



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 6, 2020 – 06:20 am BST

PDB ID : 6OTR
Title : Dimeric E.coli YoeB bound to Thermus thermophilus 70S post-cleavage (AAU)
Authors : Pavelich, I.P.; Hoffer, E.D.; Maehigashi, T.; Dunham, C.M.
Deposited on : 2019-05-03
Resolution : 3.12 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 : **FAILED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

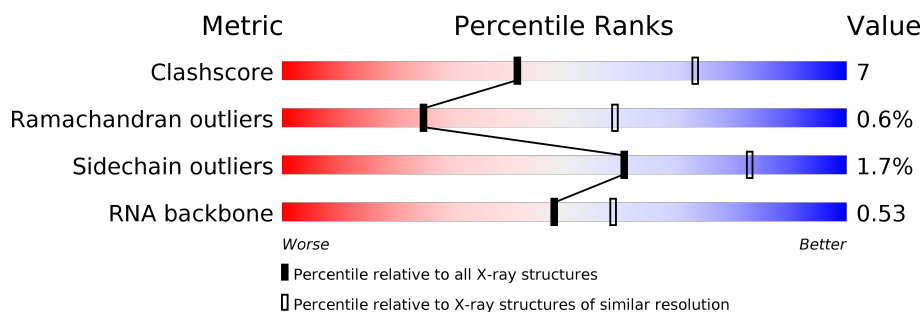
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.12 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1389 (3.14-3.10)
Ramachandran outliers	138981	1337 (3.14-3.10)
Sidechain outliers	138945	1337 (3.14-3.10)
RNA backbone	3102	1134 (3.44-2.80)












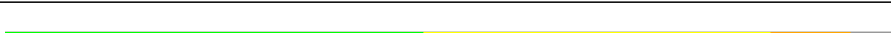


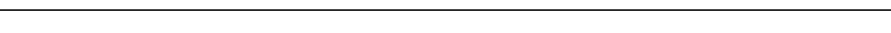




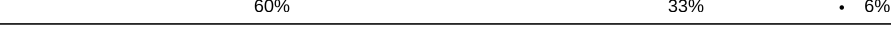





The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	QA	1521	57% 29% 11% ..
1	XA	1521	56% 31% 10% ..
2	QB	256	62% 27% . 8%
2	XB	256	57% 30% . 8%
3	QC	239	56% 27% .. 14%
3	XC	239	64% 21% . 14%
4	QD	209	77% 22% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	XD	209	
5	QE	162	
5	XE	162	
6	QF	101	
6	XF	101	
7	QG	156	
7	XG	156	
8	QH	138	
8	XH	138	
9	QI	128	
9	XI	128	
10	QJ	105	
10	XJ	105	
11	QK	129	
11	XK	129	
12	QL	132	
12	XL	132	
13	QM	126	
13	XM	126	
14	QN	61	
14	XN	61	
15	QO	89	
15	XO	89	
16	QP	88	
16	XP	88	


























Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
17	QQ	105	
17	XQ	105	
18	QR	88	
18	XR	88	
19	QS	93	
19	XS	93	
20	QT	106	
20	XT	106	
21	QU	27	
21	XU	27	
22	QV	77	
22	QW	77	
22	XV	77	
22	XW	77	
23	QX	20	
23	XX	20	
24	QY	84	
24	QZ	84	
24	XY	84	
24	XZ	84	
25	R0	85	
25	Y0	85	
26	R1	98	
26	Y1	98	
27	R2	72	















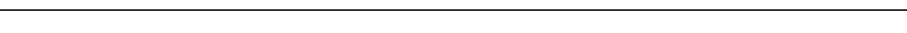




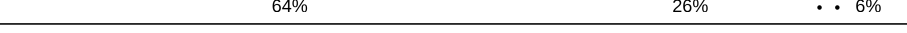





Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
27	Y2	72	
28	R3	60	
28	Y3	60	
29	R4	71	
29	Y4	71	
30	R5	60	
30	Y5	60	
31	R6	54	
31	Y6	54	
32	R7	49	
32	Y7	49	
33	R8	65	
33	Y8	65	
34	R9	37	
34	Y9	37	
35	RA	2915	
35	YA	2915	
36	RB	124	
36	YB	124	
37	RD	276	
37	YD	276	
38	RE	206	
38	YE	206	
39	RF	210	
39	YF	210	










Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
40	RG	182	
40	YG	182	
41	RH	180	
41	YH	180	
42	RI	148	
42	YI	148	
43	RN	140	
43	YN	140	
44	RO	122	
44	YO	122	
45	RP	150	
45	YP	150	
46	RQ	141	
46	YQ	141	
47	RR	118	
47	YR	118	
48	RS	112	
48	YS	112	
49	RT	146	
49	YT	146	
50	RU	118	
50	YU	118	
51	RV	101	
51	YV	101	
52	RW	113	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
52	YW	113	 89% 11%
53	RX	96	 79% 16% • •
53	YX	96	 88% 8% •
54	RY	110	 75% 21% • • •
54	YY	110	 78% 18% • •
55	RZ	206	 59% 25% • 11%
55	YZ	206	 55% 28% 5% 11%
56	ZA	3	 100%
56	ZB	3	 67% 33%

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 298517 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 rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	QA	1510	Total	C	N	O	P	0	0	0
			32452	14444	6009	10489	1510			
1	XA	1507	Total	C	N	O	P	0	0	0
			32389	14416	5999	10467	1507			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	QB	235	Total	C	N	O	S	0	0	0
			1907	1217	342	343	5			
2	XB	236	Total	C	N	O	S	0	0	0
			1915	1223	343	344	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	QC	205	Total	C	N	O	S	0	0	0
			1605	1011	313	280	1			
3	XC	205	Total	C	N	O	S	0	0	0
			1605	1011	313	280	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	QD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			
4	XD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	QE	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			
5	XE	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	QF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
6	XF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	QH	137	Total	C	N	O	S	0	0	0
			1108	700	214	192	2			
8	XH	137	Total	C	N	O	S	0	0	0
			1108	700	214	192	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	QI	127	Total	C	N	O		0	0	0
			1010	639	197	174				
9	XI	126	Total	C	N	O		0	0	0
			998	633	193	172				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	QJ	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	XJ	96	Total	C	N	O	S	0	0	0
			777	487	153	136	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	QK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			
11	XK	116	Total	C	N	O	S	0	0	0
			864	537	164	160	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	QL	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			
12	XL	122	Total	C	N	O	S	0	0	0
			956	603	193	159	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	QM	120	Total	C	N	O	S	0	0	0
			955	591	197	165	2			
13	XM	119	Total	C	N	O	S	0	0	0
			946	585	195	164	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	QO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
15	XO	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	QP	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			
16	XP	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	QQ	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			
17	XQ	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	QR	70	Total	C	N	O	0	0	0
			574	367	112	95			
18	XR	70	Total	C	N	O	0	0	0
			574	367	112	95			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	QS	83	Total	C	N	O	S	0	0	0
			665	424	124	115	2			
19	XS	83	Total	C	N	O	S	0	0	0
			665	424	124	115	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	QT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			
20	XT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	QU	25	Total	C	N	O	0	0	0
			217	134	52	31			
21	XU	25	Total	C	N	O	0	0	0
			217	134	52	31			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	QV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
22	QW	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
22	XV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
22	XW	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QX	17	Total	C	N	O	P	0	0	0
			370	167	77	110	16			
23	XX	17	Total	C	N	O	P	0	0	0
			370	167	77	110	16			

- Molecule 24 is a protein called Addiction module toxin, Txe/YoeB family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	QY	84	Total	C	N	O	S	0	0	0
			723	464	126	131	2			
24	QZ	84	Total	C	N	O	S	0	0	0
			723	464	126	131	2			
24	XY	84	Total	C	N	O	S	0	0	0
			723	464	126	131	2			
24	XZ	84	Total	C	N	O	S	0	0	0
			723	464	126	131	2			

- Molecule 25 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	R0	81	Total	C	N	O	S	0	0	0
			643	398	137	107	1			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Y0	82	Total	C	N	O	S	0	0	0
			648	401	138	108	1			

- Molecule 26 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	R1	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			
26	Y1	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			

- Molecule 27 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	R2	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			
27	Y2	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			

- Molecule 28 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
28	R3	59	Total	C	N	O	0	0	0
			469	298	90	81			
28	Y3	59	Total	C	N	O	0	0	0
			469	298	90	81			

- Molecule 29 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	R4	69	Total	C	N	O	S	0	0	0
			565	356	103	101	5			
29	Y4	69	Total	C	N	O	S	0	0	0
			565	356	103	101	5			

- Molecule 30 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	R5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
30	Y5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 31 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	R6	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			
31	Y6	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			

- Molecule 32 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	R7	47	Total	C	N	O	S	0	0	0
			409	251	102	54	2			
32	Y7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 33 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	R8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			
33	Y8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- Molecule 34 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	R9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
34	Y9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 35 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	RA	2891	Total	C	N	O	P	0	0	0
			62266	27713	11649	20014	2890			
35	YA	2878	Total	C	N	O	P	0	0	0
			61981	27587	11589	19928	2877			

- Molecule 36 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	RB	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			
36	YB	122	Total	C	N	O	P	0	0	0
			2617	1166	486	844	121			

- Molecule 37 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	RD	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			
37	YD	274	Total	C	N	O	S	0	0	0
			2135	1347	426	359	3			

- Molecule 38 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	RE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			
38	YE	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			

- Molecule 39 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	RF	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			
39	YF	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			

- Molecule 40 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	RG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			
40	YG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

- Molecule 41 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	RH	174	Total	C	N	O	S	0	0	0
			1336	848	251	236	1			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	YH	174	Total	C	N	O	S	0	0	0
			1336	848	251	236	1			

- Molecule 42 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	RI	145	Total	C	N	O	S	0	0	0
			1131	723	200	207	1			
42	YI	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

- Molecule 43 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	RN	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			
43	YN	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

- Molecule 44 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	RO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			
44	YO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 45 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	RP	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			
45	YP	147	Total	C	N	O	S	0	0	0
			1122	698	229	192	3			

- Molecule 46 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	RQ	139	Total	C	N	O	S	0	0	0
			1107	707	209	184	7			
46	YQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 47 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
47	RR	117	Total	C	N	O	0	0	0
			960	599	202	159			
47	YR	117	Total	C	N	O	0	0	0
			960	599	202	159			

- Molecule 48 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
48	RS	111	Total	C	N	O	0	0	0
			882	556	176	150			
48	YS	111	Total	C	N	O	0	0	0
			882	556	176	150			

- Molecule 49 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	RT	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			
49	YT	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	RU	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			
50	YU	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

- Molecule 51 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	RV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
51	YV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 52 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	RW	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			
52	YW	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			

- Molecule 53 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	RX	92	Total	C	N	O	S	0	0	0
			725	471	131	123				
53	YX	92	Total	C	N	O	S	0	0	0
			725	471	131	123				

- Molecule 54 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	RY	107	Total	C	N	O	S	0	0	0
			818	525	155	132	6			
54	YY	107	Total	C	N	O	S	0	0	0
			818	525	155	132	6			

- Molecule 55 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	RZ	183	Total	C	N	O	S	0	0	0
			1461	933	260	265	3			
55	YZ	183	Total	C	N	O	S	0	0	0
			1461	933	260	265	3			

- Molecule 56 is a RNA chain called CCPuro.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	ZA	3	Total	C	N	O	P	0	0	0
			74	40	13	19	2			
56	ZB	3	Total	C	N	O	P	0	0	0
			74	40	13	19	2			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QA	87	Total	Mg	0	0
			87	87		

Continued on next page...

Continued from previous page...

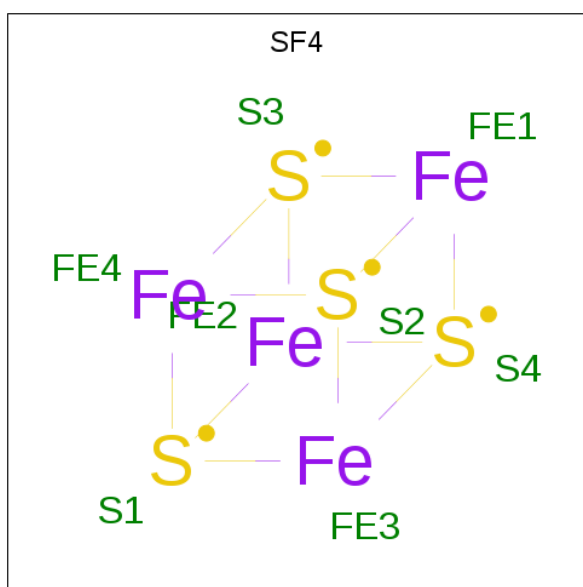
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	YV	1	Total 1	Mg 1	0	0
57	RP	1	Total 1	Mg 1	0	0
57	YA	329	Total 329	Mg 329	0	0
57	Y5	1	Total 1	Mg 1	0	0
57	YR	1	Total 1	Mg 1	0	0
57	Y9	1	Total 1	Mg 1	0	0
57	RN	1	Total 1	Mg 1	0	0
57	XE	1	Total 1	Mg 1	0	0
57	YD	2	Total 2	Mg 2	0	0
57	QV	3	Total 3	Mg 3	0	0
57	YO	1	Total 1	Mg 1	0	0
57	XA	106	Total 106	Mg 106	0	0
57	RQ	1	Total 1	Mg 1	0	0
57	R0	2	Total 2	Mg 2	0	0
57	RO	1	Total 1	Mg 1	0	0
57	YG	1	Total 1	Mg 1	0	0
57	YQ	1	Total 1	Mg 1	0	0
57	XF	1	Total 1	Mg 1	0	0
57	RR	1	Total 1	Mg 1	0	0
57	RD	1	Total 1	Mg 1	0	0
57	R5	1	Total 1	Mg 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	RA	305	Total 305	Mg 305	0	0
57	YP	1	Total 1	Mg 1	0	0
57	RE	2	Total 2	Mg 2	0	0
57	XL	1	Total 1	Mg 1	0	0
57	YB	6	Total 6	Mg 6	0	0
57	XV	4	Total 4	Mg 4	0	0
57	RB	3	Total 3	Mg 3	0	0
57	YS	1	Total 1	Mg 1	0	0
57	QE	1	Total 1	Mg 1	0	0
57	XD	1	Total 1	Mg 1	0	0
57	YE	4	Total 4	Mg 4	0	0

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).

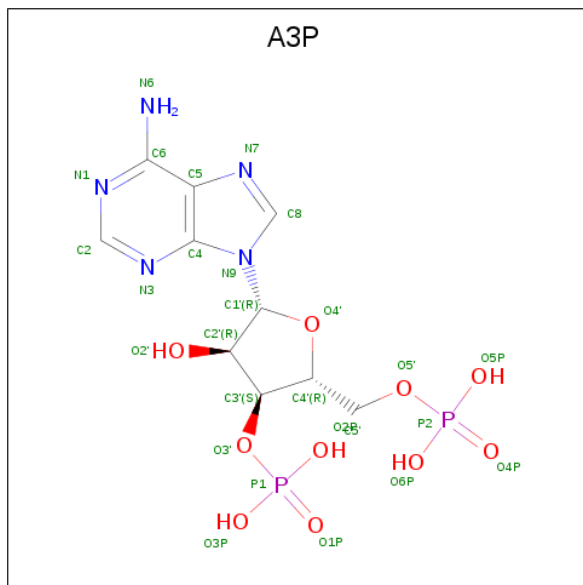


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	QD	1	Total	Fe	S	0	0
			8	4	4		
58	XD	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	Y6	1	Total	Zn	0	0
			1	1		
59	R9	1	Total	Zn	0	0
			1	1		
59	R6	1	Total	Zn	0	0
			1	1		
59	QN	1	Total	Zn	0	0
			1	1		
59	XN	1	Total	Zn	0	0
			1	1		

- Molecule 60 is ADENOSINE-3'-5'-DIPHOSPHATE (three-letter code: A3P) (formula: C₁₀H₁₅N₅O₁₀P₂).



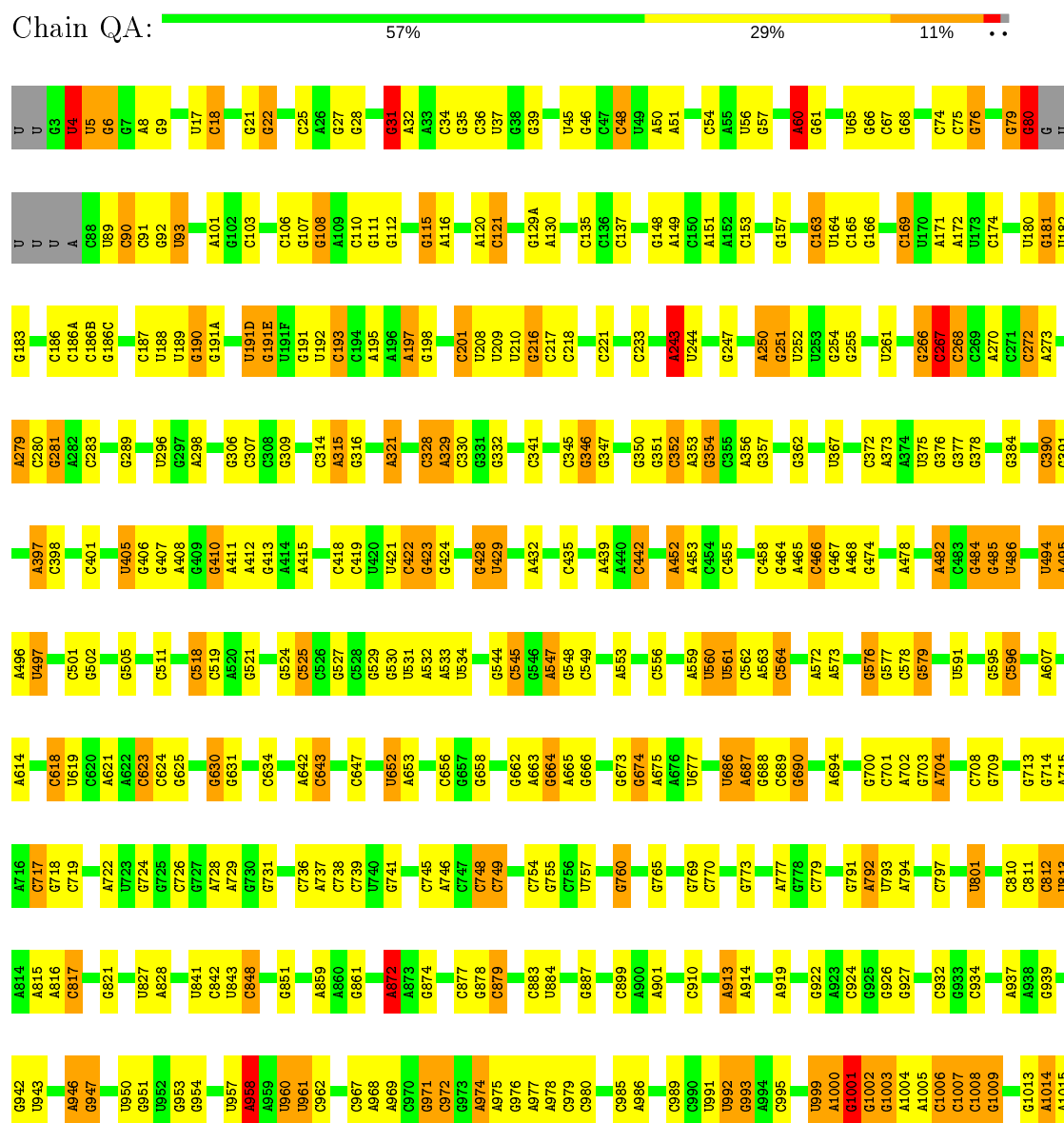
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
60	QX	1	Total	C	N	O P	0	0
			26	10	5 9	2		
60	XX	1	Total	C	N	O P	0	0
			26	10	5 9	2		

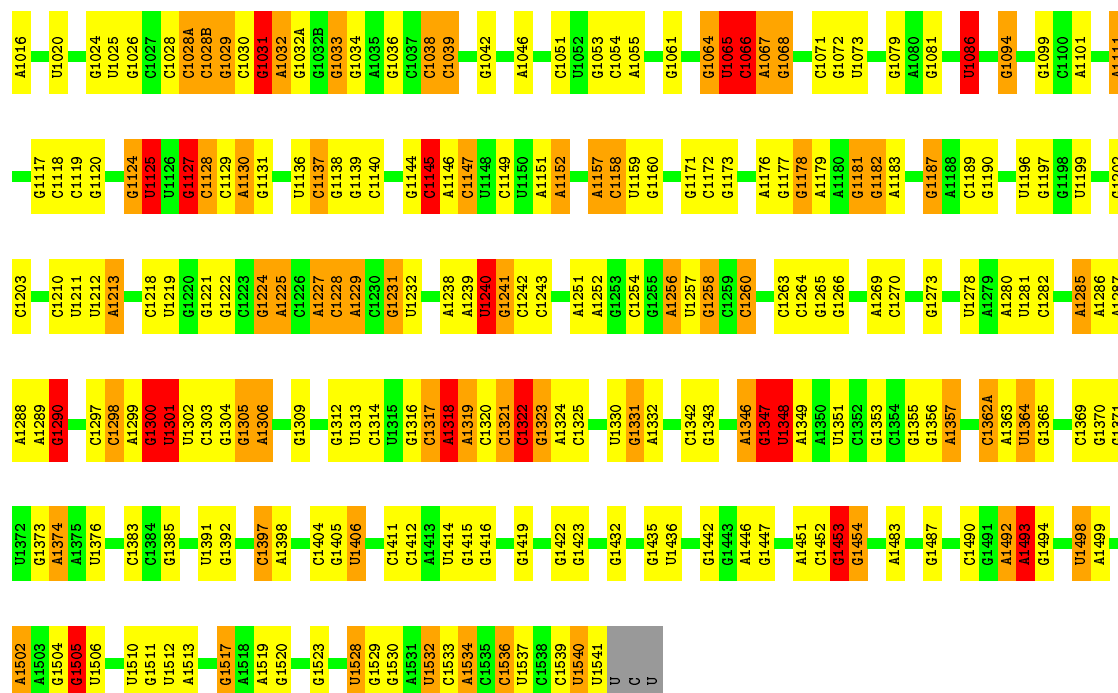
3 Residue-property plots [i](#)

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

Note EDS failed to run properly.

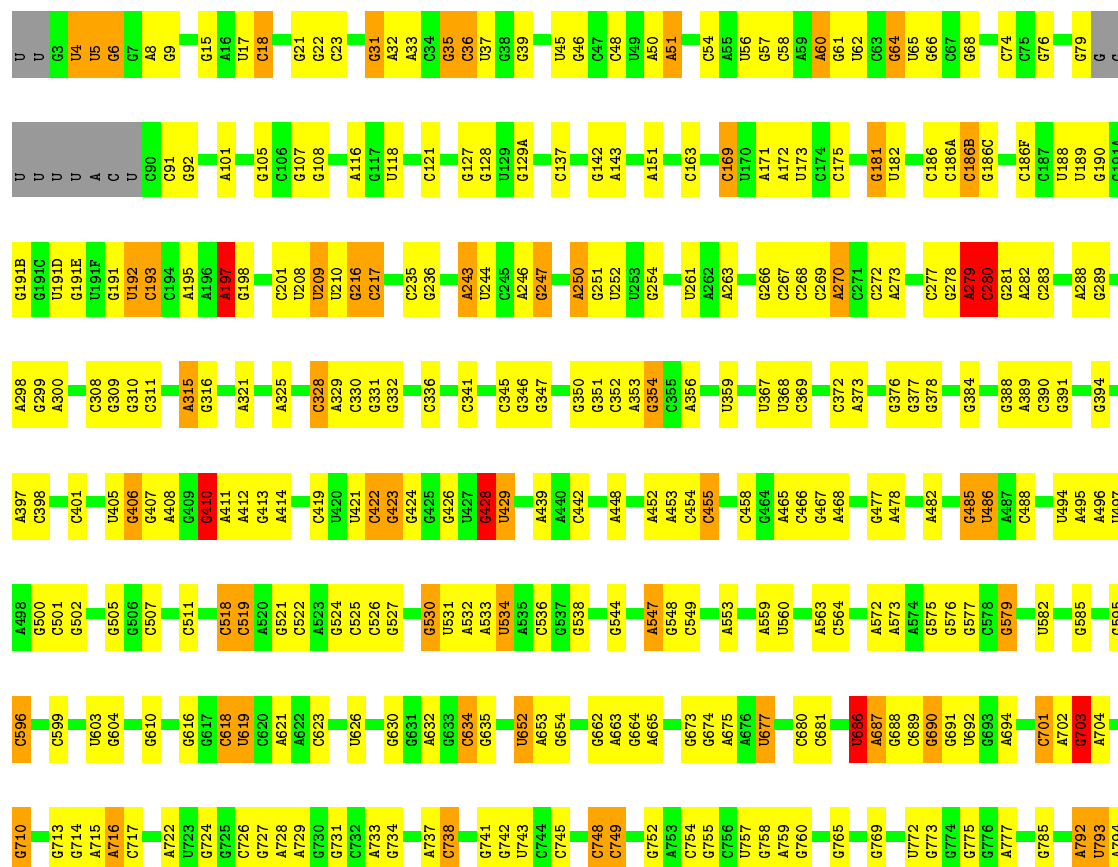
- Molecule 1: 16S rRNA

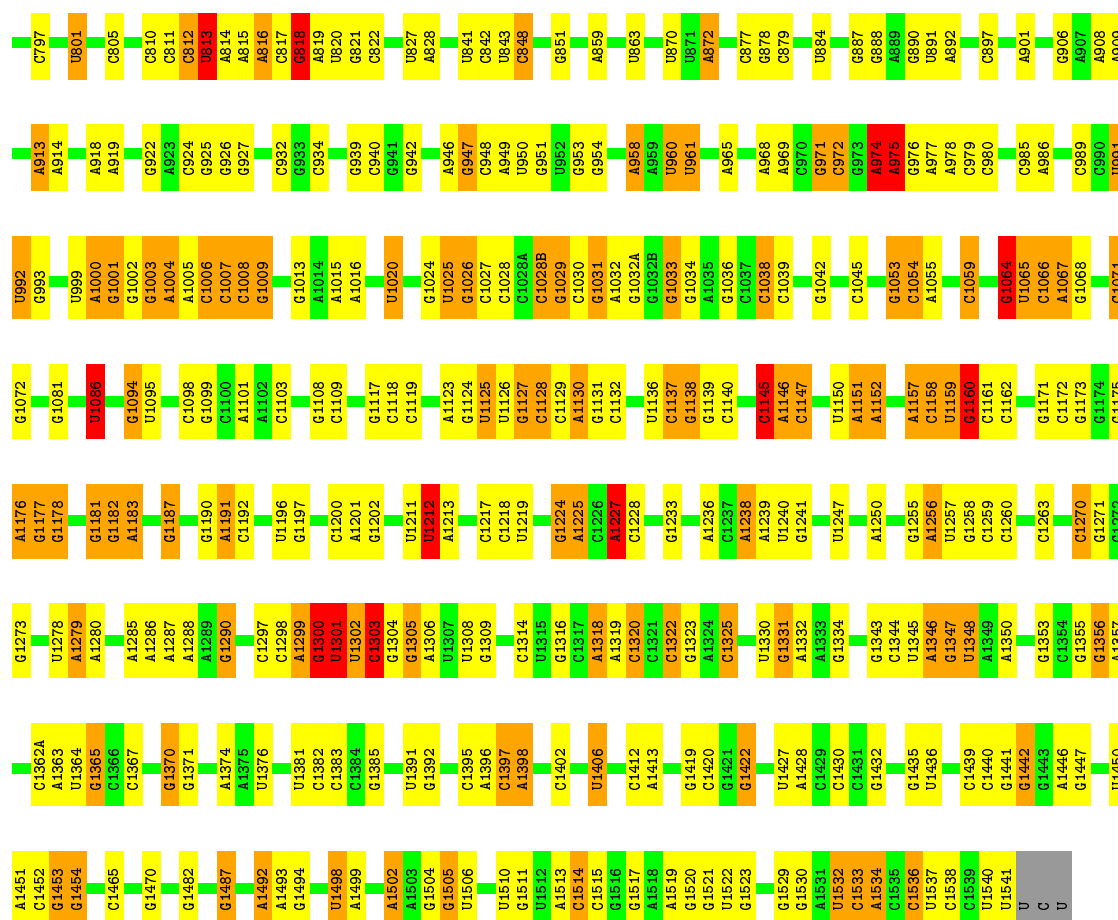




- Molecule 1: 16S rRNA

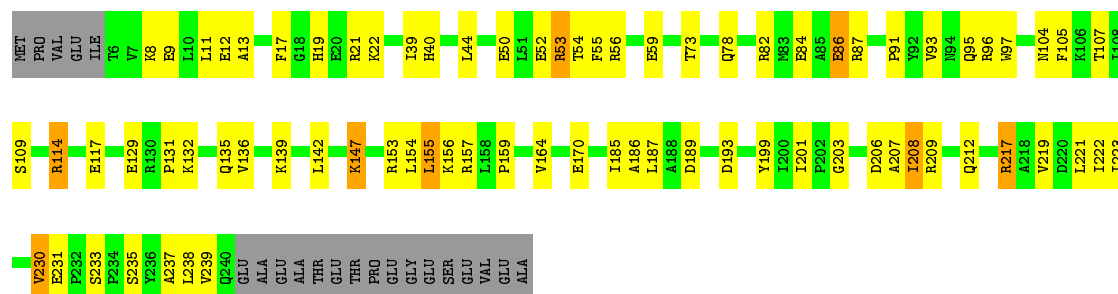
Chain XA:





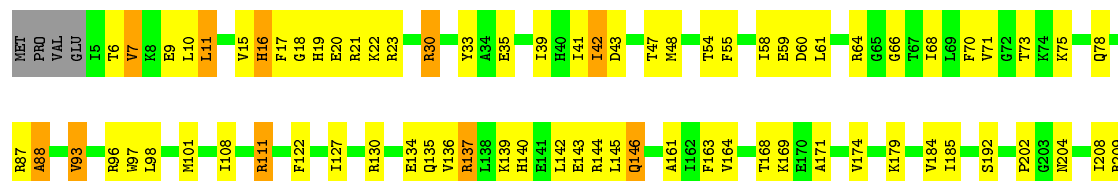
• Molecule 2: 30S ribosomal protein S2

Chain QB: 62% 27% 8%



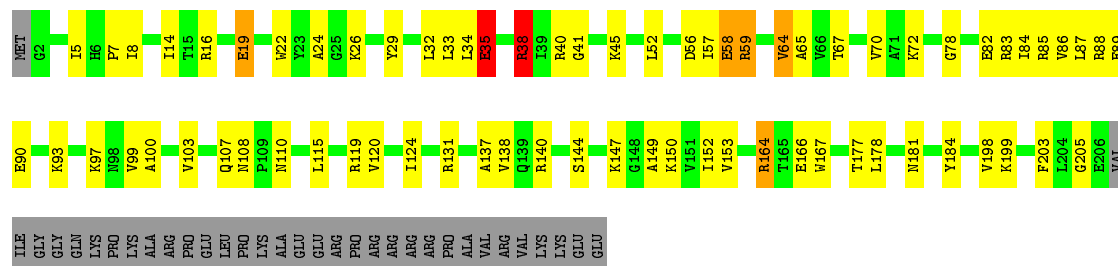
• Molecule 2: 30S ribosomal protein S2

Chain XB: 57% 30% 8%

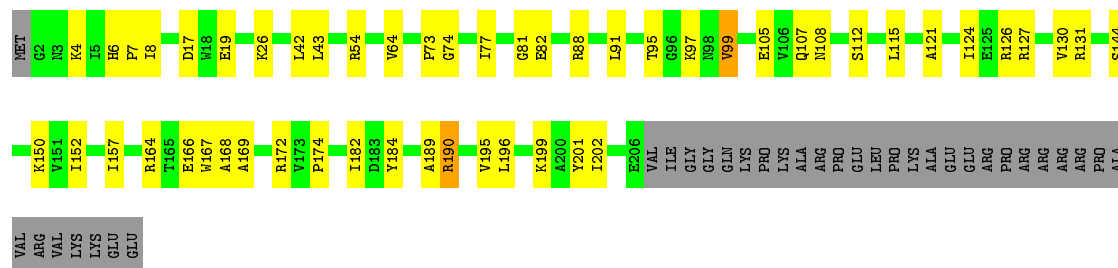




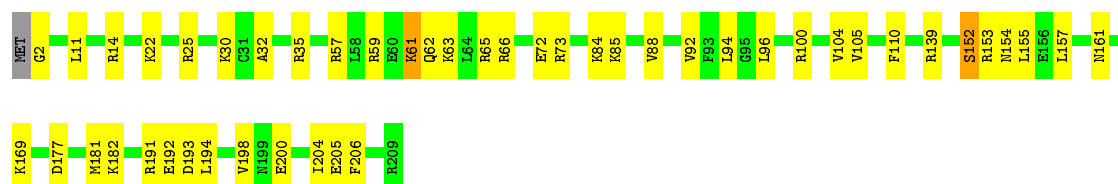
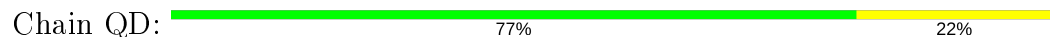
• Molecule 3: 30S ribosomal protein S3



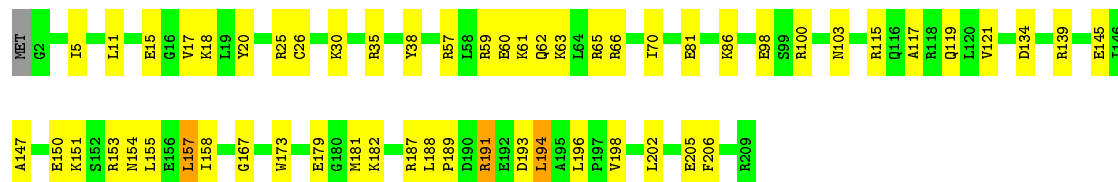
• Molecule 3: 30S ribosomal protein S3



• Molecule 4: 30S ribosomal protein S4

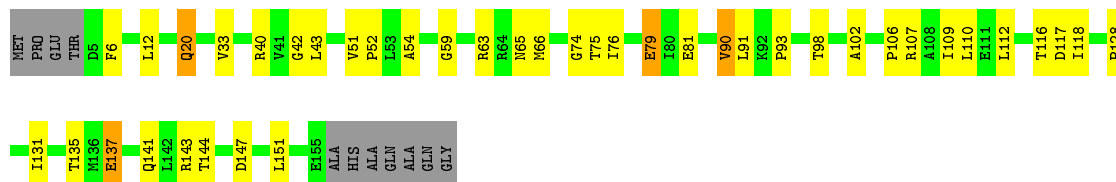


• Molecule 4: 30S ribosomal protein S4




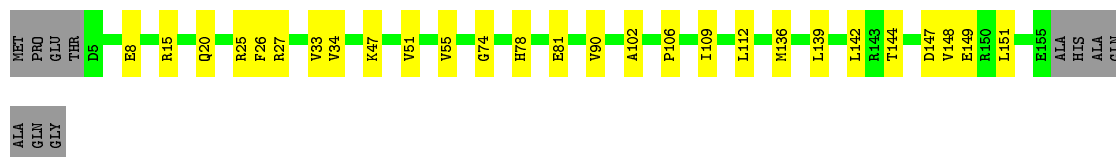
• Molecule 5: 30S ribosomal protein S5

Chain QE:  68% 23% 7%




- Molecule 5: 30S ribosomal protein S5

Chain XE:  77% 17% 7%




- Molecule 6: 30S ribosomal protein S6

Chain QF:  87% 12% 1%



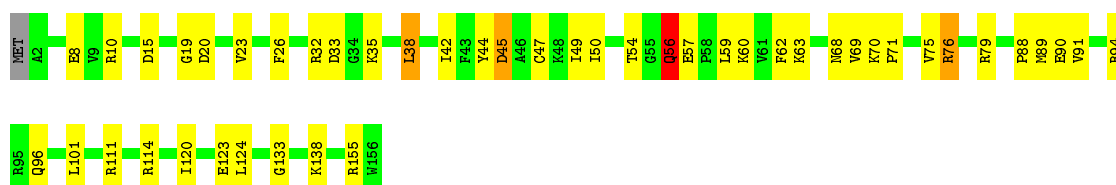
- Molecule 6: 30S ribosomal protein S6

Chain XF:  79% 21% 0%




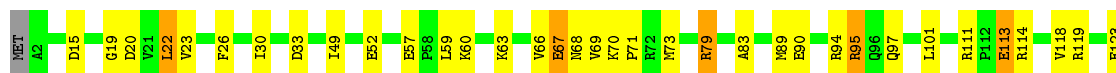
- Molecule 7: 30S ribosomal protein S7

Chain QG:  70% 27% 3%



- Molecule 7: 30S ribosomal protein S7

Chain XG:  74% 22% 4%





- Molecule 8: 30S ribosomal protein S8

Chain QH: 68% 29% ..



- Molecule 8: 30S ribosomal protein S8

Chain XH: 80% 20% .



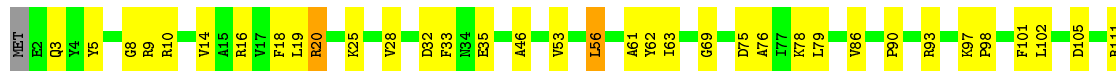
- Molecule 9: 30S ribosomal protein S9

Chain QI: 61% 33% 5% .



- Molecule 9: 30S ribosomal protein S9

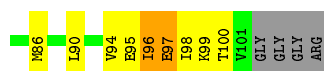
Chain XI: 69% 27% ..



- Molecule 10: 30S ribosomal protein S10

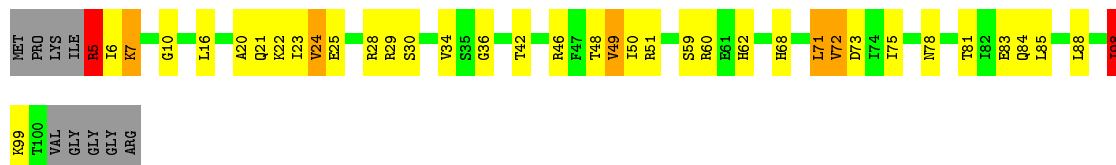
Chain QJ: 47% 39% 9% 6%





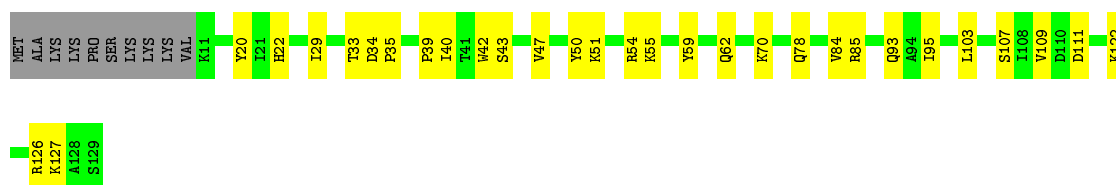
- Molecule 10: 30S ribosomal protein S10

Chain XJ: 55% 30% 5% 9%



- Molecule 11: 30S ribosomal protein S11

Chain QK: 69% 23% 8%



- Molecule 11: 30S ribosomal protein S11

Chain XK: 71% 19% 10%



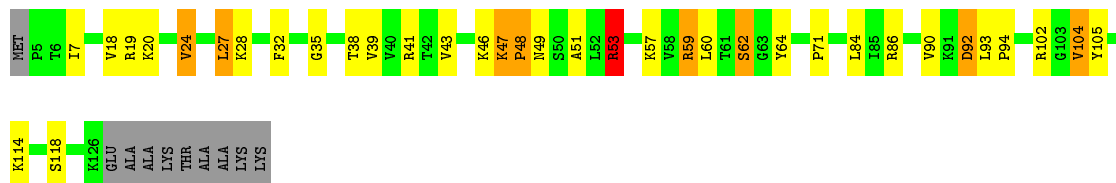
- Molecule 12: 30S ribosomal protein S12

Chain QL: 75% 18% 5%



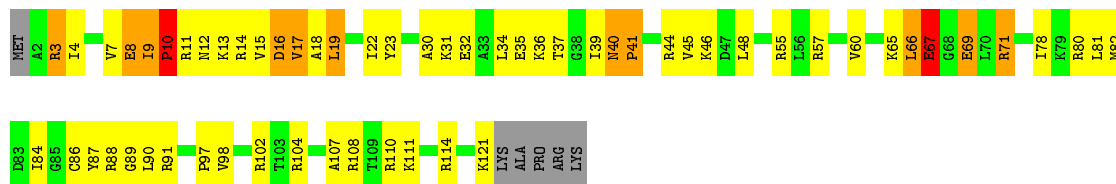
- Molecule 12: 30S ribosomal protein S12

Chain XL: 65% 20% 6% 8%



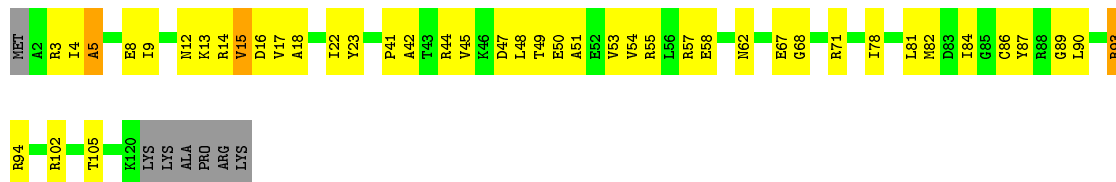
- Molecule 13: 30S ribosomal protein S13

Chain QM:  48% 37% 9% 5%




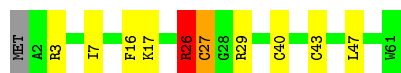
- Molecule 13: 30S ribosomal protein S13

Chain XM:  60% 33% 6%



- Molecule 14: 30S ribosomal protein S14 type Z

Chain QN:  82% 13% 3%




- Molecule 14: 30S ribosomal protein S14 type Z

Chain XN:  72% 26% 2%



- Molecule 15: 30S ribosomal protein S15

Chain QO:  83% 16% 1%




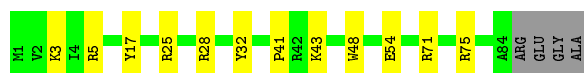
- Molecule 15: 30S ribosomal protein S15

Chain XO:  74% 19% 7%



- Molecule 16: 30S ribosomal protein S16

Chain QP:  82% 14% 5%



- Molecule 16: 30S ribosomal protein S16

Chain XP: 75% 20% 5%



- Molecule 17: 30S ribosomal protein S17

Chain QQ: 78% 17% 5%



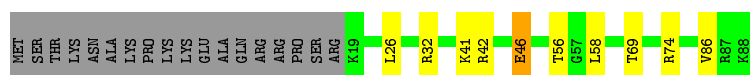
- Molecule 17: 30S ribosomal protein S17

Chain XQ: 73% 22% 5%



- Molecule 18: 30S ribosomal protein S18

Chain QR: 68% 10% 20%



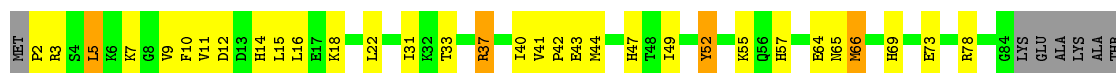
- Molecule 18: 30S ribosomal protein S18

Chain XR: 60% 18% 20%



- Molecule 19: 30S ribosomal protein S19

Chain QS: 55% 30% 11%




- Molecule 19: 30S ribosomal protein S19

Chain XS:  70% 18% 11%



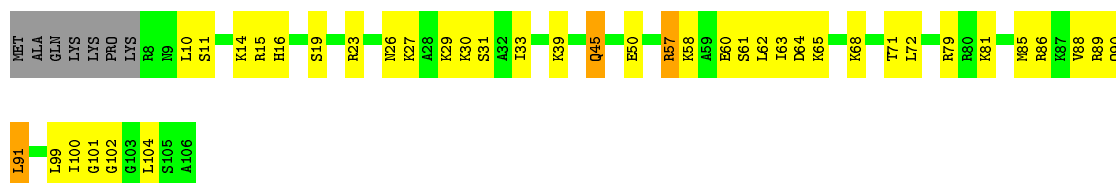
- Molecule 20: 30S ribosomal protein S20

Chain QT:  83% 9% 7%



- Molecule 20: 30S ribosomal protein S20

Chain XT:  56% 35% 7%




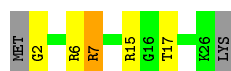
- Molecule 21: 30S ribosomal protein Thx

Chain QU:  63% 30% 7%



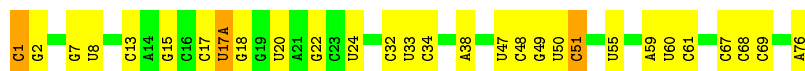
- Molecule 21: 30S ribosomal protein Thx

Chain XU:  74% 15% 7%



- Molecule 22: tRNA-fMet

Chain QV:  62% 34% 1%



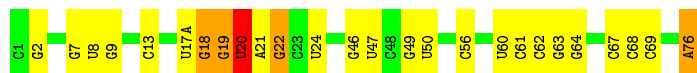
- Molecule 22: tRNA-fMet

Chain QW:  43% 44% 12%



- Molecule 22: tRNA-fMet

Chain XV:  66% 27% 5% .



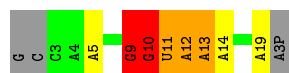
- Molecule 22: tRNA-fMet

Chain XW:  45% 43% 9% .



- Molecule 23: mRNA

Chain QX:  45% 15% 15% 10% 15%




- Molecule 23: mRNA

Chain XX:  35% 35% 15% 15%



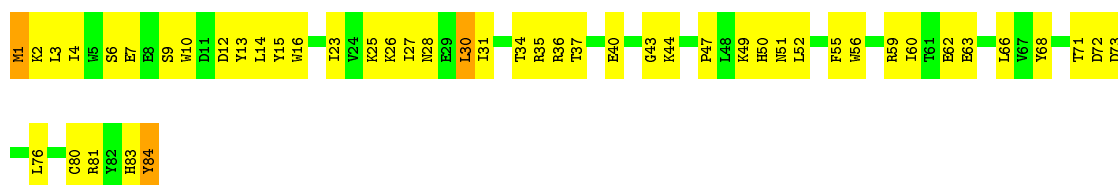
- Molecule 24: Addiction module toxin, Txe/YoeB family

Chain QY:  73% 26% .



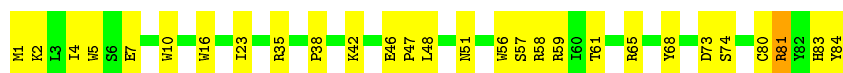
- Molecule 24: Addiction module toxin, Txe/YoeB family

Chain QZ:  43% 54% .

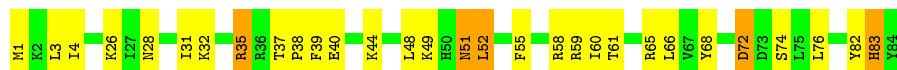


- Molecule 24: Addiction module toxin, Txe/YoeB family

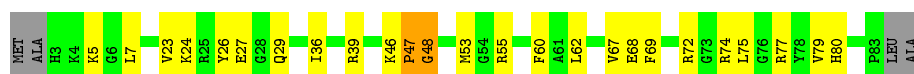
Chain XY:  67% 32% .



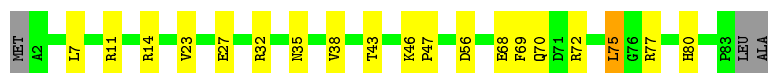
- Molecule 24: Addiction module toxin, Txe/YoeB family



- Molecule 25: 50S ribosomal protein L27



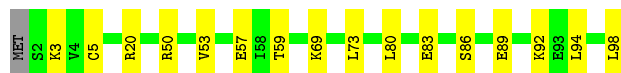
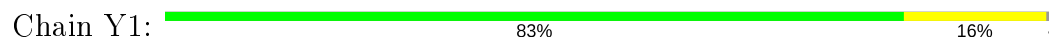
- Molecule 25: 50S ribosomal protein L27



- Molecule 26: 50S ribosomal protein L28



- Molecule 26: 50S ribosomal protein L28



- Molecule 27: 50S ribosomal protein L29



- Molecule 27: 50S ribosomal protein L29

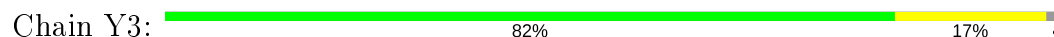




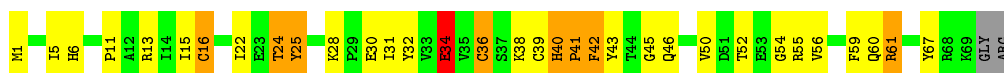
- Molecule 28: 50S ribosomal protein L30



- Molecule 28: 50S ribosomal protein L30



- Molecule 29: 50S ribosomal protein L31



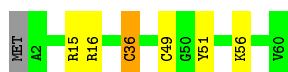
- Molecule 29: 50S ribosomal protein L31



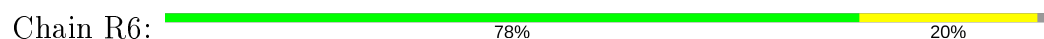
- Molecule 30: 50S ribosomal protein L32

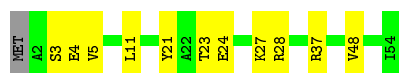


- Molecule 30: 50S ribosomal protein L32



- Molecule 31: 50S ribosomal protein L33





- Molecule 31: 50S ribosomal protein L33

Chain Y6: 83% 15% .



- Molecule 32: 50S ribosomal protein L34

Chain R7: 90% 6% .



- Molecule 32: 50S ribosomal protein L34

Chain Y7: 86% 12% .



- Molecule 33: 50S ribosomal protein L35

Chain R8: 72% 25% . .



- Molecule 33: 50S ribosomal protein L35

Chain Y8: 68% 26% 5% .



- Molecule 34: 50S ribosomal protein L36

Chain R9: 51% 35% 11% .



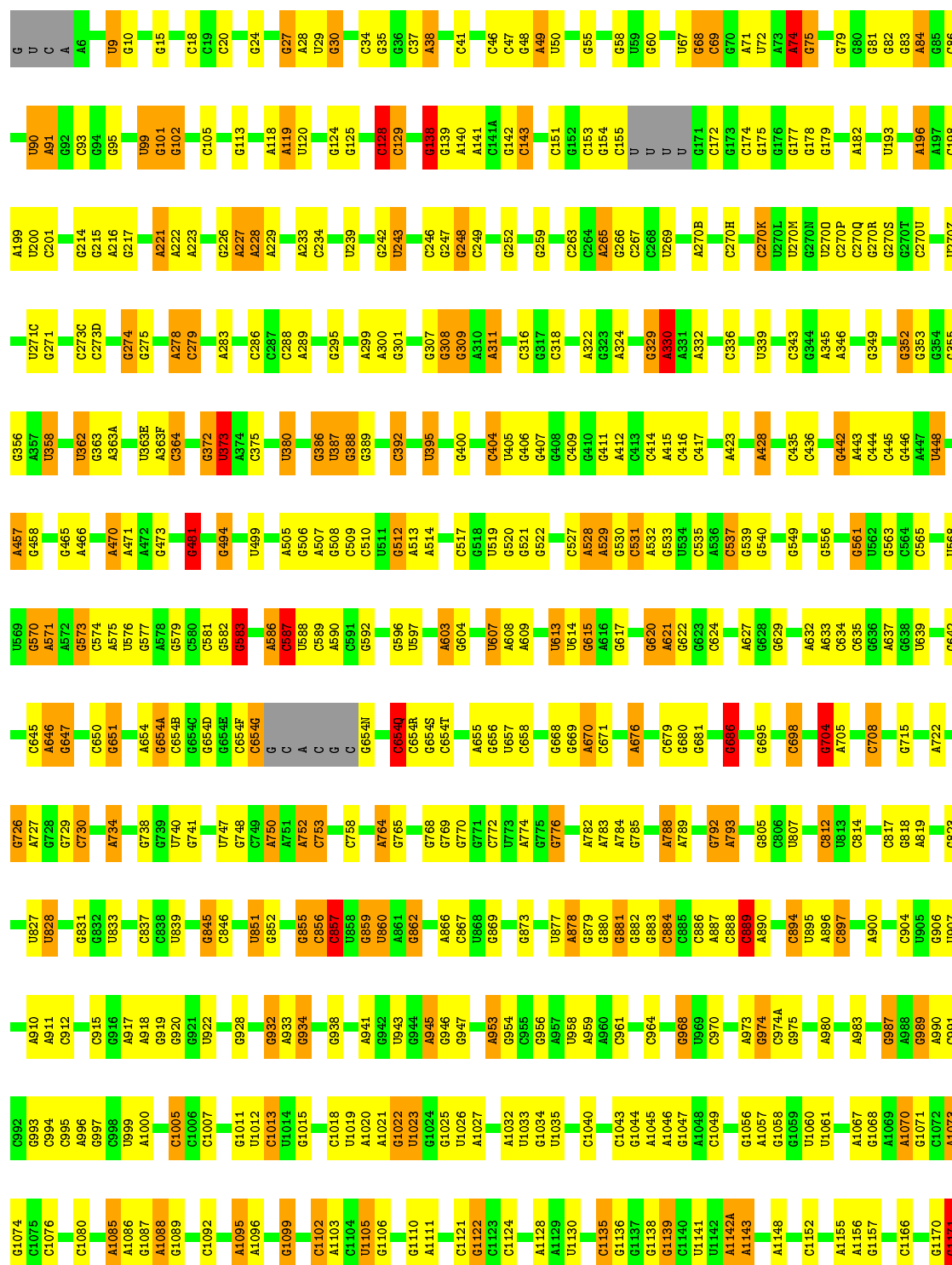
- Molecule 34: 50S ribosomal protein L36

Chain Y9: 70% 30%

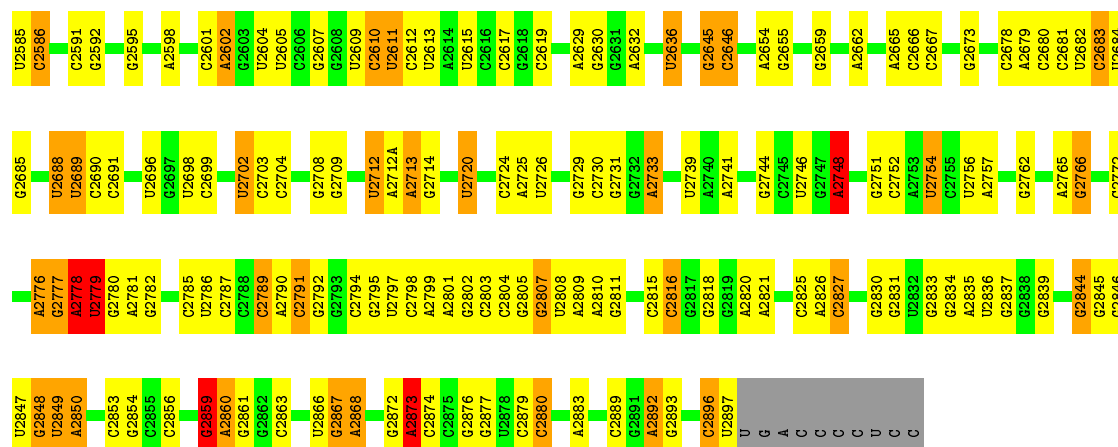


• Molecule 35: 23S rRNA

Chain RA: 56% 32% 10% ..

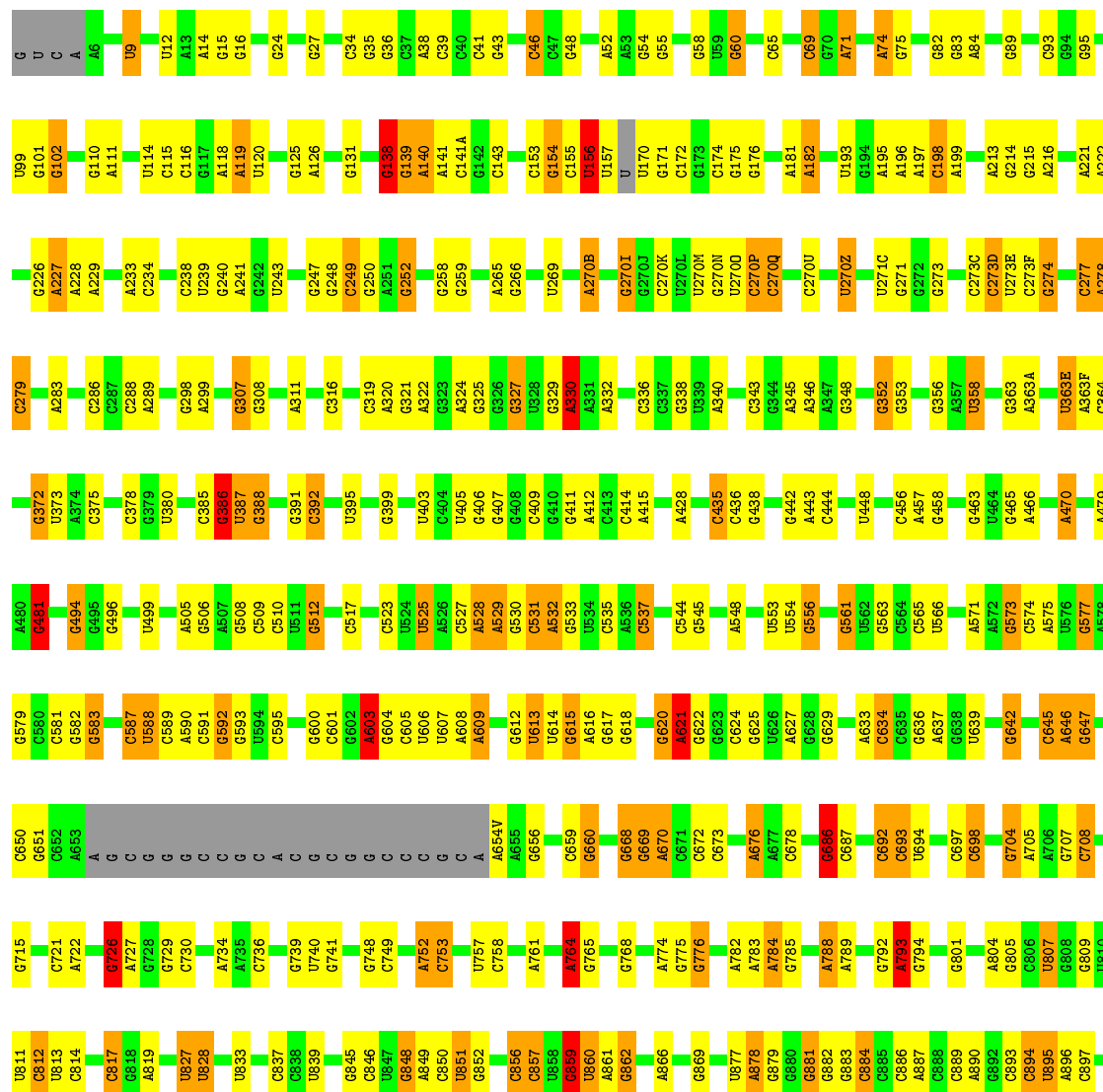


G2494	A2422	G2321	G2131	C2043	G1834	U1730	C1615	A1528	G1443	A1342	G1271	G1173
G2497	G2423	G2325	U2132	G2046	G1835	G1731	A1616	A1529	G1444	G1345	A1272	A1174
G2498	C2424	G2326	A2134	G2047	C1836	A1732	C1617	C1533	G1445	G1346	U1273	U1175
A2425	G2425	G2239	A2135	G2052	G1838	G1734	G1619	C1535	C1446	U1352	A1275	A1177
A2426	A2426	A2327	G2141	C2055	G1839	C1735	A1631	U1535	G1447	U1353	C1278	C1178
C2427	G2427	G2329	G2142	G2056	A1846	G1743	C1636	A1536	A1449	A1353	C1279	C1179
G2428	U2244	U2245	U2144	A2059	A1847	G1750	A1637	A1537	G1449A	A1354	G1280	C1180
G2429	G2429	G2246	C2146	A2060	U1851	C1751	C1638	G1538	G1450	A1359	G1281	U1188
A2430	A2430	G2247	G2147	G2061	U1963	G1755	U1639	G1539	A1451	A1360	U1282	U1187
U2431	U2431	G2248	G2148	A2062	G1964	A1756	C1640	G1541	A1453	A1361	G1283	G1191
A2432	G2250	G2253	G2149	C2063	C1965	G1756	A1641	G1542	U1454	A1365	G1285	G1196
A2435	G2253	G2253	U2150	C2065	A1966	A1757	G1642	A1543	G1455	A1366	A1286	C1196
U2438	G2259	G2260	G2156	G2069	A1970	A1762	C1644	A1545	C1458	A1367	U1287	U1197
A2439	C2260	C2261	G2157	G2080	A1971	G1764	C1648	A1547	A1460	G1368	U1288	U1198
C2440	C2261	C2261	C2161	G2086	A1972	C1771	G1649	C1550	G1461	C1370	C1290	U1199
C2441	A2266	A2266	G2162	U2086	A1872	G1772	A1652	C1551	C1467	A1378	C1293	C1202
G2442	U2272	U2272	C2163	G2087	G1878	A1772	G1653	A1554	A1471	A1379	G1294	G1203
G2444	A2273	A2273	G2164	G2088	C1879	A1773	A1654	A1558	C1474	G1380	C1295	A1204
G2445	G2274	G2274	G2165	U2089	C1880	C1774	A1657	G1560	G1475	G1385	U1300	U1205
G2446	C2275	C2275	G2166	G2090	A1881	U1775	C1657	G1562	C1478	G1386	A1302	A1214
A2448	C2276	C2276	U2167	G2091	C1882	G1776	C1658	A1566	G1479	G1388	C1304	C1304
U2449	C2279	C2279	C2168	U2092	A1885	U1779	G1667	A1567	U1482	U1391	C1305	A1220
C2450	A2283	A2283	A2170	G2093	G1888	A1780	A1668	G1568	G1483	U1394	C1306	G1228
A2451	C2284	C2284	G2171	G2094	A1889	C1781	A1669	A1569	G1484	A1395	A1307	G1228
G2454	C2285	C2285	U2172	C2095	C1890	A1786	C1670	A1570	G1485	U1396	C1233	C1233
U2457	A2286	A2286	A2173	U2098	U1891	U1786	G1678	A1571	G1488	U1397	G1310	U1234
G2458	A2287	A2287	C2178	G2099	G1899	C1790	G1674	A1572	U1489	G1400	U1312	G1236
A2459	U2291	U2291	G2183	U2100	A1900	A1791	G1678	G1573	A1490	C1404	U1313	A1241
U2460	C2292	C2292	G2184	C2103	A1901	G1792	G1681	C1574	C1493	U1405	C1314	A1242
C2461	G2293	G2293	G2184	G2104	G1906	C1797	C1686	U1578	C1499	U1406	C1315	G1243
C2465	C2294	C2294	U2189	C2108	C1909	C1800	A1689	C1585	G1502	C1407	C1317	G1244
G2468	C2295	C2295	G2190	C2111	C2021	A1801	U1693	A1586	C1505	U1415	C1319	G1248
C2469	U2296	U2296	G2191	G2112	G2022	A1802	C1694	A1587	C1506	G1416	C1320	C1251
G2470	C2297	C2297	G2192	U2113	G2023	A1803	G1695	C1588	A1507	G1417	U1326	G1252
C2471	A2298	A2298	C2196	A2114	C2026	C1804	G1697	C1598	A1508	G1418	C1327	A1253
G2472	G2304	G2304	U2197	G2115	G2027	U1805	G1699	C1600	A1509	U1419	G1328	A1254
U2473	A2305	A2305	A2198	G2116	U2028	G1816	G1699	G1601	C1510	U1420	U1329	U1255
C2474	C2306	C2306	C2205	A2117	G2029	G1817	A1698	U1602	C1513	A1421	G1332	G1256
A2475	G2307	G2307	G2209	U2119	A2030	U1818	G1699	A1603	U1514	G1429	C1333	U1263
C2476	A2309	A2309	G2210	A2120	A2031	A1819	A1700	A1608	C1430	U1430	G1334	G1264
C2477	A2310	A2310	G2211	G2123	G2032	U1820	G1703	A1609	G1523	A1437	U1338	A1265
G2481	A2311	A2311	U2212	G2124	G1929	G1824	C1708	A1610	G1524	C1428	G1339	U1267
C2482	U2312	U2312	U2213	G2125	U1930	G1827	G1725	C1611	G1526	G1429	U1340	
G2483	G2314	G2314	G2215	A2126	U1931	A1828	G1728	A1614	G1527	C1407	U1341	
G2484	C2315	C2315	A2225	G2127	C2037	G1829	G1728					
G2489	G2318	G2318	C2226	G2127	G2038	A1830	G1728					
C2490	U2319	U2319	C2226	C2128	U2041	C1830	G1728					
U2491	A2320	A2320	C2229	U2130	A2042	U1833	A1729					

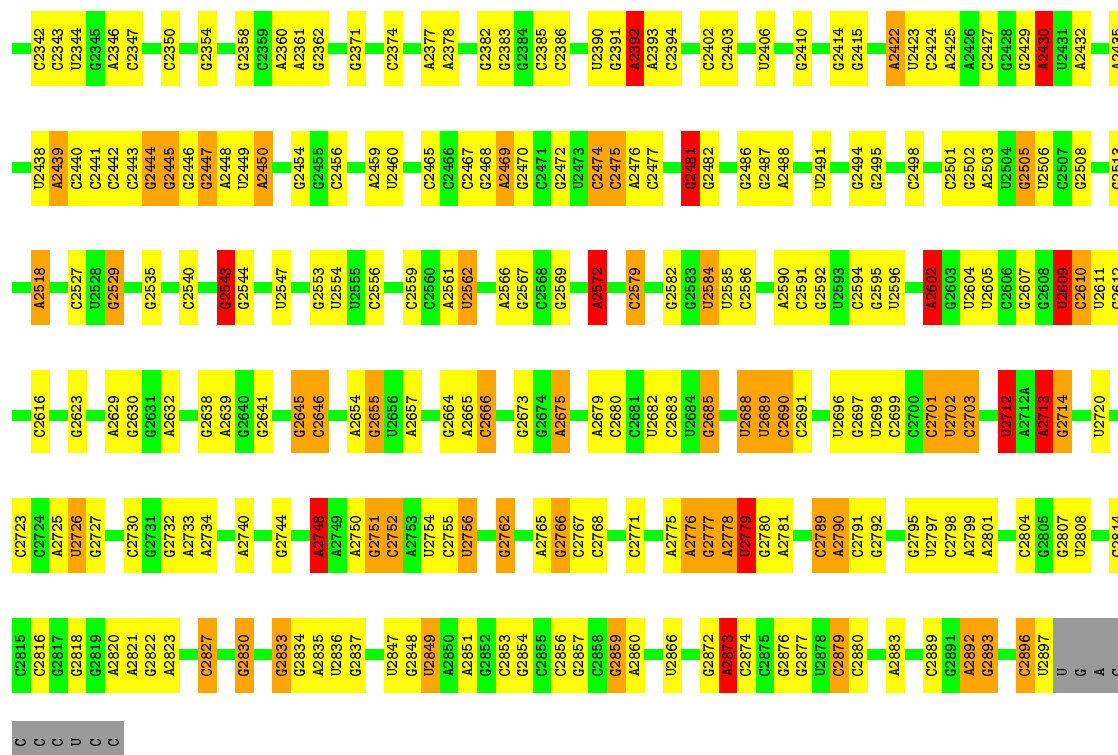


• Molecule 35: 23S rRNA

Chain YA: 57% 30% 10% ..

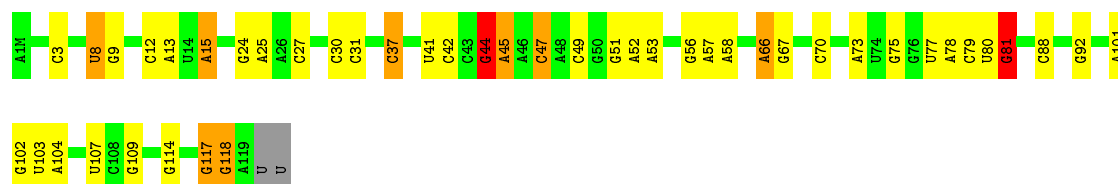


A2247	G2145	G1846	C1154	U1629	G1534	A1444A	U1340	A1254	U1159	A1070	A983	G906
G2061	C2146	A1847	A1785	C1636	U1535	A1449	U1341	U1255	U1160	G1071	A987	G907
A2052	G2147	G1858	G1756	A1637	A1536	G1449A	A1342	C1257	U1165	C1072	A988	C908
U2068	G2148	G1859	U1757	C1637	C1537	C1450	C1345	C1258	U1166	G1073	A989	A910
G2069	G2149	U1864	A1762	U1639	G1538	C1451	U1352	G1261	U1167	G1074	A990	A911
C2073	U2070	G1869	G1763	C1640	G1540	A1453	A1359	U1262	G1170	C1075	C991	C912
U2074	A1872	G1870	G1764	C1648	U1541	U1454	A1360	A1263	G1171	C1076	C992	C915
U2075	C1878	C1879	G1769	A1652	A1542	G1455	A1369	U1265	G1172	C1079	G993	G916
U2076	G1879	C1880	G1772	A1653	A1543	C1458	A1360	A1266	A1174	C1080	C994	A917
A2077	G1880	C1881	A1773	G1654	C1544	G1459	G1364	A1265	U1175	A1085	C995	A918
C1882	C1882	C1882	C1774	A1655	A1545	A1460	G1365	U1267	G1176	A1086	G997	G919
U2086	U2086	C1887	U1775	C1656	C1547	G1461	A1366	G1271	A1177	G1087	C998	U922
G2087	G2087	C1887	G1776	C1657	C1548	C1467	G1367	A1272	C1178	A1088	U999	C923
G2088	C1887	C1887	U1779	C1658	C1549	A1471	G1368	A1276	C1179	G1089	A1000	G928
U2089	A1888	A1889	A1780	G1667	A1554	G1474	C1376	A1277	C1180	C1092	G1004	G928
G1992	A1889	A1890	C1781	A1668	A1558	G1475	G1377	G1281	G1184	G1106	C1005	G929
U1993	G1896	G1896	C1782	A1669	G1559	A1476	A1378	A1286	G1185	A1095	U930	U930
C1996	G1899	G1899	A1783	G1674	G1560	C1477	G1380	A1287	G1186	A1096	G1011	G931
U1999	A1900	A1900	A1784	C1675	A1566	G1478	A1384	U1288	G1190	C1102	C1013	G932
C2105	G1906	G1906	A1785	A1676	A1567	G1478	G1385	G1294	G1191	U1105	U1019	G934
C2108	C1909	C1909	A1787	A1677	G1568	U1482	G1385	U1294	A1194	G1106	A1020	G938
G2110	G2110	G2110	C1790	G1678	A1569	G1483	U1391	C1297	G1195	G1110	A1021	G939
U2011	A1913	A1913	A1791	G1681	A1570	G1485	U1394	C1298	G1200	A1111	G1022	G940
A2019	C1914	C1914	U1794	G1687	A1572	A1488	A1395	G1299	G1200	G1112	U1023	A941
A2020	U1915	U1915	C1795	U1688	G1573	U1489	G1398	U1300	G1203	G1113	G1024	G944
C2021	C1920	C1920	G1799	A1689	C1574	A1490	C1302	A1301	A1204	G1114	G1025	A945
G2115	G1929	G1929	C1800	C1694	U1578	C1493	C1403	A1302	U1205	A1027	U1026	A946
G2116	G1930	G1930	G1801	G1695	C1585	C1493	U1405	G1303	A1210	G1122	A1028	G950
G2117	A1936	A1936	C1806	G1696	C1586	A1496	U1406	C1306	U1211	U1033	U1033	A953
U2118	A1937	A1937	A1815	G1697	A1586	U1497	U1407	A1307	G1212	G1125	G1034	G954
A2119	U1938	U1938	G1816	G1699	A1587	C1498	C1407	A1308	C1217	A1128	U1035	C955
G2120	G1940	G1940	U1817	A1698	C1588	C1499	U1415	G1309	U1220	U1130	C1041	G956
C2127	G1945	G1945	A1819	G1703	C1598	C1502	G1416	G1310	G1224	G1135	G1042	A957
C2128	U1946	U1946	U1820	G1725	C1604	C1506	G1418	G1311	A1227	G1136	G1043	U958
G2129	G1947	G1947	G1823	G1728	A1507	A1507	A1419	C1312	C1230	G1139	G1044	C961
U2130	G1948	G1948	C1827	G1729	A1508	A1508	U1420	G1313	G1231	U1141	A1045	C965
G2131	G1949	G1949	A1608	U1730	A1509	A1509	A1427	C1314	G1232	U1142	A1046	G968
U2132	G1950	G1950	A1609	U1731	A1510	A1510	C1428	C1315	G1233	A1143	G1047	U969
G2133	U1955	U1955	A1610	G1731	C1611	U1516	G1429	G1319	U1234	A1142A	C1053	C970
A2134	U1956	U1956	C1829	G1734	C1616	G1521	C1430	G1324	G1235	A1143	G1056	G971
C2137	G1959	G1959	C1830	C1735	A1617	G1522	U1433	C1327	G1236	A1148	G1057	G972
G2138	U1960	U1960	U1834	G1736	C1617	U1523	A1434	G1328	G1244	G1149	G1058	A973
C2140	C1961	C1961	C1835	C1742	A1618	U1523	G1435	U1329	G1245	A1150	G1059	G974
G2141	G1962	G1962	C1837	G1743	U1621	G1526	C1436	G1332	A1246	G1151	U1060	C974A
C2142	U1963	U1963	G1838	G1750	G1627	A1527	C1437	G1338	A1247	C1152	U1061	G975
C2143	G1964	G1964	G1839	G1750	A1628	A1528	U1439	G1339	A1253	C1153	G1064	G979
U2144										A1156		A980
A2247	G2245	G2146	C1967	U1629	G1534	A1444A	U1340	A1254	U1159	A1070	A983	G906
G2253	C2147	A1847	A1785	C1636	U1535	A1449	U1341	U1255	U1160	G1071	A987	G907
C2254	G2148	G1858	G1756	A1637	A1536	G1449A	A1342	C1257	U1165	C1072	A988	C908
G2255	G2149	G1859	U1757	C1637	C1537	C1450	C1345	C1258	U1166	G1073	A989	A910
G2256	U2068	U1864	A1762	U1639	G1538	C1451	U1352	G1261	U1167	G1074	A990	A911
U2257	G2069	G1869	G1763	C1640	G1540	A1453	A1359	U1262	G1170	C1075	C991	C912
C2258	C2073	G1870	G1764	C1648	U1541	U1454	A1360	A1263	G1171	C1076	C992	C915
G2159	U2074	A1872	G1769	A1652	A1542	G1455	A1369	U1265	G1172	C1079	G993	G916
G2160	U2075	C1878	G1772	A1653	A1543	C1458	A1360	A1266	A1174	C1080	C994	A917
G2161	U2076	G1879	A1773	G1654	C1544	G1459	G1364	A1265	U1175	A1085	C995	A918
G2162	A2077	C1880	C1774	A1655	A1545	A1460	G1365	U1267	G1176	A1086	G997	G919
C2163	C2086	C1881	C1774	C1656	C1547	G1461	A1366	G1271	A1177	G1087	C998	U922
G2165	G2087	C1882	U1775	C1657	C1548	C1467	G1367	A1272	C1178	A1088	U999	C923
G2166	G2087	C1887	G1776	C1658	C1549	A1471	G1368	A1276	C1179	G1089	A1000	G928
U2167	G2088	C1887	U1779	C1659	A1554	G1474	C1376	A1277	C1180	C1092	G1004	G928
G2168	U2089	A1888	A1780	G1667	A1558	G1475	G1377	G1281	G1184	G1106	C1005	G929
A2169	U1991	A1889	C1781	A1668	G1559	A1476	A1378	A1286	G1185	A1095	U930	U930
A2170	G1992	A1890	C1782	A1669	G1560	C1477	G1380	A1287	G1186	A1096	G1011	G931
A2171	U1993	A1899	A1783	G1674	A1566	G1478	A1384	U1288	G1190	C1102	C1013	G932
C2172	C1996	G1896	A1784	C1675	A1567	G1478	G1385	G1294	G1191	U1105	U1019	G934
C2173	U2099	G1899	A1785	A1676	G1568	U1482	G1385	U1294	A1194	G1106	A1020	G938
C2174	C1999	A1900	A1786	A1676	A1569	G1483	U1391	C1297	G1195	G1110	A1021	G939
A2175	C2105	G1906	A1787	A1677	A1570	G1485	U1394	C1298	G1200	A1111	G1022	G940
C2176	C2108	C1909	C1790	G1678	A1572	A1488	A1395	G1299	G1203	G1112	U1023	A941
C2177	G2110	G2110	A1791	G1681	A1574	U1489	G1398	U1300	A1204	G1113	G1024	G944
C2178	U2011	A1913	U1794	G1687	C1574	A1490	C1302	A1301	U1205	G1114	G1025	A945
C2286	G2111	G2111	G1799	U1688	U1578	C1493	C1403	A1302	A1210	A1027	U1026	A946
A2287	C2112	C2112	C1800	C1694	C1585	C1493	U1405	G1306	U1211	U1033	U1033	A953
C2288	G2113	G2113	G1801	G1695	C1586	A1496	U1406	A1307	G1212	G1125	G1034	G954
C2289	U2113	U2113	C1806	G1696	A1586	U1497	U1407	A1308	C1217	A1128	U1035	C955
C2290	G2114	G2114	U1794	G1697	A1587	C1498	U1415	G1309	U1220	U1130	C1041	G956
C2291	C2115	C2115	C1795	G1699	C1588	C1499	G1416	G1310	G1224	G1135	G1042	A957
C2292	G2116	G2116	G1799	A1698	C1598	C1502	G1418	G1311	A1227	G1136	G1043	U958
C2293	C2117	C2117	C1800	C1699	C1604	C1506	A1419	C1312	C1230	U1141	A1045	C961
C2294	U2022	U2022	G1801	G1699	C1604	A1507	U1420	G1313	G1231	G1139	A1046	C965
C2295	G2120	G2120	G1806	A1698	C1604	A1507	A1427	C1314	G1232	U1142	G1047	G968
C2296	C2127	C2127	A1815	G1703	C1604	A1507	C1428	C1315	U1234	A1143	C1053	C970
C2297	U2028	U2028	G1816	G1703	C1604	A1507	G1429	G1319	G1235	A1143	G1056	G971
C2298	G2029	G2029	U1817	G1703	C1604	A1507	C1429	G1327	G1236	A1148	G1057	G972
C2299	A2030	A2030	A1819	G1703	C1604	A1507	C1429	G1328	G1244	G1149	G1058	A973
C2300	G2031	G2031	G1816	U1701	C1604	A1507	C1429	G1329	G1245	A1150	G1059	G974
C2301	A2031	A2031	C1817	A1701	C1604	A1507	C1429	G1332	A1246	G1151	U1060	C974A
C2302	G2032	G2032	U1817	G1701	C1604	A1507	C1429	G1338	A1247	C1152	U1061	G975
C2303	A2033	A2033	A1819	G1703	C1604	A1507	C1429	G1339	A1253	C1153	G1064	G979
C2304	G2034	G2034	U1820	G1703	C1604	A1507	C1429	G1339	A1253	C1153	G1064	G979
C2305	U2035	U2035	G1823	G1725	C1604	A1507	C1429	G1339	A1253	C1153	G1064	G979
C2306	G2036	G2036	C1827	G1728	C1604	A1507	C1429	G1339	A1253	C1153	G1064	G979
C2307	U2037	U2037	G1829	U1730	C1604	A1507	C1429	G1339	A1253	C1153	G1064	G979
C2308	G2038	G2038	A1829	U1731	C1604	A1507	C1429	G1339	A1253	C1153	G1064	G979
C2309	U2041	U2041	C1830	G1731	C1604	A1507	C1429	G1339	A1253	C1153	G1064	G979
C2310	A2042	A2042	C1830	G1731	C1604	A1507	C1429	G1339	A1253	C1153	G1064	G979
C2311	G2043	G2043	U1834	C1734	C1604	A1507	C1429	G1339	A1253	C1153	G1064	G979
C2312	C2052	C2052	U1834	C1735	C1604	A1507	C1429	G1339	A1253	C1153	G1064	G979
C2313	G2053	G2053	C1835	C1736	C1604	A1507	C1429	G1339	A1253	C1153	G1064	G979
C2314	U2											



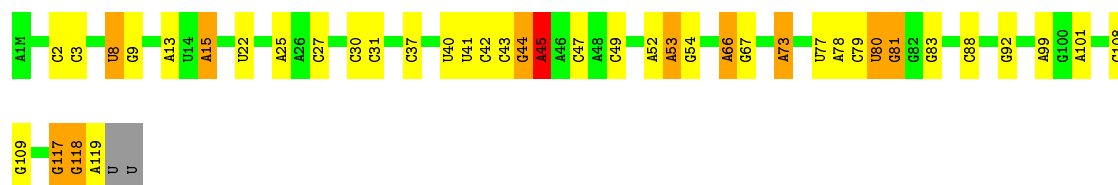
• Molecule 36: 5S rRNA

Chain RB:



• Molecule 36: 5S rRNA

Chain YB:



• Molecule 37: 50S ribosomal protein L2

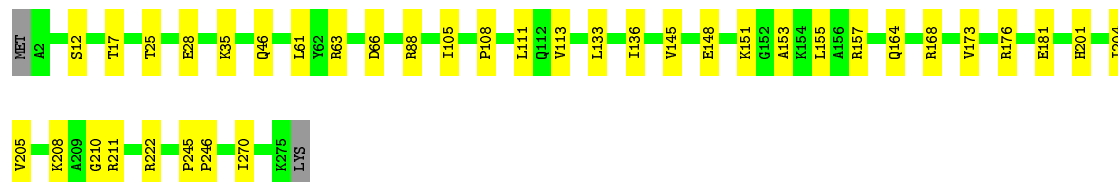
Chain RD:





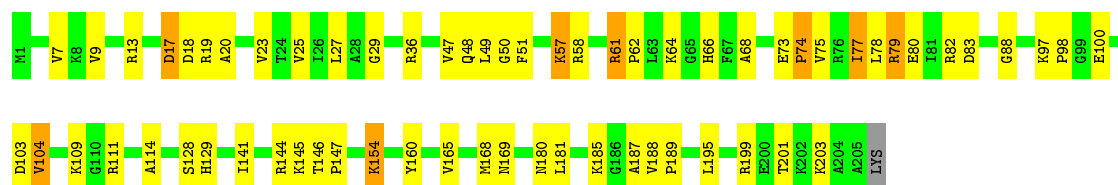
- Molecule 37: 50S ribosomal protein L2

Chain YD: 86% 13% .



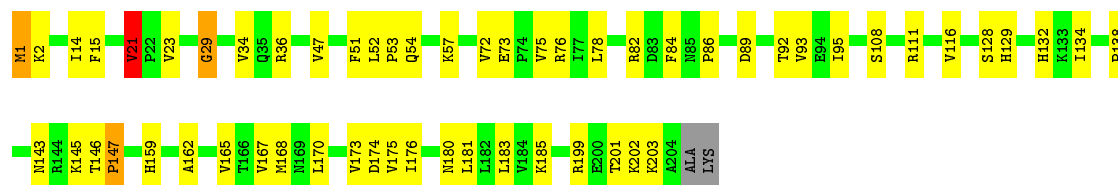
- Molecule 38: 50S ribosomal protein L3

Chain RE: 68% 27% .



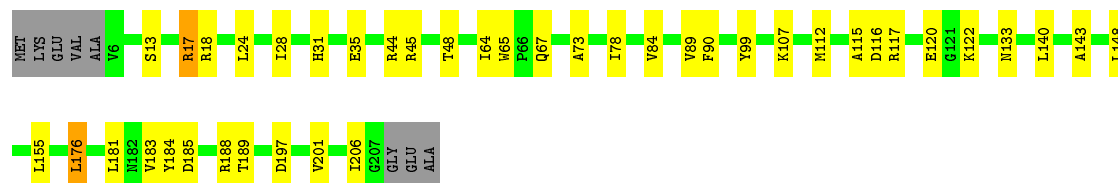
- Molecule 38: 50S ribosomal protein L3

Chain YE: 71% 26% ..



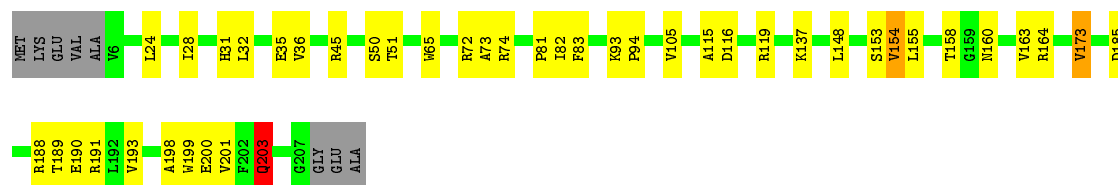
- Molecule 39: 50S ribosomal protein L4

Chain RF: 77% 19% ..



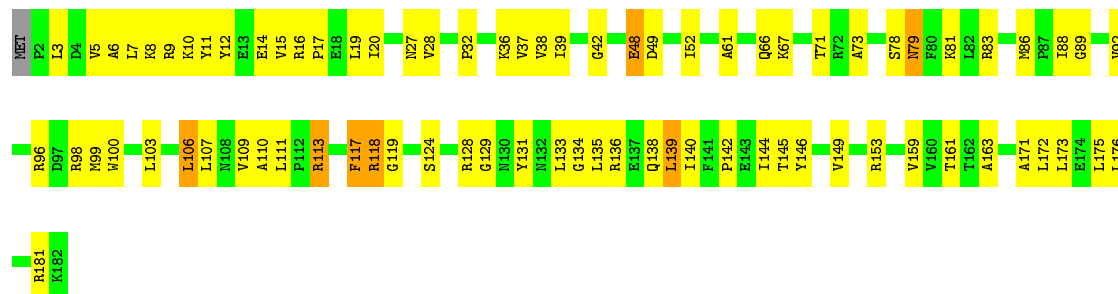
- Molecule 39: 50S ribosomal protein L4

Chain YF: 76% 19% ..



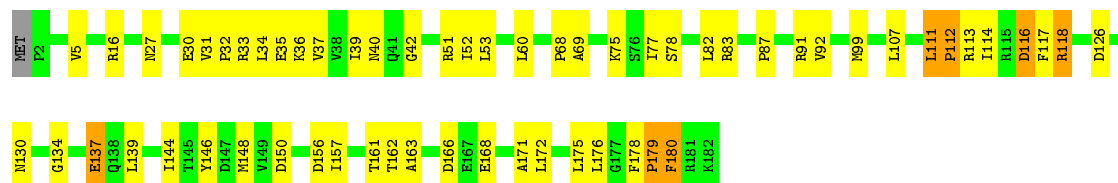
- Molecule 40: 50S ribosomal protein L5

Chain RG: 56% 40% . .



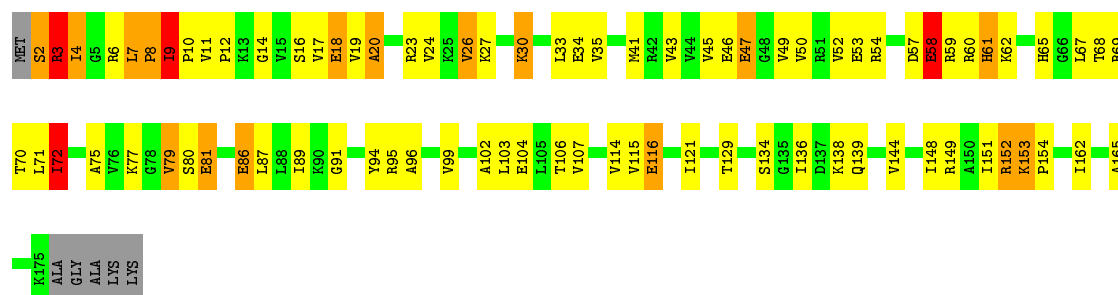
- Molecule 40: 50S ribosomal protein L5

Chain YG: 66% 29% . .



- Molecule 41: 50S ribosomal protein L6

Chain RH: 51% 35% 9% . .



- Molecule 41: 50S ribosomal protein L6

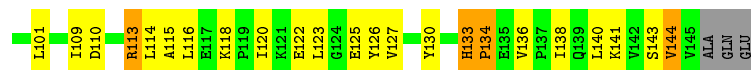
Chain YH: 73% 20% . . .





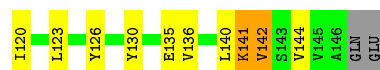
- Molecule 42: 50S ribosomal protein L9

Chain RI: 53% 36% 6% . .



- Molecule 42: 50S ribosomal protein L9

Chain YI: 68% 25% 5% . .



- Molecule 43: 50S ribosomal protein L13

Chain RN: 73% 24% . .



- Molecule 43: 50S ribosomal protein L13

Chain YN: 79% 20% .



- Molecule 44: 50S ribosomal protein L14

Chain RO: 79% 20% .



- Molecule 44: 50S ribosomal protein L14

Chain YO: 82% 18%



- Molecule 45: 50S ribosomal protein L15

Chain RP: 79% 18% ..



- Molecule 45: 50S ribosomal protein L15

Chain YP: 84% 14% .



- Molecule 46: 50S ribosomal protein L16

Chain RQ: 74% 24% ..



- Molecule 46: 50S ribosomal protein L16

Chain YQ: 80% 20%



- Molecule 47: 50S ribosomal protein L17

Chain RR: 83% 15% ..



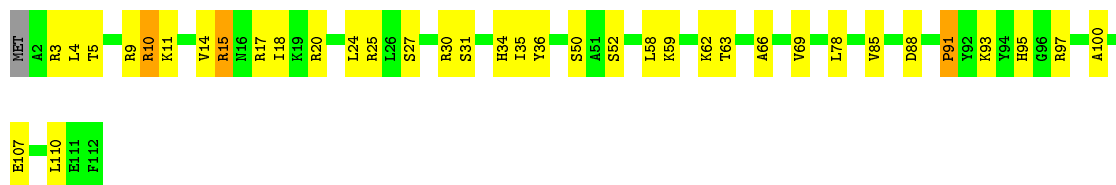
- Molecule 47: 50S ribosomal protein L17

Chain YR: 74% 25% ..



- Molecule 48: 50S ribosomal protein L18

Chain RS:  66% 30% ..



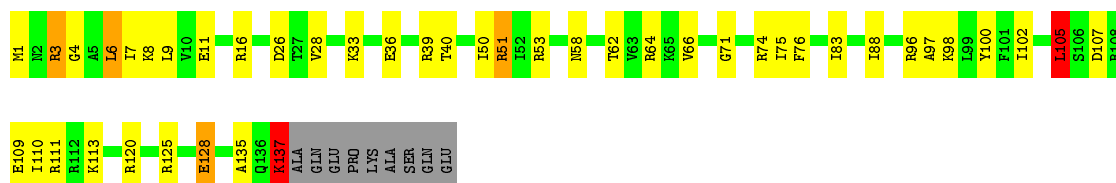
- Molecule 48: 50S ribosomal protein L18

Chain YS:  74% 25% .



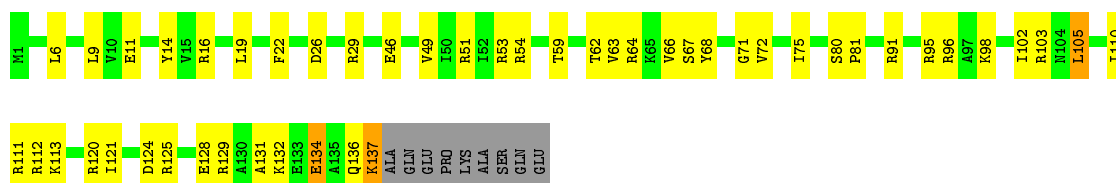
- Molecule 49: 50S ribosomal protein L19

Chain RT:  64% 26% .. 6%



- Molecule 49: 50S ribosomal protein L19

Chain YT:  61% 31% .. 6%



- Molecule 50: 50S ribosomal protein L20

Chain RU:  89% 9% ..



- Molecule 50: 50S ribosomal protein L20

Chain YU:  72% 25% ...

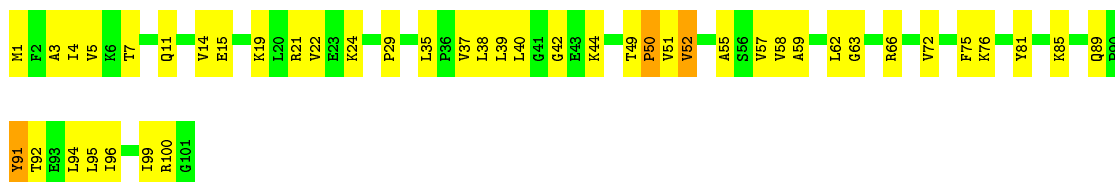


G118


- Molecule 51: 50S ribosomal protein L21

Chain RV:  73% 26%


- Molecule 51: 50S ribosomal protein L21

Chain YV:  56% 41%



- Molecule 52: 50S ribosomal protein L22

Chain RW:  88% 12%


- Molecule 52: 50S ribosomal protein L22

Chain YW:  89% 11%



- Molecule 53: 50S ribosomal protein L23

Chain RX:  79% 16%


- Molecule 53: 50S ribosomal protein L23


Chain YX:  88% 8%

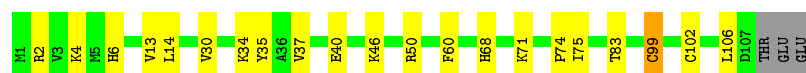

- Molecule 54: 50S ribosomal protein L24

Chain RY:  75% 21% ..



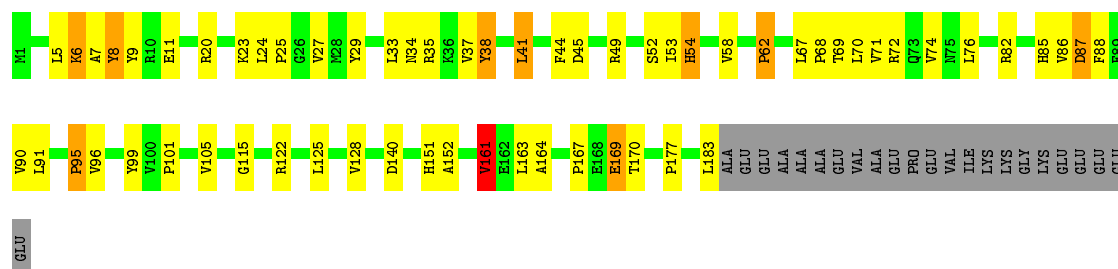
- Molecule 54: 50S ribosomal protein L24

Chain YY:  78% 18% ..



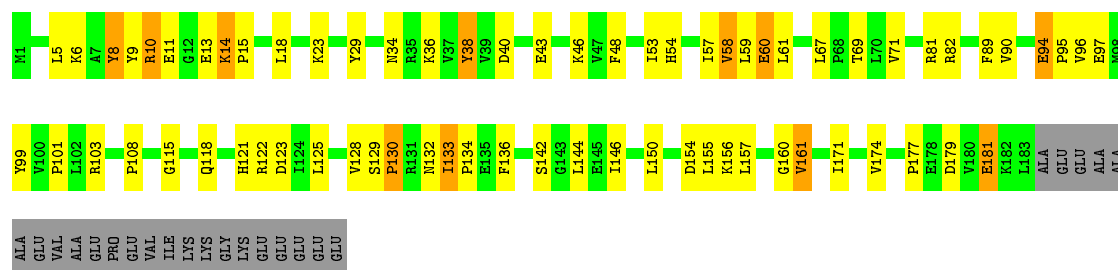
- Molecule 55: 50S ribosomal protein L25

Chain RZ:  59% 25% • 11%



- Molecule 55: 50S ribosomal protein L25

Chain YZ:  55% 28% 5% 11%



- Molecule 56: CCPuro

Chain ZA:  100%

There are no outlier residues recorded for this chain.

