



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 16, 2024 – 09:22 AM EST

PDB ID : 6NWY
Title : Modified tRNA(Pro) bound to Thermus thermophilus 70S (near-cognate)
Authors : Hoffer, E.D.; Subaramanian, S.; Hong, S.; Maehigashi, T.; Dunham, C.M.
Deposited on : 2019-02-07
Resolution : 3.50 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.21
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.004 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

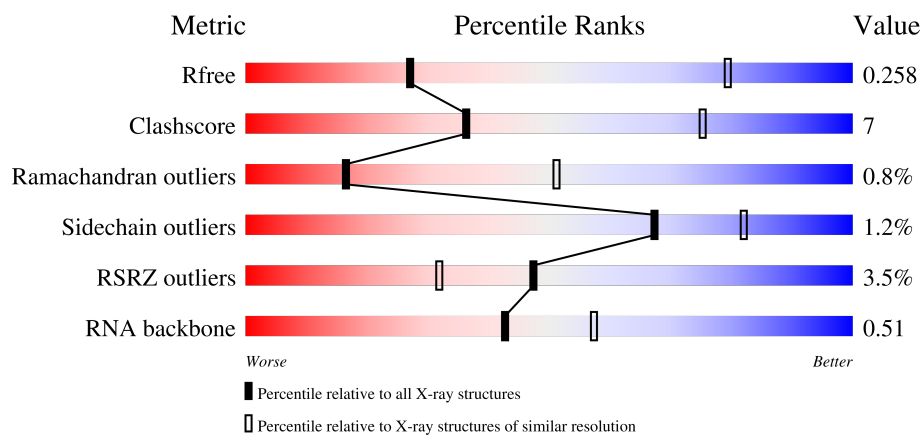
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1094 (3.56-3.44)
Clashscore	180529	1045 (3.54-3.46)
Ramachandran outliers	177936	1032 (3.54-3.46)
Sidechain outliers	177891	1033 (3.54-3.46)
RSRZ outliers	164620	1093 (3.56-3.44)
RNA backbone	3690	1089 (4.00-3.00)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	QA	1521	<div> <div>4%</div> <div>52% 38% 9% ..</div> </div>
1	XA	1521	<div> <div>%</div> <div>52% 38% 9% .</div> </div>
2	QB	256	<div> <div>2%</div> <div>66% 26% 8%</div> </div>
2	XB	256	<div> <div></div> <div>68% 24% 8%</div> </div>




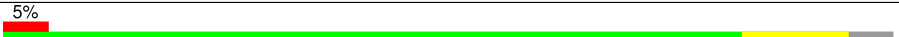
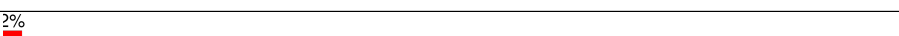
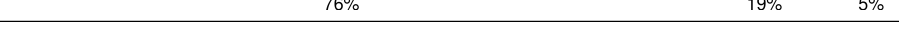
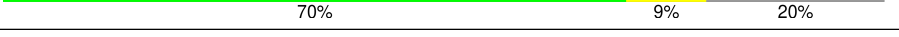




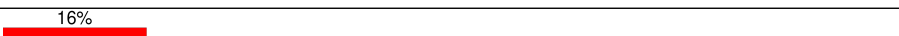

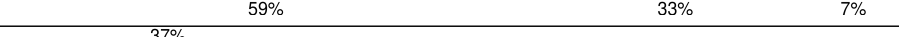





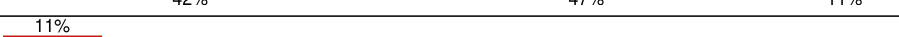





Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	QC	239	
3	XC	239	
4	QD	209	
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	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	XO	89	
16	QP	88	
16	XP	88	
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	XV	77	
23	QX	19	
23	XX	19	
24	R0	85	
24	Y0	85	
25	R1	98	
25	Y1	98	
26	R2	72	
26	Y2	72	
27	R3	60	
27	Y3	60	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	R4	71	
28	Y4	71	
29	R5	60	
29	Y5	60	
30	R6	54	
30	Y6	54	
31	R7	49	
31	Y7	49	
32	R8	65	
32	Y8	65	
33	R9	37	
33	Y9	37	
34	RA	2915	
34	YA	2915	
35	RB	122	
35	YB	122	
36	RD	276	
36	YD	276	
37	RE	206	
37	YE	206	
38	RF	210	
38	YF	210	
39	RG	182	
39	YG	182	
40	RH	180	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
40	YH	180	
41	RI	148	
41	YI	148	
42	RN	140	
42	YN	140	
43	RO	122	
43	YO	122	
44	RP	150	
44	YP	150	
45	RQ	141	
45	YQ	141	
46	RR	118	
46	YR	118	
47	RS	112	
47	YS	112	
48	RT	146	
48	YT	146	
49	RU	118	
49	YU	118	
50	RV	101	
50	YV	101	
51	RW	113	
51	YW	113	
52	RX	96	
52	YX	96	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	RY	110	
53	YY	110	
54	RZ	206	
54	YZ	206	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	MG	YA	3015	-	-	-	X
55	MG	YA	3245	-	-	-	X
56	SF4	QD	301	-	-	X	-

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 292039 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	1511	Total	C	N	O	P	0	0	0
			32469	14453	6011	10495	1510			
1	XA	1515	Total	C	N	O	P	0	0	0
			32551	14490	6022	10525	1514			

- 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	114	Total	C	N	O	S	0	0	0
			914	565	189	158	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	84	Total	C	N	O	S	0	0	0
			674	430	126	116	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 E-site tRNA-Pro.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	QV	77	Total	C	N	O	P	0	0	0
			1647	734	295	541	77			
22	XV	77	Total	C	N	O	P	0	0	0
			1647	734	295	541	77			

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QX	19	Total	C	N	O	P	0	0	0
			409	184	81	126	18			
23	XX	19	Total	C	N	O	P	0	0	0
			409	184	81	126	18			

- Molecule 24 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	R0	81	Total	C	N	O	S	0	0	0
			643	398	137	107	1			
24	Y0	82	Total	C	N	O	S	0	0	0
			648	401	138	108	1			

- Molecule 25 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	R1	95	Total	C	N	O	S	0	0	0
			746	469	148	128	1			
25	Y1	93	Total	C	N	O	S	0	0	0
			729	457	145	126	1			

- Molecule 26 is a protein called 50S ribosomal protein L29.

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Y2	68	Total	C	N	O	S	0	0	0
			575	355	117	102	1			

- Molecule 27 is a protein called 50S ribosomal protein L30.

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

- Molecule 28 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	R4	45	Total	C	N	O	S	0	0	0
			348	224	57	62	5			
28	Y4	46	Total	C	N	O	S	0	0	0
			357	229	59	64	5			

- Molecule 29 is a protein called 50S ribosomal protein L32.

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

- Molecule 30 is a protein called 50S ribosomal protein L33.

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

- Molecule 31 is a protein called 50S ribosomal protein L34.

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

- Molecule 32 is a protein called 50S ribosomal protein L35.

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

- Molecule 33 is a protein called 50S ribosomal protein L36.

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

- Molecule 34 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	RA	2882	Total	C	N	O	P	0	0	0
			62070	27627	11611	19951	2881			
34	YA	2883	Total	C	N	O	P	0	0	0
			62091	27636	11613	19960	2882			

- Molecule 35 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	RB	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			
35	YB	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

- Molecule 36 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	RD	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			
36	YD	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			

- Molecule 37 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	RE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			
37	YE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			

- Molecule 38 is a protein called 50S ribosomal protein L4.

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

- Molecule 39 is a protein called 50S ribosomal protein L5.

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

- Molecule 40 is a protein called 50S ribosomal protein L6.

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

- Molecule 41 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	RI	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			
41	YI	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

- Molecule 42 is a protein called 50S ribosomal protein L13.

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

Continued on next page...

Continued from previous page...

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

- Molecule 43 is a protein called 50S ribosomal protein L14.

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

- Molecule 44 is a protein called 50S ribosomal protein L15.

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

- Molecule 45 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	RQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
45	YQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 46 is a protein called 50S ribosomal protein L17.

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

- Molecule 47 is a protein called 50S ribosomal protein L18.

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

- Molecule 48 is a protein called 50S ribosomal protein L19.

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

- Molecule 49 is a protein called 50S ribosomal protein L20.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L22.

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

- Molecule 52 is a protein called 50S ribosomal protein L23.

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

- Molecule 53 is a protein called 50S ribosomal protein L24.

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

- Molecule 54 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	RZ	183	Total	C	N	O	S	0	0	0
			1461	933	260	265	3			
54	YZ	193	Total	C	N	O	S	0	0	0
			1529	973	270	283	3			

- Molecule 55 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	QA	87	Total	Mg	0	0
			87	87		
55	QF	1	Total	Mg	0	0
			1	1		
55	QH	2	Total	Mg	0	0
			2	2		
55	QL	1	Total	Mg	0	0
			1	1		
55	R0	2	Total	Mg	0	0
			2	2		
55	R1	1	Total	Mg	0	0
			1	1		
55	R3	1	Total	Mg	0	0
			1	1		
55	R8	1	Total	Mg	0	0
			1	1		
55	RA	429	Total	Mg	0	0
			429	429		
55	RB	11	Total	Mg	0	0
			11	11		
55	RD	1	Total	Mg	0	0
			1	1		
55	RE	4	Total	Mg	0	0
			4	4		
55	RF	2	Total	Mg	0	0
			2	2		
55	RN	1	Total	Mg	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
55	RO	1	Total 1	Mg 1	0	0
55	RP	1	Total 1	Mg 1	0	0
55	RQ	1	Total 1	Mg 1	0	0
55	XA	89	Total 89	Mg 89	0	0
55	XE	1	Total 1	Mg 1	0	0
55	Y1	1	Total 1	Mg 1	0	0
55	Y2	1	Total 1	Mg 1	0	0
55	Y5	1	Total 1	Mg 1	0	0
55	Y7	1	Total 1	Mg 1	0	0
55	Y8	1	Total 1	Mg 1	0	0
55	YA	439	Total 439	Mg 439	0	0
55	YB	8	Total 8	Mg 8	0	0
55	YD	1	Total 1	Mg 1	0	0
55	YE	2	Total 2	Mg 2	0	0
55	YF	1	Total 1	Mg 1	0	0
55	YQ	1	Total 1	Mg 1	0	0
55	YR	2	Total 2	Mg 2	0	0
55	YU	1	Total 1	Mg 1	0	0
55	YX	1	Total 1	Mg 1	0	0

- Molecule 56 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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

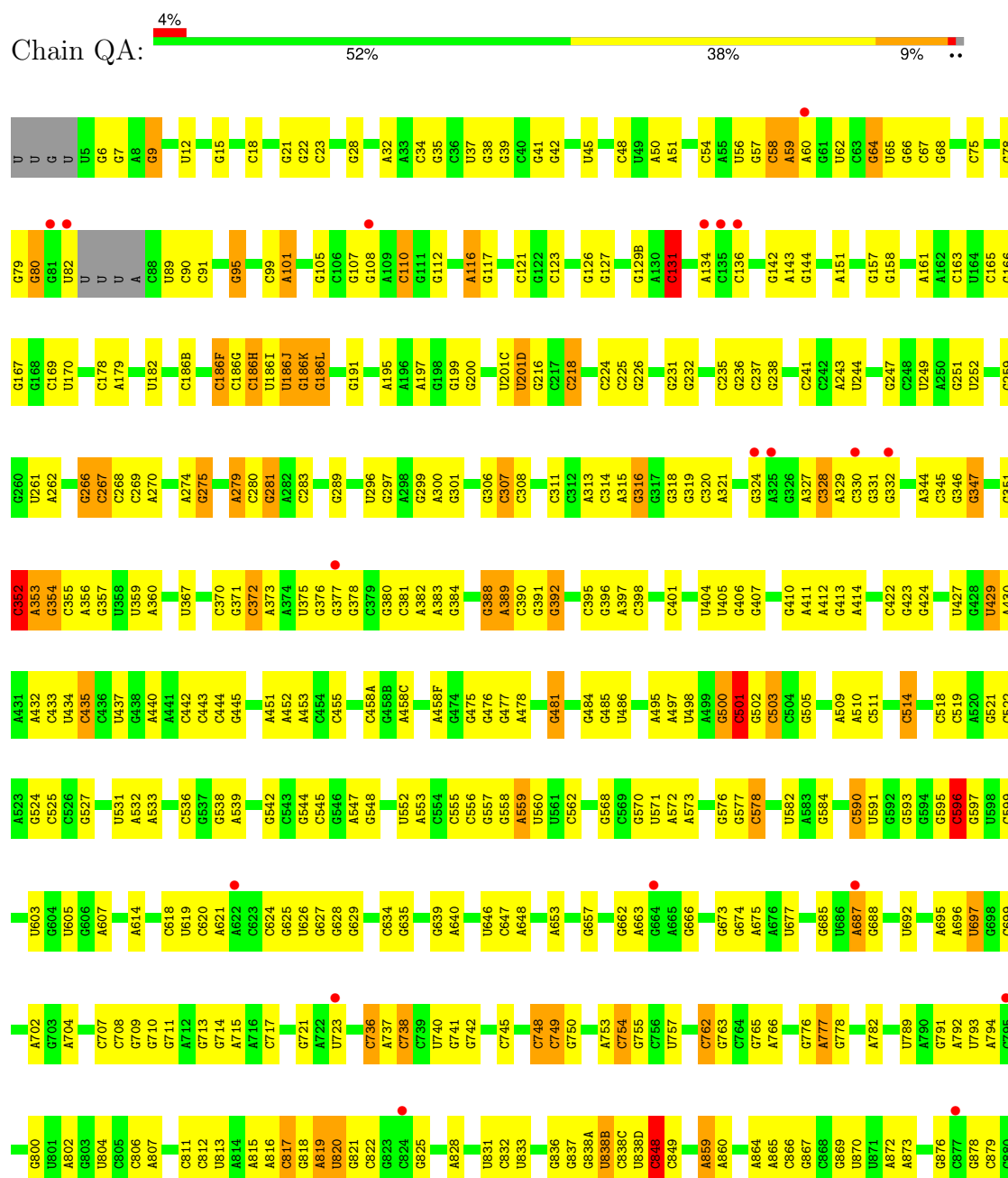
- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

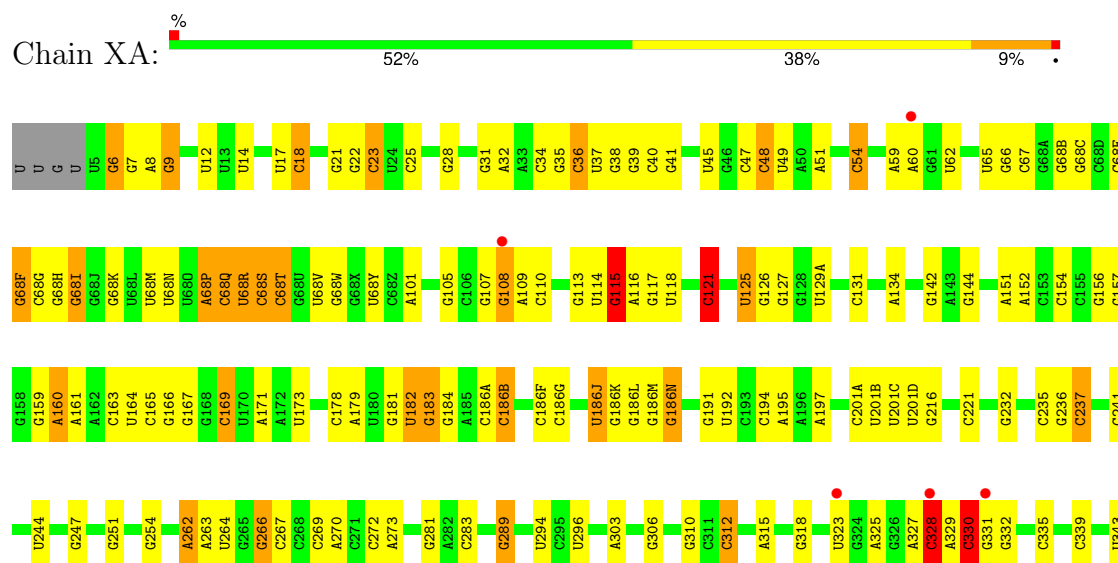
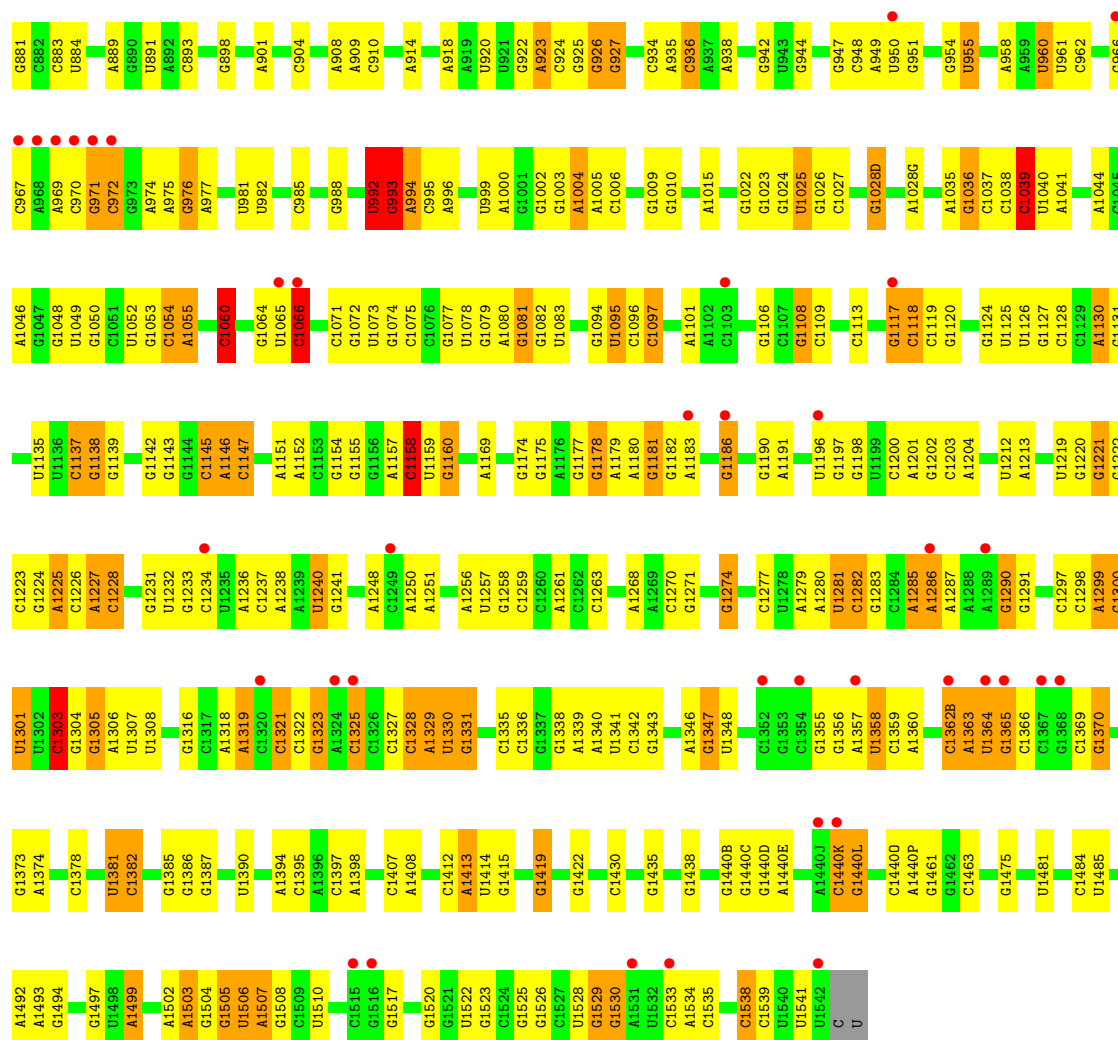
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QN	1	Total	Zn	0	0
			1	1		
57	R5	1	Total	Zn	0	0
			1	1		
57	R6	1	Total	Zn	0	0
			1	1		
57	R9	1	Total	Zn	0	0
			1	1		
57	RY	1	Total	Zn	0	0
			1	1		
57	XN	1	Total	Zn	0	0
			1	1		
57	Y5	1	Total	Zn	0	0
			1	1		
57	Y6	1	Total	Zn	0	0
			1	1		
57	Y9	1	Total	Zn	0	0
			1	1		
57	YY	1	Total	Zn	0	0
			1	1		

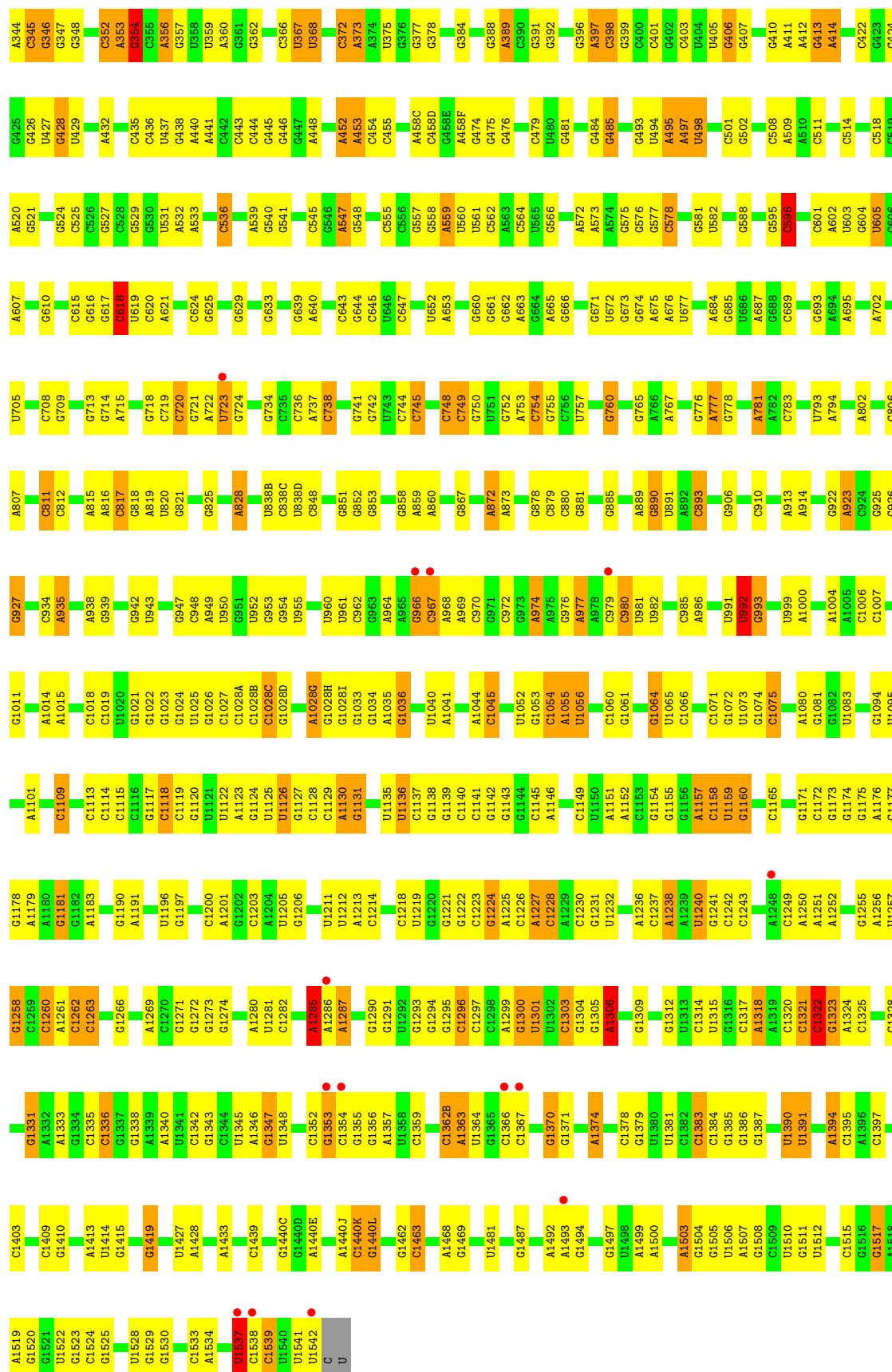
3 Residue-property plots

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

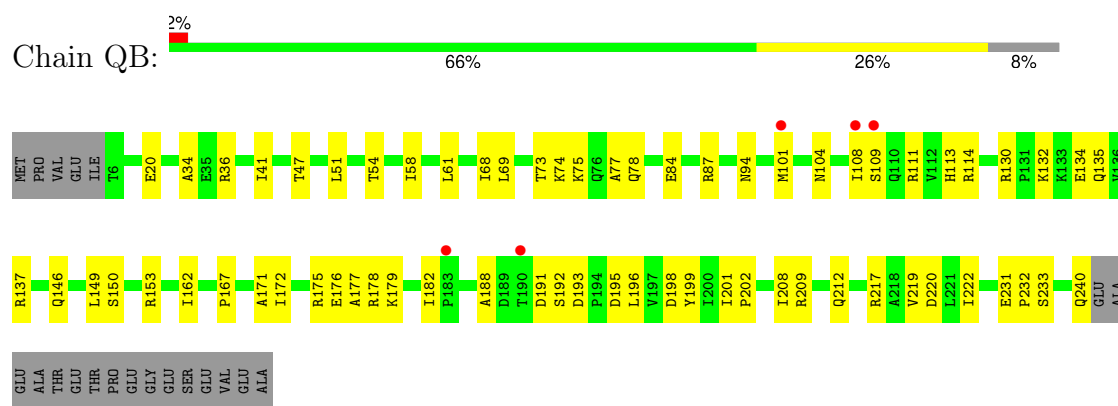
• Molecule 1: 16S rRNA



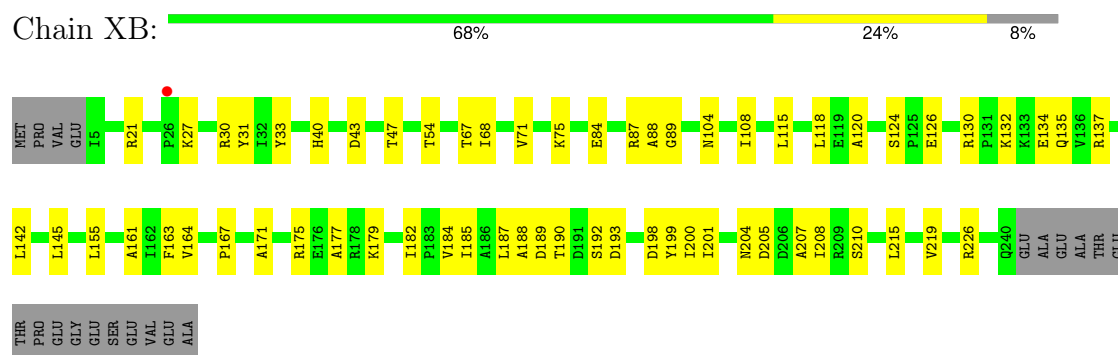




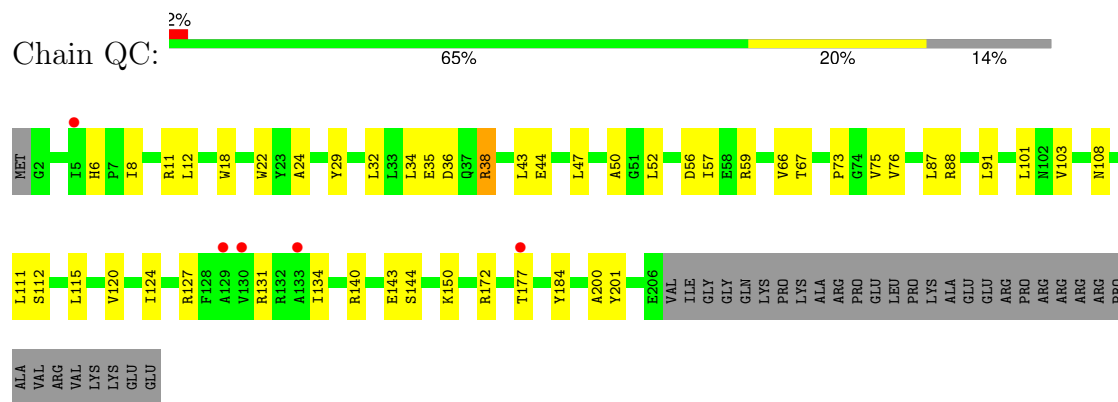
• Molecule 2: 30S ribosomal protein S2



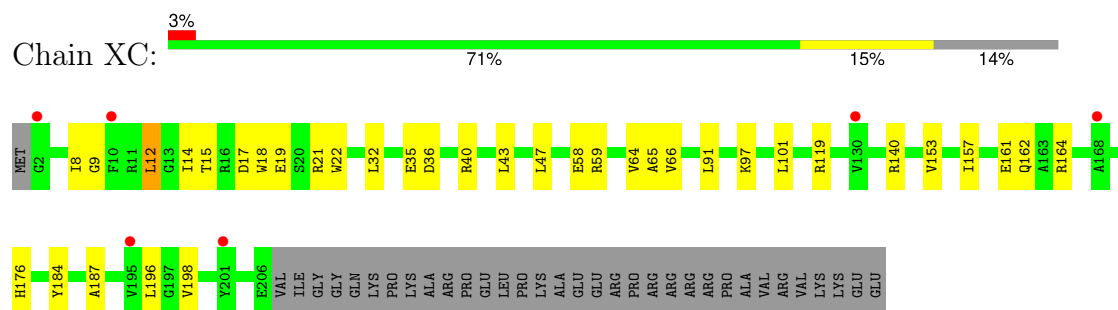
- Molecule 2: 30S ribosomal protein S2



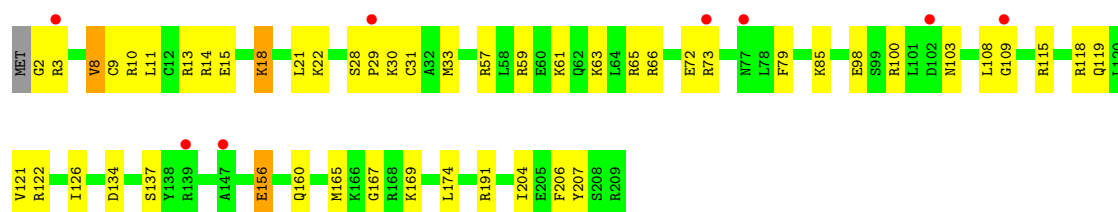
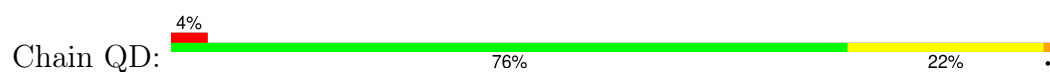
- Molecule 3: 30S ribosomal protein S3



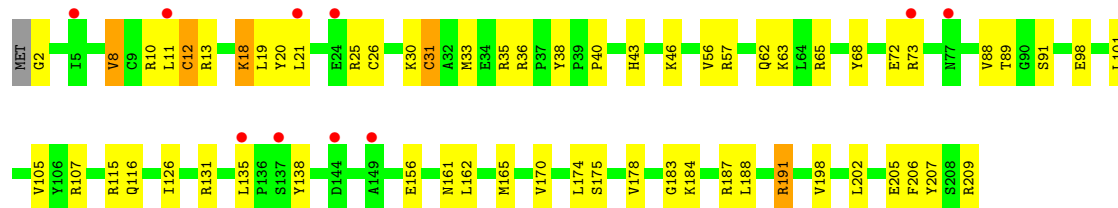
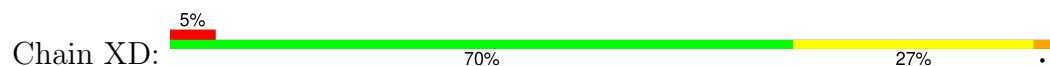
- Molecule 3: 30S ribosomal protein S3



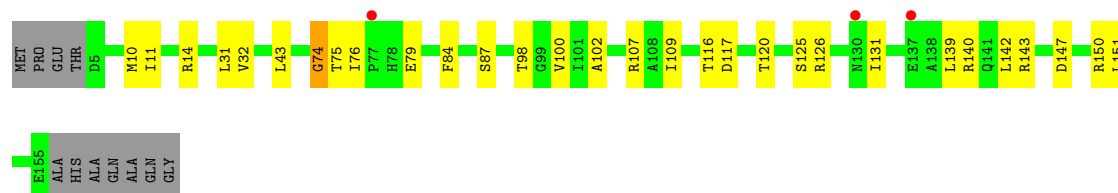
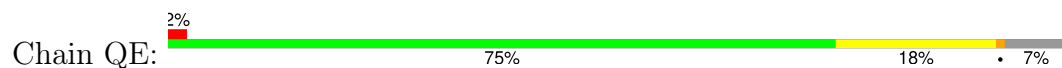
- Molecule 4: 30S ribosomal protein S4



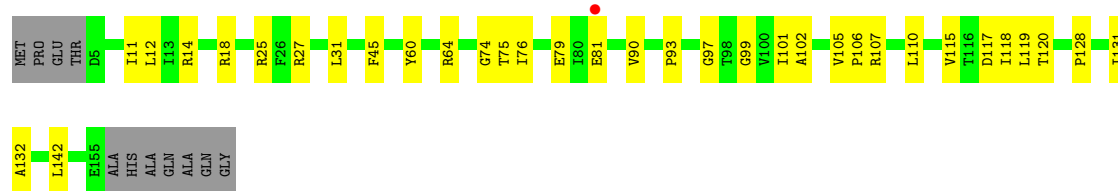
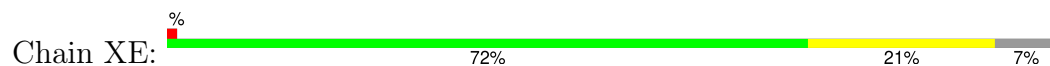
• Molecule 4: 30S ribosomal protein S4



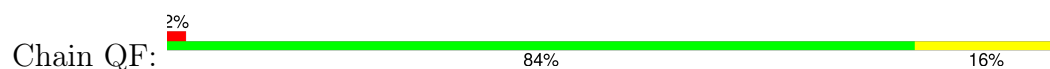
• Molecule 5: 30S ribosomal protein S5




• Molecule 5: 30S ribosomal protein S5



• Molecule 6: 30S ribosomal protein S6




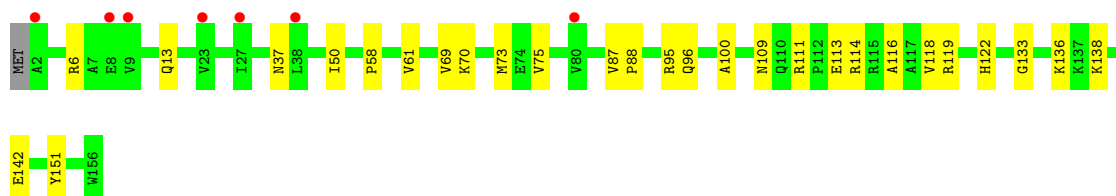
• Molecule 6: 30S ribosomal protein S6

Chain XF:  82% 18%




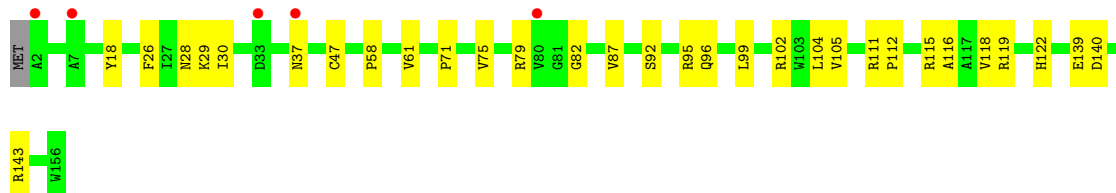
- Molecule 7: 30S ribosomal protein S7

Chain QG:  4% 81% 18%




- Molecule 7: 30S ribosomal protein S7

Chain XG:  3% 79% 20%




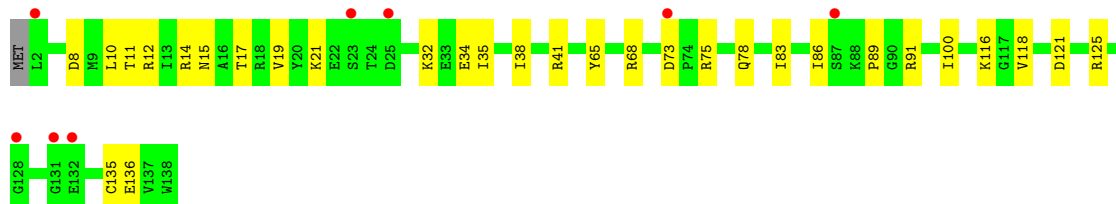
- Molecule 8: 30S ribosomal protein S8

Chain QH:  6% 80% 20%




- Molecule 8: 30S ribosomal protein S8

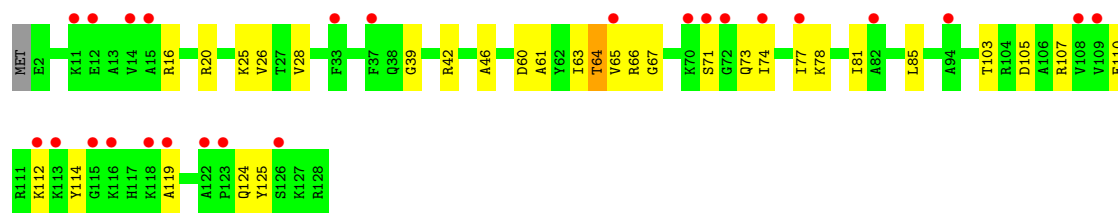
Chain XH:  6% 78% 22%



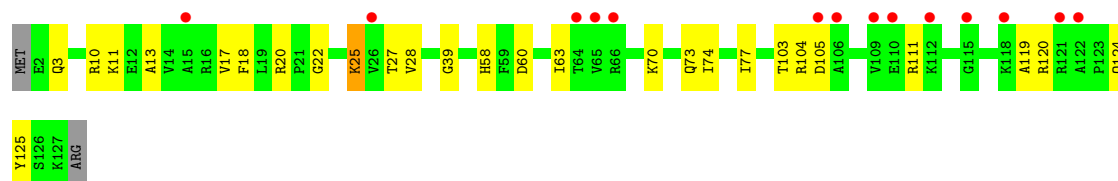
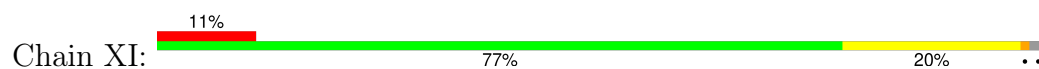
- Molecule 9: 30S ribosomal protein S9

Chain QI:  20% 75% 23%

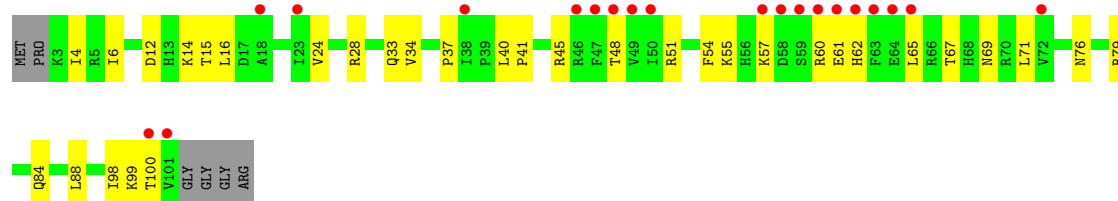




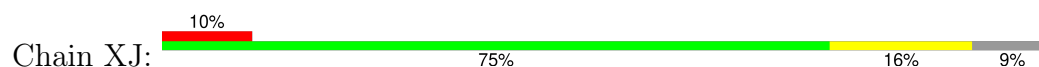
• Molecule 9: 30S ribosomal protein S9



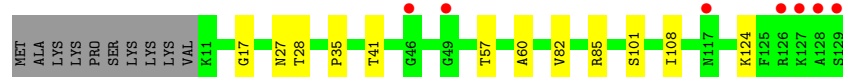
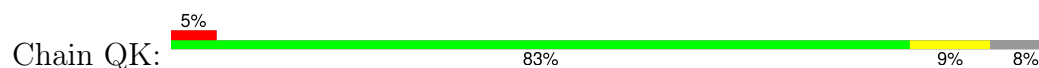
• Molecule 10: 30S ribosomal protein S10



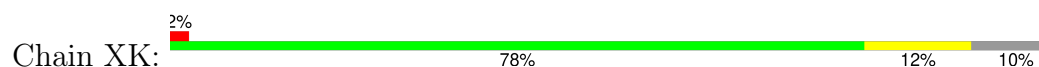
• Molecule 10: 30S ribosomal protein S10



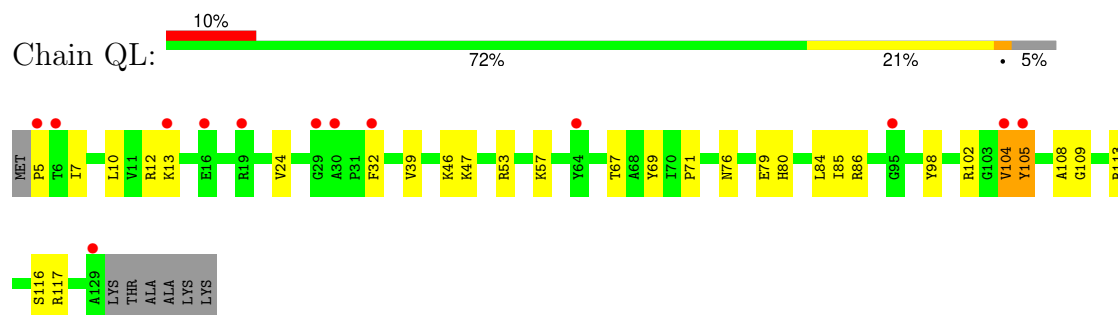
• Molecule 11: 30S ribosomal protein S11



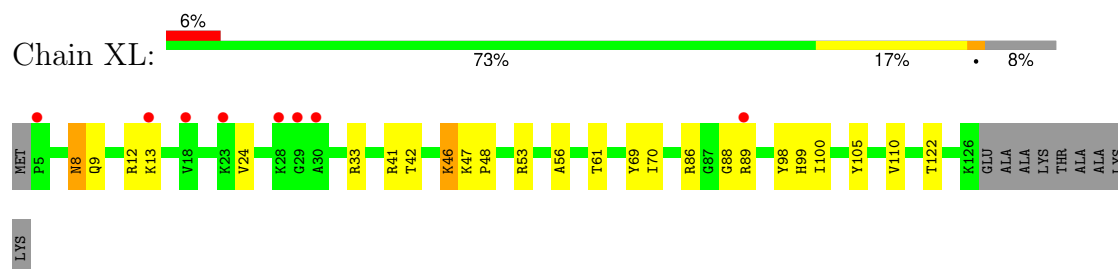
• Molecule 11: 30S ribosomal protein S11



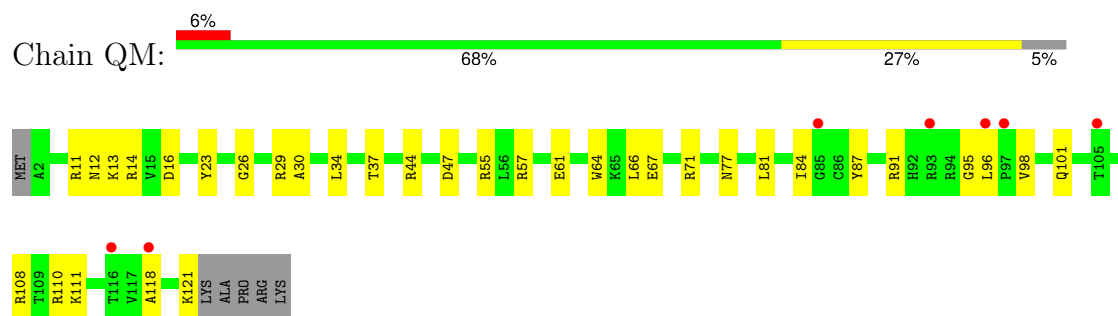
- Molecule 12: 30S ribosomal protein S12



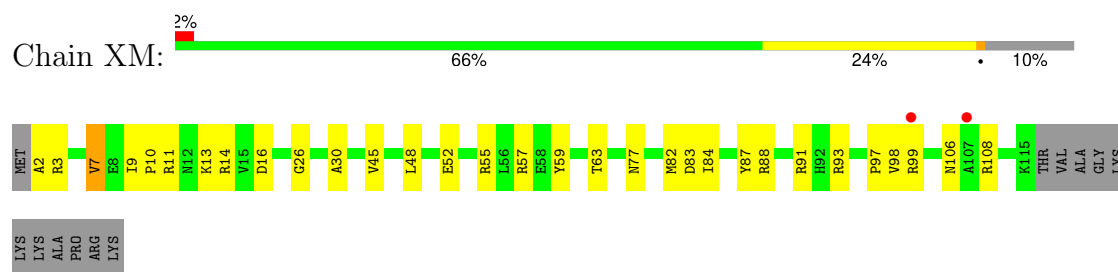
- Molecule 12: 30S ribosomal protein S12



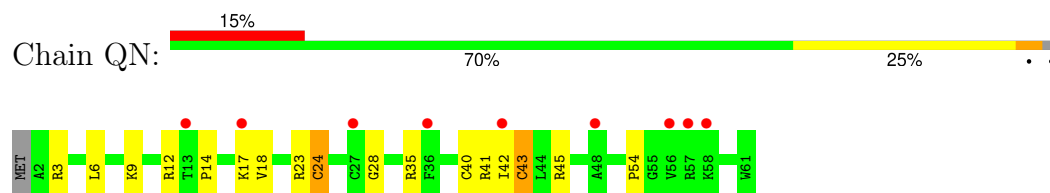
- Molecule 13: 30S ribosomal protein S13



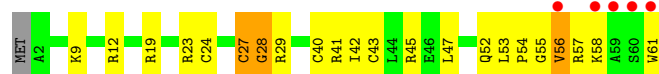
- Molecule 13: 30S ribosomal protein S13



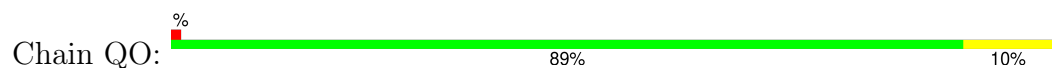
- Molecule 14: 30S ribosomal protein S14 type Z



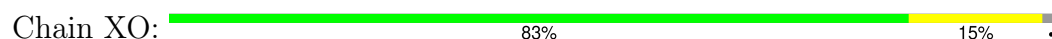
- Molecule 14: 30S ribosomal protein S14 type Z



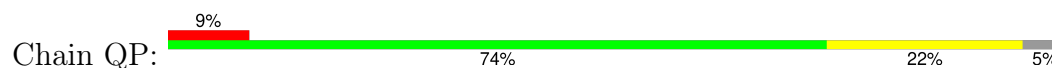
- Molecule 15: 30S ribosomal protein S15



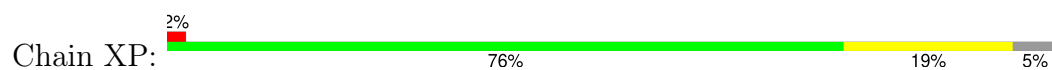
- Molecule 15: 30S ribosomal protein S15



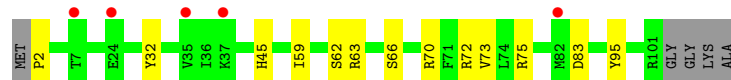
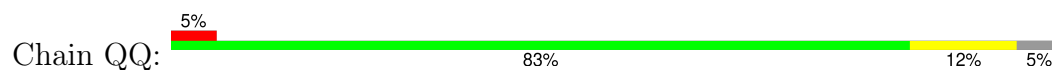
- Molecule 16: 30S ribosomal protein S16



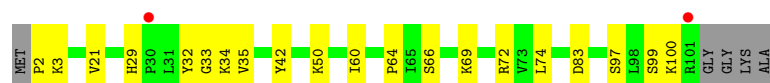
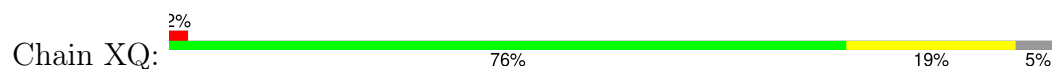
- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17

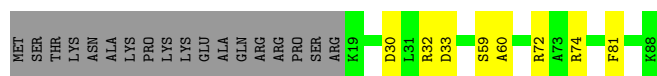


- Molecule 17: 30S ribosomal protein S17



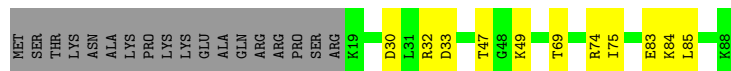
- Molecule 18: 30S ribosomal protein S18

Chain QR:  70% 9% 20%




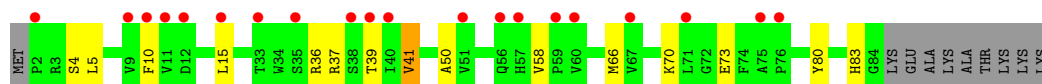
- Molecule 18: 30S ribosomal protein S18

Chain XR:  67% 13% 20%



- Molecule 19: 30S ribosomal protein S19

Chain QS:  22% 73% 15% 11%



- Molecule 19: 30S ribosomal protein S19

Chain XS:  4% 68% 23% 10%



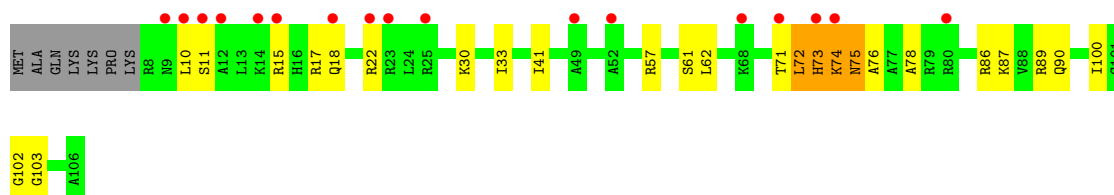
- Molecule 20: 30S ribosomal protein S20

Chain QT:  13% 70% 22% 7%

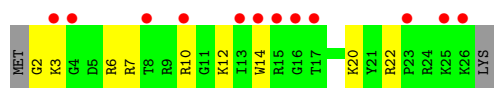


- Molecule 20: 30S ribosomal protein S20

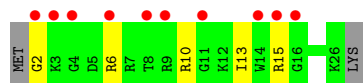
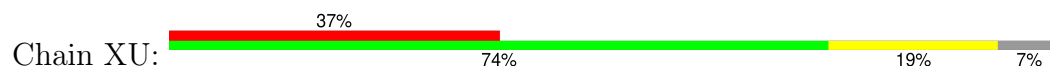
Chain XT:  16% 69% 21% 7%



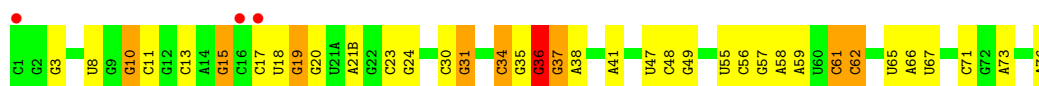
- Molecule 21: 30S ribosomal protein Thx



- Molecule 21: 30S ribosomal protein Thx



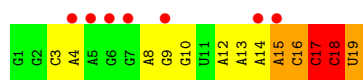
- Molecule 22: E-site tRNA-Pro



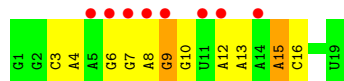
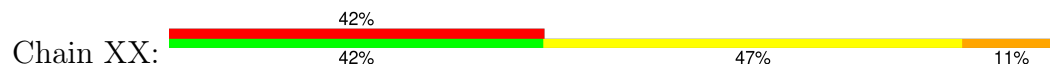
- Molecule 22: E-site tRNA-Pro



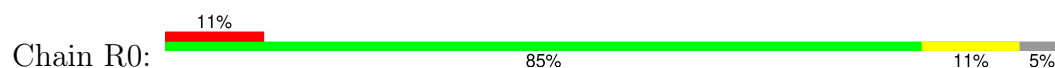
- Molecule 23: mRNA

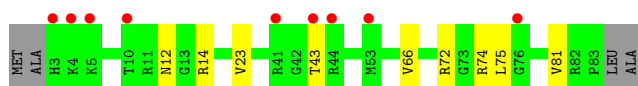


- Molecule 23: mRNA

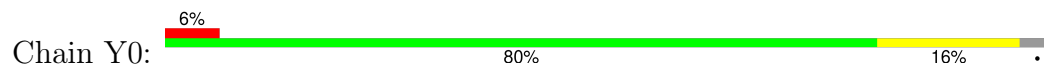


- Molecule 24: 50S ribosomal protein L27

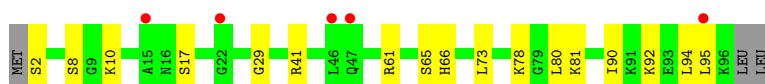
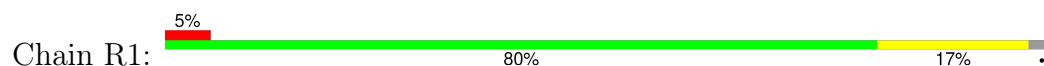




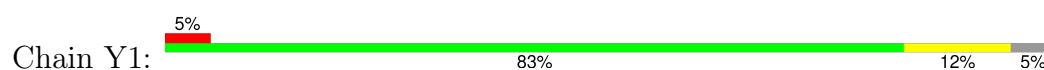
- Molecule 24: 50S ribosomal protein L27



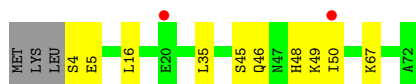
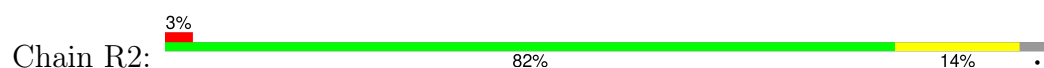
- Molecule 25: 50S ribosomal protein L28



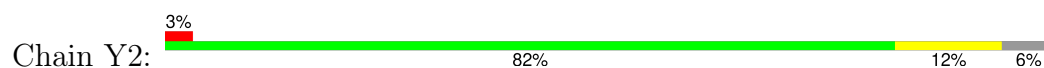
- Molecule 25: 50S ribosomal protein L28



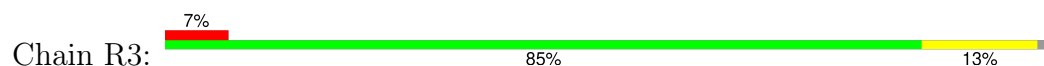
- Molecule 26: 50S ribosomal protein L29




- Molecule 26: 50S ribosomal protein L29

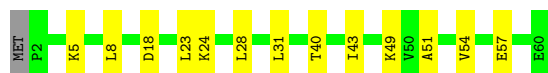


- Molecule 27: 50S ribosomal protein L30



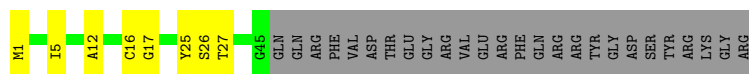
- Molecule 27: 50S ribosomal protein L30

Chain Y3:  77% 22% .



- Molecule 28: 50S ribosomal protein L31

Chain R4:  52% 11% 37%



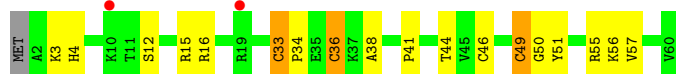
- Molecule 28: 50S ribosomal protein L31

Chain Y4:  39% 21% . . 35%



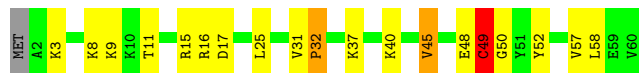
- Molecule 29: 50S ribosomal protein L32

Chain R5:  3% 68% 25% 5% .



- Molecule 29: 50S ribosomal protein L32

Chain Y5:  67% 27% . . .



- Molecule 30: 50S ribosomal protein L33

Chain R6:  72% 22% . . .



- Molecule 30: 50S ribosomal protein L33

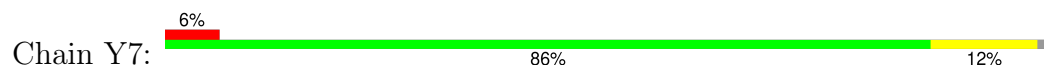
Chain Y6:  2% 65% 26% 6% . . .



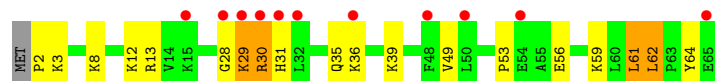
- Molecule 31: 50S ribosomal protein L34



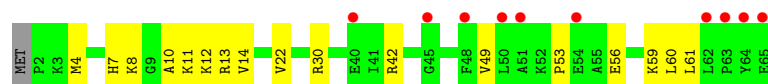
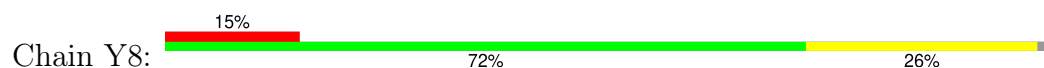
- Molecule 31: 50S ribosomal protein L34



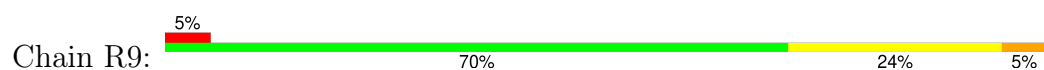
- Molecule 32: 50S ribosomal protein L35



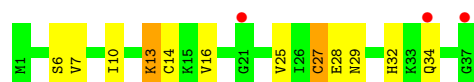
- Molecule 32: 50S ribosomal protein L35



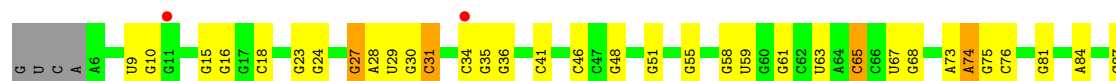
- Molecule 33: 50S ribosomal protein L36



- Molecule 33: 50S ribosomal protein L36

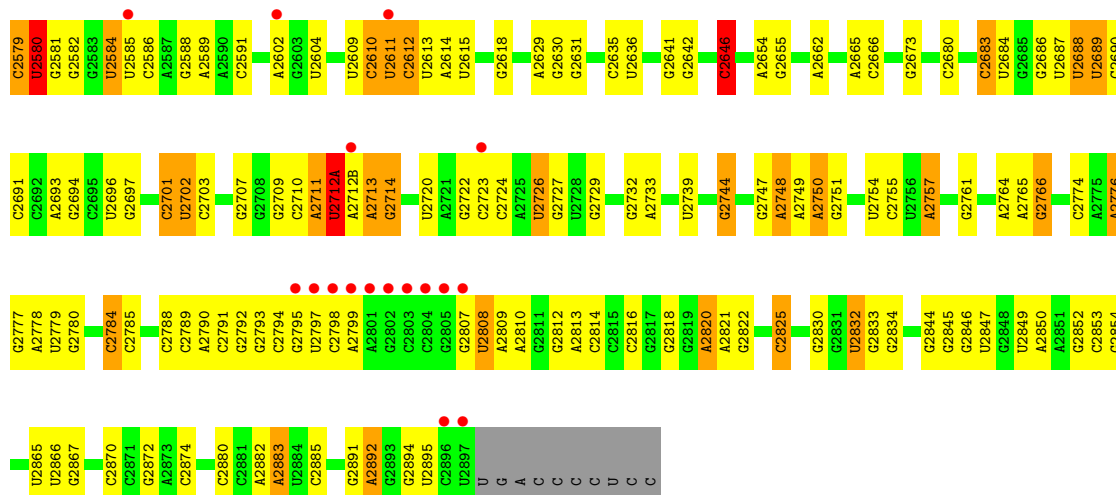


- Molecule 34: 23S rRNA

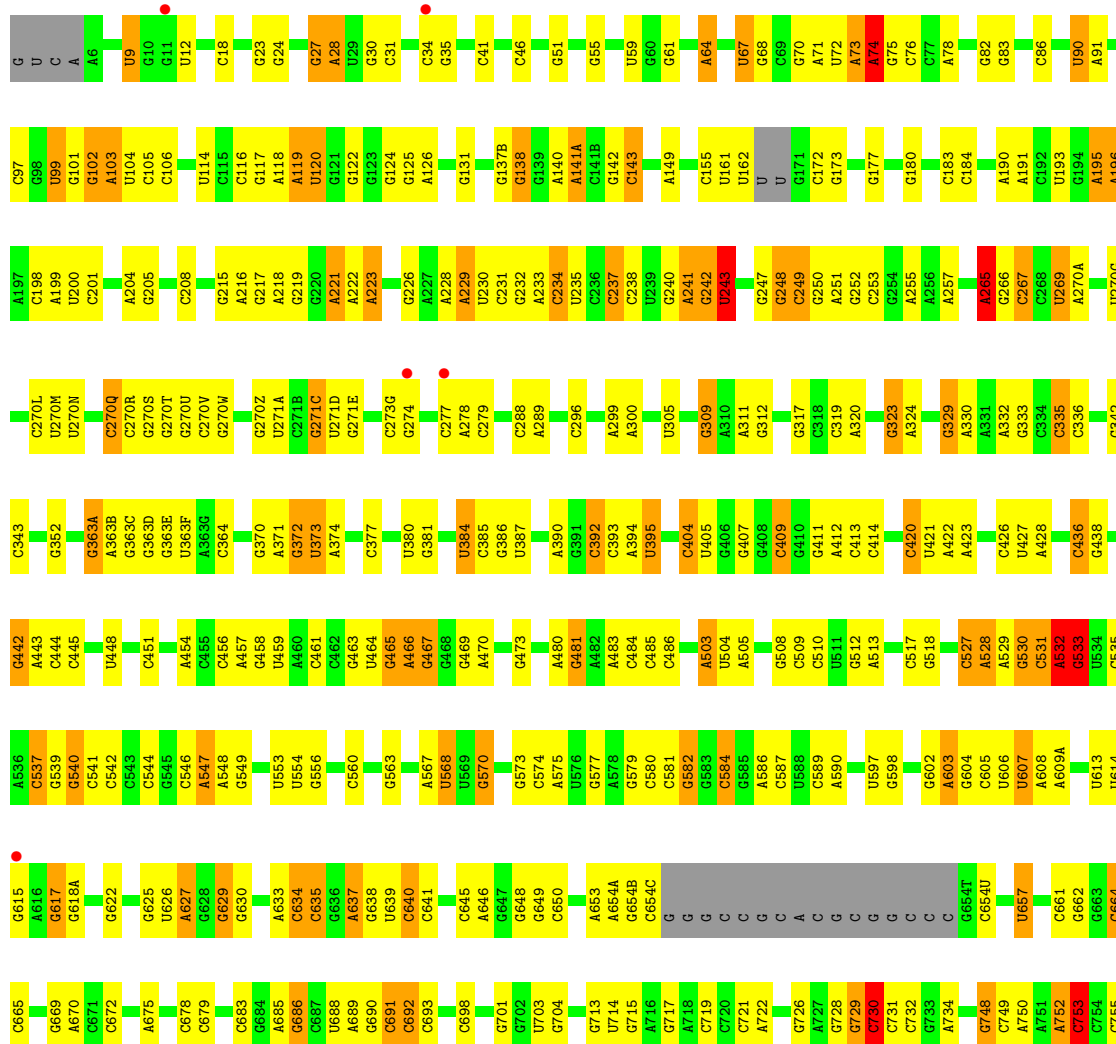


A1210	U1211	G1125	G1126	A1127	G1128	G1129	G1130	G1131	G1047	C974B	C888	C795	C687	G638	C560	G469	G363D	G208	G68
G1212	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1048	G975	C889	C796	U888	U639	G563	G469	G364	C209	G89
G1217	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1049	G976	A890	C797	G689	C540	G563	A470	C364	G214	U90
A1220	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1050	G977	C893	A300	C692	G642	U566	G481	G372	G215	G95
G1224	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1051	G978	C894	G805	G702	G645	U567	G482	G371	G216	G98
G1226	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1052	G979	U895	G806	G702	G646	U568	A483	C373B	G217	U99
A1227	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1053	A981	A896	C807	G702	G646	U568	A484	G373B	G217	U99
C1230	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1054	C982	C904	U807	G702	G646	U568	A484	G373B	G217	U99
G1231	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1055	A983	C905	G808	G702	G646	U568	A484	G373B	G217	U99
G1232	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1056	A984	C906	G809	G702	G646	U568	A484	G373B	G217	U99
G1233	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1057	C985	C907	U810	G715	G652	U574	G494	A278	G275	G101
G1234	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1058	C986	U907	U811	G716	G653	U575	G495	A278	G275	G102
G1235	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1059	G987	A910	C812	G717	G654	U576	G495	A278	G275	G103
G1238	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1060	A996	A911	C815	C721	G654B	U577	A501	C288	G276	G104
A1241	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1061	C997	C912	C816	G722	G654C	U578	A502	C288	G276	G105
A1247	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1062	C998	C913	C817	G723	G654D	U579	A503	C288	G276	G106
G1248	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1063	C999	C914	C818	G724	G654E	U580	A504	C288	G276	G107
G1249	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1064	C1000	C915	C819	G725	G654F	U581	A505	C288	G276	G108
G1250	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1065	A1008	C916	C820	G726	G654G	U582	A506	C288	G276	G109
G1251	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1066	G1003	C917	C821	G727	G654H	U583	A507	C288	G276	G110
G1252	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1067	G1004	C918	C822	G728	G654I	U584	A508	C288	G276	G111
G1253	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1068	C1005	C919	C823	G729	G654J	U585	A509	C288	G276	G112
G1254	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1069	G1006	C920	C824	G730	G654K	U586	A510	C288	G276	G113
G1255	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1070	G1007	C921	C825	G731	G654L	U587	A511	C288	G276	G114
G1256	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1071	G1008	C922	C826	G732	G654M	U588	A512	C288	G276	G115
G1257	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1072	G1009	C923	C827	G733	G654N	U589	A513	C288	G276	G116
G1258	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1073	G1010	C924	C828	G734	G654O	U590	A514	C288	G276	G117
U1263	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1074	G1011	C925	C829	G735	G654P	U591	A515	C288	G276	G118
G1264	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1075	G1012	C926	C830	G736	G654Q	U592	A516	C288	G276	G119
G1265	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1076	G1013	C927	C831	G737	G654R	U593	A517	C288	G276	G120
G1266	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1077	G1014	C928	C832	G738	G654S	U594	A518	C288	G276	G121
U1267	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1078	G1015	C929	C833	G739	G654T	U595	A519	C288	G276	G122
C1270	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1079	G1016	C930	C834	G740	G654U	U596	A520	C288	G276	G123
G1271	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1080	G1017	C931	C835	G741	G654V	U597	A521	C288	G276	G124
A1272	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1081	G1018	C932	C836	G742	G654W	U598	A522	C288	G276	G125
U1273	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1082	G1019	C933	C837	G743	G654X	U599	A523	C288	G276	G126
A1276	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1083	G1020	C934	C838	G744	G654Y	U600	A524	C288	G276	G127
A1286	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1084	G1021	C935	C839	G745	G654Z	U601	A525	C288	G276	G128
U1288	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1085	G1022	C936	C840	G746	G654A	U602	A526	C288	G276	G129
U1294	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1086	G1023	C937	C841	G747	G654B	U603	A527	C288	G276	G130
C1295	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1087	G1024	C938	C842	G748	G654C	U604	A528	C288	G276	G131
G1296	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1088	G1025	C939	C843	G749	G654D	U605	A529	C288	G276	G132
G1297	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1089	G1026	C940	C844	G750	G654E	U606	A530	C288	G276	G133
C1298	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1090	G1027	C941	C845	G751	G654F	U607	A531	C288	G276	G134
	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1091	G1028	C942	C846	G752	G654G	U608	A532	C288	G276	G135
	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1092	G1029	C943	C847	G753	G654H	U609	A533	C288	G276	G136
	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1093	G1030	C944	C848	G754	G654I	U610	A534	C288	G276	G137
	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1094	G1031	C945	C849	G755	G654J	U611	A535	C288	G276	G138
	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1095	G1032	C946	C850	G756	G654K	U612	A536	C288	G276	G139
	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1096	G1033	C947	C851	G757	G654L	U613	A537	C288	G276	G140
	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1097	G1034	C948	C852	G758	G654M	U614	A538	C288	G276	G141
	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1098	G1035	C949	C853	G759	G654N	U615	A539	C288	G276	G142
	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1099	G1036	C950	C854	G760	G654O	U616	A540	C288	G276	G143
	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1100	G1037	C951	C855	G761	G654P	U617	A541	C288	G276	G144
	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1101	G1038	C952	C856	G762	G654Q	U618	A542	C288	G276	G145
	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1102	G1039	C953	C857	G763	G654R	U619	A543	C288	G276	G146
	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1103	G1040	C954	C858	G764	G654S	U620	A544	C288	G276	G147
	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1104	G1041	C955	C859	G765	G654T	U621	A545	C288	G276	G148
	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1105	G1042	C956	C860	G766	G654U	U622	A546	C288	G276	G149
	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1106	G1043	C957	C861	G767	G654V	U623	A547	C288	G276	G150
	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1107	G1044	C958	C862	G768	G654W	U624	A548	C288	G276	G151
	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1108	G1045	C959	C863	G769	G654X	U625	A549	C288	G276	G152
	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1109	G1046	C960	C864	G770	G654Y	U626	A550	C288	G276	G153
	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1110	G1047	C961	C865	G771	G654Z	U627	A551	C288	G276	G154
	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1111	G1048	C962	C866	G772	G654A	U628	A552	C288	G276	G155
	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1112	G1049	C963	C867	G773	G654B	U629	A553	C288	G276	G156
	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1113	G1050	C964	C868	G774	G654C	U630	A554	C288	G276	G157
	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1114	G1051	C965	C869	G775	G654D	U631	A555	C288	G276	G158
	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1115	G1052	C966	C870	G776	G654E	U632	A556	C288	G276	G159
	G1216	G1125	G1126	A1127	G1128	G1129	G1130	G1131	A1116	G1053	C967	C871							

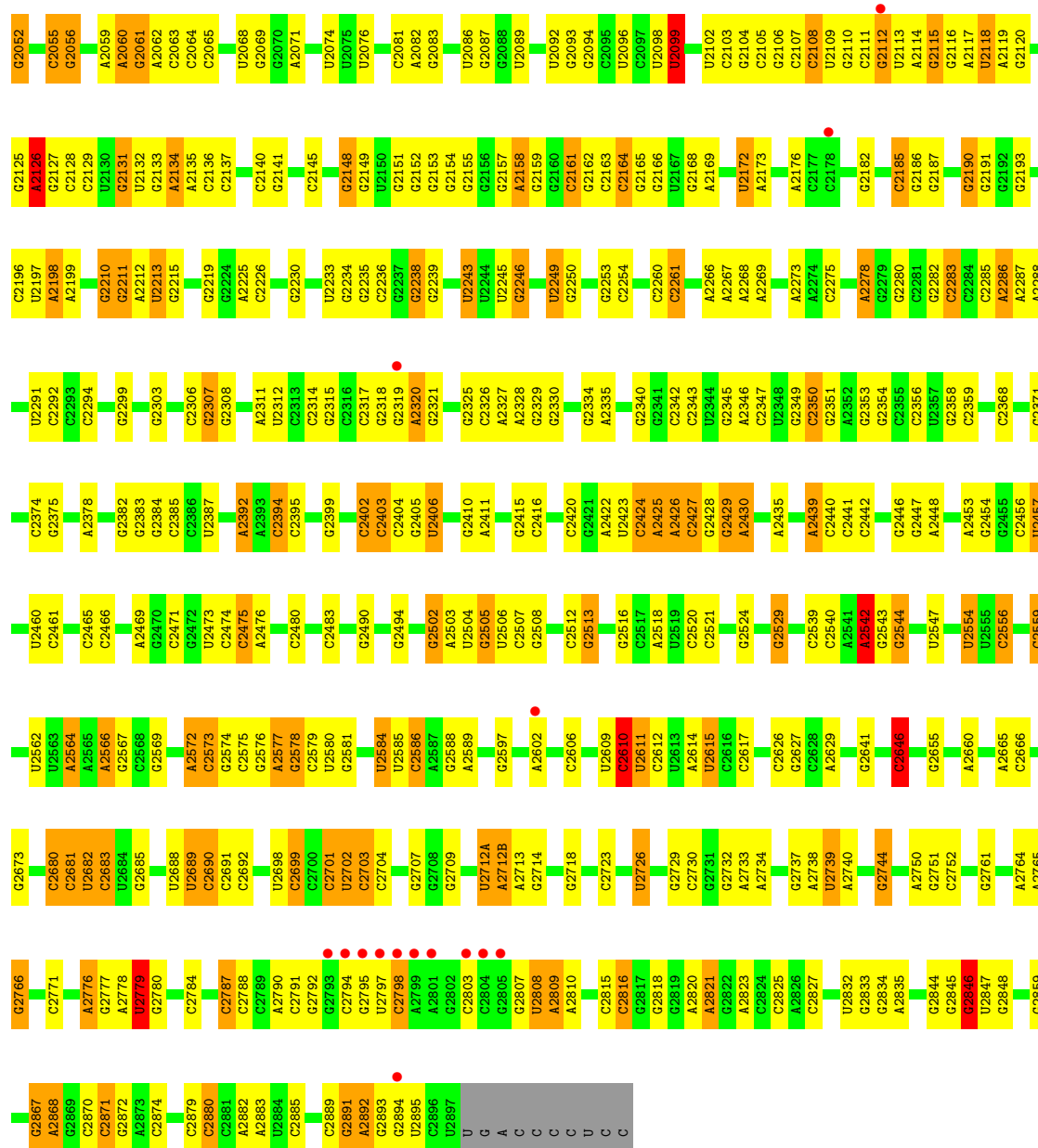
G2490	G2494	G2496	G2497	G2498	G2499	G2500	G2501	G2502	G2503	G2504	G2505	G2506	G2507	G2508	G2511	G2512	G2513	G2514	G2517	G2518	G2519	G2520	G2529	G2530	G2531	G2539	G2542	G2543	G2544	G2551	G2552	G2553	G2554	G2559	G2562	G2566	G2567	G2568	G2569	G2570	G2571	G2572	G2573	G2574	G2575	G2576	G2577	G2578	
C2402	C2403	U2406	G2410	A2411	U2419	G2422	G2423	G2424	A2425	A2426	G2427	G2428	G2429	A2430	U2431	A2432	A2433	A2434	A2435	A2439	C2440	C2441	C2442	A2443	U2449	U2449	A2450	C2456	U2460	C2463	C2466	C2467	G2468	A2469	C2470	C2471	G2472	U2473	C2474	C2475	A2478	G2479	G2480	G2481	G2482	C2483	A2488	G2489	
A2310	A2311	U2312	G2313	G2314	G2315	G2316	G2319	A2320	A2321	A2322	G2325	A2328	G2329	U2332	A2333	G2334	A2335	A2336	G2341	C2342	C2343	U2344	G2345	C2346	C2347	C2350	G2351	G2364	G2365	G2372	G2373	C2374	G2375	A2376	A2377	A2378	G2383	G2384	G2385	A2388	G2391	A2392	G2393	G2394	G2395	G2396	G2397	A2398	
U2208	C2209	G2210	G2211	G2212	G2213	G2215	G2219	G2220	G2221	G2222	G2223	G2224	G2225	G2226	C2229	G2238	G2239	U2243	U2244	U2245	G2246	A2247	C2248	U2249	G2253	C2254	C2258	A2266	G2271	C2275	A2278	C2279	G2280	C2283	A2286	A2287	A2288	U2291	C2294	C2295	U2296	C2297	G2304	A2305	C2306	G2307	A2309		
C2138	G2131	U2132	G2133	A2134	C2137	C2142	G2147	G2148	G2149	U2150	G2151	G2152	G2153	G2154	G2155	G2156	G2157	A2158	G2159	C2164	G2165	G2166	U2167	G2168	A2169	A2170	A2171	U2172	A2173	C2174	A2175	C2176	C2177	G2178	C2179	C2183	G2184	C2185	G2186	G2187	G2190	G2191	G2192	G2193	G2194	C2195	C2196	A2198	
G2056	A2059	A2060	A2061	A2062	C2063	C2064	C2065	G2069	G2070	A2071	G2072	C2073	A2077	G2080	C2081	A2082	C2085	U2086	U2089	U2092	G2093	G2094	C2095	U2096	C2097	U2098	U2099	G2100	G2101	U2102	G2103	C2104	G2105	G2106	G2107	C2108	C2111	G2112	U2113	A2114	G2115	G2116	A2117	U2118	A2119	G2120	G2123	A2126	G2127
G2208	C2209	G2210	G2211	G2212	G2213	G2215	G2219	G2220	G2221	G2222	G2223	G2224	G2225	G2226	C2229	G2238	G2239	U2243	U2244	U2245	G2246	A2247	C2248	U2249	G2253	C2254	C2258	A2266	G2271	C2275	A2278	C2279	G2280	C2283	A2286	A2287	A2288	U2291	C2294	C2295	U2296	C2297	G2304	A2305	C2306	G2307	A2309		
A2310	A2311	U2312	G2313	G2314	G2315	G2316	G2319	A2320	A2321	A2322	G2325	A2328	G2329	U2332	A2333	G2334	A2335	A2336	G2341	C2342	C2343	U2344	G2345	C2346	C2347	C2350	G2351	G2364	G2365	G2372	G2373	C2374	G2375	A2376	A2377	A2378	G2383	G2384	G2385	A2388	G2391	A2392	G2393	G2394	G2395	G2396	G2397	A2398	
C2402	C2403	U2406	G2410	A2411	U2419	G2422	G2423	G2424	A2425	A2426	G2427	G2428	G2429	A2430	U2431	A2432	A2433	A2434	A2435	A2439	C2440	C2441	C2442	A2443	U2449	U2449	A2450	C2456	U2460	C2463	C2466	C2467	G2468	A2469	C2470	C2471	G2472	U2473	C2474	C2475	A2478	G2479	G2480	G2481	G2482	C2483	A2488	G2489	
G2490	G2494	G2496	G2497	G2498	G2499	G2500	G2501	G2502	G2503	G2504	G2505	G2506	G2507	G2508	U2511	G2512	G2513	U2514	G2517	G2518	U2519	G2520	G2529	G2530	G2531	G2539	G2542	G2543	G2544	G2551	G2552	G2553	U2554	G2559	G2562	G2566	G2567	G2568	G2569	G2570	G2571	G2572	G2573	G2574	G2575	G2576	G2577	G2578	



• Molecule 34: 23S rRNA

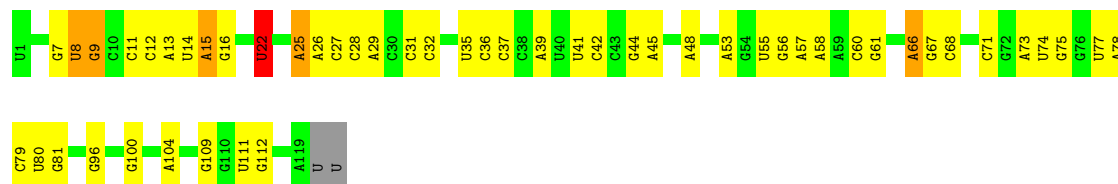






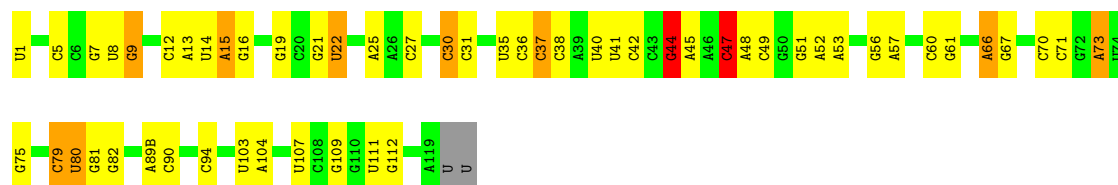
• Molecule 35: 5S rRNA

Chain RB: 57% 37% . . .

