U
26	14	1411	C
26	14	1416	G
26	14	1418	G
26	14	1419	A
26	14	1421	G
26	14	1427	A
26	14	1428	C
26	14	1444(A)	A
26	14	1445	C
26	14	1449	A
26	14	1449(A)	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	14	1451	C
26	14	1453	A
26	14	1455	G
26	14	1458	C
26	14	1459	G
26	14	1460	A
26	14	1465	G
26	14	1467	C
26	14	1469	A
26	14	1471	A
26	14	1475	G
26	14	1483	G
26	14	1493	C
26	14	1494	A
26	14	1508	A
26	14	1509	C
26	14	1510	A
26	14	1522	G
26	14	1526	G
26	14	1528	A
26	14	1534	G
26	14	1537	C
26	14	1538	G
26	14	1543	A
26	14	1544	C
26	14	1547	C
26	14	1558	A
26	14	1559	G
26	14	1560	G
26	14	1566	A
26	14	1569	A
26	14	1578	U
26	14	1582	C
26	14	1583	A
26	14	1585	C
26	14	1586	A
26	14	1588	C
26	14	1589	C
26	14	1598	C
26	14	1608	A
26	14	1609	A
26	14	1614	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	14	1616	A
26	14	1620	G
26	14	1625	C
26	14	1639	U
26	14	1647	G
26	14	1648	C
26	14	1651	G
26	14	1654	A
26	14	1669	A
26	14	1670	C
26	14	1674	G
26	14	1675	C
26	14	1700	A
26	14	1701	A
26	14	1725	G
26	14	1726	G
26	14	1730	U
26	14	1731	G
26	14	1732	A
26	14	1743	G
26	14	1756	G
26	14	1758	G
26	14	1762	A
26	14	1763	G
26	14	1764	G
26	14	1773	A
26	14	1777	U
26	14	1780	A
26	14	1782	C
26	14	1791	A
26	14	1800	C
26	14	1801	G
26	14	1816	G
26	14	1819	A
26	14	1820	U
26	14	1823	G
26	14	1828	G
26	14	1829	A
26	14	1830	C
26	14	1839	G
26	14	1847	A
26	14	1858	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	14	1878	G
26	14	1886	C
26	14	1888	G
26	14	1889	A
26	14	1899	G
26	14	1900	A
26	14	1906	G
26	14	1908	C
26	14	1909	C
26	14	1913	A
26	14	1929	G
26	14	1930	G
26	14	1936	A
26	14	1937	A
26	14	1938	A
26	14	1955	U
26	14	1963	U
26	14	1964	G
26	14	1967	C
26	14	1969	A
26	14	1970	A
26	14	1971	A
26	14	1972	A
26	14	1993	U
26	14	2020	A
26	14	2023	G
26	14	2031	A
26	14	2032	G
26	14	2033	A
26	14	2036	C
26	14	2043	C
26	14	2049	G
26	14	2055	C
26	14	2056	G
26	14	2060	A
26	14	2061	G
26	14	2062	A
26	14	2063	C
26	14	2069	G
26	14	2071	A
26	14	2093	G
26	14	2099	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	14	2100	G
26	14	2102	U
26	14	2108	C
26	14	2109	U
26	14	2114	A
26	14	2115	G
26	14	2117	A
26	14	2118	U
26	14	2119	A
26	14	2120	G
26	14	2122	U
26	14	2124	G
26	14	2125	G
26	14	2127	G
26	14	2128	C
26	14	2129	C
26	14	2131	G
26	14	2132	U
26	14	2133	G
26	14	2134	A
26	14	2135	A
26	14	2136	C
26	14	2137	C
26	14	2139	C
26	14	2140	C
26	14	2144	U
26	14	2145	C
26	14	2146	C
26	14	2147	G
26	14	2148	G
26	14	2153	G
26	14	2157	G
26	14	2158	A
26	14	2161	C
26	14	2162	G
26	14	2164	C
26	14	2165	G
26	14	2166	G
26	14	2167	U
26	14	2168	G
26	14	2171	A
26	14	2172	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	14	2173	A
26	14	2174	C
26	14	2175	C
26	14	2189	U
26	14	2190	G
26	14	2191	G
26	14	2192	G
26	14	2198	A
26	14	2207	C
26	14	2210	G
26	14	2211	G
26	14	2212	A
26	14	2213	U
26	14	2215	G
26	14	2225	A
26	14	2226	C
26	14	2238	G
26	14	2239	G
26	14	2240	C
26	14	2249	U
26	14	2251	G
26	14	2253	G
26	14	2268	A
26	14	2269	A
26	14	2273	A
26	14	2275	C
26	14	2276	G
26	14	2278	A
26	14	2280	G
26	14	2281	C
26	14	2283	C
26	14	2287	A
26	14	2288	A
26	14	2297	C
26	14	2305	A
26	14	2307	G
26	14	2309	A
26	14	2310	A
26	14	2311	A
26	14	2318	G
26	14	2321	G
26	14	2325	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	14	2333	A
26	14	2334	G
26	14	2336	A
26	14	2342	C
26	14	2346	A
26	14	2347	C
26	14	2350	C
26	14	2360	A
26	14	2372	G
26	14	2383	G
26	14	2385	C
26	14	2391	G
26	14	2392	A
26	14	2395	C
26	14	2396	G
26	14	2402	C
26	14	2403	C
26	14	2406	U
26	14	2410	G
26	14	2414	G
26	14	2422	A
26	14	2423	U
26	14	2425	A
26	14	2429	G
26	14	2430	A
26	14	2431	U
26	14	2432	A
26	14	2434	A
26	14	2435	A
26	14	2439	A
26	14	2440	C
26	14	2441	C
26	14	2448	A
26	14	2468	G
26	14	2469	A
26	14	2470	G
26	14	2475	C
26	14	2476	A
26	14	2477	C
26	14	2478	A
26	14	2482	G
26	14	2487	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	14	2492	U
26	14	2496	C
26	14	2497	A
26	14	2498	C
26	14	2501	C
26	14	2502	G
26	14	2504	U
26	14	2505	G
26	14	2507	C
26	14	2518	A
26	14	2529	G
26	14	2542	A
26	14	2543	G
26	14	2549	G
26	14	2554	U
26	14	2563	U
26	14	2564	A
26	14	2566	A
26	14	2567	G
26	14	2569	G
26	14	2573	C
26	14	2579	C
26	14	2581	G
26	14	2582	G
26	14	2585	U
26	14	2601	C
26	14	2602	A
26	14	2609	U
26	14	2610	C
26	14	2611	U
26	14	2612	C
26	14	2613	U
26	14	2617	C
26	14	2630	G
26	14	2631	G
26	14	2636	U
26	14	2648	C
26	14	2654	A
26	14	2665	A
26	14	2667	C
26	14	2673	G
26	14	2679	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	14	2689	U
26	14	2690	C
26	14	2691	C
26	14	2702	U
26	14	2703	C
26	14	2707	G
26	14	2712(A)	A
26	14	2713	A
26	14	2714	G
26	14	2726	U
26	14	2733	A
26	14	2744	G
26	14	2748	A
26	14	2750	A
26	14	2751	G
26	14	2752	C
26	14	2757	A
26	14	2758	A
26	14	2762	G
26	14	2764	A
26	14	2765	A
26	14	2766	G
26	14	2769	C
26	14	2777	G
26	14	2778	A
26	14	2787	C
26	14	2790	A
26	14	2791	C
26	14	2792	G
26	14	2793	G
26	14	2795	G
26	14	2797	U
26	14	2798	C
26	14	2799	A
26	14	2801	A
26	14	2802	G
26	14	2805	G
26	14	2808	U
26	14	2810	A
26	14	2818	G
26	14	2820	A
26	14	2821	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	14	2833	G
26	14	2834	G
26	14	2835	A
26	14	2839	G
26	14	2849	U
26	14	2860	A
26	14	2872	G
26	14	2873	A
26	14	2874	C
26	14	2880	C
26	14	2885	C
26	14	2886	G
26	14	2892	A
26	14	2893	G
26	14	2894	G
26	14	2895	U
27	1J	0	A
27	1J	7	G
27	1J	8	U
27	1J	12	C
27	1J	13	A
27	1J	15	A
27	1J	16	G
27	1J	22	U
27	1J	25	A
27	1J	26	A
27	1J	28	C
27	1J	29	A
27	1J	33	G
27	1J	40	U
27	1J	42	C
27	1J	44	G
27	1J	45	A
27	1J	51	G
27	1J	53	A
27	1J	58	A
27	1J	59	A
27	1J	73	A
27	1J	88	C
27	1J	89	G
27	1J	89(A)	A
27	1J	90	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	1J	99	A
27	1J	100	G
27	1J	102	G
27	1J	108	C
27	1J	109	G
27	1J	115	G

All (180) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	13	1	U
1	13	5	U
1	13	49	U
1	13	50	A
1	13	115	G
1	13	190	G
1	13	244	U
1	13	266	G
1	13	353	A
1	13	422	C
1	13	428	G
1	13	429	U
1	13	484	G
1	13	509	A
1	13	560	U
1	13	687	A
1	13	748	C
1	13	793	U
1	13	871	U
1	13	913	A
1	13	1025	U
1	13	1064	G
1	13	1065	U
1	13	1129	C
1	13	1256	A
1	13	1285	A
1	13	1301	U
1	13	1336	C
1	13	1397	C
1	13	1443	G
1	13	1498	U
1	13	1503	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	13	1533	C
22	1K	6	G
22	1K	21	A
22	1K	49	G
22	1K	69	A
23	2K	47	7MG
23	2K	48	U
24	3K	2	G
24	3K	34	U
25	4K	24	A
26	1H	125	G
26	1H	195	A
26	1H	196	A
26	1H	199	A
26	1H	222	A
26	1H	249	C
26	1H	404	C
26	1H	508	G
26	1H	587	C
26	1H	685	A
26	1H	746	A
26	1H	764	A
26	1H	776	G
26	1H	827	U
26	1H	845	G
26	1H	859	G
26	1H	961	C
26	1H	1022	G
26	1H	1026	U
26	1H	1081	U
26	1H	1110	G
26	1H	1178	C
26	1H	1210	A
26	1H	1275	A
26	1H	1378	A
26	1H	1379	A
26	1H	1394	U
26	1H	1396	U
26	1H	1420	U
26	1H	1451	C
26	1H	1508	A
26	1H	1509	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	1H	1558	A
26	1H	1608	A
26	1H	1609	A
26	1H	1617	C
26	1H	1757	U
26	1H	1782	C
26	1H	1799	G
26	1H	1858	G
26	1H	1900	A
26	1H	1992	G
26	1H	2060	A
26	1H	2171	A
26	1H	2172	U
26	1H	2210	G
26	1H	2211	G
26	1H	2422	A
26	1H	2439	A
26	1H	2481	G
26	1H	2566	A
26	1H	2756	U
27	16	44	G
1	1G	64	G
1	1G	80	G
1	1G	87	A
1	1G	89	U
1	1G	115	G
1	1G	250	A
1	1G	266	G
1	1G	327	A
1	1G	345	C
1	1G	412	A
1	1G	429	U
1	1G	466	C
1	1G	485	G
1	1G	509	A
1	1G	560	U
1	1G	687	A
1	1G	748	C
1	1G	793	U
1	1G	884	U
1	1G	913	A
1	1G	992	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1G	1053	G
1	1G	1064	G
1	1G	1126	U
1	1G	1145	C
1	1G	1157	A
1	1G	1285	A
1	1G	1298	C
1	1G	1300	G
1	1G	1442	G
1	1G	1449	C
1	1G	1498	U
1	1G	1533	C
24	1L	6	G
24	1L	69	A
23	2L	33	OMC
23	2L	48	U
24	3L	36	U
24	3L	58	A
25	4L	23	A
26	14	6	A
26	14	34	C
26	14	49	A
26	14	71	A
26	14	128	C
26	14	270(M)	U
26	14	278	A
26	14	310	A
26	14	503	A
26	14	685	A
26	14	752	A
26	14	764	A
26	14	774	A
26	14	877	U
26	14	893	C
26	14	960	A
26	14	1011	G
26	14	1022	G
26	14	1325	G
26	14	1379	A
26	14	1396	U
26	14	1420	U
26	14	1558	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	14	1608	A
26	14	1762	A
26	14	1819	A
26	14	1992	G
26	14	2035	G
26	14	2062	A
26	14	2212	A
26	14	2275	C
26	14	2308	G
26	14	2406	U
26	14	2425	A
26	14	2439	A
26	14	2477	C
26	14	2629	A
26	14	2689	U
26	14	2756	U
26	14	2776	A
26	14	2791	C
26	14	2859	G
27	1J	52	A
27	1J	88	C
27	1J	89	G

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

15 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
22	PSU	1K	55	22	17,21,22	1.13	1 (5%)	20,30,33	3.49	5 (25%)
23	OMC	2K	33	23	15,22,23	2.25	4 (26%)	17,31,34	1.41	3 (17%)
23	4SU	2K	8	23	14,21,22	3.10	2 (14%)	15,30,33	1.10	1 (6%)
23	7MG	2L	47	23	22,26,27	3.50	6 (27%)	28,39,42	2.52	10 (35%)
22	5MU	1K	54	22	15,22,23	2.22	3 (20%)	16,32,35	1.93	2 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	5MU	2K	55	23	15,22,23	2.18	3 (20%)	16,32,35	1.83	2 (12%)
23	4SU	2L	8	23	14,21,22	3.50	2 (14%)	15,30,33	1.11	2 (13%)
23	7MG	2K	47	23	22,26,27	3.40	7 (31%)	28,39,42	2.55	9 (32%)
23	OMC	2L	33	23	15,22,23	2.31	4 (26%)	17,31,34	1.78	3 (17%)
22	PSU	1K	39	22	17,21,22	0.97	1 (5%)	20,30,33	3.32	6 (30%)
23	PSU	2L	56	23	17,21,22	1.10	1 (5%)	20,30,33	3.51	6 (30%)
22	T6A	1K	37	22	24,34,35	2.56	4 (16%)	24,49,52	2.93	5 (20%)
22	U8U	1K	34	25,22	17,24,25	2.63	5 (29%)	19,34,37	1.51	3 (15%)
23	PSU	2K	56	23	17,21,22	1.14	1 (5%)	20,30,33	3.05	5 (25%)
23	5MU	2L	55	23	15,22,23	2.23	3 (20%)	16,32,35	1.80	2 (12%)

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
22	PSU	1K	55	22	-	0/7/25/26	0/2/2/2
23	OMC	2K	33	23	-	1/7/27/28	0/2/2/2
23	4SU	2K	8	23	-	2/5/25/26	0/2/2/2
23	7MG	2L	47	23	-	3/7/37/38	0/3/3/3
22	5MU	1K	54	22	-	0/5/25/26	0/2/2/2
23	5MU	2K	55	23	-	0/5/25/26	0/2/2/2
23	4SU	2L	8	23	-	3/5/25/26	0/2/2/2
23	7MG	2K	47	23	-	4/7/37/38	0/3/3/3
23	OMC	2L	33	23	-	3/7/27/28	0/2/2/2
22	PSU	1K	39	22	-	0/7/25/26	0/2/2/2
23	PSU	2L	56	23	-	0/7/25/26	0/2/2/2
22	T6A	1K	37	22	-	5/15/41/42	0/3/3/3
22	U8U	1K	34	25,22	-	0/7/28/29	0/2/2/2
23	PSU	2K	56	23	-	0/7/25/26	0/2/2/2
23	5MU	2L	55	23	-	0/5/25/26	0/2/2/2

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2L	47	7MG	C4-N3	11.58	1.49	1.34
23	2K	47	7MG	C4-N3	10.98	1.48	1.34
23	2L	8	4SU	C5-C4	10.44	1.50	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2K	8	4SU	C5-C4	9.26	1.48	1.38
22	1K	37	T6A	C6-N6	7.61	1.49	1.36
23	2L	8	4SU	C6-N1	7.55	1.45	1.35
23	2K	47	7MG	C5-C4	-7.30	1.24	1.39
22	1K	34	U8U	C4-N3	7.27	1.45	1.33
23	2L	47	7MG	C5-C4	-6.93	1.25	1.39
23	2K	8	4SU	C6-N1	6.68	1.44	1.35
22	1K	37	T6A	C10-N11	6.26	1.49	1.35
23	2L	33	OMC	C6-N1	5.99	1.43	1.35
22	1K	37	T6A	C10-N6	5.78	1.49	1.37
23	2L	47	7MG	C6-C5	5.71	1.49	1.41
23	2L	55	5MU	C4-C5	5.60	1.53	1.41
22	1K	54	5MU	C2-N3	5.58	1.49	1.38
22	1K	54	5MU	C4-C5	5.51	1.53	1.41
23	2L	55	5MU	C2-N3	5.49	1.49	1.38
23	2K	55	5MU	C4-C5	5.46	1.53	1.41
23	2K	47	7MG	C6-C5	5.37	1.48	1.41
23	2K	55	5MU	C2-N3	5.28	1.48	1.38
23	2K	33	OMC	C6-N1	5.23	1.42	1.35
22	1K	34	U8U	C6-C5	5.20	1.49	1.37
23	2L	47	7MG	C4-N9	-4.26	1.30	1.38
23	2K	47	7MG	C4-N9	-4.21	1.30	1.38
23	2K	33	OMC	C5-C4	4.15	1.51	1.41
23	2K	33	OMC	C2-N3	4.07	1.46	1.38
22	1K	34	U8U	C4-C5	4.06	1.50	1.41
23	2K	47	7MG	C2-N2	3.95	1.41	1.33
23	2L	33	OMC	C2-N3	3.89	1.45	1.38
23	2L	47	7MG	C2-N2	3.86	1.41	1.33
23	2L	33	OMC	C5-C4	3.81	1.50	1.41
22	1K	34	U8U	C2-S2	-3.80	1.58	1.66
22	1K	55	PSU	C4-N3	3.69	1.39	1.33
23	2L	56	PSU	C4-N3	3.67	1.39	1.33
23	2L	47	7MG	C5-N7	3.48	1.45	1.39
22	1K	39	PSU	C4-N3	3.26	1.38	1.33
23	2K	55	5MU	C4-N3	-2.95	1.27	1.33
23	2K	33	OMC	C4-N4	2.93	1.43	1.35
23	2L	55	5MU	C4-N3	-2.90	1.28	1.33
23	2K	47	7MG	C5-N7	2.90	1.44	1.39
23	2L	33	OMC	C4-N4	2.77	1.43	1.35
22	1K	54	5MU	C4-N3	-2.75	1.28	1.33
23	2K	56	PSU	C4-N3	2.62	1.37	1.33
22	1K	37	T6A	C5-C4	-2.57	1.34	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	2K	47	7MG	C2-N1	2.20	1.39	1.35
22	1K	34	U8U	O4-C4	-2.02	1.19	1.24

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	2L	56	PSU	N1-C2-N3	-12.29	118.66	128.43
22	1K	55	PSU	N1-C2-N3	-11.39	119.38	128.43
22	1K	39	PSU	N1-C2-N3	-11.30	119.45	128.43
22	1K	37	T6A	C12-N11-C10	11.11	134.61	122.75
23	2K	56	PSU	N1-C2-N3	-10.58	120.02	128.43
22	1K	55	PSU	C4-N3-C2	7.23	121.25	115.14
22	1K	39	PSU	C4-N3-C2	6.39	120.54	115.14
22	1K	54	5MU	C4-N3-C2	6.27	120.44	115.14
23	2L	56	PSU	C4-N3-C2	6.13	120.32	115.14
23	2K	56	PSU	C4-N3-C2	5.92	120.14	115.14
23	2K	47	7MG	C6-C5-C4	5.87	121.50	115.20
22	1K	37	T6A	N3-C2-N1	-5.78	119.65	128.68
23	2K	47	7MG	C5-C4-N9	5.67	114.40	106.44
22	1K	37	T6A	C2-N1-C6	5.46	121.27	116.59
23	2L	47	7MG	C4-C5-N7	5.28	115.05	106.98
23	2K	55	5MU	C4-N3-C2	5.22	119.55	115.14
23	2L	55	5MU	C4-N3-C2	5.20	119.53	115.14
22	1K	55	PSU	C5-C4-N3	-5.19	118.67	125.36
23	2L	47	7MG	C5-C4-N9	5.17	113.69	106.44
23	2L	47	7MG	C6-C5-C4	5.14	120.72	115.20
23	2K	47	7MG	C4-C5-N7	4.98	114.59	106.98
23	2K	47	7MG	C5-C4-N3	-4.68	118.84	126.49
23	2L	47	7MG	CM7-N7-C5	4.56	141.52	124.01
23	2K	55	5MU	C5-C6-N1	-4.55	117.29	122.19
22	1K	39	PSU	C5-C4-N3	-4.46	119.61	125.36
23	2L	47	7MG	C5-C4-N3	-4.44	119.25	126.49
23	2K	47	7MG	CM7-N7-C5	4.40	140.91	124.01
23	2L	55	5MU	C5-C6-N1	-4.33	117.53	122.19
23	2L	33	OMC	C2-N3-C4	4.33	120.73	116.34
23	2L	33	OMC	O2'-C2'-C1'	4.18	117.37	109.09
23	2K	56	PSU	C5-C4-N3	-3.90	120.34	125.36
22	1K	54	5MU	C5-C6-N1	-3.88	118.01	122.19
22	1K	34	U8U	C5-C4-N3	-3.86	119.59	125.25
23	2L	56	PSU	C6-N1-C2	3.82	121.67	115.36
23	2L	47	7MG	C8-N7-C5	-3.79	99.09	108.94
22	1K	55	PSU	C5-C1'-C2'	-3.72	108.69	115.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	2L	56	PSU	C5-C4-N3	-3.71	120.59	125.36
23	2K	47	7MG	C8-N7-C5	-3.56	99.68	108.94
22	1K	34	U8U	C2-N3-C4	3.54	119.55	115.93
23	2K	33	OMC	N4-C4-N3	3.52	122.06	116.49
23	2K	33	OMC	C2-N3-C4	3.46	119.85	116.34
23	2L	56	PSU	C5-C6-N1	-3.33	120.35	124.44
23	2K	8	4SU	C2-N3-C4	3.30	119.93	115.15
23	2L	47	7MG	N1-C2-N3	-3.29	120.25	125.42
22	1K	39	PSU	C6-N1-C2	3.17	120.60	115.36
23	2L	8	4SU	C2-N3-C4	2.96	119.44	115.15
22	1K	34	U8U	C6-C5-C4	2.92	120.24	115.73
23	2K	47	7MG	N1-C2-N3	-2.88	120.90	125.42
22	1K	55	PSU	C6-N1-C2	2.70	119.82	115.36
23	2L	33	OMC	N4-C4-N3	2.68	120.72	116.49
23	2K	56	PSU	C5-C6-N1	-2.60	121.25	124.44
22	1K	39	PSU	C5-C1'-C2'	-2.60	110.69	115.32
22	1K	39	PSU	C5-C6-N1	-2.59	121.25	124.44
23	2K	47	7MG	N7-C8-N9	-2.56	99.71	103.38
23	2L	56	PSU	O4'-C1'-C5	2.54	113.87	109.93
23	2L	47	7MG	C6-N1-C2	2.47	119.85	115.93
23	2L	8	4SU	C5-C4-N3	-2.45	120.55	123.83
23	2L	47	7MG	C2-N3-C4	2.30	120.26	113.89
23	2K	56	PSU	C6-N1-C2	2.29	119.14	115.36
23	2K	47	7MG	C2-N3-C4	2.25	120.12	113.89
23	2L	47	7MG	N7-C8-N9	-2.19	100.25	103.38
22	1K	37	T6A	O10-C10-N6	-2.06	120.13	123.62
23	2K	33	OMC	C5-C4-N4	-2.05	117.58	121.14
22	1K	37	T6A	C1'-N9-C4	-2.05	123.04	126.64

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	2K	33	OMC	C2'-C1'-N1-C6
23	2L	33	OMC	C2'-C1'-N1-C6
23	2L	33	OMC	O4'-C1'-N1-C6
22	1K	37	T6A	C14-C12-N11-C10
22	1K	37	T6A	N11-C12-C14-O14
22	1K	37	T6A	C13-C12-C14-O14
22	1K	37	T6A	C13-C12-C14-C15
23	2K	8	4SU	C3'-C4'-C5'-O5'
23	2K	8	4SU	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	2L	8	4SU	O4'-C4'-C5'-O5'
23	2K	47	7MG	O4'-C4'-C5'-O5'
22	1K	37	T6A	N11-C12-C14-C15
23	2L	47	7MG	C2'-C1'-N9-C8
23	2K	47	7MG	C2'-C1'-N9-C8
23	2L	8	4SU	C3'-C4'-C5'-O5'
23	2L	47	7MG	C2'-C1'-N9-C4
23	2K	47	7MG	C2'-C1'-N9-C4
23	2L	47	7MG	O4'-C1'-N9-C8
23	2K	47	7MG	O4'-C1'-N9-C8
23	2L	8	4SU	C4'-C5'-O5'-P
23	2L	33	OMC	C4'-C5'-O5'-P

There are no ring outliers.