- Molecule 56: CCPuro

Chain ZB:  67% 33%



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	213.36Å 451.70Å 607.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	146.15 – 3.12	Depositor
% Data completeness (in resolution range)	98.6 (146.15-3.12)	Depositor
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 3.13Å)	Xtriage
Refinement program	PHENIX 1.15_3459	Depositor
R, R_{free}	0.232 , 0.257	Depositor
Wilson B-factor (Å ²)	62.4	Xtriage
Anisotropy	0.211	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	298517	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.44% 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: MG, A3P, ZN, PPU, SF4

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	QA	0.52	1/36324 (0.0%)	1.39	420/56690 (0.7%)
1	XA	0.52	1/36254 (0.0%)	1.39	416/56581 (0.7%)
2	QB	0.68	1/1942 (0.1%)	1.02	9/2619 (0.3%)
2	XB	0.75	4/1950 (0.2%)	1.01	10/2630 (0.4%)
3	QC	1.04	8/1629 (0.5%)	1.01	9/2195 (0.4%)
3	XC	0.60	1/1629 (0.1%)	0.87	6/2195 (0.3%)
4	QD	0.58	1/1733 (0.1%)	0.81	5/2318 (0.2%)
4	XD	0.62	1/1733 (0.1%)	0.84	4/2318 (0.2%)
5	QE	0.66	3/1171 (0.3%)	0.80	3/1576 (0.2%)
5	XE	0.51	0/1171	0.78	1/1576 (0.1%)
6	QF	0.52	0/856	0.73	1/1154 (0.1%)
6	XF	0.57	0/856	0.76	1/1154 (0.1%)
7	QG	0.62	1/1276 (0.1%)	0.93	4/1709 (0.2%)
7	XG	0.55	0/1276	0.88	6/1709 (0.4%)
8	QH	0.61	1/1128 (0.1%)	0.79	3/1517 (0.2%)
8	XH	0.55	0/1128	0.74	0/1517
9	QI	0.88	5/1029 (0.5%)	1.05	3/1379 (0.2%)
9	XI	0.73	2/1017 (0.2%)	1.01	6/1365 (0.4%)
10	QJ	0.82	0/814	1.24	11/1095 (1.0%)
10	XJ	0.82	5/790 (0.6%)	1.01	5/1063 (0.5%)
11	QK	0.83	4/900 (0.4%)	0.88	3/1213 (0.2%)
11	XK	0.51	1/879 (0.1%)	0.76	2/1187 (0.2%)
12	QL	0.59	1/991 (0.1%)	0.83	1/1327 (0.1%)
12	XL	0.65	1/972 (0.1%)	0.93	5/1301 (0.4%)
13	QM	1.62	19/965 (2.0%)	1.53	18/1292 (1.4%)
13	XM	0.55	0/956	0.93	2/1281 (0.2%)
14	QN	0.71	2/501 (0.4%)	0.95	1/664 (0.2%)
14	XN	0.65	0/501	0.93	1/664 (0.2%)
15	QO	0.58	0/745	0.78	1/992 (0.1%)
15	XO	0.71	1/740 (0.1%)	1.06	6/987 (0.6%)
16	QP	0.45	0/721	0.80	3/970 (0.3%)
16	XP	0.58	1/721 (0.1%)	0.74	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	QQ	0.48	0/847	0.75	0/1131
17	XQ	0.52	0/847	0.73	1/1131 (0.1%)
18	QR	0.62	1/579 (0.2%)	0.88	2/768 (0.3%)
18	XR	0.55	0/579	0.93	1/768 (0.1%)
19	QS	0.86	3/680 (0.4%)	1.02	1/915 (0.1%)
19	XS	0.54	0/680	0.91	1/915 (0.1%)
20	QT	0.58	1/765 (0.1%)	0.86	1/1007 (0.1%)
20	XT	0.80	3/765 (0.4%)	1.14	4/1007 (0.4%)
21	QU	0.61	0/221	0.89	0/288
21	XU	0.66	0/221	1.01	1/288 (0.3%)
22	QV	0.55	0/1832	1.43	23/2855 (0.8%)
22	QW	0.45	0/1832	1.41	26/2855 (0.9%)
22	XV	0.54	0/1832	1.36	10/2855 (0.4%)
22	XW	0.48	0/1832	1.38	24/2855 (0.8%)
23	QX	0.51	0/417	1.27	4/650 (0.6%)
23	XX	0.51	0/417	1.31	2/650 (0.3%)
24	QY	0.60	1/743 (0.1%)	0.86	1/1002 (0.1%)
24	QZ	0.64	0/743	1.02	2/1002 (0.2%)
24	XY	0.64	0/743	0.84	0/1002
24	XZ	0.36	0/743	0.57	0/1002
25	R0	0.51	0/652	0.82	1/867 (0.1%)
25	Y0	0.45	0/657	0.67	1/874 (0.1%)
26	R1	0.66	1/770 (0.1%)	1.01	4/1022 (0.4%)
26	Y1	0.60	0/770	0.84	1/1022 (0.1%)
27	R2	0.63	1/583 (0.2%)	0.84	3/771 (0.4%)
27	Y2	0.74	2/583 (0.3%)	1.09	4/771 (0.5%)
28	R3	0.56	0/474	0.78	1/635 (0.2%)
28	Y3	0.53	0/474	0.96	3/635 (0.5%)
29	R4	1.46	6/578 (1.0%)	1.20	7/776 (0.9%)
29	Y4	0.74	1/578 (0.2%)	1.19	5/776 (0.6%)
30	R5	0.59	2/473 (0.4%)	0.67	1/639 (0.2%)
30	Y5	0.67	1/473 (0.2%)	0.73	0/639
31	R6	0.62	0/460	0.67	0/613
31	Y6	0.96	1/460 (0.2%)	1.05	3/613 (0.5%)
32	R7	0.49	0/417	0.75	0/550
32	Y7	0.45	0/426	0.65	0/561
33	R8	0.63	1/525 (0.2%)	1.01	5/691 (0.7%)
33	Y8	0.92	3/525 (0.6%)	0.87	0/691
34	R9	0.95	3/310 (1.0%)	1.56	6/407 (1.5%)
34	Y9	0.47	0/310	0.75	0/407
35	RA	0.58	10/69739 (0.0%)	1.49	1148/108870 (1.1%)
35	YA	0.60	18/69419 (0.0%)	1.50	1151/108369 (1.1%)
36	RB	0.55	0/2928	1.50	43/4568 (0.9%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
36	YB	0.54	0/2928	1.49	44/4568 (1.0%)
37	RD	0.71	7/2165 (0.3%)	0.84	5/2919 (0.2%)
37	YD	0.56	2/2185 (0.1%)	0.73	0/2944
38	RE	0.66	5/1601 (0.3%)	0.88	3/2160 (0.1%)
38	YE	0.63	1/1596 (0.1%)	0.78	1/2153 (0.0%)
39	RF	0.60	1/1620 (0.1%)	0.80	6/2194 (0.3%)
39	YF	0.61	3/1620 (0.2%)	0.79	1/2194 (0.0%)
40	RG	0.75	5/1499 (0.3%)	1.05	6/2016 (0.3%)
40	YG	0.94	7/1499 (0.5%)	1.02	8/2016 (0.4%)
41	RH	1.16	10/1362 (0.7%)	1.23	17/1841 (0.9%)
41	YH	0.88	4/1362 (0.3%)	1.00	4/1841 (0.2%)
42	RI	1.21	14/1146 (1.2%)	1.13	8/1551 (0.5%)
42	YI	0.75	2/1151 (0.2%)	1.01	5/1558 (0.3%)
43	RN	0.59	0/1131	0.88	3/1525 (0.2%)
43	YN	0.57	0/1131	0.78	0/1525
44	RO	0.70	3/943 (0.3%)	0.88	4/1269 (0.3%)
44	YO	0.62	1/943 (0.1%)	0.80	1/1269 (0.1%)
45	RP	0.73	2/1162 (0.2%)	1.02	5/1544 (0.3%)
45	YP	0.53	0/1139	0.78	1/1514 (0.1%)
46	RQ	0.69	3/1128 (0.3%)	0.89	1/1508 (0.1%)
46	YQ	0.54	0/1143	0.78	1/1527 (0.1%)
47	RR	0.59	1/974 (0.1%)	0.76	0/1302
47	YR	0.53	0/974	0.81	1/1302 (0.1%)
48	RS	0.77	1/892 (0.1%)	1.10	7/1187 (0.6%)
48	YS	0.56	1/892 (0.1%)	0.86	2/1187 (0.2%)
49	RT	0.94	5/1155 (0.4%)	1.17	9/1542 (0.6%)
49	YT	0.71	3/1155 (0.3%)	0.89	1/1542 (0.1%)
50	RU	0.58	0/982	0.68	2/1306 (0.2%)
50	YU	0.66	2/982 (0.2%)	0.84	2/1306 (0.2%)
51	RV	0.63	0/790	0.83	1/1057 (0.1%)
51	YV	0.61	0/790	0.88	4/1057 (0.4%)
52	RW	0.55	1/911 (0.1%)	0.73	0/1220
52	YW	0.54	0/911	0.70	0/1220
53	RX	0.61	1/739 (0.1%)	0.70	1/993 (0.1%)
53	YX	0.59	0/739	0.70	1/993 (0.1%)
54	RY	0.71	3/831 (0.4%)	0.74	1/1108 (0.1%)
54	YY	0.61	1/831 (0.1%)	0.89	4/1108 (0.4%)
55	RZ	0.78	7/1493 (0.5%)	0.99	6/2026 (0.3%)
55	YZ	0.99	10/1493 (0.7%)	0.99	8/2026 (0.4%)
56	ZA	0.41	0/40	1.24	0/60
56	ZB	0.45	0/40	1.35	0/60
All	All	0.61	230/323268 (0.1%)	1.33	3631/483159 (0.8%)

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	QB	0	4
2	XB	0	2
3	QC	0	2
3	XC	0	1
4	XD	0	1
7	XG	0	1
10	QJ	0	1
10	XJ	0	2
12	XL	0	3
13	QM	0	2
14	QN	0	1
18	QR	0	1
18	XR	0	2
19	XS	0	1
27	Y2	0	3
28	R3	0	1
29	R4	0	1
29	Y4	0	3
34	R9	0	1
37	RD	0	1
38	RE	0	2
38	YE	0	1
40	YG	0	1
41	RH	0	3
41	YH	0	2
42	RI	0	3
42	YI	0	2
43	RN	0	1
45	RP	0	2
46	RQ	0	1
48	RS	0	1
49	RT	0	1
50	YU	0	1
55	RZ	0	1
All	All	0	56

All (230) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	R4	34	GLU	CB-CG	-22.72	1.08	1.52
13	QM	71	ARG	CZ-NH1	18.52	1.57	1.33
41	RH	18	GLU	CG-CD	-18.50	1.24	1.51
40	YG	112	PRO	N-CD	15.77	1.70	1.47
49	RT	3	ARG	CA-CB	15.24	1.87	1.53
3	QC	35	GLU	CD-OE2	15.15	1.42	1.25
13	QM	67	GLU	CA-CB	-14.55	1.22	1.53
41	RH	8	PRO	N-CA	13.84	1.70	1.47
13	QM	41	PRO	N-CA	13.75	1.70	1.47
42	RI	8	PRO	N-CA	13.73	1.70	1.47
48	RS	91	PRO	N-CD	-13.58	1.28	1.47
13	QM	10	PRO	N-CA	13.53	1.70	1.47
29	R4	41	PRO	N-CA	13.40	1.70	1.47
3	QC	38	ARG	NE-CZ	-13.34	1.15	1.33
41	YH	10	PRO	N-CA	13.32	1.69	1.47
29	R4	34	GLU	CG-CD	-13.30	1.32	1.51
42	RI	25	TYR	CB-CG	-13.14	1.31	1.51
40	YG	179	PRO	N-CA	13.14	1.69	1.47
55	YZ	14	LYS	CB-CG	12.96	1.87	1.52
31	Y6	14	THR	CB-CG2	-12.84	1.09	1.52
3	QC	38	ARG	CZ-NH1	12.58	1.49	1.33
3	QC	64	VAL	CB-CG2	-12.17	1.27	1.52
3	QC	38	ARG	CZ-NH2	12.17	1.48	1.33
13	QM	71	ARG	NE-CZ	12.15	1.48	1.33
55	YZ	15	PRO	N-CD	12.02	1.64	1.47
3	QC	35	GLU	CB-CG	11.94	1.74	1.52
13	QM	67	GLU	CB-CG	11.83	1.74	1.52
37	RD	169	GLU	CG-CD	-11.72	1.34	1.51
49	RT	3	ARG	CD-NE	11.36	1.65	1.46
41	RH	30	LYS	CE-NZ	-11.34	1.20	1.49
41	YH	52	VAL	CB-CG1	-11.02	1.29	1.52
41	RH	81	GLU	CG-CD	-10.85	1.35	1.51
11	QK	20	TYR	CE1-CZ	-10.40	1.25	1.38
13	QM	71	ARG	CZ-NH2	-10.38	1.19	1.33
2	XB	137	ARG	CG-CD	10.35	1.77	1.51
5	QE	90	VAL	CB-CG1	10.31	1.74	1.52
41	RH	80	SER	CA-CB	10.05	1.68	1.52
12	XL	48	PRO	N-CD	-9.97	1.33	1.47
13	QM	3	ARG	CZ-NH2	9.91	1.46	1.33
35	RA	330	A	N9-C4	-9.84	1.31	1.37
55	YZ	14	LYS	CA-CB	9.82	1.75	1.53
19	QS	52	TYR	CE2-CZ	-9.73	1.25	1.38
42	RI	23	PRO	C-N	9.71	1.50	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	RT	3	ARG	CG-CD	9.71	1.76	1.51
13	QM	67	GLU	CD-OE2	-9.66	1.15	1.25
13	QM	67	GLU	CD-OE1	9.60	1.36	1.25
2	XB	137	ARG	CB-CG	9.55	1.78	1.52
9	QI	21	PRO	N-CD	-9.55	1.34	1.47
42	RI	25	TYR	CD2-CE2	-9.55	1.25	1.39
29	R4	34	GLU	CD-OE2	-9.42	1.15	1.25
45	RP	8	PRO	N-CD	-9.38	1.34	1.47
38	YE	21	VAL	CB-CG2	-9.19	1.33	1.52
33	Y8	34	TRP	CZ3-CH2	9.17	1.54	1.40
44	RO	9	GLU	CB-CG	-9.12	1.34	1.52
10	XJ	24	VAL	CB-CG1	-9.02	1.33	1.52
40	YG	111	LEU	C-N	8.97	1.51	1.34
55	YZ	94	GLU	C-N	8.96	1.51	1.34
42	RI	110	ASP	C-N	8.74	1.50	1.34
55	YZ	133	ILE	C-N	8.72	1.50	1.34
42	RI	27	ARG	CG-CD	8.71	1.73	1.51
29	Y4	40	HIS	C-N	8.71	1.50	1.34
54	YY	99	CYS	CB-SG	-8.65	1.67	1.82
55	RZ	161	VAL	CB-CG2	-8.54	1.34	1.52
46	RQ	109	VAL	CB-CG1	-8.51	1.34	1.52
9	QI	105	ASP	CB-CG	-8.48	1.33	1.51
37	RD	131	LEU	C-N	8.47	1.50	1.34
16	XP	20	VAL	CB-CG2	-8.39	1.35	1.52
49	YT	134	GLU	CB-CG	8.36	1.68	1.52
55	YZ	14	LYS	CD-CE	8.35	1.72	1.51
11	QK	20	TYR	CD1-CE1	-8.27	1.26	1.39
40	YG	83	ARG	CG-CD	8.24	1.72	1.51
40	YG	5	VAL	CB-CG1	-8.20	1.35	1.52
55	RZ	161	VAL	CB-CG1	-8.07	1.35	1.52
19	QS	52	TYR	CG-CD2	-8.03	1.28	1.39
55	YZ	130	PRO	N-CD	-8.01	1.36	1.47
40	RG	113	ARG	CD-NE	7.88	1.59	1.46
13	QM	67	GLU	C-O	7.75	1.38	1.23
10	XJ	72	VAL	CB-CG1	-7.74	1.36	1.52
33	Y8	34	TRP	CG-CD1	7.63	1.47	1.36
30	Y5	36	CYS	CB-SG	-7.62	1.69	1.82
42	RI	25	TYR	CD1-CE1	-7.61	1.27	1.39
8	QH	34	GLU	CB-CG	7.60	1.66	1.52
18	QR	46	GLU	CB-CG	7.60	1.66	1.52
9	QI	98	PRO	N-CD	-7.55	1.37	1.47
42	YI	142	VAL	CB-CG2	-7.50	1.37	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	YA	1913	A	C6-N6	-7.47	1.27	1.33
35	RA	676	A	N9-C4	-7.39	1.33	1.37
20	XT	57	ARG	CG-CD	-7.37	1.33	1.51
35	YA	2346	A	N9-C4	-7.37	1.33	1.37
35	RA	945	A	N9-C4	-7.31	1.33	1.37
13	QM	71	ARG	CD-NE	-7.29	1.34	1.46
39	YF	173	VAL	CB-CG2	-7.29	1.37	1.52
13	QM	3	ARG	CG-CD	7.25	1.70	1.51
35	YA	1913	A	C5-C4	-7.20	1.33	1.38
5	QE	79	GLU	CG-CD	-7.19	1.41	1.51
50	YU	92	ARG	CG-CD	-7.16	1.34	1.51
46	RQ	48	GLU	CD-OE2	-7.08	1.17	1.25
7	QG	71	PRO	N-CD	-7.07	1.38	1.47
5	QE	137	GLU	CB-CG	7.05	1.65	1.52
55	RZ	8	TYR	CG-CD1	-7.04	1.29	1.39
53	RX	83	VAL	CB-CG2	-7.03	1.38	1.52
42	RI	27	ARG	NE-CZ	6.99	1.42	1.33
9	XI	90	PRO	N-CD	-6.95	1.38	1.47
41	RH	81	GLU	CB-CG	6.93	1.65	1.52
40	RG	48	GLU	CB-CG	6.92	1.65	1.52
42	RI	27	ARG	CZ-NH1	-6.92	1.24	1.33
3	QC	35	GLU	CG-CD	6.91	1.62	1.51
15	XO	76	GLU	CB-CG	6.87	1.65	1.52
46	RQ	48	GLU	CD-OE1	-6.87	1.18	1.25
34	R9	11	CYS	CB-SG	-6.84	1.70	1.82
11	QK	20	TYR	CZ-OH	-6.83	1.26	1.37
35	RA	74	A	N9-C4	-6.69	1.33	1.37
35	YA	2287	A	N9-C4	-6.65	1.33	1.37
35	RA	1143	A	N9-C4	-6.62	1.33	1.37
49	YT	134	GLU	CG-CD	6.62	1.61	1.51
49	YT	137	LYS	CD-CE	-6.55	1.34	1.51
42	RI	24	GLY	N-CA	-6.54	1.36	1.46
41	YH	44	VAL	CB-CG1	-6.53	1.39	1.52
9	XI	98	PRO	N-CD	-6.52	1.38	1.47
37	RD	28	GLU	CB-CG	6.50	1.64	1.52
54	RY	99	CYS	CB-SG	-6.50	1.71	1.82
39	RF	183	VAL	CB-CG1	-6.47	1.39	1.52
24	QY	47	PRO	N-CD	-6.46	1.38	1.47
2	XB	219	VAL	CB-CG1	-6.45	1.39	1.52
3	QC	64	VAL	CB-CG1	-6.42	1.39	1.52
38	RE	104	VAL	CB-CG1	-6.41	1.39	1.52
27	R2	12	GLU	CB-CG	6.36	1.64	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	QI	17	VAL	CB-CG2	-6.30	1.39	1.52
26	R1	86	SER	C-N	6.27	1.46	1.34
40	RG	113	ARG	CZ-NH1	6.25	1.41	1.33
35	YA	2518	A	N9-C4	-6.25	1.34	1.37
2	QB	129	GLU	CB-CG	6.19	1.64	1.52
34	R9	4	ARG	CZ-NH1	-6.19	1.25	1.33
35	YA	783	A	N9-C4	-6.19	1.34	1.37
14	QN	43	CYS	CB-SG	-6.16	1.71	1.82
35	YA	2430	A	N9-C4	-6.14	1.34	1.37
13	QM	3	ARG	CD-NE	-6.13	1.36	1.46
40	RG	113	ARG	CG-CD	6.12	1.67	1.51
42	RI	27	ARG	CB-CG	6.12	1.69	1.52
55	YZ	161	VAL	CB-CG2	-6.11	1.40	1.52
19	QS	66	MET	CA-CB	6.08	1.67	1.53
12	QL	48	PRO	N-CD	-6.08	1.39	1.47
55	RZ	8	TYR	CE1-CZ	-6.08	1.30	1.38
13	QM	9	ILE	C-N	6.04	1.45	1.34
35	RA	2430	A	N9-C4	-6.04	1.34	1.37
41	RH	7	LEU	C-N	6.03	1.45	1.34
13	QM	8	GLU	CB-CG	-6.02	1.40	1.52
37	RD	132	PRO	N-CD	5.96	1.56	1.47
14	QN	27	CYS	CB-SG	-5.95	1.72	1.81
29	R4	40	HIS	C-N	5.94	1.45	1.34
41	YH	9	ILE	C-N	5.94	1.45	1.34
42	RI	7	GLU	C-N	5.93	1.45	1.34
55	RZ	95	PRO	N-CD	5.92	1.56	1.47
37	RD	171	ASP	CB-CG	-5.91	1.39	1.51
13	QM	40	ASN	C-N	5.88	1.45	1.34
39	YF	154	VAL	CB-CG2	-5.87	1.40	1.52
10	XJ	5	ARG	CG-CD	-5.86	1.37	1.51
44	YO	10	VAL	CB-CG2	-5.86	1.40	1.52
35	YA	1786	A	N9-C4	-5.82	1.34	1.37
49	RT	1	MET	SD-CE	-5.79	1.45	1.77
42	YI	103	ARG	CB-CG	5.77	1.68	1.52
40	RG	48	GLU	CG-CD	5.76	1.60	1.51
37	RD	169	GLU	CD-OE2	-5.76	1.19	1.25
4	QD	73	ARG	CG-CD	5.75	1.66	1.51
41	RH	116	GLU	CB-CG	5.72	1.63	1.52
35	YA	74	A	N9-C4	-5.71	1.34	1.37
35	YA	330	A	N9-C4	-5.71	1.34	1.37
35	YA	2392	A	N7-C5	-5.71	1.35	1.39
35	YA	1786	A	C5-C6	-5.70	1.35	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	RA	528	A	N9-C4	-5.68	1.34	1.37
13	QM	60	VAL	CB-CG1	-5.67	1.41	1.52
33	Y8	34	TRP	CE2-CZ2	5.66	1.49	1.39
39	YF	200	GLU	CB-CG	5.66	1.62	1.52
41	RH	58	GLU	CB-CG	5.64	1.62	1.52
1	XA	974	A	C6-N1	-5.64	1.31	1.35
35	YA	783	A	C5-C6	-5.63	1.35	1.41
27	Y2	69	ARG	CZ-NH1	-5.63	1.25	1.33
20	QT	91	LEU	CG-CD2	-5.62	1.31	1.51
35	RA	783	A	N9-C4	-5.60	1.34	1.37
44	RO	108	GLU	CB-CG	5.60	1.62	1.52
35	RA	586	A	N9-C4	-5.56	1.34	1.37
40	YG	178	PHE	C-N	5.55	1.44	1.34
35	YA	1913	A	C5-C6	-5.51	1.36	1.41
13	QM	90	LEU	CG-CD2	-5.48	1.31	1.51
47	RR	43	GLU	CB-CG	5.47	1.62	1.52
35	YA	74	A	N7-C5	-5.45	1.35	1.39
55	RZ	6	LYS	CE-NZ	-5.43	1.35	1.49
11	QK	47	VAL	CB-CG2	-5.43	1.41	1.52
11	XK	12	ARG	CG-CD	5.42	1.65	1.51
20	XT	57	ARG	CB-CG	-5.42	1.38	1.52
37	YD	28	GLU	CB-CG	5.41	1.62	1.52
27	Y2	69	ARG	NE-CZ	5.41	1.40	1.33
37	RD	169	GLU	CB-CG	-5.40	1.41	1.52
55	RZ	169	GLU	CB-CG	5.40	1.62	1.52
38	RE	98	PRO	N-CD	5.38	1.55	1.47
10	XJ	49	VAL	CB-CG2	-5.38	1.41	1.52
41	RH	26	VAL	CB-CG1	-5.38	1.41	1.52
2	XB	93	VAL	CB-CG2	-5.38	1.41	1.52
52	RW	78	GLU	CB-CG	5.35	1.62	1.52
40	YG	83	ARG	CB-CG	5.35	1.67	1.52
1	QA	872	A	N9-C4	-5.34	1.34	1.37
48	YS	75	GLU	CB-CG	5.32	1.62	1.52
30	R5	48	GLU	CB-CG	5.32	1.62	1.52
35	YA	71	A	N9-C4	-5.29	1.34	1.37
54	RY	49	VAL	CB-CG2	-5.29	1.41	1.52
30	R5	49	CYS	CB-SG	-5.27	1.73	1.81
54	RY	102	CYS	CB-SG	-5.26	1.73	1.81
42	RI	23	PRO	CA-C	5.25	1.63	1.52
29	R4	36	CYS	CB-SG	-5.24	1.73	1.81
34	R9	27	CYS	CB-SG	-5.21	1.73	1.81
4	XD	179	GLU	CD-OE1	-5.18	1.20	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	YA	783	A	N7-C5	-5.17	1.36	1.39
50	YU	112	ARG	CG-CD	-5.16	1.39	1.51
35	YA	74	A	C5-C6	-5.15	1.36	1.41
38	RE	27	LEU	CG-CD1	-5.13	1.32	1.51
37	YD	28	GLU	CG-CD	5.13	1.59	1.51
45	RP	95	VAL	CB-CG2	-5.12	1.42	1.52
42	RI	118	LYS	CB-CG	5.12	1.66	1.52
44	RO	107	ARG	CG-CD	5.11	1.64	1.51
35	RA	945	A	C5-C6	-5.09	1.36	1.41
33	R8	14	VAL	CB-CG1	-5.08	1.42	1.52
10	XJ	83	GLU	CB-CG	5.07	1.61	1.52
9	QI	107	ARG	CD-NE	5.06	1.55	1.46
20	XT	45	GLN	CB-CG	5.06	1.66	1.52
38	RE	58	ARG	CA-C	5.05	1.66	1.52
49	RT	3	ARG	N-CA	5.04	1.56	1.46
55	YZ	181	GLU	CB-CG	5.04	1.61	1.52
55	YZ	58	VAL	CB-CG1	-5.01	1.42	1.52
3	XC	99	VAL	CB-CG2	-5.00	1.42	1.52
38	RE	74	PRO	N-CD	-5.00	1.40	1.47