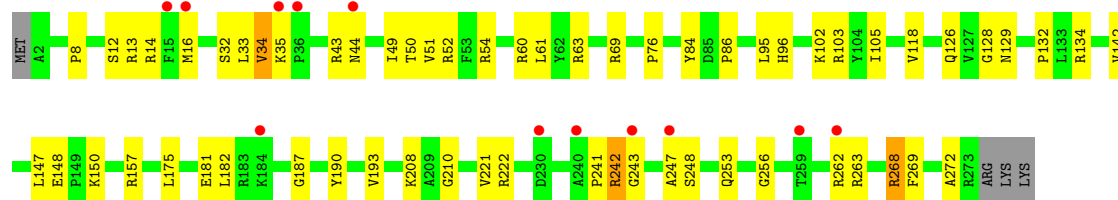
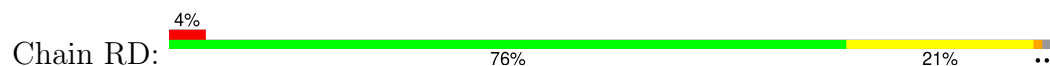


• Molecule 35: 5S rRNA

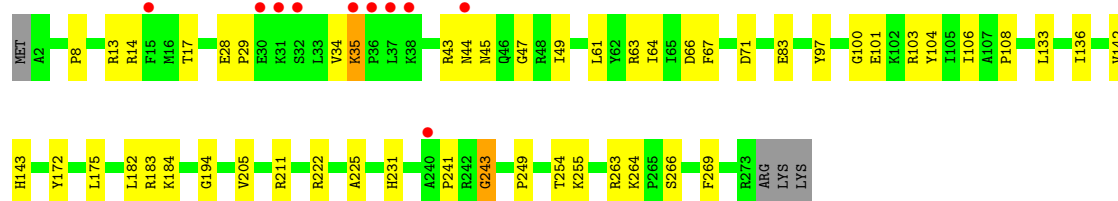
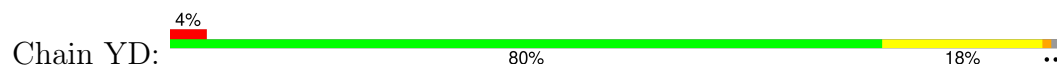
Chain YB: 53% 36% 7% . . .



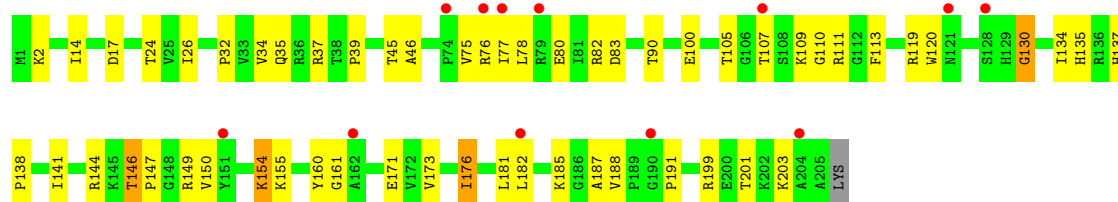
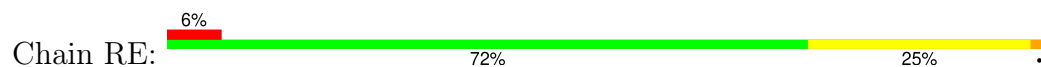
• Molecule 36: 50S ribosomal protein L2



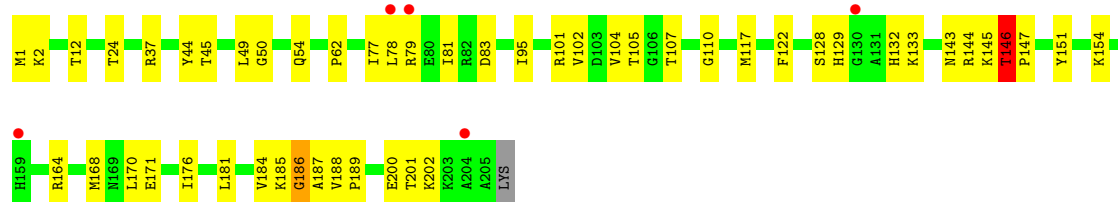
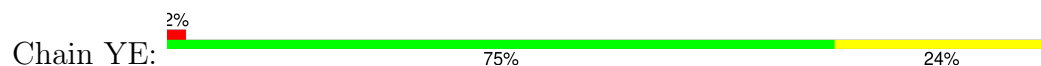
• Molecule 36: 50S ribosomal protein L2



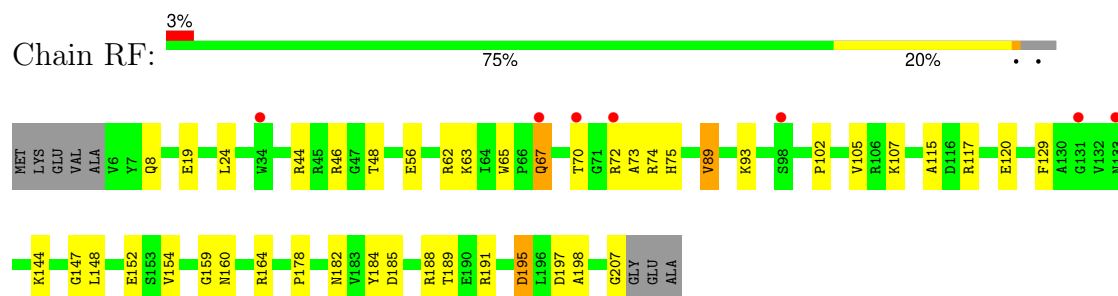
• Molecule 37: 50S ribosomal protein L3



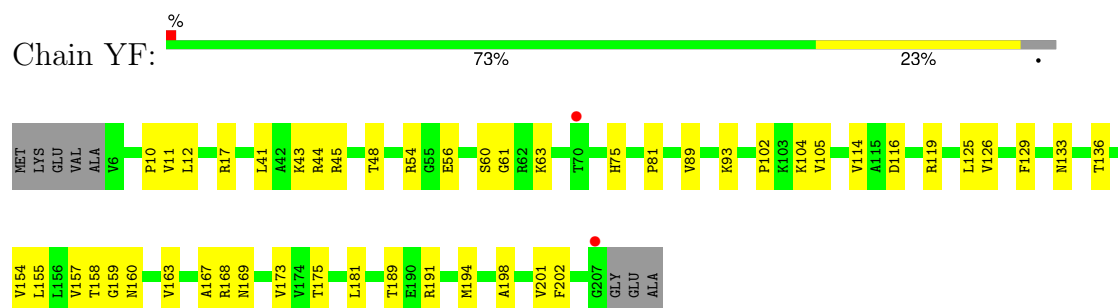
• Molecule 37: 50S ribosomal protein L3



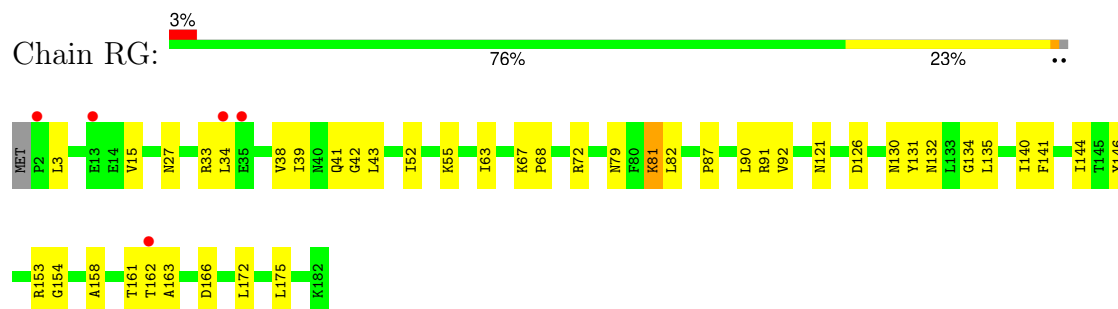
- Molecule 38: 50S ribosomal protein L4



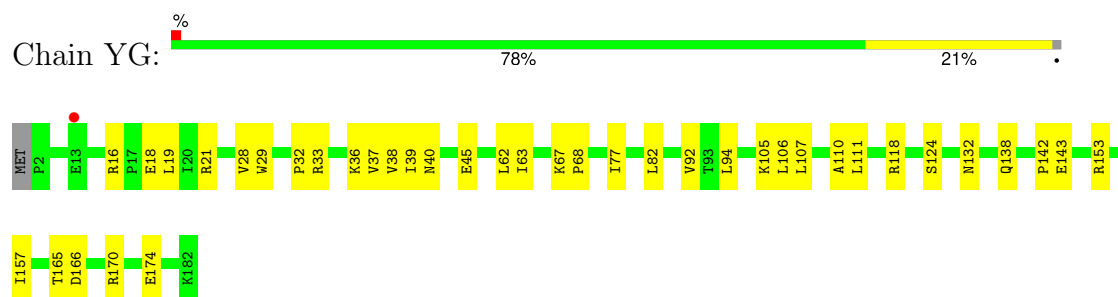
- Molecule 38: 50S ribosomal protein L4



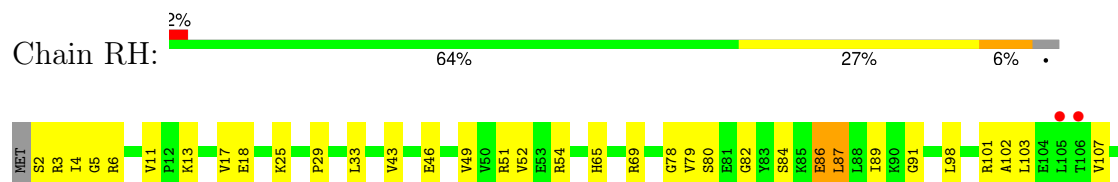
- Molecule 39: 50S ribosomal protein L5



- Molecule 39: 50S ribosomal protein L5

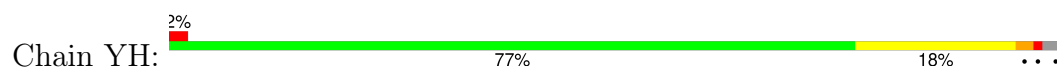



- Molecule 40: 50S ribosomal protein L6






- Molecule 40: 50S ribosomal protein L6



Chain RO:  75% 25%




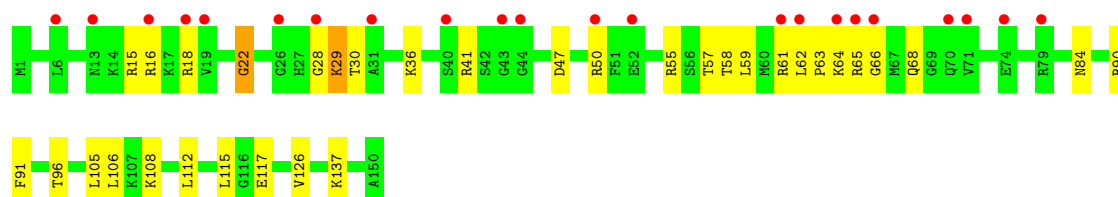
- Molecule 43: 50S ribosomal protein L14

Chain YO:  84% 16%




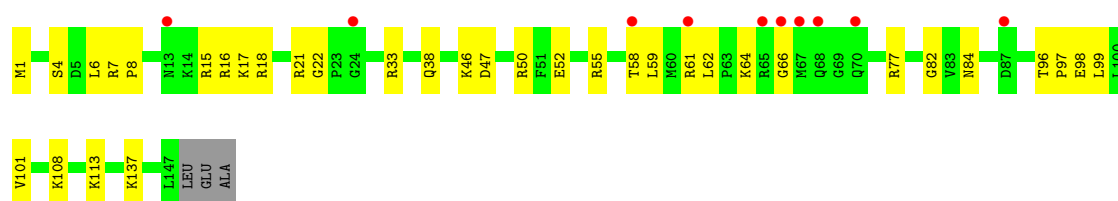
- Molecule 44: 50S ribosomal protein L15

Chain RP:  15% 77% 21%




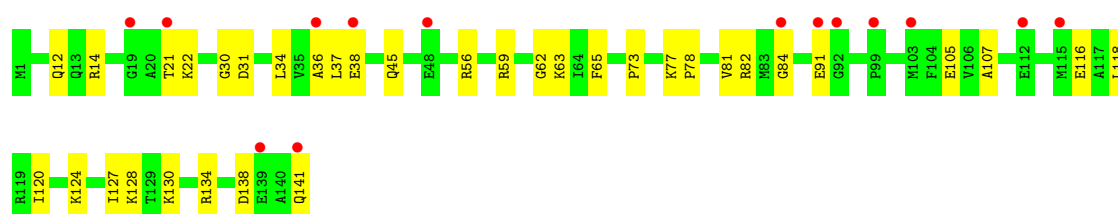
- Molecule 44: 50S ribosomal protein L15

Chain YP:  7% 75% 23%




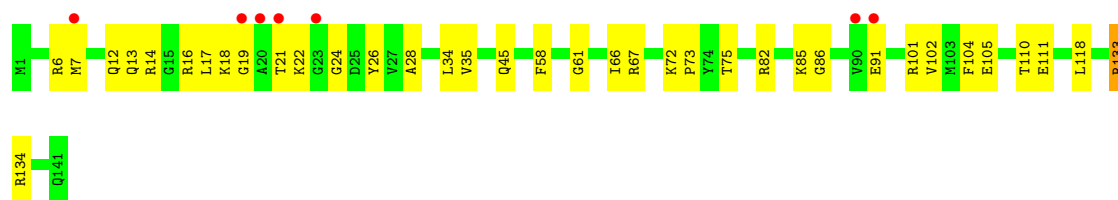
- Molecule 45: 50S ribosomal protein L16

Chain RQ:  10% 75% 25%

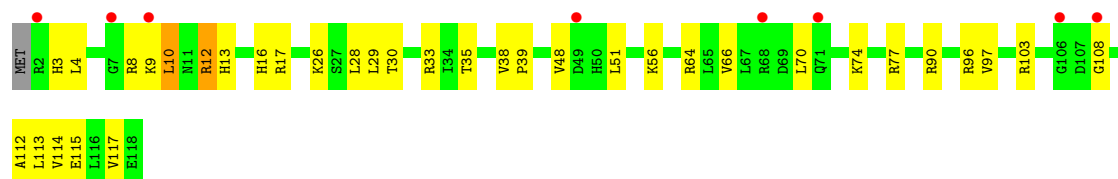


- Molecule 45: 50S ribosomal protein L16

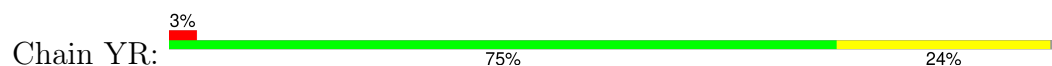
Chain YQ:  5% 74% 26%



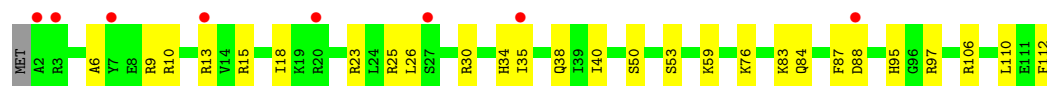
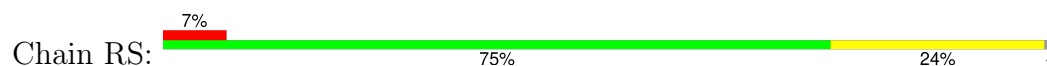
- Molecule 46: 50S ribosomal protein L17



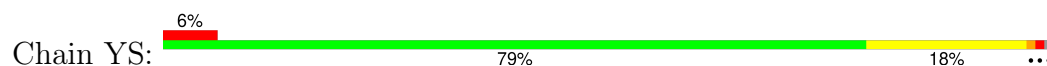
- Molecule 46: 50S ribosomal protein L17



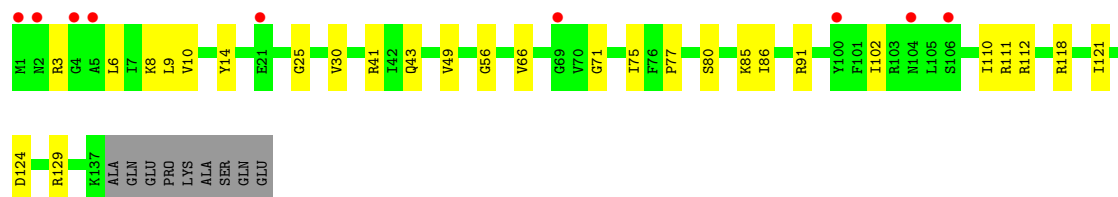
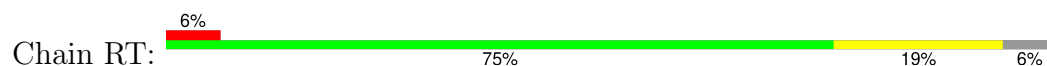
- Molecule 47: 50S ribosomal protein L18



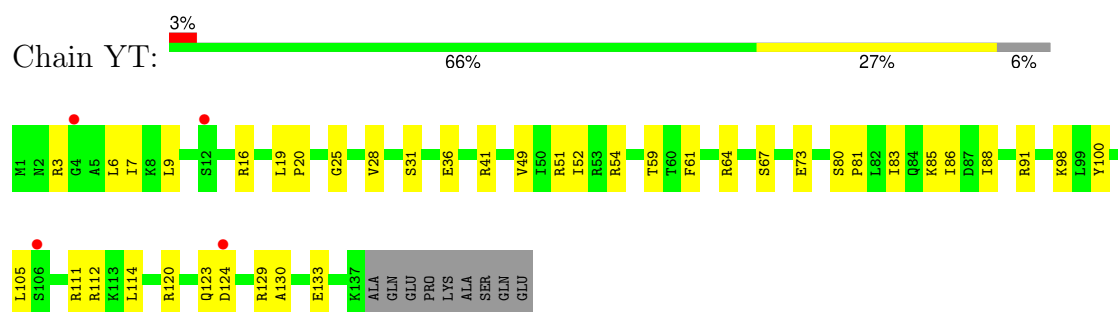
- Molecule 47: 50S ribosomal protein L18



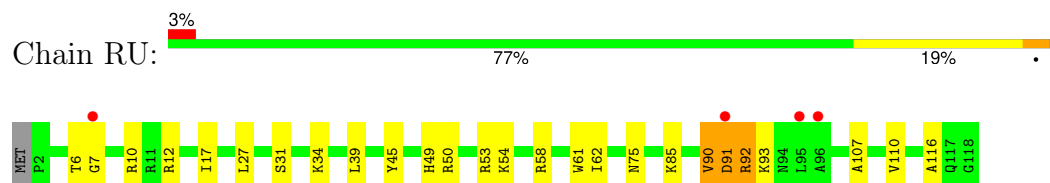
- Molecule 48: 50S ribosomal protein L19



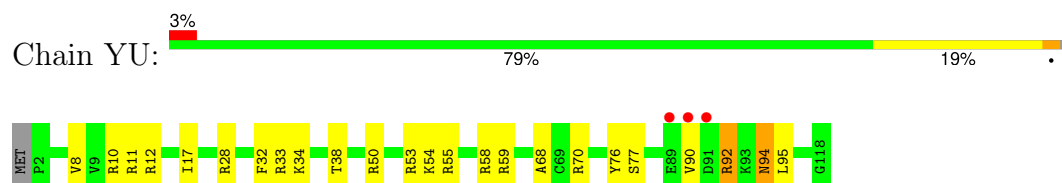
- Molecule 48: 50S ribosomal protein L19



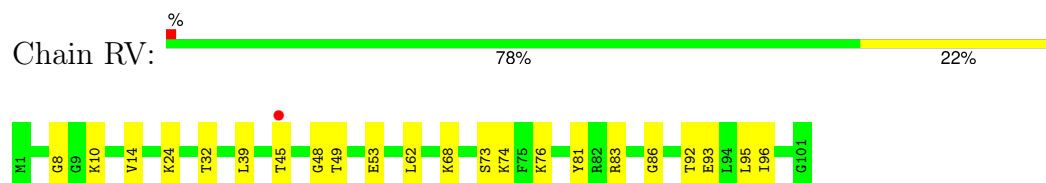
- Molecule 49: 50S ribosomal protein L20



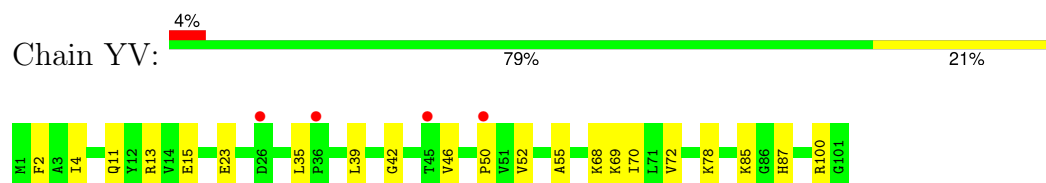
- Molecule 49: 50S ribosomal protein L20



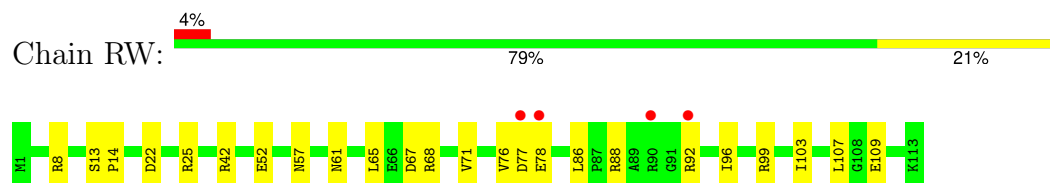
- Molecule 50: 50S ribosomal protein L21



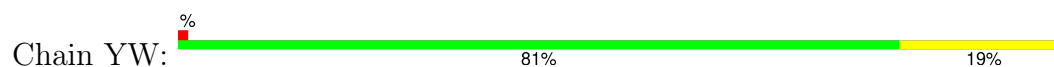
- Molecule 50: 50S ribosomal protein L21

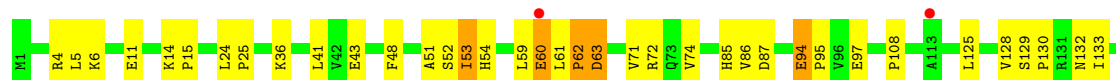


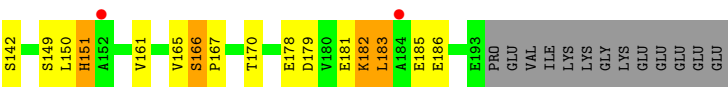
- Molecule 51: 50S ribosomal protein L22



- Molecule 51: 50S ribosomal protein L22







4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.74Å 450.26Å 626.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.94 – 3.50 49.94 – 3.50	Depositor EDS
% Data completeness (in resolution range)	97.6 (49.94-3.50) 97.5 (49.94-3.50)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.240 , 0.258 0.240 , 0.258	Depositor DCC
R_{free} test set	708492 reflections (4.57%)	wwPDB-VP
Wilson B-factor (Å ²)	75.0	Xtriage
Anisotropy	0.423	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 74.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	292039	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% 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: SF4, MG, ZN, 1MG

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	0.69	1/36343 (0.0%)	1.14	198/56720 (0.3%)
1	XA	0.77	0/36435	1.15	194/56865 (0.3%)
2	QB	0.35	0/1942	0.67	0/2619
2	XB	0.37	0/1950	0.64	1/2630 (0.0%)
3	QC	0.36	0/1629	0.66	0/2195
3	XC	0.37	0/1629	0.61	0/2195
4	QD	0.45	1/1733 (0.1%)	0.65	0/2318
4	XD	0.52	2/1733 (0.1%)	0.70	2/2318 (0.1%)
5	QE	0.37	0/1171	0.67	0/1576
5	XE	0.43	0/1171	0.62	0/1576
6	QF	0.39	0/856	0.68	0/1154
6	XF	0.41	0/856	0.62	0/1154
7	QG	0.35	0/1276	0.63	1/1709 (0.1%)
7	XG	0.36	0/1276	0.60	0/1709
8	QH	0.40	0/1128	0.62	0/1517
8	XH	0.42	0/1128	0.66	0/1517
9	QI	0.42	0/1029	0.74	0/1379
9	XI	0.36	0/1017	0.70	0/1365
10	QJ	0.35	0/814	0.67	0/1095
10	XJ	0.34	0/790	0.59	0/1063
11	QK	0.36	0/900	0.57	0/1213
11	XK	0.39	0/879	0.59	0/1187
12	QL	0.41	0/991	0.70	1/1327 (0.1%)
12	XL	0.45	0/972	0.77	2/1301 (0.2%)
13	QM	0.35	0/965	0.78	0/1292
13	XM	0.37	0/924	0.66	0/1238
14	QN	0.67	1/501 (0.2%)	0.84	3/664 (0.5%)
14	XN	0.68	1/501 (0.2%)	0.88	2/664 (0.3%)
15	QO	0.38	0/745	0.57	0/992
15	XO	0.40	0/740	0.56	0/987
16	QP	0.40	0/721	0.64	0/970
16	XP	0.38	0/721	0.66	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	QQ	0.39	0/847	0.62	0/1131
17	XQ	0.47	0/847	0.64	0/1131
18	QR	0.37	0/579	0.56	0/768
18	XR	0.39	0/579	0.58	0/768
19	QS	0.35	0/680	0.72	1/915 (0.1%)
19	XS	0.36	0/689	0.70	0/926
20	QT	0.77	2/765 (0.3%)	1.14	8/1007 (0.8%)
20	XT	0.37	0/765	0.75	2/1007 (0.2%)
21	QU	0.34	0/221	0.58	0/288
21	XU	0.32	0/221	0.54	0/288
22	QV	0.70	2/1813 (0.1%)	1.39	32/2825 (1.1%)
22	XV	0.66	0/1813	1.20	13/2825 (0.5%)
23	QX	0.99	1/459 (0.2%)	2.11	25/715 (3.5%)
23	XX	0.63	0/459	1.26	1/715 (0.1%)
24	R0	0.40	0/652	0.63	0/867
24	Y0	0.59	0/657	0.60	0/874
25	R1	0.54	0/753	0.68	0/1000
25	Y1	0.59	0/736	0.73	0/978
26	R2	0.37	0/583	0.62	0/771
26	Y2	0.47	0/577	0.62	0/764
27	R3	0.39	0/474	0.59	0/635
27	Y3	0.62	0/474	0.59	0/635
28	R4	0.33	0/357	0.60	0/483
28	Y4	1.56	2/366 (0.5%)	1.47	8/495 (1.6%)
29	R5	0.88	3/473 (0.6%)	0.79	2/639 (0.3%)
29	Y5	0.94	2/473 (0.4%)	0.77	1/639 (0.2%)
30	R6	0.96	3/460 (0.7%)	0.78	2/613 (0.3%)
30	Y6	1.33	6/460 (1.3%)	1.01	3/613 (0.5%)
31	R7	0.53	0/417	0.62	0/550
31	Y7	0.63	0/426	0.66	0/561
32	R8	0.43	0/525	0.88	3/691 (0.4%)
32	Y8	0.59	0/525	0.84	0/691
33	R9	0.62	1/310 (0.3%)	0.72	1/407 (0.2%)
33	Y9	0.63	0/310	0.73	0/407
34	RA	0.91	2/69520 (0.0%)	1.22	576/108527 (0.5%)
34	YA	1.27	23/69543 (0.0%)	1.33	807/108563 (0.7%)
35	RB	0.71	0/2878	1.14	18/4490 (0.4%)
35	YB	1.08	0/2878	1.32	38/4490 (0.8%)
36	RD	0.52	0/2165	0.71	3/2919 (0.1%)
36	YD	0.64	0/2165	0.74	4/2919 (0.1%)
37	RE	0.50	0/1601	0.83	3/2160 (0.1%)
37	YE	0.66	0/1601	0.84	3/2160 (0.1%)
38	RF	0.49	0/1620	0.70	1/2194 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	YF	0.67	0/1620	0.65	1/2194 (0.0%)
39	RG	0.40	0/1499	0.69	0/2016
39	YG	0.43	0/1499	0.68	0/2016
40	RH	0.39	0/1362	0.83	5/1841 (0.3%)
40	YH	0.58	0/1362	0.82	4/1841 (0.2%)
41	RI	0.48	2/1151 (0.2%)	0.86	6/1558 (0.4%)
41	YI	0.45	1/1151 (0.1%)	0.79	0/1558
42	RN	0.45	0/1131	0.68	1/1525 (0.1%)
42	YN	0.63	0/1131	0.70	2/1525 (0.1%)
43	RO	0.51	0/943	0.65	0/1269
43	YO	0.60	0/943	0.63	0/1269
44	RP	0.44	0/1162	0.76	1/1544 (0.1%)
44	YP	0.54	0/1139	0.83	1/1514 (0.1%)
45	RQ	0.45	0/1143	0.73	0/1527
45	YQ	0.61	0/1143	0.77	2/1527 (0.1%)
46	RR	0.48	0/974	0.68	0/1302
46	YR	0.57	0/974	0.70	0/1302
47	RS	0.39	0/892	0.66	0/1187
47	YS	0.52	0/892	0.67	0/1187
48	RT	0.43	0/1155	0.69	0/1542
48	YT	0.54	0/1155	0.72	1/1542 (0.1%)
49	RU	0.49	0/982	0.62	0/1306
49	YU	0.70	0/982	0.61	0/1306
50	RV	0.47	0/790	0.74	1/1057 (0.1%)
50	YV	0.63	0/790	0.76	1/1057 (0.1%)
51	RW	0.52	0/911	0.63	0/1220
51	YW	0.68	0/911	0.64	0/1220
52	RX	0.52	0/739	0.60	0/993
52	YX	0.66	0/739	0.68	0/993
53	RY	0.72	4/831 (0.5%)	0.66	2/1108 (0.2%)
53	YY	0.73	1/831 (0.1%)	0.72	2/1108 (0.2%)
54	RZ	0.43	0/1493	0.89	6/2026 (0.3%)
54	YZ	0.51	0/1561	0.85	5/2119 (0.2%)
All	All	0.87	61/316163 (0.0%)	1.12	2000/472822 (0.4%)

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
28	Y4	1	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
37	RE	0	1
37	YE	0	1
50	RV	0	2
54	RZ	0	1
54	YZ	0	1
All	All	1	7

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	Y4	5	ILE	CA-CB	-21.70	1.04	1.54
28	Y4	4	GLY	N-CA	-18.70	1.18	1.46
30	R6	16	CYS	CB-SG	14.24	2.06	1.82
30	Y6	16	CYS	CB-SG	-14.07	1.58	1.82
20	QT	74	LYS	CA-CB	-13.71	1.23	1.53
29	Y5	32	PRO	N-CA	13.22	1.69	1.47
30	Y6	13	CYS	CB-SG	-13.08	1.60	1.82
20	QT	73	HIS	N-CA	-12.34	1.21	1.46
14	QN	43	CYS	CB-SG	11.14	2.01	1.82
4	XD	12	CYS	CB-SG	10.96	2.00	1.82
14	XN	43	CYS	CB-SG	10.95	2.00	1.82
53	RY	102	CYS	CB-SG	-10.82	1.63	1.82
29	R5	34	PRO	N-CD	10.57	1.62	1.47
53	YY	79	CYS	CB-SG	-10.37	1.64	1.82
29	R5	33	CYS	C-N	8.95	1.51	1.34
30	Y6	40	CYS	CB-SG	8.88	1.97	1.82
30	Y6	40	CYS	C-N	8.73	1.50	1.34
33	R9	29	ASN	C-N	8.41	1.50	1.34
53	RY	79	CYS	CB-SG	8.22	1.96	1.82
30	R6	13	CYS	CB-SG	-7.94	1.68	1.82
30	R6	41	PRO	N-CD	7.50	1.58	1.47
34	RA	74	A	N9-C4	-7.27	1.33	1.37
41	RI	94	ALA	C-N	7.08	1.50	1.34
30	Y6	41	PRO	N-CD	7.04	1.57	1.47
41	RI	82	ARG	C-N	-6.80	1.18	1.34
4	QD	8	VAL	CB-CG1	6.80	1.67	1.52
34	YA	1021	A	N9-C4	-6.67	1.33	1.37
23	QX	16	C	N1-C6	6.17	1.40	1.37
53	RY	99	CYS	CB-SG	-6.08	1.72	1.82
34	RA	1601	G	O3'-P	-6.06	1.53	1.61
22	QV	36	G	N7-C5	-6.02	1.35	1.39
22	QV	34	C	N1-C2	6.00	1.46	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	YA	74	A	N9-C4	-5.98	1.34	1.37
29	Y5	31	VAL	C-N	5.92	1.45	1.34
34	YA	198	C	C4-C5	-5.86	1.38	1.43
53	RY	76	CYS	CB-SG	-5.84	1.72	1.81
1	QA	1499	A	O3'-P	5.79	1.68	1.61
4	XD	31	CYS	CB-SG	5.55	1.91	1.82
34	YA	1210	A	N9-C4	-5.52	1.34	1.37
34	YA	390	A	N9-C4	-5.47	1.34	1.37
34	YA	783	A	N9-C4	-5.41	1.34	1.37
34	YA	528	A	N9-C4	-5.40	1.34	1.37
30	Y6	51	GLU	CG-CD	-5.35	1.44	1.51
34	YA	1021	A	N3-C4	-5.35	1.31	1.34
34	YA	804	A	N9-C4	-5.33	1.34	1.37
34	YA	2015	A	N7-C5	-5.30	1.36	1.39
34	YA	582	G	N7-C5	-5.29	1.36	1.39
41	YI	109	ILE	C-N	5.28	1.46	1.34
34	YA	1253	A	N9-C4	-5.26	1.34	1.37
34	YA	2453	A	C5-C4	-5.25	1.35	1.38
34	YA	528	A	C5-C6	-5.15	1.36	1.41
29	R5	33	CYS	CB-SG	-5.15	1.73	1.81
34	YA	981	A	N7-C5	-5.12	1.36	1.39
34	YA	2025	C	N1-C6	-5.12	1.34	1.37
34	YA	451	C	N1-C6	-5.09	1.34	1.37
34	YA	2564	A	N9-C4	-5.08	1.34	1.37
34	YA	1658	C	N1-C6	-5.07	1.34	1.37
34	YA	532	A	N7-C5	-5.05	1.36	1.39
34	YA	567	A	N9-C4	-5.03	1.34	1.37
34	YA	2030	A	N9-C4	-5.03	1.34	1.37
34	YA	2542	A	N3-C4	5.01	1.37	1.34