7 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	2K	33	OMC	1	0
22	1K	54	5MU	1	0
23	2K	55	5MU	3	0
23	2K	47	7MG	2	0
23	2L	33	OMC	3	0
22	1K	37	T6A	1	0
23	2L	55	5MU	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1269 ligands modelled in this entry, 1262 are monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
61	SPE	14	3436	-	12,12,12	0.43	0	11,11,11	0.65	0
59	SF4	32	302	4	0,12,12	0.00	-	-		
59	SF4	3E	301	4	0,12,12	0.00	-	-		
58	PAR	13	1741	1	45,45,45	0.68	0	64,67,67	1.48	10 (15%)
61	SPE	1G	1703	-	12,12,12	0.35	0	11,11,11	0.76	0
61	SPE	14	3437	26	12,12,12	0.83	0	11,11,11	0.96	1 (9%)
58	PAR	1G	1702	-	45,45,45	0.67	1 (2%)	64,67,67	1.39	9 (14%)

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
61	SPE	14	3436	-	-	5/10/10/10	-
59	SF4	32	302	4	-	-	0/6/5/5
59	SF4	3E	301	4	-	-	0/6/5/5
61	SPE	14	3437	26	-	5/10/10/10	-
61	SPE	1G	1703	-	-	3/10/10/10	-
58	PAR	13	1741	1	-	5/18/94/94	0/4/4/4
58	PAR	1G	1702	-	-	1/18/94/94	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	1G	1702	PAR	C24-N24	-2.22	1.43	1.47

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	13	1741	PAR	C32-C22-C12	3.69	118.76	111.18
58	13	1741	PAR	C11-O51-C51	3.65	120.85	113.69
58	1G	1702	PAR	C14-O33-C33	-3.57	109.14	117.96
58	13	1741	PAR	C22-C12-C62	3.28	115.00	110.04
58	1G	1702	PAR	C13-O52-C52	-3.28	109.84	117.96
58	13	1741	PAR	C52-C42-C32	3.13	117.01	111.16
58	1G	1702	PAR	C11-O51-C51	3.11	119.79	113.69
58	13	1741	PAR	C14-O33-C33	-2.88	110.83	117.96
58	13	1741	PAR	O51-C11-C21	2.82	116.39	110.06
58	13	1741	PAR	O33-C14-O54	-2.80	102.86	110.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	1G	1702	PAR	O54-C14-C24	-2.69	103.99	110.06
58	13	1741	PAR	O34-C34-C24	-2.65	105.46	110.22
58	1G	1702	PAR	O51-C11-C21	2.47	115.61	110.06
58	1G	1702	PAR	O52-C13-O43	-2.43	108.80	111.43
58	1G	1702	PAR	C52-C62-C12	2.28	115.20	109.63
58	13	1741	PAR	O51-C51-C41	2.27	113.81	109.69
58	1G	1702	PAR	C22-C12-C62	2.08	113.19	110.04
61	14	3437	SPE	C6-N5-C4	-2.07	103.68	113.45
58	1G	1702	PAR	C62-C12-N12	-2.04	106.92	110.97
58	13	1741	PAR	C22-C32-C42	2.03	114.65	109.53

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	13	1741	PAR	C44-C54-C64-N64
58	13	1741	PAR	O54-C54-C64-N64
61	1G	1703	SPE	C2-C3-C4-N5
61	14	3437	SPE	C6-C7-C8-N9
61	14	3437	SPE	N9-C10-C11-C12
61	14	3436	SPE	C3-C4-N5-C6
61	1G	1703	SPE	C6-C7-C8-N9
61	14	3436	SPE	N9-C10-C11-C12
61	14	3437	SPE	N1-C2-C3-C4
61	14	3437	SPE	C10-C11-C12-N13
61	14	3436	SPE	C10-C11-C12-N13
58	13	1741	PAR	C41-C51-C61-O61
61	14	3436	SPE	N1-C2-C3-C4
58	13	1741	PAR	O51-C11-O11-C42
61	14	3436	SPE	C2-C3-C4-N5
61	1G	1703	SPE	C10-C11-C12-N13
58	1G	1702	PAR	C62-C52-O52-C13
61	14	3437	SPE	C7-C8-N9-C10
58	13	1741	PAR	C43-C33-O33-C14

There are no ring outliers.

5 monomers are involved in 13 short contacts:

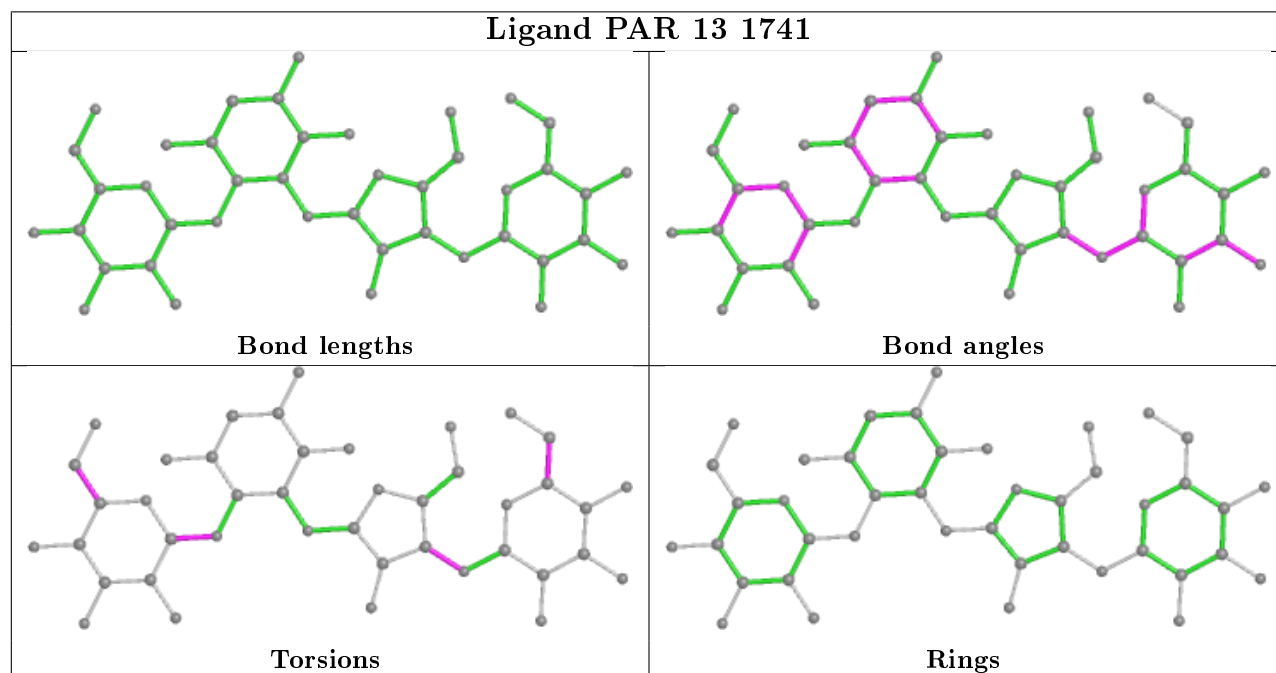
Mol	Chain	Res	Type	Clashes	Symm-Clashes
61	14	3436	SPE	2	0
59	32	302	SF4	3	0

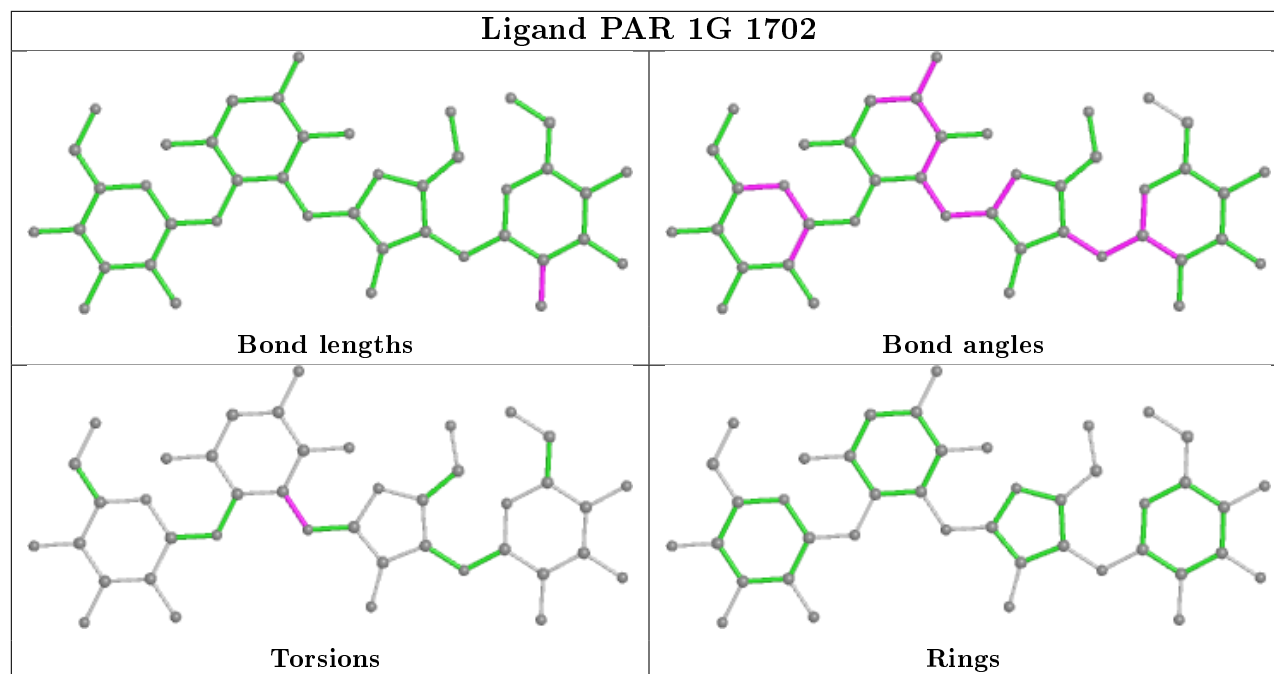
Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	3E	301	SF4	1	0
61	14	3437	SPE	6	0
58	1G	1702	PAR	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
10	1A	2
26	1H	1
4	3E	1
47	D5	1
24	1L	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1H	1055:G	O3'	1059:G	P	14.13
1	1L	72:C	O3'	73:A	P	3.25
1	1A	38:ILE	C	39:PRO	N	1.71
1	1A	76:ASN	C	77:PRO	N	1.61
1	D5	94:GLU	C	95:PRO	N	1.61
1	3E	36:ARG	C	37:PRO	N	1.19

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, 95th 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 ²)	Q<0.9
1	13	1499/1522 (98%)	-0.23	1 (0%) 95 89	57, 100, 176, 247	0
1	1G	1508/1522 (99%)	-0.17	10 (0%) 87 69	71, 119, 192, 267	0
2	12	207/256 (80%)	0.75	26 (12%) 3 1	131, 164, 184, 192	0
2	1E	231/256 (90%)	0.24	12 (5%) 27 10	112, 143, 169, 174	0
3	22	195/239 (81%)	1.21	50 (25%) 0 0	135, 160, 173, 178	0
3	2E	205/239 (85%)	0.67	22 (10%) 6 2	88, 111, 143, 151	0
4	32	208/209 (99%)	0.66	14 (6%) 17 5	92, 113, 136, 142	0
4	3E	207/209 (99%)	0.31	12 (5%) 23 7	84, 108, 132, 144	0
5	42	150/162 (92%)	0.49	11 (7%) 15 4	108, 128, 148, 160	0
5	4E	149/162 (91%)	0.30	4 (2%) 54 26	82, 103, 121, 131	0
6	52	101/101 (100%)	0.02	0 100 100	85, 104, 121, 132	0
6	5E	100/101 (99%)	0.52	7 (7%) 16 5	85, 105, 120, 132	0
7	62	138/156 (88%)	1.18	33 (23%) 0 0	116, 130, 141, 147	0
7	6E	154/156 (98%)	1.23	36 (23%) 0 0	102, 120, 150, 171	0
8	72	137/138 (99%)	0.73	15 (10%) 5 2	100, 131, 142, 149	0
8	7E	138/138 (100%)	1.07	29 (21%) 1 0	93, 110, 122, 134	0
9	82	121/128 (94%)	1.87	50 (41%) 0 0	116, 163, 174, 182	0
9	8E	126/128 (98%)	0.24	5 (3%) 38 15	87, 138, 157, 163	0
10	1A	80/105 (76%)	1.02	22 (27%) 0 0	133, 156, 169, 174	0
10	1I	94/105 (89%)	1.42	28 (29%) 0 0	81, 131, 168, 173	0
11	2A	113/129 (87%)	1.33	27 (23%) 0 0	84, 109, 124, 135	0
11	2I	111/129 (86%)	1.14	25 (22%) 0 0	72, 107, 123, 133	0
12	3A	121/132 (91%)	1.72	45 (37%) 0 0	90, 112, 135, 151	0
12	3I	122/132 (92%)	0.72	15 (12%) 4 1	66, 76, 102, 135	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	4A	109/126 (86%)	0.85	26 (23%) 0 0	123, 150, 180, 194	0
13	4I	117/126 (92%)	0.32	4 (3%) 45 19	88, 116, 131, 138	0
14	5A	59/61 (96%)	3.90	41 (69%) 0 0	137, 158, 180, 183	0
14	5I	59/61 (96%)	0.83	8 (13%) 3 1	81, 96, 114, 122	0
15	6A	87/89 (97%)	0.13	3 (3%) 45 19	84, 113, 128, 131	0
15	6I	87/89 (97%)	0.35	3 (3%) 45 19	80, 98, 113, 123	0
16	7A	84/88 (95%)	0.26	2 (2%) 59 30	92, 105, 129, 155	0
16	7I	83/88 (94%)	1.13	20 (24%) 0 0	96, 111, 137, 155	0
17	8A	99/105 (94%)	1.30	27 (27%) 0 0	97, 113, 130, 135	0
17	8I	99/105 (94%)	1.10	18 (18%) 1 0	89, 106, 115, 124	0
18	9A	67/88 (76%)	0.35	4 (5%) 21 7	92, 112, 132, 138	0
18	9I	68/88 (77%)	0.20	2 (2%) 51 23	88, 107, 131, 135	0
19	AA	65/93 (69%)	1.17	13 (20%) 1 0	162, 178, 187, 192	0
19	AI	82/93 (88%)	0.24	3 (3%) 41 17	96, 117, 138, 151	0
20	BA	99/106 (93%)	1.15	18 (18%) 1 0	90, 114, 140, 152	0
20	BI	97/106 (91%)	1.37	27 (27%) 0 0	106, 119, 145, 151	0
21	1B	22/27 (81%)	1.72	8 (36%) 0 0	127, 141, 145, 148	0
21	1F	23/27 (85%)	0.24	0 100 100	92, 99, 107, 115	0
22	1K	67/76 (88%)	0.54	5 (7%) 14 4	90, 193, 226, 233	0
23	2K	72/77 (93%)	0.03	1 (1%) 75 49	67, 92, 124, 140	0
23	2L	72/77 (93%)	0.07	0 100 100	80, 116, 152, 163	0
24	1L	66/76 (86%)	1.06	11 (16%) 1 0	145, 224, 245, 249	0
24	3K	70/76 (92%)	0.91	10 (14%) 2 1	76, 229, 251, 253	0
24	3L	72/76 (94%)	0.16	3 (4%) 36 14	85, 220, 238, 240	0
25	4K	19/30 (63%)	0.97	4 (21%) 1 0	71, 140, 219, 219	0
25	4L	19/30 (63%)	1.35	3 (15%) 2 1	98, 158, 230, 230	0
26	14	2826/2917 (96%)	-0.06	17 (0%) 89 72	50, 85, 199, 264	0
26	1H	2860/2917 (98%)	-0.10	7 (0%) 95 87	40, 69, 186, 257	0
27	16	122/122 (100%)	-0.35	1 (0%) 86 65	61, 88, 107, 197	0
27	1J	122/122 (100%)	-0.45	0 100 100	85, 119, 145, 205	0
28	7I	132/229 (57%)	0.80	20 (15%) 2 1	146, 210, 235, 243	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
29	11	273/276 (98%)	0.46	5 (1%) 68 40	41, 63, 79, 93	0
29	19	274/276 (99%)	0.59	7 (2%) 56 27	47, 73, 88, 107	0
30	21	203/206 (98%)	0.63	10 (4%) 29 11	48, 84, 120, 130	0
30	29	204/206 (99%)	1.03	39 (19%) 1 0	60, 95, 134, 149	0
31	31	202/210 (96%)	0.63	9 (4%) 33 12	46, 76, 112, 127	0
31	39	204/210 (97%)	0.56	14 (6%) 16 5	57, 101, 148, 177	0
32	41	179/182 (98%)	0.77	21 (11%) 4 1	79, 100, 134, 146	0
32	49	180/182 (98%)	1.22	48 (26%) 0 0	117, 138, 156, 174	0
33	51	174/180 (96%)	0.30	4 (2%) 60 31	77, 102, 119, 130	0
33	59	169/180 (93%)	2.48	92 (54%) 0 0	152, 196, 220, 233	0
34	61	145/148 (97%)	0.52	17 (11%) 4 1	76, 131, 149, 157	0
34	69	145/148 (97%)	0.46	12 (8%) 11 3	86, 122, 149, 156	0
35	15	137/140 (97%)	1.16	25 (18%) 1 0	81, 108, 135, 151	0
35	58	137/140 (97%)	0.86	18 (13%) 3 1	63, 85, 121, 138	0
36	25	122/122 (100%)	0.91	14 (11%) 4 1	69, 88, 105, 117	0
36	68	122/122 (100%)	0.39	3 (2%) 57 29	56, 72, 90, 99	0
37	35	147/150 (98%)	0.86	21 (14%) 2 1	58, 102, 135, 152	0
37	78	147/150 (98%)	0.57	10 (6%) 17 5	47, 80, 104, 115	0
38	45	138/141 (97%)	0.95	27 (19%) 1 0	76, 105, 124, 155	0
38	88	141/141 (100%)	0.71	10 (7%) 16 5	54, 75, 95, 123	0
39	55	118/118 (100%)	0.60	7 (5%) 22 7	65, 80, 97, 112	0
39	98	118/118 (100%)	0.81	12 (10%) 6 2	60, 78, 94, 106	0
40	65	110/112 (98%)	1.06	22 (20%) 1 0	89, 112, 132, 137	0
40	A8	111/112 (99%)	1.09	18 (16%) 1 0	72, 85, 105, 116	0
41	75	133/146 (91%)	0.40	7 (5%) 26 10	80, 96, 128, 151	0
41	B8	135/146 (92%)	0.14	5 (3%) 41 17	67, 84, 128, 139	0
42	85	116/118 (98%)	0.54	4 (3%) 45 19	63, 96, 127, 134	0
42	C8	115/118 (97%)	0.31	3 (2%) 56 27	53, 77, 102, 108	0
43	95	100/101 (99%)	1.08	22 (22%) 0 0	65, 116, 135, 142	0
43	D8	100/101 (99%)	0.89	15 (15%) 2 1	53, 101, 119, 126	0
44	A5	111/113 (98%)	0.79	5 (4%) 33 12	57, 75, 101, 137	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	E8	110/113 (97%)	0.49	8 (7%) 15 4	53, 70, 94, 106	0
45	B5	94/96 (97%)	1.09	15 (15%) 1 1	68, 83, 104, 118	0
45	F8	95/96 (98%)	0.21	1 (1%) 80 56	49, 66, 97, 110	0
46	C5	104/110 (94%)	2.12	36 (34%) 0 0	92, 118, 156, 164	0
46	G8	103/110 (93%)	0.26	5 (4%) 29 11	73, 95, 122, 130	0
47	D5	177/206 (85%)	1.81	70 (39%) 0 0	108, 148, 226, 236	0
47	H8	170/206 (82%)	1.81	65 (38%) 0 0	80, 116, 202, 210	0
48	E5	76/85 (89%)	1.15	13 (17%) 1 0	66, 88, 102, 115	0
48	I8	77/85 (90%)	0.58	5 (6%) 18 5	54, 69, 91, 102	0
49	F5	94/98 (95%)	1.21	18 (19%) 1 0	60, 83, 122, 136	0
49	J8	96/98 (97%)	0.85	9 (9%) 8 3	51, 71, 126, 138	0
50	G5	69/72 (95%)	0.44	5 (7%) 15 4	81, 104, 124, 138	0
50	K8	68/72 (94%)	0.12	1 (1%) 73 46	59, 79, 96, 120	0
51	H5	58/60 (96%)	2.04	29 (50%) 0 0	77, 99, 122, 135	0
51	L8	58/60 (96%)	0.54	2 (3%) 45 19	60, 77, 103, 110	0
52	M8	60/71 (84%)	1.54	16 (26%) 0 0	102, 143, 168, 171	0
53	J5	56/60 (93%)	0.72	7 (12%) 3 1	58, 85, 131, 141	0
53	N8	48/60 (80%)	0.36	0 100 100	46, 78, 119, 127	0
54	O8	45/54 (83%)	4.57	40 (88%) 0 0	117, 153, 171, 177	0
55	L5	47/49 (95%)	0.47	2 (4%) 35 13	47, 60, 87, 97	0
55	P8	47/49 (95%)	0.09	1 (2%) 63 34	42, 50, 72, 87	0
56	M5	64/65 (98%)	1.47	18 (28%) 0 0	68, 80, 97, 117	0
56	Q8	64/65 (98%)	0.36	0 100 100	51, 65, 80, 98	0
All	All	20730/21798 (95%)	0.42	1700 (8%) 11 3	40, 99, 184, 267	0