All (3631) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	YA	1913	A	C5-C6-N6	-21.10	106.82	123.70
13	QM	90	LEU	CB-CG-CD2	-20.03	76.94	111.00
35	RA	309	G	O5'-P-OP1	-19.70	87.06	110.70
49	RT	3	ARG	CA-CB-CG	17.17	151.18	113.40
3	QC	38	ARG	NE-CZ-NH2	-15.93	112.34	120.30
35	YA	783	A	N1-C6-N6	15.73	128.04	118.60
35	YA	1913	A	C5-C6-N1	15.38	125.39	117.70
35	YA	1913	A	N1-C6-N6	15.30	127.78	118.60
34	R9	4	ARG	CD-NE-CZ	15.20	144.88	123.60
49	RT	1	MET	CG-SD-CE	-14.60	76.83	100.20
1	XA	974	A	N1-C6-N6	-14.39	109.97	118.60
35	RA	1513	C	N3-C2-O2	-14.21	111.96	121.90
35	YA	74	A	N1-C6-N6	14.19	127.11	118.60
1	QA	1158	C	N1-C2-O2	13.87	127.22	118.90
35	YA	1786	A	N1-C6-N6	13.40	126.64	118.60
35	RA	2873	A	N7-C8-N9	13.21	120.40	113.80
35	YA	1913	A	N9-C4-C5	-13.18	100.53	105.80
35	YA	2392	A	N1-C6-N6	13.10	126.46	118.60
35	RA	1513	C	N1-C2-O2	13.04	126.72	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RA	2584	U	N3-C2-O2	-13.02	113.09	122.20
35	YA	907	U	OP1-P-O3'	-12.75	77.15	105.20
31	Y6	28	ARG	CG-CD-NE	-12.71	85.12	111.80
2	QB	155	LEU	CA-CB-CG	12.68	144.45	115.30
35	YA	1332	G	N7-C8-N9	12.52	119.36	113.10
35	YA	955	C	C5-C6-N1	12.50	127.25	121.00
13	QM	3	ARG	CD-NE-CZ	12.32	140.85	123.60
1	QA	90	C	N1-C2-O2	12.32	126.29	118.90
36	RB	117	G	C4-C5-N7	12.23	115.69	110.80
35	YA	1913	A	C8-N9-C4	12.19	110.68	105.80
35	YA	2430	A	C2-N3-C4	-12.09	104.56	110.60
35	RA	676	A	N1-C6-N6	12.07	125.84	118.60
13	QM	3	ARG	CG-CD-NE	11.93	136.86	111.80
28	Y3	35	ARG	CG-CD-NE	-11.92	86.77	111.80
35	YA	530	G	N9-C4-C5	-11.86	100.66	105.40
35	YA	955	C	C6-N1-C2	-11.86	115.56	120.30
36	RB	117	G	C5-C6-O6	-11.72	121.57	128.60
35	YA	1786	A	C5-N7-C8	-11.71	98.05	103.90
36	RB	31	C	C2-N1-C1'	11.67	131.64	118.80
35	RA	2602	A	N1-C6-N6	11.64	125.58	118.60
35	YA	1616	A	N1-C6-N6	11.58	125.55	118.60
35	YA	265	A	O4'-C1'-N9	11.57	117.46	108.20
35	RA	1786	A	C5-N7-C8	-11.54	98.13	103.90
35	RA	676	A	C5-N7-C8	-11.46	98.17	103.90
35	YA	613	U	C2-N1-C1'	11.42	131.40	117.70
1	QA	1158	C	N3-C2-O2	-11.36	113.94	121.90
1	QA	90	C	C6-N1-C2	-11.34	115.77	120.30
35	RA	1021	A	N7-C8-N9	11.33	119.46	113.80
36	RB	117	G	N9-C4-C5	-11.20	100.92	105.40
1	XA	328	C	N1-C2-O2	11.17	125.60	118.90
35	YA	783	A	C5-N7-C8	-11.12	98.34	103.90
35	RA	2688	U	N3-C2-O2	-11.06	114.46	122.20
35	YA	530	G	N1-C6-O6	11.05	126.53	119.90
3	QC	35	GLU	OE1-CD-OE2	-11.05	110.04	123.30
27	Y2	69	ARG	NE-CZ-NH2	-11.03	114.79	120.30
35	YA	2346	A	N1-C6-N6	10.91	125.15	118.60
35	YA	783	A	N7-C8-N9	10.83	119.22	113.80
35	RA	856	C	C6-N1-C2	-10.81	115.97	120.30
13	QM	90	LEU	CB-CG-CD1	10.80	129.36	111.00
35	RA	2312	U	C5-C6-N1	10.78	128.09	122.70
35	RA	676	A	N7-C8-N9	10.74	119.17	113.80
1	QA	1322	C	N1-C2-O2	10.72	125.33	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	XA	754	C	C2-N1-C1'	10.70	130.57	118.80
35	YA	783	A	C8-N9-C4	-10.70	101.52	105.80
1	XA	359	U	C5-C6-N1	10.66	128.03	122.70
35	YA	828	U	N3-C2-O2	-10.65	114.75	122.20
35	YA	2688	U	N3-C2-O2	-10.65	114.75	122.20
35	YA	1786	A	C4-C5-N7	10.64	116.02	110.70
35	YA	74	A	C5-N7-C8	-10.63	98.59	103.90
40	RG	173	LEU	CA-CB-CG	10.63	139.74	115.30
35	RA	527	C	N3-C2-O2	-10.60	114.48	121.90
1	XA	975	A	N1-C6-N6	10.56	124.93	118.60
35	RA	613	U	N3-C2-O2	-10.55	114.81	122.20
35	RA	837	C	C6-N1-C2	-10.50	116.10	120.30
1	QA	1125	U	C4-C5-C6	10.46	125.97	119.70
36	RB	31	C	N1-C2-O2	10.45	125.17	118.90
35	RA	856	C	C5-C6-N1	10.43	126.21	121.00
14	XN	12	ARG	CG-CD-NE	-10.41	89.94	111.80
35	YA	878	A	O5'-P-OP1	10.41	123.19	110.70
35	YA	621	A	C5-N7-C8	-10.40	98.70	103.90
1	QA	268	C	C6-N1-C2	-10.40	116.14	120.30
35	YA	2403	C	C6-N1-C2	-10.38	116.15	120.30
35	YA	74	A	N7-C8-N9	10.37	118.99	113.80
35	RA	530	G	N1-C6-O6	10.37	126.12	119.90
35	YA	2508	G	N1-C6-O6	10.33	126.10	119.90
35	YA	621	A	N7-C8-N9	10.32	118.96	113.80
35	YA	909	A	O5'-P-OP2	-10.31	96.42	105.70
1	QA	1028	C	C2-N1-C1'	10.28	130.11	118.80
35	RA	1407	C	C6-N1-C2	-10.27	116.19	120.30
35	RA	708	C	C6-N1-C2	-10.26	116.19	120.30
35	YA	1913	A	C4-C5-N7	10.25	115.83	110.70
35	RA	1786	A	N7-C8-N9	10.24	118.92	113.80
1	QA	79	G	C2-N3-C4	10.21	117.00	111.90
1	QA	1158	C	C2-N1-C1'	10.19	130.01	118.80
35	YA	828	U	C5-C4-O4	10.18	132.01	125.90
1	QA	1523	G	O5'-P-OP1	-10.17	96.54	105.70
1	XA	4	U	C2-N1-C1'	10.17	129.91	117.70
34	R9	1	MET	CG-SD-CE	10.17	116.47	100.20
35	YA	1342	A	C2-N3-C4	-10.11	105.55	110.60
35	RA	528	A	C2-N3-C4	-10.10	105.55	110.60
35	YA	139	G	N1-C6-O6	-10.10	113.84	119.90
36	YB	31	C	C2-N1-C1'	10.09	129.90	118.80
1	XA	1158	C	C2-N1-C1'	10.09	129.90	118.80
1	QA	328	C	C2-N1-C1'	10.08	129.89	118.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RA	2474	C	C2-N1-C1'	10.08	129.89	118.80
35	YA	2584	U	N3-C2-O2	-10.07	115.15	122.20
35	RA	74	A	C2-N3-C4	-10.05	105.58	110.60
35	RA	837	C	C5-C6-N1	10.05	126.02	121.00
35	RA	330	A	C2-N3-C4	-10.03	105.59	110.60
40	RG	106	LEU	CA-CB-CG	10.01	138.33	115.30
42	RI	27	ARG	CD-NE-CZ	9.99	137.59	123.60
35	RA	1407	C	C2-N1-C1'	9.95	129.74	118.80
35	YA	624	C	C6-N1-C2	-9.93	116.33	120.30
13	QM	66	LEU	N-CA-C	-9.92	84.21	111.00
35	RA	2474	C	C6-N1-C2	-9.91	116.34	120.30
35	RA	676	A	C2-N3-C4	-9.90	105.65	110.60
35	YA	74	A	C8-N9-C4	-9.90	101.84	105.80
35	RA	878	A	O5'-P-OP1	9.89	122.57	110.70
35	YA	530	G	C5-C6-O6	-9.88	122.67	128.60
35	YA	692	C	C6-N1-C2	-9.88	116.35	120.30
1	QA	79	G	N1-C6-O6	-9.87	113.98	119.90
35	RA	945	A	N1-C6-N6	9.86	124.52	118.60
1	QA	1301	U	C2-N1-C1'	9.86	129.53	117.70
35	YA	856	C	C6-N1-C2	-9.83	116.37	120.30
29	R4	34	GLU	CG-CD-OE2	-9.82	98.66	118.30
35	RA	1786	A	C4-C5-N7	9.81	115.61	110.70
35	RA	783	A	C5-N7-C8	-9.78	99.01	103.90
48	RS	20	ARG	CG-CD-NE	-9.78	91.27	111.80
35	RA	1021	A	C5-N7-C8	-9.76	99.02	103.90
35	RA	2873	A	C5-N7-C8	-9.75	99.02	103.90
35	RA	1313	U	C2-N1-C1'	9.72	129.36	117.70
1	XA	1502	A	N7-C8-N9	9.71	118.66	113.80
35	RA	530	G	C5-C6-O6	-9.71	122.77	128.60
35	RA	1021	A	C8-N9-C4	-9.68	101.93	105.80
35	YA	140	A	N7-C8-N9	9.68	118.64	113.80
1	QA	1301	U	C5-C6-N1	9.67	127.53	122.70
35	RA	1143	A	C2-N3-C4	-9.65	105.78	110.60
34	R9	4	ARG	NE-CZ-NH1	-9.65	115.48	120.30
35	RA	1616	A	C5-N7-C8	-9.64	99.08	103.90
1	QA	328	C	N1-C2-O2	9.63	124.68	118.90
35	YA	52	A	N1-C6-N6	9.63	124.38	118.60
35	YA	1332	G	C5-N7-C8	-9.62	99.49	104.30
1	XA	36	C	C6-N1-C2	-9.61	116.46	120.30
15	XO	88	ARG	CG-CD-NE	-9.59	91.66	111.80
35	YA	621	A	N1-C6-N6	9.57	124.34	118.60
35	YA	1332	G	C8-N9-C4	-9.57	102.57	106.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	RB	117	G	N1-C6-O6	9.55	125.63	119.90
35	YA	1698	A	N1-C6-N6	9.51	124.31	118.60
35	RA	774	A	C2-N3-C4	-9.49	105.85	110.60
15	XO	88	ARG	NE-CZ-NH2	-9.46	115.57	120.30
35	YA	71	A	N1-C6-N6	9.45	124.27	118.60
1	XA	1145	C	N1-C2-O2	9.42	124.55	118.90
35	YA	1407	C	C6-N1-C2	-9.39	116.54	120.30
1	XA	974	A	C5-C6-N1	9.38	122.39	117.70
35	YA	2430	A	N1-C6-N6	9.34	124.20	118.60
35	YA	1913	A	C6-N1-C2	-9.34	113.00	118.60
35	RA	2094	G	C6-N1-C2	-9.33	119.50	125.10
35	RA	783	A	N1-C6-N6	9.33	124.20	118.60
1	QA	1147	C	N1-C2-O2	9.32	124.49	118.90
34	R9	10	ILE	C-N-CA	9.32	145.00	121.70
5	QE	81	GLU	OE1-CD-OE2	-9.30	112.14	123.30
35	YA	1678	G	C5-N7-C8	-9.29	99.65	104.30
35	YA	758	C	C6-N1-C2	-9.28	116.59	120.30
35	YA	1678	G	C4-C5-N7	9.28	114.51	110.80
35	YA	1313	U	C2-N1-C1'	9.27	128.82	117.70
35	RA	1513	C	N3-C4-N4	9.25	124.47	118.00
1	XA	1502	A	C5-N7-C8	-9.23	99.29	103.90
14	QN	26	ARG	CG-CD-NE	9.22	131.16	111.80
1	QA	90	C	N3-C2-O2	-9.17	115.48	121.90
35	YA	2584	U	C2-N1-C1'	9.14	128.67	117.70
35	YA	1881	C	C5-C6-N1	9.13	125.57	121.00
1	QA	999	U	C2-N1-C1'	9.13	128.65	117.70
1	XA	1301	U	C2-N1-C1'	9.12	128.65	117.70
36	YB	31	C	N1-C2-O2	9.12	124.37	118.90
40	YG	112	PRO	CA-N-CD	-9.12	98.74	111.50
35	YA	527	C	C6-N1-C2	-9.09	116.66	120.30
35	RA	1616	A	N7-C8-N9	9.09	118.34	113.80
35	YA	1210	A	N1-C6-N6	9.06	124.04	118.60
36	YB	27	C	C6-N1-C2	-9.06	116.68	120.30
35	YA	530	G	C4-C5-N7	9.05	114.42	110.80
1	QA	1066	C	C2-N1-C1'	9.04	128.75	118.80
20	XT	10	LEU	CA-CB-CG	9.04	136.09	115.30
1	QA	1028(B)	C	C6-N1-C2	-9.01	116.70	120.30
35	RA	2602	A	C4-C5-N7	8.99	115.19	110.70
35	RA	270(U)	C	N1-C2-O2	8.98	124.29	118.90
35	RA	1180	C	C6-N1-C2	-8.98	116.71	120.30
35	RA	1544	C	C2-N1-C1'	8.96	128.66	118.80
35	YA	1407	C	C2-N1-C1'	8.95	128.65	118.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	YA	1786	A	N7-C8-N9	8.91	118.25	113.80
35	RA	1678	G	C8-N9-C4	-8.85	102.86	106.40
35	YA	2748	A	N7-C8-N9	8.85	118.22	113.80
35	YA	2688	U	C5-C4-O4	8.84	131.20	125.90
35	YA	527	C	N3-C2-O2	-8.83	115.72	121.90
1	QA	1301	U	N1-C2-O2	8.83	128.98	122.80
1	XA	328	C	C2-N1-C1'	8.83	128.51	118.80
35	YA	2392	A	N7-C8-N9	8.82	118.21	113.80
35	YA	2579	C	C6-N1-C2	-8.81	116.78	120.30
35	RA	527	C	N1-C2-O2	8.80	124.18	118.90
35	RA	2873	A	C8-N9-C4	-8.80	102.28	105.80
35	YA	624	C	C5-C6-N1	8.79	125.39	121.00
35	YA	783	A	C5-C6-N6	-8.78	116.67	123.70
35	RA	2688	U	C5-C4-O4	8.78	131.17	125.90
35	YA	1332	G	C6-C5-N7	-8.78	125.13	130.40
1	QA	591	U	O5'-P-OP1	-8.78	97.80	105.70
35	RA	1152	C	C6-N1-C2	-8.78	116.79	120.30
35	RA	1513	C	C6-N1-C2	-8.78	116.79	120.30
35	RA	783	A	N7-C8-N9	8.77	118.18	113.80
35	YA	1968	G	C5-C6-O6	-8.76	123.34	128.60
35	YA	74	A	C2-N3-C4	-8.75	106.22	110.60
1	QA	1066	C	N1-C2-O2	8.75	124.15	118.90
27	Y2	14	ARG	CG-CD-NE	8.74	130.16	111.80
35	YA	140	A	C8-N9-C4	-8.74	102.30	105.80
18	QR	46	GLU	CB-CA-C	-8.73	92.94	110.40
35	YA	2346	A	C5-N7-C8	-8.72	99.54	103.90
3	XC	126	ARG	CG-CD-NE	8.72	130.11	111.80
1	QA	1066	C	C5-C6-N1	8.72	125.36	121.00
36	YB	47	C	N1-C2-O2	8.72	124.13	118.90
35	YA	621	A	C8-N9-C4	-8.72	102.31	105.80
1	XA	980	C	C2-N1-C1'	8.71	128.38	118.80
1	XA	1086	U	N1-C2-O2	8.71	128.89	122.80
35	YA	1950	G	N7-C8-N9	8.71	117.45	113.10
35	RA	1930	G	P-O3'-C3'	8.70	130.15	119.70
1	QA	999	U	OP1-P-O3'	8.70	124.34	105.20
35	YA	1180	C	C2-N1-C1'	8.70	128.37	118.80
35	RA	676	A	C5-C6-N1	-8.69	113.35	117.70
29	Y4	61	ARG	CG-CD-NE	8.69	130.05	111.80
29	R4	41	PRO	CA-N-CD	-8.67	99.36	111.50
1	XA	23	C	C6-N1-C2	-8.67	116.83	120.30
35	RA	2477	C	N1-C2-O2	8.64	124.08	118.90
1	XA	58	C	C6-N1-C2	-8.64	116.84	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RA	2827	C	C2-N1-C1'	8.62	128.28	118.80
35	YA	2873	A	N7-C8-N9	8.61	118.11	113.80
35	RA	2477	C	C2-N1-C1'	8.60	128.26	118.80
35	YA	2505	G	C5-C6-O6	8.60	133.76	128.60
35	RA	330	A	N3-C4-C5	8.59	132.81	126.80
35	YA	2430	A	C5-C6-N1	-8.59	113.41	117.70
11	XK	12	ARG	CG-CD-NE	8.58	129.83	111.80
35	RA	2094	G	N3-C2-N2	-8.58	113.89	119.90
35	RA	1881	C	C6-N1-C2	-8.58	116.87	120.30
35	YA	2456	C	C6-N1-C2	-8.58	116.87	120.30
22	QW	13	C	C2-N1-C1'	8.56	128.22	118.80
35	RA	2205	C	C6-N1-C2	-8.56	116.88	120.30
35	RA	2559	C	C6-N1-C2	-8.56	116.88	120.30
35	YA	2392	A	C6-C5-N7	-8.55	126.31	132.30
1	QA	754	C	C2-N1-C1'	8.54	128.19	118.80
35	YA	708	C	C2-N1-C1'	8.53	128.18	118.80
1	QA	1347	G	C8-N9-C1'	-8.52	115.92	127.00
35	RA	69	C	C2-N1-C1'	8.52	128.17	118.80
35	YA	774	A	C2-N3-C4	-8.52	106.34	110.60
1	XA	971	G	C8-N9-C4	8.51	109.80	106.40
35	RA	2287	A	C8-N9-C4	8.50	109.20	105.80
35	YA	530	G	C8-N9-C4	8.49	109.80	106.40
35	YA	2712	U	O4'-C1'-N1	8.49	114.99	108.20
36	RB	3	C	N1-C2-O2	8.48	123.99	118.90
35	RA	74	A	N1-C6-N6	8.47	123.68	118.60
35	YA	1332	G	C4-C5-N7	8.47	114.19	110.80
35	RA	2602	A	C5-N7-C8	-8.46	99.67	103.90
35	RA	2826	A	N1-C6-N6	8.46	123.68	118.60
35	RA	613	U	N1-C2-O2	8.46	128.72	122.80
35	YA	140	A	C5-N7-C8	-8.46	99.67	103.90
1	QA	90	C	N3-C4-N4	8.46	123.92	118.00
35	RA	2584	U	N1-C2-N3	8.46	119.97	114.90
35	RA	330	A	C5-N7-C8	-8.45	99.68	103.90
35	RA	1143	A	N1-C6-N6	8.43	123.66	118.60
35	YA	828	U	N1-C2-O2	8.43	128.70	122.80
35	YA	2602	A	C5-N7-C8	-8.43	99.69	103.90
35	RA	2474	C	N1-C2-O2	8.42	123.95	118.90
36	RB	27	C	N1-C2-O2	8.41	123.95	118.90
35	YA	527	C	C2-N1-C1'	8.41	128.05	118.80
35	YA	1956	U	N3-C2-O2	-8.41	116.31	122.20
1	QA	328	C	C5-C6-N1	8.40	125.20	121.00
1	XA	1502	A	N1-C6-N6	8.39	123.63	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	YA	603	A	N1-C6-N6	8.39	123.63	118.60
35	RA	2726	U	C2-N1-C1'	8.38	127.76	117.70
35	YA	1616	A	C5-N7-C8	-8.38	99.71	103.90
1	QA	739	C	C6-N1-C2	-8.38	116.95	120.30
35	YA	1311	G	C8-N9-C1'	-8.38	116.11	127.00
35	RA	1480	G	C5-C6-O6	8.37	133.62	128.60
1	QA	664	G	N1-C6-O6	-8.37	114.88	119.90
4	QD	73	ARG	CG-CD-NE	8.37	129.37	111.80
35	YA	895	U	C2-N1-C1'	8.37	127.74	117.70
35	YA	2167	U	C2-N1-C1'	8.37	127.74	117.70
35	YA	1950	G	C8-N9-C4	-8.36	103.06	106.40
35	RA	309	G	C8-N9-C1'	8.34	137.85	127.00
35	RA	1204	A	O4'-C1'-N9	8.34	114.87	108.20
1	QA	1347	G	C4-N9-C1'	8.34	137.34	126.50
1	QA	1240	U	C5-C6-N1	-8.33	118.53	122.70
35	RA	2726	U	C5-C4-O4	8.33	130.90	125.90
35	RA	47	C	C6-N1-C2	-8.32	116.97	120.30
35	RA	1774	C	N1-C2-O2	8.31	123.89	118.90
1	QA	90	C	C2-N3-C4	8.31	124.05	119.90
35	RA	708	C	C2-N1-C1'	8.30	127.94	118.80
35	RA	2724	C	N3-C4-C5	-8.30	118.58	121.90
1	XA	848	C	C5-C6-N1	8.29	125.15	121.00
35	YA	1004	C	C6-N1-C2	-8.29	116.98	120.30
35	YA	243	U	C5-C6-N1	8.29	126.84	122.70
2	XB	137	ARG	CG-CD-NE	8.28	129.19	111.80
35	RA	2392	A	N1-C6-N6	8.28	123.57	118.60
35	RA	828	U	N3-C2-O2	-8.27	116.41	122.20
35	YA	2873	A	C8-N9-C4	-8.26	102.50	105.80
42	YI	33	ARG	CG-CD-NE	8.26	129.14	111.80
35	RA	2094	G	C5-C6-O6	-8.25	123.65	128.60
1	QA	283	C	C6-N1-C2	-8.24	117.00	120.30
1	XA	1007	C	C5-C6-N1	8.24	125.12	121.00
1	QA	1454	G	O5'-P-OP1	-8.23	98.29	105.70
1	XA	738	C	C5-C6-N1	8.23	125.12	121.00
1	QA	90	C	N3-C4-C5	-8.23	118.61	121.90
22	QW	13	C	C6-N1-C2	-8.23	117.01	120.30
1	XA	999	U	C2-N1-C1'	8.23	127.58	117.70
35	RA	828	U	C5-C4-O4	8.23	130.84	125.90
35	YA	1311	G	C4-N9-C1'	8.23	137.20	126.50
35	RA	2602	A	C6-C5-N7	-8.22	126.54	132.30
35	RA	856	C	C2-N1-C1'	8.22	127.84	118.80
1	XA	1439	C	C6-N1-C2	-8.22	117.01	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	RD	183	ARG	CG-CD-NE	8.21	129.05	111.80
35	RA	2243	U	N3-C2-O2	-8.21	116.45	122.20
2	XB	111	ARG	CG-CD-NE	8.21	129.04	111.80
22	QV	17(A)	U	N1-C1'-C2'	-8.21	102.97	112.00
35	RA	2161	C	C2-N1-C1'	8.20	127.82	118.80
35	RA	69	C	N1-C2-O2	8.20	123.82	118.90
35	RA	74	A	C5-C6-N1	-8.20	113.60	117.70
35	RA	1241	A	N1-C6-N6	8.20	123.52	118.60
35	RA	613	U	C2-N1-C1'	8.19	127.53	117.70
1	XA	1240	U	C5-C4-O4	-8.19	120.99	125.90
1	XA	186(F)	C	C6-N1-C2	-8.19	117.03	120.30
35	YA	1700	A	C8-N9-C4	8.18	109.07	105.80
35	YA	139	G	C5-C6-O6	8.17	133.50	128.60
35	YA	1332	G	C4-N9-C1'	8.17	137.12	126.50
1	QA	1301	U	N3-C2-O2	-8.17	116.48	122.20
1	QA	1322	C	N3-C2-O2	-8.17	116.18	121.90
35	YA	1882	C	C6-N1-C2	-8.16	117.04	120.30
35	RA	1480	G	N1-C6-O6	-8.16	115.00	119.90
35	YA	69	C	C2-N1-C1'	8.15	127.77	118.80
35	RA	1950	G	N7-C8-N9	8.15	117.17	113.10
35	RA	1881	C	C2-N1-C1'	8.14	127.76	118.80
2	XB	88	ALA	N-CA-CB	8.13	121.49	110.10
1	QA	1028	C	C6-N1-C1'	-8.13	111.04	120.80
35	RA	845	G	C4-C5-N7	8.12	114.05	110.80
35	YA	1150	C	C6-N1-C2	-8.12	117.05	120.30
48	RS	10	ARG	CG-CD-NE	8.12	128.84	111.80
35	YA	1379	A	N1-C6-N6	8.12	123.47	118.60
41	YH	71	LEU	CA-CB-CG	8.11	133.96	115.30
36	RB	31	C	C6-N1-C1'	-8.11	111.07	120.80
35	YA	111	A	C8-N9-C4	8.10	109.04	105.80
35	RA	867	C	N1-C2-O2	8.10	123.76	118.90
35	YA	1306	C	C6-N1-C2	-8.09	117.06	120.30
35	YA	141(A)	C	C6-N1-C2	-8.08	117.07	120.30
1	QA	1502	A	C5-N7-C8	-8.07	99.87	103.90
35	RA	1899	G	N3-C4-C5	-8.06	124.57	128.60
35	RA	1686	C	C6-N1-C2	-8.06	117.08	120.30
35	YA	1528	A	N7-C8-N9	8.06	117.83	113.80
35	YA	907	U	N1-C2-O2	8.05	128.44	122.80
35	RA	143	C	C6-N1-C2	-8.04	117.08	120.30
35	RA	2346	A	O4'-C1'-N9	8.03	114.62	108.20
1	QA	390	C	C6-N1-C2	-8.03	117.09	120.30
35	RA	970	C	C6-N1-C2	-8.03	117.09	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	XA	1031	G	N3-C4-C5	-8.03	124.59	128.60
35	YA	1233	C	C5-C6-N1	8.02	125.01	121.00
35	YA	530	G	C6-C5-N7	-8.02	125.59	130.40
35	RA	2474	C	N3-C2-O2	-8.02	116.29	121.90
50	RU	52	ARG	CG-CD-NE	-8.02	94.97	111.80
1	XA	359	U	C6-N1-C2	-8.01	116.19	121.00
36	YB	3	C	C6-N1-C2	-8.01	117.10	120.30
35	YA	1588	C	C2-N1-C1'	8.01	127.61	118.80
35	YA	812	C	C6-N1-C2	-8.00	117.10	120.30
1	XA	410	G	C8-N9-C4	-7.99	103.20	106.40
35	RA	2029	G	C8-N9-C4	7.98	109.59	106.40
36	RB	31	C	N3-C2-O2	-7.97	116.32	121.90
1	QA	1240	U	C4-C5-C6	7.96	124.48	119.70
35	RA	828	U	N1-C2-O2	7.96	128.38	122.80
23	QX	11	U	P-O3'-C3'	7.96	129.25	119.70
1	XA	1406	U	N3-C2-O2	-7.96	116.63	122.20
35	YA	69	C	N1-C2-O2	7.96	123.67	118.90
35	RA	227	A	P-O3'-C3'	7.95	129.24	119.70
1	XA	1059	C	C6-N1-C2	-7.95	117.12	120.30
36	RB	31	C	C6-N1-C2	-7.95	117.12	120.30
1	XA	1465	C	C6-N1-C2	-7.94	117.12	120.30
35	YA	1786	A	C6-C5-N7	-7.93	126.75	132.30
1	XA	1240	U	N3-C2-O2	7.92	127.74	122.20
35	RA	1864	U	N3-C2-O2	-7.91	116.66	122.20
35	RA	265	A	N1-C6-N6	7.91	123.34	118.60
2	QB	238	LEU	CA-CB-CG	7.90	133.47	115.30
35	RA	471	A	C8-N9-C4	-7.90	102.64	105.80
1	XA	1145	C	N3-C2-O2	-7.90	116.37	121.90
35	RA	2602	A	N7-C8-N9	7.90	117.75	113.80
35	YA	2287	A	C8-N9-C4	7.90	108.96	105.80
35	RA	2726	U	N3-C2-O2	-7.88	116.69	122.20
41	YH	10	PRO	CA-N-CD	-7.88	100.47	111.50
1	XA	754	C	C6-N1-C2	-7.88	117.15	120.30
35	YA	1656	C	C6-N1-C2	-7.87	117.15	120.30
1	QA	1031	G	C4-N9-C1'	7.87	136.73	126.50
35	RA	530	G	N9-C4-C5	-7.87	102.25	105.40
35	RA	1963	U	C2-N1-C1'	7.87	127.14	117.70
35	RA	2772	C	C6-N1-C2	-7.86	117.16	120.30
35	RA	1502	C	C6-N1-C2	-7.86	117.16	120.30
35	YA	138	G	C8-N9-C4	-7.86	103.26	106.40
1	XA	108	G	C8-N9-C4	-7.86	103.26	106.40
35	YA	352	G	C2-N3-C4	7.86	115.83	111.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	YA	1024	G	C6-C5-N7	-7.86	125.69	130.40
35	YA	89	G	C8-N9-C4	-7.85	103.26	106.40
35	RA	884	C	C5-C6-N1	7.85	124.92	121.00
15	XO	13	GLN	CB-CA-C	-7.85	94.70	110.40
35	YA	2211	G	OP2-P-O3'	7.85	122.47	105.20
1	QA	1263	C	C2-N1-C1'	7.84	127.43	118.80
35	RA	2210	G	C4-N9-C1'	7.84	136.70	126.50
35	RA	2335	A	O4'-C1'-N9	7.84	114.47	108.20
35	RA	309	G	C4-N9-C1'	-7.84	116.31	126.50
41	RH	8	PRO	CA-N-CD	-7.83	100.54	111.50
35	YA	139	G	N9-C4-C5	7.83	108.53	105.40
35	RA	2459	A	N9-C4-C5	-7.82	102.67	105.80
35	YA	273(D)	C	C2-N1-C1'	7.82	127.40	118.80
35	YA	1342	A	N1-C6-N6	7.82	123.29	118.60
1	XA	442	C	C2-N1-C1'	7.82	127.40	118.80
35	YA	111	A	N9-C4-C5	-7.82	102.67	105.80
35	YA	2508	G	C5-C6-O6	-7.81	123.91	128.60
35	YA	12	U	C2-N1-C1'	7.81	127.07	117.70
35	RA	172	C	C2-N1-C1'	7.81	127.39	118.80
35	RA	1417	C	C5-C6-N1	7.80	124.90	121.00
35	RA	75	G	C8-N9-C4	-7.80	103.28	106.40
35	YA	1276	A	C8-N9-C4	-7.80	102.68	105.80
1	XA	1108	G	C4-C5-N7	-7.79	107.68	110.80
36	RB	47	C	N1-C2-O2	7.79	123.57	118.90
1	QA	181	G	P-O3'-C3'	7.79	129.04	119.70
35	YA	1621	U	C5-C4-O4	-7.79	121.23	125.90
36	YB	27	C	C2-N1-C1'	7.79	127.36	118.80
1	XA	1109	C	C6-N1-C2	-7.78	117.19	120.30
35	YA	2392	A	C5-N7-C8	-7.78	100.01	103.90
36	RB	3	C	C5-C6-N1	7.78	124.89	121.00
1	QA	1128	C	C6-N1-C2	-7.77	117.19	120.30
35	RA	676	A	C8-N9-C4	-7.77	102.69	105.80
42	RI	8	PRO	CA-N-CD	-7.77	100.62	111.50
35	RA	2403	C	C6-N1-C2	-7.77	117.19	120.30
35	YA	2477	C	C2-N1-C1'	7.77	127.35	118.80
1	QA	191(D)	U	C2-N1-C1'	7.76	127.01	117.70
35	RA	1882	C	C2-N1-C1'	7.76	127.33	118.80
35	RA	748	G	C8-N9-C4	7.76	109.50	106.40
35	YA	1881	C	C2-N3-C4	7.76	123.78	119.90
35	RA	387	U	P-O3'-C3'	7.75	129.00	119.70
35	RA	1407	C	C5-C6-N1	7.75	124.88	121.00
1	QA	797	C	C6-N1-C2	-7.75	117.20	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	YA	2827	C	C2-N1-C1'	7.75	127.32	118.80
1	XA	1240	U	C6-N1-C2	7.74	125.65	121.00
35	YA	2139	C	C2-N1-C1'	7.74	127.32	118.80
35	YA	676	A	C5-N7-C8	-7.74	100.03	103.90
35	YA	1881	C	C2-N1-C1'	7.74	127.31	118.80
35	YA	1313	U	N3-C2-O2	-7.73	116.79	122.20
35	RA	1243	G	C8-N9-C4	7.73	109.49	106.40
7	XG	95	ARG	CG-CD-NE	7.72	128.01	111.80
55	YZ	60	GLU	CA-CB-CG	7.72	130.38	113.40
1	XA	687	A	N1-C6-N6	-7.72	113.97	118.60
1	QA	186	C	C6-N1-C2	-7.71	117.21	120.30
35	RA	989	G	N3-C2-N2	-7.71	114.50	119.90
35	YA	2602	A	N7-C8-N9	7.71	117.66	113.80
13	QM	10	PRO	CA-N-CD	-7.71	100.71	111.50
35	RA	2896	C	C2-N1-C1'	7.71	127.28	118.80
35	YA	2287	A	N3-C4-C5	7.71	132.19	126.80
35	YA	708	C	C6-N1-C2	-7.71	117.22	120.30
35	YA	2602	A	C4-C5-N7	7.70	114.55	110.70
1	QA	486	U	C2-N1-C1'	7.70	126.94	117.70
22	QW	20	U	O4'-C1'-N1	7.69	114.36	108.20
35	YA	932	G	N1-C6-O6	-7.69	115.28	119.90
35	RA	93	C	C6-N1-C2	-7.69	117.22	120.30
35	RA	1241	A	C2-N3-C4	-7.69	106.76	110.60
35	YA	828	U	C2-N1-C1'	7.69	126.93	117.70
1	QA	1038	C	P-O3'-C3'	7.69	128.93	119.70
35	RA	2342	C	C6-N1-C2	-7.68	117.23	120.30
35	RA	279	C	C5-C6-N1	7.68	124.84	121.00
35	YA	2210	G	C4-N9-C1'	7.68	136.48	126.50
1	XA	137	C	C6-N1-C2	-7.68	117.23	120.30
22	QW	16	C	O5'-P-OP1	-7.68	98.79	105.70
35	YA	1482	U	C2-N1-C1'	7.67	126.91	117.70
35	RA	654(Q)	C	N1-C2-O2	7.67	123.50	118.90
1	XA	1301	U	C6-N1-C1'	-7.66	110.47	121.20
33	R8	46	ARG	CG-CD-NE	-7.66	95.71	111.80
35	YA	69	C	C6-N1-C2	-7.66	117.24	120.30
35	RA	530	G	C4-C5-N7	7.65	113.86	110.80
35	RA	1616	A	N1-C6-N6	7.65	123.19	118.60
15	XO	35	ARG	CG-CD-NE	-7.65	95.74	111.80
1	XA	1158	C	N1-C2-O2	7.64	123.49	118.90
35	RA	1698	A	N7-C8-N9	7.63	117.62	113.80
35	YA	1786	A	C5-C6-N6	-7.63	117.59	123.70
35	RA	774	A	C5-C6-N1	-7.63	113.88	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RA	828	U	C2-N1-C1'	7.63	126.86	117.70
35	RA	2092	U	P-O3'-C3'	7.63	128.86	119.70
1	QA	1260	C	C6-N1-C2	-7.63	117.25	120.30
35	YA	859	G	C8-N9-C4	7.63	109.45	106.40
35	RA	1300	U	P-O3'-C3'	7.62	128.85	119.70
1	XA	1086	U	N3-C2-O2	-7.62	116.86	122.20
44	RO	107	ARG	CG-CD-NE	7.62	127.80	111.80
35	RA	2508	G	N1-C6-O6	7.62	124.47	119.90
35	YA	1678	G	N7-C8-N9	7.62	116.91	113.10
1	QA	328	C	C6-N1-C2	-7.61	117.25	120.30
35	RA	2343	C	N1-C2-O2	7.61	123.47	118.90
1	XA	961	U	N3-C2-O2	-7.61	116.87	122.20
35	YA	2392	A	C5-C6-N1	-7.60	113.90	117.70
35	RA	1262	A	C2-N3-C4	7.60	114.40	110.60
35	YA	2585	U	N3-C2-O2	-7.60	116.88	122.20
35	RA	734	A	N1-C6-N6	7.60	123.16	118.60
35	YA	1963	U	N1-C2-O2	7.60	128.12	122.80
41	RH	2	SER	C-N-CA	7.60	140.69	121.70
1	QA	1128	C	C5-C6-N1	7.59	124.80	121.00
35	YA	624	C	C2-N1-C1'	7.59	127.15	118.80
35	RA	1956	U	N3-C2-O2	-7.59	116.89	122.20
35	RA	2211	G	OP2-P-O3'	7.59	121.89	105.20
35	YA	2074	U	N3-C2-O2	-7.59	116.89	122.20
35	RA	1678	G	N7-C8-N9	7.58	116.89	113.10
35	YA	1616	A	C4-C5-N7	7.58	114.49	110.70
22	XV	69	C	C6-N1-C2	-7.58	117.27	120.30
35	YA	603	A	N7-C8-N9	7.58	117.59	113.80
35	RA	1698	A	C5-N7-C8	-7.57	100.11	103.90
35	YA	1963	U	C2-N1-C1'	7.57	126.78	117.70
35	RA	1786	A	N1-C6-N6	7.57	123.14	118.60
1	XA	15	G	C8-N9-C4	-7.56	103.38	106.40
35	YA	2287	A	C4-N9-C1'	-7.56	112.69	126.30
35	YA	69	C	N3-C2-O2	-7.56	116.61	121.90
35	RA	1948	G	C8-N9-C4	-7.55	103.38	106.40
1	QA	999	U	N1-C2-O2	7.55	128.08	122.80
35	YA	12	U	N3-C2-O2	-7.55	116.92	122.20
35	RA	2092	U	N1-C2-O2	7.54	128.08	122.80
1	QA	877	C	C6-N1-C2	-7.54	117.28	120.30
35	YA	1947	C	C6-N1-C2	-7.54	117.29	120.30
1	XA	1191	A	O5'-P-OP1	-7.53	98.92	105.70
35	RA	2792	G	N3-C4-N9	7.53	130.52	126.00
35	YA	2518	A	N1-C6-N6	7.53	123.12	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	QA	1347	G	P-O3'-C3'	7.52	128.72	119.70
35	RA	2211	G	C4-N9-C1'	7.52	136.27	126.50
35	YA	1968	G	N1-C6-O6	7.52	124.41	119.90
35	YA	1979	C	N1-C2-O2	7.52	123.41	118.90
1	QA	197	A	P-O3'-C3'	7.51	128.72	119.70
1	QA	1124	G	P-O3'-C3'	7.51	128.71	119.70
35	RA	2211	G	P-O3'-C3'	7.51	128.71	119.70
2	XB	30	ARG	CG-CD-NE	7.51	127.57	111.80
35	YA	1629	U	N3-C2-O2	-7.51	116.94	122.20
48	RS	15	ARG	CG-CD-NE	-7.50	96.04	111.80
1	XA	972	C	C6-N1-C2	-7.50	117.30	120.30
35	YA	1170	G	N3-C4-N9	7.50	130.50	126.00
1	XA	972	C	N3-C4-C5	-7.50	118.90	121.90
12	XL	59	ARG	CG-CD-NE	7.50	127.55	111.80
35	YA	1602	U	C5-C4-O4	7.50	130.40	125.90
35	YA	1735	C	C2-N1-C1'	7.49	127.04	118.80
1	QA	957	U	C5-C6-N1	7.49	126.44	122.70
9	QI	48	GLU	CB-CA-C	7.49	125.38	110.40
35	RA	1950	G	N1-C6-O6	7.49	124.39	119.90
35	YA	1882	C	C2-N1-C1'	7.48	127.03	118.80
1	XA	818	G	P-O3'-C3'	7.47	128.67	119.70
10	QJ	29	ARG	CG-CD-NE	7.47	127.48	111.80
35	RA	143	C	C2-N1-C1'	7.46	127.01	118.80
35	RA	1241	A	C5-C6-N1	-7.46	113.97	117.70
35	RA	2229	C	C6-N1-C2	-7.46	117.32	120.30
35	YA	2318	G	N7-C8-N9	7.46	116.83	113.10
35	RA	2863	C	C6-N1-C2	-7.46	117.32	120.30
35	YA	527	C	N1-C2-O2	7.46	123.37	118.90
35	RA	945	A	C5-N7-C8	-7.45	100.17	103.90
35	RA	90	U	P-O3'-C3'	7.45	128.64	119.70
35	YA	1913	A	N3-C4-N9	7.45	133.36	127.40
35	RA	2094	G	C5-C6-N1	7.45	115.22	111.50
35	RA	2889	C	C6-N1-C2	-7.45	117.32	120.30
35	RA	1899	G	N3-C4-N9	7.44	130.47	126.00
35	YA	621	A	C4-C5-N7	7.44	114.42	110.70
35	YA	1888	G	C2-N3-C4	7.44	115.62	111.90
35	RA	527	C	C5-C4-N4	7.44	125.41	120.20
35	YA	672	C	N3-C4-C5	-7.44	118.92	121.90
35	RA	774	A	C8-N9-C4	-7.43	102.83	105.80
35	RA	953	A	N1-C6-N6	7.43	123.06	118.60
35	YA	1774	C	N1-C2-O2	7.42	123.36	118.90
1	QA	90	C	C5-C6-N1	7.42	124.71	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RA	570	G	C4-C5-N7	-7.42	107.83	110.80
13	QM	41	PRO	CA-N-CD	-7.42	101.11	111.50
1	XA	192	U	N1-C2-O2	7.42	128.00	122.80
35	RA	1251	C	C6-N1-C2	7.41	123.27	120.30
1	QA	1502	A	N7-C8-N9	7.41	117.50	113.80
35	RA	404	C	P-O3'-C3'	7.40	128.58	119.70
35	RA	859	G	P-O3'-C3'	7.40	128.58	119.70
35	RA	1544	C	N1-C2-O2	7.39	123.34	118.90
1	XA	328	C	N3-C2-O2	-7.39	116.73	121.90
35	YA	330	A	C5-N7-C8	-7.39	100.21	103.90
35	YA	1781	C	C6-N1-C1'	-7.38	111.94	120.80
1	QA	1517	G	C5-C6-O6	-7.38	124.17	128.60
35	YA	908	C	OP1-P-OP2	7.37	130.65	119.60
1	XA	1502	A	C8-N9-C4	-7.37	102.85	105.80
35	RA	286	C	C2-N1-C1'	7.36	126.90	118.80
35	YA	156	U	C5-C6-N1	7.36	126.38	122.70
48	RS	20	ARG	CB-CA-C	-7.36	95.68	110.40
35	RA	1385	G	C4-N9-C1'	-7.36	116.94	126.50
35	RA	1882	C	C6-N1-C2	-7.35	117.36	120.30
36	YB	118	G	N1-C6-O6	7.35	124.31	119.90
18	XR	53	ARG	CG-CD-NE	7.35	127.23	111.80
33	R8	40	GLU	N-CA-CB	-7.34	97.38	110.60
35	RA	1313	U	N3-C2-O2	-7.34	117.06	122.20
1	XA	197	A	P-O3'-C3'	7.34	128.51	119.70
35	YA	573	G	C5-C6-O6	-7.34	124.20	128.60
35	YA	1604	C	C6-N1-C2	-7.34	117.36	120.30
20	XT	57	ARG	CB-CG-CD	-7.33	92.53	111.60
35	RA	1528	A	N7-C8-N9	7.33	117.47	113.80
35	RA	2584	U	C6-N1-C2	-7.33	116.60	121.00
35	YA	1698	A	C2-N3-C4	-7.33	106.93	110.60
1	XA	1007	C	C2-N1-C1'	7.33	126.86	118.80
35	RA	1971	A	C2-N3-C4	7.33	114.26	110.60
9	XI	25	LYS	CD-CE-NZ	7.32	128.54	111.70
15	XO	13	GLN	CA-CB-CG	7.32	129.51	113.40
35	RA	143	C	C5-C6-N1	7.32	124.66	121.00
35	YA	270(Z)	U	C5-C6-N1	-7.32	119.04	122.70
35	YA	279	C	C2-N1-C1'	7.32	126.85	118.80
35	RA	676	A	C4-C5-N7	7.31	114.36	110.70
35	RA	845	G	N1-C6-O6	7.31	124.28	119.90
35	YA	1899	G	N3-C4-C5	-7.30	124.95	128.60
35	YA	2346	A	C2-N3-C4	-7.30	106.95	110.60
35	RA	2242	G	C8-N9-C4	7.30	109.32	106.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	RB	3	C	C2-N1-C1'	7.30	126.83	118.80
35	RA	1735	C	C6-N1-C2	-7.29	117.38	120.30
35	RA	2041	U	N1-C2-O2	7.29	127.90	122.80
35	YA	1180	C	C6-N1-C2	-7.29	117.39	120.30
35	YA	1881	C	C6-N1-C2	-7.29	117.39	120.30
35	YA	2830	G	C8-N9-C4	-7.28	103.49	106.40
1	QA	108	G	C4-N9-C1'	7.28	135.96	126.50
35	RA	2312	U	C6-N1-C2	-7.28	116.63	121.00
35	RA	2712	U	C2-N1-C1'	7.27	126.43	117.70
1	XA	1054	C	P-O3'-C3'	7.27	128.43	119.70
35	YA	1490	A	C8-N9-C4	7.26	108.71	105.80
36	YB	80	U	N3-C2-O2	-7.26	117.12	122.20
35	YA	676	A	N7-C8-N9	7.26	117.43	113.80
35	YA	2346	A	C4-C5-N7	7.26	114.33	110.70
35	YA	2286	A	N7-C8-N9	7.25	117.43	113.80
1	QA	1301	U	C6-N1-C2	-7.25	116.65	121.00
35	YA	71	A	C5-N7-C8	-7.25	100.28	103.90
35	YA	1982	C	N1-C2-O2	7.25	123.25	118.90
1	QA	1298	C	C5-C4-N4	-7.24	115.13	120.20
1	XA	325	A	O5'-P-OP2	-7.24	99.18	105.70
50	YU	112	ARG	CG-CD-NE	7.24	127.01	111.80
1	QA	1528	U	P-O3'-C3'	7.23	128.38	119.70
35	YA	1528	A	C8-N9-C4	-7.23	102.91	105.80
35	RA	2666	C	N1-C2-O2	7.23	123.24	118.90
35	RA	246	C	C6-N1-C2	-7.23	117.41	120.30
35	RA	2205	C	C5-C6-N1	7.22	124.61	121.00
35	YA	270(U)	C	N1-C2-O2	7.22	123.23	118.90
35	YA	2430	A	N7-C8-N9	7.22	117.41	113.80
1	QA	79	G	N3-C4-C5	-7.22	124.99	128.60
13	QM	67	GLU	CA-C-O	-7.22	104.93	120.10
35	RA	1947	C	N1-C2-O2	7.22	123.23	118.90
1	XA	980	C	C6-N1-C2	-7.22	117.41	120.30
40	RG	79	ASN	C-N-CA	7.22	139.74	121.70
35	YA	2572	A	N7-C8-N9	-7.21	110.19	113.80
1	XA	1108	G	C5-C6-O6	7.21	132.93	128.60
1	QA	1127	G	C4-N9-C1'	7.21	135.87	126.50
35	YA	1288	U	N3-C2-O2	-7.21	117.15	122.20
35	RA	995	C	N1-C2-O2	-7.21	114.58	118.90
35	YA	2712	U	C2-N1-C1'	7.20	126.34	117.70
22	QW	13	C	N1-C2-O2	7.20	123.22	118.90
35	RA	1196	C	C6-N1-C2	-7.20	117.42	120.30
22	QV	69	C	C6-N1-C2	-7.20	117.42	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	QL	117	ARG	CG-CD-NE	-7.20	96.69	111.80
35	RA	1523	U	C5-C6-N1	7.20	126.30	122.70
35	YA	139	G	C4-C5-N7	-7.19	107.92	110.80
35	RA	2043	C	C6-N1-C2	-7.19	117.42	120.30
35	YA	1332	G	N1-C2-N2	-7.19	109.73	116.20
35	YA	1558	A	P-O3'-C3'	7.19	128.32	119.70
35	YA	774	A	C5-C6-N1	-7.18	114.11	117.70
1	XA	186	C	C2-N1-C1'	7.18	126.70	118.80
1	XA	1158	C	C6-N1-C1'	-7.18	112.19	120.80
35	YA	1621	U	N3-C4-O4	7.18	124.42	119.40
35	YA	1950	G	C5-N7-C8	-7.18	100.71	104.30
35	YA	556	G	N7-C8-N9	7.17	116.69	113.10
35	RA	1669	A	C2-N3-C4	7.17	114.18	110.60
35	RA	279	C	C6-N1-C2	-7.17	117.43	120.30
35	RA	2868	A	N7-C8-N9	7.17	117.38	113.80
35	YA	783	A	C4-C5-N7	7.17	114.28	110.70
35	YA	1697	G	N1-C6-O6	7.17	124.20	119.90
49	RT	3	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	XA	710	G	O5'-P-OP1	7.16	119.30	110.70
1	XA	975	A	C5-N7-C8	-7.16	100.32	103.90
35	RA	1950	G	C8-N9-C4	-7.16	103.53	106.40
35	RA	603	A	P-O3'-C3'	7.16	128.29	119.70
35	YA	510	C	N1-C2-O2	7.16	123.19	118.90
22	QW	34	C	C2-N1-C1'	7.16	126.67	118.80
7	XG	79	ARG	CG-CD-NE	7.16	126.83	111.80
35	YA	907	U	OP2-P-O3'	-7.15	89.46	105.20
3	XC	190	ARG	CG-CD-NE	-7.15	96.78	111.80
35	RA	2168	G	C4-N9-C1'	7.15	135.79	126.50
35	YA	2666	C	N1-C2-O2	7.14	123.19	118.90
1	XA	1128	C	C5-C6-N1	7.14	124.57	121.00
35	YA	2392	A	C2-N3-C4	-7.14	107.03	110.60
35	RA	897	C	C6-N1-C2	-7.14	117.44	120.30
1	QA	1158	C	C6-N1-C1'	-7.14	112.23	120.80
35	RA	352	G	C8-N9-C1'	-7.14	117.72	127.00
6	QF	28	ARG	CG-CD-NE	7.13	126.78	111.80
35	RA	269	U	C2-N1-C1'	7.13	126.26	117.70
35	YA	358	U	C2-N1-C1'	7.13	126.26	117.70
35	RA	2873	A	C4-N9-C1'	7.12	139.12	126.30
1	XA	726	C	C6-N1-C2	-7.12	117.45	120.30
36	YB	31	C	C6-N1-C2	-7.12	117.45	120.30
35	RA	1198	U	N3-C2-O2	-7.12	117.22	122.20
1	QA	1502	A	C4-C5-N7	7.12	114.26	110.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RA	2318	G	N1-C6-O6	7.12	124.17	119.90
35	YA	613	U	C6-N1-C1'	-7.12	111.24	121.20
35	RA	1313	U	N1-C2-O2	7.12	127.78	122.80
35	RA	1644	C	N1-C2-O2	7.12	123.17	118.90
1	XA	18	C	C5-C6-N1	7.12	124.56	121.00
1	XA	181	G	P-O3'-C3'	7.11	128.23	119.70
1	XA	1031	G	N3-C4-N9	7.11	130.27	126.00
1	XA	754	C	C6-N1-C1'	-7.11	112.27	120.80
35	YA	676	A	C2-N3-C4	-7.11	107.05	110.60
35	YA	273(C)	C	C2-N1-C1'	7.11	126.61	118.80
35	YA	1417	C	C5-C6-N1	7.11	124.55	121.00
1	QA	328	C	P-O3'-C3'	7.10	128.22	119.70
7	QG	10	ARG	CG-CD-NE	-7.10	96.88	111.80
35	RA	1314	C	C2-N1-C1'	7.10	126.61	118.80
35	YA	807	U	N3-C4-O4	7.10	124.37	119.40
35	RA	1786	A	C6-C5-N7	-7.10	127.33	132.30
35	YA	2602	A	N1-C6-N6	7.10	122.86	118.60
35	YA	172	C	C6-N1-C2	-7.10	117.46	120.30
35	YA	12	U	N1-C2-O2	7.09	127.76	122.80
35	YA	2211	G	P-O3'-C3'	7.09	128.21	119.70
35	RA	234	C	N1-C2-O2	7.09	123.15	118.90
35	YA	1940	U	C5-C4-O4	-7.09	121.65	125.90
1	XA	848	C	C6-N1-C2	-7.08	117.47	120.30
35	YA	2168	G	N3-C4-C5	-7.08	125.06	128.60
35	RA	352	G	C4-N9-C1'	7.08	135.71	126.50
35	YA	140	A	N1-C6-N6	7.08	122.85	118.60
35	RA	2501	C	C2-N1-C1'	-7.08	111.02	118.80
35	RA	2779	U	N3-C2-O2	-7.08	117.25	122.20
35	RA	1332	G	N7-C8-N9	7.07	116.64	113.10
1	QA	1001	G	O5'-P-OP1	7.07	119.18	110.70
35	RA	2584	U	C4-C5-C6	7.07	123.94	119.70
1	XA	999	U	N3-C2-O2	-7.07	117.25	122.20
35	YA	2699	C	C6-N1-C2	-7.07	117.47	120.30
38	RE	154	LYS	CD-CE-NZ	-7.06	95.46	111.70
1	XA	974	A	C2-N3-C4	7.06	114.13	110.60
22	XV	24	U	N3-C2-O2	-7.06	117.26	122.20
2	QB	147	LYS	CB-CA-C	-7.06	96.29	110.40
36	YB	2	C	N3-C2-O2	-7.05	116.97	121.90
34	R9	11	CYS	CA-CB-SG	-7.05	101.32	114.00
35	YA	277	C	N1-C2-O2	7.04	123.13	118.90
35	RA	2861	G	C4-C5-N7	7.04	113.62	110.80
1	XA	822	C	C6-N1-C2	-7.04	117.48	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	YA	1616	A	C6-C5-N7	-7.04	127.37	132.30
35	RA	750	A	N1-C6-N6	-7.04	114.38	118.60
35	YA	277	C	C6-N1-C2	-7.04	117.48	120.30
36	YB	3	C	C5-C6-N1	7.04	124.52	121.00
35	RA	2791	C	C6-N1-C1'	7.04	129.25	120.80
1	XA	1160	G	C8-N9-C1'	-7.04	117.85	127.00
1	XA	1346	A	P-O3'-C3'	7.04	128.15	119.70
45	RP	65	ARG	CG-CD-NE	-7.04	97.02	111.80
35	YA	907	U	N3-C2-O2	-7.04	117.27	122.20
36	RB	3	C	C5-C4-N4	-7.03	115.28	120.20
35	YA	2422	A	P-O3'-C3'	7.03	128.13	119.70
1	XA	1067	A	P-O3'-C3'	7.03	128.13	119.70
1	XA	1356	G	N3-C4-N9	7.03	130.22	126.00
35	RA	1533	C	C5-C6-N1	7.03	124.51	121.00
35	YA	1171	G	P-O3'-C3'	7.03	128.13	119.70
35	YA	1407	C	C5-C6-N1	7.02	124.51	121.00
35	YA	1521	G	C8-N9-C4	-7.02	103.59	106.40
35	YA	1920	C	C5-C6-N1	7.02	124.51	121.00
35	RA	565	C	N1-C2-O2	7.02	123.11	118.90
35	RA	1616	A	C8-N9-C4	-7.02	102.99	105.80
35	YA	1406	U	N1-C2-O2	7.02	127.71	122.80
35	YA	2585	U	N3-C4-O4	-7.02	114.49	119.40
35	RA	1022	G	P-O3'-C3'	7.02	128.12	119.70
35	RA	124	G	C8-N9-C4	-7.01	103.59	106.40
1	QA	1260	C	N3-C2-O2	-7.01	116.99	121.90
35	RA	974(A)	C	N3-C2-O2	-7.01	116.99	121.90
35	RA	1558	A	P-O3'-C3'	7.01	128.11	119.70
35	YA	2210	G	C2-N3-C4	7.01	115.40	111.90
35	YA	603	A	P-O3'-C3'	7.01	128.11	119.70
1	QA	999	U	N3-C2-O2	-7.00	117.30	122.20
35	RA	783	A	C8-N9-C4	-7.00	103.00	105.80
35	YA	1835	G	C8-N9-C4	-7.00	103.60	106.40
40	YG	112	PRO	N-CA-CB	7.00	111.70	103.30
1	XA	468	A	C8-N9-C4	7.00	108.60	105.80
1	XA	1065	U	P-O3'-C3'	7.00	128.10	119.70
1	QA	1254	C	C6-N1-C2	-7.00	117.50	120.30
35	RA	2666	C	N3-C2-O2	-7.00	117.00	121.90
1	XA	4	U	C6-N1-C1'	-7.00	111.41	121.20
40	YG	179	PRO	CA-N-CD	-7.00	101.71	111.50
35	YA	2748	A	C8-N9-C4	-7.00	103.00	105.80
1	XA	1160	G	C4-N9-C1'	6.99	135.59	126.50
35	YA	1653	G	P-O3'-C3'	6.99	128.09	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	YV	91	TYR	CA-CB-CG	6.99	126.68	113.40
1	XA	1381	U	N1-C2-O2	6.99	127.69	122.80
3	QC	82	GLU	CB-CA-C	-6.99	96.43	110.40
35	RA	1152	C	N3-C4-C5	-6.99	119.11	121.90
35	YA	537	C	C2-N1-C1'	6.99	126.48	118.80
35	YA	1698	A	C5-C6-N1	-6.99	114.21	117.70
1	QA	169	C	N1-C2-O2	6.98	123.09	118.90
10	QJ	79	ARG	CB-CG-CD	6.98	129.75	111.60
1	XA	1128	C	C6-N1-C2	-6.98	117.51	120.30
1	XA	1325	C	C6-N1-C2	-6.98	117.51	120.30
1	QA	525	C	C5-C6-N1	6.98	124.49	121.00
35	RA	2508	G	C5-C6-O6	-6.98	124.42	128.60
35	YA	753	C	C6-N1-C2	-6.97	117.51	120.30
35	YA	860	U	C5-C6-N1	6.97	126.19	122.70
35	RA	1899	G	C4-N9-C1'	6.97	135.56	126.50
35	RA	1385	G	C4-C5-N7	-6.97	108.01	110.80
35	YA	2286	A	C8-N9-C4	-6.97	103.01	105.80
1	QA	1523	G	N1-C6-O6	-6.97	115.72	119.90
1	XA	330	C	N1-C2-O2	6.97	123.08	118.90
1	XA	1532	U	P-O3'-C3'	6.97	128.06	119.70
22	XV	13	C	C5-C6-N1	6.96	124.48	121.00
35	RA	867	C	N3-C2-O2	-6.96	117.03	121.90
35	RA	2866	U	N1-C2-O2	-6.96	117.93	122.80
35	YA	2118	U	C5-C6-N1	6.96	126.18	122.70
1	QA	1065	U	P-O3'-C3'	6.96	128.05	119.70
36	RB	117	G	C6-C5-N7	-6.96	126.22	130.40
1	XA	1000	A	N7-C8-N9	6.96	117.28	113.80
33	R8	40	GLU	CA-CB-CG	6.95	128.70	113.40
35	RA	1686	C	C2-N1-C1'	6.95	126.45	118.80
35	RA	1774	C	N3-C2-O2	-6.95	117.03	121.90
35	YA	1076	C	C5-C6-N1	6.95	124.48	121.00
1	QA	419	C	C2-N1-C1'	6.95	126.44	118.80
1	QA	992	U	P-O3'-C3'	6.95	128.04	119.70
35	RA	263	C	C6-N1-C2	-6.95	117.52	120.30
1	QA	1007	C	C2-N1-C1'	6.95	126.44	118.80
1	QA	115	G	P-O3'-C3'	6.94	128.03	119.70
35	RA	1171	G	P-O3'-C3'	6.94	128.03	119.70
35	YA	52	A	C5-C6-N6	-6.94	118.15	123.70
35	RA	2803	C	C6-N1-C2	-6.93	117.53	120.30
1	XA	1502	A	C4-C5-N7	6.93	114.17	110.70
55	YZ	15	PRO	CA-N-CD	-6.93	101.80	111.50
35	YA	93	C	C6-N1-C2	-6.93	117.53	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	YA	817	C	C6-N1-C2	-6.93	117.53	120.30
35	YA	930	U	N3-C2-O2	-6.93	117.35	122.20
45	RP	7	ARG	CD-NE-CZ	6.93	133.30	123.60
29	Y4	44	THR	N-CA-C	6.93	129.71	111.00
35	RA	1751	C	C6-N1-C2	-6.92	117.53	120.30
1	QA	484	G	P-O3'-C3'	6.92	128.00	119.70
35	RA	2712	U	N1-C2-O2	6.92	127.64	122.80
35	YA	1407	C	N1-C2-O2	6.92	123.05	118.90
35	YA	603	A	C5-N7-C8	-6.91	100.44	103.90
35	RA	2210	G	C8-N9-C1'	-6.91	118.02	127.00
1	XA	971	G	N7-C8-N9	-6.91	109.65	113.10
1	XA	1137	C	P-O3'-C3'	6.91	127.99	119.70
13	XM	93	ARG	CA-CB-CG	6.91	128.60	113.40
35	YA	9	U	C5-C6-N1	6.91	126.15	122.70
22	XW	61	C	C6-N1-C2	-6.91	117.54	120.30
9	QI	48	GLU	N-CA-CB	-6.90	98.18	110.60
35	YA	1332	G	N3-C2-N2	6.89	124.72	119.90
36	YB	49	C	C6-N1-C2	-6.88	117.55	120.30
1	XA	974	A	O4'-C1'-N9	6.88	113.70	108.20
35	YA	93	C	C2-N1-C1'	6.88	126.37	118.80
35	YA	837	C	C5-C6-N1	6.88	124.44	121.00
35	YA	2143	C	N1-C2-O2	6.88	123.03	118.90
1	QA	186(A)	C	C6-N1-C2	-6.88	117.55	120.30
35	YA	1742	C	C6-N1-C2	-6.88	117.55	120.30
1	QA	268	C	N3-C4-C5	-6.87	119.15	121.90
35	YA	1179	C	N1-C2-O2	6.87	123.02	118.90
35	YA	1913	A	N7-C8-N9	-6.87	110.37	113.80
35	RA	2849	U	P-O3'-C3'	6.87	127.94	119.70
35	YA	277	C	C5-C6-N1	6.87	124.43	121.00
35	RA	1505	C	C5-C6-N1	6.87	124.43	121.00
35	RA	2607	G	N3-C2-N2	6.87	124.71	119.90
35	YA	2430	A	C5-N7-C8	-6.87	100.47	103.90
35	YA	2505	G	N1-C6-O6	-6.87	115.78	119.90
35	YA	708	C	N1-C2-O2	6.86	123.02	118.90
35	RA	265	A	C5-N7-C8	-6.86	100.47	103.90
35	YA	141	A	C5-N7-C8	-6.86	100.47	103.90
35	YA	1342	A	C5-C6-N1	-6.86	114.27	117.70
35	YA	2226	C	N3-C4-N4	6.86	122.80	118.00
35	RA	1143	A	C5-N7-C8	-6.86	100.47	103.90
1	XA	328	C	P-O3'-C3'	6.86	127.93	119.70
1	QA	1145	C	C5-C6-N1	6.85	124.43	121.00
35	RA	1313	U	C6-N1-C1'	-6.85	111.61	121.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	YB	3	C	N1-C2-O2	6.85	123.01	118.90
1	XA	1038	C	P-O3'-C3'	6.85	127.92	119.70
35	YA	2144	U	P-O3'-C3'	6.85	127.92	119.70
35	YA	2666	C	N3-C2-O2	-6.85	117.11	121.90
36	YB	31	C	C6-N1-C1'	-6.85	112.58	120.80
35	RA	2403	C	N3-C4-C5	-6.85	119.16	121.90
48	RS	20	ARG	N-CA-CB	6.85	122.92	110.60
35	YA	1022	G	P-O3'-C3'	6.85	127.92	119.70
35	YA	2559	C	C6-N1-C2	-6.84	117.56	120.30
35	RA	894	C	N1-C2-O2	6.84	123.00	118.90
1	XA	108	G	N7-C8-N9	6.84	116.52	113.10
35	YA	758	C	N3-C2-O2	-6.83	117.12	121.90
35	YA	1496	A	N1-C6-N6	6.83	122.70	118.60
35	RA	38	A	C5-C6-N1	6.83	121.11	117.70
35	RA	1827	C	C6-N1-C2	-6.83	117.57	120.30
1	QA	1028(A)	C	C6-N1-C2	-6.83	117.57	120.30
35	YA	48	G	C4-C5-N7	-6.83	108.07	110.80
35	RA	1830	C	N1-C2-O2	6.83	123.00	118.90
35	YA	2713	A	N1-C6-N6	6.83	122.69	118.60
1	QA	1003	G	C4-N9-C1'	6.82	135.37	126.50
1	QA	1067	A	P-O3'-C3'	6.82	127.89	119.70
35	RA	20	C	C6-N1-C2	-6.82	117.57	120.30
35	RA	1248	G	C5-C6-O6	-6.82	124.51	128.60
1	XA	992	U	P-O3'-C3'	6.81	127.88	119.70
35	YA	286	C	C2-N1-C1'	6.81	126.30	118.80
35	YA	1267	U	N3-C2-O2	-6.81	117.43	122.20
36	YB	43	C	N3-C2-O2	-6.81	117.13	121.90
1	QA	1298	C	N1-C2-O2	6.81	122.98	118.90
1	XA	999	U	N1-C2-O2	6.81	127.57	122.80
22	XV	67	C	C6-N1-C2	-6.81	117.58	120.30
35	YA	2527	C	C2-N1-C1'	6.81	126.29	118.80
35	YA	48	G	C5-C6-O6	6.80	132.68	128.60
35	YA	528	A	C2-N3-C4	-6.80	107.20	110.60
35	RA	330	A	C4-C5-N7	6.80	114.10	110.70
1	XA	536	C	C6-N1-C2	-6.80	117.58	120.30
35	YA	1505	C	C6-N1-C2	-6.80	117.58	120.30
35	YA	2666	C	C6-N1-C2	-6.80	117.58	120.30
35	RA	859	G	C4-N9-C1'	-6.80	117.66	126.50
12	XL	53	ARG	CG-CD-NE	6.80	126.08	111.80
35	YA	74	A	C5-C6-N6	-6.80	118.26	123.70
35	YA	1774	C	N3-C2-O2	-6.80	117.14	121.90
35	YA	2321	G	C8-N9-C4	-6.80	103.68	106.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	YA	2475	C	C2-N1-C1'	-6.80	111.32	118.80
10	XJ	71	LEU	CA-CB-CG	6.79	130.93	115.30
35	RA	1644	C	N3-C2-O2	-6.79	117.14	121.90
1	XA	654	G	C8-N9-C4	-6.79	103.68	106.40
9	XI	56	LEU	CA-CB-CG	6.79	130.92	115.30
35	YA	2572	A	N1-C6-N6	-6.79	114.52	118.60
35	YA	783	A	C2-N3-C4	-6.79	107.20	110.60
1	QA	193	C	C5-C6-N1	6.79	124.39	121.00
1	XA	405	U	N1-C2-O2	6.79	127.55	122.80
35	YA	269	U	C2-N1-C1'	6.79	125.84	117.70
35	YA	1516	U	C6-N1-C2	-6.79	116.93	121.00
35	RA	1528	A	N1-C6-N6	6.78	122.67	118.60
35	YA	2712	U	C6-N1-C1'	-6.78	111.70	121.20
35	RA	339	U	N3-C2-O2	-6.78	117.45	122.20
1	QA	1039	C	C5-C6-N1	6.78	124.39	121.00
1	QA	979	C	C6-N1-C2	-6.77	117.59	120.30
1	QA	946	A	N9-C4-C5	-6.77	103.09	105.80
35	YA	1616	A	C2-N3-C4	-6.77	107.22	110.60
35	RA	445	C	C6-N1-C2	-6.77	117.59	120.30
35	RA	2545	G	C8-N9-C4	-6.76	103.69	106.40
1	XA	1158	C	N3-C2-O2	-6.76	117.17	121.90
35	YA	958	U	C6-N1-C2	-6.76	116.94	121.00
35	RA	2391	G	N1-C6-O6	-6.76	115.84	119.90
35	RA	2772	C	C5-C6-N1	6.76	124.38	121.00
35	RA	2896	C	C5-C6-N1	6.76	124.38	121.00
1	XA	74	C	C2-N1-C1'	6.76	126.24	118.80
35	YA	71	A	C2-N3-C4	-6.76	107.22	110.60
35	RA	1407	C	N3-C4-C5	-6.76	119.20	121.90
35	RA	2380	C	C6-N1-C2	-6.75	117.60	120.30
1	XA	816	A	C8-N9-C4	-6.75	103.10	105.80
7	XG	67	GLU	N-CA-CB	6.75	122.75	110.60
35	YA	2584	U	N1-C2-N3	6.75	118.95	114.90
35	RA	1300	U	OP2-P-O3'	6.75	120.04	105.20
36	YB	31	C	N3-C2-O2	-6.75	117.18	121.90
35	RA	2294	C	C2-N1-C1'	6.74	126.22	118.80
9	QI	55	ALA	CB-CA-C	6.74	120.21	110.10
35	YA	2318	G	C5-N7-C8	-6.74	100.93	104.30
35	RA	1698	A	C2-N3-C4	-6.74	107.23	110.60
35	YA	1024	G	N3-C4-N9	6.74	130.04	126.00
35	YA	2311	A	OP1-P-O3'	6.74	120.02	105.20
1	QA	79	G	C5-C6-N1	6.73	114.87	111.50
35	RA	507	A	N1-C6-N6	6.73	122.64	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	YA	1616	A	N7-C8-N9	6.73	117.17	113.80
35	YA	2752	C	N1-C2-O2	6.73	122.94	118.90
35	YA	1607	C	N3-C2-O2	6.73	126.61	121.90
22	QV	51	C	C6-N1-C2	-6.73	117.61	120.30
22	XW	60	U	C2-N1-C1'	6.73	125.77	117.70
35	YA	837	C	N1-C2-O2	6.73	122.94	118.90
37	RD	112	GLN	CA-CB-CG	6.72	128.19	113.40
39	YF	203	GLN	CA-CB-CG	6.72	128.19	113.40
13	QM	66	LEU	C-N-CA	6.72	138.50	121.70
1	XA	687	A	P-O3'-C3'	6.72	127.76	119.70
22	QV	1	C	P-O3'-C3'	6.72	127.76	119.70
35	YA	479	A	N1-C6-N6	-6.72	114.57	118.60
35	YA	708	C	C5-C6-N1	6.72	124.36	121.00
35	RA	1658	C	C5-C6-N1	6.71	124.36	121.00
1	XA	60	A	P-O3'-C3'	6.71	127.75	119.70
35	YA	573	G	N1-C6-O6	6.71	123.93	119.90
41	YH	50	VAL	CB-CA-C	6.71	124.15	111.40
35	RA	1505	C	C6-N1-C2	-6.71	117.62	120.30
35	YA	2174	C	N1-C2-O2	6.71	122.92	118.90
22	QW	13	C	N3-C2-O2	-6.71	117.21	121.90
35	YA	2244	U	N3-C4-O4	6.70	124.09	119.40
35	YA	1899	G	N3-C4-N9	6.70	130.02	126.00
1	QA	328	C	C6-N1-C1'	-6.70	112.76	120.80
35	RA	2571	C	C6-N1-C2	-6.70	117.62	120.30
35	RA	1085	A	P-O3'-C3'	6.70	127.74	119.70
1	XA	419	C	C5-C6-N1	6.70	124.35	121.00
35	YA	139	G	C8-N9-C4	-6.70	103.72	106.40
35	RA	1598	C	N1-C2-O2	6.69	122.92	118.90
35	RA	1011	G	C4-N9-C1'	-6.69	117.80	126.50
51	RV	43	GLU	CB-CA-C	6.69	123.79	110.40
1	XA	1006	C	N1-C2-O2	6.69	122.92	118.90
35	RA	279	C	C2-N1-C1'	6.69	126.16	118.80
35	RA	2226	C	N1-C2-O2	6.69	122.91	118.90
1	XA	1031	G	C4-N9-C1'	6.68	135.19	126.50
35	YA	74	A	C4-C5-N7	6.68	114.04	110.70
35	RA	1234	U	N3-C2-O2	-6.68	117.52	122.20
35	RA	499	U	N3-C2-O2	-6.68	117.52	122.20
35	YA	1735	C	C5-C6-N1	6.68	124.34	121.00
35	YA	288	C	C5-C6-N1	6.68	124.34	121.00
35	RA	2481	G	P-O3'-C3'	6.67	127.71	119.70
35	RA	2816	C	C6-N1-C2	-6.67	117.63	120.30
1	XA	1298	C	N1-C2-O2	6.67	122.90	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	QA	754	C	N1-C2-O2	6.67	122.90	118.90
35	RA	75	G	N9-C4-C5	6.67	108.07	105.40
35	YA	2244	U	C5-C6-N1	6.67	126.03	122.70
35	RA	2787	C	C6-N1-C2	-6.67	117.63	120.30
1	QA	1517	G	N1-C6-O6	6.67	123.90	119.90
1	QA	779	C	N3-C4-C5	6.66	124.56	121.90
22	QW	34	C	C6-N1-C2	-6.66	117.63	120.30
35	YA	736	C	C5-C6-N1	6.66	124.33	121.00
35	YA	2128	C	C2-N1-C1'	6.66	126.13	118.80
1	QA	1260	C	N1-C2-O2	6.66	122.89	118.90
35	RA	1013	C	C6-N1-C2	-6.66	117.64	120.30
35	RA	1616	A	C4-C5-N7	6.66	114.03	110.70
39	RF	17	ARG	CG-CD-NE	6.66	125.78	111.80
22	QW	61	C	O5'-P-OP2	-6.65	99.71	105.70
35	YA	330	A	C2-N3-C4	-6.65	107.27	110.60
35	YA	1800	C	C6-N1-C2	6.65	122.96	120.30
35	RA	774	A	N7-C8-N9	6.65	117.13	113.80
35	RA	2602	A	N9-C4-C5	-6.65	103.14	105.80
1	XA	442	C	C5-C6-N1	6.65	124.33	121.00
35	YA	1159	U	C5-C6-N1	6.65	126.03	122.70
1	QA	307	C	N1-C2-O2	6.65	122.89	118.90
1	QA	442	C	C2-N1-C1'	6.64	126.11	118.80
48	RS	110	LEU	CA-CB-CG	6.64	130.58	115.30
44	RO	107	ARG	CD-NE-CZ	6.64	132.90	123.60
1	QA	1014	A	C4-N9-C1'	6.64	138.25	126.30
1	QA	687	A	P-O3'-C3'	6.64	127.66	119.70
22	QW	13	C	C5-C6-N1	6.64	124.32	121.00
35	RA	758	C	C6-N1-C2	-6.64	117.64	120.30
35	YA	2092	U	C5-C4-O4	6.63	129.88	125.90
35	RA	2059	A	N1-C6-N6	-6.63	114.62	118.60
35	RA	91	A	N1-C6-N6	6.63	122.58	118.60
35	RA	2572	A	C8-N9-C4	6.63	108.45	105.80
35	YA	174	C	C2-N1-C1'	6.63	126.09	118.80
35	YA	1979	C	N3-C2-O2	-6.63	117.26	121.90
35	YA	1992	G	P-O3'-C3'	6.63	127.66	119.70
35	YA	2143	C	N3-C2-O2	-6.63	117.26	121.90
35	RA	436	C	C6-N1-C2	-6.63	117.65	120.30
35	YA	1776	G	C2-N3-C4	6.62	115.21	111.90
35	YA	36	G	N3-C4-C5	-6.62	125.29	128.60
35	RA	1102	C	C2-N1-C1'	6.62	126.08	118.80
35	YA	807	U	C6-N1-C2	-6.62	117.03	121.00
2	QB	230	VAL	C-N-CA	6.62	138.24	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RA	1961	C	N3-C4-C5	6.62	124.55	121.90
1	QA	1502	A	C6-C5-N7	-6.61	127.67	132.30
35	RA	1342	A	C2-N3-C4	-6.61	107.30	110.60
35	RA	1881	C	C5-C6-N1	6.61	124.30	121.00
35	YA	138	G	N7-C8-N9	6.61	116.40	113.10
35	RA	2559	C	C5-C6-N1	6.60	124.30	121.00
35	YA	1687	G	N1-C6-O6	-6.60	115.94	119.90
35	RA	1950	G	C4-N9-C1'	6.60	135.08	126.50
1	QA	169	C	C2-N1-C1'	6.60	126.06	118.80
35	RA	74	A	N3-C4-C5	6.59	131.42	126.80
35	RA	2490	G	C4-C5-N7	6.59	113.44	110.80
35	RA	1965	C	C5-C4-N4	-6.59	115.58	120.20
35	YA	316	C	C6-N1-C2	-6.59	117.66	120.30
35	YA	2666	C	C2-N1-C1'	6.59	126.05	118.80
4	XD	157	LEU	N-CA-C	6.59	128.79	111.00
35	YA	176	G	C8-N9-C4	6.59	109.04	106.40
35	YA	2501	C	C5-C6-N1	-6.59	117.71	121.00
35	RA	105	C	C6-N1-C2	-6.58	117.67	120.30
35	YA	438	G	C8-N9-C4	6.58	109.03	106.40
1	QA	989	C	C6-N1-C2	-6.58	117.67	120.30
1	QA	1125	U	N3-C4-O4	6.58	124.01	119.40
1	XA	209	U	N1-C2-O2	6.58	127.41	122.80
35	RA	2585	U	C2-N1-C1'	6.58	125.59	117.70
1	QA	1528	U	C2-N1-C1'	6.58	125.59	117.70
35	RA	193	U	N3-C2-O2	-6.58	117.60	122.20
41	RH	3	ARG	N-CA-C	-6.58	93.25	111.00
1	XA	169	C	N1-C2-O2	6.58	122.84	118.90
41	RH	18	GLU	N-CA-CB	-6.57	98.77	110.60
35	RA	2392	A	N7-C8-N9	6.57	117.09	113.80
1	XA	1126	U	C5-C6-N1	6.57	125.98	122.70
35	YA	273(D)	C	C5-C6-N1	6.57	124.28	121.00
35	YA	288	C	C2-N1-C1'	6.57	126.03	118.80
35	RA	2604	U	N1-C2-O2	6.57	127.40	122.80
35	RA	2026	C	C5-C6-N1	6.57	124.28	121.00
35	YA	2830	G	N7-C8-N9	6.57	116.38	113.10
1	QA	1321	C	C6-N1-C2	6.56	122.93	120.30
35	YA	1306	C	N3-C4-C5	-6.56	119.27	121.90
35	YA	2508	G	C6-C5-N7	-6.56	126.46	130.40
1	QA	1325	C	C2-N1-C1'	6.56	126.02	118.80
35	RA	1513	C	N3-C4-C5	-6.56	119.28	121.90
35	RA	2497	A	N1-C6-N6	6.56	122.53	118.60
1	XA	530	G	N3-C4-N9	6.56	129.94	126.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RA	894	C	C6-N1-C2	-6.56	117.68	120.30
35	YA	286	C	N1-C2-O2	6.56	122.83	118.90
1	XA	975	A	C4-C5-N7	6.56	113.98	110.70
1	QA	547	A	P-O3'-C3'	6.55	127.56	119.70
35	YA	74	A	C6-C5-N7	-6.55	127.71	132.30
1	QA	1007	C	C5-C6-N1	6.55	124.28	121.00
35	RA	945	A	C4-C5-N7	6.55	113.97	110.70
35	YA	2688	U	N1-C2-N3	6.55	118.83	114.90
35	YA	2226	C	C6-N1-C2	-6.55	117.68	120.30
1	QA	974	A	O4'-C1'-N9	6.54	113.44	108.20
35	RA	417	C	C6-N1-C2	-6.54	117.68	120.30
35	YA	2077	A	N9-C4-C5	-6.54	103.18	105.80
35	YA	2874	C	C2-N1-C1'	6.54	126.00	118.80
1	QA	1014	A	C8-N9-C1'	-6.54	115.92	127.70
35	RA	308	G	C8-N9-C4	6.54	109.02	106.40
42	RI	4	ILE	CB-CA-C	-6.54	98.52	111.60
35	YA	1961	C	C6-N1-C2	6.54	122.92	120.30
1	QA	1003	G	C8-N9-C1'	-6.54	118.50	127.00
1	XA	748	C	P-O3'-C3'	6.54	127.54	119.70
36	YB	15	A	OP1-P-O3'	6.54	119.58	105.20
35	YA	141	A	N1-C6-N6	6.53	122.52	118.60
35	YA	1914	C	C6-N1-C2	-6.53	117.69	120.30
1	QA	748	C	P-O3'-C3'	6.53	127.54	119.70
35	RA	2610	C	P-O3'-C3'	6.53	127.54	119.70
35	RA	242	G	C8-N9-C4	6.53	109.01	106.40
35	RA	1950	G	C5-N7-C8	-6.53	101.03	104.30
35	RA	1514	U	C2-N1-C1'	6.53	125.53	117.70
36	RB	51	G	N1-C6-O6	-6.52	115.99	119.90
36	RB	118	G	C4-N9-C1'	6.52	134.98	126.50
1	QA	115	G	N3-C4-C5	-6.52	125.34	128.60
35	RA	774	A	N1-C2-N3	6.52	132.56	129.30
35	RA	817	C	C6-N1-C2	-6.51	117.69	120.30
35	RA	2095	C	C6-N1-C2	-6.51	117.69	120.30
35	YA	2585	U	C5-C4-O4	6.51	129.81	125.90
1	QA	1066	C	C6-N1-C1'	-6.51	112.99	120.80
35	RA	2118	U	C2-N1-C1'	6.51	125.51	117.70
35	RA	2447	G	P-O3'-C3'	6.51	127.51	119.70
35	RA	2477	C	C6-N1-C1'	-6.51	112.99	120.80
35	YA	2210	G	C8-N9-C1'	-6.51	118.53	127.00
35	RA	2242	G	N9-C4-C5	-6.51	102.80	105.40
35	YA	512	G	P-O3'-C3'	6.51	127.51	119.70
22	QW	1	C	C6-N1-C2	-6.51	117.70	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	YA	1956	U	N1-C2-O2	6.51	127.36	122.80
35	RA	1920	C	C5-C6-N1	6.50	124.25	121.00
35	RA	2128	C	C5-C6-N1	6.50	124.25	121.00
35	RA	2459	A	C8-N9-C4	6.50	108.40	105.80
35	RA	2861	G	N9-C4-C5	-6.50	102.80	105.40
35	RA	1320	C	N1-C2-O2	6.50	122.80	118.90
1	QA	328	C	N3-C2-O2	-6.50	117.35	121.90
35	RA	1725	G	C4-N9-C1'	6.50	134.95	126.50
1	XA	36	C	C5-C6-N1	6.50	124.25	121.00
1	QA	419	C	C5-C6-N1	6.50	124.25	121.00
1	XA	5	U	P-O3'-C3'	6.50	127.49	119.70
35	RA	1544	C	C6-N1-C1'	-6.49	113.01	120.80
35	RA	2585	U	N1-C2-O2	6.49	127.34	122.80
1	XA	1502	A	C6-C5-N7	-6.49	127.75	132.30
22	XW	71	C	C6-N1-C2	-6.49	117.70	120.30
35	YA	1314	C	N1-C2-O2	6.49	122.80	118.90
35	YA	2318	G	N1-C6-O6	6.49	123.80	119.90
1	QA	754	C	C6-N1-C1'	-6.49	113.01	120.80
35	YA	93	C	C5-C6-N1	6.49	124.25	121.00
35	RA	1196	C	N3-C4-C5	-6.49	119.30	121.90
36	RB	31	C	C5-C6-N1	6.49	124.24	121.00
1	XA	812	C	P-O3'-C3'	6.49	127.49	119.70
35	YA	1678	G	N1-C6-O6	6.49	123.79	119.90
35	RA	2827	C	C5-C6-N1	6.49	124.24	121.00
35	RA	2287	A	N9-C4-C5	-6.48	103.21	105.80
35	RA	1021	A	C2-N3-C4	-6.48	107.36	110.60
5	XE	136	MET	CA-CB-CG	-6.48	102.28	113.30
35	RA	1294	U	N3-C2-O2	-6.48	117.67	122.20
35	RA	2605	U	C5-C4-O4	6.48	129.79	125.90
40	RG	113	ARG	NE-CZ-NH2	6.48	123.54	120.30
22	XV	68	C	C6-N1-C2	-6.48	117.71	120.30
35	YA	141	A	N7-C8-N9	6.48	117.04	113.80
1	QA	36	C	C6-N1-C2	-6.48	117.71	120.30
35	RA	1283	G	N1-C6-O6	-6.48	116.01	119.90
36	YB	80	U	N1-C2-O2	6.48	127.33	122.80
35	YA	270(Q)	C	N1-C2-O2	6.48	122.79	118.90
16	QP	32	TYR	CA-CB-CG	6.47	125.70	113.40
35	RA	1533	C	N1-C2-O2	6.47	122.78	118.90
1	XA	1381	U	C2-N1-C1'	6.47	125.47	117.70
1	QA	1228	C	C6-N1-C2	-6.47	117.71	120.30
35	RA	274	G	C8-N9-C4	-6.47	103.81	106.40
41	YH	23	ARG	CG-CD-NE	6.47	125.39	111.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	YA	1899	G	C2-N3-C4	6.47	115.13	111.90
35	YA	2032	G	N1-C6-O6	6.47	123.78	119.90
1	QA	792	A	P-O3'-C3'	6.47	127.46	119.70
35	YA	535	C	C6-N1-C2	-6.47	117.71	120.30
1	XA	1157	A	P-O3'-C3'	6.46	127.46	119.70
35	RA	1698	A	C5-C6-N1	-6.46	114.47	117.70
35	YA	1258	C	C5-C6-N1	6.46	124.23	121.00
1	XA	328	C	C6-N1-C1'	-6.46	113.05	120.80
35	RA	1021	A	C4-C5-N7	6.46	113.93	110.70
35	RA	1021	A	N1-C6-N6	6.46	122.47	118.60
35	RA	845	G	C6-C5-N7	-6.45	126.53	130.40
1	XA	913	A	P-O3'-C3'	6.45	127.44	119.70
23	QX	9	G	C8-N9-C4	6.45	108.98	106.40
35	RA	527	C	N3-C4-N4	-6.45	113.49	118.00
35	RA	1979	C	N3-C2-O2	-6.45	117.39	121.90
35	YA	1950	G	C4-C5-N7	6.45	113.38	110.80
35	RA	1899	G	C6-C5-N7	-6.45	126.53	130.40
1	XA	792	A	P-O3'-C3'	6.45	127.44	119.70
35	YA	1437	C	C6-N1-C2	-6.44	117.72	120.30
35	YA	1996	C	C6-N1-C2	6.44	122.88	120.30
1	QA	634	C	C6-N1-C2	-6.44	117.72	120.30
35	YA	2639	A	N7-C8-N9	6.44	117.02	113.80
35	YA	2726	U	N1-C2-O2	6.44	127.31	122.80
35	YA	537	C	C6-N1-C2	-6.44	117.72	120.30
1	QA	419	C	C6-N1-C2	-6.43	117.73	120.30
35	YA	1314	C	C2-N1-C1'	6.43	125.88	118.80
1	QA	193	C	C6-N1-C2	-6.43	117.73	120.30
35	RA	2346	A	N1-C6-N6	6.43	122.46	118.60
35	YA	2594	C	N3-C4-C5	6.43	124.47	121.90
24	QZ	63	GLU	N-CA-CB	6.43	122.17	110.60
35	YA	274	G	C8-N9-C1'	6.43	135.35	127.00
1	QA	1033	G	P-O3'-C3'	6.42	127.41	119.70
35	RA	193	U	N1-C2-O2	6.42	127.30	122.80
35	RA	119	A	P-O3'-C3'	6.42	127.41	119.70
35	RA	2699	C	C6-N1-C2	-6.42	117.73	120.30
35	YA	2392	A	C8-N9-C4	-6.42	103.23	105.80
35	YA	2851	A	N1-C6-N6	6.42	122.45	118.60
1	QA	1498	U	P-O3'-C3'	6.42	127.40	119.70
36	RB	79	C	C6-N1-C2	-6.42	117.73	120.30
35	RA	2827	C	C6-N1-C2	-6.42	117.73	120.30
35	RA	2889	C	C2-N1-C1'	6.42	125.86	118.80
1	XA	4	U	N1-C2-O2	6.42	127.29	122.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	YB	66	A	P-O3'-C3'	6.42	127.40	119.70
40	YG	146	TYR	CA-CB-CG	6.42	125.59	113.40
35	RA	217	G	C5-C6-N1	6.41	114.71	111.50
35	YA	1940	U	N3-C4-O4	6.41	123.89	119.40
35	YA	1963	U	C5-C6-N1	6.41	125.90	122.70
1	QA	1147	C	N3-C2-O2	-6.41	117.42	121.90
16	QP	54	GLU	CA-CB-CG	6.41	127.49	113.40
35	RA	1725	G	C8-N9-C1'	-6.41	118.67	127.00
35	YA	2178	C	C2-N1-C1'	6.41	125.84	118.80
1	QA	428	G	P-O3'-C3'	6.40	127.38	119.70
35	RA	947	G	C4-C5-N7	-6.40	108.24	110.80
35	RA	2244	U	N3-C4-O4	6.40	123.88	119.40
1	QA	1066	C	C2-N3-C4	6.40	123.10	119.90
1	QA	1158	C	C6-N1-C2	-6.40	117.74	120.30
35	RA	2766	G	C4-N9-C1'	6.40	134.82	126.50
35	RA	1640	C	N1-C2-O2	6.40	122.74	118.90
35	YA	1200	C	C6-N1-C2	-6.40	117.74	120.30
35	YA	2562	U	N3-C2-O2	-6.40	117.72	122.20
35	YA	2607	G	N1-C2-N2	-6.40	110.44	116.20
35	RA	527	C	C2-N1-C1'	6.39	125.83	118.80
35	RA	603	A	N7-C8-N9	6.39	117.00	113.80
36	RB	27	C	N3-C2-O2	-6.39	117.42	121.90
1	XA	252	U	C5-C6-N1	6.39	125.90	122.70
35	RA	529	A	C8-N9-C4	-6.39	103.24	105.80
35	RA	1588	C	N1-C2-O2	6.39	122.73	118.90
1	XA	1538	C	C6-N1-C2	-6.39	117.74	120.30
35	YA	856	C	C2-N1-C1'	6.39	125.83	118.80
35	RA	828	U	N3-C4-O4	-6.39	114.93	119.40
35	RA	1533	C	C6-N1-C2	-6.39	117.75	120.30
10	XJ	83	GLU	CB-CA-C	-6.39	97.62	110.40
42	YI	115	ALA	N-CA-CB	6.39	119.05	110.10
35	YA	1234	U	N3-C2-O2	-6.39	117.73	122.20
1	XA	4	U	C5-C6-N1	6.39	125.89	122.70
1	XA	186	C	C6-N1-C2	-6.39	117.75	120.30
35	YA	2137	C	C6-N1-C2	-6.38	117.75	120.30
35	RA	1934	C	C2-N1-C1'	6.38	125.82	118.80
22	XV	13	C	C6-N1-C2	-6.38	117.75	120.30
27	Y2	15	LYS	CA-CB-CG	6.38	127.44	113.40
1	QA	186	C	C2-N1-C1'	6.38	125.81	118.80
35	RA	1306	C	C5-C6-N1	6.38	124.19	121.00
35	RA	2128	C	C2-N1-C1'	6.38	125.82	118.80
35	RA	2794	C	C5-C6-N1	6.38	124.19	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	YA	1945	G	C8-N9-C4	-6.38	103.85	106.40
1	QA	79	G	N3-C2-N2	-6.38	115.44	119.90
1	QA	1346	A	P-O3'-C3'	6.38	127.35	119.70
35	RA	2798	C	C6-N1-C2	-6.38	117.75	120.30
35	YA	529	A	C8-N9-C4	-6.38	103.25	105.80
35	YA	298	G	N1-C6-O6	6.37	123.72	119.90
35	YA	1394	U	C5-C6-N1	6.37	125.89	122.70
35	RA	2318	G	C5-C6-O6	-6.37	124.78	128.60
35	YA	2559	C	N1-C2-O2	6.37	122.72	118.90
35	RA	624	C	C6-N1-C2	-6.37	117.75	120.30
35	RA	1668	A	N1-C6-N6	-6.37	114.78	118.60
1	XA	547	A	P-O3'-C3'	6.37	127.34	119.70
35	YA	642	G	C8-N9-C4	-6.37	103.85	106.40
1	QA	960	U	C2-N1-C1'	6.37	125.34	117.70
35	RA	18	C	C6-N1-C2	-6.37	117.75	120.30
35	RA	2392	A	C8-N9-C4	-6.37	103.25	105.80
35	RA	270(Q)	C	N1-C2-O2	6.36	122.72	118.90
1	QA	812	C	P-O3'-C3'	6.36	127.33	119.70
35	YA	1757	U	C5-C6-N1	-6.36	119.52	122.70
1	XA	247	G	C8-N9-C4	-6.36	103.86	106.40
35	YA	2169	A	C4-N9-C1'	6.36	137.74	126.30
35	RA	1950	G	C6-C5-N7	-6.35	126.59	130.40
1	XA	1007	C	P-O3'-C3'	6.35	127.32	119.70
35	YA	2808	U	N1-C2-O2	6.35	127.25	122.80
1	QA	739	C	N3-C4-C5	-6.35	119.36	121.90
35	RA	1385	G	N3-C4-N9	-6.35	122.19	126.00
35	YA	2559	C	C2-N1-C1'	6.35	125.79	118.80
35	RA	2439	A	P-O3'-C3'	6.35	127.32	119.70
1	XA	91	C	N3-C2-O2	-6.35	117.45	121.90
35	YA	1835	G	N3-C4-C5	-6.35	125.42	128.60
35	YA	2232	U	C5-C4-O4	6.35	129.71	125.90
1	QA	999	U	C6-N1-C1'	-6.35	112.31	121.20
35	RA	1385	G	C8-N9-C1'	6.35	135.25	127.00
35	RA	1965	C	N3-C4-N4	6.35	122.44	118.00
35	YA	2572	A	C8-N9-C4	6.35	108.34	105.80
35	RA	494	G	N3-C4-C5	-6.35	125.43	128.60
35	RA	128	C	C6-N1-C2	-6.34	117.76	120.30
35	YA	1496	A	N7-C8-N9	6.34	116.97	113.80
35	YA	2342	C	C6-N1-C2	-6.34	117.76	120.30
35	YA	2232	U	C6-N1-C2	-6.34	117.19	121.00
35	YA	1598	C	N1-C2-O2	6.34	122.70	118.90
35	YA	2859	G	C8-N9-C4	-6.34	103.86	106.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	QA	1203	C	C6-N1-C2	-6.34	117.77	120.30
35	RA	708	C	C5-C6-N1	6.34	124.17	121.00
35	YA	1143	A	C2-N3-C4	-6.34	107.43	110.60
1	XA	534	U	O5'-P-OP2	-6.33	100.00	105.70
1	QA	5	U	P-O3'-C3'	6.33	127.30	119.70
8	QH	42	GLU	N-CA-CB	-6.33	99.20	110.60
39	RF	99	TYR	CA-CB-CG	6.33	125.43	113.40
1	XA	283	C	N1-C2-O2	6.33	122.70	118.90
1	XA	1515	C	C6-N1-C2	-6.33	117.77	120.30
1	QA	1028	C	N1-C2-O2	6.33	122.70	118.90
35	RA	513	A	N1-C6-N6	6.33	122.40	118.60
35	RA	1406	U	N1-C2-O2	6.33	127.23	122.80
35	RA	2086	U	O5'-P-OP2	-6.33	100.00	105.70
1	XA	1108	G	N9-C4-C5	6.33	107.93	105.40
13	QM	3	ARG	NE-CZ-NH2	-6.32	117.14	120.30
35	YA	2392	A	C4-C5-N7	6.32	113.86	110.70
35	YA	2006	C	C5-C6-N1	6.32	124.16	121.00
1	QA	1031	G	C8-N9-C1'	-6.32	118.78	127.00
35	YA	363(E)	U	N1-C2-O2	6.32	127.22	122.80
35	RA	227	A	C8-N9-C4	-6.32	103.27	105.80
35	RA	1528	A	C5-N7-C8	-6.32	100.74	103.90
35	YA	884	C	C5-C6-N1	6.32	124.16	121.00
1	XA	1033	G	P-O3'-C3'	6.32	127.28	119.70
35	YA	2447	G	P-O3'-C3'	6.32	127.28	119.70
35	RA	2490	G	N7-C8-N9	6.31	116.26	113.10
35	YA	676	A	N1-C6-N6	6.31	122.39	118.60
1	QA	268	C	C5-C6-N1	6.31	124.16	121.00
36	RB	117	G	C8-N9-C4	6.31	108.92	106.40
1	XA	455	C	C6-N1-C2	-6.31	117.78	120.30
1	QA	1079	G	C5-C6-O6	6.31	132.38	128.60
1	QA	442	C	C5-C6-N1	6.30	124.15	121.00
35	YA	1075	C	C5-C6-N1	6.30	124.15	121.00
35	YA	1406	U	N3-C2-O2	-6.30	117.79	122.20
35	RA	2847	U	C5-C6-N1	6.30	125.85	122.70
42	RI	144	VAL	C-N-CA	6.30	137.45	121.70
35	YA	2043	C	C6-N1-C2	-6.30	117.78	120.30
1	QA	1086	U	C2-N1-C1'	6.30	125.26	117.70
35	RA	2504	U	C5-C6-N1	6.30	125.85	122.70
38	RE	199	ARG	CG-CD-NE	-6.30	98.58	111.80
49	RT	3	ARG	CD-NE-CZ	6.30	132.42	123.60
1	XA	585	G	C8-N9-C4	-6.30	103.88	106.40
1	XA	91	C	N1-C2-O2	6.29	122.68	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	YA	1735	C	N1-C2-O2	6.29	122.68	118.90
35	RA	845	G	C5-N7-C8	-6.29	101.15	104.30
44	RO	107	ARG	CA-CB-CG	6.29	127.25	113.40
1	XA	1498	U	P-O3'-C3'	6.29	127.25	119.70
1	QA	135	C	C6-N1-C2	-6.29	117.78	120.30
35	YA	634	C	C6-N1-C2	-6.29	117.78	120.30
35	YA	2503	A	C2-N3-C4	6.29	113.75	110.60
22	QW	67	C	C6-N1-C2	-6.29	117.78	120.30
35	YA	972	G	N1-C6-O6	-6.29	116.13	119.90
35	YA	783	A	C6-C5-N7	-6.29	127.90	132.30
35	YA	828	U	N3-C4-O4	-6.29	115.00	119.40
35	RA	748	G	N7-C8-N9	-6.28	109.96	113.10
35	YA	269	U	N1-C2-O2	6.28	127.20	122.80
35	YA	2287	A	C4-C5-C6	-6.28	113.86	117.00
1	QA	485	G	P-O3'-C3'	6.28	127.24	119.70
1	XA	186	C	C5-C6-N1	6.28	124.14	121.00
35	YA	2585	U	N1-C2-O2	6.28	127.20	122.80
35	YA	2827	C	N1-C2-O2	6.28	122.67	118.90
35	RA	2474	C	C6-N1-C1'	-6.28	113.27	120.80
35	YA	2168	G	N3-C4-N9	6.28	129.77	126.00
35	RA	1204	A	C2-N3-C4	-6.28	107.46	110.60
35	YA	1781	C	C2-N1-C1'	6.28	125.70	118.80
35	YA	74	A	P-O3'-C3'	6.28	127.23	119.70
26	R1	97	LEU	C-N-CA	6.27	137.38	121.70
35	RA	2831	G	C8-N9-C4	-6.27	103.89	106.40
23	XX	4	A	C8-N9-C4	-6.27	103.29	105.80
35	YA	2163	C	C6-N1-C2	-6.27	117.79	120.30
35	YA	955	C	C2-N3-C4	6.27	123.04	119.90
1	QA	614	A	C8-N9-C4	-6.27	103.29	105.80
35	RA	1956	U	N1-C2-O2	6.27	127.19	122.80
35	RA	2128	C	N1-C2-O2	6.27	122.66	118.90
36	RB	102	G	N1-C6-O6	-6.27	116.14	119.90
35	RA	242	G	C4-N9-C1'	-6.27	118.35	126.50
35	YA	2442	C	C6-N1-C2	-6.27	117.79	120.30
35	RA	2211	G	C8-N9-C1'	-6.27	118.86	127.00
1	XA	137	C	C2-N1-C1'	6.26	125.69	118.80
1	QA	749	C	C6-N1-C2	-6.26	117.80	120.30
35	RA	2029	G	N9-C4-C5	-6.26	102.89	105.40
35	YA	2403	C	N3-C4-C5	-6.26	119.39	121.90
36	YB	31	C	C5-C6-N1	6.26	124.13	121.00
35	RA	2712	U	C6-N1-C1'	-6.26	112.44	121.20
35	YA	2655	G	O4'-C1'-N9	6.26	113.21	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	QA	1532	U	P-O3'-C3'	6.26	127.21	119.70
35	RA	75	G	N3-C4-C5	-6.26	125.47	128.60
35	RA	1157	G	N9-C4-C5	-6.26	102.90	105.40
35	RA	49	A	P-O3'-C3'	6.25	127.21	119.70
35	RA	860	U	C5-C6-N1	6.25	125.83	122.70
35	YA	2856	C	C6-N1-C2	-6.25	117.80	120.30
35	RA	772	C	C5-C6-N1	6.25	124.13	121.00
1	QA	435	C	C5-C6-N1	6.25	124.13	121.00
36	RB	3	C	C4-C5-C6	-6.25	114.27	117.40
35	RA	2666	C	C2-N1-C1'	6.25	125.67	118.80
1	XA	1147	C	C6-N1-C1'	-6.25	113.30	120.80
1	QA	1031	G	N3-C4-C5	-6.25	125.47	128.60
35	RA	933	A	N7-C8-N9	6.25	116.92	113.80
35	RA	2477	C	N3-C2-O2	-6.25	117.53	121.90
35	RA	2559	C	N1-C2-O2	6.25	122.65	118.90
35	YA	965	C	C6-N1-C2	-6.24	117.80	120.30
2	QB	142	LEU	CA-CB-CG	6.24	129.66	115.30
35	RA	1407	C	N1-C2-O2	6.24	122.64	118.90
35	RA	2666	C	C6-N1-C2	-6.24	117.80	120.30
1	QA	106	C	C6-N1-C2	-6.24	117.80	120.30
1	QA	817	C	C6-N1-C2	6.24	122.80	120.30
35	YA	2572	A	C5-N7-C8	6.24	107.02	103.90
35	RA	1157	G	C6-C5-N7	-6.24	126.66	130.40
35	RA	1334	G	C8-N9-C4	-6.24	103.91	106.40
35	RA	2733	A	C8-N9-C1'	-6.24	116.47	127.70
35	RA	2815	C	C6-N1-C2	-6.24	117.81	120.30
35	YA	2318	G	C4-C5-N7	6.24	113.30	110.80
35	RA	2712	U	O4'-C1'-N1	6.24	113.19	108.20
35	RA	2792	G	N3-C4-C5	-6.24	125.48	128.60
35	YA	2584	U	C4-C5-C6	6.24	123.44	119.70
35	YA	2257	U	C6-N1-C2	6.23	124.74	121.00
35	RA	2294	C	C6-N1-C2	-6.23	117.81	120.30
35	RA	2688	U	N1-C2-N3	6.23	118.64	114.90
35	RA	676	A	C6-C5-N7	-6.23	127.94	132.30
35	RA	856	C	C2-N3-C4	6.23	123.01	119.90
1	XA	677	U	N3-C2-O2	-6.23	117.84	122.20
35	YA	16	G	C8-N9-C4	-6.23	103.91	106.40
35	YA	2178	C	C6-N1-C2	-6.23	117.81	120.30
1	QA	960	U	P-O3'-C3'	6.23	127.17	119.70
49	RT	3	ARG	N-CA-CB	6.23	121.81	110.60
35	YA	969	U	O5'-P-OP1	-6.23	100.10	105.70
35	YA	2590	A	C8-N9-C4	6.23	108.29	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RA	105	C	C2-N1-C1'	6.22	125.65	118.80
35	RA	270(U)	C	N3-C2-O2	-6.22	117.54	121.90
35	RA	1365	A	N9-C4-C5	-6.22	103.31	105.80
1	XA	1439	C	C5-C6-N1	6.22	124.11	121.00
22	XW	32	C	C6-N1-C2	-6.22	117.81	120.30
35	RA	615	G	C6-C5-N7	6.22	134.13	130.40
22	QV	15	G	C5-C6-O6	6.21	132.33	128.60
35	RA	193	U	C2-N1-C1'	6.21	125.16	117.70
35	YA	1152	C	C6-N1-C2	-6.21	117.81	120.30
29	R4	34	GLU	CG-CD-OE1	6.21	130.72	118.30
41	RH	18	GLU	CB-CA-C	6.21	122.82	110.40
35	YA	603	A	C6-C5-N7	-6.21	127.95	132.30
35	RA	934	G	N3-C4-C5	-6.21	125.50	128.60
35	RA	1179	C	C2-N1-C1'	6.21	125.63	118.80
1	QA	560	U	N1-C1'-C2'	-6.21	105.17	112.00
35	RA	1243	G	N9-C4-C5	-6.21	102.92	105.40
35	YA	250	G	N3-C2-N2	6.21	124.25	119.90
35	RA	1931	U	C5-C6-N1	6.21	125.80	122.70
35	RA	2559	C	C2-N1-C1'	6.21	125.63	118.80
35	YA	1474	C	C2-N1-C1'	6.21	125.63	118.80
35	RA	1199	U	C5-C4-O4	-6.21	122.18	125.90
1	XA	1157	A	C4-N9-C1'	6.21	137.47	126.30
35	RA	1314	C	N1-C2-O2	6.20	122.62	118.90
41	RH	116	GLU	CB-CA-C	6.20	122.81	110.40
1	XA	1356	G	C4-C5-N7	6.20	113.28	110.80
1	XA	1432	G	N1-C6-O6	6.20	123.62	119.90
35	YA	119	A	P-O3'-C3'	6.20	127.14	119.70
35	YA	41	C	C5-C6-N1	6.20	124.10	121.00
35	RA	288	C	C2-N1-C1'	6.20	125.62	118.80
35	RA	933	A	C5-N7-C8	-6.20	100.80	103.90
1	QA	1128	C	C2-N1-C1'	6.20	125.62	118.80
35	YA	1262	A	C2-N3-C4	6.20	113.70	110.60
42	YI	104	GLN	N-CA-CB	-6.20	99.44	110.60
1	XA	999	U	C6-N1-C2	-6.20	117.28	121.00
35	RA	881	G	N3-C4-N9	6.20	129.72	126.00
1	QA	79	G	C6-N1-C2	-6.19	121.38	125.10
35	RA	2307	G	O4'-C1'-N9	6.19	113.15	108.20
35	YA	494	G	N3-C4-C5	-6.19	125.50	128.60
35	YA	1816	G	C2-N3-C4	6.19	115.00	111.90
35	YA	279	C	C6-N1-C2	-6.19	117.82	120.30
1	QA	60	A	P-O3'-C3'	6.19	127.13	119.70
35	RA	1574	C	C6-N1-C2	-6.19	117.83	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	YA	2584	U	C6-N1-C2	-6.19	117.29	121.00
1	XA	754	C	N1-C2-O2	6.18	122.61	118.90
1	XA	1031	G	C2-N3-C4	6.18	114.99	111.90
1	XA	1279	A	N7-C8-N9	6.18	116.89	113.80
1	QA	1306	A	N7-C8-N9	6.18	116.89	113.80
3	QC	35	GLU	CA-CB-CG	6.18	127.00	113.40
35	RA	783	A	C4-C5-N7	6.18	113.79	110.70
35	RA	881	G	C4-N9-C1'	6.18	134.54	126.50
1	XA	1240	U	N1-C2-N3	-6.18	111.19	114.90
35	RA	769	G	C2-N3-C4	6.18	114.99	111.90
1	QA	1254	C	C5-C6-N1	6.18	124.09	121.00
35	RA	2791	C	C2-N1-C1'	-6.18	112.00	118.80
35	RA	239	U	N1-C2-O2	6.18	127.12	122.80
35	RA	512	G	P-O3'-C3'	6.18	127.11	119.70
35	RA	1210	A	C5-N7-C8	-6.18	100.81	103.90
35	RA	2094	G	C2-N3-C4	6.18	114.99	111.90
36	RB	15	A	OP1-P-O3'	6.18	118.79	105.20
39	RF	176	LEU	CA-CB-CG	6.17	129.50	115.30
35	YA	804	A	N1-C6-N6	-6.17	114.90	118.60
35	RA	2791	C	N1-C2-N3	6.17	123.52	119.20
35	YA	1233	C	N1-C2-O2	6.17	122.60	118.90
3	QC	35	GLU	CG-CD-OE1	-6.17	105.96	118.30
36	RB	3	C	C6-N1-C1'	-6.17	113.39	120.80
35	YA	352	G	C8-N9-C1'	-6.17	118.98	127.00
35	YA	1754	C	C6-N1-C2	6.17	122.77	120.30
35	YA	2430	A	N1-C2-N3	6.17	132.38	129.30
1	QA	754	C	C5-C6-N1	6.17	124.08	121.00
35	RA	1157	G	C4-C5-N7	6.17	113.27	110.80
35	YA	1776	G	N3-C4-N9	6.17	129.70	126.00
35	YA	1640	C	N1-C2-O2	6.17	122.60	118.90
35	YA	2595	G	C5-C6-N1	6.17	114.58	111.50
8	QH	85	ARG	CG-CD-NE	6.17	124.75	111.80
1	QA	1127	G	C8-N9-C1'	-6.16	118.99	127.00
35	RA	528	A	C5-C6-N1	-6.16	114.62	117.70
1	XA	961	U	N1-C2-N3	6.16	118.60	114.90
35	YA	953	A	N1-C6-N6	6.16	122.30	118.60
35	RA	2794	C	C2-N1-C1'	6.16	125.58	118.80
35	RA	2859	G	C8-N9-C4	-6.16	103.94	106.40
35	RA	650	C	C6-N1-C2	-6.16	117.84	120.30
35	RA	2685	G	N9-C4-C5	6.16	107.86	105.40
35	YA	794	G	N3-C4-C5	-6.16	125.52	128.60
1	QA	958	A	C8-N9-C4	6.16	108.26	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RA	1499	C	C2-N1-C1'	6.16	125.57	118.80
35	YA	1319	G	C6-C5-N7	-6.16	126.70	130.40
1	QA	561	U	O4'-C1'-N1	6.16	113.13	108.20
1	XA	979	C	C2-N1-C1'	6.16	125.57	118.80
3	XC	126	ARG	CA-CB-CG	6.16	126.94	113.40
35	YA	74	A	C5-C6-N1	-6.15	114.62	117.70
35	YA	330	A	N7-C8-N9	6.15	116.88	113.80
35	YA	811	U	C5-C6-N1	-6.15	119.62	122.70
1	QA	913	A	P-O3'-C3'	6.15	127.08	119.70
1	QA	1348	U	C2-N1-C1'	-6.15	110.32	117.70
35	RA	1406	U	C2-N1-C1'	6.15	125.08	117.70
35	RA	2726	U	C6-N1-C2	-6.15	117.31	121.00
35	YA	556	G	C6-C5-N7	-6.15	126.71	130.40
1	QA	328	C	C2-N3-C4	6.15	122.97	119.90
1	XA	328	C	C5-C6-N1	6.15	124.07	121.00
35	RA	1102	C	C6-N1-C2	-6.15	117.84	120.30
35	YA	954	G	C4-N9-C1'	6.15	134.49	126.50
35	YA	1950	G	N1-C6-O6	6.15	123.59	119.90
35	RA	1152	C	C2-N1-C1'	6.14	125.56	118.80
35	YA	2689	U	N3-C4-O4	-6.14	115.10	119.40
35	RA	2873	A	N1-C2-N3	6.14	132.37	129.30
35	YA	2503	A	N1-C2-N3	-6.14	126.23	129.30
1	QA	1490	C	C6-N1-C2	-6.14	117.84	120.30
35	YA	43	G	C8-N9-C4	6.14	108.86	106.40
22	QW	71	C	C6-N1-C2	-6.14	117.84	120.30
35	RA	549	G	N3-C4-C5	-6.14	125.53	128.60
35	YA	698	C	C6-N1-C2	6.14	122.75	120.30
1	QA	1031	G	O5'-P-OP1	-6.14	100.18	105.70
35	RA	1698	A	N1-C6-N6	6.14	122.28	118.60
35	RA	2825	C	C6-N1-C2	-6.14	117.84	120.30
1	XA	186	C	N1-C2-O2	6.14	122.58	118.90
1	XA	975	A	N7-C8-N9	6.14	116.87	113.80
35	YA	1064	C	C6-N1-C2	-6.14	117.85	120.30
35	RA	473	G	C8-N9-C4	6.13	108.85	106.40
35	RA	2416	C	C6-N1-C2	-6.13	117.85	120.30
1	XA	428	G	P-O3'-C3'	6.13	127.06	119.70
1	XA	919	A	N1-C6-N6	-6.13	114.92	118.60
35	YA	2287	A	C2-N3-C4	-6.13	107.53	110.60
22	QW	32	C	C6-N1-C2	-6.13	117.85	120.30
35	YA	1152	C	C5-C6-N1	6.13	124.06	121.00
36	YB	27	C	C5-C6-N1	6.13	124.06	121.00
35	YA	2501	C	C2-N1-C1'	-6.12	112.06	118.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	RB	117	G	N3-C4-N9	6.12	129.67	126.00
35	YA	1609	A	O4'-C1'-N9	6.12	113.10	108.20
35	YA	2688	U	C2-N1-C1'	6.12	125.05	117.70
54	YY	40	GLU	CA-CB-CG	6.12	126.87	113.40
35	YA	213	A	C5-C6-N1	6.12	120.76	117.70
35	YA	2112	G	O4'-C1'-N9	6.12	113.10	108.20
49	RT	105	LEU	CA-CB-CG	6.12	129.37	115.30
1	XA	137	C	C5-C6-N1	6.12	124.06	121.00
35	RA	1781	C	N3-C2-O2	-6.12	117.62	121.90
35	RA	2311	A	OP1-P-O3'	6.12	118.65	105.20
35	YA	52	A	C4-C5-N7	6.12	113.76	110.70
35	RA	647	G	N3-C4-C5	-6.11	125.54	128.60
35	RA	695	G	C5-C6-N1	-6.11	108.44	111.50
35	RA	1204	A	C5-C6-N1	-6.11	114.64	117.70
1	QA	306	G	N1-C6-O6	6.11	123.57	119.90
35	RA	2391	G	C5-C6-O6	6.11	132.27	128.60
1	XA	1064	G	O4'-C1'-N9	6.11	113.09	108.20
35	RA	884	C	C6-N1-C2	-6.11	117.86	120.30
35	RA	1649	G	N3-C4-C5	-6.11	125.55	128.60
35	RA	1781	C	C2-N1-C1'	6.11	125.52	118.80
35	RA	2092	U	C6-N1-C1'	-6.11	112.64	121.20
35	YA	1313	U	C6-N1-C1'	-6.11	112.65	121.20
35	RA	1404	C	C6-N1-C2	-6.11	117.86	120.30
35	YA	2077	A	C8-N9-C4	6.11	108.24	105.80
35	YA	2609	U	C6-N1-C2	6.11	124.66	121.00
1	QA	115	G	C2-N3-C4	6.11	114.95	111.90
35	RA	2062	A	N1-C2-N3	-6.11	126.25	129.30
35	YA	114	U	C2-N1-C1'	6.10	125.03	117.70
1	XA	596	C	N1-C2-O2	6.10	122.56	118.90
1	XA	1006	C	C5-C6-N1	6.10	124.05	121.00
35	YA	2594	C	C6-N1-C2	6.10	122.74	120.30
34	R9	13	LYS	CA-CB-CG	6.10	126.82	113.40
1	XA	1147	C	C2-N1-C1'	6.10	125.51	118.80
35	RA	99	U	N1-C2-O2	6.10	127.07	122.80
35	RA	1899	G	C4-C5-C6	6.10	122.46	118.80
35	RA	2321	G	C4-N9-C1'	6.10	134.43	126.50
51	YV	44	LYS	N-CA-CB	-6.10	99.62	110.60
35	YA	2137	C	C2-N1-C1'	6.10	125.50	118.80
35	RA	1385	G	C6-C5-N7	6.09	134.06	130.40
35	YA	2178	C	C5-C6-N1	6.09	124.05	121.00
35	YA	2456	C	C5-C6-N1	6.09	124.05	121.00
35	RA	79	G	C8-N9-C4	-6.09	103.96	106.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RA	676	A	N3-C4-C5	6.09	131.06	126.80
35	YA	1728	G	N3-C4-C5	-6.09	125.56	128.60
1	QA	1447	G	N3-C4-N9	6.09	129.65	126.00
35	YA	2321	G	C4-N9-C1'	6.09	134.42	126.50
35	RA	1370	C	C5-C6-N1	6.09	124.04	121.00
1	XA	458	C	C6-N1-C2	-6.09	117.87	120.30
22	XW	75	C	C6-N1-C2	-6.09	117.86	120.30
1	QA	560	U	P-O3'-C3'	6.08	127.00	119.70
1	XA	980	C	N1-C2-O2	6.08	122.55	118.90
35	YA	2688	U	C4-C5-C6	6.08	123.35	119.70
1	XA	410	G	P-O3'-C3'	6.08	127.00	119.70
35	YA	153	C	N1-C2-O2	6.08	122.55	118.90
42	YI	141	LYS	CB-CA-C	-6.08	98.24	110.40
35	YA	234	C	C6-N1-C2	-6.08	117.87	120.30
36	RB	8	U	C6-N1-C2	-6.08	117.35	121.00
35	RA	647	G	C8-N9-C4	-6.08	103.97	106.40
35	YA	642	G	N9-C4-C5	6.08	107.83	105.40
35	YA	2041	U	N1-C2-O2	6.08	127.05	122.80
1	QA	1009	G	O5'-P-OP1	6.07	117.99	110.70
35	RA	1417	C	C6-N1-C2	-6.07	117.87	120.30
1	QA	704	A	C8-N9-C4	-6.07	103.37	105.80
35	RA	9	U	C2-N1-C1'	6.07	124.98	117.70
35	RA	2847	U	N1-C2-O2	6.07	127.05	122.80
35	YA	1776	G	N3-C4-C5	-6.07	125.56	128.60
1	QA	486	U	N3-C2-O2	-6.07	117.95	122.20
1	QA	1094	G	N9-C1'-C2'	-6.07	105.33	112.00
35	YA	2286	A	C5-N7-C8	-6.07	100.87	103.90
35	RA	945	A	N3-C4-C5	6.07	131.05	126.80
1	XA	975	A	C6-C5-N7	-6.07	128.06	132.30
35	YA	613	U	C6-N1-C2	-6.07	117.36	121.00
35	YA	1306	C	C2-N3-C4	6.07	122.93	119.90
35	YA	2477	C	C6-N1-C1'	-6.07	113.52	120.80
35	YA	2814	C	C6-N1-C2	-6.06	117.88	120.30
35	RA	74	A	N3-C4-N9	-6.06	122.55	127.40
35	YA	1000	A	C8-N9-C4	-6.06	103.38	105.80
1	QA	1502	A	N1-C6-N6	6.06	122.24	118.60
22	QV	17	C	C6-N1-C1'	6.06	128.07	120.80
35	RA	9	U	C5-C6-N1	6.06	125.73	122.70
35	YA	1488	G	C8-N9-C4	-6.06	103.98	106.40
35	YA	2689	U	C5-C6-N1	-6.06	119.67	122.70
35	YA	1915	U	N3-C2-O2	-6.06	117.96	122.20
35	YA	859	G	P-O3'-C3'	6.05	126.97	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RA	1640	C	C6-N1-C2	-6.05	117.88	120.30
35	RA	2144	U	OP1-P-O3'	6.05	118.51	105.20
4	XD	191	ARG	CG-CD-NE	6.05	124.50	111.80
35	RA	2476	A	C8-N9-C4	-6.05	103.38	105.80
35	YA	895	U	C6-N1-C1'	-6.05	112.73	121.20
35	RA	770	G	C8-N9-C4	-6.05	103.98	106.40
35	RA	1864	U	C6-N1-C2	-6.05	117.37	121.00
35	RA	2688	U	C4-C5-C6	6.04	123.33	119.70
19	XS	14	HIS	N-CA-C	-6.04	94.68	111.00
13	QM	71	ARG	CG-CD-NE	-6.04	99.11	111.80
35	RA	1790	C	C6-N1-C2	6.04	122.72	120.30
1	XA	191(E)	G	N1-C6-O6	-6.04	116.27	119.90
1	XA	749	C	C6-N1-C2	-6.04	117.88	120.30
35	RA	933	A	N1-C6-N6	6.04	122.22	118.60
35	YA	672	C	C6-N1-C2	-6.04	117.88	120.30
35	YA	2422	A	OP1-P-O3'	6.04	118.49	105.20
1	QA	1145	C	C2-N1-C1'	6.04	125.44	118.80
41	RH	86	GLU	CB-CA-C	-6.04	98.32	110.40
1	XA	1356	G	N9-C4-C5	-6.04	102.98	105.40
35	YA	2561	A	C2-N3-C4	6.04	113.62	110.60
35	YA	2360	A	N1-C6-N6	-6.04	114.98	118.60
35	RA	2311	A	P-O3'-C3'	6.04	126.94	119.70
35	YA	2073	C	C6-N1-C2	-6.04	117.89	120.30
1	QA	397	A	C8-N9-C4	-6.03	103.39	105.80
1	QA	656	C	C6-N1-C2	-6.03	117.89	120.30
35	RA	93	C	C5-C6-N1	6.03	124.02	121.00
35	RA	494	G	N3-C4-N9	6.03	129.62	126.00
35	RA	1180	C	C2-N1-C1'	6.03	125.43	118.80
35	YA	1313	U	N1-C2-O2	6.03	127.02	122.80
35	RA	445	C	N3-C4-C5	-6.03	119.49	121.90
35	YA	2316	C	C6-N1-C2	-6.03	117.89	120.30
35	RA	1523	U	C6-N1-C2	-6.03	117.38	121.00
55	RZ	82	ARG	CA-CB-CG	6.03	126.66	113.40
1	XA	54	C	C6-N1-C2	-6.03	117.89	120.30
1	XA	252	U	C2-N1-C1'	6.03	124.93	117.70
35	RA	738	G	N3-C4-N9	6.02	129.61	126.00
35	RA	1950	G	O4'-C1'-N9	6.02	113.02	108.20
1	XA	1158	C	C6-N1-C2	-6.02	117.89	120.30
35	YA	2776	A	P-O3'-C3'	6.02	126.93	119.70
35	RA	615	G	C4-N9-C1'	-6.02	118.67	126.50
1	XA	315	A	OP2-P-O3'	6.02	118.45	105.20
1	XA	960	U	P-O3'-C3'	6.02	126.93	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	QA	91	C	C5-C6-N1	6.02	124.01	121.00
35	RA	1499	C	N1-C2-O2	6.02	122.51	118.90
35	YA	1521	G	N3-C4-C5	-6.02	125.59	128.60
35	RA	995	C	N3-C2-O2	6.02	126.11	121.90
35	RA	2244	U	C6-N1-C2	-6.02	117.39	121.00
35	YA	1588	C	C6-N1-C1'	-6.02	113.58	120.80
35	YA	1656	C	C5-C6-N1	6.02	124.01	121.00
35	YA	1698	A	C5-N7-C8	-6.02	100.89	103.90
1	XA	1227	A	N1-C6-N6	6.02	122.21	118.60
35	YA	692	C	P-O3'-C3'	6.02	126.92	119.70
35	YA	2444	G	C5-C6-O6	6.02	132.21	128.60
35	RA	1210	A	N1-C6-N6	6.02	122.21	118.60
35	YA	2604	U	C5-C6-N1	6.02	125.71	122.70
35	RA	912	C	C2-N1-C1'	6.01	125.42	118.80
35	RA	2161	C	C5-C6-N1	6.01	124.01	121.00
35	YA	1407	C	N3-C2-O2	-6.01	117.69	121.90
1	XA	64	G	C8-N9-C4	6.01	108.81	106.40
1	QA	250	A	P-O3'-C3'	6.01	126.91	119.70
35	RA	603	A	C8-N9-C4	-6.01	103.39	105.80
1	XA	1356	G	C6-C5-N7	-6.01	126.79	130.40
35	RA	69	C	C6-N1-C1'	-6.01	113.59	120.80
35	RA	1346	G	C8-N9-C4	6.01	108.80	106.40
35	RA	2032	G	C4-N9-C1'	-6.01	118.69	126.50
35	YA	775	G	N9-C4-C5	6.01	107.80	105.40
35	YA	1338	G	C8-N9-C4	-6.01	104.00	106.40
35	RA	855	G	C4-C5-N7	-6.01	108.40	110.80
1	XA	1334	G	C8-N9-C4	-6.00	104.00	106.40
1	XA	743	U	N1-C2-O2	6.00	127.00	122.80
2	XB	111	ARG	N-CA-CB	-6.00	99.79	110.60
35	YA	2889	C	C2-N1-C1'	6.00	125.40	118.80
35	RA	2794	C	C6-N1-C2	-6.00	117.90	120.30
35	YA	2346	A	N3-C4-C5	6.00	131.00	126.80
1	QA	958	A	O5'-P-OP2	-6.00	100.30	105.70
35	RA	30	G	C8-N9-C4	-6.00	104.00	106.40
35	RA	686	G	C4-C5-N7	6.00	113.20	110.80
35	YA	2210	G	N3-C4-N9	6.00	129.60	126.00
54	YY	40	GLU	CB-CA-C	-6.00	98.41	110.40
35	RA	435	C	N1-C2-O2	6.00	122.50	118.90
35	RA	1694	C	P-O3'-C3'	6.00	126.90	119.70
35	RA	2779	U	C5-C6-N1	-6.00	119.70	122.70
1	XA	1000	A	P-O3'-C3'	6.00	126.90	119.70
35	YA	110	G	C8-N9-C4	6.00	108.80	106.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	QA	279	A	P-O3'-C3'	6.00	126.89	119.70
35	RA	2465	C	C6-N1-C2	-6.00	117.90	120.30
1	XA	1162	C	C6-N1-C2	-6.00	117.90	120.30
35	YA	1261	C	C6-N1-C2	5.99	122.70	120.30
35	YA	286	C	C6-N1-C1'	-5.99	113.61	120.80
35	YA	860	U	C6-N1-C2	-5.99	117.41	121.00
35	YA	2798	C	C6-N1-C2	-5.99	117.90	120.30
35	YA	2896	C	C6-N1-C2	-5.99	117.90	120.30
35	RA	1879	C	C6-N1-C2	-5.99	117.90	120.30
35	RA	349	G	C2-N3-C4	5.99	114.89	111.90
35	YA	1437	C	C2-N1-C1'	5.99	125.39	118.80
35	YA	2371	G	C8-N9-C4	-5.99	104.00	106.40
35	RA	2342	C	C5-C6-N1	5.99	123.99	121.00
1	XA	1138	G	C8-N9-C1'	-5.99	119.22	127.00
1	QA	174	C	C6-N1-C2	-5.99	117.91	120.30
35	RA	1640	C	C5-C6-N1	5.99	123.99	121.00
35	YA	2501	C	C2-N3-C4	-5.99	116.91	119.90
4	QD	192	GLU	CA-CB-CG	5.98	126.56	113.40
1	XA	186(B)	C	C6-N1-C2	-5.98	117.91	120.30
35	YA	1342	A	N1-C2-N3	5.98	132.29	129.30
40	YG	180	PHE	CB-CG-CD1	5.98	124.98	120.80
1	QA	153	C	C6-N1-C2	-5.97	117.91	120.30
35	RA	248	G	N1-C6-O6	5.97	123.48	119.90
35	YA	1881	C	N1-C2-O2	5.97	122.48	118.90
20	QT	91	LEU	CB-CG-CD2	-5.97	100.85	111.00
35	RA	530	G	C6-C5-N7	-5.97	126.82	130.40
35	RA	615	G	C2-N3-C4	5.97	114.88	111.90
36	RB	44	G	C4-N9-C1'	-5.97	118.74	126.50
1	QA	1300	G	P-O3'-C3'	5.97	126.86	119.70
35	RA	2696	U	N3-C2-O2	-5.96	118.03	122.20
36	RB	102	G	C5-C6-O6	5.96	132.18	128.60
1	XA	341	C	C6-N1-C2	-5.96	117.92	120.30
1	XA	1138	G	C4-N9-C1'	5.96	134.25	126.50
35	YA	1586	A	N7-C8-N9	5.96	116.78	113.80
35	YA	2322	A	N1-C6-N6	5.96	122.18	118.60
1	QA	556	C	C6-N1-C2	-5.96	117.92	120.30
35	YA	1135	C	C4-C5-C6	-5.96	114.42	117.40
35	YA	2032	G	C5-C6-O6	-5.96	125.02	128.60
35	YA	2168	G	C4-N9-C1'	5.96	134.25	126.50
35	RA	729	G	C8-N9-C4	-5.96	104.02	106.40
41	RH	18	GLU	CB-CG-CD	-5.96	98.11	114.20
1	XA	1263	C	N1-C2-O2	5.96	122.47	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	YA	1694	C	P-O3'-C3'	5.96	126.85	119.70
35	RA	2272	U	C6-N1-C2	5.96	124.57	121.00
35	RA	2448	A	N1-C6-N6	5.96	122.17	118.60
1	XA	575	G	N7-C8-N9	-5.96	110.12	113.10
1	QA	31	G	P-O3'-C3'	5.96	126.85	119.70
1	XA	1028	C	C6-N1-C1'	5.96	127.95	120.80
1	XA	419	C	C2-N1-C1'	5.95	125.35	118.80
35	YA	1261	C	N3-C4-C5	5.95	124.28	121.90
35	RA	845	G	P-O3'-C3'	5.95	126.84	119.70
35	YA	352	G	P-O3'-C3'	5.95	126.84	119.70
35	YA	288	C	N1-C2-O2	5.95	122.47	118.90
26	R1	82	LEU	C-N-CA	5.95	136.57	121.70
35	YA	1299	G	C5-C6-O6	-5.95	125.03	128.60
35	YA	2605	U	N3-C2-O2	-5.95	118.04	122.20
35	RA	2130	U	O4'-C1'-N1	5.95	112.96	108.20
35	YA	174	C	N1-C2-O2	5.95	122.47	118.90
22	QW	68	C	C2-N1-C1'	5.94	125.34	118.80
35	YA	2028	U	C4-C5-C6	5.94	123.27	119.70
1	XA	250	A	P-O3'-C3'	5.94	126.83	119.70
35	YA	403	U	N1-C2-O2	5.94	126.96	122.80
35	RA	1021	A	C6-C5-N7	-5.94	128.14	132.30
35	RA	2128	C	C6-N1-C2	-5.94	117.92	120.30
35	RA	814	C	N3-C4-C5	-5.94	119.53	121.90
35	RA	265	A	N7-C8-N9	5.94	116.77	113.80
35	RA	1950	G	C4-C5-N7	5.93	113.17	110.80
35	YA	1233	C	C2-N3-C4	5.93	122.87	119.90
35	YA	2062	A	C2-N3-C4	5.93	113.57	110.60
1	XA	410	G	OP1-P-O3'	5.93	118.25	105.20
1	XA	1502	A	C5-C6-N6	-5.93	118.95	123.70
35	YA	739	G	C8-N9-C4	-5.93	104.03	106.40
35	YA	2346	A	C5-C6-N1	-5.93	114.73	117.70
29	R4	67	TYR	CA-CB-CG	5.93	124.67	113.40
35	RA	818	G	N3-C4-N9	5.93	129.56	126.00
35	RA	1427	A	P-O3'-C3'	5.93	126.82	119.70
35	YA	1676	A	C8-N9-C4	-5.93	103.43	105.80
35	RA	1658	C	C6-N1-C2	-5.93	117.93	120.30
1	XA	897	C	C6-N1-C2	-5.93	117.93	120.30
35	YA	2128	C	N1-C2-O2	5.93	122.46	118.90
35	RA	1588	C	C2-N1-C1'	5.93	125.32	118.80
35	RA	2605	U	N3-C2-O2	-5.93	118.05	122.20
1	XA	31	G	P-O3'-C3'	5.93	126.81	119.70
22	QW	69	C	C6-N1-C2	-5.93	117.93	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	QA	596	C	C2-N1-C1'	5.92	125.32	118.80
35	RA	894	C	N3-C2-O2	-5.92	117.75	121.90
35	RA	2238	G	C8-N9-C4	-5.92	104.03	106.40
35	RA	1364	G	C6-C5-N7	-5.92	126.85	130.40
35	RA	2542	A	N1-C6-N6	5.92	122.15	118.60
35	YA	1899	G	C5-C6-O6	-5.92	125.05	128.60
23	QX	10	G	O5'-P-OP1	-5.92	100.37	105.70
35	RA	1180	C	C5-C6-N1	5.92	123.96	121.00
35	RA	1948	G	N3-C4-C5	-5.92	125.64	128.60
35	RA	2212	A	O5'-P-OP1	-5.92	100.37	105.70
1	XA	848	C	C2-N1-C1'	5.92	125.31	118.80
35	YA	2518	A	C5-N7-C8	-5.92	100.94	103.90
35	YA	2723	C	N3-C4-C5	-5.92	119.53	121.90
35	RA	708	C	N1-C2-O2	5.92	122.45	118.90
35	RA	1248	G	C8-N9-C4	5.92	108.77	106.40
1	QA	1028(B)	C	C5-C6-N1	5.92	123.96	121.00
35	RA	954	G	N1-C6-O6	-5.92	116.35	119.90
35	RA	2831	G	N9-C4-C5	5.92	107.77	105.40
1	XA	341	C	C5-C6-N1	5.92	123.96	121.00
1	XA	872	A	C2-N3-C4	-5.92	107.64	110.60
1	QA	674	G	C8-N9-C4	-5.92	104.03	106.40
35	RA	654(Q)	C	C5-C6-N1	5.92	123.96	121.00
35	RA	2584	U	N1-C2-O2	5.92	126.94	122.80
35	YA	352	G	C4-N9-C1'	5.92	134.19	126.50
1	XA	1053	G	C8-N9-C4	5.92	108.77	106.40
35	YA	1838	C	N1-C2-O2	-5.92	115.35	118.90
35	YA	621	A	C5-C6-N1	-5.91	114.74	117.70
1	QA	267	C	C5-C6-N1	5.91	123.95	121.00
35	RA	1781	C	N1-C2-O2	5.91	122.45	118.90
35	YA	1830	C	N1-C2-O2	5.91	122.45	118.90
1	QA	1412	C	C6-N1-C2	-5.91	117.94	120.30
35	RA	1475	G	N3-C4-N9	5.91	129.54	126.00
35	YA	1687	G	C5-C6-O6	5.91	132.14	128.60
35	RA	2043	C	C2-N1-C1'	5.91	125.30	118.80
29	R4	22	ILE	C-N-CA	5.90	136.45	121.70
22	XW	61	C	O5'-P-OP2	-5.90	100.39	105.70
35	YA	1203	G	C5-C6-O6	5.90	132.14	128.60
1	QA	1313	U	O5'-P-OP2	-5.90	100.39	105.70
22	XW	22	G	O4'-C1'-N9	5.90	112.92	108.20
35	YA	481	G	O4'-C1'-N9	5.90	112.92	108.20
35	YA	1075	C	C6-N1-C2	-5.90	117.94	120.30
1	QA	1317	C	C2-N1-C1'	5.89	125.28	118.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	YA	1297	C	C6-N1-C2	-5.89	117.94	120.30
35	RA	510	C	N1-C2-O2	5.89	122.44	118.90
35	RA	1776	G	N3-C4-N9	5.89	129.53	126.00
35	RA	2168	G	C8-N9-C1'	-5.89	119.34	127.00
35	RA	2551	C	C6-N1-C2	-5.89	117.94	120.30
35	YA	634	C	C5-C6-N1	5.89	123.95	121.00
35	YA	2167	U	N1-C2-O2	5.89	126.92	122.80
35	YA	911	A	N1-C6-N6	5.89	122.14	118.60
1	QA	1423	G	N3-C4-C5	-5.89	125.66	128.60
1	XA	455	C	N3-C2-O2	-5.89	117.78	121.90
35	YA	1675	C	N3-C2-O2	-5.89	117.78	121.90
35	YA	678	C	C6-N1-C2	-5.88	117.95	120.30
35	RA	1502	C	C5-C6-N1	5.88	123.94	121.00
1	XA	419	C	C6-N1-C2	-5.88	117.95	120.30
1	QA	1086	U	C5-C6-N1	5.88	125.64	122.70
1	QA	1086	U	C6-N1-C2	-5.88	117.47	121.00
35	RA	1191	G	C8-N9-C4	5.88	108.75	106.40
35	YA	1499	C	C2-N1-C1'	5.88	125.27	118.80
35	RA	1437	C	C2-N1-C1'	5.88	125.27	118.80
35	RA	1735	C	C2-N1-C1'	5.88	125.27	118.80
1	XA	1007	C	N1-C2-O2	5.88	122.43	118.90
1	XA	1381	U	C5-C4-O4	5.88	129.43	125.90
35	RA	2211	G	N3-C4-N9	5.88	129.53	126.00
1	XA	442	C	N1-C2-O2	5.88	122.42	118.90
1	QA	1493	A	C8-N9-C4	-5.87	103.45	105.80
35	RA	1786	A	N9-C4-C5	-5.87	103.45	105.80
1	XA	690	G	N7-C8-N9	5.87	116.04	113.10
35	YA	52	A	N9-C4-C5	-5.87	103.45	105.80
35	YA	2712	U	N1-C2-O2	5.87	126.91	122.80
35	RA	1964	G	C8-N9-C4	5.87	108.75	106.40
1	XA	971	G	N3-C4-C5	5.87	131.53	128.60
35	YA	775	G	C8-N9-C4	-5.87	104.05	106.40
1	XA	1053	G	C5-C6-O6	-5.87	125.08	128.60
35	RA	1544	C	C5-C6-N1	5.87	123.93	121.00
35	RA	1888	G	C2-N3-C4	5.87	114.83	111.90
15	XO	77	ARG	CD-NE-CZ	5.87	131.81	123.60
35	YA	1475	G	C4-N9-C1'	5.87	134.12	126.50
35	YA	1427	A	P-O3'-C3'	5.86	126.74	119.70
35	RA	2874	C	C2-N1-C1'	5.86	125.25	118.80
35	RA	1005	C	C6-N1-C2	-5.86	117.96	120.30
35	RA	2126	A	C2-N3-C4	5.86	113.53	110.60
35	RA	2099	U	N3-C2-O2	-5.86	118.10	122.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RA	2377	A	OP1-P-O3'	5.86	118.09	105.20
35	YA	2513	G	C4-C5-N7	5.86	113.14	110.80
35	RA	2161	C	C6-N1-C2	-5.86	117.96	120.30
35	RA	2733	A	C4-N9-C1'	5.86	136.84	126.30
40	RG	173	LEU	CB-CA-C	5.86	121.33	110.20
1	XA	193	C	C5-C6-N1	5.86	123.93	121.00
35	YA	565	C	C5-C4-N4	-5.85	116.10	120.20
35	YA	1992	G	C8-N9-C4	-5.85	104.06	106.40
35	RA	2196	C	C6-N1-C2	-5.85	117.96	120.30
35	RA	2688	U	N1-C2-O2	5.85	126.90	122.80
35	RA	2873	A	C2-N3-C4	-5.85	107.67	110.60
35	YA	2527	C	C5-C6-N1	5.85	123.93	121.00
35	RA	79	G	N9-C4-C5	5.85	107.74	105.40
43	RN	12	ARG	CG-CD-NE	5.85	124.08	111.80
1	XA	209	U	C2-N1-C1'	5.85	124.72	117.70
35	YA	12	U	C6-N1-C1'	-5.85	113.01	121.20
35	RA	873	G	C2-N3-C4	5.85	114.82	111.90
35	YA	1342	A	C5-N7-C8	-5.85	100.98	103.90
35	YA	2602	A	C5-C6-N6	-5.85	119.02	123.70
35	RA	851	U	N3-C2-O2	-5.84	118.11	122.20
1	XA	455	C	N1-C2-O2	5.84	122.41	118.90
2	XB	135	GLN	CB-CA-C	-5.84	98.71	110.40
35	YA	143	C	C5-C6-N1	5.84	123.92	121.00
35	YA	613	U	O4'-C1'-N1	5.84	112.88	108.20
35	YA	930	U	N1-C2-O2	5.84	126.89	122.80
35	YA	2210	G	N3-C4-C5	-5.84	125.68	128.60
1	QA	1423	G	C8-N9-C4	-5.84	104.06	106.40
1	QA	120	A	N1-C6-N6	5.84	122.10	118.60
33	R8	40	GLU	CB-CA-C	5.84	122.08	110.40
2	XB	137	ARG	CA-CB-CG	5.84	126.25	113.40
35	YA	621	A	C6-N1-C2	5.84	122.10	118.60
35	YA	997	G	C8-N9-C4	-5.84	104.06	106.40
35	YA	512	G	OP2-P-O3'	5.83	118.04	105.20
1	XA	1151	A	O4'-C1'-N9	5.83	112.87	108.20
45	RP	8	PRO	CA-N-CD	5.83	119.86	111.70
35	RA	2080	G	C2-N3-C4	5.83	114.81	111.90
1	QA	1007	C	OP1-P-O3'	5.83	118.02	105.20
35	RA	2573	C	N1-C2-O2	5.83	122.39	118.90
1	XA	410	G	N9-C4-C5	5.83	107.73	105.40
4	XD	145	GLU	CA-CB-CG	5.83	126.22	113.40
35	YA	894	C	C5-C6-N1	5.83	123.91	121.00
35	YA	1020	A	N1-C2-N3	-5.83	126.39	129.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	YA	82	G	C5-C6-O6	5.82	132.09	128.60
1	QA	1222	G	C5-C6-N1	-5.82	108.59	111.50
35	RA	2605	U	N3-C4-O4	-5.82	115.33	119.40
1	XA	1263	C	C2-N1-C1'	5.82	125.20	118.80
35	YA	435	C	N1-C2-O2	5.82	122.39	118.90
22	QV	17(A)	U	P-O3'-C3'	5.82	126.68	119.70
22	XW	65	C	C6-N1-C2	-5.82	117.97	120.30
1	QA	183	G	N3-C4-N9	5.82	129.49	126.00
1	QA	346	G	C4-N9-C1'	5.82	134.06	126.50
1	XA	818	G	C8-N9-C1'	-5.82	119.44	127.00
1	XA	1228	C	C6-N1-C2	-5.82	117.97	120.30
35	RA	2896	C	C6-N1-C2	-5.81	117.97	120.30
35	RA	2427	C	C6-N1-C2	5.81	122.62	120.30
35	YA	1695	G	N9-C4-C5	-5.81	103.08	105.40
1	XA	1128	C	C2-N1-C1'	5.81	125.19	118.80
1	QA	458	C	C6-N1-C2	-5.81	117.98	120.30
35	RA	752	A	P-O3'-C3'	5.81	126.67	119.70
35	RA	1443	G	N3-C4-C5	-5.81	125.70	128.60
35	RA	2393	A	C8-N9-C4	-5.81	103.48	105.80
3	XC	127	ARG	N-CA-C	5.81	126.68	111.00
1	QA	960	U	N1-C2-O2	5.81	126.86	122.80
35	RA	172	C	C5-C6-N1	5.80	123.90	121.00
35	YA	234	C	N3-C2-O2	-5.80	117.84	121.90
35	YA	729	G	N3-C2-N2	-5.80	115.84	119.90
35	YA	1256	G	C4-N9-C1'	5.80	134.05	126.50
35	YA	1258	C	C6-N1-C2	-5.80	117.98	120.30
35	RA	265	A	O4'-C1'-N9	5.80	112.84	108.20
35	RA	769	G	C5-C6-N1	5.80	114.40	111.50
1	QA	1432	G	N1-C6-O6	5.80	123.38	119.90
35	RA	1241	A	C6-C5-N7	-5.80	128.24	132.30
35	YA	1882	C	C5-C6-N1	5.80	123.90	121.00
35	RA	1930	G	OP2-P-O3'	5.80	117.96	105.20
35	RA	2868	A	C8-N9-C4	-5.80	103.48	105.80
1	QA	1066	C	C6-N1-C2	-5.79	117.98	120.30
35	RA	1011	G	C6-C5-N7	5.79	133.88	130.40
35	RA	2371	G	C5-C6-O6	5.79	132.08	128.60
35	RA	686	G	C5-C6-O6	-5.79	125.12	128.60
42	RI	25	TYR	N-CA-CB	-5.79	100.17	110.60
35	YA	1021	A	C2-N3-C4	-5.79	107.70	110.60
35	RA	1475	G	N3-C4-C5	-5.79	125.70	128.60
35	RA	2447	G	N1-C6-O6	5.79	123.38	119.90
35	YA	343	C	C2-N1-C1'	5.79	125.17	118.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	YA	860	U	C2-N1-C1'	5.79	124.65	117.70
48	YS	23	ARG	N-CA-CB	-5.79	100.18	110.60
1	XA	1279	A	C8-N9-C4	-5.79	103.48	105.80
12	XL	48	PRO	CA-N-CD	5.79	119.81	111.70
35	YA	2316	C	C2-N1-C1'	5.79	125.17	118.80
1	QA	197	A	N1-C6-N6	5.79	122.07	118.60
35	RA	128	C	P-O3'-C3'	5.79	126.65	119.70
36	YB	22	U	N3-C2-O2	-5.79	118.15	122.20
1	QA	1373	G	N1-C6-O6	-5.79	116.43	119.90
1	XA	389	A	C8-N9-C4	-5.79	103.48	105.80
35	YA	2253	G	N9-C4-C5	-5.79	103.08	105.40
10	QJ	74	ILE	C-N-CA	5.79	136.16	121.70
35	RA	311	A	N1-C6-N6	5.79	122.07	118.60
35	RA	528	A	N1-C2-N3	5.79	132.19	129.30
35	YA	240	G	N9-C4-C5	5.79	107.71	105.40
35	YA	2307	G	O4'-C1'-N9	5.78	112.83	108.20
22	QV	1	C	C2'-C3'-O3'	5.78	122.95	113.70
35	RA	1248	G	N9-C4-C5	-5.78	103.09	105.40
35	RA	494	G	C6-C5-N7	-5.78	126.93	130.40
35	RA	2394	C	C2-N1-C1'	5.78	125.16	118.80
1	XA	1300	G	P-O3'-C3'	5.78	126.63	119.70
1	QA	455	C	C5-C6-N1	5.78	123.89	121.00
1	QA	1532	U	OP2-P-O3'	5.78	117.91	105.20
35	RA	860	U	N3-C4-O4	5.78	123.44	119.40
35	RA	1121	C	C6-N1-C2	-5.78	117.99	120.30
35	YA	274	G	C4-N9-C1'	-5.78	118.99	126.50
1	XA	971	G	C4-N9-C1'	-5.77	118.99	126.50
35	RA	2326	C	C6-N1-C2	-5.77	117.99	120.30
35	YA	141	A	C2-N3-C4	-5.77	107.71	110.60
22	QV	34	C	N1-C2-O2	5.77	122.36	118.90
1	QA	75	C	C6-N1-C2	-5.77	117.99	120.30
1	QA	108	G	C8-N9-C1'	-5.77	119.50	127.00
35	RA	1152	C	C5-C6-N1	5.77	123.89	121.00
1	XA	980	C	C6-N1-C1'	-5.77	113.88	120.80
35	YA	2321	G	N3-C4-C5	-5.77	125.72	128.60
35	YA	2748	A	C5-N7-C8	-5.77	101.02	103.90
1	QA	1411	C	C6-N1-C2	-5.77	117.99	120.30
35	RA	676	A	C6-N1-C2	5.77	122.06	118.60
1	QA	435	C	C2-N1-C1'	5.77	125.14	118.80
35	RA	686	G	N3-C2-N2	5.77	123.94	119.90
2	XB	111	ARG	CB-CA-C	5.77	121.93	110.40
35	RA	1407	C	C2-N3-C4	5.76	122.78	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	XA	388	G	N1-C6-O6	-5.76	116.44	119.90
9	XI	20	ARG	CA-CB-CG	-5.76	100.72	113.40
27	R2	15	LYS	N-CA-CB	5.76	120.97	110.60
35	YA	1930	G	N1-C6-O6	5.76	123.36	119.90
1	QA	243	A	P-O3'-C3'	5.76	126.61	119.70
36	YB	30	C	C6-N1-C2	-5.76	118.00	120.30
35	RA	1005	C	C2-N1-C1'	5.76	125.14	118.80
35	RA	1102	C	C5-C6-N1	5.76	123.88	121.00
1	XA	596	C	C6-N1-C2	-5.76	118.00	120.30
1	XA	1532	U	OP2-P-O3'	5.76	117.87	105.20
35	YA	115	C	C6-N1-C2	-5.76	118.00	120.30
36	YB	99	A	C8-N9-C4	-5.76	103.50	105.80
35	RA	2161	C	C6-N1-C1'	-5.76	113.89	120.80
35	YA	1004	C	N3-C4-C5	-5.76	119.60	121.90
35	YA	1786	A	C4-N9-C1'	5.76	136.66	126.30
1	QA	779	C	N1-C2-O2	5.76	122.35	118.90
1	QA	1536	C	C6-N1-C2	-5.76	118.00	120.30
1	QA	943	U	N3-C2-O2	-5.75	118.17	122.20
1	XA	442	C	C6-N1-C2	-5.75	118.00	120.30
1	XA	785	G	C8-N9-C4	5.75	108.70	106.40
35	YA	672	C	C2-N3-C4	5.75	122.78	119.90
35	YA	1786	A	N9-C4-C5	-5.75	103.50	105.80
35	YA	2579	C	N3-C4-C5	-5.75	119.60	121.90
1	QA	1008	C	C5-C6-N1	5.75	123.88	121.00
1	XA	1533	C	C6-N1-C2	-5.75	118.00	120.30
35	RA	1559	G	P-O3'-C3'	5.75	126.60	119.70
35	YA	1021	A	C5-N7-C8	-5.75	101.03	103.90
35	YA	1233	C	C2-N1-C1'	5.75	125.12	118.80
35	YA	388	G	O4'-C1'-N9	5.75	112.80	108.20
1	QA	971	G	C4-N9-C1'	-5.75	119.03	126.50
35	RA	570	G	N9-C4-C5	5.75	107.70	105.40
35	RA	758	C	N3-C2-O2	-5.75	117.88	121.90
35	YA	2169	A	C8-N9-C1'	-5.75	117.36	127.70
35	RA	473	G	N9-C4-C5	-5.74	103.10	105.40
35	RA	911	A	C8-N9-C4	-5.74	103.50	105.80
35	RA	1502	C	C2-N1-C1'	5.74	125.12	118.80
1	XA	947	G	N7-C8-N9	5.74	115.97	113.10
35	YA	2028	U	N3-C4-O4	5.74	123.42	119.40
35	YA	270(U)	C	C2-N1-C1'	5.74	125.11	118.80
35	YA	556	G	N1-C6-O6	5.74	123.34	119.90
35	YA	2827	C	C5-C6-N1	5.74	123.87	121.00
1	QA	251	G	N1-C6-O6	5.74	123.34	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RA	179	G	C8-N9-C4	-5.74	104.10	106.40
35	RA	1774	C	C6-N1-C2	-5.74	118.00	120.30
35	YA	2287	A	C8-N9-C1'	5.74	138.03	127.70
1	XA	1470	G	C8-N9-C4	5.74	108.69	106.40
1	QA	664	G	C5-C6-O6	5.74	132.04	128.60
35	RA	174	C	C6-N1-C2	-5.74	118.01	120.30
35	RA	265	A	C4-C5-N7	5.74	113.57	110.70
35	RA	1011	G	C8-N9-C1'	5.74	134.46	127.00
35	RA	1437	C	C6-N1-C2	-5.74	118.01	120.30
35	YA	812	C	N3-C4-C5	-5.74	119.61	121.90
36	YB	101	A	N1-C6-N6	-5.74	115.16	118.60
35	RA	2776	A	P-O3'-C3'	5.73	126.58	119.70
35	RA	1669	A	C5-C6-N1	5.73	120.57	117.70
1	XA	279	A	P-O3'-C3'	5.73	126.58	119.70
35	RA	234	C	N3-C2-O2	-5.73	117.89	121.90
22	QV	68	C	C2-N1-C1'	5.73	125.10	118.80
35	RA	2284	C	C6-N1-C2	-5.73	118.01	120.30
1	XA	175	C	C6-N1-C2	-5.73	118.01	120.30
35	YA	1314	C	C5-C6-N1	5.73	123.86	121.00
1	QA	972	C	C6-N1-C2	-5.72	118.01	120.30
35	RA	1022	G	N1-C6-O6	-5.72	116.47	119.90
35	RA	1631	A	N1-C6-N6	5.72	122.03	118.60
35	RA	2490	G	C5-N7-C8	-5.72	101.44	104.30
42	RI	77	LEU	CA-CB-CG	5.72	128.47	115.30
41	RH	61	HIS	CB-CA-C	-5.72	98.95	110.40
35	YA	859	G	C2-N3-C4	-5.72	109.04	111.90
1	QA	1086	U	N3-C2-O2	-5.72	118.20	122.20
35	RA	1970	A	C8-N9-C4	-5.72	103.51	105.80
35	YA	2099	U	C2-N1-C1'	5.72	124.56	117.70
35	YA	893	C	C6-N1-C2	-5.72	118.01	120.30
35	RA	1430	C	C5-C6-N1	5.72	123.86	121.00
2	XB	18	GLY	N-CA-C	5.72	127.39	113.10
35	YA	2167	U	C6-N1-C1'	-5.72	113.20	121.20
1	QA	1301	U	C6-N1-C1'	-5.71	113.20	121.20
1	XA	1160	G	O4'-C1'-N9	-5.71	103.63	108.20
35	RA	2827	C	C6-N1-C1'	-5.71	113.94	120.80
35	RA	2844	G	C6-C5-N7	-5.71	126.97	130.40
35	YA	1627	G	N1-C6-O6	5.71	123.33	119.90
35	RA	330	A	N1-C6-N6	5.71	122.03	118.60
1	QA	1231	G	N1-C6-O6	-5.71	116.47	119.90
35	YA	687	C	N3-C2-O2	-5.71	117.90	121.90
35	YA	859	G	N3-C4-C5	5.71	131.45	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	XA	336	C	C6-N1-C2	-5.71	118.02	120.30
35	YA	761	A	N1-C6-N6	5.71	122.02	118.60
41	RH	2	SER	CB-CA-C	5.71	120.94	110.10
35	RA	2584	U	C5-C4-O4	5.70	129.32	125.90
1	XA	686	U	C5-C6-N1	-5.70	119.85	122.70
22	XV	20	U	C2-N1-C1'	5.70	124.55	117.70
35	YA	859	G	C5-C6-N1	-5.70	108.65	111.50
35	YA	2607	G	N3-C2-N2	5.70	123.89	119.90
35	RA	141	A	N7-C8-N9	5.70	116.65	113.80
35	RA	1936	A	N1-C6-N6	5.70	122.02	118.60
40	YG	78	SER	N-CA-CB	5.70	119.05	110.50
1	QA	4	U	C2-N3-C4	5.70	130.42	127.00
35	RA	2474	C	C5-C6-N1	5.70	123.85	121.00
35	YA	955	C	N3-C4-N4	5.70	121.99	118.00
1	QA	1298	C	N3-C4-C5	5.69	124.18	121.90
35	YA	851	U	N3-C2-O2	-5.69	118.21	122.20
1	QA	1357	A	N7-C8-N9	5.69	116.65	113.80
35	RA	343	C	C2-N1-C1'	5.69	125.06	118.80
1	QA	848	C	C6-N1-C2	-5.69	118.02	120.30
35	RA	2318	G	C4-C5-N7	5.69	113.08	110.80
35	YA	2278	A	O4'-C1'-N9	5.69	112.75	108.20
35	YA	2108	C	C6-N1-C2	-5.69	118.03	120.30
35	RA	1979	C	N1-C2-O2	5.69	122.31	118.90
35	YA	198	C	C6-N1-C2	-5.69	118.03	120.30
35	YA	1076	C	C2-N1-C1'	5.69	125.06	118.80
1	QA	812	C	N1-C2-O2	5.69	122.31	118.90
35	RA	1407	C	C6-N1-C1'	-5.69	113.98	120.80
36	RB	66	A	P-O3'-C3'	5.69	126.52	119.70
1	XA	91	C	C6-N1-C2	-5.69	118.03	120.30
1	XA	1160	G	N3-C4-N9	5.68	129.41	126.00
35	YA	686	G	N9-C4-C5	-5.68	103.13	105.40
35	YA	862	G	N3-C4-C5	-5.68	125.76	128.60
35	RA	881	G	C8-N9-C1'	-5.68	119.61	127.00
35	RA	1345	C	C6-N1-C2	-5.68	118.03	120.30
39	RF	44	ARG	CG-CD-NE	5.68	123.73	111.80
22	XV	18	G	C4-N9-C1'	-5.68	119.11	126.50
35	YA	2559	C	C5-C6-N1	5.68	123.84	121.00
35	RA	2827	C	N1-C2-O2	5.68	122.31	118.90
35	YA	2444	G	C5-C6-N1	-5.68	108.66	111.50
1	XA	1028(B)	C	C6-N1-C2	-5.68	118.03	120.30
1	QA	1149	C	C6-N1-C2	-5.68	118.03	120.30
35	RA	86	C	C6-N1-C2	-5.68	118.03	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RA	2607	G	N1-C2-N2	-5.68	111.09	116.20
35	RA	41	C	N1-C2-O2	5.68	122.31	118.90
35	RA	932	G	C5-C6-O6	5.68	132.00	128.60
35	RA	1364	G	N1-C6-O6	5.68	123.31	119.90
35	YA	71	A	C4-C5-N7	5.68	113.54	110.70
35	YA	601	C	C6-N1-C2	-5.68	118.03	120.30
1	QA	674	G	N7-C8-N9	5.67	115.94	113.10
1	XA	331	G	C4-C5-N7	5.67	113.07	110.80
35	YA	1559	G	P-O3'-C3'	5.67	126.51	119.70
35	YA	1786	A	N9-C1'-C2'	5.67	121.38	114.00
1	QA	1362(A)	C	N3-C2-O2	-5.67	117.93	121.90
35	RA	613	U	C6-N1-C1'	-5.67	113.26	121.20
35	YA	603	A	C4-C5-N7	5.67	113.54	110.70
35	RA	1289	C	C5-C6-N1	5.67	123.83	121.00
1	XA	727	G	C4-C5-N7	-5.67	108.53	110.80
1	XA	818	G	C4-N9-C1'	5.67	133.87	126.50
4	XD	145	GLU	CB-CA-C	-5.67	99.06	110.40
35	YA	804	A	C8-N9-C4	5.67	108.07	105.80
35	YA	1505	C	C5-C6-N1	5.67	123.83	121.00
1	XA	58	C	C5-C6-N1	5.67	123.83	121.00
1	XA	428	G	N1-C6-O6	-5.67	116.50	119.90
35	YA	273(D)	C	N1-C2-O2	5.67	122.30	118.90
1	XA	793	U	C5-C6-N1	-5.66	119.87	122.70
35	YA	1496	A	C5-N7-C8	-5.66	101.07	103.90
35	YA	1772	G	N3-C4-N9	5.66	129.40	126.00
35	YA	2701	C	C6-N1-C2	-5.66	118.03	120.30
35	RA	223	A	N1-C6-N6	-5.66	115.20	118.60
35	RA	528	A	N3-C4-N9	-5.66	122.87	127.40
1	XA	1441	G	N1-C6-O6	5.66	123.30	119.90
35	YA	2019	A	N1-C6-N6	5.66	122.00	118.60
35	RA	1142(A)	A	N1-C6-N6	5.66	122.00	118.60
36	RB	102	G	C4-C5-N7	-5.66	108.53	110.80
35	YA	2191	G	P-O3'-C3'	5.66	126.49	119.70
27	R2	15	LYS	CD-CE-NZ	5.66	124.71	111.70
35	RA	1642	G	C8-N9-C4	-5.66	104.14	106.40
35	RA	1695	G	N1-C6-O6	5.66	123.30	119.90
35	YA	974(A)	C	N3-C2-O2	-5.66	117.94	121.90
35	YA	2602	A	C4-N9-C1'	5.66	136.48	126.30
35	RA	2481	G	OP2-P-O3'	5.66	117.64	105.20
1	XA	1325	C	C2-N1-C1'	5.66	125.02	118.80
35	YA	633	A	N1-C6-N6	5.66	121.99	118.60
35	RA	2430	A	N9-C4-C5	-5.65	103.54	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	YP	35	HIS	N-CA-C	5.65	126.27	111.00
46	YQ	59	ARG	CA-CB-CG	5.65	125.84	113.40
55	YZ	10	ARG	CG-CD-NE	-5.65	99.93	111.80
1	QA	1263	C	C6-N1-C1'	-5.65	114.02	120.80
35	RA	201	C	C6-N1-C2	-5.65	118.04	120.30
35	YA	1178	C	N1-C2-O2	5.65	122.29	118.90
35	YA	2208	U	N3-C2-O2	-5.65	118.25	122.20
39	RF	99	TYR	CB-CA-C	5.65	121.70	110.40
35	YA	2857	G	C8-N9-C4	-5.65	104.14	106.40
1	QA	1453	G	C4-C5-N7	5.65	113.06	110.80
35	RA	708	C	N3-C2-O2	-5.65	117.95	121.90
35	RA	1365	A	N1-C6-N6	5.65	121.99	118.60
35	YA	243	U	N1-C2-O2	5.65	126.75	122.80
35	YA	529	A	C2-N3-C4	5.65	113.42	110.60
35	YA	1204	A	O4'-C1'-N9	5.65	112.72	108.20
35	RA	343	C	C6-N1-C2	-5.65	118.04	120.30
1	QA	115	G	C5-C6-N1	5.64	114.32	111.50
1	QA	1006	C	C6-N1-C2	-5.64	118.04	120.30
10	QJ	100	THR	C-N-CA	5.64	135.81	121.70
35	RA	105	C	C5-C6-N1	5.64	123.82	121.00
35	RA	1241	A	C5-N7-C8	-5.64	101.08	103.90
1	XA	341	C	C2-N1-C1'	5.64	125.01	118.80
35	YA	2392	A	C4-C5-C6	5.64	119.82	117.00
35	RA	1397	U	C5-C4-O4	5.64	129.28	125.90
35	RA	1513	C	C5-C4-N4	-5.64	116.25	120.20
1	XA	575	G	C4-C5-N7	-5.64	108.54	110.80
35	YA	2032	G	N9-C1'-C2'	-5.64	105.79	112.00
45	RP	7	ARG	CG-CD-NE	5.64	123.65	111.80
35	YA	817	C	N3-C4-C5	-5.64	119.64	121.90
1	QA	877	C	C5-C6-N1	5.64	123.82	121.00
35	RA	286	C	N1-C2-O2	5.64	122.28	118.90
35	YA	213	A	C2-N3-C4	5.64	113.42	110.60
35	YA	1653	G	OP2-P-O3'	5.64	117.61	105.20
35	RA	1544	C	C2-N3-C4	5.64	122.72	119.90
35	YA	375	C	C6-N1-C2	-5.64	118.05	120.30
1	XA	619	U	C2-N1-C1'	-5.63	110.94	117.70
36	YB	53	A	C8-N9-C4	-5.63	103.55	105.80
1	XA	243	A	P-O3'-C3'	5.63	126.46	119.70
35	YA	352	G	N3-C4-N9	5.63	129.38	126.00
1	XA	518	C	P-O3'-C3'	5.63	126.46	119.70
1	QA	283	C	C5-C6-N1	5.63	123.81	121.00
1	QA	1187	G	N3-C4-C5	-5.63	125.78	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	XA	980	C	N3-C2-O2	-5.63	117.96	121.90
1	QA	191(D)	U	C6-N1-C1'	-5.63	113.32	121.20
22	QV	15	G	N1-C6-O6	-5.63	116.52	119.90
35	RA	75	G	N1-C6-O6	-5.63	116.52	119.90
35	RA	1828	G	N3-C2-N2	5.63	123.84	119.90
36	RB	107	U	C6-N1-C2	-5.63	117.62	121.00
1	XA	1190	G	OP2-P-O3'	5.63	117.58	105.20
35	YA	2639	A	C5-N7-C8	-5.63	101.09	103.90
35	RA	812	C	C6-N1-C2	-5.63	118.05	120.30
35	YA	1379	A	C5-N7-C8	-5.63	101.09	103.90
1	QA	1086	U	N1-C2-O2	5.62	126.74	122.80
22	QV	34	C	C5-C6-N1	5.62	123.81	121.00
36	YB	118	G	C6-C5-N7	-5.62	127.03	130.40
13	QM	3	ARG	N-CA-CB	5.62	120.72	110.60
35	RA	1293	C	C6-N1-C2	-5.62	118.05	120.30
35	YA	647	G	N3-C4-N9	5.62	129.37	126.00
35	YA	1394	U	C6-N1-C2	-5.62	117.63	121.00
35	YA	2655	G	C4-N9-C1'	-5.62	119.19	126.50
49	RT	51	ARG	CG-CD-NE	5.62	123.60	111.80
1	XA	690	G	O4'-C1'-N9	5.62	112.70	108.20
35	YA	794	G	N3-C4-N9	5.62	129.37	126.00
35	YA	2318	G	C6-C5-N7	-5.62	127.03	130.40
35	RA	828	U	C6-N1-C1'	-5.62	113.33	121.20
35	RA	1273	U	N3-C2-O2	-5.62	118.27	122.20
35	YA	270(Q)	C	N3-C2-O2	-5.62	117.97	121.90
35	YA	1267	U	C2-N1-C1'	5.62	124.44	117.70
1	QA	1001	G	O5'-P-OP2	-5.62	100.64	105.70
35	RA	2346	A	C2-N3-C4	-5.62	107.79	110.60
55	RZ	169	GLU	CA-CB-CG	5.62	125.76	113.40
35	YA	1700	A	N7-C8-N9	-5.62	110.99	113.80
35	RA	887	A	N7-C8-N9	5.62	116.61	113.80
1	XA	632	A	N7-C8-N9	5.62	116.61	113.80
1	XA	872	A	N1-C6-N6	5.62	121.97	118.60
4	QD	193	ASP	N-CA-CB	5.61	120.70	110.60
35	RA	2041	U	N3-C2-O2	-5.61	118.27	122.20
35	YA	14	A	N1-C6-N6	5.61	121.97	118.60
29	Y4	56	VAL	C-N-CA	5.61	135.73	121.70
35	RA	2065	C	C5-C6-N1	5.61	123.81	121.00
1	XA	15	G	N7-C8-N9	5.61	115.90	113.10
35	RA	2584	U	C2-N1-C1'	5.61	124.43	117.70
35	RA	2685	G	C4-C5-N7	-5.61	108.56	110.80
35	YA	1602	U	N3-C4-C5	-5.61	111.24	114.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RA	845	G	C5-C6-O6	-5.61	125.24	128.60
1	XA	1161	C	C2-N1-C1'	5.61	124.97	118.80
35	YA	1203	G	N1-C6-O6	-5.61	116.54	119.90
35	RA	2032	G	C8-N9-C1'	5.60	134.29	127.00
35	YA	1616	A	C5-C6-N6	-5.60	119.22	123.70
35	YA	2346	A	C6-N1-C2	5.60	121.96	118.60
1	QA	390	C	C5-C6-N1	5.60	123.80	121.00
1	QA	797	C	C5-C6-N1	5.60	123.80	121.00
35	YA	692	C	N3-C2-O2	-5.60	117.98	121.90
35	RA	27	G	C5-C6-O6	-5.60	125.24	128.60
35	RA	352	G	N3-C4-N9	5.60	129.36	126.00
35	RA	2211	G	N3-C4-C5	-5.60	125.80	128.60
1	XA	681	C	C6-N1-C2	-5.60	118.06	120.30
35	YA	752	A	P-O3'-C3'	5.60	126.42	119.70
2	QB	96	ARG	CD-NE-CZ	5.60	131.44	123.60
22	QV	17	C	C2-N1-C1'	-5.60	112.64	118.80
36	RB	77	U	N1-C2-O2	5.60	126.72	122.80
35	RA	1233	C	C5-C6-N1	5.60	123.80	121.00
35	YA	1638	C	N3-C4-C5	-5.60	119.66	121.90
35	RA	1678	G	C5-N7-C8	-5.59	101.50	104.30
35	RA	2571	C	C5-C6-N1	5.59	123.80	121.00
1	XA	1381	U	N3-C2-O2	-5.59	118.28	122.20
1	QA	1447	G	C6-C5-N7	-5.59	127.05	130.40
35	RA	1187	G	N1-C6-O6	5.59	123.25	119.90
35	RA	2473	U	N1-C2-O2	5.59	126.71	122.80
1	XA	814	A	C8-N9-C4	5.59	108.04	105.80
35	YA	2723	C	C6-N1-C2	-5.59	118.06	120.30
35	YA	603	A	C8-N9-C4	-5.59	103.56	105.80
35	YA	721	C	N1-C2-O2	5.59	122.25	118.90
35	YA	1543	A	N1-C6-N6	-5.59	115.25	118.60
35	YA	2144	U	OP1-P-O3'	5.59	117.50	105.20
1	QA	596	C	C6-N1-C2	-5.59	118.06	120.30
24	QZ	63	GLU	N-CA-C	-5.59	95.92	111.00
35	RA	358	U	N3-C2-O2	-5.59	118.29	122.20
35	RA	1762	A	C4-N9-C1'	5.58	136.35	126.30
1	QA	943	U	N1-C2-O2	5.58	126.71	122.80
35	RA	695	G	N1-C6-O6	5.58	123.25	119.90
35	RA	989	G	C4-C5-N7	-5.58	108.57	110.80
35	RA	2808	U	N1-C2-O2	5.58	126.71	122.80
35	YA	1179	C	C2-N1-C1'	5.58	124.94	118.80
35	RA	2392	A	C6-C5-N7	-5.58	128.39	132.30
35	YA	1257	C	C6-N1-C2	-5.58	118.07	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RA	2006	C	N1-C2-O2	5.58	122.25	118.90
1	XA	979	C	N1-C2-O2	5.58	122.25	118.90
35	YA	1836	C	N1-C2-O2	5.58	122.25	118.90
35	RA	1930	G	N3-C2-N2	5.58	123.80	119.90
35	YA	2253	G	N1-C6-O6	5.58	123.25	119.90
35	RA	772	C	C6-N1-C2	-5.58	118.07	120.30
35	RA	1833	U	N3-C2-O2	-5.58	118.30	122.20
1	XA	681	C	C5-C6-N1	5.58	123.79	121.00
35	YA	2360	A	C5-C6-N6	5.57	128.16	123.70
35	RA	2602	A	C4-N9-C1'	5.57	136.33	126.30
35	YA	2879	C	N3-C4-N4	5.57	121.90	118.00
36	RB	70	C	C6-N1-C2	-5.57	118.07	120.30
1	XA	108	G	C2-N3-C4	5.57	114.69	111.90
1	QA	545	C	C6-N1-C2	-5.57	118.07	120.30
35	RA	74	A	O4'-C1'-N9	-5.57	103.75	108.20
35	RA	528	A	N3-C4-C5	5.57	130.70	126.80
35	RA	1914	C	C6-N1-C2	-5.57	118.07	120.30
35	RA	2350	C	N1-C2-O2	5.57	122.24	118.90
35	YA	958	U	N3-C4-C5	-5.57	111.26	114.60
36	YB	3	C	C2-N3-C4	5.57	122.68	119.90
35	YA	979	G	N1-C6-O6	5.56	123.24	119.90
1	QA	1137	C	P-O3'-C3'	5.56	126.38	119.70
35	RA	1326	U	N3-C2-O2	-5.56	118.31	122.20
35	RA	2602	A	C5-C6-N6	-5.56	119.25	123.70
35	RA	2689	U	C5-C4-O4	5.56	129.24	125.90
1	XA	884	U	C5-C4-O4	-5.56	122.56	125.90
7	XG	95	ARG	NE-CZ-NH2	-5.56	117.52	120.30
35	YA	859	G	N7-C8-N9	-5.56	110.32	113.10
35	YA	2454	G	N7-C8-N9	-5.56	110.32	113.10
35	RA	2394	C	C6-N1-C2	-5.56	118.08	120.30
35	YA	954	G	C8-N9-C1'	-5.56	119.77	127.00
35	YA	1498	C	C2-N1-C1'	5.56	124.92	118.80
1	QA	455	C	C6-N1-C2	-5.56	118.08	120.30
1	QA	1227	A	N1-C6-N6	5.56	121.94	118.60
35	RA	2232	U	C5-C4-O4	5.56	129.24	125.90
1	XA	277	C	C6-N1-C2	-5.56	118.08	120.30
35	RA	845	G	N9-C4-C5	-5.56	103.18	105.40
1	XA	354	G	C8-N9-C4	-5.56	104.18	106.40
35	YA	2253	G	C5-C6-O6	-5.55	125.27	128.60
35	YA	2318	G	C8-N9-C4	-5.55	104.18	106.40
4	QD	192	GLU	CB-CA-C	-5.55	99.29	110.40
35	RA	537	C	N1-C2-O2	5.55	122.23	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RA	1882	C	C5-C6-N1	5.55	123.78	121.00
1	XA	816	A	N9-C4-C5	5.55	108.02	105.80
1	QA	201	C	C6-N1-C2	-5.55	118.08	120.30
35	RA	2490	G	C4-N9-C1'	5.55	133.72	126.50
35	YA	2827	C	C6-N1-C2	-5.55	118.08	120.30
35	YA	801	G	N1-C6-O6	-5.55	116.57	119.90
1	QA	791	G	N1-C6-O6	5.55	123.23	119.90
35	RA	358	U	N1-C2-O2	5.55	126.68	122.80
35	RA	428	A	C6-C5-N7	-5.55	128.42	132.30
35	RA	1332	G	C8-N9-C4	-5.55	104.18	106.40
35	RA	1394	U	C6-N1-C1'	5.55	128.97	121.20
35	RA	2873	A	C6-C5-N7	-5.55	128.42	132.30
35	YA	2255	G	C8-N9-C4	5.55	108.62	106.40
1	QA	1383	C	N1-C2-O2	5.54	122.23	118.90
35	RA	989	G	N9-C4-C5	5.54	107.62	105.40
35	RA	1143	A	N3-C4-C5	5.54	130.68	126.80
35	YA	1186	G	N1-C6-O6	5.54	123.23	119.90
22	QW	28	C	C6-N1-C2	-5.54	118.08	120.30
35	RA	2688	U	C6-N1-C2	-5.54	117.67	121.00
35	YA	48	G	N9-C4-C5	5.54	107.62	105.40
35	YA	89	G	N9-C4-C5	5.54	107.62	105.40
35	YA	2089	U	N3-C4-O4	5.54	123.28	119.40
1	QA	80	G	N7-C8-N9	5.54	115.87	113.10
35	RA	1308	A	C8-N9-C4	5.54	108.02	105.80
35	RA	1619	G	C4-C5-N7	5.54	113.02	110.80
36	RB	118	G	C8-N9-C1'	-5.54	119.80	127.00
1	XA	863	U	N3-C2-O2	-5.54	118.32	122.20
35	YA	525	U	N3-C2-O2	-5.54	118.32	122.20
35	YA	2238	G	N3-C4-C5	-5.54	125.83	128.60
36	YB	54	G	N3-C2-N2	-5.54	116.02	119.90
1	QA	1202	G	N1-C6-O6	-5.54	116.58	119.90
35	YA	1474	C	C6-N1-C2	-5.54	118.08	120.30
35	RA	288	C	C5-C6-N1	5.54	123.77	121.00
35	RA	945	A	C2-N3-C4	-5.54	107.83	110.60
35	YA	46	C	C6-N1-C2	-5.54	118.08	120.30
35	YA	2253	G	C8-N9-C4	5.54	108.61	106.40
35	RA	1099	G	C8-N9-C4	-5.54	104.19	106.40
35	RA	270(Q)	C	N3-C2-O2	-5.53	118.03	121.90
35	RA	2504	U	C6-N1-C2	-5.53	117.68	121.00
35	RA	2751	G	C8-N9-C1'	-5.53	119.81	127.00
35	YA	1774	C	C2-N1-C1'	5.53	124.89	118.80
35	YA	2294	C	C2-N1-C1'	5.53	124.89	118.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	QA	999	U	P-O3'-C3'	5.53	126.34	119.70
35	RA	1598	C	N3-C2-O2	-5.53	118.03	121.90
1	XA	507	C	C6-N1-C2	-5.53	118.09	120.30
35	YA	1256	G	C8-N9-C1'	-5.53	119.81	127.00
35	YA	1806	C	C6-N1-C2	-5.53	118.09	120.30
35	RA	1210	A	C2-N3-C4	-5.53	107.84	110.60
35	YA	2430	A	N3-C4-C5	5.53	130.67	126.80
35	YA	2679	A	N9-C4-C5	-5.53	103.59	105.80
35	RA	1965	C	N1-C2-O2	-5.53	115.58	118.90
35	RA	2318	G	C6-C5-N7	-5.53	127.08	130.40
1	XA	716	A	C8-N9-C4	-5.53	103.59	105.80
35	YA	139	G	N3-C4-C5	-5.53	125.84	128.60
35	YA	1281	G	C6-C5-N7	-5.53	127.08	130.40
35	YA	1936	A	C4-C5-N7	5.53	113.46	110.70
36	YB	73	A	N1-C6-N6	-5.53	115.28	118.60
35	YA	561	G	N3-C2-N2	5.52	123.77	119.90
35	YA	1678	G	C6-C5-N7	-5.52	127.09	130.40
35	RA	330	A	N3-C4-N9	-5.52	122.98	127.40
1	XA	754	C	N3-C2-O2	-5.52	118.03	121.90
22	XW	60	U	C6-N1-C1'	-5.52	113.47	121.20
35	YA	171	G	N1-C6-O6	5.52	123.21	119.90
35	YA	615	G	C4-C5-N7	-5.52	108.59	110.80
35	YA	912	C	N1-C2-O2	5.52	122.21	118.90
35	YA	1152	C	C2-N1-C1'	5.52	124.88	118.80
55	YZ	155	LEU	CA-CB-CG	5.52	128.00	115.30
1	QA	717	C	N1-C2-O2	5.52	122.21	118.90
35	RA	1023	U	N3-C2-O2	-5.52	118.34	122.20
36	YB	3	C	C2-N1-C1'	5.52	124.87	118.80
35	RA	2646	C	C5-C6-N1	5.52	123.76	121.00
35	YA	990	A	C5-N7-C8	-5.52	101.14	103.90
35	YA	2775	A	N1-C6-N6	5.52	121.91	118.60
35	RA	153	C	O5'-P-OP1	-5.52	100.73	105.70
35	RA	528	A	C5-N7-C8	-5.52	101.14	103.90
36	RB	75	G	N3-C4-C5	-5.52	125.84	128.60
35	YA	1121	C	C6-N1-C2	-5.52	118.09	120.30
35	RA	2063	C	C2-N1-C1'	5.52	124.87	118.80
1	QA	919	A	N1-C6-N6	-5.51	115.29	118.60
35	RA	2585	U	C6-N1-C1'	-5.51	113.48	121.20
1	XA	37	U	N3-C2-O2	-5.51	118.34	122.20
1	XA	280	C	C6-N1-C2	5.51	122.50	120.30
35	RA	90	U	C5-C4-O4	5.51	129.21	125.90
1	QA	1282	C	C5-C6-N1	5.51	123.76	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RA	9	U	N1-C2-O2	5.51	126.66	122.80
35	RA	1342	A	N1-C6-N6	5.51	121.91	118.60
1	QA	452	A	O4'-C1'-N9	5.51	112.61	108.20
35	RA	2678	C	C6-N1-C2	-5.51	118.10	120.30
1	XA	805	C	N1-C2-O2	5.51	122.20	118.90
22	QV	17(A)	U	C3'-C2'-C1'	5.50	105.90	101.50
55	RZ	62	PRO	C-N-CA	5.50	135.46	121.70
35	YA	1607	C	N3-C4-N4	5.50	121.85	118.00
10	QJ	79	ARG	CB-CA-C	5.50	121.40	110.40
35	RA	1880	C	C5-C6-N1	5.50	123.75	121.00
35	RA	2688	U	C2-N1-C1'	5.50	124.30	117.70
1	XA	1381	U	C2-N3-C4	5.50	130.30	127.00
35	YA	1881	C	N3-C4-N4	5.50	121.85	118.00
35	RA	1670	C	C6-N1-C2	-5.50	118.10	120.30
35	YA	2553	G	N3-C4-C5	-5.50	125.85	128.60
1	QA	1001	G	OP1-P-OP2	-5.50	111.35	119.60
35	RA	1899	G	C8-N9-C1'	-5.50	119.85	127.00
35	RA	2689	U	P-O3'-C3'	5.50	126.30	119.70
15	QO	41	GLU	CA-CB-CG	5.50	125.49	113.40
35	RA	587	C	P-O3'-C3'	5.50	126.30	119.70
35	RA	1370	C	C2-N1-C1'	5.50	124.85	118.80
35	YA	1640	C	C2-N1-C1'	5.50	124.84	118.80
35	YA	2432	A	N1-C6-N6	5.50	121.90	118.60
1	QA	54	C	C6-N1-C2	-5.49	118.10	120.30
35	RA	513	A	C5-C6-N6	-5.49	119.31	123.70
35	RA	592	G	N1-C6-O6	-5.49	116.60	119.90
1	XA	1398	A	C8-N9-C4	-5.49	103.60	105.80
20	XT	72	LEU	CA-CB-CG	5.49	127.94	115.30
35	YA	930	U	C5-C4-O4	5.49	129.20	125.90
35	YA	1217	C	C5-C6-N1	5.49	123.75	121.00
55	YZ	38	TYR	CA-CB-CG	5.49	123.84	113.40
1	XA	1031	G	C8-N9-C1'	-5.49	119.86	127.00
35	RA	2766	G	C8-N9-C1'	-5.49	119.86	127.00
1	XA	1157	A	OP2-P-O3'	5.49	117.28	105.20
35	YA	143	C	N1-C2-O2	5.49	122.19	118.90
35	YA	1012	U	N3-C4-O4	-5.49	115.56	119.40
35	RA	269	U	C5-C6-N1	5.49	125.44	122.70
35	RA	730	C	C6-N1-C2	-5.49	118.11	120.30
35	RA	1241	A	O4'-C1'-N9	5.49	112.59	108.20
35	YA	140	A	C4-C5-N7	5.49	113.44	110.70
35	YA	1815	A	N9-C4-C5	-5.49	103.61	105.80
35	YA	2244	U	C5-C4-O4	-5.49	122.61	125.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	XA	971	G	C2-N3-C4	-5.49	109.16	111.90
35	YA	1379	A	C4-C5-N7	5.49	113.44	110.70
35	RA	1378	A	N1-C6-N6	-5.49	115.31	118.60
1	XA	1147	C	N1-C2-O2	5.49	122.19	118.90
35	YA	2239	G	N9-C4-C5	-5.49	103.21	105.40
35	RA	1839	G	C2-N3-C4	5.48	114.64	111.90
1	XA	92	G	C4-N9-C1'	5.48	133.63	126.50
1	QA	190	G	P-O3'-C3'	5.48	126.28	119.70
35	YA	827	U	C5-C6-N1	-5.48	119.96	122.70
1	QA	135	C	N1-C2-O2	5.48	122.19	118.90
35	RA	193	U	C6-N1-C2	-5.48	117.71	121.00
35	RA	1076	C	C6-N1-C2	-5.48	118.11	120.30
36	RB	8	U	C5-C6-N1	5.48	125.44	122.70
35	YA	1769	G	N3-C2-N2	-5.48	116.06	119.90
1	QA	221	C	C6-N1-C2	-5.48	118.11	120.30
7	QG	76	ARG	CG-CD-NE	-5.48	100.29	111.80
35	RA	356	G	C4-N9-C1'	5.48	133.62	126.50
1	QA	1031	G	N3-C4-N9	5.48	129.29	126.00
35	RA	1614	A	N1-C6-N6	5.48	121.89	118.60
35	RA	1828	G	N1-C2-N2	-5.48	111.27	116.20
55	RZ	38	TYR	CA-CB-CG	5.48	123.81	113.40
1	QA	455	C	C2-N1-C1'	5.48	124.82	118.80
35	YA	2167	U	C5-C6-N1	5.48	125.44	122.70
2	QB	86	GLU	CB-CA-C	5.47	121.35	110.40
35	RA	1400	G	C8-N9-C4	-5.47	104.21	106.40
1	XA	1157	A	C8-N9-C1'	-5.47	117.85	127.70
35	RA	2601	C	N3-C4-C5	5.47	124.09	121.90
1	XA	772	U	N3-C2-O2	-5.47	118.37	122.20
1	XA	960	U	N3-C2-O2	-5.47	118.37	122.20
35	YA	588	U	C5-C4-O4	-5.47	122.62	125.90
35	YA	2808	U	C5-C6-N1	5.47	125.44	122.70
35	RA	889	C	C2-N1-C1'	5.47	124.81	118.80
2	XB	16	HIS	CB-CA-C	-5.47	99.47	110.40
35	YA	71	A	N7-C8-N9	5.47	116.53	113.80
35	RA	1735	C	C5-C6-N1	5.46	123.73	121.00
35	RA	2803	C	C5-C6-N1	5.46	123.73	121.00
1	XA	680	C	C6-N1-C2	-5.46	118.11	120.30
35	YA	240	G	C4-C5-N7	-5.46	108.61	110.80
35	YA	2168	G	C8-N9-C4	-5.46	104.22	106.40
35	RA	738	G	N3-C4-C5	-5.46	125.87	128.60
35	YA	270(Z)	U	N3-C2-O2	-5.46	118.38	122.20
35	YA	1180	C	C6-N1-C1'	-5.46	114.25	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	XA	369	C	C6-N1-C2	-5.46	118.12	120.30
1	XA	754	C	C5-C6-N1	5.46	123.73	121.00
1	XA	989	C	C6-N1-C2	-5.46	118.12	120.30
55	YZ	8	TYR	CA-CB-CG	5.46	123.77	113.40
35	RA	239	U	N3-C2-O2	-5.46	118.38	122.20
35	RA	527	C	C6-N1-C2	-5.46	118.12	120.30
35	YA	1112	G	N1-C6-O6	-5.46	116.63	119.90
3	QC	35	GLU	CG-CD-OE2	-5.45	107.39	118.30
35	RA	404	C	OP2-P-O3'	5.45	117.20	105.20
35	RA	817	C	N3-C4-C5	-5.45	119.72	121.90
35	YA	198	C	C5-C6-N1	5.45	123.73	121.00
1	QA	418	C	N3-C4-C5	-5.45	119.72	121.90
22	QW	25	C	C6-N1-C2	-5.45	118.12	120.30
10	XJ	7	LYS	N-CA-CB	-5.45	100.79	110.60
35	YA	606	U	N3-C2-O2	-5.45	118.38	122.20
1	QA	1317	C	C6-N1-C1'	-5.45	114.26	120.80
35	YA	618	G	C8-N9-C4	-5.45	104.22	106.40
35	YA	669	G	C4-N9-C1'	5.45	133.59	126.50
35	YA	1167	U	C2-N1-C1'	5.45	124.24	117.70
35	YA	528	A	N1-C6-N6	5.45	121.87	118.60
35	YA	530	G	N3-C4-N9	5.45	129.27	126.00
36	YB	44	G	C4-N9-C1'	-5.45	119.42	126.50
1	QA	54	C	C5-C6-N1	5.45	123.72	121.00
1	XA	1453	G	C4-N9-C1'	5.45	133.58	126.50
35	YA	2610	C	P-O3'-C3'	5.45	126.23	119.70
22	XV	62	C	C6-N1-C2	-5.44	118.12	120.30
35	YA	270(P)	C	C5-C6-N1	5.44	123.72	121.00
28	Y3	35	ARG	CD-NE-CZ	5.44	131.22	123.60
35	YA	2037	G	C8-N9-C4	-5.44	104.22	106.40
35	YA	2609	U	C5-C6-N1	-5.44	119.98	122.70
1	QA	90	C	C2-N1-C1'	5.44	124.78	118.80
1	QA	497	U	N1-C2-O2	5.44	126.61	122.80
35	RA	1642	G	N7-C8-N9	5.44	115.82	113.10
35	YA	1080	C	C5-C6-N1	5.44	123.72	121.00
1	XA	1201	A	C8-N9-C4	5.44	107.98	105.80
35	YA	2124	G	C4-N9-C1'	5.44	133.57	126.50
35	RA	2509	G	C6-C5-N7	-5.44	127.14	130.40
35	YA	1588	C	C5-C6-N1	5.44	123.72	121.00
35	YA	1159	U	N1-C2-O2	5.44	126.61	122.80
1	QA	960	U	C5-C6-N1	5.43	125.42	122.70
35	RA	1314	C	C6-N1-C1'	-5.43	114.28	120.80
35	YA	2756	U	N3-C4-O4	5.43	123.20	119.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RA	512	G	OP2-P-O3'	5.43	117.15	105.20
35	RA	2451	A	C8-N9-C4	-5.43	103.63	105.80
35	YA	243	U	C2-N3-C4	5.43	130.26	127.00
1	QA	186	C	N1-C2-O2	5.43	122.16	118.90
35	YA	1786	A	C2-N3-C4	-5.43	107.89	110.60
1	QA	701	C	N1-C2-O2	5.43	122.16	118.90
22	XW	68	C	N1-C2-O2	5.43	122.16	118.90
35	YA	1950	G	C6-C5-N7	-5.43	127.14	130.40
1	XA	1038	C	N3-C2-O2	-5.43	118.10	121.90
35	YA	2527	C	N1-C2-O2	5.43	122.16	118.90
35	RA	141	A	N1-C6-N6	5.43	121.86	118.60
35	RA	151	C	N1-C2-O2	5.43	122.16	118.90
35	RA	897	C	C5-C6-N1	5.43	123.71	121.00
35	RA	1880	C	N1-C2-O2	5.43	122.16	118.90
35	RA	2798	C	C5-C6-N1	5.43	123.71	121.00
31	Y6	28	ARG	CB-CG-CD	5.43	125.71	111.60
35	YA	595	C	C6-N1-C2	-5.43	118.13	120.30
35	YA	1327	C	C6-N1-C2	-5.43	118.13	120.30
35	YA	1417	C	C2-N1-C1'	5.43	124.77	118.80
35	RA	758	C	C2-N1-C1'	5.42	124.77	118.80
35	RA	2243	U	N1-C2-O2	5.42	126.60	122.80
35	RA	2346	A	N7-C8-N9	5.42	116.51	113.80
35	YA	621	A	C6-C5-N7	-5.42	128.50	132.30
35	YA	1920	C	N1-C2-O2	5.42	122.15	118.90
35	RA	349	G	N3-C4-C5	-5.42	125.89	128.60
1	XA	1332	A	C8-N9-C4	-5.42	103.63	105.80
35	YA	676	A	C8-N9-C4	-5.42	103.63	105.80
35	YA	944	G	C8-N9-C1'	-5.42	119.95	127.00
35	YA	2286	A	N1-C6-N6	5.42	121.85	118.60
35	RA	1265	A	N1-C6-N6	5.42	121.85	118.60
35	RA	2724	C	C6-N1-C2	-5.42	118.13	120.30
35	YA	60	G	C8-N9-C4	5.42	108.57	106.40
1	QA	1321	C	N3-C4-C5	5.42	124.07	121.90
35	RA	1135	C	N1-C2-O2	5.42	122.15	118.90
35	RA	1480	G	N1-C2-N2	5.42	121.08	116.20
35	RA	2518	A	N1-C6-N6	5.42	121.85	118.60
1	XA	616	G	C8-N9-C4	-5.42	104.23	106.40
35	YA	1950	G	C4-N9-C1'	5.42	133.54	126.50
35	YA	2092	U	N3-C2-O2	-5.42	118.41	122.20
35	YA	2646	C	C6-N1-C2	-5.42	118.13	120.30
1	XA	530	G	N3-C4-C5	-5.42	125.89	128.60
35	RA	1437	C	C5-C6-N1	5.42	123.71	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	YA	845	G	N9-C4-C5	-5.42	103.23	105.40
1	QA	560	U	C3'-C2'-C1'	5.41	105.83	101.50
7	QG	56	GLN	CB-CA-C	5.41	121.23	110.40
35	RA	172	C	C6-N1-C1'	-5.41	114.30	120.80
36	YB	45	A	N9-C4-C5	-5.41	103.64	105.80
35	RA	1891	G	N3-C4-C5	-5.41	125.89	128.60
41	RH	77	LYS	CD-CE-NZ	5.41	124.15	111.70
35	YA	1319	G	N1-C6-O6	5.41	123.15	119.90
35	YA	2226	C	C5-C6-N1	5.41	123.71	121.00
22	QW	8	U	O4'-C1'-N1	5.41	112.53	108.20
35	RA	1805	U	C6-N1-C2	-5.41	117.75	121.00
35	YA	496	G	C4-C5-N7	5.41	112.96	110.80
35	YA	2311	A	P-O3'-C3'	5.41	126.19	119.70
1	QA	415	A	C8-N9-C4	-5.41	103.64	105.80
1	QA	1364	U	N1-C2-O2	5.41	126.59	122.80
35	YA	463	G	C5-C6-O6	5.41	131.85	128.60
35	YA	2346	A	N7-C8-N9	5.41	116.50	113.80
35	RA	1288	U	O5'-P-OP2	-5.41	100.83	105.70
41	RH	19	VAL	C-N-CA	5.41	135.22	121.70
35	YA	82	G	C4-C5-N7	-5.41	108.64	110.80
35	YA	955	C	C2-N1-C1'	5.41	124.75	118.80
1	QA	130	A	C8-N9-C4	5.41	107.96	105.80
10	QJ	43	ARG	CA-CB-CG	-5.41	101.51	113.40
35	RA	364	C	C6-N1-C2	-5.41	118.14	120.30
35	RA	428	A	N1-C6-N6	5.41	121.84	118.60
35	RA	1474	C	C2-N1-C1'	5.41	124.75	118.80
35	YA	1488	G	N3-C4-C5	-5.41	125.90	128.60
1	QA	1149	C	C5-C6-N1	5.40	123.70	121.00
35	RA	1233	C	N1-C2-O2	5.40	122.14	118.90
35	RA	2346	A	C5-C6-N1	-5.40	115.00	117.70
43	RN	12	ARG	CB-CG-CD	5.40	125.65	111.60
35	YA	974	G	C8-N9-C4	5.40	108.56	106.40
35	RA	1170	G	C4-N9-C1'	5.40	133.52	126.50
35	RA	1800	C	C6-N1-C2	5.40	122.46	120.30
35	YA	1839	G	C4-N9-C1'	5.40	133.52	126.50
35	RA	1529	A	N1-C2-N3	5.40	132.00	129.30
1	QA	1157	A	OP2-P-O3'	5.40	117.07	105.20
26	R1	77	ALA	CB-CA-C	5.40	118.20	110.10
35	RA	270(K)	C	C2-N1-C1'	5.40	124.74	118.80
35	RA	2461	C	C2-N1-C1'	5.40	124.74	118.80
1	XA	805	C	N3-C4-C5	5.40	124.06	121.90
1	XA	1161	C	C6-N1-C2	-5.40	118.14	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RA	1092	C	C6-N1-C2	-5.40	118.14	120.30
35	RA	2232	U	N3-C2-O2	-5.40	118.42	122.20
35	YA	273(D)	C	C6-N1-C2	-5.40	118.14	120.30
35	RA	1797	C	C5-C6-N1	5.39	123.70	121.00
35	RA	2144	U	P-O3'-C3'	5.39	126.17	119.70
42	RI	115	ALA	N-CA-CB	5.39	117.65	110.10
1	XA	727	G	C5-C6-O6	5.39	131.84	128.60
35	YA	2415	G	N1-C6-O6	5.39	123.14	119.90
22	QV	51	C	C5-C6-N1	5.39	123.70	121.00
35	RA	1455	G	C8-N9-C4	-5.39	104.24	106.40
38	RE	57	LYS	N-CA-C	5.39	125.56	111.00
35	YA	953	A	C5-C6-N6	-5.39	119.39	123.70
35	RA	823	G	N9-C4-C5	-5.39	103.24	105.40
35	RA	1698	A	C4-C5-N7	5.39	113.40	110.70
35	YA	1180	C	C5-C6-N1	5.39	123.69	121.00
35	RA	859	G	C8-N9-C1'	5.39	134.01	127.00
35	RA	1528	A	C4-C5-N7	5.39	113.39	110.70
35	RA	1888	G	N3-C4-C5	-5.39	125.91	128.60
35	YA	131	G	N3-C4-C5	-5.39	125.91	128.60
35	YA	358	U	C6-N1-C1'	-5.39	113.65	121.20
35	RA	837	C	N1-C2-O2	5.39	122.13	118.90
1	XA	186(A)	C	N1-C2-O2	5.39	122.13	118.90
3	XC	126	ARG	CD-NE-CZ	5.39	131.14	123.60
7	XG	22	LEU	CA-CB-CG	5.39	127.69	115.30
35	YA	1574	C	C6-N1-C2	-5.39	118.15	120.30
35	YA	2318	G	O4'-C1'-N9	5.39	112.51	108.20
55	YZ	130	PRO	CA-N-CD	5.39	119.24	111.70
35	RA	2261	C	C6-N1-C2	-5.38	118.15	120.30
35	YA	944	G	C4-N9-C1'	5.38	133.50	126.50
35	YA	1989	G	C5-C6-O6	-5.38	125.37	128.60
1	QA	1125	U	N3-C4-C5	-5.38	111.37	114.60
7	XG	95	ARG	CD-NE-CZ	5.38	131.14	123.60
1	XA	331	G	N1-C6-O6	5.38	123.13	119.90
35	YA	378	C	C6-N1-C2	-5.38	118.15	120.30
35	YA	1342	A	O4'-C1'-N9	5.38	112.50	108.20
35	YA	2139	C	C6-N1-C1'	-5.38	114.34	120.80
35	YA	2513	G	N9-C4-C5	-5.38	103.25	105.40
35	RA	2294	C	C5-C6-N1	5.38	123.69	121.00
1	XA	932	C	C2-N1-C1'	5.38	124.72	118.80
35	YA	974	G	N7-C8-N9	-5.38	110.41	113.10
35	YA	2474	C	N1-C2-O2	5.38	122.12	118.90
1	QA	883	C	C6-N1-C2	-5.38	118.15	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	XA	1045	C	C2-N1-C1'	5.38	124.71	118.80
1	QA	1007	C	P-O3'-C3'	5.37	126.15	119.70
22	QV	59	A	N7-C8-N9	5.37	116.49	113.80
42	YI	10	GLU	C-N-CA	5.37	135.13	121.70
35	RA	1248	G	C5-C6-N1	5.37	114.19	111.50
35	RA	1304	C	C2-N1-C1'	5.37	124.71	118.80
35	YA	556	G	C5-N7-C8	-5.37	101.61	104.30
35	YA	2604	U	C2-N1-C1'	5.37	124.15	117.70
1	QA	314	C	C6-N1-C2	-5.37	118.15	120.30
35	RA	2469	A	N1-C6-N6	5.37	121.82	118.60
35	RA	2896	C	N1-C2-O2	5.37	122.12	118.90
35	YA	1246	A	C8-N9-C4	5.37	107.95	105.80
35	YA	2454	G	C2-N3-C4	5.37	114.58	111.90
51	YV	15	GLU	CA-CB-CG	-5.37	101.58	113.40
1	QA	121	C	C6-N1-C2	5.37	122.45	120.30
35	RA	20	C	N3-C4-C5	-5.37	119.75	121.90
1	XA	1538	C	N3-C2-O2	-5.37	118.14	121.90
35	YA	1338	G	N3-C4-C5	-5.37	125.92	128.60
35	RA	38	A	C2-N3-C4	5.37	113.28	110.60
35	RA	1404	C	C2-N1-C1'	5.37	124.70	118.80
1	QA	812	C	C6-N1-C2	-5.37	118.15	120.30
29	R4	43	TYR	CB-CA-C	5.37	121.13	110.40
1	QA	494	U	C5-C6-N1	5.36	125.38	122.70
35	RA	968	G	N3-C4-N9	5.36	129.22	126.00
49	YT	105	LEU	CA-CB-CG	5.36	127.64	115.30
35	RA	945	A	C6-N1-C2	5.36	121.82	118.60
35	RA	2685	G	N3-C2-N2	-5.36	116.15	119.90
35	YA	1376	C	C2-N3-C4	-5.36	117.22	119.90
1	QA	1232	U	C5-C4-O4	-5.36	122.68	125.90
35	RA	193	U	C5-C6-N1	5.36	125.38	122.70
35	RA	2518	A	C5-N7-C8	-5.36	101.22	103.90
35	RA	2751	G	C4-N9-C1'	5.36	133.47	126.50
3	XC	126	ARG	CB-CG-CD	5.36	125.54	111.60
22	XW	3	C	C6-N1-C2	-5.36	118.16	120.30
29	Y4	45	GLY	C-N-CA	5.36	135.10	121.70
35	YA	928	G	C4-N9-C1'	5.36	133.47	126.50
35	YA	950	G	C8-N9-C4	5.36	108.54	106.40
35	YA	1430	C	N1-C2-O2	5.36	122.12	118.90
35	RA	214	G	O4'-C1'-N9	5.36	112.49	108.20
36	RB	3	C	N3-C4-N4	5.36	121.75	118.00
35	YA	850	C	C6-N1-C2	-5.36	118.16	120.30
1	XA	500	G	N9-C4-C5	-5.36	103.26	105.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	YA	634	C	N3-C4-N4	5.36	121.75	118.00
35	YA	809	G	C8-N9-C4	-5.36	104.26	106.40
35	YA	1286	A	O4'-C1'-N9	5.36	112.49	108.20
35	YA	2247	A	C4-C5-N7	5.36	113.38	110.70
35	YA	2752	C	N3-C2-O2	-5.36	118.15	121.90
1	QA	980	C	N1-C2-O2	5.36	122.11	118.90
44	RO	107	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	XA	797	C	C6-N1-C2	-5.36	118.16	120.30
35	YA	1000	A	N7-C8-N9	5.36	116.48	113.80
35	YA	1092	C	C6-N1-C2	-5.36	118.16	120.30
35	YA	1130	U	C6-N1-C2	-5.36	117.79	121.00
35	RA	471	A	N7-C8-N9	5.35	116.48	113.80
35	RA	1138	G	N9-C4-C5	5.35	107.54	105.40
35	RA	1698	A	C8-N9-C4	-5.35	103.66	105.80
42	RI	38	LEU	CA-CB-CG	5.35	127.61	115.30
35	YA	2675	A	N7-C8-N9	5.35	116.48	113.80
35	RA	596	G	N1-C6-O6	-5.35	116.69	119.90
35	RA	1880	C	C2-N3-C4	5.35	122.58	119.90
35	YA	1110	G	N3-C4-N9	-5.35	122.79	126.00
22	QV	38	A	C8-N9-C4	5.35	107.94	105.80
1	QA	1111	A	C6-N1-C2	5.35	121.81	118.60
35	RA	373	U	O4'-C1'-N1	5.35	112.48	108.20
35	RA	436	C	C2-N1-C1'	5.35	124.68	118.80
35	RA	1864	U	N1-C2-O2	5.35	126.55	122.80
35	YA	1294	U	C5-C6-N1	5.35	125.38	122.70
35	YA	2543	G	N1-C6-O6	-5.35	116.69	119.90
35	YA	1474	C	N1-C2-O2	5.35	122.11	118.90
35	YA	2851	A	C5-C6-N6	-5.35	119.42	123.70
48	YS	23	ARG	CG-CD-NE	5.35	123.03	111.80
35	YA	356	G	N3-C4-C5	-5.34	125.93	128.60
5	QE	137	GLU	CA-CB-CG	5.34	125.16	113.40
1	XA	1465	C	N3-C4-C5	-5.34	119.76	121.90
36	YB	108	C	C6-N1-C2	5.34	122.44	120.30
35	RA	2748	A	N7-C8-N9	5.34	116.47	113.80
1	XA	1538	C	N1-C2-O2	5.34	122.11	118.90
35	YA	845	G	N1-C2-N3	-5.34	120.69	123.90
35	YA	1345	C	C5-C6-N1	5.34	123.67	121.00
35	RA	933	A	C4-C5-N7	5.34	113.37	110.70
12	XL	92	ASP	CB-CG-OD1	5.34	123.11	118.30
35	YA	678	C	C5-C6-N1	5.34	123.67	121.00
35	YA	1153	C	C6-N1-C2	-5.34	118.17	120.30
35	YA	1502	C	C6-N1-C2	-5.34	118.17	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RA	859	G	O4'-C1'-N9	5.34	112.47	108.20
35	RA	974(A)	C	C6-N1-C2	-5.34	118.17	120.30
35	RA	1467	C	C2-N1-C1'	5.34	124.67	118.80
1	XA	91	C	C5-C6-N1	5.34	123.67	121.00
1	XA	690	G	C4-N9-C1'	5.34	133.44	126.50
20	XT	91	LEU	CB-CG-CD2	-5.34	101.93	111.00
35	YA	2766	G	N3-C4-N9	5.34	129.20	126.00
35	RA	288	C	N1-C2-O2	5.33	122.10	118.90
1	XA	1259	C	C6-N1-C2	-5.33	118.17	120.30
22	XW	28	C	C6-N1-C2	-5.33	118.17	120.30
1	QA	1202	G	C5-C6-O6	5.33	131.80	128.60
35	RA	2497	A	C5-C6-N6	-5.33	119.43	123.70
35	YA	736	C	C4-C5-C6	-5.33	114.73	117.40
1	QA	1225	A	C4-N9-C1'	5.33	135.90	126.30
35	RA	2319	G	N3-C4-N9	5.33	129.20	126.00
36	RB	81	G	C8-N9-C4	-5.33	104.27	106.40
1	XA	619	U	C6-N1-C1'	5.33	128.66	121.20
35	YA	881	G	C4-N9-C1'	5.33	133.43	126.50
35	YA	2174	C	N3-C2-O2	-5.33	118.17	121.90
35	YA	2561	A	C5-C6-N1	5.33	120.37	117.70
1	QA	614	A	N7-C8-N9	5.33	116.47	113.80
1	XA	1303	C	N1-C2-O2	5.33	122.10	118.90
35	YA	1170	G	N3-C4-C5	-5.33	125.94	128.60
35	YA	1306	C	C5-C6-N1	5.33	123.67	121.00
35	RA	69	C	C6-N1-C2	-5.33	118.17	120.30
35	RA	1166	C	C5-C6-N1	5.33	123.66	121.00
35	YA	1909	C	C2-N1-C1'	5.33	124.66	118.80
35	YA	1963	U	C6-N1-C1'	-5.33	113.74	121.20
1	QA	962	C	C6-N1-C2	-5.33	118.17	120.30
35	RA	1307	A	C8-N9-C4	5.33	107.93	105.80
35	RA	1979	C	C6-N1-C2	-5.33	118.17	120.30
35	YA	544	C	C6-N1-C2	-5.33	118.17	120.30
35	YA	697	C	C5-C4-N4	-5.33	116.47	120.20
1	XA	1225	A	C4-N9-C1'	5.33	135.89	126.30
35	YA	707	G	N3-C4-C5	-5.33	125.94	128.60
35	RA	2059	A	C5-C6-N6	5.32	127.96	123.70
35	YA	213	A	N1-C2-N3	-5.32	126.64	129.30
35	YA	2139	C	C6-N1-C2	-5.32	118.17	120.30
22	XW	11	A	C8-N9-C1'	-5.32	118.12	127.70
1	XA	801	U	N3-C2-O2	-5.32	118.48	122.20
35	RA	243	U	C5-C6-N1	5.32	125.36	122.70
1	XA	690	G	C8-N9-C4	-5.32	104.27	106.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	YA	154	G	C4-N9-C1'	5.32	133.41	126.50
35	YA	1433	U	N1-C2-O2	5.32	126.52	122.80
1	QA	1397	C	C2-N1-C1'	-5.32	112.95	118.80
35	RA	2164	C	C6-N1-C2	-5.32	118.17	120.30
35	RA	2702	U	N1-C2-O2	5.32	126.52	122.80
35	YA	1488	G	C4-N9-C1'	5.32	133.41	126.50
35	RA	695	G	C4-C5-C6	5.31	121.99	118.80
25	Y0	75	LEU	CA-CB-CG	5.31	127.52	115.30
35	YA	894	C	N1-C2-O2	5.31	122.09	118.90
35	YA	1467	C	C6-N1-C2	-5.31	118.18	120.30
35	YA	2790	A	O4'-C1'-N9	-5.31	103.95	108.20
1	QA	201	C	P-O3'-C3'	5.31	126.07	119.70
22	QW	13	C	C6-N1-C1'	-5.31	114.43	120.80
35	RA	286	C	C6-N1-C1'	-5.31	114.43	120.80
35	RA	615	G	C8-N9-C1'	5.31	133.90	127.00
23	XX	12	A	P-O3'-C3'	5.31	126.07	119.70
55	YZ	60	GLU	CB-CA-C	-5.31	99.78	110.40
1	QA	174	C	C5-C6-N1	5.31	123.65	121.00
1	QA	1453	G	C6-N1-C2	5.31	128.28	125.10
35	RA	2306	C	N1-C2-O2	5.31	122.08	118.90
1	XA	1071	C	O5'-P-OP1	-5.31	100.92	105.70
35	YA	1433	U	N3-C2-O2	-5.31	118.49	122.20
1	QA	1282	C	C6-N1-C2	-5.30	118.18	120.30
29	R4	54	GLY	N-CA-C	5.30	126.36	113.10
35	RA	1963	U	C6-N1-C2	-5.30	117.82	121.00
21	XU	7	ARG	N-CA-CB	-5.30	101.05	110.60
1	XA	519	C	C6-N1-C2	5.30	122.42	120.30
35	YA	1640	C	C5-C6-N1	5.30	123.65	121.00
47	YR	86	ARG	CG-CD-NE	-5.30	100.66	111.80
35	RA	654(A)	G	O4'-C1'-N9	5.30	112.44	108.20
35	RA	881	G	C6-C5-N7	-5.30	127.22	130.40
35	RA	1241	A	C4-C5-N7	5.30	113.35	110.70
35	RA	1771	C	C6-N1-C2	-5.30	118.18	120.30
35	YA	273(D)	C	C6-N1-C1'	-5.30	114.44	120.80
35	YA	392	C	N1-C2-O2	5.30	122.08	118.90
35	YA	1011	G	C6-C5-N7	5.30	133.58	130.40
35	RA	823	G	C8-N9-C4	5.30	108.52	106.40
35	RA	2607	G	N1-C6-O6	-5.30	116.72	119.90
1	XA	217	C	C6-N1-C2	-5.30	118.18	120.30
35	YA	1734	C	C6-N1-C2	-5.30	118.18	120.30
35	YA	1827	C	N3-C2-O2	-5.30	118.19	121.90
35	RA	2708	G	C8-N9-C4	5.30	108.52	106.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	XA	311	C	C6-N1-C2	-5.30	118.18	120.30
35	YA	609	A	C2-N3-C4	5.30	113.25	110.60
35	YA	1846	G	OP2-P-O3'	5.30	116.85	105.20
1	QA	135	C	C5-C6-N1	5.29	123.65	121.00
1	QA	749	C	C5-C6-N1	5.29	123.65	121.00
35	RA	2611	U	N3-C2-O2	5.29	125.91	122.20
35	YA	1881	C	N3-C4-C5	-5.29	119.78	121.90
28	R3	39	ASP	C-N-CA	5.29	134.93	121.70
35	RA	1507	A	C8-N9-C4	-5.29	103.68	105.80
35	YA	1398	C	C2-N1-C1'	5.29	124.62	118.80
35	YA	2343	C	C2-N1-C1'	5.29	124.62	118.80
25	R0	48	GLY	N-CA-C	5.29	126.32	113.10
35	RA	2451	A	N9-C4-C5	5.29	107.92	105.80
35	YA	1834	U	C5-C4-O4	-5.29	122.73	125.90
35	YA	154	G	C8-N9-C1'	-5.29	120.12	127.00
35	RA	2739	U	C6-N1-C2	-5.29	117.83	121.00
35	YA	2590	A	N9-C4-C5	-5.29	103.69	105.80
22	QV	32	C	N1-C2-O2	5.29	122.07	118.90
35	RA	1488	G	C8-N9-C4	-5.29	104.28	106.40
35	RA	2164	C	C5-C6-N1	5.29	123.64	121.00
35	RA	2787	C	C5-C6-N1	5.29	123.64	121.00
9	XI	19	LEU	C-N-CA	5.29	134.91	121.70
9	XI	33	PHE	CB-CA-C	5.29	120.97	110.40
35	YA	757	U	N3-C2-O2	-5.29	118.50	122.20
35	YA	1675	C	N1-C2-O2	5.29	122.07	118.90
35	YA	2714	G	C4-C5-N7	-5.29	108.69	110.80
1	QA	1228	C	C5-C6-N1	5.28	123.64	121.00
35	RA	1157	G	N1-C6-O6	5.28	123.07	119.90
1	XA	1439	C	C2-N1-C1'	5.28	124.61	118.80
35	YA	1267	U	N1-C2-O2	5.28	126.50	122.80
1	QA	722	A	C8-N9-C4	-5.28	103.69	105.80
1	QA	1357	A	C8-N9-C4	-5.28	103.69	105.80
35	RA	671	C	N3-C4-C5	-5.28	119.79	121.90
35	YA	591	C	C6-N1-C2	-5.28	118.19	120.30
35	YA	1992	G	OP2-P-O3'	5.28	116.82	105.20
35	RA	1640	C	C2-N1-C1'	5.28	124.61	118.80
31	Y6	14	THR	OG1-CB-CG2	-5.28	97.86	110.00
35	YA	1588	C	N1-C2-O2	5.28	122.07	118.90
35	YA	1819	A	P-O3'-C3'	5.28	126.03	119.70
1	QA	1290	G	C6-C5-N7	-5.28	127.23	130.40
35	RA	84	A	C8-N9-C4	5.28	107.91	105.80
35	RA	273(C)	C	C2-N1-C1'	5.28	124.61	118.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RA	880	G	C8-N9-C4	-5.28	104.29	106.40
35	RA	1233	C	C2-N1-C1'	5.28	124.61	118.80
35	RA	2055	C	N1-C2-O2	5.28	122.07	118.90
35	YA	1385	G	N1-C6-O6	-5.28	116.73	119.90
35	YA	1549	C	C2-N1-C1'	5.28	124.61	118.80
35	YA	1735	C	C6-N1-C1'	-5.28	114.47	120.80
35	RA	2559	C	N3-C4-C5	-5.28	119.79	121.90
35	RA	2712(A)	A	N7-C8-N9	5.28	116.44	113.80
1	XA	51	A	C8-N9-C4	5.28	107.91	105.80
1	XA	759	A	C8-N9-C4	5.28	107.91	105.80
35	YA	93	C	C2-N3-C4	5.28	122.54	119.90
35	YA	141	A	C4-C5-N7	5.28	113.34	110.70
35	YA	930	U	C2-N1-C1'	5.28	124.03	117.70
40	YG	35	GLU	N-CA-CB	-5.28	101.11	110.60
35	YA	1950	G	O4'-C1'-N9	5.27	112.42	108.20
35	RA	953	A	C5-C6-N6	-5.27	119.48	123.70
1	XA	1217	C	O5'-P-OP1	5.27	117.03	110.70
35	YA	2579	C	C5-C6-N1	5.27	123.64	121.00
35	RA	2343	C	C4-C5-C6	-5.27	114.76	117.40
1	QA	442	C	N1-C2-O2	5.27	122.06	118.90
1	QA	482	A	N7-C8-N9	5.27	116.43	113.80
35	RA	650	C	C5-C6-N1	5.27	123.64	121.00
35	RA	953	A	N9-C4-C5	-5.27	103.69	105.80
35	RA	974(A)	C	C2-N1-C1'	5.27	124.59	118.80
35	RA	2347	C	C6-N1-C1'	-5.27	114.48	120.80
1	XA	1132	C	N1-C2-O2	5.27	122.06	118.90
35	YA	9	U	C6-N1-C2	-5.27	117.84	121.00
35	YA	1909	C	C6-N1-C2	-5.27	118.19	120.30
35	YA	2306	C	C2-N3-C4	5.27	122.53	119.90
1	QA	1406	U	N3-C2-O2	-5.27	118.51	122.20
35	YA	1080	C	C6-N1-C2	-5.27	118.19	120.30
35	YA	1959	G	C8-N9-C4	-5.27	104.29	106.40
35	YA	2292	C	C6-N1-C2	-5.27	118.19	120.30
1	QA	518	C	P-O3'-C3'	5.27	126.02	119.70
35	RA	1528	A	C6-C5-N7	-5.27	128.61	132.30
35	RA	748	G	C4-N9-C1'	-5.26	119.66	126.50
35	YA	512	G	N9-C4-C5	5.26	107.51	105.40
35	YA	1076	C	C6-N1-C2	-5.26	118.19	120.30
36	YB	8	U	N3-C2-O2	-5.26	118.52	122.20
35	RA	845	G	OP1-P-O3'	5.26	116.78	105.20
49	RT	137	LYS	CG-CD-CE	5.26	127.69	111.90
1	QA	187	C	C6-N1-C2	-5.26	118.20	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	QA	939	G	C8-N9-C4	5.26	108.50	106.40
35	RA	395	U	N1-C2-O2	5.26	126.48	122.80
35	RA	537	C	C6-N1-C2	-5.26	118.19	120.30
1	XA	108	G	C4-N9-C1'	5.26	133.34	126.50
35	YA	932	G	C5-C6-O6	5.26	131.76	128.60
35	YA	1125	G	C2-N3-C4	-5.26	109.27	111.90
35	YA	1701	A	N1-C6-N6	-5.26	115.44	118.60
1	QA	266	G	C8-N9-C1'	-5.26	120.16	127.00
35	RA	2342	C	C2-N1-C1'	5.26	124.59	118.80
35	YA	577	G	C6-C5-N7	-5.26	127.24	130.40
1	QA	93	U	C6-N1-C2	-5.26	117.84	121.00
1	QA	1523	G	C5-C6-N1	5.26	114.13	111.50
35	RA	2431	U	C6-N1-C2	-5.26	117.84	121.00
36	RB	37	C	N1-C2-O2	5.26	122.06	118.90
35	YA	587	C	P-O3'-C3'	5.26	126.01	119.70
1	QA	980	C	C6-N1-C2	-5.26	118.20	120.30
35	RA	568	U	C6-N1-C2	-5.26	117.85	121.00
35	RA	774	A	N3-C4-N9	-5.26	123.19	127.40
1	XA	331	G	C5-C6-O6	-5.26	125.45	128.60
1	XA	1187	G	C4-N9-C1'	5.25	133.33	126.50
1	XA	1482	G	C2-N3-C4	-5.25	109.27	111.90
35	RA	528	A	N1-C6-N6	5.25	121.75	118.60
1	XA	1007	C	C6-N1-C2	-5.25	118.20	120.30
1	XA	1094	G	C2-N3-C4	5.25	114.53	111.90
35	YA	1977	A	N1-C6-N6	5.25	121.75	118.60
35	YA	2390	U	N3-C4-O4	5.25	123.08	119.40
1	QA	243	A	N1-C6-N6	-5.25	115.45	118.60
1	QA	1066	C	C4-C5-C6	-5.25	114.77	117.40
8	QH	42	GLU	CB-CA-C	5.25	120.90	110.40
35	RA	792	G	N7-C8-N9	5.25	115.72	113.10
35	RA	2501	C	N3-C4-N4	-5.25	114.32	118.00
22	XW	61	C	C5-C6-N1	5.25	123.62	121.00
35	YA	2232	U	N3-C4-C5	-5.25	111.45	114.60
22	QW	34	C	C5-C6-N1	5.25	123.62	121.00
35	RA	1562	A	C2-N3-C4	5.25	113.22	110.60
35	YA	176	G	N7-C8-N9	-5.25	110.47	113.10
35	YA	273(F)	C	C6-N1-C2	-5.25	118.20	120.30
35	YA	2362	G	C2-N3-C4	5.25	114.53	111.90
10	QJ	80	LYS	CA-CB-CG	5.25	124.94	113.40
35	RA	1786	A	C4-N9-C1'	5.25	135.75	126.30
1	XA	485	G	N3-C4-N9	-5.25	122.85	126.00
35	RA	2636	U	C2-N1-C1'	5.25	123.99	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	YA	71	A	C6-C5-N7	-5.25	128.63	132.30
35	YA	2105	C	C5-C6-N1	5.25	123.62	121.00
35	RA	2093	G	N3-C2-N2	-5.24	116.23	119.90
35	RA	2163	C	C6-N1-C2	-5.24	118.20	120.30
35	YA	1125	G	C5-C6-N1	-5.24	108.88	111.50
35	RA	1955	U	N3-C2-O2	-5.24	118.53	122.20
35	YA	660	G	C5-C6-O6	5.24	131.75	128.60
35	RA	753	C	C6-N1-C2	-5.24	118.20	120.30
1	XA	1007	C	OP1-P-O3'	5.24	116.73	105.20
35	YA	270(I)	G	C8-N9-C4	-5.24	104.30	106.40
35	YA	348	G	C8-N9-C4	-5.24	104.30	106.40
35	YA	928	G	N3-C4-C5	-5.24	125.98	128.60
35	YA	2632	A	C8-N9-C4	-5.24	103.70	105.80
35	YA	1041	C	C6-N1-C2	-5.24	118.20	120.30
35	YA	2247	A	N9-C4-C5	-5.24	103.70	105.80
35	YA	2616	C	N3-C4-C5	-5.24	119.80	121.90
35	RA	2702	U	N3-C2-O2	-5.24	118.54	122.20
1	XA	1000	A	C6-C5-N7	-5.24	128.63	132.30
35	YA	2028	U	N3-C4-C5	-5.24	111.46	114.60
1	QA	690	G	C4-N9-C1'	5.23	133.30	126.50
35	YA	391	G	N1-C6-O6	5.23	123.04	119.90
35	YA	804	A	C5-C6-N6	5.23	127.89	123.70
1	QA	529	G	N3-C2-N2	5.23	123.56	119.90
1	QA	643	C	C5-C6-N1	5.23	123.62	121.00
1	QA	1000	A	P-O3'-C3'	5.23	125.98	119.70
35	RA	1314	C	C5-C6-N1	5.23	123.62	121.00
35	YA	352	G	N3-C4-C5	-5.23	125.98	128.60
1	QA	1203	C	C2-N1-C1'	5.23	124.55	118.80
27	R2	44	LEU	CA-CB-CG	5.23	127.33	115.30
35	RA	1095	A	C4-N9-C1'	5.23	135.72	126.30
35	RA	2444	G	C8-N9-C4	5.23	108.49	106.40
1	XA	563	A	N9-C4-C5	-5.23	103.71	105.80
35	YA	2168	G	N7-C8-N9	5.23	115.72	113.10
50	RU	86	ALA	N-CA-CB	5.23	117.42	110.10
35	YA	2896	C	C5-C6-N1	5.23	123.61	121.00
35	RA	583	G	N3-C4-C5	-5.23	125.99	128.60
35	RA	1499	C	C6-N1-C1'	-5.23	114.53	120.80
35	RA	2036	C	C6-N1-C2	-5.23	118.21	120.30
35	YA	2320	A	C8-N9-C4	-5.23	103.71	105.80
35	YA	2775	A	C5-C6-N6	-5.23	119.52	123.70
1	XA	703	G	OP2-P-O3'	5.23	116.70	105.20
35	YA	2596	U	C5-C4-O4	-5.23	122.76	125.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	YY	40	GLU	N-CA-CB	5.23	120.01	110.60
1	QA	137	C	C6-N1-C2	-5.22	118.21	120.30
1	QA	486	U	N1-C2-O2	5.22	126.46	122.80
35	RA	380	U	C6-N1-C2	-5.22	117.86	121.00
35	RA	2191	G	P-O3'-C3'	5.22	125.97	119.70
37	RD	169	GLU	CA-CB-CG	-5.22	101.91	113.40
1	QA	1199	U	C5-C4-O4	5.22	129.03	125.90
1	XA	486	U	C5-C4-O4	-5.22	122.77	125.90
1	XA	1038	C	N1-C2-O2	5.22	122.03	118.90
10	XJ	5	ARG	CB-CG-CD	-5.22	98.02	111.60
22	XW	61	C	C2-N1-C1'	5.22	124.54	118.80
54	RY	53	PRO	C-N-CA	5.22	134.75	121.70
35	YA	273(C)	C	C6-N1-C1'	-5.22	114.53	120.80
35	YA	2041	U	N3-C2-O2	-5.22	118.55	122.20
1	QA	37	U	N1-C2-N3	5.22	118.03	114.90
35	RA	113	G	C8-N9-C1'	5.22	133.79	127.00
35	RA	1170	G	C6-C5-N7	-5.22	127.27	130.40
22	XW	11	A	C4-N9-C1'	5.22	135.70	126.30
36	RB	44	G	C8-N9-C1'	5.22	133.78	127.00
35	YA	748	G	C2-N3-C4	5.22	114.51	111.90
1	QA	169	C	C6-N1-C1'	-5.22	114.54	120.80
1	QA	330	C	C6-N1-C2	-5.22	118.21	120.30
1	QA	883	C	N3-C4-C5	-5.22	119.81	121.90
35	RA	82	G	C8-N9-C4	-5.22	104.31	106.40
35	RA	2287	A	N1-C6-N6	5.22	121.73	118.60
13	XM	5	ALA	N-CA-CB	-5.22	102.80	110.10
35	YA	41	C	C2-N3-C4	5.22	122.51	119.90
35	YA	856	C	P-O3'-C3'	5.22	125.96	119.70
35	RA	1370	C	C6-N1-C2	-5.21	118.21	120.30
35	YA	669	G	C8-N9-C1'	-5.21	120.22	127.00
1	QA	1187	G	C4-N9-C1'	5.21	133.28	126.50
24	QY	47	PRO	CA-N-CD	5.21	119.00	111.70
1	XA	485	G	OP2-P-O3'	5.21	116.67	105.20
35	YA	2584	U	C6-N1-C1'	-5.21	113.90	121.20
35	YA	2889	C	C6-N1-C2	-5.21	118.22	120.30
1	XA	738	C	C6-N1-C2	-5.21	118.22	120.30
35	YA	307	G	C8-N9-C4	-5.21	104.31	106.40
35	RA	373	U	N1-C2-O2	5.21	126.45	122.80
35	YA	537	C	C5-C6-N1	5.21	123.61	121.00
1	QA	93	U	C5-C6-N1	5.21	125.30	122.70
1	QA	879	C	C6-N1-C2	-5.21	118.22	120.30
22	QV	24	U	N3-C2-O2	-5.21	118.55	122.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	XA	1430	C	C6-N1-C2	-5.21	118.22	120.30
1	XA	1492	A	O5'-P-OP1	5.21	116.95	110.70
35	YA	386	G	C5-C6-O6	5.21	131.72	128.60
35	RA	1170	G	N7-C8-N9	5.21	115.70	113.10
35	RA	1318	C	C2-N1-C1'	5.21	124.53	118.80
35	YA	1999	C	C6-N1-C2	-5.21	118.22	120.30
35	YA	2167	U	N3-C2-O2	-5.21	118.56	122.20
35	RA	2619	C	C6-N1-C2	-5.21	118.22	120.30
35	RA	1803	A	C8-N9-C4	-5.20	103.72	105.80
41	RH	72	ILE	N-CA-CB	5.20	122.77	110.80
35	YA	327	G	C6-C5-N7	-5.20	127.28	130.40
35	YA	676	A	O4'-C1'-N9	5.20	112.36	108.20
35	YA	2061	G	C8-N9-C4	-5.20	104.32	106.40
35	RA	84	A	N9-C4-C5	-5.20	103.72	105.80
1	XA	442	C	C6-N1-C1'	-5.20	114.56	120.80
1	XA	980	C	C5-C6-N1	5.20	123.60	121.00
1	XA	999	U	C5-C6-N1	5.20	125.30	122.70
35	YA	2444	G	N9-C4-C5	5.20	107.48	105.40
1	QA	482	A	C8-N9-C4	-5.20	103.72	105.80
35	RA	597	U	C5-C4-O4	5.20	129.02	125.90
35	RA	1839	G	C5-C6-O6	-5.20	125.48	128.60
35	RA	2856	C	C5-C6-N1	5.20	123.60	121.00
45	RP	26	GLY	N-CA-C	-5.20	100.11	113.10
35	RA	316	C	C6-N1-C2	-5.20	118.22	120.30
35	RA	392	C	C2-N1-C1'	5.20	124.52	118.80
1	XA	888	G	C8-N9-C4	-5.20	104.32	106.40
35	YA	621	A	C2-N3-C4	-5.20	108.00	110.60
35	YA	1669	A	C4-N9-C1'	5.20	135.65	126.30
35	YA	1945	G	N7-C8-N9	5.20	115.70	113.10
35	YA	2057	A	N1-C6-N6	-5.20	115.48	118.60
35	YA	2762	G	C8-N9-C4	-5.20	104.32	106.40
35	RA	1475	G	C6-C5-N7	-5.19	127.28	130.40
1	XA	1420	C	C5-C6-N1	5.19	123.60	121.00
35	YA	1735	C	N3-C4-N4	5.19	121.64	118.00
35	YA	2266	A	N1-C6-N6	-5.19	115.48	118.60
35	RA	670	A	C8-N9-C4	-5.19	103.72	105.80
35	RA	698	C	C6-N1-C2	5.19	122.38	120.30
35	RA	1329	U	C5-C4-O4	-5.19	122.78	125.90
35	RA	1488	G	N3-C4-C5	-5.19	126.00	128.60
35	RA	2099	U	N1-C2-O2	5.19	126.43	122.80
35	RA	2253	G	N9-C4-C5	-5.19	103.32	105.40
35	RA	2321	G	C8-N9-C1'	-5.19	120.25	127.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RA	2689	U	N3-C4-O4	-5.19	115.77	119.40
35	RA	2712(A)	A	C5-N7-C8	-5.19	101.30	103.90
1	XA	186(F)	C	C6-N1-C1'	5.19	127.03	120.80
1	XA	1212	U	O5'-P-OP1	-5.19	101.03	105.70
35	YA	636	G	N1-C6-O6	5.19	123.02	119.90
35	YA	1024	G	N3-C4-C5	-5.19	126.00	128.60
1	QA	652	U	N3-C2-O2	-5.19	118.57	122.20
1	QA	690	G	O4'-C1'-N9	5.19	112.35	108.20
22	QV	67	C	C6-N1-C2	-5.19	118.22	120.30
35	RA	2259	G	C6-C5-N7	-5.19	127.28	130.40
41	RH	20	ALA	N-CA-CB	-5.19	102.83	110.10
48	RS	20	ARG	CD-NE-CZ	5.19	130.87	123.60
1	XA	1514	C	C5-C6-N1	5.19	123.59	121.00
35	YA	269	U	C5-C6-N1	5.19	125.30	122.70
1	QA	1007	C	C6-N1-C2	-5.19	118.22	120.30
35	RA	2779	U	O4'-C1'-N1	5.19	112.35	108.20
36	YB	22	U	C6-N1-C2	-5.19	117.89	121.00
44	YO	49	ARG	CD-NE-CZ	5.19	130.86	123.60
35	RA	1776	G	N3-C4-C5	-5.19	126.01	128.60
35	RA	2046	G	C6-C5-N7	-5.19	127.29	130.40
35	RA	2678	C	C5-C6-N1	5.19	123.59	121.00
1	XA	1001	G	O5'-P-OP1	5.19	116.92	110.70
17	XQ	75	ARG	N-CA-CB	-5.19	101.26	110.60
35	YA	156	U	C2-N3-C4	5.19	130.11	127.00
35	YA	2604	U	N3-C4-O4	5.19	123.03	119.40
36	YB	53	A	N7-C8-N9	5.19	116.39	113.80
35	YA	325	G	C8-N9-C4	5.19	108.47	106.40
36	YB	77	U	C2-N1-C1'	5.19	123.92	117.70
1	QA	341	C	C2-N1-C1'	5.18	124.50	118.80
33	R8	46	ARG	CB-CA-C	-5.18	100.03	110.40
35	YA	2159	G	N3-C4-N9	-5.18	122.89	126.00
35	YA	2827	C	C6-N1-C1'	-5.18	114.58	120.80
1	QA	1008	C	C2-N1-C1'	5.18	124.50	118.80
35	RA	537	C	C2-N1-C1'	5.18	124.50	118.80
35	RA	1443	G	C8-N9-C4	-5.18	104.33	106.40
35	RA	2874	C	N1-C2-O2	5.18	122.01	118.90
36	RB	37	C	N3-C2-O2	-5.18	118.27	121.90
1	XA	626	U	C5-C6-N1	5.18	125.29	122.70
35	YA	528	A	C5-C6-N1	-5.18	115.11	117.70
35	YA	764	A	N1-C6-N6	-5.18	115.49	118.60
35	YA	708	C	C6-N1-C1'	-5.18	114.58	120.80
1	QA	180	U	N1-C2-O2	5.18	126.43	122.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	QA	883	C	C2-N1-C1'	5.18	124.50	118.80
35	RA	1708	C	C6-N1-C2	-5.18	118.23	120.30
1	XA	309	G	C8-N9-C4	-5.18	104.33	106.40
36	YB	27	C	N3-C2-O2	-5.18	118.27	121.90
5	QE	79	GLU	CG-CD-OE2	-5.18	107.95	118.30
1	XA	191(B)	G	N1-C6-O6	-5.18	116.79	119.90
1	XA	872	A	C5-N7-C8	-5.18	101.31	103.90
35	YA	140	A	C6-C5-N7	-5.18	128.68	132.30
35	YA	241	A	C8-N9-C4	-5.18	103.73	105.80
35	YA	2804	C	C6-N1-C2	-5.18	118.23	120.30
35	YA	2814	C	C2-N1-C1'	5.18	124.50	118.80
35	RA	1397	U	N1-C2-O2	-5.17	119.18	122.80
35	YA	1947	C	N3-C2-O2	-5.17	118.28	121.90
35	YA	2623	G	N3-C4-N9	5.17	129.10	126.00
1	QA	1517	G	C4-C5-N7	5.17	112.87	110.80
35	RA	2527	C	C2-N1-C1'	5.17	124.49	118.80
35	YA	527	C	C5-C4-N4	5.17	123.82	120.20
1	QA	1079	G	N1-C6-O6	-5.17	116.80	119.90
1	QA	1318	A	C8-N9-C4	5.17	107.87	105.80
35	YA	214	G	C4-C5-N7	-5.17	108.73	110.80
51	YV	52	VAL	N-CA-C	-5.17	97.04	111.00
16	QP	32	TYR	CB-CA-C	5.17	120.74	110.40
26	R1	82	LEU	CA-CB-CG	5.17	127.19	115.30
35	RA	2471	C	N1-C2-O2	5.17	122.00	118.90
1	XA	526	C	N1-C2-O2	5.17	122.00	118.90
1	XA	1447	G	C4-N9-C1'	5.17	133.22	126.50
35	YA	1332	G	C8-N9-C1'	-5.17	120.28	127.00
35	YA	1950	G	C5-C6-O6	-5.17	125.50	128.60
35	RA	2419	U	C6-N1-C2	-5.17	117.90	121.00
1	XA	1453	G	C8-N9-C1'	-5.17	120.28	127.00
35	YA	1886	C	C6-N1-C2	-5.17	118.23	120.30
35	YA	2527	C	C6-N1-C2	-5.17	118.23	120.30
40	YG	126	ASP	N-CA-CB	-5.17	101.30	110.60
1	QA	1453	G	N1-C2-N3	-5.17	120.80	123.90
2	QB	53	ARG	CD-NE-CZ	5.17	130.83	123.60
35	RA	987	G	N9-C4-C5	5.16	107.47	105.40
35	RA	2896	C	C6-N1-C1'	-5.16	114.61	120.80
1	XA	979	C	N3-C2-O2	-5.16	118.29	121.90
35	RA	1170	G	C8-N9-C4	-5.16	104.33	106.40
35	YA	1823	G	C5-C6-O6	5.16	131.70	128.60
35	YA	2430	A	C6-C5-N7	-5.16	128.69	132.30
35	YA	2444	G	C4-C5-N7	-5.16	108.73	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RA	856	C	C2'-C3'-O3'	5.16	121.96	113.70
12	XL	28	LYS	CA-CB-CG	5.16	124.75	113.40
1	QA	272	C	C6-N1-C2	-5.16	118.24	120.30
22	QW	22	G	O4'-C1'-N9	5.16	112.33	108.20
22	QW	68	C	C5-C6-N1	5.16	123.58	121.00
35	RA	1018	C	C6-N1-C2	-5.16	118.24	120.30
41	RH	4	ILE	N-CA-CB	-5.16	98.93	110.80
1	XA	54	C	C2-N1-C1'	5.16	124.47	118.80
35	YA	811	U	C6-N1-C2	5.16	124.09	121.00
35	YA	1823	G	C4-C5-N7	-5.16	108.74	110.80
1	QA	27	G	C8-N9-C4	-5.16	104.34	106.40
35	RA	2756	U	OP1-P-O3'	5.16	116.55	105.20
1	QA	267	C	C6-N1-C2	-5.16	118.24	120.30
1	QA	1260	C	C2-N1-C1'	5.16	124.47	118.80
35	RA	274	G	N7-C8-N9	5.16	115.68	113.10
35	YA	2212	A	N1-C6-N6	5.16	121.69	118.60
35	RA	537	C	C5-C6-N1	5.15	123.58	121.00
1	XA	1536	C	N1-C2-O2	5.15	121.99	118.90
22	XW	5	G	N3-C4-N9	5.15	129.09	126.00
35	YA	2232	U	N1-C2-N3	5.15	117.99	114.90
35	RA	355	G	N3-C4-C5	-5.15	126.02	128.60
37	RD	13	ARG	CG-CD-NE	5.15	122.62	111.80
22	XW	69	C	N1-C2-O2	5.15	121.99	118.90
1	QA	1254	C	N3-C4-C5	-5.15	119.84	121.90
13	QM	55	ARG	CG-CD-NE	-5.15	100.98	111.80
35	RA	198	C	C6-N1-C2	-5.15	118.24	120.30
35	RA	894	C	C2-N1-C1'	5.15	124.47	118.80
35	RA	1819	A	P-O3'-C3'	5.15	125.88	119.70
35	RA	2610	C	C6-N1-C2	5.15	122.36	120.30
35	RA	2645	G	C4-N9-C1'	5.15	133.20	126.50
1	XA	918	A	C8-N9-C4	-5.15	103.74	105.80
1	XA	974	A	C6-C5-N7	5.15	135.91	132.30
35	YA	197	A	C5-C6-N6	-5.15	119.58	123.70
1	QA	252	U	C2-N1-C1'	5.15	123.88	117.70
1	XA	775	G	N1-C6-O6	5.15	122.99	119.90
35	YA	2342	C	C2-N1-C1'	5.15	124.46	118.80
35	YA	2685	G	C4-C5-N7	-5.15	108.74	110.80
3	QC	107	GLN	C-N-CA	5.15	134.57	121.70
35	RA	1909	C	C2-N1-C1'	5.15	124.46	118.80
35	YA	1011	G	C4-N9-C1'	-5.15	119.81	126.50
35	YA	1638	C	C6-N1-C2	-5.15	118.24	120.30
11	QK	70	LYS	CA-CB-CG	5.15	124.72	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	QX	11	U	C2-N1-C1'	5.15	123.88	117.70
35	RA	1446	C	C6-N1-C2	-5.15	118.24	120.30
1	XA	394	G	C5-C6-O6	5.15	131.69	128.60
10	QJ	79	ARG	CA-CB-CG	-5.14	102.08	113.40
35	RA	654(Q)	C	C6-N1-C2	-5.14	118.24	120.30
35	RA	1210	A	N7-C8-N9	5.14	116.37	113.80
1	XA	722	A	N1-C6-N6	5.14	121.69	118.60
35	YA	1499	C	N1-C2-O2	5.14	121.99	118.90
35	YA	1920	C	C6-N1-C2	-5.14	118.24	120.30
35	YA	2342	C	C5-C6-N1	5.14	123.57	121.00
1	QA	801	U	N3-C2-O2	-5.14	118.60	122.20
11	QK	20	TYR	CG-CD2-CE2	-5.14	117.19	121.30
35	RA	2443	C	N3-C2-O2	-5.14	118.30	121.90
1	XA	1028	C	C2-N1-C1'	-5.14	113.14	118.80
35	YA	1566	A	N1-C6-N6	5.14	121.69	118.60
35	YA	686	G	C4-C5-N7	5.14	112.86	110.80
1	QA	486	U	C6-N1-C2	-5.14	117.92	121.00
1	QA	1373	G	C5-C6-O6	5.14	131.68	128.60
3	QC	82	GLU	CA-CB-CG	5.14	124.71	113.40
35	RA	1542	G	N1-C6-O6	-5.14	116.82	119.90
53	RX	48	LYS	CA-CB-CG	5.14	124.71	113.40
1	XA	21	G	C8-N9-C4	5.14	108.45	106.40
35	YA	1769	G	C8-N9-C4	-5.14	104.34	106.40
35	YA	1817	G	C2-N3-C4	5.14	114.47	111.90
50	YU	92	ARG	O-C-N	-5.14	114.48	122.70
1	QA	999	U	C5-C6-N1	5.14	125.27	122.70
1	QA	1229	A	O5'-P-OP2	-5.14	101.08	105.70
1	QA	1374	A	N1-C2-N3	5.14	131.87	129.30
22	QV	13	C	C5-C6-N1	5.14	123.57	121.00
35	RA	1253	A	C5-C6-N6	-5.14	119.59	123.70
35	RA	1528	A	C8-N9-C4	-5.14	103.75	105.80
35	YA	881	G	N3-C4-N9	5.14	129.08	126.00
35	YA	2177	C	C6-N1-C2	-5.14	118.25	120.30
35	YA	2454	G	C8-N9-C4	5.14	108.45	106.40
1	QA	1540	U	N1-C2-O2	5.13	126.39	122.80
4	QD	14	ARG	CD-NE-CZ	-5.13	116.41	123.60
35	RA	1043	C	C6-N1-C2	-5.13	118.25	120.30
35	RA	1779	U	C2-N1-C1'	5.13	123.86	117.70
35	RA	2094	G	N3-C4-C5	-5.13	126.03	128.60
1	XA	8	A	C8-N9-C4	5.13	107.85	105.80
35	YA	848	G	N3-C4-C5	-5.13	126.03	128.60
35	YA	1085	A	P-O3'-C3'	5.13	125.86	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	YB	78	A	C5-C6-N1	5.13	120.27	117.70
35	RA	2613	U	C5-C4-O4	5.13	128.98	125.90
1	XA	654	G	N9-C4-C5	5.13	107.45	105.40
22	XW	36	U	C6-N1-C2	-5.13	117.92	121.00
35	YA	788	A	N9-C4-C5	-5.13	103.75	105.80
35	YA	1102	C	C6-N1-C2	-5.13	118.25	120.30
35	YA	1496	A	C8-N9-C4	-5.13	103.75	105.80
35	RA	267	C	N1-C2-O2	5.13	121.98	118.90
35	RA	859	G	N7-C8-N9	-5.13	110.53	113.10
49	RT	6	LEU	CA-CB-CG	5.13	127.10	115.30
1	XA	610	G	C8-N9-C4	-5.13	104.35	106.40
35	RA	1143	A	N1-C2-N3	5.13	131.86	129.30
35	RA	2430	A	C8-N9-C4	5.13	107.85	105.80
35	YA	1012	U	C5-C6-N1	-5.13	120.14	122.70
35	YA	1835	G	N9-C4-C5	5.13	107.45	105.40
35	RA	69	C	C5-C6-N1	5.13	123.56	121.00
35	RA	388	G	N1-C6-O6	5.13	122.98	119.90
35	RA	1138	G	N3-C2-N2	-5.13	116.31	119.90
35	RA	1762	A	C8-N9-C1'	-5.13	118.47	127.70
35	RA	1776	G	C8-N9-C1'	-5.13	120.33	127.00
1	XA	330	C	C2-N1-C1'	5.13	124.44	118.80
35	YA	2312	U	O5'-P-OP1	-5.13	101.08	105.70
35	YA	2320	A	N7-C8-N9	5.13	116.36	113.80
1	QA	91	C	C6-N1-C2	-5.12	118.25	120.30
1	QA	36	C	C5-C6-N1	5.12	123.56	121.00
1	XA	354	G	N7-C8-N9	5.12	115.66	113.10
35	YA	647	G	C5-C6-N1	5.12	114.06	111.50
35	YA	650	C	C5-C6-N1	5.12	123.56	121.00
35	YA	2481	G	P-O3'-C3'	5.12	125.85	119.70
1	QA	442	C	C6-N1-C2	-5.12	118.25	120.30
1	QA	947	G	N1-C6-O6	5.12	122.97	119.90
35	RA	1614	A	N7-C8-N9	5.12	116.36	113.80
35	RA	2791	C	C5-C4-N4	5.12	123.78	120.20
35	YA	561	G	N1-C2-N2	-5.12	111.59	116.20
1	XA	486	U	N1-C2-O2	5.12	126.38	122.80
1	QA	1240	U	C2-N3-C4	-5.12	123.93	127.00
35	RA	141	A	C5-N7-C8	-5.12	101.34	103.90
1	XA	186(F)	C	N3-C4-C5	-5.12	119.85	121.90
11	XK	12	ARG	CA-CB-CG	5.12	124.66	113.40
35	YA	193	U	N3-C4-O4	5.12	122.98	119.40
35	YA	1404	C	N1-C2-O2	5.12	121.97	118.90
35	YA	1882	C	N3-C4-C5	-5.12	119.85	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RA	2569	G	C6-C5-N7	-5.12	127.33	130.40
35	YA	2755	C	C5-C6-N1	5.12	123.56	121.00
1	XA	488	C	C5-C6-N1	5.12	123.56	121.00
1	XA	793	U	N3-C2-O2	-5.12	118.62	122.20
35	YA	1834	U	N3-C4-O4	5.12	122.98	119.40
35	RA	943	U	N3-C4-O4	5.11	122.98	119.40
1	XA	92	G	C8-N9-C1'	-5.11	120.35	127.00
35	YA	1276	A	N7-C8-N9	5.11	116.36	113.80
35	RA	1505	C	C2-N1-C1'	5.11	124.42	118.80
35	RA	1964	G	N7-C8-N9	-5.11	110.54	113.10
35	RA	2804	C	C2-N1-C1'	5.11	124.42	118.80
35	YA	74	A	N3-C4-N9	-5.11	123.31	127.40
1	QA	525	C	N3-C4-N4	5.11	121.58	118.00
35	RA	2667	C	C6-N1-C2	-5.11	118.26	120.30
35	RA	2826	A	C6-C5-N7	-5.11	128.72	132.30
35	YA	1640	C	C2-N3-C4	5.11	122.46	119.90
35	YA	2391	G	C5-C6-O6	5.11	131.67	128.60
1	XA	35	G	N3-C4-C5	-5.11	126.05	128.60
1	QA	405	U	C2-N1-C1'	5.11	123.83	117.70
35	RA	837	C	C2-N1-C1'	5.11	124.42	118.80
35	RA	2250	G	C8-N9-C4	-5.11	104.36	106.40
35	RA	2602	A	C6-N1-C2	5.11	121.67	118.60
35	RA	2896	C	C2-N3-C4	5.11	122.45	119.90
1	XA	813	U	C5-C4-O4	-5.11	122.83	125.90
1	XA	974	A	C4-C5-C6	-5.11	114.45	117.00
1	XA	1521	G	N3-C4-N9	5.11	129.06	126.00
35	YA	1578	U	N3-C2-O2	-5.11	118.62	122.20
35	YA	1607	C	C5-C4-N4	-5.11	116.62	120.20
35	RA	2501	C	C6-N1-C1'	5.11	126.93	120.80
35	RA	2720	U	C5-C4-O4	5.11	128.96	125.90
35	RA	2861	G	C6-C5-N7	-5.11	127.34	130.40
1	XA	677	U	N1-C2-O2	5.11	126.37	122.80
35	YA	141	A	C5-C6-N1	-5.11	115.15	117.70
35	YA	1698	A	N7-C8-N9	5.11	116.35	113.80
1	XA	1301	U	O4'-C1'-N1	5.10	112.28	108.20
35	YA	1528	A	C5-N7-C8	-5.10	101.35	103.90
35	RA	2720	U	N1-C2-O2	5.10	126.37	122.80
39	RF	18	ARG	CG-CD-NE	-5.10	101.08	111.80
6	XF	28	ARG	CB-CG-CD	-5.10	98.33	111.60
22	XW	39	C	N1-C2-O2	5.10	121.96	118.90
35	YA	968	G	N3-C4-N9	5.10	129.06	126.00
36	YB	117	G	N1-C6-O6	-5.10	116.84	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RA	196	A	O4'-C1'-N9	5.10	112.28	108.20
1	XA	793	U	C5-C4-O4	5.10	128.96	125.90
1	QA	1182	G	OP2-P-O3'	5.10	116.41	105.20
35	RA	2062	A	N1-C6-N6	-5.10	115.54	118.60
35	RA	2604	U	C2-N1-C1'	5.10	123.82	117.70
35	YA	143	C	C2-N1-C1'	5.10	124.41	118.80
35	YA	2688	U	N1-C2-O2	5.10	126.37	122.80
1	QA	435	C	C2-N3-C4	5.10	122.45	119.90
1	QA	932	C	C6-N1-C2	-5.10	118.26	120.30
35	RA	1786	A	N9-C1'-C2'	5.10	120.62	114.00
35	RA	2615	U	N1-C2-O2	5.10	126.37	122.80
22	XV	22	G	C8-N9-C4	-5.10	104.36	106.40
1	QA	191(E)	G	C4-C5-N7	5.09	112.84	110.80
19	QS	5	LEU	CA-CB-CG	5.09	127.02	115.30
35	RA	2108	C	C2-N1-C1'	5.09	124.40	118.80
40	RG	139	LEU	CA-CB-CG	-5.09	103.58	115.30
35	YA	1478	G	C8-N9-C4	-5.09	104.36	106.40
35	YA	2056	G	N3-C4-N9	5.09	129.06	126.00
1	XA	1395	C	N1-C2-O2	5.09	121.96	118.90
1	QA	1067	A	C2-N3-C4	5.09	113.14	110.60
22	QW	68	C	C6-N1-C2	-5.09	118.26	120.30
35	RA	676	A	N3-C4-N9	-5.09	123.33	127.40
35	RA	704	G	C5-C6-O6	-5.09	125.55	128.60
35	RA	2559	C	C2-N3-C4	5.09	122.45	119.90
1	XA	863	U	C5-C4-O4	5.09	128.96	125.90
35	YA	2459	A	C8-N9-C4	5.09	107.84	105.80
35	YA	2734	A	N1-C6-N6	5.09	121.65	118.60
36	YB	47	C	N3-C2-O2	-5.09	118.33	121.90
53	YX	24	GLY	N-CA-C	-5.09	100.37	113.10
35	RA	375	C	C6-N1-C2	-5.09	118.26	120.30
35	RA	1040	C	C6-N1-C2	-5.09	118.27	120.30
55	RZ	161	VAL	CB-CA-C	5.09	121.07	111.40
26	Y1	80	LEU	C-N-CA	5.09	134.42	121.70
35	YA	182	A	C8-N9-C4	-5.09	103.76	105.80
35	YA	1264	G	C8-N9-C4	-5.09	104.36	106.40
35	YA	2112	G	C8-N9-C1'	5.09	133.62	127.00
35	YA	2873	A	N1-C2-N3	5.09	131.84	129.30
36	YB	118	G	N3-C2-N2	-5.09	116.34	119.90
1	QA	1127	G	N3-C4-C5	-5.09	126.06	128.60
35	RA	1824	G	N9-C4-C5	-5.09	103.36	105.40
35	RA	2318	G	C4-N9-C1'	5.09	133.12	126.50
22	QW	22	G	C8-N9-C1'	5.09	133.61	127.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RA	654(Q)	C	C2-N1-C1'	5.09	124.39	118.80
35	RA	887	A	C8-N9-C4	-5.09	103.77	105.80
35	RA	904	C	C2-N1-C1'	5.09	124.39	118.80
1	XA	74	C	C6-N1-C1'	-5.09	114.70	120.80
1	XA	1008	C	C5-C6-N1	5.09	123.54	121.00
35	YA	139	G	C6-C5-N7	5.09	133.45	130.40
35	YA	556	G	C8-N9-C4	-5.09	104.36	106.40
35	YA	1678	G	N3-C4-C5	5.09	131.14	128.60
35	YA	1775	U	C5-C4-O4	-5.09	122.85	125.90
35	YA	1896	G	C8-N9-C4	-5.09	104.37	106.40
1	QA	1008	C	C6-N1-C2	-5.08	118.27	120.30
1	QA	1492	A	O5'-P-OP1	5.08	116.80	110.70
35	RA	2863	C	C2-N1-C1'	5.08	124.39	118.80
22	XW	12	G	C8-N9-C4	-5.08	104.37	106.40
35	YA	171	G	N9-C4-C5	-5.08	103.37	105.40
35	YA	707	G	C4-N9-C1'	5.08	133.11	126.50
35	YA	1365	A	C8-N9-C4	5.08	107.83	105.80
1	QA	1539	C	C6-N1-C2	-5.08	118.27	120.30
10	QJ	54	PHE	N-CA-CB	5.08	119.75	110.60
35	RA	74	A	C5-N7-C8	-5.08	101.36	103.90
35	RA	179	G	N3-C2-N2	-5.08	116.34	119.90
35	RA	889	C	C6-N1-C2	-5.08	118.27	120.30
1	XA	33	A	C8-N9-C4	-5.08	103.77	105.80
35	YA	385	C	C6-N1-C2	-5.08	118.27	120.30
35	YA	1915	U	N1-C2-O2	5.08	126.36	122.80
35	YA	2294	C	C6-N1-C2	-5.08	118.27	120.30
35	RA	2062	A	C2-N3-C4	5.08	113.14	110.60
1	XA	1001	G	OP1-P-OP2	-5.08	111.98	119.60
1	XA	1150	U	C5-C6-N1	5.08	125.24	122.70
1	QA	623	C	N1-C2-O2	5.08	121.95	118.90
1	QA	971	G	C4-C5-N7	-5.08	108.77	110.80
1	QA	1007	C	N1-C2-O2	5.08	121.95	118.90
35	RA	1406	U	C5-C6-N1	5.08	125.24	122.70
35	RA	2092	U	N1-C2-N3	-5.08	111.85	114.90
35	YA	620	G	C8-N9-C4	-5.08	104.37	106.40
35	RA	2347	C	C2-N1-C1'	5.08	124.39	118.80
35	YA	273	G	C2-N3-C4	5.08	114.44	111.90
1	QA	18	C	C5-C6-N1	5.08	123.54	121.00
22	QV	34	C	C2-N3-C4	5.08	122.44	119.90
30	R5	48	GLU	CB-CA-C	-5.08	100.25	110.40
35	RA	2189	U	N1-C2-O2	5.08	126.35	122.80
35	YA	774	A	N1-C6-N6	5.08	121.64	118.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	YA	1299	G	C4-C5-N7	5.08	112.83	110.80
35	YA	2392	A	C5-C6-N6	-5.08	119.64	123.70
22	QV	59	A	C8-N9-C4	-5.07	103.77	105.80
35	RA	248	G	C5-C6-O6	-5.07	125.56	128.60
35	RA	1327	C	N1-C2-O2	5.07	121.94	118.90
41	RH	153	LYS	N-CA-C	5.07	124.70	111.00
43	RN	127	ASP	C-N-CA	-5.07	109.02	121.70
35	YA	1143	A	C5-N7-C8	-5.07	101.36	103.90
54	YY	50	ARG	CG-CD-NE	5.07	122.46	111.80
35	RA	2490	G	N1-C6-O6	5.07	122.94	119.90
27	Y2	69	ARG	CB-CA-C	-5.07	100.26	110.40
35	YA	2069	G	N3-C2-N2	-5.07	116.35	119.90
35	RA	987	G	C8-N9-C4	-5.07	104.37	106.40
1	XA	315	A	P-O3'-C3'	5.07	125.78	119.70
1	XA	1007	C	C2-N3-C4	5.07	122.44	119.90
35	YA	928	G	C8-N9-C4	-5.07	104.37	106.40
35	YA	1482	U	C6-N1-C1'	-5.07	114.10	121.20
35	YA	1930	G	C8-N9-C4	5.07	108.43	106.40
35	RA	198	C	N3-C4-C5	-5.07	119.87	121.90
35	RA	2726	U	N1-C2-N3	5.07	117.94	114.90
1	XA	596	C	N3-C2-O2	-5.07	118.35	121.90
1	QA	79	G	N1-C2-N2	5.07	120.76	116.20
1	QA	1051	C	C6-N1-C2	-5.07	118.27	120.30
35	RA	1342	A	C5-C6-N1	-5.07	115.17	117.70
35	RA	1774	C	C5-C6-N1	5.07	123.53	121.00
35	YA	2142	C	C6-N1-C2	-5.07	118.27	120.30
35	YA	2506	U	C5-C6-N1	-5.07	120.17	122.70
1	QA	556	C	C5-C6-N1	5.07	123.53	121.00
1	QA	971	G	C8-N9-C1'	5.07	133.59	127.00
1	QA	1157	A	P-O3'-C3'	5.07	125.78	119.70
13	QM	67	GLU	C-N-CA	-5.07	111.66	122.30
35	RA	1551	C	C6-N1-C2	-5.07	118.27	120.30
35	RA	2602	A	C5-C6-N1	-5.07	115.17	117.70
36	YB	31	C	C2-N3-C4	5.07	122.43	119.90
35	YA	2474	C	C6-N1-C2	-5.06	118.27	120.30
1	QA	37	U	C6-N1-C2	-5.06	117.96	121.00
1	QA	961	U	O5'-P-OP1	-5.06	101.14	105.70
13	QM	3	ARG	CB-CA-C	-5.06	100.27	110.40
35	RA	1846	G	O4'-C1'-N9	5.06	112.25	108.20
35	RA	2473	U	N3-C2-O2	-5.06	118.66	122.20
35	RA	2873	A	C8-N9-C1'	-5.06	118.59	127.70
55	RZ	41	LEU	CA-CB-CG	5.06	126.94	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	QA	1306	A	C5-N7-C8	-5.06	101.37	103.90
10	QJ	75	ILE	N-CA-C	5.06	124.67	111.00
35	RA	1980	G	N3-C4-C5	-5.06	126.07	128.60
35	RA	2720	U	C2-N3-C4	5.06	130.04	127.00
35	YA	812	C	C5-C6-N1	5.06	123.53	121.00
1	QA	108	G	N7-C8-N9	5.06	115.63	113.10
35	RA	153	C	C6-N1-C2	-5.06	118.28	120.30
35	RA	856	C	N3-C4-C5	-5.06	119.88	121.90
35	RA	1338	G	N3-C4-C5	-5.06	126.07	128.60
35	RA	2311	A	C2-N3-C4	5.06	113.13	110.60
35	RA	2683	C	C2-N1-C1'	5.06	124.37	118.80
1	QA	563	A	C4-N9-C1'	5.06	135.40	126.30
1	QA	810	C	C2-N1-C1'	5.06	124.36	118.80
22	QW	71	C	C5-C6-N1	5.06	123.53	121.00
35	RA	416	C	C5-C6-N1	5.06	123.53	121.00
35	RA	457	A	C8-N9-C4	-5.06	103.78	105.80
35	RA	1406	U	C6-N1-C1'	-5.06	114.12	121.20
35	RA	1824	G	C4-C5-N7	5.06	112.82	110.80
35	RA	1881	C	C2-N3-C4	5.06	122.43	119.90
1	XA	1402	C	C6-N1-C2	-5.06	118.28	120.30
1	XA	1027	C	C2-N1-C1'	5.06	124.36	118.80
35	YA	9	U	C2-N1-C1'	5.06	123.77	117.70
1	QA	1006	C	C5-C6-N1	5.05	123.53	121.00
11	QK	107	SER	N-CA-CB	5.05	118.08	110.50
13	QM	3	ARG	CA-CB-CG	5.05	124.52	113.40
35	RA	530	G	C8-N9-C4	5.05	108.42	106.40
35	RA	1267	U	C2-N1-C1'	5.05	123.76	117.70
1	XA	308	C	C6-N1-C2	-5.05	118.28	120.30
35	YA	2559	C	N3-C2-O2	-5.05	118.36	121.90
35	RA	2118	U	C6-N1-C1'	-5.05	114.12	121.20
29	Y4	61	ARG	CB-CA-C	5.05	120.51	110.40
35	YA	592	G	N3-C4-C5	-5.05	126.07	128.60
1	QA	1127	G	N3-C4-N9	5.05	129.03	126.00
35	RA	138	G	C2-N3-C4	5.05	114.43	111.90
35	RA	1326	U	N1-C2-O2	5.05	126.34	122.80
35	RA	2092	U	C6-N1-C2	5.05	124.03	121.00
35	RA	2550	G	N1-C6-O6	5.05	122.93	119.90
35	YA	1509	C	C6-N1-C2	-5.05	118.28	120.30
35	YA	1658	C	C5-C6-N1	5.05	123.53	121.00
1	QA	1068	G	N7-C8-N9	5.05	115.62	113.10
35	RA	1395	A	O4'-C1'-N9	5.05	112.24	108.20
37	RD	263	ARG	CG-CD-NE	-5.05	101.19	111.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	XW	3	C	C5-C6-N1	5.05	123.53	121.00
35	YA	915	C	C6-N1-C2	-5.05	118.28	120.30
35	YA	1880	C	C2-N1-C1'	5.05	124.35	118.80
35	RA	2553	G	N1-C2-N2	-5.05	111.66	116.20
35	RA	2571	C	C2-N1-C1'	5.05	124.35	118.80
1	XA	283	C	N3-C2-O2	-5.05	118.37	121.90
35	YA	1439	A	N1-C6-N6	5.05	121.63	118.60
35	RA	1407	C	N3-C2-O2	-5.05	118.37	121.90
35	RA	2099	U	C2-N1-C1'	5.05	123.76	117.70
1	XA	634	C	C6-N1-C2	-5.05	118.28	120.30
35	YA	2556	C	N1-C2-O2	5.05	121.93	118.90
35	YA	238	C	C6-N1-C2	-5.04	118.28	120.30
35	RA	1544	C	C6-N1-C2	-5.04	118.28	120.30
35	RA	1805	U	N1-C2-N3	5.04	117.93	114.90
35	RA	2089	U	C5-C6-N1	5.04	125.22	122.70
10	QJ	21	GLN	C-N-CA	-5.04	109.10	121.70
13	QM	19	LEU	CB-CG-CD1	-5.04	102.43	111.00
1	XA	960	U	N1-C2-O2	5.04	126.33	122.80
1	XA	1348	U	N1-C2-O2	5.04	126.33	122.80
35	YA	141	A	C6-C5-N7	-5.04	128.77	132.30
35	YA	239	U	N3-C2-O2	-5.04	118.67	122.20
35	RA	172	C	C6-N1-C2	-5.04	118.28	120.30
41	RH	116	GLU	CA-CB-CG	5.04	124.49	113.40
35	YA	2137	C	C5-C6-N1	5.04	123.52	121.00
1	QA	74	C	C6-N1-C2	-5.04	118.28	120.30
35	RA	1266	G	C8-N9-C4	5.04	108.42	106.40
35	RA	2545	G	N3-C4-C5	-5.04	126.08	128.60
35	YA	1913	A	C2-N3-C4	5.04	113.12	110.60
35	YA	2762	G	N3-C4-C5	-5.04	126.08	128.60
35	RA	101	G	OP1-P-O3'	5.04	116.28	105.20
35	RA	1152	C	C2-N3-C4	5.04	122.42	119.90
35	RA	2063	C	N3-C2-O2	-5.04	118.37	121.90
1	XA	31	G	C4-N9-C1'	5.04	133.05	126.50
9	XI	53	VAL	C-N-CA	5.04	134.29	121.70
35	YA	2529	G	C4-N9-C1'	5.04	133.05	126.50
35	RA	2508	G	C6-C5-N7	-5.04	127.38	130.40
35	YA	1784	A	N1-C6-N6	-5.04	115.58	118.60
35	YA	2688	U	N3-C4-O4	-5.04	115.88	119.40
35	RA	2448	A	C8-N9-C4	5.03	107.81	105.80
35	RA	2861	G	C5-C6-O6	-5.03	125.58	128.60
22	XW	43	A	C6-N1-C2	-5.03	115.58	118.60
35	YA	1088	A	N7-C8-N9	5.03	116.32	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	YA	2501	C	N3-C4-C5	5.03	123.91	121.90
35	YA	270(B)	A	C8-N9-C4	-5.03	103.79	105.80
35	RA	561	G	C8-N9-C1'	5.03	133.54	127.00
1	XA	810	C	N1-C2-O2	5.03	121.92	118.90
22	XW	39	C	C6-N1-C2	-5.03	118.29	120.30
2	QB	207	ALA	C-N-CA	5.03	134.27	121.70
35	RA	729	G	N3-C2-N2	-5.03	116.38	119.90
1	XA	209	U	N3-C2-O2	-5.03	118.68	122.20
1	XA	468	A	N9-C4-C5	-5.03	103.79	105.80
1	XA	500	G	N3-C4-N9	5.03	129.02	126.00
35	YA	436	C	C6-N1-C2	-5.03	118.29	120.30
35	YA	656	G	C8-N9-C4	5.03	108.41	106.40
35	YA	1376	C	N3-C4-C5	5.03	123.91	121.90
35	RA	248	G	C4-C5-N7	5.03	112.81	110.80
35	RA	1909	C	C6-N1-C2	-5.03	118.29	120.30
35	RA	68	G	N3-C4-C5	-5.02	126.09	128.60
35	RA	308	G	N9-C4-C5	-5.02	103.39	105.40
35	YA	654(V)	A	N1-C6-N6	-5.02	115.59	118.60
35	YA	726	G	C8-N9-C4	5.02	108.41	106.40
35	RA	86	C	C2-N1-C1'	5.02	124.32	118.80
10	XJ	7	LYS	CB-CA-C	5.02	120.44	110.40
28	Y3	35	ARG	N-CA-CB	-5.02	101.56	110.60
35	YA	156	U	C2-N1-C1'	5.02	123.73	117.70
35	YA	258	G	C4-C5-N7	-5.02	108.79	110.80
35	YA	1652	A	C5-N7-C8	-5.02	101.39	103.90
3	QC	164	ARG	CG-CD-NE	5.02	122.34	111.80
35	YA	1024	G	N7-C8-N9	5.02	115.61	113.10
1	QA	330	C	C5-C6-N1	5.02	123.51	121.00
35	RA	857	C	C6-N1-C2	-5.02	118.29	120.30
35	RA	1143	A	C4-C5-N7	5.02	113.21	110.70
35	RA	1909	C	C5-C6-N1	5.02	123.51	121.00
1	XA	1000	A	C5-N7-C8	-5.02	101.39	103.90
35	YA	277	C	C2-N3-C4	5.02	122.41	119.90
35	YA	1655	A	N9-C4-C5	-5.02	103.79	105.80
38	YE	72	VAL	C-N-CA	-5.02	109.15	121.70
35	RA	920	G	C8-N9-C4	5.02	108.41	106.40
35	RA	2778	A	C8-N9-C4	5.02	107.81	105.80
35	RA	2839	G	N1-C6-O6	5.02	122.91	119.90
35	RA	2859	G	P-O3'-C3'	5.02	125.72	119.70
1	XA	1344	C	C5-C6-N1	5.02	123.51	121.00
35	YA	1190	G	C8-N9-C4	-5.02	104.39	106.40
35	YA	1762	A	N7-C8-N9	5.02	116.31	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	QA	233	C	C6-N1-C2	-5.02	118.29	120.30
1	QA	812	C	N3-C2-O2	-5.02	118.39	121.90
1	QA	1505	G	N3-C4-N9	-5.02	122.99	126.00
35	RA	355	G	N3-C4-N9	5.02	129.01	126.00
35	RA	1764	G	N9-C4-C5	5.01	107.41	105.40
46	RQ	25	ASP	CB-CG-OD1	5.01	122.81	118.30
35	YA	856	C	N3-C2-O2	-5.01	118.39	121.90
1	QA	108	G	C8-N9-C4	-5.01	104.39	106.40
7	QG	38	LEU	CA-CB-CG	5.01	126.83	115.30
35	YA	265	A	C4-C5-N7	5.01	113.20	110.70
35	YA	2508	G	N3-C2-N2	-5.01	116.39	119.90
18	QR	26	LEU	CA-CB-CG	5.01	126.82	115.30
35	RA	248	G	C6-C5-N7	-5.01	127.39	130.40
35	RA	270(U)	C	C6-N1-C2	-5.01	118.30	120.30
1	XA	1502	A	C4-N9-C1'	5.01	135.32	126.30
35	YA	784	A	C5-C6-N6	5.01	127.71	123.70
35	YA	793	A	C8-N9-C1'	5.01	136.72	127.70
35	YA	2027	G	N3-C4-C5	-5.01	126.09	128.60
35	RA	217	G	N1-C6-O6	-5.01	116.89	119.90
35	RA	481	G	O4'-C1'-N9	5.01	112.21	108.20
35	YA	1787	A	N1-C6-N6	-5.01	115.59	118.60
1	QA	1290	G	C8-N9-C4	-5.01	104.40	106.40
13	QM	69	GLU	CB-CA-C	5.01	120.41	110.40
35	RA	535	C	C6-N1-C2	-5.01	118.30	120.30
35	YA	1377	G	C2-N3-C4	-5.01	109.40	111.90
35	YA	2163	C	C5-C6-N1	5.01	123.50	121.00
35	RA	2604	U	N3-C2-O2	-5.00	118.70	122.20
1	XA	1200	C	N1-C2-O2	5.00	121.90	118.90
35	YA	193	U	C2-N1-C1'	5.00	123.71	117.70
35	YA	1043	C	C6-N1-C2	-5.00	118.30	120.30
35	YA	2779	U	O4'-C1'-N1	5.00	112.20	108.20
35	RA	945	A	C5-C6-N6	-5.00	119.70	123.70
35	RA	2704	C	N1-C2-O2	5.00	121.90	118.90
1	XA	877	C	C6-N1-C2	-5.00	118.30	120.30
35	YA	2808	U	N3-C2-O2	-5.00	118.70	122.20
1	QA	163	C	C6-N1-C2	-5.00	118.30	120.30
1	QA	647	C	C6-N1-C2	-5.00	118.30	120.30
1	QA	1416	G	C5-C6-N1	5.00	114.00	111.50
35	RA	587	C	C6-N1-C2	-5.00	118.30	120.30
35	RA	2441	C	N1-C2-O2	5.00	121.90	118.90
35	YA	399	G	C5-C6-N1	5.00	114.00	111.50
35	YA	1407	C	C6-N1-C1'	-5.00	114.80	120.80