All (2000) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	QT	74	LYS	N-CA-CB	21.28	148.91	110.60
23	QX	17	C	C6-N1-C2	-19.01	112.70	120.30
22	QV	35	G	C8-N9-C4	-16.76	99.70	106.40
28	Y4	5	ILE	CB-CA-C	16.14	143.88	111.60
34	YA	2453	A	N1-C2-N3	-15.63	121.48	129.30
23	QX	18	C	O5'-P-OP1	-15.31	91.92	105.70
37	RE	146	THR	C-N-CD	-15.29	86.97	120.60
54	RZ	166	SER	C-N-CD	-14.13	89.52	120.60
37	YE	146	THR	C-N-CD	-14.12	89.53	120.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	QX	15	A	P-O3'-C3'	-13.61	103.37	119.70
40	RH	86	GLU	CB-CA-C	-12.84	84.72	110.40
54	YZ	166	SER	C-N-CD	-12.60	92.88	120.60
1	XA	1301	U	C2-N1-C1'	12.40	132.58	117.70
1	XA	1158	C	N1-C2-O2	11.98	126.09	118.90
1	QA	1301	U	C2-N1-C1'	11.78	131.84	117.70
23	QX	18	C	N1-C2-O2	11.78	125.97	118.90
1	QA	754	C	C2-N1-C1'	11.76	131.74	118.80
1	QA	754	C	N1-C2-O2	11.76	125.96	118.90
1	XA	1158	C	C2-N1-C1'	11.73	131.70	118.80
23	QX	18	C	C2-N1-C1'	11.72	131.69	118.80
22	QV	35	G	O5'-P-OP1	-11.31	95.52	105.70
34	YA	856	C	C6-N1-C2	-11.28	115.79	120.30
22	QV	35	G	N7-C8-N9	11.26	118.73	113.10
23	QX	18	C	C6-N1-C1'	-11.00	107.60	120.80
1	XA	1301	U	N1-C2-O2	10.97	130.48	122.80
34	YA	2542	A	N9-C4-C5	-10.95	101.42	105.80
34	RA	856	C	C6-N1-C2	-10.75	116.00	120.30
1	QA	1301	U	N1-C2-O2	10.56	130.20	122.80
34	RA	828	U	C2-N1-C1'	10.38	130.15	117.70
1	XA	754	C	C2-N1-C1'	10.29	130.12	118.80
23	QX	17	C	C5-C6-N1	10.27	126.13	121.00
34	RA	1313	U	C2-N1-C1'	10.17	129.91	117.70
34	RA	1407	C	C6-N1-C2	-10.17	116.23	120.30
34	YA	1658	C	C5-C6-N1	10.05	126.03	121.00
34	YA	537	C	C5-C6-N1	10.04	126.02	121.00
34	RA	120	U	N3-C2-O2	-10.00	115.20	122.20
34	YA	2063	C	N1-C2-O2	10.00	124.90	118.90
34	RA	1762	A	C6-N1-C2	-9.99	112.61	118.60
34	RA	828	U	N1-C2-O2	9.94	129.76	122.80
34	YA	1653	G	N1-C6-O6	-9.92	113.95	119.90
1	XA	1301	U	N3-C2-O2	-9.90	115.27	122.20
30	Y6	43	CYS	N-CA-CB	-9.84	92.89	110.60
1	XA	121	C	C2-N3-C4	-9.83	114.98	119.90
1	QA	1301	U	N3-C2-O2	-9.80	115.34	122.20
34	RA	120	U	N1-C2-O2	9.70	129.59	122.80
34	YA	2032	G	C5-N7-C8	-9.66	99.47	104.30
34	YA	1956	U	N3-C2-O2	-9.64	115.45	122.20
1	QA	754	C	N3-C2-O2	-9.60	115.18	121.90
34	YA	1914	C	N1-C2-O2	9.55	124.63	118.90
34	RA	1407	C	C2-N1-C1'	9.52	129.28	118.80
37	YE	146	THR	C-N-CA	9.52	161.97	122.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	QX	17	C	C2-N1-C1'	9.48	129.23	118.80
34	YA	1788	C	C5-C6-N1	9.47	125.74	121.00
34	RA	1314	C	C2-N1-C1'	9.44	129.18	118.80
1	XA	618	C	N1-C2-O2	9.44	124.56	118.90
34	YA	1535	U	N1-C2-O2	9.39	129.37	122.80
1	XA	1158	C	N3-C2-O2	-9.37	115.34	121.90
34	YA	1653	G	N3-C4-C5	-9.31	123.95	128.60
34	YA	837	C	C6-N1-C2	-9.23	116.61	120.30
34	YA	1914	C	C2-N1-C1'	9.20	128.92	118.80
34	YA	860	U	N3-C2-O2	-9.19	115.77	122.20
34	RA	1640	C	N1-C2-O2	9.16	124.40	118.90
34	RA	2143	C	N3-C2-O2	-9.16	115.49	121.90
23	QX	18	C	N3-C4-N4	9.15	124.41	118.00
1	QA	1358	U	N3-C2-O2	-9.15	115.80	122.20
54	RZ	166	SER	C-N-CA	9.14	160.39	122.00
34	YA	2544	G	C5-N7-C8	-9.13	99.73	104.30
34	RA	856	C	C5-C6-N1	9.11	125.56	121.00
30	R6	16	CYS	CA-CB-SG	9.10	130.39	114.00
34	YA	2868	A	N7-C8-N9	9.10	118.35	113.80
20	QT	74	LYS	N-CA-C	-9.09	86.46	111.00
20	QT	73	HIS	N-CA-C	9.07	135.49	111.00
1	QA	618	C	N1-C2-O2	9.07	124.34	118.90
22	QV	34	C	N1-C2-O2	8.99	124.30	118.90
34	RA	1417	C	C5-C6-N1	8.99	125.50	121.00
1	QA	1358	U	N1-C2-O2	8.96	129.07	122.80
34	YA	120	U	N3-C2-O2	-8.95	115.93	122.20
1	QA	90	C	C2-N1-C1'	8.93	128.62	118.80
34	YA	856	C	C5-C6-N1	8.93	125.46	121.00
34	YA	1314	C	C2-N1-C1'	8.91	128.60	118.80
1	XA	1301	U	C5-C6-N1	8.91	127.15	122.70
28	Y4	39	CYS	C-N-CA	8.90	143.96	121.70
34	YA	1313	U	C2-N1-C1'	8.89	128.37	117.70
34	RA	1632	A	C5-N7-C8	-8.89	99.45	103.90
28	Y4	5	ILE	N-CA-C	-8.88	87.02	111.00
34	YA	2544	G	C4-C5-N7	8.87	114.35	110.80
35	YB	31	C	N1-C2-O2	8.85	124.21	118.90
1	QA	1395	C	C2-N1-C1'	8.83	128.51	118.80
34	RA	1535	U	C2-N1-C1'	8.79	128.25	117.70
34	YA	1535	U	C2-N1-C1'	8.79	128.25	117.70
34	YA	753	C	C5-C6-N1	8.77	125.38	121.00
34	YA	2063	C	N3-C2-O2	-8.75	115.78	121.90
1	XA	1019	C	N3-C2-O2	-8.70	115.81	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	QA	136	C	C2-N1-C1'	8.66	128.33	118.80
34	YA	1640	C	N1-C2-O2	8.64	124.09	118.90
34	YA	198	C	C5-C6-N1	8.63	125.31	121.00
34	YA	795	C	C6-N1-C2	-8.62	116.85	120.30
34	RA	1882	C	C2-N1-C1'	8.61	128.28	118.80
35	RB	11	C	N1-C2-O2	8.61	124.06	118.90
34	YA	31	C	C5-C6-N1	8.61	125.30	121.00
34	RA	828	U	N3-C2-O2	-8.60	116.18	122.20
34	RA	889	C	O4'-C1'-N1	8.58	115.06	108.20
34	RA	456	C	C2-N1-C1'	8.57	128.23	118.80
34	YA	343	C	C6-N1-C2	-8.56	116.88	120.30
34	RA	1135	C	N1-C2-O2	8.55	124.03	118.90
34	YA	1407	C	C2-N1-C1'	8.55	128.20	118.80
34	YA	1658	C	C6-N1-C2	-8.54	116.88	120.30
34	RA	613	U	N1-C2-O2	8.54	128.78	122.80
1	XA	221	C	N1-C2-O2	8.51	124.00	118.90
54	YZ	166	SER	C-N-CA	8.51	157.72	122.00
1	XA	1539	C	N3-C2-O2	-8.50	115.95	121.90
2	XB	89	GLY	C-N-CA	8.49	142.92	121.70
34	RA	1407	C	C5-C6-N1	8.45	125.23	121.00
34	YA	2808	U	N3-C2-O2	-8.45	116.28	122.20
30	Y6	43	CYS	CB-CA-C	8.43	127.27	110.40
37	RE	146	THR	C-N-CA	8.43	157.41	122.00
22	QV	35	G	N9-C4-C5	8.43	108.77	105.40
34	RA	669	G	C4-N9-C1'	8.39	137.41	126.50
34	YA	1653	G	C6-N1-C2	-8.38	120.07	125.10
34	YA	2712(B)	A	N7-C8-N9	8.34	117.97	113.80
34	YA	1535	U	N3-C2-O2	-8.34	116.36	122.20
34	YA	2726	U	N3-C2-O2	-8.32	116.38	122.20
34	RA	613	U	N3-C2-O2	-8.31	116.38	122.20
1	XA	1383	C	N1-C2-O2	8.31	123.89	118.90
4	XD	18	LYS	CD-CE-NZ	8.30	130.79	111.70
34	YA	97	C	C6-N1-C2	-8.29	116.98	120.30
34	YA	2542	A	C8-N9-C4	8.29	109.12	105.80
22	QV	35	G	C4-N9-C1'	8.26	137.24	126.50
34	YA	120	U	N1-C2-O2	8.24	128.57	122.80
1	XA	1348	U	N1-C2-O2	8.24	128.57	122.80
34	YA	343	C	C5-C6-N1	8.24	125.12	121.00
34	YA	661	C	C6-N1-C2	-8.23	117.01	120.30
34	YA	1264	G	C8-N9-C4	-8.22	103.11	106.40
34	YA	1313	U	N3-C2-O2	-8.21	116.45	122.20
1	XA	1019	C	N1-C2-O2	8.20	123.82	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	QA	754	C	C6-N1-C1'	-8.19	110.97	120.80
34	YA	2453	A	C2-N3-C4	8.18	114.69	110.60
1	XA	498	U	N3-C2-O2	-8.18	116.48	122.20
34	RA	1535	U	N3-C2-O2	-8.17	116.48	122.20
1	XA	312	C	N3-C2-O2	-8.14	116.20	121.90
36	YD	34	VAL	N-CA-C	-8.14	89.02	111.00
22	XV	15	G	C4-N9-C1'	8.13	137.07	126.50
34	YA	2868	A	C8-N9-C4	-8.12	102.55	105.80
35	YB	27	C	N1-C2-O2	8.12	123.77	118.90
1	QA	1348	U	N1-C2-O2	8.12	128.48	122.80
34	RA	1535	U	N1-C2-O2	8.09	128.46	122.80
34	RA	1804	C	C6-N1-C2	-8.07	117.07	120.30
34	YA	749	C	N1-C2-O2	8.07	123.74	118.90
34	RA	1914	C	C2-N1-C1'	8.05	127.65	118.80
1	XA	1158	C	C6-N1-C2	-8.05	117.08	120.30
1	XA	738	C	C5-C6-N1	8.04	125.02	121.00
1	XA	1301	U	C6-N1-C1'	-8.03	109.95	121.20
22	QV	36	G	C5'-C4'-O4'	8.03	118.74	109.10
29	Y5	32	PRO	CA-N-CD	-8.03	100.26	111.50
34	YA	1135	C	N1-C2-O2	8.02	123.71	118.90
34	YA	2739	U	N3-C2-O2	-8.01	116.59	122.20
34	RA	1313	U	N1-C2-O2	8.01	128.41	122.80
40	RH	152	ARG	C-N-CA	7.99	141.68	121.70
34	YA	1788	C	C6-N1-C2	-7.99	117.10	120.30
23	QX	19	U	C4-C5-C6	7.99	124.50	119.70
34	RA	1313	U	N3-C2-O2	-7.99	116.61	122.20
1	XA	1158	C	C6-N1-C1'	-7.99	111.21	120.80
40	YH	151	ILE	N-CA-C	-7.98	89.45	111.00
34	YA	2542	A	C2-N3-C4	-7.98	106.61	110.60
34	RA	856	C	C2-N1-C1'	7.98	127.58	118.80
34	YA	2465	C	C5-C6-N1	7.98	124.99	121.00
34	YA	373	U	N3-C2-O2	-7.97	116.62	122.20
34	YA	2712(B)	A	C8-N9-C4	-7.94	102.63	105.80
1	QA	307	C	N1-C2-O2	7.93	123.66	118.90
34	YA	198	C	C6-N1-C2	-7.93	117.13	120.30
34	YA	1407	C	C6-N1-C2	-7.92	117.13	120.30
34	YA	795	C	C5-C6-N1	7.92	124.96	121.00
34	RA	613	U	C2-N1-C1'	7.91	127.20	117.70
34	YA	2726	U	C2-N1-C1'	7.91	127.19	117.70
34	YA	2815	C	C6-N1-C2	-7.90	117.14	120.30
34	YA	856	C	C2-N1-C1'	7.89	127.48	118.80
34	YA	2465	C	C6-N1-C2	-7.88	117.15	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	RA	753	C	C5-C6-N1	7.88	124.94	121.00
34	RA	1804	C	C5-C6-N1	7.88	124.94	121.00
34	YA	915	C	C2-N1-C1'	7.87	127.46	118.80
34	RA	2210	G	C4-N9-C1'	7.87	136.73	126.50
34	YA	837	C	C5-C6-N1	7.87	124.94	121.00
34	YA	1979	C	C6-N1-C2	-7.87	117.15	120.30
34	RA	1417	C	C2-N1-C1'	7.87	127.45	118.80
1	XA	754	C	C6-N1-C1'	-7.87	111.36	120.80
22	QV	30	C	C6-N1-C2	-7.86	117.16	120.30
34	YA	392	C	C6-N1-C2	-7.86	117.16	120.30
34	YA	1882	C	C6-N1-C2	-7.85	117.16	120.30
34	YA	2416	C	C6-N1-C2	-7.85	117.16	120.30
34	RA	31	C	C5-C6-N1	7.84	124.92	121.00
34	RA	2542	A	C2-N3-C4	-7.84	106.68	110.60
34	RA	1406	U	C2-N1-C1'	7.84	127.10	117.70
34	YA	889	C	O4'-C1'-N1	7.84	114.47	108.20
34	YA	2808	U	N1-C2-O2	7.84	128.29	122.80
34	YA	2210	G	C4-N9-C1'	7.83	136.67	126.50
1	XA	1328	C	N3-C2-O2	-7.82	116.43	121.90
34	YA	930	U	C2-N1-C1'	7.82	127.08	117.70
34	YA	120	U	C2-N1-C1'	7.81	127.07	117.70
34	YA	1640	C	C2-N1-C1'	7.81	127.39	118.80
34	YA	97	C	C5-C6-N1	7.80	124.90	121.00
34	RA	2847	U	N1-C2-O2	7.80	128.26	122.80
34	YA	2416	C	C5-C6-N1	7.79	124.90	121.00
34	RA	1914	C	N1-C2-O2	7.78	123.56	118.90
34	YA	530	G	O4'-C1'-N9	7.77	114.42	108.20
34	YA	1640	C	C6-N1-C2	-7.75	117.20	120.30
28	Y4	5	ILE	N-CA-CB	7.75	128.62	110.80
28	Y4	3	GLU	C-N-CA	-7.75	106.03	122.30
1	XA	618	C	N3-C2-O2	-7.73	116.49	121.90
34	RA	1180	C	C2-N1-C1'	7.72	127.29	118.80
1	QA	1301	U	C6-N1-C1'	-7.71	110.40	121.20
1	XA	1383	C	N3-C2-O2	-7.70	116.51	121.90
34	YA	1437	C	C6-N1-C2	-7.69	117.22	120.30
34	YA	2712(A)	U	N3-C2-O2	-7.69	116.82	122.20
41	RI	82	ARG	C-N-CA	-7.69	102.48	121.70
34	YA	1313	U	N1-C2-O2	7.68	128.18	122.80
34	RA	1078	U	N1-C2-O2	7.68	128.18	122.80
34	RA	456	C	N1-C2-O2	7.67	123.50	118.90
34	YA	2666	C	N1-C2-O2	7.67	123.50	118.90
1	QA	330	C	N1-C2-O2	7.66	123.50	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	YA	1914	C	N3-C2-O2	-7.66	116.54	121.90
34	RA	912	C	C2-N1-C1'	7.65	127.21	118.80
34	YA	2063	C	C2-N1-C1'	7.64	127.20	118.80
34	YA	2394	C	N1-C2-O2	7.64	123.48	118.90
34	RA	2295	C	C5-C6-N1	7.64	124.82	121.00
35	YB	37	C	N3-C2-O2	-7.64	116.56	121.90
34	YA	1598	C	C2-N1-C1'	7.63	127.20	118.80
34	YA	1375	C	C5-C6-N1	7.62	124.81	121.00
34	YA	12	U	N3-C2-O2	-7.62	116.87	122.20
34	YA	860	U	C2-N1-C1'	7.62	126.84	117.70
14	QN	24	CYS	CA-CB-SG	7.61	127.70	114.00
1	XA	125	U	N1-C2-N3	7.58	119.45	114.90
35	RB	11	C	N3-C2-O2	-7.58	116.59	121.90
34	RA	676	A	N7-C8-N9	7.58	117.59	113.80
1	XA	1322	C	N1-C2-O2	7.57	123.44	118.90
1	QA	1358	U	C2-N1-C1'	7.56	126.77	117.70
34	YA	930	U	N1-C2-O2	7.56	128.09	122.80
34	YA	1534	G	N3-C4-C5	-7.55	124.82	128.60
20	QT	73	HIS	N-CA-CB	7.54	124.18	110.60
34	RA	2847	U	N3-C2-O2	-7.54	116.92	122.20
1	XA	221	C	N3-C2-O2	-7.54	116.62	121.90
34	YA	2787	C	C2-N1-C1'	7.54	127.09	118.80
1	QA	754	C	C6-N1-C2	-7.53	117.29	120.30
35	YB	47	C	N1-C2-O2	7.53	123.42	118.90
34	YA	1640	C	N3-C2-O2	-7.52	116.63	121.90
34	YA	806	C	N1-C2-O2	7.52	123.41	118.90
34	YA	1180	C	C5-C6-N1	7.51	124.76	121.00
34	YA	2044	C	C6-N1-C2	-7.51	117.30	120.30
34	RA	1474	C	C6-N1-C2	-7.50	117.30	120.30
34	RA	2179	C	N1-C2-O2	7.50	123.40	118.90
34	YA	1892	C	C6-N1-C2	-7.49	117.30	120.30
34	YA	1534	G	N3-C4-N9	7.48	130.49	126.00
34	YA	183	C	C6-N1-C2	-7.47	117.31	120.30
34	YA	797	C	C5-C6-N1	7.47	124.73	121.00
34	RA	120	U	C2-N1-C1'	7.46	126.66	117.70
23	QX	19	U	N3-C4-C5	-7.46	110.12	114.60
34	RA	749	C	N1-C2-O2	7.46	123.38	118.90
34	RA	456	C	C6-N1-C2	-7.46	117.32	120.30
34	RA	1881	C	C2-N1-C1'	7.46	127.00	118.80
34	YA	860	U	N1-C2-O2	7.45	128.02	122.80
34	YA	856	C	N1-C2-O2	7.45	123.37	118.90
34	YA	2321	G	C4-N9-C1'	7.43	136.16	126.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	RA	2168	G	C4-N9-C1'	7.43	136.16	126.50
34	YA	1882	C	C2-N1-C1'	7.43	126.97	118.80
34	YA	640	C	C5-C6-N1	7.43	124.71	121.00
34	YA	753	C	C6-N1-C2	-7.41	117.33	120.30
34	RA	1640	C	N3-C2-O2	-7.41	116.71	121.90
1	QA	1301	U	C5-C6-N1	7.40	126.40	122.70
36	RD	34	VAL	N-CA-C	-7.39	91.04	111.00
34	YA	930	U	N3-C2-O2	-7.39	117.02	122.20
34	YA	2032	G	C8-N9-C1'	7.39	136.61	127.00
35	YB	30	C	C6-N1-C2	-7.39	117.34	120.30
34	YA	2108	C	N1-C2-O2	7.39	123.33	118.90
34	YA	1180	C	C6-N1-C2	-7.38	117.35	120.30
1	QA	307	C	N3-C2-O2	-7.37	116.74	121.90
34	YA	41	C	C6-N1-C2	-7.37	117.35	120.30
34	RA	1180	C	C5-C6-N1	7.35	124.68	121.00
34	YA	2044	C	C5-C6-N1	7.35	124.67	121.00
34	RA	1774	C	N1-C2-O2	7.34	123.31	118.90
23	QX	18	C	O5'-P-OP2	7.34	119.51	110.70
34	RA	1406	U	C5-C6-N1	7.34	126.37	122.70
1	XA	115	G	P-O3'-C3'	7.33	128.50	119.70
34	RA	2712(A)	U	C2'-C3'-O3'	7.33	125.63	109.50
34	RA	2814	C	N1-C2-O2	7.33	123.30	118.90
34	YA	1656	C	C6-N1-C2	-7.32	117.37	120.30
34	RA	1741	C	N1-C2-O2	7.32	123.29	118.90
34	YA	1314	C	C6-N1-C2	-7.31	117.38	120.30
1	XA	1348	U	N3-C2-O2	-7.31	117.09	122.20
34	RA	2143	C	C6-N1-C2	-7.30	117.38	120.30
34	RA	2701	C	C6-N1-C2	-7.30	117.38	120.30
34	YA	2726	U	N1-C2-O2	7.30	127.91	122.80
34	RA	1267	U	N3-C2-O2	-7.30	117.09	122.20
1	QA	136	C	N1-C2-O2	7.29	123.28	118.90
1	XA	1149	C	N3-C2-O2	-7.29	116.80	121.90
34	YA	1774	C	C2-N1-C1'	7.29	126.81	118.80
1	QA	618	C	N3-C2-O2	-7.28	116.80	121.90
34	RA	1956	U	N3-C2-O2	-7.28	117.10	122.20
34	YA	1598	C	N1-C2-O2	7.28	123.27	118.90
34	RA	63	U	O4'-C1'-N1	7.27	114.02	108.20
34	YA	974(B)	C	C2-N1-C1'	7.27	126.79	118.80
34	RA	1774	C	C6-N1-C2	-7.26	117.40	120.30
1	QA	1263	C	C2-N1-C1'	7.25	126.78	118.80
34	RA	669	G	C8-N9-C1'	-7.23	117.60	127.00
34	RA	2703	C	C2-N1-C1'	7.23	126.75	118.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	XA	125	U	C6-N1-C2	-7.23	116.66	121.00
1	QA	620	C	N1-C2-O2	7.23	123.24	118.90
35	YB	31	C	N3-C2-O2	-7.22	116.84	121.90
34	YA	1375	C	C6-N1-C2	-7.22	117.41	120.30
34	RA	721	C	C2-N1-C1'	7.22	126.74	118.80
1	XA	514	C	C2-N1-C1'	7.22	126.74	118.80
34	YA	640	C	C6-N1-C2	-7.22	117.41	120.30
34	RA	114	U	C2-N1-C1'	7.21	126.36	117.70
34	YA	114	U	C2-N1-C1'	7.21	126.35	117.70
34	YA	2870	C	C6-N1-C2	-7.20	117.42	120.30
34	YA	1956	U	N1-C2-O2	7.19	127.84	122.80
1	XA	1306	A	C8-N9-C4	-7.19	102.92	105.80
34	YA	1407	C	C5-C6-N1	7.19	124.60	121.00
1	XA	1395	C	C2-N1-C1'	7.18	126.70	118.80
34	RA	2006	C	C2-N1-C1'	7.18	126.69	118.80
1	QA	136	C	C6-N1-C2	-7.17	117.43	120.30
35	YB	37	C	N1-C2-O2	7.16	123.20	118.90
22	QV	35	G	N3-C4-C5	-7.16	125.02	128.60
34	YA	650	C	C5-C6-N1	7.16	124.58	121.00
34	YA	1636	C	C6-N1-C2	-7.16	117.44	120.30
34	RA	2321	G	C4-N9-C1'	7.16	135.80	126.50
34	YA	265	A	O4'-C1'-N9	7.15	113.92	108.20
34	YA	1267	U	C2-N1-C1'	7.15	126.28	117.70
34	YA	1882	C	C5-C6-N1	7.15	124.58	121.00
34	YA	466	A	C8-N9-C4	-7.15	102.94	105.80
34	YA	1804	C	C6-N1-C2	-7.15	117.44	120.30
23	QX	17	C	N3-C2-O2	-7.15	116.90	121.90
36	YD	35	LYS	CA-CB-CG	7.14	129.12	113.40
22	QV	30	C	C2-N1-C1'	7.14	126.66	118.80
34	YA	2211	G	C4-N9-C1'	7.14	135.78	126.50
34	RA	1498	C	C2-N1-C1'	7.14	126.65	118.80
34	YA	2666	C	N3-C2-O2	-7.14	116.90	121.90
34	YA	1306	C	C5-C6-N1	7.13	124.57	121.00
34	RA	828	U	C5-C6-N1	7.13	126.26	122.70
1	QA	1228	C	C2-N1-C1'	7.12	126.64	118.80
1	XA	1537	U	OP1-P-O3'	7.12	120.86	105.20
34	YA	140	A	N7-C8-N9	7.12	117.36	113.80
34	RA	139	G	O4'-C1'-N9	-7.12	102.51	108.20
34	YA	1830	C	C2-N1-C1'	7.12	126.63	118.80
34	YA	806	C	C6-N1-C2	-7.10	117.46	120.30
34	YA	2666	C	C6-N1-C2	-7.10	117.46	120.30
34	RA	753	C	C6-N1-C2	-7.09	117.46	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	YA	1534	G	C4-N9-C1'	7.09	135.72	126.50
34	YA	2063	C	C6-N1-C2	-7.09	117.46	120.30
34	YA	2584	U	C2-N1-C1'	7.09	126.21	117.70
1	XA	498	U	N1-C2-O2	7.08	127.76	122.80
34	YA	1793	C	C6-N1-C2	-7.08	117.47	120.30
34	YA	31	C	C6-N1-C2	-7.08	117.47	120.30
1	QA	1027	C	C2-N1-C1'	7.08	126.58	118.80
1	QA	241	C	C2-N1-C1'	7.08	126.58	118.80
34	RA	2726	U	C2-N1-C1'	7.08	126.19	117.70
34	RA	1774	C	N3-C2-O2	-7.07	116.95	121.90
34	YA	231	C	C2-N1-C1'	7.06	126.57	118.80
34	RA	2580	U	C2-N1-C1'	7.06	126.17	117.70
34	YA	1506	C	C2-N1-C1'	7.05	126.56	118.80
22	XV	15	G	N3-C4-C5	-7.05	125.07	128.60
34	YA	1830	C	C5-C6-N1	7.05	124.53	121.00
34	RA	2832	U	P-O3'-C3'	7.05	128.16	119.70
34	YA	1407	C	N1-C2-O2	7.05	123.13	118.90
34	YA	2542	A	C4-C5-N7	7.04	114.22	110.70
1	QA	435	C	C5-C6-N1	7.04	124.52	121.00
34	YA	2559	C	C2-N1-C1'	7.04	126.54	118.80
1	XA	962	C	C6-N1-C2	-7.03	117.49	120.30
34	YA	721	C	C2-N1-C1'	7.03	126.53	118.80
1	QA	748	C	P-O3'-C3'	7.02	128.12	119.70
34	RA	2874	C	C2-N1-C1'	7.01	126.51	118.80
34	YA	2185	C	C6-N1-C2	-7.01	117.50	120.30
34	RA	2210	G	C8-N9-C1'	-7.00	117.90	127.00
34	YA	607	U	N1-C2-O2	7.00	127.70	122.80
34	YA	1370	C	C2-N1-C1'	7.00	126.50	118.80
34	YA	2041	U	C5-C6-N1	7.00	126.20	122.70
34	YA	537	C	C6-N1-C2	-7.00	117.50	120.30
34	YA	2032	G	N3-C4-N9	-7.00	121.80	126.00
34	RA	2683	C	N1-C2-O2	6.99	123.10	118.90
41	RI	82	ARG	O-C-N	6.99	133.89	122.70
1	XA	368	U	N3-C2-O2	-6.99	117.31	122.20
34	YA	1474	C	C2-N1-C1'	6.99	126.49	118.80
34	RA	795	C	C6-N1-C2	-6.99	117.50	120.30
34	RA	537	C	C5-C6-N1	6.97	124.48	121.00
34	YA	1332	G	C6-C5-N7	-6.97	126.22	130.40
34	YA	2712(A)	U	P-O3'-C3'	6.97	128.06	119.70
1	XA	1260	C	N1-C2-O2	6.97	123.08	118.90
34	RA	2211	G	C4-N9-C1'	6.96	135.55	126.50
35	YB	1	U	N3-C2-O2	-6.96	117.33	122.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	YA	1915	U	N1-C2-O2	6.96	127.67	122.80
34	YA	1105	U	C2-N1-C1'	6.96	126.05	117.70
1	QA	1066	C	N1-C2-O2	6.95	123.07	118.90
34	YA	1741	C	C2-N1-C1'	6.95	126.44	118.80
34	YA	2507	C	C6-N1-C2	-6.95	117.52	120.30
34	RA	2814	C	N3-C2-O2	-6.94	117.05	121.90
1	QA	1036	G	N3-C4-N9	6.93	130.16	126.00
34	YA	1830	C	C6-N1-C2	-6.93	117.53	120.30
34	YA	1306	C	C6-N1-C2	-6.93	117.53	120.30
1	QA	186(H)	C	C6-N1-C2	-6.93	117.53	120.30
34	RA	2229	C	C6-N1-C2	-6.93	117.53	120.30
20	QT	73	HIS	CB-CA-C	-6.93	96.55	110.40
34	YA	2712(A)	U	C6-N1-C2	-6.92	116.84	121.00
34	YA	1506	C	N1-C2-O2	6.92	123.05	118.90
34	YA	2617	C	N1-C2-O2	6.92	123.05	118.90
34	YA	2559	C	C6-N1-C2	-6.92	117.53	120.30
1	XA	992	U	P-O3'-C3'	6.91	127.99	119.70
34	RA	1135	C	C2-N1-C1'	6.90	126.39	118.80
35	YB	30	C	N1-C2-O2	6.90	123.04	118.90
34	RA	1686	C	C2-N1-C1'	6.90	126.39	118.80
34	YA	2083	G	N3-C4-N9	6.89	130.13	126.00
34	YA	1022	G	P-O3'-C3'	6.89	127.97	119.70
22	QV	36	G	C6-C5-N7	-6.88	126.27	130.40
34	YA	1135	C	C2-N1-C1'	6.88	126.37	118.80
34	RA	2128	C	C2-N1-C1'	6.88	126.36	118.80
34	YA	607	U	N3-C2-O2	-6.88	117.39	122.20
34	YA	1026	U	P-O3'-C3'	6.88	127.95	119.70
34	RA	904	C	N1-C2-O2	6.87	123.03	118.90
1	XA	1260	C	N3-C2-O2	-6.87	117.09	121.90
23	QX	18	C	C5-C4-N4	-6.87	115.39	120.20
34	RA	2559	C	N1-C2-O2	6.87	123.02	118.90
41	RI	131	LYS	N-CA-C	6.87	129.54	111.00
34	RA	721	C	N1-C2-O2	6.86	123.02	118.90
23	QX	18	C	N1-C2-N3	-6.86	114.40	119.20
34	RA	2703	C	C5-C6-N1	6.86	124.43	121.00
34	YA	2196	C	C2-N1-C1'	6.86	126.34	118.80
34	RA	1267	U	N1-C2-O2	6.86	127.60	122.80
34	YA	537	C	C2-N1-C1'	6.85	126.34	118.80
34	YA	2688	U	C2-N1-C1'	6.85	125.92	117.70
1	XA	1537	U	P-O3'-C3'	6.85	127.92	119.70
34	RA	372	G	OP2-P-O3'	6.85	120.27	105.20
34	RA	1314	C	C6-N1-C2	-6.85	117.56	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	YA	1781	C	N1-C2-O2	6.85	123.01	118.90
34	YA	2065	C	C6-N1-C2	-6.85	117.56	120.30
34	YA	2889	C	N1-C2-O2	6.85	123.01	118.90
35	YB	27	C	C6-N1-C2	-6.85	117.56	120.30
34	YA	1656	C	C5-C6-N1	6.84	124.42	121.00
1	XA	1149	C	N1-C2-O2	6.84	123.00	118.90
34	YA	271(C)	G	P-O3'-C3'	6.84	127.91	119.70
34	RA	1694	C	P-O3'-C3'	6.84	127.91	119.70
34	RA	1632	A	C4-C5-N7	6.83	114.11	110.70
34	RA	343	C	C6-N1-C2	-6.83	117.57	120.30
1	XA	962	C	C5-C6-N1	6.83	124.41	121.00
34	RA	828	U	C6-N1-C1'	-6.82	111.65	121.20
34	YA	141(A)	A	N7-C8-N9	6.82	117.21	113.80
34	YA	1558	A	P-O3'-C3'	6.82	127.89	119.70
34	RA	1314	C	N1-C2-O2	6.82	122.99	118.90
34	YA	846	C	P-O3'-C3'	6.82	127.88	119.70
34	YA	2210	G	C8-N9-C1'	-6.82	118.14	127.00
1	QA	1036	G	C4-N9-C1'	6.81	135.36	126.50
34	RA	1598	C	N1-C2-O2	6.81	122.98	118.90
34	RA	2544	G	C5-N7-C8	-6.80	100.90	104.30
34	YA	1892	C	C5-C6-N1	6.80	124.40	121.00
1	QA	330	C	C6-N1-C2	-6.80	117.58	120.30
1	XA	1064	G	P-O3'-C3'	6.80	127.86	119.70
1	XA	645	C	N1-C2-O2	6.80	122.98	118.90
34	YA	1920	C	C5-C6-N1	6.79	124.39	121.00
34	RA	1836	C	C6-N1-C2	-6.79	117.58	120.30
34	YA	2739	U	N1-C2-O2	6.79	127.55	122.80
34	RA	1914	C	N3-C2-O2	-6.78	117.15	121.90
34	YA	1516	U	C2-N1-C1'	6.78	125.84	117.70
23	QX	19	U	C5-C4-O4	6.78	129.97	125.90
34	YA	2666	C	C2-N1-C1'	6.78	126.26	118.80
35	YB	27	C	N3-C2-O2	-6.78	117.16	121.90
34	RA	2321	G	N3-C4-C5	-6.78	125.21	128.60
34	RA	456	C	C5-C6-N1	6.77	124.39	121.00
1	QA	992	U	P-O3'-C3'	6.77	127.82	119.70
34	RA	837	C	C5-C6-N1	6.77	124.38	121.00
34	YA	1881	C	C2-N1-C1'	6.77	126.24	118.80
35	YB	1	U	N1-C2-O2	6.77	127.54	122.80
1	XA	1296	C	N1-C2-O2	6.76	122.96	118.90
1	QA	330	C	C5-C6-N1	6.76	124.38	121.00
34	YA	41	C	C5-C6-N1	6.76	124.38	121.00
34	YA	1830	C	N1-C2-O2	6.76	122.96	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	RA	1064	C	C6-N1-C2	-6.76	117.60	120.30
1	XA	368	U	N1-C2-O2	6.76	127.53	122.80
34	RA	2507	C	C5-C6-N1	6.75	124.38	121.00
34	RA	2043	C	C5-C6-N1	6.75	124.38	121.00
34	RA	2499	C	C2-N3-C4	-6.75	116.53	119.90
1	XA	1325	C	C2-N1-C1'	6.75	126.22	118.80
34	RA	2064	C	C6-N1-C2	-6.75	117.60	120.30
42	YN	114	ARG	N-CA-C	-6.75	92.78	111.00
34	YA	537	C	N1-C2-O2	6.74	122.94	118.90
35	YB	79	C	C6-N1-C2	-6.74	117.60	120.30
34	RA	976	C	C6-N1-C2	-6.74	117.61	120.30
34	YA	985	C	C5-C6-N1	6.74	124.37	121.00
35	RB	11	C	C2-N1-C1'	6.73	126.20	118.80
1	XA	221	C	C6-N1-C2	-6.73	117.61	120.30
34	YA	1774	C	C6-N1-C2	-6.73	117.61	120.30
34	YA	2465	C	C2-N1-C1'	6.73	126.20	118.80
34	YA	141(A)	A	C5-N7-C8	-6.72	100.54	103.90
1	QA	972	C	C6-N1-C2	-6.72	117.61	120.30
34	RA	459	U	N1-C2-O2	6.72	127.50	122.80
34	YA	650	C	C6-N1-C2	-6.71	117.61	120.30
34	RA	1762	A	C5-C6-N1	6.71	121.05	117.70
34	YA	1332	G	N7-C8-N9	6.71	116.45	113.10
34	RA	2394	C	N1-C2-O2	6.70	122.92	118.90
1	XA	121	C	C5-C4-N4	-6.70	115.51	120.20
34	YA	465	G	C8-N9-C4	-6.70	103.72	106.40
22	QV	30	C	C5-C6-N1	6.70	124.35	121.00
34	RA	1417	C	C6-N1-C2	-6.69	117.62	120.30
40	YH	152	ARG	C-N-CA	6.68	138.41	121.70
34	YA	637	A	P-O3'-C3'	6.68	127.72	119.70
35	RB	27	C	N1-C2-O2	6.68	122.91	118.90
34	YA	1498	C	C2-N1-C1'	6.67	126.14	118.80
34	RA	2814	C	C2-N1-C1'	6.67	126.14	118.80
20	QT	74	LYS	CA-C-O	6.67	134.10	120.10
1	XA	1036	G	N3-C4-C5	-6.66	125.27	128.60
34	RA	1078	U	C2-N1-C1'	6.66	125.69	117.70
35	YB	80	U	N3-C2-O2	-6.66	117.54	122.20
34	RA	1558	A	P-O3'-C3'	6.65	127.69	119.70
34	RA	1882	C	C6-N1-C2	-6.65	117.64	120.30
34	RA	234	C	N1-C2-O2	6.65	122.89	118.90
34	RA	537	C	C2-N1-C1'	6.65	126.11	118.80
34	YA	2032	G	N7-C8-N9	6.65	116.42	113.10
1	QA	91	C	C2-N1-C1'	6.65	126.11	118.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	QA	596	C	C6-N1-C2	-6.65	117.64	120.30
34	YA	1914	C	C6-N1-C1'	-6.65	112.82	120.80
34	RA	1506	C	N1-C2-O2	6.64	122.89	118.90
34	YA	2032	G	C4-C5-N7	6.64	113.46	110.80
34	YA	2701	C	C6-N1-C2	-6.64	117.64	120.30
34	YA	758	C	C6-N1-C2	-6.64	117.64	120.30
1	QA	90	C	N1-C2-O2	6.64	122.88	118.90
34	YA	1332	G	C4-N9-C1'	6.64	135.13	126.50
34	YA	2703	C	C2-N1-C1'	6.64	126.10	118.80
1	QA	1075	C	N1-C2-O2	6.63	122.88	118.90
22	QV	34	C	C2-N1-C1'	6.63	126.10	118.80
34	RA	676	A	C8-N9-C4	-6.63	103.15	105.80
34	YA	2610	C	P-O3'-C3'	6.63	127.66	119.70
1	QA	501	C	C6-N1-C2	-6.63	117.65	120.30
34	YA	857	C	C2-N1-C1'	6.63	126.09	118.80
1	XA	754	C	N1-C2-O2	6.62	122.87	118.90
34	YA	2681	C	P-O3'-C3'	6.62	127.64	119.70
34	RA	2442	C	C6-N1-C2	-6.61	117.66	120.30
34	RA	1304	C	C6-N1-C2	-6.61	117.66	120.30
34	RA	67	U	C5-C6-N1	6.61	126.00	122.70
1	XA	962	C	C2-N1-C1'	6.61	126.07	118.80
34	YA	1411	C	C6-N1-C2	-6.61	117.66	120.30
22	QV	34	C	C6-N1-C1'	-6.60	112.88	120.80
34	YA	373	U	N1-C2-O2	6.60	127.42	122.80
1	QA	308	C	N1-C2-O2	6.60	122.86	118.90
34	RA	2847	U	C2-N1-C1'	6.60	125.62	117.70
1	QA	1158	C	C6-N1-C2	-6.60	117.66	120.30
19	QS	41	VAL	N-CA-C	6.60	128.82	111.00
34	YA	1474	C	C6-N1-C2	-6.60	117.66	120.30
34	YA	2779	U	C2-N1-C1'	6.60	125.62	117.70
34	YA	2460	U	C5-C6-N1	6.59	126.00	122.70
34	RA	1306	C	C5-C6-N1	6.58	124.29	121.00
34	RA	2559	C	C2-N1-C1'	6.58	126.04	118.80
34	YA	974(B)	C	N1-C2-O2	6.58	122.84	118.90
34	RA	1102	C	N1-C2-O2	6.57	122.84	118.90
34	YA	2453	A	N9-C4-C5	-6.57	103.17	105.80
34	YA	635	C	C6-N1-C2	-6.57	117.67	120.30
34	RA	1533	C	C2-N1-C1'	6.57	126.03	118.80
35	YB	1	U	C2-N1-C1'	6.57	125.58	117.70
34	YA	634	C	C6-N1-C2	-6.57	117.67	120.30
34	YA	12	U	N1-C2-O2	6.57	127.39	122.80
1	QA	1060	C	C2-N1-C1'	6.56	126.02	118.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	RA	637	A	P-O3'-C3'	6.56	127.57	119.70
34	YA	544	C	C6-N1-C2	-6.56	117.68	120.30
34	YA	1805	U	C6-N1-C2	-6.55	117.07	121.00
1	QA	838(B)	U	N3-C2-O2	-6.55	117.61	122.20
34	RA	856	C	N1-C2-O2	6.55	122.83	118.90
1	XA	201(A)	C	C2-N1-C1'	6.55	126.00	118.80
34	YA	466	A	N7-C8-N9	6.55	117.07	113.80
34	RA	2128	C	C5-C6-N1	6.54	124.27	121.00
14	XN	28	GLY	N-CA-C	6.54	129.46	113.10
34	RA	1306	C	C6-N1-C2	-6.54	117.68	120.30
34	YA	2584	U	N3-C2-O2	-6.54	117.62	122.20
1	XA	443	C	C2-N1-C1'	6.54	125.99	118.80
34	YA	856	C	N3-C2-O2	-6.54	117.32	121.90
34	YA	392	C	C5-C6-N1	6.54	124.27	121.00
34	YA	1012	U	P-O3'-C3'	6.54	127.54	119.70
34	RA	426	C	N1-C2-O2	6.53	122.82	118.90
34	YA	363(F)	U	C2-N1-C1'	6.53	125.54	117.70
1	XA	514	C	C5-C6-N1	6.53	124.27	121.00
20	QT	74	LYS	CA-C-N	-6.53	102.84	117.20
34	YA	1445	C	C6-N1-C2	-6.53	117.69	120.30
34	YA	2043	C	C5-C6-N1	6.53	124.26	121.00
34	YA	998	C	C6-N1-C2	-6.53	117.69	120.30
34	RA	2043	C	C6-N1-C2	-6.52	117.69	120.30
34	YA	1264	G	N7-C8-N9	6.52	116.36	113.10
34	RA	1267	U	C2-N1-C1'	6.52	125.52	117.70
22	QV	15	G	N3-C4-C5	-6.51	125.34	128.60
34	YA	834	C	C6-N1-C2	-6.51	117.69	120.30
1	QA	503	C	C6-N1-C2	-6.51	117.69	120.30
1	QA	1348	U	C2-N1-C1'	6.51	125.51	117.70
34	RA	2683	C	N3-C2-O2	-6.50	117.35	121.90
34	YA	384	U	N3-C2-O2	-6.50	117.65	122.20
23	QX	19	U	N1-C1'-C2'	-6.49	104.86	112.00
34	RA	846	C	P-O3'-C3'	6.49	127.49	119.70
1	QA	58	C	C5-C6-N1	6.49	124.24	121.00
34	YA	2506	U	N1-C2-O2	6.49	127.34	122.80
34	RA	1294	U	N3-C2-O2	-6.49	117.66	122.20
1	XA	1322	C	C2-N1-C1'	6.49	125.93	118.80
34	YA	1881	C	C6-N1-C2	-6.49	117.71	120.30
34	RA	1474	C	C2-N1-C1'	6.48	125.93	118.80
34	RA	1640	C	C2-N1-C1'	6.48	125.93	118.80
34	YA	2588	G	C4-C5-N7	6.48	113.39	110.80
34	YA	2816	C	C6-N1-C2	-6.48	117.71	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	YB	27	C	C2-N1-C1'	6.48	125.92	118.80
1	QA	267	C	N1-C2-O2	6.47	122.78	118.90
34	RA	2559	C	C6-N1-C2	-6.47	117.71	120.30
54	RZ	62	PRO	C-N-CA	6.47	137.86	121.70
1	XA	110	C	N1-C2-O2	6.47	122.78	118.90
34	RA	2580	U	N3-C2-O2	-6.46	117.68	122.20
1	QA	443	C	N1-C2-O2	6.46	122.78	118.90
1	QA	1395	C	N1-C2-O2	6.46	122.78	118.90
34	YA	2439	A	P-O3'-C3'	6.46	127.45	119.70
1	QA	962	C	C2-N1-C1'	6.45	125.90	118.80
34	RA	2825	C	N1-C2-O2	6.45	122.77	118.90
34	YA	2784	C	C5-C6-N1	6.45	124.22	121.00
34	YA	672	C	C6-N1-C2	-6.44	117.72	120.30
1	QA	618	C	C2-N1-C1'	6.44	125.89	118.80
34	YA	2646	C	C5-C6-N1	6.44	124.22	121.00
34	YA	1804	C	C5-C6-N1	6.44	124.22	121.00
34	RA	2507	C	C6-N1-C2	-6.44	117.72	120.30
1	XA	121	C	N3-C4-C5	6.44	124.47	121.90
34	RA	459	U	N3-C2-O2	-6.43	117.70	122.20
34	YA	459	U	C2-N1-C1'	6.43	125.42	117.70
1	QA	699	C	C6-N1-C2	-6.43	117.73	120.30
34	YA	1234	U	N3-C2-O2	-6.43	117.70	122.20
34	YA	1404	C	C6-N1-C2	-6.43	117.73	120.30
34	YA	749	C	N3-C2-O2	-6.43	117.40	121.90
1	QA	91	C	N1-C2-O2	6.42	122.75	118.90
34	YA	806	C	N3-C2-O2	-6.42	117.40	121.90
34	YA	2064	C	C6-N1-C2	-6.42	117.73	120.30
1	QA	1325	C	N1-C2-O2	6.42	122.75	118.90
34	YA	2032	G	C8-N9-C4	-6.42	103.83	106.40
34	YA	2825	C	C6-N1-C2	-6.42	117.73	120.30
1	QA	754	C	C5-C6-N1	6.42	124.21	121.00
34	RA	1313	U	C6-N1-C1'	-6.42	112.22	121.20
34	YA	484	C	C6-N1-C2	-6.42	117.73	120.30
22	QV	36	G	C5-C6-O6	-6.41	124.75	128.60
42	RN	114	ARG	N-CA-C	-6.41	93.69	111.00
34	YA	140	A	C8-N9-C4	-6.41	103.24	105.80
34	YA	1045	A	P-O3'-C3'	6.41	127.39	119.70
34	RA	755	C	C5-C6-N1	6.41	124.20	121.00
34	YA	533	G	C8-N9-C4	-6.41	103.84	106.40
22	QV	36	G	N1-C6-O6	6.40	123.74	119.90
1	QA	838(B)	U	N1-C2-O2	6.40	127.28	122.80
34	RA	837	C	C6-N1-C2	-6.40	117.74	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	YA	1881	C	C5-C6-N1	6.40	124.20	121.00
34	RA	229	A	P-O3'-C3'	6.40	127.38	119.70
30	R6	13	CYS	CA-CB-SG	-6.39	102.49	114.00
34	YA	183	C	C2-N1-C1'	6.39	125.83	118.80
34	RA	1314	C	C6-N1-C1'	-6.39	113.13	120.80
34	RA	31	C	C6-N1-C2	-6.39	117.74	120.30
34	RA	758	C	C6-N1-C2	-6.39	117.74	120.30
34	YA	1653	G	C5-C6-N1	6.39	114.69	111.50
53	RY	99	CYS	CA-CB-SG	6.39	125.50	114.00
1	XA	738	C	C6-N1-C2	-6.39	117.75	120.30
34	YA	613	U	C2-N1-C1'	6.38	125.36	117.70
1	QA	307	C	C6-N1-C2	-6.38	117.75	120.30
1	XA	68(S)	C	C6-N1-C2	-6.38	117.75	120.30
1	XA	368	U	C2-N1-C1'	6.38	125.36	117.70
1	QA	1348	U	N3-C2-O2	-6.38	117.73	122.20
34	YA	2065	C	C5-C6-N1	6.38	124.19	121.00
34	YA	183	C	N1-C2-O2	6.38	122.73	118.90
1	QA	1036	G	N3-C4-C5	-6.38	125.41	128.60
34	RA	1882	C	C5-C6-N1	6.38	124.19	121.00
22	XV	15	G	N3-C4-N9	6.38	129.83	126.00
34	YA	1498	C	N1-C2-O2	6.38	122.72	118.90
34	RA	1544	C	N1-C2-O2	6.37	122.72	118.90
34	YA	2107	C	N1-C2-O2	6.37	122.72	118.90
34	YA	1333	C	C5-C6-N1	6.37	124.18	121.00
1	QA	1263	C	N1-C2-O2	6.36	122.72	118.90
1	QA	1538	C	P-O3'-C3'	6.36	127.34	119.70
34	RA	208	C	C6-N1-C2	-6.36	117.75	120.30
23	QX	18	C	C2-N3-C4	6.36	123.08	119.90
34	RA	1022	G	C2'-C3'-O3'	6.36	123.88	113.70
34	YA	783	A	C5-N7-C8	-6.36	100.72	103.90
34	YA	1013	C	C6-N1-C2	-6.36	117.76	120.30
34	YA	2688	U	N3-C2-O2	-6.36	117.75	122.20
1	QA	1395	C	C6-N1-C2	-6.36	117.76	120.30
34	RA	2126	A	P-O3'-C3'	6.36	127.33	119.70
34	RA	1078	U	N3-C2-O2	-6.35	117.75	122.20
1	QA	1109	C	N1-C2-O2	6.35	122.71	118.90
34	YA	528	A	C5-N7-C8	-6.35	100.72	103.90
22	XV	15	G	C8-N9-C1'	-6.35	118.74	127.00
34	RA	2814	C	C6-N1-C2	-6.35	117.76	120.30
34	YA	661	C	C5-C6-N1	6.35	124.17	121.00
34	RA	1474	C	N1-C2-O2	6.35	122.71	118.90
34	RA	2043	C	C2-N1-C1'	6.34	125.78	118.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	QA	1325	C	N3-C2-O2	-6.34	117.46	121.90
1	XA	221	C	C2-N1-C1'	6.33	125.77	118.80
34	YA	1893	C	N1-C2-O2	6.33	122.70	118.90
34	RA	343	C	C5-C6-N1	6.33	124.16	121.00
34	YA	1408	C	C6-N1-C2	-6.33	117.77	120.30
1	XA	618	C	C2-N1-C1'	6.33	125.76	118.80
34	RA	965	C	C2-N1-C1'	6.32	125.75	118.80
1	QA	936	C	N1-C2-O2	6.32	122.69	118.90
34	YA	1402	C	C6-N1-C2	-6.32	117.77	120.30
34	RA	1956	U	N1-C2-O2	6.32	127.22	122.80
34	RA	2785	C	C6-N1-C2	-6.32	117.77	120.30
34	RA	459	U	C2-N1-C1'	6.32	125.28	117.70
34	YA	384	U	N1-C2-O2	6.32	127.22	122.80
34	RA	1180	C	C6-N1-C2	-6.31	117.78	120.30
34	YA	392	C	C2-N1-C1'	6.31	125.74	118.80
34	YA	242	G	P-O3'-C3'	6.31	127.27	119.70
34	YA	1653	G	P-O3'-C3'	6.31	127.27	119.70
34	YA	1406	U	C2-N1-C1'	6.31	125.27	117.70
40	YH	82	GLY	N-CA-C	6.31	128.87	113.10
34	RA	1915	U	N3-C2-O2	-6.30	117.79	122.20
42	YN	48	MET	CG-SD-CE	-6.30	90.11	100.20
34	RA	2168	G	N3-C4-C5	-6.30	125.45	128.60
1	QA	433	C	C6-N1-C2	-6.30	117.78	120.30
34	YA	1180	C	C2-N1-C1'	6.30	125.73	118.80
34	YA	1404	C	C2-N1-C1'	6.30	125.73	118.80
12	QL	104	VAL	C-N-CA	6.29	137.43	121.70
34	RA	242	G	P-O3'-C3'	6.29	127.25	119.70
34	RA	1899	G	N3-C4-N9	6.29	129.78	126.00
1	XA	972	C	C6-N1-C2	-6.29	117.78	120.30
34	YA	404	C	P-O3'-C3'	6.29	127.25	119.70
34	YA	752	A	P-O3'-C3'	6.29	127.24	119.70
1	XA	1306	A	N7-C8-N9	6.28	116.94	113.80
34	YA	985	C	C2-N1-C1'	6.28	125.71	118.80
1	QA	90	C	C6-N1-C2	-6.28	117.79	120.30
34	YA	2559	C	C5-C6-N1	6.28	124.14	121.00
1	XA	18	C	C5-C6-N1	6.28	124.14	121.00
1	XA	1383	C	C6-N1-C2	-6.28	117.79	120.30
34	RA	2295	C	C6-N1-C2	-6.27	117.79	120.30
34	YA	1026	U	OP1-P-O3'	6.27	119.00	105.20
34	YA	1774	C	C5-C6-N1	6.27	124.14	121.00
1	QA	962	C	N1-C2-O2	6.27	122.66	118.90
34	YA	1915	U	N3-C2-O2	-6.27	117.81	122.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	RA	271(C)	G	P-O3'-C3'	6.27	127.22	119.70
1	XA	1260	C	C6-N1-C2	-6.27	117.79	120.30
34	RA	915	C	C2-N1-C1'	6.26	125.69	118.80
34	RA	104	U	N1-C2-O2	6.26	127.18	122.80
1	XA	1290	G	C4-N9-C1'	6.26	134.64	126.50
1	XA	736	C	C6-N1-C2	-6.26	117.80	120.30
34	YA	1833	U	N3-C2-O2	-6.26	117.82	122.20
34	RA	1950	G	C4-N9-C1'	6.26	134.63	126.50
34	RA	2179	C	N3-C2-O2	-6.26	117.52	121.90
34	YA	1411	C	C5-C6-N1	6.25	124.13	121.00
34	RA	1087	G	O4'-C1'-N9	-6.25	103.20	108.20
34	RA	229	A	OP2-P-O3'	6.25	118.94	105.20
34	RA	537	C	C6-N1-C2	-6.25	117.80	120.30
34	RA	2439	A	P-O3'-C3'	6.25	127.20	119.70
34	RA	456	C	N3-C2-O2	-6.25	117.53	121.90
34	YA	985	C	N1-C2-O2	6.24	122.64	118.90
34	YA	691	C	C6-N1-C2	-6.24	117.80	120.30
34	YA	2766	G	C4-N9-C1'	6.24	134.61	126.50
35	RB	27	C	N3-C2-O2	-6.24	117.53	121.90
1	QA	455	C	N1-C2-O2	6.24	122.64	118.90
1	XA	1158	C	C5-C6-N1	6.24	124.12	121.00
34	YA	2211	G	C8-N9-C1'	-6.24	118.89	127.00
1	XA	54	C	N1-C2-O2	6.23	122.64	118.90
34	RA	2542	A	N9-C4-C5	-6.23	103.31	105.80
34	YA	377	C	C5-C6-N1	6.23	124.11	121.00
1	QA	1097	C	N1-C2-O2	6.23	122.64	118.90
34	YA	1982	C	C2-N1-C1'	6.23	125.65	118.80
35	YB	30	C	C2-N1-C1'	6.23	125.65	118.80
34	RA	1920	C	C5-C6-N1	6.22	124.11	121.00
34	YA	834	C	C5-C6-N1	6.22	124.11	121.00
34	YA	1437	C	C5-C6-N1	6.22	124.11	121.00
34	YA	393	C	C6-N1-C2	-6.22	117.81	120.30
34	YA	1950	G	C4-N9-C1'	6.22	134.59	126.50
22	QV	36	G	N7-C8-N9	6.22	116.21	113.10
1	QA	960	U	C2-N1-C1'	6.22	125.16	117.70
1	QA	1228	C	N1-C2-O2	6.22	122.63	118.90
34	RA	269	U	N3-C2-O2	-6.22	117.85	122.20
22	XV	31	G	C4-N9-C1'	6.22	134.58	126.50
34	YA	904	C	N3-C2-O2	-6.22	117.55	121.90
34	RA	1983	C	C6-N1-C2	-6.21	117.81	120.30
38	RF	197	ASP	N-CA-C	-6.21	94.22	111.00
34	YA	1992	G	P-O3'-C3'	6.21	127.16	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RB	22	U	C2-N1-C1'	6.21	125.16	117.70
34	YA	915	C	C6-N1-C2	-6.21	117.82	120.30
22	QV	30	C	N1-C2-O2	6.21	122.62	118.90
34	RA	1304	C	C2-N1-C1'	6.21	125.63	118.80
34	YA	613	U	N1-C2-O2	6.21	127.14	122.80
34	YA	2211	G	N3-C4-N9	6.21	129.72	126.00
34	YA	2099	U	C5-C6-N1	6.20	125.80	122.70
34	YA	2108	C	N3-C2-O2	-6.20	117.56	121.90
34	YA	1178	C	C6-N1-C2	-6.20	117.82	120.30
1	QA	328	C	P-O3'-C3'	6.20	127.13	119.70
34	YA	420	C	C2-N1-C1'	6.20	125.61	118.80
1	XA	893	C	N1-C2-O2	6.19	122.62	118.90
34	YA	1653	G	N3-C4-N9	6.19	129.71	126.00
34	YA	2006	C	N1-C2-O2	6.19	122.61	118.90
1	QA	252	U	N3-C2-O2	-6.18	117.87	122.20
34	RA	2128	C	N1-C2-O2	6.18	122.61	118.90
7	QG	73	MET	N-CA-CB	-6.18	99.47	110.60
34	YA	2126	A	P-O3'-C3'	6.18	127.12	119.70
1	QA	620	C	C2-N1-C1'	6.18	125.59	118.80
1	XA	241	C	C2-N1-C1'	6.18	125.59	118.80
35	RB	66	A	P-O3'-C3'	6.17	127.11	119.70
34	RA	1533	C	N1-C2-O2	6.17	122.60	118.90
34	RA	1498	C	N1-C2-O2	6.17	122.60	118.90
34	RA	1312	U	P-O3'-C3'	6.16	127.10	119.70
1	XA	68(R)	U	N1-C2-O2	6.16	127.11	122.80
34	RA	2825	C	N3-C2-O2	-6.16	117.59	121.90
34	YA	974(B)	C	P-O3'-C3'	6.15	127.08	119.70
35	YB	47	C	N3-C2-O2	-6.15	117.59	121.90
1	QA	90	C	C6-N1-C1'	-6.15	113.42	120.80
35	RB	11	C	C6-N1-C2	-6.15	117.84	120.30
22	QV	36	G	C4-C5-N7	6.15	113.26	110.80
34	RA	200	U	N3-C2-O2	-6.15	117.90	122.20
34	YA	114	U	C5-C6-N1	6.15	125.77	122.70
34	YA	229	A	P-O3'-C3'	6.14	127.07	119.70
34	YA	1982	C	C5-C6-N1	6.14	124.07	121.00
34	YA	198	C	C2-N1-C1'	6.14	125.55	118.80
34	YA	420	C	N1-C2-O2	6.14	122.58	118.90
22	QV	15	G	C4-N9-C1'	6.14	134.48	126.50
1	XA	18	C	C6-N1-C2	-6.13	117.85	120.30
34	YA	985	C	C6-N1-C2	-6.13	117.85	120.30
34	YA	1267	U	N3-C2-O2	-6.13	117.91	122.20
34	YA	669	G	C4-N9-C1'	6.13	134.47	126.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	RI	10	GLU	C-N-CA	6.13	137.02	121.70
1	XA	618	C	C6-N1-C2	-6.13	117.85	120.30
1	XA	620	C	N1-C2-O2	6.12	122.58	118.90
34	RA	923	C	C5-C6-N1	6.12	124.06	121.00
34	RA	2703	C	N1-C2-O2	6.12	122.57	118.90
34	YA	2320	A	C2-N3-C4	6.12	113.66	110.60
34	RA	222	A	P-O3'-C3'	6.12	127.04	119.70
1	XA	237	C	N3-C4-C5	-6.12	119.45	121.90
1	XA	525	C	C5-C6-N1	6.12	124.06	121.00
23	QX	16	C	C6-N1-C2	-6.12	117.85	120.30
34	RA	269	U	N1-C2-O2	6.12	127.08	122.80
34	RA	2480	C	N3-C2-O2	-6.11	117.62	121.90
1	QA	1036	G	C8-N9-C1'	-6.11	119.06	127.00
1	QA	1039	C	N3-C2-O2	-6.11	117.62	121.90
1	QA	91	C	C6-N1-C2	-6.11	117.86	120.30
1	QA	1395	C	C6-N1-C1'	-6.11	113.47	120.80
34	RA	385	C	C6-N1-C2	-6.11	117.86	120.30
35	YB	27	C	C5-C6-N1	6.11	124.05	121.00
34	YA	2889	C	C6-N1-C2	-6.10	117.86	120.30
34	RA	2295	C	C2-N1-C1'	6.10	125.51	118.80
23	QX	17	C	N1-C2-N3	6.10	123.47	119.20
34	RA	1549	C	C2-N1-C1'	6.10	125.51	118.80
34	RA	1882	C	N1-C2-O2	6.10	122.56	118.90
1	XA	514	C	C6-N1-C2	-6.10	117.86	120.30
34	YA	2787	C	N1-C2-O2	6.10	122.56	118.90
1	QA	381	C	N1-C2-O2	6.09	122.56	118.90
34	RA	2043	C	N1-C2-O2	6.09	122.56	118.90
22	QV	62	C	C5-C6-N1	6.09	124.05	121.00
1	QA	1109	C	N3-C2-O2	-6.09	117.64	121.90
34	RA	912	C	N1-C2-O2	6.09	122.56	118.90
34	RA	1915	U	N1-C2-O2	6.09	127.06	122.80
34	RA	1314	C	C5-C6-N1	6.09	124.05	121.00
34	RA	1427	A	P-O3'-C3'	6.09	127.01	119.70
36	RD	33	LEU	CA-CB-CG	6.09	129.31	115.30
34	YA	1314	C	C5-C6-N1	6.09	124.05	121.00
34	YA	2776	A	P-O3'-C3'	6.09	127.01	119.70
34	RA	2471	C	C6-N1-C2	-6.09	117.87	120.30
34	RA	1742	C	C6-N1-C2	-6.08	117.87	120.30
1	XA	68(S)	C	C5-C6-N1	6.08	124.04	121.00
1	QA	90	C	C5-C6-N1	6.08	124.04	121.00
34	RA	2456	C	C6-N1-C2	-6.08	117.87	120.30
34	RA	2776	A	P-O3'-C3'	6.08	126.99	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	YA	2260	C	C6-N1-C2	-6.08	117.87	120.30
1	QA	1113	C	C6-N1-C2	-6.08	117.87	120.30
34	RA	1462	C	N3-C2-O2	-6.08	117.65	121.90
22	XV	40	G	C4-N9-C1'	6.08	134.40	126.50
34	RA	912	C	C6-N1-C2	-6.08	117.87	120.30
34	RA	2168	G	C8-N9-C1'	-6.07	119.10	127.00
1	XA	54	C	N3-C2-O2	-6.07	117.65	121.90
34	YA	2889	C	C5-C6-N1	6.07	124.04	121.00
34	YA	456	C	N1-C2-O2	6.07	122.54	118.90
34	RA	2471	C	C2-N1-C1'	6.07	125.47	118.80
1	XA	201(A)	C	N1-C2-O2	6.07	122.54	118.90
34	YA	1506	C	C5-C6-N1	6.07	124.03	121.00
34	YA	2474	C	N1-C2-O2	6.07	122.54	118.90
34	YA	1121	C	C6-N1-C2	-6.06	117.88	120.30
1	QA	736	C	C6-N1-C2	-6.06	117.88	120.30
34	RA	372	G	P-O3'-C3'	6.06	126.97	119.70
34	RA	876	C	N1-C2-O2	6.06	122.53	118.90
34	RA	1658	C	C5-C6-N1	6.06	124.03	121.00
34	YA	2506	U	C2-N1-C1'	6.06	124.97	117.70
34	RA	2210	G	N3-C4-N9	6.05	129.63	126.00
34	RA	2512	C	C5-C6-N1	6.05	124.03	121.00
34	RA	2254	C	C6-N1-C2	-6.05	117.88	120.30
34	YA	1544	C	N1-C2-O2	6.05	122.53	118.90
34	YA	2041	U	C6-N1-C2	-6.05	117.37	121.00
1	QA	1027	C	N1-C2-O2	6.05	122.53	118.90
34	YA	2712(A)	U	N1-C2-O2	6.05	127.03	122.80
1	QA	1075	C	C2-N1-C1'	6.05	125.45	118.80
34	YA	1894	C	C6-N1-C2	-6.05	117.88	120.30
1	QA	687	A	P-O3'-C3'	6.04	126.95	119.70
1	QA	1325	C	C2-N1-C1'	6.04	125.45	118.80
1	XA	1322	C	N3-C2-O2	-6.04	117.67	121.90
34	RA	2544	G	C4-C5-N7	6.04	113.21	110.80
40	RH	87	LEU	N-CA-CB	-6.04	98.33	110.40
1	XA	582	U	N3-C2-O2	-6.04	117.97	122.20
34	YA	1535	U	C6-N1-C1'	-6.04	112.75	121.20
34	RA	1950	G	O4'-C1'-N9	6.03	113.02	108.20
34	YA	333	G	C4-N9-C1'	6.03	134.34	126.50
34	YA	200	U	N3-C2-O2	-6.02	117.98	122.20
34	RA	2307	G	C4-N9-C1'	6.02	134.32	126.50
1	XA	723	U	N1-C2-O2	6.02	127.01	122.80
34	YA	1799	G	P-O3'-C3'	6.02	126.92	119.70
34	YA	1462	C	N1-C2-O2	6.02	122.51	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	YA	634	C	C5-C6-N1	6.01	124.01	121.00
34	RA	2006	C	C6-N1-C2	-6.01	117.89	120.30
1	XA	1395	C	C6-N1-C2	-6.01	117.90	120.30
34	YA	1636	C	N3-C2-O2	-6.01	117.69	121.90
34	RA	1899	G	N1-C2-N2	-6.01	110.79	116.20
34	RA	2053	G	C4-C5-N7	6.01	113.20	110.80
34	RA	1135	C	N3-C2-O2	-6.01	117.70	121.90
34	RA	2032	G	C5-N7-C8	-6.00	101.30	104.30
1	QA	697	U	N3-C2-O2	-6.00	118.00	122.20
34	RA	9	U	N3-C2-O2	-6.00	118.00	122.20
41	RI	130	TYR	C-N-CA	6.00	136.70	121.70
34	YA	2210	G	N3-C4-N9	6.00	129.60	126.00
1	XA	1114	C	C6-N1-C2	-5.99	117.90	120.30
34	YA	755	C	C6-N1-C2	-5.99	117.90	120.30
22	QV	31	G	C4-N9-C1'	5.99	134.28	126.50
34	RA	1982	C	N1-C2-O2	5.99	122.49	118.90
34	YA	2868	A	C5-N7-C8	-5.99	100.91	103.90
1	QA	455	C	C2-N1-C1'	5.98	125.38	118.80
34	RA	904	C	N3-C2-O2	-5.98	117.71	121.90
1	XA	455	C	C2-N1-C1'	5.98	125.38	118.80
34	YA	1893	C	N3-C2-O2	-5.98	117.71	121.90
35	YB	66	A	P-O3'-C3'	5.98	126.88	119.70
1	QA	960	U	N1-C2-O2	5.98	126.98	122.80
34	RA	669	G	N3-C4-N9	5.98	129.59	126.00
34	YA	806	C	C5-C6-N1	5.97	123.99	121.00
34	YA	1427	A	P-O3'-C3'	5.97	126.87	119.70
35	YB	31	C	C2-N1-C1'	5.97	125.37	118.80
34	RA	1370	C	N1-C2-O2	5.96	122.48	118.90
34	YA	923	C	C5-C6-N1	5.96	123.98	121.00
34	YA	1297	C	C6-N1-C2	-5.96	117.92	120.30
34	YA	1417	C	C5-C6-N1	5.96	123.98	121.00
34	RA	1799	G	P-O3'-C3'	5.96	126.85	119.70
34	RA	2766	G	C4-N9-C1'	5.95	134.24	126.50
41	RI	82	ARG	CA-C-N	-5.95	104.10	117.20
34	RA	766	C	C6-N1-C2	-5.95	117.92	120.30
34	RA	1741	C	C2-N1-C1'	5.95	125.35	118.80
34	YA	2226	C	N1-C2-O2	5.95	122.47	118.90
1	QA	993	G	N3-C4-N9	5.95	129.57	126.00
34	RA	1533	C	C5-C6-N1	5.95	123.97	121.00
34	RA	74	A	N3-C4-N9	-5.95	122.64	127.40
34	YA	74	A	O4'-C1'-N9	-5.95	103.44	108.20
34	YA	1534	G	C2-N3-C4	5.94	114.87	111.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	RA	752	A	P-O3'-C3'	5.94	126.83	119.70
1	XA	1301	U	C6-N1-C2	-5.94	117.43	121.00
34	YA	104	U	N3-C2-O2	-5.94	118.04	122.20
34	RA	1130	U	P-O3'-C3'	5.94	126.83	119.70
34	RA	1468	C	C6-N1-C2	-5.94	117.92	120.30
1	XA	328	C	P-O3'-C3'	5.94	126.83	119.70
35	YB	47	C	C2-N1-C1'	5.94	125.33	118.80
1	QA	186(H)	C	C6-N1-C1'	5.94	127.92	120.80
34	RA	806	C	C6-N1-C2	-5.94	117.92	120.30
34	RA	41	C	C2-N1-C1'	5.93	125.33	118.80
1	XA	498	U	C2-N1-C1'	5.93	124.82	117.70
34	YA	1333	C	C6-N1-C2	-5.93	117.93	120.30
34	RA	2726	U	N1-C2-O2	5.93	126.95	122.80
34	RA	2229	C	N3-C4-C5	-5.93	119.53	121.90
34	RA	1774	C	C2-N1-C1'	5.93	125.32	118.80
34	RA	2784	C	C5-C6-N1	5.93	123.96	121.00
34	YA	99	U	P-O3'-C3'	5.93	126.81	119.70
34	RA	1462	C	N1-C2-O2	5.92	122.45	118.90
22	QV	31	G	N3-C4-C5	-5.92	125.64	128.60
35	YB	30	C	C5-C6-N1	5.92	123.96	121.00
34	RA	2065	C	C5-C6-N1	5.92	123.96	121.00
34	YA	530	G	N1-C6-O6	-5.92	116.35	119.90
34	YA	2321	G	C8-N9-C4	-5.92	104.03	106.40
34	RA	1644	C	C6-N1-C2	-5.92	117.93	120.30
34	RA	63	U	C4'-C3'-O3'	5.91	124.82	113.00
34	YA	1362	C	C6-N1-C2	-5.91	117.94	120.30
28	Y4	5	ILE	CA-CB-CG1	5.91	122.22	111.00
34	YA	198	C	N1-C2-O2	5.91	122.44	118.90
34	YA	2483	C	C6-N1-C2	-5.91	117.94	120.30
1	QA	1060	C	C6-N1-C2	-5.90	117.94	120.30
1	XA	1036	G	N3-C4-N9	5.90	129.54	126.00
34	YA	2507	C	C5-C6-N1	5.90	123.95	121.00
34	RA	1833	U	N3-C2-O2	-5.90	118.07	122.20
34	YA	1694	C	P-O3'-C3'	5.90	126.78	119.70
34	YA	2544	G	N7-C8-N9	5.90	116.05	113.10
1	QA	955	U	C5-C6-N1	5.90	125.65	122.70
34	RA	2580	U	N1-C2-O2	5.90	126.93	122.80
34	RA	1779	U	C2-N1-C1'	5.89	124.77	117.70
34	YA	377	C	C6-N1-C2	-5.89	117.94	120.30
34	RA	544	C	C2-N1-C1'	5.89	125.28	118.80
34	RA	141(B)	C	C6-N1-C2	-5.89	117.94	120.30
34	RA	624	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(°)
34	YA	1013	C	C5-C6-N1	5.89	123.94	121.00
34	YA	974(B)	C	N3-C2-O2	-5.88	117.78	121.90
34	YA	2566	A	P-O3'-C3'	5.88	126.76	119.70
34	YA	967	C	C6-N1-C2	-5.88	117.95	120.30
1	QA	866	C	C5-C6-N1	5.88	123.94	121.00
34	YA	97	C	C2-N1-C1'	5.88	125.27	118.80
34	RA	1045	A	P-O3'-C3'	5.88	126.75	119.70
34	RA	138	G	O4'-C1'-N9	5.87	112.90	108.20
34	RA	634	C	C6-N1-C2	-5.87	117.95	120.30
34	RA	2006	C	N1-C2-O2	5.87	122.42	118.90
34	YA	143	C	C5-C6-N1	5.87	123.94	121.00
34	YA	957	A	C5-C6-N6	-5.87	119.00	123.70
34	RA	1741	C	N3-C2-O2	-5.87	117.79	121.90
34	RA	209	C	C5-C6-N1	5.87	123.93	121.00
34	YA	731	C	C6-N1-C2	-5.86	117.95	120.30
34	RA	1376	C	C5-C6-N1	5.86	123.93	121.00
34	YA	528	A	C4-C5-N7	5.86	113.63	110.70
1	XA	962	C	N1-C2-O2	5.86	122.42	118.90
34	YA	2703	C	C5-C6-N1	5.86	123.93	121.00
1	QA	1228	C	C6-N1-C2	-5.86	117.96	120.30
1	XA	1539	C	N3-C4-N4	-5.86	113.90	118.00
54	RZ	59	LEU	CA-CB-CG	5.86	128.77	115.30
34	YA	2243	U	N3-C2-O2	-5.85	118.10	122.20
34	RA	676	A	C5-N7-C8	-5.85	100.97	103.90
1	XA	1260	C	C2-N1-C1'	5.85	125.24	118.80
34	YA	67	U	C5-C6-N1	5.85	125.63	122.70
34	RA	2666	C	C6-N1-C2	-5.85	117.96	120.30
34	YA	1920	C	C6-N1-C2	-5.85	117.96	120.30
34	YA	2243	U	N1-C2-N3	5.85	118.41	114.90
34	YA	2504	U	N1-C2-O2	5.85	126.89	122.80
34	YA	976	C	C6-N1-C2	-5.85	117.96	120.30
4	XD	8	VAL	CG1-CB-CG2	5.84	120.25	110.90
34	YA	195	A	P-O3'-C3'	5.84	126.71	119.70
34	RA	2689	U	P-O3'-C3'	5.84	126.71	119.70
34	YA	267	C	C5-C6-N1	5.84	123.92	121.00
34	RA	512	G	P-O3'-C3'	5.84	126.71	119.70
34	RA	1644	C	N3-C2-O2	-5.84	117.81	121.90
34	YA	221	A	P-O3'-C3'	5.84	126.71	119.70
34	YA	2321	G	N3-C4-C5	-5.84	125.68	128.60
34	YA	1915	U	C2-N1-C1'	5.84	124.71	117.70
1	QA	1323	G	N3-C4-N9	5.83	129.50	126.00
34	RA	834	C	C6-N1-C2	-5.83	117.97	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	XA	891	U	N3-C2-O2	-5.83	118.12	122.20
1	QA	1303	C	C2-N1-C1'	5.83	125.22	118.80
1	QA	1290	G	C4-N9-C1'	5.83	134.08	126.50
34	RA	2517	C	C6-N1-C2	-5.83	117.97	120.30
1	XA	993	G	C4-N9-C1'	5.83	134.08	126.50
34	YA	2779	U	N3-C2-O2	-5.83	118.12	122.20
1	XA	1113	C	C6-N1-C2	-5.83	117.97	120.30
1	XA	1296	C	N3-C2-O2	-5.83	117.82	121.90
1	QA	136	C	C5-C6-N1	5.83	123.91	121.00
34	RA	650	C	C6-N1-C2	-5.82	117.97	120.30
34	YA	486	C	C6-N1-C2	-5.82	117.97	120.30
34	YA	503	A	OP2-P-O3'	5.82	118.01	105.20
34	YA	1437	C	C2-N1-C1'	5.82	125.21	118.80
34	YA	2211	G	N3-C4-C5	-5.82	125.69	128.60
34	YA	2254	C	C6-N1-C2	-5.82	117.97	120.30
32	R8	62	LEU	CA-CB-CG	5.82	128.69	115.30
34	YA	1293	C	C5-C6-N1	5.82	123.91	121.00
34	RA	2582	G	C4-N9-C1'	5.82	134.06	126.50
34	YA	1314	C	N1-C2-O2	5.82	122.39	118.90
34	YA	2615	U	C2-N1-C1'	5.82	124.68	117.70
34	YA	2815	C	C5-C6-N1	5.82	123.91	121.00
28	Y4	5	ILE	CA-CB-CG2	-5.82	99.27	110.90
1	QA	582	U	N3-C2-O2	-5.81	118.13	122.20
34	RA	2688	U	C2-N1-C1'	5.81	124.67	117.70
34	YA	580	C	C5-C6-N1	5.81	123.91	121.00
34	YA	930	U	C5-C6-N1	5.81	125.61	122.70
34	YA	967	C	C5-C6-N1	5.81	123.91	121.00
34	YA	1234	U	N1-C2-O2	5.81	126.87	122.80
1	QA	1285	A	P-O3'-C3'	5.81	126.67	119.70
34	YA	672	C	C5-C6-N1	5.81	123.91	121.00
34	YA	859	G	P-O3'-C3'	5.81	126.67	119.70
34	RA	1819	A	P-O3'-C3'	5.81	126.67	119.70
34	RA	2785	C	C5-C6-N1	5.80	123.90	121.00
34	YA	234	C	N1-C2-O2	5.80	122.38	118.90
34	YA	503	A	P-O3'-C3'	5.80	126.66	119.70
1	QA	1060	C	C5-C6-N1	5.80	123.90	121.00
34	RA	209	C	C6-N1-C2	-5.80	117.98	120.30
34	RA	776	G	C4-N9-C1'	5.80	134.04	126.50
34	YA	1293	C	C6-N1-C2	-5.80	117.98	120.30
12	XL	47	LYS	N-CA-C	5.80	126.66	111.00
34	YA	556	G	C6-C5-N7	-5.80	126.92	130.40
34	YA	2808	U	C2-N1-C1'	5.80	124.66	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	RA	1474	C	C5-C6-N1	5.79	123.90	121.00
1	QA	1499	A	P-O3'-C3'	5.79	126.65	119.70
34	YA	485	C	C6-N1-C2	-5.79	117.98	120.30
34	YA	1534	G	C8-N9-C1'	-5.79	119.47	127.00
34	RA	392	C	C2-N1-C1'	5.79	125.17	118.80
34	RA	1920	C	C6-N1-C2	-5.79	117.98	120.30
34	YA	114	U	N1-C2-O2	5.79	126.85	122.80
34	YA	758	C	N3-C2-O2	-5.79	117.85	121.90
34	YA	1519	G	C4-N9-C1'	5.79	134.03	126.50
34	YA	1537	C	C6-N1-C2	-5.78	117.99	120.30
1	QA	433	C	N3-C2-O2	-5.78	117.85	121.90
34	YA	2739	U	C6-N1-C2	-5.78	117.53	121.00
1	XA	1322	C	C6-N1-C2	-5.78	117.99	120.30
34	RA	2175	C	C5-C6-N1	5.78	123.89	121.00
34	YA	1988	C	C6-N1-C2	-5.78	117.99	120.30
34	RA	9	U	N1-C2-O2	5.77	126.84	122.80
34	RA	1658	C	C6-N1-C2	-5.77	117.99	120.30
34	RA	2646	C	C6-N1-C2	-5.77	117.99	120.30
34	RA	797	C	C5-C6-N1	5.77	123.88	121.00
34	RA	1881	C	N1-C2-O2	5.77	122.36	118.90
34	RA	669	G	N3-C4-C5	-5.76	125.72	128.60
34	RA	1430	C	C5-C6-N1	5.76	123.88	121.00
1	QA	618	C	C6-N1-C2	-5.76	118.00	120.30
34	YA	426	C	N1-C2-O2	5.76	122.36	118.90
34	RA	1430	C	C6-N1-C2	-5.76	118.00	120.30
34	YA	1188	U	N1-C2-O2	5.76	126.83	122.80
34	YA	1468	C	C6-N1-C2	-5.76	118.00	120.30
34	RA	1762	A	N1-C2-N3	5.75	132.18	129.30
34	YA	1314	C	C6-N1-C1'	-5.75	113.89	120.80
1	QA	1066	C	C2-N1-C1'	5.75	125.13	118.80
34	YA	155	C	C6-N1-C2	-5.75	118.00	120.30
34	YA	2784	C	C6-N1-C2	-5.75	118.00	120.30
34	YA	140	A	C5-N7-C8	-5.75	101.03	103.90
34	YA	613	U	N3-C2-O2	-5.75	118.18	122.20
1	QA	620	C	N3-C2-O2	-5.75	117.88	121.90
34	YA	2504	U	N3-C2-O2	-5.75	118.18	122.20
34	RA	1258	C	C6-N1-C2	-5.74	118.00	120.30
22	XV	56	C	N1-C2-O2	5.74	122.35	118.90
34	YA	196	A	O4'-C1'-N9	5.74	112.80	108.20
34	YA	267	C	C6-N1-C2	-5.74	118.00	120.30
34	YA	721	C	C6-N1-C2	-5.74	118.00	120.30
34	YA	1474	C	C5-C6-N1	5.74	123.87	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	YA	1979	C	C5-C6-N1	5.74	123.87	121.00
1	QA	838(B)	U	C2-N1-C1'	5.74	124.59	117.70
34	RA	1304	C	C5-C6-N1	5.74	123.87	121.00
34	YA	234	C	N3-C2-O2	-5.74	117.88	121.90
34	YA	1313	U	C6-N1-C1'	-5.74	113.16	121.20
34	YA	2576	G	C4-N9-C1'	5.74	133.96	126.50
1	XA	312	C	C6-N1-C2	-5.74	118.00	120.30
1	XA	1149	C	C6-N1-C2	-5.74	118.00	120.30
1	XA	596	C	C6-N1-C2	-5.73	118.01	120.30
22	XV	15	G	C8-N9-C4	-5.73	104.11	106.40
34	YA	1012	U	OP2-P-O3'	5.73	117.81	105.20
34	YA	2089	U	C5-C6-N1	5.73	125.57	122.70
34	YA	2870	C	N3-C2-O2	-5.73	117.89	121.90
34	YA	1102	C	N1-C2-O2	5.73	122.34	118.90
1	QA	136	C	N3-C2-O2	-5.73	117.89	121.90
34	RA	976	C	C5-C6-N1	5.73	123.86	121.00
34	RA	1078	U	C5-C6-N1	5.73	125.56	122.70
34	RA	1404	C	N1-C2-O2	5.73	122.34	118.90
34	YA	1140	C	N1-C2-O2	5.73	122.34	118.90
14	QN	43	CYS	CB-CA-C	5.72	121.85	110.40
34	RA	384	U	N1-C2-O2	5.72	126.81	122.80
34	RA	1075	C	N3-C2-O2	-5.72	117.89	121.90
35	RB	27	C	C2-N1-C1'	5.72	125.10	118.80
34	YA	2506	U	N3-C2-O2	-5.72	118.19	122.20
34	YA	1679	U	N3-C2-O2	-5.72	118.19	122.20
34	RA	856	C	P-O3'-C3'	5.72	126.56	119.70
34	RA	1406	U	N1-C2-O2	5.72	126.80	122.80
34	YA	485	C	C5-C6-N1	5.72	123.86	121.00
34	RA	234	C	N3-C2-O2	-5.71	117.90	121.90
34	RA	1882	C	C6-N1-C1'	-5.71	113.95	120.80
34	RA	1899	G	N3-C2-N2	5.71	123.90	119.90
34	YA	2490	G	C4-N9-C1'	5.71	133.92	126.50
34	RA	640	C	C5-C6-N1	5.71	123.86	121.00
34	RA	2060	A	P-O3'-C3'	5.70	126.54	119.70
34	RA	2584	U	N3-C2-O2	-5.70	118.21	122.20
1	XA	330	C	N1-C2-O2	5.70	122.32	118.90
1	QA	353	A	OP2-P-O3'	5.70	117.74	105.20
34	RA	2321	G	C8-N9-C4	-5.70	104.12	106.40
34	YA	640	C	C2-N1-C1'	5.70	125.07	118.80
34	YA	965	C	C5-C6-N1	5.70	123.85	121.00
34	RA	1914	C	C6-N1-C2	-5.70	118.02	120.30
35	YB	60	C	C6-N1-C2	-5.70	118.02	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	YA	1233	C	C6-N1-C2	-5.70	118.02	120.30
34	RA	1404	C	C6-N1-C2	-5.69	118.02	120.30
1	XA	596	C	N1-C2-O2	5.69	122.31	118.90
1	XA	736	C	C5-C6-N1	5.69	123.84	121.00
34	YA	1819	A	P-O3'-C3'	5.69	126.53	119.70
34	YA	1982	C	N1-C2-O2	5.69	122.31	118.90
1	QA	960	U	N3-C2-O2	-5.68	118.22	122.20
34	RA	2226	C	N1-C2-O2	5.68	122.31	118.90
35	RB	60	C	C5-C6-N1	5.68	123.84	121.00
34	YA	363(F)	U	N1-C2-O2	5.68	126.78	122.80
34	RA	2566	A	P-O3'-C3'	5.68	126.51	119.70
34	RA	2512	C	C6-N1-C2	-5.68	118.03	120.30
34	RA	2584	U	C2-N1-C1'	5.67	124.51	117.70
34	YA	2584	U	N1-C2-O2	5.67	126.77	122.80
34	RA	1005	C	C2-N1-C1'	5.67	125.04	118.80
34	YA	2588	G	C6-C5-N7	-5.67	127.00	130.40
34	RA	1295	C	C6-N1-C2	-5.67	118.03	120.30
1	XA	993	G	C8-N9-C1'	-5.67	119.63	127.00
34	YA	1775	U	C5-C4-O4	-5.67	122.50	125.90
34	RA	65	C	N1-C2-O2	5.67	122.30	118.90
34	YA	2098	U	N1-C2-O2	5.67	126.77	122.80
45	YQ	19	GLY	N-CA-C	-5.67	98.93	113.10
1	XA	1262	C	C5-C6-N1	5.67	123.83	121.00
34	RA	271(C)	G	OP2-P-O3'	5.66	117.66	105.20
34	YA	1399	C	C6-N1-C2	-5.66	118.03	120.30
34	YA	231	C	C6-N1-C1'	-5.66	114.01	120.80
34	YA	1774	C	N1-C2-O2	5.66	122.30	118.90
34	YA	1930	G	OP2-P-O3'	5.66	117.65	105.20
34	YA	2048	G	C4-N9-C1'	5.66	133.86	126.50
34	RA	2726	U	N3-C2-O2	-5.66	118.24	122.20
34	YA	1267	U	N1-C2-O2	5.66	126.76	122.80
22	QV	62	C	C6-N1-C2	-5.66	118.04	120.30
34	YA	1806	C	C6-N1-C2	-5.66	118.04	120.30
35	YB	30	C	N3-C2-O2	-5.66	117.94	121.90
34	YA	1686	C	C2-N1-C1'	5.65	125.02	118.80
34	YA	2723	C	C6-N1-C2	-5.65	118.04	120.30
34	RA	1632	A	N7-C8-N9	5.64	116.62	113.80
1	XA	23	C	C5-C6-N1	5.64	123.82	121.00
22	QV	31	G	C8-N9-C4	-5.64	104.14	106.40
34	RA	2701	C	C5-C6-N1	5.64	123.82	121.00
34	YA	1992	G	OP2-P-O3'	5.64	117.61	105.20
34	RA	104	U	N3-C2-O2	-5.64	118.25	122.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	RA	1513	C	C5-C6-N1	5.64	123.82	121.00
34	YA	183	C	N3-C2-O2	-5.64	117.95	121.90
34	YA	544	C	C5-C6-N1	5.64	123.82	121.00
34	YA	1407	C	N3-C2-O2	-5.64	117.95	121.90
1	QA	936	C	N3-C2-O2	-5.63	117.96	121.90
1	XA	68(R)	U	N3-C2-O2	-5.63	118.26	122.20
1	XA	1285	A	P-O3'-C3'	5.63	126.46	119.70
34	YA	106	C	C6-N1-C2	-5.63	118.05	120.30
37	YE	186	GLY	N-CA-C	5.63	127.18	113.10
34	YA	363(F)	U	N3-C2-O2	-5.63	118.26	122.20
34	YA	2294	C	N1-C2-O2	5.63	122.28	118.90
34	RA	2168	G	N3-C4-N9	5.63	129.38	126.00
1	XA	1203	C	N1-C2-O2	5.63	122.28	118.90
35	YB	70	C	C6-N1-C2	-5.63	118.05	120.30
34	RA	1407	C	N1-C2-O2	5.63	122.28	118.90
34	YA	384	U	C2-N1-C1'	5.63	124.45	117.70
34	YA	1085	A	P-O3'-C3'	5.63	126.45	119.70
35	YB	71	C	N1-C2-O2	5.63	122.28	118.90
36	YD	241	PRO	C-N-CA	5.62	135.76	121.70
1	XA	1290	G	N3-C4-N9	5.62	129.37	126.00
34	YA	1844	C	C6-N1-C2	-5.62	118.05	120.30
20	QT	73	HIS	CA-CB-CG	5.62	123.15	113.60
34	RA	689	A	C5-C6-N1	5.62	120.51	117.70
34	YA	2368	C	C6-N1-C2	-5.62	118.05	120.30
1	XA	68(T)	C	N1-C2-O2	5.62	122.27	118.90
34	YA	584	C	C2-N1-C1'	5.62	124.98	118.80
34	YA	243	U	C5-C6-N1	5.62	125.51	122.70
34	YA	1398	C	N1-C2-O2	5.62	122.27	118.90
1	QA	1225	A	C4-N9-C1'	5.62	136.41	126.30
34	YA	1535	U	O4'-C1'-N1	5.62	112.69	108.20
1	QA	23	C	C6-N1-C2	-5.61	118.05	120.30
35	RB	60	C	C6-N1-C2	-5.61	118.06	120.30
34	YA	319	C	N1-C2-O2	5.61	122.27	118.90
1	QA	267	C	N3-C2-O2	-5.61	117.97	121.90
1	XA	748	C	P-O3'-C3'	5.61	126.43	119.70
34	YA	964	C	C6-N1-C2	-5.61	118.06	120.30
34	RA	2211	G	C8-N9-C1'	-5.61	119.71	127.00
1	XA	68(R)	U	C2-N1-C1'	5.61	124.43	117.70
34	YA	1786	A	C4-N9-C1'	5.61	136.39	126.30
34	RA	2542	A	C8-N9-C4	5.60	108.04	105.80
34	YA	2457	U	N3-C2-O2	-5.60	118.28	122.20
44	RP	59	LEU	CA-CB-CG	5.60	128.18	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	XA	435	C	C5-C6-N1	5.60	123.80	121.00
34	RA	1417	C	N1-C2-O2	5.60	122.26	118.90
34	RA	1982	C	C2-N1-C1'	5.60	124.96	118.80
34	RA	1934	C	N1-C2-O2	5.60	122.26	118.90
34	YA	231	C	N1-C2-O2	5.60	122.26	118.90
34	YA	2559	C	N1-C2-O2	5.60	122.26	118.90
1	QA	525	C	C5-C6-N1	5.60	123.80	121.00
22	XV	31	G	N3-C4-C5	-5.60	125.80	128.60
22	QV	15	G	N3-C4-N9	5.59	129.35	126.00
22	XV	15	G	N7-C8-N9	5.59	115.90	113.10
34	RA	1881	C	C6-N1-C2	-5.59	118.06	120.30
34	YA	1742	C	C6-N1-C2	-5.59	118.06	120.30
35	YB	38	C	C6-N1-C2	-5.59	118.06	120.30
35	YB	60	C	C5-C6-N1	5.59	123.79	121.00
34	RA	420	C	C2-N1-C1'	5.59	124.94	118.80
35	YB	37	C	C6-N1-C2	-5.58	118.07	120.30
35	YB	94	C	C6-N1-C2	-5.58	118.07	120.30
34	YA	1430	C	C5-C6-N1	5.58	123.79	121.00
1	XA	154	C	N1-C2-O2	5.58	122.25	118.90
34	YA	1683	C	C5-C6-N1	5.58	123.79	121.00
1	QA	891	U	N3-C2-O2	-5.58	118.30	122.20
34	RA	2065	C	C6-N1-C2	-5.58	118.07	120.30
34	YA	2460	U	N1-C2-O2	5.58	126.70	122.80
1	QA	503	C	C2-N1-C1'	5.57	124.93	118.80
34	RA	76	C	C6-N1-C2	-5.57	118.07	120.30
34	YA	797	C	C6-N1-C2	-5.57	118.07	120.30
34	YA	2008	C	C6-N1-C2	-5.57	118.07	120.30
34	YA	2516	G	N3-C4-C5	-5.57	125.81	128.60
34	RA	2128	C	C6-N1-C2	-5.57	118.07	120.30
34	YA	409	C	N1-C2-O2	5.57	122.24	118.90
34	YA	2032	G	N3-C4-C5	5.57	131.38	128.60
34	YA	1644	C	N3-C2-O2	-5.57	118.00	121.90
34	RA	102	G	P-O3'-C3'	5.56	126.37	119.70
34	RA	2559	C	N3-C2-O2	-5.56	118.01	121.90
34	RA	1881	C	C5-C6-N1	5.56	123.78	121.00
1	XA	645	C	N3-C2-O2	-5.56	118.01	121.90
34	YA	2832	U	OP2-P-O3'	5.55	117.42	105.20
1	QA	241	C	C6-N1-C2	-5.55	118.08	120.30
34	YA	385	C	C2-N1-C1'	5.55	124.91	118.80
1	QA	993	G	C4-N9-C1'	5.55	133.72	126.50
34	YA	1398	C	C6-N1-C2	-5.55	118.08	120.30
1	XA	1113	C	C5-C6-N1	5.55	123.77	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	R5	34	PRO	CA-N-CD	-5.55	103.73	111.50
34	YA	2099	U	N1-C2-O2	5.55	126.68	122.80
28	Y4	39	CYS	N-CA-C	-5.54	96.03	111.00
32	R8	61	LEU	C-N-CA	5.54	135.56	121.70
34	RA	384	U	C2-N1-C1'	5.54	124.35	117.70
34	YA	1383	C	N1-C2-O2	5.54	122.23	118.90
34	YA	2161	C	N1-C2-O2	5.54	122.23	118.90
1	XA	455	C	N1-C2-O2	5.54	122.22	118.90
34	YA	2321	G	C8-N9-C1'	-5.54	119.80	127.00
34	YA	2889	C	C2-N1-C1'	5.54	124.90	118.80
34	RA	99	U	P-O3'-C3'	5.54	126.35	119.70
34	RA	1264	G	C8-N9-C4	-5.54	104.18	106.40
1	QA	458(A)	C	C6-N1-C2	-5.54	118.08	120.30
34	RA	624	C	C6-N1-C2	-5.54	118.08	120.30
34	YA	2061	G	C4-N9-C1'	5.54	133.70	126.50
1	QA	762	C	C6-N1-C2	-5.54	118.09	120.30
1	QA	381	C	N3-C2-O2	-5.53	118.03	121.90
1	XA	1322	C	C5-C6-N1	5.53	123.77	121.00
34	YA	544	C	C2-N1-C1'	5.53	124.88	118.80
34	YA	1290	C	C6-N1-C2	-5.53	118.09	120.30
34	YA	2846	G	C8-N9-C4	-5.53	104.19	106.40
54	YZ	62	PRO	C-N-CA	5.53	135.52	121.70
34	YA	2827	C	C5-C6-N1	5.53	123.77	121.00
34	RA	1857	G	C8-N9-C4	-5.53	104.19	106.40
34	RA	2559	C	C5-C6-N1	5.53	123.76	121.00
34	RA	2874	C	N1-C2-O2	5.53	122.22	118.90
1	XA	125	U	O4'-C1'-N1	5.53	112.62	108.20
1	XA	811	C	N3-C2-O2	-5.53	118.03	121.90
40	RH	153	LYS	N-CA-C	5.53	125.92	111.00
34	YA	267	C	N1-C2-O2	5.53	122.22	118.90
34	YA	2453	A	C5-C6-N6	-5.53	119.28	123.70
1	QA	443	C	C2-N1-C1'	5.52	124.88	118.80
34	YA	9	U	N1-C2-O2	5.52	126.67	122.80
34	YA	1658	C	C2-N1-C1'	5.52	124.88	118.80
34	YA	2107	C	N3-C2-O2	-5.52	118.03	121.90
34	YA	1549	C	C6-N1-C2	-5.52	118.09	120.30
34	YA	904	C	N1-C2-O2	5.52	122.21	118.90
1	QA	455	C	C5-C6-N1	5.52	123.76	121.00
34	YA	104	U	N1-C2-O2	5.52	126.66	122.80
34	YA	1653	G	C4-N9-C1'	5.52	133.67	126.50
44	YP	59	LEU	CA-CB-CG	5.52	127.99	115.30
34	RA	1742	C	N1-C2-O2	5.51	122.21	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	YA	102	G	P-O3'-C3'	5.51	126.32	119.70
34	YA	2506	U	C5-C6-N1	5.51	125.46	122.70
34	YA	2871	C	C6-N1-C2	-5.51	118.09	120.30
1	QA	597	G	C4-C5-N7	5.51	113.00	110.80
1	QA	136	C	C6-N1-C1'	-5.51	114.19	120.80
34	RA	1376	C	C2-N1-C1'	5.51	124.86	118.80
34	RA	1632	A	C8-N9-C4	-5.51	103.59	105.80
34	RA	1786	A	N7-C8-N9	5.51	116.56	113.80
34	RA	2295	C	N1-C2-O2	5.51	122.21	118.90
1	XA	353	A	OP2-P-O3'	5.51	117.33	105.20
34	YA	1598	C	N3-C2-O2	-5.51	118.04	121.90
1	QA	697	U	N1-C2-O2	5.51	126.66	122.80
1	QA	1158	C	C2-N1-C1'	5.51	124.86	118.80
34	RA	1611	C	C6-N1-C2	-5.51	118.10	120.30
34	RA	2226	C	C6-N1-C2	-5.51	118.10	120.30
34	RA	2591	C	C6-N1-C2	-5.51	118.10	120.30
1	XA	1290	G	C8-N9-C1'	-5.51	119.84	127.00
34	RA	1549	C	N1-C2-O2	5.50	122.20	118.90
34	YA	2098	U	N3-C2-O2	-5.50	118.35	122.20
34	YA	2771	C	N1-C2-O2	5.50	122.20	118.90
34	RA	2316	C	C5-C6-N1	5.50	123.75	121.00
1	XA	525	C	C6-N1-C2	-5.50	118.10	120.30
34	YA	923	C	C6-N1-C2	-5.50	118.10	120.30
34	YA	998	C	C5-C6-N1	5.50	123.75	121.00
34	YA	1947	C	C6-N1-C2	-5.50	118.10	120.30
34	YA	2048	G	C8-N9-C1'	-5.50	119.84	127.00
34	YA	2576	G	N3-C4-N9	5.50	129.30	126.00
34	RA	974(B)	C	P-O3'-C3'	5.50	126.30	119.70
34	YA	641	C	N1-C2-O2	5.50	122.20	118.90
34	YA	2512	C	C5-C6-N1	5.50	123.75	121.00
23	QX	17	C	N3-C4-C5	-5.50	119.70	121.90
34	YA	1295	C	N3-C2-O2	-5.50	118.05	121.90
34	YA	1140	C	C2-N1-C1'	5.50	124.84	118.80
34	YA	2099	U	C2-N1-C1'	5.50	124.29	117.70
34	RA	2666	C	N1-C2-O2	5.49	122.20	118.90
1	QA	1181	G	N1-C6-O6	-5.49	116.61	119.90
34	YA	1290	C	C5-C6-N1	5.49	123.75	121.00
34	YA	2048	G	N3-C4-N9	5.49	129.29	126.00
23	QX	19	U	O4'-C1'-N1	5.49	112.59	108.20
34	RA	2053	G	N9-C4-C5	-5.49	103.20	105.40
1	QA	64	G	P-O3'-C3'	5.49	126.28	119.70
34	RA	856	C	N3-C2-O2	-5.48	118.06	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	QA	988	G	N1-C6-O6	-5.48	116.61	119.90
1	XA	1297	C	N1-C2-O2	5.48	122.19	118.90
1	QA	548	G	C6-C5-N7	-5.48	127.11	130.40
34	YA	657	U	N3-C2-O2	-5.48	118.36	122.20
34	RA	1064	C	C5-C6-N1	5.48	123.74	121.00
34	RA	2720	U	N3-C2-O2	-5.48	118.37	122.20
34	YA	510	C	N1-C2-O2	5.48	122.19	118.90
1	QA	1407	C	C6-N1-C2	-5.47	118.11	120.30
1	XA	1403	C	C6-N1-C2	-5.47	118.11	120.30
34	RA	1786	A	C4-N9-C1'	5.47	136.15	126.30
34	RA	2784	C	C6-N1-C2	-5.47	118.11	120.30
34	RA	1180	C	N1-C2-O2	5.47	122.18	118.90
34	RA	1611	C	C5-C6-N1	5.47	123.73	121.00
34	YA	413	C	N1-C2-O2	5.47	122.18	118.90
34	RA	665	C	C6-N1-C2	-5.47	118.11	120.30
34	YA	1575	C	C5-C6-N1	5.47	123.73	121.00
34	RA	825	C	C6-N1-C2	-5.46	118.11	120.30
34	RA	1644	C	N1-C2-O2	5.46	122.18	118.90
34	YA	2317	C	C6-N1-C2	-5.46	118.11	120.30
1	XA	1539	C	C5-C4-N4	5.46	124.02	120.20
34	YA	1775	U	N3-C4-O4	5.46	123.22	119.40
1	QA	1366	C	C6-N1-C2	-5.46	118.12	120.30
1	QA	590	C	C2-N1-C1'	5.46	124.80	118.80
1	QA	1430	C	C6-N1-C2	-5.46	118.12	120.30
34	RA	120	U	C6-N1-C2	-5.46	117.72	121.00
34	RA	1075	C	N1-C2-O2	5.46	122.17	118.90
34	RA	2254	C	C5-C6-N1	5.46	123.73	121.00
34	YA	1844	C	C5-C6-N1	5.46	123.73	121.00
34	RA	641	C	C2-N1-C1'	5.45	124.80	118.80
34	RA	1535	U	C6-N1-C1'	-5.45	113.57	121.20
34	RA	1741	C	C6-N1-C2	-5.45	118.12	120.30
34	YA	1363	C	C6-N1-C2	-5.45	118.12	120.30
34	RA	456	C	C6-N1-C1'	-5.45	114.27	120.80
34	RA	2142	C	N1-C2-O2	5.45	122.17	118.90
1	XA	514	C	N1-C2-O2	5.45	122.17	118.90
34	YA	986	C	C6-N1-C2	-5.45	118.12	120.30
34	YA	1549	C	C2-N1-C1'	5.45	124.79	118.80
34	RA	1762	A	C8-N9-C4	-5.44	103.62	105.80
34	YA	393	C	C5-C6-N1	5.44	123.72	121.00
34	YA	1157	G	C6-C5-N7	-5.44	127.13	130.40
34	YA	2683	C	N1-C2-O2	5.44	122.17	118.90
50	RV	48	GLY	C-N-CA	5.44	135.30	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	YA	1135	C	N3-C2-O2	-5.44	118.09	121.90
34	RA	208	C	C5-C6-N1	5.44	123.72	121.00
34	YA	30	G	N3-C4-N9	5.44	129.26	126.00
34	RA	74	A	C4-C5-C6	-5.44	114.28	117.00
34	YA	2294	C	C5-C6-N1	5.44	123.72	121.00
34	RA	2064	C	C2-N1-C1'	5.43	124.78	118.80
1	XA	1190	G	C6-N1-C2	-5.43	121.84	125.10
34	YA	584	C	N1-C2-O2	5.43	122.16	118.90
34	RA	2579	C	C6-N1-C2	-5.43	118.13	120.30
34	YA	2043	C	C6-N1-C2	-5.43	118.13	120.30
23	XX	16	C	O5'-P-OP2	-5.43	100.81	105.70
34	YA	669	G	C8-N9-C1'	-5.43	119.94	127.00
1	QA	54	C	N3-C2-O2	-5.43	118.10	121.90
1	XA	1539	C	C6-N1-C1'	5.43	127.31	120.80
34	RA	1774	C	C5-C6-N1	5.42	123.71	121.00
34	YA	208	C	C5-C6-N1	5.42	123.71	121.00
34	YA	2254	C	C5-C6-N1	5.42	123.71	121.00
1	QA	1263	C	C6-N1-C1'	-5.42	114.30	120.80
34	RA	265	A	O4'-C1'-N9	5.42	112.53	108.20
1	XA	943	U	N1-C2-O2	5.42	126.59	122.80
1	QA	1301	U	C6-N1-C2	-5.42	117.75	121.00
34	RA	676	A	O4'-C1'-N9	5.42	112.53	108.20
34	RA	2073	C	C6-N1-C2	-5.42	118.13	120.30
34	YA	335	C	C6-N1-C2	-5.42	118.13	120.30
34	RA	1506	C	N3-C2-O2	-5.41	118.11	121.90
34	RA	1836	C	C5-C6-N1	5.41	123.71	121.00
1	XA	993	G	C6-C5-N7	-5.41	127.15	130.40
34	YA	1233	C	C5-C6-N1	5.41	123.71	121.00
34	RA	1437	C	C6-N1-C2	-5.41	118.14	120.30
34	RA	2008	C	C6-N1-C2	-5.41	118.14	120.30
34	YA	657	U	N1-C2-O2	5.41	126.59	122.80
34	RA	221	A	P-O3'-C3'	5.41	126.19	119.70
12	XL	46	LYS	C-N-CA	-5.41	108.18	121.70
34	RA	2456	C	C5-C6-N1	5.40	123.70	121.00
34	YA	691	C	C5-C6-N1	5.40	123.70	121.00
34	YA	1781	C	N3-C2-O2	-5.40	118.12	121.90
34	YA	2474	C	N3-C2-O2	-5.40	118.12	121.90
1	QA	58	C	C6-N1-C2	-5.40	118.14	120.30
1	QA	738	C	C5-C6-N1	5.40	123.70	121.00
34	YA	957	A	C4-C5-N7	5.40	113.40	110.70
34	YA	1343	G	C4-N9-C1'	5.40	133.52	126.50
1	QA	522	C	N1-C2-O2	5.40	122.14	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	QV	13	C	N1-C2-O2	5.40	122.14	118.90
34	RA	2108	C	N1-C2-O2	5.40	122.14	118.90
35	YB	71	C	C2-N1-C1'	5.40	124.74	118.80
34	YA	1402	C	C5-C6-N1	5.40	123.70	121.00
34	RA	1914	C	C6-N1-C1'	-5.39	114.33	120.80
22	XV	40	G	C8-N9-C1'	-5.39	119.99	127.00
34	RA	1407	C	C6-N1-C1'	-5.39	114.33	120.80
34	YA	1640	C	C5-C6-N1	5.39	123.70	121.00
48	YT	114	LEU	CA-CB-CG	5.39	127.70	115.30
34	YA	1021	A	C8-N9-C4	-5.39	103.64	105.80
34	YA	1468	C	C5-C6-N1	5.39	123.70	121.00
34	RA	634	C	N1-C2-O2	5.39	122.13	118.90
34	RA	1126	A	C6-N1-C2	5.39	121.83	118.60
34	RA	1830	C	N1-C2-O2	5.39	122.13	118.90
34	YA	2036	C	C2-N1-C1'	5.39	124.73	118.80
40	YH	155	SER	N-CA-C	5.39	125.55	111.00
34	YA	461	C	C5-C6-N1	5.39	123.69	121.00
34	RA	420	C	N1-C2-O2	5.38	122.13	118.90
34	RA	2496	C	O5'-P-OP1	-5.38	100.86	105.70
34	YA	897	C	C2-N1-C1'	5.38	124.72	118.80
34	YA	2576	G	C8-N9-C1'	-5.38	120.00	127.00
34	YA	2787	C	C6-N1-C1'	-5.38	114.34	120.80
34	RA	270(L)	C	N1-C2-O2	5.38	122.13	118.90
34	RA	1598	C	C2-N1-C1'	5.38	124.72	118.80
34	YA	2646	C	C6-N1-C2	-5.38	118.15	120.30
34	YA	2779	U	N1-C2-O2	5.38	126.57	122.80
34	RA	1762	A	N3-C4-C5	-5.38	123.03	126.80
34	RA	2063	C	N1-C2-O2	5.38	122.13	118.90
1	XA	455	C	C6-N1-C2	-5.38	118.15	120.30
34	YA	445	C	C6-N1-C2	-5.38	118.15	120.30
34	RA	1640	C	C6-N1-C2	-5.38	118.15	120.30
34	YA	2032	G	C4-C5-C6	-5.38	115.57	118.80
1	XA	615	C	C6-N1-C2	-5.37	118.15	120.30
1	XA	723	U	N3-C2-O2	-5.37	118.44	122.20
34	YA	2107	C	C6-N1-C2	-5.37	118.15	120.30
35	YB	51	G	N1-C6-O6	-5.37	116.68	119.90
1	QA	218	C	C6-N1-C2	-5.37	118.15	120.30
1	XA	1045	C	N1-C2-O2	5.37	122.12	118.90
34	YA	1644	C	N1-C2-O2	5.37	122.12	118.90
34	RA	2517	C	N3-C4-C5	-5.37	119.75	121.90
34	YA	1598	C	C5-C6-N1	5.37	123.69	121.00
34	YA	2043	C	N1-C2-O2	5.37	122.12	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	YA	2809	A	N7-C8-N9	5.37	116.48	113.80
1	XA	443	C	C6-N1-C2	-5.37	118.15	120.30
34	YA	183	C	C5-C6-N1	5.37	123.68	121.00
1	QA	514	C	N1-C2-O2	5.37	122.12	118.90
14	QN	43	CYS	CA-CB-SG	-5.37	104.34	114.00
34	RA	1158	C	N1-C2-O2	5.37	122.12	118.90
34	RA	1534	G	N3-C4-N9	5.37	129.22	126.00
34	YA	1679	U	C2-N1-C1'	5.37	124.14	117.70
34	YA	2320	A	N3-C4-N9	5.37	131.69	127.40
22	QV	36	G	C8-N9-C4	-5.36	104.25	106.40
34	RA	1513	C	C6-N1-C2	-5.36	118.16	120.30
14	XN	58	LYS	N-CA-C	-5.36	96.52	111.00
34	YA	2008	C	C5-C6-N1	5.36	123.68	121.00
23	QX	19	U	C2-N1-C1'	-5.36	111.27	117.70
34	YA	729	G	N3-C2-N2	-5.36	116.15	119.90
1	QA	1395	C	C5-C6-N1	5.36	123.68	121.00
34	RA	1788	C	C6-N1-C2	-5.36	118.16	120.30
1	XA	891	U	N1-C2-O2	5.36	126.55	122.80
34	YA	541	C	C6-N1-C2	-5.36	118.16	120.30
34	YA	2210	G	N3-C4-C5	-5.36	125.92	128.60
34	YA	2471	C	C2-N1-C1'	5.36	124.69	118.80
34	YA	2681	C	OP2-P-O3'	5.36	116.99	105.20
35	RB	22	U	N3-C2-O2	-5.36	118.45	122.20
34	YA	1411	C	C2-N1-C1'	5.36	124.69	118.80
1	QA	1066	C	C5-C6-N1	5.36	123.68	121.00
34	RA	1306	C	C2-N1-C1'	5.36	124.69	118.80
34	RA	2089	U	N1-C2-O2	5.36	126.55	122.80
34	YA	1021	A	C5-N7-C8	-5.36	101.22	103.90
34	RA	1544	C	N3-C2-O2	-5.36	118.15	121.90
34	RA	1988	C	C5-C6-N1	5.36	123.68	121.00
34	YA	12	U	C2-N1-C1'	5.36	124.13	117.70
34	YA	2032	G	C4-N9-C1'	-5.36	119.54	126.50
34	RA	1313	U	C5-C6-N1	5.35	125.38	122.70
34	RA	1947	C	C6-N1-C2	-5.35	118.16	120.30
34	YA	2395	C	C5-C6-N1	5.35	123.68	121.00
34	RA	1445	C	C5-C6-N1	5.35	123.67	121.00
1	XA	1056	U	N3-C2-O2	-5.35	118.46	122.20
34	YA	1957	C	N3-C2-O2	-5.35	118.16	121.90
34	YA	2889	C	N3-C2-O2	-5.35	118.16	121.90
1	QA	54	C	C6-N1-C2	-5.35	118.16	120.30
1	QA	241	C	N1-C2-O2	5.35	122.11	118.90
34	RA	797	C	C6-N1-C2	-5.35	118.16	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	RA	1797	C	C6-N1-C2	-5.35	118.16	120.30
34	RA	2115	G	C4-N9-C1'	5.35	133.45	126.50
34	RA	2703	C	C6-N1-C2	-5.35	118.16	120.30
34	RA	1375	C	C6-N1-C2	-5.35	118.16	120.30
34	RA	2307	G	O4'-C1'-N9	5.35	112.48	108.20
34	YA	1793	C	C5-C6-N1	5.34	123.67	121.00
34	YA	2542	A	N1-C6-N6	5.34	121.81	118.60
1	QA	131	C	N3-C2-O2	-5.34	118.16	121.90
34	RA	487	C	N1-C2-O2	5.34	122.10	118.90
34	RA	1741	C	C5-C6-N1	5.34	123.67	121.00
20	XT	10	LEU	CA-CB-CG	5.34	127.58	115.30
34	YA	1166	C	C5-C6-N1	5.34	123.67	121.00
34	YA	2033	A	O5'-P-OP2	-5.34	100.89	105.70
34	RA	1526	G	C4-N9-C1'	5.34	133.44	126.50
34	YA	2026	C	C5-C6-N1	5.34	123.67	121.00
34	RA	721	C	C5-C6-N1	5.34	123.67	121.00
34	RA	817	C	C6-N1-C2	-5.34	118.17	120.30
1	XA	1348	U	C2-N1-C1'	5.34	124.10	117.70
34	RA	1049	C	C6-N1-C2	-5.33	118.17	120.30
1	QA	848	C	N1-C2-O2	5.33	122.10	118.90
34	RA	200	U	N1-C2-O2	5.33	126.53	122.80
34	RA	384	U	N3-C2-O2	-5.33	118.47	122.20
34	RA	2321	G	C8-N9-C1'	-5.33	120.07	127.00
1	XA	354	G	C4-N9-C1'	5.33	133.43	126.50
34	YA	459	U	N1-C2-O2	5.33	126.53	122.80
34	YA	1102	C	N3-C2-O2	-5.33	118.17	121.90
33	R9	32	HIS	CB-CA-C	5.33	121.06	110.40
1	QA	1158	C	N3-C2-O2	-5.33	118.17	121.90
34	RA	721	C	C6-N1-C1'	-5.33	114.41	120.80
1	XA	1109	C	N1-C2-O2	5.33	122.10	118.90
34	YA	2359	C	C5-C6-N1	5.33	123.66	121.00
34	RA	67	U	C2-N1-C1'	5.33	124.09	117.70
34	YA	1004	C	C5-C6-N1	5.33	123.66	121.00
34	RA	2115	G	N3-C4-N9	5.32	129.19	126.00
1	QA	352	C	N1-C2-O2	5.32	122.09	118.90
34	YA	1506	C	C6-N1-C2	-5.32	118.17	120.30
34	RA	580	C	C6-N1-C2	-5.32	118.17	120.30
34	RA	1691	C	C5-C6-N1	5.32	123.66	121.00
34	YA	2043	C	C2-N1-C1'	5.32	124.65	118.80
34	RA	2568	C	C5-C6-N1	5.32	123.66	121.00
34	RA	1781	C	C2-N1-C1'	5.32	124.65	118.80
1	XA	1390	U	N3-C2-O2	-5.32	118.48	122.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	YA	535	C	C5-C6-N1	5.32	123.66	121.00
34	YA	1157	G	C4-N9-C1'	5.32	133.41	126.50
34	RA	665	C	C5-C6-N1	5.31	123.66	121.00
1	XA	1296	C	C6-N1-C2	-5.31	118.17	120.30
35	YB	22	U	N1-C2-O2	5.31	126.52	122.80
35	RB	22	U	N1-C2-O2	5.31	126.52	122.80
34	YA	1805	U	C5-C6-N1	5.31	125.36	122.70
34	YA	2874	C	N1-C2-O2	5.31	122.09	118.90
34	RA	634	C	C5-C6-N1	5.31	123.66	121.00
34	RA	141(B)	C	C5-C6-N1	5.31	123.65	121.00
1	XA	110	C	N3-C2-O2	-5.31	118.19	121.90
34	YA	241	A	OP1-P-O3'	5.31	116.88	105.20
35	YB	44	G	C4-N9-C1'	-5.31	119.60	126.50
45	YQ	17	LEU	CB-CA-C	-5.31	100.11	110.20
34	YA	2395	C	C6-N1-C2	-5.31	118.18	120.30
1	XA	910	C	C5-C6-N1	5.30	123.65	121.00
34	YA	248	G	C8-N9-C4	-5.30	104.28	106.40
34	YA	542	C	C6-N1-C2	-5.30	118.18	120.30
34	YA	1990	C	C6-N1-C2	-5.30	118.18	120.30
34	YA	2236	C	N1-C2-O2	5.30	122.08	118.90
34	RA	503	A	P-O3'-C3'	5.30	126.06	119.70
34	YA	641	C	C6-N1-C2	-5.30	118.18	120.30
34	YA	2320	A	C4-N9-C1'	5.30	135.84	126.30
34	YA	481	G	O4'-C1'-N9	5.30	112.44	108.20
1	QA	904	C	N1-C2-O2	5.30	122.08	118.90
1	QA	252	U	N1-C2-O2	5.30	126.51	122.80
34	RA	1445	C	C6-N1-C2	-5.30	118.18	120.30
1	QA	435	C	C6-N1-C2	-5.29	118.18	120.30
34	RA	2089	U	C5-C6-N1	5.29	125.35	122.70
34	YA	556	G	C4-N9-C1'	5.29	133.38	126.50
1	QA	514	C	C6-N1-C2	-5.29	118.18	120.30
22	QV	36	G	C5-N7-C8	-5.29	101.66	104.30
34	RA	537	C	N1-C2-O2	5.29	122.08	118.90
34	YA	836	G	C8-N9-C4	-5.29	104.28	106.40
34	YA	1398	C	C5-C6-N1	5.29	123.65	121.00
34	RA	1506	C	C6-N1-C2	-5.29	118.18	120.30
34	YA	2682	U	N1-C2-O2	5.29	126.50	122.80
34	RA	1611	C	C2-N1-C1'	5.29	124.62	118.80
34	YA	1385	G	O4'-C1'-N9	5.29	112.43	108.20
34	RA	2089	U	N3-C2-O2	-5.28	118.50	122.20
34	YA	2236	C	C5-C6-N1	5.28	123.64	121.00
34	YA	420	C	N3-C2-O2	-5.28	118.20	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	YA	1463	C	C6-N1-C2	-5.28	118.19	120.30
34	RA	1437	C	C2-N1-C1'	5.28	124.61	118.80
1	XA	68(S)	C	C2-N1-C1'	5.28	124.61	118.80
34	YA	556	G	N3-C4-N9	5.28	129.17	126.00
34	YA	692	C	C6-N1-C2	-5.28	118.19	120.30
34	RA	192	C	N3-C2-O2	-5.28	118.21	121.90
34	RA	846	C	OP2-P-O3'	5.28	116.81	105.20
34	RA	1313	U	C6-N1-C2	-5.28	117.83	121.00
34	YA	1407	C	C6-N1-C1'	-5.28	114.47	120.80
34	YA	1864	U	N1-C2-O2	5.28	126.49	122.80
34	YA	2350	C	C2-N1-C1'	5.28	124.61	118.80
35	YB	51	G	C5-C6-O6	5.28	131.77	128.60
34	RA	1982	C	C5-C6-N1	5.28	123.64	121.00
1	XA	186(B)	C	C5-C6-N1	5.28	123.64	121.00
34	YA	1267	U	C5-C6-N1	5.28	125.34	122.70
34	YA	1766	U	N3-C2-O2	-5.28	118.51	122.20
34	YA	2798	C	N1-C2-O2	5.28	122.06	118.90
35	RB	27	C	C6-N1-C2	-5.27	118.19	120.30
34	YA	1370	C	N1-C2-O2	5.27	122.06	118.90
1	QA	1234	C	C6-N1-C2	-5.27	118.19	120.30
34	RA	1526	G	C8-N9-C1'	-5.27	120.15	127.00
34	YA	692	C	C5-C6-N1	5.27	123.64	121.00
34	YA	1257	C	C6-N1-C2	-5.27	118.19	120.30
34	YA	1920	C	C2-N1-C1'	5.27	124.60	118.80
1	QA	597	G	N9-C4-C5	-5.27	103.29	105.40
34	RA	2615	U	C2-N1-C1'	5.27	124.03	117.70
34	YA	229	A	OP2-P-O3'	5.27	116.80	105.20
34	YA	840	C	C6-N1-C2	-5.27	118.19	120.30
34	RA	1509	C	OP1-P-O3'	5.27	116.80	105.20
34	YA	1135	C	C6-N1-C1'	-5.27	114.48	120.80
34	YA	1742	C	C5-C6-N1	5.27	123.63	121.00
34	YA	2699	C	N1-C2-O2	5.27	122.06	118.90
1	XA	723	U	C2-N1-C1'	5.27	124.02	117.70
34	YA	1298	C	C5-C6-N1	5.27	123.63	121.00
34	YA	2539	C	N1-C2-O2	5.27	122.06	118.90
54	YZ	151	HIS	N-CA-C	5.27	125.22	111.00
34	RA	650	C	C2-N1-C1'	5.26	124.59	118.80
34	RA	692	C	C2-N1-C1'	5.26	124.59	118.80
34	RA	74	A	C4-N9-C1'	-5.26	116.83	126.30
34	RA	2666	C	C2-N1-C1'	5.26	124.59	118.80
1	XA	689	C	C2-N1-C1'	5.26	124.59	118.80
34	RA	1153	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	XA	283	C	C6-N1-C2	-5.26	118.20	120.30
34	YA	2556	C	N1-C2-O2	5.26	122.05	118.90
1	QA	555	C	C6-N1-C2	-5.25	118.20	120.30
1	QA	745	C	C6-N1-C2	-5.25	118.20	120.30
1	XA	266	G	P-O3'-C3'	5.25	126.00	119.70
34	YA	2798	C	C6-N1-C2	-5.25	118.20	120.30
35	YB	31	C	C6-N1-C2	-5.25	118.20	120.30
34	RA	1549	C	C6-N1-C2	-5.25	118.20	120.30
34	YA	1295	C	N1-C2-O2	5.25	122.05	118.90
34	YA	1931	U	N3-C2-O2	-5.25	118.53	122.20
34	RA	2179	C	C2-N1-C1'	5.25	124.57	118.80
1	XA	966	G	C4-N9-C1'	-5.25	119.68	126.50
1	QA	962	C	C6-N1-C2	-5.25	118.20	120.30
34	RA	1830	C	C6-N1-C2	-5.24	118.20	120.30
1	XA	37	U	N3-C2-O2	-5.24	118.53	122.20
34	YA	1653	G	C8-N9-C4	-5.24	104.30	106.40
34	RA	1708	C	C6-N1-C2	-5.24	118.20	120.30
54	RZ	178	GLU	C-N-CA	5.24	134.81	121.70
34	YA	2063	C	C5-C6-N1	5.24	123.62	121.00
34	YA	1779	U	C2-N1-C1'	5.24	123.98	117.70
34	RA	1332	G	C4-N9-C1'	5.24	133.31	126.50
34	RA	1971	A	C2-N3-C4	5.24	113.22	110.60
1	XA	993	G	N3-C4-N9	5.24	129.14	126.00
1	QA	519	C	N1-C2-O2	5.23	122.04	118.90
34	YA	2129	C	N1-C2-O2	5.23	122.04	118.90
34	YA	664	C	C6-N1-C2	-5.23	118.21	120.30
34	YA	752	A	OP2-P-O3'	5.23	116.71	105.20
34	YA	856	C	C2-N3-C4	5.23	122.52	119.90
34	RA	666	G	N3-C4-N9	5.23	129.14	126.00
34	RA	1102	C	C5-C6-N1	5.23	123.61	121.00
34	YA	1957	C	N1-C2-O2	5.23	122.03	118.90
1	XA	328	C	OP2-P-O3'	5.22	116.69	105.20
34	YA	2787	C	C5-C6-N1	5.22	123.61	121.00
34	RA	876	C	N3-C2-O2	-5.22	118.24	121.90
34	RA	2646	C	C5-C6-N1	5.22	123.61	121.00
1	XA	536	C	C6-N1-C2	-5.22	118.21	120.30
34	YA	1526	G	C4-N9-C1'	5.22	133.29	126.50
34	RA	2755	C	C5-C6-N1	5.22	123.61	121.00
34	RA	31	C	C2-N1-C1'	5.22	124.54	118.80
34	RA	613	U	C6-N1-C1'	-5.22	113.90	121.20
34	RA	1930	G	P-O3'-C3'	5.22	125.96	119.70
34	YA	1083	U	N3-C2-O2	-5.22	118.55	122.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	RA	2588	G	C4-C5-N7	5.21	112.89	110.80
34	YA	273(G)	C	C6-N1-C2	-5.21	118.22	120.30
1	XA	1463	C	C6-N1-C2	-5.21	118.22	120.30
34	YA	1598	C	C6-N1-C1'	-5.21	114.55	120.80
34	YA	528	A	N1-C6-N6	5.21	121.72	118.60
34	RA	2137	C	C2-N1-C1'	5.21	124.53	118.80
1	XA	970	C	C6-N1-C2	-5.21	118.22	120.30
1	XA	1539	C	C2-N1-C1'	-5.21	113.07	118.80
34	YA	635	C	C5-C6-N1	5.21	123.60	121.00
35	YB	44	G	C8-N9-C1'	5.21	133.77	127.00
1	XA	1306	A	O4'-C1'-N9	5.20	112.36	108.20
34	YA	1145	C	C6-N1-C2	-5.20	118.22	120.30
34	RA	2582	G	C8-N9-C1'	-5.20	120.24	127.00
1	XA	1383	C	C2-N1-C1'	5.20	124.52	118.80
34	RA	2874	C	C6-N1-C1'	-5.20	114.56	120.80
34	RA	2544	G	N7-C8-N9	5.20	115.70	113.10
1	XA	943	U	N3-C2-O2	-5.20	118.56	122.20
34	YA	530	G	C4-C5-N7	-5.20	108.72	110.80
34	RA	2063	C	C6-N1-C2	-5.19	118.22	120.30
34	YA	816	C	C5-C6-N1	5.19	123.60	121.00
34	YA	1178	C	C5-C6-N1	5.19	123.60	121.00
1	QA	891	U	N1-C2-O2	5.19	126.43	122.80
34	YA	1021	A	C2-N3-C4	-5.19	108.00	110.60
34	YA	1652	A	N1-C6-N6	5.19	121.71	118.60
34	YA	2685	G	N3-C4-N9	-5.19	122.89	126.00
53	YY	79	CYS	N-CA-CB	5.19	119.94	110.60
34	RA	339	U	N3-C2-O2	-5.18	118.57	122.20
22	XV	15	G	C2-N3-C4	5.18	114.49	111.90
34	YA	915	C	C6-N1-C1'	-5.18	114.58	120.80
34	RA	915	C	C6-N1-C2	-5.18	118.23	120.30
34	RA	976	C	C2-N1-C1'	5.18	124.50	118.80
34	YA	721	C	C5-C6-N1	5.18	123.59	121.00
34	YA	730	C	C6-N1-C2	-5.18	118.23	120.30
34	YA	1519	G	C6-C5-N7	-5.18	127.29	130.40
34	YA	2299	G	C4-N9-C1'	5.18	133.24	126.50
1	QA	110	C	N1-C2-O2	5.18	122.01	118.90
1	QA	590	C	C6-N1-C2	-5.18	118.23	120.30
34	YA	2544	G	C5-C6-O6	-5.18	125.49	128.60
34	YA	2456	C	C6-N1-C2	-5.18	118.23	120.30
34	RA	510	C	C5-C6-N1	5.18	123.59	121.00
34	YA	2798	C	C2-N1-C1'	5.18	124.50	118.80
35	RB	31	C	C6-N1-C2	-5.18	118.23	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	YA	1598	C	C6-N1-C2	-5.18	118.23	120.30
34	YA	1684	C	C6-N1-C2	-5.18	118.23	120.30
34	YA	1839	G	C4-N9-C1'	5.18	133.23	126.50
34	RA	1474	C	N3-C2-O2	-5.17	118.28	121.90
1	XA	620	C	N3-C2-O2	-5.17	118.28	121.90
34	RA	1776	G	N3-C4-N9	5.17	129.10	126.00
34	RA	1806	C	C6-N1-C2	-5.17	118.23	120.30
1	XA	241	C	N1-C2-O2	5.17	122.00	118.90
34	RA	1899	G	N3-C4-C5	-5.17	126.02	128.60
34	RA	1950	G	C8-N9-C1'	-5.17	120.28	127.00
34	RA	1294	U	N1-C2-O2	5.16	126.42	122.80
1	XA	1054	C	N1-C2-O2	5.16	122.00	118.90
36	YD	243	GLY	N-CA-C	5.16	126.01	113.10
34	RA	1526	G	N3-C4-N9	5.16	129.10	126.00
34	YA	2006	C	N3-C2-O2	-5.16	118.29	121.90
34	RA	9	U	C2-N1-C1'	5.16	123.89	117.70
34	RA	1830	C	C2-N1-C1'	5.16	124.48	118.80
34	YA	1256	G	N3-C4-N9	5.16	129.10	126.00
34	YA	2442	C	C6-N1-C2	-5.16	118.24	120.30
1	QA	330	C	N3-C2-O2	-5.16	118.29	121.90
1	QA	442	C	C6-N1-C2	-5.16	118.24	120.30
1	QA	833	U	N3-C2-O2	-5.16	118.59	122.20
34	YA	105	C	C6-N1-C2	-5.16	118.24	120.30
34	RA	2307	G	C8-N9-C1'	-5.16	120.30	127.00
34	YA	1881	C	N1-C2-O2	5.16	121.99	118.90
1	QA	224	C	N1-C2-O2	5.16	121.99	118.90
34	RA	1130	U	OP1-P-O3'	5.16	116.54	105.20
34	YA	333	G	C8-N9-C1'	-5.16	120.30	127.00
34	YA	2584	U	O4'-C1'-N1	5.16	112.32	108.20
34	RA	1788	C	C2-N1-C1'	5.15	124.47	118.80
34	YA	2006	C	C6-N1-C2	-5.15	118.24	120.30
1	QA	1440(O)	C	N3-C2-O2	-5.15	118.29	121.90
34	YA	1683	C	C6-N1-C2	-5.15	118.24	120.30
1	QA	308	C	N3-C2-O2	-5.15	118.30	121.90
34	RA	41	C	C6-N1-C2	-5.15	118.24	120.30
34	RA	1467	C	C6-N1-C2	-5.15	118.24	120.30
34	YA	634	C	N1-C2-O2	5.15	121.99	118.90
34	RA	2089	U	C2-N1-C1'	5.15	123.88	117.70
34	RA	2142	C	N3-C2-O2	-5.15	118.30	121.90
34	YA	9	U	C2-N1-C1'	5.15	123.88	117.70
34	RA	635	C	C6-N1-C2	-5.15	118.24	120.30
34	RA	1506	C	C2-N1-C1'	5.14	124.46	118.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	XT	72	LEU	CA-CB-CG	5.14	127.13	115.30
1	XA	68(S)	C	N1-C2-O2	5.14	121.98	118.90
34	YA	2689	U	P-O3'-C3'	5.14	125.87	119.70
50	YV	35	LEU	CA-CB-CG	5.14	127.13	115.30
1	QA	1097	C	C5-C6-N1	5.14	123.57	121.00
34	RA	2306	C	C6-N1-C2	-5.14	118.24	120.30
34	YA	1157	G	C8-N9-C1'	-5.14	120.32	127.00
34	YA	1950	G	C6-C5-N7	-5.14	127.32	130.40
34	YA	2420	C	C5-C6-N1	5.14	123.57	121.00
34	YA	2579	C	N1-C2-O2	5.14	121.98	118.90
34	YA	1767	C	C5-C6-N1	5.14	123.57	121.00
34	YA	2460	U	C2-N1-C1'	5.14	123.87	117.70
53	RY	99	CYS	CB-CA-C	-5.14	100.13	110.40
34	YA	1218	C	C6-N1-C2	-5.14	118.25	120.30
34	YA	1533	C	N1-C2-O2	5.14	121.98	118.90
34	RA	74	A	N3-C4-C5	5.13	130.40	126.80
34	YA	531	C	O5'-P-OP1	-5.13	101.08	105.70
34	YA	976	C	C5-C6-N1	5.13	123.57	121.00
34	YA	1950	G	C8-N9-C1'	-5.13	120.33	127.00
1	QA	1290	G	C8-N9-C1'	-5.13	120.33	127.00
34	RA	1505	C	N3-C2-O2	-5.13	118.31	121.90
36	RD	241	PRO	C-N-CA	5.13	134.53	121.70
34	YA	689	A	C5-C6-N1	5.13	120.27	117.70
34	YA	2137	C	N1-C2-O2	5.13	121.98	118.90
34	YA	2704	C	C2-N1-C1'	5.13	124.44	118.80
34	RA	1157	G	N3-C4-N9	5.13	129.08	126.00
32	R8	28	GLY	N-CA-C	5.13	125.92	113.10
34	RA	640	C	C6-N1-C2	-5.13	118.25	120.30
34	YA	894	C	N1-C2-O2	5.13	121.98	118.90
34	YA	99	U	OP2-P-O3'	5.13	116.48	105.20
34	YA	1158	C	N1-C2-O2	5.13	121.97	118.90
34	YA	1914	C	C6-N1-C2	-5.13	118.25	120.30
34	YA	2453	A	C6-N1-C2	5.13	121.68	118.60
34	YA	2040	C	C5-C6-N1	5.12	123.56	121.00
34	YA	2680	C	C2-N1-C1'	5.12	124.44	118.80
34	RA	659	C	C6-N1-C2	-5.12	118.25	120.30
34	RA	806	C	C2-N1-C1'	5.12	124.44	118.80
34	RA	1404	C	C2-N1-C1'	5.12	124.44	118.80
34	RA	2551	C	N1-C2-O2	5.12	121.97	118.90
34	YA	459	U	N3-C2-O2	-5.12	118.61	122.20
34	YA	1101	U	N1-C2-O2	5.12	126.39	122.80
34	YA	2844	G	C4-N9-C1'	5.12	133.16	126.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	YA	2885	C	C6-N1-C2	-5.12	118.25	120.30
34	YA	749	C	C2-N1-C1'	5.12	124.43	118.80
34	YA	2712(A)	U	C5-C6-N1	5.12	125.26	122.70
1	XA	1439	C	C6-N1-C2	-5.12	118.25	120.30
34	YA	1417	C	C2-N1-C1'	5.12	124.43	118.80
1	QA	514	C	C5-C6-N1	5.12	123.56	121.00
34	RA	63	U	OP1-P-O3'	5.12	116.46	105.20
1	XA	744	C	C6-N1-C2	-5.12	118.25	120.30
29	R5	34	PRO	N-CA-CB	5.12	109.44	103.30
34	RA	1370	C	N3-C2-O2	-5.12	118.32	121.90
1	XA	1391	U	N3-C2-O2	-5.12	118.62	122.20
30	Y6	13	CYS	CA-CB-SG	-5.11	104.80	114.00
34	YA	1332	G	C8-N9-C1'	-5.11	120.35	127.00
22	QV	10	G	P-O3'-C3'	5.11	125.83	119.70
34	RA	974(B)	C	C2-N1-C1'	5.11	124.42	118.80
34	YA	838	C	C6-N1-C2	-5.11	118.26	120.30
34	YA	868	U	C2-N1-C1'	5.11	123.83	117.70
34	YA	2108	C	C6-N1-C2	-5.11	118.26	120.30
34	YA	1157	G	C4-C5-N7	5.11	112.84	110.80
34	RA	2784	C	N1-C2-O2	5.11	121.96	118.90
1	XA	328	C	C2-N1-C1'	5.11	124.42	118.80
1	XA	738	C	C2-N1-C1'	5.11	124.42	118.80
34	YA	2885	C	C5-C6-N1	5.11	123.55	121.00
34	RA	1178	C	P-O3'-C3'	5.11	125.83	119.70
34	RA	1516	U	C2-N1-C1'	5.11	123.83	117.70
34	YA	1516	U	N3-C2-O2	-5.11	118.63	122.20
34	YA	1982	C	C6-N1-C2	-5.11	118.26	120.30
34	YA	2326	C	C6-N1-C2	-5.11	118.26	120.30
38	YF	133	ASN	N-CA-C	-5.11	97.22	111.00
1	QA	18	C	C5-C6-N1	5.10	123.55	121.00
34	RA	691	C	C6-N1-C2	-5.10	118.26	120.30
34	YA	999	U	N3-C2-O2	-5.10	118.63	122.20
34	YA	2424	C	C5-C4-N4	-5.10	116.63	120.20
34	YA	2794	C	N1-C2-O2	5.10	121.96	118.90
34	YA	404	C	OP2-P-O3'	5.10	116.42	105.20
1	QA	1290	G	N3-C4-N9	5.10	129.06	126.00
34	RA	2636	U	N3-C2-O2	-5.10	118.63	122.20
35	RB	71	C	C2-N1-C1'	5.10	124.41	118.80
34	YA	1330	C	C6-N1-C2	-5.10	118.26	120.30
22	XV	31	G	C8-N9-C4	-5.10	104.36	106.40
1	XA	647	C	C6-N1-C2	-5.09	118.26	120.30
1	XA	754	C	C5-C6-N1	5.09	123.55	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	YA	1147	C	C6-N1-C2	-5.09	118.26	120.30
34	YA	1899	G	N1-C2-N2	-5.09	111.61	116.20
1	QA	1060	C	N1-C2-O2	5.09	121.96	118.90
1	XA	1165	C	C6-N1-C2	-5.09	118.26	120.30
34	YA	237	C	N1-C2-O2	5.09	121.95	118.90
1	QA	1358	U	C5-C6-N1	5.09	125.25	122.70
34	RA	1333	C	N1-C2-O2	5.09	121.95	118.90
34	RA	1417	C	N3-C4-N4	5.09	121.56	118.00
1	XA	955	U	C5-C6-N1	5.09	125.25	122.70
34	YA	914	C	C6-N1-C2	-5.09	118.26	120.30
34	YA	1370	C	C6-N1-C1'	-5.09	114.69	120.80
34	RA	231	C	N1-C2-O2	5.09	121.95	118.90
34	RA	1233	C	C6-N1-C2	-5.09	118.27	120.30
1	XA	1290	G	N3-C4-C5	-5.09	126.06	128.60
23	QX	18	C	C5'-C4'-O4'	5.08	115.20	109.10
34	YA	2044	C	C2-N1-C1'	5.08	124.39	118.80
22	QV	34	C	C5-C4-N4	-5.08	116.64	120.20
34	RA	766	C	C5-C6-N1	5.08	123.54	121.00
34	YA	177	G	C4-N9-C1'	5.08	133.11	126.50
34	YA	683	C	N1-C2-O2	5.08	121.95	118.90
34	YA	1864	U	N3-C2-O2	-5.08	118.64	122.20
1	QA	1285	A	OP2-P-O3'	5.08	116.38	105.20
1	XA	1075	C	C6-N1-C2	-5.08	118.27	120.30
34	YA	1332	G	C4-C5-N7	5.08	112.83	110.80
34	RA	904	C	C2-N1-C1'	5.08	124.39	118.80
34	RA	2210	G	N3-C4-C5	-5.08	126.06	128.60
34	RA	2636	U	N1-C2-O2	5.08	126.35	122.80
34	YA	465	G	N3-C4-C5	-5.08	126.06	128.60
34	RA	1526	G	C6-C5-N7	-5.08	127.36	130.40
54	RZ	12	GLY	N-CA-C	-5.08	100.41	113.10
1	XA	1018	C	N1-C2-O2	5.08	121.95	118.90
34	YA	719	C	C6-N1-C2	-5.07	118.27	120.30
1	QA	201(D)	U	C2-N1-C1'	5.07	123.79	117.70
34	RA	1830	C	C5-C6-N1	5.07	123.54	121.00
1	XA	241	C	C5-C6-N1	5.07	123.54	121.00
34	RA	2480	C	N1-C2-O2	5.07	121.94	118.90
1	XA	1336	C	OP2-P-O3'	5.07	116.36	105.20
34	YA	372	G	C4-N9-C1'	-5.07	119.91	126.50
34	YA	2036	C	C6-N1-C2	-5.07	118.27	120.30
1	QA	500	G	C4-N9-C1'	5.07	133.09	126.50
34	RA	319	C	C2-N1-C1'	5.07	124.37	118.80
34	RA	1312	U	OP2-P-O3'	5.07	116.35	105.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	YA	372	G	O4'-C1'-N9	5.07	112.25	108.20
34	YA	753	C	N1-C2-O2	5.07	121.94	118.90
34	YA	2816	C	C5-C6-N1	5.07	123.53	121.00
1	QA	1440(O)	C	N1-C2-O2	5.07	121.94	118.90
34	RA	2320	A	C2-N3-C4	5.07	113.13	110.60
34	RA	2579	C	C5-C6-N1	5.07	123.53	121.00
34	YA	641	C	C2-N1-C1'	5.07	124.37	118.80
34	YA	1394	U	C6-N1-C1'	5.07	128.29	121.20
34	YA	76	C	C6-N1-C2	-5.06	118.27	120.30
34	YA	533	G	N3-C4-C5	-5.06	126.07	128.60
34	RA	2471	C	N1-C2-O2	5.06	121.94	118.90
34	YA	537	C	C4-C5-C6	-5.06	114.87	117.40
34	RA	1178	C	N1-C2-O2	5.06	121.94	118.90
34	YA	114	U	N3-C2-O2	-5.06	118.66	122.20
34	YA	242	G	OP2-P-O3'	5.06	116.33	105.20
34	YA	436	C	C6-N1-C2	-5.06	118.28	120.30
34	YA	1741	C	C6-N1-C2	-5.06	118.28	120.30
1	QA	201(D)	U	N1-C2-O2	5.06	126.34	122.80
40	RH	155	SER	N-CA-C	5.06	124.66	111.00
34	YA	1398	C	C2-N1-C1'	5.06	124.36	118.80
34	YA	2870	C	C5-C6-N1	5.06	123.53	121.00
34	RA	2186	G	C4-N9-C1'	5.06	133.07	126.50
1	QA	1054	C	N1-C2-O2	5.05	121.93	118.90
1	QA	1225	A	N3-C4-N9	5.05	131.44	127.40
34	RA	1611	C	N1-C2-O2	5.05	121.93	118.90
37	RE	146	THR	N-CA-C	5.05	124.64	111.00
34	YA	2461	C	C2-N1-C1'	5.05	124.36	118.80
34	YA	1318	C	C5-C6-N1	5.05	123.53	121.00
34	RA	856	C	C2-N3-C4	5.05	122.42	119.90
34	YA	1958	C	C5-C6-N1	5.05	123.52	121.00
34	RA	2115	G	N3-C4-C5	-5.05	126.08	128.60
35	RB	68	C	C6-N1-C2	-5.05	118.28	120.30
1	XA	36	C	C6-N1-C2	-5.05	118.28	120.30
34	YA	626	U	C5-C6-N1	5.05	125.22	122.70
34	YA	1383	C	N3-C2-O2	-5.05	118.37	121.90
34	YA	2083	G	C5-C6-O6	-5.05	125.57	128.60
34	RA	2870	C	C6-N1-C2	-5.04	118.28	120.30
34	RA	1187	G	C8-N9-C4	-5.04	104.38	106.40
34	YA	2056	G	C4-N9-C1'	5.04	133.05	126.50
34	YA	2261	C	C2-N1-C1'	5.04	124.34	118.80
1	QA	1027	C	C6-N1-C1'	-5.04	114.75	120.80
34	RA	1686	C	C6-N1-C2	-5.04	118.28	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	RA	2103	C	N1-C2-O2	5.04	121.92	118.90
34	RA	2116	G	C8-N9-C4	-5.04	104.39	106.40
34	YA	510	C	C2-N1-C1'	5.04	124.34	118.80
34	RA	1345	C	C6-N1-C2	-5.04	118.29	120.30
34	RA	2350	C	C5-C6-N1	5.04	123.52	121.00
34	YA	857	C	C6-N1-C2	-5.04	118.29	120.30
35	RB	22	U	C5-C6-N1	5.03	125.22	122.70
34	RA	2343	C	C2-N1-C1'	5.03	124.33	118.80
34	RA	2724	C	N1-C2-O2	5.03	121.92	118.90
34	YA	486	C	C5-C6-N1	5.03	123.52	121.00
34	YA	2703	C	N1-C2-O2	5.03	121.92	118.90
34	RA	1258	C	C5-C6-N1	5.03	123.52	121.00
34	YA	1306	C	N1-C2-O2	5.03	121.92	118.90
34	YA	1432	C	C5-C6-N1	5.03	123.52	121.00
34	RA	1241	A	O4'-C1'-N9	5.03	112.22	108.20
34	RA	2164	C	N1-C2-O2	5.03	121.92	118.90
34	YA	1887	C	C6-N1-C2	-5.03	118.29	120.30
34	RA	1742	C	C5-C6-N1	5.03	123.51	121.00
34	YA	755	C	C5-C6-N1	5.03	123.51	121.00
34	YA	2083	G	C6-C5-N7	-5.03	127.38	130.40
23	QX	16	C	C5-C4-N4	5.02	123.72	120.20
34	YA	2752	C	N1-C2-O2	5.02	121.91	118.90
1	XA	330	C	C5-C6-N1	5.02	123.51	121.00
1	XA	1539	C	O4'-C1'-N1	5.02	112.22	108.20
34	YA	732	C	C5-C6-N1	5.02	123.51	121.00
1	QA	1075	C	C5-C6-N1	5.02	123.51	121.00
34	RA	267	C	C6-N1-C2	-5.02	118.29	120.30
34	YA	1533	C	C2-N1-C1'	5.02	124.32	118.80
1	XA	745	C	C6-N1-C2	-5.02	118.29	120.30
34	YA	560	C	C6-N1-C2	-5.02	118.29	120.30
34	YA	731	C	C5-C6-N1	5.02	123.51	121.00
34	YA	1404	C	N1-C2-O2	5.02	121.91	118.90
1	QA	514	C	C2-N1-C1'	5.02	124.32	118.80
34	RA	1417	C	C6-N1-C1'	-5.02	114.78	120.80
34	YA	974(B)	C	C6-N1-C1'	-5.02	114.78	120.80
34	RA	2149	G	N1-C2-N2	-5.01	111.69	116.20
54	YZ	63	ASP	CB-CG-OD1	5.01	122.81	118.30
34	RA	1375	C	C5-C6-N1	5.01	123.51	121.00
34	YA	1675	C	N3-C2-O2	-5.01	118.39	121.90
34	YA	731	C	C2-N1-C1'	5.01	124.31	118.80
34	YA	1882	C	N1-C2-O2	5.01	121.91	118.90
34	YA	2342	C	C2-N1-C1'	5.01	124.31	118.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	YY	79	CYS	CA-CB-SG	5.01	123.02	114.00
34	RA	392	C	C6-N1-C2	-5.01	118.30	120.30
34	YA	1786	A	C8-N9-C1'	-5.01	118.68	127.70
34	YA	2286	A	N7-C8-N9	5.01	116.30	113.80
1	QA	910	C	C6-N1-C2	-5.01	118.30	120.30
34	YA	540	G	C4-N9-C1'	5.01	133.01	126.50
34	RA	392	C	C5-C6-N1	5.01	123.50	121.00
34	YA	1406	U	N1-C2-O2	5.01	126.31	122.80
34	YA	783	A	C4-C5-N7	5.00	113.20	110.70
34	YA	944	G	C4-N9-C1'	5.00	133.01	126.50
34	YA	2803	C	N1-C2-O2	5.00	121.90	118.90
34	RA	231	C	C2-N1-C1'	5.00	124.30	118.80
34	RA	976	C	N1-C2-O2	5.00	121.90	118.90
34	YA	253	C	C5-C6-N1	5.00	123.50	121.00
34	RA	1178	C	C6-N1-C2	-5.00	118.30	120.30
34	YA	1544	C	N3-C2-O2	-5.00	118.40	121.90
34	YA	2474	C	C6-N1-C2	-5.00	118.30	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
28	Y4	5	ILE	CA