All (1700) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
46	C5	59	GLY	14.7
14	5A	38	GLY	12.9
33	59	96	ALA	12.6
46	C5	49	VAL	12.1
52	M8	40	HIS	11.7
43	D8	37	VAL	11.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
14	5A	39	LEU	11.3
12	3A	64	TYR	10.9
33	59	17	VAL	10.7
9	82	115	GLY	10.0
46	C5	58	GLY	9.9
46	C5	50	ARG	9.8
19	AA	68	GLY	9.3
54	O8	13	CYS	9.3
14	5A	26	ARG	9.2
14	5A	25	VAL	9.2
54	O8	19	ARG	9.1
14	5A	34	TYR	8.8
12	3A	28	LYS	8.8
54	O8	14	THR	8.4
37	35	110	TYR	8.3
40	A8	110	LEU	8.2
54	O8	52	VAL	8.2
54	O8	20	ASN	8.1
54	O8	34	LEU	7.9
46	C5	60	PHE	7.9
14	5A	30	ALA	7.8
54	O8	53	LYS	7.7
12	3A	27	LEU	7.6
14	5A	37	PHE	7.5
10	1A	47	PHE	7.4
47	D5	142	SER	7.4
33	59	170	ARG	7.4
47	H8	113	ALA	7.4
50	G5	44	LEU	7.2
54	O8	26	ASN	7.2
13	4A	102	ARG	7.2
33	59	83	TYR	7.1
46	C5	29	GLU	7.1
33	59	168	PRO	7.1
54	O8	50	ARG	7.1
54	O8	42	TRP	7.0
14	5A	53	LEU	7.0
54	O8	43	CYS	7.0
33	59	99	VAL	7.0
7	6E	81	GLY	7.0
33	59	107	VAL	6.9
46	C5	47	LYS	6.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
45	B5	69	TYR	6.9
47	D5	9	TYR	6.9
14	5A	41	ARG	6.8
54	O8	18	ARG	6.8
14	5A	31	ARG	6.7
12	3A	19	ARG	6.6
3	22	6	HIS	6.6
9	82	109	VAL	6.6
33	59	87	LEU	6.6
14	5A	51	GLY	6.6
10	1A	54	PHE	6.5
33	59	33	LEU	6.5
46	C5	63	LYS	6.5
46	C5	61	ILE	6.4
26	14	888	C	6.4
10	1A	62	HIS	6.4
25	4L	25	A	6.3
33	59	128	PRO	6.3
14	5A	35	ARG	6.3
14	5A	42	ILE	6.3
41	B8	106	SER	6.3
2	12	62	ALA	6.3
24	1L	71	C	6.2
24	1L	1	G	6.2
12	3A	63	GLY	6.2
19	AA	67	VAL	6.2
33	59	169	VAL	6.2
22	1K	76	A	6.1
7	62	16	LEU	6.1
33	59	103	LEU	6.1
7	6E	80	VAL	6.1
7	6E	85	TYR	6.1
10	1A	65	LEU	6.1
33	59	95	ARG	6.0
7	6E	84	ASN	6.0
10	1I	10	GLY	5.9
33	59	105	LEU	5.9
52	M8	41	PRO	5.9
33	59	164	TYR	5.8
54	O8	49	HIS	5.8
12	3A	62	SER	5.8
7	6E	83	ALA	5.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	12	72	GLY	5.8
7	6E	78	ARG	5.7
32	49	139	LEU	5.7
33	59	76	VAL	5.7
3	22	39	ILE	5.7
10	1I	22	LYS	5.7
16	7I	32	TYR	5.7
45	B5	68	ARG	5.7
46	C5	46	LYS	5.6
19	AA	40	ILE	5.6
12	3A	20	LYS	5.6
12	3I	64	TYR	5.6
12	3A	68	ALA	5.6
45	B5	79	ALA	5.6
47	D5	155	LEU	5.6
6	5E	46	ARG	5.6
12	3A	21	LYS	5.6
32	49	138	GLN	5.5
47	D5	146	ILE	5.5
51	H5	6	VAL	5.5
14	5A	6	LEU	5.5
52	M8	31	ILE	5.5
32	49	90	LEU	5.5
33	59	115	VAL	5.4
10	1A	61	GLU	5.4
34	69	1	MET	5.4
2	1E	10	LEU	5.4
54	O8	32	ASN	5.4
12	3A	32	PHE	5.4
9	82	116	LYS	5.3
33	59	25	LYS	5.3
14	5A	33	VAL	5.3
33	59	26	VAL	5.3
33	59	106	THR	5.3
10	1A	59	SER	5.3
3	22	198	VAL	5.3
14	5A	58	LYS	5.3
31	39	10	PRO	5.2
28	71	175	VAL	5.2
47	H8	165	VAL	5.2
47	D5	112	ARG	5.2
20	BA	9	ASN	5.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
29	19	26	LYS	5.2
46	C5	48	ALA	5.2
38	88	104	PHE	5.2
33	59	130	ARG	5.2
47	D5	121	HIS	5.2
12	3I	61	THR	5.2
47	D5	69	THR	5.2
33	59	90	LYS	5.2
19	AI	71	LEU	5.1
3	22	177	THR	5.1
54	O8	12	GLU	5.1
47	H8	96	VAL	5.1
33	59	162	ILE	5.1
24	3K	6	G	5.1
54	O8	25	LYS	5.1
7	6E	79	ARG	5.1
47	D5	68	PRO	5.0
2	12	152	PHE	5.0
47	D5	179	ASP	5.0
13	4A	111	LYS	5.0
14	5A	50	LYS	5.0
13	4A	95	GLY	5.0
33	59	114	VAL	5.0
46	C5	44	ILE	5.0
14	5A	44	LEU	5.0
33	59	171	LEU	5.0
51	H5	26	LEU	5.0
10	1A	48	THR	5.0
14	5A	23	ARG	5.0
3	2E	193	TYR	5.0
47	H8	147	GLY	5.0
32	49	133	LEU	5.0
33	59	94	TYR	4.9
10	1A	49	VAL	4.9
30	29	77	ILE	4.9
52	M8	22	ILE	4.9
19	AA	53	ASN	4.9
54	O8	23	THR	4.9
25	4K	25	A	4.9
30	29	76	ARG	4.9
9	82	110	GLU	4.9
9	82	123	PRO	4.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
11	2A	75	TYR	4.9
46	C5	53	PRO	4.9
52	M8	66	SER	4.9
10	1A	63	PHE	4.8
35	15	9	VAL	4.8
38	88	33	GLY	4.8
33	59	89	ILE	4.8
9	82	102	LEU	4.8
32	41	80	PHE	4.8
48	I8	8	GLY	4.8
14	5A	36	PHE	4.8
14	5A	29	ARG	4.8
54	O8	22	ALA	4.8
7	6E	154	TYR	4.8
47	D5	153	SER	4.7
17	8I	36	ILE	4.7
47	H8	166	SER	4.7
43	D8	38	LEU	4.7
12	3I	20	LYS	4.7
9	82	20	ARG	4.7
47	D5	150	LEU	4.7
49	F5	91	LYS	4.7
40	A8	49	VAL	4.7
47	D5	5	LEU	4.7
33	59	153	LYS	4.7
3	22	28	GLN	4.7
33	59	16	SER	4.7
35	58	72	TYR	4.6
47	D5	70	LEU	4.6
40	A8	48	LEU	4.6
12	3I	19	ARG	4.6
37	35	71	VAL	4.6
24	3L	34	U	4.6
7	6E	82	GLY	4.6
7	6E	16	LEU	4.5
47	D5	171	ILE	4.5
54	O8	15	GLU	4.5
13	4A	103	THR	4.5
14	5A	22	THR	4.5
32	41	25	TYR	4.5
40	65	60	GLY	4.5
3	22	186	PHE	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
47	H8	70	LEU	4.5
2	12	165	VAL	4.5
29	19	27	THR	4.5
32	49	62	LEU	4.5
14	5A	10	ALA	4.5
3	22	35	GLU	4.5
7	62	61	VAL	4.4
10	1I	94	VAL	4.4
46	C5	56	PRO	4.4
14	5A	47	LEU	4.4
51	H5	30	ARG	4.4
54	O8	31	PRO	4.4
54	O8	10	LEU	4.4
47	H8	146	ILE	4.4
20	BI	55	ILE	4.4
50	G5	43	GLN	4.4
47	D5	144	LEU	4.4
54	O8	16	CYS	4.4
3	22	53	ALA	4.4
33	59	49	VAL	4.4
33	59	88	LEU	4.4
45	B5	92	LEU	4.4
30	21	88	GLY	4.4
51	H5	15	TYR	4.3
43	D8	1	MET	4.3
2	12	133	LYS	4.3
47	H8	104	PHE	4.3
33	59	155	SER	4.3
10	1A	51	ARG	4.3
8	7E	63	LEU	4.3
30	29	78	LEU	4.3
56	M5	12	LYS	4.3
53	J5	56	LYS	4.3
3	22	101	LEU	4.3
12	3A	23	LYS	4.3
16	7I	35	LYS	4.3
44	E8	92	ARG	4.3
20	BI	72	LEU	4.3
32	49	34	LEU	4.3
28	71	176	GLY	4.3
17	8A	7	THR	4.3
16	7I	48	TRP	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
28	71	13	LYS	4.3
13	4A	98	VAL	4.2
33	59	123	PHE	4.2
2	12	224	GLN	4.2
38	45	104	PHE	4.2
19	AA	62	ILE	4.2
14	5A	46	GLU	4.2
47	D5	51	ALA	4.2
12	3A	69	TYR	4.2
33	59	132	ARG	4.2
30	29	71	GLY	4.2
40	65	55	ALA	4.2
47	H8	153	SER	4.2
47	D5	96	VAL	4.2
54	O8	29	ASN	4.2
47	H8	38	TYR	4.2
10	1I	90	LEU	4.2
51	H5	28	LEU	4.2
41	75	106	SER	4.2
12	3A	85	ILE	4.2
47	D5	125	LEU	4.1
49	J8	70	VAL	4.1
43	95	1	MET	4.1
47	H8	98	MET	4.1
9	82	36	TYR	4.1
26	1H	1536	A	4.1
47	H8	8	TYR	4.1
47	H8	155	LEU	4.1
30	29	69	LYS	4.1
9	82	50	LEU	4.1
32	49	152	LEU	4.1
9	82	53	VAL	4.1
13	4A	101	GLN	4.1
11	2I	42	TRP	4.1
40	65	58	LEU	4.1
47	H8	144	LEU	4.1
10	1A	55	LYS	4.1
13	4I	96	LEU	4.1
7	6E	149	ARG	4.1
7	62	42	ILE	4.1
19	AA	71	LEU	4.1
35	58	15	LEU	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
54	O8	21	TYR	4.1
31	31	6	VAL	4.1
33	59	72	ILE	4.1
47	H8	161	VAL	4.0
32	49	142	PRO	4.0
54	O8	9	LEU	4.0
30	29	3	GLY	4.0
28	71	27	HIS	4.0
46	C5	45	VAL	4.0
32	49	92	VAL	4.0
25	4L	10	G	4.0
36	25	1	MET	4.0
47	D5	173	ALA	4.0
48	E5	8	GLY	4.0
47	D5	168	GLU	4.0
3	2E	200	ALA	4.0
33	59	10	PRO	4.0
17	8A	23	VAL	4.0
33	59	34	GLU	4.0
54	O8	33	LYS	4.0
48	E5	12	ASN	4.0
2	12	163	PHE	4.0
38	45	102	VAL	3.9
32	49	39	ILE	3.9
32	49	177	GLY	3.9
10	1I	95	GLU	3.9
10	1I	65	LEU	3.9
39	55	101	ALA	3.9
24	3L	35	U	3.9
10	1I	72	VAL	3.9
20	BA	10	LEU	3.9
51	H5	5	LYS	3.9
2	12	134	GLU	3.9
8	7E	95	VAL	3.9
14	5A	52	GLN	3.9
17	8I	98	LEU	3.9
40	65	56	LEU	3.9
52	M8	58	ARG	3.9
8	7E	109	ILE	3.9
53	J5	55	ARG	3.9
3	22	8	ILE	3.9
26	14	229	A	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
26	14	2799	A	3.9
33	59	125	VAL	3.9
7	62	41	ARG	3.9
40	65	108	GLY	3.9
33	59	98	LEU	3.9
47	H8	1	MET	3.9
2	1E	232	PRO	3.8
47	H8	164	ALA	3.8
9	82	114	TYR	3.8
44	A5	6	ILE	3.8
10	1I	88	LEU	3.8
28	71	181	PRO	3.8
37	35	106	LEU	3.8
10	1A	60	ARG	3.8
3	22	155	GLY	3.8
35	15	8	GLN	3.8
38	45	103	MET	3.8
14	5A	24	CYS	3.8
3	22	60	ALA	3.8
24	3K	36	U	3.8
12	3A	15	ARG	3.8
30	29	28	ALA	3.8
26	14	2802	G	3.8
11	2A	14	VAL	3.8
21	1B	13	ILE	3.8
30	29	67	PHE	3.8
47	H8	111	VAL	3.8
4	3E	96	LEU	3.8
30	29	73	GLU	3.8
47	H8	157	LEU	3.8
14	5A	54	PRO	3.8
49	F5	5	CYS	3.8
10	1I	96	ILE	3.8
14	5A	49	HIS	3.8
27	16	1(M)	A	3.8
33	59	97	ARG	3.8
11	2A	25	TYR	3.8
30	29	70	ALA	3.8
33	59	131	VAL	3.8
49	F5	62	VAL	3.8
26	14	2795	G	3.8
33	59	124	GLU	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
35	15	84	LYS	3.7
24	1L	3	G	3.7
39	55	70	LEU	3.7
55	L5	1	MET	3.7
9	8E	126	SER	3.7
17	8A	9	VAL	3.7
32	41	88	ILE	3.7
33	59	45	VAL	3.7
47	D5	117	LEU	3.7
54	O8	36	LEU	3.7
46	C5	86	ARG	3.7
56	M5	40	GLU	3.7
38	45	100	GLY	3.7
47	D5	50	GLN	3.7
2	12	164	VAL	3.7
47	H8	5	LEU	3.7
56	M5	22	VAL	3.7
12	3A	30	ALA	3.7
12	3A	65	GLU	3.7
17	8A	22	LEU	3.7
32	49	175	LEU	3.7
37	35	123	LEU	3.7
48	E5	71	ASP	3.7
49	F5	28	GLY	3.7
7	6E	86	GLN	3.7
10	1A	57	LYS	3.7
40	A8	112	PHE	3.7
11	2A	83	ILE	3.7
47	H8	106	GLY	3.7
20	BA	42	GLN	3.7
14	5A	59	ALA	3.7
3	22	23	TYR	3.7
34	69	35	LEU	3.7
18	9A	84	LYS	3.6
12	3A	33	ARG	3.6
11	2I	48	ILE	3.6
20	BI	41	ILE	3.6
28	71	32	LEU	3.6
32	49	82	LEU	3.6
45	B5	89	ILE	3.6
33	59	111	HIS	3.6
3	22	10	PHE	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	22	190	ARG	3.6
30	29	29	GLY	3.6
10	1A	64	GLU	3.6
12	3A	55	VAL	3.6
17	8A	6	LEU	3.6
54	O8	40	CYS	3.6
46	C5	65	ALA	3.6
47	H8	168	GLU	3.6
56	M5	16	ILE	3.6
1	1G	82	U	3.6
21	1B	14	TRP	3.6
40	A8	68	GLN	3.6
3	2E	94	LEU	3.6
32	41	34	LEU	3.6
33	59	32	GLU	3.6
33	59	29	PRO	3.6
8	72	133	LEU	3.6
29	11	111	LEU	3.6
33	59	4	ILE	3.6
38	45	17	LEU	3.6
47	D5	141	VAL	3.6
3	22	184	TYR	3.5
17	8A	32	TYR	3.5
9	82	120	ARG	3.5
10	1A	46	ARG	3.5
13	4A	94	ARG	3.5
34	61	107	VAL	3.5
35	15	85	ILE	3.5
40	65	20	ARG	3.5
46	G8	89	PHE	3.5
20	BI	40	ALA	3.5
56	M5	64	TYR	3.5
33	59	11	VAL	3.5
51	H5	9	VAL	3.5
17	8A	27	PHE	3.5
32	49	178	PHE	3.5
47	H8	134	PRO	3.5
30	29	181	LEU	3.5
5	42	90	VAL	3.5
20	BI	100	ILE	3.5
24	1L	70	C	3.5
56	M5	34	TRP	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
14	5A	55	GLY	3.5
38	45	33	GLY	3.5
11	2I	50	TYR	3.5
47	D5	152	ALA	3.5
46	C5	51	VAL	3.5
24	3K	45	G	3.5
38	45	99	PRO	3.5
47	D5	95	PRO	3.5
46	C5	30	VAL	3.5
52	M8	13	ARG	3.5
10	1A	58	ASP	3.5
3	22	96	GLY	3.4
33	59	71	LEU	3.4
24	3K	70	C	3.4
3	22	7	PRO	3.4
47	H8	169	GLU	3.4
10	1A	56	HIS	3.4
13	4A	87	TYR	3.4
17	8I	95	TYR	3.4
30	29	51	PHE	3.4
30	29	4	ILE	3.4
35	58	85	ILE	3.4
40	A8	59	LYS	3.4
13	4A	110	ARG	3.4
10	1A	53	PRO	3.4
40	65	57	LYS	3.4
5	42	109	ILE	3.4
12	3A	24	VAL	3.4
35	15	98	VAL	3.4
32	49	23	PHE	3.4
54	O8	30	THR	3.4
14	5A	17	LYS	3.4
8	7E	59	LEU	3.4
45	B5	66	LEU	3.4
43	95	4	ILE	3.4
33	59	81	GLU	3.4
37	78	71	VAL	3.4
49	F5	61	ARG	3.4
35	15	73	THR	3.4
47	D5	8	TYR	3.4
45	B5	13	LEU	3.4
8	7E	46	LYS	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	3E	3	ARG	3.4
9	82	79	LEU	3.4
1	1G	1202	G	3.4
12	3I	28	LYS	3.4
12	3A	29	GLY	3.4
35	15	51	PHE	3.4
40	65	109	GLY	3.4
33	59	122	THR	3.4
46	C5	2	ARG	3.3
13	4A	96	LEU	3.3
8	7E	58	TYR	3.3
35	15	12	ARG	3.3
3	22	94	LEU	3.3
31	31	123	LEU	3.3
43	D8	99	ILE	3.3
38	45	65	PHE	3.3
25	4L	9	G	3.3
11	2A	21	ILE	3.3
12	3A	31	PRO	3.3
20	BI	44	ALA	3.3
28	71	19	ILE	3.3
32	41	23	PHE	3.3
38	45	22	LYS	3.3
37	78	106	LEU	3.3
3	22	187	ALA	3.3
16	7I	19	ILE	3.3
35	58	16	ILE	3.3
17	8A	21	VAL	3.3
32	49	160	VAL	3.3
26	1H	163	U	3.3
33	59	100	GLY	3.3
47	D5	114	GLY	3.3
32	49	179	PRO	3.3
47	H8	74	VAL	3.3
52	M8	3	GLU	3.3
24	1L	72	C	3.3
35	15	72	TYR	3.3
7	62	5	ARG	3.3
40	A8	44	LYS	3.3
21	1B	2	GLY	3.3
47	D5	143	GLY	3.3
40	65	40	ILE	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	59	159	GLU	3.3
6	5E	63	TYR	3.3
35	15	87	LEU	3.3
43	D8	54	GLY	3.3
32	49	109	VAL	3.3
43	95	14	VAL	3.3
10	1I	33	GLN	3.3
13	4A	92	HIS	3.3
3	22	197	GLY	3.3
26	1H	2476	A	3.3
33	51	9	ILE	3.3
38	88	132	VAL	3.3
32	49	176	LEU	3.3
12	3A	98	TYR	3.2
33	59	151	ILE	3.2
47	H8	141	VAL	3.2
21	1B	22	ARG	3.2
35	15	48	MET	3.2
30	29	49	LEU	3.2
51	H5	53	LEU	3.2
51	H5	48	GLU	3.2
13	4A	88	ARG	3.2
13	4A	90	LEU	3.2
20	BI	17	ARG	3.2
17	8I	23	VAL	3.2
37	35	125	VAL	3.2
17	8A	8	GLY	3.2
43	D8	45	THR	3.2
11	2I	71	LYS	3.2
9	82	31	GLN	3.2
28	71	31	GLU	3.2
51	H5	19	GLN	3.2
20	BA	8	ARG	3.2
2	12	92	TYR	3.2
7	62	28	ASN	3.2
46	C5	52	SER	3.2
12	3I	63	GLY	3.2
40	A8	58	LEU	3.2
26	14	2141	G	3.2
7	62	62	PHE	3.2
33	59	15	VAL	3.2
35	15	92	ALA	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	29	151	TYR	3.2
17	8A	92	ARG	3.2
47	D5	134	PRO	3.2
47	D5	176	PRO	3.2
51	H5	2	PRO	3.2
13	4A	117	VAL	3.2
9	82	92	TYR	3.2
11	2I	25	TYR	3.2
11	2I	98	LEU	3.2
14	5I	39	LEU	3.2
54	O8	11	LEU	3.2
32	41	52	ILE	3.2
12	3A	97	ARG	3.2
20	BI	59	ALA	3.2
2	1E	14	GLY	3.2
43	95	16	PRO	3.2
17	8A	71	PHE	3.2
46	C5	62	GLU	3.2
11	2I	68	ALA	3.1
13	4A	115	LYS	3.1
9	82	30	GLY	3.1
47	H8	99	TYR	3.1
7	6E	99	LEU	3.1
32	49	155	MET	3.1
9	82	59	PHE	3.1
40	65	112	PHE	3.1
41	75	50	ILE	3.1
46	C5	42	VAL	3.1
7	62	12	LEU	3.1
17	8I	27	PHE	3.1
34	61	111	PRO	3.1
43	D8	98	GLU	3.1
3	2E	189	ALA	3.1
20	BA	99	LEU	3.1
32	49	89	GLY	3.1
8	72	2	LEU	3.1
12	3A	16	GLU	3.1
14	5A	45	ARG	3.1
32	41	137	GLU	3.1
37	78	110	TYR	3.1
31	39	14	PRO	3.1
16	7I	36	ILE	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	59	93	GLY	3.1
47	H8	2	GLU	3.1
7	6E	12	LEU	3.1
16	7I	6	LEU	3.1
34	61	130	TYR	3.1
9	82	21	PRO	3.1
16	7I	28	ARG	3.1
20	BI	43	LEU	3.1
33	59	79	VAL	3.1
54	O8	48	VAL	3.1
3	22	32	LEU	3.1
7	62	101	LEU	3.1
8	72	112	LEU	3.1
12	3A	93	LEU	3.1
38	45	130	LYS	3.1
47	H8	156	LYS	3.1
47	D5	156	LYS	3.1
36	25	42	SER	3.1
4	32	186	LEU	3.1
8	7E	133	LEU	3.1
12	3I	17	LYS	3.1
17	8I	45	HIS	3.1
2	1E	96	ARG	3.1
30	29	150	VAL	3.0
47	H8	149	SER	3.0
12	3A	46	LYS	3.0
16	7I	49	LEU	3.0
32	49	135	LEU	3.0
56	M5	61	LEU	3.0
21	1B	6	ARG	3.0
7	6E	151	TYR	3.0
7	62	27	ILE	3.0
24	3K	71	C	3.0
29	11	112	GLN	3.0
14	5A	56	VAL	3.0
12	3A	56	ALA	3.0
32	49	36	LYS	3.0
47	D5	7	ALA	3.0
34	61	128	LEU	3.0
41	75	1	MET	3.0
16	7A	32	TYR	3.0
3	22	64	VAL	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
49	F5	70	VAL	3.0
47	H8	66	SER	3.0
7	62	76	ARG	3.0
3	22	31	HIS	3.0
37	35	108	LYS	3.0
33	59	9	ILE	3.0
43	95	96	ILE	3.0
35	58	55	VAL	3.0
40	A8	37	ALA	3.0
43	95	94	LEU	3.0
3	22	199	LYS	3.0
43	95	99	ILE	3.0
7	62	37	ASN	3.0
33	59	86	GLU	3.0
47	D5	162	GLU	3.0
47	H8	133	ILE	3.0
11	2A	84	VAL	3.0
9	82	106	ALA	3.0
16	7I	7	ALA	3.0
18	9I	78	LEU	3.0
35	58	73	THR	3.0
47	H8	67	LEU	3.0
3	2E	190	ARG	3.0
11	2A	91	ARG	3.0
6	5E	9	VAL	3.0
33	59	13	LYS	3.0
42	85	90	VAL	3.0
1	1G	1029	G	3.0
24	3K	34	U	3.0
16	7I	30	GLY	3.0
2	12	96	ARG	3.0
3	2E	79	ARG	3.0
7	62	73	MET	3.0
4	32	128	VAL	3.0
9	82	65	VAL	3.0
10	1I	34	VAL	3.0
47	D5	126	VAL	3.0
47	D5	151	HIS	3.0
33	59	165	ALA	3.0
11	2I	66	LEU	3.0
34	69	12	LEU	3.0
43	95	12	TYR	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
29	19	44	ASN	3.0
32	41	48	GLU	3.0
8	72	79	VAL	3.0
12	3A	18	VAL	3.0
8	7E	112	LEU	2.9
18	9A	43	PHE	2.9
13	4I	6	GLY	2.9
32	49	149	VAL	2.9
29	19	2	ALA	2.9
11	2I	63	LEU	2.9
47	D5	108	PRO	2.9
17	8A	95	TYR	2.9
31	39	199	TRP	2.9
46	C5	64	GLU	2.9
10	1A	44	VAL	2.9
11	2I	70	LYS	2.9
38	45	6	ARG	2.9
3	22	42	LEU	2.9
12	3A	60	LEU	2.9
13	4A	107	ALA	2.9
20	BI	80	ARG	2.9
54	O8	47	THR	2.9
2	12	155	LEU	2.9
14	5A	48	ALA	2.9
24	1L	31	A	2.9
32	41	26	GLN	2.9
4	32	187	ARG	2.9
7	6E	72	ARG	2.9
56	M5	6	THR	2.9
38	45	37	LEU	2.9
47	D5	172	ALA	2.9
32	49	137	GLU	2.9
12	3I	7	ILE	2.9
3	2E	151	VAL	2.9
11	2I	43	SER	2.9
32	49	159	VAL	2.9
42	85	40	PHE	2.9
6	5E	14	LEU	2.9
3	22	30	ARG	2.9
8	7E	131	GLY	2.9
12	3I	91	LYS	2.9
54	O8	44	ARG	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	12	129	GLU	2.9
4	32	17	VAL	2.9
2	12	102	LEU	2.9
51	H5	11	SER	2.9
8	72	74	PRO	2.9
11	2A	35	PRO	2.9
50	K8	43	GLN	2.9
3	22	201	TYR	2.9
10	1I	46	ARG	2.9
17	8A	11	VAL	2.9
33	59	141	VAL	2.9
47	H8	109	ALA	2.9
47	D5	28	MET	2.9
34	61	103	ARG	2.8
3	2E	60	ALA	2.8
3	22	188	LEU	2.8
3	22	189	ALA	2.8
25	4K	13	A	2.8
34	61	123	LEU	2.8
14	5A	32	SER	2.8
33	59	134	SER	2.8
39	98	34	ILE	2.8
46	C5	84	ARG	2.8
37	78	91	PHE	2.8
14	5A	60	SER	2.8
47	H8	114	GLY	2.8
33	59	113	VAL	2.8
33	59	133	VAL	2.8
43	95	44	LYS	2.8
47	D5	91	LEU	2.8
48	I8	84	LEU	2.8
56	M5	50	LEU	2.8
9	82	122	ALA	2.8
30	29	131	ALA	2.8
47	H8	103	ARG	2.8
1	1G	1226	C	2.8
2	12	223	ILE	2.8
10	1I	36	GLY	2.8
12	3A	17	LYS	2.8
12	3A	88	GLY	2.8
33	59	85	LYS	2.8
46	C5	54	LYS	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
8	7E	10	LEU	2.8
46	C5	43	ASN	2.8
47	H8	163	LEU	2.8
47	D5	61	LEU	2.8
29	11	262	ARG	2.8
30	29	56	PRO	2.8
48	E5	46	LYS	2.8
17	8A	59	ILE	2.8
9	82	37	PHE	2.8
45	B5	26	TYR	2.8
47	D5	59	LEU	2.8
30	29	79	ARG	2.8
51	H5	55	ARG	2.8
52	M8	20	ASN	2.8
4	32	146	ILE	2.8
48	E5	42	GLY	2.8
35	15	41	ASP	2.8
5	4E	152	ARG	2.8
9	82	19	LEU	2.8
18	9A	46	GLU	2.8
30	21	195	LEU	2.8
38	45	34	LEU	2.8
49	J8	80	LEU	2.8
52	M8	32	TYR	2.8
11	2A	19	ALA	2.8
26	14	2797	U	2.8
8	7E	6	ILE	2.8
40	65	35	ILE	2.8
7	6E	153	HIS	2.8
32	49	35	GLU	2.8
33	59	129	THR	2.8
51	H5	37	LEU	2.8
20	BI	45	GLN	2.8
33	59	46	GLU	2.8
33	59	101	ARG	2.8
48	E5	45	PHE	2.8
7	6E	60	LYS	2.8
9	82	32	ASP	2.8
10	1I	64	GLU	2.8
17	8I	99	SER	2.8
56	M5	29	LYS	2.8
2	1E	187	LEU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
17	8A	10	VAL	2.8
38	45	97	VAL	2.8
39	98	113	LEU	2.8
41	B8	104	ASN	2.7
46	C5	5	MET	2.7
8	72	83	ILE	2.7
17	8A	36	ILE	2.7
33	59	12	PRO	2.7
35	15	86	PRO	2.7
11	2I	82	VAL	2.7
22	1K	5	C	2.7
23	2K	1	C	2.7
4	32	169	LYS	2.7
14	5A	11	LYS	2.7
15	6A	15	PHE	2.7
45	F8	89	ILE	2.7
30	29	74	PRO	2.7
47	D5	83	PRO	2.7
8	72	129	VAL	2.7
29	19	18	VAL	2.7
35	58	52	VAL	2.7
17	8I	44	ALA	2.7
46	C5	69	ALA	2.7
47	H8	21	ALA	2.7
17	8I	37	LYS	2.7
46	C5	81	LYS	2.7
9	82	34	ASN	2.7
10	1I	23	ILE	2.7
11	2A	108	ILE	2.7
20	BA	41	ILE	2.7
3	22	43	LEU	2.7
12	3A	84	LEU	2.7
20	BA	45	GLN	2.7
28	71	11	LEU	2.7
32	49	41	GLN	2.7
43	D8	39	LEU	2.7
53	J5	45	VAL	2.7
8	72	98	LYS	2.7
47	H8	131	ARG	2.7
52	M8	25	TYR	2.7
11	2A	95	ILE	2.7
7	62	9	VAL	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
49	J8	21	ARG	2.7
39	98	109	ALA	2.7
14	5I	8	GLU	2.7
38	45	105	GLU	2.7
47	D5	119	GLU	2.7
56	M5	9	GLY	2.7
16	7I	4	ILE	2.7
56	M5	58	ILE	2.7
51	H5	20	LYS	2.7
2	12	43	ASP	2.7
7	62	104	LEU	2.7
37	35	77	ARG	2.7
47	D5	76	LEU	2.7
11	2A	20	TYR	2.7
49	F5	69	LYS	2.7
51	H5	10	LYS	2.7
48	I8	82	ARG	2.7
3	2E	66	VAL	2.7
32	49	150	ASP	2.7
47	H8	105	VAL	2.7
3	22	100	ALA	2.7
43	95	27	ALA	2.7
8	72	86	ILE	2.7
11	2A	18	ARG	2.7
20	BA	84	LEU	2.7
32	41	135	LEU	2.7
32	49	107	LEU	2.7
39	98	114	VAL	2.7
51	H5	31	LEU	2.7
9	82	52	ALA	2.7
19	AA	38	SER	2.7
17	8A	91	ARG	2.7
11	2A	40	ILE	2.7
37	35	75	ILE	2.7
52	M8	43	TYR	2.7
6	5E	55	ASP	2.7
20	BA	104	LEU	2.7
32	49	161	THR	2.7
34	61	114	LEU	2.7
43	95	5	VAL	2.7
51	H5	4	LEU	2.7
8	7E	48	TYR	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
47	D5	57	ILE	2.6
28	71	21	THR	2.6
12	3A	94	PRO	2.6
19	AA	76	PRO	2.6
47	H8	25	PRO	2.6
32	49	136	ARG	2.6
7	62	26	PHE	2.6
11	2I	73	MET	2.6
33	59	136	ILE	2.6
33	59	167	GLU	2.6
34	61	77	LEU	2.6
35	58	61	ARG	2.6
34	69	83	ALA	2.6
40	65	19	LYS	2.6
37	78	114	ILE	2.6
20	BI	18	GLN	2.6
12	3A	89	ARG	2.6
36	25	58	VAL	2.6
16	7I	22	THR	2.6
44	E8	104	THR	2.6
12	3A	26	ALA	2.6
20	BI	87	LYS	2.6
20	BI	95	ALA	2.6
24	3K	65	C	2.6
33	59	92	ILE	2.6
38	45	64	ILE	2.6
41	B8	48	ILE	2.6
9	82	96	LEU	2.6
14	5A	21	TYR	2.6
20	BA	53	LEU	2.6
35	15	26	LEU	2.6
38	88	17	LEU	2.6
43	D8	25	LEU	2.6
43	95	73	SER	2.6
11	2I	47	VAL	2.6
12	3A	90	VAL	2.6
28	71	41	VAL	2.6
31	39	114	VAL	2.6
33	59	127	GLU	2.6
30	29	141	ILE	2.6
30	21	151	TYR	2.6
30	29	75	VAL	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
31	39	131	GLY	2.6
32	49	15	VAL	2.6
34	69	3	VAL	2.6
47	D5	27	VAL	2.6
12	3I	94	PRO	2.6
33	59	55	PRO	2.6
24	1L	2	G	2.6
33	59	41	MET	2.6
38	45	7	MET	2.6
49	F5	66	HIS	2.6
39	98	98	LEU	2.6
2	1E	15	VAL	2.6
17	8A	57	VAL	2.6
30	21	89	ASP	2.6
49	F5	2	SER	2.6
7	62	43	PHE	2.6
9	8E	101	PHE	2.6
17	8I	28	PRO	2.6
46	C5	92	ASN	2.6
16	7I	18	ARG	2.6
49	F5	21	ARG	2.6
22	1K	73	A	2.6
7	62	97	GLN	2.6
10	1A	50	ILE	2.6
37	35	124	LYS	2.6
47	D5	46	LYS	2.6
49	F5	7	ILE	2.6
7	6E	59	LEU	2.6
10	1I	71	LEU	2.6
32	49	94	LEU	2.6
33	59	161	GLY	2.6
40	65	24	LEU	2.6
40	65	49	VAL	2.6
47	D5	56	VAL	2.6
3	22	167	TRP	2.6
5	42	121	LYS	2.6
12	3A	48	PRO	2.6
35	58	74	ARG	2.6
50	G5	37	PHE	2.6
9	82	38	GLN	2.6
43	95	18	LEU	2.6
7	62	146	GLU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	29	34	VAL	2.6
38	88	27	VAL	2.6
47	H8	140	ASP	2.6
13	4A	97	PRO	2.6
2	1E	208	ILE	2.5
17	8A	43	LEU	2.5
24	3L	12	U	2.5
30	29	52	LEU	2.5
47	H8	125	LEU	2.5
47	D5	60	GLU	2.5
9	8E	127	LYS	2.5
30	29	116	VAL	2.5
38	88	102	VAL	2.5
11	2I	75	TYR	2.5
38	45	32	TYR	2.5
5	4E	45	PHE	2.5
10	1I	11	PHE	2.5
28	71	170	ALA	2.5
37	35	51	PHE	2.5
7	62	88	PRO	2.5
35	15	126	PRO	2.5
47	H8	158	PRO	2.5
31	39	172	TRP	2.5
7	62	30	ILE	2.5
11	2I	29	ILE	2.5
33	59	14	GLY	2.5
43	D8	40	LEU	2.5
51	H5	8	LEU	2.5
51	H5	23	LEU	2.5
52	M8	30	GLU	2.5
20	BI	56	MET	2.5
49	F5	10	LYS	2.5
2	12	193	ASP	2.5
3	2E	153	VAL	2.5
8	7E	137	VAL	2.5
34	69	21	VAL	2.5
26	14	2146	C	2.5
3	22	133	ALA	2.5
40	65	87	PHE	2.5
50	G5	45	SER	2.5
53	J5	2	ALA	2.5
7	62	74	GLU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
8	7E	47	GLY	2.5
36	25	19	ILE	2.5
51	H5	43	ILE	2.5
56	M5	21	LYS	2.5
35	15	116	LEU	2.5
2	12	101	MET	2.5
30	29	198	VAL	2.5
38	45	66	ILE	2.5
9	82	85	LEU	2.5
20	BA	13	LEU	2.5
34	69	72	LEU	2.5
41	75	99	LEU	2.5
42	85	25	TRP	2.5
35	15	130	HIS	2.5
33	59	160	LYS	2.5
40	65	33	LYS	2.5
47	D5	6	LYS	2.5
30	29	50	GLY	2.5
47	D5	79	ARG	2.5
34	69	4	ILE	2.5
4	3E	135	LEU	2.5
30	21	49	LEU	2.5
9	82	54	ASP	2.5
30	21	51	PHE	2.5
3	22	132	ARG	2.5
21	1B	9	ARG	2.5
36	25	33	ALA	2.5
38	88	32	TYR	2.5
44	E8	90	ARG	2.5
48	E5	76	GLY	2.5
12	3A	100	ILE	2.5
30	29	30	PRO	2.5
34	69	80	PRO	2.5
40	A8	35	ILE	2.5
47	H8	57	ILE	2.5
17	8A	31	LEU	2.5
31	31	196	LEU	2.5
12	3A	83	VAL	2.5
33	59	24	VAL	2.5
34	61	131	LYS	2.5
35	15	46	VAL	2.5
37	35	46	LYS	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
49	J8	69	LYS	2.5
14	5I	37	PHE	2.5
14	5A	61	TRP	2.5
11	2I	96	ARG	2.5
47	H8	97	GLU	2.5
14	5I	13	THR	2.5
16	7I	39	TYR	2.5
2	1E	201	ILE	2.5
3	22	154	SER	2.5
32	41	139	LEU	2.5
51	H5	13	ILE	2.5
10	1I	7	LYS	2.5
17	8I	10	VAL	2.5
47	H8	39	VAL	2.5
9	82	93	ARG	2.5
9	82	8	GLY	2.5
12	3A	35	GLY	2.5
33	59	102	ALA	2.5
36	25	11	ALA	2.5
54	O8	39	TYR	2.5
2	12	131	PRO	2.5
2	12	71	VAL	2.5
6	5E	88	VAL	2.5
20	BI	15	ARG	2.5
30	21	7	VAL	2.5
1	1G	1225	A	2.5
35	15	13	TRP	2.5
49	J8	42	GLN	2.5
47	H8	107	THR	2.5
48	E5	75	LEU	2.5
30	29	1	MET	2.4
14	5A	4	LYS	2.4
36	68	53	LYS	2.4
20	BI	42	GLN	2.4
3	2E	196	LEU	2.4
31	39	9	ILE	2.4
32	41	164	GLU	2.4
41	B8	114	LEU	2.4
48	E5	21	LEU	2.4
47	H8	95	PRO	2.4
47	D5	52	SER	2.4
48	E5	9	SER	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	2E	72	LYS	2.4
8	7E	44	PHE	2.4
8	72	61	VAL	2.4
9	82	108	VAL	2.4
12	3I	11	VAL	2.4
22	1K	71	C	2.4
26	14	2794	C	2.4
34	69	19	VAL	2.4
39	98	48	VAL	2.4
56	M5	14	VAL	2.4
7	6E	5	ARG	2.4
14	5I	29	ARG	2.4
32	49	63	ILE	2.4
37	35	111	ARG	2.4
7	6E	136	LYS	2.4
11	2A	70	LYS	2.4
53	J5	10	LYS	2.4
4	3E	110	PHE	2.4
17	8A	19	VAL	2.4
35	58	51	PHE	2.4
35	15	53	VAL	2.4
31	31	133	ASN	2.4
7	62	32	ARG	2.4
34	69	36	ALA	2.4
42	C8	4	ALA	2.4
31	39	148	LEU	2.4
37	78	138	LEU	2.4
7	62	17	VAL	2.4
38	45	106	VAL	2.4
47	H8	90	VAL	2.4
11	2I	49	GLY	2.4
51	H5	29	ARG	2.4
10	1I	97	GLU	2.4
43	95	3	ALA	2.4
20	BA	48	LYS	2.4
33	59	140	LYS	2.4
11	2A	66	LEU	2.4
43	95	20	LEU	2.4
11	2A	31	THR	2.4
24	1L	23	A	2.4
7	62	91	VAL	2.4
17	8A	85	VAL	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
8	7E	64	LYS	2.4
49	F5	92	LYS	2.4