There are no chirality outliers.

All (56) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	QB	114	ARG	Peptide
2	QB	131	PRO	Peptide
2	QB	153	ARG	Peptide
2	QB	217	ARG	Sidechain
3	QC	35	GLU	Sidechain
3	QC	38	ARG	Sidechain
10	QJ	35	SER	Peptide
13	QM	66	LEU	Peptide
13	QM	67	GLU	Mainchain
14	QN	26	ARG	Sidechain
18	QR	46	GLU	Sidechain
28	R3	3	ARG	Mainchain
29	R4	34	GLU	Sidechain
34	R9	4	ARG	Sidechain
37	RD	183	ARG	Sidechain
38	RE	146	THR	Peptide
38	RE	17	ASP	Peptide
41	RH	3	ARG	Mainchain
41	RH	58	GLU	Peptide
41	RH	79	VAL	Peptide
42	RI	116	LEU	Peptide
42	RI	13	GLY	Mainchain
42	RI	27	ARG	Sidechain
43	RN	126	PRO	Mainchain
45	RP	147	LEU	Peptide
45	RP	7	ARG	Sidechain
46	RQ	5	ARG	Sidechain
48	RS	10	ARG	Sidechain
49	RT	110	ILE	Peptide
55	RZ	161	VAL	Mainchain
2	XB	30	ARG	Sidechain
2	XB	42	ILE	Peptide
3	XC	107	GLN	Peptide
4	XD	167	GLY	Peptide
7	XG	95	ARG	Sidechain
10	XJ	29	ARG	Peptide
10	XJ	98	ILE	Peptide
12	XL	104	VAL	Peptide
12	XL	53	ARG	Sidechain
12	XL	59	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
18	XR	53	ARG	Sidechain
18	XR	54	ARG	Sidechain
19	XS	23	ASN	Peptide
27	Y2	14	ARG	Sidechain
27	Y2	70	GLN	Peptide
27	Y2	71	ASN	Peptide
29	Y4	39	CYS	Mainchain
29	Y4	55	ARG	Peptide
29	Y4	61	ARG	Sidechain
38	YE	146	THR	Peptide
40	YG	180	PHE	Sidechain
41	YH	51	ARG	Mainchain,Peptide
42	YI	100	ALA	Mainchain
42	YI	33	ARG	Sidechain
50	YU	92	ARG	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	QA	32452	0	16383	225	0
1	XA	32389	0	16350	231	0
2	QB	1907	0	1958	58	0
2	XB	1915	0	1969	82	0
3	QC	1605	0	1668	46	0
3	XC	1605	0	1668	30	0
4	QD	1703	0	1766	30	0
4	XD	1703	0	1767	43	0
5	QE	1155	0	1213	28	0
5	XE	1155	0	1213	18	0
6	QF	843	0	857	7	0
6	XF	843	0	857	16	0
7	QG	1257	0	1296	42	0
7	XG	1257	0	1296	25	0
8	QH	1108	0	1165	31	0
8	XH	1108	0	1165	18	0
9	QI	1010	0	1037	49	0
9	XI	998	0	1024	29	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	QJ	801	0	849	72	0
10	XJ	777	0	816	29	0
11	QK	885	0	904	18	0
11	XK	864	0	881	14	0
12	QL	975	0	1062	24	0
12	XL	956	0	1046	32	0
13	QM	955	0	1021	78	0
13	XM	946	0	1007	43	0
14	QN	492	0	530	5	0
14	XN	492	0	529	16	0
15	QO	734	0	771	6	0
15	XO	729	0	768	16	0
16	QP	705	0	725	11	0
16	XP	705	0	725	12	0
17	QQ	834	0	904	12	0
17	XQ	834	0	904	16	0
18	QR	574	0	644	6	0
18	XR	574	0	644	7	0
19	QS	665	0	686	47	0
19	XS	665	0	686	18	0
20	QT	763	0	861	10	0
20	XT	763	0	861	30	0
21	QU	217	0	234	6	0
21	XU	217	0	234	7	0
22	QV	1640	0	837	2	0
22	QW	1640	0	837	19	0
22	XV	1640	0	837	7	0
22	XW	1640	0	837	8	0
23	QX	370	0	186	3	0
23	XX	370	0	186	5	0
24	QY	723	0	713	37	0
24	QZ	723	0	713	81	0
24	XY	723	0	713	21	0
24	XZ	723	0	713	55	0
25	R0	643	0	667	23	0
25	Y0	648	0	672	14	0
26	R1	763	0	848	23	0
26	Y1	763	0	848	10	0
27	R2	581	0	629	8	0
27	Y2	581	0	629	18	0
28	R3	469	0	518	8	0
28	Y3	469	0	518	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	R4	565	0	561	32	0
29	Y4	565	0	557	25	0
30	R5	459	0	480	8	0
30	Y5	459	0	480	3	0
31	R6	453	0	475	11	0
31	Y6	453	0	474	4	0
32	R7	409	0	454	5	0
32	Y7	418	0	467	5	0
33	R8	517	0	582	12	0
33	Y8	517	0	582	20	0
34	R9	307	0	336	15	0
34	Y9	307	0	336	7	0
35	RA	62266	0	31389	339	0
35	YA	61981	0	31240	292	0
36	RB	2617	0	1328	15	0
36	YB	2617	0	1328	6	0
37	RD	2115	0	2195	69	0
37	YD	2135	0	2221	25	0
38	RE	1568	0	1634	50	0
38	YE	1563	0	1629	41	0
39	RF	1585	0	1632	25	0
39	YF	1585	0	1631	35	0
40	RG	1474	0	1535	82	0
40	YG	1474	0	1535	44	0
41	RH	1336	0	1418	121	0
41	YH	1336	0	1418	29	0
42	RI	1131	0	1218	76	0
42	YI	1136	0	1223	44	0
43	RN	1104	0	1180	23	0
43	YN	1104	0	1180	21	0
44	RO	933	0	996	18	0
44	YO	933	0	996	21	0
45	RP	1145	0	1228	23	0
45	YP	1122	0	1206	15	0
46	RQ	1107	0	1166	26	0
46	YQ	1122	0	1179	21	0
47	RR	960	0	1021	15	0
47	YR	960	0	1020	19	0
48	RS	882	0	943	38	0
48	YS	882	0	943	17	0
49	RT	1141	0	1202	34	0
49	YT	1141	0	1202	37	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	RU	964	0	1022	10	0
50	YU	964	0	1022	37	0
51	RV	779	0	852	20	0
51	YV	779	0	852	50	0
52	RW	900	0	964	10	0
52	YW	900	0	964	17	0
53	RX	725	0	778	13	0
53	YX	725	0	778	7	0
54	RY	818	0	913	14	0
54	YY	818	0	913	12	0
55	RZ	1461	0	1493	44	0
55	YZ	1461	0	1493	58	0
56	ZA	74	0	51	0	0
56	ZB	74	0	51	1	0
57	QA	87	0	0	0	0
57	QE	1	0	0	0	0
57	QV	3	0	0	0	0
57	R0	2	0	0	0	0
57	R5	1	0	0	0	0
57	RA	305	0	0	0	0
57	RB	3	0	0	0	0
57	RD	1	0	0	0	0
57	RE	2	0	0	0	0
57	RN	1	0	0	0	0
57	RO	1	0	0	0	0
57	RP	1	0	0	0	0
57	RQ	1	0	0	0	0
57	RR	1	0	0	0	0
57	XA	106	0	0	0	0
57	XD	1	0	0	0	0
57	XE	1	0	0	0	0
57	XF	1	0	0	0	0
57	XL	1	0	0	0	0
57	XV	4	0	0	0	0
57	Y5	1	0	0	0	0
57	Y9	1	0	0	0	0
57	YA	329	0	0	0	0
57	YB	6	0	0	0	0
57	YD	2	0	0	0	0
57	YE	4	0	0	0	0
57	YG	1	0	0	0	0
57	YO	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	YP	1	0	0	0	0
57	YQ	1	0	0	0	0
57	YR	1	0	0	0	0
57	YS	1	0	0	0	0
57	YV	1	0	0	0	0
58	QD	8	0	0	0	0
58	XD	8	0	0	0	0
59	QN	1	0	0	0	0
59	R6	1	0	0	0	0
59	R9	1	0	0	0	0
59	XN	1	0	0	0	0
59	Y6	1	0	0	0	0
60	QX	26	0	11	5	0
60	XX	26	0	11	2	0
All	All	298517	0	202833	3434	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 7.

All (3434) 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)
5:QE:90:VAL:CG1	5:QE:90:VAL:CB	1.74	1.63
2:XB:137:ARG:CD	2:XB:137:ARG:CG	1.77	1.62
49:RT:3:ARG:CD	49:RT:3:ARG:CG	1.76	1.62
13:QM:67:GLU:CG	13:QM:67:GLU:CB	1.74	1.62
55:YZ:14:LYS:CA	55:YZ:14:LYS:CB	1.75	1.62
2:XB:137:ARG:CG	2:XB:137:ARG:CB	1.78	1.61
3:QC:35:GLU:CB	3:QC:35:GLU:CG	1.74	1.61
24:XZ:48:LEU:CB	24:XZ:52:LEU:HG	1.25	1.57
19:QS:41:VAL:CG1	19:QS:42:PRO:HD2	1.34	1.56
49:RT:3:ARG:CA	49:RT:3:ARG:CB	1.87	1.52
10:QJ:6:ILE:CD1	10:QJ:98:ILE:HA	1.41	1.51
55:YZ:14:LYS:CG	55:YZ:14:LYS:CB	1.87	1.49
13:QM:41:PRO:CA	13:QM:41:PRO:N	1.70	1.49
24:XZ:48:LEU:HB3	24:XZ:52:LEU:CG	1.41	1.48
42:RI:8:PRO:CA	42:RI:8:PRO:N	1.70	1.47
41:RH:8:PRO:CG	41:RH:69:ARG:HD3	1.44	1.46
19:QS:41:VAL:HG12	19:QS:42:PRO:CD	1.47	1.42
41:RH:8:PRO:N	41:RH:8:PRO:CA	1.70	1.41
40:YG:112:PRO:CD	40:YG:112:PRO:N	1.69	1.38

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:YH:10:PRO:CA	41:YH:10:PRO:N	1.69	1.35
42:YI:92:VAL:HB	42:YI:120:ILE:CG2	1.55	1.35
12:XL:47:LYS:CG	12:XL:48:PRO:HD2	1.53	1.35
40:YG:179:PRO:CA	40:YG:179:PRO:N	1.69	1.33
29:R4:41:PRO:CA	29:R4:41:PRO:N	1.70	1.32
13:QM:10:PRO:N	13:QM:10:PRO:CA	1.70	1.29
19:QS:41:VAL:CG1	19:QS:42:PRO:CD	2.06	1.29
10:QJ:8:LEU:CD1	10:QJ:96:ILE:HA	1.61	1.28
44:YO:68:GLU:OE1	44:YO:78:ARG:HD3	1.28	1.28
10:QJ:8:LEU:HD11	10:QJ:96:ILE:CG2	1.64	1.27
51:RV:49:THR:OG1	51:RV:50:PRO:HD3	1.14	1.26
37:RD:6:PHE:CE1	37:RD:13:ARG:NH2	2.02	1.26
60:XX:101:A3P:C1'	60:XX:101:A3P:O4'	1.67	1.25
2:XB:87:ARG:NH1	2:XB:233:SER:HB2	1.51	1.25
51:YV:49:THR:OG1	51:YV:50:PRO:HD3	1.26	1.25
9:QI:19:LEU:HG	9:QI:59:PHE:CE1	1.74	1.22
12:XL:47:LYS:CB	12:XL:48:PRO:HD2	1.72	1.19
7:XG:68:ASN:O	7:XG:138:LYS:HE2	1.43	1.19
24:XZ:48:LEU:CB	24:XZ:52:LEU:CG	2.09	1.18
60:QX:101:A3P:C1'	60:QX:101:A3P:O4'	1.66	1.17
41:RH:10:PRO:HG3	41:RH:49:VAL:HA	1.21	1.17
41:RH:8:PRO:HG3	41:RH:69:ARG:CD	1.73	1.17
51:RV:49:THR:OG1	51:RV:50:PRO:CD	1.93	1.16
9:QI:50:LEU:HD23	9:QI:53:VAL:HG11	1.26	1.16
41:RH:8:PRO:CG	41:RH:69:ARG:CD	2.24	1.16
38:RE:73:GLU:HG2	38:RE:74:PRO:CD	1.74	1.16
42:YI:92:VAL:HB	42:YI:120:ILE:HG22	1.20	1.15
41:RH:8:PRO:HG3	41:RH:69:ARG:HD3	1.24	1.15
51:YV:52:VAL:CG2	51:YV:55:ALA:HB3	1.76	1.15
19:QS:55:LYS:NZ	24:QZ:36:ARG:HH22	1.45	1.15
10:QJ:8:LEU:CD1	10:QJ:96:ILE:HG22	1.76	1.14
24:XZ:48:LEU:O	24:XZ:52:LEU:HB2	1.48	1.13
2:XB:87:ARG:HH12	2:XB:233:SER:CB	1.60	1.13
2:XB:87:ARG:NH1	2:XB:233:SER:CB	2.11	1.13
41:RH:35:VAL:HG11	41:RH:71:LEU:HD13	1.13	1.12
10:QJ:8:LEU:HD11	10:QJ:96:ILE:HG22	1.15	1.12
38:RE:103:ASP:OD2	38:RE:201:THR:HA	1.47	1.11
10:QJ:6:ILE:HD12	10:QJ:98:ILE:HA	1.18	1.11
33:Y8:26:LYS:HG2	33:Y8:48:PHE:HD2	1.13	1.10
24:QZ:43:GLY:HA2	24:QZ:59:ARG:NE	1.65	1.09
10:QJ:6:ILE:HD11	10:QJ:98:ILE:HA	1.17	1.09

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:XL:18:VAL:HG11	12:XL:20:LYS:HE3	1.31	1.09
41:RH:8:PRO:HG2	41:RH:69:ARG:HD3	1.27	1.09
10:QJ:6:ILE:HD12	10:QJ:97:GLU:O	1.48	1.09
24:XZ:48:LEU:HB3	24:XZ:52:LEU:CD2	1.82	1.09
10:QJ:8:LEU:HD11	10:QJ:96:ILE:CB	1.81	1.09
37:RD:76:PRO:CA	37:RD:118:VAL:HG23	1.84	1.08
10:QJ:8:LEU:HD11	10:QJ:96:ILE:CA	1.84	1.08
10:QJ:8:LEU:HD12	10:QJ:96:ILE:HA	1.31	1.08
12:XL:47:LYS:HG3	12:XL:48:PRO:HD2	1.08	1.08
13:QM:8:GLU:C	13:QM:10:PRO:HD2	1.74	1.07
41:RH:7:LEU:O	41:RH:7:LEU:HD23	1.52	1.07
10:QJ:6:ILE:HG23	10:QJ:97:GLU:O	1.52	1.07
10:QJ:8:LEU:HD11	10:QJ:96:ILE:HA	1.33	1.07
38:RE:73:GLU:CG	38:RE:74:PRO:CD	2.31	1.07
37:RD:76:PRO:HA	37:RD:118:VAL:HG23	1.08	1.06
41:RH:54:ARG:HD2	41:RH:61:HIS:CB	1.85	1.06
52:YW:11:ARG:NH2	52:YW:98:LYS:HB3	1.70	1.06
38:RE:73:GLU:HG2	38:RE:74:PRO:HD2	1.09	1.05
13:QM:13:LYS:HG3	13:QM:17:VAL:HG21	1.36	1.05
24:QZ:43:GLY:CA	24:QZ:59:ARG:HG2	1.86	1.05
10:QJ:6:ILE:CD1	10:QJ:98:ILE:CA	2.35	1.04
42:YI:92:VAL:CB	42:YI:120:ILE:CG2	2.36	1.03
50:YU:92:ARG:HD2	51:YV:11:GLN:CD	1.76	1.03
24:XZ:48:LEU:HB2	24:XZ:52:LEU:HG	1.40	1.02
41:RH:46:GLU:HB3	41:RH:49:VAL:HB	1.40	1.02
12:XL:47:LYS:CB	12:XL:48:PRO:CD	2.36	1.02
26:R1:78:LYS:NZ	35:RA:270(R):G:H21	1.58	1.02
38:RE:57:LYS:HG2	38:RE:57:LYS:O	1.54	1.02
52:YW:11:ARG:NH2	52:YW:98:LYS:HD3	1.74	1.02
2:XB:6:THR:HG22	2:XB:7:VAL:H	1.25	1.02
41:RH:35:VAL:HG11	41:RH:71:LEU:CD1	1.90	1.01
2:XB:87:ARG:HH12	2:XB:233:SER:HB2	1.02	1.01
38:RE:73:GLU:CG	38:RE:74:PRO:HD2	1.91	1.01
24:QZ:10:TRP:CD1	24:QZ:14:LEU:HD13	1.96	1.00
35:RA:2112:G:H21	35:RA:2169:A:N6	1.57	1.00
50:YU:92:ARG:CD	51:YV:11:GLN:HB2	1.91	1.00
10:QJ:8:LEU:HD21	10:QJ:96:ILE:HG22	1.44	0.99
44:YO:78:ARG:NH2	49:YT:103:ARG:NH2	2.10	0.99
37:YD:181:GLU:OE2	37:YD:270:ILE:CG2	2.10	0.99
42:YI:92:VAL:HB	42:YI:120:ILE:HG21	1.42	0.99
21:XU:6:ARG:NH1	21:XU:15:ARG:HH21	1.61	0.98