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
37	RE	146	THR	Peptide
50	RV	49	THR	Mainchain,Peptide
54	RZ	166	SER	Peptide
28	Y4	5	ILE	Mainchain
37	YE	146	THR	Peptide
54	YZ	166	SER	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	32469	0	16393	389	0
1	XA	32551	0	16433	382	1
2	QB	1907	0	1958	40	0
2	XB	1915	0	1968	37	0
3	QC	1605	0	1668	31	0
3	XC	1605	0	1668	22	0
4	QD	1703	0	1763	55	0
4	XD	1703	0	1763	47	0
5	QE	1155	0	1213	20	0
5	XE	1155	0	1213	22	0
6	QF	843	0	857	9	0
6	XF	843	0	857	11	0
7	QG	1257	0	1296	21	0
7	XG	1257	0	1296	23	0
8	QH	1108	0	1165	20	0
8	XH	1108	0	1165	23	0
9	QI	1010	0	1037	22	0
9	XI	998	0	1024	21	0
10	QJ	801	0	849	22	0
10	XJ	777	0	816	13	0
11	QK	885	0	904	7	0
11	XK	864	0	881	11	0
12	QL	975	0	1062	23	0
12	XL	956	0	1046	14	0
13	QM	955	0	1021	27	0
13	XM	914	0	971	23	0
14	QN	492	0	532	18	0
14	XN	492	0	531	16	0
15	QO	734	0	771	5	0
15	XO	729	0	768	10	0
16	QP	705	0	725	13	0
16	XP	705	0	725	12	0
17	QQ	834	0	904	12	0
17	XQ	834	0	904	12	0
18	QR	574	0	644	5	0
18	XR	574	0	644	11	0
19	QS	665	0	686	14	0
19	XS	674	0	699	16	0
20	QT	763	0	861	17	0
20	XT	763	0	861	17	0
21	QU	217	0	234	8	0
21	XU	217	0	234	4	0
22	QV	1647	0	834	23	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	XV	1647	0	834	18	0
23	QX	409	0	209	13	0
23	XX	409	0	209	6	0
24	R0	643	0	667	6	0
24	Y0	648	0	672	14	0
25	R1	746	0	826	21	0
25	Y1	729	0	802	7	0
26	R2	581	0	629	7	0
26	Y2	575	0	624	5	0
27	R3	469	0	518	6	0
27	Y3	469	0	518	10	0
28	R4	348	0	354	6	0
28	Y4	357	0	362	12	0
29	R5	459	0	477	23	0
29	Y5	459	0	476	17	0
30	R6	453	0	474	7	0
30	Y6	453	0	473	13	0
31	R7	409	0	454	9	0
31	Y7	418	0	467	7	0
32	R8	517	0	582	19	0
32	Y8	517	0	582	16	0
33	R9	307	0	335	9	0
33	Y9	307	0	336	17	0
34	RA	62070	0	31284	607	0
34	YA	62091	0	31294	489	0
35	RB	2573	0	1306	26	0
35	YB	2573	0	1306	24	0
36	RD	2115	0	2195	50	0
36	YD	2115	0	2195	39	0
37	RE	1568	0	1634	36	0
37	YE	1568	0	1633	34	0
38	RF	1585	0	1632	30	0
38	YF	1585	0	1632	31	0
39	RG	1474	0	1535	32	0
39	YG	1474	0	1535	24	0
40	RH	1336	0	1418	57	0
40	YH	1336	0	1418	21	0
41	RI	1136	0	1223	32	1
41	YI	1136	0	1223	25	0
42	RN	1104	0	1180	14	0
42	YN	1104	0	1180	15	0
43	RO	933	0	996	21	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	YO	933	0	996	14	0
44	RP	1145	0	1228	27	0
44	YP	1122	0	1206	28	0
45	RQ	1122	0	1179	23	0
45	YQ	1122	0	1179	25	0
46	RR	960	0	1021	31	0
46	YR	960	0	1021	19	0
47	RS	882	0	943	20	0
47	YS	882	0	943	18	0
48	RT	1141	0	1202	17	0
48	YT	1141	0	1202	27	0
49	RU	964	0	1022	25	0
49	YU	964	0	1022	22	0
50	RV	779	0	852	14	0
50	YV	779	0	852	12	0
51	RW	900	0	964	17	0
51	YW	900	0	964	16	0
52	RX	725	0	778	9	0
52	YX	725	0	778	14	0
53	RY	818	0	911	24	0
53	YY	818	0	910	21	0
54	RZ	1461	0	1493	32	0
54	YZ	1529	0	1551	29	0
55	QA	87	0	0	0	0
55	QF	1	0	0	0	0
55	QH	2	0	0	0	0
55	QL	1	0	0	0	0
55	R0	2	0	0	0	0
55	R1	1	0	0	0	0
55	R3	1	0	0	0	0
55	R8	1	0	0	0	0
55	RA	429	0	0	0	0
55	RB	11	0	0	0	0
55	RD	1	0	0	0	0
55	RE	4	0	0	0	0
55	RF	2	0	0	0	0
55	RN	1	0	0	0	0
55	RO	1	0	0	0	0
55	RP	1	0	0	0	0
55	RQ	1	0	0	0	0
55	XA	89	0	0	0	0
55	XE	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	Y1	1	0	0	0	0
55	Y2	1	0	0	0	0
55	Y5	1	0	0	0	0
55	Y7	1	0	0	0	0
55	Y8	1	0	0	0	0
55	YA	439	0	0	0	0
55	YB	8	0	0	0	0
55	YD	1	0	0	0	0
55	YE	2	0	0	0	0
55	YF	1	0	0	0	0
55	YQ	1	0	0	0	0
55	YR	2	0	0	0	0
55	YU	1	0	0	0	0
55	YX	1	0	0	0	0
56	QD	8	0	0	2	0
56	XD	8	0	0	0	0
57	QN	1	0	0	0	0
57	R5	1	0	0	0	0
57	R6	1	0	0	0	0
57	R9	1	0	0	0	0
57	RY	1	0	0	0	0
57	XN	1	0	0	0	0
57	Y5	1	0	0	0	0
57	Y6	1	0	0	0	0
57	Y9	1	0	0	0	0
57	YY	1	0	0	1	0
All	All	292039	0	197760	3309	1

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 (3309) 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)
14:QN:24:CYS:SG	14:QN:40:CYS:HB2	1.24	1.78
40:RH:98:LEU:CD2	40:RH:125:VAL:HG11	1.44	1.45
29:Y5:32:PRO:N	29:Y5:32:PRO:CA	1.69	1.44
30:R6:16:CYS:SG	30:R6:16:CYS:CB	2.06	1.44
14:QN:24:CYS:SG	14:QN:40:CYS:CB	2.14	1.35
34:RA:1789:A:OP1	36:RD:222:ARG:HG3	1.26	1.29
46:RR:12:ARG:CG	46:RR:16:HIS:CD2	2.17	1.27