51	H5	7	LYS	2.4
54	O8	17	LYS	2.4
54	O8	35	GLU	2.4
51	H5	21	ALA	2.4
8	7E	45	ILE	2.4
10	1I	8	LEU	2.4
17	8I	59	ILE	2.4
30	29	195	LEU	2.4
44	A5	103	ILE	2.4
47	H8	59	LEU	2.4
7	62	118	VAL	2.4
11	2A	28	THR	2.4
14	5I	51	GLY	2.4
15	6A	88	ARG	2.4
32	49	141	PHE	2.4
39	55	21	TYR	2.4
47	H8	167	PRO	2.4
11	2A	42	TRP	2.4
33	59	91	GLY	2.4
36	25	41	ALA	2.4
2	12	185	ILE	2.4
3	2E	101	LEU	2.4
36	25	25	LEU	2.4
41	75	48	ILE	2.4
43	D8	35	LEU	2.4
1	1G	973	G	2.4
4	32	166	LYS	2.4
38	45	98	LYS	2.4
51	H5	35	ARG	2.4
9	82	26	VAL	2.4
40	A8	45	GLY	2.4
47	D5	147	GLY	2.4
17	8A	82	MET	2.4
4	3E	21	LEU	2.4
8	7E	107	LEU	2.4
29	19	270	ILE	2.4
31	31	181	LEU	2.4
47	H8	41	LEU	2.4
38	45	10	ARG	2.4
30	29	96	PHE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	61	126	TYR	2.4
34	69	144	VAL	2.4
10	1A	67	THR	2.4
30	21	90	THR	2.4
47	D5	107	THR	2.4
2	12	97	TRP	2.4
9	82	46	ALA	2.4
38	88	28	ALA	2.4
7	62	22	LEU	2.4
9	8E	128	ARG	2.4
9	82	56	LEU	2.4
11	2A	96	ARG	2.4
16	7I	8	ARG	2.4
32	41	94	LEU	2.4
35	15	91	LEU	2.4
3	2E	166	GLU	2.3
48	I8	69	PHE	2.3
47	H8	128	VAL	2.3
9	82	7	THR	2.3
37	78	1	MET	2.3
4	3E	111	ALA	2.3
9	82	71	SER	2.3
13	4I	102	ARG	2.3
46	C5	87	LYS	2.3
11	2A	48	ILE	2.3
13	4A	25	ILE	2.3
31	31	41	LEU	2.3
39	55	4	LEU	2.3
46	G8	92	ASN	2.3
13	4A	73	GLU	2.3
17	8I	29	HIS	2.3
8	7E	53	VAL	2.3
13	4I	87	TYR	2.3
32	49	146	TYR	2.3
41	75	35	LYS	2.3
53	J5	28	PRO	2.3
37	35	15	ARG	2.3
7	62	2	ALA	2.3
2	12	118	LEU	2.3
3	22	152	ILE	2.3
12	3I	27	LEU	2.3
14	5I	44	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
29	11	165	ILE	2.3
33	51	171	LEU	2.3
40	65	48	LEU	2.3
40	65	82	ILE	2.3
26	1H	2062	A	2.3
49	F5	60	PHE	2.3
26	14	277	C	2.3
43	95	46	VAL	2.3
52	M8	33	VAL	2.3
33	59	163	TYR	2.3
7	6E	144	MET	2.3
8	7E	22	GLU	2.3
8	7E	35	ILE	2.3
10	1I	38	ILE	2.3
40	A8	43	GLU	2.3
49	J8	90	ILE	2.3
3	22	20	SER	2.3
9	82	111	ARG	2.3
12	3A	99	HIS	2.3
13	4A	80	ARG	2.3
28	71	58	VAL	2.3
36	25	121	VAL	2.3
47	H8	82	ARG	2.3
47	D5	32	HIS	2.3
7	6E	73	MET	2.3
39	98	94	TYR	2.3
15	6I	56	LEU	2.3
16	7A	33	ILE	2.3
37	35	138	LEU	2.3
49	J8	82	LEU	2.3
20	BA	14	LYS	2.3
46	C5	4	LYS	2.3
49	F5	32	LYS	2.3
12	3I	62	SER	2.3
39	98	32	GLY	2.3
38	88	106	VAL	2.3
40	A8	85	VAL	2.3
1	13	344	A	2.3
24	3K	23	A	2.3
24	3K	32	C	2.3
7	62	31	MET	2.3
2	12	187	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	6E	22	LEU	2.3
54	O8	27	LYS	2.3
46	C5	75	ILE	2.3
8	72	131	GLY	2.3
10	1A	52	GLY	2.3
20	BA	83	ARG	2.3
45	B5	28	PHE	2.3
11	2I	81	ASP	2.3
17	8A	51	TYR	2.3
49	F5	71	TYR	2.3
4	3E	23	GLY	2.3
7	6E	143	ARG	2.3
9	82	74	ILE	2.3
13	4A	100	GLY	2.3
20	BI	101	GLY	2.3
39	98	33	ARG	2.3
37	78	130	PHE	2.3
32	49	108	ASN	2.3
7	6E	87	VAL	2.3
12	3A	66	VAL	2.3
40	A8	46	VAL	2.3
32	41	35	GLU	2.3
46	C5	28	LYS	2.3
48	I8	68	GLU	2.3
47	D5	148	ASP	2.3
2	1E	196	LEU	2.3
4	32	176	LEU	2.3
32	49	83	ARG	2.3
3	22	124	ILE	2.3
11	2I	83	ILE	2.3
35	15	75	TYR	2.3
7	6E	26	PHE	2.3
32	49	80	PHE	2.3
2	1E	165	VAL	2.3
43	95	15	GLU	2.3
2	12	26	PRO	2.3
8	7E	119	LEU	2.3
32	41	7	LEU	2.3
33	59	108	GLY	2.3
45	B5	46	ALA	2.3
4	3E	138	TYR	2.3
8	72	111	ILE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
22	1K	75	C	2.3
41	75	102	ILE	2.3
26	1H	2790	A	2.3
35	58	84	LYS	2.3
37	35	64	LYS	2.3
3	22	15	THR	2.2
14	5I	25	VAL	2.2
31	39	126	VAL	2.2
37	35	95	VAL	2.2
37	35	126	VAL	2.2
33	59	84	SER	2.2
34	61	113	ARG	2.2
7	62	70	LYS	2.2
8	7E	130	GLY	2.2
28	71	185	LEU	2.2
40	A8	105	ALA	2.2
32	49	11	TYR	2.2
9	82	35	GLU	2.2
3	22	59	ARG	2.2
32	49	95	ARG	2.2
36	25	17	ARG	2.2
37	78	79	ARG	2.2
24	1L	24	G	2.2
29	19	4	LYS	2.2
5	42	31	LEU	2.2
9	82	80	GLY	2.2
9	82	94	ALA	2.2
15	6I	70	LEU	2.2
33	59	117	PRO	2.2
34	61	140	LEU	2.2
39	98	75	LEU	2.2
39	55	29	LEU	2.2
44	E8	93	ALA	2.2
47	D5	55	HIS	2.2
7	6E	103	TRP	2.2
38	45	69	PHE	2.2
50	G5	41	ILE	2.2
9	82	125	TYR	2.2
26	1H	654(Q)	C	2.2
3	2E	198	VAL	2.2
4	32	178	VAL	2.2
32	49	5	VAL	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	49	37	VAL	2.2
36	68	66	LYS	2.2
44	A5	98	LYS	2.2
10	1I	85	LEU	2.2
33	59	166	GLY	2.2
40	A8	80	LEU	2.2
5	42	81	GLU	2.2
43	D8	4	ILE	2.2
5	4E	24	ARG	2.2
9	82	51	ARG	2.2
17	8I	92	ARG	2.2
24	1L	65	C	2.2
52	M8	21	VAL	2.2
31	39	147	GLY	2.2
3	2E	65	ALA	2.2
7	6E	134	ALA	2.2
20	BA	16	HIS	2.2
20	BA	40	ALA	2.2
47	H8	7	ALA	2.2
49	J8	94	LEU	2.2
32	49	102	PHE	2.2
1	1G	1031	G	2.2
11	2A	85	ARG	2.2
26	14	1509	C	2.2
32	41	54	GLU	2.2
39	98	102	GLU	2.2
54	O8	51	GLU	2.2
3	22	131	ARG	2.2
7	6E	62	PHE	2.2
8	72	101	PRO	2.2
10	1I	47	PHE	2.2
11	2A	89	ALA	2.2
19	AA	4	SER	2.2
47	D5	149	SER	2.2
56	M5	62	LEU	2.2
12	3A	13	LYS	2.2
28	71	193	ILE	2.2
30	29	149	ARG	2.2
32	41	142	PRO	2.2
32	41	178	PHE	2.2
37	78	124	LYS	2.2
38	45	68	ILE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	42	133	TYR	2.2
43	95	81	TYR	2.2
45	B5	29	TRP	2.2
47	H8	86	VAL	2.2
2	1E	94	ASN	2.2
7	62	148	ASN	2.2
8	72	119	LEU	2.2
20	BI	91	LEU	2.2
5	4E	89	ILE	2.2
9	82	76	ALA	2.2
19	AI	75	ALA	2.2
20	BI	38	LYS	2.2
46	G8	94	LYS	2.2
56	M5	5	LYS	2.2
47	D5	92	SER	2.2
26	14	2801	A	2.2
33	51	61	HIS	2.2
35	58	11	PRO	2.2
19	AA	11	VAL	2.2
31	39	6	VAL	2.2
36	25	32	TYR	2.2
47	H8	58	VAL	2.2
7	62	130	GLY	2.2
8	72	84	ARG	2.2
45	B5	86	GLY	2.2
47	H8	72	ARG	2.2
53	J5	54	GLY	2.2
54	O8	28	ARG	2.2
4	3E	176	LEU	2.2
9	82	47	LEU	2.2
28	71	196	LEU	2.2
56	M5	10	ALA	2.2
37	35	35	HIS	2.2
46	C5	57	GLN	2.2
24	1L	73	A	2.2
3	22	26	LYS	2.2
4	32	68	TYR	2.2
16	7I	51	VAL	2.2
17	8A	42	TYR	2.2
32	49	25	TYR	2.2
35	58	54	VAL	2.2
44	A5	38	TYR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	6E	32	ARG	2.2
45	B5	33	LYS	2.2
31	31	131	GLY	2.2
38	45	19	GLY	2.2
24	3K	33	U	2.2
26	14	274	G	2.2
34	61	68	LEU	2.2
39	55	65	LEU	2.2
43	95	39	LEU	2.2
10	1I	74	ILE	2.2
40	65	37	ALA	2.2
46	G8	100	ALA	2.2
17	8I	91	ARG	2.2
37	35	65	ARG	2.2
54	O8	45	LYS	2.2
11	2I	59	TYR	2.2
25	4K	15	A	2.2
49	J8	62	VAL	2.2
43	95	75	PHE	2.1
44	E8	69	LEU	2.1
4	3E	158	ILE	2.1
10	1I	50	ILE	2.1
19	AA	55	LYS	2.1
3	22	89	GLU	2.1
13	4A	91	ARG	2.1
48	E5	55	ARG	2.1
35	58	46	VAL	2.1
35	58	53	VAL	2.1
3	22	33	LEU	2.1
3	22	196	LEU	2.1
4	3E	162	LEU	2.1
4	32	97	LEU	2.1
30	21	52	LEU	2.1
44	E8	86	LEU	2.1
45	B5	21	PHE	2.1
6	5E	8	ILE	2.1
8	7E	111	ILE	2.1
11	2I	69	ALA	2.1
19	AA	75	ALA	2.1
20	BI	54	LYS	2.1
1	1G	1030	C	2.1
3	2E	21	ARG	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
15	6I	63	ARG	2.1
32	49	118	ARG	2.1
7	6E	88	PRO	2.1
51	H5	12	PRO	2.1
56	M5	4	MET	2.1
3	22	93	LYS	2.1
4	32	19	LEU	2.1
31	39	12	LEU	2.1
43	95	74	LYS	2.1
47	D5	82	ARG	2.1
11	2I	80	VAL	2.1
36	68	98	VAL	2.1
47	H8	121	HIS	2.1
47	D5	66	SER	2.1
51	L8	59	VAL	2.1
55	L5	46	VAL	2.1
32	49	105	LYS	2.1
15	6A	31	LEU	2.1
32	41	82	LEU	2.1
47	D5	38	TYR	2.1
12	3A	7	ILE	2.1
13	4A	84	ILE	2.1
20	BI	90	GLN	2.1
20	BA	15	ARG	2.1
45	B5	8	ILE	2.1
51	H5	32	GLN	2.1
52	M8	23	GLU	2.1
5	42	66	MET	2.1
8	7E	93	VAL	2.1
34	61	144	VAL	2.1
3	2E	128	PHE	2.1
41	B8	105	LEU	2.1
42	C8	83	LEU	2.1
42	85	74	LEU	2.1
9	82	87	GLN	2.1
28	71	173	ALA	2.1
49	F5	18	ILE	2.1
7	6E	131	LYS	2.1
30	21	32	PRO	2.1
33	59	82	GLY	2.1
37	35	22	GLY	2.1
47	H8	108	PRO	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	22	76	VAL	2.1
10	1I	19	SER	2.1
11	2A	54	ARG	2.1
17	8A	38	ARG	2.1
30	29	135	HIS	2.1
3	2E	90	GLU	2.1
5	42	45	PHE	2.1
5	42	119	LEU	2.1
17	8I	42	TYR	2.1
19	AA	77	THR	2.1
30	29	40	GLU	2.1
44	E8	109	GLU	2.1
47	D5	154	ASP	2.1
5	42	62	ALA	2.1
31	39	146	ALA	2.1
26	1H	2793	G	2.1
35	58	83	LYS	2.1
10	1I	66	ARG	2.1
11	2A	109	VAL	2.1
32	41	72	ARG	2.1
43	D8	5	VAL	2.1
43	D8	46	VAL	2.1
47	H8	126	VAL	2.1
48	E5	39	ARG	2.1
4	3E	24	GLU	2.1
7	6E	139	GLU	2.1
20	BI	16	HIS	2.1
26	14	2139	C	2.1
47	D5	11	GLU	2.1
35	15	15	LEU	2.1
40	65	73	LEU	2.1
48	E5	59	LEU	2.1
19	AI	79	THR	2.1
30	29	2	LYS	2.1
36	25	53	LYS	2.1
38	45	93	TYR	2.1
9	82	55	ALA	2.1
18	9I	20	ALA	2.1
26	14	1026	U	2.1
3	22	88	ARG	2.1
8	7E	9	MET	2.1
8	7E	37	ARG	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
47	D5	80	ARG	2.1
42	C8	90	VAL	2.1
16	7I	27	LYS	2.1
7	62	13	GLN	2.1
16	7I	59	TRP	2.1
40	A8	73	LEU	2.1
40	65	110	LEU	2.1
8	7E	65	TYR	2.1
11	2I	36	ASP	2.1
3	2E	100	ALA	2.1
7	6E	54	THR	2.1
28	7I	25	ALA	2.1
33	59	121	ILE	2.1
13	4A	99	ARG	2.1
29	11	210	GLY	2.1
44	E8	68	ARG	2.1
47	D5	115	GLY	2.1
43	95	47	VAL	2.1
44	A5	17	VAL	2.1
47	D5	178	GLU	2.1
20	BI	58	LYS	2.1
20	BA	98	PRO	2.1
33	51	39	PRO	2.1
2	12	105	PHE	2.1
36	25	99	PHE	2.1
3	22	22	TRP	2.0
3	2E	61	ALA	2.0
12	3I	15	ARG	2.0
21	1B	15	ARG	2.0
31	31	9	ILE	2.0
32	41	46	ALA	2.0
34	61	88	ILE	2.0
8	7E	135	CYS	2.0
9	8E	8	GLY	2.0
17	8I	8	GLY	2.0
17	8I	33	GLY	2.0
26	14	2506	U	2.0
35	58	75	TYR	2.0
40	A8	72	ALA	2.0
47	D5	20	ARG	2.0
47	H8	22	GLY	2.0
47	D5	145	GLU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
10	1I	37	PRO	2.0
16	7I	20	VAL	2.0
21	1B	23	PRO	2.0
28	7I	165	ASN	2.0
30	29	54	GLN	2.0
51	L8	23	LEU	2.0
1	1G	1061	G	2.0
1	1G	1535	C	2.0
4	32	49	ARG	2.0
12	3A	70	ILE	2.0
4	32	16	GLY	2.0
20	BI	96	GLY	2.0
36	25	43	VAL	2.0
40	65	85	VAL	2.0
35	15	44	PRO	2.0
38	88	99	PRO	2.0
55	P8	1	MET	2.0
47	H8	136	PHE	2.0
9	82	121	ARG	2.0
13	4A	108	ARG	2.0
11	2I	16	SER	2.0
16	7I	31	LYS	2.0
34	61	79	ILE	2.0
46	G8	96	ILE	2.0
49	F5	37	ILE	2.0
34	61	83	ALA	2.0
26	14	1536	A	2.0
13	4A	105	THR	2.0
2	1E	71	VAL	2.0
7	6E	141	VAL	2.0
20	BI	85	MET	2.0
51	H5	47	VAL	2.0
28	7I	8	ARG	2.0
30	29	53	PRO	2.0
31	39	192	LEU	2.0
35	58	116	LEU	2.0
39	98	10	LEU	2.0
3	2E	26	LYS	2.0
11	2A	92	GLU	2.0
12	3I	29	GLY	2.0
30	29	134	ILE	2.0
38	45	38	GLU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
39	55	6	SER	2.0
5	42	105	VAL	2.0
11	2A	30	VAL	2.0
25	4K	14	A	2.0
20	BI	86	ARG	2.0
31	31	72	ARG	2.0
37	35	50	ARG	2.0
17	8A	30	PRO	2.0
18	9A	44	LEU	2.0
33	59	112	PRO	2.0
33	59	138	LYS	2.0
43	D8	44	LYS	2.0
47	H8	24	LEU	2.0
47	D5	177	PRO	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, 95th 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 ²)	Q<0.9
22	PSU	1K	55	20/21	0.87	0.16	107,127,140,145	0
23	4SU	2L	8	20/21	0.88	0.16	107,118,124,125	0
23	OMC	2L	33	21/22	0.90	0.19	94,103,107,109	0
23	PSU	2L	56	20/21	0.91	0.10	109,121,126,126	0
23	7MG	2L	47	24/25	0.92	0.14	118,128,137,141	0
22	5MU	1K	54	21/22	0.92	0.16	104,125,133,143	0
23	PSU	2K	56	20/21	0.92	0.12	91,101,110,117	0
22	PSU	1K	39	20/21	0.93	0.21	94,112,118,120	0
23	7MG	2K	47	24/25	0.94	0.15	96,101,113,116	0
22	T6A	1K	37	32/33	0.94	0.20	81,92,114,116	0
23	4SU	2K	8	20/21	0.94	0.17	89,95,101,103	0
23	5MU	2L	55	21/22	0.94	0.14	115,122,127,130	0
23	5MU	2K	55	21/22	0.95	0.14	98,105,112,114	0
22	U8U	1K	34	23/24	0.96	0.17	83,98,108,110	0
23	OMC	2K	33	21/22	0.96	0.21	73,79,82,94	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, 95th 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 ²)	Q<0.9
57	MG	13	1678	1/1	0.02	0.16	112,112,112,112	0
57	MG	1H	3445	1/1	0.18	0.12	92,92,92,92	0
57	MG	1H	3081	1/1	0.19	0.45	83,83,83,83	0
57	MG	13	1704	1/1	0.32	0.13	106,106,106,106	0
57	MG	14	3393	1/1	0.32	0.08	165,165,165,165	0
57	MG	1H	3180	1/1	0.34	0.42	90,90,90,90	0
57	MG	1G	1673	1/1	0.34	0.14	115,115,115,115	0
57	MG	14	3350	1/1	0.39	0.16	101,101,101,101	0
57	MG	14	3115	1/1	0.40	0.78	87,87,87,87	0
57	MG	14	3377	1/1	0.47	0.10	131,131,131,131	0
57	MG	1H	3113	1/1	0.48	0.26	81,81,81,81	0
57	MG	1G	1609	1/1	0.50	0.87	92,92,92,92	0
57	MG	14	3163	1/1	0.51	0.38	93,93,93,93	0
57	MG	14	3422	1/1	0.52	0.24	108,108,108,108	0
57	MG	1H	3154	1/1	0.53	0.23	58,58,58,58	0
57	MG	1H	3157	1/1	0.54	0.38	89,89,89,89	0
57	MG	13	1709	1/1	0.54	0.26	99,99,99,99	0
57	MG	1H	3454	1/1	0.54	0.07	111,111,111,111	0
57	MG	1H	3520	1/1	0.54	0.10	105,105,105,105	0
57	MG	1G	1642	1/1	0.55	0.28	99,99,99,99	0
57	MG	14	3355	1/1	0.56	0.10	104,104,104,104	0
57	MG	1H	3145	1/1	0.56	0.53	80,80,80,80	0
57	MG	14	3127	1/1	0.56	1.02	87,87,87,87	0
57	MG	1G	1686	1/1	0.57	0.13	106,106,106,106	0
57	MG	13	1679	1/1	0.57	0.30	99,99,99,99	0
57	MG	1H	3237	1/1	0.57	0.46	81,81,81,81	0
57	MG	1G	1678	1/1	0.58	0.11	111,111,111,111	0
57	MG	14	3154	1/1	0.58	0.40	95,95,95,95	0
57	MG	1H	3050	1/1	0.59	0.38	72,72,72,72	0
57	MG	1H	3007	1/1	0.59	0.31	81,81,81,81	0
57	MG	13	1643	1/1	0.59	0.23	101,101,101,101	0
57	MG	1H	3141	1/1	0.59	0.29	83,83,83,83	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	13	1739	1/1	0.59	0.06	121,121,121,121	0
57	MG	1H	3120	1/1	0.60	0.18	88,88,88,88	0
57	MG	14	3008	1/1	0.60	0.21	77,77,77,77	0
57	MG	1H	3230	1/1	0.60	0.36	82,82,82,82	0
57	MG	E5	101	1/1	0.60	0.58	89,89,89,89	0
57	MG	14	3208	1/1	0.61	0.95	88,88,88,88	0
57	MG	1H	3339	1/1	0.61	0.12	106,106,106,106	0
57	MG	1H	3150	1/1	0.61	0.70	98,98,98,98	0
57	MG	14	3132	1/1	0.61	0.44	82,82,82,82	0
57	MG	14	3430	1/1	0.61	0.19	107,107,107,107	0
57	MG	1H	3205	1/1	0.62	0.60	79,79,79,79	0
57	MG	1H	3500	1/1	0.62	0.14	94,94,94,94	0
57	MG	14	3384	1/1	0.63	0.14	78,78,78,78	0
57	MG	14	3433	1/1	0.64	0.26	114,114,114,114	0
57	MG	13	1685	1/1	0.64	0.16	90,90,90,90	0
57	MG	1H	3442	1/1	0.64	0.09	103,103,103,103	0
57	MG	14	3347	1/1	0.64	0.10	88,88,88,88	0
57	MG	13	1738	1/1	0.64	0.10	133,133,133,133	0
57	MG	14	3114	1/1	0.64	0.22	70,70,70,70	0
57	MG	1H	3503	1/1	0.64	0.12	91,91,91,91	0
57	MG	14	3332	1/1	0.65	0.09	102,102,102,102	0
57	MG	14	3064	1/1	0.65	0.48	63,63,63,63	0
57	MG	14	3376	1/1	0.65	0.23	102,102,102,102	0
57	MG	1H	3451	1/1	0.65	0.08	102,102,102,102	0
57	MG	14	3426	1/1	0.65	0.16	104,104,104,104	0
57	MG	C5	201	1/1	0.65	0.10	113,113,113,113	0
57	MG	1J	208	1/1	0.65	0.10	103,103,103,103	0
57	MG	14	3166	1/1	0.65	0.46	79,79,79,79	0
57	MG	14	3266	1/1	0.65	0.08	107,107,107,107	0
57	MG	13	1671	1/1	0.66	0.51	79,79,79,79	0
57	MG	14	3135	1/1	0.66	0.32	79,79,79,79	0
57	MG	1H	3211	1/1	0.66	0.46	78,78,78,78	0
57	MG	14	3152	1/1	0.66	0.17	78,78,78,78	0
57	MG	14	3344	1/1	0.66	0.09	93,93,93,93	0
57	MG	14	3434	1/1	0.66	0.12	110,110,110,110	0
57	MG	1H	3079	1/1	0.66	0.34	63,63,63,63	0
57	MG	1H	3388	1/1	0.66	0.13	55,55,55,55	0
57	MG	13	1723	1/1	0.66	0.07	128,128,128,128	0
57	MG	1H	3204	1/1	0.66	0.20	91,91,91,91	0
57	MG	14	3395	1/1	0.67	0.10	118,118,118,118	0
57	MG	14	3122	1/1	0.67	0.37	75,75,75,75	0
57	MG	14	3387	1/1	0.67	0.14	83,83,83,83	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	14	3176	1/1	0.67	0.20	82,82,82,82	0
57	MG	1H	3496	1/1	0.67	0.16	89,89,89,89	0
57	MG	1H	3004	1/1	0.67	0.51	89,89,89,89	0
57	MG	1H	3423	1/1	0.67	0.18	84,84,84,84	0
57	MG	14	3429	1/1	0.67	0.30	95,95,95,95	0
57	MG	1H	3487	1/1	0.68	0.11	85,85,85,85	0
57	MG	14	3017	1/1	0.68	0.34	119,119,119,119	0
57	MG	1H	3499	1/1	0.68	0.09	112,112,112,112	0
57	MG	1H	3511	1/1	0.68	0.16	101,101,101,101	0
57	MG	1H	3234	1/1	0.68	0.20	79,79,79,79	0
57	MG	13	1729	1/1	0.68	0.11	110,110,110,110	0
57	MG	14	3277	1/1	0.68	0.16	84,84,84,84	0
57	MG	35	201	1/1	0.69	0.22	75,75,75,75	0
57	MG	1H	3085	1/1	0.69	0.28	70,70,70,70	0
57	MG	31	301	1/1	0.69	0.13	63,63,63,63	0
57	MG	14	3407	1/1	0.69	0.12	123,123,123,123	0
57	MG	13	1673	1/1	0.69	0.40	84,84,84,84	0
57	MG	13	1662	1/1	0.69	0.50	89,89,89,89	0
57	MG	1H	3422	1/1	0.69	0.33	65,65,65,65	0
57	MG	1H	3065	1/1	0.69	0.53	65,65,65,65	0
57	MG	1H	3216	1/1	0.69	0.27	82,82,82,82	0
57	MG	1H	3428	1/1	0.70	0.09	89,89,89,89	0
57	MG	1H	3130	1/1	0.70	0.47	63,63,63,63	0
57	MG	14	3385	1/1	0.70	0.16	67,67,67,67	0
57	MG	16	208	1/1	0.70	0.39	85,85,85,85	0
57	MG	14	3212	1/1	0.70	0.32	75,75,75,75	0
57	MG	14	3173	1/1	0.70	0.45	79,79,79,79	0
57	MG	13	1668	1/1	0.70	0.29	66,66,66,66	0
57	MG	4I	200	1/1	0.70	0.23	95,95,95,95	0
57	MG	14	3435	1/1	0.70	0.20	92,92,92,92	0
57	MG	1H	3177	1/1	0.70	0.90	82,82,82,82	0
57	MG	1H	3419	1/1	0.70	0.15	86,86,86,86	0
57	MG	14	3109	1/1	0.71	0.43	67,67,67,67	0
57	MG	14	3264	1/1	0.71	0.14	93,93,93,93	0
57	MG	14	3207	1/1	0.71	0.37	70,70,70,70	0
57	MG	14	3164	1/1	0.71	0.33	78,78,78,78	0
57	MG	1H	3135	1/1	0.71	0.49	79,79,79,79	0
57	MG	1G	1635	1/1	0.71	0.20	105,105,105,105	0
57	MG	14	3138	1/1	0.71	0.67	78,78,78,78	0
57	MG	14	3161	1/1	0.71	0.41	78,78,78,78	0
57	MG	14	3330	1/1	0.71	0.14	94,94,94,94	0
57	MG	14	3110	1/1	0.71	0.24	69,69,69,69	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1G	1671	1/1	0.72	0.17	112,112,112,112	0
57	MG	1H	3168	1/1	0.72	0.49	80,80,80,80	0
57	MG	14	3291	1/1	0.72	0.21	85,85,85,85	0
57	MG	14	3252	1/1	0.72	0.18	90,90,90,90	0
57	MG	14	3409	1/1	0.72	0.22	88,88,88,88	0
57	MG	1H	3227	1/1	0.72	0.28	72,72,72,72	0
57	MG	1H	3225	1/1	0.72	0.43	71,71,71,71	0
57	MG	1H	3006	1/1	0.72	0.28	74,74,74,74	0
57	MG	1H	3195	1/1	0.72	0.31	55,55,55,55	0
57	MG	1G	1682	1/1	0.72	0.05	123,123,123,123	0
57	MG	14	3366	1/1	0.73	0.23	82,82,82,82	0
57	MG	13	1737	1/1	0.73	0.11	99,99,99,99	0
57	MG	1H	3075	1/1	0.73	0.29	76,76,76,76	0
57	MG	1H	3172	1/1	0.73	0.30	83,83,83,83	0
57	MG	1H	3171	1/1	0.73	0.38	73,73,73,73	0
57	MG	13	1669	1/1	0.73	0.53	95,95,95,95	0
57	MG	14	3417	1/1	0.73	0.12	108,108,108,108	0
57	MG	14	3406	1/1	0.73	0.12	101,101,101,101	0
57	MG	14	3181	1/1	0.73	0.30	75,75,75,75	0
57	MG	16	205	1/1	0.73	0.18	69,69,69,69	0
57	MG	14	3185	1/1	0.73	0.41	86,86,86,86	0
57	MG	14	3023	1/1	0.73	0.27	76,76,76,76	0
57	MG	7A	101	1/1	0.73	0.26	114,114,114,114	0
57	MG	1H	3458	1/1	0.73	0.10	82,82,82,82	0
57	MG	1H	3267	1/1	0.73	0.10	56,56,56,56	0
57	MG	14	3151	1/1	0.74	0.29	70,70,70,70	0
57	MG	1H	3396	1/1	0.74	0.22	59,59,59,59	0
57	MG	1G	1644	1/1	0.74	0.20	106,106,106,106	0
57	MG	1H	3444	1/1	0.74	0.11	74,74,74,74	0
57	MG	14	3211	1/1	0.74	0.09	81,81,81,81	0
57	MG	1G	1668	1/1	0.74	0.09	124,124,124,124	0
57	MG	14	3118	1/1	0.74	0.44	61,61,61,61	0
57	MG	13	1714	1/1	0.74	0.09	122,122,122,122	0
57	MG	13	1660	1/1	0.74	0.23	88,88,88,88	0
57	MG	13	1674	1/1	0.74	0.36	92,92,92,92	0
57	MG	13	1637	1/1	0.74	0.32	74,74,74,74	0
57	MG	14	3073	1/1	0.74	0.31	78,78,78,78	0
57	MG	1H	3476	1/1	0.74	0.21	82,82,82,82	0
57	MG	4L	101	1/1	0.74	0.32	131,131,131,131	0
57	MG	1H	3226	1/1	0.74	0.31	71,71,71,71	0
57	MG	14	3128	1/1	0.74	0.41	89,89,89,89	0
57	MG	P8	101	1/1	0.74	0.56	71,71,71,71	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	16	203	1/1	0.75	0.21	82,82,82,82	0
57	MG	1H	3395	1/1	0.75	0.14	68,68,68,68	0
61	SPE	14	3436	13/13	0.75	0.25	83,88,93,94	0
57	MG	1H	3217	1/1	0.75	0.64	82,82,82,82	0
57	MG	1H	3522	1/1	0.75	0.14	110,110,110,110	0
57	MG	1H	3415	1/1	0.75	0.14	72,72,72,72	0
57	MG	1H	3118	1/1	0.75	0.15	69,69,69,69	0
57	MG	1G	1699	1/1	0.75	0.07	133,133,133,133	0
57	MG	1H	3063	1/1	0.75	0.27	100,100,100,100	0
57	MG	1H	3243	1/1	0.76	0.17	82,82,82,82	0
57	MG	14	3100	1/1	0.76	0.27	71,71,71,71	0
57	MG	1H	3196	1/1	0.76	0.38	77,77,77,77	0
57	MG	14	3432	1/1	0.76	0.13	116,116,116,116	0
57	MG	14	3080	1/1	0.76	0.25	68,68,68,68	0
57	MG	14	3103	1/1	0.76	0.43	96,96,96,96	0
57	MG	1H	3053	1/1	0.76	0.46	75,75,75,75	0
57	MG	1H	3479	1/1	0.76	0.10	83,83,83,83	0
57	MG	1G	1675	1/1	0.76	0.08	103,103,103,103	0
57	MG	14	3398	1/1	0.76	0.13	76,76,76,76	0
57	MG	1G	1618	1/1	0.76	0.69	78,78,78,78	0
57	MG	14	3098	1/1	0.76	0.35	77,77,77,77	0
57	MG	1H	3374	1/1	0.76	0.11	83,83,83,83	0
57	MG	13	1727	1/1	0.76	0.13	90,90,90,90	0
57	MG	1H	3414	1/1	0.76	0.14	105,105,105,105	0
57	MG	14	3197	1/1	0.76	0.61	77,77,77,77	0
57	MG	1H	3516	1/1	0.77	0.14	102,102,102,102	0
57	MG	1H	3352	1/1	0.77	0.12	57,57,57,57	0
57	MG	14	3379	1/1	0.77	0.14	84,84,84,84	0
57	MG	1H	3488	1/1	0.77	0.28	105,105,105,105	0
57	MG	13	1706	1/1	0.77	0.08	117,117,117,117	0
57	MG	1H	3363	1/1	0.77	0.12	96,96,96,96	0
57	MG	1H	3203	1/1	0.77	0.24	74,74,74,74	0
57	MG	14	3258	1/1	0.77	0.07	79,79,79,79	0
57	MG	14	3274	1/1	0.77	0.05	85,85,85,85	0
57	MG	14	3060	1/1	0.77	0.30	98,98,98,98	0
57	MG	14	3156	1/1	0.77	0.17	87,87,87,87	0
57	MG	13	1676	1/1	0.77	0.47	93,93,93,93	0
57	MG	1H	3277	1/1	0.77	0.16	71,71,71,71	0
57	MG	14	3428	1/1	0.77	0.29	119,119,119,119	0
57	MG	1H	3389	1/1	0.77	0.14	88,88,88,88	0
57	MG	1H	3123	1/1	0.77	0.37	65,65,65,65	0
57	MG	1H	3153	1/1	0.77	0.44	77,77,77,77	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1H	3003	1/1	0.77	0.37	65,65,65,65	0
57	MG	14	3067	1/1	0.78	0.23	78,78,78,78	0
57	MG	14	3326	1/1	0.78	0.09	77,77,77,77	0
57	MG	1H	3105	1/1	0.78	0.23	72,72,72,72	0
57	MG	1H	3129	1/1	0.78	0.20	76,76,76,76	0
57	MG	14	3348	1/1	0.78	0.11	96,96,96,96	0
57	MG	1H	3089	1/1	0.78	0.20	38,38,38,38	0
57	MG	14	3382	1/1	0.78	0.12	66,66,66,66	0
57	MG	1H	3241	1/1	0.78	0.22	58,58,58,58	0
57	MG	14	3139	1/1	0.78	0.31	68,68,68,68	0
57	MG	1H	3309	1/1	0.78	0.23	54,54,54,54	0
57	MG	1H	3518	1/1	0.78	0.11	96,96,96,96	0
57	MG	14	3134	1/1	0.78	0.33	85,85,85,85	0
57	MG	14	3168	1/1	0.78	0.24	89,89,89,89	0
57	MG	1H	3163	1/1	0.78	0.44	91,91,91,91	0
57	MG	1H	3206	1/1	0.78	0.56	93,93,93,93	0
57	MG	14	3257	1/1	0.78	0.16	69,69,69,69	0
57	MG	14	3342	1/1	0.78	0.09	113,113,113,113	0
57	MG	13	1661	1/1	0.78	0.19	90,90,90,90	0
57	MG	1G	1634	1/1	0.79	0.72	85,85,85,85	0
57	MG	14	3187	1/1	0.79	0.25	117,117,117,117	0
57	MG	14	3381	1/1	0.79	0.31	79,79,79,79	0
57	MG	1G	1632	1/1	0.79	0.09	91,91,91,91	0
57	MG	52	201	1/1	0.79	0.15	129,129,129,129	0
57	MG	14	3276	1/1	0.79	0.10	120,120,120,120	0
57	MG	1G	1694	1/1	0.79	0.12	113,113,113,113	0
57	MG	1H	3170	1/1	0.79	0.34	80,80,80,80	0
57	MG	1H	3111	1/1	0.79	0.61	79,79,79,79	0
57	MG	1H	3434	1/1	0.79	0.17	95,95,95,95	0
57	MG	19	301	1/1	0.79	0.42	48,48,48,48	0
57	MG	14	3421	1/1	0.79	0.10	97,97,97,97	0
57	MG	1G	1688	1/1	0.79	0.24	113,113,113,113	0
57	MG	1H	3198	1/1	0.79	0.23	79,79,79,79	0
57	MG	13	1647	1/1	0.79	0.47	88,88,88,88	0
57	MG	1G	1680	1/1	0.79	0.07	123,123,123,123	0
57	MG	14	3175	1/1	0.79	0.21	88,88,88,88	0
57	MG	1J	207	1/1	0.79	0.15	97,97,97,97	0
57	MG	1H	3421	1/1	0.80	0.06	82,82,82,82	0
57	MG	14	3339	1/1	0.80	0.10	107,107,107,107	0
57	MG	1H	3144	1/1	0.80	0.61	102,102,102,102	0
57	MG	14	3142	1/1	0.80	0.29	80,80,80,80	0
57	MG	1G	1663	1/1	0.80	0.23	98,98,98,98	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1H	3329	1/1	0.80	0.08	85,85,85,85	0
57	MG	1H	3224	1/1	0.80	0.33	85,85,85,85	0
57	MG	1G	1637	1/1	0.80	0.16	103,103,103,103	0
57	MG	1G	1636	1/1	0.80	0.33	90,90,90,90	0
57	MG	13	1664	1/1	0.80	0.46	78,78,78,78	0
57	MG	14	3108	1/1	0.80	0.28	72,72,72,72	0
57	MG	1H	3405	1/1	0.80	0.09	66,66,66,66	0
57	MG	1G	1693	1/1	0.80	0.07	129,129,129,129	0
57	MG	1H	3368	1/1	0.80	0.12	69,69,69,69	0
57	MG	1H	3391	1/1	0.80	0.13	89,89,89,89	0
57	MG	14	3271	1/1	0.80	0.06	94,94,94,94	0
57	MG	13	1711	1/1	0.80	0.16	74,74,74,74	0
57	MG	1H	3350	1/1	0.80	0.11	74,74,74,74	0
57	MG	1H	3497	1/1	0.80	0.10	107,107,107,107	0
57	MG	1G	1690	1/1	0.80	0.06	117,117,117,117	0