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:2757:A:N1	41:RH:67:LEU:HD22	1.79	0.98
42:RI:133:HIS:HB3	42:RI:134:PRO:HD3	1.45	0.98
7:QG:68:ASN:O	7:QG:138:LYS:HE2	1.60	0.98
44:YO:78:ARG:HH21	49:YT:103:ARG:NH2	1.61	0.97
33:Y8:26:LYS:HG2	33:Y8:48:PHE:CD2	1.98	0.97
19:XS:11:VAL:HB	19:XS:13:ASP:OD1	1.63	0.97
24:XZ:52:LEU:H	24:XZ:52:LEU:HD22	1.24	0.97
19:QS:55:LYS:NZ	24:QZ:36:ARG:NH2	2.12	0.97
24:QZ:43:GLY:C	24:QZ:59:ARG:HG2	1.83	0.97
1:XA:1302:U:C5	13:XM:17:VAL:HG11	2.00	0.96
51:RV:37:VAL:O	51:RV:51:VAL:CG2	2.13	0.96
24:XZ:48:LEU:CG	24:XZ:52:LEU:HG	1.94	0.96
51:YV:49:THR:OG1	51:YV:50:PRO:CD	2.12	0.96
37:YD:181:GLU:OE2	37:YD:270:ILE:HG23	1.66	0.96
13:XM:3:ARG:HD2	29:Y4:34:GLU:HG3	1.44	0.96
19:QS:55:LYS:HZ2	24:QZ:36:ARG:NH2	1.61	0.96
24:QZ:12:ASP:HB2	24:QZ:80:CYS:SG	2.05	0.96
51:RV:49:THR:HG1	51:RV:50:PRO:HD3	1.18	0.95
12:XL:47:LYS:HB2	12:XL:48:PRO:CD	1.96	0.95
13:XM:53:VAL:HG12	13:XM:57:ARG:HH12	1.30	0.95
44:YO:78:ARG:HH21	49:YT:103:ARG:HH21	1.13	0.95
12:XL:47:LYS:HG3	12:XL:48:PRO:CD	1.96	0.95
10:QJ:8:LEU:CD2	10:QJ:96:ILE:HG22	1.96	0.95
41:RH:10:PRO:HB3	41:RH:50:VAL:HG22	1.46	0.95
7:QG:69:VAL:C	7:QG:138:LYS:HD3	1.86	0.95
51:YV:52:VAL:HG21	51:YV:55:ALA:HB3	1.43	0.95
24:QZ:43:GLY:HA2	24:QZ:59:ARG:HE	1.24	0.95
10:QJ:6:ILE:CD1	10:QJ:97:GLU:O	2.15	0.95
24:XZ:48:LEU:HD13	24:XZ:52:LEU:CD1	1.97	0.95
55:YZ:129:SER:OG	55:YZ:130:PRO:CD	2.16	0.94
9:QI:19:LEU:HG	9:QI:59:PHE:HE1	1.31	0.94
19:QS:41:VAL:HG13	19:QS:42:PRO:CD	1.96	0.94
26:R1:78:LYS:NZ	35:RA:270(R):G:N2	2.16	0.94
13:QM:13:LYS:HG3	13:QM:17:VAL:CG2	1.98	0.94
9:QI:50:LEU:HA	9:QI:53:VAL:HG12	1.49	0.93
41:RH:54:ARG:HD2	41:RH:61:HIS:HB2	1.48	0.93
33:R8:15:LYS:HG3	45:RP:65:ARG:HH11	1.32	0.93
12:QL:33:ARG:HD2	12:QL:60:LEU:HD13	1.50	0.93
10:QJ:8:LEU:CD1	10:QJ:96:ILE:CA	2.44	0.93
50:YU:92:ARG:HD3	50:YU:95:LEU:HD12	1.48	0.93
13:QM:13:LYS:O	13:QM:17:VAL:CG1	2.17	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:YG:77:ILE:HB	40:YG:82:LEU:HD12	1.51	0.92
40:RG:145:THR:O	40:RG:146:TYR:CD2	2.22	0.92
7:XG:69:VAL:O	7:XG:138:LYS:HD3	1.70	0.92
55:YZ:129:SER:OG	55:YZ:130:PRO:HD2	1.69	0.92
26:R1:78:LYS:HZ3	35:RA:270(R):G:H21	1.14	0.92
38:RE:73:GLU:HG3	38:RE:74:PRO:HD3	1.50	0.92
42:RI:113:ARG:HH11	42:RI:113:ARG:HG2	1.32	0.92
9:XI:16:ARG:NH1	9:XI:18:PHE:HZ	1.66	0.92
21:XU:6:ARG:HH11	21:XU:15:ARG:HH21	1.02	0.91
38:RE:73:GLU:CG	38:RE:74:PRO:HD3	1.99	0.91
13:QM:9:ILE:N	13:QM:10:PRO:HD2	1.80	0.91
24:XZ:1:MET:HB2	24:XZ:35:ARG:CG	2.01	0.91
4:XD:150:GLU:HA	4:XD:153:ARG:HB2	1.53	0.91
44:YO:68:GLU:OE1	44:YO:78:ARG:CD	2.18	0.91
41:RH:86:GLU:HG2	41:RH:86:GLU:O	1.69	0.90
13:QM:13:LYS:O	13:QM:17:VAL:HG13	1.69	0.90
51:YV:66:ARG:C	51:YV:91:TYR:HE2	1.73	0.90
26:R1:78:LYS:HZ3	35:RA:270(R):G:N2	1.69	0.90
55:RZ:52:SER:O	55:RZ:53:ILE:HG13	1.69	0.90
50:YU:92:ARG:HD2	51:YV:11:GLN:OE1	1.72	0.90
10:QJ:6:ILE:HD12	10:QJ:98:ILE:CA	2.00	0.89
37:RD:123:ALA:HB3	37:RD:131:LEU:HD11	1.52	0.89
9:QI:21:PRO:HA	9:QI:59:PHE:HB3	1.54	0.89
24:QY:5:TRP:CZ2	24:QZ:10:TRP:CH2	2.61	0.89
10:XJ:6:ILE:HD11	10:XJ:98:ILE:HG12	1.54	0.89
10:QJ:7:LYS:HA	10:QJ:71:LEU:HA	1.52	0.88
20:QT:45:GLN:HA	20:QT:91:LEU:HD21	1.56	0.88
12:XL:18:VAL:CG1	12:XL:20:LYS:HE3	2.02	0.88
41:RH:54:ARG:HD2	41:RH:61:HIS:HB3	1.56	0.88
39:YF:28:ILE:HG12	39:YF:119:ARG:HH22	1.37	0.88
10:QJ:22:LYS:HE2	10:QJ:90:LEU:HD22	1.54	0.88
38:RE:57:LYS:CG	38:RE:57:LYS:O	2.16	0.88
42:RI:9:LEU:HD11	42:RI:12:LEU:HB2	1.55	0.88
24:QZ:1:MET:HB2	24:QZ:73:ASP:C	1.94	0.87
33:R8:15:LYS:HG3	45:RP:65:ARG:NH1	1.88	0.87
7:QG:69:VAL:HA	7:QG:138:LYS:HD3	1.55	0.87
41:RH:8:PRO:HG3	41:RH:69:ARG:HD2	1.55	0.87
24:QZ:10:TRP:NE1	24:QZ:14:LEU:CD1	2.37	0.87
24:QZ:43:GLY:HA2	24:QZ:59:ARG:CG	2.04	0.87
10:QJ:8:LEU:HD21	10:QJ:96:ILE:CG2	2.04	0.87
39:YF:65:TRP:CH2	39:YF:72:ARG:HD2	2.10	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:YI:117:GLU:O	42:YI:118:LYS:HG2	1.75	0.87
7:QG:69:VAL:O	7:QG:138:LYS:HD3	1.74	0.87
37:RD:6:PHE:CD1	37:RD:13:ARG:NH2	2.41	0.87
13:QM:67:GLU:CG	13:QM:67:GLU:CA	2.51	0.86
42:RI:109:ILE:HG23	42:RI:130:TYR:OH	1.75	0.86
40:YG:114:ILE:HB	40:YG:117:PHE:HB2	1.57	0.86
42:YI:92:VAL:CB	42:YI:120:ILE:HG22	2.01	0.86
29:R4:40:HIS:N	29:R4:41:PRO:HD3	1.89	0.86
9:QI:50:LEU:HD23	9:QI:53:VAL:CG1	2.04	0.86
19:QS:64:GLU:HG2	29:R4:56:VAL:HG23	1.58	0.86
48:RS:62:LYS:HD2	48:RS:97:ARG:NH1	1.90	0.86
24:QZ:1:MET:HB2	24:QZ:73:ASP:O	1.75	0.86
40:RG:9:ARG:HH11	40:RG:9:ARG:HG3	1.38	0.86
4:XD:153:ARG:HD3	4:XD:181:MET:CE	2.06	0.86
12:QL:33:ARG:HD3	12:QL:61:THR:HB	1.55	0.86
24:QZ:44:LYS:HD3	24:QZ:59:ARG:HD3	1.56	0.85
24:QZ:43:GLY:HA2	24:QZ:59:ARG:CD	2.06	0.85
10:QJ:6:ILE:HD11	10:QJ:98:ILE:CA	2.00	0.85
10:QJ:8:LEU:CG	10:QJ:96:ILE:HG22	2.05	0.85
7:QG:69:VAL:CA	7:QG:138:LYS:HD3	2.05	0.85
51:RV:52:VAL:HG21	51:RV:55:ALA:HB3	1.58	0.85
51:YV:52:VAL:HG23	51:YV:55:ALA:HB3	1.57	0.85
24:XZ:1:MET:HB2	24:XZ:35:ARG:HG2	1.58	0.85
51:RV:37:VAL:O	51:RV:51:VAL:HG22	1.74	0.84
50:YU:92:ARG:HD2	51:YV:11:GLN:HB2	1.58	0.84
41:RH:6:ARG:CD	41:RH:54:ARG:HH12	1.89	0.84
44:RO:104:ARG:O	44:RO:107:ARG:HB3	1.77	0.84
52:YW:11:ARG:HH21	52:YW:98:LYS:HD3	1.40	0.84
9:QI:21:PRO:HA	9:QI:59:PHE:CB	2.07	0.84
24:QZ:1:MET:CG	24:QZ:2:LYS:H	1.91	0.84
19:QS:41:VAL:HG13	19:QS:42:PRO:HD3	1.57	0.84
24:QZ:12:ASP:CB	24:QZ:80:CYS:SG	2.66	0.84
12:XL:49:ASN:ND2	12:XL:92:ASP:OD2	2.11	0.83
2:QB:95:GLN:CG	2:QB:147:LYS:HE3	2.08	0.83
24:QZ:15:TYR:CE2	24:QZ:81:ARG:NH2	2.46	0.83
9:XI:16:ARG:NH1	9:XI:18:PHE:CZ	2.46	0.83
10:QJ:21:GLN:HA	10:QJ:24:VAL:HG13	1.59	0.83
24:QZ:43:GLY:CA	24:QZ:59:ARG:CG	2.55	0.83
8:QH:87:SER:HB2	8:QH:93:VAL:H	1.42	0.83
41:RH:10:PRO:CG	41:RH:49:VAL:HA	2.07	0.83
24:QY:44:LYS:NZ	24:QY:59:ARG:NH1	2.26	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:XY:83:HIS:O	24:XY:84:TYR:CD1	2.32	0.83
24:XZ:48:LEU:HB2	24:XZ:52:LEU:CB	2.09	0.83
24:QY:48:LEU:HD13	24:QY:52:LEU:CD2	2.09	0.82
1:XA:1299:A:C6	1:XA:1301:U:N3	2.46	0.82
24:XZ:48:LEU:HB3	24:XZ:52:LEU:HG	0.83	0.82
24:QY:44:LYS:HZ2	24:QY:59:ARG:NH1	1.78	0.82
41:RH:10:PRO:HG3	41:RH:49:VAL:CA	2.08	0.82
35:YA:2748:A:H8	41:YH:63:SER:HB3	1.44	0.82
2:QB:95:GLN:HG2	2:QB:147:LYS:HE3	1.60	0.82
51:RV:37:VAL:O	51:RV:51:VAL:HG23	1.78	0.82
35:RA:2112:G:H21	35:RA:2169:A:H61	1.24	0.82
44:RO:36:GLY:HA3	44:RO:109:LYS:HD3	1.61	0.82
29:R4:52:THR:O	29:R4:52:THR:HG22	1.80	0.81
55:YZ:128:VAL:HG21	55:YZ:161:VAL:HG12	1.62	0.81
42:RI:123:LEU:HD21	42:RI:144:VAL:HG11	1.61	0.81
49:RT:3:ARG:HA	49:RT:3:ARG:CB	2.08	0.81
2:XB:87:ARG:NH1	2:XB:233:SER:OG	2.14	0.81
35:RA:676:A:H8	35:RA:2069:G:H21	1.28	0.81
7:XG:89:MET:HG2	7:XG:155:ARG:HG2	1.60	0.81
1:XA:1238:A:N7	1:XA:1301:U:O4	2.12	0.81
12:XL:47:LYS:HB2	12:XL:48:PRO:HD3	1.62	0.81
52:YW:11:ARG:NH2	52:YW:98:LYS:CD	2.43	0.80
8:XH:109:ILE:HD11	8:XH:120:THR:HB	1.64	0.80
52:YW:11:ARG:NH2	52:YW:98:LYS:CB	2.45	0.80
10:QJ:6:ILE:HD12	10:QJ:97:GLU:C	2.01	0.80
20:XT:99:LEU:HG	20:XT:100:ILE:HG12	1.63	0.80
24:QY:5:TRP:HZ2	24:QZ:10:TRP:CH2	1.99	0.80
39:YF:154:VAL:HG12	39:YF:191:ARG:HB3	1.62	0.80
43:RN:3:THR:HG21	50:RU:61:TRP:HE1	1.47	0.80
9:QI:50:LEU:CD2	9:QI:53:VAL:HG11	2.09	0.80
10:QJ:6:ILE:CD1	10:QJ:99:LYS:H	1.95	0.80
2:XB:6:THR:CG2	2:XB:7:VAL:H	1.93	0.80
24:QZ:10:TRP:NE1	24:QZ:14:LEU:HD13	1.94	0.80
55:YZ:103:ARG:HG2	55:YZ:136:PHE:HB2	1.62	0.80
7:XG:68:ASN:O	7:XG:138:LYS:CE	2.29	0.79
13:XM:53:VAL:HG12	13:XM:57:ARG:NH1	1.97	0.79
25:R0:27:GLU:HG3	25:R0:68:GLU:HA	1.65	0.79
55:YZ:103:ARG:HG3	55:YZ:136:PHE:CD2	2.17	0.79
19:XS:17:GLU:O	19:XS:21:GLU:HB2	1.83	0.79
1:QA:1422:G:H5"	44:RO:48:PRO:HB3	1.65	0.78
60:QX:101:A3P:O2P	24:QY:59:ARG:NH1	2.15	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:RN:74:ARG:HH21	43:RN:85:ILE:HD11	1.49	0.78
52:RW:14:PRO:HG2	52:RW:78:GLU:OE1	1.84	0.78
40:YG:139:LEU:O	40:YG:139:LEU:HD13	1.82	0.78
4:XD:20:TYR:HD2	4:XD:26:CYS:HB3	1.49	0.78
49:YT:131:ALA:O	49:YT:136:GLN:NE2	2.17	0.78
40:RG:138:GLN:HG3	40:RG:139:LEU:HD12	1.65	0.78
24:QY:44:LYS:HD2	24:QY:59:ARG:HH11	1.48	0.78
55:RZ:54:HIS:HB3	55:RZ:101:PRO:HD3	1.66	0.78
13:QM:84:ILE:HG23	13:QM:86:CYS:H	1.47	0.78
24:QZ:43:GLY:HA2	24:QZ:59:ARG:HG2	1.62	0.78
24:QZ:1:MET:CG	24:QZ:2:LYS:N	2.44	0.78
37:RD:76:PRO:HA	37:RD:118:VAL:CG2	2.02	0.78
49:YT:128:GLU:O	49:YT:132:LYS:HB2	1.84	0.78
21:XU:6:ARG:HD3	21:XU:15:ARG:HE	1.48	0.77
55:YZ:103:ARG:CG	55:YZ:136:PHE:HB2	2.13	0.77
1:QA:80:G:N1	1:QA:89:U:O2	2.18	0.77
10:QJ:7:LYS:HB3	10:QJ:71:LEU:HD12	1.67	0.77
19:QS:40:ILE:HA	19:QS:44:MET:SD	2.24	0.77
24:XZ:48:LEU:HD13	24:XZ:52:LEU:HD11	1.66	0.77
8:QH:46:LYS:HG3	8:QH:64:LYS:CG	2.13	0.77
19:QS:55:LYS:CE	24:QZ:36:ARG:HH22	1.97	0.77
24:XZ:48:LEU:CD1	24:XZ:52:LEU:HG	2.14	0.77
10:QJ:6:ILE:HD11	10:QJ:99:LYS:H	1.49	0.77
42:RI:24:GLY:HA2	42:RI:27:ARG:HG2	1.65	0.77
1:XA:1299:A:C6	1:XA:1301:U:C2	2.73	0.77
2:XB:15:VAL:O	2:XB:17:PHE:CD2	2.38	0.77
7:QG:68:ASN:C	7:QG:138:LYS:HE2	2.05	0.77
19:XS:32:LYS:HG2	19:XS:50:ALA:HB3	1.66	0.77
33:R8:15:LYS:CG	45:RP:65:ARG:NH1	2.48	0.76
35:RA:1857:G:H21	35:RA:1885:A:H62	1.33	0.76
19:XS:11:VAL:CB	19:XS:13:ASP:OD1	2.34	0.76
51:YV:49:THR:HG1	51:YV:50:PRO:HD3	1.50	0.76
38:YE:14:ILE:HG13	38:YE:21:VAL:HG23	1.65	0.76
19:QS:55:LYS:HZ2	24:QZ:36:ARG:HH22	1.11	0.76
24:QZ:10:TRP:HE1	24:QZ:14:LEU:HD11	1.51	0.76
35:RA:2086:U:OP2	37:RD:263:ARG:NH1	2.19	0.76
4:XD:153:ARG:HD3	4:XD:181:MET:HE2	1.67	0.76
24:XY:38:PRO:O	24:XY:68:TYR:OH	2.04	0.76
50:YU:92:ARG:HD2	51:YV:11:GLN:CG	2.15	0.76
46:YQ:139:GLU:OE2	55:YZ:122:ARG:HG2	1.85	0.76
55:YZ:10:ARG:HD3	55:YZ:38:TYR:HB3	1.66	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:2720:U:H3	35:RA:2873:A:H2	1.31	0.76
35:RA:2873:A:H8	47:RR:6:SER:H	1.33	0.76
1:QA:1330:U:H4'	13:QM:23:TYR:HD1	1.51	0.75
25:Y0:27:GLU:HG3	25:Y0:68:GLU:HA	1.68	0.75
41:RH:46:GLU:N	41:RH:49:VAL:O	2.19	0.75
7:XG:69:VAL:C	7:XG:138:LYS:HD3	2.06	0.75
10:XJ:30:SER:HB2	10:XJ:81:THR:HG21	1.68	0.75
1:QA:1534:A:N6	23:QX:10:G:C6	2.54	0.75
2:QB:87:ARG:HH21	2:QB:233:SER:HB3	1.51	0.75
41:RH:54:ARG:CZ	41:RH:62:LYS:HG2	2.17	0.75
48:RS:11:LYS:HE2	48:RS:91:PRO:HG3	1.67	0.75
1:XA:1178:G:H5''	9:XI:93:ARG:HH22	1.52	0.75
2:QB:209:ARG:NH1	2:QB:212:GLN:OE1	2.19	0.75
26:R1:50:ARG:NH1	26:R1:57:GLU:OE2	2.18	0.75
1:XA:1147:C:HO2'	9:XI:5:TYR:HH	1.34	0.74
9:QI:104:ARG:NH1	9:QI:105:ASP:O	2.20	0.74
40:RG:9:ARG:HG3	40:RG:9:ARG:NH1	1.97	0.74
43:RN:61:ARG:HG3	43:RN:61:ARG:O	1.87	0.74
12:QL:117:ARG:HB2	12:QL:122:THR:HB	1.69	0.74
10:XJ:49:VAL:HG23	14:XN:41:ARG:HB2	1.68	0.74
39:RF:120:GLU:HG3	39:RF:122:LYS:HG2	1.68	0.74
24:XZ:48:LEU:CB	24:XZ:52:LEU:CB	2.64	0.74
37:RD:123:ALA:O	37:RD:131:LEU:HD21	1.88	0.74
41:RH:71:LEU:C	41:RH:71:LEU:HD12	2.07	0.74
35:YA:1728:G:N7	35:YA:1731:G:N2	2.34	0.74
24:QY:44:LYS:HZ2	24:QY:59:ARG:HH11	1.33	0.74
24:XZ:1:MET:CB	24:XZ:35:ARG:CG	2.66	0.74
24:XZ:1:MET:CB	24:XZ:35:ARG:HG2	2.17	0.74
35:YA:2141:G:H1	35:YA:2150:U:H3	0.79	0.74
52:YW:11:ARG:CZ	52:YW:98:LYS:HB3	2.17	0.74
50:YU:92:ARG:HD2	51:YV:11:GLN:CB	2.18	0.73
35:YA:676:A:H8	35:YA:2069:G:H21	1.35	0.73
48:RS:63:THR:HA	48:RS:97:ARG:HB3	1.71	0.73
24:XZ:1:MET:HB2	24:XZ:35:ARG:HD3	1.69	0.73
24:XZ:52:LEU:N	24:XZ:52:LEU:HD22	2.01	0.73
8:QH:46:LYS:HG3	8:QH:64:LYS:HG3	1.69	0.73
15:QO:40:SER:HB2	35:RA:715:G:H21	1.53	0.73
24:QZ:36:ARG:HG3	24:QZ:37:THR:HG23	1.68	0.73
24:QZ:9:SER:OG	24:QZ:10:TRP:N	2.21	0.73
42:YI:92:VAL:CG2	42:YI:120:ILE:CG2	2.65	0.73
24:QZ:1:MET:HG2	24:QZ:2:LYS:N	2.01	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:R9:22:ARG:HH12	35:RA:2741:A:H5''	1.53	0.73
37:RD:147:LEU:HD11	37:RD:183:ARG:CZ	2.19	0.73
2:XB:15:VAL:O	2:XB:17:PHE:HD2	1.72	0.73
9:XI:16:ARG:HH12	9:XI:18:PHE:HZ	1.32	0.73
37:YD:181:GLU:OE2	37:YD:270:ILE:HG21	1.87	0.73
24:XZ:48:LEU:HB2	24:XZ:52:LEU:CG	2.04	0.73
1:QA:664:G:H22	1:QA:741:G:H1	1.37	0.73
5:QE:102:ALA:HB1	5:QE:106:PRO:HG2	1.71	0.73
42:RI:123:LEU:HD21	42:RI:144:VAL:CG1	2.18	0.73
46:RQ:24:GLY:H	46:RQ:101:ARG:HH11	1.33	0.73
55:RZ:128:VAL:HG23	55:RZ:161:VAL:HG12	1.69	0.73
19:XS:11:VAL:HG12	19:XS:13:ASP:H	1.53	0.73
24:XZ:52:LEU:H	24:XZ:52:LEU:CD2	2.01	0.73
24:QZ:83:HIS:O	24:QZ:84:TYR:OXT	2.06	0.73
24:XZ:37:THR:OG1	24:XZ:40:GLU:O	2.05	0.73
39:YF:65:TRP:CZ2	39:YF:72:ARG:HD2	2.23	0.73
19:XS:11:VAL:HG11	19:XS:16:LEU:HB2	1.71	0.73
24:XZ:1:MET:HB2	24:XZ:35:ARG:CD	2.19	0.73
25:R0:36:ILE:CD1	25:R0:39:ARG:HH21	2.01	0.72
25:R0:36:ILE:HD13	25:R0:39:ARG:HH21	1.52	0.72
42:RI:3:VAL:HG23	42:RI:38:LEU:HA	1.71	0.72
40:YG:16:ARG:HH21	40:YG:31:VAL:HG11	1.54	0.72
29:Y4:58:ARG:HG3	29:Y4:59:PHE:HD1	1.53	0.72
39:YF:65:TRP:CH2	39:YF:72:ARG:CD	2.72	0.72
55:YZ:23:LYS:HD3	55:YZ:40:ASP:HA	1.71	0.72
50:YU:19:LYS:HA	50:YU:22:LYS:HE2	1.70	0.72
35:YA:2833:G:C2	38:YE:57:LYS:HE2	2.25	0.72
51:YV:66:ARG:C	51:YV:91:TYR:CE2	2.60	0.72
7:QG:91:VAL:HG12	7:QG:96:GLN:HG3	1.72	0.72
42:RI:72:LEU:HD21	42:RI:101:LEU:HD21	1.70	0.72
1:XA:1130:A:O2'	9:XI:3:GLN:NE2	2.23	0.72
29:R4:28:LYS:NZ	29:R4:30:GLU:O	2.23	0.72
42:RI:77:LEU:HD22	42:RI:101:LEU:HD13	1.72	0.72
42:RI:125:GLU:HA	42:RI:141:LYS:HG3	1.72	0.72
35:RA:2245:U:H5'	35:RA:2246:G:H5'	1.72	0.71
24:XZ:52:LEU:HB3	24:XZ:55:PHE:HB2	1.73	0.71
33:Y8:26:LYS:HA	33:Y8:48:PHE:HE2	1.54	0.71
3:QC:57:ILE:HG23	3:QC:64:VAL:HG11	1.72	0.71
4:XD:188:LEU:HD12	4:XD:189:PRO:HD2	1.72	0.71
40:YG:107:LEU:HA	40:YG:111:LEU:HD12	1.71	0.71
41:RH:52:VAL:HB	41:RH:69:ARG:NH2	2.05	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:XU:6:ARG:HH11	21:XU:15:ARG:NH2	1.84	0.71
50:YU:92:ARG:HD3	51:YV:11:GLN:HB2	1.71	0.71
2:XB:6:THR:HG22	2:XB:7:VAL:N	2.04	0.71
35:YA:2114:A:N1	35:YA:2170:A:N6	2.38	0.71
39:YF:116:ASP:OD1	39:YF:119:ARG:NH2	2.20	0.71
21:QU:4:GLY:HA2	21:QU:15:ARG:HH22	1.56	0.71
55:RZ:53:ILE:HG22	55:RZ:71:VAL:O	1.91	0.71
13:QM:23:TYR:CE2	13:QM:71:ARG:HG2	2.26	0.71
42:RI:79:ILE:CD1	42:RI:140:LEU:HD21	2.20	0.71
4:XD:62:GLN:HE22	4:XD:65:ARG:HH21	1.39	0.71
16:XP:69:THR:HA	16:XP:72:ARG:HG2	1.73	0.71
51:YV:7:THR:HG23	51:YV:22:VAL:HG21	1.73	0.71
9:XI:78:LYS:HZ1	9:XI:101:PHE:HD1	1.36	0.70
24:QZ:44:LYS:CD	24:QZ:59:ARG:HD3	2.21	0.70
40:RG:135:LEU:HD21	40:RG:140:ILE:HD11	1.73	0.70
1:XA:686:U:H1'	11:XK:42:TRP:HE1	1.57	0.70
1:QA:1309:G:OP1	13:QM:88:ARG:NH1	2.24	0.70
48:RS:30:ARG:HG2	48:RS:97:ARG:HH21	1.56	0.70
1:XA:1502:A:H2	1:XA:1505:G:H1	1.39	0.70
42:RI:123:LEU:CD2	42:RI:144:VAL:CG1	2.68	0.70
47:RR:65:LEU:HA	47:RR:68:ARG:HH11	1.55	0.70
5:XE:144:THR:HG1	5:XE:147:ASP:H	1.38	0.70
42:RI:113:ARG:HG2	42:RI:113:ARG:NH1	2.06	0.70
1:XA:1071:C:OP1	5:XE:27:ARG:NH2	2.24	0.70
50:YU:92:ARG:HD3	50:YU:95:LEU:CD1	2.22	0.70
2:QB:91:PRO:HG2	2:QB:155:LEU:HB2	1.72	0.70
10:QJ:5:ARG:NH1	10:QJ:73:ASP:OD2	2.23	0.70
25:R0:60:PHE:HE1	25:R0:62:LEU:HD23	1.55	0.70
40:RG:39:ILE:HB	40:RG:92:VAL:HG12	1.73	0.70
24:QY:48:LEU:HD13	24:QY:52:LEU:HD23	1.72	0.70
41:RH:8:PRO:CD	41:RH:69:ARG:CD	2.70	0.70
55:RZ:6:LYS:HZ1	55:RZ:62:PRO:HD3	1.56	0.70
35:YA:1342:A:H2	35:YA:1602:U:H3	1.37	0.70
40:RG:66:GLN:OE1	40:RG:98:ARG:NH1	2.25	0.70
4:XD:187:ARG:NH2	4:XD:193:ASP:OD2	2.25	0.70
12:XL:27:LEU:HD23	12:XL:62:SER:HB3	1.72	0.70
2:QB:185:ILE:HG22	2:QB:199:TYR:HB2	1.74	0.70
24:QY:5:TRP:NE1	24:QZ:10:TRP:CZ3	2.60	0.70
35:RA:2401:U:H3	35:RA:2415:G:H1	1.39	0.70
1:XA:1348:U:H3	1:XA:1374:A:H2	1.38	0.70
35:RA:259:G:H21	35:RA:621:A:H8	1.37	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:YF:51:THR:O	39:YF:93:LYS:NZ	2.24	0.69
9:QI:50:LEU:HA	9:QI:53:VAL:CG1	2.22	0.69
22:XW:50:U:H3	22:XW:64:G:H1	1.39	0.69
4:QD:153:ARG:HD3	4:QD:181:MET:SD	2.33	0.69
6:QF:2:ARG:HD3	6:QF:92:LYS:HE2	1.75	0.69
42:RI:123:LEU:CD2	42:RI:144:VAL:HG11	2.22	0.69
33:R8:25:MET:HG3	45:RP:64:LYS:HB3	1.74	0.69
4:QD:169:LYS:HB2	6:XF:21:LEU:HD21	1.73	0.69
41:RH:26:VAL:HG12	41:RH:33:LEU:H	1.56	0.69
42:RI:9:LEU:HG	42:RI:11:ASN:H	1.58	0.69
2:XB:71:VAL:HB	2:XB:164:VAL:HG12	1.75	0.69
19:XS:11:VAL:CG1	19:XS:13:ASP:OD1	2.41	0.69
1:QA:686:U:H1'	11:QK:42:TRP:HE1	1.58	0.69
35:RA:2777:G:H5''	35:RA:2778:A:H5'	1.73	0.69
35:RA:67:U:H3	35:RA:74:A:H2	1.39	0.69
35:YA:2777:G:H5''	35:YA:2778:A:H5'	1.74	0.69
55:YZ:129:SER:OG	55:YZ:130:PRO:HD3	1.93	0.69
38:RE:7:VAL:HG23	38:RE:51:PHE:HE2	1.58	0.69
46:RQ:24:GLY:N	46:RQ:101:ARG:HH11	1.90	0.69
1:XA:1086:U:H3	1:XA:1099:G:H22	1.38	0.69
18:XR:87:ARG:HG2	18:XR:87:ARG:O	1.93	0.69
46:RQ:17:LEU:HD23	46:RQ:39:PRO:HB2	1.74	0.69
55:YZ:43:GLU:HA	55:YZ:46:LYS:HE2	1.72	0.69
24:QZ:10:TRP:NE1	24:QZ:14:LEU:HD11	2.04	0.69
24:QZ:43:GLY:CA	24:QZ:59:ARG:HE	2.02	0.69
45:RP:95:VAL:HB	45:RP:125:VAL:HG23	1.75	0.69
36:YB:80:U:H2'	36:YB:81:G:H21	1.56	0.69
40:YG:161:THR:HG22	40:YG:163:ALA:H	1.58	0.69
19:QS:3:ARG:HH21	19:QS:9:VAL:HB	1.57	0.69
55:YZ:99:TYR:HB3	55:YZ:123:ASP:OD2	1.93	0.69
17:QQ:66:SER:O	17:QQ:70:ARG:NH1	2.26	0.69
37:RD:8:PRO:HB3	37:RD:14:ARG:HB3	1.74	0.69
41:RH:9:ILE:HG13	41:RH:10:PRO:HD2	1.75	0.69
10:QJ:50:ILE:HG13	10:QJ:60:ARG:HH12	1.57	0.68
24:QZ:26:LYS:NZ	24:QZ:60:ILE:O	2.25	0.68
1:XA:1299:A:C5	1:XA:1301:U:C2	2.82	0.68
4:XD:157:LEU:HD23	4:XD:158:ILE:HG23	1.75	0.68
4:XD:191:ARG:HG2	4:XD:191:ARG:O	1.92	0.68
29:Y4:58:ARG:HG3	29:Y4:59:PHE:N	2.08	0.68
35:YA:2720:U:H3	35:YA:2873:A:H2	1.42	0.68
42:YI:92:VAL:CG2	42:YI:120:ILE:HG23	2.23	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:RH:7:LEU:N	41:RH:8:PRO:CD	2.56	0.68
48:RS:30:ARG:HG2	48:RS:97:ARG:NH2	2.07	0.68
35:YA:252:G:OP2	45:YP:50:ARG:NH2	2.27	0.68
50:YU:92:ARG:CD	50:YU:95:LEU:HD12	2.20	0.68
35:RA:888:C:H4'	35:RA:889:C:H5	1.58	0.68
41:RH:7:LEU:O	41:RH:7:LEU:CD2	2.36	0.68
47:YR:83:ILE:HG23	47:YR:86:ARG:HH21	1.57	0.68
35:YA:1339:G:H5''	53:YX:16:LYS:HD2	1.74	0.68
42:RI:130:TYR:HB3	42:RI:136:VAL:HG13	1.74	0.68
38:YE:36:ARG:NH2	38:YE:86:PRO:O	2.21	0.68
37:RD:76:PRO:CA	37:RD:118:VAL:CG2	2.65	0.68
13:XM:3:ARG:NH2	40:YG:113:ARG:HH21	1.91	0.68
29:R4:36:CYS:O	29:R4:41:PRO:HG2	1.94	0.68
35:RA:2512:C:O2'	38:RE:154:LYS:NZ	2.24	0.68
8:XH:113:SER:HB2	8:XH:134:ILE:HD11	1.75	0.68
13:XM:5:ALA:HB2	13:XM:22:ILE:HD13	1.76	0.68
13:QM:97:PRO:HA	13:QM:110:ARG:HD3	1.76	0.68
35:RA:2292:C:OP1	48:RS:17:ARG:NH2	2.26	0.68
2:XB:168:THR:HG23	2:XB:192:SER:HB3	1.76	0.68
1:QA:971:G:N2	1:QA:1363:A:OP2	2.26	0.68
24:QY:5:TRP:CZ2	24:QZ:10:TRP:HH2	2.10	0.68
35:RA:2112:G:N2	35:RA:2169:A:H61	1.91	0.68
40:RG:106:LEU:HD13	40:RG:111:LEU:HD11	1.76	0.68
40:RG:111:LEU:HB3	40:RG:117:PHE:CE1	2.29	0.68
33:Y8:6:THR:HG22	33:Y8:63:PRO:HD2	1.76	0.68
44:YO:78:ARG:NH2	49:YT:103:ARG:HH22	1.91	0.68
52:YW:11:ARG:HH21	52:YW:98:LYS:CD	2.03	0.68
3:QC:131:ARG:NH1	3:QC:166:GLU:OE1	2.27	0.68
10:QJ:6:ILE:HD11	10:QJ:99:LYS:N	2.08	0.68
30:R5:19:ARG:NH2	35:RA:1264:G:OP1	2.25	0.68
1:XA:974:A:N3	14:XM:31:ARG:NH1	2.42	0.68
51:YV:52:VAL:HG21	51:YV:55:ALA:CB	2.20	0.68
2:QB:209:ARG:HH21	2:QB:239:VAL:HG22	1.59	0.67
26:R1:75:GLU:HB3	26:R1:76:ARG:HD2	1.75	0.67
1:XA:1125:U:OP2	1:XA:1145:C:N4	2.26	0.67
55:YZ:103:ARG:HG3	55:YZ:136:PHE:HD2	1.56	0.67
9:QI:50:LEU:HD21	9:QI:85:LEU:HD21	1.75	0.67
13:QM:13:LYS:O	13:QM:17:VAL:HG11	1.94	0.67
15:QO:70:LEU:HD21	15:QO:77:ARG:HG3	1.76	0.67
38:RE:50:GLY:HA2	38:RE:78:LEU:HA	1.76	0.67
41:RH:8:PRO:CD	41:RH:69:ARG:HD3	2.24	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:RH:8:PRO:HD2	41:RH:69:ARG:NE	2.09	0.67
24:XZ:49:LYS:O	24:XZ:52:LEU:HD23	1.94	0.67
10:QJ:42:THR:HG22	10:QJ:68:HIS:HA	1.76	0.67
1:QA:1330:U:H4'	13:QM:23:TYR:CD1	2.29	0.67
31:R6:37:ARG:HA	31:R6:48:VAL:HA	1.74	0.67
42:RI:133:HIS:HB3	42:RI:134:PRO:CD	2.23	0.67
4:XD:150:GLU:HG2	4:XD:153:ARG:NH2	2.08	0.67
15:XO:54:ARG:O	15:XO:58:MET:HG3	1.94	0.67
1:QA:1224:G:O2'	19:QS:78:ARG:NH2	2.27	0.67
40:RG:32:PRO:HB2	40:RG:172:LEU:HD13	1.74	0.67
17:XQ:88:TYR:OH	17:XQ:92:ARG:NH2	2.27	0.67
49:YT:29:ARG:HG3	49:YT:46:GLU:HB2	1.77	0.67
7:QG:68:ASN:O	7:QG:138:LYS:CE	2.38	0.67
24:QZ:44:LYS:CE	24:QZ:59:ARG:HD3	2.24	0.67
41:RH:6:ARG:CD	41:RH:54:ARG:NH1	2.57	0.67
2:XB:217:ARG:HG3	2:XB:217:ARG:HH11	1.60	0.67
15:XO:40:SER:HB2	35:YA:715:G:H21	1.59	0.67
37:RD:121:PRO:HB3	37:RD:135:PHE:CE2	2.29	0.67
40:RG:111:LEU:O	40:RG:117:PHE:CD1	2.47	0.67
45:RP:126:VAL:HG12	45:RP:145:PRO:HD2	1.74	0.67
13:XM:3:ARG:HD2	29:Y4:34:GLU:CG	2.24	0.67
5:QE:79:GLU:O	5:QE:79:GLU:HG2	1.94	0.67
35:RA:2031:A:O2'	35:RA:2454:G:N2	2.27	0.67
24:XZ:59:ARG:HG2	24:XZ:65:ARG:CZ	2.25	0.67
35:YA:1165:U:H3	35:YA:1184:G:H1	1.43	0.67
41:YH:35:VAL:HG21	41:YH:72:ILE:HG12	1.77	0.67
51:YV:52:VAL:CG2	51:YV:55:ALA:CB	2.66	0.67
13:QM:14:ARG:HE	13:QM:16:ASP:CG	1.98	0.67
2:XB:111:ARG:HD2	2:XB:145:LEU:HD21	1.75	0.67
31:Y6:33:LYS:HB3	31:Y6:51:GLU:HG2	1.77	0.67
1:QA:1318:A:H4'	19:QS:11:VAL:HG21	1.75	0.67
35:RA:1817:G:OP1	37:RD:88:ARG:NH2	2.27	0.67
40:RG:161:THR:HG22	40:RG:163:ALA:H	1.59	0.67
49:YT:129:ARG:HG3	49:YT:132:LYS:HE3	1.77	0.67
9:QI:19:LEU:HG	9:QI:59:PHE:CD1	2.29	0.67
41:RH:10:PRO:HB2	41:RH:12:PRO:HD3	1.76	0.67
2:XB:87:ARG:CZ	2:XB:233:SER:HB2	2.23	0.67
9:XI:8:GLY:HA2	9:XI:79:LEU:HD23	1.77	0.67
13:XM:23:TYR:HD2	13:XM:67:GLU:HA	1.60	0.67
35:RA:704:G:O2'	35:RA:726:G:N2	2.28	0.66
27:Y2:70:GLN:HB2	27:Y2:71:ASN:HB2	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:QL:33:ARG:HD2	12:QL:60:LEU:CD1	2.24	0.66
17:QQ:48:GLU:HB2	17:QQ:50:LYS:HB2	1.78	0.66
35:RA:2571:C:H5'	35:RA:2572:A:H5''	1.76	0.66
35:RA:458:G:N2	35:RA:470:A:OP2	2.27	0.66
38:RE:141:ILE:HA	38:RE:154:LYS:HE2	1.77	0.66
42:RI:69:LYS:HA	42:RI:136:VAL:HG21	1.76	0.66
24:XZ:48:LEU:CD1	24:XZ:52:LEU:CD1	2.73	0.66
24:QZ:28:ASN:HA	24:QZ:31:ILE:HG12	1.77	0.66
40:RG:111:LEU:O	40:RG:117:PHE:CE1	2.48	0.66
11:XK:54:ARG:HH12	22:XW:39:C:H4'	1.61	0.66
42:YI:91:SER:OG	42:YI:119:PRO:HB3	1.95	0.66
51:YV:66:ARG:O	51:YV:91:TYR:HE2	1.79	0.66
1:QA:1502:A:H2	1:QA:1505:G:H1	1.42	0.66
3:QC:19:GLU:HB3	3:QC:40:ARG:HH22	1.61	0.66
24:QZ:15:TYR:HE2	24:QZ:81:ARG:HH21	1.39	0.66
1:XA:553:A:H5''	12:XL:24:VAL:HG21	1.77	0.66
37:YD:168:ARG:HG2	37:YD:173:VAL:HG13	1.76	0.66
1:QA:218:C:H5'	1:QA:466:C:H42	1.58	0.66
35:RA:2111:C:OP1	35:RA:2145:C:N4	2.29	0.66
40:YG:33:ARG:H	40:YG:162:THR:HB	1.61	0.66
3:QC:34:LEU:HD22	3:QC:38:ARG:HH21	1.60	0.66
13:QM:23:TYR:HE2	13:QM:71:ARG:CG	2.09	0.66
13:QM:23:TYR:HE2	13:QM:71:ARG:HG2	1.60	0.66
41:RH:68:THR:O	41:RH:71:LEU:HG	1.96	0.66
1:XA:677:U:H3	1:XA:713:G:H22	1.44	0.66
35:RA:654(D):G:H1	35:RA:654(Q):C:H42	1.44	0.66
55:RZ:52:SER:O	55:RZ:52:SER:OG	2.06	0.66
35:YA:2701:C:H3'	35:YA:2702:U:H5''	1.76	0.66
35:YA:2849:U:OP1	49:YT:95:ARG:NH1	2.29	0.66
1:QA:1317:C:OP2	14:QN:17:LYS:NZ	2.29	0.66
35:RA:68:G:H21	35:RA:74:A:H5'	1.59	0.66
41:RH:23:ARG:HD2	41:RH:34:GLU:HB2	1.77	0.66
27:Y2:61:LEU:O	27:Y2:65:ASN:HB2	1.96	0.66
29:Y4:58:ARG:HG3	29:Y4:59:PHE:H	1.59	0.66
35:YA:2358:G:H1	45:YP:55:ARG:HH12	1.44	0.66
35:RA:2304:G:H22	35:RA:2312:U:H3	1.42	0.65
3:QC:137:ALA:HA	3:QC:140:ARG:HH11	1.61	0.65
3:QC:29:TYR:HA	3:QC:32:LEU:HD12	1.78	0.65
37:RD:6:PHE:HE1	37:RD:13:ARG:NH2	1.84	0.65
42:RI:125:GLU:OE1	42:RI:125:GLU:N	2.28	0.65
55:RZ:6:LYS:NZ	55:RZ:62:PRO:HD3	2.11	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:XB:142:LEU:O	2:XB:146:GLN:HB2	1.96	0.65
35:YA:2768:C:O2'	43:YN:89:LYS:NZ	2.29	0.65
42:YI:100:ALA:O	42:YI:104:GLN:CB	2.45	0.65
38:RE:47:VAL:O	38:RE:80:GLU:HA	1.96	0.65
42:RI:130:TYR:HB3	42:RI:136:VAL:CG1	2.27	0.65
3:XC:108:ASN:ND2	3:XC:144:SER:OG	2.29	0.65
8:XH:100:ILE:HD12	8:XH:112:LEU:HD21	1.78	0.65
51:YV:38:LEU:HD12	51:YV:38:LEU:N	2.12	0.65
10:QJ:9:ARG:HG2	10:QJ:69:ASN:OD1	1.96	0.65
13:QM:86:CYS:SG	13:QM:87:TYR:N	2.70	0.65
35:RA:2468:G:N2	35:RA:2482:G:OP2	2.30	0.65
36:RB:30:C:H1'	36:RB:57:A:H61	1.60	0.65
55:YZ:48:PHE:HE1	55:YZ:71:VAL:HG11	1.61	0.65
1:QA:677:U:H3	1:QA:713:G:H22	1.43	0.65
7:QG:69:VAL:HA	7:QG:138:LYS:CD	2.27	0.65
19:QS:3:ARG:NH1	19:QS:5:LEU:HB3	2.11	0.65
22:QW:58:A:H2	22:QW:60:U:H2'	1.62	0.65
41:RH:17:VAL:HG11	41:RH:50:VAL:HG11	1.78	0.65
37:RD:147:LEU:HD21	37:RD:183:ARG:HH22	1.61	0.65
35:YA:443:A:C5	39:YF:45:ARG:HD2	2.32	0.65
12:QL:47:LYS:CB	12:QL:48:PRO:HD3	2.28	0.64
1:XA:191:G:O2'	20:XT:101:GLY:O	2.14	0.64
1:QA:1221:G:OP1	1:QA:1321:C:N4	2.31	0.64
42:RI:69:LYS:HG2	42:RI:136:VAL:HG23	1.79	0.64
1:XA:1302:U:C6	13:XM:17:VAL:HG11	2.32	0.64
41:YH:24:VAL:HB	41:YH:35:VAL:HG23	1.79	0.64
8:QH:46:LYS:HG3	8:QH:64:LYS:HG2	1.79	0.64
1:XA:1299:A:N6	1:XA:1301:U:H3	1.94	0.64
3:XC:189:ALA:HB3	3:XC:196:LEU:H	1.63	0.64
37:RD:183:ARG:HG3	37:RD:269:PHE:O	1.97	0.64
52:YW:11:ARG:HH22	52:YW:98:LYS:HD3	1.63	0.64
34:R9:11:CYS:SG	34:R9:14:CYS:N	2.59	0.64
35:RA:635:C:H41	45:RP:79:ARG:HH12	1.43	0.64
24:QZ:62:GLU:O	24:QZ:62:GLU:HG2	1.97	0.64
41:RH:46:GLU:HG3	41:RH:47:GLU:N	2.12	0.64
4:XD:98:GLU:HA	4:XD:103:ASN:HD22	1.62	0.64
5:QE:90:VAL:CG1	5:QE:90:VAL:CA	2.74	0.64
13:QM:10:PRO:HB2	13:QM:18:ALA:HB1	1.79	0.64
9:XI:5:TYR:HE1	9:XI:16:ARG:HB2	1.61	0.64
51:YV:51:VAL:O	51:YV:51:VAL:HG23	1.97	0.64
35:RA:833:U:O2	45:RP:55:ARG:NH1	2.30	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:RH:54:ARG:NH2	41:RH:57:ASP:OD1	2.30	0.64
27:Y2:21:LEU:HD13	27:Y2:64:LEU:HA	1.79	0.64
33:Y8:26:LYS:HA	33:Y8:48:PHE:CE2	2.32	0.64
41:YH:12:PRO:O	41:YH:15:VAL:HG12	1.97	0.64
55:YZ:97:GLU:HB3	55:YZ:125:LEU:HD11	1.79	0.64
40:RG:27:ASN:OD1	40:RG:28:VAL:N	2.31	0.64
41:RH:6:ARG:NE	41:RH:54:ARG:HH12	1.95	0.64
24:QZ:1:MET:HG3	24:QZ:2:LYS:H	1.63	0.64
35:RA:2112:G:N2	35:RA:2169:A:N6	2.39	0.64
51:RV:95:LEU:HD13	51:RV:97:LYS:HE3	1.80	0.64
35:YA:2833:G:N1	38:YE:57:LYS:HE2	2.12	0.64
1:QA:157:G:H1	1:QA:164:U:H3	1.46	0.63
13:QM:67:GLU:CD	13:QM:67:GLU:CB	2.64	0.63
12:XL:41:ARG:HH21	12:XL:43:VAL:HG12	1.63	0.63
3:QC:56:ASP:HB2	3:QC:67:THR:HB	1.80	0.63
9:QI:112:LYS:HA	9:QI:119:ALA:HB2	1.80	0.63
13:QM:14:ARG:O	13:QM:17:VAL:HG13	1.98	0.63
35:YA:2849:U:O2'	35:YA:2866:U:O2	2.16	0.63
1:XA:1178:G:OP2	9:XI:93:ARG:NH2	2.31	0.63
20:XT:100:ILE:HG22	20:XT:102:GLY:H	1.64	0.63
35:YA:2680:C:OP2	38:YE:111:ARG:NH2	2.30	0.63
42:YI:100:ALA:O	42:YI:104:GLN:HB2	1.97	0.63
42:YI:123:LEU:HB2	42:YI:142:VAL:HG23	1.80	0.63
50:YU:92:ARG:O	50:YU:94:ASN:N	2.26	0.63
2:QB:105:PHE:O	2:QB:109:SER:OG	2.15	0.63
42:RI:62:LYS:HG3	42:RI:133:HIS:ND1	2.14	0.63
35:RA:1339:G:H5''	53:RX:16:LYS:HD2	1.80	0.63
27:Y2:69:ARG:HG3	27:Y2:70:GLN:HG3	1.80	0.63
1:QA:405:U:O4	4:QD:2:GLY:N	2.32	0.63
1:QA:910:C:H5''	12:QL:97:ARG:HH22	1.63	0.63
30:R5:16:ARG:NH1	30:R5:17:ASP:OD1	2.32	0.63
40:RG:15:VAL:HG13	40:RG:175:LEU:HB2	1.79	0.63
43:RN:16:ILE:HG21	43:RN:26:LEU:HD11	1.80	0.63
55:RZ:25:PRO:HB2	55:RZ:85:HIS:HD2	1.63	0.63
22:QW:71:C:HO2'	35:RA:1851:U:HO2'	1.43	0.63
41:RH:35:VAL:CG1	41:RH:71:LEU:HD13	2.08	0.63
55:RZ:6:LYS:HZ2	55:RZ:8:TYR:HD1	1.45	0.63
18:QR:56:THR:HB	18:QR:58:LEU:HD12	1.81	0.63
35:RA:2119:A:N6	35:RA:2170:A:N7	2.47	0.63
37:RD:75:ILE:C	37:RD:118:VAL:CG2	2.66	0.63
55:RZ:6:LYS:NZ	55:RZ:7:ALA:O	2.31	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:XR:51:LEU:HD13	18:XR:55:ARG:HE	1.64	0.63
26:Y1:86:SER:OG	26:Y1:89:GLU:OE1	2.16	0.63
24:QY:44:LYS:CD	24:QY:59:ARG:HH11	2.12	0.63
24:XZ:48:LEU:HB3	24:XZ:52:LEU:HD23	1.78	0.63
27:Y2:29:LYS:HD3	27:Y2:57:ILE:HD13	1.81	0.63
39:YF:160:ASN:HB3	39:YF:163:VAL:HG22	1.80	0.63
1:QA:1086:U:H3	1:QA:1099:G:H22	1.46	0.63
24:QY:5:TRP:NE1	24:QZ:10:TRP:HZ3	1.96	0.63
24:XY:4:ILE:HA	24:XZ:3:LEU:O	1.98	0.63
26:R1:78:LYS:HZ1	35:RA:270(R):G:N2	1.92	0.62
43:YN:6:PRO:HG3	43:YN:41:ASP:HB2	1.82	0.62
13:QM:23:TYR:CE2	13:QM:71:ARG:CG	2.82	0.62
13:QM:23:TYR:HB3	13:QM:71:ARG:HH21	1.63	0.62
38:YE:57:LYS:HG3	38:YE:57:LYS:O	1.97	0.62
38:YE:54:GLN:HB2	38:YE:76:ARG:HG3	1.81	0.62
1:QA:468:A:H5''	16:QP:75:ARG:HH12	1.62	0.62
13:QM:12:ASN:HB2	13:QM:46:LYS:HE2	1.81	0.62
38:RE:141:ILE:HA	38:RE:154:LYS:CE	2.28	0.62
39:RF:13:SER:O	39:RF:17:ARG:NH1	2.31	0.62
46:RQ:65:PHE:HB2	46:RQ:105:GLU:HB3	1.82	0.62
9:QI:26:VAL:HG12	9:QI:61:ALA:HB3	1.80	0.62
10:QJ:6:ILE:CG2	10:QJ:97:GLU:O	2.40	0.62
35:RA:2091:U:OP1	42:RI:27:ARG:NH1	2.32	0.62
54:RY:13:VAL:HG12	54:RY:74:PRO:HA	1.81	0.62
35:YA:768:G:O2'	35:YA:1379:A:N6	2.33	0.62
41:YH:3:ARG:HH12	41:YH:65:HIS:CE1	2.17	0.62
55:YZ:128:VAL:HG23	55:YZ:160:GLY:O	1.99	0.62
7:QG:69:VAL:C	7:QG:138:LYS:CD	2.66	0.62
2:XB:19:HIS:HB2	2:XB:204:ASN:HD21	1.63	0.62
11:QK:22:HIS:HB3	11:QK:29:ILE:HG23	1.81	0.62
9:XI:20:ARG:NH2	9:XI:62:TYR:HB2	2.15	0.62
14:XN:7:ILE:HG22	14:XN:23:ARG:HD3	1.80	0.62
24:XY:83:HIS:O	24:XY:84:TYR:CG	2.53	0.62
2:QB:95:GLN:HG2	2:QB:147:LYS:CE	2.29	0.62
41:YH:9:ILE:HD11	41:YH:69:ARG:HG2	1.82	0.62
24:QY:48:LEU:HD13	24:QY:52:LEU:HD22	1.79	0.62
35:RA:1342:A:H2	35:RA:1602:U:H3	1.47	0.62
37:RD:123:ALA:HB3	37:RD:131:LEU:CD1	2.29	0.62
47:RR:97:VAL:HG22	47:RR:114:VAL:HG12	1.82	0.62
4:XD:153:ARG:HD2	4:XD:181:MET:SD	2.39	0.62
1:QA:1252:A:H61	1:QA:1285:A:H61	1.48	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:QB:230:VAL:HG12	2:QB:231:GLU:H	1.64	0.62
55:RZ:8:TYR:O	55:RZ:38:TYR:N	2.32	0.62
35:YA:2306:C:H5'	35:YA:2307:G:H5''	1.82	0.62
35:YA:2795:G:H21	35:YA:2801:A:H62	1.45	0.62
40:RG:118:ARG:O	40:RG:181:ARG:HG2	2.00	0.61
55:RZ:105:VAL:H	55:RZ:140:ASP:HB2	1.65	0.61
2:XB:47:THR:HA	2:XB:202:PRO:HG2	1.82	0.61
24:XZ:49:LYS:O	24:XZ:52:LEU:CD2	2.47	0.61
25:Y0:23:VAL:HG13	25:Y0:38:VAL:HG12	1.82	0.61
32:R7:7:PRO:HB2	35:RA:1309:G:H4'	1.83	0.61
40:RG:139:LEU:HD11	40:RG:149:VAL:HG11	1.82	0.61
42:RI:81:VAL:HG21	42:RI:88:ILE:CD1	2.29	0.61
1:QA:1240:U:C4	7:QG:32:ARG:HD2	2.35	0.61
24:QZ:72:ASP:OD1	24:QZ:73:ASP:N	2.31	0.61
35:RA:1816:G:O6	37:RD:35:LYS:NZ	2.28	0.61
25:Y0:7:LEU:HB3	46:YQ:85:LYS:HG3	1.83	0.61
37:YD:12:SER:HB3	37:YD:208:LYS:HB3	1.82	0.61
47:YR:78:LYS:HE3	47:YR:83:ILE:HD11	1.82	0.61
1:QA:1031:G:N2	1:QA:1032:A:N3	2.49	0.61
41:RH:149:ARG:HG2	41:RH:149:ARG:O	2.00	0.61
42:RI:79:ILE:HD13	42:RI:140:LEU:HD21	1.81	0.61
1:QA:924:C:O2'	1:QA:1502:A:N6	2.34	0.61
35:RA:1490:A:O2'	37:RD:99:ASP:OD1	2.17	0.61
35:RA:2392:A:H2	35:RA:2424:C:H42	1.48	0.61
35:RA:768:G:O2'	35:RA:1379:A:N6	2.33	0.61
42:RI:21:VAL:HG21	42:RI:26:ALA:HB2	1.82	0.61
42:RI:4:ILE:HG23	42:RI:18:VAL:HA	1.82	0.61
2:XB:6:THR:CG2	2:XB:7:VAL:HG13	2.30	0.61
1:QA:673:G:H5''	6:QF:87:ARG:NH1	2.16	0.61
11:QK:78:GLN:O	11:QK:103:LEU:HA	1.99	0.61
41:RH:149:ARG:HH21	41:RH:154:PRO:CB	2.14	0.61
49:RT:36:GLU:O	49:RT:36:GLU:CD	2.39	0.61
35:RA:138:G:O6	53:RX:40:LYS:NZ	2.34	0.61
24:XZ:51:ASN:OD1	24:XZ:51:ASN:N	2.32	0.61
55:YZ:128:VAL:HG22	55:YZ:132:ASN:HB3	1.81	0.61
1:QA:674:G:H2'	1:QA:675:A:H8	1.65	0.61
12:QL:28:LYS:HD3	12:QL:62:SER:HB2	1.82	0.61
18:QR:41:LYS:HD3	18:QR:42:ARG:HG3	1.81	0.61
41:RH:115:VAL:HG11	41:RH:148:ILE:HG22	1.82	0.61
41:RH:54:ARG:CD	41:RH:61:HIS:CB	2.73	0.61
3:XC:43:LEU:HD21	3:XC:91:LEU:HD11	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:XH:37:ARG:O	8:XH:41:ARG:HB2	2.01	0.61
4:QD:177:ASP:HB3	4:QD:182:LYS:HG3	1.83	0.61
35:RA:993:G:OP1	50:RU:50:ARG:NH2	2.33	0.61
1:XA:1159:U:O2'	1:XA:1160:G:N7	2.33	0.61
1:XA:1350:A:O2'	7:XG:33:ASP:OD1	2.18	0.61
4:XD:153:ARG:CD	4:XD:181:MET:SD	2.89	0.61
1:QA:217:C:O2'	1:QA:466:C:N4	2.33	0.61
24:QY:64:HIS:HA	24:QY:82:TYR:O	2.00	0.61
43:RN:115:ARG:HA	43:RN:118:LYS:HD2	1.83	0.61
1:XA:522:C:H41	12:XL:53:ARG:HH22	1.48	0.61
4:XD:194:LEU:HD12	4:XD:196:LEU:HG	1.82	0.61
16:XP:57:ARG:HH21	16:XP:79:VAL:HA	1.66	0.61
29:Y4:58:ARG:NH2	29:Y4:59:PHE:HE1	1.98	0.61
42:YI:123:LEU:N	42:YI:123:LEU:HD23	2.16	0.61
49:YT:124:ASP:OD1	49:YT:125:ARG:N	2.33	0.61
55:YZ:181:GLU:OE1	55:YZ:181:GLU:N	2.33	0.61
10:QJ:48:THR:HA	10:QJ:62:HIS:HB3	1.83	0.61
24:QY:50:HIS:O	24:QY:51:ASN:OD1	2.18	0.61
37:RD:147:LEU:HD11	37:RD:183:ARG:NH1	2.16	0.61
37:RD:17:THR:HB	37:RD:205:VAL:H	1.66	0.61
41:YH:19:VAL:HG23	41:YH:24:VAL:HG22	1.81	0.61
17:QQ:66:SER:OG	17:QQ:67:LYS:O	2.18	0.60
24:QY:48:LEU:CD1	24:QY:52:LEU:HD23	2.30	0.60
35:RA:642:G:H21	35:RA:646:A:H2	1.47	0.60
1:QA:1422:G:H4'	44:RO:49:ARG:HH22	1.65	0.60
42:YI:123:LEU:HA	42:YI:142:VAL:HG21	1.82	0.60
8:QH:25:ASP:HB3	8:QH:58:TYR:HD2	1.66	0.60
29:R4:34:GLU:OE1	29:R4:34:GLU:N	2.34	0.60
35:RA:1689:A:H62	35:RA:1698:A:H2	1.49	0.60
35:RA:1110:G:H4'	41:RH:3:ARG:HE	1.66	0.60
35:YA:987:G:O2'	35:YA:1000:A:N3	2.31	0.60
9:QI:29:ASN:OD1	9:QI:64:THR:OG1	2.19	0.60
13:QM:81:LEU:O	13:QM:89:GLY:HA3	2.01	0.60
35:RA:629:G:N3	35:RA:639:U:O2'	2.34	0.60
37:RD:182:LEU:H	37:RD:272:ALA:HB3	1.66	0.60
41:RH:6:ARG:HD2	41:RH:54:ARG:NH1	2.15	0.60
35:YA:994:C:OP1	50:YU:53:ARG:NH2	2.33	0.60
55:YZ:69:THR:HG22	55:YZ:90:VAL:HG22	1.82	0.60
4:QD:30:LYS:HG2	4:QD:35:ARG:HH21	1.67	0.60
13:QM:16:ASP:N	13:QM:16:ASP:OD1	2.33	0.60
13:QM:35:GLU:OE2	13:QM:39:ILE:N	2.34	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YA:273(E):U:H3	35:YA:363(A):A:H61	1.48	0.60
10:QJ:78:ASN:O	10:QJ:81:THR:OG1	2.20	0.60
13:QM:3:ARG:HH12	40:RG:113:ARG:HH21	1.49	0.60
19:QS:64:GLU:CG	29:R4:56:VAL:HG23	2.31	0.60
1:XA:413:G:N2	1:XA:429:U:OP2	2.34	0.60
16:XP:32:TYR:HE2	16:XP:35:LYS:HB2	1.66	0.60
24:XZ:48:LEU:C	24:XZ:52:LEU:HB2	2.21	0.60
1:QA:1266:G:N2	1:QA:1269:A:OP2	2.35	0.60
41:RH:46:GLU:HG3	41:RH:47:GLU:H	1.65	0.60
42:RI:58:LEU:O	42:RI:62:LYS:HB2	2.01	0.60
12:XL:62:SER:HB2	12:XL:64:TYR:CD2	2.35	0.60
43:YN:21:LYS:HE2	43:YN:26:LEU:HD22	1.83	0.60
13:QM:9:ILE:N	13:QM:10:PRO:CD	2.60	0.60
41:RH:50:VAL:O	41:RH:50:VAL:HG23	2.01	0.60
41:RH:79:VAL:HA	41:RH:136:ILE:HD11	1.84	0.60
1:XA:971:G:N2	1:XA:1363:A:OP2	2.33	0.60
5:XE:102:ALA:HB1	5:XE:106:PRO:HG2	1.83	0.60
10:XJ:42:THR:HG22	10:XJ:68:HIS:HA	1.84	0.60
13:XM:45:VAL:O	13:XM:48:LEU:HD22	2.02	0.60
41:YH:19:VAL:HG21	41:YH:43:VAL:HG11	1.82	0.60
1:QA:76:G:H1	1:QA:93:U:H3	1.50	0.60
13:QM:31:LYS:HA	13:QM:34:LEU:HB2	1.83	0.60
35:RA:2298:A:H62	35:RA:2318:G:H8	1.50	0.60
48:RS:97:ARG:HA	48:RS:100:ALA:HB3	1.84	0.60
2:XB:7:VAL:HB	2:XB:11:LEU:HD12	1.84	0.60
1:QA:362:G:H5''	12:QL:61:THR:HG21	1.82	0.60
1:XA:414:A:OP2	1:XA:428:G:N2	2.32	0.60
52:YW:11:ARG:NH2	52:YW:98:LYS:CG	2.65	0.60
54:YY:99:CYS:SG	54:YY:106:LEU:HD11	2.42	0.60
1:QA:410:G:H21	1:QA:432:A:H62	1.50	0.59
1:QA:468:A:OP1	16:QP:75:ARG:NH2	2.35	0.59
35:RA:586:A:H5'	39:RF:89:VAL:HG11	1.82	0.59
37:RD:147:LEU:HD21	37:RD:183:ARG:NH2	2.17	0.59
40:RG:138:GLN:CG	40:RG:139:LEU:HD12	2.31	0.59
1:XA:765:G:N2	1:XA:813:U:OP2	2.35	0.59
20:XT:26:ASN:HA	20:XT:29:LYS:HG2	1.83	0.59
2:QB:8:LYS:HD3	2:QB:9:GLU:H	1.68	0.59
7:QG:20:ASP:HB3	7:QG:23:VAL:HG12	1.82	0.59
10:QJ:78:ASN:OD1	10:QJ:80:LYS:HB2	2.03	0.59
38:RE:77:ILE:HG21	38:RE:195:LEU:HD22	1.84	0.59
40:RG:48:GLU:O	40:RG:48:GLU:CD	2.40	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:RH:54:ARG:CD	41:RH:61:HIS:HB3	2.29	0.59
12:XL:62:SER:HB2	12:XL:64:TYR:HD2	1.67	0.59
35:YA:2068:U:H3	35:YA:2430:A:H2	1.50	0.59
41:YH:44:VAL:H	41:YH:52:VAL:HG22	1.67	0.59
28:R3:40:THR:HG22	28:R3:42:ALA:H	1.67	0.59
36:RB:49:C:OP2	48:RS:30:ARG:NH1	2.35	0.59
1:XA:1422:G:H5'	44:YO:48:PRO:HB3	1.83	0.59
29:R4:36:CYS:HB2	29:R4:39:CYS:SG	2.42	0.59
45:RP:19:VAL:HG23	45:RP:27:HIS:HB3	1.84	0.59
26:Y1:89:GLU:HA	26:Y1:92:LYS:HB2	1.83	0.59
35:YA:1779:U:OP2	35:YA:1784:A:N6	2.33	0.59
35:YA:2298:A:H62	35:YA:2318:G:H8	1.49	0.59
19:QS:31:ILE:HB	19:QS:49:ILE:HA	1.83	0.59
44:YO:120:GLU:OE1	49:YT:67:SER:OG	2.18	0.59
3:QC:150:LYS:HE3	3:QC:167:TRP:HE1	1.67	0.59
34:R9:11:CYS:HB2	34:R9:13:LYS:HE2	1.84	0.59
38:RE:23:VAL:HG12	38:RE:185:LYS:HA	1.85	0.59
38:RE:36:ARG:HH12	38:RE:88:GLY:HA2	1.66	0.59
35:YA:704:G:O2'	35:YA:726:G:N2	2.32	0.59
22:QW:51:C:H42	22:QW:63:G:H1	1.49	0.59
24:QY:44:LYS:CE	24:QY:59:ARG:NH1	2.66	0.59
25:R0:26:TYR:HE2	35:RA:857:C:H1'	1.67	0.59
29:R4:6:HIS:HE2	40:RG:67:LYS:H	1.51	0.59
48:RS:11:LYS:HE2	48:RS:91:PRO:CG	2.32	0.59
2:XB:127:ILE:HD12	2:XB:130:ARG:HB2	1.85	0.59
10:XJ:98:ILE:O	10:XJ:99:LYS:HD3	2.03	0.59
35:RA:2010:G:H5''	52:RW:42:ARG:HB2	1.85	0.59
35:RA:2816:C:O2	35:RA:2883:A:O2'	2.19	0.59
40:RG:37:VAL:HG23	40:RG:159:VAL:HG12	1.85	0.59
41:RH:24:VAL:HG11	41:RH:72:ILE:HD12	1.85	0.59
35:YA:1019:U:H3	35:YA:1142(A):A:H62	1.50	0.59
42:YI:92:VAL:HG23	42:YI:120:ILE:HG23	1.85	0.59
36:RB:80:U:H2'	36:RB:81:G:H21	1.67	0.59
39:RF:116:ASP:OD2	45:RP:1:MET:N	2.32	0.59
42:RI:127:VAL:O	42:RI:127:VAL:HG13	2.03	0.59
1:XA:544:G:OP1	4:XD:59:ARG:NH2	2.36	0.59
1:XA:1009:G:H1	1:XA:1020:U:H3	1.51	0.59
1:XA:728:A:N6	15:XO:54:ARG:HD3	2.18	0.59
3:XC:131:ARG:HH12	3:XC:168:ALA:HB2	1.68	0.59
1:QA:544:G:OP1	4:QD:59:ARG:NH2	2.35	0.58
10:QJ:38:ILE:HD11	10:QJ:71:LEU:HB3	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:QL:76:ASN:HD21	12:QL:108:ALA:H	1.47	0.58
35:RA:1300:U:H4'	35:RA:1301:A:H5'	1.85	0.58
7:XG:49:ILE:HD13	7:XG:118:VAL:HG12	1.84	0.58
24:XY:2:LYS:HB2	24:XY:74:SER:HB3	1.84	0.58
1:QA:1316:G:N2	1:QA:1319:A:OP2	2.36	0.58
2:QB:135:GLN:OE1	2:QB:135:GLN:N	2.36	0.58
7:QG:56:GLN:OE1	7:QG:57:GLU:N	2.35	0.58
36:RB:45:A:OP2	40:RG:96:ARG:NH2	2.35	0.58
37:RD:75:ILE:C	37:RD:118:VAL:HG22	2.24	0.58
37:RD:76:PRO:N	37:RD:118:VAL:CG2	2.66	0.58
41:RH:86:GLU:O	41:RH:86:GLU:CG	2.50	0.58
55:RZ:11:GLU:OE2	55:RZ:35:ARG:NH2	2.36	0.58
2:XB:223:ILE:HA	2:XB:226:ARG:HG2	1.83	0.58
28:Y3:39:ASP:OD1	28:Y3:44:ARG:NH2	2.36	0.58
55:YZ:6:LYS:HG3	55:YZ:8:TYR:HE2	1.68	0.58
55:YZ:94:GLU:HG2	55:YZ:95:PRO:HD2	1.86	0.58
3:QC:153:VAL:HG22	3:QC:198:VAL:HG22	1.84	0.58
1:XA:710:G:H5''	6:XF:54:LYS:HE2	1.85	0.58
17:XQ:66:SER:O	17:XQ:70:ARG:NH1	2.36	0.58
20:XT:11:SER:HB3	20:XT:14:LYS:HE2	1.85	0.58
33:Y8:29:LYS:O	33:Y8:31:HIS:N	2.30	0.58
34:Y9:6:SER:OG	34:Y9:6:SER:O	2.20	0.58
35:YA:458:G:N2	35:YA:470:A:OP2	2.28	0.58
19:QS:52:TYR:HD2	19:QS:57:HIS:CG	2.21	0.58
35:RA:2306:C:H5'	35:RA:2307:G:H5''	1.84	0.58
33:R8:8:LYS:NZ	35:RA:243:U:OP2	2.31	0.58
35:RA:2848:G:O2'	35:RA:2867:G:N2	2.36	0.58
20:XT:85:MET:HA	20:XT:88:VAL:HG22	1.86	0.58
24:XZ:59:ARG:HG2	24:XZ:65:ARG:NE	2.18	0.58
38:YE:167:VAL:HG22	38:YE:170:LEU:HD11	1.86	0.58
39:YF:199:TRP:O	39:YF:203:GLN:HB2	2.04	0.58
3:QC:164:ARG:NH1	3:QC:166:GLU:OE2	2.37	0.58
10:QJ:6:ILE:CD1	10:QJ:99:LYS:N	2.63	0.58
33:R8:18:ALA:HB3	35:RA:651:G:H5'	1.86	0.58
35:RA:726:G:HO2'	35:RA:727:A:H8	1.51	0.58
2:XB:213:LEU:C	2:XB:213:LEU:HD23	2.23	0.58
22:XW:21:A:H61	22:XW:46:G:H2'	1.69	0.58
50:YU:92:ARG:CD	51:YV:11:GLN:OE1	2.50	0.58
2:QB:95:GLN:CB	2:QB:147:LYS:HE3	2.34	0.58
3:QC:108:ASN:ND2	3:QC:144:SER:OG	2.36	0.58
38:RE:141:ILE:CA	38:RE:154:LYS:HE2	2.34	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:QG:69:VAL:O	7:QG:138:LYS:CD	2.48	0.58
29:R4:13:ARG:N	29:R4:24:THR:OG1	2.29	0.58
2:XB:163:PHE:HA	2:XB:185:ILE:O	2.04	0.58
4:XD:30:LYS:HA	4:XD:35:ARG:HE	1.67	0.58
35:YA:1689:A:H62	35:YA:1698:A:H2	1.52	0.58
35:YA:138:G:N2	53:YX:44:GLU:OE1	2.33	0.58
35:RA:1980:G:O2'	35:RA:1982:C:OP2	2.21	0.58
1:XA:742:G:OP2	15:XO:35:ARG:NH2	2.36	0.58
7:XG:138:LYS:O	7:XG:142:GLU:HG3	2.04	0.58
17:XQ:11:VAL:HG12	17:XQ:85:VAL:HG12	1.85	0.58
40:YG:39:ILE:HG12	40:YG:157:ILE:HD12	1.86	0.58
5:QE:143:ARG:NE	8:QH:77:GLU:OE2	2.37	0.58
13:QM:44:ARG:O	13:QM:48:LEU:HD21	2.04	0.58
7:XG:71:PRO:HB3	7:XG:138:LYS:HG3	1.85	0.58
35:YA:1980:G:O2'	35:YA:1982:C:OP2	2.22	0.58
35:YA:2816:C:O2	35:YA:2883:A:O2'	2.21	0.58
9:XI:18:PHE:O	9:XI:61:ALA:HA	2.04	0.57
55:YZ:9:TYR:HE2	55:YZ:61:LEU:HD23	1.67	0.57
34:R9:11:CYS:HB2	34:R9:13:LYS:H	1.69	0.57
30:R5:3:LYS:HE3	35:RA:2577:A:H5'	1.87	0.57
35:RA:2680:C:H5'	38:RE:189:PRO:HA	1.85	0.57
41:RH:54:ARG:CD	41:RH:61:HIS:HB2	2.30	0.57
48:RS:24:LEU:HB2	48:RS:85:VAL:HG12	1.86	0.57
1:XA:618:C:H5'	1:XA:619:U:H5''	1.85	0.57
2:XB:19:HIS:O	2:XB:39:ILE:HD13	2.04	0.57
10:XJ:25:GLU:HA	10:XJ:28:ARG:HG2	1.85	0.57
22:XV:76:A:O3'	35:YA:2602:A:N6	2.38	0.57
22:XW:16:C:H4'	22:XW:60:U:H4'	1.86	0.57
24:XZ:59:ARG:HA	24:XZ:65:ARG:HD3	1.85	0.57
35:YA:2299:G:OP1	40:YG:75:LYS:NZ	2.37	0.57
12:QL:47:LYS:HB3	12:QL:48:PRO:HD3	1.86	0.57
13:QM:3:ARG:HA	13:QM:7:VAL:O	2.04	0.57
35:RA:1266:G:O5'	52:RW:15:ARG:NH2	2.36	0.57
1:XA:925:G:H1	1:XA:1391:U:H3	1.50	0.57
2:XB:54:THR:HG22	2:XB:58:ILE:HD11	1.87	0.57
26:Y1:50:ARG:HG2	26:Y1:59:THR:HG23	1.85	0.57
28:Y3:29:ARG:NH2	35:YA:932:G:OP2	2.36	0.57
40:YG:77:ILE:HB	40:YG:82:LEU:CD1	2.30	0.57
21:QU:12:LYS:HB2	21:QU:22:ARG:HD3	1.84	0.57
24:QY:44:LYS:HD2	24:QY:59:ARG:NH1	2.15	0.57
48:RS:78:LEU:HD11	48:RS:107:GLU:HB3	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:XE:33:VAL:HG13	5:XE:112:LEU:HD12	1.85	0.57
24:XZ:48:LEU:CD1	24:XZ:52:LEU:CG	2.83	0.57
38:YE:143:ASN:HB2	38:YE:147:PRO:HD2	1.87	0.57
39:RF:185:ASP:OD1	39:RF:188:ARG:NH1	2.36	0.57
51:RV:39:LEU:HD12	51:RV:47:VAL:HG22	1.85	0.57
2:XB:217:ARG:CG	2:XB:217:ARG:HH11	2.13	0.57
29:Y4:58:ARG:CG	29:Y4:59:PHE:H	2.18	0.57
41:YH:5:GLY:HA2	41:YH:69:ARG:HG3	1.85	0.57
24:QY:17:GLN:HG2	24:QY:24:VAL:HG11	1.87	0.57
40:RG:17:PRO:HA	40:RG:20:ILE:HD12	1.87	0.57
2:XB:87:ARG:NH2	2:XB:220:ASP:OD2	2.37	0.57
20:XT:65:LYS:HA	20:XT:68:LYS:HG3	1.85	0.57
32:Y7:11:LYS:HE2	35:YA:686:G:H5''	1.85	0.57
45:YP:94:GLU:HG3	45:YP:124:LYS:HB3	1.87	0.57
2:QB:21:ARG:HB3	2:QB:39:ILE:HD13	1.86	0.57
24:XY:7:GLU:OE2	24:XZ:35:ARG:HD3	2.05	0.57
51:YV:58:VAL:HG13	51:YV:100:ARG:HH12	1.70	0.57
1:QA:1351:U:H3	1:QA:1371:G:H1	1.52	0.57
24:QZ:60:ILE:HD11	24:QZ:66:LEU:HD13	1.87	0.57
35:RA:918:A:N3	36:RB:80:U:O2'	2.36	0.57
55:RZ:45:ASP:O	55:RZ:49:ARG:HG3	2.04	0.57
41:YH:28:GLY:HA3	41:YH:79:VAL:HB	1.85	0.57
40:RG:113:ARG:HH12	40:RG:142:PRO:HA	1.68	0.57
41:RH:24:VAL:HG21	41:RH:72:ILE:CD1	2.34	0.57
48:YS:105:ALA:HB1	48:YS:110:LEU:HD23	1.87	0.57
1:QA:1224:G:O2'	1:QA:1322:C:OP1	2.22	0.57
1:QA:413:G:N2	1:QA:429:U:OP2	2.37	0.57
7:QG:69:VAL:HA	7:QG:138:LYS:CE	2.35	0.57
13:QM:102:ARG:HH21	13:QM:104:ARG:HD2	1.70	0.57
35:RA:10:G:N2	35:RA:2802:G:OP1	2.38	0.57
37:YD:17:THR:HB	37:YD:205:VAL:H	1.69	0.57
40:YG:118:ARG:O	40:YG:118:ARG:HD2	2.05	0.57
45:YP:65:ARG:O	45:YP:68:GLN:NE2	2.38	0.57
50:YU:92:ARG:CD	51:YV:11:GLN:CB	2.75	0.57
13:QM:65:LYS:HB2	13:QM:69:GLU:HG3	1.86	0.56
14:QN:26:ARG:HH21	14:QN:47:LEU:HD21	1.70	0.56
35:RA:84:A:N6	35:RA:102:G:O2'	2.38	0.56
41:RH:58:GLU:HB2	41:RH:61:HIS:CG	2.40	0.56
1:XA:1534:A:N1	23:XX:10:G:C6	2.72	0.56
2:XB:16:HIS:O	2:XB:17:PHE:CD2	2.58	0.56
35:RA:300:A:OP1	54:RY:86:ARG:NH2	2.38	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:RG:11:TYR:HA	40:RG:15:VAL:HG23	1.87	0.56
38:RE:181:LEU:HD11	49:RT:7:ILE:HD12	1.87	0.56
1:XA:673:G:H2'	1:XA:674:G:C8	2.40	0.56
1:QA:953:G:N7	13:QM:104:ARG:NH2	2.52	0.56
35:RA:2141:G:H1	35:RA:2150:U:H3	1.53	0.56
55:RZ:33:LEU:HD12	55:RZ:34:ASN:H	1.70	0.56
11:XK:41:THR:HG21	11:XK:71:LYS:HB3	1.86	0.56
29:Y4:14:ILE:HB	29:Y4:22:ILE:HB	1.88	0.56
1:QA:1231:G:O3'	9:QI:126:SER:OG	2.22	0.56
16:QP:17:TYR:HE1	16:QP:41:PRO:HG3	1.71	0.56
42:RI:109:ILE:HG23	42:RI:130:TYR:CZ	2.40	0.56
41:YH:61:HIS:HD2	41:YH:64:LEU:HD12	1.71	0.56
42:RI:72:LEU:HD11	42:RI:101:LEU:HD11	1.88	0.56
25:Y0:46:LYS:HG2	25:Y0:47:PRO:HD2	1.87	0.56
30:Y5:16:ARG:NH2	35:YA:517:C:OP1	2.37	0.56
35:YA:2467:C:O2	46:YQ:124:LYS:NZ	2.38	0.56
4:QD:85:LYS:HG2	4:QD:92:VAL:HG11	1.88	0.56
41:RH:8:PRO:HD2	41:RH:69:ARG:CZ	2.35	0.56
35:YA:1266:G:O5'	52:YW:15:ARG:NH2	2.38	0.56
35:YA:996:A:OP2	50:YU:92:ARG:NH2	2.27	0.56
24:QY:44:LYS:NZ	24:QY:59:ARG:HH12	2.03	0.56
42:RI:113:ARG:HG3	42:RI:113:ARG:O	2.06	0.56
5:XE:15:ARG:HD2	5:XE:26:PHE:CG	2.41	0.56
10:XJ:6:ILE:O	10:XJ:71:LEU:HA	2.06	0.56
24:XZ:48:LEU:HD13	24:XZ:52:LEU:CG	2.35	0.56
35:YA:336:C:O2'	54:YY:35:TYR:OH	2.23	0.56
46:YQ:48:GLU:HG3	46:YQ:51:ARG:HE	1.70	0.56
5:QE:42:GLY:HA3	5:QE:66:MET:HG2	1.86	0.56
8:QH:51:VAL:HG11	8:QH:60:ARG:HH21	1.70	0.56
12:QL:53:ARG:HG3	12:QL:93:LEU:HD21	1.88	0.56
15:QO:7:GLU:HA	15:QO:10:LYS:HG2	1.86	0.56
25:R0:60:PHE:HE1	25:R0:62:LEU:CD2	2.19	0.56
38:RE:61:ARG:N	38:RE:62:PRO:HD2	2.21	0.56
42:RI:136:VAL:HG13	42:RI:136:VAL:O	2.04	0.56
38:YE:23:VAL:HG12	38:YE:185:LYS:HA	1.86	0.56
51:YV:37:VAL:HG11	51:YV:40:LEU:HG	1.88	0.56
1:QA:1178:G:N2	1:QA:1181:G:N7	2.54	0.56
41:RH:17:VAL:HG23	41:RH:45:VAL:HG11	1.88	0.56
43:RN:95:PRO:O	43:RN:97:ARG:N	2.39	0.56
48:RS:66:ALA:CB	48:RS:97:ARG:HB2	2.36	0.56
55:RZ:6:LYS:HG3	55:RZ:8:TYR:HE1	1.71	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:XH:91:ARG:NE	17:XQ:32:TYR:O	2.36	0.56
13:XM:102:ARG:HE	13:XM:105:THR:HG22	1.71	0.56
25:Y0:77:ARG:NH2	35:YA:857:C:OP2	2.38	0.56
39:YF:198:ALA:HA	39:YF:201:VAL:HG22	1.87	0.56
35:YA:2305:A:H5''	40:YG:134:GLY:HA3	1.88	0.56
8:QH:9:MET:HG3	8:QH:26:VAL:HG21	1.88	0.56
10:QJ:6:ILE:HD12	10:QJ:98:ILE:N	2.20	0.56
29:R4:31:ILE:HD12	40:RG:142:PRO:HB2	1.88	0.56
41:RH:70:THR:O	41:RH:70:THR:HG23	2.05	0.56
35:RA:1649:G:O2'	47:RR:107:ASP:OD1	2.21	0.56
54:RY:44:ILE:HG12	54:RY:64:GLU:HG2	1.87	0.56
1:XA:1302:U:O4	13:XM:14:ARG:NH1	2.39	0.56
35:YA:2572:A:H62	38:YE:145:LYS:HE2	1.71	0.56
35:YA:993:G:OP1	50:YU:50:ARG:NH2	2.36	0.56
40:YG:32:PRO:HB2	40:YG:172:LEU:HD12	1.87	0.56
3:QC:70:VAL:HG12	3:QC:72:LYS:H	1.71	0.56
10:QJ:76:ASN:ND2	10:QJ:78:ASN:HD22	2.04	0.56
41:RH:68:THR:HA	41:RH:71:LEU:HD21	1.87	0.56
24:XZ:48:LEU:HB2	24:XZ:52:LEU:HB3	1.88	0.56
26:Y1:3:LYS:NZ	35:YA:1364:G:OP1	2.32	0.56
35:RA:1728:G:H8	35:RA:1732:A:H62	1.54	0.55
35:RA:2393:A:H4'	45:RP:62:LEU:H	1.70	0.55
38:RE:17:ASP:O	38:RE:19:ARG:N	2.38	0.55
1:XA:1256:A:OP2	3:XC:26:LYS:NZ	2.38	0.55
3:XC:74:GLY:HA2	3:XC:77:ILE:HG12	1.87	0.55
14:XN:23:ARG:NH1	14:XN:28:GLY:O	2.38	0.55
32:Y7:24:THR:HG23	32:Y7:27:GLY:H	1.70	0.55
35:YA:2495:G:H5''	46:YQ:82:ARG:HG2	1.88	0.55
1:QA:1014:A:H4'	19:QS:14:HIS:CE1	2.41	0.55
1:QA:1073:U:O2	2:QB:104:ASN:ND2	2.39	0.55
35:RA:2130:U:O2	35:RA:2133:G:O2'	2.24	0.55
37:RD:85:ASP:OD2	37:RD:88:ARG:NH1	2.40	0.55
26:Y1:53:VAL:HG21	26:Y1:94:LEU:HD11	1.88	0.55
35:YA:668:G:H2'	35:YA:670:A:H62	1.71	0.55
35:YA:443:A:C6	39:YF:45:ARG:HD2	2.41	0.55
42:YI:92:VAL:CB	42:YI:120:ILE:HG21	2.19	0.55
35:YA:906:G:O2'	46:YQ:67:ARG:NH2	2.36	0.55
7:QG:123:GLU:OE2	7:QG:133:GLY:N	2.36	0.55
40:RG:145:THR:O	40:RG:146:TYR:CG	2.60	0.55
41:RH:68:THR:HA	41:RH:71:LEU:CD2	2.36	0.55
46:RQ:134:ARG:HH12	55:RZ:122:ARG:CZ	2.19	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:RV:34:GLU:HG2	51:RV:56:SER:HB3	1.88	0.55
2:XB:209:ARG:NH2	2:XB:238:LEU:O	2.39	0.55
35:YA:1678:G:N2	35:YA:1990:C:O2	2.40	0.55
41:YH:88:LEU:O	41:YH:88:LEU:HD12	2.06	0.55
55:YZ:57:ILE:O	55:YZ:69:THR:OG1	2.22	0.55
5:QE:43:LEU:O	5:QE:65:ASN:ND2	2.40	0.55
25:R0:23:VAL:HG21	35:RA:857:C:H4'	1.89	0.55
25:R0:55:ARG:NH2	35:RA:2364:C:OP1	2.38	0.55
35:RA:2795:G:H21	35:RA:2801:A:H62	1.55	0.55
35:RA:307:G:H21	35:RA:330:A:H62	1.54	0.55
24:XY:1:MET:HE2	24:XY:35:ARG:HA	1.88	0.55
24:XZ:59:ARG:CZ	24:XZ:65:ARG:NH2	2.70	0.55
51:YV:29:PRO:HB3	51:YV:63:GLY:HA2	1.88	0.55
1:QA:967:C:H4'	9:QI:125:TYR:HE1	1.72	0.55
9:QI:42:ARG:NH1	9:QI:71:SER:OG	2.40	0.55
13:XM:49:THR:HG22	13:XM:51:ALA:H	1.70	0.55
14:XN:34:TYR:CE2	14:XN:44:LEU:CD1	2.90	0.55
33:Y8:12:LYS:NZ	35:YA:249:C:O2	2.36	0.55
44:YO:80:ASP:OD2	49:YT:64:ARG:NH2	2.39	0.55
11:QK:127:LYS:HG2	23:QX:9:G:H3'	1.89	0.55
35:RA:577:G:O2'	35:RA:1254:A:OP1	2.23	0.55
55:RZ:58:VAL:HA	55:RZ:68:PRO:HA	1.87	0.55
1:XA:582:U:OP2	1:XA:758:G:N1	2.26	0.55
2:XB:9:GLU:HB3	2:XB:48:MET:CE	2.36	0.55
20:XT:60:GLU:HB2	20:XT:81:LYS:HD2	1.89	0.55
51:YV:62:LEU:HD21	51:YV:95:LEU:HB2	1.89	0.55
55:YZ:13:GLU:HB3	55:YZ:18:LEU:HD21	1.87	0.55
1:QA:673:G:H2'	1:QA:674:G:C8	2.41	0.55
2:QB:136:VAL:HG23	2:QB:139:LYS:HB2	1.89	0.55
2:QB:22:LYS:HD3	2:QB:40:HIS:NE2	2.21	0.55
10:QJ:6:ILE:HD13	10:QJ:99:LYS:H	1.72	0.55
44:RO:80:ASP:OD2	49:RT:64:ARG:NH2	2.40	0.55
12:XL:53:ARG:NH1	12:XL:92:ASP:OD1	2.40	0.55
15:XO:7:GLU:HA	15:XO:10:LYS:HD2	1.89	0.55
1:XA:280:C:N4	17:XQ:91:ARG:HH12	2.05	0.55
37:YD:153:ALA:O	37:YD:157:ARG:NH2	2.36	0.55
43:YN:21:LYS:HD3	43:YN:138:LEU:CD2	2.36	0.55
33:Y8:57:ARG:NE	45:YP:48:PRO:O	2.38	0.55
1:QA:1065:U:O5'	1:QA:1190:G:N2	2.40	0.55
2:QB:209:ARG:NH2	2:QB:239:VAL:HG22	2.21	0.55
3:QC:88:ARG:HB3	3:QC:99:VAL:HG11	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:QI:82:ALA:HA	9:QI:85:LEU:HD12	1.89	0.55
40:RG:138:GLN:HB3	40:RG:153:ARG:O	2.07	0.55
1:XA:1247:U:H3	1:XA:1290:G:H1	1.54	0.55
55:YZ:103:ARG:HG3	55:YZ:136:PHE:HB2	1.88	0.55
12:QL:60:LEU:HD12	12:QL:62:SER:H	1.72	0.55
35:RA:1667:G:O2'	35:RA:1669:A:N6	2.39	0.55
40:RG:15:VAL:HG13	40:RG:175:LEU:CB	2.36	0.55
35:RA:994:C:OP1	50:RU:53:ARG:NH1	2.40	0.55
55:RZ:24:LEU:HB2	55:RZ:41:LEU:HB3	1.88	0.55
5:XE:139:LEU:HA	5:XE:142:LEU:HD12	1.89	0.55
2:QB:93:VAL:HG21	2:QB:97:TRP:HD1	1.71	0.55
13:QM:10:PRO:C	13:QM:10:PRO:N	2.55	0.55
28:R3:7:LYS:HE3	28:R3:32:GLN:HA	1.88	0.55
35:RA:607:U:H3	35:RA:621:A:H2	1.54	0.55
48:RS:30:ARG:CG	48:RS:97:ARG:HH21	2.20	0.55
55:RZ:67:LEU:HD12	55:RZ:90:VAL:HG21	1.87	0.55
1:XA:1238:A:C8	1:XA:1301:U:O4	2.59	0.55
1:XA:946:A:H2'	1:XA:947:G:C8	2.41	0.55
11:XK:24:SER:HG	11:XK:27:ASN:H	1.54	0.55
1:QA:186(B):C:H2'	1:QA:186(C):G:H8	1.72	0.54
1:QA:474:G:OP2	16:QP:75:ARG:NH1	2.32	0.54
41:RH:52:VAL:O	41:RH:69:ARG:NH2	2.40	0.54
42:RI:14:ASP:O	42:RI:16:GLY:N	2.36	0.54
54:RY:102:CYS:SG	54:RY:103:GLY:N	2.80	0.54
9:XI:46:ALA:HA	9:XI:78:LYS:HB3	1.87	0.54
42:YI:91:SER:OG	42:YI:119:PRO:CB	2.56	0.54
42:RI:123:LEU:HD23	42:RI:144:VAL:CG1	2.37	0.54
48:RS:11:LYS:HG3	48:RS:91:PRO:HD3	1.89	0.54
1:XA:455:C:H42	1:XA:477:G:H1	1.55	0.54
24:XY:4:ILE:HD11	24:XY:74:SER:HB2	1.88	0.54
51:YV:1:MET:HA	51:YV:42:GLY:HA3	1.89	0.54
35:YA:338:G:OP1	54:YY:4:LYS:NZ	2.39	0.54
1:QA:689:C:H3'	1:QA:690:G:H21	1.71	0.54
19:QS:10:PHE:HE1	19:QS:16:LEU:HD13	1.70	0.54
35:RA:2100:G:H1	35:RA:2189:U:H3	1.54	0.54
44:RO:22:ILE:HD11	44:RO:42:SER:HB2	1.90	0.54
46:RQ:109:VAL:HG12	46:RQ:113:GLN:HG3	1.89	0.54
18:XR:32:ARG:HA	18:XR:69:THR:HG21	1.89	0.54
9:QI:27:THR:O	9:QI:27:THR:OG1	2.23	0.54
13:QM:40:ASN:OD1	13:QM:41:PRO:HD2	2.06	0.54
1:QA:1312:G:H5'	19:QS:5: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:R2:22:GLU:HG2	27:R2:64:LEU:HD11	1.89	0.54
25:R0:24:LYS:HG3	35:RA:2355:C:H4'	1.88	0.54
41:RH:14:GLY:O	41:RH:16:SER:OG	2.26	0.54
45:RP:96:THR:HA	45:RP:126:VAL:HG22	1.88	0.54
4:XD:17:VAL:HG21	4:XD:63:LYS:HD2	1.89	0.54
38:YE:53:PRO:HA	38:YE:75:VAL:HG12	1.90	0.54
52:YW:4:LYS:HE2	52:YW:6:ILE:HD11	1.89	0.54
4:QD:65:ARG:HD3	4:QD:72:GLU:OE1	2.08	0.54
11:QK:62:GLN:HB3	11:QK:93:GLN:HG2	1.89	0.54
13:QM:31:LYS:O	13:QM:34:LEU:N	2.40	0.54
30:R5:48:GLU:HA	30:R5:60:VAL:HG11	1.89	0.54
35:RA:1139:G:H21	35:RA:1143:A:H8	1.56	0.54
35:RA:2135:A:H62	35:RA:2156:G:H21	1.55	0.54
35:RA:2306:C:N4	40:RG:42:GLY:O	2.40	0.54
35:RA:956:G:OP2	46:RQ:14:ARG:NH2	2.40	0.54
1:XA:1299:A:N6	1:XA:1301:U:N3	2.52	0.54
4:XD:98:GLU:OE1	4:XD:103:ASN:ND2	2.41	0.54
6:XF:46:ARG:HD3	6:XF:60:PHE:CD2	2.42	0.54
1:XA:1239:A:O2'	7:XG:114:ARG:O	2.22	0.54
1:XA:279:A:OP2	17:XQ:95:TYR:OH	2.25	0.54
55:YZ:133:ILE:HD12	55:YZ:133:ILE:O	2.06	0.54
3:QC:14:ILE:HD11	3:QC:178:LEU:HD22	1.89	0.54
17:QQ:17:LYS:NZ	17:QQ:47:PRO:O	2.39	0.54
35:RA:481:G:O2'	35:RA:506:G:N2	2.41	0.54
51:RV:62:LEU:HD11	51:RV:95:LEU:HG	1.89	0.54
35:YA:2141:G:O6	35:YA:2150:U:O4	2.24	0.54
49:YT:129:ARG:HG3	49:YT:132:LYS:CE	2.36	0.54
53:YX:53:LYS:NZ	53:YX:55:ASN:OD1	2.40	0.54
1:QA:861:G:HO2'	1:QA:874:G:HO2'	1.56	0.54
8:QH:87:SER:OG	8:QH:87:SER:O	2.22	0.54
15:QO:87:ILE:HG22	15:QO:88:ARG:H	1.73	0.54
35:RA:24:G:O2'	52:RW:78:GLU:O	2.23	0.54
11:XK:62:GLN:HB3	11:XK:93:GLN:HG3	1.90	0.54
34:Y9:19:ARG:HG2	35:YA:2756:U:H5''	1.88	0.54
55:YZ:157:LEU:HG	55:YZ:161:VAL:HG23	1.88	0.54
3:QC:35:GLU:CB	3:QC:35:GLU:CD	2.72	0.54
24:QZ:34:THR:CG2	24:QZ:68:TYR:CE1	2.91	0.54
29:R4:42:PHE:O	29:R4:42:PHE:HD1	1.91	0.54
35:RA:1693:U:O2	37:RD:14:ARG:NH1	2.40	0.54
35:RA:372:G:HO2'	35:RA:400:G:H1	1.53	0.54
37:RD:121:PRO:HB3	37:RD:135:PHE:HE2	1.69	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:RF:143:ALA:HB1	39:RF:148:LEU:HB2	1.89	0.54
42:RI:62:LYS:HG3	42:RI:133:HIS:CE1	2.43	0.54
4:XD:20:TYR:CD2	4:XD:26:CYS:HB3	2.37	0.54
24:XY:7:GLU:OE2	24:XZ:35:ARG:CD	2.55	0.54
35:YA:2141:G:N2	35:YA:2150:U:O2	2.34	0.54
35:YA:321:G:O2'	35:YA:340:A:N3	2.41	0.54
41:YH:54:ARG:HB3	41:YH:65:HIS:ND1	2.22	0.54
47:YR:22:ARG:O	47:YR:26:LYS:HG2	2.07	0.54
7:QG:89:MET:SD	7:QG:155:ARG:HB2	2.48	0.54
9:QI:105:ASP:CG	9:QI:107:ARG:HE	2.11	0.54
24:QZ:26:LYS:O	24:QZ:30:LEU:HD12	2.08	0.54
24:QZ:44:LYS:HE2	24:QZ:59:ARG:HD3	1.89	0.54
35:RA:1286:A:O2'	35:RA:1288:U:OP2	2.23	0.54
35:RA:1857:G:N2	35:RA:1885:A:H62	2.03	0.54
44:RO:112:MET:HA	44:RO:115:VAL:HG22	1.89	0.54
1:XA:1356:G:H2'	1:XA:1357:A:C8	2.43	0.54
1:XA:254:G:O2'	17:XQ:16:GLN:O	2.24	0.54
35:YA:1011:G:OP2	50:YU:66:ASN:ND2	2.40	0.54
38:YE:36:ARG:NH2	38:YE:89:ASP:OD2	2.38	0.54
2:QB:209:ARG:HH22	2:QB:237:ALA:N	2.05	0.54
7:QG:60:LYS:HE3	7:QG:63:LYS:HD2	1.89	0.54
13:QM:65:LYS:NZ	29:R4:52:THR:OG1	2.40	0.54
35:RA:2853:C:H2'	35:RA:2854:G:H8	1.72	0.54
42:RI:81:VAL:HG21	42:RI:88:ILE:HD11	1.90	0.54
49:RT:50:ILE:HD11	49:RT:100:TYR:HA	1.88	0.54
55:RZ:152:ALA:HB3	55:RZ:167:PRO:HA	1.89	0.54
2:XB:101:MET:HA	2:XB:108:ILE:HG13	1.90	0.54
35:YA:2445:G:OP1	39:YF:74:ARG:NH1	2.39	0.54
25:R0:74:ARG:NH2	36:RB:12:C:N3	2.56	0.53
35:YA:2291:U:O2'	35:YA:2374:C:O2	2.25	0.53
35:YA:583:G:OP2	50:YU:10:ARG:NH1	2.39	0.53
41:YH:10:PRO:N	41:YH:10:PRO:C	2.57	0.53
1:QA:254:G:O2'	17:QQ:16:GLN:O	2.25	0.53
1:QA:878:G:H5'	8:QH:89:PRO:HG2	1.90	0.53
2:QB:73:THR:OG1	2:QB:170:GLU:OE1	2.21	0.53
19:QS:44:MET:O	19:QS:47:HIS:ND1	2.32	0.53
26:R1:51:VAL:HG11	26:R1:74:VAL:HG21	1.90	0.53
37:RD:146:GLU:HB2	37:RD:189:CYS:HB3	1.90	0.53
41:RH:149:ARG:HH21	41:RH:154:PRO:HB2	1.73	0.53
27:Y2:40:SER:OG	27:Y2:41:ILE:N	2.40	0.53
35:YA:1667:G:O2'	35:YA:1669:A:N6	2.41	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:YE:14:ILE:CD1	38:YE:173:VAL:HG11	2.38	0.53
41:YH:54:ARG:HH21	41:YH:57:ASP:HA	1.72	0.53
35:YA:1035:U:OP1	41:YH:59:ARG:NE	2.41	0.53
9:QI:128:ARG:NH2	22:QV:33:U:OP2	2.39	0.53
12:QL:47:LYS:CB	12:QL:48:PRO:CD	2.85	0.53
25:R0:48:GLY:O	25:R0:80:HIS:ND1	2.42	0.53
35:RA:1105:U:H2'	35:RA:1106:G:H8	1.73	0.53
35:RA:958:U:OP2	46:RQ:14:ARG:NH1	2.41	0.53
43:RN:22:THR:HG23	43:RN:62:VAL:HG23	1.89	0.53
3:XC:164:ARG:NH1	3:XC:166:GLU:OE2	2.42	0.53
1:XA:728:A:N6	15:XO:54:ARG:CD	2.71	0.53
55:YZ:67:LEU:HD22	55:YZ:90:VAL:HG11	1.90	0.53
10:QJ:54:PHE:CD2	10:QJ:55:LYS:HB3	2.43	0.53
13:QM:45:VAL:HA	13:QM:48:LEU:HG	1.89	0.53
35:RA:1080:C:N4	35:RA:1088:A:OP1	2.41	0.53
40:RG:117:PHE:O	40:RG:117:PHE:HD2	1.92	0.53
2:XB:6:THR:CG2	2:XB:7:VAL:N	2.67	0.53
1:XA:599:C:O2'	8:XH:129:VAL:O	2.24	0.53
20:XT:19:SER:O	20:XT:23:ARG:HB2	2.09	0.53
20:XT:50:GLU:HB2	20:XT:99:LEU:HD11	1.89	0.53
35:YA:1817:G:OP1	37:YD:88:ARG:NH1	2.40	0.53
3:QC:65:ALA:HA	3:QC:100:ALA:HB3	1.88	0.53
32:R7:47:ARG:HH12	53:RX:60:ARG:HH12	1.57	0.53
35:RA:1111:A:O2'	41:RH:2:SER:O	2.25	0.53
35:RA:807:U:O2'	35:RA:2060:A:N1	2.39	0.53
35:RA:2209:C:O2'	35:RA:2211:G:N2	2.42	0.53
40:RG:49:ASP:HB3	40:RG:52:ILE:HG22	1.91	0.53
41:RH:61:HIS:O	41:RH:65:HIS:HB2	2.09	0.53
48:RS:14:VAL:O	48:RS:18:ILE:HG12	2.08	0.53
35:YA:2296:U:OP2	48:YS:9:ARG:NH1	2.41	0.53
33:Y8:64:TYR:HH	35:YA:592:G:HO2'	1.55	0.53
35:YA:993:G:N3	51:YV:89:GLN:NE2	2.55	0.53
54:YY:14:LEU:HB2	54:YY:75:ILE:HD11	1.91	0.53
40:RG:16:ARG:O	40:RG:20:ILE:HG13	2.09	0.53
46:RQ:35:VAL:HG22	46:RQ:102:VAL:HA	1.90	0.53
2:XB:19:HIS:HB2	2:XB:204:ASN:ND2	2.23	0.53
3:XC:42:LEU:HD23	3:XC:43:LEU:HD23	1.90	0.53
7:XG:26:PHE:O	7:XG:30:ILE:HG12	2.08	0.53
9:QI:19:LEU:CG	9:QI:59:PHE:HE1	2.11	0.53
19:QS:52:TYR:CD2	19:QS:57:HIS:CG	2.97	0.53
24:QY:44:LYS:NZ	24:QY:59:ARG:HH11	1.94	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:RD:77:ALA:HA	37:RD:97:TYR:HA	1.89	0.53
1:XA:714:G:H2'	1:XA:715:A:C8	2.44	0.53
12:XL:46:LYS:HG2	12:XL:47:LYS:N	2.24	0.53
39:YF:148:LEU:HD11	39:YF:193:VAL:HG21	1.91	0.53
48:YS:89:ARG:HH22	48:YS:93:LYS:HA	1.74	0.53
50:YU:90:VAL:HG12	50:YU:91:ASP:H	1.74	0.53
50:YU:91:ASP:O	50:YU:95:LEU:N	2.42	0.53
55:YZ:144:LEU:HD11	55:YZ:150:LEU:HD23	1.91	0.53
1:QA:993:G:H2'	1:QA:995:C:H41	1.74	0.53
2:QB:164:VAL:O	2:QB:186:ALA:HA	2.08	0.53
2:QB:84:GLU:HB3	2:QB:219:VAL:HG11	1.90	0.53
13:QM:8:GLU:C	13:QM:10:PRO:CD	2.64	0.53
35:RA:1568:G:OP2	37:RD:63:ARG:NH2	2.42	0.53
43:RN:54:VAL:HB	43:RN:122:VAL:HG22	1.90	0.53
1:XA:426:G:OP1	4:XD:38:TYR:OH	2.25	0.53
2:XB:9:GLU:HB3	2:XB:48:MET:HE1	1.90	0.53
19:XS:11:VAL:HG12	19:XS:13:ASP:N	2.21	0.53
35:YA:2162:G:O2'	35:YA:2173:A:OP2	2.23	0.53
39:YF:185:ASP:OD1	39:YF:188:ARG:NH1	2.42	0.53
41:YH:101:ARG:NH2	41:YH:116:GLU:OE1	2.42	0.53
41:YH:4:ILE:HG22	41:YH:69:ARG:HD2	1.90	0.53
54:YY:83:THR:HG21	54:YY:99:CYS:SG	2.49	0.53
1:QA:700:G:H4'	1:QA:704:A:H1'	1.89	0.53
4:QD:32:ALA:HA	4:QD:35:ARG:HB2	1.90	0.53
35:RA:2484:G:H1'	46:RQ:124:LYS:HD2	1.91	0.53
41:RH:91:GLY:HA3	41:RH:94:TYR:HB2	1.90	0.53
50:RU:86:ALA:HB3	50:RU:88:ILE:HD12	1.90	0.53
2:XB:60:ASP:CG	2:XB:64:ARG:HH12	2.11	0.53
2:XB:6:THR:HG22	2:XB:7:VAL:HG13	1.91	0.53
9:XI:86:VAL:HG21	9:XI:102:LEU:HD11	1.91	0.53
22:XV:63:G:OP1	25:Y0:11:ARG:NH2	2.41	0.53
35:YA:226:G:H21	35:YA:228:A:H62	1.57	0.53
39:YF:50:SER:HB2	39:YF:94:PRO:HD3	1.90	0.53
55:YZ:146:ILE:HA	55:YZ:174:VAL:HG13	1.90	0.53
1:QA:1221:G:H5''	1:QA:1321:C:H42	1.74	0.53
35:RA:1681:G:O2'	35:RA:1762:A:O2'	2.27	0.53
37:RD:132:PRO:HG3	37:RD:190:TYR:CE1	2.44	0.53
42:RI:126:TYR:O	42:RI:140:LEU:O	2.25	0.53
35:RA:2012:G:OP1	52:RW:11:ARG:NH2	2.42	0.53
1:XA:1534:A:C6	23:XX:10:G:O6	2.62	0.53
13:QM:87:TYR:H	19:QS:73:GLU:HB3	1.74	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:QZ:12:ASP:HB3	24:QZ:80:CYS:SG	2.47	0.52
35:RA:2572:A:OP1	35:RA:2574:G:O2'	2.26	0.52
42:RI:9:LEU:H	42:RI:9:LEU:CD2	2.22	0.52
1:XA:56:U:H2'	1:XA:57:G:H8	1.72	0.52
9:XI:9:ARG:HG2	9:XI:14:VAL:HG12	1.91	0.52
35:YA:1254:A:H5''	35:YA:1255:U:H5'	1.90	0.52
5:QE:93:PRO:HG2	8:QH:105:ARG:HE	1.74	0.52
17:QQ:66:SER:OG	17:QQ:69:LYS:HB3	2.09	0.52
22:QW:50:U:H3	22:QW:64:G:H1	1.56	0.52
35:RA:2328:A:H2'	35:RA:2329:G:C8	2.44	0.52
35:RA:974:G:O2'	35:RA:975:G:N7	2.32	0.52
29:R4:6:HIS:CD2	40:RG:66:GLN:HA	2.44	0.52
48:RS:66:ALA:HB2	48:RS:97:ARG:HB2	1.91	0.52
1:XA:954:G:H21	1:XA:1227:A:H62	1.55	0.52
1:XA:1098:C:OP2	2:XB:144:ARG:NH1	2.42	0.52
10:XJ:51:ARG:H	10:XJ:60:ARG:HA	1.74	0.52
13:XM:53:VAL:CG1	13:XM:57:ARG:HH12	2.13	0.52
1:XA:1224:G:O2'	19:XS:78:ARG:NH2	2.43	0.52
35:YA:1105:U:H2'	35:YA:1106:G:H8	1.75	0.52
35:YA:2287:A:H62	35:YA:2344:U:H3	1.57	0.52
38:YE:34:VAL:HG11	38:YE:78:LEU:HD21	1.91	0.52
1:QA:578:C:O2'	1:QA:728:A:N3	2.39	0.52
9:QI:46:ALA:HA	9:QI:78:LYS:HB2	1.90	0.52
10:QJ:7:LYS:HB3	10:QJ:71:LEU:CD1	2.37	0.52
35:RA:221:A:N1	35:RA:265:A:O2'	2.41	0.52
35:RA:581:C:H2'	35:RA:582:G:H8	1.74	0.52
35:RA:698:C:O2'	35:RA:734:A:N6	2.41	0.52
52:RW:24:ILE:HG22	52:RW:35:ILE:HD11	1.92	0.52
53:RX:57:LEU:HD11	53:RX:78:LYS:HD2	1.90	0.52
1:XA:127:G:O2'	17:XQ:2:PRO:O	2.27	0.52
49:YT:51:ARG:HG2	49:YT:98:LYS:HE2	1.90	0.52
50:YU:97:ASP:OD2	50:YU:101:ARG:NH1	2.42	0.52
1:QA:1111:A:N1	3:QC:177:THR:HG22	2.25	0.52
4:QD:152:SER:HA	4:QD:155:LEU:HD23	1.92	0.52
35:RA:2100:G:O6	35:RA:2189:U:O4	2.27	0.52
35:RA:2688:U:OP1	35:RA:2713:A:N6	2.42	0.52
35:RA:442:G:H1'	39:RF:48:THR:HG21	1.92	0.52
37:RD:75:ILE:O	37:RD:118:VAL:HG22	2.09	0.52
41:RH:43:VAL:HG23	41:RH:43:VAL:O	2.09	0.52
41:RH:6:ARG:HB2	41:RH:65:HIS:CD2	2.44	0.52
42:RI:73:GLU:O	42:RI:73:GLU:HG2	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:RQ:52:VAL:O	46:RQ:56:ARG:HG2	2.10	0.52
49:RT:105:LEU:HD12	49:RT:109:GLU:HG3	1.91	0.52
49:RT:6:LEU:HA	49:RT:9:LEU:HB2	1.91	0.52
1:XA:1003:G:H3'	1:XA:1004:A:H8	1.73	0.52
2:XB:75:LYS:HA	2:XB:78:GLN:HG3	1.91	0.52
20:XT:58:LYS:HA	20:XT:61:SER:OG	2.10	0.52
24:XZ:28:ASN:HB3	24:XZ:32:LYS:HE3	1.91	0.52
46:YQ:140:ALA:HA	55:YZ:53:ILE:HD11	1.91	0.52
5:QE:110:LEU:HD13	5:QE:118:ILE:HG21	1.90	0.52
27:R2:65:ASN:ND2	35:RA:72:U:O4	2.43	0.52
39:RF:89:VAL:HG13	39:RF:90:PHE:H	1.75	0.52
40:RG:111:LEU:HB3	40:RG:117:PHE:CZ	2.44	0.52
43:RN:103:VAL:HG21	43:RN:120:LEU:HD22	1.92	0.52
54:RY:68:HIS:HB3	54:RY:71:LYS:HG3	1.92	0.52
55:RZ:74:VAL:HG22	55:RZ:86:VAL:HG12	1.92	0.52
2:XB:215:LEU:O	2:XB:219:VAL:HG12	2.09	0.52
17:XQ:43:LEU:HD13	17:XQ:68:ARG:CZ	2.39	0.52
29:Y4:58:ARG:CZ	29:Y4:59:PHE:HE1	2.21	0.52
38:YE:15:PHE:H	49:YT:14:TYR:HE1	1.57	0.52
35:RA:1528:A:OP2	35:RA:1542:G:N1	2.42	0.52
37:RD:133:LEU:HD23	37:RD:136:ILE:HD12	1.90	0.52
37:RD:4:LYS:HE2	37:RD:18:VAL:HG13	1.90	0.52
49:RT:62:THR:HG22	49:RT:75:ILE:HG12	1.91	0.52
55:RZ:41:LEU:HA	55:RZ:44:PHE:HB3	1.92	0.52
29:Y4:14:ILE:HD13	29:Y4:31:ILE:HB	1.90	0.52
20:QT:76:ALA:HB1	20:QT:80:ARG:HH12	1.74	0.52
33:R8:29:LYS:O	33:R8:31:HIS:N	2.41	0.52
35:RA:1818:U:H2'	37:RD:157:ARG:HG2	1.91	0.52
47:RR:79:LEU:HA	47:RR:83:ILE:HD12	1.91	0.52
51:RV:14:VAL:HB	51:RV:96:ILE:HD13	1.91	0.52
1:XA:1182:G:H4'	1:XA:1183:A:H5'	1.91	0.52
2:XB:223:ILE:HD12	2:XB:226:ARG:HB2	1.91	0.52
9:XI:5:TYR:CE1	9:XI:16:ARG:HB2	2.42	0.52
38:YE:47:VAL:HG11	38:YE:86:PRO:HD2	1.92	0.52
55:YZ:53:ILE:HD12	55:YZ:53:ILE:H	1.73	0.52
2:QB:54:THR:HG21	2:QB:201:ILE:HG13	1.92	0.52
10:QJ:6:ILE:O	10:QJ:72:VAL:HG22	2.10	0.52
19:QS:55:LYS:HZ1	24:QZ:36:ARG:NH2	2.02	0.52
35:RA:2291:U:O2'	35:RA:2374:C:O2	2.28	0.52
35:RA:2526:G:H1	35:RA:2537:U:H3	1.58	0.52
40:RG:109:VAL:HG12	40:RG:113:ARG:HD2	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:RG:9:ARG:HH11	40:RG:9:ARG:CG	2.14	0.52
49:RT:3:ARG:CA	49:RT:3:ARG:HB2	2.23	0.52
1:XA:1325:C:H4'	21:XU:17:THR:HG21	1.92	0.52
35:YA:1021:A:H61	35:YA:1142(A):A:H61	1.58	0.52
35:YA:807:U:O2'	35:YA:2060:A:N1	2.42	0.52
1:QA:922:G:H4'	5:QE:20:GLN:HA	1.92	0.52
1:QA:1072:G:H21	2:QB:107:THR:HG21	1.74	0.52
8:QH:109:ILE:HD11	8:QH:120:THR:HB	1.90	0.52
29:R4:39:CYS:C	29:R4:41:PRO:HD3	2.30	0.52
41:RH:104:GLU:HG2	41:RH:114:VAL:HG12	1.92	0.52
38:YE:116:VAL:HG21	38:YE:138:PRO:HB3	1.92	0.52
46:YQ:104:PHE:HE2	46:YQ:125:LEU:HD11	1.75	0.52
4:QD:92:VAL:HG12	4:QD:96:LEU:HD11	1.92	0.52
8:QH:46:LYS:CG	8:QH:64:LYS:HG2	2.39	0.52
4:XD:15:GLU:OE2	4:XD:59:ARG:NH1	2.43	0.52
27:Y2:38:GLN:HB3	27:Y2:44:LEU:HB3	1.92	0.52
44:YO:1:MET:HB2	44:YO:32:TYR:HB3	1.92	0.52
46:YQ:60:ARG:HD3	55:YZ:179:ASP:OD1	2.10	0.52
35:RA:2112:G:N2	35:RA:2169:A:C6	2.76	0.51
35:RA:620:G:H5''	35:RA:620:G:N3	2.25	0.51
37:RD:96:HIS:CD2	37:RD:102:LYS:HE2	2.45	0.51
48:RS:27:SER:HA	48:RS:88:ASP:HB3	1.91	0.51
51:RV:59:ALA:HB1	51:RV:94:LEU:HB3	1.92	0.51
26:Y1:20:ARG:NH1	35:YA:387:U:OP2	2.41	0.51
35:YA:1341:U:OP2	35:YA:1394:U:O2'	2.25	0.51
3:QC:120:VAL:O	3:QC:124:ILE:HG13	2.10	0.51
19:QS:18:LYS:HE2	19:QS:22:LEU:HD21	1.92	0.51
4:XD:153:ARG:HD3	4:XD:181:MET:SD	2.49	0.51
8:XH:19:VAL:HG13	8:XH:21:LYS:HG3	1.92	0.51
10:XJ:5:ARG:NH1	10:XJ:71:LEU:HD11	2.25	0.51
18:XR:70:ILE:O	18:XR:74:ARG:HB2	2.10	0.51
23:XX:5:A:H2'	23:XX:6:G:H8	1.75	0.51
35:YA:1638:C:O2	35:YA:2698:U:O2'	2.28	0.51
22:QW:76:A:O2'	35:RA:2394:C:N3	2.43	0.51
37:RD:69:ARG:HH22	37:RD:117:VAL:HG22	1.75	0.51
39:RF:31:HIS:NE2	39:RF:35:GLU:OE1	2.44	0.51
40:RG:15:VAL:HG21	40:RG:176:LEU:HG	1.93	0.51
41:RH:87:LEU:HD22	41:RH:162:ILE:HG22	1.92	0.51
3:XC:182:ILE:HA	3:XC:202:ILE:O	2.10	0.51
3:XC:64:VAL:HB	3:XC:99:VAL:HG22	1.92	0.51
22:XW:14:A:N7	22:XW:22:G:N2	2.58	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Y1:73:LEU:HD21	26:Y1:98:LEU:HG	1.93	0.51
51:YV:58:VAL:HG13	51:YV:100:ARG:NH1	2.25	0.51
42:RI:9:LEU:HD23	42:RI:9:LEU:N	2.26	0.51
49:RT:102:ILE:HA	49:RT:105:LEU:HD23	1.93	0.51
55:RZ:70:LEU:HB2	55:RZ:91:LEU:HD21	1.92	0.51
35:YA:1028:A:N3	35:YA:2486:G:O2'	2.43	0.51
35:YA:414:C:O2	35:YA:1864:U:O2'	2.27	0.51
39:YF:65:TRP:CZ2	39:YF:72:ARG:CD	2.92	0.51
2:QB:13:ALA:C	2:QB:17:PHE:HE2	2.14	0.51
2:QB:19:HIS:CE1	2:QB:206:ASP:HB2	2.46	0.51
13:QM:97:PRO:CA	13:QM:110:ARG:HD3	2.38	0.51
34:R9:27:CYS:SG	34:R9:28:GLU:N	2.83	0.51
39:RF:28:ILE:HG23	39:RF:112:MET:HB3	1.92	0.51
40:RG:107:LEU:HA	40:RG:111:LEU:HD12	1.92	0.51
35:RA:2684:U:O2'	44:RO:68:GLU:OE2	2.27	0.51
49:RT:33:LYS:HE3	49:RT:40:THR:HG21	1.92	0.51
11:XK:18:ARG:HG2	11:XK:81:ASP:HB2	1.93	0.51
11:XK:84:VAL:HG11	11:XK:95:ILE:HD11	1.91	0.51
35:YA:2683:C:OP1	49:YT:53:ARG:NH2	2.43	0.51
1:QA:401:C:O2'	1:QA:621:A:N3	2.39	0.51
8:QH:100:ILE:O	8:QH:125:ARG:NH2	2.43	0.51
24:QZ:36:ARG:HG3	24:QZ:37:THR:N	2.26	0.51
46:RQ:37:LEU:HD11	46:RQ:130:LYS:HB2	1.91	0.51
1:XA:1125:U:O4	10:XJ:5:ARG:NH2	2.43	0.51
5:XE:148:VAL:HG12	5:XE:149:GLU:HG3	1.91	0.51
6:XF:21:LEU:O	6:XF:25:ILE:HG13	2.11	0.51
21:XU:6:ARG:HD3	21:XU:15:ARG:NE	2.20	0.51
35:YA:2547:U:O2	44:YO:23:ARG:NH2	2.43	0.51
46:YQ:65:PHE:HB2	46:YQ:105:GLU:HB2	1.93	0.51
55:YZ:89:PHE:CE2	55:YZ:96:VAL:HG21	2.46	0.51
1:QA:422:C:O2'	1:QA:423:G:N2	2.44	0.51
13:QM:88:ARG:HB2	13:QM:98:VAL:HG13	1.91	0.51
25:R0:27:GLU:HA	25:R0:67:VAL:HG12	1.93	0.51
29:R4:52:THR:CG2	29:R4:52:THR:O	2.52	0.51
35:RA:1067:A:N6	35:RA:1068:G:O6	2.44	0.51
25:R0:60:PHE:CE2	35:RA:2365:G:H4'	2.46	0.51
2:XB:16:HIS:CD2	2:XB:210:SER:HB2	2.45	0.51
1:XA:410:G:H3'	4:XD:25:ARG:HH12	1.76	0.51
1:XA:1314:C:N4	19:XS:2:PRO:O	2.43	0.51
35:YA:1080:C:N4	35:YA:1088:A:OP1	2.43	0.51
39:YF:28:ILE:HG12	39:YF:119:ARG:NH2	2.18	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:YV:52:VAL:HG23	51:YV:55:ALA:CB	2.34	0.51
10:QJ:55:LYS:O	10:QJ:55:LYS:HG3	2.11	0.51
43:RN:16:ILE:HB	43:RN:54:VAL:HG22	1.91	0.51
1:XA:1413:A:H2	1:XA:1487:G:H22	1.58	0.51
13:XM:4:ILE:HD11	13:XM:53:VAL:HG13	1.91	0.51
13:XM:90:LEU:HA	13:XM:93:ARG:HB3	1.93	0.51
32:Y7:7:PRO:HB2	35:YA:1309:G:H4'	1.92	0.51
40:YG:31:VAL:O	40:YG:33:ARG:NH1	2.43	0.51
35:YA:2690:C:OP1	47:YR:17:ARG:NH1	2.44	0.51
49:YT:16:ARG:HE	49:YT:19:LEU:HD11	1.75	0.51
1:QA:1179:A:H4'	9:QI:103:THR:HA	1.92	0.51
1:QA:618:C:H5'	1:QA:619:U:H5''	1.93	0.51
24:QY:5:TRP:CE2	24:QZ:10:TRP:CZ3	2.98	0.51
37:RD:10:THR:OG1	37:RD:13:ARG:HG2	2.10	0.51
24:XY:5:TRP:HB3	24:XY:10:TRP:HB2	1.93	0.51
28:Y3:6:VAL:HA	28:Y3:56:VAL:HG12	1.93	0.51
35:YA:156:U:H3	35:YA:170:U:H3	1.59	0.51
35:YA:2789:C:O2'	35:YA:2893:G:N2	2.42	0.51
42:YI:109:ILE:HG23	42:YI:130:TYR:CE1	2.46	0.51
48:YS:25:ARG:NH2	48:YS:42:ASP:OD1	2.44	0.51
1:QA:56:U:H2'	1:QA:57:G:H8	1.75	0.51
35:RA:414:C:O2	35:RA:1864:U:O2'	2.27	0.51
35:RA:888:C:H4'	35:RA:889:C:C5	2.43	0.51
41:RH:95:ARG:H	41:RH:106:THR:HG1	1.58	0.51
42:RI:133:HIS:CB	42:RI:134:PRO:HD3	2.31	0.51
55:RZ:125:LEU:HG	55:RZ:164:ALA:HB3	1.92	0.51
2:XB:6:THR:HG23	2:XB:217:ARG:HD2	1.93	0.51
10:XJ:34:VAL:HG12	10:XJ:75:ILE:H	1.76	0.51
35:YA:2540:C:O2'	35:YA:2740:A:N3	2.38	0.51
1:QA:642:A:N3	8:QH:113:SER:OG	2.44	0.50
2:QB:114:ARG:HD3	2:QB:117:GLU:OE1	2.10	0.50
13:QM:14:ARG:NE	13:QM:16:ASP:OD2	2.33	0.50
49:RT:125:ARG:NH2	49:RT:128:GLU:HG3	2.25	0.50
35:YA:1799:G:H8	37:YD:181:GLU:OE1	1.94	0.50
46:YQ:78:PRO:HG2	46:YQ:81:VAL:HG21	1.92	0.50
1:QA:662:G:H2'	1:QA:663:A:C8	2.45	0.50
10:QJ:8:LEU:CD1	10:QJ:96:ILE:CG2	2.50	0.50
25:R0:47:PRO:HG3	25:R0:53:MET:HB2	1.93	0.50
35:RA:1340:U:OP1	53:RX:16:LYS:NZ	2.43	0.50
35:RA:776:G:N7	35:RA:793:A:O2'	2.44	0.50
40:RG:111:LEU:HB3	40:RG:117:PHE:HE1	1.76	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:1305:G:OP1	21:XU:2:GLY:N	2.44	0.50
1:XA:975:A:N1	10:XJ:48:THR:OG1	2.44	0.50
2:XB:88:ALA:HB2	2:XB:219:VAL:HG23	1.91	0.50
4:XD:150:GLU:HG2	4:XD:153:ARG:CZ	2.41	0.50
24:XZ:44:LYS:NZ	24:XZ:59:ARG:HE	2.10	0.50
24:XZ:26:LYS:NZ	24:XZ:60:ILE:O	2.31	0.50
26:Y1:50:ARG:NH1	26:Y1:57:GLU:OE2	2.44	0.50
35:YA:2771:C:H5''	38:YE:202:LYS:HZ2	1.76	0.50
51:YV:35:LEU:HB2	51:YV:57:VAL:HG13	1.93	0.50
1:QA:985:C:H2'	1:QA:986:A:C8	2.46	0.50
5:QE:90:VAL:CG2	5:QE:90:VAL:CG1	2.82	0.50
7:QG:91:VAL:CG1	7:QG:96:GLN:HG3	2.40	0.50
24:QZ:23:ILE:O	24:QZ:27:ILE:HG12	2.11	0.50
24:QZ:47:PRO:HB3	24:QZ:56:TRP:CE2	2.47	0.50
44:RO:111:PHE:HB3	44:RO:114:ILE:HD13	1.94	0.50
1:XA:674:G:H2'	1:XA:675:A:H8	1.75	0.50
4:XD:11:LEU:HD13	4:XD:66:ARG:HD3	1.92	0.50
5:XE:81:GLU:HG2	5:XE:90:VAL:HG22	1.93	0.50
6:XF:5:GLU:HG3	6:XF:93:SER:HB2	1.93	0.50
12:XL:38:THR:HG23	12:XL:39:VAL:HG23	1.93	0.50
35:YA:1020:A:N6	35:YA:1141:U:O2'	2.44	0.50
35:YA:698:C:O2'	35:YA:734:A:N6	2.44	0.50
49:YT:128:GLU:O	49:YT:132:LYS:CB	2.58	0.50
52:YW:65:LEU:HD12	52:YW:68:ARG:HH21	1.77	0.50
13:QM:8:GLU:O	13:QM:10:PRO:HD2	2.08	0.50
49:RT:51:ARG:HG3	49:RT:98:LYS:HG2	1.91	0.50
1:XA:1128:C:H1'	1:XA:1146:A:H61	1.77	0.50
13:XM:23:TYR:CD2	13:XM:67:GLU:HA	2.45	0.50
29:Y4:47:GLN:HG2	29:Y4:49:PHE:HB3	1.94	0.50
35:YA:2638:G:OP2	38:YE:82:ARG:NH1	2.40	0.50
6:QF:94:GLN:HB3	18:QR:32:ARG:HD3	1.93	0.50
24:QZ:71:THR:OG1	24:QZ:72:ASP:N	2.43	0.50
41:RH:18:GLU:HG3	41:RH:27:LYS:NZ	2.26	0.50
3:QC:41:GLY:O	3:QC:45:LYS:HG2	2.11	0.50
1:QA:191:G:O2'	20:QT:101:GLY:O	2.26	0.50
24:QZ:49:LYS:O	24:QZ:51:ASN:N	2.41	0.50
34:R9:3:VAL:HG21	35:RA:2539:C:H4'	1.94	0.50
35:RA:81:G:HO2'	35:RA:295:G:HO2'	1.56	0.50
4:XD:70:ILE:HG21	4:XD:100:ARG:NH1	2.27	0.50
1:XA:922:G:H4'	5:XE:20:GLN:HA	1.94	0.50
13:XM:13:LYS:HA	13:XM:44:ARG:HH11	1.77	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:XT:100:ILE:HG22	20:XT:102:GLY:N	2.25	0.50
31:Y6:25:LYS:HD2	31:Y6:34:LEU:HD13	1.92	0.50
35:YA:2304:G:H22	35:YA:2312:U:H3	1.59	0.50
35:YA:531:C:OP1	35:YA:561:G:N1	2.44	0.50
1:QA:501:C:H2'	1:QA:502:G:H8	1.77	0.50
7:QG:15:ASP:HB3	7:QG:19:GLY:H	1.77	0.50
8:QH:113:SER:HB2	8:QH:134:ILE:HD11	1.92	0.50
26:R1:91:LYS:HD2	26:R1:92:LYS:HG2	1.93	0.50
28:R3:15:TYR:O	28:R3:20:LYS:NZ	2.44	0.50
48:RS:63:THR:HA	48:RS:97:ARG:CB	2.40	0.50
1:XA:978:A:H61	1:XA:1316:G:H1'	1.77	0.50
13:XM:78:ILE:O	13:XM:82:MET:HG3	2.12	0.50
1:XA:728:A:C6	15:XO:54:ARG:CD	2.94	0.50
30:Y5:36:CYS:SG	30:Y5:49:CYS:HB3	2.51	0.50
33:Y8:48:PHE:CE1	33:Y8:50:LEU:HD22	2.46	0.50
40:YG:166:ASP:OD1	40:YG:166:ASP:N	2.44	0.50
1:QA:1028(B):C:H3'	1:QA:1029:G:H4'	1.93	0.50
1:QA:708:C:H2'	1:QA:709:G:H8	1.76	0.50
1:QA:770:C:O2'	1:QA:899:C:N3	2.41	0.50
35:RA:2148:G:H2'	35:RA:2149:G:H8	1.77	0.50
35:RA:2859:G:H2'	35:RA:2860:A:C8	2.47	0.50
41:RH:45:VAL:HG22	41:RH:50:VAL:HG12	1.93	0.50
41:RH:52:VAL:HB	41:RH:69:ARG:CZ	2.42	0.50
1:XA:235:C:H2'	1:XA:236:G:H8	1.76	0.50
8:XH:6:ILE:HB	8:XH:85:ARG:NH1	2.27	0.50
1:XA:1119:C:OP2	9:XI:9:ARG:NH2	2.44	0.50
25:Y0:23:VAL:HG21	35:YA:857:C:H4'	1.94	0.50
35:YA:2011:U:OP1	52:YW:42:ARG:NH1	2.43	0.50
35:YA:566:U:H5''	45:YP:29:LYS:HE3	1.94	0.50
39:YF:32:LEU:HD11	39:YF:105:VAL:HG13	1.93	0.50
3:QC:152:ILE:HD11	3:QC:199:LYS:HD2	1.93	0.50
60:QX:101:A3P:O2P	24:QY:44:LYS:NZ	2.44	0.50
28:R3:26:LEU:O	28:R3:35:ARG:HD3	2.12	0.50
41:RH:96:ALA:HB1	41:RH:103:LEU:HD21	1.93	0.50
49:RT:36:GLU:CD	49:RT:39:ARG:HH21	2.15	0.50
52:RW:22:ASP:OD1	52:RW:25:ARG:NH1	2.38	0.50
1:XA:662:G:H2'	1:XA:663:A:C8	2.47	0.50
1:XA:827:U:H3	1:XA:872:A:H62	1.59	0.50
1:XA:376:G:H5''	16:XP:5:ARG:HB2	1.94	0.50
49:YT:11:GLU:N	49:YT:11:GLU:OE2	2.43	0.50
19:QS:41:VAL:HG12	19:QS:42:PRO:HD2	0.56	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:RH:52:VAL:HG12	41:RH:65:HIS:CD2	2.46	0.49
42:RI:126:TYR:HB2	42:RI:140:LEU:O	2.12	0.49
1:XA:1534:A:N1	23:XX:10:G:O6	2.44	0.49
2:XB:140:HIS:HA	2:XB:143:GLU:HG3	1.94	0.49
12:XL:90:VAL:HB	12:XL:93:LEU:HB2	1.93	0.49
35:YA:2675:A:H61	35:YA:2732:G:H1	1.60	0.49
38:YE:176:ILE:HB	38:YE:181:LEU:HB2	1.93	0.49
44:YO:68:GLU:HG3	44:YO:78:ARG:HG3	1.93	0.49
1:QA:946:A:H2'	1:QA:947:G:C8	2.46	0.49
5:QE:102:ALA:O	5:QE:107:ARG:NH2	2.43	0.49
8:QH:10:LEU:HD22	8:QH:83:ILE:HD11	1.94	0.49
33:R8:6:THR:HG22	33:R8:63:PRO:HD2	1.94	0.49
35:RA:589:C:H2'	35:RA:590:A:C8	2.46	0.49
48:RS:31:SER:O	48:RS:97:ARG:NH2	2.42	0.49
52:RW:10:VAL:HG13	52:RW:101:SER:HB3	1.94	0.49
2:XB:6:THR:HG23	2:XB:7:VAL:HG13	1.94	0.49
4:XD:153:ARG:CD	4:XD:181:MET:HE2	2.38	0.49
14:YN:34:TYR:CE2	14:YN:44:LEU:HD13	2.47	0.49
24:XY:73:ASP:OD1	24:XY:73:ASP:N	2.44	0.49
38:YE:14:ILE:HD11	38:YE:173:VAL:HG11	1.94	0.49
55:YZ:115:GLY:HA2	55:YZ:177:PRO:HD3	1.94	0.49
6:QF:76:ALA:HB1	6:QF:80:ARG:HH21	1.77	0.49
8:QH:102:ARG:HH22	8:QH:105:ARG:NH1	2.11	0.49
11:QK:51:LYS:HA	11:QK:55:LYS:HD3	1.94	0.49
26:R1:90:ILE:HG13	26:R1:94:LEU:HD11	1.93	0.49
35:RA:1032:A:H2	35:RA:1122:G:H22	1.59	0.49
35:RA:278:A:H61	35:RA:362:U:H3	1.60	0.49
1:XA:1376:U:P	7:XG:94:ARG:HH12	2.36	0.49
2:XB:174:VAL:HG12	2:XB:184:VAL:HG11	1.93	0.49
6:XF:6:VAL:HB	6:XF:63:TYR:HB2	1.94	0.49
42:YI:123:LEU:N	42:YI:123:LEU:CD2	2.76	0.49
42:YI:7:GLU:HA	42:YI:15:VAL:HG22	1.93	0.49
51:YV:59:ALA:HB2	51:YV:96:ILE:HD13	1.92	0.49
35:YA:1342:A:OP1	53:YX:36:LYS:NZ	2.45	0.49
3:QC:59:ARG:HG3	3:QC:64:VAL:CG2	2.43	0.49
30:R5:16:ARG:NH2	35:RA:517:C:OP1	2.40	0.49
35:RA:839:U:H1'	35:RA:1191:G:H1'	1.95	0.49
35:RA:573:G:N1	35:RA:2031:A:OP2	2.31	0.49
43:RN:42:TRP:CD1	43:RN:48:MET:HE1	2.47	0.49
1:XA:664:G:H22	1:XA:741:G:H1	1.59	0.49
35:YA:1992:G:N2	35:YA:1996:C:O2'	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YA:270(I):G:H1	35:YA:270(Q):C:H42	1.60	0.49
35:YA:481:G:O2'	35:YA:506:G:N2	2.44	0.49
44:YO:87:ILE:HD12	44:YO:91:LEU:HA	1.95	0.49
1:QA:1306:A:N6	1:QA:1331:G:O2'	2.45	0.49
1:QA:1356:G:H2'	1:QA:1357:A:C8	2.47	0.49
1:QA:967:C:H4'	9:QI:125:TYR:CE1	2.46	0.49
2:QB:136:VAL:HA	2:QB:139:LYS:HB2	1.94	0.49
3:QC:138:VAL:HG13	3:QC:149:ALA:HB3	1.95	0.49
19:QS:40:ILE:HG21	19:QS:66:MET:O	2.13	0.49
24:QY:59:ARG:HA	24:QY:65:ARG:HD3	1.94	0.49
24:QY:5:TRP:CZ2	24:QZ:10:TRP:CZ3	3.00	0.49
37:RD:72:LYS:NZ	37:RD:99:ASP:OD2	2.40	0.49
38:RE:50:GLY:CA	38:RE:78:LEU:HA	2.40	0.49
41:RH:7:LEU:N	41:RH:8:PRO:HD2	2.27	0.49
35:RA:446:G:OP1	50:RU:3:ARG:NH1	2.44	0.49
1:XA:1219:U:OP1	14:XN:19:ARG:NH2	2.44	0.49
3:XC:130:VAL:HG11	3:XC:157:ILE:HG23	1.94	0.49
9:XI:75:ASP:HA	9:XI:78:LYS:HG2	1.95	0.49
35:YA:1791:A:N6	35:YA:1828:G:O2'	2.45	0.49
35:YA:247:G:H4'	35:YA:386:G:C5	2.48	0.49
35:YA:642:G:N2	35:YA:645:C:OP2	2.45	0.49
37:YD:133:LEU:HD23	37:YD:136:ILE:HD12	1.93	0.49
52:YW:11:ARG:HH22	52:YW:98:LYS:CG	2.25	0.49
1:QA:309:G:O2'	1:QA:607:A:N1	2.44	0.49
1:QA:67:C:H2'	1:QA:68:G:C8	2.47	0.49
19:QS:10:PHE:HE2	19:QS:12:ASP:HB3	1.78	0.49
19:QS:15:LEU:HD22	19:QS:33:THR:HG21	1.94	0.49
1:QA:958:A:C5	19:QS:55:LYS:HB2	2.48	0.49
29:R4:5:ILE:HG23	29:R4:6:HIS:ND1	2.28	0.49
35:RA:2147:G:H2'	35:RA:2148:G:C8	2.48	0.49
35:RA:465:G:H2'	35:RA:466:A:C8	2.48	0.49
37:RD:132:PRO:HB2	37:RD:134:ARG:HG2	1.94	0.49
37:RD:169:GLU:O	37:RD:169:GLU:HG3	2.13	0.49
46:RQ:110:THR:HG22	46:RQ:113:GLN:HG2	1.95	0.49
1:XA:128:G:O2'	17:XQ:3:LYS:NZ	2.32	0.49
7:XG:97:GLN:HG2	7:XG:101:LEU:HD13	1.95	0.49
15:XO:77:ARG:HA	15:XO:80:ALA:HB3	1.94	0.49
39:YF:65:TRP:CH2	39:YF:72:ARG:HD3	2.48	0.49
6:QF:28:ARG:O	6:QF:32:ASN:ND2	2.44	0.49
24:QZ:1:MET:CE	24:QZ:35:ARG:HG3	2.43	0.49
35:RA:1102:C:H2'	35:RA:1103:A:H8	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:RT:28:VAL:HG23	49:RT:88:ILE:HA	1.95	0.49
1:XA:6:G:H4'	1:XA:298:A:H4'	1.94	0.49
14:YN:34:TYR:CD2	14:YN:44:LEU:HD12	2.47	0.49
35:YA:1042:G:H1	35:YA:1113:U:H3	1.59	0.49
36:YB:37:C:O2	48:YS:95:HIS:NE2	2.40	0.49
42:YI:93:THR:OG1	42:YI:96:ASP:N	2.41	0.49
10:QJ:9:ARG:O	10:QJ:94:VAL:HG13	2.13	0.49
35:RA:686:G:N2	35:RA:788:A:H61	2.11	0.49
38:RE:109:LYS:O	38:RE:111:ARG:NH1	2.44	0.49
41:RH:24:VAL:HG21	41:RH:72:ILE:HD11	1.94	0.49
35:RA:2296:U:OP2	48:RS:9:ARG:NH1	2.46	0.49
2:XB:21:ARG:O	2:XB:23:ARG:N	2.44	0.49
4:XD:191:ARG:CG	4:XD:191:ARG:O	2.60	0.49
7:XG:67:GLU:HA	7:XG:70:LYS:HD3	1.94	0.49
1:QA:255:G:H4'	17:QQ:17:LYS:HD3	1.94	0.49
11:QK:84:VAL:HG21	11:QK:95:ILE:HD11	1.95	0.49
14:QN:26:ARG:HE	14:QN:47:LEU:HD11	1.77	0.49
31:R6:11:LEU:HB2	31:R6:21:TYR:HB2	1.95	0.49
41:RH:4:ILE:C	41:RH:6:ARG:H	2.15	0.49
1:XA:1013:G:N2	1:XA:1016:A:OP2	2.45	0.49
1:XA:261:U:OP2	20:XT:79:ARG:NH1	2.43	0.49
4:XD:117:ALA:O	4:XD:121:VAL:HG23	2.12	0.49
13:XM:68:GLY:HA3	40:YG:116:ASP:OD1	2.13	0.49
35:YA:1210:A:H5'	35:YA:1211:U:H2'	1.93	0.49
22:QW:63:G:H2'	22:QW:64:G:C8	2.48	0.49
24:QZ:10:TRP:O	24:QZ:14:LEU:N	2.43	0.49
25:R0:72:ARG:HB3	25:R0:75:LEU:HB2	1.95	0.49
35:RA:1019:U:OP1	35:RA:1035:U:O2'	2.30	0.49
47:RR:96:ARG:NH1	47:RR:117:VAL:HA	2.28	0.49
1:XA:263:A:OP2	20:XT:79:ARG:NH2	2.46	0.49
1:XA:406:G:H21	4:XD:119:GLN:HE22	1.60	0.49
24:XY:48:LEU:HD11	24:XY:57:SER:HB3	1.95	0.49
26:Y1:69:LYS:HD3	26:Y1:98:LEU:HD21	1.95	0.49
35:YA:1827:C:OP2	37:YD:222:ARG:NH1	2.45	0.49
44:YO:19:ILE:HG22	44:YO:43:VAL:HA	1.95	0.49
48:YS:66:ALA:HA	48:YS:69:VAL:HG12	1.94	0.49
2:QB:82:ARG:O	2:QB:86:GLU:HB2	2.11	0.48
5:QE:137:GLU:O	5:QE:141:GLN:HG3	2.13	0.48
21:QU:3:LYS:O	21:QU:15:ARG:NH1	2.41	0.48
29:R4:50:VAL:HG12	29:R4:52:THR:H	1.77	0.48
48:RS:36:TYR:CD1	48:RS:52:SER:HB2	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:192:U:H2'	1:XA:193:C:C6	2.48	0.48
1:XA:689:C:H3'	1:XA:690:G:H21	1.77	0.48
1:XA:745:C:OP1	1:XA:851:G:O2'	2.31	0.48
2:XB:68:ILE:HD12	2:XB:161:ALA:HB3	1.94	0.48
1:XA:1202:G:O4'	14:XN:29:ARG:NH1	2.46	0.48
40:YG:137:GLU:HG3	40:YG:137:GLU:O	2.12	0.48
35:YA:1142(A):A:H4'	43:YN:25:ARG:HH22	1.76	0.48
44:YO:8:LEU:HD13	44:YO:82:ASN:HB3	1.95	0.48
3:QC:58:GLU:H	3:QC:64:VAL:HG13	1.77	0.48
3:QC:86:VAL:O	3:QC:89:GLU:HB3	2.13	0.48
4:QD:11:LEU:HB3	4:QD:66:ARG:HD3	1.94	0.48
5:QE:116:THR:OG1	5:QE:117:ASP:N	2.44	0.48
24:QZ:25:LYS:HA	24:QZ:25:LYS:HD2	1.63	0.48
31:R6:5:VAL:HA	31:R6:27:LYS:HD2	1.95	0.48
35:RA:1309:G:HO2'	35:RA:1611:C:HO2'	1.60	0.48
35:RA:2315:G:OP1	40:RG:36:LYS:NZ	2.42	0.48
40:RG:131:TYR:HE1	40:RG:133:LEU:HB3	1.78	0.48
40:RG:135:LEU:HD21	40:RG:140:ILE:CD1	2.41	0.48
48:RS:11:LYS:HE2	48:RS:91:PRO:HD3	1.95	0.48
51:RV:58:VAL:HG22	51:RV:98:GLU:HG2	1.95	0.48
1:XA:1064:G:H1'	1:XA:1066:C:C6	2.48	0.48
1:XA:1147:C:O2'	9:XI:5:TYR:OH	2.14	0.48
26:Y1:69:LYS:NZ	35:YA:372:G:OP2	2.36	0.48
39:YF:31:HIS:NE2	39:YF:35:GLU:OE1	2.46	0.48
41:YH:90:LYS:HD3	41:YH:159:GLU:HG2	1.95	0.48
24:QZ:3:LEU:HD11	24:QZ:31:ILE:HG21	1.96	0.48
35:RA:579:G:O2'	35:RA:2019:A:OP1	2.30	0.48
35:RA:2853:C:H2'	35:RA:2854:G:C8	2.48	0.48
38:RE:9:VAL:HB	38:RE:25:VAL:HG23	1.95	0.48
40:RG:11:TYR:HA	40:RG:15:VAL:CG2	2.43	0.48
41:RH:46:GLU:CB	41:RH:49:VAL:HB	2.29	0.48
45:RP:7:ARG:HA	45:RP:8:PRO:HD2	1.63	0.48
1:XA:579:G:H5'	1:XA:728:A:H1'	1.95	0.48
2:XB:111:ARG:HG3	2:XB:145:LEU:HD22	1.95	0.48
2:XB:16:HIS:O	2:XB:17:PHE:CG	2.66	0.48
2:XB:20:GLU:O	2:XB:39:ILE:HG23	2.13	0.48
17:XQ:45:HIS:CD2	17:XQ:47:PRO:HG3	2.48	0.48
20:XT:29:LYS:HD2	20:XT:71:THR:HG21	1.95	0.48
28:Y3:43:ILE:O	28:Y3:47:VAL:HG23	2.13	0.48
35:YA:1528:A:OP2	35:YA:1542:G:N1	2.47	0.48
33:Y8:63:PRO:HB2	35:YA:593:G:H4'	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:YI:100:ALA:O	42:YI:104:GLN:HB3	2.13	0.48
9:QI:21:PRO:HA	9:QI:59:PHE:HB2	1.91	0.48
10:QJ:7:LYS:HB2	10:QJ:70:ARG:O	2.14	0.48
13:QM:13:LYS:CG	13:QM:17:VAL:CG2	2.81	0.48
1:QA:375:U:O2	16:QP:28:ARG:NH1	2.46	0.48
29:R4:13:ARG:HG3	29:R4:30:GLU:HG2	1.94	0.48
29:R4:42:PHE:C	29:R4:42:PHE:CD1	2.85	0.48
35:RA:1571:A:H2'	35:RA:1572:A:C8	2.49	0.48
31:R6:24:GLU:OE2	35:RA:2285:C:N4	2.44	0.48
36:RB:44:G:H1'	36:RB:47:C:H42	1.78	0.48
41:RH:71:LEU:HD12	41:RH:72:ILE:N	2.27	0.48
48:RS:31:SER:HG	48:RS:34:HIS:H	1.59	0.48
9:XI:28:VAL:HG12	9:XI:63:ILE:HB	1.96	0.48
12:XL:35:GLY:HA3	12:XL:60:LEU:HD23	1.96	0.48
16:XP:43:LYS:HG2	16:XP:48:TRP:CD2	2.48	0.48
35:YA:2177:C:H2'	35:YA:2178:C:H6	1.78	0.48