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:QL:104:VAL:O	12:QL:105:TYR:CD2	1.90	1.24
40:RH:98:LEU:HD21	40:RH:125:VAL:CG1	1.66	1.23
40:RH:103:LEU:HD11	40:RH:123:PHE:CZ	1.72	1.22
46:RR:12:ARG:HD3	46:RR:16:HIS:NE2	1.53	1.21
46:RR:12:ARG:CG	46:RR:16:HIS:HD2	1.50	1.19
46:RR:12:ARG:HG2	46:RR:16:HIS:CD2	1.76	1.19
46:RR:12:ARG:HD3	46:RR:16:HIS:CD2	1.82	1.14
46:RR:12:ARG:CD	46:RR:16:HIS:CD2	2.31	1.14
1:XA:372:C:N4	1:XA:389:A:H62	1.48	1.11
34:YA:2611:U:H6	34:YA:2611:U:H5'	1.15	1.11
25:R1:90:ILE:HG22	25:R1:94:LEU:HD11	1.19	1.09
1:XA:372:C:H42	1:XA:389:A:N6	1.51	1.06
4:XD:18:LYS:NZ	4:XD:31:CYS:SG	2.26	1.06
14:YN:27:CYS:SG	14:YN:28:GLY:N	2.28	1.06
40:RH:87:LEU:O	40:RH:131:VAL:HG23	1.54	1.05
26:R2:48:HIS:HE2	26:R2:49:LYS:HE2	1.21	1.02
34:RA:1093:G:N2	34:RA:1098:A:H62	1.58	1.01
26:R2:48:HIS:NE2	26:R2:49:LYS:HE2	1.74	1.00
46:RR:12:ARG:HG2	46:RR:16:HIS:HD2	1.12	0.99
34:RA:1542:G:O6	34:RA:1543:A:N6	1.97	0.98
25:R1:95:LEU:O	25:R1:95:LEU:HD23	1.64	0.97
34:RA:1247:A:N1	34:RA:1249:U:O2	1.99	0.96
30:R6:13:CYS:SG	30:R6:14:THR:N	2.39	0.96
1:QA:372:C:N4	1:QA:389:A:H62	1.64	0.95
35:RB:22:U:H3	35:RB:61:G:H1	1.08	0.95
34:RA:2808:U:H3	34:RA:2892:A:H62	0.97	0.95
34:YA:2611:U:H5'	34:YA:2611:U:C6	2.02	0.95
29:R5:16:ARG:CD	34:RA:1263:U:H5''	1.97	0.94
1:QA:62:U:H3	1:QA:105:G:H1	0.95	0.94
34:RA:1093:G:H21	34:RA:1098:A:N6	1.66	0.94
34:YA:1652:A:N6	34:YA:1653:G:N1	2.17	0.93
22:XV:8:U:H3	22:XV:14:A:N6	1.66	0.93
34:RA:1035:U:H3	34:RA:1120:G:H1	1.14	0.93
1:XA:1238:A:N6	1:XA:1301:U:H3	1.66	0.93
34:RA:2094:G:OP1	41:RI:22:LYS:HE3	1.70	0.91
34:YA:2099:U:H3	34:YA:2190:G:H1	1.00	0.91
1:QA:372:C:H42	1:QA:389:A:N6	1.69	0.91
1:XA:45:U:H3	1:XA:396:G:H1	1.19	0.90
1:XA:927:G:H1	1:XA:1390:U:H3	1.10	0.90
25:R1:90:ILE:HA	25:R1:94:LEU:CD1	2.00	0.90
34:YA:1165:U:H3	34:YA:1184:G:H1	1.15	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:YA:2068:U:H3	34:YA:2430:A:H2	1.15	0.90
22:XV:8:U:H3	22:XV:14:A:H62	1.20	0.89
1:XA:1304:G:H21	1:XA:1333:A:H62	1.15	0.89
25:R1:90:ILE:CG2	25:R1:94:LEU:HD11	2.03	0.89
29:Y5:48:GLU:OE2	51:YW:37:ARG:NH1	2.05	0.88
1:XA:741:G:P	15:XO:35:ARG:HH21	1.96	0.88
34:RA:855:G:H1	34:RA:922:U:H3	1.20	0.88
34:RA:2508:G:H1	34:RA:2580:U:H3	1.21	0.88
1:XA:152:A:N6	1:XA:169:C:C4	2.43	0.87
1:QA:1066:C:H42	1:QA:1191:A:N6	1.72	0.87
34:RA:2680:C:OP2	37:RE:111:ARG:NH2	2.08	0.87
34:RA:585:G:N2	34:RA:1256:G:C6	2.42	0.86
34:RA:2808:U:H3	34:RA:2892:A:N6	1.73	0.86
33:Y9:13:LYS:HD2	33:Y9:13:LYS:O	1.76	0.86
1:QA:249:U:H3	1:QA:275:G:H1	1.19	0.86
1:XA:12:U:H3	1:XA:22:G:H1	1.24	0.86
40:RH:103:LEU:HD11	40:RH:123:PHE:CE1	2.09	0.85
1:XA:157:G:H1	1:XA:164:U:H3	1.21	0.85
34:YA:270(A):A:N6	34:YA:271(A):U:O2	2.09	0.85
1:XA:437:U:H3	1:XA:495:A:H62	1.21	0.85
34:YA:1419:A:H62	34:YA:1578:U:H3	1.23	0.85
34:RA:1482:U:H3	34:RA:1512:G:H1	1.25	0.85
34:RA:2475:C:H42	34:RA:2529:G:H22	1.22	0.84
4:QD:61:LYS:HE2	4:QD:206:PHE:CE2	2.11	0.84
16:QP:37:GLY:HA3	16:QP:50:LYS:O	1.77	0.84
34:RA:139:G:N2	34:RA:141(A):A:C6	2.45	0.84
34:RA:2542:A:O2'	34:RA:2543:G:H8	1.60	0.84
40:YH:9:ILE:HG21	40:YH:49:VAL:HB	1.56	0.84
1:QA:372:C:H42	1:QA:389:A:H62	0.88	0.84
34:RA:1093:G:H21	34:RA:1098:A:H62	0.86	0.84
35:RB:8:U:H3	35:RB:112:G:H1	1.21	0.84
34:YA:2542:A:H2	34:YA:2544:G:O6	1.61	0.84
40:RH:103:LEU:CD1	40:RH:123:PHE:CZ	2.61	0.84
1:XA:244:U:H3	1:XA:893:C:H42	1.22	0.84
35:YB:73:A:H62	35:YB:103:U:H3	1.26	0.83
34:RA:1247:A:C6	34:RA:1249:U:O2	2.31	0.83
29:R5:16:ARG:HD2	34:RA:1263:U:H5''	1.57	0.83
34:RA:2475:C:H42	34:RA:2529:G:N2	1.75	0.83
34:RA:2123:G:H1	34:RA:2175:C:H42	1.26	0.83
1:QA:401:C:C5	4:QD:73:ARG:NH2	2.48	0.82
1:QA:782:A:H62	1:QA:800:G:H21	1.27	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:RA:2751:G:C4	40:RH:3:ARG:HB3	2.14	0.82
1:XA:560:U:H5'	1:XA:566:G:N2	1.95	0.82
34:RA:586:A:H5'	38:RF:89:VAL:HG21	1.63	0.81
4:QD:61:LYS:HE2	4:QD:206:PHE:HE2	1.45	0.81
1:QA:15:G:H1	1:QA:920:U:H3	1.25	0.81
29:Y5:45:VAL:HG21	29:Y5:58:LEU:HD21	1.63	0.81
34:YA:1652:A:N6	34:YA:1653:G:C6	2.49	0.81
40:YH:9:ILE:CG2	40:YH:49:VAL:HB	2.11	0.80
40:RH:98:LEU:HD21	40:RH:125:VAL:HG11	0.81	0.80
1:XA:289:G:N2	1:XA:312:C:O2	2.14	0.80
25:R1:90:ILE:HG22	25:R1:94:LEU:CD1	2.06	0.80
46:RR:12:ARG:HG3	46:RR:16:HIS:HD2	1.47	0.80
34:RA:1632:A:N6	34:RA:1762:A:C2	2.49	0.80
34:RA:2852:G:H1	34:RA:2865:U:H3	1.26	0.80
40:RH:89:ILE:CD1	40:RH:131:VAL:HG22	2.12	0.80
41:RI:84:GLY:HA3	41:RI:89:TYR:OH	1.82	0.80
29:R5:16:ARG:HD3	34:RA:1263:U:H5''	1.63	0.79
35:RB:35:U:OP2	35:RB:36:C:OP2	1.98	0.79
34:RA:978:G:N2	34:RA:986:C:C2	2.50	0.79
1:QA:766:A:H62	1:QA:813:U:H3	1.27	0.79
4:QD:18:LYS:NZ	56:QD:301:SF4:S4	2.55	0.79
40:RH:98:LEU:CG	40:RH:125:VAL:HG11	2.13	0.78
1:QA:80:G:H1	1:QA:89:U:H3	1.30	0.78
1:QA:401:C:H5	4:QD:73:ARG:NH2	1.82	0.78
34:YA:59:U:H3	34:YA:68:G:H1	1.32	0.78
34:RA:2094:G:OP1	41:RI:22:LYS:CE	2.32	0.77
34:RA:676:A:H8	34:RA:2069:G:H21	1.33	0.77
34:RA:990:A:OP2	34:RA:991:C:OP2	2.03	0.77
34:RA:2291:U:H3	34:RA:2341:G:H1	1.28	0.77
40:RH:98:LEU:CD2	40:RH:125:VAL:CG1	2.41	0.77
34:RA:585:G:C2	34:RA:1256:G:C6	2.73	0.77
40:RH:87:LEU:O	40:RH:131:VAL:CG2	2.32	0.77
34:RA:1276:A:O2'	46:RR:12:ARG:NH1	2.18	0.77
1:XA:575:G:N2	1:XA:880:C:O2	2.17	0.77
34:YA:2508:G:H1	34:YA:2580:U:H3	1.31	0.77
50:RV:45:THR:O	50:RV:45:THR:HG22	1.83	0.77
25:R1:90:ILE:HA	25:R1:94:LEU:HD12	1.67	0.76
1:QA:819:A:N7	1:QA:1529:G:N1	2.34	0.76
41:RI:92:VAL:O	41:RI:120:ILE:HB	1.85	0.76
54:YZ:183:LEU:HD23	54:YZ:183:LEU:O	1.85	0.76
34:RA:2475:C:N4	34:RA:2529:G:H22	1.83	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:RA:526:A:OP1	34:RA:527:C:OP1	2.03	0.75
34:RA:2747:G:H21	34:RA:2757:A:H62	1.32	0.75
41:RI:92:VAL:HB	41:RI:120:ILE:CG2	2.16	0.75
10:QJ:79:ARG:NH1	10:QJ:79:ARG:O	2.20	0.75
33:Y9:27:CYS:SG	33:Y9:29:ASN:N	2.58	0.75
33:Y9:29:ASN:ND2	33:Y9:32:HIS:NE2	2.35	0.75
34:RA:1789:A:OP1	36:RD:222:ARG:CG	2.21	0.74
34:RA:2641:G:N2	34:RA:2774:C:C2	2.55	0.74
34:YA:2245:U:H6	34:YA:2245:U:H5''	1.52	0.74
34:YA:855:G:H1	34:YA:922:U:H3	1.34	0.74
32:R8:35:GLN:NE2	32:R8:36:LYS:HE2	2.02	0.74
34:RA:1165:U:H3	34:RA:1184:G:H1	1.35	0.74
34:RA:1234:U:C2'	34:RA:1235:G:H5'	2.17	0.74
1:XA:244:U:H3	1:XA:893:C:N4	1.85	0.74
1:XA:1304:G:N2	1:XA:1333:A:H62	1.85	0.74
1:QA:1066:C:H42	1:QA:1191:A:H62	1.32	0.74
1:QA:663:A:H61	1:QA:742:G:H1	1.36	0.73
1:QA:1066:C:N4	1:QA:1191:A:H62	1.84	0.73
1:XA:152:A:N6	1:XA:169:C:N4	2.36	0.73
34:RA:139:G:N2	34:RA:141(A):A:N6	2.36	0.73
34:YA:1215:G:H1	34:YA:1234:U:H3	1.36	0.73
34:RA:2542:A:O2'	34:RA:2543:G:C8	2.37	0.73
34:RA:2061:G:H5''	34:RA:2503:A:C2	2.24	0.72
34:RA:1632:A:N6	34:RA:1762:A:H2	1.87	0.72
2:QB:172:ILE:O	2:QB:176:GLU:HB2	1.88	0.72
34:YA:2611:U:H6	34:YA:2611:U:C5'	1.99	0.72
34:RA:141(A):A:H8	34:RA:1595:G:H21	1.37	0.72
1:QA:60:A:H62	1:QA:110:C:N4	1.88	0.72
36:RD:96:HIS:CE1	36:RD:102:LYS:HE2	2.24	0.71
1:XA:765:G:H1	1:XA:812:C:HO2'	1.37	0.71
1:QA:778:G:H1	1:QA:804:U:H3	1.38	0.71
34:YA:1612:C:C2	34:YA:1620:G:N2	2.59	0.71
9:QI:16:ARG:HB3	9:QI:64:THR:HG23	1.73	0.71
45:RQ:65:PHE:HB2	45:RQ:105:GLU:HB2	1.72	0.71
34:YA:1433:U:H3	34:YA:1560:G:H1	1.37	0.71
34:YA:574:C:N3	37:YE:145:LYS:NZ	2.35	0.71
1:XA:323:U:H3	1:XA:327:A:H62	1.39	0.71
34:RA:978:G:C2	34:RA:986:C:C2	2.79	0.70
2:XB:120:ALA:O	2:XB:124:SER:HB2	1.92	0.70
34:RA:1768:U:H3	34:RA:1984:G:H1	1.40	0.70
34:YA:2403:C:N4	34:YA:2415:G:C6	2.60	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:152:A:H62	1:XA:169:C:N4	1.90	0.70
12:QL:104:VAL:O	12:QL:105:TYR:HD2	1.68	0.70
2:QB:54:THR:HG22	2:QB:199:TYR:HB3	1.74	0.69
4:XD:57:ARG:HB3	4:XD:206:PHE:HB2	1.72	0.69
34:RA:1632:A:H61	34:RA:1762:A:H2	1.39	0.69
4:XD:12:CYS:SG	4:XD:19:LEU:HB2	2.33	0.69
4:QD:61:LYS:CE	4:QD:206:PHE:CE2	2.75	0.69
14:QN:24:CYS:SG	14:QN:40:CYS:CA	2.81	0.69
40:RH:103:LEU:CD1	40:RH:123:PHE:CE1	2.75	0.69
1:QA:819:A:N7	1:QA:1529:G:C2	2.61	0.69
34:RA:1234:U:O2'	34:RA:1235:G:H5'	1.93	0.69
29:R5:15:ARG:NH2	34:RA:2022:U:OP2	2.26	0.69
36:YD:35:LYS:HB2	36:YD:63:ARG:HA	1.75	0.69
1:QA:927:G:H1	1:QA:1390:U:H3	1.40	0.68
36:RD:8:PRO:HB3	36:RD:14:ARG:HB3	1.75	0.68
30:Y6:6:ARG:NH1	34:YA:2285:C:OP2	2.25	0.68
1:XA:289:G:N1	1:XA:312:C:N3	2.41	0.68
34:RA:1791:A:N6	34:RA:1828:G:O2'	2.25	0.68
42:RN:16:ILE:HB	42:RN:54:VAL:HG12	1.75	0.68
53:RY:99:CYS:HB2	53:RY:103:GLY:H	1.58	0.68
1:XA:68(F):G:H1	1:XA:68(V):U:H3	1.39	0.68
34:YA:2392:A:H2	34:YA:2424:C:H42	1.41	0.68
1:QA:60:A:N6	1:QA:110:C:N4	2.41	0.68
3:XC:43:LEU:O	3:XC:47:LEU:HB2	1.93	0.68
22:XV:8:U:N3	22:XV:14:A:N6	2.34	0.68
34:YA:2185:C:H2'	34:YA:2186:G:H8	1.58	0.68
41:RI:81:VAL:HG21	41:RI:88:ILE:HD12	1.75	0.68
45:RQ:38:GLU:HG2	45:RQ:127:ILE:HG23	1.74	0.68
34:YA:2245:U:H5''	34:YA:2245:U:C6	2.29	0.67
34:YA:2542:A:C2	34:YA:2544:G:O6	2.46	0.67
4:QD:3:ARG:HH22	4:QD:100:ARG:HH22	1.42	0.67
34:RA:2576:G:H3'	34:RA:2576:G:N3	2.09	0.67
34:YA:1154:G:OP2	49:YU:58:ARG:NH2	2.27	0.67
38:RF:154:VAL:HG12	38:RF:191:ARG:HB2	1.77	0.67
1:XA:1238:A:H62	1:XA:1301:U:H3	0.80	0.67
1:QA:437:U:H3	1:QA:495:A:H62	1.42	0.67
42:YN:131:GLN:OE1	42:YN:134:ARG:NH2	2.27	0.67
1:XA:107:G:N7	20:XT:15:ARG:NH2	2.43	0.67
45:YQ:16:ARG:HH21	45:YQ:18:LYS:HD3	1.59	0.67
5:QE:139:LEU:HA	5:QE:142:LEU:HD12	1.77	0.67
34:RA:784:A:OP2	34:RA:2589:A:OP1	2.13	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:RI:92:VAL:HB	41:RI:120:ILE:HG21	1.74	0.67
34:RA:2343:C:HO2'	34:RA:2373:G:HO2'	1.37	0.67
40:RH:101:ARG:HH12	40:RH:123:PHE:H	1.43	0.67
54:RZ:52:SER:O	54:RZ:54:HIS:N	2.28	0.67
22:QV:37:1MG:HM13	23:QX:16:C:C6	2.30	0.67
4:QD:31:CYS:SG	4:QD:33:MET:HB2	2.35	0.66
33:Y9:13:LYS:HD2	33:Y9:13:LYS:C	2.14	0.66
54:RZ:112:ARG:HG3	54:RZ:114:GLY:H	1.59	0.66
1:XA:1119:C:H2'	1:XA:1120:G:H8	1.60	0.66
1:XA:1238:A:N7	1:XA:1301:U:O4	2.27	0.66
22:XV:65:U:H2'	22:XV:66:A:H8	1.59	0.66
32:Y8:8:LYS:NZ	34:YA:243:U:OP1	2.28	0.66
53:YY:79:CYS:SG	57:YY:201:ZN:ZN	1.84	0.66
1:XA:1512:U:H3	1:XA:1523:G:H1	1.43	0.66
34:RA:139:G:N3	34:RA:141(A):A:N1	2.43	0.66
2:XB:185:ILE:HG22	2:XB:199:TYR:HB2	1.78	0.66
1:QA:765:G:H1	1:QA:812:C:HO2'	1.42	0.66
34:RA:981:A:H2	34:RA:2027:G:N3	1.93	0.66
1:XA:1300:G:O2'	1:XA:1303:C:N4	2.29	0.66
34:YA:1187:G:H8	34:YA:1187:G:O5'	1.79	0.66
34:RA:2751:G:N3	40:RH:3:ARG:HG2	2.10	0.66
1:XA:186(G):C:H42	1:XA:186(M):G:H1	1.43	0.66
1:QA:815:A:O4'	1:QA:817:C:N4	2.29	0.66
34:RA:27:G:N2	34:RA:513:A:OP2	2.29	0.66
40:RH:18:GLU:HB2	40:RH:25:LYS:HB2	1.78	0.66
1:XA:560:U:H5'	1:XA:566:G:H21	1.60	0.66
1:XA:1320:C:H42	19:XS:36:ARG:HG3	1.59	0.66
40:YH:84:SER:HB2	40:YH:132:ARG:HD2	1.78	0.66
9:XI:18:PHE:HB3	9:XI:20:ARG:HH12	1.60	0.66
34:RA:1052:C:O5'	34:RA:1052:C:H6	1.79	0.65
29:Y5:16:ARG:NH2	34:YA:517:C:OP1	2.28	0.65
2:QB:167:PRO:O	2:QB:171:ALA:HB2	1.96	0.65
34:RA:2508:G:O6	34:RA:2580:U:O4	2.15	0.65
34:RA:2641:G:C2	34:RA:2774:C:N3	2.65	0.65
34:RA:2641:G:N1	34:RA:2774:C:N3	2.43	0.65
1:QA:1127:G:N3	1:QA:1147:C:N4	2.44	0.65
1:QA:266:G:H5'	1:QA:268:C:H41	1.60	0.65
1:QA:766:A:N6	1:QA:813:U:H3	1.94	0.65
34:RA:962:G:OP1	34:RA:963:U:OP2	2.13	0.65
34:RA:1824:G:HO2'	36:RD:248:SER:HG	1.40	0.65
51:RW:88:ARG:HB2	51:RW:92:ARG:HB3	1.77	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:674:G:H2'	1:XA:675:A:H8	1.61	0.65
20:XT:86:ARG:O	20:XT:90:GLN:NE2	2.30	0.65
34:YA:530:G:O2'	34:YA:532:A:N7	2.29	0.65
50:RV:62:LEU:HD11	50:RV:95:LEU:HB2	1.77	0.65
1:QA:401:C:OP2	4:QD:73:ARG:NE	2.29	0.65
38:RF:147:GLY:O	38:RF:191:ARG:NH1	2.29	0.65
40:RH:89:ILE:HD11	40:RH:131:VAL:HG22	1.76	0.65
1:XA:375:U:H4'	16:XP:6:LEU:HD11	1.78	0.65
1:XA:438:G:H21	1:XA:497:A:H62	1.45	0.65
1:XA:1386:G:H2'	1:XA:1387:G:H8	1.61	0.65
34:YA:2680:C:H5'	37:YE:189:PRO:HA	1.79	0.65
13:QM:14:ARG:HG2	13:QM:44:ARG:HD3	1.78	0.65
34:RA:675:A:O2'	38:RF:67:GLN:NE2	2.29	0.65
34:RA:2641:G:N1	34:RA:2774:C:C4	2.65	0.65
29:Y5:48:GLU:CD	51:YW:37:ARG:HH12	1.99	0.65
1:QA:982:U:H3	1:QA:1223:C:H42	1.44	0.65
4:QD:121:VAL:HG22	4:QD:126:ILE:HG13	1.79	0.65
34:RA:229:A:H4'	34:RA:230:U:H5'	1.78	0.65
34:YA:703:U:H3	34:YA:728:G:H1	1.44	0.65
1:QA:942:G:H1	1:QA:1341:U:H3	1.45	0.65
1:XA:1261:A:H62	1:XA:1274:G:H21	1.45	0.65
54:RZ:10:ARG:HD2	54:RZ:38:TYR:HB3	1.79	0.65
4:XD:20:TYR:HA	4:XD:26:CYS:SG	2.37	0.65
22:XV:8:U:O4	22:XV:14:A:N7	2.30	0.65
47:YS:106:ARG:HB2	47:YS:110:LEU:HD23	1.78	0.65
34:RA:811:U:HO2'	34:RA:1250:G:HO2'	1.35	0.64
37:RE:75:VAL:HG23	37:RE:76:ARG:HG2	1.79	0.64
1:QA:860:A:N3	8:QH:18:ARG:NH1	2.44	0.64
2:QB:177:ALA:HB1	2:QB:182:ILE:HB	1.78	0.64
34:RA:331:A:N6	34:RA:1210:A:OP2	2.30	0.64
8:XH:14:ARG:HB3	8:XH:83:ILE:HD11	1.79	0.64
35:YB:90:C:H5'	45:YQ:18:LYS:HA	1.80	0.64
41:RI:92:VAL:HB	41:RI:120:ILE:HB	1.80	0.64
29:Y5:16:ARG:NH1	29:Y5:17:ASP:OD1	2.30	0.64
34:YA:1252:G:N3	49:YU:33:ARG:NH1	2.45	0.64
34:YA:1392:A:N6	52:YX:15:GLU:OE2	2.30	0.64
34:YA:2402:C:H6	34:YA:2402:C:O5'	1.80	0.64
4:QD:18:LYS:HG3	4:QD:33:MET:HG3	1.78	0.64
25:Y1:87:PRO:HA	25:Y1:90:ILE:HG22	1.80	0.64
1:QA:1291:G:H4'	9:QI:39:GLY:HA3	1.80	0.64
4:QD:9:CYS:SG	4:QD:22:LYS:NZ	2.71	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:RA:2542:A:C2	34:RA:2544:G:O6	2.50	0.64
1:QA:624:C:H2'	1:QA:625:G:H8	1.62	0.64
1:QA:1074:G:H1	1:QA:1083:U:H3	1.45	0.64
9:XI:17:VAL:HG12	9:XI:63:ILE:HD12	1.79	0.64
32:R8:8:LYS:NZ	34:RA:243:U:OP1	2.29	0.64
1:XA:1323:G:H5''	13:XM:99:ARG:HH21	1.61	0.64
34:YA:138:G:N2	52:YX:44:GLU:OE2	2.29	0.64
34:YA:414:C:O2	34:YA:1864:U:O2'	2.16	0.64
34:YA:2086:U:OP2	36:YD:263:ARG:NH1	2.29	0.64
1:QA:12:U:H3	1:QA:22:G:H1	1.46	0.64
34:RA:811:U:H3'	44:RP:22:GLY:HA2	1.80	0.64
34:RA:1654:A:H8	34:RA:1654:A:H5''	1.61	0.64
34:YA:1270:C:H5''	34:YA:1271:G:H5'	1.79	0.64
34:YA:1307:A:C6	34:YA:1622:G:O6	2.51	0.64
2:QB:132:LYS:HA	2:QB:135:GLN:HB2	1.78	0.64
34:RA:1026:U:H1'	34:RA:1027:A:H5''	1.80	0.64
34:YA:2425:A:H4'	34:YA:2426:A:H5''	1.79	0.64
1:QA:1415:G:H1	1:QA:1485:U:H3	1.44	0.64
34:RA:1818:U:OP2	36:RD:157:ARG:NH1	2.31	0.64
40:RH:6:ARG:HH22	40:RH:54:ARG:HD3	1.62	0.64
10:XJ:50:ILE:HA	10:XJ:60:ARG:HB2	1.79	0.64
36:RD:60:ARG:HD3	36:RD:86:PRO:HB2	1.80	0.63
45:RQ:81:VAL:HG12	45:RQ:82:ARG:HG2	1.80	0.63
1:XA:160:A:N1	1:XA:343:U:O2'	2.30	0.63
1:QA:1221:G:OP1	1:QA:1321:C:N4	2.31	0.63
54:RZ:52:SER:O	54:RZ:54:HIS:ND1	2.32	0.63
2:XB:54:THR:HG22	2:XB:199:TYR:HB3	1.81	0.63
32:Y8:22:VAL:HB	32:Y8:53:PRO:HB3	1.80	0.63
5:QE:140:ARG:O	5:QE:143:ARG:NH1	2.32	0.63
34:RA:1012:U:OP1	49:RU:75:ASN:ND2	2.31	0.63
40:RH:78:GLY:HA2	40:RH:82:GLY:HA3	1.79	0.63
41:RI:84:GLY:HA3	41:RI:89:TYR:CZ	2.33	0.63
34:YA:1695:G:N7	36:YD:14:ARG:NH2	2.47	0.63
34:YA:2701:C:H3'	34:YA:2702:U:H5''	1.80	0.63
44:YP:4:SER:O	44:YP:7:ARG:NH2	2.32	0.63
1:QA:346:G:OP1	48:RT:41:ARG:NH2	2.32	0.63
5:QE:79:GLU:O	8:QH:104:ARG:NH1	2.32	0.63
17:XQ:29:HIS:HB3	17:XQ:33:GLY:H	1.64	0.63
28:Y4:22:ILE:HG22	28:Y4:23:GLU:HG3	1.80	0.63
34:RA:1022:G:N7	34:RA:1140:C:N4	2.46	0.63
24:Y0:72:ARG:HE	24:Y0:75:LEU:HD12	1.64	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:RE:109:LYS:HE3	37:RE:191:PRO:HA	1.79	0.63
1:XA:166:G:H2'	1:XA:167:G:H8	1.64	0.63
34:YA:2006:C:O2'	34:YA:2823:A:N3	2.31	0.63
1:QA:619:U:N3	4:QD:134:ASP:OD1	2.30	0.63
34:RA:1247:A:OP2	44:RP:15:ARG:NH2	2.32	0.63
4:XD:8:VAL:HA	4:XD:11:LEU:HD13	1.81	0.63
32:R8:35:GLN:HE22	32:R8:36:LYS:HE2	1.62	0.62
34:YA:1186:G:H8	34:YA:1186:G:O5'	1.82	0.62
34:YA:1607:C:N4	34:YA:1622:G:OP2	2.32	0.62
34:YA:1995:U:O2	43:YO:3:GLN:NE2	2.32	0.62
1:QA:674:G:H2'	1:QA:675:A:H8	1.64	0.62
21:QU:12:LYS:HB3	21:QU:22:ARG:HD2	1.80	0.62
34:RA:998:C:OP2	49:RU:58:ARG:NH1	2.32	0.62
37:RE:119:ARG:HG3	37:RE:160:TYR:CD1	2.34	0.62
34:RA:2102:U:H3	34:RA:2187:G:H1	1.46	0.62
34:YA:627:A:N7	44:YP:84:ASN:ND2	2.46	0.62
54:YZ:52:SER:O	54:YZ:54:HIS:N	2.32	0.62
34:RA:139:G:C2	34:RA:141(A):A:N6	2.67	0.62
34:RA:2641:G:C2	34:RA:2774:C:C2	2.88	0.62
47:RS:83:LYS:HG3	47:RS:84:GLN:HG3	1.81	0.62
1:XA:345:C:O2'	1:XA:346:G:N2	2.33	0.62
1:QA:1198:G:H21	10:QJ:54:PHE:HE1	1.48	0.62
7:QG:118:VAL:O	7:QG:122:HIS:ND1	2.32	0.62
29:R5:51:TYR:CE1	29:R5:56:LYS:HB3	2.35	0.62
45:RQ:37:LEU:HD11	45:RQ:130:LYS:HG2	1.81	0.62
53:RY:99:CYS:CB	53:RY:103:GLY:H	2.12	0.62
1:QA:1066:C:N4	1:QA:1191:A:N6	2.43	0.62
27:R3:49:LYS:NZ	34:RA:851:U:OP1	2.31	0.62
34:YA:270(A):A:OP2	34:YA:270(Z):G:N2	2.28	0.62
34:YA:2547:U:O2	43:YO:23:ARG:NH2	2.33	0.62
41:YI:80:PRO:HB2	41:YI:146:ALA:HB2	1.81	0.62
34:RA:1314:C:OP1	34:RA:1332:G:OP1	2.17	0.62
1:XA:954:G:H21	1:XA:1227:A:H62	1.48	0.62
1:XA:1179:A:H4'	9:XI:103:THR:HA	1.80	0.62
1:XA:1510:U:H3	1:XA:1525:G:H1	1.48	0.62
34:YA:780:G:H21	34:YA:783:A:H62	1.48	0.62
34:YA:1612:C:C2	34:YA:1620:G:C2	2.88	0.62
36:YD:264:LYS:HG2	36:YD:266:SER:H	1.64	0.62
1:QA:262:A:H5''	20:QT:76:ALA:HB2	1.82	0.62
1:QA:553:A:H5''	12:QL:24:VAL:HG11	1.82	0.62
1:QA:570:G:H2'	1:QA:571:U:H6	1.64	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:1077:G:N2	1:QA:1080:A:OP2	2.33	0.62
47:YS:23:ARG:NH2	47:YS:84:GLN:OE1	2.33	0.62
1:QA:1073:U:O2	2:QB:104:ASN:ND2	2.32	0.62
29:R5:3:LYS:O	34:RA:2056:G:N2	2.30	0.62
1:XA:289:G:N2	1:XA:312:C:C2	2.68	0.62
1:XA:1007:C:N3	1:XA:1023:G:N2	2.48	0.62
38:YF:160:ASN:HB3	38:YF:163:VAL:HG12	1.81	0.62
22:QV:19:G:H1'	22:QV:56:C:H42	1.65	0.61
25:R1:95:LEU:O	25:R1:95:LEU:CD2	2.45	0.61
54:RZ:72:ARG:NH2	54:RZ:97:GLU:O	2.33	0.61
34:YA:269:U:C5	34:YA:271(A):U:C4	2.88	0.61
34:YA:768:G:O2'	34:YA:1379:A:N6	2.32	0.61
37:RE:141:ILE:O	37:RE:154:LYS:NZ	2.33	0.61
8:XH:17:THR:O	8:XH:78:GLN:NE2	2.32	0.61
32:Y8:11:LYS:HB3	32:Y8:60:LEU:HD11	1.82	0.61
34:YA:2126:A:N6	34:YA:2163:C:O2'	2.34	0.61
50:YV:72:VAL:HB	50:YV:85:LYS:HB3	1.82	0.61
27:R3:12:PRO:HB2	27:R3:20:LYS:HD3	1.82	0.61
34:RA:259:G:H21	34:RA:621:A:H8	1.48	0.61
34:RA:1664:A:H61	34:RA:1996:C:N4	1.99	0.61
34:RA:1859:A:N6	34:RA:1883:G:O2'	2.33	0.61
1:XA:339:C:OP2	43:YO:97:ARG:NH1	2.33	0.61
1:XA:749:C:H2'	1:XA:750:G:H8	1.64	0.61
1:XA:1157:A:H2'	1:XA:1181:G:H22	1.65	0.61
15:XO:88:ARG:NH1	34:YA:713:G:OP2	2.33	0.61
34:YA:814:C:O2'	34:YA:1225:C:N3	2.33	0.61
44:RP:47:ASP:OD2	44:RP:50:ARG:NH2	2.33	0.61
16:XP:6:LEU:HB2	16:XP:17:TYR:HB3	1.82	0.61
42:YN:112:LEU:O	42:YN:116:LEU:HB2	1.99	0.61
28:R4:16:CYS:SG	28:R4:17:GLY:N	2.73	0.61
1:XA:437:U:H3	1:XA:495:A:N6	1.96	0.61
36:RD:96:HIS:HE1	36:RD:102:LYS:HE2	1.64	0.61
34:YA:955:C:OP1	45:YQ:85:LYS:NZ	2.33	0.61
41:YI:30:LEU:HB3	41:YI:36:ALA:HB3	1.80	0.61
1:QA:992:U:H3	1:QA:1044:A:H62	1.47	0.61
1:QA:1316:G:H4'	14:QN:18:VAL:HG11	1.83	0.61
45:RQ:63:LYS:HD2	54:RZ:175:VAL:HG21	1.82	0.61
1:XA:881:G:OP2	12:XL:9:GLN:NE2	2.33	0.61
32:Y8:12:LYS:NZ	34:YA:249:C:O2	2.32	0.61
16:QP:53:VAL:HG12	16:QP:79:VAL:HG12	1.82	0.61
34:RA:300:A:OP1	53:RY:86:ARG:NH2	2.34	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:RR:74:LYS:HD3	46:RR:77:ARG:HH21	1.66	0.61
1:XA:1324:A:OP2	13:XM:99:ARG:NH2	2.33	0.61
54:YZ:181:GLU:O	54:YZ:182:LYS:O	2.19	0.61
1:QA:766:A:N7	1:QA:813:U:O4	2.34	0.61
1:QA:1306:A:N6	1:QA:1331:G:O2'	2.33	0.61
34:RA:1638:C:O3'	34:RA:2709:G:N2	2.34	0.61
53:RY:76:CYS:SG	53:RY:80:GLY:N	2.74	0.61
34:YA:265:A:N6	34:YA:427:U:O2'	2.34	0.61
35:YB:37:C:O2	47:YS:95:HIS:NE2	2.27	0.61
7:QG:133:GLY:HA2	7:QG:136:LYS:HE2	1.83	0.60
7:QG:138:LYS:HE2	7:QG:142:GLU:HG3	1.83	0.60
13:QM:57:ARG:O	13:QM:61:GLU:HB2	2.01	0.60
54:RZ:3:TYR:HB2	54:RZ:57:ILE:HG22	1.81	0.60
34:YA:2010:G:H5''	51:YW:42:ARG:HB2	1.81	0.60
34:RA:2641:G:H2'	34:RA:2642:G:H8	1.66	0.60
48:RT:77:PRO:HG2	48:RT:80:SER:HB3	1.82	0.60
1:XA:68(I):G:H21	1:XA:68(T):C:H41	1.47	0.60
34:YA:960:A:H61	45:YQ:82:ARG:HH12	1.48	0.60
34:RA:626:U:H3	44:RP:105:LEU:HA	1.66	0.60
34:RA:994:C:OP1	49:RU:53:ARG:NH2	2.35	0.60
4:XD:25:ARG:NE	4:XD:30:LYS:O	2.33	0.60
34:YA:688:U:H6	34:YA:688:U:O5'	1.85	0.60
34:YA:750:A:C2	34:YA:753:C:C6	2.89	0.60
34:YA:2402:C:H6	34:YA:2402:C:C5'	2.14	0.60
34:RA:2483:C:N3	45:RQ:124:LYS:NZ	2.49	0.60
39:RG:72:ARG:HA	39:RG:87:PRO:HA	1.82	0.60
34:YA:1093:G:H21	34:YA:1098:A:H62	1.48	0.60
34:YA:2572:A:OP1	34:YA:2574:G:O2'	2.20	0.60
35:YB:48:A:OP2	47:YS:30:ARG:NH2	2.34	0.60
37:YE:1:MET:HG3	37:YE:200:GLU:HG2	1.82	0.60
2:XB:163:PHE:HA	2:XB:185:ILE:O	2.01	0.60
34:YA:1669:A:H2'	34:YA:1669:A:N3	2.17	0.60
34:RA:2808:U:C2	34:RA:2892:A:N6	2.70	0.60
28:Y4:1:MET:N	35:YB:44:G:OP1	2.33	0.60
34:YA:1224:G:N2	34:YA:1227:A:OP2	2.31	0.60
41:RI:92:VAL:HB	41:RI:120:ILE:CB	2.30	0.60
1:XA:1118:C:OP1	9:XI:104:ARG:NH1	2.34	0.60
39:YG:16:ARG:NH2	39:YG:28:VAL:O	2.35	0.60
44:YP:58:THR:O	44:YP:61:ARG:NH2	2.34	0.60
51:YW:6:ILE:HG12	51:YW:104:THR:HG23	1.84	0.60
51:YW:30:GLU:O	51:YW:34:ASN:ND2	2.34	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:RA:585:G:C2	34:RA:1256:G:O6	2.55	0.60
34:RA:1234:U:H2'	34:RA:1235:G:H5'	1.83	0.60
46:RR:97:VAL:HG22	46:RR:114:VAL:HG12	1.84	0.60
4:XD:13:ARG:HG3	4:XD:40:PRO:HD3	1.84	0.60
34:YA:987:G:O2'	34:YA:1000:A:N3	2.30	0.60
40:YH:89:ILE:O	40:YH:129:THR:OG1	2.19	0.60
1:QA:1261:A:H62	1:QA:1274:G:H21	1.50	0.60
32:R8:12:LYS:NZ	34:RA:249:C:O2	2.35	0.60
2:XB:67:THR:HG21	2:XB:155:LEU:HG	1.84	0.60
2:XB:126:GLU:OE2	2:XB:130:ARG:NH1	2.34	0.60
13:XM:3:ARG:O	13:XM:57:ARG:NH2	2.35	0.60
34:RA:1827:C:OP2	36:RD:222:ARG:NH1	2.35	0.60
1:XA:545:C:OP2	4:XD:65:ARG:NH2	2.35	0.60
34:YA:811:U:O4	44:YP:21:ARG:NH2	2.34	0.60
34:YA:1340:U:OP2	52:YX:78:LYS:NZ	2.32	0.60
38:YF:11:VAL:HG22	38:YF:125:LEU:HB2	1.84	0.60
10:QJ:6:ILE:HG22	10:QJ:98:ILE:HG22	1.84	0.59
32:R8:56:GLU:HA	32:R8:59:LYS:HE2	1.83	0.59
1:XA:760:G:N2	17:XQ:97:SER:OG	2.35	0.59
5:XE:79:GLU:HG3	5:XE:93:PRO:HD2	1.84	0.59
34:YA:782:A:O2'	36:YD:225:ALA:O	2.19	0.59
34:YA:2108:C:N3	34:YA:2182:G:N2	2.50	0.59
47:YS:4:LEU:HD11	47:YS:12:PHE:HE2	1.67	0.59
1:QA:544:G:OP1	4:QD:59:ARG:NH2	2.35	0.59
11:XK:17:GLY:HA2	11:XK:35:PRO:HD3	1.83	0.59
30:Y6:6:ARG:HH21	30:Y6:24:GLU:HG3	1.65	0.59
31:Y7:3:ARG:NE	34:YA:1613:G:O2'	2.36	0.59
1:QA:178:C:H2'	1:QA:179:A:H8	1.66	0.59
1:QA:545:C:OP2	4:QD:65:ARG:NH2	2.36	0.59
34:RA:825:C:O2	44:RP:55:ARG:NH2	2.36	0.59
34:RA:2701:C:H3'	34:RA:2702:U:H5''	1.84	0.59
37:RE:201:THR:HG22	37:RE:203:LYS:H	1.66	0.59
41:RI:88:ILE:HG22	41:RI:90:GLY:H	1.66	0.59
1:XA:520:A:H62	1:XA:529:G:H21	1.50	0.59
34:YA:994:C:OP1	49:YU:53:ARG:NH2	2.36	0.59
34:YA:1988:C:N4	34:YA:1989:G:O6	2.35	0.59
51:YW:33:ARG:NH2	51:YW:52:GLU:OE1	2.35	0.59
34:RA:2820:A:N3	34:RA:2820:A:H2'	2.17	0.59
46:RR:12:ARG:HG3	46:RR:16:HIS:CD2	2.25	0.59
28:Y4:5:ILE:HD13	28:Y4:5:ILE:N	2.17	0.59
34:YA:2055:C:O2	34:YA:2572:A:N6	2.35	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:RA:530:G:O2'	34:RA:532:A:N7	2.34	0.59
40:RH:89:ILE:HD11	40:RH:131:VAL:CG2	2.32	0.59
1:XA:410:G:H21	1:XA:432:A:H62	1.50	0.59
8:XH:100:ILE:HD11	8:XH:125:ARG:HB3	1.84	0.59
34:YA:1216:G:OP1	49:YU:11:ARG:NH2	2.32	0.59
34:YA:1433:U:O4	34:YA:1560:G:O6	2.21	0.59
37:YE:143:ASN:OD1	37:YE:143:ASN:N	2.35	0.59
53:YY:79:CYS:HB2	53:YY:81:LYS:HG2	1.83	0.59
31:R7:9:ARG:NE	34:RA:1310:G:OP2	2.34	0.59
34:RA:572:A:H61	34:RA:2029:G:H21	1.50	0.59
34:RA:659:C:H2'	34:RA:660:G:H8	1.66	0.59
22:XV:30:C:H2'	22:XV:31:G:H8	1.66	0.59
36:YD:61:LEU:O	36:YD:63:ARG:NH1	2.36	0.59
41:YI:9:LEU:HD21	41:YI:35:LEU:HD12	1.84	0.59
34:RA:2085:C:H4'	36:RD:262:ARG:HH21	1.66	0.59
34:RA:2542:A:H2	34:RA:2544:G:O6	1.86	0.59
35:RB:37:C:O2	47:RS:95:HIS:NE2	2.35	0.59
41:RI:93:THR:O	41:RI:97:ILE:HG13	2.03	0.59
46:RR:51:LEU:HG	46:RR:66:VAL:HG23	1.85	0.59
8:XH:91:ARG:NH1	17:XQ:32:TYR:O	2.35	0.59
25:Y1:39:LYS:NZ	34:YA:205:G:O6	2.35	0.59
34:YA:83:G:N2	34:YA:103:A:OP2	2.34	0.59
1:QA:782:A:H62	1:QA:800:G:N2	1.98	0.59
4:QD:98:GLU:OE1	4:QD:103:ASN:ND2	2.36	0.59
34:RA:1066:U:N3	34:RA:1069:A:OP2	2.34	0.59
40:RH:107:VAL:O	40:RH:152:ARG:NH2	2.35	0.59
43:RO:88:ASN:ND2	43:RO:90:GLN:OE1	2.36	0.59
23:QX:8:A:H2'	23:QX:9:G:H8	1.68	0.59
10:XJ:10:GLY:HA3	10:XJ:16:LEU:HD21	1.84	0.59
34:YA:2475:C:H42	34:YA:2529:G:H22	1.50	0.59
34:YA:2502:G:H5''	34:YA:2503:A:H5''	1.85	0.59
38:YF:168:ARG:HG2	38:YF:175:THR:HG21	1.84	0.59
34:RA:2576:G:O2'	34:RA:2579:C:OP2	2.16	0.59
13:XM:3:ARG:HH12	13:XM:11:ARG:HH21	1.51	0.59
19:XS:63:THR:OG1	19:XS:65:ASN:OD1	2.21	0.59
34:YA:1800:C:OP2	36:YD:183:ARG:NH1	2.34	0.59
54:YZ:151:HIS:HB3	54:YZ:170:THR:HA	1.85	0.59
1:QA:1071:C:H2'	1:QA:1072:G:H8	1.67	0.58
29:R5:33:CYS:CB	29:R5:46:CYS:SG	2.90	0.58
34:RA:2134:A:O2'	34:RA:2159:G:N3	2.36	0.58
34:RA:2448:A:OP2	34:RA:2499:C:OP2	2.21	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:RH:152:ARG:HG2	40:RH:153:LYS:HG2	1.84	0.58
33:Y9:6:SER:HB3	34:YA:2466:C:H5''	1.85	0.58
3:QC:108:ASN:ND2	3:QC:144:SER:OG	2.36	0.58
5:QE:75:THR:OG1	5:QE:76:ILE:N	2.35	0.58
38:RF:148:LEU:HD13	38:RF:191:ARG:HH11	1.68	0.58
1:XA:406:G:H1	1:XA:436:C:H42	1.51	0.58
1:XA:578:C:H5''	1:XA:578:C:H6	1.68	0.58
34:YA:1930:G:N2	34:YA:1969:A:OP2	2.35	0.58
34:RA:309:G:N3	34:RA:329:G:O2'	2.36	0.58
1:XA:1463:C:H4'	48:YT:112:ARG:HH21	1.68	0.58
34:YA:1789:A:OP2	36:YD:222:ARG:NH1	2.36	0.58
1:QA:976:G:O4'	1:QA:1363:A:N6	2.36	0.58
2:QB:78:GLN:O	2:QB:94:ASN:ND2	2.37	0.58
34:RA:946:G:O6	34:RA:972:G:N2	2.36	0.58
34:RA:1637:A:H4'	34:RA:2711:A:O2'	2.03	0.58
1:XA:49:U:H3	1:XA:362:G:H1'	1.69	0.58
1:XA:1130:A:O2'	9:XI:3:GLN:OE1	2.22	0.58
34:YA:27:G:N2	34:YA:513:A:OP2	2.36	0.58
34:YA:776:G:N7	34:YA:793:A:O2'	2.36	0.58
34:YA:1667:G:O2'	34:YA:1991:U:O4	2.21	0.58
36:YD:35:LYS:H	36:YD:64:ILE:HG12	1.68	0.58
6:QF:23:LYS:NZ	6:QF:42:GLU:OE1	2.36	0.58
34:RA:2086:U:OP2	36:RD:263:ARG:NH1	2.36	0.58
34:RA:2729:G:H1'	37:RE:187:ALA:HB2	1.86	0.58
5:XE:18:ARG:NH1	5:XE:25:ARG:O	2.36	0.58
22:XV:49:G:H1	22:XV:65:U:H3	1.52	0.58
24:Y0:33:ALA:O	34:YA:2353:G:O2'	2.22	0.58
32:Y8:42:ARG:NH1	34:YA:2349:G:OP2	2.36	0.58
34:YA:269:U:C6	34:YA:271(A):U:C4	2.91	0.58
37:YE:50:GLY:HA2	37:YE:77:ILE:HA	1.85	0.58
37:YE:128:SER:OG	37:YE:129:HIS:N	2.35	0.58
43:YO:80:ASP:OD2	48:YT:64:ARG:NH2	2.34	0.58
30:R6:16:CYS:SG	30:R6:42:TRP:HB2	2.44	0.58
1:XA:578:C:H5''	1:XA:578:C:C6	2.38	0.58
1:XA:643:C:H2'	1:XA:644:G:H8	1.67	0.58
3:XC:9:GLY:HA2	3:XC:12:LEU:HD13	1.83	0.58
34:YA:180:G:N2	34:YA:215:G:O6	2.36	0.58
4:QD:59:ARG:HH12	4:QD:66:ARG:HH22	1.51	0.58
34:RA:654(B):G:N2	34:RA:654(U):C:O2	2.36	0.58
34:RA:863:A:O3'	35:RB:100:G:N2	2.37	0.58
50:RV:24:LYS:HA	50:RV:92:THR:HG23	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:RX:25:LYS:HD3	52:RX:80:ILE:HD11	1.86	0.58
53:RY:99:CYS:HB2	53:RY:103:GLY:N	2.18	0.58
34:YA:141(A):A:H8	34:YA:1595:G:H21	1.50	0.58
1:QA:736:C:OP1	18:QR:72:ARG:NH2	2.37	0.58
1:QA:1268:A:N3	21:QU:20:LYS:NZ	2.51	0.58
43:RO:1:MET:HB2	43:RO:32:TYR:HB3	1.84	0.58
54:RZ:30:ASN:HB3	54:RZ:90:VAL:HG22	1.86	0.58
13:XM:11:ARG:O	13:XM:13:LYS:NZ	2.35	0.58
17:XQ:99:SER:OG	17:XQ:100:LYS:N	2.37	0.58
20:XT:71:THR:OG1	20:XT:72:LEU:N	2.36	0.58
1:QA:1233:G:OP2	9:QI:124:GLN:NE2	2.36	0.58
1:QA:1522:U:H2'	1:QA:1523:G:H8	1.69	0.58
10:QJ:40:LEU:HD11	10:QJ:71:LEU:HB2	1.86	0.58
22:QV:37:IMG:H3'	22:QV:38:A:H8	1.69	0.58
34:RA:197:A:N6	34:RA:2430:A:C8	2.72	0.58
34:RA:2431:U:N3	34:RA:2434:A:OP2	2.31	0.58
34:RA:2808:U:O4	34:RA:2892:A:N7	2.36	0.58
1:XA:825:G:O2'	8:XH:12:ARG:NH2	2.37	0.58
34:YA:392:C:H5''	34:YA:409:C:H5''	1.85	0.58
34:YA:442:G:H1'	38:YF:48:THR:HG21	1.86	0.58
34:YA:2683:C:O2	43:YO:70:LYS:NZ	2.28	0.58
41:YI:3:VAL:HG12	41:YI:38:LEU:HA	1.85	0.58
3:QC:91:LEU:HD12	3:QC:101:LEU:HD11	1.85	0.57
27:R3:30:ARG:NH1	34:RA:1184:G:OP1	2.37	0.57
34:RA:1653:G:N7	46:RR:9:LYS:HB2	2.18	0.57
34:RA:2314:C:H2'	34:RA:2315:G:H8	1.69	0.57
39:RG:15:VAL:HG22	39:RG:175:LEU:HD22	1.86	0.57
5:XE:11:ILE:HG21	5:XE:105:VAL:HG22	1.86	0.57
34:YA:662:G:OP1	44:YP:15:ARG:NH1	2.36	0.57
34:YA:1068:G:O2'	34:YA:1096:A:N3	2.37	0.57
34:YA:2118:U:H3	34:YA:2148:G:H4'	1.67	0.57
34:YA:2788:C:O2'	34:YA:2809:A:N3	2.32	0.57
34:RA:265:A:N6	34:RA:428:A:N7	2.52	0.57
34:RA:2712(A):U:O2	34:RA:2712(A):U:H5''	2.05	0.57
41:RI:115:ALA:HB2	41:RI:131:LYS:HE3	1.85	0.57
1:XA:1304:G:H21	1:XA:1333:A:N6	1.93	0.57
27:Y3:24:LYS:NZ	34:YA:933:A:OP1	2.36	0.57
34:YA:2131:G:H1'	34:YA:2158:A:H61	1.69	0.57
34:YA:2508:G:O6	34:YA:2580:U:O4	2.22	0.57
46:YR:56:LYS:O	46:YR:88:ARG:NH2	2.36	0.57
48:YT:36:GLU:OE1	48:YT:41:ARG:NH1	2.37	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:881:G:OP1	12:QL:13:LYS:NZ	2.37	0.57
4:QD:167:GLY:O	4:QD:169:LYS:NZ	2.36	0.57
12:QL:113:ARG:HH21	12:QL:116:SER:HB2	1.68	0.57
34:RA:585:G:N2	34:RA:1256:G:C5	2.71	0.57
34:RA:1789:A:P	36:RD:222:ARG:HG3	2.40	0.57
35:RB:9:G:OP1	47:RS:15:ARG:NH1	2.37	0.57
37:RE:26:ILE:HG23	37:RE:182:LEU:HB3	1.86	0.57
49:RU:6:THR:OG1	49:RU:7:GLY:N	2.37	0.57
1:XA:708:C:OP1	11:XK:85:ARG:NH2	2.35	0.57
1:XA:1028(B):C:O2	1:XA:1028(I):G:N2	2.37	0.57
2:XB:115:LEU:HD12	2:XB:145:LEU:HB3	1.86	0.57
20:XT:30:LYS:HA	20:XT:33:ILE:HD12	1.87	0.57
34:YA:2134:A:H8	34:YA:2157:G:H21	1.53	0.57
34:YA:2880:C:O2'	46:YR:90:ARG:NH1	2.37	0.57
39:YG:29:TRP:O	39:YG:33:ARG:NH1	2.37	0.57
40:YH:9:ILE:HD12	40:YH:51:ARG:HG2	1.85	0.57
1:QA:1408:A:O2'	34:RA:1916:A:N6	2.34	0.57
34:RA:1856:G:O6	34:RA:1857:G:N2	2.37	0.57
40:RH:149:ARG:HA	40:RH:162:ILE:HD11	1.85	0.57
1:XA:1440(K):C:O2'	1:XA:1440(L):G:N2	2.37	0.57
1:XA:1507:A:H2'	1:XA:1508:G:H8	1.70	0.57
8:XH:11:THR:O	8:XH:15:ASN:ND2	2.37	0.57
34:YA:2312:U:O2	39:YG:40:ASN:ND2	2.35	0.57
1:QA:995:C:H2'	1:QA:996:A:H8	1.70	0.57
10:QJ:45:ARG:HB3	10:QJ:65:LEU:HB3	1.85	0.57
34:RA:1454:U:O2'	34:RA:1455:G:N7	2.36	0.57
8:XH:8:ASP:OD2	8:XH:12:ARG:NH2	2.37	0.57
34:YA:2219:G:OP1	36:YD:172:TYR:OH	2.22	0.57
34:YA:2871:C:OP1	46:YR:50:HIS:NE2	2.37	0.57
1:QA:677:U:O2	1:QA:777:A:O2'	2.22	0.57
1:QA:1060:C:H4'	10:QJ:51:ARG:HB3	1.86	0.57
1:QA:1240:U:O4	7:QG:109:ASN:ND2	2.37	0.57
2:QB:74:LYS:HG3	2:QB:77:ALA:HB3	1.87	0.57
7:QG:50:ILE:HG12	7:QG:61:VAL:HG11	1.86	0.57
9:QI:67:GLY:O	9:QI:73:GLN:NE2	2.38	0.57
26:R2:4:SER:OG	26:R2:5:GLU:N	2.37	0.57
34:RA:514:A:N3	34:RA:581:C:O2'	2.35	0.57
45:RQ:12:GLN:HB2	45:RQ:73:PRO:HD2	1.87	0.57
1:XA:1158:C:H2'	1:XA:1159:U:H4'	1.87	0.57
1:XA:1414:U:H2'	1:XA:1415:G:H8	1.70	0.57
3:XC:17:ASP:OD1	3:XC:21:ARG:NH2	2.37	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:YA:1113:U:H5'	40:YH:2:SER:HB3	1.85	0.57
34:YA:1307:A:C6	34:YA:1622:G:C6	2.93	0.57
36:YD:28:GLU:HG2	36:YD:29:PRO:HD3	1.86	0.57
1:QA:237:C:H2'	1:QA:238:G:H8	1.69	0.57
1:QA:1505:G:H4'	1:QA:1506:U:H5''	1.85	0.57
2:QB:219:VAL:HA	2:QB:222:ILE:HD12	1.85	0.57
10:QJ:24:VAL:HG21	10:QJ:37:PRO:HG3	1.87	0.57
32:R8:13:ARG:HG2	44:RP:63:PRO:HB3	1.85	0.57
34:RA:1528:A:OP2	34:RA:1542:G:O6	2.23	0.57
34:RA:2744:G:N2	40:RH:143:GLN:OE1	2.37	0.57
43:RO:71:ARG:NE	43:RO:105:GLU:OE2	2.36	0.57
1:XA:1252:A:H61	1:XA:1285:A:H61	1.53	0.57
34:YA:2882:A:OP1	46:YR:96:ARG:NH1	2.37	0.57
46:YR:57:ARG:NH1	46:YR:59:ASP:OD2	2.38	0.57
1:QA:944:G:H21	1:QA:1339:A:H62	1.52	0.57
34:RA:2683:C:N3	34:RA:2727:G:O2'	2.36	0.57
3:XC:36:ASP:OD1	3:XC:59:ARG:NH2	2.34	0.57
34:YA:1566:A:OP1	36:YD:211:ARG:NH1	2.37	0.57
36:YD:184:LYS:HB3	36:YD:269:PHE:HB3	1.86	0.57
53:YY:30:VAL:HG22	53:YY:37:VAL:HG12	1.87	0.57
1:QA:1440(K):C:O2'	1:QA:1440(L):G:N2	2.36	0.57
9:XI:10:ARG:HG3	9:XI:11:LYS:HG2	1.86	0.57
34:YA:974(A):G:C4	34:YA:989:G:N2	2.72	0.57
1:QA:9:G:N7	1:QA:558:G:O2'	2.38	0.57
1:QA:570:G:O4'	1:QA:820:U:C6	2.58	0.57
13:QM:91:ARG:HD2	13:QM:96:LEU:HD22	1.87	0.57
34:RA:2406:U:OP2	34:RA:2411:A:N6	2.38	0.57
1:XA:1131:G:H1	1:XA:1143:G:H21	1.53	0.57
34:YA:886:C:O2'	34:YA:889:C:N4	2.35	0.57
40:YH:155:SER:OG	40:YH:156:ALA:N	2.36	0.57
1:QA:401:C:C6	4:QD:73:ARG:NH2	2.73	0.56
17:XQ:3:LYS:HB2	17:XQ:60:ILE:HD11	1.86	0.56
30:Y6:3:SER:OG	30:Y6:4:GLU:N	2.37	0.56
30:Y6:19:ARG:HH21	30:Y6:52:VAL:HG21	1.68	0.56
34:YA:184:C:O2'	34:YA:217:G:N3	2.35	0.56
1:QA:60:A:N6	1:QA:110:C:C4	2.73	0.56
1:QA:1316:G:N1	1:QA:1319:A:OP2	2.37	0.56
2:QB:130:ARG:O	2:QB:135:GLN:NE2	2.37	0.56
9:QI:64:THR:OG1	9:QI:66:ARG:NH1	2.37	0.56
28:R4:1:MET:N	35:RB:39:A:N1	2.53	0.56
34:RA:495:G:N3	51:RW:61:ASN:ND2	2.53	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:RA:1251:C:OP2	49:RU:10:ARG:NH1	2.38	0.56
34:RA:2816:C:O2	34:RA:2883:A:O2'	2.21	0.56
39:RG:144:ILE:HG22	39:RG:146:TYR:H	1.69	0.56
1:XA:427:U:OP2	4:XD:36:ARG:NH1	2.38	0.56
1:XA:1317:C:O2	19:XS:37:ARG:NH2	2.38	0.56
11:XK:15:ALA:HA	11:XK:77:MET:HA	1.86	0.56
15:XO:88:ARG:NH2	34:YA:714:U:OP2	2.38	0.56
34:YA:1812:A:H2'	34:YA:1813:G:H8	1.69	0.56
1:QA:708:C:H2'	1:QA:709:G:H8	1.70	0.56
2:QB:87:ARG:NH1	2:QB:220:ASP:OD2	2.38	0.56
25:R1:29:GLY:O	34:RA:2396:G:O2'	2.23	0.56
34:RA:978:G:C2	34:RA:986:C:N3	2.73	0.56
34:RA:1066:U:H2'	34:RA:1067:A:H3'	1.87	0.56
34:RA:2635:C:H5''	37:RE:78:LEU:HA	1.86	0.56
35:RB:35:U:OP2	35:RB:36:C:P	2.62	0.56
40:RH:29:PRO:HD2	40:RH:79:VAL:HB	1.86	0.56
44:RP:58:THR:O	44:RP:61:ARG:NH2	2.38	0.56
54:RZ:127:LYS:HB3	54:RZ:162:GLU:HB2	1.86	0.56
1:XA:405:U:O4	4:XD:2:GLY:N	2.37	0.56
1:XA:413:G:H1'	1:XA:428:G:H21	1.70	0.56
8:XH:73:ASP:OD1	8:XH:75:ARG:NH1	2.38	0.56
10:XJ:40:LEU:HD11	10:XJ:71:LEU:HB2	1.87	0.56
37:YE:49:LEU:HD22	37:YE:81:ILE:HD11	1.85	0.56
45:YQ:24:GLY:H	45:YQ:101:ARG:HD2	1.70	0.56
46:YR:14:SER:OG	46:YR:15:SER:N	2.38	0.56
53:YY:76:CYS:HB3	53:YY:79:CYS:SG	2.45	0.56
33:R9:6:SER:HB2	34:RA:2466:C:H5''	1.88	0.56
1:XA:118:U:O5'	1:XA:118:U:H6	1.88	0.56
1:XA:754:C:OP1	15:XO:72:ARG:NH2	2.38	0.56
8:XH:32:LYS:HA	8:XH:35:ILE:HD12	1.86	0.56
9:XI:111:ARG:NH1	14:XN:61:TRP:O	2.33	0.56
34:YA:2068:U:N3	34:YA:2430:A:H2	1.95	0.56
1:QA:825:G:O2'	8:QH:12:ARG:NH2	2.37	0.56
8:QH:12:ARG:HD2	8:QH:26:VAL:HG12	1.88	0.56
31:R7:29:LYS:HA	31:R7:32:LYS:HG3	1.88	0.56
34:RA:768:G:O2'	34:RA:1379:A:N6	2.39	0.56
37:RE:34:VAL:HG21	37:RE:77:ILE:HD11	1.88	0.56
45:RQ:138:ASP:O	45:RQ:141:GLN:NE2	2.39	0.56
49:RU:50:ARG:O	49:RU:54:LYS:NZ	2.39	0.56
53:RY:30:VAL:HG12	53:RY:37:VAL:HG23	1.87	0.56
1:XA:272:C:H2'	1:XA:273:A:H8	1.70	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:YA:748:G:C8	34:YA:750:A:C8	2.94	0.56
34:RA:1035:U:O2	34:RA:1120:G:N2	2.31	0.56
35:RB:104:A:OP1	54:RZ:72:ARG:NH1	2.38	0.56
37:RE:39:PRO:HD3	37:RE:45:THR:HG22	1.87	0.56
1:XA:407:G:OP1	4:XD:115:ARG:NH1	2.38	0.56
34:YA:2847:U:OP1	48:YT:98:LYS:NZ	2.37	0.56
39:YG:37:VAL:HG13	39:YG:94:LEU:HB2	1.85	0.56
54:YZ:52:SER:O	54:YZ:54:HIS:ND1	2.38	0.56
34:RA:793:A:OP2	34:RA:2071:A:O2'	2.23	0.56
34:RA:1297:C:H2'	34:RA:1298:C:H6	1.71	0.56
34:RA:2061:G:H5''	34:RA:2503:A:N1	2.20	0.56
38:RF:195:ASP:N	38:RF:195:ASP:OD1	2.38	0.56
41:RI:26:ALA:HA	41:RI:30:LEU:HB2	1.88	0.56
43:YO:107:ARG:NH2	48:YT:36:GLU:O	2.39	0.56
1:QA:200:G:N2	1:QA:218:C:O2	2.38	0.56
12:QL:71:PRO:O	12:QL:102:ARG:NH1	2.39	0.56
13:QM:11:ARG:HG3	13:QM:12:ASN:H	1.71	0.56
38:RF:117:ARG:NH1	38:RF:120:GLU:OE2	2.38	0.56
1:XA:152:A:N6	1:XA:169:C:N3	2.54	0.56
1:XA:684:A:O2'	11:XK:39:PRO:O	2.21	0.56
24:Y0:23:VAL:HG21	34:YA:857:C:H4'	1.88	0.56
34:YA:1918:A:O2'	34:YA:1920:C:N4	2.38	0.56
42:YN:63:THR:OG1	42:YN:64:GLY:N	2.39	0.56
1:QA:186(J):U:O2'	17:QQ:63:ARG:NH2	2.38	0.56
34:RA:1022:G:N2	34:RA:1141:U:N3	2.54	0.56
42:RN:22:THR:OG1	42:RN:23:LEU:N	2.39	0.56
1:XA:8:A:N1	4:XD:209:ARG:NH1	2.53	0.56
1:XA:605:U:H6	1:XA:605:U:O5'	1.88	0.56
4:XD:205:GLU:OE1	5:XE:107:ARG:NH1	2.39	0.56
34:YA:2291:U:O2'	34:YA:2374:C:O2	2.24	0.56
1:QA:259:G:OP2	20:QT:83:ARG:NH1	2.38	0.56
1:XA:38:G:N2	1:XA:397:A:OP1	2.39	0.56
1:XA:776:G:N2	1:XA:802:A:OP2	2.38	0.56
3:XC:14:ILE:HG22	3:XC:15:THR:HG23	1.88	0.56
34:YA:664:C:OP1	44:YP:18:ARG:NH1	2.39	0.56
41:YI:130:TYR:HB3	41:YI:136:VAL:HG13	1.86	0.56
1:QA:1236:A:OP1	21:QU:10:ARG:NH1	2.39	0.55
34:RA:180:G:N2	34:RA:215:G:O6	2.39	0.55
34:RA:566:U:H5''	44:RP:29:LYS:HE3	1.88	0.55
34:RA:1658:C:OP1	37:RE:135:HIS:NE2	2.39	0.55
39:RG:126:ASP:OD2	39:RG:130:ASN:ND2	2.36	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:RI:86:THR:O	41:RI:122:GLU:HG2	2.05	0.55
34:YA:2375:G:N2	34:YA:2378:A:OP2	2.34	0.55
39:YG:77:ILE:HG22	39:YG:82:LEU:HB2	1.89	0.55
1:QA:791:G:O6	1:QA:792:A:N6	2.39	0.55
1:QA:993:G:O2'	1:QA:994:A:N7	2.37	0.55
2:QB:195:ASP:O	8:QH:68:ARG:NH2	2.39	0.55
25:R1:90:ILE:CA	25:R1:94:LEU:HD12	2.35	0.55
34:RA:494:G:OP1	51:RW:8:ARG:NH1	2.39	0.55
35:RB:48:A:OP2	47:RS:30:ARG:NH2	2.39	0.55
53:RY:47:LYS:NZ	53:RY:48:ALA:O	2.37	0.55
34:YA:1728:G:N1	34:YA:1730:U:OP2	2.39	0.55
35:YB:90:C:OP2	45:YQ:16:ARG:NH1	2.38	0.55
34:RA:815:C:OP2	50:RV:83:ARG:NH1	2.38	0.55
34:RA:1025:G:N7	34:RA:1135:C:H1'	2.21	0.55
43:RO:106:LEU:HB3	43:RO:111:PHE:HB2	1.87	0.55
44:RP:90:ARG:HG3	44:RP:91:PHE:HD1	1.71	0.55
14:YN:23:ARG:NH1	14:YN:24:CYS:O	2.40	0.55
28:Y4:24:THR:O	39:YG:105:LYS:NZ	2.38	0.55
34:YA:527:C:N4	34:YA:2779:U:OP2	2.39	0.55
34:YA:956:G:OP2	45:YQ:14:ARG:NH2	2.39	0.55
42:YN:129:PRO:O	42:YN:134:ARG:NH1	2.33	0.55
1:QA:806:C:H2'	1:QA:807:A:H8	1.70	0.55
24:R0:74:ARG:NH2	34:RA:2334:G:O6	2.39	0.55
43:RO:19:ILE:HG22	43:RO:43:VAL:HG12	1.88	0.55
23:XX:6:G:H2'	23:XX:7:G:C8	2.42	0.55
34:YA:335:C:OP2	53:YY:84:ARG:NH2	2.40	0.55
34:YA:1246:A:OP1	44:YP:15:ARG:NH2	2.38	0.55
34:YA:2690:C:OP1	46:YR:17:ARG:NH2	2.40	0.55
48:YT:51:ARG:HD2	48:YT:100:TYR:HE1	1.72	0.55
1:QA:116:A:H61	1:QA:313:A:H1'	1.71	0.55
1:QA:677:U:H3	1:QA:713:G:H22	1.53	0.55
1:QA:1438:G:OP1	20:QT:34:LYS:NZ	2.40	0.55
40:RH:33:LEU:HD11	40:RH:136:ILE:HG13	1.87	0.55
43:RO:14:THR:HG21	43:RO:86:ILE:HD12	1.88	0.55
1:XA:323:U:O4	1:XA:327:A:N7	2.40	0.55
1:XA:890:G:O2'	1:XA:906:G:O6	2.24	0.55
1:XA:1291:G:OP1	7:XG:37:ASN:ND2	2.39	0.55
32:Y8:12:LYS:NZ	34:YA:247:G:O6	2.36	0.55
34:YA:2406:U:OP2	34:YA:2411:A:N6	2.39	0.55
43:YO:87:ILE:HD12	43:YO:91:LEU:HA	1.89	0.55
48:YT:3:ARG:HG3	48:YT:6:LEU:HB2	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:YU:92:ARG:HH11	50:YV:11:GLN:HB2	1.71	0.55
1:QA:673:G:H2'	1:QA:674:G:C8	2.42	0.55
9:QI:46:ALA:HA	9:QI:78:LYS:HB3	1.88	0.55
34:RA:288:C:H2'	34:RA:289:A:H8	1.71	0.55
34:RA:1075:C:OP1	45:RQ:59:ARG:NH1	2.36	0.55
34:RA:2581:G:C6	34:RA:2610:C:N3	2.75	0.55
38:RF:117:ARG:NH2	38:RF:189:THR:O	2.40	0.55
47:RS:106:ARG:HA	47:RS:110:LEU:HD21	1.88	0.55
4:QD:11:LEU:HD13	4:QD:66:ARG:HD2	1.88	0.55
29:R5:16:ARG:NH2	34:RA:517:C:OP1	2.40	0.55
34:RA:729:G:C6	36:RD:208:LYS:HB2	2.42	0.55
34:RA:1660:C:H2'	34:RA:1661:G:H8	1.71	0.55
34:RA:1675:C:H6	34:RA:1675:C:O5'	1.89	0.55
1:XA:927:G:N2	1:XA:1390:U:O2	2.32	0.55
33:Y9:14:CYS:HA	33:Y9:27:CYS:HB2	1.88	0.55
34:YA:998:C:OP2	49:YU:58:ARG:NH1	2.40	0.55
34:YA:1203:G:O6	34:YA:1204:A:N6	2.40	0.55
38:YF:56:GLU:OE2	38:YF:93:LYS:NZ	2.36	0.55
1:QA:626:U:H2'	1:QA:627:G:H8	1.71	0.55
1:QA:1507:A:C2	1:QA:1530:G:C4	2.95	0.55
3:QC:108:ASN:HB3	3:QC:111:LEU:HB2	1.89	0.55
34:RA:2463:C:C2	34:RA:2488:A:C2	2.95	0.55
40:RH:86:GLU:HG3	40:RH:165:ALA:HB3	1.89	0.55
43:RO:112:MET:HA	43:RO:115:VAL:HG22	1.88	0.55
1:XA:59:A:H2	1:XA:330:C:H42	1.54	0.55
41:YI:131:LYS:HG2	41:YI:135:GLU:HG3	1.87	0.55
26:R2:35:LEU:HD23	26:R2:50:ILE:HG12	1.88	0.55
47:RS:25:ARG:HH21	47:RS:40:ILE:HG13	1.70	0.55
24:Y0:19:LYS:NZ	34:YA:2261:C:OP1	2.34	0.55
34:YA:483:A:O2'	53:YY:49:VAL:O	2.25	0.55
34:YA:2403:C:C4	34:YA:2415:G:N1	2.75	0.55
1:QA:107:G:H3'	1:QA:108:G:H21	1.71	0.55
1:QA:542:G:OP1	4:QD:10:ARG:NH1	2.34	0.55
31:R7:23:ARG:O	31:R7:28:ARG:NH1	2.40	0.55
33:Y9:16:VAL:HG12	33:Y9:25:VAL:HG12	1.88	0.55
1:QA:578:C:H6	1:QA:578:C:H5''	1.71	0.54
1:QA:954:G:H4'	13:QM:121:LYS:HB3	1.89	0.54
34:RA:834:C:H2'	34:RA:835:A:H8	1.72	0.54
43:RO:104:ARG:NH2	43:RO:121:VAL:O	2.40	0.54
1:XA:45:U:O4	1:XA:396:G:O6	2.25	0.54
1:XA:564:C:O2'	8:XH:91:ARG:NH2	2.39	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:1261:A:H62	1:XA:1274:G:N2	2.04	0.54
1:XA:1312:G:H5'	19:XS:5:LEU:HD11	1.88	0.54
34:YA:219:G:N3	34:YA:234:C:O2'	2.35	0.54
34:YA:2473:U:OP1	34:YA:2529:G:N2	2.39	0.54
41:YI:129:THR:HA	41:YI:137:PRO:HA	1.89	0.54
53:YY:83:THR:HG21	53:YY:99:CYS:SG	2.48	0.54
8:QH:64:LYS:HG2	8:QH:79:VAL:HG11	1.90	0.54
13:QM:67:GLU:OE1	13:QM:71:ARG:NH1	2.40	0.54
14:QN:24:CYS:SG	14:QN:40:CYS:N	2.80	0.54
31:R7:7:PRO:HB2	34:RA:1309:G:H4'	1.89	0.54
34:RA:2511:U:O2'	37:RE:138:PRO:O	2.25	0.54
45:RQ:45:GLN:NE2	45:RQ:91:GLU:O	2.40	0.54
1:XA:398:C:H2'	1:XA:399:G:H8	1.72	0.54
54:YZ:149:SER:OG	54:YZ:150:LEU:N	2.40	0.54
1:QA:634:C:H2'	1:QA:635:G:H8	1.73	0.54
34:RA:783:A:H8	34:RA:784:A:H4'	1.72	0.54
34:RA:982:C:O5'	34:RA:982:C:H6	1.90	0.54
34:RA:2845:G:H2'	34:RA:2846:G:H8	1.72	0.54
43:RO:22:ILE:HB	43:RO:40:VAL:HG13	1.89	0.54
47:RS:34:HIS:ND1	47:RS:53:SER:OG	2.40	0.54
51:RW:67:ASP:N	51:RW:67:ASP:OD1	2.39	0.54
54:RZ:128:VAL:HG23	54:RZ:161:VAL:HG12	1.89	0.54
2:XB:187:LEU:HA	2:XB:201:ILE:HB	1.90	0.54
6:XF:87:ARG:NH1	18:XR:75:ILE:O	2.40	0.54
7:XG:29:LYS:HE2	7:XG:102:ARG:HB3	1.89	0.54
25:Y1:52:ARG:NH2	34:YA:2213:U:O2	2.41	0.54
30:Y6:40:CYS:HB3	30:Y6:43:CYS:HB3	1.88	0.54
34:YA:116:C:O2'	34:YA:126:A:N3	2.33	0.54
34:YA:1328:G:O5'	34:YA:1328:G:H8	1.89	0.54
1:QA:1360:A:OP2	14:QN:35:ARG:NH1	2.40	0.54
5:QE:151:LEU:HD12	8:QH:79:VAL:HG12	1.89	0.54
12:QL:53:ARG:HB3	12:QL:69:TYR:HE1	1.73	0.54
14:QN:6:LEU:HB3	14:QN:23:ARG:HH12	1.72	0.54
34:RA:270(V):C:H2'	34:RA:270(W):G:H8	1.73	0.54
34:RA:819:A:OP2	34:RA:1187:G:N2	2.40	0.54
34:RA:2490:G:H2'	34:RA:2490:G:N3	2.22	0.54
35:RB:22:U:O4	35:RB:61:G:O6	2.26	0.54
1:XA:318:G:HO2'	1:XA:1468:A:HO2'	1.54	0.54
1:XA:1394:A:N6	1:XA:1500:A:O2'	2.30	0.54
22:XV:31:G:H22	22:XV:39:C:H42	1.54	0.54
34:YA:24:G:O2'	51:YW:78:GLU:O	2.25	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:YA:323:G:HO2'	34:YA:1205:U:H3	1.56	0.54
34:YA:867:C:N3	34:YA:912:C:O2'	2.40	0.54
34:YA:958:U:OP2	45:YQ:14:ARG:NH1	2.40	0.54
34:YA:2848:G:O2'	34:YA:2867:G:N2	2.38	0.54
1:QA:231:G:H2'	1:QA:232:G:H8	1.73	0.54
1:QA:458(F):A:OP1	16:QP:75:ARG:NH1	2.39	0.54
34:RA:392:C:H5''	34:RA:409:C:H5''	1.89	0.54
37:RE:2:LYS:NZ	37:RE:100:GLU:OE2	2.40	0.54
34:YA:1657:C:H4'	37:YE:133:LYS:HB3	1.89	0.54
40:YH:2:SER:O	40:YH:2:SER:OG	2.24	0.54
54:YZ:97:GLU:HB3	54:YZ:125:LEU:HD11	1.90	0.54
1:QA:266:G:O2'	1:QA:268:C:OP2	2.21	0.54
3:QC:88:ARG:HG2	3:QC:101:LEU:HD13	1.90	0.54
33:R9:14:CYS:HA	33:R9:27:CYS:HB2	1.88	0.54
34:RA:484:C:P	53:RY:50:ARG:HG2	2.48	0.54
34:RA:687:C:H42	34:RA:787:U:H4'	1.73	0.54
50:RV:62:LEU:HB2	50:RV:93:GLU:HG3	1.88	0.54
1:XA:107:G:H3'	1:XA:108:G:H21	1.72	0.54
1:XA:356:A:O2'	1:XA:367:U:O2'	2.21	0.54
1:XA:1240:U:OP1	7:XG:119:ARG:NH2	2.41	0.54
34:YA:581:C:H2'	34:YA:582:G:H8	1.72	0.54
34:YA:784:A:OP2	34:YA:2589:A:OP1	2.25	0.54
46:YR:104:ARG:NH1	46:YR:107:ASP:OD1	2.40	0.54
34:RA:1546:C:H5'	34:RA:1547:C:H5'	1.90	0.54
34:RA:2808:U:N3	34:RA:2892:A:N6	2.39	0.54
38:RF:63:LYS:NZ	38:RF:75:HIS:O	2.33	0.54
53:RY:6:HIS:O	53:RY:97:ARG:NH2	2.39	0.54
1:XA:1221:G:H4'	19:XS:77:THR:HG21	1.88	0.54
26:Y2:36:ARG:NH2	52:YX:8:ILE:O	2.41	0.54
34:YA:579:G:O2'	34:YA:2019:A:OP1	2.25	0.54
34:YA:2577:A:H5''	34:YA:2578:G:H5'	1.88	0.54
51:YW:69:LEU:HD13	51:YW:107:LEU:HD23	1.89	0.54
1:QA:191:G:O2'	20:QT:101:GLY:O	2.22	0.54
3:QC:11:ARG:NH2	3:QC:177:THR:O	2.40	0.54
22:QV:19:G:OP2	22:QV:20:G:N2	2.41	0.54
1:XA:453:A:H5'	16:XP:75:ARG:HH22	1.73	0.54
45:YQ:45:GLN:NE2	45:YQ:91:GLU:O	2.40	0.54
1:QA:296:U:O2'	1:QA:556:C:O2	2.24	0.54
1:QA:1106:G:H4'	3:QC:172:ARG:HG3	1.89	0.54
34:RA:240:G:O2'	34:RA:257:A:N6	2.41	0.54
34:RA:1202:C:HO2'	38:RF:184:TYR:HH	1.56	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:RA:1676:A:C2	34:RA:1993:U:H5'	2.43	0.54
1:XA:9:G:N7	1:XA:558:G:O2'	2.41	0.54
7:XG:71:PRO:O	7:XG:96:GLN:NE2	2.41	0.54
27:Y3:8:LEU:HD13	27:Y3:23:LEU:HD11	1.90	0.54
32:Y8:7:HIS:NE2	34:YA:251:A:OP1	2.38	0.54
34:YA:602:G:HO2'	34:YA:604:G:HO2'	1.50	0.54
34:YA:861:A:N3	35:YB:79:C:O2'	2.40	0.54
34:YA:971:C:O2'	34:YA:983:A:N3	2.32	0.54
34:YA:1709:U:O2'	34:YA:2859:G:N3	2.35	0.54
54:YZ:53:ILE:HG22	54:YZ:71:VAL:HG13	1.90	0.54
1:QA:938:A:O3'	7:QG:95:ARG:NH2	2.41	0.54
10:QJ:40:LEU:HD13	10:QJ:69:ASN:HB3	1.90	0.54
29:R5:33:CYS:N	29:R5:38:ALA:O	2.28	0.54
34:RA:59:U:H3	34:RA:68:G:H1	1.55	0.54
34:RA:987:G:O2'	34:RA:1000:A:N3	2.35	0.54
34:RA:1681:G:O2'	34:RA:1762:A:O2'	2.26	0.54
34:RA:2468:G:OP2	34:RA:2468:G:N2	2.41	0.54
46:RR:33:ARG:NH2	46:RR:115:GLU:OE1	2.41	0.54
34:YA:1664:A:H61	34:YA:1996:C:H42	1.56	0.54
39:YG:19:LEU:HD23	39:YG:32:PRO:HD2	1.89	0.54
54:YZ:108:PRO:HA	54:YZ:142:SER:HA	1.88	0.54
3:QC:108:ASN:HD22	3:QC:111:LEU:HD23	1.72	0.53
19:QS:4:SER:OG	19:QS:5:LEU:N	2.41	0.53
33:R9:25:VAL:HB	33:R9:34:GLN:HB2	1.90	0.53
34:RA:1068:G:N2	34:RA:1095:A:O2'	2.41	0.53
2:XB:192:SER:OG	2:XB:193:ASP:N	2.40	0.53
34:YA:270(G):U:H3	34:YA:270(U):G:H1	1.56	0.53
34:YA:1296:G:OP1	34:YA:2709:G:O2'	2.19	0.53
34:YA:2540:C:O2'	34:YA:2740:A:N3	2.34	0.53
29:R5:36:CYS:SG	29:R5:49:CYS:HB3	2.49	0.53
34:RA:662:G:OP1	44:RP:15:ARG:NH1	2.41	0.53
34:RA:1019:U:OP1	34:RA:1035:U:O2'	2.21	0.53
16:XP:37:GLY:HA3	16:XP:50:LYS:O	2.09	0.53
35:YB:73:A:N7	35:YB:103:U:O4	2.40	0.53
41:YI:68:LEU:HA	41:YI:71:ILE:HG22	1.90	0.53
1:QA:112:G:H1	1:QA:315:A:H61	1.57	0.53
34:RA:605:C:O2	34:RA:657:U:O2'	2.26	0.53
34:RA:1247:A:C6	34:RA:1249:U:C2	2.96	0.53
35:RB:57:A:OP2	35:RB:58:A:OP2	2.27	0.53
36:RD:44:ASN:N	36:RD:44:ASN:OD1	2.41	0.53
1:XA:1354:C:H2'	1:XA:1355:G:H8	1.73	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:XH:86:ILE:HD11	8:XH:136:GLU:HG2	1.89	0.53
25:Y1:2:SER:N	34:YA:1364:G:N7	2.56	0.53
29:Y5:3:LYS:HG3	34:YA:2611:U:C4	2.42	0.53
33:Y9:29:ASN:ND2	33:Y9:32:HIS:CD2	2.77	0.53
34:YA:2125:G:N1	34:YA:2172:U:OP1	2.42	0.53
45:YQ:28:ALA:N	45:YQ:105:GLU:OE2	2.41	0.53
54:YZ:11:GLU:O	54:YZ:36:LYS:NZ	2.36	0.53
1:QA:754:C:OP1	15:QO:72:ARG:NH2	2.40	0.53
34:RA:918:A:N3	35:RB:80:U:O2'	2.39	0.53
34:RA:2291:U:O2'	34:RA:2374:C:O2	2.27	0.53
1:XA:1306:A:N6	1:XA:1331:G:O2'	2.41	0.53
17:XQ:83:ASP:N	17:XQ:83:ASP:OD1	2.40	0.53
30:Y6:35:GLU:OE2	30:Y6:50:ARG:NH1	2.42	0.53
31:Y7:8:ASN:ND2	34:YA:770:G:OP1	2.40	0.53
34:YA:2403:C:N4	34:YA:2415:G:N1	2.57	0.53
54:YZ:129:SER:OG	54:YZ:132:ASN:OD1	2.24	0.53
46:RR:56:LYS:NZ	46:RR:90:ARG:O	2.41	0.53
1:XA:1028(D):G:O2'	1:XA:1028(G):A:N6	2.40	0.53
18:XR:47:THR:HG22	18:XR:85:LEU:HD13	1.90	0.53
24:Y0:20:ARG:HD3	34:YA:2356:C:H4'	1.91	0.53
34:YA:906:G:HO2'	45:YQ:67:ARG:HH21	1.56	0.53
1:QA:357:G:O2'	41:YI:89:TYR:O	2.25	0.53
6:QF:97:PHE:HB2	18:QR:32:ARG:HE	1.73	0.53
27:R3:12:PRO:HA	27:R3:15:TYR:HD2	1.73	0.53
29:R5:16:ARG:HD3	34:RA:1263:U:C5'	2.37	0.53
34:RA:2306:C:N4	39:RG:42:GLY:O	2.42	0.53
38:RF:185:ASP:OD1	38:RF:188:ARG:NH1	2.42	0.53
46:RR:103:ARG:NH1	46:RR:108:GLY:O	2.40	0.53
51:RW:14:PRO:HG2	51:RW:78:GLU:HG3	1.90	0.53
1:XA:860:A:H61	1:XA:872:A:H62	1.57	0.53
1:QA:320:C:HO2'	1:QA:1435:G:HO2'	1.57	0.53
1:QA:430:A:OP1	4:QD:9:CYS:HB2	2.08	0.53
4:QD:98:GLU:HA	4:QD:103:ASN:HD22	1.73	0.53
25:R1:41:ARG:NH2	34:RA:1365:A:O4'	2.42	0.53
34:RA:23:G:N2	51:RW:77:ASP:OD1	2.36	0.53
38:RF:107:LYS:HE3	38:RF:207:GLY:H	1.73	0.53
1:XA:624:C:H2'	1:XA:625:G:H8	1.73	0.53
1:XA:719:C:N3	18:XR:74:ARG:NH2	2.51	0.53
28:Y4:7:PRO:HG3	39:YG:62:LEU:HA	1.91	0.53
28:Y4:11:PRO:HA	28:Y4:25:TYR:HA	1.90	0.53
34:YA:703:U:O4	34:YA:728:G:O6	2.27	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:591:U:OP1	8:QH:30:ARG:NH1	2.42	0.53
1:QA:938:A:H4'	7:QG:95:ARG:HH12	1.74	0.53
31:R7:39:ARG:NH1	34:RA:459:U:OP2	2.42	0.53
34:RA:2784:C:O2'	37:RE:37:ARG:NH1	2.42	0.53
47:RS:18:ILE:HD13	47:RS:88:ASP:HA	1.90	0.53
1:XA:1232:U:OP1	9:XI:124:GLN:NE2	2.42	0.53
2:XB:132:LYS:HA	2:XB:135:GLN:HB2	1.89	0.53
7:XG:18:TYR:OH	7:XG:47:CYS:SG	2.64	0.53
29:Y5:57:VAL:O	46:YR:33:ARG:NH2	2.34	0.53
34:YA:1215:G:O6	34:YA:1234:U:O4	2.27	0.53
47:YS:26:LEU:HB3	47:YS:87:PHE:HA	1.90	0.53
9:QI:71:SER:HA	9:QI:74:ILE:HG12	1.90	0.53
34:RA:139:G:H22	34:RA:1596:A:H4'	1.73	0.53
34:RA:2328:A:H2'	34:RA:2329:G:C8	2.44	0.53
37:RE:171:GLU:HB3	37:RE:185:LYS:HE2	1.90	0.53
42:RN:39:ARG:NH1	42:RN:48:MET:SD	2.82	0.53
40:YH:103:LEU:HB3	40:YH:115:VAL:HG22	1.91	0.53
1:QA:570:G:H2'	1:QA:571:U:C6	2.44	0.53
7:QG:111:ARG:HH11	7:QG:119:ARG:HA	1.73	0.53
34:RA:380:U:H2'	34:RA:381:G:H8	1.74	0.53
34:RA:468:G:O2'	38:RF:62:ARG:NH2	2.42	0.53
34:RA:2100:G:H8	34:RA:2100:G:O5'	1.92	0.53
1:XA:127:G:O2'	17:XQ:2:PRO:O	2.27	0.53
1:XA:548:G:H5'	4:XD:73:ARG:HH22	1.74	0.53
1:XA:977:A:N6	1:XA:1224:G:OP1	2.41	0.53
34:YA:86:C:OP1	53:YY:33:LYS:NZ	2.42	0.53
34:YA:2307:G:N1	39:YG:45:GLU:OE2	2.36	0.53
36:YD:17:THR:HB	36:YD:205:VAL:H	1.74	0.53
1:QA:373:A:O2'	1:QA:451:A:N6	2.42	0.52
2:QB:109:SER:O	2:QB:113:HIS:ND1	2.41	0.52
22:QV:55:U:N3	22:QV:58:A:OP2	2.39	0.52
22:QV:65:U:H2'	22:QV:66:A:H8	1.74	0.52
32:R8:2:PRO:O	34:RA:666:G:N2	2.42	0.52
34:RA:184:C:O2'	34:RA:217:G:N3	2.39	0.52
34:RA:1025:G:C8	34:RA:1135:C:H1'	2.43	0.52
34:RA:1782:C:H42	34:RA:2586:C:H42	1.57	0.52
34:RA:2319:G:N1	34:RA:2334:G:OP2	2.39	0.52
50:RV:76:LYS:HB2	50:RV:81:TYR:HB3	1.90	0.52
1:XA:68(P):A:C5	1:XA:68(Q):C:H1'	2.44	0.52
1:XA:186(B):C:O2'	20:XT:89:ARG:NH2	2.42	0.52
11:XK:83:ILE:HD13	11:XK:109:VAL:HB	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:YA:1473:G:H1	34:YA:1520:U:H3	1.57	0.52
1:QA:614:A:OP2	4:QD:85:LYS:NZ	2.34	0.52
1:QA:955:U:O2	19:QS:83:HIS:NE2	2.39	0.52
7:QG:114:ARG:O	7:QG:119:ARG:NH2	2.42	0.52
10:QJ:33:GLN:O	10:QJ:76:ASN:ND2	2.43	0.52
24:R0:23:VAL:HG21	34:RA:857:C:H4'	1.90	0.52
30:R6:9:LEU:HD13	30:R6:51:GLU:HB2	1.90	0.52
34:RA:48:G:N2	34:RA:177:G:OP2	2.37	0.52
34:RA:303:U:H2'	34:RA:304:G:H8	1.74	0.52
34:RA:664:C:OP1	44:RP:18:ARG:NH2	2.39	0.52
34:RA:1788:C:OP1	36:RD:222:ARG:NH2	2.43	0.52
39:RG:166:ASP:OD2	39:RG:166:ASP:N	2.42	0.52
34:YA:729:G:OP2	36:YD:13:ARG:NH1	2.42	0.52
49:YU:28:ARG:NH1	49:YU:38:THR:OG1	2.42	0.52
2:QB:209:ARG:NH1	2:QB:240:GLN:OE1	2.42	0.52
23:QX:17:C:C4	23:QX:18:C:C5	2.97	0.52
29:R5:49:CYS:SG	29:R5:50:GLY:N	2.82	0.52
34:RA:1116:C:H2'	34:RA:1117:G:H8	1.74	0.52
44:RP:29:LYS:HD3	44:RP:30:THR:HG23	1.92	0.52
1:XA:947:G:HO2'	1:XA:1306:A:HO2'	1.57	0.52
1:XA:1295:G:O3'	13:XM:14:ARG:NH1	2.42	0.52
3:XC:32:LEU:O	3:XC:59:ARG:NH2	2.42	0.52
47:YS:61:ASN:ND2	47:YS:64:GLU:OE1	2.42	0.52
23:QX:14:A:H8	23:QX:14:A:O5'	1.92	0.52
34:RA:1482:U:O4	34:RA:1512:G:O6	2.26	0.52
40:RH:125:VAL:HG22	40:RH:125:VAL:O	2.08	0.52
1:XA:1073:U:O2	2:XB:104:ASN:ND2	2.40	0.52
36:YD:67:PHE:HE1	36:YD:106:ILE:HD11	1.75	0.52
37:YE:176:ILE:HG13	37:YE:181:LEU:HB2	1.92	0.52
39:YG:170:ARG:NH1	39:YG:174:GLU:OE1	2.43	0.52
1:QA:352:C:O2'	1:QA:354:G:OP1	2.21	0.52
7:QG:13:GLN:OE1	9:QI:42:ARG:NH2	2.42	0.52
29:R5:46:CYS:HB3	29:R5:49:CYS:SG	2.50	0.52
34:RA:979:G:N2	34:RA:985:C:N4	2.56	0.52
34:RA:1026:U:C4	34:RA:1125:G:O6	2.62	0.52
34:RA:1815:A:OP2	36:RD:54:ARG:NH2	2.42	0.52
34:RA:2224:G:OP1	36:RD:268:ARG:HD3	2.10	0.52
34:RA:2448:A:OP2	34:RA:2498:C:OP2	2.27	0.52
39:RG:41:GLN:HB2	39:RG:90:LEU:HB2	1.92	0.52
48:RT:6:LEU:HA	48:RT:9:LEU:HB2	1.91	0.52
34:YA:605:C:O2	34:YA:657:U:O2'	2.26	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:YA:1478:G:H2'	34:YA:1479:G:H8	1.74	0.52
34:YA:1701:A:OP1	34:YA:1763:G:N1	2.37	0.52
34:YA:2099:U:O4	34:YA:2190:G:O6	2.27	0.52
34:YA:2573:C:OP1	34:YA:2575:C:OP2	2.26	0.52
1:QA:864:A:H2'	1:QA:865:A:C8	2.45	0.52
1:QA:1005:A:O2'	1:QA:1036:G:N2	2.43	0.52
1:QA:1358:U:H5''	14:QN:35:ARG:H	1.74	0.52
38:RF:65:TRP:NE1	38:RF:73:ALA:O	2.42	0.52
43:RO:24:VAL:HG13	43:RO:33:ALA:HB2	1.91	0.52
54:RZ:24:LEU:HD11	54:RZ:83:PRO:HB2	1.90	0.52
54:RZ:27:VAL:HG22	54:RZ:85:HIS:HE1	1.74	0.52
1:XA:708:C:H2'	1:XA:709:G:H8	1.75	0.52
5:XE:110:LEU:HD13	5:XE:118:ILE:HG21	1.90	0.52
45:YQ:21:THR:OG1	45:YQ:22:LYS:N	2.42	0.52
1:QA:789:U:H6	1:QA:789:U:O5'	1.93	0.52
1:QA:859:A:OP2	1:QA:869:G:N1	2.39	0.52
9:QI:112:LYS:HA	9:QI:119:ALA:HB2	1.92	0.52
24:R0:66:VAL:O	24:R0:81:VAL:HA	2.10	0.52
34:RA:615:G:N2	38:RF:44:ARG:O	2.43	0.52
34:RA:1247:A:N6	34:RA:1249:U:O2	2.43	0.52
34:RA:2208:U:O2'	36:RD:150:LYS:O	2.28	0.52
34:RA:2506:U:O2	34:RA:2506:U:H2'	2.10	0.52
34:RA:2641:G:H2'	34:RA:2642:G:C8	2.44	0.52
1:XA:719:C:H1'	18:XR:49:LYS:HB2	1.90	0.52
31:Y7:28:ARG:NH2	34:YA:1368:G:OP1	2.42	0.52
32:Y8:49:VAL:HG23	32:Y8:53:PRO:HD3	1.91	0.52
34:YA:617:G:OP2	38:YF:43:LYS:NZ	2.32	0.52
12:QL:85:ILE:HD11	12:QL:98:TYR:HB3	1.92	0.52
34:RA:2010:G:H5''	51:RW:42:ARG:HB2	1.92	0.52
34:RA:2258:C:O2'	34:RA:2427:C:OP2	2.28	0.52
34:RA:2375:G:N2	34:RA:2378:A:OP2	2.41	0.52
48:RT:30:VAL:HG12	48:RT:86:ILE:HG23	1.92	0.52
1:XA:8:A:N6	4:XD:205:GLU:O	2.43	0.52
1:XA:1345:U:H5''	9:XI:120:ARG:HH11	1.75	0.52
8:XH:121:ASP:OD1	8:XH:121:ASP:N	2.42	0.52
9:XI:25:LYS:HE3	9:XI:60:ASP:HB3	1.92	0.52
34:YA:780:G:N2	34:YA:783:A:H62	2.08	0.52
34:YA:831:G:O2'	44:YP:38:GLN:OE1	2.28	0.52
34:YA:2292:C:OP2	47:YS:17:ARG:NH1	2.42	0.52
2:QB:61:LEU:HD21	2:QB:68:ILE:HD11	1.91	0.52
5:QE:147:ASP:HA	5:QE:150:ARG:HD2	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:QR:30:ASP:HB3	18:QR:33:ASP:HB2	1.92	0.52
33:R9:27:CYS:SG	33:R9:28:GLU:N	2.83	0.52
34:RA:579:G:O2'	34:RA:2019:A:OP1	2.27	0.52
45:RQ:81:VAL:O	45:RQ:82:ARG:NE	2.34	0.52
1:XA:1080:A:H5'	5:XE:14:ARG:HH21	1.74	0.52
1:XA:1172:C:H2'	1:XA:1173:G:H8	1.74	0.52
1:XA:1255:G:O2'	1:XA:1258:G:N3	2.36	0.52
7:XG:92:SER:O	7:XG:96:GLN:HB2	2.10	0.52
34:YA:873:G:N2	34:YA:905:U:O2	2.42	0.52
34:YA:2019:A:O2'	49:YU:34:LYS:NZ	2.43	0.52
1:QA:1040:U:H2'	1:QA:1041:A:H8	1.75	0.52
4:QD:122:ARG:NH1	4:QD:122:ARG:O	2.43	0.52
34:RA:372:G:N2	34:RA:401:A:OP2	2.37	0.52
34:RA:458:G:O2'	34:RA:469:G:O6	2.25	0.52
34:RA:2144:U:O2'	34:RA:2147:G:O6	2.28	0.52
42:RN:35:ARG:HG3	42:RN:37:LYS:HG2	1.91	0.52
44:RP:84:ASN:ND2	44:RP:117:GLU:OE2	2.43	0.52
5:XE:76:ILE:HB	5:XE:142:LEU:HD21	1.92	0.52
1:QA:395:C:N4	1:QA:396:G:O6	2.43	0.51
1:QA:1022:G:H2'	1:QA:1023:G:H8	1.75	0.51
1:QA:1286:A:N6	1:QA:1355:G:OP1	2.44	0.51
4:QD:15:GLU:OE2	4:QD:66:ARG:NH2	2.42	0.51
14:QN:24:CYS:HB2	14:QN:28:GLY:H	1.73	0.51
34:RA:385:C:O2'	34:RA:388:G:N2	2.42	0.51
43:RO:23:ARG:NH2	43:RO:28:SER:O	2.43	0.51
47:RS:26:LEU:O	47:RS:88:ASP:HB3	2.10	0.51
53:RY:19:LYS:HZ1	53:RY:20:TYR:HE2	1.49	0.51
53:RY:76:CYS:HB2	53:RY:99:CYS:SG	2.51	0.51
1:XA:1266:G:N2	1:XA:1269:A:OP2	2.35	0.51
3:XC:22:TRP:HA	10:XJ:93:GLY:HA2	1.92	0.51
34:YA:2846:G:N1	34:YA:2871:C:O2	2.43	0.51
35:YB:44:G:O2'	35:YB:47:C:N4	2.43	0.51
36:YD:8:PRO:HB3	36:YD:14:ARG:HG2	1.92	0.51
38:YF:198:ALA:HA	38:YF:201:VAL:HG12	1.91	0.51
1:QA:313:A:H2'	1:QA:314:C:C6	2.46	0.51
1:QA:951:G:N3	1:QA:970:C:O2'	2.40	0.51
34:RA:981:A:C2	34:RA:2027:G:N3	2.75	0.51
53:RY:67:LEU:HD22	53:RY:71:LYS:HD2	1.91	0.51
1:XA:925:G:H1	1:XA:1391:U:H3	1.58	0.51
2:XB:43:ASP:O	2:XB:47:THR:OG1	2.23	0.51
13:XM:82:MET:O	13:XM:93:ARG:NH2	2.43	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:XP:4:ILE:HB	16:XP:66:PRO:HB3	1.92	0.51
37:YE:78:LEU:HG	37:YE:79:ARG:HD2	1.91	0.51
48:YT:19:LEU:HD22	48:YT:86:ILE:HD12	1.92	0.51
1:QA:377:G:H2'	1:QA:378:G:H8	1.75	0.51
1:QA:392:G:OP2	16:QP:8:ARG:NH2	2.37	0.51
2:QB:84:GLU:OE2	2:QB:87:ARG:NH2	2.43	0.51
20:QT:71:THR:OG1	20:QT:72:LEU:N	2.43	0.51
28:R4:26:SER:OG	28:R4:27:THR:N	2.43	0.51
34:RA:1216:G:OP2	49:RU:12:ARG:NH2	2.40	0.51
34:RA:1651:G:H4'	46:RR:39:PRO:HG2	1.92	0.51
40:RH:103:LEU:HG	40:RH:123:PHE:CE1	2.45	0.51
45:RQ:21:THR:OG1	45:RQ:22:LYS:N	2.43	0.51
1:XA:639:G:H2'	1:XA:640:A:H8	1.74	0.51
4:XD:187:ARG:NH1	4:XD:188:LEU:O	2.43	0.51
30:Y6:34:LEU:N	30:Y6:51:GLU:OE1	2.44	0.51
45:YQ:67:ARG:O	45:YQ:101:ARG:NH2	2.44	0.51
30:R6:6:ARG:NH1	30:R6:24:GLU:OE2	2.43	0.51
34:RA:566:U:H5''	44:RP:29:LYS:CE	2.40	0.51
34:RA:1824:G:OP1	36:RD:52:ARG:NH2	2.38	0.51
40:RH:103:LEU:CG	40:RH:123:PHE:CE1	2.94	0.51
41:RI:86:THR:HA	41:RI:123:LEU:CB	2.40	0.51
47:RS:6:ALA:HA	47:RS:9:ARG:HG2	1.92	0.51
1:XA:235:C:H2'	1:XA:236:G:H8	1.75	0.51
1:XA:1074:G:H1	1:XA:1083:U:H3	1.58	0.51
34:YA:584:C:OP2	49:YU:10:ARG:NH2	2.43	0.51
34:YA:807:U:O2'	34:YA:2060:A:N1	2.40	0.51
34:YA:1286:A:N6	34:YA:1289:C:C2	2.78	0.51
34:YA:1792:G:H5'	36:YD:205:VAL:HG13	1.93	0.51
1:QA:123:C:OP1	1:QA:311:C:O2'	2.27	0.51
1:QA:427:U:OP1	4:QD:13:ARG:NH2	2.40	0.51
1:QA:1151:A:H5'	10:QJ:41:PRO:HA	1.92	0.51
1:QA:1238:A:H62	1:QA:1301:U:H3	1.59	0.51
1:QA:1259:C:O2'	1:QA:1283:G:N2	2.38	0.51
7:QG:69:VAL:HG13	7:QG:100:ALA:HB1	1.93	0.51
1:XA:1367:C:H4'	10:XJ:48:THR:HG21	1.90	0.51
22:XV:55:U:N3	22:XV:58:A:OP2	2.38	0.51
28:Y4:6:HIS:CE1	39:YG:67:LYS:H	2.28	0.51
32:Y8:30:ARG:HE	44:YP:62:LEU:HD12	1.76	0.51
34:YA:2152:G:H2'	34:YA:2153:G:H8	1.75	0.51
53:YY:76:CYS:SG	53:YY:79:CYS:SG	3.08	0.51
25:R1:10:LYS:NZ	25:R1:65:SER:OG	2.41	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:RA:748:G:OP1	34:RA:2612:C:N4	2.44	0.51
34:RA:1567:A:OP2	36:RD:84:TYR:OH	2.28	0.51
34:RA:2795:G:N2	34:RA:2799:A:OP2	2.44	0.51
41:RI:86:THR:HA	41:RI:123:LEU:HB2	1.92	0.51
41:RI:94:ALA:HA	41:RI:97:ILE:HD12	1.93	0.51
42:RN:3:THR:HG21	49:RU:61:TRP:HE1	1.75	0.51
1:XA:59:A:H3'	1:XA:331:G:H22	1.74	0.51
1:XA:935:A:O2'	1:XA:1383:C:N3	2.43	0.51
1:XA:992:U:H3	1:XA:1044:A:H62	1.57	0.51
10:XJ:26:ALA:O	10:XJ:84:GLN:NE2	2.43	0.51
36:YD:108:PRO:HB3	36:YD:143:HIS:CE1	2.46	0.51
52:YX:25:LYS:HA	52:YX:81:VAL:O	2.11	0.51
1:QA:15:G:O6	1:QA:920:U:O4	2.29	0.51
1:QA:778:G:O6	1:QA:804:U:O4	2.28	0.51
34:RA:1990:C:H2'	34:RA:1991:U:C6	2.45	0.51
34:RA:2169:A:N6	34:RA:2170:A:N1	2.59	0.51
37:RE:110:GLY:HA2	37:RE:161:GLY:HA3	1.92	0.51
39:RG:52:ILE:HG22	39:RG:55:LYS:HD2	1.92	0.51
1:XA:21:G:H2'	1:XA:22:G:C8	2.46	0.51
2:XB:198:ASP:OD1	8:XH:68:ARG:NH2	2.44	0.51
27:Y3:31:LEU:HG	34:YA:989:G:OP1	2.10	0.51
34:YA:693:C:O2'	34:YA:1353:A:N3	2.37	0.51
34:YA:1012:U:OP2	49:YU:70:ARG:NH2	2.39	0.51
34:YA:1435:G:N2	34:YA:1477:A:O2'	2.42	0.51
34:YA:1824:G:N3	36:YD:254:THR:OG1	2.44	0.51
42:YN:97:ARG:HA	42:YN:100:GLU:HB2	1.92	0.51
1:QA:249:U:O4	1:QA:275:G:O6	2.28	0.51
1:QA:1081:G:H2'	1:QA:1082:G:H8	1.75	0.51
8:QH:32:LYS:HA	8:QH:35:ILE:HD12	1.92	0.51
5:XE:102:ALA:HB1	5:XE:106:PRO:HG2	1.93	0.51
34:YA:1670:C:H6	34:YA:1670:C:O5'	1.94	0.51
1:QA:878:G:H5'	8:QH:89:PRO:HG2	1.92	0.51
1:QA:1233:G:O2'	1:QA:1365:G:OP1	2.28	0.51
32:R8:30:ARG:O	32:R8:30:ARG:HG2	2.11	0.51
34:RA:1041:C:H2'	34:RA:1042:G:H8	1.76	0.51
34:RA:1759:A:HO2'	34:RA:2714:G:HO2'	1.59	0.51
34:RA:2014:A:O3'	51:RW:92:ARG:NH2	2.44	0.51
36:RD:147:LEU:HD12	36:RD:148:GLU:HG3	1.93	0.51
39:RG:121:ASN:O	39:RG:131:TYR:OH	2.26	0.51
6:XF:9:VAL:HB	6:XF:87:ARG:HB2	1.92	0.51
34:YA:960:A:C8	34:YA:962:G:C8	2.99	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:YF:63:LYS:NZ	38:YF:75:HIS:O	2.33	0.51
38:YF:154:VAL:HG22	38:YF:191:ARG:HB2	1.93	0.51
1:QA:556:C:H2'	1:QA:557:G:H8	1.76	0.51
5:QE:10:MET:HA	5:QE:32:VAL:HG12	1.93	0.51
12:QL:39:VAL:HG12	12:QL:57:LYS:HG2	1.93	0.51
12:QL:104:VAL:O	12:QL:105:TYR:CG	2.57	0.51
22:QV:36:G:C2	23:QX:17:C:O2	2.64	0.51
34:RA:1288:U:O3'	34:RA:1647:G:N2	2.44	0.51
44:RP:57:THR:OG1	44:RP:58:THR:N	2.44	0.51
48:RT:3:ARG:HG3	48:RT:6:LEU:HB2	1.92	0.51
1:XA:352:C:O2'	1:XA:354:G:OP1	2.24	0.51
1:XA:1537:U:H3	23:XX:9:G:H1	1.59	0.51
2:XB:167:PRO:O	2:XB:171:ALA:HB2	2.11	0.51
3:XC:58:GLU:HB2	3:XC:65:ALA:HB3	1.91	0.51
34:YA:547:A:H2'	34:YA:548:A:C8	2.46	0.51
1:QA:235:C:H2'	1:QA:236:G:H8	1.75	0.50
3:QC:150:LYS:HB3	3:QC:201:TYR:HB2	1.93	0.50
32:R8:8:LYS:HB3	32:R8:12:LYS:HE3	1.94	0.50
34:RA:2397:G:O6	34:RA:2419:U:O2	2.29	0.50
36:RD:175:LEU:O	36:RD:182:LEU:HA	2.12	0.50
42:RN:39:ARG:NH2	42:RN:41:ASP:OD1	2.44	0.50
47:RS:35:ILE:HD11	47:RS:97:ARG:HD2	1.92	0.50
50:RV:8:GLY:O	50:RV:10:LYS:NZ	2.42	0.50
1:XA:428:G:OP2	4:XD:10:ARG:NH1	2.39	0.50
1:XA:672:U:H2'	1:XA:673:G:H8	1.76	0.50
1:XA:828:A:H62	1:XA:858:G:H21	1.59	0.50
1:XA:1338:G:N3	22:XV:41:A:O2'	2.44	0.50
4:XD:19:LEU:HB3	4:XD:21:LEU:HD23	1.92	0.50
7:XG:111:ARG:HD3	7:XG:112:PRO:HD2	1.93	0.50
34:YA:2508:G:O2'	34:YA:2554:U:O2'	2.29	0.50
41:YI:1:MET:HG2	41:YI:23:PRO:HB3	1.92	0.50
12:QL:46:LYS:HD2	12:QL:47:LYS:HB2	1.93	0.50
22:QV:49:G:H1	22:QV:65:U:H3	1.59	0.50
53:RY:19:LYS:NZ	53:RY:20:TYR:CE2	2.71	0.50
1:XA:373:A:H61	1:XA:391:G:H1'	1.75	0.50
1:XA:1034:G:H2'	1:XA:1035:A:C8	2.47	0.50
3:XC:157:ILE:HD12	3:XC:164:ARG:HG3	1.94	0.50
8:XH:21:LYS:O	8:XH:65:TYR:OH	2.28	0.50
34:YA:1286:A:C6	34:YA:1289:C:C2	2.99	0.50
2:QB:111:ARG:HH11	2:QB:114:ARG:HH12	1.60	0.50
2:QB:208:ILE:O	2:QB:212:GLN:HB2	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:QC:57:ILE:HG22	3:QC:66:VAL:HG22	1.93	0.50
34:RA:58:G:H5'	52:RX:74:PRO:HB3	1.92	0.50
1:XA:1500:A:H5''	1:XA:1508:G:H5''	1.93	0.50
40:YH:85:LYS:HB3	40:YH:133:VAL:HG13	1.93	0.50
34:RA:321:G:O2'	34:RA:340:A:N3	2.42	0.50
34:RA:1953:A:O2'	34:RA:2559:C:O2	2.29	0.50
34:RA:2185:C:H2'	34:RA:2186:G:H8	1.77	0.50
1:XA:410:G:N2	1:XA:432:A:H62	2.10	0.50
8:XH:38:ILE:HD12	8:XH:41:ARG:HH21	1.76	0.50
34:YA:530:G:C6	34:YA:2022:U:OP1	2.65	0.50
34:YA:662:G:H5''	44:YP:17:LYS:HG2	1.92	0.50
1:QA:603:U:H3	1:QA:635:G:H1	1.60	0.50
1:QA:692:U:OP1	11:QK:124:LYS:NZ	2.37	0.50
34:RA:1297:C:H2'	34:RA:1298:C:C6	2.46	0.50
34:RA:2178:C:H2'	34:RA:2179:C:H6	1.76	0.50
1:XA:1386:G:H2'	1:XA:1387:G:C8	2.43	0.50
3:XC:19:GLU:O	3:XC:40:ARG:NH2	2.44	0.50
20:XT:75:ASN:N	20:XT:75:ASN:OD1	2.44	0.50
24:Y0:41:ARG:NH2	34:YA:2387:U:O2'	2.45	0.50
34:YA:581:C:H2'	34:YA:582:G:C8	2.47	0.50
34:YA:2148:G:H2'	34:YA:2149:G:H8	1.76	0.50
40:YH:113:VAL:HG11	40:YH:151:ILE:HD12	1.94	0.50
52:YX:53:LYS:HG2	52:YX:82:GLN:HB3	1.93	0.50
1:QA:1261:A:H62	1:QA:1274:G:N2	2.09	0.50
1:QA:1342:C:H2'	1:QA:1343:G:C8	2.47	0.50
1:QA:1484:C:HO2'	34:RA:1960:A:HO2'	1.53	0.50
13:QM:84:ILE:HG12	19:QS:66:MET:CE	2.41	0.50
22:QV:37:IMG:HM13	23:QX:16:C:N1	2.26	0.50
31:R7:34:ARG:NH1	34:RA:466:A:OP1	2.45	0.50
34:RA:505:A:OP2	34:RA:1235:G:OP1	2.29	0.50
34:RA:2490:G:N2	34:RA:2490:G:OP2	2.45	0.50
1:XA:159:G:H21	1:XA:161:A:H8	1.60	0.50
1:XA:181:G:N2	1:XA:182:U:O4	2.36	0.50
1:XA:745:C:OP1	1:XA:851:G:O2'	2.30	0.50
2:XB:118:LEU:HD23	2:XB:142:LEU:HB2	1.94	0.50
18:XR:32:ARG:HA	18:XR:69:THR:HG21	1.92	0.50
28:Y4:16:CYS:HB3	28:Y4:33:VAL:HB	1.93	0.50
34:YA:458:G:O2'	34:YA:469:G:O6	2.29	0.50
34:YA:630:G:N2	34:YA:633:A:OP2	2.42	0.50
34:YA:2076:U:OP2	34:YA:2238:G:N2	2.37	0.50
34:YA:2808:U:C2	34:YA:2892:A:N6	2.79	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:1338:G:N3	22:QV:41:A:O2'	2.44	0.50
34:RA:1422:G:H1	34:RA:1576:U:H3	1.60	0.50
34:RA:2751:G:C4	40:RH:3:ARG:CB	2.90	0.50
36:RD:69:ARG:NH1	36:RD:128:GLY:O	2.42	0.50
42:RN:9:VAL:HG11	42:RN:39:ARG:HH12	1.77	0.50
42:RN:112:LEU:O	42:RN:116:LEU:HB2	2.10	0.50
4:XD:107:ARG:HB3	4:XD:174:LEU:HD11	1.93	0.50
34:YA:255:A:O2'	34:YA:384:U:OP1	2.27	0.50
34:YA:305:U:O4	34:YA:312:G:O6	2.30	0.50
34:YA:919:G:N2	34:YA:2269:A:OP2	2.44	0.50
37:YE:101:ARG:NE	37:YE:171:GLU:OE2	2.41	0.50
38:YF:10:PRO:HB3	38:YF:17:ARG:HH21	1.76	0.50
19:QS:10:PHE:HZ	19:QS:15:LEU:HD11	1.76	0.50
34:RA:947:G:H2'	34:RA:948:G:H8	1.75	0.50
34:RA:1405:U:H2'	34:RA:1406:U:H6	1.76	0.50
34:RA:1654:A:N1	34:RA:2048:G:O2'	2.44	0.50
34:RA:2572:A:OP1	34:RA:2574:G:O2'	2.25	0.50
5:XE:81:GLU:HG2	5:XE:90:VAL:HG23	1.94	0.50
9:XI:22:GLY:N	9:XI:58:HIS:O	2.37	0.50
10:XJ:53:PRO:HB3	14:YN:42:ILE:HG12	1.94	0.50
33:Y9:27:CYS:HB3	33:Y9:32:HIS:HB2	1.94	0.50
34:YA:28:A:HO2'	34:YA:582:G:HO2'	1.56	0.50
34:YA:2692:C:O2	34:YA:2847:U:O2'	2.27	0.50
51:YW:86:LEU:HD22	51:YW:96:ILE:HD11	1.93	0.50
53:YY:28:LYS:NZ	53:YY:64:GLU:OE2	2.35	0.50
1:QA:279:A:OP2	17:QQ:95:TYR:OH	2.27	0.50
13:QM:84:ILE:HG12	19:QS:66:MET:HE3	1.94	0.50
34:RA:764:A:H5'	36:RD:210:GLY:HA2	1.93	0.50
36:RD:126:GLN:O	36:RD:129:ASN:ND2	2.41	0.50
1:XA:126:G:OP1	1:XA:633:G:N2	2.42	0.50
1:XA:444:C:H2'	1:XA:445:G:C8	2.46	0.50
20:XT:74:LYS:O	20:XT:76:ALA:N	2.44	0.50
34:YA:962:G:H2'	34:YA:963:U:C6	2.47	0.50
34:YA:1682:G:OP1	34:YA:1699:G:N1	2.44	0.50
1:QA:243:A:N6	1:QA:281:G:O2'	2.43	0.49
1:QA:1305:G:OP2	21:QU:2:GLY:N	2.45	0.49
1:QA:1510:U:H3	1:QA:1525:G:H1	1.59	0.49
2:QB:146:GLN:HG3	2:QB:153:ARG:HH22	1.77	0.49
2:QB:178:ARG:NH2	2:QB:198:ASP:OD1	2.39	0.49
13:QM:16:ASP:N	13:QM:16:ASP:OD1	2.44	0.49
34:RA:1882:C:H3'	34:RA:1883:G:H8	1.75	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:XH:19:VAL:HG23	8:XH:21:LYS:HG3	1.94	0.49
29:Y5:25:LEU:HG	51:YW:19:LEU:HD12	1.94	0.49
35:YB:36:C:H42	35:YB:49:C:H1'	1.77	0.49
1:XA:1122:U:O4	1:XA:1123:A:N6	2.45	0.49
34:YA:1791:A:N6	34:YA:1828:G:O2'	2.44	0.49
34:YA:2729:G:H1'	37:YE:187:ALA:HB2	1.94	0.49
43:YO:63:VAL:HG12	43:YO:106:LEU:HD21	1.93	0.49
1:QA:1117:G:H21	1:QA:1180:A:H1'	1.76	0.49
1:QA:1203:C:H2'	1:QA:1204:A:H8	1.78	0.49
1:QA:1304:G:OP1	21:QU:10:ARG:NH2	2.45	0.49
4:QD:61:LYS:HD3	4:QD:206:PHE:CD2	2.46	0.49
20:QT:56:MET:HG3	20:QT:84:LEU:HD21	1.94	0.49
20:QT:66:ALA:O	20:QT:71:THR:OG1	2.28	0.49
24:R0:12:ASN:ND2	34:RA:2278:A:OP2	2.45	0.49
28:R4:5:ILE:HB	39:RG:67:LYS:HD2	1.94	0.49
1:XA:757:U:O2'	1:XA:879:C:O2	2.30	0.49
1:XA:1071:C:H2'	1:XA:1072:G:H8	1.76	0.49
1:XA:1124:G:H1'	10:XJ:38:ILE:HD12	1.95	0.49
4:XD:88:VAL:HG13	5:XE:97:GLY:HA3	1.94	0.49
5:XE:101:ILE:O	5:XE:120:THR:OG1	2.30	0.49
7:XG:58:PRO:HA	7:XG:61:VAL:HG12	1.92	0.49
33:Y9:27:CYS:SG	33:Y9:28:GLU:N	2.84	0.49
34:YA:124:G:N2	34:YA:126:A:O2'	2.46	0.49
34:YA:1653:G:O6	46:YR:11:ASN:N	2.43	0.49
34:YA:1901:A:OP2	36:YD:255:LYS:NZ	2.34	0.49
34:YA:2198:A:OP1	41:YI:33:ARG:NH2	2.46	0.49
1:QA:776:G:N2	1:QA:802:A:OP2	2.45	0.49
23:QX:3:C:H2'	23:QX:4:A:C8	2.47	0.49
24:R0:72:ARG:HE	24:R0:75:LEU:HD12	1.76	0.49
25:R1:90:ILE:HA	25:R1:94:LEU:CG	2.42	0.49
34:RA:1147:C:H2'	34:RA:1148:A:H8	1.77	0.49
1:XA:269:C:H2'	1:XA:270:A:H8	1.77	0.49
23:XX:6:G:H2'	23:XX:7:G:H8	1.75	0.49
34:YA:1668:A:H62	34:YA:1991:U:H3	1.60	0.49
37:YE:1:MET:N	37:YE:83:ASP:O	2.36	0.49
54:YZ:6:LYS:NZ	54:YZ:43:GLU:OE1	2.39	0.49
1:QA:1128:C:O2'	1:QA:1130:A:N7	2.45	0.49
30:R6:18:ARG:O	30:R6:20:ASN:ND2	2.44	0.49
34:RA:270(S):G:H2'	34:RA:270(T):G:H8	1.78	0.49
34:RA:290:G:H1	34:RA:350:U:H3	1.60	0.49
34:RA:586:A:C5'	38:RF:89:VAL:HG21	2.37	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:RA:2148:G:H2'	34:RA:2149:G:C8	2.48	0.49
34:RA:2306:C:H2'	34:RA:2307:G:H21	1.76	0.49
40:RH:89:ILE:HD12	40:RH:131:VAL:HG22	1.94	0.49
7:XG:140:ASP:OD2	7:XG:143:ARG:NH1	2.45	0.49
36:YD:97:TYR:HB2	36:YD:101:GLU:O	2.13	0.49
1:QA:766:A:N6	1:QA:813:U:N3	2.48	0.49
1:QA:1268:A:H5'	21:QU:20:LYS:HG2	1.95	0.49
13:QM:84:ILE:HG12	19:QS:66:MET:SD	2.53	0.49
25:R1:78:LYS:HZ3	34:RA:270(T):G:H1'	1.77	0.49
33:R9:11:CYS:SG	33:R9:14:CYS:N	2.85	0.49
34:RA:1668:A:N3	34:RA:1670:C:N4	2.60	0.49
39:RG:135:LEU:O	39:RG:154:GLY:HA3	2.13	0.49
50:RV:45:THR:O	50:RV:45:THR:CG2	2.55	0.49
1:XA:186(A):C:H5'	20:XT:78:ALA:HB1	1.95	0.49
1:XA:652:U:O4	1:XA:752:G:O2'	2.28	0.49
7:XG:115:ARG:HB2	7:XG:118:VAL:HG12	1.94	0.49
7:XG:118:VAL:HG22	7:XG:122:HIS:CE1	2.48	0.49
20:XT:41:ILE:HD13	20:XT:87:LYS:HG2	1.95	0.49
26:Y2:16:LEU:O	26:Y2:67:LYS:NZ	2.45	0.49
28:Y4:31:ILE:HG21	39:YG:142:PRO:HB2	1.93	0.49
32:Y8:10:ALA:O	32:Y8:14:VAL:HB	2.13	0.49
34:YA:793:A:OP2	34:YA:2071:A:O2'	2.30	0.49
34:YA:959:A:N3	34:YA:2457:U:O2'	2.36	0.49
34:YA:2245:U:H5'	34:YA:2246:G:H5'	1.93	0.49
44:YP:52:GLU:OE1	44:YP:55:ARG:NH1	2.46	0.49
1:QA:475:G:H2'	1:QA:476:G:H8	1.78	0.49
1:QA:762:C:H2'	1:QA:763:G:H8	1.76	0.49
3:QC:35:GLU:HA	3:QC:38:ARG:HH21	1.77	0.49
6:QF:35:ALA:HB1	6:QF:65:VAL:HG21	1.95	0.49
34:RA:505:A:HO2'	34:RA:509:C:HO2'	1.58	0.49
34:RA:690:G:H21	36:RD:43:ARG:HH21	1.61	0.49
34:RA:1652:A:C2	34:RA:2006:C:N3	2.80	0.49
1:XA:557:G:H2'	1:XA:558:G:C8	2.48	0.49
1:XA:925:G:O2'	1:XA:927:G:OP1	2.24	0.49
6:XF:61:LEU:HD23	6:XF:63:TYR:HE2	1.77	0.49
19:XS:12:ASP:HB2	19:XS:37:ARG:HE	1.77	0.49
19:XS:40:ILE:HD13	19:XS:71:LEU:HD21	1.95	0.49
30:Y6:23:THR:OG1	30:Y6:24:GLU:N	2.42	0.49
34:YA:71:A:N3	34:YA:73:A:N6	2.60	0.49
34:YA:288:C:H2'	34:YA:289:A:H8	1.77	0.49
34:YA:577:G:O2'	34:YA:1254:A:OP1	2.31	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:YA:1153:C:H5'	49:YU:76:TYR:HE2	1.77	0.49
34:YA:1212:G:O2'	34:YA:1236:G:N2	2.39	0.49
34:YA:2092:U:OP2	41:YI:27:ARG:NH2	2.42	0.49
34:YA:2131:G:N3	34:YA:2158:A:N6	2.61	0.49
1:QA:1049:U:H4'	1:QA:1050:G:H5''	1.94	0.49
34:RA:577:G:O2'	34:RA:1254:A:OP1	2.30	0.49
34:RA:1224:G:N2	34:RA:1227:A:OP2	2.36	0.49
34:RA:1265:A:H61	34:RA:2013:A:H5''	1.77	0.49
34:RA:1837:C:O2'	34:RA:1927:A:N3	2.36	0.49
43:RO:88:ASN:HD21	43:RO:90:GLN:HB2	1.78	0.49
51:RW:22:ASP:OD1	51:RW:25:ARG:NH1	2.45	0.49
1:XA:474:G:H2'	1:XA:475:G:H8	1.77	0.49
4:XD:56:VAL:HG13	4:XD:57:ARG:HD2	1.94	0.49
4:XD:72:GLU:OE2	4:XD:207:TYR:OH	2.19	0.49
34:YA:2744:G:H21	40:YH:143:GLN:HE22	1.61	0.49
45:YQ:66:ILE:HA	45:YQ:104:PHE:HA	1.95	0.49
1:QA:126:G:OP1	1:QA:605:U:O2'	2.25	0.49
1:QA:1096:C:H2'	1:QA:1097:C:H6	1.78	0.49
3:QC:47:LEU:HD11	3:QC:87:LEU:HD21	1.95	0.49
4:QD:79:PHE:HE1	4:QD:204:ILE:HD13	1.77	0.49
34:RA:1116:C:H2'	34:RA:1117:G:C8	2.48	0.49
34:RA:1181:C:H2'	34:RA:1182:A:H8	1.78	0.49
34:RA:2581:G:N2	34:RA:2581:G:OP2	2.44	0.49
45:RQ:36:ALA:HB1	45:RQ:127:ILE:HG21	1.94	0.49
1:XA:14:U:N3	1:XA:17:U:OP2	2.42	0.49
1:XA:107:G:OP1	1:XA:325:A:N6	2.46	0.49
1:QA:59:A:H5''	1:QA:60:A:H5''	1.95	0.49
1:QA:1281:U:H5''	1:QA:1282:C:H5	1.78	0.49
5:QE:87:SER:OG	5:QE:125:SER:OG	2.27	0.49
34:RA:180:G:N1	34:RA:214:G:O6	2.46	0.49
34:RA:441:U:O2	38:RF:46:ARG:NH2	2.45	0.49
34:RA:848:G:H2'	34:RA:849:A:C8	2.48	0.49
34:RA:975:G:N2	34:RA:1156:A:O2'	2.46	0.49
53:RY:76:CYS:SG	53:RY:79:CYS:CA	2.94	0.49
1:XA:191:G:N2	20:XT:103:GLY:O	2.34	0.49
1:XA:1384:C:H2'	1:XA:1385:G:H8	1.77	0.49
15:XO:10:LYS:HA	15:XO:13:GLN:HG2	1.95	0.49
48:YT:28:VAL:HG12	48:YT:88:ILE:HA	1.95	0.49
1:QA:1270:C:H2'	1:QA:1271:G:C8	2.48	0.48
2:QB:69:LEU:HB3	2:QB:162:ILE:HG22	1.94	0.48
34:RA:566:U:H5''	44:RP:29:LYS:NZ	2.28	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:RA:820:A:N3	34:RA:943:U:O2'	2.39	0.48
34:RA:1086:A:O2'	34:RA:1087:G:N7	2.43	0.48
34:RA:1454:U:O2	46:RR:64:ARG:NE	2.41	0.48
54:RZ:163:LEU:HD22	54:RZ:167:PRO:HG3	1.95	0.48
1:XA:62:U:H3	1:XA:105:G:H1	1.61	0.48
1:XA:714:G:H2'	1:XA:715:A:C8	2.48	0.48
1:XA:1500:A:OP1	1:XA:1508:G:OP1	2.31	0.48
13:XM:88:ARG:HD2	13:XM:98:VAL:HB	1.95	0.48
13:XM:91:ARG:NE	13:XM:97:PRO:O	2.46	0.48
34:YA:587:C:O2	44:YP:33:ARG:NH2	2.36	0.48
34:YA:1165:U:O4	34:YA:1184:G:O6	2.30	0.48
1:QA:570:G:H1'	1:QA:820:U:H5	1.77	0.48
4:QD:72:GLU:OE2	4:QD:207:TYR:OH	2.29	0.48
5:QE:84:PHE:N	5:QE:87:SER:O	2.45	0.48
17:QQ:66:SER:O	17:QQ:70:ARG:NH1	2.46	0.48
18:QR:59:SER:OG	18:QR:60:ALA:N	2.46	0.48
34:RA:560:C:O2	49:RU:49:HIS:NE2	2.46	0.48
34:RA:1315:C:O2'	34:RA:1392:A:N3	2.40	0.48
34:RA:2291:U:O4	34:RA:2341:G:O6	2.31	0.48
40:RH:3:ARG:HH12	40:RH:5:GLY:HA2	1.77	0.48
1:XA:1115:C:H1'	9:XI:111:ARG:HH21	1.78	0.48
1:XA:1175:G:H2'	1:XA:1176:A:H8	1.78	0.48
4:XD:20:TYR:HD1	4:XD:26:CYS:HB3	1.78	0.48
31:Y7:7:PRO:HA	34:YA:686:G:C8	2.47	0.48
33:Y9:14:CYS:HB3	33:Y9:27:CYS:HB2	1.95	0.48
34:YA:860:U:H1'	34:YA:2268:A:H5'	1.94	0.48
34:YA:2403:C:C4	34:YA:2415:G:C2	3.01	0.48
41:YI:129:THR:HG22	41:YI:137:PRO:HB3	1.95	0.48
54:YZ:24:LEU:HD23	54:YZ:41:LEU:HG	1.94	0.48
1:QA:1507:A:C2	1:QA:1530:G:N9	2.81	0.48
34:RA:1024:G:HO2'	34:RA:1144:G:HO2'	1.59	0.48
40:RH:3:ARG:HG3	40:RH:3:ARG:O	2.13	0.48
43:RO:15:GLY:O	43:RO:47:ILE:N	2.45	0.48
53:RY:15:VAL:HA	53:RY:72:VAL:HA	1.94	0.48
1:XA:922:G:H2'	1:XA:923:A:C8	2.48	0.48
48:YT:31:SER:OG	48:YT:85:LYS:NZ	2.44	0.48
1:QA:1137:C:O2'	1:QA:1138:G:N2	2.46	0.48
1:QA:1291:G:H5'	7:QG:37:ASN:HD21	1.77	0.48
1:QA:1357:A:H5'	10:QJ:45:ARG:HH12	1.78	0.48
34:RA:358:U:H2'	34:RA:359:A:H8	1.79	0.48
34:RA:483:A:O2'	53:RY:49:VAL:O	2.30	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:RA:1608:A:C5	34:RA:1611:C:C4	3.01	0.48
34:RA:2195:C:H2'	34:RA:2196:C:C6	2.49	0.48
34:RA:2295:C:OP1	47:RS:10:ARG:NH1	2.46	0.48
44:RP:106:LEU:HD13	44:RP:112:LEU:HD13	1.95	0.48
1:XA:781:A:O2'	1:XA:1522:U:O2	2.30	0.48
1:XA:1230:C:H2'	1:XA:1231:G:H8	1.77	0.48
6:XF:82:ARG:HB3	6:XF:85:VAL:HG12	1.95	0.48
20:XT:73:HIS:HB3	20:XT:74:LYS:H	1.47	0.48
34:YA:675:A:OP1	38:YF:63:LYS:NZ	2.39	0.48
34:YA:2099:U:O2	34:YA:2190:G:N2	2.37	0.48
36:YD:108:PRO:HB3	36:YD:143:HIS:HE1	1.77	0.48
41:YI:77:LEU:HD13	41:YI:101:LEU:HB3	1.96	0.48
54:YZ:130:PRO:HA	54:YZ:133:ILE:HD11	1.96	0.48
1:QA:117:G:H8	1:QA:117:G:O5'	1.96	0.48
7:QG:111:ARG:NH1	7:QG:113:GLU:OE1	2.43	0.48
10:QJ:4:ILE:HG12	10:QJ:100:THR:HG22	1.96	0.48
11:QK:82:VAL:HG13	11:QK:108:ILE:HA	1.95	0.48
20:QT:54:LYS:HE3	20:QT:100:ILE:HG21	1.95	0.48
20:QT:67:ALA:O	20:QT:73:HIS:ND1	2.39	0.48
34:RA:1525:G:H2'	34:RA:1526:G:H8	1.77	0.48
34:RA:2489:G:O2'	34:RA:2518:A:N6	2.47	0.48
35:RB:75:G:H4'	54:RZ:36:LYS:HE2	1.96	0.48
54:RZ:61:LEU:HD23	54:RZ:67:LEU:HD23	1.94	0.48
6:XF:5:GLU:HA	6:XF:63:TYR:O	2.14	0.48
16:XP:40:ASP:HB3	16:XP:48:TRP:HB2	1.94	0.48
19:XS:36:ARG:HB2	19:XS:72:GLY:HA3	1.94	0.48
32:Y8:13:ARG:HD2	44:YP:61:ARG:HG3	1.95	0.48
34:YA:363(B):A:H2'	34:YA:363(C):G:H8	1.78	0.48
34:YA:1193:G:OP2	44:YP:16:ARG:NH2	2.42	0.48
34:YA:1307:A:N1	34:YA:1622:G:C6	2.81	0.48
34:YA:1802:A:H2'	34:YA:1803:A:C8	2.48	0.48
34:YA:2816:C:O2	34:YA:2883:A:O2'	2.27	0.48
47:YS:4:LEU:HD22	47:YS:8:GLU:CD	2.34	0.48
48:YT:52:ILE:HG13	48:YT:61:PHE:HB3	1.96	0.48
1:QA:261:U:OP2	20:QT:80:ARG:NH2	2.47	0.48
1:QA:819:A:C8	1:QA:1529:G:N1	2.81	0.48
1:QA:976:G:OP2	1:QA:1358:U:O2'	2.30	0.48
34:RA:521:G:H2'	34:RA:522:G:H8	1.77	0.48
34:RA:571:A:O5'	34:RA:2030:A:N6	2.43	0.48
34:RA:2314:C:H5'	39:RG:38:VAL:HG11	1.96	0.48
4:XD:63:LYS:HD2	4:XD:198:VAL:HG12	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:XM:3:ARG:HD2	13:XM:7:VAL:HG12	1.96	0.48
26:Y2:4:SER:OG	26:Y2:5:GLU:N	2.39	0.48
34:YA:1174:A:H2'	34:YA:1175:U:H4'	1.94	0.48
34:YA:2250:G:C4	45:YQ:82:ARG:HG3	2.48	0.48
1:QA:1342:C:H4'	9:QI:125:TYR:HB3	1.95	0.48
5:QE:74:GLY:O	5:QE:116:THR:OG1	2.31	0.48
29:R5:4:HIS:O	34:RA:2056:G:N2	2.47	0.48
34:RA:1586:A:H3'	34:RA:1587:A:H8	1.79	0.48
34:RA:2450:A:H62	34:RA:2501:C:H42	1.61	0.48
38:RF:48:THR:O	38:RF:48:THR:OG1	2.32	0.48
40:RH:43:VAL:HG23	40:RH:52:VAL:HG12	1.95	0.48
40:RH:46:GLU:HB2	40:RH:49:VAL:HG23	1.95	0.48
49:RU:90:VAL:O	49:RU:92:ARG:N	2.35	0.48
53:RY:13:VAL:HA	53:RY:74:PRO:HA	1.96	0.48
1:XA:28:G:O2'	1:XA:296:U:OP1	2.30	0.48
1:XA:372:C:H42	1:XA:389:A:H62	0.68	0.48
1:XA:520:A:H62	1:XA:529:G:N2	2.11	0.48
1:XA:693:G:H22	22:XV:37:1MG:HN21	1.60	0.48
4:XD:89:THR:OG1	5:XE:97:GLY:O	2.27	0.48
4:XD:91:SER:HB2	4:XD:191:ARG:HD2	1.95	0.48
32:Y8:13:ARG:NH2	34:YA:250:G:OP2	2.47	0.48
34:YA:993:G:N2	50:YV:23:GLU:OE2	2.46	0.48
34:YA:1087:G:O6	34:YA:1089:G:N2	2.44	0.48
34:YA:1419:A:N7	34:YA:1578:U:O4	2.47	0.48
34:YA:1980:G:O2'	34:YA:1982:C:OP2	2.25	0.48
39:YG:68:PRO:HB3	39:YG:92:VAL:HB	1.95	0.48
46:YR:3:HIS:O	46:YR:5:LYS:N	2.47	0.48
34:RA:514:A:H2'	34:RA:515:A:H8	1.79	0.48
34:RA:685:A:OP1	34:RA:686:G:N2	2.45	0.48
1:XA:114:U:H2'	1:XA:115:G:C8	2.48	0.48
1:XA:346:G:OP1	48:YT:41:ARG:NH2	2.39	0.48
1:XA:410:G:OP1	4:XD:30:LYS:NZ	2.47	0.48
1:XA:737:A:H2'	1:XA:738:C:H6	1.79	0.48
1:XA:938:A:O3'	7:XG:95:ARG:NH2	2.47	0.48
1:XA:1223:C:H5''	1:XA:1224:G:H5''	1.95	0.48
5:XE:60:TYR:OH	5:XE:64:ARG:NH2	2.47	0.48
24:Y0:11:ARG:O	24:Y0:14:ARG:NH2	2.43	0.48
25:Y1:83:GLU:HG3	25:Y1:85:LEU:H	1.78	0.48
34:YA:2787:C:H1'	37:YE:62:PRO:HG3	1.96	0.48
37:YE:117:MET:HA	37:YE:122:PHE:H	1.79	0.48
38:YF:116:ASP:OD2	44:YP:1:MET:N	2.43	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:YG:107:LEU:HA	39:YG:111:LEU:HD12	1.95	0.48
1:QA:1299:A:H2'	1:QA:1301:U:H1'	1.96	0.48
1:QA:1318:A:H1'	19:QS:37:ARG:HE	1.79	0.48
25:R1:2:SER:N	34:RA:1364:G:OP2	2.46	0.48
34:RA:23:G:OP1	34:RA:504:U:N3	2.38	0.48
34:RA:597:U:H2'	34:RA:598:G:C8	2.49	0.48
34:RA:2245:U:H5''	34:RA:2246:G:H5'	1.96	0.48
34:RA:2473:U:OP1	34:RA:2529:G:N2	2.46	0.48
38:RF:159:GLY:O	38:RF:164:ARG:NH2	2.41	0.48
42:RN:60:ILE:HD12	42:RN:60:ILE:HA	1.81	0.48
1:XA:618:C:H5'	1:XA:619:U:H5''	1.96	0.48
2:XB:30:ARG:NH1	2:XB:31:TYR:OH	2.46	0.48
3:XC:153:VAL:HB	3:XC:196:LEU:HD21	1.95	0.48
15:XO:39:LEU:HG	15:XO:56:LEU:HD12	1.96	0.48
34:YA:480:A:O2'	53:YY:46:LYS:O	2.32	0.48
34:YA:1338:G:N7	52:YX:62:LYS:NZ	2.59	0.48
34:YA:2115:G:N2	34:YA:2164:C:OP2	2.47	0.48
40:YH:70:THR:O	40:YH:74:ASN:ND2	2.47	0.48
45:YQ:35:VAL:HG12	45:YQ:102:VAL:HG22	1.94	0.48
1:QA:501:C:OP1	12:QL:117:ARG:NH2	2.47	0.48
1:QA:1250:A:H4'	9:QI:67:GLY:HA2	1.96	0.48
5:QE:102:ALA:O	5:QE:107:ARG:NH2	2.45	0.48
34:RA:862:G:O2'	35:RB:78:A:N3	2.47	0.48
34:RA:1052:C:H2'	34:RA:1053:C:C5	2.49	0.48
34:RA:2085:C:H4'	36:RD:262:ARG:NH2	2.29	0.48
34:RA:2156:G:O6	34:RA:2157:G:N2	2.47	0.48
39:RG:126:ASP:OD1	39:RG:130:ASN:N	2.43	0.48
1:XA:192:U:H4'	20:XT:57:ARG:HD3	1.96	0.48
1:XA:605:U:H5	1:XA:605:U:OP2	1.97	0.48
1:XA:767:A:O2'	1:XA:1524:C:O2	2.27	0.48
1:XA:949:A:O2'	1:XA:1363:A:OP2	2.31	0.48
9:XI:73:GLN:O	9:XI:77:ILE:HG12	2.14	0.48
22:XV:8:U:C2	22:XV:14:A:N6	2.82	0.48
30:Y6:19:ARG:NH1	34:YA:2399:G:O2'	2.47	0.48
37:YE:37:ARG:O	37:YE:45:THR:HA	2.13	0.48
39:YG:63:ILE:HG22	39:YG:143:GLU:HB2	1.95	0.48
1:QA:407:G:H5''	4:QD:115:ARG:HE	1.78	0.47
1:QA:815:A:H4'	1:QA:817:C:C5	2.48	0.47
2:QB:47:THR:HG23	2:QB:202:PRO:HG2	1.96	0.47
3:QC:50:ALA:HB2	3:QC:75:VAL:HB	1.96	0.47
34:RA:1411:C:H42	34:RA:1591:G:H22	1.62	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:RT:91:ARG:NH2	48:RT:124:ASP:OD2	2.47	0.47
1:XA:1370:G:H2'	1:XA:1371:G:H8	1.79	0.47
17:XQ:66:SER:H	17:XQ:69:LYS:HB3	1.78	0.47
20:XT:61:SER:OG	20:XT:62:LEU:N	2.47	0.47
34:YA:363(D):G:H2'	34:YA:363(E):G:H8	1.78	0.47
34:YA:2105:C:H2'	34:YA:2106:G:C8	2.49	0.47
34:YA:2427:C:H5'	34:YA:2429:G:H5'	1.96	0.47
35:YB:12:C:O4'	35:YB:15:A:N6	2.47	0.47
37:YE:102:VAL:O	37:YE:170:LEU:N	2.45	0.47
1:QA:161:A:H2	1:QA:347:G:H21	1.62	0.47
3:QC:34:LEU:O	3:QC:38:ARG:NE	2.43	0.47
4:QD:108:LEU:HD22	4:QD:174:LEU:HD13	1.96	0.47
13:QM:26:GLY:O	13:QM:30:ALA:CB	2.62	0.47
34:RA:839:U:H3	34:RA:939:G:H1	1.62	0.47
34:RA:1058:G:H2'	34:RA:1059:G:C8	2.49	0.47
34:RA:2693:A:H2'	34:RA:2694:G:H8	1.78	0.47
47:RS:26:LEU:HB3	47:RS:87:PHE:HA	1.96	0.47
49:RU:17:ILE:HG13	49:RU:39:LEU:HD12	1.95	0.47
16:XP:6:LEU:HD13	16:XP:17:TYR:CG	2.49	0.47
19:XS:4:SER:HB2	19:XS:7:LYS:HG2	1.95	0.47
34:YA:2154:G:H2'	34:YA:2155:G:H8	1.79	0.47
35:YB:9:G:OP1	47:YS:25:ARG:NH1	2.40	0.47
50:YV:13:ARG:NH1	50:YV:15:GLU:OE2	2.45	0.47
50:YV:52:VAL:HG21	50:YV:55:ALA:HB3	1.95	0.47
53:YY:11:ASP:OD1	53:YY:11:ASP:N	2.43	0.47
1:QA:1318:A:H1'	19:QS:37:ARG:HH21	1.80	0.47
29:R5:12:SER:O	29:R5:16:ARG:HB2	2.14	0.47
38:RF:102:PRO:HB2	38:RF:105:VAL:HG23	1.95	0.47
1:XA:426:G:OP1	4:XD:38:TYR:OH	2.28	0.47
1:XA:458(F):A:HO2'	16:XP:82:GLN:H	1.60	0.47
2:XB:71:VAL:HB	2:XB:164:VAL:HG12	1.96	0.47
4:XD:175:SER:O	4:XD:183:GLY:HA2	2.15	0.47
4:XD:175:SER:HB3	4:XD:184:LYS:HB3	1.96	0.47
47:YS:25:ARG:HG3	47:YS:88:ASP:HB2	1.96	0.47
1:QA:21:G:H2'	1:QA:22:G:C8	2.49	0.47
1:QA:269:C:H2'	1:QA:270:A:H8	1.79	0.47
1:QA:1186:G:O2'	9:QI:110:GLU:OE2	2.27	0.47
9:QI:20:ARG:HG3	9:QI:60:ASP:HB2	1.96	0.47
12:QL:7:ILE:HD11	17:QQ:32:TYR:HB3	1.94	0.47
25:R1:17:SER:O	25:R1:17:SER:OG	2.29	0.47
34:RA:442:G:N2	38:RF:48:THR:OG1	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:RA:1203:G:O6	34:RA:1204:A:N6	2.48	0.47
34:RA:2845:G:OP1	48:RT:56:GLY:N	2.48	0.47
37:RE:105:THR:OG1	37:RE:199:ARG:NH1	2.48	0.47
1:XA:974:A:OP2	14:XN:29:ARG:NH2	2.48	0.47
29:Y5:52:TYR:OH	34:YA:2883:A:OP1	2.20	0.47
34:YA:1286:A:C6	34:YA:1289:C:N3	2.83	0.47
34:YA:1792:G:O2'	34:YA:1830:C:OP1	2.32	0.47
45:YQ:75:THR:HB	45:YQ:86:GLY:HA3	1.96	0.47
1:QA:1052:U:O2'	1:QA:1055:A:OP2	2.28	0.47
31:R7:24:THR:HG23	31:R7:27:GLY:H	1.79	0.47
34:RA:1068:G:O6	34:RA:1069:A:N6	2.48	0.47
34:RA:1270:C:H5''	34:RA:1271:G:H5'	1.97	0.47
34:RA:1542:G:O6	34:RA:1543:A:C6	2.67	0.47
34:RA:2328:A:H2'	34:RA:2329:G:H8	1.79	0.47
41:RI:51:ILE:HA	41:RI:54:GLN:HG2	1.95	0.47
2:XB:204:ASN:OD1	2:XB:205:ASP:N	2.48	0.47
27:Y3:18:ASP:OD1	27:Y3:18:ASP:N	2.46	0.47
34:YA:28:A:N6	34:YA:512:G:O2'	2.47	0.47
34:YA:730:C:OP1	34:YA:1775:U:O2'	2.25	0.47
34:YA:974(A):G:C4	34:YA:1186:G:C2	3.03	0.47
34:YA:1535:U:H2'	34:YA:1536:A:C8	2.49	0.47
1:QA:1221:G:H5'	19:QS:36:ARG:HH22	1.78	0.47
11:QK:17:GLY:HA2	11:QK:35:PRO:HD3	1.97	0.47
12:QL:5:PRO:HG2	12:QL:10:LEU:HD21	1.96	0.47
34:RA:99:U:O4	53:RY:8:LYS:NZ	2.46	0.47
34:RA:534:U:H3	34:RA:559:G:H1	1.63	0.47
34:RA:1148:A:H2'	34:RA:1149:G:H8	1.80	0.47
1:XA:303:A:HO2'	1:XA:555:C:HO2'	1.59	0.47
1:XA:734:G:H21	18:XR:75:ILE:HD13	1.80	0.47
2:XB:84:GLU:HG3	2:XB:215:LEU:HB3	1.96	0.47
7:XG:99:LEU:HD12	7:XG:102:ARG:HD2	1.96	0.47
13:XM:83:ASP:OD2	13:XM:84:ILE:N	2.46	0.47
27:Y3:51:ALA:HA	27:Y3:54:VAL:HG12	1.96	0.47
34:YA:137(B):G:N3	52:YX:41:ASN:ND2	2.61	0.47
37:YE:105:THR:HG21	37:YE:164:ARG:HH21	1.78	0.47
41:YI:88:ILE:HG22	41:YI:90:GLY:H	1.80	0.47
1:QA:1251:A:N3	1:QA:1369:C:O2'	2.46	0.47
1:QA:1328:C:H4'	13:QM:29:ARG:HD3	1.96	0.47
11:QK:27:ASN:OD1	11:QK:28:THR:N	2.47	0.47
17:QQ:83:ASP:N	17:QQ:83:ASP:OD1	2.47	0.47
33:R9:11:CYS:N	33:R9:14:CYS:SG	2.83	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:RA:581:C:H2'	34:RA:582:G:H8	1.79	0.47
34:RA:978:G:N1	34:RA:986:C:N3	2.62	0.47
34:RA:1843:C:O2'	36:RD:256:GLY:O	2.28	0.47
34:RA:2096:U:H3	34:RA:2193:G:H1	1.61	0.47
34:RA:2118:U:H3	34:RA:2148:G:H4'	1.80	0.47
34:RA:2749:A:H3'	34:RA:2750:A:H2'	1.96	0.47
34:RA:2751:G:N7	40:RH:2:SER:OG	2.46	0.47
46:RR:26:LYS:O	46:RR:30:THR:OG1	2.24	0.47
49:RU:6:THR:HG21	49:RU:10:ARG:HH12	1.79	0.47
49:RU:90:VAL:HG13	50:RV:39:LEU:HD22	1.97	0.47
52:RX:64:LYS:HD2	52:RX:73:ARG:HH12	1.77	0.47
1:XA:403:C:H42	1:XA:547:A:H5'	1.80	0.47
1:XA:616:G:H2'	1:XA:617:G:H8	1.78	0.47
1:XA:1503:A:O2'	23:XX:15:A:N6	2.44	0.47
22:XV:19:G:OP1	22:XV:20:G:N2	2.48	0.47
34:YA:586:A:H5'	38:YF:89:VAL:HG21	1.96	0.47
34:YA:821:A:N6	34:YA:972:G:O2'	2.47	0.47
34:YA:958:U:O2	35:YB:89(B):A:O2'	2.25	0.47
34:YA:1689:A:H62	34:YA:1698:A:H2	1.63	0.47
34:YA:2589:A:N1	34:YA:2606:C:N4	2.63	0.47
36:YD:35:LYS:HG3	36:YD:63:ARG:HG3	1.96	0.47
43:YO:120:GLU:OE1	48:YT:67:SER:OG	2.33	0.47
47:YS:11:LYS:HG3	47:YS:15:ARG:HE	1.80	0.47
1:QA:749:C:H2'	1:QA:750:G:H8	1.80	0.47
1:QA:1035:A:H2'	1:QA:1036:G:H8	1.80	0.47
1:QA:1237:C:H5''	1:QA:1238:A:C8	2.50	0.47
1:QA:1329:A:H62	21:QU:7:ARG:HH12	1.62	0.47
8:QH:120:THR:OG1	8:QH:121:ASP:N	2.47	0.47
16:QP:21:VAL:HG23	16:QP:33:ILE:HB	1.96	0.47
17:QQ:62:SER:OG	17:QQ:72:ARG:NE	2.47	0.47
34:RA:2150:U:H2'	34:RA:2151:G:H8	1.79	0.47
34:RA:2852:G:O6	34:RA:2865:U:O4	2.32	0.47
1:XA:413:G:H21	1:XA:428:G:H1'	1.79	0.47
1:XA:427:U:O2'	1:XA:541:G:OP1	2.29	0.47
1:XA:1028(H):G:H2'	1:XA:1028(I):G:C8	2.50	0.47
2:XB:184:VAL:HG23	2:XB:198:ASP:H	1.79	0.47
34:YA:422:A:H8	34:YA:422:A:O5'	1.97	0.47
34:YA:1058:G:H2'	34:YA:1059:G:H8	1.80	0.47
34:YA:1728:G:H8	34:YA:1732:A:H62	1.62	0.47
34:YA:2584:U:H2'	34:YA:2585:U:H2'	1.96	0.47
34:YA:2611:U:C6	34:YA:2611:U:C5'	2.86	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:YH:18:GLU:HB3	40:YH:25:LYS:HG2	1.96	0.47
41:YI:20:ASP:OD2	41:YI:20:ASP:N	2.43	0.47
1:QA:316:G:OP2	1:QA:351:G:O2'	2.31	0.47
1:QA:542:G:O3'	4:QD:14:ARG:NH2	2.48	0.47
1:QA:982:U:H5''	14:QN:6:LEU:HD11	1.96	0.47
10:QJ:67:THR:O	10:QJ:67:THR:OG1	2.32	0.47
15:QO:26:GLU:HA	15:QO:29:VAL:HG12	1.97	0.47
34:RA:2377:A:H4'	47:RS:112:PHE:HA	1.97	0.47
40:RH:6:ARG:HE	40:RH:65:HIS:HB3	1.80	0.47
41:RI:83:ALA:C	41:RI:89:TYR:CE2	2.88	0.47
1:XA:942:G:N2	9:XI:124:GLN:OE1	2.44	0.47
1:XA:1522:U:H2'	1:XA:1523:G:H8	1.79	0.47
13:XM:14:ARG:HG2	13:XM:16:ASP:H	1.79	0.47
14:XN:23:ARG:NH1	14:XN:28:GLY:HA2	2.29	0.47
28:Y4:23:GLU:O	28:Y4:25:TYR:N	2.46	0.47
34:YA:223:A:O2'	34:YA:420:C:O2	2.25	0.47
34:YA:380:U:H2'	34:YA:381:G:H8	1.80	0.47
34:YA:1779:U:OP2	34:YA:1784:A:N6	2.43	0.47
34:YA:2011:U:OP2	51:YW:16:LYS:NZ	2.35	0.47
38:YF:157:VAL:HG13	38:YF:194:MET:HB3	1.97	0.47
6:QF:24:GLU:OE1	6:QF:28:ARG:NH1	2.48	0.47
8:QH:108:GLY:HA3	8:QH:138:TRP:HB3	1.97	0.47
25:R1:2:SER:O	25:R1:61:ARG:NH1	2.47	0.47
34:RA:414:C:O2	34:RA:1864:U:O2'	2.30	0.47
34:RA:2249:U:N3	34:RA:2253:G:OP2	2.48	0.47
1:XA:925:G:O6	1:XA:1391:U:O4	2.33	0.47
1:XA:967:C:O3'	9:XI:125:TYR:OH	2.27	0.47
1:XA:1525:G:OP1	11:XK:120:ARG:NH1	2.41	0.47
12:XL:12:ARG:HH21	12:XL:13:LYS:HE3	1.79	0.47
17:XQ:21:VAL:N	17:XQ:42:TYR:O	2.40	0.47
22:XV:76:A:N6	34:YA:2422:A:O4'	2.47	0.47
34:YA:238:C:O2'	34:YA:608:A:N3	2.34	0.47
34:YA:363(A):G:H2'	34:YA:363(B):A:H8	1.79	0.47
34:YA:635:C:O2'	34:YA:639:U:OP1	2.29	0.47
38:YF:12:LEU:HB3	38:YF:126:VAL:HG12	1.95	0.47
1:QA:1048:G:O2'	1:QA:1050:G:OP1	2.34	0.46
1:QA:1298:C:N4	7:QG:113:GLU:O	2.48	0.46
2:QB:134:GLU:HA	2:QB:137:ARG:HG2	1.96	0.46
4:QD:156:GLU:O	4:QD:160:GLN:N	2.48	0.46
8:QH:91:ARG:NE	17:QQ:32:TYR:O	2.40	0.46
22:QV:37:1MG:C8	22:QV:38:A:C8	3.04	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:RA:659:C:H2'	34:RA:660:G:C8	2.49	0.46
34:RA:956:G:OP2	45:RQ:14:ARG:NH2	2.36	0.46
34:RA:1102:C:H2'	34:RA:1103:A:H8	1.79	0.46
34:RA:1783:A:OP1	34:RA:1784:A:OP2	2.33	0.46
35:RB:15:A:H5'	35:RB:16:G:C8	2.49	0.46
37:RE:24:THR:HG21	37:RE:188:VAL:HG22	1.97	0.46
40:RH:11:VAL:HG12	40:RH:13:LYS:HG2	1.97	0.46
51:RW:68:ARG:NH2	51:RW:109:GLU:OE2	2.48	0.46
1:XA:1127:G:N2	1:XA:1145:C:O2	2.47	0.46
4:XD:18:LYS:HZ3	4:XD:33:MET:HG3	1.80	0.46
4:XD:62:GLN:HE22	4:XD:65:ARG:HH21	1.62	0.46
12:XL:8:ASN:O	12:XL:12:ARG:HB2	2.15	0.46
22:XV:19:G:H2'	34:YA:2112:G:C6	2.50	0.46
33:Y9:14:CYS:CA	33:Y9:27:CYS:HB2	2.44	0.46
34:YA:28:A:O2'	34:YA:582:G:O2'	2.30	0.46
34:YA:963:U:H1'	34:YA:2250:G:O6	2.15	0.46
42:YN:16:ILE:HG21	42:YN:26:LEU:HD11	1.97	0.46
1:QA:407:G:H5'	4:QD:115:ARG:HH21	1.80	0.46
1:QA:1004:A:N6	1:QA:1025:U:O3'	2.47	0.46
7:QG:70:LYS:HB2	7:QG:96:GLN:HB3	1.97	0.46
16:QP:40:ASP:OD1	16:QP:43:LYS:N	2.46	0.46
34:RA:144:C:H2'	34:RA:145:G:H8	1.80	0.46
34:RA:2151:G:H2'	34:RA:2152:G:H8	1.81	0.46
34:RA:2153:G:H2'	34:RA:2154:G:H8	1.80	0.46
34:RA:2185:C:H2'	34:RA:2186:G:C8	2.51	0.46
40:RH:126:PRO:HG2	40:RH:130:ARG:HG3	1.96	0.46
52:RX:72:LYS:NZ	52:RX:73:ARG:O	2.38	0.46
1:XA:413:G:H4'	1:XA:414:A:H5''	1.97	0.46
1:XA:673:G:H2'	1:XA:674:G:C8	2.51	0.46
1:XA:1419:G:H1	1:XA:1481:U:H3	1.62	0.46
2:XB:188:ALA:HB3	2:XB:200:ILE:HD11	1.97	0.46
16:XP:20:VAL:HG12	16:XP:35:LYS:HA	1.97	0.46
31:Y7:33:ARG:NH1	34:YA:467:G:OP1	2.47	0.46
34:YA:296:C:O3'	53:YY:95:LYS:NZ	2.48	0.46
34:YA:373:U:H1'	34:YA:423:A:N3	2.30	0.46
34:YA:805:G:N2	34:YA:829:A:OP1	2.47	0.46
41:YI:72:LEU:HD12	41:YI:138:ILE:HD12	1.97	0.46
1:QA:75:C:H42	1:QA:95:G:H1	1.62	0.46
1:QA:976:G:N1	1:QA:1362(B):C:OP2	2.37	0.46
1:QA:1097:C:O2'	1:QA:1169:A:N3	2.37	0.46
34:RA:630:G:N2	34:RA:633:A:OP2	2.35	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:RA:979:G:N2	34:RA:985:C:C4	2.84	0.46
34:RA:1070:A:O2'	34:RA:1097:U:O3'	2.32	0.46
38:RF:24:LEU:HD12	38:RF:115:ALA:HB2	1.96	0.46
40:RH:123:PHE:HE2	40:RH:133:VAL:HG22	1.80	0.46
46:RR:28:LEU:HD23	46:RR:48:VAL:HG21	1.98	0.46
54:RZ:182:LYS:HA	54:RZ:182:LYS:HD2	1.75	0.46
1:XA:186(F):C:N3	1:XA:186(N):G:N2	2.63	0.46
7:XG:75:VAL:HA	7:XG:87:VAL:O	2.16	0.46
34:YA:840:C:H2'	34:YA:841:A:H8	1.79	0.46
34:YA:2152:G:H2'	34:YA:2153:G:C8	2.49	0.46
38:YF:60:SER:OG	38:YF:61:GLY:N	2.49	0.46
1:QA:599:C:O2'	8:QH:129:VAL:O	2.27	0.46
1:QA:1000:A:N1	1:QA:1041:A:N6	2.64	0.46
1:QA:1227:A:OP1	19:QS:80:TYR:OH	2.30	0.46
9:QI:28:VAL:HA	9:QI:63:ILE:HB	1.97	0.46
22:QV:61:C:H2'	22:QV:62:C:H6	1.80	0.46
25:R1:90:ILE:HA	25:R1:94:LEU:HD11	1.93	0.46
29:R5:12:SER:HB3	34:RA:2020:A:H5'	1.97	0.46
32:R8:30:ARG:HH21	44:RP:62:LEU:HD12	1.81	0.46
34:RA:1657:C:H2'	34:RA:1658:C:H6	1.80	0.46
1:XA:6:G:H2'	5:XE:119:LEU:HD21	1.98	0.46
1:XA:165:C:H2'	1:XA:166:G:C8	2.51	0.46
1:XA:640:A:O2'	8:XH:116:LYS:NZ	2.49	0.46
1:XA:948:C:H2'	1:XA:949:A:H8	1.80	0.46
1:XA:979:C:O2	14:XN:19:ARG:NH2	2.40	0.46
8:XH:86:ILE:HD12	8:XH:135:CYS:HA	1.97	0.46
34:YA:309:G:N3	34:YA:329:G:O2'	2.47	0.46
34:YA:363(C):G:H2'	34:YA:363(D):G:H8	1.80	0.46
34:YA:974(A):G:C6	34:YA:1186:G:N1	2.84	0.46
34:YA:984:A:H5''	34:YA:985:C:H5	1.81	0.46
34:YA:1753:G:N2	34:YA:1758:G:N7	2.62	0.46
34:YA:2403:C:N3	34:YA:2415:G:C2	2.83	0.46
44:YP:98:GLU:HA	44:YP:101:VAL:HG12	1.96	0.46
1:QA:186(H):C:O2	1:QA:186(L):G:N1	2.49	0.46
1:QA:324:G:N2	1:QA:327:A:OP2	2.48	0.46
1:QA:707:C:H2'	1:QA:708:C:H6	1.81	0.46
1:QA:898:G:N2	1:QA:901:A:OP2	2.45	0.46
3:QC:66:VAL:HB	3:QC:101:LEU:HG	1.98	0.46
4:QD:57:ARG:HB3	4:QD:206:PHE:HB2	1.97	0.46
9:QI:105:ASP:HB3	9:QI:107:ARG:HE	1.80	0.46
26:R2:48:HIS:ND1	34:RA:95:G:O2'	2.38	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:R5:57:VAL:O	46:RR:33:ARG:NH1	2.39	0.46
34:RA:1363:C:O2'	34:RA:1809:A:N3	2.39	0.46
34:RA:2195:C:H2'	34:RA:2196:C:H6	1.80	0.46
1:XA:186(F):C:H42	1:XA:186(N):G:H1	1.61	0.46
10:XJ:78:ASN:HB2	10:XJ:81:THR:HG23	1.97	0.46
17:XQ:34:LYS:NZ	17:XQ:35:VAL:O	2.46	0.46
34:YA:589:C:H2'	34:YA:590:A:C8	2.50	0.46
34:YA:1669:A:N3	34:YA:1669:A:C2'	2.78	0.46
38:YF:41:LEU:HA	38:YF:44:ARG:HG2	1.98	0.46
1:QA:359:U:H2'	1:QA:360:A:H8	1.79	0.46
1:QA:410:G:H21	1:QA:432:A:H62	1.62	0.46
1:QA:628:G:H2'	1:QA:629:G:H8	1.80	0.46
1:QA:663:A:N6	1:QA:742:G:H1	2.10	0.46
1:QA:972:C:H4'	10:QJ:57:LYS:HB2	1.98	0.46
8:QH:121:ASP:OD2	8:QH:125:ARG:NH1	2.48	0.46
13:QM:91:ARG:HD2	13:QM:96:LEU:HB3	1.98	0.46
34:RA:1181:C:H2'	34:RA:1182:A:C8	2.49	0.46
34:RA:1316:U:H2'	34:RA:1317:A:H8	1.80	0.46
34:RA:2845:G:H2'	34:RA:2846:G:C8	2.51	0.46
34:RA:2882:A:OP1	46:RR:96:ARG:NH1	2.47	0.46
41:RI:88:ILE:HG22	41:RI:90:GLY:N	2.31	0.46
1:XA:36:C:O2'	1:XA:501:C:OP1	2.33	0.46
1:XA:737:A:H2'	1:XA:738:C:C6	2.50	0.46
1:XA:1071:C:OP1	5:XE:27:ARG:NH2	2.49	0.46
13:XM:59:TYR:O	13:XM:63:THR:OG1	2.25	0.46
34:YA:517:C:O2'	51:YW:18:ARG:NH2	2.48	0.46
34:YA:1363:C:O2'	34:YA:1809:A:N3	2.38	0.46
34:YA:2404:C:O3'	44:YP:77:ARG:NH2	2.49	0.46
40:YH:89:ILE:HD11	40:YH:94:TYR:HB3	1.98	0.46
2:QB:101:MET:HA	2:QB:108:ILE:HG13	1.97	0.46
13:QM:47:ASP:OD1	13:QM:47:ASP:N	2.48	0.46
34:RA:65:C:H1'	34:RA:456:C:H42	1.81	0.46
34:RA:971:C:O2'	34:RA:983:A:N3	2.38	0.46
34:RA:1543:A:H1'	34:RA:1545(A):A:H5''	1.97	0.46
37:RE:14:ILE:HD11	37:RE:173:VAL:HG11	1.97	0.46
38:RF:56:GLU:OE2	38:RF:93:LYS:NZ	2.49	0.46
49:RU:27:LEU:HD22	49:RU:31:SER:HB2	1.97	0.46
1:XA:444:C:H2'	1:XA:445:G:H8	1.81	0.46
1:XA:1014:A:H2'	1:XA:1015:A:C8	2.50	0.46
22:XV:1:C:H2'	22:XV:2:G:H8	1.81	0.46
34:YA:1255:U:N3	34:YA:2060:A:OP2	2.44	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:YA:1652:A:N6	34:YA:1653:G:H1	2.10	0.46
35:YB:73:A:N6	35:YB:103:U:H3	2.04	0.46
42:YN:47:ALA:HB2	42:YN:112:LEU:HD11	1.98	0.46
43:YO:78:ARG:NE	48:YT:73:GLU:OE1	2.45	0.46
1:QA:359:U:H2'	1:QA:360:A:C8	2.51	0.46
9:QI:26:VAL:HG12	9:QI:61:ALA:HB3	1.98	0.46
10:QJ:48:THR:HG22	10:QJ:62:HIS:HB3	1.98	0.46
20:QT:54:LYS:HZ3	20:QT:57:ARG:HE	1.64	0.46
32:R8:29:LYS:O	32:R8:31:HIS:N	2.45	0.46
34:RA:16:G:C6	34:RA:525:U:N3	2.84	0.46
34:RA:2635:C:O2'	37:RE:80:GLU:OE1	2.26	0.46
34:RA:2812:G:H2'	34:RA:2813:A:H8	1.81	0.46
37:RE:14:ILE:HB	48:RT:14:TYR:HE2	1.81	0.46
38:RF:182:ASN:OD1	38:RF:182:ASN:N	2.46	0.46
40:RH:84:SER:HA	40:RH:134:SER:HA	1.97	0.46
2:XB:118:LEU:HB3	2:XB:142:LEU:HD13	1.98	0.46
6:XF:36:ARG:NH2	6:XF:38:GLU:OE2	2.49	0.46
13:XM:45:VAL:HG23	13:XM:48:LEU:HD12	1.98	0.46
26:Y2:28:LYS:HD3	26:Y2:28:LYS:HA	1.77	0.46
34:YA:1953:A:O2'	34:YA:2559:C:O2	2.28	0.46
40:YH:137:ASP:OD2	40:YH:138:LYS:N	2.48	0.46
43:YO:64:ARG:HB2	43:YO:83:ALA:HB3	1.98	0.46
54:YZ:74:VAL:HG22	54:YZ:86:VAL:HG23	1.97	0.46
1:QA:373:A:H61	1:QA:391:G:H1'	1.80	0.46
1:QA:593:G:H1	1:QA:646:U:H3	1.64	0.46
1:QA:710:G:H2'	1:QA:711:G:H8	1.80	0.46
1:QA:864:A:O2'	1:QA:1078:U:O4	2.26	0.46
1:QA:883:C:N4	1:QA:884:U:O4	2.49	0.46
1:QA:1463:C:H5''	48:RT:112:ARG:HE	1.79	0.46
3:QC:184:TYR:HA	3:QC:200:ALA:O	2.15	0.46
16:QP:59:TRP:HA	16:QP:62:VAL:HG22	1.97	0.46
34:RA:1247:A:N1	34:RA:1249:U:C2	2.81	0.46
43:RO:104:ARG:NH2	48:RT:43:GLN:OE1	2.49	0.46
52:RX:90:GLU:HA	52:RX:93:GLU:HG2	1.97	0.46
54:RZ:67:LEU:HD13	54:RZ:68:PRO:HD2	1.96	0.46
1:XA:581:G:OP1	15:XO:65:ARG:NH1	2.33	0.46
2:XB:175:ARG:HH22	2:XB:179:LYS:HZ1	1.64	0.46
12:XL:53:ARG:HB3	12:XL:69:TYR:HE1	1.79	0.46
31:Y7:7:PRO:HA	34:YA:686:G:H8	1.80	0.46
34:YA:1891:G:O2'	34:YA:2235:G:O2'	2.32	0.46
34:YA:2314:C:H2'	34:YA:2315:G:C8	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:YX:64:LYS:HZ2	52:YX:73:ARG:HE	1.63	0.46
1:QA:157:G:H2'	1:QA:158:G:H8	1.81	0.46
1:QA:1385:G:H2'	1:QA:1386:G:H8	1.81	0.46
5:QE:98:THR:N	5:QE:117:ASP:OD1	2.40	0.46
13:QM:26:GLY:O	13:QM:30:ALA:HB2	2.15	0.46
25:R1:90:ILE:CA	25:R1:94:LEU:CD1	2.84	0.46
34:RA:1048:A:N6	34:RA:1111:A:N3	2.64	0.46
34:RA:2310:A:N6	39:RG:79:ASN:HD22	2.14	0.46
34:RA:2514:U:H3	34:RA:2570:G:H1	1.63	0.46
37:RE:46:ALA:HB1	37:RE:80:GLU:HG2	1.98	0.46
46:RR:38:VAL:HG12	46:RR:112:ALA:HB2	1.96	0.46
1:XA:448:A:OP2	1:XA:485:G:N1	2.39	0.46
1:XA:603:U:H2'	1:XA:604:G:H8	1.80	0.46
1:XA:806:C:H2'	1:XA:807:A:H8	1.80	0.46
11:XK:31:THR:HA	11:XK:42:TRP:HA	1.97	0.46
21:XU:6:ARG:HH21	21:XU:15:ARG:HH22	1.64	0.46
41:YI:4:ILE:HG22	41:YI:18:VAL:HB	1.98	0.46
48:YT:91:ARG:NH2	48:YT:124:ASP:OD2	2.48	0.46
1:QA:657:G:H4'	15:QO:28:GLN:HG2	1.97	0.45
1:QA:666:G:H1	1:QA:740:U:H3	1.62	0.45
1:QA:949:A:HO2'	1:QA:971:G:H1	1.64	0.45
2:QB:73:THR:O	2:QB:75:LYS:NZ	2.50	0.45
5:QE:87:SER:OG	5:QE:125:SER:O	2.32	0.45
11:QK:57:THR:HG23	11:QK:60:ALA:H	1.81	0.45
18:QR:74:ARG:HD3	18:QR:81:PHE:HA	1.98	0.45
34:RA:271(E):G:H2'	34:RA:272:G:H8	1.80	0.45
34:RA:414:C:H2'	34:RA:415:A:H8	1.81	0.45
34:RA:1654:A:O2'	37:RE:113:PHE:O	2.19	0.45
34:RA:2037:G:H2'	34:RA:2038:G:C8	2.51	0.45
34:RA:2618:G:H21	37:RE:150:VAL:HG21	1.80	0.45
35:RB:74:U:H1'	54:RZ:34:ASN:HD21	1.81	0.45
51:RW:86:LEU:HD22	51:RW:96:ILE:HD11	1.98	0.45
1:XA:264:U:O2'	17:XQ:64:PRO:O	2.31	0.45
1:XA:407:G:O2'	4:XD:116:GLN:OE1	2.33	0.45
34:YA:597:U:H2'	34:YA:598:G:H8	1.81	0.45
45:YQ:133:ARG:HG3	45:YQ:134:ARG:H	1.80	0.45
48:YT:16:ARG:HH21	48:YT:81:PRO:HA	1.80	0.45
1:QA:922:G:H2'	1:QA:923:A:C8	2.52	0.45
1:QA:1250:A:N3	1:QA:1370:G:O2'	2.44	0.45
9:QI:114:TYR:HB2	10:QJ:60:ARG:HB2	1.98	0.45
10:QJ:12:ASP:O	10:QJ:16:LEU:HB3	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:R0:43:THR:HG21	34:RA:2336:A:H61	1.81	0.45
34:RA:81:G:HO2'	34:RA:295:G:HO2'	1.50	0.45
34:RA:513:A:O2'	34:RA:1217:C:OP1	2.30	0.45
34:RA:1147:C:H2'	34:RA:1148:A:C8	2.51	0.45
39:RG:68:PRO:HB3	39:RG:92:VAL:HB	1.98	0.45
1:XA:1124:G:O2'	1:XA:1126:U:O4	2.28	0.45
2:XB:68:ILE:HG22	2:XB:161:ALA:HB3	1.98	0.45
34:YA:1174:A:H2	34:YA:1176:G:H4'	1.81	0.45
34:YA:1612:C:N3	34:YA:1620:G:N1	2.65	0.45
34:YA:2315:G:OP1	39:YG:36:LYS:NZ	2.40	0.45
34:YA:2730:C:O2'	37:YE:168:MET:O	2.32	0.45
44:YP:96:THR:HG22	44:YP:99:LEU:HD22	1.98	0.45
49:YU:90:VAL:HG22	50:YV:39:LEU:HB3	1.98	0.45
1:QA:1177:G:H2'	1:QA:1178:G:C4	2.51	0.45
4:QD:22:LYS:HG3	56:QD:301:SF4:S1	2.56	0.45
11:QK:101:SER:O	11:QK:101:SER:OG	2.30	0.45
15:QO:39:LEU:HD22	15:QO:56:LEU:HD13	1.97	0.45
34:RA:589:C:H2'	34:RA:590:A:C8	2.52	0.45
34:RA:2463:C:C2	34:RA:2488:A:H2	2.35	0.45
34:RA:2722:G:H5''	34:RA:2820:A:N7	2.31	0.45
1:XA:881:G:P	12:XL:12:ARG:HH22	2.40	0.45
2:XB:207:ALA:O	2:XB:210:SER:OG	2.28	0.45
9:XI:28:VAL:HG12	9:XI:63:ILE:HB	1.98	0.45
34:YA:2151:G:H2'	34:YA:2152:G:H8	1.80	0.45
34:YA:2641:G:H5''	42:YN:76:SER:HB3	1.97	0.45
36:YD:133:LEU:HD23	36:YD:136:ILE:HD12	1.98	0.45
46:YR:33:ARG:HA	46:YR:114:VAL:O	2.17	0.45
1:QA:28:G:O2'	1:QA:296:U:OP1	2.31	0.45
1:QA:370:C:H2'	1:QA:371:G:C8	2.51	0.45
7:QG:116:ALA:HA	7:QG:119:ARG:HE	1.82	0.45
13:QM:108:ARG:HA	13:QM:111:LYS:HB2	1.97	0.45
34:RA:665:C:H2'	34:RA:666:G:H8	1.81	0.45
34:RA:2308:G:H22	34:RA:2311:A:H2	1.64	0.45
36:RD:247:ALA:HA	36:RD:253:GLN:HA	1.98	0.45
43:RO:63:VAL:HB	43:RO:102:VAL:HG13	1.98	0.45
49:RU:45:TYR:O	49:RU:49:HIS:ND1	2.49	0.45
1:XA:603:U:H2'	1:XA:604:G:C8	2.51	0.45
1:XA:1304:G:OP1	21:XU:2:GLY:N	2.50	0.45
1:XA:1356:G:H2'	1:XA:1357:A:H8	1.82	0.45
2:XB:27:LYS:HD2	2:XB:193:ASP:HB2	1.97	0.45
4:XD:162:LEU:HD12	4:XD:178:VAL:HG13	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:XL:46:LYS:HG3	12:XL:48:PRO:HD2	1.98	0.45
15:XO:64:ARG:HH12	15:XO:68:ARG:HH22	1.63	0.45
1:QA:99:C:H2'	1:QA:101:A:C8	2.51	0.45
1:QA:165:C:H2'	1:QA:166:G:H8	1.81	0.45
1:QA:1347:G:O2'	1:QA:1373:G:O6	2.33	0.45
34:RA:809:G:H2'	34:RA:810:U:C6	2.51	0.45
34:RA:890:A:H2'	34:RA:892:G:H8	1.82	0.45
34:RA:1230:C:H2'	34:RA:1231:G:H8	1.82	0.45
35:RB:7:G:H21	47:RS:38:GLN:HE22	1.64	0.45
36:RD:13:ARG:NH1	36:RD:16:MET:SD	2.90	0.45
53:RY:28:LYS:HG3	53:RY:40:GLU:HG2	1.99	0.45
1:XA:34:C:H2'	1:XA:35:G:H8	1.81	0.45
1:XA:595:G:H1'	1:XA:596:C:H5	1.81	0.45
4:XD:30:LYS:HB3	4:XD:35:ARG:HH22	1.81	0.45
20:XT:11:SER:O	20:XT:11:SER:OG	2.28	0.45
36:YD:71:ASP:HB2	36:YD:103:ARG:HH12	1.82	0.45
38:YF:155:LEU:HB2	38:YF:189:THR:HG21	1.99	0.45
1:QA:244:U:H3	1:QA:893:C:H42	1.64	0.45
1:QA:947:G:HO2'	1:QA:1306:A:HO2'	1.59	0.45
2:QB:233:SER:O	2:QB:233:SER:OG	2.34	0.45
34:RA:172:C:H2'	34:RA:173:G:C8	2.52	0.45
34:RA:581:C:H2'	34:RA:582:G:C8	2.51	0.45
34:RA:626:U:H5'	34:RA:627:A:H5''	1.97	0.45
34:RA:2641:G:P	42:RN:74:ARG:HE	2.39	0.45
36:RD:132:PRO:HA	36:RD:190:TYR:HA	1.99	0.45
41:RI:123:LEU:HD12	41:RI:142:VAL:HG13	1.98	0.45
50:RV:14:VAL:HB	50:RV:96:ILE:HG12	1.98	0.45
51:RW:76:VAL:HG22	51:RW:103:ILE:HG23	1.98	0.45
1:XA:269:C:H2'	1:XA:270:A:C8	2.52	0.45
1:XA:327:A:O2'	1:XA:328:C:O4'	2.29	0.45
1:XA:1128:C:O2'	1:XA:1130:A:N7	2.50	0.45
1:XA:1151:A:H2'	1:XA:1152:A:H8	1.82	0.45
4:XD:21:LEU:N	4:XD:26:CYS:SG	2.89	0.45
33:Y9:25:VAL:HG22	33:Y9:34:GLN:HB3	1.98	0.45
34:YA:122:G:OP1	34:YA:149:A:O2'	2.31	0.45
34:YA:606:U:OP2	38:YF:104:LYS:NZ	2.43	0.45
34:YA:1636:C:H2'	34:YA:1637:A:C8	2.51	0.45
34:YA:1657:C:H2'	34:YA:1658:C:C6	2.51	0.45
35:YB:104:A:OP1	54:YZ:72:ARG:NH1	2.49	0.45
38:YF:54:ARG:HD2	38:YF:81:PRO:HD3	1.98	0.45
45:YQ:13:GLN:O	45:YQ:72:LYS:NZ	2.38	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:YU:8:VAL:HG22	49:YU:12:ARG:HE	1.82	0.45
51:YW:46:PHE:O	51:YW:50:VAL:HG23	2.16	0.45
1:QA:950:U:H3	1:QA:1231:G:H1	1.65	0.45
1:QA:1174:G:H2'	1:QA:1175:G:H8	1.81	0.45
1:QA:1412:C:H2'	1:QA:1413:A:C8	2.51	0.45
4:QD:85:LYS:HA	4:QD:85:LYS:HD2	1.73	0.45
32:R8:13:ARG:HD2	44:RP:61:ARG:HE	1.81	0.45
34:RA:249:C:O5'	34:RA:2394:C:O2'	2.35	0.45
34:RA:1400:G:H2'	34:RA:1401:G:H8	1.81	0.45
34:RA:1789:A:H5''	36:RD:221:VAL:HA	1.99	0.45
36:RD:208:LYS:HG3	36:RD:210:GLY:H	1.82	0.45
48:RT:102:ILE:HD12	48:RT:110:ILE:HD12	1.99	0.45
1:XA:125:U:H2'	1:XA:126:G:C8	2.52	0.45
1:XA:619:U:H5'	4:XD:131:ARG:HH21	1.82	0.45
4:XD:43:HIS:HB3	4:XD:46:LYS:HD2	1.98	0.45
7:XG:26:PHE:O	7:XG:30:ILE:HG12	2.17	0.45
7:XG:139:GLU:OE1	7:XG:143:ARG:NH2	2.49	0.45
8:XH:121:ASP:HB2	8:XH:125:ARG:HH21	1.82	0.45
12:XL:110:VAL:H	12:XL:122:THR:HG22	1.82	0.45
25:Y1:40:ARG:HG2	25:Y1:41:ARG:H	1.81	0.45
28:Y4:5:ILE:N	28:Y4:5:ILE:CD1	2.79	0.45
34:YA:172:C:H2'	34:YA:173:G:C8	2.52	0.45
34:YA:748:G:C8	34:YA:750:A:N7	2.85	0.45
34:YA:1682:G:OP2	34:YA:1699:G:N2	2.44	0.45
34:YA:2162:G:H2'	34:YA:2163:C:C2	2.52	0.45
42:YN:91:LEU:HD23	42:YN:91:LEU:HA	1.81	0.45
42:YN:137:LYS:HD3	42:YN:138:LEU:HG	1.99	0.45
48:YT:54:ARG:HA	48:YT:59:THR:HG23	1.99	0.45
49:YU:17:ILE:HG13	49:YU:32:PHE:HE1	1.82	0.45
1:QA:1338:G:H21	22:QV:41:A:H1'	1.80	0.45
34:RA:65:C:H5'	52:RX:71:GLY:HA3	1.98	0.45
34:RA:1608:A:C8	34:RA:1611:C:N4	2.84	0.45
34:RA:1662:C:O2'	34:RA:2687:U:OP1	2.34	0.45
34:RA:1689:A:H2'	34:RA:1690:A:H8	1.82	0.45
34:RA:2448:A:OP1	34:RA:2499:C:OP1	2.34	0.45
37:RE:111:ARG:HD3	37:RE:160:TYR:CE2	2.52	0.45
39:RG:81:LYS:HD2	39:RG:81:LYS:HA	1.74	0.45
40:RH:98:LEU:CG	40:RH:125:VAL:CG1	2.91	0.45
40:RH:124:GLU:HG3	40:RH:124:GLU:O	2.17	0.45
50:RV:68:LYS:HD2	50:RV:68:LYS:HA	1.70	0.45
54:RZ:54:HIS:HB3	54:RZ:101:PRO:HD3	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:985:C:H2'	1:XA:986:A:C8	2.51	0.45
24:Y0:41:ARG:O	34:YA:2330:G:N2	2.47	0.45
34:YA:2031:A:O2'	34:YA:2454:G:N2	2.49	0.45
35:YB:14:U:O3'	35:YB:107:U:O2'	2.29	0.45
37:YE:171:GLU:HB2	37:YE:185:LYS:HG3	1.98	0.45
1:QA:62:U:O4	1:QA:105:G:O6	2.35	0.45
1:QA:765:G:N1	1:QA:812:C:O2'	2.44	0.45
16:QP:4:ILE:HD13	16:QP:21:VAL:HG12	1.97	0.45
17:QQ:59:ILE:HG22	17:QQ:73:VAL:HA	1.98	0.45
31:R7:18:PHE:HB2	31:R7:43:THR:HG21	1.99	0.45
34:RA:1518:C:H2'	34:RA:1519:G:H8	1.82	0.45
34:RA:1687:G:N2	34:RA:1702:G:O6	2.50	0.45
34:RA:1838:C:O2	34:RA:1898:U:C4	2.70	0.45
34:RA:1939:U:OP1	34:RA:2604:U:O2'	2.35	0.45
34:RA:2099:U:H2'	34:RA:2100:G:C8	2.51	0.45
39:RG:161:THR:HG22	39:RG:163:ALA:H	1.82	0.45
41:RI:80:PRO:HB2	41:RI:146:ALA:HB2	1.97	0.45
43:RO:106:LEU:HA	43:RO:109:LYS:HB2	1.99	0.45
48:RT:118:ARG:HH11	48:RT:121:ILE:HG21	1.81	0.45
53:RY:28:LYS:NZ	53:RY:40:GLU:OE2	2.38	0.45
1:XA:778:G:H21	11:XK:120:ARG:HB3	1.81	0.45
1:XA:977:A:O2'	1:XA:979:C:OP2	2.28	0.45
1:XA:1228:C:P	13:XM:108:ARG:HH12	2.40	0.45
27:Y3:23:LEU:HD12	27:Y3:28:LEU:HB2	1.98	0.45
34:YA:2032:G:N2	37:YE:146:THR:OG1	2.48	0.45
36:YD:44:ASN:HB3	36:YD:49:ILE:HG22	1.98	0.45
1:QA:382:A:H2'	1:QA:383:A:H8	1.81	0.45
1:QA:1095:U:P	1:QA:1108:G:H1	2.40	0.45
2:QB:193:ASP:OD2	2:QB:193:ASP:N	2.50	0.45
3:QC:6:HIS:HE1	3:QC:8:ILE:HD12	1.82	0.45
3:QC:24:ALA:HB1	3:QC:32:LEU:HD21	1.99	0.45
6:QF:12:PRO:HD3	6:QF:58:GLY:HA2	1.99	0.45
33:R9:35:ARG:NH2	34:RA:2539:C:O2'	2.49	0.45
39:RG:81:LYS:HB3	39:RG:82:LEU:H	1.59	0.45
40:RH:126:PRO:HG2	40:RH:130:ARG:CG	2.46	0.45
41:RI:79:ILE:HG23	41:RI:142:VAL:HA	1.99	0.45
1:XA:68(C):G:H1	1:XA:68(Y):U:H3	1.64	0.45
1:XA:186(M):G:H2'	1:XA:186(N):G:C8	2.52	0.45
1:XA:741:G:H5'	1:XA:742:G:OP2	2.17	0.45
1:XA:985:C:H2'	1:XA:986:A:H8	1.82	0.45
1:XA:1342:C:H2'	1:XA:1343:G:C8	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:XS:53:ASN:ND2	19:XS:76:PRO:O	2.48	0.45
27:Y3:40:THR:HB	27:Y3:43:ILE:HG12	1.98	0.45
1:QA:237:C:H2'	1:QA:238:G:C8	2.51	0.44
1:QA:685:G:N1	1:QA:704:A:OP2	2.41	0.44
8:QH:112:LEU:HD11	8:QH:133:LEU:HD12	1.99	0.44
33:R9:19:ARG:NH2	34:RA:2754:U:O3'	2.50	0.44
34:RA:18:C:O2'	34:RA:553:U:OP1	2.33	0.44
34:RA:139:G:C2	34:RA:141(A):A:C6	3.04	0.44
34:RA:1127:A:N7	34:RA:2488:A:O2'	2.45	0.44
34:RA:2342:C:O2'	34:RA:2374:C:OP1	2.33	0.44
34:RA:2687:U:H3	34:RA:2722:G:H1	1.66	0.44
36:RD:95:LEU:HB2	36:RD:103:ARG:O	2.17	0.44
37:RE:32:PRO:HA	37:RE:90:THR:HA	1.99	0.44
1:XA:1224:G:O2'	1:XA:1322:C:OP2	2.36	0.44
1:XA:1414:U:H2'	1:XA:1415:G:C8	2.50	0.44
2:XB:33:TYR:HB2	2:XB:43:ASP:HB2	1.99	0.44
12:XL:24:VAL:HG13	12:XL:98:TYR:HE1	1.82	0.44
32:Y8:42:ARG:NH2	34:YA:2382:G:H21	2.14	0.44
33:Y9:27:CYS:SG	33:Y9:29:ASN:HB3	2.57	0.44
34:YA:775:G:H4'	34:YA:776:G:H5'	1.98	0.44
34:YA:783:A:H8	34:YA:784:A:H4'	1.82	0.44
34:YA:1266:G:O2'	34:YA:2012:G:O6	2.22	0.44
34:YA:1499:C:H2'	34:YA:1500:G:H8	1.82	0.44
34:YA:2402:C:C5'	34:YA:2402:C:C6	2.97	0.44
34:YA:2809:A:H2'	34:YA:2810:A:C8	2.52	0.44
43:YO:44:LYS:HA	43:YO:44:LYS:HD3	1.72	0.44
54:YZ:5:LEU:HB2	54:YZ:59:LEU:HD12	1.98	0.44
1:QA:37:U:HO2'	1:QA:500:G:HO2'	1.64	0.44
1:QA:166:G:H2'	1:QA:167:G:H8	1.82	0.44
1:QA:647:C:H2'	1:QA:648:A:H8	1.81	0.44
1:QA:948:C:H2'	1:QA:949:A:H8	1.82	0.44
22:QV:76:A:N6	34:RA:2422:A:O4'	2.50	0.44
34:RA:780:G:H21	34:RA:783:A:H62	1.65	0.44
34:RA:966:G:H4'	34:RA:2271:G:H22	1.83	0.44
34:RA:1509:C:N3	34:RA:1511:A:N6	2.65	0.44
34:RA:2531:A:H61	34:RA:2662:A:H61	1.64	0.44
34:RA:2630:G:H2'	34:RA:2631:G:C8	2.52	0.44
54:RZ:97:GLU:HB3	54:RZ:125:LEU:HD11	2.00	0.44
1:XA:1499:A:H8	1:XA:1499:A:O5'	2.00	0.44
7:XG:79:ARG:HH21	7:XG:82:GLY:HA2	1.82	0.44
34:YA:532:A:H4'	34:YA:533:G:C8	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:YA:2005:A:O2'	34:YA:2049:G:OP1	2.30	0.44
1:QA:67:C:H2'	1:QA:68:G:C8	2.53	0.44
1:QA:626:U:H2'	1:QA:627:G:C8	2.51	0.44
2:QB:178:ARG:NH1	2:QB:196:LEU:O	2.49	0.44
6:QF:47:ARG:HD2	6:QF:57:GLN:HB3	2.00	0.44
29:R5:41:PRO:O	29:R5:44:THR:OG1	2.27	0.44
34:RA:29:U:H2'	34:RA:30:G:C8	2.53	0.44
34:RA:84:A:N1	34:RA:98:G:O2'	2.38	0.44
34:RA:494:G:H21	51:RW:57:ASN:HD21	1.63	0.44
34:RA:2498:C:OP2	34:RA:2499:C:OP2	2.36	0.44
40:RH:86:GLU:O	40:RH:164:TYR:HB2	2.17	0.44
43:RO:76:ALA:HB3	48:RT:75:ILE:HG12	1.99	0.44
1:XA:1462:G:H5''	48:YT:111:ARG:HH22	1.81	0.44
1:XA:1499:A:O5'	1:XA:1499:A:C8	2.70	0.44
12:XL:88:GLY:H	12:XL:98:TYR:HA	1.82	0.44
24:Y0:38:VAL:HG22	24:Y0:59:LEU:HB2	1.98	0.44
29:Y5:32:PRO:N	29:Y5:32:PRO:C	2.61	0.44
34:YA:568:U:H5''	34:YA:568:U:H6	1.82	0.44
42:YN:21:LYS:HD2	42:YN:26:LEU:HD13	1.98	0.44
48:YT:25:GLY:N	48:YT:49:VAL:O	2.42	0.44
50:YV:2:PHE:H	50:YV:42:GLY:HA3	1.82	0.44
1:QA:269:C:H2'	1:QA:270:A:C8	2.52	0.44
1:QA:318:G:H2'	1:QA:319:G:H8	1.83	0.44
1:QA:1080:A:OP1	5:QE:14:ARG:NH2	2.47	0.44
34:RA:28:A:HO2'	34:RA:582:G:HO2'	1.58	0.44
34:RA:861:A:N3	35:RB:79:C:O2'	2.51	0.44
34:RA:2319:G:N2	34:RA:2334:G:OP1	2.51	0.44
34:RA:2809:A:OP2	34:RA:2891:G:N1	2.45	0.44
35:RB:25:A:H2'	35:RB:26:A:H8	1.83	0.44
41:RI:4:ILE:HG23	41:RI:39:ALA:HB2	2.00	0.44
48:RT:25:GLY:H	48:RT:49:VAL:HG13	1.82	0.44
54:RZ:115:GLY:H	54:RZ:177:PRO:HG3	1.83	0.44
1:XA:673:G:O3'	6:XF:87:ARG:NH2	2.50	0.44
1:XA:1354:C:H2'	1:XA:1355:G:C8	2.53	0.44
1:XA:1356:G:H2'	1:XA:1357:A:C8	2.52	0.44
3:XC:18:TRP:CE2	14:YN:55:GLY:HA2	2.53	0.44
13:XM:2:ALA:HB3	13:XM:9:ILE:HG21	2.00	0.44
34:YA:190:A:N3	34:YA:679:C:O2'	2.44	0.44
34:YA:1549:C:O2'	34:YA:1733:G:N2	2.42	0.44
34:YA:2102:U:H3	34:YA:2187:G:H1	1.64	0.44
34:YA:2303:G:N3	39:YG:132:ASN:ND2	2.64	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:YR:100:LEU:HD11	46:YR:113:LEU:HG	2.00	0.44
1:QA:502:G:H2'	1:QA:503:C:O4'	2.18	0.44
1:QA:707:C:OP1	11:QK:85:ARG:NH1	2.51	0.44
4:QD:61:LYS:HD2	4:QD:207:TYR:CZ	2.53	0.44
34:RA:299:A:N3	34:RA:319:C:O2'	2.38	0.44
34:RA:679:C:H2'	34:RA:680:G:H8	1.82	0.44
34:RA:1796:U:H2'	34:RA:1797:C:H6	1.82	0.44
34:RA:1851:U:H3	34:RA:1891:G:H1	1.65	0.44
34:RA:1992:G:C5	34:RA:1997:G:C6	3.05	0.44
36:RD:61:LEU:HD23	36:RD:61:LEU:HA	1.83	0.44
39:RG:135:LEU:HD11	39:RG:140:ILE:HD11	2.00	0.44
51:RW:65:LEU:HD12	51:RW:68:ARG:HH21	1.83	0.44
1:XA:1427:U:H2'	1:XA:1428:A:C8	2.52	0.44
16:XP:22:THR:OG1	16:XP:23:ASP:N	2.50	0.44
18:XR:85:LEU:HD12	18:XR:85:LEU:HA	1.83	0.44
34:YA:840:C:H2'	34:YA:841:A:C8	2.53	0.44
34:YA:1859:A:N6	34:YA:1883:G:O2'	2.51	0.44
38:YF:167:ALA:HB1	38:YF:173:VAL:HG11	1.99	0.44
45:YQ:12:GLN:HB2	45:YQ:73:PRO:HD2	2.00	0.44
1:QA:476:G:H2'	1:QA:477:G:H8	1.82	0.44
2:QB:51:LEU:HD23	2:QB:201:ILE:HD12	1.99	0.44
27:R3:18:ASP:OD1	27:R3:18:ASP:N	2.48	0.44
34:RA:373:U:H2'	34:RA:374:A:H8	1.83	0.44
34:RA:1441:G:H2'	34:RA:1442:G:H8	1.82	0.44
34:RA:1791:A:H61	34:RA:1828:G:HO2'	1.61	0.44
34:RA:2094:G:OP1	41:RI:22:LYS:HE2	2.13	0.44
34:RA:2580:U:H5'	37:RE:130:GLY:O	2.18	0.44
36:RD:12:SER:HB2	36:RD:208:LYS:HB3	1.99	0.44
41:RI:84:GLY:CA	41:RI:89:TYR:OH	2.61	0.44
1:XA:1174:G:H2'	1:XA:1175:G:C8	2.53	0.44
1:XA:1271:G:H5'	1:XA:1314:C:H5''	1.99	0.44
2:XB:189:ASP:OD1	2:XB:189:ASP:N	2.49	0.44
4:XD:57:ARG:NH2	4:XD:205:GLU:OE1	2.51	0.44
30:Y6:29:ASN:ND2	34:YA:2286:A:OP1	2.50	0.44
34:YA:270(R):C:H5''	41:YI:45:LYS:HD3	1.99	0.44
34:YA:828:U:O2	34:YA:828:U:H3'	2.17	0.44
34:YA:1006:C:H5'	42:YN:28:THR:HG23	1.99	0.44
34:YA:1500:G:O2'	36:YD:100:GLY:O	2.27	0.44
34:YA:1853:A:N3	34:YA:2233:U:O2'	2.46	0.44
34:YA:2109:U:H2'	34:YA:2110:G:C8	2.52	0.44
45:YQ:58:PHE:HD2	45:YQ:61:GLY:HA3	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:YY:13:VAL:HG12	53:YY:74:PRO:HA	1.99	0.44
1:QA:59:A:H3'	1:QA:331:G:H22	1.82	0.44
1:QA:297:G:N2	1:QA:300:A:OP2	2.51	0.44
1:QA:949:A:H2'	1:QA:950:U:H6	1.83	0.44
1:QA:1220:G:H2'	1:QA:1221:G:H8	1.82	0.44
1:QA:1440(B):G:H21	1:QA:1440(P):A:H62	1.65	0.44
10:QJ:28:ARG:HE	10:QJ:34:VAL:HG12	1.83	0.44
13:QM:95:GLY:HA2	13:QM:110:ARG:HH21	1.83	0.44
22:QV:71:C:O2	34:RA:1851:U:O2'	2.36	0.44
34:RA:1138:G:H21	42:RN:106:MET:HG2	1.83	0.44
34:RA:2294:C:H2'	34:RA:2295:C:H6	1.82	0.44
40:RH:4:ILE:HD12	40:RH:6:ARG:HB2	1.99	0.44
1:XA:59:A:H5'	1:XA:60:A:H5''	1.99	0.44
1:XA:294:U:OP1	1:XA:610:G:O2'	2.32	0.44
1:XA:964:A:N3	10:XJ:55:LYS:NZ	2.62	0.44
4:XD:68:TYR:OH	4:XD:98:GLU:OE2	2.33	0.44
34:YA:1151:G:O2'	49:YU:77:SER:O	2.33	0.44
34:YA:2153:G:H2'	34:YA:2154:G:H8	1.82	0.44
46:YR:29:LEU:HD13	46:YR:79:LEU:HD22	1.99	0.44
1:QA:444:C:H2'	1:QA:445:G:C8	2.53	0.44
1:QA:927:G:N2	1:QA:1390:U:O2	2.33	0.44
1:QA:1022:G:H2'	1:QA:1023:G:C8	2.52	0.44
3:QC:112:SER:HB3	3:QC:115:LEU:HD12	2.00	0.44
34:RA:1053:C:O5'	34:RA:1053:C:H6	2.00	0.44
34:RA:1276:A:H1'	46:RR:16:HIS:HE1	1.83	0.44
34:RA:1695:G:H1'	36:RD:8:PRO:O	2.17	0.44
34:RA:2081:C:H2'	34:RA:2082:A:H8	1.83	0.44
34:RA:2097:C:C6	34:RA:2097:C:OP2	2.71	0.44
34:RA:2097:C:OP2	34:RA:2097:C:H6	2.00	0.44
34:RA:2287:A:N6	34:RA:2344:U:H3	2.16	0.44
34:RA:2850:A:OP2	34:RA:2866:U:N3	2.51	0.44
36:RD:181:GLU:HA	36:RD:272:ALA:HB3	1.99	0.44
1:XA:40:C:H2'	1:XA:41:G:H8	1.82	0.44
1:XA:1230:C:H2'	1:XA:1231:G:C8	2.53	0.44
26:Y2:58:ALA:O	26:Y2:62:THR:OG1	2.30	0.44
39:YG:124:SER:O	39:YG:124:SER:OG	2.35	0.44
39:YG:138:GLN:OE1	39:YG:153:ARG:N	2.43	0.44
1:QA:401:C:O2'	1:QA:621:A:N3	2.47	0.44
1:QA:538:G:H2'	1:QA:539:A:H8	1.83	0.44
1:QA:595:G:H1'	1:QA:596:C:H5	1.83	0.44
1:QA:662:G:H2'	1:QA:663:A:C8	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:1203:C:H2'	1:QA:1204:A:C8	2.53	0.44
5:QE:43:LEU:HD13	5:QE:109:ILE:HD11	1.99	0.44
19:QS:50:ALA:HA	19:QS:58:VAL:O	2.17	0.44
22:QV:37:1MG:C5	22:QV:38:A:C4	3.06	0.44
34:RA:31:C:O2'	34:RA:1238:G:OP1	2.35	0.44
34:RA:997:G:OP1	49:RU:93:LYS:HD3	2.18	0.44
34:RA:1068:G:N2	34:RA:1095:A:O3'	2.51	0.44
34:RA:1790:C:OP2	34:RA:1828:G:N1	2.48	0.44
34:RA:1962:C:O2'	34:RA:1964:G:OP2	2.28	0.44
34:RA:2098:U:O2	34:RA:2098:U:H2'	2.17	0.44
36:RD:50:THR:OG1	36:RD:51:VAL:N	2.50	0.44
1:XA:575:G:N1	1:XA:880:C:N3	2.55	0.44
1:XA:1251:A:H2'	1:XA:1252:A:C8	2.53	0.44
1:XA:1342:C:H2'	1:XA:1343:G:H8	1.83	0.44
1:XA:1427:U:H2'	1:XA:1428:A:H8	1.83	0.44
3:XC:66:VAL:HB	3:XC:101:LEU:HD13	2.00	0.44
16:XP:19:ILE:HG13	16:XP:36:ILE:HD11	2.00	0.44
18:XR:47:THR:O	18:XR:83:GLU:N	2.51	0.44
20:XT:100:ILE:HG23	20:XT:102:GLY:H	1.81	0.44
34:YA:1853:A:H2'	34:YA:1854:A:C8	2.53	0.44
38:YF:102:PRO:HB2	38:YF:105:VAL:HG23	1.99	0.44
51:YW:35:ILE:O	51:YW:39:THR:OG1	2.27	0.44
53:YY:28:LYS:N	53:YY:38:ILE:O	2.45	0.44
1:QA:1204:A:OP1	14:QN:3:ARG:NH2	2.51	0.43
25:R1:90:ILE:HA	25:R1:94:LEU:HG	1.99	0.43
34:RA:117:G:OP1	34:RA:124:G:N1	2.44	0.43
34:RA:265:A:N7	34:RA:428:A:N6	2.65	0.43
34:RA:707:G:H1	34:RA:724:U:H3	1.66	0.43
45:RQ:34:LEU:HB2	45:RQ:118:LEU:HD12	1.99	0.43
51:RW:71:VAL:HA	51:RW:107:LEU:HD23	2.00	0.43
52:RX:55:ASN:HB2	52:RX:80:ILE:HG23	2.00	0.43
1:XA:48:C:OP2	1:XA:115:G:OP1	2.35	0.43
1:XA:1291:G:H4'	9:XI:39:GLY:HA3	1.99	0.43
5:XE:31:LEU:HD13	5:XE:45:PHE:HD1	1.83	0.43
15:XO:53:HIS:NE2	34:YA:715:G:O6	2.49	0.43
36:YD:142:VAL:HA	36:YD:194:GLY:H	1.83	0.43
37:YE:102:VAL:N	37:YE:170:LEU:O	2.46	0.43
1:QA:1503:A:N3	23:QX:15:A:N6	2.65	0.43
5:QE:100:VAL:O	5:QE:107:ARG:NH1	2.48	0.43
16:QP:55:ARG:HD2	16:QP:55:ARG:HA	1.79	0.43
23:QX:14:A:C8	23:QX:14:A:OP2	2.70	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:R4:12:ALA:H	28:R4:25:TYR:HA	1.83	0.43
34:RA:1084:A:H2'	34:RA:1085:A:C4	2.53	0.43
34:RA:2246:G:H2'	34:RA:2247:A:H8	1.82	0.43
34:RA:2392:A:H2	34:RA:2424:C:H42	1.66	0.43
34:RA:2576:G:N3	34:RA:2576:G:C3'	2.80	0.43
41:RI:79:ILE:HD12	41:RI:80:PRO:HD2	2.00	0.43
3:XC:187:ALA:HB3	3:XC:198:VAL:HG13	2.00	0.43
5:XE:105:VAL:HG11	5:XE:132:ALA:HB2	1.99	0.43
12:XL:33:ARG:NH2	12:XL:61:THR:OG1	2.51	0.43
28:Y4:37:SER:HA	28:Y4:41:PRO:HD2	1.98	0.43
32:Y8:56:GLU:OE1	32:Y8:59:LYS:NZ	2.36	0.43
34:YA:748:G:N9	34:YA:750:A:N7	2.66	0.43
34:YA:2031:A:HO2'	34:YA:2454:G:H21	1.66	0.43
34:YA:2821:A:OP1	37:YE:110:GLY:N	2.47	0.43
35:YB:5:C:OP1	35:YB:61:G:O2'	2.28	0.43
37:YE:37:ARG:NH1	37:YE:44:TYR:OH	2.48	0.43
39:YG:106:LEU:HD12	39:YG:110:ALA:HB3	1.99	0.43
44:YP:21:ARG:HB3	44:YP:22:GLY:H	1.67	0.43
1:QA:355:C:O2'	1:QA:388:G:N3	2.36	0.43
1:QA:406:G:H21	4:QD:119:GLN:HE22	1.66	0.43
1:QA:559:A:H4'	1:QA:560:U:H5''	2.00	0.43
1:QA:673:G:O3'	6:QF:87:ARG:NH2	2.50	0.43
1:QA:881:G:P	12:QL:12:ARG:HH22	2.41	0.43
34:RA:691:C:H2'	34:RA:692:C:H6	1.82	0.43
34:RA:1165:U:O4	34:RA:1184:G:O6	2.36	0.43
34:RA:1182:A:H2'	34:RA:1183:G:H8	1.83	0.43
34:RA:1385:G:O2'	34:RA:1396:U:O2	2.32	0.43
34:RA:2313:C:H5''	39:RG:91:ARG:HH21	1.83	0.43
37:RE:176:ILE:HG13	37:RE:181:LEU:HB2	2.00	0.43
1:XA:1409:C:H2'	1:XA:1410:G:H8	1.82	0.43
24:Y0:12:ASN:ND2	34:YA:2278:A:OP2	2.51	0.43
29:Y5:48:GLU:CD	51:YW:37:ARG:NH1	2.67	0.43
30:Y6:3:SER:HB3	30:Y6:6:ARG:HB3	2.00	0.43
35:YB:75:G:H21	54:YZ:85:HIS:CD2	2.36	0.43
47:YS:4:LEU:HD11	47:YS:12:PHE:CE2	2.51	0.43
1:QA:57:G:H2'	1:QA:58:C:H6	1.84	0.43
2:QB:54:THR:O	2:QB:58:ILE:HG12	2.18	0.43
6:QF:14:LEU:HD12	6:QF:18:GLN:CD	2.38	0.43
29:R5:12:SER:O	29:R5:16:ARG:CB	2.67	0.43
34:RA:29:U:H2'	34:RA:30:G:H8	1.83	0.43
34:RA:273(E):C:N4	34:RA:363(D):G:O6	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:RA:922:U:H2'	34:RA:923:C:C6	2.54	0.43
34:RA:1525:G:H2'	34:RA:1526:G:C8	2.53	0.43
34:RA:2294:C:OP2	47:RS:13:ARG:NH2	2.52	0.43
34:RA:2311:A:C8	39:RG:82:LEU:HD21	2.53	0.43
37:RE:171:GLU:H	37:RE:185:LYS:HB2	1.84	0.43
40:RH:80:SER:O	40:RH:80:SER:OG	2.31	0.43
46:RR:29:LEU:HD12	46:RR:70:LEU:HD21	1.99	0.43
46:RR:35:THR:HG22	46:RR:113:LEU:HD13	2.01	0.43
1:XA:25:C:C4	1:XA:558:G:N2	2.86	0.43
1:XA:67:C:O2'	1:XA:171:A:N3	2.40	0.43
1:XA:605:U:OP2	1:XA:605:U:C5	2.70	0.43
1:XA:1135:U:H4'	1:XA:1136:U:H5	1.83	0.43
27:Y3:18:ASP:HB2	27:Y3:49:LYS:HE2	1.99	0.43
31:Y7:34:ARG:NH1	34:YA:466:A:OP1	2.51	0.43
34:YA:530:G:N1	34:YA:2022:U:OP1	2.52	0.43
34:YA:629:G:N3	34:YA:639:U:O2'	2.51	0.43
34:YA:2047:U:O2'	34:YA:2823:A:N1	2.47	0.43
41:YI:81:VAL:HG11	41:YI:88:ILE:HD13	1.99	0.43
44:YP:97:PRO:O	44:YP:98:GLU:HG3	2.18	0.43
49:YU:55:ARG:O	49:YU:59:ARG:HG2	2.18	0.43
1:QA:501:C:H2'	1:QA:502:G:C8	2.54	0.43
1:QA:674:G:H2'	1:QA:675:A:C8	2.48	0.43
1:QA:1414:U:H2'	1:QA:1415:G:H8	1.83	0.43
3:QC:131:ARG:HH11	3:QC:134:ILE:HG21	1.83	0.43
8:QH:82:HIS:N	8:QH:138:TRP:OXT	2.41	0.43
9:QI:65:VAL:HG11	9:QI:73:GLN:HG3	2.01	0.43
26:R2:16:LEU:H	26:R2:67:LYS:NZ	2.16	0.43
34:RA:947:G:H2'	34:RA:948:G:C8	2.53	0.43
34:RA:1814:G:H5'	36:RD:51:VAL:HG11	2.01	0.43
34:RA:2315:G:H2'	34:RA:2316:C:C6	2.54	0.43
34:RA:2425:A:H4'	34:RA:2426:A:H5''	2.00	0.43
34:RA:2504:U:H6	34:RA:2504:U:O5'	2.02	0.43
34:RA:2584:U:H2'	34:RA:2585:U:H2'	2.00	0.43
39:RG:43:LEU:HD21	39:RG:153:ARG:HB2	1.99	0.43
43:RO:15:GLY:HA3	43:RO:50:GLY:HA3	1.99	0.43
48:RT:6:LEU:O	48:RT:10:VAL:HG23	2.19	0.43
1:XA:186(J):U:O2	17:XQ:72:ARG:NH2	2.52	0.43
1:XA:713:G:H2'	1:XA:714:G:C8	2.53	0.43
1:XA:765:G:N1	1:XA:812:C:O2'	2.40	0.43
9:XI:70:LYS:O	9:XI:74:ILE:HG13	2.19	0.43
18:XR:49:LYS:HB3	18:XR:49:LYS:HE2	1.85	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:YA:90:U:H1'	34:YA:91:A:C8	2.54	0.43
34:YA:320:A:N3	38:YF:169:ASN:ND2	2.67	0.43
34:YA:463:G:O2'	34:YA:465:G:O6	2.36	0.43
35:YB:9:G:P	47:YS:25:ARG:HH12	2.42	0.43
39:YG:165:THR:OG1	39:YG:166:ASP:N	2.52	0.43
41:YI:101:LEU:HD11	41:YI:109:ILE:HD13	2.00	0.43
1:QA:865:A:N3	1:QA:918:A:O2'	2.42	0.43
1:QA:1038:C:N3	1:QA:1039:C:N4	2.67	0.43
3:QC:12:LEU:HG	3:QC:18:TRP:HE1	1.83	0.43
4:QD:191:ARG:HA	4:QD:191:ARG:HD2	1.72	0.43
20:QT:58:LYS:O	20:QT:61:SER:OG	2.26	0.43
44:RP:96:THR:HA	44:RP:126:VAL:HB	2.01	0.43
54:RZ:48:PHE:HA	54:RZ:51:ALA:HB3	2.01	0.43
54:RZ:53:ILE:HG22	54:RZ:71:VAL:HG13	1.99	0.43
54:RZ:156:LYS:HE3	54:RZ:156:LYS:HB3	1.74	0.43
1:XA:7:G:O2'	5:XE:120:THR:O	2.36	0.43
1:XA:377:G:H2'	1:XA:378:G:H8	1.83	0.43
1:XA:601:C:H2'	1:XA:602:A:H8	1.83	0.43
1:XA:1374:A:O2'	7:XG:28:ASN:O	2.37	0.43
12:XL:86:ARG:HH21	12:XL:99:HIS:CD2	2.37	0.43
14:XN:40:CYS:SG	14:XN:41:ARG:N	2.91	0.43
34:YA:240:G:O2'	34:YA:257:A:N6	2.51	0.43
34:YA:2081:C:H2'	34:YA:2082:A:H8	1.83	0.43
34:YA:2581:G:N1	34:YA:2610:C:O2'	2.47	0.43
34:YA:2646:C:OP2	34:YA:2732:G:O2'	2.24	0.43
44:YP:64:LYS:O	44:YP:66:GLY:N	2.51	0.43
48:YT:19:LEU:HD21	48:YT:83:ILE:HD11	2.00	0.43
1:QA:131:C:OP2	1:QA:186(K):G:O2'	2.35	0.43
1:QA:382:A:H2'	1:QA:383:A:C8	2.54	0.43
1:QA:736:C:H2'	1:QA:737:A:C8	2.53	0.43
1:QA:1119:C:H2'	1:QA:1120:G:H8	1.83	0.43
2:QB:188:ALA:HB1	2:QB:192:SER:HB2	2.01	0.43
23:QX:14:A:O5'	23:QX:14:A:C8	2.70	0.43
34:RA:1148:A:H2'	34:RA:1149:G:C8	2.54	0.43
34:RA:1528:A:H2'	34:RA:1529:A:H8	1.84	0.43
38:RF:152:GLU:OE1	38:RF:191:ARG:NE	2.52	0.43
42:RN:28:THR:O	42:RN:32:THR:OG1	2.24	0.43
49:RU:91:ASP:O	49:RU:93:LYS:N	2.50	0.43
1:XA:129(A):U:H3	1:XA:232:G:H1	1.67	0.43
1:XA:262:A:H2'	1:XA:263:A:C8	2.54	0.43
1:XA:1205:U:H2'	1:XA:1206:G:H8	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:XK:82:VAL:HB	11:XK:108:ILE:HA	2.01	0.43
24:Y0:72:ARG:CB	24:Y0:75:LEU:HB2	2.49	0.43
33:Y9:10:ILE:N	33:Y9:14:CYS:SG	2.84	0.43
34:YA:947:G:N3	34:YA:984:A:C2	2.87	0.43
34:YA:974(A):G:C5	34:YA:1186:G:C2	3.07	0.43
36:YD:143:HIS:ND1	36:YD:194:GLY:O	2.40	0.43
39:YG:18:GLU:OE1	39:YG:21:ARG:NH2	2.50	0.43
48:YT:120:ARG:HA	48:YT:123:GLN:HB2	2.01	0.43
53:YY:76:CYS:CB	53:YY:79:CYS:SG	3.07	0.43
1:QA:451:A:N7	1:QA:481:G:N1	2.67	0.43
1:QA:819:A:N7	1:QA:1529:G:C6	2.87	0.43
1:QA:1003:G:H2'	1:QA:1004:A:H4'	2.00	0.43
7:QG:75:VAL:HA	7:QG:88:PRO:HA	2.00	0.43
12:QL:76:ASN:HD21	12:QL:108:ALA:HB3	1.84	0.43
13:QM:29:ARG:HH21	13:QM:64:TRP:HE1	1.67	0.43
13:QM:87:TYR:OH	13:QM:91:ARG:NH2	2.47	0.43
14:QN:6:LEU:HD23	14:QN:9:LYS:HD3	2.00	0.43
34:RA:578:A:OP1	34:RA:1255:U:O2'	2.36	0.43
34:RA:1140:C:O3'	42:RN:25:ARG:NH2	2.44	0.43
34:RA:1732:A:H3'	34:RA:1733:G:H8	1.82	0.43
34:RA:2133:G:N2	34:RA:2157:G:H2'	2.33	0.43
43:RO:15:GLY:HA2	43:RO:47:ILE:HG22	2.00	0.43
3:XC:64:VAL:HG13	3:XC:97:LYS:HD2	2.01	0.43
32:Y8:60:LEU:HD12	32:Y8:60:LEU:HA	1.81	0.43
34:YA:363(B):A:H2'	34:YA:363(C):G:C8	2.52	0.43
34:YA:2148:G:H2'	34:YA:2149:G:C8	2.54	0.43
47:YS:14:VAL:O	47:YS:18:ILE:HG12	2.18	0.43
48:YT:16:ARG:NH2	48:YT:83:ILE:O	2.51	0.43
1:QA:380:G:N2	1:QA:383:A:OP2	2.42	0.43
1:QA:401:C:H5	4:QD:73:ARG:HH22	1.60	0.43
1:QA:411:A:OP1	4:QD:30:LYS:NZ	2.49	0.43
1:QA:708:C:H2'	1:QA:709:G:C8	2.53	0.43
3:QC:43:LEU:HG	3:QC:47:LEU:HD22	2.00	0.43
13:QM:34:LEU:HA	13:QM:37:THR:HG22	2.01	0.43
19:QS:70:LYS:N	19:QS:73:GLU:OE1	2.52	0.43
22:QV:23:C:H2'	22:QV:24:G:C8	2.54	0.43
34:RA:1370:C:O2'	34:RA:1811:G:O2'	2.34	0.43
34:RA:1995:U:H3'	34:RA:1996:C:H2'	2.01	0.43
34:RA:2630:G:H2'	34:RA:2631:G:H8	1.84	0.43
35:RB:8:U:O2	35:RB:112:G:N2	2.43	0.43
1:XA:851:G:H2'	1:XA:852:G:H8	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y0:26:TYR:N	24:Y0:29:GLN:OE1	2.52	0.43
34:YA:688:U:H1'	34:YA:786:C:O2'	2.19	0.43
34:YA:2140:C:H2'	34:YA:2141:G:H8	1.83	0.43
38:YF:158:THR:OG1	38:YF:159:GLY:N	2.51	0.43
40:YH:152:ARG:HA	40:YH:152:ARG:HD3	1.80	0.43
34:RA:1179:C:H2'	34:RA:1180:C:H6	1.84	0.43
34:RA:1539:G:H2'	34:RA:1540:G:H8	1.83	0.43
34:RA:2470:G:OP1	45:RQ:56:ARG:NH2	2.43	0.43
37:RE:35:GLN:HB2	37:RE:37:ARG:HH21	1.84	0.43
40:RH:46:GLU:OE1	40:RH:51:ARG:NH1	2.52	0.43
54:RZ:130:PRO:HA	54:RZ:133:ILE:HD11	2.01	0.43
1:XA:445:G:H2'	1:XA:446:G:H8	1.84	0.43
7:XG:102:ARG:HA	7:XG:105:VAL:HG22	2.01	0.43
11:XK:109:VAL:HG11	18:XR:84:LYS:HD2	2.01	0.43
27:Y3:5:LYS:HE3	27:Y3:57:GLU:HB3	1.99	0.43
34:YA:18:C:O2'	34:YA:553:U:OP1	2.31	0.43
34:YA:964:C:O2'	34:YA:2273:A:N3	2.37	0.43
34:YA:1600:C:OP1	52:YX:58:HIS:NE2	2.42	0.43
34:YA:2249:U:N3	34:YA:2253:G:OP2	2.46	0.43
38:YF:48:THR:O	38:YF:48:THR:OG1	2.36	0.43
54:YZ:85:HIS:NE2	54:YZ:87:ASP:OD1	2.52	0.43
1:QA:908:A:H2'	1:QA:909:A:H8	1.84	0.42
1:QA:1145:C:O2'	1:QA:1146:A:N7	2.47	0.42
2:QB:150:SER:HA	2:QB:153:ARG:HH21	1.83	0.42
3:QC:140:ARG:HA	3:QC:143:GLU:HG2	2.01	0.42
6:QF:78:GLU:HA	6:QF:81:ILE:HG12	2.01	0.42
10:QJ:61:GLU:HG3	14:QN:45:ARG:HH12	1.84	0.42
15:QO:64:ARG:NH1	34:RA:715:G:OP1	2.52	0.42
34:RA:532:A:H4'	34:RA:533:G:C8	2.53	0.42
34:RA:807:U:OP1	44:RP:36:LYS:HD3	2.19	0.42
37:RE:134:ILE:HD12	37:RE:134:ILE:HA	1.85	0.42
45:RQ:77:LYS:NZ	45:RQ:84:GLY:O	2.40	0.42
53:RY:79:CYS:N	53:RY:102:CYS:SG	2.92	0.42
1:XA:17:U:H2'	1:XA:18:C:H6	1.83	0.42
1:XA:815:A:O4'	1:XA:817:C:N4	2.52	0.42
10:XJ:99:LYS:HA	10:XJ:99:LYS:HD2	1.73	0.42
34:YA:603:A:N1	34:YA:625:G:O2'	2.49	0.42
34:YA:2808:U:N3	34:YA:2892:A:N6	2.67	0.42
54:YZ:48:PHE:HA	54:YZ:51:ALA:HB3	2.00	0.42
1:QA:757:U:O2'	1:QA:879:C:O2	2.35	0.42
3:QC:29:TYR:OH	14:QN:54:PRO:O	2.37	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:QD:100:ARG:HG3	4:QD:137:SER:HA	2.00	0.42
8:QH:10:LEU:HG	8:QH:83:ILE:HD11	1.99	0.42
12:QL:57:LYS:HA	12:QL:67:THR:HA	2.00	0.42
34:RA:30:G:H2'	34:RA:31:C:C6	2.53	0.42
36:RD:13:ARG:HD2	36:RD:13:ARG:HA	1.80	0.42
37:RE:109:LYS:HG2	37:RE:191:PRO:HB3	2.00	0.42
37:RE:120:TRP:CD2	37:RE:155:LYS:HB3	2.54	0.42
44:RP:65:ARG:O	44:RP:68:GLN:NE2	2.52	0.42
1:XA:948:C:OP2	13:XM:106:ASN:ND2	2.48	0.42
1:XA:1314:C:H2'	1:XA:1315:U:H6	1.84	0.42
1:XA:1384:C:H2'	1:XA:1385:G:C8	2.54	0.42
7:XG:116:ALA:HA	7:XG:119:ARG:HE	1.83	0.42
29:Y5:8:LYS:NZ	34:YA:2055:C:OP1	2.45	0.42
34:YA:691:C:H2'	34:YA:692:C:H6	1.85	0.42
34:YA:1935:G:H1'	34:YA:1964:G:N2	2.34	0.42
34:YA:2446:G:H2'	34:YA:2447:G:H5''	2.01	0.42
37:YE:144:ARG:HG3	37:YE:145:LYS:H	1.84	0.42
1:QA:1071:C:H2'	1:QA:1072:G:C8	2.52	0.42
3:QC:22:TRP:HH2	3:QC:32:LEU:HD13	1.85	0.42
5:QE:102:ALA:H	5:QE:107:ARG:NH2	2.18	0.42
22:QV:19:G:H4'	22:QV:57:G:H1	1.85	0.42
23:QX:14:A:C8	23:QX:14:A:P	3.12	0.42
34:RA:1021:A:H62	34:RA:1022:G:H21	1.67	0.42
1:XA:662:G:H2'	1:XA:663:A:C8	2.54	0.42
1:XA:1052:U:O2'	1:XA:1055:A:OP2	2.29	0.42
1:XA:1314:C:H2'	1:XA:1315:U:C6	2.55	0.42
2:XB:87:ARG:HH21	2:XB:219:VAL:HG13	1.84	0.42
13:XM:9:ILE:HA	13:XM:10:PRO:HD3	1.90	0.42
13:XM:52:GLU:HA	13:XM:55:ARG:HG2	2.00	0.42
19:XS:36:ARG:NH2	19:XS:72:GLY:O	2.52	0.42
20:XT:17:ARG:HE	20:XT:17:ARG:HB3	1.73	0.42
34:YA:816:C:O2'	34:YA:932:G:O6	2.36	0.42
34:YA:1782:C:H42	34:YA:2586:C:N4	2.16	0.42
34:YA:2151:G:H2'	34:YA:2152:G:C8	2.54	0.42
35:YB:111:U:H2'	35:YB:112:G:H8	1.85	0.42
40:YH:159:GLU:HG2	40:YH:169:VAL:HG21	2.01	0.42
51:YW:57:ASN:O	51:YW:61:ASN:HB2	2.19	0.42
1:QA:477:G:H2'	1:QA:478:A:H8	1.83	0.42
1:QA:1028(D):G:N2	1:QA:1028(G):A:OP2	2.53	0.42
1:QA:1219:U:H2'	1:QA:1220:G:C8	2.54	0.42
4:QD:15:GLU:HG2	4:QD:63:LYS:HB3	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:QE:126:ARG:HA	5:QE:131:ILE:HD11	2.01	0.42
7:QG:75:VAL:HG12	7:QG:88:PRO:HB3	2.01	0.42
12:QL:79:GLU:OE2	12:QL:80:HIS:NE2	2.53	0.42
17:QQ:45:HIS:H	17:QQ:72:ARG:HA	1.84	0.42
19:QS:39:THR:HG22	19:QS:41:VAL:HG22	2.01	0.42
22:QV:61:C:H2'	22:QV:62:C:C6	2.53	0.42
23:QX:15:A:O2'	23:QX:17:C:OP2	2.37	0.42
34:RA:894:C:H2'	34:RA:895:U:C6	2.55	0.42
34:RA:2378:A:O3'	47:RS:23:ARG:NH1	2.52	0.42
46:RR:8:ARG:HD2	46:RR:10:LEU:HD21	2.01	0.42
1:XA:1218:C:H2'	1:XA:1219:U:C6	2.54	0.42
3:XC:8:ILE:HG12	3:XC:184:TYR:HB3	2.02	0.42
14:XN:23:ARG:NH1	14:XN:24:CYS:HB3	2.34	0.42
33:Y9:32:HIS:CD2	33:Y9:32:HIS:N	2.87	0.42
34:YA:117:G:OP2	34:YA:119:A:O2'	2.27	0.42
34:YA:690:G:O2'	36:YD:43:ARG:NH1	2.53	0.42
34:YA:2245:U:H6	34:YA:2245:U:C5'	2.29	0.42
53:YY:79:CYS:SG	53:YY:81:LYS:HE2	2.60	0.42
13:QM:66:LEU:HB3	13:QM:67:GLU:H	1.71	0.42
34:RA:504:U:H5''	34:RA:505:A:H5'	2.02	0.42
34:RA:511:U:H4'	34:RA:1235:G:H4'	2.00	0.42
34:RA:1728:G:H8	34:RA:1732:A:H62	1.67	0.42
34:RA:2748:A:H62	34:RA:2754:U:H3	1.67	0.42
34:RA:2853:C:H2'	34:RA:2854:G:H8	1.84	0.42
35:RB:28:C:H2'	35:RB:29:A:H8	1.85	0.42
35:RB:28:C:H2'	35:RB:29:A:C8	2.54	0.42
36:RD:49:ILE:HD11	36:RD:52:ARG:HA	2.00	0.42
51:RW:13:SER:HA	51:RW:99:ARG:HB2	2.01	0.42
1:XA:401:C:O2'	1:XA:621:A:N3	2.43	0.42
1:XA:501:C:H2'	1:XA:502:G:C8	2.54	0.42
1:XA:674:G:H2'	1:XA:675:A:C8	2.49	0.42
1:XA:878:G:H5'	8:XH:89:PRO:HG2	2.00	0.42
1:XA:1060:C:H2'	1:XA:1061:G:H8	1.85	0.42
7:XG:99:LEU:HD12	7:XG:99:LEU:HA	1.93	0.42
19:XS:19:VAL:HA	19:XS:22:LEU:HB2	2.01	0.42
32:Y8:4:MET:HG3	32:Y8:61:LEU:HD11	2.01	0.42
34:YA:639:U:H3	34:YA:649:G:H1	1.67	0.42
34:YA:750:A:C2	34:YA:753:C:N1	2.88	0.42
40:YH:9:ILE:HG22	40:YH:49:VAL:HB	1.96	0.42
42:YN:40:PRO:HB3	49:YU:68:ALA:HB2	2.02	0.42
44:YP:82:GLY:HA2	44:YP:113:LYS:O	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:YR:35:THR:HA	46:YR:112:ALA:O	2.19	0.42
1:QA:1118:C:H1'	1:QA:1179:A:C5	2.54	0.42
1:QA:1220:G:O3'	19:QS:36:ARG:NH2	2.53	0.42
2:QB:175:ARG:O	2:QB:179:LYS:HG3	2.20	0.42
9:QI:103:THR:O	9:QI:103:THR:OG1	2.37	0.42
14:QN:41:ARG:HG3	14:QN:42:ILE:HG13	2.01	0.42
20:QT:14:LYS:HA	20:QT:17:ARG:HG2	2.02	0.42
34:RA:24:G:O2'	51:RW:78:GLU:O	2.24	0.42
34:RA:336:C:HO2'	53:RY:35:TYR:HH	1.67	0.42
34:RA:863:A:H2'	34:RA:864:G:C8	2.55	0.42
34:RA:1051:G:C5	34:RA:1052:C:C4	3.08	0.42
34:RA:2014:A:H2	34:RA:2613:U:N3	2.17	0.42
34:RA:2105:C:H2'	34:RA:2106:G:C8	2.55	0.42
34:RA:2710:C:H2'	34:RA:2711:A:C8	2.55	0.42
49:RU:85:LYS:HE2	49:RU:116:ALA:HA	2.01	0.42
54:RZ:67:LEU:HD12	54:RZ:90:VAL:HB	2.02	0.42
1:XA:17:U:H2'	1:XA:18:C:C6	2.54	0.42
1:XA:186(A):C:H2'	1:XA:186(B):C:C6	2.54	0.42
1:XA:1517:G:N3	34:YA:1919:A:O2'	2.47	0.42
6:XF:27:GLN:HA	6:XF:30:LEU:HD12	2.02	0.42
34:YA:664:C:H2'	34:YA:665:C:H6	1.85	0.42
34:YA:750:A:H2	34:YA:753:C:C6	2.34	0.42
34:YA:906:G:OP1	45:YQ:26:TYR:OH	2.34	0.42
34:YA:2521:C:O2'	34:YA:2564:A:N3	2.38	0.42
47:YS:34:HIS:O	47:YS:97:ARG:NH2	2.52	0.42
1:QA:56:U:H2'	1:QA:57:G:C8	2.55	0.42
1:QA:375:U:OP1	16:QP:69:THR:OG1	2.29	0.42
1:QA:502:G:OP1	12:QL:117:ARG:N	2.53	0.42
1:QA:552:U:O2'	12:QL:86:ARG:O	2.31	0.42
1:QA:926:G:O6	23:QX:19:U:H3'	2.19	0.42
1:QA:1158:C:H1'	2:QB:132:LYS:HD3	2.02	0.42
1:QA:1381:U:H1'	1:QA:1382:C:H5'	2.01	0.42
4:QD:59:ARG:HH12	4:QD:66:ARG:NH2	2.16	0.42
31:R7:12:ARG:HH21	31:R7:44:PRO:HB3	1.84	0.42
34:RA:589:C:H2'	34:RA:590:A:H8	1.84	0.42
34:RA:1518:C:H2'	34:RA:1519:G:C8	2.54	0.42
34:RA:2296:U:OP2	47:RS:9:ARG:NH1	2.52	0.42
36:RD:142:VAL:HG23	36:RD:193:VAL:HA	2.02	0.42
1:XA:411:A:OP1	4:XD:30:LYS:NZ	2.45	0.42
1:XA:693:G:N2	22:XV:37:1MG:HN21	2.17	0.42
2:XB:177:ALA:HB1	2:XB:182:ILE:HB	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:XC:119:ARG:HG2	3:XC:140:ARG:HH22	1.85	0.42
5:XE:99:GLY:N	5:XE:117:ASP:OD1	2.47	0.42
14:YN:53:LEU:HD12	14:YN:54:PRO:HD2	2.01	0.42
34:YA:848:G:H2'	34:YA:849:A:C8	2.55	0.42
34:YA:1858:G:O2'	34:YA:1884:A:N6	2.53	0.42
38:YF:114:VAL:HG11	38:YF:202:PHE:CZ	2.55	0.42
48:YT:6:LEU:HA	48:YT:9:LEU:HB2	2.02	0.42
1:QA:737:A:H2'	1:QA:738:C:C6	2.55	0.42
1:QA:1060:C:OP1	14:QN:45:ARG:NH2	2.41	0.42
7:QG:58:PRO:HA	7:QG:61:VAL:HG12	2.01	0.42
8:QH:21:LYS:HE2	8:QH:21:LYS:HB2	1.91	0.42
22:QV:56:C:N4	22:QV:57:G:O6	2.53	0.42
32:R8:39:LYS:NZ	34:RA:2351:G:O6	2.49	0.42
32:R8:61:LEU:HD12	32:R8:62:LEU:HG	2.02	0.42
34:RA:514:A:H2'	34:RA:515:A:C8	2.54	0.42
34:RA:2308:G:H1	34:RA:2311:A:H2	1.68	0.42
34:RA:2712(A):U:O2	34:RA:2712(A):U:H3'	2.19	0.42
36:RD:32:SER:C	36:RD:34:VAL:H	2.23	0.42
53:RY:92:ASN:OD1	53:RY:92:ASN:N	2.53	0.42
1:XA:178:C:H2'	1:XA:179:A:H8	1.84	0.42
1:XA:183:G:H2'	1:XA:184:G:H8	1.84	0.42
1:XA:454:C:H41	1:XA:479:C:H42	1.65	0.42
1:XA:1060:C:OP1	14:YN:45:ARG:NH2	2.53	0.42
9:XI:13:ALA:HB1	9:XI:73:GLN:HG3	2.01	0.42
12:XL:42:THR:HA	12:XL:53:ARG:O	2.19	0.42
21:XU:6:ARG:NH2	21:XU:15:ARG:HH22	2.16	0.42
30:Y6:40:CYS:HB3	30:Y6:43:CYS:CB	2.50	0.42
34:YA:2291:U:H2'	34:YA:2292:C:C6	2.55	0.42
36:YD:83:GLU:OE1	36:YD:104:TYR:OH	2.31	0.42
37:YE:102:VAL:HG23	37:YE:200:GLU:HA	2.02	0.42
44:YP:46:LYS:HB3	44:YP:46:LYS:HE3	1.78	0.42
45:YQ:110:THR:OG1	45:YQ:111:GLU:N	2.53	0.42
52:YX:25:LYS:HB3	52:YX:80:ILE:HD11	2.00	0.42
1:QA:324:G:OP1	20:QT:70:SER:OG	2.35	0.42
1:QA:570:G:O4'	1:QA:820:U:H6	2.02	0.42
1:QA:762:C:H2'	1:QA:763:G:C8	2.54	0.42
1:QA:1307:U:OP1	13:QM:101:GLN:NE2	2.53	0.42
1:QA:1386:G:H2'	1:QA:1387:G:H8	1.85	0.42
2:QB:34:ALA:H	2:QB:41:ILE:HB	1.84	0.42
20:QT:10:LEU:HD23	20:QT:10:LEU:HA	1.86	0.42
33:R9:29:ASN:HB3	33:R9:32:HIS:CD2	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:RA:30:G:H2'	34:RA:31:C:H6	1.85	0.42
34:RA:303:U:H2'	34:RA:304:G:C8	2.55	0.42
34:RA:587:C:C2	34:RA:671:C:O4'	2.73	0.42
34:RA:1779:U:OP2	34:RA:1784:A:N6	2.35	0.42
34:RA:2431:U:P	34:RA:2432:A:OP2	2.77	0.42
34:RA:2474:C:H5''	34:RA:2475:C:H5	1.84	0.42
34:RA:2646:C:OP2	34:RA:2732:G:O2'	2.25	0.42
38:RF:8:GLN:NE2	38:RF:19:GLU:OE1	2.51	0.42
38:RF:70:THR:HG23	38:RF:72:ARG:H	1.85	0.42
40:RH:126:PRO:HB2	40:RH:127:GLU:H	1.68	0.42
1:XA:156:G:H2'	1:XA:157:G:H8	1.85	0.42
1:XA:624:C:H2'	1:XA:625:G:C8	2.55	0.42
1:XA:1347:G:N2	1:XA:1374:A:OP2	2.34	0.42
7:XG:104:LEU:HD23	7:XG:104:LEU:HA	1.90	0.42
19:XS:30:LEU:HD13	19:XS:48:THR:HG23	2.01	0.42
21:XU:10:ARG:HA	21:XU:13:ILE:HG22	2.01	0.42
22:XV:9:G:O2'	22:XV:10:G:N7	2.53	0.42
34:YA:320:A:H2'	38:YF:136:THR:HG21	2.02	0.42
34:YA:513:A:O2'	34:YA:1217:C:OP1	2.38	0.42
34:YA:648:G:O2'	34:YA:2351:G:OP1	2.26	0.42
34:YA:654(C):C:H42	34:YA:654(U):C:N4	2.18	0.42
34:YA:2096:U:H3	34:YA:2193:G:H1	1.68	0.42
44:YP:15:ARG:HD3	44:YP:15:ARG:HA	1.85	0.42
45:YQ:34:LEU:HB2	45:YQ:118:LEU:HD22	2.01	0.42
1:QA:41:G:H2'	1:QA:42:G:H8	1.84	0.42
1:QA:56:U:H2'	1:QA:57:G:H8	1.85	0.42
1:QA:142:G:H2'	1:QA:143:A:C8	2.54	0.42
1:QA:404:U:O4	4:QD:2:GLY:N	2.53	0.42
1:QA:406:G:H21	4:QD:119:GLN:NE2	2.18	0.42
1:QA:714:G:H2'	1:QA:715:A:C8	2.55	0.42
1:QA:1232:U:H5''	9:QI:124:GLN:HG3	2.02	0.42
1:QA:1440(B):G:N2	1:QA:1461:G:O6	2.52	0.42
2:QB:231:GLU:HA	2:QB:232:PRO:HD3	1.87	0.42
12:QL:102:ARG:HB3	12:QL:109:GLY:HA2	2.01	0.42
13:QM:29:ARG:HD2	13:QM:29:ARG:HA	1.79	0.42
32:R8:49:VAL:HG23	32:R8:53:PRO:HD3	2.02	0.42
32:R8:64:TYR:HB3	34:RA:625:G:P	2.60	0.42
36:RD:76:PRO:HB3	36:RD:118:VAL:HG22	2.02	0.42
39:RG:34:LEU:HD21	39:RG:172:LEU:HD21	2.02	0.42
1:XA:310:G:OP2	16:XP:27:LYS:NZ	2.43	0.42
1:XA:335:C:O2'	1:XA:1433:A:N3	2.46	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:950:U:H3	1:XA:1231:G:H1	1.67	0.42
29:Y5:9:LYS:NZ	34:YA:2019:A:OP2	2.34	0.42
34:YA:442:G:N2	38:YF:48:THR:OG1	2.53	0.42
34:YA:822:U:H2'	34:YA:823:G:H8	1.85	0.42
34:YA:1024:G:OP2	34:YA:1025:G:C2'	2.68	0.42
34:YA:2105:C:H2'	34:YA:2106:G:H8	1.85	0.42
34:YA:2282:G:H5''	34:YA:2283:C:O4'	2.20	0.42
34:YA:2314:C:H5'	39:YG:38:VAL:HG21	2.01	0.42
37:YE:2:LYS:HD2	37:YE:95:ILE:HG22	2.02	0.42
37:YE:24:THR:HG22	37:YE:186:GLY:H	1.83	0.42
46:YR:87:TYR:OH	46:YR:117:VAL:O	2.31	0.42
47:YS:18:ILE:HG21	47:YS:88:ASP:HA	2.02	0.42
49:YU:94:ASN:HD22	49:YU:94:ASN:C	2.23	0.42
1:QA:376:G:H5''	16:QP:5:ARG:HB2	2.01	0.41
1:QA:815:A:O4'	1:QA:817:C:C4	2.72	0.41
3:QC:120:VAL:O	3:QC:124:ILE:HG12	2.20	0.41
7:QG:87:VAL:HG23	7:QG:151:TYR:HB3	2.02	0.41
34:RA:414:C:H2'	34:RA:415:A:C8	2.54	0.41
34:RA:2562:U:H4'	43:RO:25:LEU:HD21	2.02	0.41
34:RA:2576:G:P	34:RA:2576:G:N2	2.93	0.41
34:RA:2577:A:H5''	34:RA:2578:G:H5'	2.01	0.41
38:RF:178:PRO:HB3	38:RF:198:ALA:HB2	2.02	0.41
41:RI:84:GLY:N	41:RI:89:TYR:CE2	2.89	0.41
45:RQ:62:GLY:HA2	54:RZ:116:VAL:HG21	2.01	0.41
1:XA:22:G:H2'	1:XA:23:C:C6	2.55	0.41
1:XA:121:C:N4	1:XA:237:C:H41	2.18	0.41
1:XA:272:C:H2'	1:XA:273:A:C8	2.54	0.41
1:XA:475:G:H2'	1:XA:476:G:H8	1.84	0.41
1:XA:741:G:H3'	1:XA:742:G:H8	1.84	0.41
1:XA:1040:U:H2'	1:XA:1041:A:C8	2.55	0.41
2:XB:75:LYS:HA	2:XB:75:LYS:HD3	1.85	0.41
4:XD:105:VAL:HG21	4:XD:126:ILE:HD13	2.02	0.41
5:XE:128:PRO:HA	5:XE:131:ILE:HG12	2.02	0.41
6:XF:22:GLU:OE2	6:XF:84:ASN:ND2	2.40	0.41
34:YA:191:A:HO2'	34:YA:678:C:HO2'	1.67	0.41
34:YA:467:G:O2'	34:YA:796:C:O2'	2.27	0.41
34:YA:2086:U:H2'	34:YA:2087:G:C8	2.55	0.41
34:YA:2306:C:H3'	34:YA:2307:G:H5''	2.01	0.41
34:YA:2845:G:H2'	34:YA:2846:G:C8	2.54	0.41
36:YD:45:ASN:O	36:YD:47:GLY:N	2.52	0.41
42:YN:5:VAL:HA	42:YN:6:PRO:HD3	1.93	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:YP:47:ASP:OD2	44:YP:50:ARG:NH1	2.53	0.41
46:YR:104:ARG:HD2	46:YR:109:ALA:HB3	2.01	0.41
1:QA:60:A:N6	1:QA:110:C:H42	2.14	0.41
1:QA:1154:G:H2'	1:QA:1155:G:H8	1.85	0.41
1:QA:1355:G:H2'	1:QA:1356:G:C8	2.55	0.41
3:QC:73:PRO:HA	3:QC:76:VAL:HG22	2.01	0.41
7:QG:6:ARG:HA	7:QG:6:ARG:HD3	1.75	0.41
34:RA:87:C:H5''	34:RA:88:G:H5'	2.01	0.41
34:RA:997:G:H3'	49:RU:58:ARG:HH12	1.85	0.41
34:RA:1225:C:O2'	50:RV:86:GLY:N	2.36	0.41
34:RA:1600:C:OP1	52:RX:58:HIS:NE2	2.51	0.41
39:RG:39:ILE:HB	39:RG:92:VAL:HG13	2.02	0.41
44:RP:84:ASN:HA	44:RP:115:LEU:O	2.20	0.41
46:RR:13:HIS:O	46:RR:17:ARG:HB2	2.20	0.41
47:RS:50:SER:O	47:RS:76:LYS:NZ	2.41	0.41
1:XA:1028(C):C:H42	1:XA:1028(I):G:H1	1.68	0.41
1:XA:1318:A:H4'	19:XS:11:VAL:HG11	2.02	0.41
1:XA:1510:U:H2'	1:XA:1511:G:C8	2.55	0.41
5:XE:75:THR:HG22	5:XE:117:ASP:O	2.21	0.41
34:YA:639:U:H2'	34:YA:640:C:C6	2.54	0.41
34:YA:1028:A:OP2	34:YA:1126:A:N6	2.51	0.41
34:YA:2475:C:H42	34:YA:2529:G:N2	2.17	0.41
34:YA:2698:U:H2'	34:YA:2699:C:C6	2.54	0.41
36:YD:66:ASP:OD1	36:YD:103:ARG:NH1	2.53	0.41
37:YE:201:THR:OG1	37:YE:202:LYS:N	2.53	0.41
39:YG:39:ILE:HG12	39:YG:157:ILE:HD12	2.02	0.41
41:YI:50:ARG:HA	41:YI:50:ARG:HD3	1.80	0.41
43:YO:70:LYS:HE2	43:YO:70:LYS:HB3	1.81	0.41
54:YZ:185:GLU:O	54:YZ:186:GLU:C	2.58	0.41
1:QA:7:G:O2'	5:QE:120:THR:O	2.34	0.41
1:QA:37:U:O2'	1:QA:500:G:O2'	2.30	0.41
1:QA:370:C:H2'	1:QA:371:G:H8	1.84	0.41
1:QA:584:G:H1	1:QA:757:U:H3	1.69	0.41
1:QA:924:C:H2'	1:QA:925:G:C8	2.55	0.41
1:QA:958:A:N3	1:QA:985:C:O2'	2.42	0.41
1:QA:1151:A:H2'	1:QA:1152:A:C8	2.56	0.41
1:QA:1160:G:OP1	2:QB:132:LYS:NZ	2.48	0.41
1:QA:1308:U:OP1	13:QM:98:VAL:N	2.54	0.41
4:QD:109:GLY:HA3	4:QD:165:MET:HG2	2.02	0.41
28:R4:25:TYR:HE2	39:RG:3:LEU:HG	1.85	0.41
34:RA:674:G:H1'	38:RF:74:ARG:HD2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:RA:1999:C:OP1	34:RA:2723:C:O2'	2.37	0.41
34:RA:2145:C:H2'	34:RA:2147:G:C2	2.55	0.41
34:RA:2309:A:H2'	34:RA:2310:A:C4	2.56	0.41
45:RQ:116:GLU:O	45:RQ:120:ILE:HG12	2.20	0.41
49:RU:107:ALA:HA	49:RU:110:VAL:HG12	2.01	0.41
1:XA:493:G:N2	1:XA:494:U:O4	2.53	0.41
1:XA:676:A:H2'	1:XA:677:U:H6	1.84	0.41
1:XA:1141:C:H2'	1:XA:1142:G:H8	1.85	0.41
1:XA:1242:C:H2'	1:XA:1243:C:H6	1.85	0.41
1:XA:1287:A:H2	1:XA:1353:G:H1'	1.85	0.41
4:XD:101:LEU:HD22	4:XD:138:TYR:HB3	2.01	0.41
4:XD:161:ASN:O	4:XD:165:MET:HB2	2.21	0.41
6:XF:39:LYS:HB2	6:XF:64:GLN:HB3	2.01	0.41
33:Y9:7:VAL:O	34:YA:1031:G:O2'	2.25	0.41
34:YA:142:G:H2'	34:YA:143:C:C6	2.56	0.41
34:YA:1210:A:H5''	34:YA:1211:U:H3'	2.02	0.41
34:YA:1791:A:H3'	34:YA:1792:G:H8	1.85	0.41
44:YP:7:ARG:HA	44:YP:8:PRO:HD2	1.97	0.41
49:YU:50:ARG:O	49:YU:54:LYS:NZ	2.38	0.41
53:YY:102:CYS:SG	53:YY:103:GLY:N	2.94	0.41
1:QA:707:C:H2'	1:QA:708:C:C6	2.55	0.41
9:QL:77:ILE:O	9:QL:81:ILE:HG12	2.20	0.41
12:QL:104:VAL:O	12:QL:105:TYR:CE2	2.63	0.41
14:QN:6:LEU:HD23	14:QN:6:LEU:HA	1.84	0.41
21:QU:3:LYS:HD3	21:QU:14:TRP:CG	2.55	0.41
29:R5:3:LYS:HG2	34:RA:2611:U:C5	2.56	0.41
34:RA:1636:C:H2'	34:RA:1637:A:C8	2.55	0.41
34:RA:2174:C:H2'	34:RA:2175:C:C6	2.55	0.41
34:RA:2641:G:C6	34:RA:2774:C:N4	2.89	0.41
39:RG:63:ILE:HD13	39:RG:141:PHE:HB3	2.02	0.41
50:RV:32:THR:O	50:RV:32:THR:OG1	2.37	0.41
1:XA:22:G:O2'	1:XA:913:A:N1	2.46	0.41
1:XA:605:U:O5'	1:XA:605:U:C6	2.70	0.41
1:XA:999:U:H2'	1:XA:1000:A:C8	2.55	0.41
1:XA:1222:G:OP1	19:XS:78:ARG:NH1	2.53	0.41
2:XB:115:LEU:HB2	2:XB:145:LEU:HD23	2.02	0.41
3:XC:8:ILE:HD11	3:XC:184:TYR:H	1.84	0.41
14:XN:24:CYS:SG	14:XN:40:CYS:N	2.93	0.41
14:XN:47:LEU:HD23	14:XN:47:LEU:HA	1.86	0.41
24:Y0:72:ARG:HB3	24:Y0:75:LEU:HB2	2.02	0.41
34:YA:223:A:N6	34:YA:374:A:O2'	2.43	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:YA:685:A:C2	34:YA:787:U:H1'	2.55	0.41
34:YA:996:A:O3'	49:YU:92:ARG:NH2	2.53	0.41
34:YA:1252:G:H21	49:YU:33:ARG:HH11	1.68	0.41
37:YE:132:HIS:CD2	37:YE:132:HIS:O	2.73	0.41
1:QA:34:C:H2'	1:QA:35:G:H8	1.85	0.41
1:QA:186(J):U:H3	17:QQ:63:ARG:HG2	1.85	0.41
1:QA:696:A:H2'	1:QA:697:U:H6	1.86	0.41
1:QA:831:U:H2'	1:QA:832:C:H6	1.86	0.41
13:QM:37:THR:O	13:QM:55:ARG:NH2	2.53	0.41
27:R3:4:LEU:HD21	27:R3:56:VAL:HB	2.02	0.41
32:R8:12:LYS:NZ	34:RA:247:G:O6	2.38	0.41
34:RA:1234:U:H2'	34:RA:1235:G:C5'	2.48	0.41
34:RA:1716:U:O2	34:RA:1743:G:O6	2.38	0.41
34:RA:1841:U:H2'	34:RA:1842:G:H8	1.85	0.41
34:RA:2191:G:H2'	34:RA:2191:G:N3	2.35	0.41
41:RI:143:SER:HB2	41:RI:144:VAL:H	1.64	0.41
44:RP:41:ARG:HD3	44:RP:41:ARG:HA	1.82	0.41
44:RP:137:LYS:HA	44:RP:137:LYS:HD3	1.86	0.41
49:RU:27:LEU:O	49:RU:31:SER:HB3	2.20	0.41
53:RY:99:CYS:HB3	53:RY:102:CYS:H	1.85	0.41
54:RZ:24:LEU:HA	54:RZ:25:PRO:HD3	1.92	0.41
1:XA:718:G:OP2	1:XA:720:C:N4	2.52	0.41
1:XA:1236:A:H4'	1:XA:1304:G:H4'	2.02	0.41
1:XA:1237:C:H5''	1:XA:1238:A:C8	2.56	0.41
1:XA:1440(K):C:OP1	1:XA:1440(L):G:N1	2.54	0.41
11:XK:51:LYS:HE2	11:XK:51:LYS:HB2	1.93	0.41
14:XN:47:LEU:HD22	14:XN:52:GLN:HB2	2.02	0.41
23:XX:8:A:H2'	23:XX:9:G:C8	2.55	0.41
34:YA:1173:G:H4'	34:YA:1174:A:C8	2.55	0.41
40:YH:86:GLU:H	40:YH:86:GLU:HG2	1.51	0.41
54:YZ:6:LYS:O	54:YZ:62:PRO:HD3	2.20	0.41
1:QA:127:G:HO2'	17:QQ:2:PRO:N	2.17	0.41
1:QA:225:C:H2'	1:QA:226:G:H8	1.84	0.41
1:QA:377:G:H2'	1:QA:378:G:C8	2.55	0.41
1:QA:475:G:H2'	1:QA:476:G:C8	2.56	0.41
1:QA:1009:G:H2'	1:QA:1010:G:H8	1.86	0.41
3:QC:76:VAL:HG21	3:QC:103:VAL:HG11	2.03	0.41
8:QH:3:THR:OG1	8:QH:4:ASP:N	2.54	0.41
22:QV:3:G:O2'	34:RA:1851:U:OP1	2.38	0.41
29:R5:33:CYS:SG	29:R5:46:CYS:HB2	2.60	0.41
34:RA:1149:G:H2'	34:RA:1150:C:H6	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:RA:1664:A:H61	34:RA:1996:C:H42	1.65	0.41
34:RA:2183:C:H2'	34:RA:2184:G:H8	1.85	0.41
36:RD:268:ARG:HG3	36:RD:269:PHE:CD2	2.55	0.41
40:RH:91:GLY:HA2	40:RH:160:LYS:HG2	2.03	0.41
1:XA:501:C:H2'	1:XA:502:G:H8	1.86	0.41
1:XA:1160:G:O6	1:XA:1177:G:N2	2.53	0.41
13:XM:9:ILE:HA	13:XM:9:ILE:HD13	1.93	0.41
27:Y3:31:LEU:HD23	27:Y3:31:LEU:HA	1.87	0.41
34:YA:67:U:H3	34:YA:74:A:H2	1.69	0.41
34:YA:305:U:C4	34:YA:312:G:O6	2.73	0.41
34:YA:1889:A:N3	34:YA:2086:U:O2'	2.52	0.41
35:YB:30:C:H1'	35:YB:57:A:H61	1.85	0.41
1:QA:405:U:P	4:QD:118:ARG:HH12	2.43	0.41
1:QA:628:G:H2'	1:QA:629:G:C8	2.56	0.41
1:QA:1300:G:O2'	1:QA:1303:C:N4	2.47	0.41
2:QB:75:LYS:HA	2:QB:75:LYS:HD3	1.83	0.41
13:QM:77:ASN:O	13:QM:81:LEU:HG	2.21	0.41
34:RA:271(E):G:H2'	34:RA:272:G:C8	2.55	0.41
34:RA:642:G:H21	34:RA:646:A:H2	1.67	0.41
34:RA:1029:A:OP1	45:RQ:128:LYS:NZ	2.43	0.41
34:RA:1537:C:H2'	34:RA:1538:G:C8	2.56	0.41
34:RA:2751:G:N3	40:RH:3:ARG:CB	2.84	0.41
37:RE:134:ILE:HD12	37:RE:137:HIS:HB2	2.02	0.41
39:RG:141:PHE:HB2	39:RG:144:ILE:HD13	2.03	0.41
48:RT:66:VAL:HA	48:RT:71:GLY:HA2	2.02	0.41
49:RU:39:LEU:HD23	49:RU:39:LEU:HA	1.93	0.41
49:RU:58:ARG:HH11	49:RU:93:LYS:NZ	2.18	0.41
1:XA:359:U:H2'	1:XA:360:A:H8	1.84	0.41
1:XA:605:U:H6	1:XA:605:U:C5'	2.33	0.41
1:XA:1028(C):C:N4	1:XA:1028(I):G:H1	2.18	0.41
1:XA:1250:A:N3	1:XA:1370:G:O2'	2.46	0.41
29:Y5:11:THR:HG23	29:Y5:15:ARG:HD2	2.02	0.41
29:Y5:58:LEU:HD23	46:YR:113:LEU:HD11	2.03	0.41
34:YA:336:C:HO2'	53:YY:35:TYR:HH	1.68	0.41
34:YA:698:C:O2'	34:YA:734:A:N6	2.53	0.41
34:YA:945:A:H2'	34:YA:945:A:N3	2.36	0.41
34:YA:2867:G:O2'	34:YA:2868:A:H8	2.04	0.41
36:YD:44:ASN:OD1	36:YD:44:ASN:N	2.53	0.41
37:YE:104:VAL:HG11	37:YE:188:VAL:HG12	2.03	0.41
48:YT:3:ARG:O	48:YT:7:ILE:HG12	2.21	0.41
54:YZ:178:GLU:HB3	54:YZ:179:ASP:H	1.60	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:434:U:H2'	1:QA:435:C:C6	2.56	0.41
1:QA:1347:G:N2	1:QA:1374:A:OP2	2.39	0.41
2:QB:20:GLU:HG3	2:QB:191:ASP:HB2	2.02	0.41
2:QB:167:PRO:O	2:QB:171:ALA:CB	2.67	0.41
4:QD:122:ARG:HA	4:QD:122:ARG:HD2	1.90	0.41
34:RA:171:G:H2'	34:RA:172:C:C6	2.56	0.41
34:RA:690:G:H21	36:RD:43:ARG:NH2	2.18	0.41
34:RA:946:G:H2'	34:RA:947:G:H8	1.85	0.41
34:RA:1569:A:H2'	34:RA:1570:A:C8	2.56	0.41
42:RN:97:ARG:HA	42:RN:100:GLU:HB2	2.02	0.41
45:RQ:31:ASP:OD2	45:RQ:134:ARG:NH2	2.54	0.41
45:RQ:34:LEU:HD13	45:RQ:118:LEU:HD12	2.03	0.41
46:RR:96:ARG:HB2	46:RR:117:VAL:HG12	2.02	0.41
48:RT:8:LYS:HB2	48:RT:8:LYS:HE2	1.86	0.41
54:RZ:5:LEU:H	54:RZ:59:LEU:HA	1.85	0.41
1:XA:539:A:H2'	1:XA:540:G:H8	1.85	0.41
2:XB:40:HIS:HB2	2:XB:190:THR:HG21	2.01	0.41
5:XE:110:LEU:HB3	5:XE:115:VAL:HB	2.03	0.41
13:XM:87:TYR:OH	13:XM:91:ARG:NH1	2.53	0.41
15:XO:26:GLU:HG3	15:XO:81:LEU:HD22	2.03	0.41
34:YA:270(V):C:H2'	34:YA:270(W):G:H8	1.86	0.41
34:YA:922:U:H2'	34:YA:923:C:C6	2.56	0.41
34:YA:993:G:H4'	50:YV:70:ILE:HD11	2.02	0.41
34:YA:2475:C:N4	34:YA:2529:G:H22	2.17	0.41
34:YA:2810:A:H61	34:YA:2891:G:H2'	1.86	0.41
36:YD:231:HIS:CD2	36:YD:249:PRO:HG3	2.56	0.41
1:QA:110:C:O2'	16:QP:25:ARG:O	2.29	0.41
1:QA:186(B):C:OP1	20:QT:82:SER:OG	2.33	0.41
1:QA:186(F):C:H2'	1:QA:186(G):C:C6	2.56	0.41
1:QA:639:G:H2'	1:QA:640:A:C8	2.56	0.41
1:QA:757:U:OP1	1:QA:822:C:O2'	2.38	0.41
1:QA:936:C:H1'	1:QA:1382:C:H42	1.86	0.41
1:QA:1330:U:H4'	13:QM:23:TYR:CD2	2.56	0.41
3:QC:12:LEU:HG	3:QC:18:TRP:NE1	2.36	0.41
3:QC:36:ASP:OD1	3:QC:59:ARG:NH2	2.53	0.41
4:QD:8:VAL:HG13	4:QD:21:LEU:HD12	2.02	0.41
9:QI:25:LYS:O	9:QI:60:ASP:HA	2.21	0.41
22:QV:23:C:H2'	22:QV:24:G:H8	1.85	0.41
25:R1:8:SER:HB3	25:R1:66:HIS:CD2	2.55	0.41
25:R1:80:LEU:HD12	25:R1:81:LYS:HB2	2.03	0.41
26:R2:45:SER:OG	26:R2:46:GLN:N	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:R5:51:TYR:HD1	29:R5:55:ARG:O	2.03	0.41
34:RA:177:G:H5'	34:RA:178:G:C8	2.56	0.41
34:RA:270(F):G:H1	34:RA:270(V):C:H42	1.69	0.41
34:RA:747:U:O2	34:RA:2014:A:H1'	2.21	0.41
34:RA:851:U:H2'	34:RA:852:G:H8	1.86	0.41
34:RA:1400:G:H2'	34:RA:1401:G:C8	2.55	0.41
34:RA:2128:C:O2'	34:RA:2173:A:N3	2.43	0.41
34:RA:2581:G:C5	34:RA:2610:C:C4	3.09	0.41
34:RA:2684:U:O2'	43:RO:68:GLU:OE2	2.32	0.41
34:RA:2788:C:O2'	34:RA:2809:A:N3	2.53	0.41
35:RB:75:G:H21	54:RZ:85:HIS:HD1	1.68	0.41
36:RD:35:LYS:HB3	36:RD:63:ARG:HA	2.03	0.41
40:RH:123:PHE:HD2	40:RH:123:PHE:HA	1.77	0.41
41:RI:14:ASP:HB3	41:RI:15:VAL:H	1.65	0.41
49:RU:34:LYS:HD3	49:RU:34:LYS:HA	1.72	0.41
54:RZ:151:HIS:HB2	54:RZ:170:THR:HA	2.02	0.41
1:XA:396:G:O2'	1:XA:398:C:OP1	2.28	0.41
1:XA:445:G:H2'	1:XA:446:G:C8	2.55	0.41
1:XA:452:A:O2'	1:XA:453:A:O5'	2.36	0.41
1:XA:548:G:H5'	4:XD:73:ARG:NH2	2.36	0.41
1:XA:559:A:H4'	1:XA:560:U:H3'	2.03	0.41
1:XA:1055:A:O2'	3:XC:161:GLU:O	2.26	0.41
1:XA:1109:C:OP2	3:XC:176:HIS:ND1	2.54	0.41
1:XA:1324:A:H5''	1:XA:1362(B):C:H5'	2.02	0.41
1:XA:1366:C:O3'	10:XJ:60:ARG:NH2	2.53	0.41
3:XC:35:GLU:HB3	3:XC:59:ARG:HH22	1.85	0.41
6:XF:12:PRO:HD3	6:XF:58:GLY:HA2	2.02	0.41
9:XI:10:ARG:CZ	9:XI:105:ASP:HB2	2.51	0.41
13:XM:26:GLY:O	13:XM:30:ALA:HB2	2.20	0.41
20:XT:18:GLN:HE21	20:XT:22:ARG:NH2	2.19	0.41
24:Y0:23:VAL:HA	24:Y0:38:VAL:HG12	2.02	0.41
25:Y1:43:TYR:HD2	34:YA:2230:G:H5''	1.85	0.41
29:Y5:49:CYS:SG	29:Y5:50:GLY:N	2.93	0.41
30:Y6:46:HIS:ND1	34:YA:2371:G:O2'	2.42	0.41
34:YA:218:A:N1	34:YA:235:U:H4'	2.36	0.41
34:YA:270(Q):C:H1'	41:YI:50:ARG:HH22	1.86	0.41
34:YA:363(C):G:H2'	34:YA:363(D):G:C8	2.55	0.41
34:YA:589:C:H2'	34:YA:590:A:H8	1.85	0.41
34:YA:860:U:OP2	34:YA:916:G:N1	2.53	0.41
34:YA:870:A:OP1	45:YQ:6:ARG:NH2	2.37	0.41
34:YA:1196:C:O2'	34:YA:1228:G:O2'	2.24	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:YA:1853:A:N6	34:YA:1889:A:N7	2.68	0.41
34:YA:2103:C:H2'	34:YA:2104:G:H8	1.86	0.41
35:YB:48:A:H2'	35:YB:49:C:C6	2.56	0.41
38:YF:157:VAL:HG21	38:YF:181:LEU:HD13	2.03	0.41
41:YI:143:SER:HB2	41:YI:144:VAL:H	1.60	0.41
48:YT:19:LEU:HA	48:YT:20:PRO:HD3	1.91	0.41
52:YX:34:ALA:O	52:YX:77:LYS:NZ	2.54	0.41
1:QA:57:G:H2'	1:QA:58:C:C6	2.56	0.41
1:QA:318:G:H2'	1:QA:319:G:C8	2.56	0.41
1:QA:737:A:H2'	1:QA:738:C:H6	1.86	0.41
1:QA:838(A):G:H1	1:QA:848:C:H42	1.68	0.41
1:QA:999:U:O4	1:QA:1000:A:N6	2.54	0.41
4:QD:28:SER:HA	4:QD:29:PRO:HD3	1.96	0.41
29:R5:36:CYS:HG	29:R5:49:CYS:HB3	1.86	0.41
32:R8:35:GLN:NE2	32:R8:36:LYS:CE	2.80	0.41
34:RA:557:U:H2'	34:RA:558:G:H8	1.86	0.41
34:RA:1130:U:O2	37:RE:149:ARG:NH2	2.38	0.41
34:RA:1405:U:H2'	34:RA:1406:U:C6	2.56	0.41
34:RA:1669:A:N3	34:RA:1669:A:H2'	2.34	0.41
34:RA:1773:A:HO2'	34:RA:1978:A:H61	1.69	0.41
34:RA:1853:A:N6	34:RA:1889:A:N7	2.69	0.41
34:RA:2194:G:C2'	34:RA:2195:C:H5'	2.50	0.41
34:RA:2696:U:H2'	34:RA:2697:G:C8	2.56	0.41
39:RG:33:ARG:H	39:RG:162:THR:HG22	1.85	0.41
1:XA:23:C:OP2	1:XA:561:U:N3	2.40	0.41
1:XA:40:C:H2'	1:XA:41:G:C8	2.55	0.41
3:XC:91:LEU:HD22	3:XC:101:LEU:HD21	2.03	0.41
4:XD:170:VAL:HB	4:XD:174:LEU:HD12	2.02	0.41
12:XL:56:ALA:HB2	12:XL:70:ILE:HD11	2.03	0.41
34:YA:64:A:OP1	52:YX:73:ARG:NH1	2.54	0.41
34:YA:82:G:H5''	34:YA:296:C:H5'	2.03	0.41
34:YA:2513:G:O2'	37:YE:151:TYR:OH	2.20	0.41
38:YF:116:ASP:OD1	38:YF:119:ARG:NH2	2.52	0.41
44:YP:137:LYS:HA	44:YP:137:LYS:HD3	1.86	0.41
46:YR:56:LYS:NZ	46:YR:90:ARG:O	2.53	0.41
52:YX:92:LEU:HD23	52:YX:92:LEU:HA	1.86	0.41
53:YY:39:VAL:HG23	53:YY:42:VAL:HB	2.01	0.41
54:YZ:4:ARG:NH1	54:YZ:60:GLU:OE2	2.54	0.41
1:QA:836:G:H2'	1:QA:837:G:C8	2.56	0.40
1:QA:1525:G:H2'	1:QA:1526:G:H8	1.85	0.40
12:QL:32:PHE:HB3	12:QL:84:LEU:HD21	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:QN:12:ARG:HE	14:QN:14:PRO:HD2	1.86	0.40
17:QQ:75:ARG:HA	17:QQ:75:ARG:HD2	1.88	0.40
34:RA:270(A):A:OP2	34:RA:270(Z):G:N2	2.54	0.40
34:RA:1598:C:H5'	52:RX:36:LYS:HB2	2.02	0.40
34:RA:2688:U:OP1	34:RA:2713:A:N6	2.54	0.40
34:RA:2810:A:H61	34:RA:2891:G:H2'	1.87	0.40
35:RB:55:U:O2'	39:RG:27:ASN:ND2	2.51	0.40
39:RG:132:ASN:HD22	39:RG:158:ALA:HA	1.86	0.40
40:RH:103:LEU:HD11	40:RH:123:PHE:CE2	2.45	0.40
40:RH:126:PRO:HD2	40:RH:131:VAL:HA	2.03	0.40
47:RS:59:LYS:HA	47:RS:59:LYS:HD2	1.94	0.40
1:XA:939:G:H4'	7:XG:102:ARG:NH2	2.36	0.40
1:XA:1249:C:O2'	9:XI:73:GLN:NE2	2.51	0.40
1:XA:1309:G:O3'	13:XM:77:ASN:ND2	2.48	0.40
8:XH:10:LEU:HD12	8:XH:83:ILE:HD12	2.03	0.40
34:YA:394:A:H2'	34:YA:395:U:O4'	2.21	0.40
34:YA:423:A:H8	34:YA:423:A:O5'	2.03	0.40
34:YA:443:A:N7	38:YF:45:ARG:HD3	2.36	0.40
34:YA:974(A):G:C5	34:YA:1186:G:N2	2.89	0.40
34:YA:1307:A:N6	34:YA:1622:G:O6	2.54	0.40
34:YA:2578:G:OP1	34:YA:2614:A:N6	2.51	0.40
43:YO:71:ARG:HH21	43:YO:77:ILE:HG21	1.86	0.40
48:YT:130:ALA:HA	48:YT:133:GLU:HG2	2.04	0.40
54:YZ:24:LEU:HA	54:YZ:25:PRO:HD3	1.87	0.40
1:QA:819:A:C5	1:QA:1529:G:C6	3.10	0.40
1:QA:838(A):G:N2	1:QA:849:C:O2	2.54	0.40
1:QA:1096:C:H2'	1:QA:1097:C:C6	2.56	0.40
10:QJ:99:LYS:HA	10:QJ:99:LYS:HD3	1.79	0.40
22:QV:37:1MG:C2	22:QV:38:A:H1'	2.56	0.40
34:RA:925:C:H2'	34:RA:926:A:H8	1.86	0.40
34:RA:1798:U:O2'	34:RA:1802:A:N3	2.48	0.40
34:RA:2844:G:H3'	34:RA:2845:G:H8	1.87	0.40
34:RA:2853:C:H2'	34:RA:2854:G:C8	2.56	0.40
36:RD:105:ILE:HD12	36:RD:105:ILE:HA	1.91	0.40
36:RD:134:ARG:N	36:RD:187:GLY:O	2.54	0.40
40:RH:103:LEU:O	40:RH:114:VAL:HA	2.22	0.40
44:RP:28:GLY:C	44:RP:30:THR:H	2.24	0.40
50:RV:73:SER:OG	50:RV:74:LYS:N	2.53	0.40
1:XA:68(B):G:H2'	1:XA:68(C):G:H8	1.87	0.40
1:XA:1320:C:H2'	1:XA:1321:C:C6	2.57	0.40
8:XH:34:GLU:O	8:XH:38:ILE:HG12	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:YA:237:C:O2	34:YA:609(A):A:O2'	2.35	0.40
34:YA:270(S):G:H2'	34:YA:270(T):G:H8	1.86	0.40
34:YA:436:C:H2'	34:YA:438:G:C8	2.56	0.40
34:YA:918:A:N3	35:YB:80:U:O2'	2.53	0.40
34:YA:1009:A:OP2	34:YA:1010:A:OP2	2.40	0.40
34:YA:2052:G:O2'	37:YE:144:ARG:O	2.38	0.40
34:YA:2503:A:O2'	34:YA:2505:G:OP2	2.31	0.40
36:YD:172:TYR:HB3	36:YD:184:LYS:HG2	2.04	0.40
37:YE:154:LYS:HD2	37:YE:154:LYS:HA	1.87	0.40
40:YH:115:VAL:HG21	40:YH:148:ILE:HD11	2.02	0.40
41:YI:121:LYS:HD3	41:YI:121:LYS:HA	1.67	0.40
44:YP:6:LEU:HD23	44:YP:6:LEU:HA	1.90	0.40
53:YY:12:THR:HA	53:YY:26:LYS:HA	2.03	0.40
54:YZ:94:GLU:HA	54:YZ:95:PRO:HD2	1.75	0.40
1:QA:157:G:H2'	1:QA:158:G:C8	2.56	0.40
1:QA:1077:G:N2	1:QA:1079:G:H3'	2.36	0.40
1:QA:1142:G:H3'	1:QA:1143:G:H8	1.86	0.40
1:QA:1277:C:HO2'	1:QA:1279:A:H8	1.66	0.40
1:QA:1419:G:H1	1:QA:1481:U:H3	1.69	0.40
5:QE:11:ILE:HG21	5:QE:31:LEU:HD23	2.02	0.40
10:QJ:14:LYS:HD3	10:QJ:15:THR:HG23	2.02	0.40
16:QP:14:ASN:OD1	16:QP:16:HIS:NE2	2.54	0.40
32:R8:3:LYS:H	32:R8:3:LYS:HG2	1.71	0.40
34:RA:172:C:H2'	34:RA:173:G:H8	1.85	0.40
34:RA:949:C:H2'	34:RA:950:G:C8	2.56	0.40
34:RA:1053:C:H2'	34:RA:1054:A:C8	2.56	0.40
34:RA:1418:G:N1	34:RA:1579:A:OP2	2.42	0.40
34:RA:2304:G:O2'	39:RG:134:GLY:N	2.53	0.40
40:RH:102:ALA:HA	40:RH:117:PRO:HD3	2.03	0.40
45:RQ:30:GLY:HA2	45:RQ:107:ALA:HB2	2.03	0.40
49:RU:58:ARG:O	49:RU:62:ILE:HG12	2.20	0.40
1:XA:68(G):C:H2'	1:XA:68(H):G:C8	2.56	0.40
1:XA:165:C:H2'	1:XA:166:G:H8	1.86	0.40
1:XA:783:C:OP1	1:XA:1515:C:O2'	2.37	0.40
1:XA:1028(I):G:H2'	1:XA:1033:G:C8	2.56	0.40
1:XA:1321:C:H5''	1:XA:1322:C:H5''	2.02	0.40
2:XB:104:ASN:O	2:XB:108:ILE:HG12	2.21	0.40
2:XB:134:GLU:HG3	2:XB:137:ARG:NE	2.37	0.40
34:YA:2074:U:O2'	34:YA:2597:G:O2'	2.33	0.40
34:YA:2626:C:H2'	34:YA:2627:G:C8	2.57	0.40
34:YA:2737:G:H2'	34:YA:2738:A:C8	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YB:48:A:H4'	47:YS:95:HIS:HD2	1.85	0.40
50:YV:68:LYS:HD3	50:YV:68:LYS:HA	1.75	0.40
1:QA:45:U:H5''	1:QA:307:C:H1'	2.03	0.40
1:QA:429:U:H3'	4:QD:9:CYS:SG	2.62	0.40
1:QA:736:C:H2'	1:QA:737:A:H8	1.85	0.40
1:QA:1363:A:H4'	1:QA:1364:U:H5''	2.03	0.40
3:QC:56:ASP:HB3	3:QC:67:THR:HG23	2.02	0.40
10:QJ:84:GLN:O	10:QJ:88:LEU:HB2	2.22	0.40
34:RA:1364:G:N2	34:RA:1367:A:OP2	2.37	0.40
34:RA:1375:C:H2'	34:RA:1376:C:H6	1.87	0.40
34:RA:1388:G:O2'	34:RA:1525:G:O2'	2.27	0.40
34:RA:2364:C:H2'	34:RA:2365:G:O4'	2.21	0.40
46:RR:3:HIS:HB3	46:RR:4:LEU:H	1.64	0.40
1:XA:113:G:H2'	1:XA:114:U:C6	2.56	0.40
1:XA:677:U:O2	1:XA:777:A:O2'	2.37	0.40
1:XA:952:U:H2'	1:XA:953:G:H8	1.85	0.40
1:XA:1152:A:H5''	10:XJ:13:HIS:CD2	2.57	0.40
1:XA:1154:G:H2'	1:XA:1155:G:H8	1.87	0.40
1:XA:1262:C:H2'	1:XA:1263:C:C6	2.56	0.40
1:XA:1293:G:H2'	1:XA:1294:G:H8	1.87	0.40
2:XB:88:ALA:O	2:XB:226:ARG:NH1	2.46	0.40
2:XB:188:ALA:HB1	2:XB:192:SER:HB3	2.03	0.40
4:XD:202:LEU:HA	4:XD:205:GLU:HB2	2.03	0.40
8:XH:34:GLU:HB3	8:XH:118:VAL:HG11	2.03	0.40
12:XL:70:ILE:HG13	12:XL:100:ILE:HG13	2.03	0.40
34:YA:828:U:O2	34:YA:828:U:C2'	2.70	0.40
34:YA:2197:U:H1'	34:YA:2198:A:C8	2.56	0.40
36:YD:61:LEU:HD23	36:YD:61:LEU:HA	1.94	0.40
50:YV:69:LYS:HA	50:YV:87:HIS:O	2.21	0.40
54:YZ:14:LYS:HA	54:YZ:15:PRO:HD3	1.93	0.40
1:QA:299:G:H2'	1:QA:300:A:C8	2.57	0.40
1:QA:1306:A:N6	1:QA:1331:G:HO2'	2.20	0.40
1:QA:1385:G:H2'	1:QA:1386:G:C8	2.56	0.40
3:QC:44:GLU:HA	3:QC:52:LEU:HD21	2.03	0.40
4:QD:3:ARG:HE	4:QD:118:ARG:HD2	1.85	0.40
20:QT:74:LYS:O	20:QT:76:ALA:N	2.55	0.40
30:R6:29:ASN:HD22	34:RA:2286:A:P	2.44	0.40
34:RA:848:G:C2	34:RA:933:A:H1'	2.57	0.40
34:RA:1352:U:O2'	34:RA:1570:A:N3	2.52	0.40
34:RA:1358:G:H21	34:RA:1373:A:H62	1.69	0.40
34:RA:2150:U:H2'	34:RA:2151:G:C8	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:RA:2310:A:H61	39:RG:79:ASN:HD22	1.67	0.40
35:RB:111:U:H2'	35:RB:112:G:H8	1.85	0.40
38:RF:160:ASN:OD1	38:RF:160:ASN:N	2.54	0.40
41:RI:40:THR:OG1	41:RI:41:GLU:N	2.54	0.40
44:RP:64:LYS:O	44:RP:66:GLY:N	2.55	0.40
1:XA:21:G:H2'	1:XA:22:G:H8	1.87	0.40
1:XA:685:G:N2	1:XA:705:U:O4	2.55	0.40
1:XA:980:C:O3'	14:YN:9:LYS:NZ	2.43	0.40
1:XA:1021:G:H2'	1:XA:1022:G:C8	2.57	0.40
18:XR:30:ASP:OD2	18:XR:33:ASP:N	2.54	0.40
19:XS:66:MET:HE2	19:XS:66:MET:HB3	2.00	0.40
23:XX:3:C:H2'	23:XX:4:A:C8	2.56	0.40
34:YA:172:C:H2'	34:YA:173:G:H8	1.86	0.40
34:YA:570:G:H2'	34:YA:2030:A:C5	2.57	0.40
34:YA:1309:G:HO2'	34:YA:1611:C:HO2'	1.56	0.40
36:YD:175:LEU:O	36:YD:182:LEU:HA	2.22	0.40
42:YN:34:LEU:O	42:YN:49:GLY:HA3	2.21	0.40
48:YT:80:SER:HA	48:YT:81:PRO:HD3	1.96	0.40
49:YU:95:LEU:HG	50:YV:4:ILE:HD13	2.02	0.40
50:YV:100:ARG:HE	50:YV:100:ARG:HB2	1.70	0.40
54:YZ:5:LEU:HB3	54:YZ:6:LYS:H	1.72	0.40
54:YZ:128:VAL:HG22	54:YZ:161:VAL:HG22	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:RI:89:TYR:O	1:XA:357:G:O2'[4_555]	1.70	0.50