57	MG	14	3146	1/1	0.80	0.28	75,75,75,75	0
57	MG	1H	3043	1/1	0.80	0.40	75,75,75,75	0
57	MG	1G	1704	1/1	0.80	0.20	84,84,84,84	0
57	MG	14	3133	1/1	0.80	1.00	88,88,88,88	0
57	MG	14	3007	1/1	0.80	0.26	60,60,60,60	0
57	MG	1H	3332	1/1	0.80	0.16	102,102,102,102	0
57	MG	14	3069	1/1	0.80	0.46	86,86,86,86	0
57	MG	1H	3074	1/1	0.81	0.38	64,64,64,64	0
57	MG	1H	3341	1/1	0.81	0.12	78,78,78,78	0
57	MG	14	3285	1/1	0.81	0.06	108,108,108,108	0
57	MG	1H	3125	1/1	0.81	0.20	56,56,56,56	0
57	MG	14	3074	1/1	0.81	0.27	69,69,69,69	0
57	MG	14	3131	1/1	0.81	0.29	64,64,64,64	0
57	MG	1G	1605	1/1	0.81	0.39	104,104,104,104	0
57	MG	13	1675	1/1	0.81	0.47	101,101,101,101	0
57	MG	1H	3083	1/1	0.81	0.84	83,83,83,83	0
57	MG	1H	3470	1/1	0.81	0.08	83,83,83,83	0
57	MG	1G	1697	1/1	0.81	0.09	128,128,128,128	0
57	MG	1G	1670	1/1	0.81	0.06	134,134,134,134	0
57	MG	41	201	1/1	0.81	0.12	69,69,69,69	0
57	MG	14	3202	1/1	0.81	0.49	84,84,84,84	0
57	MG	1G	1669	1/1	0.81	0.09	105,105,105,105	0
57	MG	1H	3106	1/1	0.81	0.23	87,87,87,87	0
57	MG	14	3183	1/1	0.81	0.30	103,103,103,103	0
57	MG	1H	3486	1/1	0.81	0.07	95,95,95,95	0
57	MG	14	3091	1/1	0.81	0.09	78,78,78,78	0
57	MG	1H	3401	1/1	0.81	0.09	64,64,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1H	3055	1/1	0.81	0.18	48,48,48,48	0
57	MG	1H	3386	1/1	0.81	0.18	42,42,42,42	0
57	MG	1H	3308	1/1	0.81	0.14	50,50,50,50	0
57	MG	1H	3222	1/1	0.82	0.14	69,69,69,69	0
57	MG	13	1628	1/1	0.82	0.32	91,91,91,91	0
57	MG	1H	3456	1/1	0.82	0.06	94,94,94,94	0
57	MG	1H	3197	1/1	0.82	0.51	77,77,77,77	0
57	MG	13	1649	1/1	0.82	0.42	75,75,75,75	0
57	MG	14	3404	1/1	0.82	0.16	97,97,97,97	0
57	MG	14	3155	1/1	0.82	0.16	78,78,78,78	0
57	MG	1H	3367	1/1	0.82	0.08	66,66,66,66	0
61	SPE	14	3437	13/13	0.82	0.29	59,68,73,74	0
57	MG	1J	205	1/1	0.82	0.15	73,73,73,73	0
57	MG	14	3075	1/1	0.82	0.16	73,73,73,73	0
57	MG	14	3072	1/1	0.82	0.27	94,94,94,94	0
57	MG	1H	3431	1/1	0.82	0.09	98,98,98,98	0
57	MG	1H	3201	1/1	0.82	0.75	104,104,104,104	0
57	MG	1H	3020	1/1	0.82	0.14	73,73,73,73	0
57	MG	1H	3408	1/1	0.82	0.12	67,67,67,67	0
57	MG	39	302	1/1	0.82	0.20	74,74,74,74	0
57	MG	14	3295	1/1	0.82	0.10	60,60,60,60	0
57	MG	14	3386	1/1	0.82	0.09	74,74,74,74	0
57	MG	1H	3119	1/1	0.82	0.39	83,83,83,83	0
57	MG	1H	3038	1/1	0.82	0.32	50,50,50,50	0
57	MG	14	3262	1/1	0.82	0.14	83,83,83,83	0
57	MG	14	3298	1/1	0.82	0.11	86,86,86,86	0
57	MG	14	3412	1/1	0.82	0.10	97,97,97,97	0
57	MG	14	3345	1/1	0.82	0.16	99,99,99,99	0
57	MG	14	3221	1/1	0.82	0.20	62,62,62,62	0
57	MG	88	203	1/1	0.83	0.33	79,79,79,79	0
57	MG	1H	3191	1/1	0.83	0.27	58,58,58,58	0
57	MG	1H	3298	1/1	0.83	0.11	51,51,51,51	0
57	MG	1H	3236	1/1	0.83	0.31	67,67,67,67	0
57	MG	1H	3071	1/1	0.83	0.22	79,79,79,79	0
57	MG	5I	101	1/1	0.83	0.10	79,79,79,79	0
57	MG	14	3368	1/1	0.83	0.09	88,88,88,88	0
57	MG	14	3230	1/1	0.83	0.17	63,63,63,63	0
57	MG	1H	3134	1/1	0.83	0.14	57,57,57,57	0
57	MG	1H	3483	1/1	0.83	0.17	91,91,91,91	0
57	MG	14	3278	1/1	0.83	0.09	102,102,102,102	0
57	MG	14	3391	1/1	0.83	0.23	99,99,99,99	0
57	MG	13	1670	1/1	0.83	0.30	82,82,82,82	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	14	3243	1/1	0.83	0.15	58,58,58,58	0
57	MG	1G	1683	1/1	0.83	0.13	121,121,121,121	0
57	MG	1H	3453	1/1	0.83	0.12	93,93,93,93	0
57	MG	14	3198	1/1	0.83	0.43	81,81,81,81	0
57	MG	1H	3347	1/1	0.83	0.10	67,67,67,67	0
57	MG	1H	3156	1/1	0.83	0.15	83,83,83,83	0
57	MG	1H	3161	1/1	0.83	0.38	67,67,67,67	0
57	MG	1H	3376	1/1	0.83	0.15	66,66,66,66	0
57	MG	1H	3066	1/1	0.83	0.26	60,60,60,60	0
57	MG	14	3214	1/1	0.83	0.70	80,80,80,80	0
57	MG	14	3225	1/1	0.83	0.07	73,73,73,73	0
57	MG	1H	3407	1/1	0.83	0.09	72,72,72,72	0
57	MG	14	3184	1/1	0.83	0.26	78,78,78,78	0
57	MG	1H	3504	1/1	0.83	0.07	109,109,109,109	0
57	MG	1H	3229	1/1	0.83	0.49	90,90,90,90	0
57	MG	1H	3485	1/1	0.83	0.06	77,77,77,77	0
57	MG	1H	3517	1/1	0.83	0.07	91,91,91,91	0
57	MG	1H	3223	1/1	0.83	0.43	85,85,85,85	0
57	MG	13	1728	1/1	0.83	0.05	117,117,117,117	0
57	MG	1G	1674	1/1	0.83	0.08	107,107,107,107	0
57	MG	1H	3176	1/1	0.83	0.14	83,83,83,83	0
57	MG	14	3005	1/1	0.83	0.26	54,54,54,54	0
57	MG	1H	3220	1/1	0.83	0.45	89,89,89,89	0
57	MG	14	3204	1/1	0.83	0.22	72,72,72,72	0
57	MG	14	3003	1/1	0.83	0.27	78,78,78,78	0
57	MG	1H	3049	1/1	0.83	0.25	62,62,62,62	0
57	MG	1H	3523	1/1	0.83	0.11	82,82,82,82	0
57	MG	1H	3406	1/1	0.84	0.08	85,85,85,85	0
57	MG	14	3256	1/1	0.84	0.13	83,83,83,83	0
57	MG	1H	3420	1/1	0.84	0.12	69,69,69,69	0
57	MG	1H	3136	1/1	0.84	0.41	116,116,116,116	0
57	MG	1H	3140	1/1	0.84	0.20	54,54,54,54	0
57	MG	1H	3162	1/1	0.84	0.29	60,60,60,60	0
57	MG	1G	1691	1/1	0.84	0.05	133,133,133,133	0
57	MG	1H	3506	1/1	0.84	0.08	106,106,106,106	0
57	MG	14	3107	1/1	0.84	0.36	54,54,54,54	0
57	MG	1H	3373	1/1	0.84	0.09	80,80,80,80	0
57	MG	14	3215	1/1	0.84	1.26	86,86,86,86	0
57	MG	1G	1610	1/1	0.84	0.23	91,91,91,91	0
57	MG	1H	3178	1/1	0.84	0.43	63,63,63,63	0
57	MG	14	3099	1/1	0.84	0.18	78,78,78,78	0
57	MG	14	3418	1/1	0.84	0.07	90,90,90,90	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1H	3147	1/1	0.84	0.39	84,84,84,84	0
57	MG	13	1732	1/1	0.84	0.08	114,114,114,114	0
57	MG	1H	3084	1/1	0.84	0.20	62,62,62,62	0
57	MG	14	3414	1/1	0.84	0.12	97,97,97,97	0
57	MG	14	3343	1/1	0.84	0.06	80,80,80,80	0
57	MG	14	3267	1/1	0.84	0.06	82,82,82,82	0
57	MG	14	3318	1/1	0.84	0.12	89,89,89,89	0
57	MG	14	3153	1/1	0.84	0.59	90,90,90,90	0
57	MG	13	1627	1/1	0.84	0.48	71,71,71,71	0
57	MG	14	3427	1/1	0.84	0.08	65,65,65,65	0
57	MG	1H	3274	1/1	0.84	0.14	97,97,97,97	0
57	MG	13	1724	1/1	0.84	0.11	117,117,117,117	0
57	MG	14	3389	1/1	0.84	0.07	93,93,93,93	0
57	MG	1H	3525	1/1	0.84	0.22	68,68,68,68	0
57	MG	14	3063	1/1	0.84	0.24	67,67,67,67	0
57	MG	1G	1657	1/1	0.84	0.06	121,121,121,121	0
57	MG	16	201	1/1	0.84	0.25	62,62,62,62	0
57	MG	14	3213	1/1	0.84	0.71	87,87,87,87	0
57	MG	1H	3164	1/1	0.85	0.41	69,69,69,69	0
57	MG	1H	3502	1/1	0.85	0.18	141,141,141,141	0
57	MG	14	3286	1/1	0.85	0.11	73,73,73,73	0
57	MG	14	3157	1/1	0.85	0.32	92,92,92,92	0
57	MG	14	3170	1/1	0.85	0.58	81,81,81,81	0
57	MG	1H	3482	1/1	0.85	0.09	94,94,94,94	0
57	MG	13	1665	1/1	0.85	0.69	82,82,82,82	0
57	MG	14	3061	1/1	0.85	0.31	61,61,61,61	0
57	MG	1H	3346	1/1	0.85	0.10	92,92,92,92	0
57	MG	1H	3433	1/1	0.85	0.14	72,72,72,72	0
57	MG	1H	3242	1/1	0.85	0.47	90,90,90,90	0
57	MG	1G	1621	1/1	0.85	0.42	82,82,82,82	0
57	MG	14	3425	1/1	0.85	0.13	91,91,91,91	0
57	MG	14	3399	1/1	0.85	0.09	123,123,123,123	0
57	MG	14	3130	1/1	0.85	0.24	66,66,66,66	0
57	MG	1H	3058	1/1	0.85	0.17	60,60,60,60	0
57	MG	16	206	1/1	0.85	0.12	77,77,77,77	0
60	ZN	C5	202	1/1	0.85	0.06	165,165,165,165	0
57	MG	14	3419	1/1	0.85	0.06	110,110,110,110	0
57	MG	13	1650	1/1	0.85	0.41	75,75,75,75	0
57	MG	1H	3061	1/1	0.85	0.28	53,53,53,53	0
57	MG	1H	3194	1/1	0.85	0.10	63,63,63,63	0
57	MG	14	3323	1/1	0.85	0.11	81,81,81,81	0
57	MG	1H	3481	1/1	0.85	0.11	103,103,103,103	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	14	3006	1/1	0.85	0.32	75,75,75,75	0
57	MG	14	3111	1/1	0.85	0.19	58,58,58,58	0
57	MG	1G	1641	1/1	0.85	0.59	103,103,103,103	0
57	MG	1H	3489	1/1	0.85	0.32	73,73,73,73	0
57	MG	13	1733	1/1	0.85	0.11	101,101,101,101	0
57	MG	1H	3128	1/1	0.85	0.42	85,85,85,85	0
57	MG	14	3196	1/1	0.85	0.51	71,71,71,71	0
57	MG	1G	1647	1/1	0.85	0.10	97,97,97,97	0
57	MG	13	1659	1/1	0.85	0.15	126,126,126,126	0
57	MG	32	301	1/1	0.85	0.47	113,113,113,113	0
57	MG	1G	1654	1/1	0.85	0.30	108,108,108,108	0
57	MG	1G	1606	1/1	0.85	0.13	73,73,73,73	0
57	MG	14	3328	1/1	0.85	0.08	81,81,81,81	0
57	MG	14	3380	1/1	0.85	0.08	78,78,78,78	0
57	MG	13	1654	1/1	0.85	0.41	101,101,101,101	0
57	MG	1H	3148	1/1	0.85	0.37	83,83,83,83	0
57	MG	1H	3394	1/1	0.85	0.11	49,49,49,49	0
57	MG	14	3117	1/1	0.85	0.47	64,64,64,64	0
57	MG	1H	3235	1/1	0.86	0.20	71,71,71,71	0
57	MG	1H	3046	1/1	0.86	0.13	33,33,33,33	0
57	MG	1J	202	1/1	0.86	0.28	92,92,92,92	0
57	MG	14	3254	1/1	0.86	0.10	77,77,77,77	0
57	MG	1H	3492	1/1	0.86	0.15	78,78,78,78	0
57	MG	14	3255	1/1	0.86	0.13	79,79,79,79	0
57	MG	13	1740	1/1	0.86	0.06	98,98,98,98	0
57	MG	21	302	1/1	0.86	0.25	72,72,72,72	0
57	MG	14	3049	1/1	0.86	1.18	83,83,83,83	0
57	MG	1H	3443	1/1	0.86	0.10	75,75,75,75	0
57	MG	1H	3137	1/1	0.86	0.43	70,70,70,70	0
57	MG	1H	3005	1/1	0.86	0.21	68,68,68,68	0
57	MG	13	1622	1/1	0.86	0.26	63,63,63,63	0
57	MG	14	3165	1/1	0.86	0.66	77,77,77,77	0
57	MG	1H	3101	1/1	0.86	0.41	78,78,78,78	0
57	MG	1H	3512	1/1	0.86	0.13	87,87,87,87	0
57	MG	1H	3383	1/1	0.86	0.10	68,68,68,68	0
57	MG	14	3373	1/1	0.86	0.12	65,65,65,65	0
57	MG	78	201	1/1	0.86	0.10	66,66,66,66	0
57	MG	1H	3320	1/1	0.86	0.08	58,58,58,58	0
57	MG	14	3401	1/1	0.86	0.15	110,110,110,110	0
57	MG	1H	3240	1/1	0.86	0.38	73,73,73,73	0
57	MG	I8	101	1/1	0.86	0.09	85,85,85,85	0
57	MG	1H	3392	1/1	0.86	0.15	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1H	3457	1/1	0.86	0.16	84,84,84,84	0
57	MG	1H	3498	1/1	0.86	0.20	98,98,98,98	0
57	MG	14	3077	1/1	0.86	0.22	52,52,52,52	0
57	MG	1H	3080	1/1	0.86	0.17	80,80,80,80	0
57	MG	14	3408	1/1	0.86	0.13	92,92,92,92	0
57	MG	1J	206	1/1	0.86	0.24	94,94,94,94	0
57	MG	1H	3513	1/1	0.86	0.15	53,53,53,53	0
57	MG	14	3312	1/1	0.86	0.16	92,92,92,92	0
57	MG	1G	1695	1/1	0.86	0.23	107,107,107,107	0
57	MG	13	1710	1/1	0.86	0.07	96,96,96,96	0
57	MG	1H	3271	1/1	0.86	0.19	51,51,51,51	0
57	MG	1H	3133	1/1	0.86	0.23	55,55,55,55	0
57	MG	14	3137	1/1	0.86	0.53	99,99,99,99	0
57	MG	1H	3174	1/1	0.86	0.23	55,55,55,55	0
57	MG	1G	1667	1/1	0.86	0.11	103,103,103,103	0
57	MG	14	3025	1/1	0.86	0.12	80,80,80,80	0
57	MG	14	3125	1/1	0.87	0.21	81,81,81,81	0
57	MG	13	1726	1/1	0.87	0.08	74,74,74,74	0
57	MG	1H	3521	1/1	0.87	0.12	82,82,82,82	0
57	MG	1H	3108	1/1	0.87	0.24	64,64,64,64	0
57	MG	14	3416	1/1	0.87	0.13	102,102,102,102	0
57	MG	1G	1656	1/1	0.87	0.08	100,100,100,100	0
57	MG	1H	3008	1/1	0.87	0.39	82,82,82,82	0
57	MG	14	3076	1/1	0.87	0.45	81,81,81,81	0
57	MG	13	1651	1/1	0.87	0.29	98,98,98,98	0
57	MG	14	3209	1/1	0.87	0.17	83,83,83,83	0
57	MG	1H	3002	1/1	0.87	0.21	48,48,48,48	0
57	MG	1G	1611	1/1	0.87	0.65	76,76,76,76	0
57	MG	1H	3412	1/1	0.87	0.10	75,75,75,75	0
57	MG	13	1616	1/1	0.87	0.48	74,74,74,74	0
57	MG	14	3403	1/1	0.87	0.12	84,84,84,84	0
57	MG	14	3336	1/1	0.87	0.09	94,94,94,94	0
57	MG	14	3088	1/1	0.87	0.49	87,87,87,87	0
57	MG	1G	1659	1/1	0.87	0.04	115,115,115,115	0
57	MG	14	3177	1/1	0.87	0.45	101,101,101,101	0
57	MG	1H	3192	1/1	0.87	0.34	75,75,75,75	0
57	MG	1H	3001	1/1	0.87	0.39	84,84,84,84	0
57	MG	14	3200	1/1	0.87	0.15	89,89,89,89	0
57	MG	14	3411	1/1	0.87	0.04	105,105,105,105	0
57	MG	13	1683	1/1	0.87	0.05	93,93,93,93	0
57	MG	13	1610	1/1	0.87	0.38	82,82,82,82	0
57	MG	1G	1615	1/1	0.87	0.21	86,86,86,86	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	14	3275	1/1	0.87	0.10	65,65,65,65	0
57	MG	1H	3213	1/1	0.87	0.29	71,71,71,71	0
57	MG	1H	3384	1/1	0.87	0.08	67,67,67,67	0
57	MG	1H	3477	1/1	0.87	0.14	83,83,83,83	0
57	MG	1H	3348	1/1	0.87	0.10	111,111,111,111	0
57	MG	14	3084	1/1	0.87	0.27	79,79,79,79	0
57	MG	1H	3455	1/1	0.87	0.15	76,76,76,76	0
57	MG	1H	3375	1/1	0.87	0.10	79,79,79,79	0
57	MG	14	3268	1/1	0.87	0.15	82,82,82,82	0
57	MG	1H	3314	1/1	0.87	0.08	68,68,68,68	0
57	MG	13	1730	1/1	0.88	0.09	94,94,94,94	0
57	MG	14	3424	1/1	0.88	0.09	109,109,109,109	0
57	MG	14	3210	1/1	0.88	0.29	91,91,91,91	0
57	MG	1H	3452	1/1	0.88	0.10	72,72,72,72	0
57	MG	14	3413	1/1	0.88	0.15	107,107,107,107	0
57	MG	1H	3126	1/1	0.88	0.43	86,86,86,86	0
57	MG	13	1712	1/1	0.88	0.07	89,89,89,89	0
57	MG	14	3143	1/1	0.88	0.17	57,57,57,57	0
57	MG	13	1635	1/1	0.88	0.24	81,81,81,81	0
57	MG	1H	3057	1/1	0.88	0.38	75,75,75,75	0
57	MG	13	1613	1/1	0.88	0.13	87,87,87,87	0
57	MG	14	3172	1/1	0.88	0.39	77,77,77,77	0
57	MG	14	3273	1/1	0.88	0.09	86,86,86,86	0
57	MG	14	3129	1/1	0.88	0.42	118,118,118,118	0
57	MG	1H	3379	1/1	0.88	0.09	73,73,73,73	0
57	MG	14	3431	1/1	0.88	0.25	116,116,116,116	0
57	MG	13	1620	1/1	0.88	0.53	86,86,86,86	0
57	MG	2L	102	1/1	0.88	0.18	132,132,132,132	0
57	MG	13	1615	1/1	0.88	0.24	88,88,88,88	0
57	MG	13	1700	1/1	0.88	0.12	102,102,102,102	0
57	MG	1H	3410	1/1	0.88	0.10	83,83,83,83	0
57	MG	1G	1679	1/1	0.88	0.09	94,94,94,94	0
57	MG	13	1713	1/1	0.88	0.08	86,86,86,86	0
57	MG	1H	3515	1/1	0.88	0.19	58,58,58,58	0
57	MG	1H	3069	1/1	0.88	0.41	69,69,69,69	0
57	MG	1H	3165	1/1	0.88	0.29	64,64,64,64	0
57	MG	13	1694	1/1	0.88	0.14	82,82,82,82	0
57	MG	14	3159	1/1	0.88	0.11	79,79,79,79	0
57	MG	1H	3212	1/1	0.88	0.27	65,65,65,65	0
57	MG	14	3167	1/1	0.88	0.32	78,78,78,78	0
57	MG	13	1696	1/1	0.88	0.05	93,93,93,93	0
57	MG	1H	3010	1/1	0.88	0.37	39,39,39,39	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	14	3236	1/1	0.88	0.28	44,44,44,44	0
57	MG	1H	3362	1/1	0.88	0.13	100,100,100,100	0
57	MG	1G	1649	1/1	0.88	0.14	113,113,113,113	0
57	MG	16	204	1/1	0.88	0.06	59,59,59,59	0
57	MG	1H	3082	1/1	0.88	0.27	71,71,71,71	0
57	MG	14	3390	1/1	0.88	0.22	94,94,94,94	0
57	MG	1H	3296	1/1	0.88	0.08	91,91,91,91	0
57	MG	13	1617	1/1	0.88	0.14	51,51,51,51	0
61	SPE	1G	1703	13/13	0.88	0.09	90,107,113,114	0
57	MG	1G	1646	1/1	0.88	0.10	86,86,86,86	0
57	MG	13	1731	1/1	0.88	0.05	112,112,112,112	0
57	MG	1H	3142	1/1	0.88	0.29	68,68,68,68	0
57	MG	1H	3460	1/1	0.89	0.06	96,96,96,96	0
57	MG	1G	1625	1/1	0.89	0.08	99,99,99,99	0
57	MG	14	3148	1/1	0.89	0.39	85,85,85,85	0
57	MG	1H	3181	1/1	0.89	0.24	65,65,65,65	0
57	MG	14	3223	1/1	0.89	0.10	87,87,87,87	0
57	MG	14	3402	1/1	0.89	0.08	78,78,78,78	0
57	MG	14	3346	1/1	0.89	0.08	99,99,99,99	0
57	MG	1G	1676	1/1	0.89	0.09	93,93,93,93	0
57	MG	14	3388	1/1	0.89	0.07	85,85,85,85	0
57	MG	1H	3480	1/1	0.89	0.07	87,87,87,87	0
57	MG	13	1655	1/1	0.89	0.50	82,82,82,82	0
57	MG	14	3144	1/1	0.89	0.32	102,102,102,102	0
57	MG	13	1684	1/1	0.89	0.08	85,85,85,85	0
57	MG	1H	3098	1/1	0.89	0.41	46,46,46,46	0
57	MG	14	3024	1/1	0.89	0.07	81,81,81,81	0
57	MG	14	3160	1/1	0.89	0.18	65,65,65,65	0
57	MG	1H	3086	1/1	0.89	0.18	53,53,53,53	0
57	MG	1G	1664	1/1	0.89	0.05	80,80,80,80	0
57	MG	14	3282	1/1	0.89	0.06	90,90,90,90	0
57	MG	14	3299	1/1	0.89	0.11	79,79,79,79	0
57	MG	14	3203	1/1	0.89	0.53	79,79,79,79	0
57	MG	14	3241	1/1	0.89	0.05	78,78,78,78	0
57	MG	13	1719	1/1	0.89	0.04	81,81,81,81	0
57	MG	16	202	1/1	0.89	0.23	82,82,82,82	0
57	MG	14	3374	1/1	0.89	0.12	92,92,92,92	0
57	MG	1H	3246	1/1	0.89	0.09	55,55,55,55	0
57	MG	1H	3221	1/1	0.89	0.24	73,73,73,73	0
57	MG	1J	204	1/1	0.89	0.09	89,89,89,89	0
57	MG	1H	3424	1/1	0.89	0.04	101,101,101,101	0
57	MG	1H	3149	1/1	0.89	0.24	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	13	1658	1/1	0.89	0.25	82,82,82,82	0
57	MG	1H	3256	1/1	0.89	0.13	47,47,47,47	0
57	MG	1G	1648	1/1	0.89	0.16	115,115,115,115	0
57	MG	1G	1629	1/1	0.89	0.52	85,85,85,85	0
57	MG	14	3070	1/1	0.89	0.22	52,52,52,52	0
57	MG	1H	3215	1/1	0.89	0.13	63,63,63,63	0
57	MG	1H	3435	1/1	0.89	0.06	62,62,62,62	0
57	MG	14	3001	1/1	0.89	0.17	57,57,57,57	0
57	MG	1H	3509	1/1	0.89	0.12	47,47,47,47	0
57	MG	1H	3371	1/1	0.89	0.10	56,56,56,56	0
57	MG	13	1629	1/1	0.89	0.21	72,72,72,72	0
57	MG	14	3263	1/1	0.90	0.09	71,71,71,71	0
57	MG	14	3158	1/1	0.90	0.24	66,66,66,66	0
57	MG	1H	3331	1/1	0.90	0.12	70,70,70,70	0
57	MG	14	3319	1/1	0.90	0.07	95,95,95,95	0
57	MG	14	3349	1/1	0.90	0.13	83,83,83,83	0
57	MG	13	1618	1/1	0.90	0.20	48,48,48,48	0
57	MG	14	3042	1/1	0.90	0.19	65,65,65,65	0
57	MG	14	3083	1/1	0.90	0.15	72,72,72,72	0
57	MG	13	1657	1/1	0.90	0.15	68,68,68,68	0
57	MG	14	3405	1/1	0.90	0.07	108,108,108,108	0
57	MG	1H	3062	1/1	0.90	0.13	38,38,38,38	0
57	MG	1H	3268	1/1	0.90	0.17	59,59,59,59	0
57	MG	1G	1614	1/1	0.90	0.60	88,88,88,88	0
57	MG	14	3307	1/1	0.90	0.15	66,66,66,66	0
57	MG	13	1631	1/1	0.90	0.09	78,78,78,78	0
57	MG	13	1725	1/1	0.90	0.04	115,115,115,115	0
57	MG	14	3296	1/1	0.90	0.12	72,72,72,72	0
57	MG	1J	201	1/1	0.90	0.29	73,73,73,73	0
57	MG	14	3327	1/1	0.90	0.09	82,82,82,82	0
57	MG	1G	1612	1/1	0.90	0.15	106,106,106,106	0
57	MG	14	3397	1/1	0.90	0.17	96,96,96,96	0
57	MG	1H	3490	1/1	0.90	0.07	89,89,89,89	0
57	MG	1G	1692	1/1	0.90	0.12	101,101,101,101	0
57	MG	14	3057	1/1	0.90	0.25	49,49,49,49	0
57	MG	14	3279	1/1	0.90	0.08	58,58,58,58	0
57	MG	1G	1643	1/1	0.90	0.54	83,83,83,83	0
57	MG	1H	3013	1/1	0.90	0.27	40,40,40,40	0
57	MG	1G	1687	1/1	0.90	0.08	111,111,111,111	0
57	MG	1H	3303	1/1	0.90	0.17	48,48,48,48	0
57	MG	14	3120	1/1	0.90	0.18	78,78,78,78	0
57	MG	1H	3505	1/1	0.90	0.14	100,100,100,100	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	13	1626	1/1	0.90	0.33	84,84,84,84	0
57	MG	1H	3484	1/1	0.90	0.09	105,105,105,105	0
57	MG	1G	1628	1/1	0.90	0.31	113,113,113,113	0
57	MG	1H	3336	1/1	0.90	0.14	62,62,62,62	0
57	MG	14	3245	1/1	0.90	0.14	63,63,63,63	0
57	MG	1H	3109	1/1	0.90	0.31	59,59,59,59	0
57	MG	13	1641	1/1	0.90	0.19	81,81,81,81	0
57	MG	1H	3334	1/1	0.90	0.10	77,77,77,77	0
57	MG	14	3260	1/1	0.90	0.11	106,106,106,106	0
57	MG	1H	3103	1/1	0.90	0.32	61,61,61,61	0
57	MG	14	3354	1/1	0.90	0.14	60,60,60,60	0
57	MG	1H	3244	1/1	0.90	0.42	74,74,74,74	0
57	MG	14	3227	1/1	0.90	0.15	58,58,58,58	0
57	MG	1H	3088	1/1	0.90	0.42	80,80,80,80	0
57	MG	14	3193	1/1	0.90	0.13	45,45,45,45	0
57	MG	13	1656	1/1	0.90	0.38	74,74,74,74	0
57	MG	1H	3037	1/1	0.90	0.54	75,75,75,75	0
57	MG	1H	3409	1/1	0.90	0.07	85,85,85,85	0
57	MG	14	3186	1/1	0.90	0.16	108,108,108,108	0
57	MG	14	3169	1/1	0.90	0.31	85,85,85,85	0
57	MG	1H	3429	1/1	0.90	0.10	88,88,88,88	0
57	MG	25	201	1/1	0.90	0.05	115,115,115,115	0
57	MG	1H	3321	1/1	0.90	0.46	86,86,86,86	0
57	MG	1H	3294	1/1	0.90	0.16	54,54,54,54	0
57	MG	1G	1639	1/1	0.90	0.54	78,78,78,78	0
57	MG	1H	3416	1/1	0.90	0.06	89,89,89,89	0
57	MG	13	1708	1/1	0.90	0.16	65,65,65,65	0
57	MG	1H	3115	1/1	0.90	0.10	61,61,61,61	0
57	MG	13	1695	1/1	0.90	0.10	106,106,106,106	0
57	MG	88	202	1/1	0.90	0.32	66,66,66,66	0
57	MG	42	201	1/1	0.90	0.21	120,120,120,120	0
57	MG	1H	3127	1/1	0.90	0.12	91,91,91,91	0
57	MG	13	1722	1/1	0.90	0.09	87,87,87,87	0
57	MG	14	3316	1/1	0.90	0.13	69,69,69,69	0
57	MG	14	3420	1/1	0.90	0.07	107,107,107,107	0
57	MG	1H	3404	1/1	0.90	0.13	71,71,71,71	0
57	MG	1G	1619	1/1	0.90	0.10	102,102,102,102	0
57	MG	1H	3508	1/1	0.90	0.10	117,117,117,117	0
57	MG	13	1640	1/1	0.90	0.28	92,92,92,92	0
57	MG	14	3121	1/1	0.90	0.12	61,61,61,61	0
57	MG	14	3358	1/1	0.90	0.15	86,86,86,86	0
57	MG	14	3119	1/1	0.90	0.20	81,81,81,81	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	14	3022	1/1	0.90	0.13	81,81,81,81	0
57	MG	14	3009	1/1	0.90	0.34	57,57,57,57	0
57	MG	14	3090	1/1	0.91	0.35	86,86,86,86	0
57	MG	14	3095	1/1	0.91	0.18	62,62,62,62	0
57	MG	13	1735	1/1	0.91	0.07	100,100,100,100	0
57	MG	1H	3202	1/1	0.91	0.45	73,73,73,73	0
57	MG	14	3309	1/1	0.91	0.14	55,55,55,55	0
57	MG	14	3313	1/1	0.91	0.05	105,105,105,105	0
57	MG	1H	3351	1/1	0.91	0.09	68,68,68,68	0
57	MG	1H	3228	1/1	0.91	0.15	60,60,60,60	0
57	MG	13	1672	1/1	0.91	0.15	88,88,88,88	0
57	MG	14	3188	1/1	0.91	0.50	72,72,72,72	0
57	MG	39	301	1/1	0.91	0.18	89,89,89,89	0
57	MG	1H	3310	1/1	0.91	0.18	70,70,70,70	0
57	MG	2K	101	1/1	0.91	0.11	100,100,100,100	0
57	MG	14	3251	1/1	0.91	0.09	80,80,80,80	0
57	MG	14	3297	1/1	0.91	0.17	71,71,71,71	0
57	MG	14	3015	1/1	0.91	0.29	63,63,63,63	0
57	MG	1H	3104	1/1	0.91	0.13	43,43,43,43	0
57	MG	16	209	1/1	0.91	0.47	76,76,76,76	0
57	MG	14	3011	1/1	0.91	0.18	44,44,44,44	0
57	MG	14	3201	1/1	0.91	0.20	88,88,88,88	0
57	MG	1G	1604	1/1	0.91	0.17	127,127,127,127	0
57	MG	1G	1696	1/1	0.91	0.07	128,128,128,128	0
57	MG	14	3237	1/1	0.91	0.26	51,51,51,51	0
57	MG	14	3359	1/1	0.91	0.08	93,93,93,93	0
57	MG	1H	3193	1/1	0.91	0.26	61,61,61,61	0
57	MG	13	1720	1/1	0.91	0.15	109,109,109,109	0
57	MG	13	1645	1/1	0.91	0.28	92,92,92,92	0
57	MG	1H	3124	1/1	0.91	0.21	61,61,61,61	0
57	MG	1H	3427	1/1	0.91	0.10	67,67,67,67	0
57	MG	14	3039	1/1	0.91	0.71	89,89,89,89	0
57	MG	1H	3122	1/1	0.91	0.09	52,52,52,52	0
57	MG	1H	3447	1/1	0.91	0.24	70,70,70,70	0
57	MG	13	1677	1/1	0.91	0.47	77,77,77,77	0
57	MG	1H	3185	1/1	0.91	0.49	64,64,64,64	0
57	MG	1H	3138	1/1	0.91	0.14	54,54,54,54	0
57	MG	1H	3117	1/1	0.91	0.18	60,60,60,60	0
57	MG	14	3392	1/1	0.91	0.07	63,63,63,63	0
57	MG	1H	3190	1/1	0.91	0.38	91,91,91,91	0
57	MG	14	3396	1/1	0.91	0.03	126,126,126,126	0
57	MG	1G	1652	1/1	0.91	0.15	81,81,81,81	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1H	3301	1/1	0.91	0.17	45,45,45,45	0
57	MG	1G	1630	1/1	0.91	0.37	72,72,72,72	0
57	MG	13	1697	1/1	0.91	0.07	84,84,84,84	0
57	MG	14	3180	1/1	0.91	0.41	91,91,91,91	0
57	MG	1G	1689	1/1	0.91	0.06	116,116,116,116	0
57	MG	14	3423	1/1	0.91	0.07	120,120,120,120	0
57	MG	1H	3231	1/1	0.91	0.49	66,66,66,66	0
57	MG	14	3369	1/1	0.91	0.10	91,91,91,91	0
57	MG	13	1701	1/1	0.91	0.12	108,108,108,108	0
57	MG	1H	3151	1/1	0.91	0.55	80,80,80,80	0
57	MG	1H	3093	1/1	0.91	0.09	56,56,56,56	0
57	MG	1H	3132	1/1	0.91	0.23	65,65,65,65	0
57	MG	1H	3251	1/1	0.91	0.16	48,48,48,48	0
57	MG	1H	3116	1/1	0.91	0.16	53,53,53,53	0
57	MG	1H	3270	1/1	0.91	0.15	50,50,50,50	0
57	MG	45	202	1/1	0.91	0.44	64,64,64,64	0
57	MG	1G	1624	1/1	0.91	0.13	95,95,95,95	0
57	MG	14	3357	1/1	0.92	0.08	105,105,105,105	0
57	MG	1H	3345	1/1	0.92	0.06	102,102,102,102	0
57	MG	14	3289	1/1	0.92	0.13	74,74,74,74	0
57	MG	1H	3403	1/1	0.92	0.07	99,99,99,99	0
57	MG	1H	3340	1/1	0.92	0.05	76,76,76,76	0
57	MG	1H	3051	1/1	0.92	0.11	60,60,60,60	0
57	MG	1H	3299	1/1	0.92	0.13	48,48,48,48	0
57	MG	1H	3312	1/1	0.92	0.15	44,44,44,44	0
57	MG	13	1686	1/1	0.92	0.17	76,76,76,76	0
57	MG	14	3113	1/1	0.92	0.18	52,52,52,52	0
57	MG	16	207	1/1	0.92	0.33	74,74,74,74	0
57	MG	1H	3253	1/1	0.92	0.08	42,42,42,42	0
57	MG	Q8	300	1/1	0.92	0.12	80,80,80,80	0
57	MG	14	3020	1/1	0.92	0.12	75,75,75,75	0
57	MG	14	3141	1/1	0.92	0.28	95,95,95,95	0
57	MG	1H	3034	1/1	0.92	0.21	46,46,46,46	0
57	MG	1H	3100	1/1	0.92	0.54	68,68,68,68	0
57	MG	1H	3064	1/1	0.92	0.07	51,51,51,51	0
57	MG	1H	3519	1/1	0.92	0.18	116,116,116,116	0
57	MG	14	3302	1/1	0.92	0.11	58,58,58,58	0
57	MG	1G	1608	1/1	0.92	0.37	93,93,93,93	0
57	MG	14	3224	1/1	0.92	0.24	45,45,45,45	0
57	MG	1H	3146	1/1	0.92	0.16	52,52,52,52	0
57	MG	1H	3077	1/1	0.92	0.42	80,80,80,80	0
57	MG	1H	3023	1/1	0.92	0.17	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	14	3190	1/1	0.92	0.37	59,59,59,59	0
57	MG	1G	1662	1/1	0.92	0.13	91,91,91,91	0
57	MG	1H	3094	1/1	0.92	0.15	33,33,33,33	0
57	MG	1H	3432	1/1	0.92	0.11	93,93,93,93	0
57	MG	1H	3390	1/1	0.92	0.20	64,64,64,64	0