40:YG:40:ASN:HB3	40:YG:156:ASP:HB2	1.95	0.48
40:YG:60:LEU:HD11	40:YG:92:VAL:HG11	1.95	0.48
50:YU:27:LEU:HD13	50:YU:30:LYS:HB2	1.94	0.48
1:QA:1031:G:H21	1:QA:1032:A:H1'	1.79	0.48
1:QA:1064:G:H1'	1:QA:1066:C:C6	2.48	0.48
1:QA:1330:U:H3'	1:QA:1331:G:O4'	2.13	0.48
4:QD:154:ASN:O	4:QD:154:ASN:ND2	2.46	0.48
5:QE:90:VAL:CG1	5:QE:90:VAL:HB	2.18	0.48
35:RA:1542:G:O6	35:RA:1543:A:N6	2.46	0.48
38:RE:73:GLU:HG3	38:RE:74:PRO:CD	2.16	0.48
40:RG:5:VAL:HG23	40:RG:8:LYS:HB3	1.96	0.48
1:XA:1412:C:H2'	1:XA:1413:A:C8	2.49	0.48
2:XB:217:ARG:CG	2:XB:217:ARG:NH1	2.74	0.48
10:XJ:48:THR:O	10:XJ:48:THR:OG1	2.29	0.48
39:YF:24:LEU:HD23	39:YF:115:ALA:HA	1.95	0.48
7:QG:79:ARG:NH2	22:QW:33:U:O3'	2.44	0.48
9:QI:13:ALA:HB2	9:QI:68:GLY:HA3	1.95	0.48
29:R4:1:MET:HG2	40:RG:98:ARG:NH2	2.29	0.48
35:RA:2850:A:N7	35:RA:2868:A:O2'	2.40	0.48
35:RA:514:A:N3	35:RA:581:C:O2'	2.40	0.48
41:RH:86:GLU:HG3	41:RH:165:ALA:H	1.78	0.48
45:RP:101:VAL:HG11	45:RP:108:LYS:HG2	1.94	0.48
46:RQ:1:MET:SD	46:RQ:45:GLN:HG3	2.53	0.48
47:RR:96:ARG:HH12	47:RR:117:VAL:HA	1.79	0.48
48:RS:30:ARG:CG	48:RS:97:ARG:NH2	2.75	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:XL:46:LYS:HG2	12:XL:47:LYS:H	1.78	0.48
24:XZ:58:ARG:O	24:XZ:66:LEU:N	2.43	0.48
29:Y4:34:GLU:OE2	40:YG:113:ARG:NE	2.47	0.48
35:YA:764:A:H5'	37:YD:210:GLY:HA2	1.94	0.48
39:YF:154:VAL:HG23	39:YF:173:VAL:HG12	1.95	0.48
35:YA:2306:C:N4	40:YG:42:GLY:O	2.39	0.48
47:YR:33:ARG:HD3	47:YR:113:LEU:HD11	1.95	0.48
51:YV:21:ARG:NE	51:YV:91:TYR:CE1	2.82	0.48
1:QA:6:G:H4'	1:QA:298:A:H4'	1.96	0.48
9:QI:20:ARG:O	9:QI:59:PHE:HB2	2.13	0.48
31:R6:3:SER:OG	31:R6:4:GLU:N	2.45	0.48
35:RA:1285:G:N2	35:RA:1328:G:H5''	2.29	0.48
6:XF:37:VAL:HA	6:XF:65:VAL:HG12	1.96	0.48
29:Y4:58:ARG:CG	29:Y4:59:PHE:HD1	2.23	0.48
35:YA:84:A:N6	35:YA:102:G:O2'	2.46	0.48
35:YA:909:A:OP2	46:YQ:22:LYS:NZ	2.34	0.48
38:YE:93:VAL:HG22	38:YE:175:VAL:HG13	1.96	0.48
1:QA:769:G:H4'	1:QA:1513:A:H4'	1.94	0.48
13:QM:19:LEU:HD23	13:QM:19:LEU:H	1.78	0.48
19:QS:55:LYS:HE3	24:QZ:36:ARG:HH22	1.76	0.48
35:RA:764:A:H5'	37:RD:210:GLY:HA2	1.96	0.48
40:RG:6:ALA:O	40:RG:10:LYS:N	2.40	0.48
46:RQ:66:ILE:HA	46:RQ:104:PHE:HA	1.95	0.48
54:RY:83:THR:OG1	54:RY:84:ARG:N	2.46	0.48
1:XA:538:G:H5''	12:XL:114:LYS:HB2	1.95	0.48
35:YA:2666:C:O2	41:YH:152:ARG:NH2	2.47	0.48
47:YR:24:GLN:HG2	47:YR:44:LEU:HD22	1.95	0.48
1:QA:321:A:N6	1:QA:329:A:OP2	2.47	0.48
8:QH:14:ARG:NH2	8:QH:83:ILE:O	2.46	0.48
1:QA:1349:A:OP1	9:QI:120:ARG:HB2	2.14	0.48
9:QI:53:VAL:O	9:QI:53:VAL:HG22	2.14	0.48
32:R7:47:ARG:HH22	53:RX:60:ARG:NH2	2.11	0.48
35:RA:1171:G:O2'	35:RA:1173:G:O4'	2.30	0.48
35:RA:2729:G:H1'	38:RE:187:ALA:HB2	1.95	0.48
35:RA:2789:C:H1'	35:RA:2892:A:H2	1.79	0.48
46:RQ:19:GLY:H	46:RQ:98:LYS:NZ	2.11	0.48
51:RV:34:GLU:HG3	51:RV:58:VAL:HG12	1.95	0.48
2:XB:142:LEU:HD22	2:XB:146:GLN:NE2	2.28	0.48
1:XA:619:U:N3	4:XD:134:ASP:OD1	2.46	0.48
24:XZ:48:LEU:CD1	24:XZ:52:LEU:HD12	2.43	0.48
38:YE:92:THR:OG1	38:YE:93:VAL:N	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:YN:21:LYS:HD3	43:YN:138:LEU:HD23	1.94	0.48
55:YZ:23:LYS:HE3	55:YZ:40:ASP:HB2	1.96	0.48
3:QC:152:ILE:HG12	3:QC:199:LYS:HB2	1.95	0.48
17:QQ:45:HIS:CD2	17:QQ:47:PRO:HG3	2.49	0.48
19:QS:3:ARG:NH2	19:QS:9:VAL:HB	2.28	0.48
44:RO:93:PRO:HD3	44:RO:114:ILE:HD11	1.96	0.48
55:RZ:69:THR:HG21	55:RZ:88:PHE:HB3	1.95	0.48
1:XA:985:C:H2'	1:XA:986:A:C8	2.49	0.48
2:XB:73:THR:HB	2:XB:169:LYS:HE3	1.96	0.48
5:XE:144:THR:OG1	5:XE:147:ASP:N	2.30	0.48
35:YA:2096:U:H3	35:YA:2193:G:H1	1.62	0.48
35:YA:181:A:H1'	35:YA:435:C:H5'	1.96	0.48
40:YG:130:ASN:OD1	40:YG:161:THR:N	2.47	0.48
41:YH:42:ARG:O	41:YH:52:VAL:HG11	2.14	0.48
42:YI:24:GLY:O	42:YI:28:ASN:HB2	2.14	0.48
1:QA:1494:G:H5'	24:QY:47:PRO:HG2	1.96	0.47
1:QA:745:C:OP1	1:QA:851:G:O2'	2.28	0.47
7:QG:70:LYS:HB2	7:QG:96:GLN:HB3	1.95	0.47
9:QI:10:ARG:HG2	9:QI:75:ASP:HB2	1.95	0.47
34:R9:11:CYS:HB2	34:R9:13:LYS:HB2	1.96	0.47
35:RA:29:U:H5''	50:RU:7:GLY:HA2	1.96	0.47
40:RG:37:VAL:HG12	40:RG:99:MET:HG3	1.95	0.47
49:RT:107:ASP:OD1	49:RT:109:GLU:HG2	2.13	0.47
54:RY:49:VAL:HG21	54:RY:61:ILE:HG13	1.96	0.47
55:RZ:9:TYR:HA	55:RZ:37:VAL:HG12	1.95	0.47
1:XA:811:C:O2'	1:XA:901:A:N1	2.47	0.47
3:XC:91:LEU:O	3:XC:95:THR:HG22	2.14	0.47
22:XW:1:C:H2'	22:XW:2:G:H8	1.79	0.47
36:YB:40:U:H1'	36:YB:45:A:H61	1.78	0.47
40:YG:51:ARG:HG3	40:YG:52:ILE:HG13	1.96	0.47
43:YN:26:LEU:HG	43:YN:30:ILE:HD11	1.95	0.47
49:YT:62:THR:HG22	49:YT:75:ILE:HG23	1.96	0.47
1:QA:8:A:N6	4:QD:205:GLU:O	2.47	0.47
12:QL:84:LEU:HD23	12:QL:101:VAL:HG11	1.96	0.47
22:QW:50:U:H3	22:QW:64:G:H22	1.62	0.47
35:RA:392:C:H5''	35:RA:409:C:H5''	1.97	0.47
42:RI:122:GLU:HA	42:RI:122:GLU:OE2	2.14	0.47
35:RA:2683:C:OP1	49:RT:53:ARG:NH2	2.47	0.47
55:RZ:6:LYS:HG3	55:RZ:8:TYR:CE1	2.48	0.47
1:XA:890:G:O2'	1:XA:906:G:O6	2.24	0.47
29:Y4:58:ARG:CG	29:Y4:59:PHE:N	2.70	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YA:1342:A:H5''	53:YX:55:ASN:HD22	1.79	0.47
35:YA:1754:C:OP1	49:YT:96:ARG:NH1	2.48	0.47
39:YF:72:ARG:HG2	39:YF:73:ALA:H	1.78	0.47
42:YI:102:SER:HA	42:YI:107:VAL:O	2.13	0.47
51:YV:51:VAL:O	51:YV:51:VAL:CG2	2.61	0.47
51:YV:1:MET:HG3	51:YV:99:ILE:HD11	1.96	0.47
2:QB:73:THR:O	2:QB:78:GLN:NE2	2.39	0.47
7:QG:38:LEU:O	7:QG:42:ILE:HG13	2.14	0.47
12:QL:114:LYS:O	12:QL:117:ARG:NH1	2.47	0.47
27:R2:65:ASN:O	27:R2:69:ARG:HD2	2.15	0.47
35:RA:1057:A:H2'	35:RA:1058:G:H8	1.79	0.47
35:RA:2786:U:O2'	38:RE:62:PRO:O	2.28	0.47
2:XB:16:HIS:C	2:XB:17:PHE:CD2	2.87	0.47
2:XB:55:PHE:HD1	2:XB:58:ILE:HD12	1.78	0.47
4:XD:202:LEU:HA	4:XD:205:GLU:HG2	1.95	0.47
35:YA:299:A:N3	35:YA:319:C:O2'	2.40	0.47
1:QA:1013:G:N2	1:QA:1016:A:OP2	2.46	0.47
3:QC:181:ASN:HB3	3:QC:205:GLY:H	1.79	0.47
1:QA:107:G:O6	20:QT:15:ARG:HD3	2.15	0.47
34:R9:11:CYS:SG	34:R9:12:ASP:N	2.86	0.47
35:RA:581:C:H2'	35:RA:582:G:C8	2.49	0.47
36:RB:44:G:O2'	36:RB:47:C:N4	2.46	0.47
37:RD:12:SER:HB2	37:RD:208:LYS:HB3	1.95	0.47
37:RD:142:VAL:HG23	37:RD:193:VAL:HA	1.94	0.47
49:RT:4:GLY:O	49:RT:8:LYS:NZ	2.48	0.47
18:XR:59:SER:OG	18:XR:60:ALA:N	2.48	0.47
50:YU:29:SER:OG	50:YU:30:LYS:NZ	2.42	0.47
2:QB:52:GLU:HG3	2:QB:56:ARG:NH1	2.30	0.47
2:QB:55:PHE:O	2:QB:59:GLU:HG2	2.14	0.47
11:QK:50:TYR:CE2	11:QK:54:ARG:NH1	2.83	0.47
25:R0:29:GLN:NE2	35:RA:922:U:O2'	2.47	0.47
35:RA:2416:C:H5''	45:RP:64:LYS:HE2	1.95	0.47
35:RA:2845:G:H2'	35:RA:2846:G:H8	1.80	0.47
37:RD:145:VAL:HG11	37:RD:175:LEU:HD11	1.96	0.47
41:RH:4:ILE:HG23	41:RH:6:ARG:HG2	1.97	0.47
45:RP:107:LYS:HB2	45:RP:110:TYR:CD2	2.50	0.47
1:XA:818:G:O2'	1:XA:820:U:OP2	2.23	0.47
8:XH:85:ARG:HD3	8:XH:88:LYS:HG2	1.96	0.47
11:XK:83:ILE:HG23	11:XK:109:VAL:HG13	1.97	0.47
35:YA:2392:A:C8	45:YP:61:ARG:HG2	2.49	0.47
35:YA:974:G:O2'	35:YA:975:G:N7	2.35	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:YG:163:ALA:HB1	40:YG:168:GLU:HG3	1.95	0.47
51:YV:19:LYS:HA	51:YV:94:LEU:O	2.15	0.47
35:YA:24:G:O2'	52:YW:78:GLU:O	2.30	0.47
54:YY:34:LYS:HD3	54:YY:34:LYS:HA	1.68	0.47
54:YY:68:HIS:HB3	54:YY:71:LYS:HG3	1.97	0.47
1:QA:1014:A:H3'	1:QA:1015:A:C8	2.50	0.47
1:QA:272:C:H2'	1:QA:273:A:H8	1.78	0.47
1:QA:464:G:N1	1:QA:467:G:OP2	2.46	0.47
1:QA:1061:G:OP1	10:QJ:59:SER:OG	2.32	0.47
19:QS:65:ASN:OD1	19:QS:66:MET:HG2	2.14	0.47
36:RB:37:C:O2	48:RS:95:HIS:NE2	2.48	0.47
1:XA:1015:A:H2'	1:XA:1016:A:C8	2.50	0.47
25:Y0:70:GLN:OE1	25:Y0:80:HIS:NE2	2.48	0.47
35:YA:579:G:O2'	35:YA:2019:A:OP1	2.30	0.47
35:YA:2175:C:H2'	35:YA:2176:A:H8	1.79	0.47
35:YA:2006:C:O2'	35:YA:2823:A:N3	2.47	0.47
35:YA:2822:G:OP1	38:YE:159:HIS:NE2	2.48	0.47
47:YR:36:THR:HG22	47:YR:37:THR:H	1.80	0.47
16:QP:71:ARG:HH11	16:QP:75:ARG:HE	1.61	0.47
29:R4:42:PHE:C	29:R4:42:PHE:HD1	2.17	0.47
35:RA:1791:A:N6	35:RA:1828:G:O2'	2.44	0.47
40:RG:135:LEU:CD2	40:RG:140:ILE:HD11	2.42	0.47
41:RH:6:ARG:O	41:RH:69:ARG:NH2	2.48	0.47
1:XA:1316:G:N2	1:XA:1318:A:H3'	2.29	0.47
1:XA:769:G:H4'	1:XA:1513:A:H4'	1.97	0.47
5:XE:78:HIS:CE1	5:XE:142:LEU:HD23	2.50	0.47
10:XJ:10:GLY:HA3	10:XJ:16:LEU:HD11	1.97	0.47
13:XM:81:LEU:O	13:XM:89:GLY:HA3	2.15	0.47
13:XM:86:CYS:SG	13:XM:87:TYR:N	2.87	0.47
20:XT:89:ARG:HD2	20:XT:104:LEU:HD21	1.96	0.47
22:XV:76:A:OP1	35:YA:2439:A:N6	2.46	0.47
30:Y5:51:TYR:CE2	30:Y5:56:LYS:HD3	2.49	0.47
35:YA:1139:G:O2'	35:YA:1143:A:N6	2.45	0.47
35:YA:2010:G:H5''	52:YW:42:ARG:HB2	1.96	0.47
35:YA:2123:G:H2'	35:YA:2124:G:C8	2.49	0.47
35:YA:1049:C:N4	35:YA:2751:G:O6	2.48	0.47
35:YA:851:U:H2'	35:YA:852:G:H8	1.80	0.47
40:YG:37:VAL:HG23	40:YG:99:MET:HE3	1.97	0.47
10:QJ:8:LEU:HG	10:QJ:94:VAL:HG12	1.97	0.47
41:RH:53:GLU:HA	41:RH:65:HIS:CE1	2.49	0.47
45:RP:100:LEU:O	45:RP:105:LEU:N	2.38	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:XF:46:ARG:HD3	6:XF:60:PHE:HD2	1.78	0.47
8:XH:6:ILE:HB	8:XH:85:ARG:HH12	1.80	0.47
10:XJ:20:ALA:HA	10:XJ:23:ILE:HD12	1.97	0.47
11:XK:124:LYS:HD2	11:XK:125:PHE:CE1	2.50	0.47
13:XM:3:ARG:HA	13:XM:8:GLU:HA	1.96	0.47
13:XM:58:GLU:O	13:XM:62:ASN:HB2	2.13	0.47
20:XT:27:LYS:O	20:XT:31:SER:OG	2.30	0.47
35:YA:1019:U:OP1	35:YA:1035:U:O2'	2.23	0.47
35:YA:2712:U:H2'	35:YA:2713:A:H5'	1.96	0.47
40:YG:144:ILE:HG23	40:YG:148:MET:HE3	1.96	0.47
33:Y8:7:HIS:CD2	45:YP:50:ARG:HD3	2.50	0.47
1:QA:1240:U:H4'	7:QG:38:LEU:HD21	1.97	0.47
7:QG:75:VAL:HA	7:QG:88:PRO:HA	1.97	0.47
13:QM:108:ARG:CZ	13:QM:114:ARG:HG3	2.45	0.47
13:QM:16:ASP:OD1	13:QM:41:PRO:O	2.33	0.47
35:RA:1385:G:O2'	35:RA:1386:C:O4'	2.33	0.47
35:RA:531:C:OP1	35:RA:561:G:N1	2.47	0.47
40:RG:117:PHE:C	40:RG:119:GLY:H	2.18	0.47
42:RI:88:ILE:HG22	42:RI:90:GLY:O	2.14	0.47
43:RN:24:GLY:O	43:RN:28:THR:HG23	2.14	0.47
45:RP:81:GLN:HB3	45:RP:106:LEU:HD12	1.96	0.47
45:RP:65:ARG:O	45:RP:68:GLN:NE2	2.48	0.47
1:XA:652:U:O4	1:XA:752:G:O2'	2.25	0.47
7:XG:97:GLN:CG	7:XG:101:LEU:HD13	2.45	0.47
1:QA:405:U:H5''	1:QA:495:A:H2	1.80	0.47
2:QB:87:ARG:NH1	2:QB:219:VAL:HG13	2.29	0.47
13:QM:23:TYR:CE2	13:QM:71:ARG:HG3	2.50	0.47
48:RS:66:ALA:HA	48:RS:69:VAL:HG12	1.97	0.47
49:RT:66:VAL:HA	49:RT:71:GLY:HA2	1.97	0.47
1:XA:1016:A:OP1	14:YN:15:LYS:NZ	2.43	0.47
3:XC:82:GLU:OE2	3:XC:82:GLU:N	2.43	0.47
24:XZ:58:ARG:NE	24:XZ:68:TYR:OH	2.48	0.47
35:YA:392:C:H5''	35:YA:409:C:H5''	1.96	0.47
39:YF:155:LEU:HB2	39:YF:189:THR:HG21	1.95	0.47
43:YN:95:PRO:O	43:YN:97:ARG:N	2.44	0.47
47:YR:79:LEU:HA	47:YR:83:ILE:HD12	1.97	0.47
1:QA:501:C:H2'	1:QA:502:G:C8	2.50	0.47
5:QE:51:VAL:HG13	5:QE:52:PRO:HD3	1.96	0.47
35:RA:1678:G:N2	35:RA:1989:G:H22	2.13	0.47
39:RF:117:ARG:HD3	39:RF:120:GLU:OE2	2.15	0.47
35:RA:301:G:OP2	54:RY:84:ARG:NH2	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:45:U:H2'	1:XA:46:G:C8	2.50	0.47
7:XG:15:ASP:HB3	7:XG:19:GLY:H	1.79	0.47
1:XA:1343:G:H1'	9:XI:121:ARG:HE	1.80	0.47
13:XM:14:ARG:H	13:XM:44:ARG:HD3	1.79	0.47
1:XA:1494:G:H5'	24:XY:47:PRO:HG2	1.96	0.47
24:XZ:3:LEU:HD11	24:XZ:31:ILE:HG21	1.97	0.47
35:YA:1806:C:O2	37:YD:46:GLN:NE2	2.48	0.47
35:YA:2212:A:H1'	35:YA:2215:G:C5	2.50	0.47
35:YA:954:G:H5'	46:YQ:13:GLN:HB3	1.96	0.47
55:YZ:108:PRO:HA	55:YZ:142:SER:HA	1.97	0.47
1:QA:186(B):C:H2'	1:QA:186(C):G:C8	2.50	0.46
1:QA:674:G:H2'	1:QA:675:A:C8	2.48	0.46
3:QC:24:ALA:HB3	3:QC:32:LEU:HD11	1.97	0.46
8:QH:34:GLU:OE1	8:QH:37:ARG:NH2	2.48	0.46
31:R6:23:THR:OG1	31:R6:24:GLU:N	2.47	0.46
35:RA:1296:G:OP1	35:RA:2709:G:O2'	2.31	0.46
41:RH:17:VAL:HG23	41:RH:45:VAL:CG1	2.45	0.46
1:XA:246:A:N1	1:XA:278:G:O2'	2.43	0.46
1:XA:692:U:O2'	1:XA:694:A:N7	2.43	0.46
20:XT:99:LEU:HD23	20:XT:99:LEU:H	1.80	0.46
35:YA:1434:A:H61	35:YA:1558:A:H62	1.61	0.46
1:QA:1453:G:H2'	20:QT:39:LYS:HE2	1.96	0.46
1:QA:243:A:N6	1:QA:281:G:O2'	2.47	0.46
2:QB:212:GLN:HG3	2:QB:235:SER:HB3	1.97	0.46
4:QD:57:ARG:HB3	4:QD:206:PHE:HB2	1.98	0.46
9:QI:5:TYR:HA	9:QI:17:VAL:O	2.15	0.46
35:RA:1600:C:OP1	53:RX:58:HIS:NE2	2.40	0.46
35:RA:2112:G:H22	35:RA:2170:A:H61	1.63	0.46
35:RA:27:G:HO2'	35:RA:28:A:H8	1.62	0.46
41:RH:107:VAL:HG21	41:RH:151:ILE:HG21	1.97	0.46
38:RE:20:ALA:N	44:RO:72:PRO:O	2.45	0.46
1:XA:1305:G:HO2'	1:XA:1306:A:H8	1.61	0.46
1:XA:674:G:H2'	1:XA:675:A:C8	2.50	0.46
1:XA:991:U:O4	1:XA:1212:U:O2'	2.28	0.46
20:XT:23:ARG:NH1	20:XT:27:LYS:HE2	2.31	0.46
22:XV:19:G:H3'	22:XV:20:U:H5	1.80	0.46
35:YA:629:G:N3	35:YA:639:U:O2'	2.48	0.46
38:YE:29:GLY:H	38:YE:180:ASN:HB3	1.80	0.46
55:YZ:6:LYS:HG3	55:YZ:8:TYR:CE2	2.49	0.46
1:QA:1119:C:H2'	1:QA:1120:G:H8	1.79	0.46
1:QA:45:U:H2'	1:QA:46:G:C8	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:545:C:H5'	4:QD:72:GLU:HG2	1.96	0.46
7:QG:45:ASP:O	7:QG:49:ILE:HG13	2.15	0.46
35:RA:571:A:H5'	35:RA:2030:A:H62	1.80	0.46
35:RA:686:G:H21	35:RA:788:A:H61	1.63	0.46
41:RH:99:VAL:HB	41:RH:102:ALA:HB3	1.97	0.46
41:RH:8:PRO:HD2	41:RH:69:ARG:CD	2.42	0.46
44:RO:105:GLU:OE2	44:RO:105:GLU:N	2.46	0.46
46:RQ:24:GLY:N	46:RQ:101:ARG:NH1	2.60	0.46
46:RQ:67:ARG:HE	46:RQ:102:VAL:HB	1.80	0.46
1:XA:1255:G:H5''	3:XC:26:LYS:HZ2	1.80	0.46
1:XA:1510:U:H2'	1:XA:1511:G:C8	2.50	0.46
2:XB:35:GLU:OE2	2:XB:39:ILE:N	2.49	0.46
2:XB:61:LEU:HG	2:XB:66:GLY:HA3	1.97	0.46
12:XL:39:VAL:HB	12:XL:57:LYS:HD3	1.97	0.46
27:Y2:38:GLN:NE2	27:Y2:44:LEU:HD23	2.31	0.46
32:Y7:5:TRP:NE1	32:Y7:7:PRO:HG3	2.31	0.46
35:YA:2584:U:H5'	56:ZB:3:PPU:H103	1.98	0.46
35:YA:299:A:N1	35:YA:322:A:O2'	2.39	0.46
41:YH:40:GLU:OE2	41:YH:60:ARG:NH2	2.48	0.46
1:QA:861:G:O2'	1:QA:874:G:O2'	2.30	0.46
2:QB:8:LYS:H	2:QB:11:LEU:HD12	1.80	0.46
7:QG:47:CYS:HA	7:QG:50:ILE:HG22	1.96	0.46
7:QG:91:VAL:O	7:QG:96:GLN:NE2	2.49	0.46
16:QP:43:LYS:HG2	16:QP:48:TRP:CD2	2.50	0.46
29:R4:40:HIS:NE2	29:R4:45:GLY:HA3	2.30	0.46
35:RA:2731:G:OP1	38:RE:169:ASN:ND2	2.48	0.46
35:RA:608:A:H2'	35:RA:609:A:C8	2.50	0.46
39:RF:107:LYS:HE3	39:RF:206:ILE:HA	1.97	0.46
29:R4:25:TYR:CZ	40:RG:3:LEU:HD21	2.50	0.46
48:RS:93:LYS:HD3	48:RS:95:HIS:HB2	1.98	0.46
35:RA:24:G:H5''	52:RW:8:ARG:HH22	1.80	0.46
36:RB:104:A:OP1	55:RZ:72:ARG:NH2	2.48	0.46
1:XA:1270:C:H2'	1:XA:1271:G:C8	2.50	0.46
1:XA:56:U:H2'	1:XA:57:G:C8	2.50	0.46
2:XB:54:THR:O	2:XB:58:ILE:HG13	2.14	0.46
3:XC:150:LYS:HB3	3:XC:201:TYR:HB2	1.96	0.46
24:XZ:49:LYS:HA	24:XZ:49:LYS:HD2	1.67	0.46
29:Y4:57:GLU:HA	29:Y4:60:GLN:HB2	1.97	0.46
32:Y7:24:THR:O	32:Y7:28:ARG:HG3	2.16	0.46
35:YA:2258:C:O2'	35:YA:2427:C:OP2	2.28	0.46
49:YT:6:LEU:HA	49:YT:9:LEU:HB2	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:QL:59:ARG:HA	12:QL:65:GLU:HA	1.97	0.46
13:QM:19:LEU:HD11	13:QM:30:ALA:HA	1.98	0.46
1:QA:1318:A:H1'	19:QS:37:ARG:HH21	1.81	0.46
35:RA:247:G:H4'	35:RA:386:G:C5	2.51	0.46
35:RA:270(H):C:H42	35:RA:270(R):G:H1	1.63	0.46
42:RI:97:ILE:HG12	42:RI:140:LEU:HD11	1.97	0.46
2:XB:59:GLU:HB3	2:XB:221:LEU:HD21	1.97	0.46
3:XC:19:GLU:OE1	3:XC:54:ARG:HG3	2.15	0.46
13:XM:49:THR:HG22	13:XM:51:ALA:N	2.30	0.46
6:XF:87:ARG:NH1	18:XR:75:ILE:O	2.49	0.46
35:YA:1782:C:H1'	35:YA:2609:U:H5''	1.97	0.46
35:YA:918:A:N3	36:YB:80:U:O2'	2.45	0.46
43:YN:12:ARG:HB3	43:YN:50:ASP:OD2	2.15	0.46
1:QA:1189:C:OP1	10:QJ:51:ARG:NH2	2.43	0.46
1:QA:1323:G:H2'	1:QA:1324:A:C8	2.51	0.46
2:QB:13:ALA:HA	2:QB:17:PHE:CE2	2.50	0.46
33:R8:62:LEU:HB3	33:R8:65:GLU:HB2	1.98	0.46
35:RA:1105:U:H2'	35:RA:1106:G:C8	2.51	0.46
35:RA:2098:U:H3	35:RA:2191:G:H1	1.63	0.46
35:RA:300:A:O2'	35:RA:318:C:O2	2.31	0.46
35:RA:632:A:H2'	35:RA:633:A:C8	2.50	0.46
40:RG:103:LEU:O	40:RG:106:LEU:HB3	2.15	0.46
40:RG:73:ALA:HB2	40:RG:88:ILE:HD11	1.97	0.46
42:RI:8:PRO:C	42:RI:8:PRO:N	2.62	0.46
51:RV:68:LYS:H	51:RV:68:LYS:HD2	1.79	0.46
1:XA:192:U:H2'	1:XA:193:C:H6	1.81	0.46
7:XG:113:GLU:HB2	7:XG:119:ARG:HG2	1.98	0.46
35:YA:227:A:OP1	45:YP:76:LYS:NZ	2.27	0.46
35:YA:776:G:N7	35:YA:793:A:O2'	2.49	0.46
44:YO:70:LYS:HE2	44:YO:70:LYS:HB2	1.70	0.46
47:YR:56:LYS:NZ	47:YR:90:ARG:O	2.48	0.46
2:QB:154:LEU:O	2:QB:155:LEU:HB3	2.15	0.46
1:QA:738:C:H5''	6:QF:69:GLU:HB2	1.96	0.46
7:QG:69:VAL:CA	7:QG:138:LYS:CD	2.87	0.46
37:RD:133:LEU:HD11	37:RD:145:VAL:HG13	1.98	0.46
40:RG:7:LEU:HD23	40:RG:100:TRP:HE3	1.80	0.46
44:RO:2:ILE:HB	44:RO:33:ALA:HB3	1.97	0.46
1:XA:924:C:O2'	1:XA:1502:A:N6	2.49	0.46
7:XG:111:ARG:HD2	7:XG:123:GLU:HB2	1.98	0.46
9:XI:10:ARG:HD3	9:XI:75:ASP:HB3	1.98	0.46
1:XA:1279:A:H5''	10:XJ:7:LYS:HE3	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:XK:21:ILE:HB	11:XK:84:VAL:HG12	1.98	0.46
35:YA:2315:G:OP1	40:YG:36:LYS:NZ	2.37	0.46
35:YA:2638:G:P	38:YE:82:ARG:HH12	2.39	0.46
1:QA:630:G:H3'	1:QA:631:G:H8	1.81	0.46
1:QA:937:A:O2'	7:QG:76:ARG:NH2	2.49	0.46
4:QD:96:LEU:HB3	4:QD:139:ARG:HH12	1.81	0.46
7:QG:90:GLU:CD	7:QG:90:GLU:H	2.17	0.46
9:QI:113:LYS:H	9:QI:119:ALA:HA	1.81	0.46
24:QY:44:LYS:CE	24:QY:59:ARG:HH11	2.25	0.46
35:RA:1139:G:O2'	35:RA:1143:A:N6	2.49	0.46
37:RD:4:LYS:HB2	37:RD:18:VAL:HG13	1.98	0.46
3:XC:189:ALA:CB	3:XC:196:LEU:H	2.27	0.46
6:XF:61:LEU:HD23	6:XF:63:TYR:HE2	1.80	0.46
13:XM:51:ALA:O	13:XM:55:ARG:HG3	2.15	0.46
27:Y2:41:ILE:HG13	27:Y2:43:GLN:HG3	1.97	0.46
35:YA:2148:G:H2'	35:YA:2149:G:H8	1.81	0.46
35:YA:277:C:H3'	35:YA:278:A:H8	1.81	0.46
44:YO:34:THR:HG22	44:YO:35:VAL:H	1.80	0.46
1:QA:1510:U:H2'	1:QA:1511:G:C8	2.51	0.46
1:QA:985:C:H2'	1:QA:986:A:H8	1.81	0.46
7:QG:120:ILE:O	7:QG:124:LEU:HD12	2.16	0.46
27:R2:25:VAL:O	27:R2:29:LYS:HG2	2.16	0.46
35:RA:2314:C:H5'	40:RG:38:VAL:HG11	1.96	0.46
41:RH:59:ARG:HA	41:RH:62:LYS:HE2	1.98	0.46
43:RN:12:ARG:HG2	43:RN:13:TRP:N	2.31	0.46
1:XA:958:A:N3	1:XA:985:C:O2'	2.40	0.46
1:XA:1330:U:H4'	13:XM:23:TYR:CD1	2.50	0.46
15:XO:36:ILE:HD13	15:XO:60:VAL:HG12	1.98	0.46
35:YA:1194:A:N7	45:YP:15:ARG:NH1	2.63	0.46
25:Y0:14:ARG:NH2	35:YA:2279:G:N7	2.58	0.46
35:YA:2688:U:OP1	35:YA:2713:A:N6	2.48	0.46
38:YE:132:HIS:O	38:YE:134:ILE:HG12	2.16	0.46
39:YF:32:LEU:O	39:YF:36:VAL:HG23	2.15	0.46
41:YH:127:GLU:HG2	41:YH:128:PRO:HD2	1.97	0.46
43:YN:40:PRO:HB3	50:YU:68:ALA:HB2	1.98	0.46
55:YZ:14:LYS:C	55:YZ:14:LYS:CB	2.77	0.46
34:R9:25:VAL:HG22	34:R9:34:GLN:HB2	1.98	0.46
35:RA:2275:C:H1'	46:RQ:85:LYS:HA	1.98	0.46
42:RI:113:ARG:CG	42:RI:113:ARG:NH1	2.73	0.46
49:RT:11:GLU:OE1	49:RT:11:GLU:N	2.41	0.46
1:XA:62:U:H3	1:XA:105:G:H1	1.63	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:1392:G:N2	1:XA:1502:A:H8	2.14	0.46
1:XA:908:A:H2'	1:XA:909:A:C8	2.51	0.46
7:XG:59:LEU:O	7:XG:63:LYS:HG3	2.16	0.46
20:XT:45:GLN:N	20:XT:91:LEU:HD21	2.31	0.46
3:QC:52:LEU:HA	3:QC:70:VAL:HG22	1.97	0.45
9:QI:71:SER:HA	9:QI:74:ILE:HG22	1.98	0.45
11:QK:34:ASP:HB2	11:QK:35:PRO:CD	2.46	0.45
24:QY:16:TRP:NE1	24:QY:80:CYS:O	2.37	0.45
24:QZ:44:LYS:NZ	24:QZ:59:ARG:NH1	2.64	0.45
24:QZ:62:GLU:CG	24:QZ:62:GLU:O	2.65	0.45
35:RA:1550:C:H5'	35:RA:1733:G:H22	1.81	0.45
39:RF:155:LEU:HB2	39:RF:189:THR:HG21	1.98	0.45
39:RF:64:ILE:HD11	39:RF:78:ILE:HG23	1.97	0.45
42:RI:109:ILE:CG2	42:RI:130:TYR:CZ	3.00	0.45
1:XA:501:C:H2'	1:XA:502:G:H8	1.81	0.45
2:XB:21:ARG:HD2	2:XB:22:LYS:HB3	1.98	0.45
35:YA:2148:G:H2'	35:YA:2149:G:C8	2.51	0.45
35:YA:839:U:H1'	35:YA:1191:G:H1'	1.97	0.45
1:QA:1001:G:H2'	1:QA:1002:G:C8	2.50	0.45
1:QA:148:G:H2'	1:QA:149:A:C8	2.50	0.45
1:QA:171:A:H2'	1:QA:172:A:C8	2.51	0.45
1:QA:713:G:H2'	1:QA:714:G:C8	2.52	0.45
13:QM:14:ARG:O	13:QM:16:ASP:N	2.49	0.45
24:QZ:34:THR:HG21	24:QZ:68:TYR:CE1	2.52	0.45
31:R6:37:ARG:HB2	31:R6:48:VAL:HG12	1.98	0.45
35:RA:2502:G:H5''	35:RA:2503:A:H5''	1.98	0.45
42:RI:114:LEU:O	42:RI:114:LEU:HD23	2.15	0.45
53:RX:90:GLU:N	53:RX:90:GLU:OE1	2.47	0.45
1:XA:107:G:O6	20:XT:15:ARG:NH1	2.44	0.45
1:XA:1123:A:H4'	10:XJ:36:GLY:HA3	1.97	0.45
1:XA:269:C:H2'	1:XA:270:A:C8	2.50	0.45
1:XA:118:U:H3'	1:XA:288:A:H61	1.81	0.45
1:XA:413:G:O2'	1:XA:428:G:N2	2.49	0.45
1:XA:737:A:H2'	1:XA:738:C:C6	2.51	0.45
1:XA:948:C:H2'	1:XA:949:A:H8	1.81	0.45
13:XM:84:ILE:HG23	13:XM:86:CYS:H	1.80	0.45
8:QH:54:ASP:HB2	8:QH:56:LYS:NZ	2.31	0.45
24:QZ:27:ILE:HG23	24:QZ:66:LEU:HD21	1.98	0.45
29:R4:15:ILE:HD11	29:R4:32:TYR:HD2	1.81	0.45
35:RA:373:U:H1'	35:RA:423:A:N3	2.32	0.45
35:RA:519:U:H2'	35:RA:520:G:H8	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:RD:73:VAL:HA	37:RD:119:ALA:O	2.17	0.45
38:RE:77:ILE:HG21	38:RE:195:LEU:CD2	2.45	0.45
41:RH:30:LYS:HE2	41:RH:30:LYS:HB2	1.68	0.45
41:RH:45:VAL:O	41:RH:45:VAL:HG12	2.16	0.45
54:RY:14:LEU:HB2	54:RY:75:ILE:HD11	1.98	0.45
1:XA:1103:C:OP1	2:XB:96:ARG:NH2	2.49	0.45
9:XI:32:ASP:N	9:XI:35:GLU:OE1	2.27	0.45
9:XI:114:TYR:CE2	10:XJ:59:SER:HA	2.52	0.45
15:XO:3:ILE:HD12	15:XO:8:LYS:HD2	1.99	0.45
16:XP:71:ARG:HH11	16:XP:75:ARG:HH21	1.63	0.45
35:YA:2159:G:H2'	35:YA:2160:G:C8	2.52	0.45
35:YA:2702:U:O2	35:YA:2703:C:N4	2.50	0.45
35:YA:693:C:H2'	35:YA:694:U:C6	2.52	0.45
43:YN:83:LYS:HA	43:YN:83:LYS:HD2	1.70	0.45
43:RN:118:LYS:O	43:RN:121:LYS:NZ	2.49	0.45
55:RZ:152:ALA:N	55:RZ:169:GLU:O	2.48	0.45
1:XA:1172:C:H2'	1:XA:1173:G:H8	1.82	0.45
1:XA:1435:G:H2'	1:XA:1436:U:C6	2.51	0.45
1:XA:501:C:H2'	1:XA:502:G:C8	2.52	0.45
2:XB:70:PHE:HD1	2:XB:163:PHE:HB3	1.81	0.45
11:XK:20:TYR:HB2	11:XK:31:THR:HG23	1.97	0.45
19:XS:25:LYS:HA	19:XS:25:LYS:HD2	1.70	0.45
1:XA:1318:A:C5'	19:XS:3:ARG:HH12	2.29	0.45
35:YA:2446:G:N2	35:YA:2449:U:O2	2.47	0.45
35:YA:859:G:HO2'	35:YA:916:G:H1	1.61	0.45
42:YI:140:LEU:HD12	42:YI:141:LYS:N	2.32	0.45
45:YP:138:LEU:HD23	45:YP:145:PRO:HB3	1.96	0.45
35:YA:2393:A:O2'	45:YP:60:MET:O	2.30	0.45
1:QA:1300:G:O2'	1:QA:1301:U:O5'	2.33	0.45
1:QA:1404:C:H2'	1:QA:1405:G:C8	2.52	0.45
2:QB:155:LEU:HD22	2:QB:157:ARG:O	2.17	0.45
2:QB:193:ASP:OD2	2:QB:193:ASP:N	2.48	0.45
3:QC:85:ARG:O	3:QC:89:GLU:N	2.50	0.45
5:QE:144:THR:OG1	5:QE:147:ASP:OD1	2.32	0.45
19:QS:43:GLU:O	19:QS:47:HIS:CE1	2.70	0.45
60:QX:101:A3P:N6	24:QY:49:LYS:O	2.49	0.45
35:RA:48:G:N1	35:RA:177:G:OP2	2.41	0.45
35:RA:2023:G:OP2	35:RA:2617:C:H4'	2.17	0.45
35:RA:2183:C:H2'	35:RA:2184:G:H8	1.81	0.45
41:RH:72:ILE:O	41:RH:75:ALA:HB3	2.16	0.45
1:XA:1233:G:O2'	1:XA:1365:G:OP1	2.35	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:634:C:H2'	1:XA:635:G:H8	1.82	0.45
1:XA:878:G:H5'	8:XH:89:PRO:HG2	1.97	0.45
13:XM:14:ARG:HH21	13:XM:42:ALA:HA	1.81	0.45
13:XM:23:TYR:CE2	13:XM:71:ARG:HG3	2.51	0.45
24:XY:42:LYS:O	24:XY:58:ARG:NH1	2.49	0.45
35:YA:589:C:H2'	35:YA:590:A:C8	2.52	0.45
44:YO:119:PRO:HB2	49:YT:68:TYR:CZ	2.50	0.45
35:YA:833:U:O2	45:YP:55:ARG:NH2	2.50	0.45
51:YV:4:ILE:HD12	51:YV:39:LEU:HD22	1.99	0.45
54:YY:30:VAL:HG22	54:YY:37:VAL:HG12	1.98	0.45
11:QK:50:TYR:CD2	11:QK:54:ARG:NH1	2.85	0.45
13:QM:23:TYR:HE2	13:QM:71:ARG:HG3	1.82	0.45
11:QK:109:VAL:HG12	18:QR:86:VAL:HA	1.97	0.45
19:QS:3:ARG:HH12	19:QS:5:LEU:HB3	1.82	0.45
26:R1:69:LYS:O	26:R1:73:LEU:HG	2.17	0.45
35:RA:851:U:H2'	35:RA:852:G:H8	1.81	0.45
41:RH:7:LEU:N	41:RH:8:PRO:HD3	2.30	0.45
55:RZ:41:LEU:O	55:RZ:45:ASP:N	2.45	0.45
1:XA:1355:G:H2'	1:XA:1356:G:H8	1.81	0.45
1:XA:142:G:H2'	1:XA:143:A:H8	1.81	0.45
1:XA:448:A:H62	1:XA:486:U:H3	1.64	0.45
1:XA:715:A:H2'	1:XA:716:A:C8	2.51	0.45
24:XY:16:TRP:CZ2	24:XY:81:ARG:HG3	2.52	0.45
35:YA:1113:U:H2'	35:YA:1114:G:H8	1.81	0.45
35:YA:2291:U:H2'	35:YA:2292:C:C6	2.51	0.45
37:YD:145:VAL:HB	37:YD:155:LEU:HB2	1.99	0.45
42:YI:130:TYR:HB3	42:YI:136:VAL:HG13	1.97	0.45
42:YI:66:GLU:OE1	42:YI:67:ARG:HG2	2.17	0.45
1:QA:1151:A:H1'	10:QJ:39:PRO:HB2	1.98	0.45
1:QA:1210:C:O2'	1:QA:1213:A:O2'	2.34	0.45
1:QA:1355:G:H2'	1:QA:1356:G:H8	1.82	0.45
1:QA:757:U:O2'	1:QA:879:C:O2	2.34	0.45
4:QD:63:LYS:HE3	4:QD:198:VAL:HG22	1.99	0.45
13:QM:13:LYS:HG3	13:QM:17:VAL:HG22	1.94	0.45
13:QM:14:ARG:O	13:QM:17:VAL:CG1	2.64	0.45
28:R3:55:ARG:HE	28:R3:55:ARG:HA	1.82	0.45
1:XA:1371:G:O3'	9:XI:69:GLY:HA3	2.17	0.45
1:XA:950:U:H2'	1:XA:951:G:C8	2.52	0.45
24:XZ:61:THR:O	24:XZ:65:ARG:NH1	2.50	0.45
33:Y8:30:ARG:NH1	35:YA:2394:C:OP1	2.50	0.45
35:YA:532:A:N1	35:YA:2035:G:N2	2.64	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YA:320:A:H4'	35:YA:322:A:N7	2.32	0.45
38:YE:29:GLY:HA3	38:YE:51:PHE:HE1	1.82	0.45
40:YG:179:PRO:N	40:YG:179:PRO:C	2.61	0.45
48:YS:25:ARG:HG3	48:YS:88:ASP:HB2	1.98	0.45
51:YV:5:VAL:HG11	51:YV:35:LEU:HD13	1.98	0.45
1:QA:31:G:O2'	1:QA:48:C:N4	2.49	0.45
4:QD:62:GLN:HE22	4:QD:65:ARG:HH21	1.64	0.45
10:QJ:7:LYS:HB3	10:QJ:71:LEU:CG	2.46	0.45
1:QA:1228:C:P	13:QM:108:ARG:HH12	2.40	0.45
34:R9:22:ARG:HD2	34:R9:35:ARG:NH1	2.32	0.45
35:RA:30:G:O2'	35:RA:1214:A:N3	2.47	0.45
26:R1:78:LYS:HE2	35:RA:270(S):G:H1'	1.99	0.45
35:RA:587:C:OP2	45:RP:21:ARG:NH1	2.26	0.45
38:RE:64:LYS:O	38:RE:68:ALA:N	2.48	0.45
41:RH:89:ILE:O	41:RH:129:THR:OG1	2.35	0.45
3:XC:81:GLY:N	3:XC:82:GLU:OE2	2.49	0.45
4:XD:173:TRP:HB3	4:XD:187:ARG:HH21	1.80	0.45
1:XA:728:A:N7	15:XO:54:ARG:NH1	2.65	0.45
35:YA:2392:A:H2	35:YA:2424:C:H42	1.64	0.45
35:YA:414:C:H2'	35:YA:415:A:C8	2.52	0.45
48:YS:39:ILE:HD12	48:YS:85:VAL:HG11	1.99	0.45
5:QE:147:ASP:O	5:QE:151:LEU:HG	2.16	0.45
8:QH:95:VAL:HB	8:QH:99:GLU:HG3	1.99	0.45
15:QO:56:LEU:O	15:QO:60:VAL:HG23	2.17	0.45
19:QS:66:MET:HA	19:QS:69:HIS:HD2	1.81	0.45
26:R1:82:LEU:HB3	26:R1:83:GLU:H	1.54	0.45
35:RA:2746:U:H5"	41:RH:138:LYS:HD2	1.99	0.45
42:RI:12:LEU:HD22	42:RI:19:VAL:HB	1.99	0.45
1:XA:454:C:H5'	16:XP:71:ARG:HH22	1.82	0.45
9:XI:10:ARG:HH11	9:XI:105:ASP:HB2	1.81	0.45
24:XY:56:TRP:HB2	24:XY:68:TYR:CE1	2.51	0.45
35:YA:1571:A:H2'	35:YA:1572:A:C8	2.52	0.45
38:YE:57:LYS:CG	38:YE:57:LYS:O	2.63	0.45
39:YF:65:TRP:CZ3	39:YF:72:ARG:HD2	2.51	0.45
47:YR:38:VAL:HG13	47:YR:39:PRO:HD3	1.98	0.45
54:YY:13:VAL:HG12	54:YY:74:PRO:HA	1.98	0.45
55:YZ:128:VAL:CG2	55:YZ:161:VAL:HG12	2.39	0.45
1:QA:352:C:O2'	1:QA:354:G:OP1	2.30	0.45
2:QB:219:VAL:O	2:QB:222:ILE:HG13	2.17	0.45
3:QC:84:ILE:O	3:QC:88:ARG:HG3	2.16	0.45
9:QI:17:VAL:HG21	9:QI:80:GLY:O	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:QM:78:ILE:O	13:QM:82:MET:HG3	2.17	0.45
27:R2:28:LYS:HD3	27:R2:53:LEU:HD11	1.99	0.45
35:RA:2103:C:H2'	35:RA:2104:G:H8	1.82	0.45
35:RA:414:C:H2'	35:RA:415:A:C8	2.52	0.45
37:RD:148:GLU:HB2	37:RD:151:LYS:HD2	1.99	0.45
40:RG:61:ALA:HB2	40:RG:67:LYS:HA	1.99	0.45
48:RS:11:LYS:CE	48:RS:91:PRO:HG3	2.43	0.45
49:RT:74:ARG:HG2	49:RT:76:PHE:CZ	2.52	0.45
1:XA:1382:C:H2'	1:XA:1383:C:H6	1.82	0.45
1:XA:1440:C:O2'	1:XA:1442:G:N2	2.50	0.45
6:XF:70:ASP:OD1	6:XF:70:ASP:N	2.47	0.45
8:XH:110:ALA:HB3	8:XH:121:ASP:HB3	1.97	0.45
8:XH:14:ARG:NH2	8:XH:83:ILE:O	2.47	0.45
9:XI:8:GLY:HA3	9:XI:76:ALA:O	2.17	0.45
10:XJ:34:VAL:HB	10:XJ:73:ASP:O	2.16	0.45
27:Y2:38:GLN:NE2	27:Y2:41:ILE:HD11	2.31	0.45
29:Y4:28:LYS:HB2	29:Y4:31:ILE:HD11	1.99	0.45
35:YA:116:C:O2'	35:YA:126:A:N3	2.44	0.45
35:YA:2245:U:H5''	35:YA:2246:G:H5'	1.99	0.45
40:YG:150:ASP:N	40:YG:150:ASP:OD1	2.36	0.45
35:YA:2727:G:O2'	44:YO:70:LYS:NZ	2.50	0.45
1:QA:17:U:H2'	1:QA:18:C:C6	2.52	0.44
1:QA:946:A:H2'	1:QA:947:G:H8	1.82	0.44
2:QB:233:SER:OG	2:QB:233:SER:O	2.35	0.44
2:QB:50:GLU:O	2:QB:54:THR:HG23	2.17	0.44
22:QW:19:G:H2'	35:RA:2112:G:H1'	1.99	0.44
24:QZ:44:LYS:NZ	24:QZ:59:ARG:HH11	2.16	0.44
33:R8:33:ASN:HB3	33:R8:41:ILE:HD11	1.99	0.44
35:RA:2441:C:OP2	35:RA:2586:C:O2'	2.30	0.44
39:RF:197:ASP:O	39:RF:201:VAL:HG23	2.18	0.44
40:RG:139:LEU:HD21	40:RG:146:TYR:HA	1.98	0.44
41:RH:18:GLU:HG3	41:RH:27:LYS:HZ2	1.82	0.44
49:RT:3:ARG:CA	49:RT:3:ARG:HB3	2.23	0.44
49:RT:96:ARG:HG2	49:RT:97:ALA:N	2.31	0.44
1:XA:1320:C:O2	19:XS:36:ARG:NH2	2.51	0.44
1:XA:1355:G:H2'	1:XA:1356:G:C8	2.52	0.44
22:XV:50:U:H3	22:XV:64:G:H1	1.65	0.44
25:Y0:27:GLU:HB2	25:Y0:69:PHE:HD2	1.82	0.44
35:YA:2108:C:OP1	35:YA:2150:U:O2'	2.35	0.44
35:YA:2657:A:H62	35:YA:2664:G:H21	1.65	0.44
35:YA:2730:C:O2'	38:YE:168:MET:O	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:XM:3:ARG:HH21	40:YG:113:ARG:HH21	1.62	0.44
42:YI:120:ILE:O	42:YI:120:ILE:HG23	2.17	0.44
3:QC:110:ASN:OD1	3:QC:140:ARG:NH2	2.50	0.44
3:QC:87:LEU:HA	3:QC:87:LEU:HD13	1.88	0.44
4:QD:92:VAL:O	4:QD:96:LEU:HD12	2.17	0.44
1:QA:4:U:H3	8:QH:102:ARG:NH1	2.14	0.44
27:R2:25:VAL:HG23	27:R2:57:ILE:HG23	2.00	0.44
28:R3:44:ARG:HA	28:R3:47:VAL:HG22	2.00	0.44
35:RA:1388:G:O2'	35:RA:1525:G:O2'	2.29	0.44
35:RA:2103:C:H2'	35:RA:2104:G:C8	2.53	0.44
41:RH:58:GLU:HB2	41:RH:61:HIS:H	1.82	0.44
46:RQ:68:ILE:HG22	46:RQ:101:ARG:HE	1.83	0.44
36:RB:114:G:HO2'	48:RS:50:SER:HG	1.59	0.44
35:RA:997:G:H5''	50:RU:92:ARG:NH1	2.33	0.44
54:RY:19:LYS:HE3	54:RY:20:TYR:CZ	2.52	0.44
2:XB:98:LEU:O	2:XB:101:MET:HG3	2.16	0.44
2:XB:136:VAL:HG13	2:XB:139:LYS:HB3	1.99	0.44
2:XB:21:ARG:HE	2:XB:21:ARG:HB3	1.47	0.44
31:Y6:8:LYS:HD3	33:Y8:34:TRP:CE2	2.52	0.44
37:YD:66:ASP:HB3	37:YD:105:ILE:HG22	1.99	0.44
1:QA:1064:G:OP2	1:QA:1385:G:O2'	2.29	0.44
1:QA:1391:U:H2'	1:QA:1392:G:C8	2.52	0.44
1:QA:377:G:OP1	16:QP:5:ARG:NH1	2.45	0.44
1:QA:56:U:H2'	1:QA:57:G:C8	2.51	0.44
40:RG:7:LEU:HA	40:RG:10:LYS:HB3	1.99	0.44
42:RI:9:LEU:N	42:RI:9:LEU:CD2	2.80	0.44
35:RA:2880:C:O3'	47:RR:90:ARG:NH1	2.50	0.44
48:RS:30:ARG:HD2	48:RS:97:ARG:HE	1.82	0.44
49:RT:7:ILE:HA	49:RT:7:ILE:HD13	1.75	0.44
1:XA:1270:C:H2'	1:XA:1271:G:H8	1.82	0.44
4:XD:153:ARG:CD	4:XD:181:MET:CE	2.87	0.44
11:XK:34:ASP:OD1	11:XK:38:ASN:N	2.50	0.44
8:XH:91:ARG:HD2	12:XL:7:ILE:HG13	1.99	0.44
15:XO:15:PHE:HD2	15:XO:30:ALA:HB2	1.82	0.44
16:XP:74:LEU:HB3	16:XP:79:VAL:HG11	1.98	0.44
18:XR:34:TYR:CD2	18:XR:35:ARG:HG3	2.53	0.44
22:XW:65:C:H2'	22:XW:66:C:C6	2.52	0.44
27:Y2:37:PHE:HE2	53:YX:47:PHE:HZ	1.64	0.44
31:Y6:8:LYS:HD3	33:Y8:34:TRP:CD2	2.53	0.44
35:YA:577:G:O2'	35:YA:1254:A:OP1	2.33	0.44
35:YA:336:C:H4'	54:YY:6:HIS:CE1	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YA:523:C:O2	35:YA:553:U:O2'	2.35	0.44
49:YT:111:ARG:C	49:YT:113:LYS:H	2.21	0.44
1:QA:1256:A:OP2	3:QC:26:LYS:NZ	2.32	0.44
1:QA:1435:G:H2'	1:QA:1436:U:C6	2.53	0.44
1:QA:811:C:O2'	1:QA:901:A:N1	2.45	0.44
2:QB:53:ARG:HG2	2:QB:56:ARG:NH2	2.32	0.44
8:QH:13:ILE:O	8:QH:17:THR:HG23	2.18	0.44
26:R1:92:LYS:HD3	26:R1:95:LEU:HD12	1.99	0.44
35:RA:1202:C:O2'	39:RF:184:TYR:OH	2.34	0.44
35:RA:1210:A:H5''	35:RA:1211:U:H3'	1.99	0.44
35:RA:2659:G:N2	35:RA:2662:A:OP2	2.46	0.44
36:RB:114:G:O2'	48:RS:50:SER:OG	2.21	0.44
42:RI:80:PRO:HA	42:RI:143:SER:O	2.18	0.44
1:XA:310:G:H4'	16:XP:31:LYS:HD2	1.99	0.44
4:XD:151:LYS:HE2	4:XD:151:LYS:H	1.82	0.44
9:XI:93:ARG:HH21	9:XI:97:LYS:HD3	1.82	0.44
22:XV:21:A:H61	22:XV:46:G:H2'	1.83	0.44
22:XW:43:A:H2'	22:XW:44:A:C8	2.53	0.44
27:Y2:15:LYS:N	27:Y2:67:LYS:HZ1	2.16	0.44
35:YA:1171:G:O2'	35:YA:1173:G:O4'	2.33	0.44
35:YA:1418:G:OP1	35:YA:1588:C:O2'	2.34	0.44
35:YA:2328:A:H2'	35:YA:2329:G:C8	2.52	0.44
35:YA:2579:C:H4'	38:YE:134:ILE:HG13	1.99	0.44
35:YA:859:G:N2	35:YA:917:A:OP2	2.48	0.44
37:YD:25:THR:HG21	37:YD:113:VAL:HG21	1.98	0.44
39:YF:153:SER:HB2	39:YF:190:GLU:H	1.83	0.44
48:YS:76:LYS:HB2	48:YS:76:LYS:HE2	1.75	0.44
55:YZ:133:ILE:HA	55:YZ:134:PRO:HD3	1.80	0.44
9:QI:9:ARG:HB2	9:QI:104:ARG:NE	2.33	0.44
11:QK:34:ASP:HB3	11:QK:40:ILE:HD11	1.99	0.44
12:QL:76:ASN:N	12:QL:76:ASN:OD1	2.47	0.44
1:QA:1229:A:P	13:QM:114:ARG:HD3	2.57	0.44
22:QW:18:G:H4'	22:QW:60:U:C2	2.53	0.44
24:QY:14:LEU:HD21	24:QZ:28:ASN:HD22	1.83	0.44
35:RA:2681:C:OP2	38:RE:109:LYS:NZ	2.44	0.44
35:RA:309:G:N3	35:RA:329:G:O2'	2.44	0.44
35:RA:539:G:H2'	35:RA:540:G:H8	1.82	0.44
35:RA:704:G:H1'	35:RA:727:A:N6	2.32	0.44
35:RA:959:A:N3	35:RA:2457:U:O2'	2.43	0.44
43:RN:6:PRO:HG3	43:RN:41:ASP:HB2	2.00	0.44
47:RR:96:ARG:O	47:RR:114:VAL:HA	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:RZ:151:HIS:HA	55:RZ:170:THR:HA	2.00	0.44
3:XC:152:ILE:HG12	3:XC:167:TRP:HD1	1.81	0.44
8:XH:119:LEU:HD23	8:XH:124:ALA:HA	2.00	0.44
35:YA:583:G:H5''	50:YU:10:ARG:HH12	1.83	0.44
35:YA:582:G:H2'	35:YA:583:G:H8	1.82	0.44
35:YA:919:G:N2	35:YA:2269:A:OP2	2.51	0.44
47:YR:28:LEU:HD23	47:YR:48:VAL:HG11	1.99	0.44
49:YT:128:GLU:O	49:YT:132:LYS:N	2.51	0.44
1:QA:1348:U:H4'	9:QI:120:ARG:NE	2.32	0.44
7:QG:44:TYR:HE2	9:QI:41:VAL:HG11	1.82	0.44
10:QJ:82:ILE:O	10:QJ:86:MET:HB2	2.17	0.44
1:QA:553:A:H5''	12:QL:24:VAL:HG21	1.98	0.44
13:QM:44:ARG:O	13:QM:48:LEU:CD2	2.66	0.44
35:RA:2748:A:H2	35:RA:2754:U:H3	1.65	0.44
35:RA:443:A:N7	39:RF:45:ARG:HG3	2.32	0.44
41:RH:6:ARG:HH11	41:RH:6:ARG:HG3	1.82	0.44
42:RI:120:ILE:HD13	42:RI:120:ILE:HG21	1.70	0.44
1:XA:1064:G:OP2	1:XA:1385:G:O2'	2.27	0.44
1:XA:1177:G:N2	1:XA:1181:G:O6	2.51	0.44
1:XA:269:C:H2'	1:XA:270:A:H8	1.83	0.44
2:XB:16:HIS:HD2	2:XB:204:ASN:H	1.66	0.44
6:XF:50:TYR:OH	6:XF:87:ARG:NH1	2.47	0.44
12:XL:51:ALA:HB3	12:XL:53:ARG:HE	1.82	0.44
20:XT:60:GLU:HA	20:XT:63:ILE:HD12	2.00	0.44
29:Y4:48:ARG:HB3	29:Y4:51:ASP:HB3	2.00	0.44
35:YA:1022:G:OP2	43:YN:69:GLN:NE2	2.43	0.44
35:YA:1568:G:OP2	37:YD:63:ARG:NH2	2.47	0.44
35:YA:600:G:N2	35:YA:605:C:O3'	2.51	0.44
42:YI:117:GLU:HG3	42:YI:117:GLU:O	2.17	0.44
49:YT:102:ILE:HA	49:YT:105:LEU:HD23	1.99	0.44
51:YV:72:VAL:HG23	51:YV:85:LYS:HB3	2.00	0.44
52:YW:36:LEU:HD13	52:YW:47:VAL:HG23	2.00	0.44
4:QD:88:VAL:O	4:QD:92:VAL:HG23	2.17	0.44
5:QE:59:GLY:O	5:QE:63:ARG:HG3	2.18	0.44
7:QG:15:ASP:OD1	7:QG:44:TYR:OH	2.36	0.44
7:QG:79:ARG:HG3	7:QG:79:ARG:O	2.18	0.44
8:QH:86:ILE:HD11	8:QH:136:GLU:HG2	2.00	0.44
24:QY:4:ILE:HB	24:QY:76:LEU:HG	2.00	0.44
26:R1:11:ARG:NH2	35:RA:1365:A:O2'	2.49	0.44
35:RA:521:G:H2'	35:RA:522:G:H8	1.83	0.44
41:RH:102:ALA:HB2	41:RH:116:GLU:OE1	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:RH:86:GLU:N	41:RH:86:GLU:OE1	2.38	0.44
42:RI:92:VAL:O	42:RI:120:ILE:HG22	2.18	0.44
55:RZ:27:VAL:HG12	55:RZ:85:HIS:HE1	1.83	0.44
1:XA:1025:U:H2'	1:XA:1026:G:C8	2.52	0.44
1:XA:407:G:H2'	1:XA:408:A:H8	1.82	0.44
7:XG:57:GLU:OE1	7:XG:60:LYS:NZ	2.47	0.44
13:XM:16:ASP:HB3	13:XM:41:PRO:HB3	1.99	0.44
29:Y4:43:TYR:CE1	40:YG:179:PRO:HG3	2.53	0.44
35:YA:2037:G:H2'	35:YA:2038:G:C8	2.53	0.44
35:YA:2836:U:H2'	35:YA:2837:G:C8	2.53	0.44
47:YR:38:VAL:HG22	47:YR:42:LYS:HE2	2.00	0.44
47:YR:41:ALA:HB1	47:YR:97:VAL:HG21	1.99	0.44
50:YU:50:ARG:HH12	51:YV:72:VAL:HG12	1.82	0.44
50:YU:92:ARG:CG	50:YU:95:LEU:HD12	2.48	0.44
1:QA:1072:G:N2	2:QB:107:THR:HG21	2.33	0.44
3:QC:78:GLY:HA3	3:QC:83:ARG:HB3	1.99	0.44
5:QE:33:VAL:HG13	5:QE:112:LEU:HD12	1.99	0.44
8:QH:20:TYR:CE1	8:QH:76:PRO:HG2	2.52	0.44
26:R1:60:PHE:HB3	26:R1:62:VAL:HG23	1.99	0.44
35:RA:2125:G:H21	35:RA:2173:A:H62	1.65	0.44
35:RA:2591:C:H2'	35:RA:2592:G:C8	2.52	0.44
35:RA:389:G:N1	45:RP:71:VAL:HG12	2.32	0.44
41:RH:71:LEU:C	41:RH:71:LEU:CD1	2.78	0.44
47:RR:65:LEU:HD23	47:RR:68:ARG:NH1	2.33	0.44
48:RS:11:LYS:HE2	48:RS:91:PRO:CD	2.47	0.44
43:RN:40:PRO:HB3	50:RU:68:ALA:HB2	1.99	0.44
55:RZ:115:GLY:HA2	55:RZ:177:PRO:HD3	2.00	0.44
1:XA:17:U:H2'	1:XA:18:C:C6	2.53	0.44
5:XE:20:GLN:OE1	5:XE:25:ARG:CZ	2.66	0.44
10:XJ:50:ILE:HA	10:XJ:60:ARG:HB2	1.99	0.44
33:Y8:10:ALA:HB3	33:Y8:62:LEU:HD21	1.98	0.44
33:Y8:46:ARG:HG3	33:Y8:47:LYS:O	2.18	0.44
34:Y9:25:VAL:HB	34:Y9:34:GLN:HB2	2.00	0.44
35:YA:2645:G:N2	35:YA:2767:C:OP2	2.50	0.44
35:YA:581:C:H2'	35:YA:582:G:C8	2.53	0.44
40:YG:60:LEU:HD12	40:YG:68:PRO:HG3	2.00	0.44
55:YZ:58:VAL:HG23	55:YZ:67:LEU:C	2.38	0.44
1:QA:1512:U:H2'	1:QA:1513:A:C8	2.52	0.44
1:QA:579:G:H5'	1:QA:728:A:H1'	1.99	0.44
2:QB:155:LEU:HD21	2:QB:159:PRO:HD3	2.00	0.44
11:QK:59:TYR:O	11:QK:62:GLN:HG2	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:QZ:37:THR:OG1	24:QZ:40:GLU:O	2.34	0.44
24:QZ:83:HIS:C	24:QZ:84:TYR:OXT	2.56	0.44
26:R1:40:ARG:HH12	26:R1:42:GLN:HE21	1.64	0.44
35:RA:582:G:H2'	35:RA:583:G:C8	2.53	0.44
40:RG:124:SER:HB2	40:RG:131:TYR:CE2	2.53	0.44
42:RI:67:ARG:O	42:RI:71:ILE:HG12	2.18	0.44
44:RO:47:ILE:HD12	44:RO:48:PRO:O	2.18	0.44
48:RS:4:LEU:O	48:RS:9:ARG:NH2	2.51	0.44
54:RY:35:TYR:CE2	54:RY:69:ALA:HB3	2.52	0.44
2:XB:171:ALA:HA	2:XB:174:VAL:HG22	1.99	0.44
5:XE:51:VAL:O	5:XE:55:VAL:HG23	2.18	0.44
7:XG:49:ILE:HA	7:XG:52:GLU:HG2	1.99	0.44
10:XJ:21:GLN:OE1	10:XJ:22:LYS:HG2	2.18	0.44
10:XJ:46:ARG:HD3	14:XN:61:TRP:CH2	2.53	0.44
20:XT:58:LYS:O	20:XT:62:LEU:HD12	2.18	0.44
37:YD:17:THR:O	37:YD:211:ARG:NH2	2.42	0.44
38:YE:108:SER:HG	38:YE:162:ALA:N	2.16	0.44
40:YG:139:LEU:HD13	40:YG:139:LEU:C	2.38	0.44
42:YI:120:ILE:HD11	42:YI:126:TYR:CD2	2.53	0.44
49:YT:66:VAL:HA	49:YT:71:GLY:HA2	1.98	0.44
55:YZ:6:LYS:CD	55:YZ:60:GLU:HB2	2.48	0.44
5:QE:75:THR:OG1	5:QE:76:ILE:N	2.47	0.43
7:QG:59:LEU:O	7:QG:62:PHE:HB3	2.18	0.43
17:QQ:13:ASP:OD2	17:QQ:14:LYS:NZ	2.50	0.43
35:RA:987:G:O2'	35:RA:1000:A:N3	2.42	0.43
35:RA:1332:G:H21	35:RA:1610:A:H8	1.66	0.43
35:RA:1638:C:O2	35:RA:2698:U:O2'	2.36	0.43
35:RA:2134:A:N6	35:RA:2157:G:O2'	2.51	0.43
35:RA:226:G:H21	35:RA:228:A:H62	1.64	0.43
39:RF:65:TRP:NE1	39:RF:73:ALA:O	2.41	0.43
40:RG:16:ARG:O	40:RG:20:ILE:CD1	2.66	0.43
42:RI:59:ALA:O	42:RI:62:LYS:HB3	2.18	0.43
48:RS:62:LYS:HD2	48:RS:97:ARG:HH11	1.72	0.43
3:XC:150:LYS:HG3	3:XC:169:ALA:HB2	1.99	0.43
12:XL:104:VAL:HG12	12:XL:105:TYR:H	1.83	0.43
13:XM:3:ARG:HG2	13:XM:3:ARG:O	2.18	0.43
24:XY:61:THR:O	24:XY:65:ARG:NH1	2.50	0.43
35:YA:2487:G:H2'	35:YA:2488:A:H8	1.81	0.43
35:YA:2713:A:OP1	47:YR:14:SER:OG	2.24	0.43
40:YG:172:LEU:HD23	40:YG:176:LEU:HD13	1.99	0.43
40:YG:68:PRO:HB3	40:YG:92:VAL:HB	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:YP:45:LEU:HD12	45:YP:46:LYS:O	2.18	0.43
1:QA:1172:C:H2'	1:QA:1173:G:H8	1.83	0.43
1:QA:1264:C:H2'	1:QA:1265:G:H8	1.84	0.43
1:QA:736:C:H2'	1:QA:737:A:C8	2.53	0.43
8:QH:87:SER:OG	8:QH:132:GLU:OE2	2.35	0.43
12:QL:117:ARG:NH2	12:QL:124:LYS:HD2	2.34	0.43
24:QY:59:ARG:HB2	24:QY:65:ARG:NH1	2.32	0.43
24:QZ:30:LEU:O	24:QZ:34:THR:OG1	2.27	0.43
35:RA:2148:G:H2'	35:RA:2149:G:C8	2.53	0.43
35:RA:2873:A:H8	47:RR:6:SER:N	2.07	0.43
37:RD:96:HIS:HD2	37:RD:102:LYS:HE2	1.82	0.43
38:RE:144:ARG:HB3	38:RE:145:LYS:H	1.51	0.43
41:RH:41:MET:HE2	41:RH:52:VAL:HG13	2.00	0.43
42:RI:12:LEU:HB3	42:RI:19:VAL:HG11	2.00	0.43
51:RV:34:GLU:OE2	51:RV:100:ARG:NH2	2.51	0.43
55:RZ:183:LEU:H	55:RZ:183:LEU:HD23	1.83	0.43
55:RZ:91:LEU:HD11	55:RZ:96:VAL:HG21	2.00	0.43
9:XI:111:ARG:HG2	9:XI:112:LYS:O	2.17	0.43
10:XJ:48:THR:HG22	10:XJ:62:HIS:HB3	2.00	0.43
13:XM:50:GLU:O	13:XM:54:VAL:HG23	2.18	0.43
13:XM:84:ILE:HD12	13:XM:84:ILE:HA	1.67	0.43
23:XX:4:A:H2'	23:XX:5:A:O4'	2.18	0.43
35:YA:1056:G:H4'	35:YA:1086:A:H1'	1.99	0.43
35:YA:1991:U:H2'	35:YA:1992:G:H5''	1.99	0.43
35:YA:38:A:H2'	35:YA:39:C:C6	2.53	0.43
37:YD:245:PRO:HA	37:YD:246:PRO:HD3	1.89	0.43
48:YS:27:SER:HA	48:YS:88:ASP:HB3	2.00	0.43
55:YZ:128:VAL:CG2	55:YZ:132:ASN:HB3	2.49	0.43
4:QD:94:LEU:HD11	4:QD:200:GLU:HG2	2.00	0.43
5:QE:131:ILE:O	5:QE:135:THR:HG23	2.17	0.43
5:QE:79:GLU:HB2	5:QE:91:LEU:O	2.18	0.43
30:R5:4:HIS:O	35:RA:2056:G:N2	2.51	0.43
37:RD:182:LEU:HD12	37:RD:272:ALA:HB2	2.00	0.43
40:RG:106:LEU:HA	40:RG:110:ALA:HB3	2.00	0.43
43:RN:95:PRO:C	43:RN:97:ARG:H	2.21	0.43
46:RQ:79:LEU:HD23	46:RQ:79:LEU:HA	1.73	0.43
49:RT:16:ARG:NH1	49:RT:83:ILE:O	2.35	0.43
1:XA:501:C:H1'	1:XA:549:C:H1'	2.01	0.43
6:XF:22:GLU:OE1	6:XF:84:ASN:HB2	2.18	0.43
14:XN:29:ARG:HD3	14:XN:40:CYS:HB2	2.00	0.43
33:Y8:28:GLY:HA3	33:Y8:44:LYS:HD3	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YA:1728:G:N7	35:YA:1731:G:C2	2.85	0.43
35:YA:581:C:H2'	35:YA:582:G:H8	1.83	0.43
48:YS:10:ARG:HE	48:YS:10:ARG:HB3	1.54	0.43
55:YZ:54:HIS:CD2	55:YZ:101:PRO:HG3	2.53	0.43
1:QA:714:G:H2'	1:QA:715:A:C8	2.54	0.43
3:QC:59:ARG:HG3	3:QC:64:VAL:HG23	2.01	0.43
4:QD:61:LYS:HB3	4:QD:61:LYS:HE3	1.85	0.43
13:QM:84:ILE:HD11	19:QS:66:MET:HB3	2.01	0.43
25:R0:77:ARG:NH2	35:RA:857:C:OP2	2.51	0.43
1:QA:1483:A:H1'	35:RA:1948:G:H1'	2.00	0.43
35:RA:855:G:H1	35:RA:922:U:H3	1.64	0.43
38:RE:128:SER:OG	38:RE:129:HIS:N	2.50	0.43
40:RG:83:ARG:O	40:RG:86:MET:HG2	2.18	0.43
43:RN:23:LEU:HD13	43:RN:60:ILE:HD12	2.00	0.43
55:RZ:9:TYR:HE2	55:RZ:35:ARG:HE	1.66	0.43
35:YA:2243:U:H2'	35:YA:2244:U:C6	2.53	0.43
33:Y8:27:THR:OG1	35:YA:2361:A:O5'	2.36	0.43
28:Y3:49:LYS:NZ	35:YA:851:U:OP1	2.42	0.43
43:YN:30:ILE:HG23	43:YN:52:VAL:HG11	2.01	0.43
48:YS:5:THR:OG1	48:YS:6:ALA:N	2.51	0.43
49:YT:49:VAL:HG22	49:YT:63:VAL:HG22	2.00	0.43
35:YA:2685:G:OP2	49:YT:51:ARG:NH2	2.51	0.43
1:QA:1127:G:H2'	1:QA:1128:C:C6	2.54	0.43
1:QA:1218:C:H2'	1:QA:1219:U:C6	2.53	0.43
1:QA:216:G:H2'	1:QA:217:C:C6	2.54	0.43
1:QA:658:G:OP1	15:QO:8:LYS:NZ	2.47	0.43
2:QB:208:ILE:H	2:QB:208:ILE:HD12	1.82	0.43
3:QC:119:ARG:HD2	3:QC:119:ARG:HA	1.76	0.43
10:QJ:25:GLU:HB3	10:QJ:29:ARG:CZ	2.48	0.43
13:QM:107:ALA:HB3	13:QM:111:LYS:HD3	2.00	0.43
31:R6:24:GLU:HB3	33:R8:34:TRP:CZ3	2.53	0.43
26:R1:78:LYS:CE	35:RA:270(R):G:H21	2.28	0.43
35:RA:299:A:N1	35:RA:322:A:O2'	2.45	0.43
37:RD:131:LEU:HD12	37:RD:131:LEU:N	2.33	0.43
1:XA:1300:G:O2'	1:XA:1303:C:N4	2.52	0.43
7:XG:73:MET:HG2	7:XG:90:GLU:HA	1.99	0.43
19:XS:37:ARG:HG2	19:XS:37:ARG:H	1.62	0.43
24:XY:16:TRP:CE2	24:XY:23:ILE:HG21	2.53	0.43
29:Y4:16:CYS:HB3	29:Y4:20:ASN:HB3	2.00	0.43
35:YA:2086:U:H2'	35:YA:2087:G:C8	2.54	0.43
42:YI:66:GLU:OE2	42:YI:67:ARG:NH1	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:YV:24:LYS:HA	51:YV:92:THR:OG1	2.18	0.43
1:QA:390:C:H2'	1:QA:391:G:C8	2.53	0.43
1:QA:1290:G:OP1	7:QG:35:LYS:NZ	2.52	0.43
10:QJ:6:ILE:HD11	10:QJ:98:ILE:C	2.38	0.43
13:QM:4:ILE:CD1	13:QM:57:ARG:HA	2.49	0.43
24:QZ:6:SER:OG	24:QZ:7:GLU:N	2.52	0.43
35:RA:1073:A:H2'	35:RA:1074:G:H8	1.84	0.43
35:RA:1353:A:H2'	35:RA:1354:A:C8	2.54	0.43
35:RA:200:U:O2	35:RA:386:G:N2	2.52	0.43
37:RD:16:MET:HG3	37:RD:207:GLY:HA3	1.99	0.43
1:XA:452:A:O2'	1:XA:453:A:O4'	2.34	0.43
2:XB:9:GLU:HG3	2:XB:10:LEU:N	2.33	0.43
13:XM:89:GLY:O	13:XM:93:ARG:HB3	2.18	0.43
16:XP:49:LEU:HD11	16:XP:73:LEU:HD22	2.01	0.43
1:XA:192:U:O2'	20:XT:57:ARG:HG3	2.18	0.43
35:YA:1794:U:H2'	35:YA:1795:C:C6	2.54	0.43
13:XM:93:ARG:NH1	35:YA:887:A:OP1	2.51	0.43
42:YI:9:LEU:HD11	42:YI:35:LEU:HD13	2.01	0.43
43:YN:67:LEU:O	43:YN:88:GLU:HG3	2.19	0.43
1:QA:1376:U:OP1	7:QG:94:ARG:NH1	2.42	0.43
1:QA:25:C:H5'	1:QA:524:G:H1'	2.01	0.43
1:QA:80:G:C2	1:QA:89:U:O2	2.71	0.43
1:QA:694:A:HO2'	22:QW:38:A:HO2'	1.54	0.43
22:QW:43:A:H2'	22:QW:44:A:C8	2.53	0.43
35:RA:1819:A:H5''	37:RD:161:THR:HG21	2.00	0.43
35:RA:2086:U:H2'	35:RA:2087:G:C8	2.53	0.43
35:RA:2469:A:H2	35:RA:2481:G:H21	1.66	0.43
35:RA:2844:G:H3'	35:RA:2845:G:H8	1.83	0.43
35:RA:747:U:H5'	52:RW:90:ARG:HH21	1.84	0.43
41:RH:151:ILE:HG22	41:RH:153:LYS:HG2	2.01	0.43
41:RH:52:VAL:HG12	41:RH:65:HIS:NE2	2.34	0.43
42:RI:125:GLU:HG3	42:RI:141:LYS:CD	2.49	0.43
1:XA:272:C:H2'	1:XA:273:A:H8	1.84	0.43
6:XF:69:GLU:CD	6:XF:69:GLU:H	2.21	0.43
24:XZ:38:PRO:HB2	24:XZ:39:PHE:CD1	2.53	0.43
34:Y9:11:CYS:HB3	34:Y9:14:CYS:H	1.82	0.43
47:YR:97:VAL:HA	47:YR:113:LEU:O	2.19	0.43
1:QA:1130:A:N6	1:QA:1144:G:H21	2.17	0.43
1:QA:28:G:O2'	1:QA:296:U:OP1	2.30	0.43
1:QA:576:G:N2	1:QA:760:G:OP2	2.51	0.43
1:QA:765:G:N2	1:QA:813:U:OP2	2.46	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:QB:156:LYS:HB2	2:QB:156:LYS:HE2	1.86	0.43
22:QW:43:A:H2'	22:QW:44:A:H8	1.84	0.43
28:R3:8:LEU:HG	28:R3:28:LEU:HD23	2.00	0.43
29:R4:55:ARG:CD	29:R4:59:PHE:CD1	3.02	0.43
37:RD:125:ILE:HG22	37:RD:125:ILE:O	2.19	0.43
37:RD:206:LEU:O	37:RD:211:ARG:HD3	2.18	0.43
38:RE:13:ARG:HE	49:RT:58:ASN:HB2	1.83	0.43
41:RH:121:ILE:HG13	41:RH:134:SER:O	2.18	0.43
41:RH:87:LEU:HD23	41:RH:87:LEU:HA	1.74	0.43
48:RS:35:ILE:HD13	48:RS:66:ALA:HB2	2.01	0.43
1:XA:454:C:H5'	16:XP:71:ARG:NH2	2.33	0.43
1:XA:701:C:O2	1:XA:703:G:N1	2.51	0.43
3:XC:73:PRO:HG3	3:XC:105:GLU:HB3	2.00	0.43
4:XD:63:LYS:HE3	4:XD:198:VAL:HG12	2.00	0.43
12:XL:93:LEU:HA	12:XL:94:PRO:HD3	1.87	0.43
20:XT:19:SER:O	20:XT:23:ARG:CB	2.66	0.43
51:YV:3:ALA:HB3	51:YV:14:VAL:HG22	2.01	0.43
55:YZ:121:HIS:HB2	55:YZ:171:ILE:HA	2.00	0.43
4:QD:22:LYS:HE3	4:QD:25:ARG:HG2	2.01	0.43
10:QJ:16:LEU:HD22	10:QJ:70:ARG:HG2	2.01	0.43
11:QK:85:ARG:HG2	11:QK:111:ASP:O	2.19	0.43
22:QW:22:G:H2'	22:QW:23:C:C6	2.54	0.43
24:QY:36:ARG:HG3	24:QY:37:THR:HG23	2.00	0.43
1:QA:958:A:OP1	24:QZ:36:ARG:NH1	2.52	0.43
24:QZ:52:LEU:HB3	24:QZ:55:PHE:HB2	2.01	0.43
29:R4:16:CYS:HB2	29:R4:36:CYS:SG	2.58	0.43
29:R4:60:GLN:HB2	29:R4:61:ARG:HD3	2.00	0.43
34:R9:30:PRO:HB2	35:RA:2527:C:H5'	2.00	0.43
35:RA:1434:A:H61	35:RA:1558:A:N6	2.17	0.43
35:RA:1971:A:C8	37:RD:241:PRO:HB3	2.53	0.43
40:RG:117:PHE:CD2	40:RG:117:PHE:O	2.70	0.43
42:RI:9:LEU:HD23	42:RI:10:GLU:H	1.83	0.43
46:RQ:32:TYR:CE2	46:RQ:133:ARG:HG3	2.54	0.43
47:RR:65:LEU:HA	47:RR:68:ARG:NH1	2.29	0.43
51:RV:59:ALA:HA	51:RV:95:LEU:O	2.19	0.43
1:XA:401:C:O2'	1:XA:621:A:N3	2.40	0.43
1:XA:953:G:H5'	1:XA:965:A:H61	1.83	0.43
12:XL:71:PRO:O	12:XL:102:ARG:NH1	2.51	0.43
35:YA:2030:A:H4'	35:YA:2031:A:C8	2.54	0.43
42:YI:117:GLU:O	42:YI:118:LYS:CG	2.57	0.43
46:YQ:138:ASP:CG	55:YZ:81:ARG:HH12	2.23	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:YZ:14:LYS:N	55:YZ:14:LYS:CB	2.65	0.43
1:QA:1371:G:OP2	9:QI:11:LYS:NZ	2.52	0.43
1:QA:452:A:O2'	1:QA:453:A:O4'	2.34	0.43
1:QA:666:G:H5'	1:QA:726:C:H1'	2.01	0.43
30:R5:20:ARG:HA	30:R5:23:HIS:ND1	2.34	0.43
32:R7:47:ARG:HH22	53:RX:60:ARG:CZ	2.32	0.43
1:XA:1308:U:H2'	1:XA:1309:G:H8	1.83	0.43
1:XA:173:U:O2	1:XA:197:A:N6	2.52	0.43
2:XB:16:HIS:HB3	2:XB:17:PHE:H	1.17	0.43
3:XC:121:ALA:O	3:XC:124:ILE:HG13	2.19	0.43
4:XD:147:ALA:HA	4:XD:182:LYS:HA	2.01	0.43
1:XA:1224:G:HO2'	19:XS:78:ARG:NH2	2.17	0.43
42:YI:107:VAL:H	42:YI:107:VAL:HG22	1.62	0.43
50:YU:76:TYR:O	50:YU:80:ILE:HG12	2.18	0.43
51:YV:21:ARG:NE	51:YV:91:TYR:HE1	2.16	0.43
11:QK:33:THR:HG22	11:QK:39:PRO:HA	2.00	0.42
23:QX:12:A:H2'	23:QX:13:A:C8	2.54	0.42
24:QZ:4:ILE:HB	24:QZ:76:LEU:HA	2.01	0.42
32:R7:37:LYS:HG2	35:RA:458:G:C8	2.54	0.42
35:RA:1570:A:H2'	35:RA:1571:A:C8	2.53	0.42
35:RA:1995:U:O2	44:RO:3:GLN:NE2	2.51	0.42
35:RA:654(G):C:N3	35:RA:654(N):G:N1	2.62	0.42
38:RE:114:ALA:HB3	38:RE:160:TYR:HB3	2.01	0.42
39:RF:176:LEU:HD21	39:RF:181:LEU:HA	2.00	0.42
39:RF:89:VAL:H	39:RF:89:VAL:HG12	1.61	0.42
40:RG:138:GLN:OE1	40:RG:153:ARG:HB2	2.18	0.42
41:RH:10:PRO:CB	41:RH:12:PRO:HD3	2.46	0.42
49:RT:111:ARG:O	49:RT:113:LYS:N	2.52	0.42
1:XA:171:A:H2'	1:XA:172:A:C8	2.54	0.42
2:XB:233:SER:HA	2:XB:234:PRO:HD2	1.92	0.42
3:XC:112:SER:HB3	3:XC:115:LEU:HD12	2.00	0.42
4:XD:5:ILE:HA	4:XD:115:ARG:HH22	1.84	0.42
35:YA:2847:U:OP1	49:YT:98:LYS:NZ	2.46	0.42
35:YA:259:G:H21	35:YA:621:A:H8	1.67	0.42
40:YG:34:LEU:HG	40:YG:99:MET:HE1	2.01	0.42
1:QA:377:G:H2'	1:QA:378:G:C8	2.54	0.42
2:QB:219:VAL:O	2:QB:223:ILE:HG13	2.19	0.42
9:QI:73:GLN:O	9:QI:77:ILE:HG12	2.19	0.42
13:QM:121:LYS:HA	13:QM:121:LYS:HD3	1.91	0.42
35:RA:1252:G:OP2	50:RU:14:HIS:NE2	2.52	0.42
35:RA:2595:G:N2	35:RA:2598:A:OP2	2.45	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:2679:A:H4'	38:RE:165:VAL:HG11	2.00	0.42
35:RA:2785:C:O2'	38:RE:66:HIS:HD2	2.02	0.42
36:RB:103:U:O2'	55:RZ:29:TYR:OH	2.27	0.42
1:XA:1028(B):C:H3'	1:XA:1029:G:H4'	2.01	0.42
1:XA:1322:C:OP1	19:XS:78:ARG:NH2	2.33	0.42
1:XA:728:A:C8	15:XO:54:ARG:NH1	2.87	0.42
2:XB:93:VAL:HG21	2:XB:97:TRP:HD1	1.84	0.42
4:XD:57:ARG:HB3	4:XD:206:PHE:HB2	2.00	0.42
20:XT:30:LYS:HA	20:XT:33:ILE:HD12	2.00	0.42
35:YA:2591:C:H2'	35:YA:2592:G:C8	2.54	0.42
35:YA:372:G:O2'	35:YA:373:U:OP2	2.37	0.42
42:YI:135:GLU:HG2	42:YI:136:VAL:N	2.34	0.42
47:YR:65:LEU:HA	47:YR:68:ARG:HD2	2.01	0.42
50:YU:93:LYS:H	50:YU:93:LYS:HD2	1.84	0.42
2:QB:12:GLU:O	2:QB:17:PHE:HD2	2.02	0.42
6:QF:23:LYS:HE2	6:QF:61:LEU:HD21	2.00	0.42
17:QQ:83:ASP:OD1	17:QQ:83:ASP:N	2.52	0.42
18:QR:32:ARG:HA	18:QR:69:THR:HG21	2.01	0.42
24:QZ:10:TRP:HE1	24:QZ:14:LEU:CD1	2.09	0.42
30:R5:40:LYS:HZ2	30:R5:46:CYS:HB2	1.83	0.42
35:RA:1188:U:H4'	51:RV:79:VAL:HG22	2.01	0.42
35:RA:177:G:H3'	35:RA:178:G:H8	1.84	0.42
35:RA:655:A:H4'	35:RA:656:G:H5'	2.01	0.42
35:RA:750:A:OP1	35:RA:1615:C:N4	2.51	0.42
37:RD:25:THR:HG21	37:RD:113:VAL:HG21	2.01	0.42
37:RD:132:PRO:HB2	37:RD:134:ARG:CG	2.49	0.42
38:RE:104:VAL:HG11	38:RE:188:VAL:HG23	2.01	0.42
1:XA:1250:A:N3	1:XA:1370:G:O2'	2.41	0.42
1:XA:1299:A:C5	1:XA:1301:U:O2	2.72	0.42
1:XA:1192:C:O2	5:XE:25:ARG:NH2	2.52	0.42
10:XJ:24:VAL:CG1	10:XJ:72:VAL:HG11	2.49	0.42
27:Y2:14:ARG:O	27:Y2:15:LYS:HB3	2.20	0.42
27:Y2:16:LEU:HD23	27:Y2:21:LEU:HG	2.01	0.42
35:YA:1309:G:O2'	35:YA:1611:C:O2'	2.31	0.42
35:YA:1434:A:H61	35:YA:1558:A:N6	2.17	0.42
35:YA:2377:A:H2'	35:YA:2378:A:C8	2.53	0.42
43:YN:95:PRO:C	43:YN:97:ARG:H	2.23	0.42
35:YA:2292:C:OP1	48:YS:17:ARG:NH2	2.52	0.42
1:QA:103:C:OP2	20:QT:14:LYS:NZ	2.50	0.42
1:QA:1305:G:N2	1:QA:1331:G:H2'	2.34	0.42
3:QC:90:GLU:OE1	3:QC:93:LYS:HD2	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:1239:A:O2'	7:QG:114:ARG:O	2.28	0.42
9:QI:114:TYR:HE2	10:QJ:59:SER:HA	1.85	0.42
22:QW:62:C:H2'	22:QW:63:G:H8	1.84	0.42
35:RA:1020:A:N6	35:RA:1141:U:O2'	2.52	0.42
35:RA:521:G:H2'	35:RA:522:G:C8	2.55	0.42
37:RD:232:PRO:HB3	37:RD:244:ARG:NH1	2.34	0.42
38:RE:48:GLN:HB3	38:RE:78:LEU:HD11	2.01	0.42
53:RX:34:ALA:O	53:RX:77:LYS:NZ	2.41	0.42
1:XA:1522:U:H2'	1:XA:1523:G:H8	1.84	0.42
1:XA:280:C:H41	17:XQ:91:ARG:HH12	1.67	0.42
24:XZ:4:ILE:HB	24:XZ:76:LEU:HA	1.99	0.42
24:XZ:82:TYR:HB3	24:XZ:83:HIS:H	1.71	0.42
35:YA:1790:C:H2'	35:YA:1791:A:C5	2.54	0.42
35:YA:2779:U:H1'	35:YA:2781:A:C5	2.54	0.42
37:YD:201:HIS:O	37:YD:204:ILE:HG12	2.19	0.42
39:YF:158:THR:O	39:YF:164:ARG:NH1	2.52	0.42
42:YI:68:LEU:HD21	42:YI:109:ILE:HD11	2.00	0.42
1:QA:1355:G:H2'	1:QA:1356:G:C8	2.55	0.42
1:QA:501:C:H1'	1:QA:549:C:H1'	2.00	0.42
4:QD:84:LYS:HD2	4:QD:84:LYS:HA	1.78	0.42
1:QA:562:C:O2'	12:QL:16:GLU:O	2.32	0.42
14:QN:29:ARG:HD3	14:QN:40:CYS:HB2	2.01	0.42
35:RA:657:U:H2'	35:RA:658:C:C6	2.54	0.42
38:RE:75:VAL:HG23	38:RE:77:ILE:O	2.19	0.42
35:RA:2305:A:H5''	40:RG:134:GLY:HA3	2.02	0.42
1:XA:142:G:H2'	1:XA:143:A:C8	2.54	0.42
1:XA:422:C:HO2'	1:XA:423:G:N2	2.18	0.42
2:XB:17:PHE:CD1	2:XB:17:PHE:O	2.73	0.42
3:XC:190:ARG:H	3:XC:195:VAL:HG23	1.84	0.42
29:Y4:41:PRO:HA	29:Y4:44:THR:HG21	2.02	0.42
35:YA:1403:C:H5''	35:YA:1471:A:H1'	2.02	0.42
35:YA:1636:C:H2'	35:YA:1637:A:C8	2.54	0.42
35:YA:2183:C:H2'	35:YA:2184:G:C8	2.55	0.42
22:XV:76:A:N6	35:YA:2450:A:O2'	2.53	0.42
35:YA:2469:A:O2'	46:YQ:56:ARG:HD3	2.19	0.42
35:YA:642:G:H21	35:YA:646:A:H2	1.67	0.42
48:YS:12:PHE:O	48:YS:16:ASN:ND2	2.52	0.42
49:YT:22:PHE:HA	49:YT:91:ARG:HH12	1.85	0.42
51:YV:76:LYS:HB2	51:YV:81:TYR:HB3	2.00	0.42
55:YZ:8:TYR:HD1	55:YZ:38:TYR:CZ	2.38	0.42
1:QA:954:G:H21	1:QA:1227:A:H62	1.66	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:QG:111:ARG:HD2	7:QG:123:GLU:OE1	2.20	0.42
24:QZ:10:TRP:HA	24:QZ:13:TYR:HB3	2.01	0.42
35:RA:964:C:O2'	35:RA:2273:A:N3	2.41	0.42
35:RA:2777:G:OP2	35:RA:2781:A:O2'	2.31	0.42
35:RA:2809:A:H2'	35:RA:2810:A:C8	2.55	0.42
40:RG:7:LEU:O	40:RG:11:TYR:N	2.45	0.42
48:RS:3:ARG:HG2	48:RS:4:LEU:HD13	2.01	0.42
1:XA:1127:G:H2'	1:XA:1128:C:C6	2.55	0.42
1:XA:1151:A:H2'	1:XA:1152:A:C8	2.53	0.42
2:XB:222:ILE:O	2:XB:226:ARG:HG2	2.20	0.42
3:XC:172:ARG:HG2	3:XC:174:PRO:HD3	2.02	0.42
12:XL:32:PHE:HE1	12:XL:86:ARG:HG3	1.84	0.42
25:Y0:72:ARG:HB3	25:Y0:75:LEU:HB2	2.01	0.42
35:YA:1435:G:N2	35:YA:1477:A:O2'	2.50	0.42
35:YA:2469:A:H2	35:YA:2481:G:H21	1.66	0.42
35:YA:2641:G:P	43:YN:74:ARG:HH21	2.41	0.42
35:YA:673:C:H5''	39:YF:81:PRO:HD2	2.00	0.42
38:YE:54:GLN:HA	38:YE:54:GLN:HE21	1.85	0.42
42:YI:72:LEU:HD11	42:YI:101:LEU:HD21	2.01	0.42
50:YU:44:ASN:HD21	51:YV:75:PHE:HB3	1.85	0.42
55:YZ:128:VAL:CG1	55:YZ:133:ILE:HG22	2.49	0.42
1:QA:261:U:OP2	20:QT:79:ARG:NH2	2.53	0.42
1:QA:377:G:H2'	1:QA:378:G:H8	1.84	0.42
1:QA:737:A:H2'	1:QA:738:C:C6	2.55	0.42
8:QH:12:ARG:NH1	8:QH:27:PRO:HD3	2.35	0.42
13:QM:31:LYS:O	13:QM:32:GLU:C	2.57	0.42
19:QS:10:PHE:CE2	19:QS:12:ASP:HB3	2.55	0.42
35:RA:2037:G:H2'	35:RA:2038:G:C8	2.55	0.42
35:RA:2291:U:H2'	35:RA:2292:C:C6	2.55	0.42
35:RA:2805:G:H2'	35:RA:2807:G:C8	2.55	0.42
35:RA:448:U:H1'	39:RF:84:VAL:HG21	2.02	0.42
38:RE:111:ARG:HB2	38:RE:160:TYR:O	2.20	0.42
39:RF:17:ARG:N	39:RF:17:ARG:HD3	2.35	0.42
42:RI:58:LEU:O	42:RI:62:LYS:CB	2.66	0.42
46:RQ:60:ARG:HA	55:RZ:177:PRO:HB2	2.02	0.42
1:XA:1299:A:N1	1:XA:1301:U:C4	2.88	0.42
1:XA:757:U:O2'	1:XA:879:C:O2	2.38	0.42
1:XA:690:G:H22	11:XK:55:LYS:NZ	2.18	0.42
13:XM:102:ARG:HE	13:XM:105:THR:CG2	2.33	0.42
14:XN:34:TYR:CD2	14:XN:44:LEU:CD1	3.03	0.42
24:XY:51:ASN:OD1	24:XY:51:ASN:N	2.51	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:XZ:48:LEU:HD13	24:XZ:52:LEU:HD12	1.90	0.42
35:YA:1057:A:H2'	35:YA:1058:G:C8	2.54	0.42
35:YA:749:C:H5'	35:YA:1271:G:H1'	2.01	0.42
35:YA:2789:C:H1'	35:YA:2892:A:H2	1.85	0.42
35:YA:608:A:H2'	35:YA:609:A:C8	2.54	0.42
40:YG:27:ASN:HB3	40:YG:30:GLU:HG3	2.00	0.42
42:YI:4:ILE:HG12	42:YI:18:VAL:HG22	2.01	0.42
49:YT:54:ARG:HA	49:YT:59:THR:HG23	2.00	0.42
55:YZ:95:PRO:HA	55:YZ:129:SER:HA	2.02	0.42
1:QA:1071:C:H2'	1:QA:1072:G:H8	1.84	0.42
1:QA:1304:G:N1	1:QA:1332:A:OP2	2.53	0.42
10:QJ:8:LEU:HD12	10:QJ:8:LEU:HA	1.80	0.42
26:R1:53:VAL:HB	26:R1:58:ILE:HD12	2.02	0.42
35:RA:1889:A:N3	35:RA:2086:U:O2'	2.53	0.42
35:RA:2546:U:H5''	35:RA:2547:U:H5'	2.02	0.42
35:RA:589:C:H2'	35:RA:590:A:H8	1.85	0.42
25:R0:26:TYR:CE2	35:RA:857:C:H1'	2.52	0.42
37:RD:130:ALA:C	37:RD:131:LEU:HD12	2.39	0.42
55:RZ:29:TYR:HE2	55:RZ:87:ASP:HB3	1.84	0.42
1:XA:1175:G:H2'	1:XA:1176:A:C8	2.55	0.42
1:XA:1392:G:H21	1:XA:1502:A:H8	1.68	0.42
1:XA:713:G:H2'	1:XA:714:G:C8	2.55	0.42
1:XA:985:C:H2'	1:XA:986:A:H8	1.83	0.42
3:XC:7:PRO:HG2	3:XC:184:TYR:HB2	2.00	0.42
7:XG:22:LEU:HD21	7:XG:66:VAL:HG21	2.02	0.42
20:XT:86:ARG:O	20:XT:90:GLN:HG2	2.19	0.42
35:YA:1224:G:N2	35:YA:1227:A:OP2	2.48	0.42
35:YA:817:C:H4'	35:YA:932:G:C5	2.55	0.42
38:YE:201:THR:HG22	38:YE:203:LYS:H	1.85	0.42
49:YT:91:ARG:HB2	49:YT:121:ILE:HD11	2.02	0.42
1:QA:1125:U:P	1:QA:1145:C:H42	2.43	0.42
1:QA:1151:A:H2'	1:QA:1152:A:H8	1.85	0.42
1:QA:1241:G:H2'	1:QA:1242:C:H6	1.84	0.42
1:QA:1414:U:H2'	1:QA:1415:G:H8	1.85	0.42
1:QA:112:G:H22	1:QA:315:A:H2	1.66	0.42
1:QA:624:C:H2'	1:QA:625:G:H8	1.85	0.42
2:QB:189:ASP:HB3	2:QB:203:GLY:O	2.20	0.42
3:QC:22:TRP:CZ3	3:QC:32:LEU:HD13	2.55	0.42
4:QD:200:GLU:O	4:QD:204:ILE:HG12	2.19	0.42
5:QE:33:VAL:HG21	5:QE:109:ILE:HG12	2.02	0.42
13:QM:11:ARG:HA	13:QM:45:VAL:CG1	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:QM:34:LEU:O	13:QM:37:THR:OG1	2.38	0.42
19:QS:65:ASN:OD1	19:QS:65:ASN:N	2.48	0.42
35:RA:1007:C:H5''	43:RN:35:ARG:NH1	2.35	0.42
35:RA:1394:U:H4'	35:RA:1603:A:H4'	2.01	0.42
35:RA:2543:G:H2'	35:RA:2544:G:C8	2.55	0.42
35:RA:2632:A:O2'	35:RA:2811:G:O2'	2.30	0.42
35:RA:576:U:H2'	35:RA:577:G:C8	2.55	0.42
40:RG:139:LEU:HA	40:RG:144:ILE:CD1	2.50	0.42
41:RH:144:VAL:O	41:RH:148:ILE:HG23	2.20	0.42
42:RI:75:LEU:HD12	42:RI:75:LEU:HA	1.86	0.42
35:RA:1007:C:H5''	43:RN:35:ARG:HH11	1.83	0.42
49:RT:96:ARG:CG	49:RT:97:ALA:N	2.82	0.42
1:XA:891:U:H2'	1:XA:892:A:H8	1.84	0.42
5:XE:33:VAL:HG21	5:XE:109:ILE:HG12	2.02	0.42
19:XS:50:ALA:HA	19:XS:58:VAL:O	2.20	0.42
35:YA:2115:G:OP1	35:YA:2167:U:N3	2.35	0.42
39:YF:72:ARG:HG2	39:YF:73:ALA:N	2.35	0.42
48:YS:94:TYR:OH	48:YS:106:ARG:NH2	2.52	0.42
55:YZ:133:ILE:C	55:YZ:133:ILE:HD12	2.41	0.42
55:YZ:5:LEU:O	55:YZ:59:LEU:HA	2.20	0.42
1:QA:950:U:H2'	1:QA:951:G:C8	2.54	0.42
5:QE:98:THR:N	5:QE:117:ASP:OD2	2.52	0.42
10:QJ:24:VAL:HG23	10:QJ:25:GLU:HG3	2.01	0.42
13:QM:23:TYR:HB3	13:QM:71:ARG:NH2	2.34	0.42
35:RA:336:C:O2'	54:RY:35:TYR:OH	2.38	0.42
40:RG:32:PRO:HB3	40:RG:163:ALA:HB2	2.01	0.42
41:RH:11:VAL:N	41:RH:12:PRO:HD3	2.35	0.42
48:RS:25:ARG:HG3	48:RS:88:ASP:HB2	2.02	0.42
1:XA:1071:C:H2'	1:XA:1072:G:H8	1.85	0.42
1:XA:216:G:H2'	1:XA:217:C:C6	2.55	0.42
1:XA:422:C:O2'	1:XA:423:G:N2	2.52	0.42
1:XA:728:A:H2'	1:XA:729:A:C8	2.55	0.42
2:XB:42:ILE:HG22	2:XB:43:ASP:C	2.40	0.42
2:XB:179:LYS:HA	8:XH:72:PRO:HG3	2.00	0.42
10:XJ:85:LEU:HA	10:XJ:85:LEU:HD23	1.91	0.42
27:Y2:58:ALA:O	27:Y2:62:THR:HG23	2.19	0.42
27:Y2:16:LEU:H	27:Y2:67:LYS:HZ1	1.66	0.42
35:YA:1230:C:H2'	35:YA:1231:G:C8	2.55	0.42
35:YA:612:G:O2'	35:YA:616:A:N1	2.48	0.42
40:YG:69:ALA:HB3	40:YG:91:ARG:HH12	1.85	0.42
42:YI:40:THR:O	42:YI:44:LEU:HB2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:YN:61:ARG:CG	43:YN:61:ARG:HH11	2.33	0.42
47:YR:63:ARG:HH11	47:YR:76:VAL:HG23	1.85	0.42
48:YS:15:ARG:HG2	48:YS:19:LYS:HE3	2.00	0.42
1:QA:950:U:H2'	1:QA:951:G:H8	1.85	0.41
10:QJ:22:LYS:NZ	10:QJ:90:LEU:HB2	2.35	0.41
11:QK:34:ASP:HB2	11:QK:35:PRO:HD2	2.02	0.41
24:QZ:44:LYS:HD3	24:QZ:59:ARG:CD	2.38	0.41
25:R0:5:LYS:HA	25:R0:5:LYS:HD3	1.65	0.41
35:RA:1636:C:H2'	35:RA:1637:A:C8	2.55	0.41
35:RA:2375:G:N2	35:RA:2377:A:H3'	2.34	0.41
35:RA:2636:U:OP1	38:RE:79:ARG:HG3	2.19	0.41
40:RG:171:ALA:O	40:RG:175:LEU:HG	2.20	0.41
42:RI:125:GLU:N	42:RI:125:GLU:CD	2.73	0.41
46:RQ:66:ILE:HG13	46:RQ:66:ILE:H	1.49	0.41
49:RT:111:ARG:C	49:RT:113:LYS:H	2.23	0.41
1:XA:35:G:H2'	1:XA:36:C:C6	2.55	0.41
13:XM:14:ARG:HB2	13:XM:17:VAL:HG22	2.01	0.41
15:XO:5:LYS:HG2	15:XO:9:GLN:HG2	2.02	0.41
29:Y4:58:ARG:CZ	29:Y4:59:PHE:CE1	3.02	0.41
35:YA:1316:U:H2'	35:YA:1317:A:C8	2.55	0.41
35:YA:813:U:H2'	35:YA:814:C:H6	1.85	0.41
38:YE:1:MET:HG3	38:YE:84:PHE:HA	2.02	0.41
47:YR:8:ARG:HD3	47:YR:10:LEU:HD21	2.02	0.41
51:YV:5:VAL:HG13	51:YV:35:LEU:HB3	2.01	0.41
1:QA:34:C:H2'	1:QA:35:G:H8	1.84	0.41
1:QA:376:G:H5''	16:QP:5:ARG:HD2	2.02	0.41
1:QA:524:G:H2'	1:QA:525:C:C6	2.55	0.41
1:QA:643:C:H4'	8:QH:31:PHE:CE1	2.54	0.41
20:QT:76:ALA:HB1	20:QT:80:ARG:NH1	2.35	0.41
25:R0:69:PHE:CE2	25:R0:79:VAL:HG22	2.54	0.41
27:R2:12:GLU:OE1	27:R2:15:LYS:HD2	2.21	0.41
27:R2:63:VAL:HA	27:R2:66:GLU:HG2	2.02	0.41
35:RA:2141:G:N2	35:RA:2150:U:O2	2.44	0.41
35:RA:2343:C:O2'	35:RA:2373:G:O2'	2.24	0.41
36:RB:24:G:O6	36:RB:56:G:O2'	2.37	0.41
37:RD:123:ALA:CB	37:RD:131:LEU:HD11	2.35	0.41
40:RG:78:SER:O	40:RG:78:SER:OG	2.36	0.41
42:RI:136:VAL:O	42:RI:136:VAL:CG1	2.68	0.41
49:RT:26:ASP:OD2	49:RT:120:ARG:NH2	2.49	0.41
1:XA:1300:G:O2'	1:XA:1301:U:O5'	2.32	0.41
3:XC:6:HIS:CE1	3:XC:8:ILE:HG12	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:XJ:49:VAL:HG21	14:XN:41:ARG:O	2.20	0.41
35:YA:195:A:H61	35:YA:198:C:H3'	1.85	0.41
35:YA:2175:C:H2'	35:YA:2176:A:C8	2.55	0.41
35:YA:307:G:H21	35:YA:330:A:H62	1.68	0.41
35:YA:659:C:H2'	35:YA:660:G:H8	1.85	0.41
35:YA:2052:G:H4'	38:YE:143:ASN:O	2.20	0.41
39:YF:137:LYS:HA	39:YF:137:LYS:HD2	1.86	0.41
40:YG:171:ALA:O	40:YG:175:LEU:HG	2.20	0.41
45:YP:19:VAL:HG12	45:YP:27:HIS:HB3	2.02	0.41
46:YQ:110:THR:HG23	46:YQ:113:GLN:H	1.85	0.41
50:YU:72:HIS:ND1	50:YU:110:VAL:HG11	2.34	0.41
1:QA:377:G:OP1	16:QP:3:LYS:HD3	2.19	0.41
1:QA:827:U:H3	1:QA:872:A:H62	1.67	0.41
2:QB:187:LEU:HD12	2:QB:201:ILE:O	2.20	0.41
3:QC:97:LYS:HD3	3:QC:97:LYS:HA	1.75	0.41
9:QI:48:GLU:OE2	9:QI:51:ARG:HD3	2.20	0.41
10:QJ:78:ASN:ND2	10:QJ:80:LYS:HD3	2.35	0.41
19:QS:43:GLU:O	19:QS:47:HIS:HE1	2.04	0.41
1:QA:1493:A:C6	60:QX:101:A3P:H4'	2.55	0.41
25:R0:7:LEU:HD11	46:RQ:85:LYS:HE2	2.02	0.41
35:RA:1837:C:O2'	35:RA:1927:A:N3	2.43	0.41
35:RA:2757:A:N1	41:RH:67:LEU:CD2	2.66	0.41
35:RA:519:U:H2'	35:RA:520:G:C8	2.54	0.41
38:RE:47:VAL:HG13	38:RE:49:LEU:HD11	2.01	0.41
42:RI:13:GLY:HA3	42:RI:17:GLN:HB3	2.01	0.41
42:RI:57:ARG:O	42:RI:61:ARG:HG2	2.19	0.41
48:RS:58:LEU:HD12	48:RS:59:LYS:H	1.85	0.41
1:XA:1236:A:H4'	1:XA:1304:G:H4'	2.01	0.41
1:QA:1256:A:H1'	1:QA:1258:G:C6	2.56	0.41
3:QC:7:PRO:HG2	3:QC:184:TYR:HB2	2.02	0.41
8:QH:11:THR:HG23	8:QH:14:ARG:HH12	1.84	0.41
9:QI:9:ARG:HB2	9:QI:104:ARG:HE	1.84	0.41
13:QM:81:LEU:HA	13:QM:81:LEU:HD23	1.78	0.41
14:QN:3:ARG:O	14:QN:7:ILE:HG23	2.20	0.41
22:QW:69:C:H2'	22:QW:70:G:C8	2.56	0.41
25:R0:46:LYS:HZ2	25:R0:46:LYS:HB3	1.85	0.41
35:RA:1273:U:O2'	35:RA:1275:A:OP1	2.28	0.41
35:RA:443:A:C8	39:RF:45:ARG:HG3	2.55	0.41
35:RA:680:G:H2'	35:RA:681:G:C8	2.55	0.41
35:RA:740:U:H2'	35:RA:741:G:C8	2.55	0.41
40:RG:19:LEU:HD11	40:RG:172:LEU:HD12	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:RG:8:LYS:HE3	40:RG:12:TYR:HE2	1.85	0.41
41:RH:4:ILE:HG21	41:RH:6:ARG:NE	2.35	0.41
42:RI:5:LEU:HD13	42:RI:9:LEU:HD22	2.02	0.41
51:RV:18:LEU:HB3	51:RV:96:ILE:HD12	2.02	0.41
54:RY:50:ARG:NH1	54:RY:52:SER:OG	2.53	0.41
7:XG:79:ARG:HA	7:XG:83:ALA:O	2.20	0.41
13:XM:47:ASP:N	13:XM:47:ASP:OD1	2.54	0.41
25:Y0:32:ARG:H	25:Y0:35:ASN:ND2	2.17	0.41
29:Y4:44:THR:HB	29:Y4:47:GLN:HB2	2.01	0.41
35:YA:2438:U:O2'	35:YA:2440:C:OP1	2.33	0.41
35:YA:545:G:N2	35:YA:548:A:OP2	2.46	0.41
37:YD:148:GLU:HB2	37:YD:151:LYS:HD2	2.03	0.41
35:YA:1816:G:O6	37:YD:35:LYS:NZ	2.53	0.41
38:YE:2:LYS:HB3	38:YE:95:ILE:HD12	2.03	0.41
41:YH:77:LYS:HA	41:YH:77:LYS:HD3	1.80	0.41
42:YI:33:ARG:HA	42:YI:33:ARG:HD2	1.89	0.41
43:YN:26:LEU:O	43:YN:30:ILE:HG13	2.21	0.41
46:YQ:30:GLY:N	46:YQ:105:GLU:OE2	2.54	0.41
51:YV:5:VAL:CG1	51:YV:35:LEU:HB3	2.51	0.41
1:QA:1347:G:H2'	1:QA:1347:G:H8	1.52	0.41
4:QD:191:ARG:NH1	4:QD:194:LEU:O	2.54	0.41
13:QM:36:LYS:HA	13:QM:36:LYS:HD2	1.93	0.41
22:QW:36:U:H2'	22:QW:37:A:C8	2.56	0.41
22:QW:71:C:H2'	22:QW:72:A:C8	2.56	0.41
13:QM:80:ARG:NH2	29:R4:55:ARG:CZ	2.83	0.41
35:RA:1056:G:H21	35:RA:1103:A:H62	1.68	0.41
35:RA:1657:C:H2'	35:RA:1658:C:H6	1.85	0.41
31:R6:21:TYR:OH	35:RA:2347:C:O2'	2.37	0.41
37:RD:42:GLY:HA2	37:RD:51:VAL:HG12	2.03	0.41
35:RA:2310:A:N6	40:RG:79:ASN:OD1	2.52	0.41
41:RH:58:GLU:HB3	41:RH:60:ARG:N	2.35	0.41
42:RI:123:LEU:HD23	42:RI:144:VAL:HG13	2.00	0.41
42:RI:5:LEU:H	42:RI:5:LEU:HG	1.60	0.41
42:RI:68:LEU:HD23	42:RI:72:LEU:HB2	2.03	0.41
43:RN:21:LYS:NZ	43:RN:138:LEU:C	2.73	0.41
55:RZ:163:LEU:HA	55:RZ:163:LEU:HD23	1.95	0.41
1:XA:235:C:H2'	1:XA:236:G:C8	2.56	0.41
15:XO:53:HIS:O	15:XO:56:LEU:HB3	2.20	0.41
28:Y3:52:HIS:CG	36:YB:83:G:H4'	2.56	0.41
29:Y4:13:ARG:HB3	29:Y4:29:PRO:O	2.20	0.41
35:YA:1681:G:O2'	35:YA:1762:A:O2'	2.38	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YA:2116:G:H22	35:YA:2164:C:H41	1.68	0.41
35:YA:2183:C:H2'	35:YA:2184:G:H8	1.85	0.41
43:YN:35:ARG:HG2	43:YN:37:LYS:HG3	2.03	0.41
50:YU:88:ILE:HG13	51:YV:49:THR:HA	2.02	0.41
1:QA:1028(A):C:H2'	1:QA:1028(B):C:C6	2.54	0.41
1:QA:1251:A:N3	1:QA:1369:C:O2'	2.42	0.41
1:QA:1342:C:H2'	1:QA:1343:G:C8	2.55	0.41
1:QA:1348:U:N3	1:QA:1374:A:H2	2.18	0.41
1:QA:21:G:H2'	1:QA:22:G:C8	2.56	0.41
1:QA:564:C:P	12:QL:15:ARG:HH21	2.43	0.41
2:QB:217:ARG:HG3	2:QB:217:ARG:HH11	1.86	0.41
22:QW:22:G:H2'	22:QW:23:C:H6	1.85	0.41
35:RA:2125:G:N2	35:RA:2173:A:H62	2.18	0.41
35:RA:2212:A:H1'	35:RA:2215:G:C5	2.55	0.41
35:RA:2489:G:N2	35:RA:2491:U:O4	2.45	0.41
35:RA:2636:U:H3	35:RA:2782:G:H1	1.67	0.41
35:RA:2730:C:O2'	38:RE:168:MET:O	2.34	0.41
39:RF:140:LEU:HA	39:RF:140:LEU:HD23	1.80	0.41
43:RN:23:LEU:HD13	43:RN:60:ILE:CD1	2.50	0.41
53:RX:83:VAL:HG22	53:RX:87:GLN:HB2	2.02	0.41
1:XA:1306:A:N6	1:XA:1331:G:O2'	2.53	0.41
1:XA:299:G:H2'	1:XA:300:A:C8	2.56	0.41
1:XA:971:G:C6	1:XA:1365:G:H5'	2.55	0.41
1:XA:728:A:C6	15:XO:54:ARG:HD3	2.53	0.41
20:XT:57:ARG:HD3	20:XT:102:GLY:O	2.20	0.41
29:Y4:51:ASP:HB3	29:Y4:52:THR:H	1.72	0.41
35:YA:2111:C:OP1	35:YA:2145:C:N4	2.36	0.41
35:YA:861:A:N3	36:YB:79:C:O2'	2.53	0.41
37:YD:108:PRO:HD2	37:YD:111:LEU:HD22	2.02	0.41
50:YU:17:ILE:HG23	50:YU:39:LEU:HD12	2.03	0.41
1:QA:60:A:OP1	1:QA:111:G:N2	2.54	0.41
9:QI:28:VAL:HG12	9:QI:63:ILE:HB	2.03	0.41
10:QJ:21:GLN:O	10:QJ:24:VAL:HG22	2.21	0.41
11:QK:122:LYS:O	11:QK:126:ARG:HG2	2.20	0.41
1:QA:1316:G:N7	19:QS:7:LYS:NZ	2.68	0.41
25:R0:24:LYS:HD2	25:R0:24:LYS:HA	1.82	0.41
26:R1:50:ARG:HG2	26:R1:59:THR:HG23	2.03	0.41
26:R1:62:VAL:HG12	26:R1:63:ALA:O	2.21	0.41
34:R9:24:TYR:CE1	34:R9:35:ARG:CD	3.04	0.41
35:RA:1057:A:H2'	35:RA:1058:G:C8	2.55	0.41
35:RA:2111:C:C2	35:RA:2118:U:H1'	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:2415:G:H4'	45:RP:67:MET:H	1.85	0.41
35:RA:2438:U:O3'	35:RA:2439:A:H3'	2.20	0.41
37:RD:106:ILE:HD11	37:RD:143:HIS:HD2	1.86	0.41
38:RE:97:LYS:HG2	38:RE:100:GLU:OE1	2.20	0.41
39:RF:24:LEU:HB3	39:RF:115:ALA:HB2	2.02	0.41
40:RG:11:TYR:CE2	40:RG:16:ARG:HD2	2.56	0.41
40:RG:71:THR:N	40:RG:89:GLY:O	2.48	0.41
41:RH:58:GLU:N	41:RH:61:HIS:ND1	2.66	0.41
47:RR:38:VAL:HG12	47:RR:112:ALA:HB2	2.01	0.41
54:RY:20:TYR:HE1	54:RY:43:ASN:HA	1.86	0.41
55:RZ:99:TYR:HE1	55:RZ:125:LEU:HB2	1.85	0.41
1:XA:524:G:H2'	1:XA:525:C:C6	2.55	0.41
4:XD:61:LYS:HE2	4:XD:206:PHE:CE2	2.56	0.41
6:XF:22:GLU:OE2	6:XF:82:ARG:NE	2.52	0.41
17:XQ:84:LEU:O	17:XQ:87:LYS:HG2	2.20	0.41
35:YA:603:A:N6	35:YA:625:G:O2'	2.53	0.41
35:YA:969:U:H2'	35:YA:970:C:C6	2.56	0.41
39:YF:158:THR:HG21	39:YF:163:VAL:HG23	2.02	0.41
40:YG:53:LEU:HD21	40:YG:87:PRO:HB2	2.01	0.41
42:YI:117:GLU:CG	42:YI:117:GLU:O	2.69	0.41
1:QA:357:G:O2'	42:YI:89:TYR:O	2.38	0.41
55:YZ:11:GLU:O	55:YZ:36:LYS:NZ	2.54	0.41
1:QA:407:G:H2'	1:QA:408:A:H8	1.86	0.41
1:QA:745:C:H2'	1:QA:746:A:C8	2.55	0.41
1:QA:1314:C:N4	19:QS:2:PRO:O	2.53	0.41
24:QY:3:LEU:HD11	24:QY:31:ILE:HG21	2.03	0.41
34:R9:2:LYS:HG3	34:R9:3:VAL:HG23	2.03	0.41
35:RA:128:C:H2'	35:RA:129:C:C6	2.55	0.41
38:RE:29:GLY:HA2	38:RE:180:ASN:HB3	2.03	0.41
40:RG:7:LEU:HD12	40:RG:10:LYS:HD3	2.03	0.41
1:XA:1218:C:OP2	14:YN:9:LYS:NZ	2.54	0.41
1:XA:1308:U:H2'	1:XA:1309:G:C8	2.56	0.41
1:XA:1454:G:OP1	20:XT:39:LYS:NZ	2.35	0.41
1:XA:1059:C:OP2	3:XC:199:LYS:NZ	2.53	0.41
7:XG:20:ASP:HB3	7:XG:23:VAL:HG12	2.01	0.41
10:XJ:78:ASN:OD1	10:XJ:78:ASN:N	2.54	0.41
12:XL:32:PHE:HB3	12:XL:84:LEU:HD11	2.03	0.41
17:XQ:19:VAL:HG23	17:XQ:44:ALA:HB3	2.03	0.41
19:XS:15:LEU:O	19:XS:19:VAL:HG23	2.21	0.41
35:YA:1230:C:H2'	35:YA:1231:G:H8	1.84	0.41
35:YA:2853:C:H2'	35:YA:2854:G:H8	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YA:499:U:H5'	54:YY:46:LYS:HE3	2.02	0.41
35:YA:848:G:H2'	35:YA:849:A:C8	2.56	0.41
1:QA:1125:U:C5	10:QJ:5:ARG:NH2	2.89	0.41
1:QA:267:C:OP2	17:QQ:67:LYS:HD2	2.20	0.41
2:QB:59:GLU:HB3	2:QB:221:LEU:HD22	2.03	0.41
3:QC:131:ARG:NH2	3:QC:167:TRP:O	2.53	0.41
3:QC:8:ILE:HG23	3:QC:16:ARG:HE	1.85	0.41
13:QM:8:GLU:O	13:QM:10:PRO:CD	2.67	0.41
1:QA:1243:C:H5''	21:QU:8:THR:HG21	2.02	0.41
35:RA:1278:A:H2'	35:RA:1279:G:C8	2.56	0.41
35:RA:2305:A:H1'	40:RG:136:ARG:HG2	2.02	0.41
35:RA:2779:U:H1'	35:RA:2781:A:C5	2.56	0.41
35:RA:2779:U:H6	35:RA:2779:U:H2'	1.63	0.41
40:RG:117:PHE:C	40:RG:119:GLY:N	2.74	0.41
42:RI:123:LEU:N	42:RI:123:LEU:HD12	2.35	0.41
44:RO:24:VAL:HG13	44:RO:33:ALA:HB2	2.03	0.41
53:RX:18:TYR:HA	53:RX:21:PHE:CD2	2.56	0.41
1:XA:1129:C:H4'	1:XA:1130:A:H5'	2.03	0.41
2:XB:15:VAL:O	2:XB:17:PHE:CE2	2.73	0.41
4:XD:60:GLU:HG2	4:XD:63:LYS:HE2	2.03	0.41
4:XD:86:LYS:HA	4:XD:86:LYS:HD2	1.75	0.41
5:XE:20:GLN:OE1	5:XE:25:ARG:NE	2.54	0.41
6:XF:50:TYR:HE2	6:XF:87:ARG:HH22	1.69	0.41
11:XK:52:GLY:H	11:XK:55:LYS:HE2	1.86	0.41
16:XP:45:THR:HG22	16:XP:47:ASP:H	1.86	0.41
17:XQ:89:LEU:HA	17:XQ:92:ARG:HG2	2.03	0.41
35:YA:2443:C:H2'	35:YA:2444:G:C8	2.56	0.41
35:YA:2853:C:H2'	35:YA:2854:G:C8	2.56	0.41
35:YA:65:C:O2'	35:YA:456:C:N3	2.44	0.41
35:YA:465:G:H2'	35:YA:466:A:C8	2.55	0.41
35:YA:740:U:H2'	35:YA:741:G:C8	2.56	0.41
35:YA:2748:A:C8	41:YH:63:SER:HB3	2.36	0.41
43:YN:136:GLU:O	43:YN:137:LYS:HD2	2.21	0.41
49:YT:80:SER:HA	49:YT:81:PRO:HD3	1.91	0.41
1:QA:1289:A:OP1	21:QU:9:ARG:NH2	2.53	0.41
1:QA:1189:C:H5''	3:QC:5:ILE:HD13	2.02	0.41
35:RA:1316:U:H2'	35:RA:1317:A:H8	1.86	0.41
35:RA:448:U:C4	35:RA:583:G:H1'	2.55	0.41
35:RA:862:G:O2'	36:RB:78:A:N3	2.50	0.41
38:RE:201:THR:HG22	38:RE:203:LYS:H	1.85	0.41
41:RH:54:ARG:HB2	41:RH:61:HIS:HB3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:RI:78:THR:HA	42:RI:141:LYS:O	2.21	0.41
55:RZ:23:LYS:HB3	55:RZ:38:TYR:HD2	1.85	0.41
1:XA:1218:C:H2'	1:XA:1219:U:C6	2.56	0.41
1:XA:64:G:N2	1:XA:68:G:O6	2.48	0.41
3:XC:95:THR:OG1	3:XC:97:LYS:HB2	2.20	0.41
35:YA:922:U:H2'	35:YA:923:C:C6	2.56	0.41
35:YA:2771:C:H5''	38:YE:202:LYS:NZ	2.35	0.41
1:QA:1241:G:H2'	1:QA:1242:C:C6	2.56	0.41
4:QD:100:ARG:O	4:QD:104:VAL:HG23	2.21	0.41
5:QE:12:LEU:HD22	5:QE:128:PRO:HB2	2.03	0.41
9:QI:17:VAL:HG12	9:QI:63:ILE:HG12	2.02	0.41
12:QL:8:ASN:O	12:QL:12:ARG:HG3	2.21	0.41
1:QA:110:C:O2'	16:QP:25:ARG:O	2.35	0.41
17:QQ:85:VAL:O	17:QQ:89:LEU:HG	2.21	0.41
19:QS:52:TYR:OH	19:QS:55:LYS:O	2.39	0.41
28:R3:10:LYS:HB3	28:R3:53:LEU:HD23	2.03	0.41
29:R4:38:LYS:HD3	29:R4:38:LYS:HA	1.93	0.41
31:R6:4:GLU:O	31:R6:27:LYS:NZ	2.36	0.41
35:RA:570:G:H2'	35:RA:2030:A:C5	2.55	0.41
35:RA:2836:U:H2'	35:RA:2837:G:C8	2.56	0.41
41:RH:58:GLU:CB	41:RH:61:HIS:H	2.34	0.41
49:RT:135:ALA:HA	49:RT:137:LYS:HD2	2.02	0.41
1:XA:1396:A:H4'	1:XA:1397:C:H5''	2.03	0.41
1:XA:1427:U:H2'	1:XA:1428:A:C8	2.56	0.41
1:XA:377:G:H2'	1:XA:378:G:C8	2.56	0.41
8:XH:51:VAL:HG21	8:XH:60:ARG:HG3	2.03	0.41
13:XM:15:VAL:O	13:XM:18:ALA:HB3	2.21	0.41
25:Y0:7:LEU:HD21	46:YQ:81:VAL:HG13	2.03	0.41
37:YD:164:GLN:OE1	37:YD:176:ARG:NH2	2.46	0.41
39:YF:82:ILE:HG13	39:YF:83:PHE:HD1	1.85	0.41
44:YO:120:GLU:HG2	44:YO:122:LEU:HG	2.03	0.41
47:YR:42:LYS:HA	47:YR:45:ARG:HD3	2.03	0.41
49:YT:102:ILE:HB	49:YT:110:ILE:HD12	2.02	0.41
1:QA:165:C:H2'	1:QA:166:G:H8	1.85	0.40
7:QG:50:ILE:O	7:QG:54:THR:HG22	2.21	0.40
8:QH:46:LYS:CG	8:QH:64:LYS:CG	2.93	0.40
9:QI:19:LEU:HA	9:QI:19:LEU:HD12	1.92	0.40
10:QJ:6:ILE:HD13	10:QJ:97:GLU:O	2.14	0.40
11:QK:122:LYS:HE2	11:QK:122:LYS:HB3	1.92	0.40
13:QM:11:ARG:O	13:QM:12:ASN:OD1	2.39	0.40
26:R1:12:PRO:HB3	26:R1:43:TYR:HD1	1.86	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:679:C:H2'	35:RA:680:G:H8	1.86	0.40
41:RH:4:ILE:CG2	41:RH:6:ARG:HG2	2.51	0.40
42:RI:138:ILE:HG23	42:RI:138:ILE:O	2.21	0.40
43:RN:5:VAL:HA	43:RN:6:PRO:HD3	1.94	0.40
20:XT:16:HIS:O	20:XT:19:SER:OG	2.19	0.40
60:XX:101:A3P:O2'	24:XY:46:GLU:OE2	2.39	0.40
24:XY:59:ARG:HG3	24:XY:65:ARG:NH1	2.37	0.40
29:Y4:58:ARG:HG3	29:Y4:59:PHE:CD1	2.44	0.40
34:Y9:11:CYS:SG	34:Y9:13:LYS:HB2	2.61	0.40
35:YA:2074:U:H2'	35:YA:2075:U:C6	2.56	0.40
50:YU:74:LEU:HD11	50:YU:114:LYS:HG2	2.03	0.40
1:QA:192:U:H2'	1:QA:193:C:C6	2.56	0.40
1:QA:719:C:N3	18:QR:74:ARG:NH2	2.69	0.40
2:QB:105:PHE:HZ	2:QB:156:LYS:HA	1.86	0.40
3:QC:115:LEU:HA	3:QC:115:LEU:HD23	1.95	0.40
7:QG:26:PHE:HA	7:QG:101:LEU:HD23	2.03	0.40
10:QJ:7:LYS:HB3	10:QJ:71:LEU:CB	2.51	0.40
13:QM:22:ILE:HD11	13:QM:67:GLU:HB3	2.02	0.40
26:R1:33:LYS:HD2	35:RA:2432:A:C8	2.56	0.40
35:RA:1228:G:OP1	50:RU:13:LYS:NZ	2.46	0.40
35:RA:1536:A:H62	35:RA:1538:G:H1'	1.86	0.40
35:RA:2845:G:H2'	35:RA:2846:G:C8	2.56	0.40
35:RA:37:C:H2'	35:RA:38:A:C8	2.56	0.40
35:RA:726:G:O2'	35:RA:727:A:H8	2.04	0.40
37:RD:245:PRO:HA	37:RD:246:PRO:HD3	1.92	0.40
40:RG:129:GLY:O	40:RG:161:THR:HB	2.20	0.40
41:RH:152:ARG:HD3	41:RH:152:ARG:HA	1.95	0.40
41:RH:4:ILE:H	41:RH:4:ILE:HG22	1.52	0.40
46:RQ:66:ILE:HD12	46:RQ:67:ARG:N	2.36	0.40
47:RR:18:LEU:HD21	47:RR:22:ARG:CZ	2.52	0.40
47:RR:9:LYS:HB2	47:RR:17:ARG:NH1	2.36	0.40
44:RO:76:ALA:HB3	49:RT:75:ILE:HD12	2.02	0.40
1:XA:1191:A:OP1	3:XC:4:LYS:HE3	2.21	0.40
1:XA:186(B):C:H2'	1:XA:186(C):G:H8	1.85	0.40
1:XA:691:G:H2'	1:XA:692:U:C6	2.57	0.40
10:XJ:84:GLN:O	10:XJ:88:LEU:HB2	2.20	0.40
14:YN:48:ALA:HB2	14:YN:53:LEU:HD12	2.03	0.40
17:XQ:43:LEU:HD13	17:XQ:68:ARG:NH1	2.37	0.40
35:YA:1070:A:H5'	35:YA:1071:G:H5''	2.02	0.40
35:YA:2212:A:H4'	35:YA:2213:U:H5	1.86	0.40
35:YA:2696:U:H2'	35:YA:2697:G:C8	2.57	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:YD:61:LEU:O	37:YD:63:ARG:NH1	2.54	0.40
38:YE:128:SER:OG	38:YE:129:HIS:N	2.53	0.40
38:YE:174:ASP:HB3	38:YE:183:LEU:HD22	2.02	0.40
48:YS:18:ILE:HG21	48:YS:88:ASP:HA	2.03	0.40
53:YX:66:LEU:HD12	53:YX:66:LEU:HA	1.99	0.40
55:YZ:54:HIS:HB3	55:YZ:101:PRO:HD3	2.03	0.40
2:QB:132:LYS:HG2	2:QB:135:GLN:NE2	2.36	0.40
3:QC:147:LYS:HE3	3:QC:203:PHE:CE2	2.56	0.40
4:QD:105:VAL:HG13	4:QD:110:PHE:HB2	2.02	0.40
5:QE:51:VAL:HA	5:QE:54:ALA:HB3	2.03	0.40
9:QI:19:LEU:CG	9:QI:59:PHE:CE1	2.69	0.40
10:QJ:79:ARG:CZ	10:QJ:82:ILE:HG13	2.51	0.40
19:QS:10:PHE:CE1	19:QS:16:LEU:HD22	2.56	0.40
20:QT:58:LYS:HB2	20:QT:58:LYS:HE3	1.81	0.40
20:QT:99:LEU:HA	20:QT:99:LEU:HD23	1.93	0.40
22:QV:50:U:H2'	22:QV:51:C:C6	2.56	0.40
24:QY:5:TRP:HB2	24:QZ:3:LEU:HB2	2.04	0.40
29:R4:46:GLN:OE1	29:R4:46:GLN:HA	2.21	0.40
34:R9:36:GLN:NE2	35:RA:1124:C:O2	2.54	0.40
35:RA:1070:A:H5'	35:RA:1071:G:H5''	2.03	0.40
35:RA:142:G:H2'	35:RA:143:C:H6	1.86	0.40
37:RD:120:GLY:O	37:RD:131:LEU:HG	2.20	0.40
37:RD:75:ILE:O	37:RD:118:VAL:CG2	2.69	0.40
41:RH:46:GLU:CG	41:RH:47:GLU:H	2.33	0.40
35:RA:831:G:N2	45:RP:53:GLY:O	2.53	0.40
1:XA:390:C:H2'	1:XA:391:G:C8	2.57	0.40
2:XB:134:GLU:OE1	2:XB:137:ARG:HD3	2.22	0.40
4:XD:81:GLU:CD	4:XD:139:ARG:HH12	2.25	0.40
5:XE:8:GLU:HG3	5:XE:34:VAL:HG12	2.03	0.40
27:Y2:7:ARG:NH2	35:YA:102:G:OP1	2.55	0.40
33:Y8:48:PHE:HE1	33:Y8:50:LEU:HD22	1.85	0.40
34:Y9:18:ARG:HD2	34:Y9:23:VAL:HG22	2.04	0.40
25:Y0:56:ASP:HA	35:YA:2386:C:H4'	2.03	0.40
43:YN:71:ILE:HG21	43:YN:84:LYS:HB3	2.03	0.40
44:YO:79:PHE:HD1	49:YT:72:VAL:HG22	1.87	0.40
54:YY:46:LYS:HG3	54:YY:60:PHE:HB3	2.04	0.40
55:YZ:54:HIS:CG	55:YZ:101:PRO:HG3	2.56	0.40
1:QA:1316:G:N2	1:QA:1318:A:H3'	2.36	0.40
1:QA:407:G:H2'	1:QA:408:A:C8	2.55	0.40
9:QI:9:ARG:CB	9:QI:104:ARG:HE	2.34	0.40
10:QJ:7:LYS:HB3	10:QJ:71:LEU:HB2	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:QL:47:LYS:HB2	12:QL:48:PRO:CD	2.51	0.40
13:QM:91:ARG:HD2	13:QM:91:ARG:HA	1.88	0.40
24:QY:14:LEU:HD11	24:QZ:28:ASN:HD22	1.85	0.40
24:QZ:16:TRP:CD2	24:QZ:23:ILE:HG21	2.57	0.40
31:R6:24:GLU:HB3	33:R8:34:TRP:HZ3	1.86	0.40
34:R9:24:TYR:CZ	34:R9:35:ARG:HD3	2.56	0.40
35:RA:1289:C:H2'	35:RA:1290:C:H6	1.87	0.40
35:RA:1791:A:H3'	35:RA:1792:G:H8	1.85	0.40
40:RG:109:VAL:HG12	40:RG:113:ARG:CD	2.52	0.40
40:RG:131:TYR:CE1	40:RG:133:LEU:HB3	2.57	0.40
44:RO:108:GLU:HG3	44:RO:108:GLU:O	2.21	0.40
35:RA:1598:C:H5'	53:RX:37:THR:HG23	2.04	0.40
1:XA:1367:C:O2'	10:XJ:48:THR:HG21	2.20	0.40
1:XA:1513:A:H2'	1:XA:1514:C:C6	2.57	0.40
1:XA:35:G:N3	12:XL:118:SER:OG	2.46	0.40
1:XA:603:U:H2'	1:XA:604:G:C8	2.56	0.40
5:XE:151:LEU:HD21	8:XH:77:GLU:HG2	2.04	0.40
35:YA:2543:G:H2'	35:YA:2544:G:C8	2.56	0.40
35:YA:582:G:H2'	35:YA:583:G:C8	2.56	0.40
39:YF:154:VAL:CG2	39:YF:173:VAL:HG12	2.52	0.40
41:YH:25:LYS:HB2	41:YH:25:LYS:HE2	1.67	0.40
42:YI:86:THR:H	42:YI:123:LEU:HD21	1.87	0.40
35:YA:582:G:OP1	50:YU:14:HIS:ND1	2.54	0.40
1:QA:728:A:H2'	1:QA:729:A:C8	2.56	0.40
2:QB:19:HIS:ND1	2:QB:206:ASP:HB2	2.36	0.40
2:QB:17:PHE:HB2	2:QB:44:LEU:HD11	2.03	0.40
4:QD:157:LEU:O	4:QD:161:ASN:OD1	2.39	0.40
5:QE:6:PHE:HZ	5:QE:40:ARG:HH21	1.69	0.40
10:QJ:33:GLN:O	10:QJ:75:ILE:CG1	2.70	0.40
10:QJ:30:SER:C	10:QJ:80:LYS:HE3	2.42	0.40
12:QL:93:LEU:HA	12:QL:94:PRO:HD3	1.91	0.40
21:QU:11:GLY:O	21:QU:15:ARG:HG2	2.21	0.40
42:RI:122:GLU:CA	42:RI:122:GLU:OE2	2.70	0.40
55:RZ:5:LEU:HD12	55:RZ:5:LEU:HA	1.87	0.40
1:XA:1347:G:H22	1:XA:1374:A:P	2.45	0.40
1:XA:939:G:H2'	1:XA:940:C:C6	2.56	0.40
2:XB:11:LEU:HD23	2:XB:11:LEU:HA	1.87	0.40
13:XM:90:LEU:O	13:XM:94:ARG:HG2	2.22	0.40
24:XZ:1:MET:CB	24:XZ:35:ARG:HG3	2.50	0.40
27:Y2:16:LEU:H	27:Y2:67:LYS:NZ	2.19	0.40
34:Y9:18:ARG:NH1	34:Y9:21:GLY:O	2.55	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YA:554:U:HO2'	35:YA:556:G:H8	1.63	0.40
35:YA:813:U:H2'	35:YA:814:C:C6	2.55	0.40
35:YA:907:U:OP1	46:YQ:24:GLY:N	2.55	0.40
35:YA:839:U:H3	35:YA:939:G:H1	1.69	0.40
40:YG:111:LEU:O	40:YG:114:ILE:HD12	2.22	0.40
41:YH:44:VAL:CG1	41:YH:50:VAL:HG13	2.51	0.40
42:YI:97:ILE:O	42:YI:101:LEU:HB2	2.22	0.40
46:YQ:26:TYR:O	46:YQ:67:ARG:NH1	2.52	0.40
35:YA:956:G:H5''	46:YQ:77:LYS:HD2	2.03	0.40
49:YT:26:ASP:OD2	49:YT:120:ARG:NH2	2.54	0.40
50:YU:92:ARG:HG2	50:YU:95:LEU:HD12	2.03	0.40
51:YV:52:VAL:O	51:YV:52:VAL:CG2	2.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	QB	233/256 (91%)	205 (88%)	27 (12%)	1 (0%)	34	68
2	XB	234/256 (91%)	204 (87%)	29 (12%)	1 (0%)	34	68
3	QC	203/239 (85%)	188 (93%)	15 (7%)	0	100	100
3	XC	203/239 (85%)	191 (94%)	12 (6%)	0	100	100
4	QD	206/209 (99%)	200 (97%)	6 (3%)	0	100	100
4	XD	206/209 (99%)	197 (96%)	8 (4%)	1 (0%)	29	63
5	QE	149/162 (92%)	143 (96%)	5 (3%)	1 (1%)	22	56
5	XE	149/162 (92%)	143 (96%)	5 (3%)	1 (1%)	22	56
6	QF	99/101 (98%)	98 (99%)	1 (1%)	0	100	100
6	XF	99/101 (98%)	99 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	QG	153/156 (98%)	145 (95%)	7 (5%)	1 (1%)	22	56
7	XG	153/156 (98%)	148 (97%)	5 (3%)	0	100	100
8	QH	135/138 (98%)	130 (96%)	5 (4%)	0	100	100
8	XH	135/138 (98%)	130 (96%)	5 (4%)	0	100	100
9	QI	125/128 (98%)	108 (86%)	17 (14%)	0	100	100
9	XI	124/128 (97%)	111 (90%)	13 (10%)	0	100	100
10	QJ	97/105 (92%)	86 (89%)	10 (10%)	1 (1%)	15	48
10	XJ	94/105 (90%)	88 (94%)	6 (6%)	0	100	100
11	QK	117/129 (91%)	107 (92%)	10 (8%)	0	100	100
11	XK	114/129 (88%)	107 (94%)	7 (6%)	0	100	100
12	QL	123/132 (93%)	110 (89%)	12 (10%)	1 (1%)	19	53
12	XL	120/132 (91%)	108 (90%)	10 (8%)	2 (2%)	9	35
13	QM	118/126 (94%)	99 (84%)	17 (14%)	2 (2%)	9	35
13	XM	117/126 (93%)	100 (86%)	16 (14%)	1 (1%)	17	51
14	QN	58/61 (95%)	55 (95%)	2 (3%)	1 (2%)	9	35
14	XN	58/61 (95%)	54 (93%)	4 (7%)	0	100	100
15	QO	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
15	XO	85/89 (96%)	83 (98%)	2 (2%)	0	100	100
16	QP	82/88 (93%)	79 (96%)	3 (4%)	0	100	100
16	XP	82/88 (93%)	79 (96%)	3 (4%)	0	100	100
17	QQ	98/105 (93%)	93 (95%)	5 (5%)	0	100	100
17	XQ	98/105 (93%)	95 (97%)	3 (3%)	0	100	100
18	QR	68/88 (77%)	66 (97%)	2 (3%)	0	100	100
18	XR	68/88 (77%)	66 (97%)	2 (3%)	0	100	100
19	QS	81/93 (87%)	71 (88%)	10 (12%)	0	100	100
19	XS	81/93 (87%)	77 (95%)	3 (4%)	1 (1%)	13	43
20	QT	97/106 (92%)	92 (95%)	5 (5%)	0	100	100
20	XT	97/106 (92%)	89 (92%)	8 (8%)	0	100	100
21	QU	23/27 (85%)	23 (100%)	0	0	100	100
21	XU	23/27 (85%)	23 (100%)	0	0	100	100
24	QY	82/84 (98%)	71 (87%)	11 (13%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	QZ	82/84 (98%)	74 (90%)	7 (8%)	1 (1%)	13	43
24	XY	82/84 (98%)	76 (93%)	6 (7%)	0	100	100
24	XZ	82/84 (98%)	71 (87%)	10 (12%)	1 (1%)	13	43
25	R0	79/85 (93%)	71 (90%)	7 (9%)	1 (1%)	12	41
25	Y0	80/85 (94%)	77 (96%)	3 (4%)	0	100	100
26	R1	95/98 (97%)	84 (88%)	11 (12%)	0	100	100
26	Y1	95/98 (97%)	89 (94%)	5 (5%)	1 (1%)	14	45
27	R2	67/72 (93%)	60 (90%)	7 (10%)	0	100	100
27	Y2	67/72 (93%)	65 (97%)	2 (3%)	0	100	100
28	R3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
28	Y3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
29	R4	67/71 (94%)	46 (69%)	18 (27%)	3 (4%)	2	14
29	Y4	67/71 (94%)	49 (73%)	13 (19%)	5 (8%)	1	5
30	R5	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
30	Y5	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
31	R6	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
31	Y6	51/54 (94%)	51 (100%)	0	0	100	100
32	R7	45/49 (92%)	45 (100%)	0	0	100	100
32	Y7	46/49 (94%)	46 (100%)	0	0	100	100
33	R8	62/65 (95%)	58 (94%)	2 (3%)	2 (3%)	4	21
33	Y8	62/65 (95%)	57 (92%)	3 (5%)	2 (3%)	4	21
34	R9	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
34	Y9	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
37	RD	270/276 (98%)	256 (95%)	14 (5%)	0	100	100
37	YD	272/276 (99%)	262 (96%)	10 (4%)	0	100	100
38	RE	203/206 (98%)	177 (87%)	22 (11%)	4 (2%)	7	30
38	YE	202/206 (98%)	191 (95%)	8 (4%)	3 (2%)	10	38
39	RF	200/210 (95%)	194 (97%)	6 (3%)	0	100	100
39	YF	200/210 (95%)	188 (94%)	12 (6%)	0	100	100
40	RG	179/182 (98%)	161 (90%)	16 (9%)	2 (1%)	14	45
40	YG	179/182 (98%)	153 (86%)	25 (14%)	1 (1%)	25	59