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%)	206 (88%)	27 (12%)	0	100	100
2	XB	234/256 (91%)	202 (86%)	31 (13%)	1 (0%)	30	64
3	QC	203/239 (85%)	180 (89%)	23 (11%)	0	100	100
3	XC	203/239 (85%)	182 (90%)	21 (10%)	0	100	100
4	QD	206/209 (99%)	195 (95%)	10 (5%)	1 (0%)	25	59
4	XD	206/209 (99%)	194 (94%)	11 (5%)	1 (0%)	25	59
5	QE	149/162 (92%)	134 (90%)	14 (9%)	1 (1%)	19	53
5	XE	149/162 (92%)	140 (94%)	8 (5%)	1 (1%)	19	53
6	QF	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
6	XF	99/101 (98%)	98 (99%)	1 (1%)	0	100	100
7	QG	153/156 (98%)	145 (95%)	8 (5%)	0	100	100
7	XG	153/156 (98%)	143 (94%)	10 (6%)	0	100	100
8	QH	135/138 (98%)	127 (94%)	8 (6%)	0	100	100
8	XH	135/138 (98%)	126 (93%)	9 (7%)	0	100	100
9	QI	125/128 (98%)	109 (87%)	16 (13%)	0	100	100
9	XI	124/128 (97%)	110 (89%)	13 (10%)	1 (1%)	16	51
10	QJ	97/105 (92%)	88 (91%)	8 (8%)	1 (1%)	13	46
10	XJ	94/105 (90%)	86 (92%)	8 (8%)	0	100	100
11	QK	117/129 (91%)	108 (92%)	9 (8%)	0	100	100
11	XK	114/129 (88%)	104 (91%)	10 (9%)	0	100	100
12	QL	123/132 (93%)	98 (80%)	24 (20%)	1 (1%)	16	51
12	XL	120/132 (91%)	99 (82%)	21 (18%)	0	100	100
13	QM	118/126 (94%)	99 (84%)	17 (14%)	2 (2%)	7	36
13	XM	112/126 (89%)	101 (90%)	10 (9%)	1 (1%)	14	49
14	QN	58/61 (95%)	50 (86%)	7 (12%)	1 (2%)	7	36
14	XN	58/61 (95%)	48 (83%)	8 (14%)	2 (3%)	3	24
15	QO	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
15	XO	85/89 (96%)	81 (95%)	4 (5%)	0	100	100
16	QP	82/88 (93%)	76 (93%)	6 (7%)	0	100	100
16	XP	82/88 (93%)	78 (95%)	4 (5%)	0	100	100
17	QQ	98/105 (93%)	92 (94%)	6 (6%)	0	100	100
17	XQ	98/105 (93%)	94 (96%)	4 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	66 (82%)	15 (18%)	0	100	100
19	XS	82/93 (88%)	65 (79%)	17 (21%)	0	100	100
20	QT	97/106 (92%)	86 (89%)	8 (8%)	3 (3%)	3	26
20	XT	97/106 (92%)	84 (87%)	10 (10%)	3 (3%)	3	26
21	QU	23/27 (85%)	21 (91%)	2 (9%)	0	100	100
21	XU	23/27 (85%)	19 (83%)	4 (17%)	0	100	100
24	R0	79/85 (93%)	71 (90%)	8 (10%)	0	100	100
24	Y0	80/85 (94%)	75 (94%)	5 (6%)	0	100	100
25	R1	93/98 (95%)	76 (82%)	17 (18%)	0	100	100
25	Y1	91/98 (93%)	78 (86%)	12 (13%)	1 (1%)	12	45
26	R2	67/72 (93%)	63 (94%)	4 (6%)	0	100	100
26	Y2	66/72 (92%)	64 (97%)	2 (3%)	0	100	100
27	R3	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
27	Y3	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
28	R4	43/71 (61%)	41 (95%)	2 (5%)	0	100	100
28	Y4	44/71 (62%)	28 (64%)	13 (30%)	3 (7%)	1	11
29	R5	57/60 (95%)	49 (86%)	7 (12%)	1 (2%)	7	35
29	Y5	57/60 (95%)	49 (86%)	7 (12%)	1 (2%)	7	35
30	R6	51/54 (94%)	46 (90%)	5 (10%)	0	100	100
30	Y6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
31	R7	45/49 (92%)	43 (96%)	2 (4%)	0	100	100
31	Y7	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
32	R8	62/65 (95%)	51 (82%)	9 (14%)	2 (3%)	3	25
32	Y8	62/65 (95%)	48 (77%)	14 (23%)	0	100	100
33	R9	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
33	Y9	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
36	RD	270/276 (98%)	244 (90%)	24 (9%)	2 (1%)	19	53
36	YD	270/276 (98%)	241 (89%)	28 (10%)	1 (0%)	30	64
37	RE	203/206 (98%)	159 (78%)	39 (19%)	5 (2%)	4	29