57	MG	13	1707	1/1	0.92	0.10	56,56,56,56	0
57	MG	1H	3446	1/1	0.92	0.06	98,98,98,98	0
57	MG	14	3303	1/1	0.92	0.07	74,74,74,74	0
57	MG	1H	3219	1/1	0.92	0.20	71,71,71,71	0
57	MG	3I	201	1/1	0.92	0.24	60,60,60,60	0
60	ZN	G8	201	1/1	0.92	0.14	139,139,139,139	0
57	MG	14	3178	1/1	0.92	0.73	78,78,78,78	0
57	MG	1H	3167	1/1	0.92	0.53	98,98,98,98	0
57	MG	1H	3425	1/1	0.92	0.07	64,64,64,64	0
57	MG	14	3306	1/1	0.92	0.08	58,58,58,58	0
57	MG	14	3361	1/1	0.92	0.05	79,79,79,79	0
57	MG	14	3383	1/1	0.92	0.07	90,90,90,90	0
57	MG	1H	3102	1/1	0.92	0.21	60,60,60,60	0
57	MG	14	3259	1/1	0.92	0.10	71,71,71,71	0
57	MG	1H	3087	1/1	0.92	0.21	71,71,71,71	0
57	MG	1G	1701	1/1	0.92	0.03	111,111,111,111	0
57	MG	1G	1660	1/1	0.92	0.14	74,74,74,74	0
57	MG	13	1612	1/1	0.92	0.12	86,86,86,86	0
57	MG	1H	3370	1/1	0.92	0.08	68,68,68,68	0
57	MG	1H	3494	1/1	0.92	0.08	72,72,72,72	0
57	MG	14	3149	1/1	0.92	0.28	72,72,72,72	0
57	MG	14	3400	1/1	0.92	0.05	108,108,108,108	0
57	MG	1H	3158	1/1	0.92	0.17	71,71,71,71	0
57	MG	1H	3073	1/1	0.92	0.21	66,66,66,66	0
57	MG	1H	3209	1/1	0.92	0.60	76,76,76,76	0
57	MG	1H	3501	1/1	0.92	0.07	90,90,90,90	0
57	MG	1H	3092	1/1	0.92	0.24	61,61,61,61	0
57	MG	1H	3524	1/1	0.92	0.18	81,81,81,81	0
57	MG	13	1698	1/1	0.92	0.11	83,83,83,83	0
57	MG	1G	1602	1/1	0.92	0.33	106,106,106,106	0
57	MG	13	1717	1/1	0.92	0.11	99,99,99,99	0
57	MG	14	3041	1/1	0.92	0.20	55,55,55,55	0
57	MG	14	3333	1/1	0.92	0.17	50,50,50,50	0
57	MG	1H	3078	1/1	0.92	0.28	58,58,58,58	0
57	MG	1H	3095	1/1	0.92	0.17	70,70,70,70	0
57	MG	1H	3189	1/1	0.92	0.35	68,68,68,68	0
57	MG	1H	3418	1/1	0.92	0.10	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1G	1640	1/1	0.92	0.39	108,108,108,108	0
57	MG	13	1638	1/1	0.92	0.07	85,85,85,85	0
57	MG	14	3337	1/1	0.92	0.14	104,104,104,104	0
57	MG	1H	3397	1/1	0.92	0.19	51,51,51,51	0
57	MG	13	1682	1/1	0.92	0.11	93,93,93,93	0
57	MG	1H	3417	1/1	0.92	0.18	83,83,83,83	0
57	MG	14	3360	1/1	0.92	0.07	96,96,96,96	0
57	MG	1G	1613	1/1	0.93	0.76	89,89,89,89	0
57	MG	1G	1700	1/1	0.93	0.06	109,109,109,109	0
57	MG	1H	3155	1/1	0.93	0.15	55,55,55,55	0
57	MG	1G	1650	1/1	0.93	0.16	101,101,101,101	0
57	MG	14	3335	1/1	0.93	0.08	81,81,81,81	0
57	MG	14	3284	1/1	0.93	0.14	72,72,72,72	0
57	MG	1H	3462	1/1	0.93	0.10	94,94,94,94	0
57	MG	1H	3261	1/1	0.93	0.08	63,63,63,63	0
57	MG	1H	3430	1/1	0.93	0.08	73,73,73,73	0
57	MG	1H	3028	1/1	0.93	0.10	67,67,67,67	0
57	MG	14	3410	1/1	0.93	0.06	85,85,85,85	0
57	MG	1G	1655	1/1	0.93	0.12	110,110,110,110	0
57	MG	14	3112	1/1	0.93	0.20	83,83,83,83	0
57	MG	14	3331	1/1	0.93	0.20	90,90,90,90	0
57	MG	14	3311	1/1	0.93	0.11	67,67,67,67	0
57	MG	14	3220	1/1	0.93	0.12	54,54,54,54	0
57	MG	13	1639	1/1	0.93	0.58	70,70,70,70	0
57	MG	1H	3293	1/1	0.93	0.14	73,73,73,73	0
57	MG	14	3250	1/1	0.93	0.08	79,79,79,79	0
57	MG	88	201	1/1	0.93	0.19	76,76,76,76	0
57	MG	1H	3300	1/1	0.93	0.19	62,62,62,62	0
57	MG	1G	1677	1/1	0.93	0.17	92,92,92,92	0
57	MG	1H	3232	1/1	0.93	0.22	48,48,48,48	0
57	MG	1H	3468	1/1	0.93	0.24	82,82,82,82	0
57	MG	14	3371	1/1	0.93	0.10	107,107,107,107	0
57	MG	14	3317	1/1	0.93	0.08	82,82,82,82	0
57	MG	14	3079	1/1	0.93	0.30	48,48,48,48	0
57	MG	1H	3378	1/1	0.93	0.09	50,50,50,50	0
57	MG	2L	101	1/1	0.93	0.40	91,91,91,91	0
57	MG	14	3365	1/1	0.93	0.13	78,78,78,78	0
57	MG	1G	1681	1/1	0.93	0.06	96,96,96,96	0
57	MG	14	3068	1/1	0.93	0.41	53,53,53,53	0
57	MG	13	1667	1/1	0.93	0.67	89,89,89,89	0
57	MG	1G	1645	1/1	0.93	0.14	81,81,81,81	0
57	MG	14	3043	1/1	0.93	0.29	71,71,71,71	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	16	210	1/1	0.93	0.11	73,73,73,73	0
57	MG	1G	1620	1/1	0.93	0.19	91,91,91,91	0
57	MG	1H	3478	1/1	0.93	0.06	101,101,101,101	0
57	MG	14	3071	1/1	0.93	0.19	74,74,74,74	0
57	MG	14	3124	1/1	0.93	0.18	97,97,97,97	0
57	MG	1H	3343	1/1	0.93	0.07	78,78,78,78	0
57	MG	1H	3160	1/1	0.93	0.18	71,71,71,71	0
57	MG	14	3352	1/1	0.93	0.07	82,82,82,82	0
57	MG	14	3378	1/1	0.93	0.13	92,92,92,92	0
57	MG	1H	3076	1/1	0.93	0.24	72,72,72,72	0
57	MG	14	3094	1/1	0.93	0.65	73,73,73,73	0
57	MG	1H	3438	1/1	0.93	0.04	62,62,62,62	0
57	MG	1H	3436	1/1	0.93	0.10	70,70,70,70	0
57	MG	1G	1685	1/1	0.93	0.14	110,110,110,110	0
57	MG	14	3051	1/1	0.93	0.27	61,61,61,61	0
57	MG	14	3338	1/1	0.93	0.05	107,107,107,107	0
57	MG	14	3249	1/1	0.93	0.15	52,52,52,52	0
57	MG	14	3233	1/1	0.93	0.26	65,65,65,65	0
57	MG	M5	101	1/1	0.93	0.18	88,88,88,88	0
57	MG	1H	3393	1/1	0.93	0.11	50,50,50,50	0
57	MG	14	3415	1/1	0.93	0.15	103,103,103,103	0
57	MG	1H	3067	1/1	0.93	0.21	58,58,58,58	0
57	MG	1H	3048	1/1	0.93	0.13	45,45,45,45	0
57	MG	14	3123	1/1	0.94	0.28	83,83,83,83	0
57	MG	1H	3449	1/1	0.94	0.10	80,80,80,80	0
57	MG	1H	3184	1/1	0.94	0.24	70,70,70,70	0
57	MG	1H	3313	1/1	0.94	0.17	47,47,47,47	0
57	MG	1H	3021	1/1	0.94	0.17	49,49,49,49	0
57	MG	1H	3026	1/1	0.94	0.39	55,55,55,55	0
57	MG	14	3105	1/1	0.94	0.14	73,73,73,73	0
57	MG	13	1625	1/1	0.94	0.16	82,82,82,82	0
57	MG	1H	3366	1/1	0.94	0.17	68,68,68,68	0
57	MG	1H	3114	1/1	0.94	0.15	71,71,71,71	0
57	MG	14	3018	1/1	0.94	0.14	44,44,44,44	0
57	MG	1H	3372	1/1	0.94	0.08	89,89,89,89	0
57	MG	14	3104	1/1	0.94	0.18	78,78,78,78	0
57	MG	1H	3279	1/1	0.94	0.15	48,48,48,48	0
57	MG	13	1666	1/1	0.94	0.20	85,85,85,85	0
57	MG	14	3244	1/1	0.94	0.15	54,54,54,54	0
57	MG	1H	3358	1/1	0.94	0.18	45,45,45,45	0
58	PAR	1G	1702	42/42	0.94	0.22	83,92,100,103	0
57	MG	14	3145	1/1	0.94	0.21	90,90,90,90	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1H	3295	1/1	0.94	0.09	89,89,89,89	0
57	MG	14	3265	1/1	0.94	0.07	91,91,91,91	0
57	MG	14	3106	1/1	0.94	0.41	57,57,57,57	0
57	MG	14	3238	1/1	0.94	0.20	50,50,50,50	0
57	MG	13	1644	1/1	0.94	0.45	85,85,85,85	0
57	MG	14	3050	1/1	0.94	0.20	57,57,57,57	0
57	MG	1H	3357	1/1	0.94	0.12	52,52,52,52	0
57	MG	14	3367	1/1	0.94	0.08	106,106,106,106	0
57	MG	1H	3041	1/1	0.94	0.28	51,51,51,51	0
57	MG	1H	3035	1/1	0.94	0.11	40,40,40,40	0
57	MG	1H	3491	1/1	0.94	0.10	70,70,70,70	0
57	MG	1H	3238	1/1	0.94	0.34	80,80,80,80	0
57	MG	1H	3266	1/1	0.94	0.08	54,54,54,54	0
57	MG	1H	3356	1/1	0.94	0.11	54,54,54,54	0
57	MG	13	1687	1/1	0.94	0.06	103,103,103,103	0
57	MG	1G	1666	1/1	0.94	0.14	100,100,100,100	0
57	MG	1H	3510	1/1	0.94	0.14	39,39,39,39	0
57	MG	1H	3283	1/1	0.94	0.15	71,71,71,71	0
57	MG	14	3038	1/1	0.94	0.21	52,52,52,52	0
57	MG	13	1716	1/1	0.94	0.10	71,71,71,71	0
57	MG	1G	1626	1/1	0.94	0.19	83,83,83,83	0
57	MG	14	3097	1/1	0.94	0.26	97,97,97,97	0
57	MG	14	3269	1/1	0.94	0.05	78,78,78,78	0
57	MG	14	3232	1/1	0.94	0.14	66,66,66,66	0
57	MG	14	3010	1/1	0.94	0.25	57,57,57,57	0
57	MG	1H	3337	1/1	0.94	0.05	86,86,86,86	0
57	MG	1H	3288	1/1	0.94	0.08	54,54,54,54	0
57	MG	1G	1623	1/1	0.94	0.21	115,115,115,115	0
57	MG	1H	3475	1/1	0.94	0.12	97,97,97,97	0
57	MG	14	3362	1/1	0.94	0.06	114,114,114,114	0
57	MG	13	1633	1/1	0.94	0.22	73,73,73,73	0
57	MG	1H	3469	1/1	0.94	0.14	58,58,58,58	0
57	MG	14	3162	1/1	0.94	0.40	74,74,74,74	0
57	MG	14	3029	1/1	0.94	0.21	57,57,57,57	0
57	MG	14	3218	1/1	0.94	0.09	65,65,65,65	0
57	MG	1H	3441	1/1	0.94	0.06	105,105,105,105	0
57	MG	13	1691	1/1	0.94	0.12	92,92,92,92	0
57	MG	1H	3099	1/1	0.94	0.44	56,56,56,56	0
57	MG	14	3205	1/1	0.94	0.45	59,59,59,59	0
57	MG	14	3033	1/1	0.94	0.33	80,80,80,80	0
57	MG	13	1681	1/1	0.94	0.14	59,59,59,59	0
57	MG	13	1642	1/1	0.94	0.13	103,103,103,103	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1H	3259	1/1	0.94	0.17	54,54,54,54	0
57	MG	13	1634	1/1	0.94	0.36	75,75,75,75	0
57	MG	1H	3175	1/1	0.94	0.29	64,64,64,64	0
57	MG	14	3292	1/1	0.94	0.12	74,74,74,74	0
57	MG	1H	3131	1/1	0.94	0.50	83,83,83,83	0
57	MG	21	301	1/1	0.94	0.14	59,59,59,59	0
57	MG	14	3150	1/1	0.94	0.12	63,63,63,63	0
57	MG	14	3035	1/1	0.94	0.41	58,58,58,58	0
57	MG	14	3304	1/1	0.94	0.10	74,74,74,74	0
57	MG	14	3046	1/1	0.94	0.45	79,79,79,79	0
57	MG	1H	3173	1/1	0.94	0.22	59,59,59,59	0
57	MG	1H	3507	1/1	0.94	0.08	57,57,57,57	0
57	MG	14	3054	1/1	0.94	0.25	79,79,79,79	0
57	MG	1H	3285	1/1	0.94	0.14	55,55,55,55	0
57	MG	13	1715	1/1	0.94	0.06	76,76,76,76	0
57	MG	1H	3107	1/1	0.94	0.12	60,60,60,60	0
57	MG	1H	3245	1/1	0.94	0.11	47,47,47,47	0
57	MG	1H	3239	1/1	0.94	0.10	67,67,67,67	0
57	MG	13	1653	1/1	0.94	0.33	73,73,73,73	0
57	MG	1H	3276	1/1	0.94	0.10	78,78,78,78	0
57	MG	14	3340	1/1	0.94	0.09	107,107,107,107	0
57	MG	1H	3009	1/1	0.94	0.54	71,71,71,71	0
57	MG	1H	3474	1/1	0.94	0.09	93,93,93,93	0
57	MG	1H	3218	1/1	0.94	0.21	37,37,37,37	0
57	MG	1G	1684	1/1	0.94	0.06	96,96,96,96	0
57	MG	13	1718	1/1	0.94	0.09	90,90,90,90	0
57	MG	1H	3030	1/1	0.94	0.10	39,39,39,39	0
57	MG	14	3321	1/1	0.94	0.08	69,69,69,69	0
57	MG	1H	3473	1/1	0.94	0.13	95,95,95,95	0
57	MG	1H	3365	1/1	0.94	0.16	67,67,67,67	0
57	MG	1G	1658	1/1	0.95	0.06	104,104,104,104	0
57	MG	14	3136	1/1	0.95	0.46	92,92,92,92	0
57	MG	1H	3326	1/1	0.95	0.10	62,62,62,62	0
57	MG	1G	1665	1/1	0.95	0.05	91,91,91,91	0
57	MG	14	3058	1/1	0.95	0.34	84,84,84,84	0
57	MG	14	3174	1/1	0.95	0.08	89,89,89,89	0
57	MG	14	3085	1/1	0.95	0.25	88,88,88,88	0
57	MG	1G	1653	1/1	0.95	0.11	97,97,97,97	0
57	MG	1H	3257	1/1	0.95	0.14	43,43,43,43	0
57	MG	14	3272	1/1	0.95	0.09	71,71,71,71	0
57	MG	14	3065	1/1	0.95	0.10	47,47,47,47	0
57	MG	1H	3381	1/1	0.95	0.11	74,74,74,74	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	14	3179	1/1	0.95	0.32	77,77,77,77	0
57	MG	14	3030	1/1	0.95	0.36	57,57,57,57	0
57	MG	13	1611	1/1	0.95	0.25	70,70,70,70	0
57	MG	1H	3493	1/1	0.95	0.05	101,101,101,101	0
57	MG	1H	3514	1/1	0.95	0.05	98,98,98,98	0
57	MG	1G	1616	1/1	0.95	0.13	94,94,94,94	0
57	MG	14	3062	1/1	0.95	0.25	59,59,59,59	0
57	MG	14	3021	1/1	0.95	0.35	38,38,38,38	0
57	MG	14	3028	1/1	0.95	0.33	45,45,45,45	0
57	MG	14	3053	1/1	0.95	0.07	95,95,95,95	0
57	MG	13	1624	1/1	0.95	0.32	59,59,59,59	0
57	MG	14	3353	1/1	0.95	0.08	83,83,83,83	0
57	MG	1G	1617	1/1	0.95	0.11	116,116,116,116	0
57	MG	1H	3068	1/1	0.95	0.40	72,72,72,72	0
57	MG	14	3195	1/1	0.95	0.25	78,78,78,78	0
57	MG	1H	3249	1/1	0.95	0.13	63,63,63,63	0
57	MG	1H	3316	1/1	0.95	0.07	78,78,78,78	0
57	MG	14	3126	1/1	0.95	0.28	72,72,72,72	0
57	MG	1H	3054	1/1	0.95	0.35	52,52,52,52	0
57	MG	1H	3110	1/1	0.95	0.23	79,79,79,79	0
57	MG	14	3320	1/1	0.95	0.09	53,53,53,53	0
57	MG	1H	3377	1/1	0.95	0.09	76,76,76,76	0
57	MG	1G	1638	1/1	0.95	0.14	127,127,127,127	0
57	MG	1H	3096	1/1	0.95	0.15	64,64,64,64	0
57	MG	2K	102	1/1	0.95	0.17	78,78,78,78	0
57	MG	1H	3182	1/1	0.95	0.57	60,60,60,60	0
57	MG	1H	3052	1/1	0.95	0.18	59,59,59,59	0
57	MG	14	3370	1/1	0.95	0.06	97,97,97,97	0
57	MG	1H	3017	1/1	0.95	0.29	62,62,62,62	0
57	MG	13	1703	1/1	0.95	0.13	70,70,70,70	0
57	MG	13	1688	1/1	0.95	0.10	109,109,109,109	0
57	MG	14	3247	1/1	0.95	0.09	52,52,52,52	0
57	MG	14	3363	1/1	0.95	0.09	107,107,107,107	0
58	PAR	13	1741	42/42	0.95	0.24	64,71,75,82	0
57	MG	1H	3289	1/1	0.95	0.12	59,59,59,59	0
57	MG	1H	3159	1/1	0.95	0.13	80,80,80,80	0
57	MG	1H	3139	1/1	0.95	0.35	71,71,71,71	0
57	MG	1H	3355	1/1	0.95	0.09	59,59,59,59	0
57	MG	1H	3344	1/1	0.95	0.08	103,103,103,103	0
57	MG	1H	3459	1/1	0.95	0.13	75,75,75,75	0
57	MG	1H	3467	1/1	0.95	0.03	84,84,84,84	0
57	MG	14	3192	1/1	0.95	0.28	74,74,74,74	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1H	3039	1/1	0.95	0.20	33,33,33,33	0
57	MG	14	3246	1/1	0.95	0.13	61,61,61,61	0
57	MG	1H	3282	1/1	0.95	0.04	71,71,71,71	0
57	MG	1H	3472	1/1	0.95	0.04	83,83,83,83	0
57	MG	31	302	1/1	0.95	0.16	77,77,77,77	0
57	MG	1H	3019	1/1	0.95	0.23	32,32,32,32	0
57	MG	1H	3233	1/1	0.95	0.08	93,93,93,93	0
57	MG	1H	3269	1/1	0.95	0.16	41,41,41,41	0
57	MG	14	3334	1/1	0.95	0.10	60,60,60,60	0
57	MG	14	3300	1/1	0.95	0.09	89,89,89,89	0
57	MG	1H	3260	1/1	0.95	0.19	42,42,42,42	0
57	MG	14	3329	1/1	0.95	0.06	105,105,105,105	0
57	MG	14	3092	1/1	0.95	0.26	66,66,66,66	0
57	MG	1H	3143	1/1	0.95	0.37	50,50,50,50	0
57	MG	14	3189	1/1	0.95	0.33	51,51,51,51	0
57	MG	14	3351	1/1	0.95	0.11	78,78,78,78	0
57	MG	1H	3047	1/1	0.95	0.15	55,55,55,55	0
57	MG	1J	203	1/1	0.95	0.26	73,73,73,73	0
57	MG	14	3087	1/1	0.95	0.27	76,76,76,76	0
57	MG	1H	3179	1/1	0.95	0.14	80,80,80,80	0
57	MG	14	3288	1/1	0.95	0.19	49,49,49,49	0
57	MG	1H	3200	1/1	0.95	0.26	71,71,71,71	0
57	MG	13	1721	1/1	0.95	0.17	106,106,106,106	0
57	MG	14	3290	1/1	0.95	0.22	59,59,59,59	0
57	MG	14	3036	1/1	0.95	0.27	85,85,85,85	0
57	MG	I8	102	1/1	0.95	0.05	62,62,62,62	0
57	MG	45	201	1/1	0.95	0.13	101,101,101,101	0
57	MG	14	3248	1/1	0.95	0.29	47,47,47,47	0
57	MG	13	1636	1/1	0.95	0.28	74,74,74,74	0
57	MG	14	3281	1/1	0.95	0.16	69,69,69,69	0
57	MG	13	1646	1/1	0.95	0.17	71,71,71,71	0
57	MG	14	3315	1/1	0.95	0.12	68,68,68,68	0
57	MG	1H	3284	1/1	0.95	0.07	83,83,83,83	0
57	MG	14	3283	1/1	0.95	0.07	68,68,68,68	0
57	MG	1H	3072	1/1	0.95	0.20	58,58,58,58	0
57	MG	1H	3250	1/1	0.95	0.18	41,41,41,41	0
57	MG	1H	3297	1/1	0.96	0.14	49,49,49,49	0
57	MG	14	3217	1/1	0.96	0.20	56,56,56,56	0
57	MG	1H	3461	1/1	0.96	0.06	45,45,45,45	0
57	MG	1H	3248	1/1	0.96	0.11	44,44,44,44	0
57	MG	1H	3402	1/1	0.96	0.05	85,85,85,85	0
57	MG	14	3364	1/1	0.96	0.07	92,92,92,92	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1H	3022	1/1	0.96	0.19	49,49,49,49	0
57	MG	14	3287	1/1	0.96	0.11	88,88,88,88	0
57	MG	13	1736	1/1	0.96	0.12	101,101,101,101	0
57	MG	14	3016	1/1	0.96	0.38	74,74,74,74	0
57	MG	1H	3463	1/1	0.96	0.09	81,81,81,81	0
57	MG	14	3031	1/1	0.96	0.28	73,73,73,73	0
57	MG	13	1680	1/1	0.96	0.16	64,64,64,64	0
57	MG	1H	3342	1/1	0.96	0.06	86,86,86,86	0
57	MG	14	3280	1/1	0.96	0.14	61,61,61,61	0
57	MG	1H	3275	1/1	0.96	0.18	57,57,57,57	0
57	MG	13	1699	1/1	0.96	0.09	83,83,83,83	0
57	MG	14	3078	1/1	0.96	0.29	56,56,56,56	0
57	MG	14	3089	1/1	0.96	0.24	54,54,54,54	0
57	MG	1H	3317	1/1	0.96	0.07	66,66,66,66	0
57	MG	1H	3290	1/1	0.96	0.12	55,55,55,55	0
57	MG	13	1692	1/1	0.96	0.18	72,72,72,72	0
57	MG	14	3261	1/1	0.96	0.17	59,59,59,59	0
57	MG	14	3116	1/1	0.96	0.13	88,88,88,88	0
57	MG	13	1608	1/1	0.96	0.08	76,76,76,76	0
57	MG	14	3240	1/1	0.96	0.12	73,73,73,73	0
57	MG	1G	1603	1/1	0.96	0.14	88,88,88,88	0
57	MG	1H	3070	1/1	0.96	0.34	75,75,75,75	0
57	MG	1H	3387	1/1	0.96	0.10	33,33,33,33	0
57	MG	1H	3305	1/1	0.96	0.14	63,63,63,63	0
57	MG	1H	3033	1/1	0.96	0.25	70,70,70,70	0
57	MG	1H	3112	1/1	0.96	0.26	55,55,55,55	0
57	MG	14	3082	1/1	0.96	0.49	79,79,79,79	0
57	MG	14	3096	1/1	0.96	0.20	65,65,65,65	0
57	MG	14	3140	1/1	0.96	0.13	51,51,51,51	0
57	MG	1G	1631	1/1	0.96	0.56	92,92,92,92	0
57	MG	13	1693	1/1	0.96	0.07	85,85,85,85	0
57	MG	1H	3369	1/1	0.96	0.08	44,44,44,44	0
57	MG	1H	3208	1/1	0.96	0.15	72,72,72,72	0
57	MG	1H	3335	1/1	0.96	0.14	48,48,48,48	0
57	MG	14	3234	1/1	0.96	0.18	57,57,57,57	0
57	MG	1H	3272	1/1	0.96	0.09	63,63,63,63	0
57	MG	1H	3426	1/1	0.96	0.05	74,74,74,74	0
57	MG	14	3182	1/1	0.96	0.36	74,74,74,74	0
57	MG	1H	3399	1/1	0.96	0.06	73,73,73,73	0
57	MG	1H	3471	1/1	0.96	0.12	90,90,90,90	0
57	MG	14	3044	1/1	0.96	0.18	57,57,57,57	0
57	MG	14	3219	1/1	0.96	0.10	57,57,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1H	3318	1/1	0.96	0.15	59,59,59,59	0
57	MG	14	3059	1/1	0.96	0.23	89,89,89,89	0
57	MG	13	1632	1/1	0.96	0.22	78,78,78,78	0
57	MG	13	1614	1/1	0.96	0.34	84,84,84,84	0
57	MG	14	3372	1/1	0.96	0.12	86,86,86,86	0
57	MG	1H	3183	1/1	0.96	0.21	70,70,70,70	0
57	MG	1H	3464	1/1	0.96	0.08	63,63,63,63	0
57	MG	1H	3287	1/1	0.96	0.08	71,71,71,71	0
57	MG	1H	3263	1/1	0.96	0.19	46,46,46,46	0
57	MG	1H	3214	1/1	0.96	0.47	77,77,77,77	0
57	MG	14	3102	1/1	0.96	0.56	85,85,85,85	0
57	MG	14	3394	1/1	0.96	0.05	91,91,91,91	0
57	MG	1H	3324	1/1	0.96	0.08	70,70,70,70	0
57	MG	1H	3495	1/1	0.96	0.05	97,97,97,97	0
57	MG	1H	3286	1/1	0.96	0.12	40,40,40,40	0
57	MG	14	3310	1/1	0.96	0.15	54,54,54,54	0
57	MG	1H	3024	1/1	0.96	0.24	83,83,83,83	0
57	MG	1H	3258	1/1	0.96	0.11	47,47,47,47	0
57	MG	1H	3400	1/1	0.96	0.12	53,53,53,53	0
57	MG	14	3012	1/1	0.96	0.32	57,57,57,57	0
57	MG	1H	3025	1/1	0.96	0.35	75,75,75,75	0
57	MG	13	1689	1/1	0.96	0.07	88,88,88,88	0
57	MG	1H	3338	1/1	0.96	0.11	66,66,66,66	0
57	MG	1H	3014	1/1	0.96	0.17	53,53,53,53	0
57	MG	1H	3207	1/1	0.96	0.24	92,92,92,92	0
57	MG	14	3194	1/1	0.96	0.22	80,80,80,80	0
57	MG	1G	1698	1/1	0.96	0.10	123,123,123,123	0
57	MG	13	1652	1/1	0.96	0.62	71,71,71,71	0
57	MG	13	1705	1/1	0.96	0.17	97,97,97,97	0
57	MG	14	3324	1/1	0.96	0.15	48,48,48,48	0
57	MG	1H	3042	1/1	0.96	0.26	65,65,65,65	0
57	MG	14	3314	1/1	0.96	0.16	69,69,69,69	0
57	MG	1H	3440	1/1	0.96	0.09	92,92,92,92	0
57	MG	13	1690	1/1	0.96	0.05	70,70,70,70	0
57	MG	1H	3199	1/1	0.96	0.12	61,61,61,61	0
57	MG	14	3027	1/1	0.96	0.14	66,66,66,66	0
57	MG	1H	3323	1/1	0.96	0.17	57,57,57,57	0
57	MG	1H	3307	1/1	0.96	0.14	44,44,44,44	0
57	MG	1H	3166	1/1	0.96	0.43	78,78,78,78	0
57	MG	1H	3465	1/1	0.96	0.09	67,67,67,67	0
57	MG	1H	3188	1/1	0.96	0.41	49,49,49,49	0
57	MG	13	1604	1/1	0.96	0.15	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1H	3330	1/1	0.96	0.10	71,71,71,71	0
57	MG	13	1623	1/1	0.96	0.22	76,76,76,76	0
57	MG	1H	3029	1/1	0.96	0.32	77,77,77,77	0
57	MG	1H	3315	1/1	0.97	0.10	63,63,63,63	0
57	MG	1H	3056	1/1	0.97	0.31	49,49,49,49	0
57	MG	14	3014	1/1	0.97	0.25	59,59,59,59	0
57	MG	1H	3328	1/1	0.97	0.13	47,47,47,47	0
57	MG	14	3045	1/1	0.97	0.20	53,53,53,53	0
57	MG	14	3308	1/1	0.97	0.10	94,94,94,94	0
57	MG	1H	3040	1/1	0.97	0.31	44,44,44,44	0
57	MG	14	3004	1/1	0.97	0.28	63,63,63,63	0
57	MG	1H	3448	1/1	0.97	0.07	80,80,80,80	0
57	MG	1H	3036	1/1	0.97	0.16	37,37,37,37	0
57	MG	14	3293	1/1	0.97	0.10	63,63,63,63	0
57	MG	21	303	1/1	0.97	0.09	46,46,46,46	0
57	MG	14	3253	1/1	0.97	0.07	58,58,58,58	0
57	MG	1H	3439	1/1	0.97	0.07	67,67,67,67	0
57	MG	1H	3364	1/1	0.97	0.09	44,44,44,44	0
57	MG	13	1734	1/1	0.97	0.10	94,94,94,94	0
57	MG	14	3048	1/1	0.97	0.47	51,51,51,51	0
57	MG	14	3239	1/1	0.97	0.17	77,77,77,77	0
57	MG	1G	1672	1/1	0.97	0.12	110,110,110,110	0
57	MG	1G	1651	1/1	0.97	0.11	76,76,76,76	0
57	MG	14	3081	1/1	0.97	0.15	56,56,56,56	0
57	MG	14	3199	1/1	0.97	0.38	76,76,76,76	0
57	MG	1G	1601	1/1	0.97	0.20	77,77,77,77	0
57	MG	14	3086	1/1	0.97	0.23	56,56,56,56	0
57	MG	1H	3466	1/1	0.97	0.05	72,72,72,72	0
57	MG	13	1605	1/1	0.97	0.20	71,71,71,71	0
57	MG	14	3037	1/1	0.97	0.26	65,65,65,65	0
57	MG	16	211	1/1	0.97	0.11	73,73,73,73	0
57	MG	1H	3090	1/1	0.97	0.21	42,42,42,42	0
57	MG	1H	3264	1/1	0.97	0.25	50,50,50,50	0
57	MG	14	3032	1/1	0.97	0.41	64,64,64,64	0
57	MG	1H	3247	1/1	0.97	0.14	36,36,36,36	0
57	MG	14	3375	1/1	0.97	0.07	93,93,93,93	0
57	MG	14	3026	1/1	0.97	0.29	56,56,56,56	0
57	MG	1G	1661	1/1	0.97	0.08	95,95,95,95	0
57	MG	13	1606	1/1	0.97	0.26	72,72,72,72	0
57	MG	1H	3353	1/1	0.97	0.14	48,48,48,48	0
57	MG	1H	3027	1/1	0.97	0.19	52,52,52,52	0
57	MG	14	3002	1/1	0.97	0.37	57,57,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1H	3273	1/1	0.97	0.14	78,78,78,78	0
57	MG	1H	3012	1/1	0.97	0.42	58,58,58,58	0
57	MG	1H	3265	1/1	0.97	0.08	46,46,46,46	0
57	MG	1H	3413	1/1	0.97	0.10	78,78,78,78	0
57	MG	1H	3011	1/1	0.97	0.30	56,56,56,56	0
57	MG	1H	3306	1/1	0.97	0.09	75,75,75,75	0
57	MG	1H	3186	1/1	0.97	0.26	62,62,62,62	0
57	MG	14	3171	1/1	0.97	0.34	56,56,56,56	0
57	MG	1H	3437	1/1	0.97	0.09	92,92,92,92	0
57	MG	13	1602	1/1	0.97	0.14	120,120,120,120	0
57	MG	14	3226	1/1	0.97	0.16	51,51,51,51	0
57	MG	1H	3169	1/1	0.97	0.45	91,91,91,91	0
57	MG	1H	3304	1/1	0.97	0.10	58,58,58,58	0
57	MG	14	3270	1/1	0.97	0.13	67,67,67,67	0
57	MG	1H	3411	1/1	0.97	0.07	63,63,63,63	0
57	MG	1H	3382	1/1	0.97	0.09	49,49,49,49	0
57	MG	13	1609	1/1	0.97	0.15	70,70,70,70	0
57	MG	1H	3354	1/1	0.97	0.17	60,60,60,60	0
57	MG	14	3093	1/1	0.97	0.42	84,84,84,84	0
57	MG	14	3052	1/1	0.97	0.23	54,54,54,54	0
57	MG	14	3101	1/1	0.97	0.33	87,87,87,87	0
57	MG	1H	3361	1/1	0.97	0.07	52,52,52,52	0
57	MG	14	3231	1/1	0.97	0.23	55,55,55,55	0
57	MG	1H	3262	1/1	0.97	0.18	43,43,43,43	0
57	MG	1H	3018	1/1	0.97	0.18	41,41,41,41	0
57	MG	13	1663	1/1	0.97	0.10	107,107,107,107	0
57	MG	14	3228	1/1	0.98	0.14	56,56,56,56	0
57	MG	1G	1627	1/1	0.98	0.41	87,87,87,87	0
57	MG	14	3206	1/1	0.98	0.27	85,85,85,85	0
57	MG	1H	3398	1/1	0.98	0.07	78,78,78,78	0
57	MG	14	3229	1/1	0.98	0.13	59,59,59,59	0
57	MG	1H	3252	1/1	0.98	0.09	65,65,65,65	0
57	MG	1H	3152	1/1	0.98	0.41	70,70,70,70	0
57	MG	14	3322	1/1	0.98	0.14	58,58,58,58	0
57	MG	1H	3280	1/1	0.98	0.15	36,36,36,36	0
57	MG	1G	1607	1/1	0.98	0.20	86,86,86,86	0
57	MG	14	3294	1/1	0.98	0.05	75,75,75,75	0
57	MG	1H	3210	1/1	0.98	0.18	56,56,56,56	0
57	MG	14	3040	1/1	0.98	0.25	68,68,68,68	0
57	MG	1H	3327	1/1	0.98	0.08	50,50,50,50	0
57	MG	14	3235	1/1	0.98	0.24	48,48,48,48	0
57	MG	14	3305	1/1	0.98	0.12	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1H	3016	1/1	0.98	0.19	44,44,44,44	0
57	MG	13	1648	1/1	0.98	0.16	67,67,67,67	0
57	MG	1H	3255	1/1	0.98	0.08	49,49,49,49	0
57	MG	1H	3319	1/1	0.98	0.18	57,57,57,57	0
57	MG	14	3147	1/1	0.98	0.40	69,69,69,69	0
57	MG	1H	3359	1/1	0.98	0.17	44,44,44,44	0
57	MG	13	1603	1/1	0.98	0.24	74,74,74,74	0
57	MG	1H	3044	1/1	0.98	0.36	67,67,67,67	0
57	MG	1H	3187	1/1	0.98	0.42	44,44,44,44	0
57	MG	1G	1633	1/1	0.98	0.21	118,118,118,118	0
57	MG	1H	3045	1/1	0.98	0.28	46,46,46,46	0
57	MG	14	3341	1/1	0.98	0.12	66,66,66,66	0
57	MG	1H	3254	1/1	0.98	0.08	46,46,46,46	0
57	MG	1H	3281	1/1	0.98	0.15	61,61,61,61	0
57	MG	13	1619	1/1	0.98	0.21	52,52,52,52	0
57	MG	29	301	1/1	0.98	0.35	58,58,58,58	0
57	MG	1H	3015	1/1	0.98	0.31	51,51,51,51	0
57	MG	1H	3333	1/1	0.98	0.13	77,77,77,77	0
57	MG	13	1702	1/1	0.98	0.13	85,85,85,85	0
57	MG	13	1601	1/1	0.98	0.42	80,80,80,80	0
57	MG	1H	3302	1/1	0.98	0.13	51,51,51,51	0
57	MG	1H	3311	1/1	0.98	0.09	53,53,53,53	0
57	MG	1H	3278	1/1	0.98	0.09	75,75,75,75	0
57	MG	1H	3380	1/1	0.98	0.18	55,55,55,55	0
57	MG	14	3047	1/1	0.98	0.34	65,65,65,65	0
57	MG	1H	3385	1/1	0.98	0.15	25,25,25,25	0
57	MG	14	3301	1/1	0.98	0.04	85,85,85,85	0
57	MG	14	3356	1/1	0.98	0.06	75,75,75,75	0
57	MG	14	3013	1/1	0.98	0.23	47,47,47,47	0
57	MG	14	3019	1/1	0.98	0.35	57,57,57,57	0
57	MG	14	3325	1/1	0.98	0.04	79,79,79,79	0
57	MG	13	1621	1/1	0.98	0.09	85,85,85,85	0
60	ZN	5A	101	1/1	0.98	0.09	146,146,146,146	0
57	MG	1H	3292	1/1	0.98	0.21	43,43,43,43	0
57	MG	14	3034	1/1	0.98	0.48	40,40,40,40	0
57	MG	14	3066	1/1	0.98	0.57	61,61,61,61	0
57	MG	1G	1622	1/1	0.98	0.20	125,125,125,125	0
57	MG	14	3216	1/1	0.98	0.21	52,52,52,52	0
57	MG	14	3222	1/1	0.98	0.20	59,59,59,59	0
57	MG	1H	3349	1/1	0.98	0.12	50,50,50,50	0
57	MG	1H	3097	1/1	0.98	0.06	65,65,65,65	0
57	MG	14	3191	1/1	0.98	0.26	67,67,67,67	0