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	RH	172/180 (96%)	137 (80%)	30 (17%)	5 (3%)	4	23
41	YH	172/180 (96%)	160 (93%)	9 (5%)	3 (2%)	9	35
42	RI	143/148 (97%)	121 (85%)	17 (12%)	5 (4%)	3	19
42	YI	144/148 (97%)	126 (88%)	15 (10%)	3 (2%)	7	29
43	RN	136/140 (97%)	123 (90%)	11 (8%)	2 (2%)	10	38
43	YN	136/140 (97%)	125 (92%)	10 (7%)	1 (1%)	22	56
44	RO	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
44	YO	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
45	RP	148/150 (99%)	129 (87%)	15 (10%)	4 (3%)	5	24
45	YP	145/150 (97%)	138 (95%)	7 (5%)	0	100	100
46	RQ	137/141 (97%)	122 (89%)	14 (10%)	1 (1%)	22	56
46	YQ	139/141 (99%)	132 (95%)	6 (4%)	1 (1%)	22	56
47	RR	115/118 (98%)	105 (91%)	9 (8%)	1 (1%)	17	51
47	YR	115/118 (98%)	108 (94%)	7 (6%)	0	100	100
48	RS	109/112 (97%)	87 (80%)	21 (19%)	1 (1%)	17	51
48	YS	109/112 (97%)	94 (86%)	15 (14%)	0	100	100
49	RT	135/146 (92%)	120 (89%)	15 (11%)	0	100	100
49	YT	135/146 (92%)	122 (90%)	13 (10%)	0	100	100
50	RU	115/118 (98%)	113 (98%)	2 (2%)	0	100	100
50	YU	115/118 (98%)	111 (96%)	3 (3%)	1 (1%)	17	51
51	RV	99/101 (98%)	88 (89%)	10 (10%)	1 (1%)	15	48
51	YV	99/101 (98%)	96 (97%)	2 (2%)	1 (1%)	15	48
52	RW	111/113 (98%)	105 (95%)	6 (5%)	0	100	100
52	YW	111/113 (98%)	106 (96%)	5 (4%)	0	100	100
53	RX	90/96 (94%)	86 (96%)	4 (4%)	0	100	100
53	YX	90/96 (94%)	86 (96%)	4 (4%)	0	100	100
54	RY	105/110 (96%)	99 (94%)	6 (6%)	0	100	100
54	YY	105/110 (96%)	101 (96%)	4 (4%)	0	100	100
55	RZ	181/206 (88%)	168 (93%)	12 (7%)	1 (1%)	25	59
55	YZ	181/206 (88%)	176 (97%)	5 (3%)	0	100	100
All	All	11788/12464 (95%)	10894 (92%)	822 (7%)	72 (1%)	25	59