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	YE	203/206 (98%)	163 (80%)	38 (19%)	2 (1%)	13	46
38	RF	200/210 (95%)	183 (92%)	15 (8%)	2 (1%)	13	46
38	YF	200/210 (95%)	183 (92%)	16 (8%)	1 (0%)	25	59
39	RG	179/182 (98%)	150 (84%)	28 (16%)	1 (1%)	22	56
39	YG	179/182 (98%)	152 (85%)	27 (15%)	0	100	100
40	RH	172/180 (96%)	145 (84%)	24 (14%)	3 (2%)	7	36
40	YH	172/180 (96%)	147 (86%)	20 (12%)	5 (3%)	3	27
41	RI	144/148 (97%)	115 (80%)	23 (16%)	6 (4%)	2	19
41	YI	144/148 (97%)	118 (82%)	22 (15%)	4 (3%)	4	27
42	RN	136/140 (97%)	122 (90%)	13 (10%)	1 (1%)	19	53
42	YN	136/140 (97%)	123 (90%)	12 (9%)	1 (1%)	19	53
43	RO	120/122 (98%)	109 (91%)	11 (9%)	0	100	100
43	YO	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
44	RP	148/150 (99%)	114 (77%)	31 (21%)	3 (2%)	6	33
44	YP	145/150 (97%)	116 (80%)	28 (19%)	1 (1%)	19	53
45	RQ	139/141 (99%)	120 (86%)	18 (13%)	1 (1%)	19	53
45	YQ	139/141 (99%)	111 (80%)	27 (19%)	1 (1%)	19	53
46	RR	115/118 (98%)	103 (90%)	12 (10%)	0	100	100
46	YR	115/118 (98%)	104 (90%)	10 (9%)	1 (1%)	14	49
47	RS	109/112 (97%)	94 (86%)	15 (14%)	0	100	100
47	YS	109/112 (97%)	95 (87%)	13 (12%)	1 (1%)	14	49
48	RT	135/146 (92%)	116 (86%)	19 (14%)	0	100	100
48	YT	135/146 (92%)	121 (90%)	14 (10%)	0	100	100
49	RU	115/118 (98%)	106 (92%)	6 (5%)	3 (3%)	4	28
49	YU	115/118 (98%)	109 (95%)	6 (5%)	0	100	100
50	RV	99/101 (98%)	87 (88%)	11 (11%)	1 (1%)	13	46
50	YV	99/101 (98%)	90 (91%)	8 (8%)	1 (1%)	13	46
51	RW	111/113 (98%)	104 (94%)	7 (6%)	0	100	100
51	YW	111/113 (98%)	107 (96%)	4 (4%)	0	100	100
52	RX	90/96 (94%)	85 (94%)	5 (6%)	0	100	100
52	YX	90/96 (94%)	84 (93%)	6 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	RY	105/110 (96%)	102 (97%)	3 (3%)	0	100	100
53	YY	105/110 (96%)	99 (94%)	6 (6%)	0	100	100
54	RZ	181/206 (88%)	139 (77%)	38 (21%)	4 (2%)	5	31
54	YZ	191/206 (93%)	145 (76%)	39 (20%)	7 (4%)	2	22
All	All	11414/12128 (94%)	10111 (89%)	1217 (11%)	86 (1%)	16	51