Continued on next page...

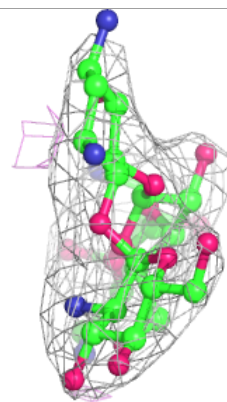
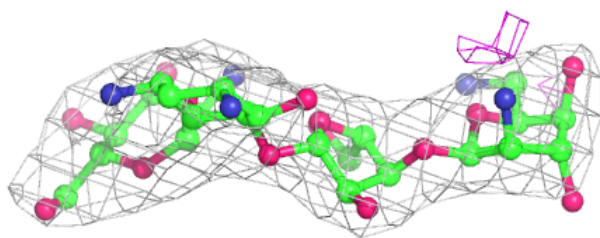
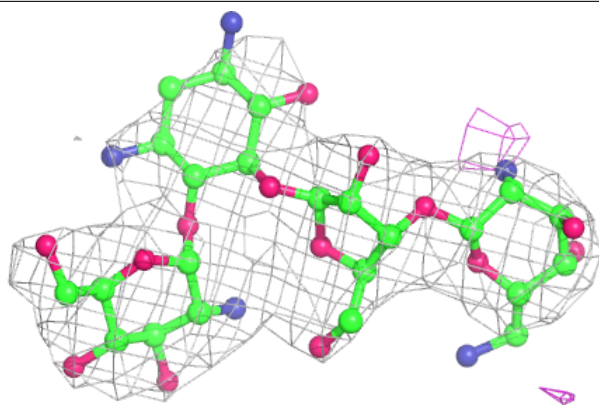
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
57	MG	1H	3322	1/1	0.98	0.06	58,58,58,58	0
57	MG	1H	3325	1/1	0.99	0.15	46,46,46,46	0
57	MG	1H	3121	1/1	0.99	0.24	39,39,39,39	0
57	MG	1H	3091	1/1	0.99	0.15	41,41,41,41	0
59	SF4	3E	301	8/8	0.99	0.21	82,91,95,98	0
57	MG	13	1607	1/1	0.99	0.20	72,72,72,72	0
57	MG	13	1630	1/1	0.99	0.34	96,96,96,96	0
57	MG	1H	3059	1/1	0.99	0.27	56,56,56,56	0
57	MG	14	3242	1/1	0.99	0.10	62,62,62,62	0
59	SF4	32	302	8/8	0.99	0.17	100,109,118,124	0
57	MG	1H	3291	1/1	0.99	0.13	59,59,59,59	0
60	ZN	5I	102	1/1	0.99	0.13	86,86,86,86	0
57	MG	1H	3032	1/1	0.99	0.25	47,47,47,47	0
57	MG	1H	3360	1/1	0.99	0.09	78,78,78,78	0
57	MG	14	3056	1/1	0.99	0.11	54,54,54,54	0
57	MG	14	3055	1/1	0.99	0.30	60,60,60,60	0
57	MG	1H	3060	1/1	0.99	0.16	35,35,35,35	0
57	MG	1H	3031	1/1	0.99	0.14	51,51,51,51	0
57	MG	1H	3450	1/1	1.00	0.06	44,44,44,44	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