All (72) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	QM	15	VAL
29	R4	25	TYR
38	RE	18	ASP
42	RI	15	VAL
42	RI	133	HIS
43	RN	126	PRO
12	XL	47	LYS
24	XZ	72	ASP
29	Y4	44	THR
29	Y4	56	VAL
29	Y4	57	GLU
33	Y8	29	LYS
33	Y8	30	ARG
40	YG	137	GLU
50	YU	93	LYS
12	QL	48	PRO
33	R8	29	LYS
45	RP	27	HIS
13	XM	15	VAL
51	YV	50	PRO
25	R0	47	PRO
29	R4	24	THR
33	R8	30	ARG
41	RH	20	ALA
48	RS	5	THR
26	Y1	83	GLU
46	YQ	28	ALA
7	QG	8	GLU
13	QM	10	PRO
24	QZ	50	HIS
38	RE	83	ASP
38	RE	147	PRO
40	RG	118	ARG
41	RH	47	GLU
41	RH	81	GLU
43	RN	96	GLU
45	RP	7	ARG
45	RP	56	SER
45	RP	57	THR
47	RR	4	LEU
2	XB	208	ILE
29	Y4	41	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
29	Y4	47	GLN
38	YE	147	PRO
41	YH	51	ARG
2	QB	208	ILE
5	QE	74	GLY
14	QN	16	PHE
38	RE	82	ARG
40	RG	81	LYS
41	RH	152	ARG
46	RQ	6	ARG
4	XD	155	LEU
5	XE	74	GLY
12	XL	27	LEU
19	XS	25	LYS
38	YE	52	LEU
43	YN	96	GLU
10	QJ	32	ALA
42	RI	13	GLY
42	YI	10	GLU
41	RH	9	ILE
55	RZ	95	PRO
42	RI	8	PRO
51	RV	50	PRO
41	YH	10	PRO
42	YI	118	LYS
29	R4	11	PRO
42	RI	134	PRO
38	YE	29	GLY
41	YH	55	PRO
42	YI	144	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	QB	203/220 (92%)	203 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	XB	204/220 (93%)	197 (97%)	7 (3%)	37	68
3	QC	159/188 (85%)	154 (97%)	5 (3%)	40	69
3	XC	159/188 (85%)	157 (99%)	2 (1%)	69	86
4	QD	180/181 (99%)	178 (99%)	2 (1%)	73	88
4	XD	180/181 (99%)	177 (98%)	3 (2%)	60	83
5	QE	116/123 (94%)	115 (99%)	1 (1%)	78	91
5	XE	116/123 (94%)	115 (99%)	1 (1%)	78	91
6	QF	90/90 (100%)	88 (98%)	2 (2%)	52	77
6	XF	90/90 (100%)	89 (99%)	1 (1%)	73	88
7	QG	126/127 (99%)	123 (98%)	3 (2%)	49	75
7	XG	126/127 (99%)	124 (98%)	2 (2%)	62	84
8	QH	118/119 (99%)	115 (98%)	3 (2%)	47	75
8	XH	118/119 (99%)	117 (99%)	1 (1%)	81	92
9	QI	98/99 (99%)	95 (97%)	3 (3%)	40	69
9	XI	97/99 (98%)	95 (98%)	2 (2%)	53	78
10	QJ	89/92 (97%)	85 (96%)	4 (4%)	27	59
10	XJ	86/92 (94%)	84 (98%)	2 (2%)	50	76
11	QK	90/99 (91%)	89 (99%)	1 (1%)	73	88
11	XK	88/99 (89%)	86 (98%)	2 (2%)	50	76
12	QL	104/109 (95%)	104 (100%)	0	100	100
12	XL	103/109 (94%)	100 (97%)	3 (3%)	42	71
13	QM	96/101 (95%)	94 (98%)	2 (2%)	53	78
13	XM	95/101 (94%)	93 (98%)	2 (2%)	53	78
14	QN	49/50 (98%)	48 (98%)	1 (2%)	55	79
14	XN	49/50 (98%)	49 (100%)	0	100	100
15	QO	79/80 (99%)	76 (96%)	3 (4%)	33	65
15	XO	79/80 (99%)	77 (98%)	2 (2%)	47	75
16	QP	72/74 (97%)	72 (100%)	0	100	100
16	XP	72/74 (97%)	72 (100%)	0	100	100
17	QQ	95/97 (98%)	92 (97%)	3 (3%)	39	69
17	XQ	95/97 (98%)	94 (99%)	1 (1%)	73	88

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	QR	61/77 (79%)	61 (100%)	0	100	100
18	XR	61/77 (79%)	58 (95%)	3 (5%)	25	57
19	QS	72/80 (90%)	71 (99%)	1 (1%)	67	85
19	XS	72/80 (90%)	72 (100%)	0	100	100
20	QT	76/82 (93%)	76 (100%)	0	100	100
20	XT	76/82 (93%)	75 (99%)	1 (1%)	69	86
21	QU	20/22 (91%)	20 (100%)	0	100	100
21	XU	20/22 (91%)	19 (95%)	1 (5%)	24	56
24	QY	78/78 (100%)	78 (100%)	0	100	100
24	QZ	78/78 (100%)	75 (96%)	3 (4%)	33	65
24	XY	78/78 (100%)	76 (97%)	2 (3%)	46	74
24	XZ	78/78 (100%)	72 (92%)	6 (8%)	13	40
25	R0	65/67 (97%)	65 (100%)	0	100	100
25	Y0	65/67 (97%)	64 (98%)	1 (2%)	65	85
26	R1	82/83 (99%)	79 (96%)	3 (4%)	34	66
26	Y1	82/83 (99%)	81 (99%)	1 (1%)	71	87
27	R2	64/67 (96%)	63 (98%)	1 (2%)	62	84
27	Y2	64/67 (96%)	63 (98%)	1 (2%)	62	84
28	R3	51/52 (98%)	51 (100%)	0	100	100
28	Y3	51/52 (98%)	51 (100%)	0	100	100
29	R4	62/63 (98%)	59 (95%)	3 (5%)	25	57
29	Y4	62/63 (98%)	62 (100%)	0	100	100
30	R5	51/52 (98%)	49 (96%)	2 (4%)	32	64
30	Y5	51/52 (98%)	50 (98%)	1 (2%)	55	79
31	R6	51/52 (98%)	50 (98%)	1 (2%)	55	79
31	Y6	51/52 (98%)	50 (98%)	1 (2%)	55	79
32	R7	40/42 (95%)	40 (100%)	0	100	100
32	Y7	41/42 (98%)	41 (100%)	0	100	100
33	R8	54/55 (98%)	54 (100%)	0	100	100
33	Y8	54/55 (98%)	54 (100%)	0	100	100
34	R9	34/34 (100%)	32 (94%)	2 (6%)	19	50

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	Y9	34/34 (100%)	33 (97%)	1 (3%)	42	71
37	RD	214/218 (98%)	209 (98%)	5 (2%)	50	76
37	YD	216/218 (99%)	216 (100%)	0	100	100
38	RE	165/166 (99%)	162 (98%)	3 (2%)	59	82
38	YE	165/166 (99%)	160 (97%)	5 (3%)	41	70
39	RF	161/166 (97%)	159 (99%)	2 (1%)	71	87
39	YF	161/166 (97%)	160 (99%)	1 (1%)	86	93
40	RG	155/156 (99%)	152 (98%)	3 (2%)	57	80
40	YG	155/156 (99%)	153 (99%)	2 (1%)	69	86
41	RH	145/148 (98%)	142 (98%)	3 (2%)	53	78
41	YH	145/148 (98%)	142 (98%)	3 (2%)	53	78
42	RI	122/124 (98%)	118 (97%)	4 (3%)	38	68
42	YI	122/124 (98%)	118 (97%)	4 (3%)	38	68
43	RN	117/119 (98%)	116 (99%)	1 (1%)	78	91
43	YN	117/119 (98%)	116 (99%)	1 (1%)	78	91
44	RO	100/100 (100%)	99 (99%)	1 (1%)	76	89
44	YO	100/100 (100%)	100 (100%)	0	100	100
45	RP	116/116 (100%)	116 (100%)	0	100	100
45	YP	114/116 (98%)	112 (98%)	2 (2%)	59	82
46	RQ	110/111 (99%)	110 (100%)	0	100	100
46	YQ	111/111 (100%)	110 (99%)	1 (1%)	78	91
47	RR	100/101 (99%)	99 (99%)	1 (1%)	76	89
47	YR	100/101 (99%)	100 (100%)	0	100	100
48	RS	87/88 (99%)	86 (99%)	1 (1%)	73	88
48	YS	87/88 (99%)	87 (100%)	0	100	100
49	RT	120/127 (94%)	117 (98%)	3 (2%)	47	75
49	YT	120/127 (94%)	117 (98%)	3 (2%)	47	75
50	RU	93/94 (99%)	93 (100%)	0	100	100
50	YU	93/94 (99%)	90 (97%)	3 (3%)	39	69
51	RV	82/82 (100%)	79 (96%)	3 (4%)	34	66
51	YV	82/82 (100%)	82 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	RW	92/92 (100%)	91 (99%)	1 (1%)	73	88
52	YW	92/92 (100%)	91 (99%)	1 (1%)	73	88
53	RX	74/78 (95%)	73 (99%)	1 (1%)	67	85
53	YX	74/78 (95%)	74 (100%)	0	100	100
54	RY	88/91 (97%)	86 (98%)	2 (2%)	50	76
54	YY	88/91 (97%)	86 (98%)	2 (2%)	50	76
55	RZ	162/179 (90%)	158 (98%)	4 (2%)	47	75
55	YZ	162/179 (90%)	156 (96%)	6 (4%)	34	66
All	All	10007/10378 (96%)	9836 (98%)	171 (2%)	60	83

All (171) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	QC	19	GLU
3	QC	33	LEU
3	QC	58	GLU
3	QC	59	ARG
3	QC	103	VAL
4	QD	61	LYS
4	QD	152	SER
5	QE	20	GLN
6	QF	24	GLU
6	QF	74	ASP
7	QG	33	ASP
7	QG	45	ASP
7	QG	56	GLN
8	QH	31	PHE
8	QH	87	SER
8	QH	127	LEU
9	QI	9	ARG
9	QI	20	ARG
9	QI	102	LEU
10	QJ	8	LEU
10	QJ	95	GLU
10	QJ	96	ILE
10	QJ	97	GLU
11	QK	43	SER
13	QM	16	ASP
13	QM	17	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	QN	27	CYS
15	QO	4	THR
15	QO	39	LEU
15	QO	62	GLN
17	QQ	24	GLU
17	QQ	86	GLU
17	QQ	92	ARG
19	QS	37	ARG
24	QZ	1	MET
24	QZ	30	LEU
24	QZ	84	TYR
26	R1	56	GLN
26	R1	87	PRO
26	R1	91	LYS
27	R2	69	ARG
29	R4	16	CYS
29	R4	42	PHE
29	R4	61	ARG
30	R5	21	SER
30	R5	36	CYS
31	R6	28	ARG
34	R9	24	TYR
34	R9	27	CYS
37	RD	111	LEU
37	RD	116	GLN
37	RD	118	VAL
37	RD	242	ARG
37	RD	273	ARG
38	RE	61	ARG
38	RE	77	ILE
38	RE	79	ARG
39	RF	67	GLN
39	RF	133	ASN
40	RG	14	GLU
40	RG	117	PHE
40	RG	128	ARG
41	RH	9	ILE
41	RH	72	ILE
41	RH	139	GLN
42	RI	4	ILE
42	RI	9	LEU
42	RI	69	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
42	RI	113	ARG
43	RN	29	LYS
44	RO	53	LYS
47	RR	18	LEU
48	RS	15	ARG
49	RT	105	LEU
49	RT	128	GLU
49	RT	137	LYS
51	RV	19	LYS
51	RV	44	LYS
51	RV	82	ARG
52	RW	113	LYS
53	RX	23	GLU
54	RY	49	VAL
54	RY	92	ASN
55	RZ	20	ARG
55	RZ	54	HIS
55	RZ	76	LEU
55	RZ	87	ASP
2	XB	7	VAL
2	XB	11	LEU
2	XB	33	TYR
2	XB	41	ILE
2	XB	122	PHE
2	XB	146	GLN
2	XB	235	SER
3	XC	17	ASP
3	XC	88	ARG
4	XD	18	LYS
4	XD	154	ASN
4	XD	194	LEU
5	XE	47	LYS
6	XF	83	ASP
7	XG	113	GLU
7	XG	143	ARG
8	XH	25	ASP
9	XI	56	LEU
9	XI	114	TYR
10	XJ	5	ARG
10	XJ	98	ILE
11	XK	11	LYS
11	XK	124	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	XL	19	ARG
12	XL	24	VAL
12	XL	62	SER
13	XM	9	ILE
13	XM	12	ASN
15	XO	13	GLN
15	XO	88	ARG
17	XQ	58	GLU
18	XR	66	LEU
18	XR	68	LYS
18	XR	84	LYS
20	XT	64	ASP
21	XU	7	ARG
24	XY	80	CYS
24	XY	81	ARG
24	XZ	35	ARG
24	XZ	51	ASN
24	XZ	52	LEU
24	XZ	72	ASP
24	XZ	74	SER
24	XZ	83	HIS
25	Y0	43	THR
26	Y1	5	CYS
27	Y2	45	SER
30	Y5	15	ARG
31	Y6	5	VAL
34	Y9	35	ARG
38	YE	1	MET
38	YE	21	VAL
38	YE	73	GLU
38	YE	165	VAL
38	YE	199	ARG
39	YF	203	GLN
40	YG	116	ASP
40	YG	118	ARG
41	YH	3	ARG
41	YH	50	VAL
41	YH	97	ARG
42	YI	7	GLU
42	YI	71	ILE
42	YI	77	LEU
42	YI	101	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
43	YN	23	LEU
45	YP	5	ASP
45	YP	52	GLU
46	YQ	1	MET
49	YT	112	ARG
49	YT	134	GLU
49	YT	137	LYS
50	YU	59	ARG
50	YU	94	ASN
50	YU	98	LEU
52	YW	28	SER
54	YY	2	ARG
54	YY	102	CYS
55	YZ	29	TYR
55	YZ	34	ASN
55	YZ	82	ARG
55	YZ	118	GLN
55	YZ	154	ASP
55	YZ	156	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
3	QC	108	ASN
10	QJ	76	ASN
37	RD	96	HIS
27	Y2	38	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1508/1521 (99%)	311 (20%)	52 (3%)
1	XA	1505/1521 (98%)	303 (20%)	50 (3%)
22	QV	77/77 (100%)	12 (15%)	4 (5%)
22	QW	76/77 (98%)	18 (23%)	1 (1%)
22	XV	76/77 (98%)	13 (17%)	3 (3%)
22	XW	76/77 (98%)	21 (27%)	1 (1%)
23	QX	16/20 (80%)	8 (50%)	2 (12%)
23	XX	16/20 (80%)	7 (43%)	1 (6%)
35	RA	2888/2915 (99%)	606 (20%)	49 (1%)

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
35	YA	2875/2915 (98%)	593 (20%)	46 (1%)
36	RB	121/124 (97%)	21 (17%)	1 (0%)
36	YB	121/124 (97%)	20 (16%)	1 (0%)
56	ZA	1/3 (33%)	0	0
56	ZB	1/3 (33%)	0	0
All	All	9357/9474 (98%)	1933 (20%)	211 (2%)

All (1933) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	4	U
1	QA	5	U
1	QA	6	G
1	QA	9	G
1	QA	22	G
1	QA	32	A
1	QA	39	G
1	QA	48	C
1	QA	50	A
1	QA	51	A
1	QA	61	G
1	QA	65	U
1	QA	66	G
1	QA	76	G
1	QA	79	G
1	QA	80	G
1	QA	90	C
1	QA	92	G
1	QA	101	A
1	QA	108	G
1	QA	116	A
1	QA	121	C
1	QA	129(A)	G
1	QA	151	A
1	QA	163	C
1	QA	169	C
1	QA	181	G
1	QA	182	U
1	QA	188	U
1	QA	189	U
1	QA	190	G
1	QA	191(A)	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	QA	191(D)	U
1	QA	191(E)	G
1	QA	195	A
1	QA	197	A
1	QA	198	G
1	QA	208	U
1	QA	209	U
1	QA	210	U
1	QA	216	G
1	QA	244	U
1	QA	247	G
1	QA	251	G
1	QA	266	G
1	QA	267	C
1	QA	268	C
1	QA	270	A
1	QA	280	C
1	QA	281	G
1	QA	289	G
1	QA	315	A
1	QA	316	G
1	QA	321	A
1	QA	328	C
1	QA	329	A
1	QA	332	G
1	QA	345	C
1	QA	346	G
1	QA	347	G
1	QA	350	G
1	QA	351	G
1	QA	352	C
1	QA	353	A
1	QA	354	G
1	QA	356	A
1	QA	367	U
1	QA	372	C
1	QA	373	A
1	QA	384	G
1	QA	397	A
1	QA	398	C
1	QA	406	G
1	QA	411	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	QA	412	A
1	QA	421	U
1	QA	422	C
1	QA	423	G
1	QA	424	G
1	QA	429	U
1	QA	439	A
1	QA	442	C
1	QA	465	A
1	QA	466	C
1	QA	478	A
1	QA	482	A
1	QA	485	G
1	QA	486	U
1	QA	494	U
1	QA	495	A
1	QA	496	A
1	QA	497	U
1	QA	505	G
1	QA	511	C
1	QA	518	C
1	QA	519	C
1	QA	521	G
1	QA	527	G
1	QA	530	G
1	QA	531	U
1	QA	532	A
1	QA	533	A
1	QA	534	U
1	QA	547	A
1	QA	548	G
1	QA	559	A
1	QA	560	U
1	QA	561	U
1	QA	564	C
1	QA	572	A
1	QA	573	A
1	QA	576	G
1	QA	577	G
1	QA	579	G
1	QA	596	C
1	QA	618	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	QA	623	C
1	QA	630	G
1	QA	652	U
1	QA	653	A
1	QA	665	A
1	QA	686	U
1	QA	688	G
1	QA	702	A
1	QA	703	G
1	QA	717	C
1	QA	718	G
1	QA	724	G
1	QA	731	G
1	QA	749	C
1	QA	755	G
1	QA	760	G
1	QA	773	G
1	QA	777	A
1	QA	792	A
1	QA	793	U
1	QA	794	A
1	QA	801	U
1	QA	813	U
1	QA	815	A
1	QA	816	A
1	QA	817	C
1	QA	821	G
1	QA	828	A
1	QA	841	U
1	QA	842	C
1	QA	843	U
1	QA	848	C
1	QA	859	A
1	QA	872	A
1	QA	884	U
1	QA	887	G
1	QA	914	A
1	QA	926	G
1	QA	927	G
1	QA	934	C
1	QA	942	G
1	QA	958	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	QA	960	U
1	QA	961	U
1	QA	968	A
1	QA	969	A
1	QA	972	C
1	QA	974	A
1	QA	975	A
1	QA	976	G
1	QA	977	A
1	QA	978	A
1	QA	991	U
1	QA	992	U
1	QA	993	G
1	QA	1000	A
1	QA	1001	G
1	QA	1002	G
1	QA	1003	G
1	QA	1004	A
1	QA	1005	A
1	QA	1006	C
1	QA	1007	C
1	QA	1008	C
1	QA	1009	G
1	QA	1020	U
1	QA	1024	G
1	QA	1025	U
1	QA	1026	G
1	QA	1029	G
1	QA	1030	C
1	QA	1031	G
1	QA	1032	A
1	QA	1032(A)	G
1	QA	1033	G
1	QA	1034	G
1	QA	1036	G
1	QA	1038	C
1	QA	1039	C
1	QA	1042	G
1	QA	1046	A
1	QA	1053	G
1	QA	1054	C
1	QA	1055	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	QA	1064	G
1	QA	1065	U
1	QA	1066	C
1	QA	1068	G
1	QA	1081	G
1	QA	1086	U
1	QA	1094	G
1	QA	1101	A
1	QA	1117	G
1	QA	1118	C
1	QA	1124	G
1	QA	1125	U
1	QA	1127	G
1	QA	1129	C
1	QA	1130	A
1	QA	1131	G
1	QA	1136	U
1	QA	1137	C
1	QA	1138	G
1	QA	1139	G
1	QA	1140	C
1	QA	1145	C
1	QA	1146	A
1	QA	1147	C
1	QA	1152	A
1	QA	1157	A
1	QA	1158	C
1	QA	1159	U
1	QA	1160	G
1	QA	1171	G
1	QA	1176	A
1	QA	1177	G
1	QA	1178	G
1	QA	1181	G
1	QA	1183	A
1	QA	1187	G
1	QA	1196	U
1	QA	1197	G
1	QA	1211	U
1	QA	1212	U
1	QA	1213	A
1	QA	1224	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	QA	1225	A
1	QA	1238	A
1	QA	1240	U
1	QA	1241	G
1	QA	1256	A
1	QA	1257	U
1	QA	1258	G
1	QA	1260	C
1	QA	1270	C
1	QA	1273	G
1	QA	1278	U
1	QA	1280	A
1	QA	1281	U
1	QA	1285	A
1	QA	1286	A
1	QA	1287	A
1	QA	1288	A
1	QA	1290	G
1	QA	1297	C
1	QA	1298	C
1	QA	1299	A
1	QA	1300	G
1	QA	1301	U
1	QA	1302	U
1	QA	1303	C
1	QA	1305	G
1	QA	1318	A
1	QA	1319	A
1	QA	1320	C
1	QA	1322	C
1	QA	1323	G
1	QA	1331	G
1	QA	1346	A
1	QA	1347	G
1	QA	1348	U
1	QA	1353	G
1	QA	1362(A)	C
1	QA	1364	U
1	QA	1365	G
1	QA	1370	G
1	QA	1397	C
1	QA	1398	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	QA	1406	U
1	QA	1419	G
1	QA	1442	G
1	QA	1446	A
1	QA	1451	A
1	QA	1452	C
1	QA	1453	G
1	QA	1454	G
1	QA	1487	G
1	QA	1492	A
1	QA	1493	A
1	QA	1499	A
1	QA	1504	G
1	QA	1505	G
1	QA	1506	U
1	QA	1517	G
1	QA	1519	A
1	QA	1520	G
1	QA	1529	G
1	QA	1530	G
1	QA	1532	U
1	QA	1533	C
1	QA	1534	A
1	QA	1536	C
1	QA	1537	U
1	QA	1540	U
1	QA	1541	U
22	QV	2	G
22	QV	7	G
22	QV	8	U
22	QV	18	G
22	QV	20	U
22	QV	22	G
22	QV	47	U
22	QV	48	C
22	QV	49	G
22	QV	55	U
22	QV	61	C
22	QV	76	A
22	QW	7	G
22	QW	8	U
22	QW	14	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	QW	15	G
22	QW	17	C
22	QW	17(A)	U
22	QW	18	G
22	QW	19	G
22	QW	20	U
22	QW	22	G
22	QW	46	G
22	QW	47	U
22	QW	49	G
22	QW	55	U
22	QW	56	C
22	QW	60	U
22	QW	61	C
22	QW	76	A
23	QX	5	A
23	QX	9	G
23	QX	10	G
23	QX	11	U
23	QX	12	A
23	QX	13	A
23	QX	14	A
23	QX	19	A
35	RA	9	U
35	RA	15	G
35	RA	34	C
35	RA	35	G
35	RA	46	C
35	RA	50	U
35	RA	55	G
35	RA	58	G
35	RA	60	G
35	RA	69	C
35	RA	71	A
35	RA	74	A
35	RA	75	G
35	RA	83	G
35	RA	91	A
35	RA	95	G
35	RA	99	U
35	RA	101	G
35	RA	102	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	RA	118	A
35	RA	119	A
35	RA	120	U
35	RA	125	G
35	RA	129	C
35	RA	138	G
35	RA	139	G
35	RA	140	A
35	RA	154	G
35	RA	155	C
35	RA	175	G
35	RA	182	A
35	RA	196	A
35	RA	199	A
35	RA	215	G
35	RA	216	A
35	RA	221	A
35	RA	222	A
35	RA	228	A
35	RA	229	A
35	RA	233	A
35	RA	248	G
35	RA	249	C
35	RA	252	G
35	RA	266	G
35	RA	270(B)	A
35	RA	270(K)	C
35	RA	270(M)	U
35	RA	270(O)	U
35	RA	270(P)	C
35	RA	270(Z)	U
35	RA	271(C)	U
35	RA	271	G
35	RA	273(D)	C
35	RA	274	G
35	RA	275	G
35	RA	278	A
35	RA	279	C
35	RA	283	A
35	RA	289	A
35	RA	308	G
35	RA	311	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	RA	324	A
35	RA	329	G
35	RA	330	A
35	RA	332	A
35	RA	345	A
35	RA	346	A
35	RA	352	G
35	RA	353	G
35	RA	358	U
35	RA	362	U
35	RA	363	G
35	RA	363(A)	A
35	RA	363(E)	U
35	RA	363(F)	A
35	RA	364	C
35	RA	372	G
35	RA	373	U
35	RA	380	U
35	RA	386	G
35	RA	388	G
35	RA	395	U
35	RA	405	U
35	RA	406	G
35	RA	407	G
35	RA	411	G
35	RA	412	A
35	RA	428	A
35	RA	442	G
35	RA	444	C
35	RA	448	U
35	RA	457	A
35	RA	470	A
35	RA	481	G
35	RA	494	G
35	RA	505	A
35	RA	508	G
35	RA	509	C
35	RA	512	G
35	RA	528	A
35	RA	529	A
35	RA	531	C
35	RA	532	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	RA	533	G
35	RA	537	C
35	RA	556	G
35	RA	563	G
35	RA	571	A
35	RA	573	G
35	RA	574	C
35	RA	575	A
35	RA	583	G
35	RA	588	U
35	RA	603	A
35	RA	604	G
35	RA	607	U
35	RA	613	U
35	RA	614	U
35	RA	615	G
35	RA	617	G
35	RA	620	G
35	RA	621	A
35	RA	622	G
35	RA	627	A
35	RA	634	C
35	RA	637	A
35	RA	645	C
35	RA	646	A
35	RA	647	G
35	RA	651	G
35	RA	654	A
35	RA	654(A)	G
35	RA	654(B)	C
35	RA	654(F)	C
35	RA	654(G)	C
35	RA	654(Q)	C
35	RA	654(R)	C
35	RA	654(S)	G
35	RA	654(T)	C
35	RA	668	G
35	RA	669	G
35	RA	670	A
35	RA	686	G
35	RA	704	G
35	RA	705	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	RA	708	C
35	RA	722	A
35	RA	726	G
35	RA	730	C
35	RA	753	C
35	RA	764	A
35	RA	765	G
35	RA	776	G
35	RA	782	A
35	RA	784	A
35	RA	785	G
35	RA	788	A
35	RA	789	A
35	RA	792	G
35	RA	793	A
35	RA	805	G
35	RA	812	C
35	RA	819	A
35	RA	827	U
35	RA	828	U
35	RA	846	C
35	RA	856	C
35	RA	857	C
35	RA	859	G
35	RA	860	U
35	RA	862	G
35	RA	866	A
35	RA	869	G
35	RA	878	A
35	RA	879	G
35	RA	881	G
35	RA	882	G
35	RA	883	G
35	RA	884	C
35	RA	886	C
35	RA	889	C
35	RA	890	A
35	RA	894	C
35	RA	895	U
35	RA	896	A
35	RA	897	C
35	RA	900	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	RA	906	G
35	RA	907	U
35	RA	910	A
35	RA	915	C
35	RA	917	A
35	RA	919	G
35	RA	928	G
35	RA	932	G
35	RA	934	G
35	RA	938	G
35	RA	941	A
35	RA	945	A
35	RA	946	G
35	RA	953	A
35	RA	961	C
35	RA	968	G
35	RA	973	A
35	RA	974	G
35	RA	980	A
35	RA	983	A
35	RA	989	G
35	RA	990	A
35	RA	991	C
35	RA	996	A
35	RA	999	U
35	RA	1005	C
35	RA	1012	U
35	RA	1013	C
35	RA	1015	G
35	RA	1022	G
35	RA	1023	U
35	RA	1025	G
35	RA	1026	U
35	RA	1027	A
35	RA	1033	U
35	RA	1034	G
35	RA	1044	G
35	RA	1045	A
35	RA	1046	A
35	RA	1047	G
35	RA	1049	C
35	RA	1060	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	RA	1061	U
35	RA	1070	A
35	RA	1073	A
35	RA	1086	A
35	RA	1087	G
35	RA	1088	A
35	RA	1089	G
35	RA	1095	A
35	RA	1096	A
35	RA	1099	G
35	RA	1105	U
35	RA	1122	G
35	RA	1128	A
35	RA	1130	U
35	RA	1135	C
35	RA	1136	G
35	RA	1139	G
35	RA	1142(A)	A
35	RA	1148	A
35	RA	1155	A
35	RA	1156	A
35	RA	1171	G
35	RA	1173	G
35	RA	1174	A
35	RA	1175	U
35	RA	1176	G
35	RA	1177	A
35	RA	1178	C
35	RA	1180	C
35	RA	1195	G
35	RA	1204	A
35	RA	1205	U
35	RA	1220	A
35	RA	1236	G
35	RA	1244	G
35	RA	1253	A
35	RA	1254	A
35	RA	1255	U
35	RA	1256	G
35	RA	1262	A
35	RA	1265	A
35	RA	1271	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	RA	1272	A
35	RA	1281	G
35	RA	1287	A
35	RA	1300	U
35	RA	1301	A
35	RA	1303	G
35	RA	1308	A
35	RA	1311	G
35	RA	1312	U
35	RA	1314	C
35	RA	1319	G
35	RA	1329	U
35	RA	1341	U
35	RA	1352	U
35	RA	1359	A
35	RA	1360	A
35	RA	1367	A
35	RA	1368	G
35	RA	1379	A
35	RA	1380	G
35	RA	1384	A
35	RA	1391	U
35	RA	1395	A
35	RA	1407	C
35	RA	1415	U
35	RA	1416	G
35	RA	1419	A
35	RA	1420	U
35	RA	1421	G
35	RA	1428	C
35	RA	1434	A
35	RA	1437	C
35	RA	1444(A)	A
35	RA	1449	A
35	RA	1449(A)	G
35	RA	1451	C
35	RA	1453	A
35	RA	1454	U
35	RA	1455	G
35	RA	1458	C
35	RA	1460	A
35	RA	1461	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	RA	1467	C
35	RA	1471	A
35	RA	1475	G
35	RA	1478	G
35	RA	1482	U
35	RA	1483	G
35	RA	1485	G
35	RA	1488	G
35	RA	1490	A
35	RA	1493	C
35	RA	1505	C
35	RA	1506	C
35	RA	1509	C
35	RA	1510	A
35	RA	1523	U
35	RA	1526	G
35	RA	1533	C
35	RA	1535	U
35	RA	1536	A
35	RA	1537	C
35	RA	1540	G
35	RA	1543	A
35	RA	1544	C
35	RA	1545	A
35	RA	1547	C
35	RA	1554	A
35	RA	1558	A
35	RA	1559	G
35	RA	1560	G
35	RA	1566	A
35	RA	1569	A
35	RA	1578	U
35	RA	1585	C
35	RA	1586	A
35	RA	1598	C
35	RA	1608	A
35	RA	1618	A
35	RA	1640	C
35	RA	1648	C
35	RA	1652	A
35	RA	1654	A
35	RA	1667	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	RA	1668	A
35	RA	1674	G
35	RA	1695	G
35	RA	1696	G
35	RA	1700	A
35	RA	1703	G
35	RA	1725	G
35	RA	1728	G
35	RA	1729	A
35	RA	1730	U
35	RA	1731	G
35	RA	1735	C
35	RA	1743	G
35	RA	1750	G
35	RA	1754	C
35	RA	1756	G
35	RA	1762	A
35	RA	1763	G
35	RA	1764	G
35	RA	1773	A
35	RA	1780	A
35	RA	1791	A
35	RA	1800	C
35	RA	1801	G
35	RA	1816	G
35	RA	1820	U
35	RA	1828	G
35	RA	1829	A
35	RA	1835	G
35	RA	1847	A
35	RA	1854	A
35	RA	1858	G
35	RA	1869	G
35	RA	1872	A
35	RA	1878	G
35	RA	1881	C
35	RA	1882	C
35	RA	1888	G
35	RA	1889	A
35	RA	1900	A
35	RA	1901	A
35	RA	1906	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	RA	1913	A
35	RA	1924	C
35	RA	1929	G
35	RA	1930	G
35	RA	1931	U
35	RA	1936	A
35	RA	1938	A
35	RA	1948	G
35	RA	1955	U
35	RA	1963	U
35	RA	1964	G
35	RA	1967	C
35	RA	1970	A
35	RA	1971	A
35	RA	1972	A
35	RA	1980	G
35	RA	1982	C
35	RA	1992	G
35	RA	1993	U
35	RA	2020	A
35	RA	2021	C
35	RA	2022	U
35	RA	2023	G
35	RA	2027	G
35	RA	2031	A
35	RA	2032	G
35	RA	2033	A
35	RA	2043	C
35	RA	2052	G
35	RA	2055	C
35	RA	2056	G
35	RA	2059	A
35	RA	2060	A
35	RA	2061	G
35	RA	2062	A
35	RA	2069	G
35	RA	2093	G
35	RA	2095	C
35	RA	2111	C
35	RA	2112	G
35	RA	2113	U
35	RA	2114	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	RA	2116	G
35	RA	2117	A
35	RA	2120	G
35	RA	2123	G
35	RA	2128	C
35	RA	2130	U
35	RA	2131	G
35	RA	2132	U
35	RA	2134	A
35	RA	2145	C
35	RA	2147	G
35	RA	2148	G
35	RA	2161	C
35	RA	2165	G
35	RA	2166	G
35	RA	2167	U
35	RA	2168	G
35	RA	2169	A
35	RA	2171	A
35	RA	2173	A
35	RA	2178	C
35	RA	2190	G
35	RA	2191	G
35	RA	2192	G
35	RA	2198	A
35	RA	2210	G
35	RA	2211	G
35	RA	2212	A
35	RA	2213	U
35	RA	2215	G
35	RA	2225	A
35	RA	2226	C
35	RA	2238	G
35	RA	2239	G
35	RA	2243	U
35	RA	2266	A
35	RA	2275	C
35	RA	2279	G
35	RA	2283	C
35	RA	2305	A
35	RA	2306	C
35	RA	2307	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	RA	2308	G
35	RA	2309	A
35	RA	2312	U
35	RA	2319	G
35	RA	2320	A
35	RA	2321	G
35	RA	2325	G
35	RA	2334	G
35	RA	2336	A
35	RA	2345	G
35	RA	2346	A
35	RA	2347	C
35	RA	2350	C
35	RA	2354	G
35	RA	2382	G
35	RA	2383	G
35	RA	2385	C
35	RA	2392	A
35	RA	2402	C
35	RA	2406	U
35	RA	2410	G
35	RA	2411	A
35	RA	2422	A
35	RA	2423	U
35	RA	2425	A
35	RA	2429	G
35	RA	2430	A
35	RA	2435	A
35	RA	2439	A
35	RA	2440	C
35	RA	2441	C
35	RA	2445	G
35	RA	2448	A
35	RA	2450	A
35	RA	2460	U
35	RA	2465	C
35	RA	2469	A
35	RA	2470	G
35	RA	2474	C
35	RA	2475	C
35	RA	2476	A
35	RA	2481	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	RA	2482	G
35	RA	2491	U
35	RA	2494	G
35	RA	2498	C
35	RA	2502	G
35	RA	2505	G
35	RA	2518	A
35	RA	2529	G
35	RA	2535	G
35	RA	2540	C
35	RA	2542	A
35	RA	2543	G
35	RA	2554	U
35	RA	2566	A
35	RA	2567	G
35	RA	2569	G
35	RA	2572	A
35	RA	2582	G
35	RA	2586	C
35	RA	2602	A
35	RA	2609	U
35	RA	2610	C
35	RA	2611	U
35	RA	2612	C
35	RA	2629	A
35	RA	2630	G
35	RA	2645	G
35	RA	2646	C
35	RA	2654	A
35	RA	2655	G
35	RA	2665	A
35	RA	2673	G
35	RA	2682	U
35	RA	2689	U
35	RA	2690	C
35	RA	2691	C
35	RA	2702	U
35	RA	2703	C
35	RA	2712	U
35	RA	2713	A
35	RA	2714	G
35	RA	2725	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	RA	2733	A
35	RA	2744	G
35	RA	2748	A
35	RA	2752	C
35	RA	2754	U
35	RA	2762	G
35	RA	2765	A
35	RA	2766	G
35	RA	2777	G
35	RA	2778	A
35	RA	2779	U
35	RA	2780	G
35	RA	2789	C
35	RA	2790	A
35	RA	2791	C
35	RA	2797	U
35	RA	2799	A
35	RA	2807	G
35	RA	2818	G
35	RA	2820	A
35	RA	2821	A
35	RA	2827	C
35	RA	2830	G
35	RA	2833	G
35	RA	2834	G
35	RA	2835	A
35	RA	2848	G
35	RA	2849	U
35	RA	2850	A
35	RA	2860	A
35	RA	2867	G
35	RA	2872	G
35	RA	2873	A
35	RA	2876	G
35	RA	2877	G
35	RA	2879	C
35	RA	2880	C
35	RA	2892	A
35	RA	2893	G
35	RA	2896	C
35	RA	2897	U
36	RB	8	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	RB	9	G
36	RB	13	A
36	RB	15	A
36	RB	25	A
36	RB	41	U
36	RB	42	C
36	RB	44	G
36	RB	45	A
36	RB	52	A
36	RB	53	A
36	RB	58	A
36	RB	67	G
36	RB	73	A
36	RB	81	G
36	RB	88	C
36	RB	92	G
36	RB	101	A
36	RB	109	G
36	RB	117	G
36	RB	118	G
1	XA	4	U
1	XA	5	U
1	XA	6	G
1	XA	9	G
1	XA	22	G
1	XA	32	A
1	XA	39	G
1	XA	48	C
1	XA	50	A
1	XA	51	A
1	XA	61	G
1	XA	65	U
1	XA	66	G
1	XA	76	G
1	XA	79	G
1	XA	101	A
1	XA	116	A
1	XA	121	C
1	XA	129(A)	G
1	XA	151	A
1	XA	163	C
1	XA	169	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	XA	182	U
1	XA	188	U
1	XA	189	U
1	XA	190	G
1	XA	191(D)	U
1	XA	195	A
1	XA	197	A
1	XA	198	G
1	XA	208	U
1	XA	209	U
1	XA	210	U
1	XA	216	G
1	XA	244	U
1	XA	247	G
1	XA	251	G
1	XA	266	G
1	XA	267	C
1	XA	268	C
1	XA	270	A
1	XA	279	A
1	XA	280	C
1	XA	281	G
1	XA	282	A
1	XA	289	G
1	XA	315	A
1	XA	316	G
1	XA	321	A
1	XA	328	C
1	XA	329	A
1	XA	332	G
1	XA	345	C
1	XA	346	G
1	XA	347	G
1	XA	350	G
1	XA	351	G
1	XA	352	C
1	XA	353	A
1	XA	354	G
1	XA	356	A
1	XA	367	U
1	XA	368	U
1	XA	372	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	XA	373	A
1	XA	384	G
1	XA	397	A
1	XA	398	C
1	XA	406	G
1	XA	411	A
1	XA	412	A
1	XA	422	C
1	XA	423	G
1	XA	424	G
1	XA	429	U
1	XA	439	A
1	XA	465	A
1	XA	466	C
1	XA	467	G
1	XA	478	A
1	XA	482	A
1	XA	485	G
1	XA	494	U
1	XA	495	A
1	XA	496	A
1	XA	497	U
1	XA	505	G
1	XA	511	C
1	XA	518	C
1	XA	519	C
1	XA	521	G
1	XA	527	G
1	XA	530	G
1	XA	531	U
1	XA	532	A
1	XA	533	A
1	XA	534	U
1	XA	547	A
1	XA	548	G
1	XA	559	A
1	XA	564	C
1	XA	572	A
1	XA	573	A
1	XA	576	G
1	XA	577	G
1	XA	579	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	XA	596	C
1	XA	618	C
1	XA	623	C
1	XA	630	G
1	XA	652	U
1	XA	653	A
1	XA	665	A
1	XA	686	U
1	XA	688	G
1	XA	701	C
1	XA	702	A
1	XA	703	G
1	XA	704	A
1	XA	724	G
1	XA	731	G
1	XA	733	A
1	XA	734	G
1	XA	749	C
1	XA	755	G
1	XA	760	G
1	XA	773	G
1	XA	777	A
1	XA	792	A
1	XA	793	U
1	XA	794	A
1	XA	801	U
1	XA	813	U
1	XA	815	A
1	XA	816	A
1	XA	817	C
1	XA	818	G
1	XA	819	A
1	XA	821	G
1	XA	828	A
1	XA	841	U
1	XA	842	C
1	XA	843	U
1	XA	848	C
1	XA	859	A
1	XA	870	U
1	XA	887	G
1	XA	913	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	XA	914	A
1	XA	926	G
1	XA	927	G
1	XA	934	C
1	XA	942	G
1	XA	958	A
1	XA	960	U
1	XA	961	U
1	XA	968	A
1	XA	969	A
1	XA	972	C
1	XA	974	A
1	XA	975	A
1	XA	976	G
1	XA	977	A
1	XA	991	U
1	XA	992	U
1	XA	993	G
1	XA	1000	A
1	XA	1001	G
1	XA	1002	G
1	XA	1003	G
1	XA	1005	A
1	XA	1006	C
1	XA	1007	C
1	XA	1008	C
1	XA	1009	G
1	XA	1020	U
1	XA	1024	G
1	XA	1025	U
1	XA	1026	G
1	XA	1029	G
1	XA	1030	C
1	XA	1031	G
1	XA	1032	A
1	XA	1032(A)	G
1	XA	1033	G
1	XA	1034	G
1	XA	1036	G
1	XA	1038	C
1	XA	1039	C
1	XA	1042	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	XA	1053	G
1	XA	1054	C
1	XA	1055	A
1	XA	1064	G
1	XA	1065	U
1	XA	1066	C
1	XA	1068	G
1	XA	1081	G
1	XA	1086	U
1	XA	1094	G
1	XA	1095	U
1	XA	1101	A
1	XA	1117	G
1	XA	1118	C
1	XA	1124	G
1	XA	1125	U
1	XA	1127	G
1	XA	1130	A
1	XA	1131	G
1	XA	1136	U
1	XA	1137	C
1	XA	1138	G
1	XA	1139	G
1	XA	1140	C
1	XA	1145	C
1	XA	1146	A
1	XA	1152	A
1	XA	1157	A
1	XA	1158	C
1	XA	1159	U
1	XA	1160	G
1	XA	1171	G
1	XA	1176	A
1	XA	1177	G
1	XA	1178	G
1	XA	1181	G
1	XA	1183	A
1	XA	1187	G
1	XA	1196	U
1	XA	1197	G
1	XA	1211	U
1	XA	1212	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	XA	1213	A
1	XA	1224	G
1	XA	1225	A
1	XA	1227	A
1	XA	1238	A
1	XA	1241	G
1	XA	1256	A
1	XA	1257	U
1	XA	1258	G
1	XA	1260	C
1	XA	1270	C
1	XA	1273	G
1	XA	1278	U
1	XA	1280	A
1	XA	1285	A
1	XA	1286	A
1	XA	1287	A
1	XA	1288	A
1	XA	1290	G
1	XA	1297	C
1	XA	1299	A
1	XA	1300	G
1	XA	1301	U
1	XA	1302	U
1	XA	1303	C
1	XA	1305	G
1	XA	1318	A
1	XA	1319	A
1	XA	1320	C
1	XA	1322	C
1	XA	1323	G
1	XA	1331	G
1	XA	1345	U
1	XA	1346	A
1	XA	1347	G
1	XA	1353	G
1	XA	1362(A)	C
1	XA	1364	U
1	XA	1365	G
1	XA	1370	G
1	XA	1397	C
1	XA	1398	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	XA	1406	U
1	XA	1419	G
1	XA	1422	G
1	XA	1442	G
1	XA	1446	A
1	XA	1450	U
1	XA	1451	A
1	XA	1452	C
1	XA	1453	G
1	XA	1454	G
1	XA	1487	G
1	XA	1492	A
1	XA	1493	A
1	XA	1499	A
1	XA	1504	G
1	XA	1505	G
1	XA	1506	U
1	XA	1517	G
1	XA	1519	A
1	XA	1520	G
1	XA	1529	G
1	XA	1530	G
1	XA	1532	U
1	XA	1533	C
1	XA	1534	A
1	XA	1536	C
1	XA	1537	U
1	XA	1540	U
1	XA	1541	U
22	XV	2	G
22	XV	7	G
22	XV	8	U
22	XV	9	G
22	XV	18	G
22	XV	19	G
22	XV	20	U
22	XV	22	G
22	XV	47	U
22	XV	49	G
22	XV	56	C
22	XV	61	C
22	XV	76	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	XW	2	G
22	XW	6	G
22	XW	8	U
22	XW	9	G
22	XW	13	C
22	XW	14	A
22	XW	15	G
22	XW	17	C
22	XW	17(A)	U
22	XW	18	G
22	XW	20	U
22	XW	22	G
22	XW	46	G
22	XW	47	U
22	XW	48	C
22	XW	49	G
22	XW	55	U
22	XW	56	C
22	XW	60	U
22	XW	61	C
22	XW	76	A
23	XX	9	G
23	XX	10	G
23	XX	11	U
23	XX	12	A
23	XX	13	A
23	XX	14	A
23	XX	19	A
35	YA	9	U
35	YA	15	G
35	YA	27	G
35	YA	34	C
35	YA	35	G
35	YA	46	C
35	YA	54	G
35	YA	55	G
35	YA	58	G
35	YA	60	G
35	YA	69	C
35	YA	71	A
35	YA	74	A
35	YA	75	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	YA	83	G
35	YA	95	G
35	YA	99	U
35	YA	101	G
35	YA	102	G
35	YA	118	A
35	YA	119	A
35	YA	120	U
35	YA	125	G
35	YA	138	G
35	YA	139	G
35	YA	140	A
35	YA	154	G
35	YA	155	C
35	YA	156	U
35	YA	157	U
35	YA	175	G
35	YA	182	A
35	YA	196	A
35	YA	199	A
35	YA	215	G
35	YA	216	A
35	YA	221	A
35	YA	222	A
35	YA	227	A
35	YA	229	A
35	YA	233	A
35	YA	248	G
35	YA	249	C
35	YA	252	G
35	YA	266	G
35	YA	270(B)	A
35	YA	270(K)	C
35	YA	270(M)	U
35	YA	270(N)	G
35	YA	270(O)	U
35	YA	270(P)	C
35	YA	270(Z)	U
35	YA	271(C)	U
35	YA	271	G
35	YA	273(D)	C
35	YA	274	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	YA	278	A
35	YA	279	C
35	YA	283	A
35	YA	289	A
35	YA	308	G
35	YA	311	A
35	YA	324	A
35	YA	327	G
35	YA	329	G
35	YA	330	A
35	YA	332	A
35	YA	345	A
35	YA	346	A
35	YA	352	G
35	YA	353	G
35	YA	358	U
35	YA	363	G
35	YA	363(E)	U
35	YA	363(F)	A
35	YA	364	C
35	YA	372	G
35	YA	380	U
35	YA	386	G
35	YA	388	G
35	YA	395	U
35	YA	405	U
35	YA	406	G
35	YA	407	G
35	YA	411	G
35	YA	412	A
35	YA	428	A
35	YA	442	G
35	YA	444	C
35	YA	448	U
35	YA	457	A
35	YA	470	A
35	YA	481	G
35	YA	494	G
35	YA	505	A
35	YA	508	G
35	YA	509	C
35	YA	512	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	YA	525	U
35	YA	528	A
35	YA	529	A
35	YA	531	C
35	YA	532	A
35	YA	533	G
35	YA	537	C
35	YA	563	G
35	YA	571	A
35	YA	573	G
35	YA	574	C
35	YA	575	A
35	YA	583	G
35	YA	588	U
35	YA	603	A
35	YA	604	G
35	YA	607	U
35	YA	613	U
35	YA	614	U
35	YA	615	G
35	YA	617	G
35	YA	620	G
35	YA	621	A
35	YA	622	G
35	YA	627	A
35	YA	634	C
35	YA	637	A
35	YA	645	C
35	YA	646	A
35	YA	647	G
35	YA	651	G
35	YA	668	G
35	YA	669	G
35	YA	670	A
35	YA	686	G
35	YA	693	C
35	YA	705	A
35	YA	708	C
35	YA	722	A
35	YA	726	G
35	YA	727	A
35	YA	730	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	YA	753	C
35	YA	764	A
35	YA	765	G
35	YA	776	G
35	YA	782	A
35	YA	784	A
35	YA	785	G
35	YA	788	A
35	YA	789	A
35	YA	792	G
35	YA	793	A
35	YA	805	G
35	YA	812	C
35	YA	819	A
35	YA	827	U
35	YA	828	U
35	YA	846	C
35	YA	856	C
35	YA	857	C
35	YA	859	G
35	YA	860	U
35	YA	862	G
35	YA	866	A
35	YA	869	G
35	YA	878	A
35	YA	879	G
35	YA	881	G
35	YA	882	G
35	YA	883	G
35	YA	884	C
35	YA	886	C
35	YA	889	C
35	YA	890	A
35	YA	894	C
35	YA	895	U
35	YA	896	A
35	YA	897	C
35	YA	906	G
35	YA	907	U
35	YA	910	A
35	YA	915	C
35	YA	917	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	YA	919	G
35	YA	928	G
35	YA	932	G
35	YA	934	G
35	YA	938	G
35	YA	941	A
35	YA	945	A
35	YA	946	G
35	YA	953	A
35	YA	955	C
35	YA	961	C
35	YA	968	G
35	YA	973	A
35	YA	974	G
35	YA	980	A
35	YA	983	A
35	YA	989	G
35	YA	990	A
35	YA	991	C
35	YA	996	A
35	YA	997	G
35	YA	999	U
35	YA	1005	C
35	YA	1012	U
35	YA	1013	C
35	YA	1022	G
35	YA	1023	U
35	YA	1025	G
35	YA	1026	U
35	YA	1027	A
35	YA	1033	U
35	YA	1034	G
35	YA	1044	G
35	YA	1045	A
35	YA	1046	A
35	YA	1047	G
35	YA	1049	C
35	YA	1053	C
35	YA	1060	U
35	YA	1061	U
35	YA	1064	C
35	YA	1070	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	YA	1073	A
35	YA	1079	C
35	YA	1086	A
35	YA	1087	G
35	YA	1088	A
35	YA	1089	G
35	YA	1095	A
35	YA	1096	A
35	YA	1105	U
35	YA	1122	G
35	YA	1128	A
35	YA	1130	U
35	YA	1135	C
35	YA	1136	G
35	YA	1139	G
35	YA	1142	U
35	YA	1142(A)	A
35	YA	1148	A
35	YA	1156	A
35	YA	1171	G
35	YA	1173	G
35	YA	1174	A
35	YA	1175	U
35	YA	1177	A
35	YA	1178	C
35	YA	1180	C
35	YA	1195	G
35	YA	1204	A
35	YA	1205	U
35	YA	1210	A
35	YA	1212	G
35	YA	1220	A
35	YA	1236	G
35	YA	1244	G
35	YA	1247	A
35	YA	1253	A
35	YA	1254	A
35	YA	1255	U
35	YA	1256	G
35	YA	1262	A
35	YA	1265	A
35	YA	1271	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	YA	1272	A
35	YA	1281	G
35	YA	1300	U
35	YA	1301	A
35	YA	1303	G
35	YA	1308	A
35	YA	1314	C
35	YA	1319	G
35	YA	1324	G
35	YA	1329	U
35	YA	1352	U
35	YA	1359	A
35	YA	1360	A
35	YA	1367	A
35	YA	1368	G
35	YA	1379	A
35	YA	1380	G
35	YA	1384	A
35	YA	1385	G
35	YA	1391	U
35	YA	1395	A
35	YA	1407	C
35	YA	1415	U
35	YA	1416	G
35	YA	1419	A
35	YA	1420	U
35	YA	1421	G
35	YA	1428	C
35	YA	1434	A
35	YA	1437	C
35	YA	1444(A)	A
35	YA	1449	A
35	YA	1449(A)	G
35	YA	1451	C
35	YA	1453	A
35	YA	1455	G
35	YA	1458	C
35	YA	1460	A
35	YA	1461	G
35	YA	1467	C
35	YA	1471	A
35	YA	1475	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	YA	1478	G
35	YA	1482	U
35	YA	1483	G
35	YA	1485	G
35	YA	1488	G
35	YA	1490	A
35	YA	1493	C
35	YA	1505	C
35	YA	1506	C
35	YA	1508	A
35	YA	1509	C
35	YA	1510	A
35	YA	1523	U
35	YA	1526	G
35	YA	1534	G
35	YA	1535	U
35	YA	1536	A
35	YA	1537	C
35	YA	1538	G
35	YA	1540	G
35	YA	1543	A
35	YA	1544	C
35	YA	1545	A
35	YA	1547	C
35	YA	1549	C
35	YA	1554	A
35	YA	1558	A
35	YA	1559	G
35	YA	1560	G
35	YA	1566	A
35	YA	1569	A
35	YA	1578	U
35	YA	1585	C
35	YA	1586	A
35	YA	1598	C
35	YA	1608	A
35	YA	1618	A
35	YA	1640	C
35	YA	1648	C
35	YA	1652	A
35	YA	1654	A
35	YA	1667	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	YA	1668	A
35	YA	1674	G
35	YA	1695	G
35	YA	1696	G
35	YA	1700	A
35	YA	1703	G
35	YA	1725	G
35	YA	1728	G
35	YA	1729	A
35	YA	1731	G
35	YA	1735	C
35	YA	1743	G
35	YA	1750	G
35	YA	1754	C
35	YA	1756	G
35	YA	1762	A
35	YA	1763	G
35	YA	1764	G
35	YA	1773	A
35	YA	1774	C
35	YA	1780	A
35	YA	1791	A
35	YA	1800	C
35	YA	1801	G
35	YA	1816	G
35	YA	1820	U
35	YA	1828	G
35	YA	1829	A
35	YA	1835	G
35	YA	1847	A
35	YA	1858	G
35	YA	1869	G
35	YA	1872	A
35	YA	1878	G
35	YA	1881	C
35	YA	1882	C
35	YA	1888	G
35	YA	1889	A
35	YA	1900	A
35	YA	1906	G
35	YA	1913	A
35	YA	1929	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	YA	1930	G
35	YA	1936	A
35	YA	1938	A
35	YA	1948	G
35	YA	1955	U
35	YA	1963	U
35	YA	1964	G
35	YA	1967	C
35	YA	1970	A
35	YA	1971	A
35	YA	1972	A
35	YA	1980	G
35	YA	1982	C
35	YA	1992	G
35	YA	1993	U
35	YA	2020	A
35	YA	2021	C
35	YA	2023	G
35	YA	2027	G
35	YA	2031	A
35	YA	2032	G
35	YA	2033	A
35	YA	2043	C
35	YA	2055	C
35	YA	2056	G
35	YA	2059	A
35	YA	2060	A
35	YA	2061	G
35	YA	2062	A
35	YA	2069	G
35	YA	2111	C
35	YA	2112	G
35	YA	2113	U
35	YA	2114	A
35	YA	2116	G
35	YA	2117	A
35	YA	2120	G
35	YA	2123	G
35	YA	2124	G
35	YA	2126	A
35	YA	2127	G
35	YA	2128	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	YA	2130	U
35	YA	2131	G
35	YA	2132	U
35	YA	2134	A
35	YA	2145	C
35	YA	2146	C
35	YA	2147	G
35	YA	2148	G
35	YA	2161	C
35	YA	2167	U
35	YA	2168	G
35	YA	2169	A
35	YA	2170	A
35	YA	2171	A
35	YA	2173	A
35	YA	2186	G
35	YA	2190	G
35	YA	2191	G
35	YA	2192	G
35	YA	2198	A
35	YA	2210	G
35	YA	2211	G
35	YA	2212	A
35	YA	2213	U
35	YA	2215	G
35	YA	2225	A
35	YA	2226	C
35	YA	2238	G
35	YA	2239	G
35	YA	2266	A
35	YA	2275	C
35	YA	2279	G
35	YA	2283	C
35	YA	2305	A
35	YA	2306	C
35	YA	2307	G
35	YA	2308	G
35	YA	2309	A
35	YA	2310	A
35	YA	2312	U
35	YA	2320	A
35	YA	2321	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	YA	2325	G
35	YA	2334	G
35	YA	2335	A
35	YA	2336	A
35	YA	2347	C
35	YA	2350	C
35	YA	2354	G
35	YA	2382	G
35	YA	2383	G
35	YA	2385	C
35	YA	2392	A
35	YA	2402	C
35	YA	2406	U
35	YA	2410	G
35	YA	2414	G
35	YA	2423	U
35	YA	2425	A
35	YA	2429	G
35	YA	2430	A
35	YA	2435	A
35	YA	2439	A
35	YA	2441	C
35	YA	2445	G
35	YA	2448	A
35	YA	2450	A
35	YA	2460	U
35	YA	2465	C
35	YA	2468	G
35	YA	2469	A
35	YA	2470	G
35	YA	2472	G
35	YA	2474	C
35	YA	2475	C
35	YA	2476	A
35	YA	2482	G
35	YA	2491	U
35	YA	2494	G
35	YA	2498	C
35	YA	2502	G
35	YA	2505	G
35	YA	2518	A
35	YA	2529	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	YA	2535	G
35	YA	2543	G
35	YA	2554	U
35	YA	2562	U
35	YA	2566	A
35	YA	2567	G
35	YA	2569	G
35	YA	2572	A
35	YA	2582	G
35	YA	2586	C
35	YA	2602	A
35	YA	2609	U
35	YA	2611	U
35	YA	2612	C
35	YA	2629	A
35	YA	2630	G
35	YA	2645	G
35	YA	2646	C
35	YA	2654	A
35	YA	2655	G
35	YA	2665	A
35	YA	2673	G
35	YA	2682	U
35	YA	2689	U
35	YA	2690	C
35	YA	2691	C
35	YA	2702	U
35	YA	2703	C
35	YA	2712	U
35	YA	2713	A
35	YA	2714	G
35	YA	2725	A
35	YA	2726	U
35	YA	2733	A
35	YA	2744	G
35	YA	2748	A
35	YA	2750	A
35	YA	2751	G
35	YA	2752	C
35	YA	2754	U
35	YA	2762	G
35	YA	2765	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	YA	2766	G
35	YA	2777	G
35	YA	2778	A
35	YA	2779	U
35	YA	2780	G
35	YA	2789	C
35	YA	2790	A
35	YA	2791	C
35	YA	2792	G
35	YA	2797	U
35	YA	2799	A
35	YA	2807	G
35	YA	2818	G
35	YA	2820	A
35	YA	2821	A
35	YA	2827	C
35	YA	2830	G
35	YA	2833	G
35	YA	2834	G
35	YA	2835	A
35	YA	2848	G
35	YA	2849	U
35	YA	2860	A
35	YA	2872	G
35	YA	2873	A
35	YA	2876	G
35	YA	2877	G
35	YA	2879	C
35	YA	2880	C
35	YA	2892	A
35	YA	2893	G
35	YA	2896	C
35	YA	2897	U
36	YB	8	U
36	YB	9	G
36	YB	13	A
36	YB	15	A
36	YB	25	A
36	YB	41	U
36	YB	42	C
36	YB	44	G
36	YB	45	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	YB	52	A
36	YB	53	A
36	YB	67	G
36	YB	73	A
36	YB	81	G
36	YB	88	C
36	YB	92	G
36	YB	109	G
36	YB	117	G
36	YB	118	G
36	YB	119	A

All (211) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	QA	5	U
1	QA	31	G
1	QA	60	A
1	QA	115	G
1	QA	181	G
1	QA	190	G
1	QA	197	A
1	QA	201	C
1	QA	208	U
1	QA	243	A
1	QA	250	A
1	QA	279	A
1	QA	281	G
1	QA	315	A
1	QA	328	C
1	QA	410	G
1	QA	428	G
1	QA	484	G
1	QA	485	G
1	QA	518	C
1	QA	547	A
1	QA	560	U
1	QA	595	G
1	QA	687	A
1	QA	717	C
1	QA	748	C
1	QA	792	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	QA	812	C
1	QA	913	A
1	QA	960	U
1	QA	976	G
1	QA	992	U
1	QA	999	U
1	QA	1033	G
1	QA	1038	C
1	QA	1053	G
1	QA	1065	U
1	QA	1067	A
1	QA	1124	G
1	QA	1137	C
1	QA	1139	G
1	QA	1182	G
1	QA	1224	G
1	QA	1285	A
1	QA	1300	G
1	QA	1322	C
1	QA	1346	A
1	QA	1347	G
1	QA	1364	U
1	QA	1498	U
1	QA	1528	U
1	QA	1532	U
22	QV	1	C
22	QV	7	G
22	QV	17(A)	U
22	QV	60	U
22	QW	60	U
23	QX	9	G
23	QX	11	U
35	RA	49	A
35	RA	90	U
35	RA	119	A
35	RA	128	C
35	RA	227	A
35	RA	345	A
35	RA	372	G
35	RA	387	U
35	RA	404	C
35	RA	587	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	RA	603	A
35	RA	704	G
35	RA	752	A
35	RA	845	G
35	RA	856	C
35	RA	859	G
35	RA	877	U
35	RA	1022	G
35	RA	1085	A
35	RA	1171	G
35	RA	1204	A
35	RA	1286	A
35	RA	1300	U
35	RA	1311	G
35	RA	1379	A
35	RA	1427	A
35	RA	1451	C
35	RA	1558	A
35	RA	1559	G
35	RA	1694	C
35	RA	1819	A
35	RA	1900	A
35	RA	1930	G
35	RA	2092	U
35	RA	2144	U
35	RA	2191	G
35	RA	2211	G
35	RA	2311	A
35	RA	2346	A
35	RA	2439	A
35	RA	2447	G
35	RA	2481	G
35	RA	2610	C
35	RA	2689	U
35	RA	2725	A
35	RA	2776	A
35	RA	2848	G
35	RA	2849	U
35	RA	2859	G
36	RB	66	A
1	XA	5	U
1	XA	31	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	XA	60	A
1	XA	181	G
1	XA	197	A
1	XA	201	C
1	XA	243	A
1	XA	250	A
1	XA	279	A
1	XA	281	G
1	XA	315	A
1	XA	328	C
1	XA	410	G
1	XA	421	U
1	XA	428	G
1	XA	518	C
1	XA	547	A
1	XA	560	U
1	XA	595	G
1	XA	687	A
1	XA	703	G
1	XA	717	C
1	XA	733	A
1	XA	748	C
1	XA	792	A
1	XA	812	C
1	XA	818	G
1	XA	913	A
1	XA	960	U
1	XA	992	U
1	XA	1004	A
1	XA	1033	G
1	XA	1038	C
1	XA	1053	G
1	XA	1054	C
1	XA	1065	U
1	XA	1067	A
1	XA	1094	G
1	XA	1124	G
1	XA	1137	C
1	XA	1139	G
1	XA	1177	G
1	XA	1182	G
1	XA	1285	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	XA	1300	G
1	XA	1345	U
1	XA	1346	A
1	XA	1364	U
1	XA	1498	U
1	XA	1532	U
22	XV	7	G
22	XV	17(A)	U
22	XV	60	U
22	XW	60	U
23	XX	9	G
35	YA	74	A
35	YA	119	A
35	YA	345	A
35	YA	352	G
35	YA	372	G
35	YA	387	U
35	YA	587	C
35	YA	603	A
35	YA	692	C
35	YA	704	G
35	YA	726	G
35	YA	752	A
35	YA	856	C
35	YA	859	G
35	YA	877	U
35	YA	1022	G
35	YA	1085	A
35	YA	1171	G
35	YA	1379	A
35	YA	1427	A
35	YA	1451	C
35	YA	1558	A
35	YA	1559	G
35	YA	1653	G
35	YA	1694	C
35	YA	1819	A
35	YA	1900	A
35	YA	1992	G
35	YA	2032	G
35	YA	2144	U
35	YA	2166	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	YA	2191	G
35	YA	2211	G
35	YA	2311	A
35	YA	2320	A
35	YA	2335	A
35	YA	2422	A
35	YA	2447	G
35	YA	2468	G
35	YA	2481	G
35	YA	2610	C
35	YA	2689	U
35	YA	2725	A
35	YA	2776	A
35	YA	2848	G
35	YA	2859	G
36	YB	66	A

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

2 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	$\# Z > 2$
56	PPU	ZA	3	56,35	32,40,41	0.91	2 (6%)	33,57,60	1.51	6 (18%)
56	PPU	ZB	3	56,35	32,40,41	0.89	2 (6%)	33,57,60	1.44	5 (15%)

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
56	PPU	ZA	3	56,35	-	4/21/43/44	0/4/4/4
56	PPU	ZB	3	56,35	-	3/21/43/44	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	ZA	3	PPU	C5-C4	2.76	1.48	1.40
56	ZB	3	PPU	C5-C4	2.73	1.48	1.40
56	ZA	3	PPU	C6-N1	2.18	1.36	1.33
56	ZB	3	PPU	C6-N1	2.02	1.36	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	ZB	3	PPU	C4-C5-N7	-3.49	105.76	109.40
56	ZA	3	PPU	C4-C5-N7	-3.46	105.79	109.40
56	ZA	3	PPU	C3'-N3'-C	-3.34	118.18	123.21
56	ZA	3	PPU	N3-C2-N1	-3.25	123.60	128.68
56	ZB	3	PPU	N3-C2-N1	-3.24	123.61	128.68
56	ZA	3	PPU	N1-C6-N6	3.17	120.39	117.06
56	ZB	3	PPU	C10-N6-C6	-3.14	110.02	119.51
56	ZB	3	PPU	C10-N6-C9	-3.11	106.11	116.12
56	ZA	3	PPU	C10-N6-C6	-3.09	110.15	119.51
56	ZA	3	PPU	C10-N6-C9	-2.80	107.10	116.12
56	ZB	3	PPU	N1-C6-N6	2.78	119.98	117.06

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	ZB	3	PPU	CE1-CZ-OC-CM
56	ZB	3	PPU	CE2-CZ-OC-CM
56	ZA	3	PPU	CE2-CZ-OC-CM
56	ZA	3	PPU	CE1-CZ-OC-CM
56	ZA	3	PPU	C5-C6-N6-C9
56	ZB	3	PPU	C5-C6-N6-C9
56	ZA	3	PPU	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	ZB	3	PPU	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 883 ligands modelled in this entry, 879 are monoatomic - leaving 4 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
60	A3P	QX	101	23	23,28,29	5.17	7 (30%)	23,42,45	1.46	3 (13%)
58	SF4	XD	301	4	0,12,12	0.00	-	-		
58	SF4	QD	301	4	0,12,12	0.00	-	-		
60	A3P	XX	101	23	23,28,29	5.26	7 (30%)	23,42,45	1.59	4 (17%)

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
60	A3P	QX	101	23	-	2/8/30/31	0/3/3/3
58	SF4	XD	301	4	-	-	0/6/5/5
58	SF4	QD	301	4	-	-	0/6/5/5
60	A3P	XX	101	23	-	0/8/30/31	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	XX	101	A3P	O4'-C1'	18.58	1.67	1.41
60	QX	101	A3P	O4'-C1'	18.11	1.66	1.41
60	XX	101	A3P	C2'-C1'	-13.95	1.32	1.53
60	QX	101	A3P	C2'-C1'	-13.75	1.32	1.53
60	QX	101	A3P	O4'-C4'	-6.31	1.30	1.45
60	XX	101	A3P	O4'-C4'	-6.11	1.31	1.45
60	XX	101	A3P	P1-O3'	4.11	1.67	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	QX	101	A3P	P1-O3'	3.89	1.66	1.59
60	QX	101	A3P	O3'-C3'	-3.53	1.31	1.44
60	XX	101	A3P	O3'-C3'	-3.39	1.31	1.44
60	QX	101	A3P	C6-N6	3.23	1.45	1.34
60	XX	101	A3P	C6-N6	3.17	1.45	1.34
60	XX	101	A3P	C3'-C4'	2.13	1.58	1.52
60	QX	101	A3P	C2'-C3'	2.09	1.57	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	XX	101	A3P	N3-C2-N1	-4.92	120.99	128.68
60	QX	101	A3P	N3-C2-N1	-4.77	121.22	128.68
60	XX	101	A3P	C3'-C2'-C1'	3.31	107.22	99.89
60	QX	101	A3P	C4-C5-N7	-3.24	106.02	109.40
60	XX	101	A3P	C4-C5-N7	-2.87	106.40	109.40
60	QX	101	A3P	C3'-C2'-C1'	2.86	106.23	99.89
60	XX	101	A3P	C2'-C3'-C4'	2.44	107.54	103.22

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	QX	101	A3P	C3'-C4'-C5'-O5'
60	QX	101	A3P	O4'-C4'-C5'-O5'

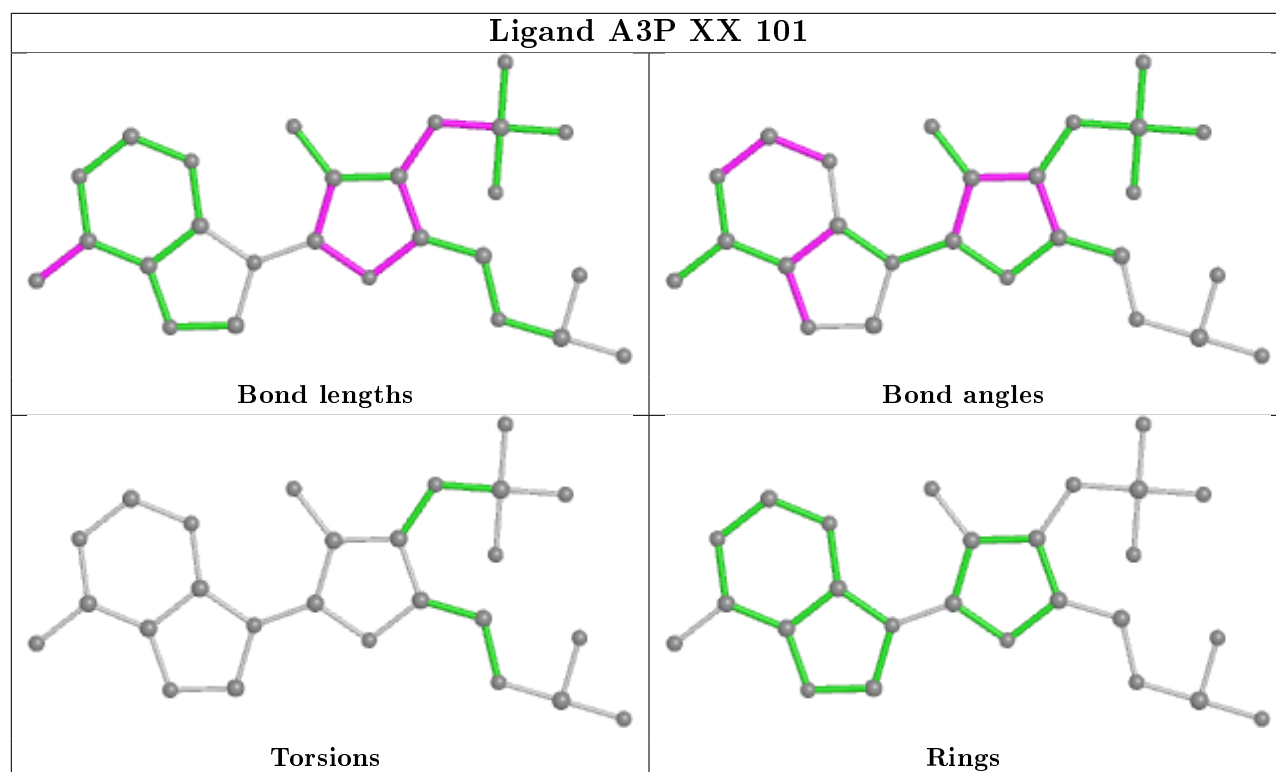
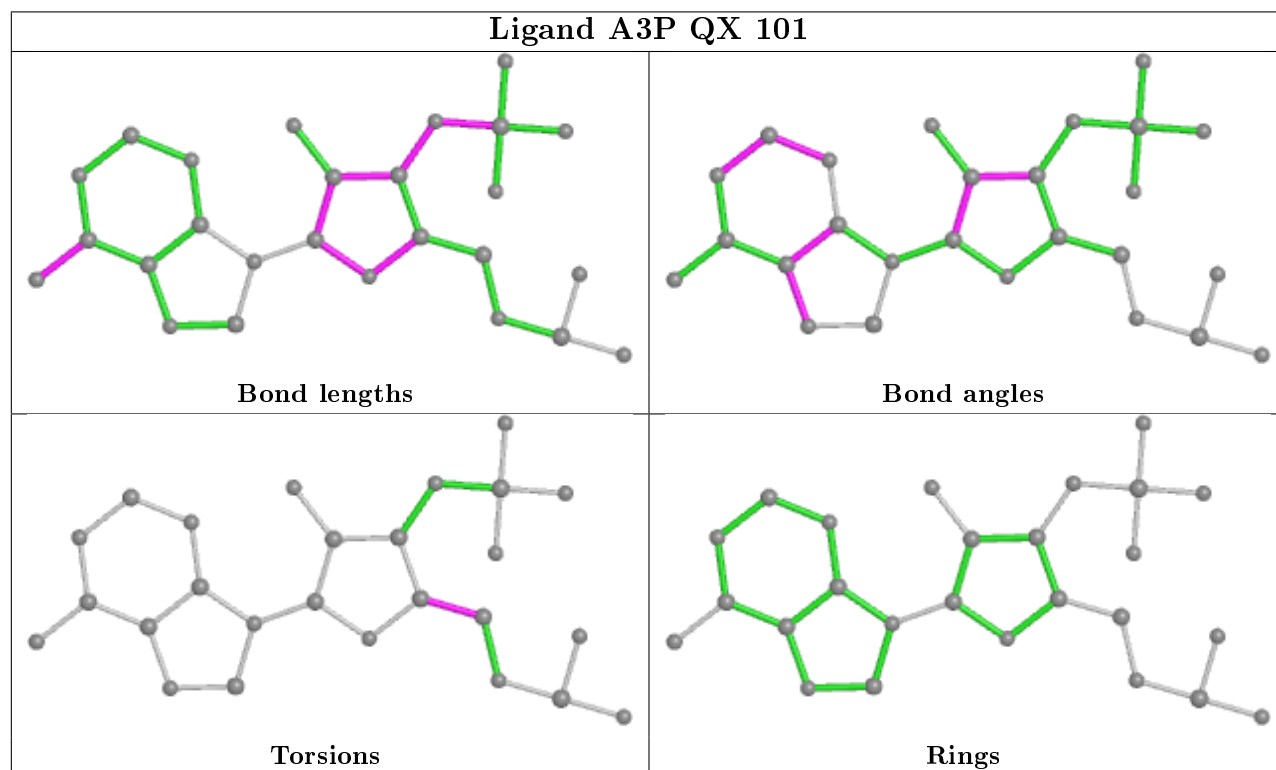
There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	QX	101	A3P	5	0
60	XX	101	A3P	2	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](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.