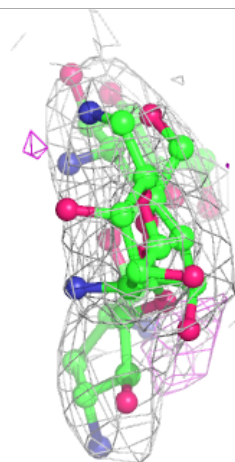
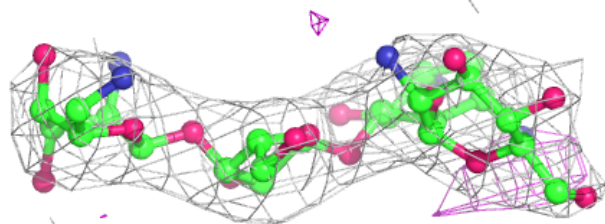
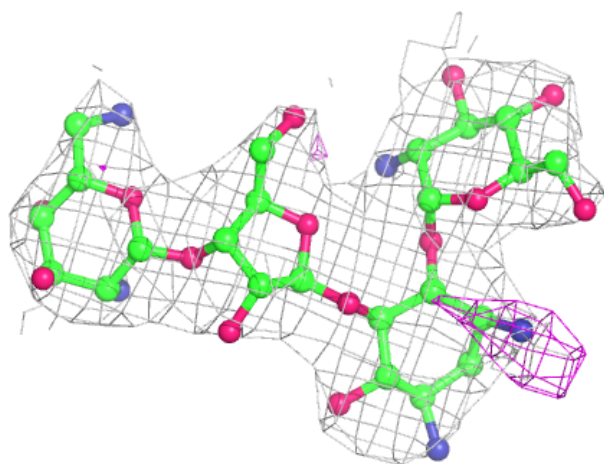
Electron density around PAR 1G 1702:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PAR 13 1741:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.