All (86) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	QL	105	TYR
20	QT	75	ASN
32	R8	30	ARG
37	RE	147	PRO
40	RH	157	TYR
41	RI	11	ASN
44	RP	108	LYS
49	RU	91	ASP
49	RU	92	ARG
54	RZ	53	ILE
4	XD	156	GLU
20	XT	74	LYS
20	XT	75	ASN
28	Y4	5	ILE
28	Y4	24	THR
37	YE	147	PRO
40	YH	157	TYR
44	YP	108	LYS
50	YV	50	PRO
54	YZ	53	ILE
54	YZ	182	LYS
14	QN	17	LYS
32	R8	29	LYS
36	RD	243	GLY
39	RG	81	LYS
40	RH	126	PRO
41	RI	132	PRO
42	RN	22	THR
44	RP	22	GLY
49	RU	90	VAL
54	RZ	167	PRO
14	XN	57	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	YD	243	GLY
40	YH	47	GLU
41	YI	122	GLU
41	YI	132	PRO
47	YS	110	LEU
54	YZ	60	GLU
54	YZ	167	PRO
13	QM	118	ALA
20	QT	74	LYS
36	RD	242	ARG
37	RE	130	GLY
38	RF	67	GLN
38	RF	129	PHE
38	YF	129	PHE
46	YR	4	LEU
10	QJ	55	LYS
29	R5	49	CYS
37	RE	17	ASP
37	RE	83	ASP
41	RI	10	GLU
41	RI	122	GLU
44	RP	29	LYS
54	RZ	52	SER
54	RZ	63	ASP
13	XM	7	VAL
20	XT	73	HIS
28	Y4	40	HIS
29	Y5	49	CYS
40	YH	152	ARG
41	YI	15	VAL
54	YZ	183	LEU
20	QT	98	PRO
37	RE	82	ARG
40	RH	156	ALA
50	RV	53	GLU
5	XE	74	GLY
14	XN	56	VAL
40	YH	156	ALA
42	YN	22	THR
54	YZ	61	LEU
4	QD	156	GLU
13	QM	13	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	RI	15	VAL
9	XI	119	ALA
25	Y1	54	ALA
37	YE	54	GLN
45	YQ	7	MET
54	YZ	94	GLU
5	QE	74	GLY
2	XB	208	ILE
45	RQ	78	PRO
41	YI	133	HIS
41	RI	119	PRO
40	YH	12	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	QB	203/220 (92%)	200 (98%)	3 (2%)	60	77
2	XB	204/220 (93%)	203 (100%)	1 (0%)	86	93
3	QC	159/188 (85%)	157 (99%)	2 (1%)	65	81
3	XC	159/188 (85%)	157 (99%)	2 (1%)	65	81
4	QD	180/181 (99%)	179 (99%)	1 (1%)	84	91
4	XD	180/181 (99%)	178 (99%)	2 (1%)	70	83
5	QE	116/123 (94%)	116 (100%)	0	100	100
5	XE	116/123 (94%)	115 (99%)	1 (1%)	75	86
6	QF	90/90 (100%)	90 (100%)	0	100	100
6	XF	90/90 (100%)	89 (99%)	1 (1%)	70	83
7	QG	126/127 (99%)	126 (100%)	0	100	100
7	XG	126/127 (99%)	126 (100%)	0	100	100
8	QH	118/119 (99%)	117 (99%)	1 (1%)	79	88
8	XH	118/119 (99%)	118 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	QI	98/99 (99%)	96 (98%)	2 (2%)	50	72
9	XI	97/99 (98%)	95 (98%)	2 (2%)	48	71
10	QJ	89/92 (97%)	89 (100%)	0	100	100
10	XJ	86/92 (94%)	86 (100%)	0	100	100
11	QK	90/99 (91%)	89 (99%)	1 (1%)	70	83
11	XK	88/99 (89%)	87 (99%)	1 (1%)	70	83
12	QL	104/109 (95%)	104 (100%)	0	100	100
12	XL	103/109 (94%)	99 (96%)	4 (4%)	27	56
13	QM	96/101 (95%)	96 (100%)	0	100	100
13	XM	92/101 (91%)	92 (100%)	0	100	100
14	QN	49/50 (98%)	48 (98%)	1 (2%)	50	72
14	XN	49/50 (98%)	46 (94%)	3 (6%)	15	43
15	QO	79/80 (99%)	77 (98%)	2 (2%)	42	67
15	XO	79/80 (99%)	79 (100%)	0	100	100
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%)	95 (100%)	0	100	100
17	XQ	95/97 (98%)	93 (98%)	2 (2%)	48	71
18	QR	61/77 (79%)	61 (100%)	0	100	100
18	XR	61/77 (79%)	61 (100%)	0	100	100
19	QS	72/80 (90%)	72 (100%)	0	100	100
19	XS	73/80 (91%)	73 (100%)	0	100	100
20	QT	76/82 (93%)	75 (99%)	1 (1%)	65	81
20	XT	76/82 (93%)	76 (100%)	0	100	100
21	QU	20/22 (91%)	19 (95%)	1 (5%)	20	49
21	XU	20/22 (91%)	20 (100%)	0	100	100
24	R0	65/67 (97%)	64 (98%)	1 (2%)	60	77
24	Y0	65/67 (97%)	65 (100%)	0	100	100
25	R1	80/83 (96%)	78 (98%)	2 (2%)	42	67
25	Y1	78/83 (94%)	77 (99%)	1 (1%)	65	81
26	R2	64/67 (96%)	64 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	Y2	64/67 (96%)	63 (98%)	1 (2%)	58	76
27	R3	51/52 (98%)	51 (100%)	0	100	100
27	Y3	51/52 (98%)	51 (100%)	0	100	100
28	R4	40/63 (64%)	40 (100%)	0	100	100
28	Y4	41/63 (65%)	39 (95%)	2 (5%)	21	50
29	R5	51/52 (98%)	50 (98%)	1 (2%)	50	72
29	Y5	51/52 (98%)	47 (92%)	4 (8%)	10	34
30	R6	51/52 (98%)	48 (94%)	3 (6%)	16	44
30	Y6	51/52 (98%)	49 (96%)	2 (4%)	27	56
31	R7	40/42 (95%)	40 (100%)	0	100	100
31	Y7	41/42 (98%)	41 (100%)	0	100	100
32	R8	54/55 (98%)	54 (100%)	0	100	100
32	Y8	54/55 (98%)	54 (100%)	0	100	100
33	R9	34/34 (100%)	34 (100%)	0	100	100
33	Y9	34/34 (100%)	32 (94%)	2 (6%)	16	44
36	RD	214/218 (98%)	212 (99%)	2 (1%)	75	86
36	YD	214/218 (98%)	214 (100%)	0	100	100
37	RE	165/166 (99%)	161 (98%)	4 (2%)	44	68
37	YE	165/166 (99%)	162 (98%)	3 (2%)	54	74
38	RF	161/166 (97%)	158 (98%)	3 (2%)	52	73
38	YF	161/166 (97%)	161 (100%)	0	100	100
39	RG	155/156 (99%)	155 (100%)	0	100	100
39	YG	155/156 (99%)	154 (99%)	1 (1%)	84	91
40	RH	145/148 (98%)	137 (94%)	8 (6%)	18	46
40	YH	145/148 (98%)	142 (98%)	3 (2%)	48	71
41	RI	122/124 (98%)	122 (100%)	0	100	100
41	YI	122/124 (98%)	118 (97%)	4 (3%)	33	61
42	RN	117/119 (98%)	116 (99%)	1 (1%)	75	86
42	YN	117/119 (98%)	115 (98%)	2 (2%)	56	75
43	RO	100/100 (100%)	100 (100%)	0	100	100
43	YO	100/100 (100%)	97 (97%)	3 (3%)	36	63

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	RP	116/116 (100%)	115 (99%)	1 (1%)	75	86
44	YP	114/116 (98%)	114 (100%)	0	100	100
45	RQ	111/111 (100%)	111 (100%)	0	100	100
45	YQ	111/111 (100%)	110 (99%)	1 (1%)	75	86
46	RR	100/101 (99%)	98 (98%)	2 (2%)	50	72
46	YR	100/101 (99%)	99 (99%)	1 (1%)	73	84
47	RS	87/88 (99%)	87 (100%)	0	100	100
47	YS	87/88 (99%)	85 (98%)	2 (2%)	45	69
48	RT	120/127 (94%)	117 (98%)	3 (2%)	42	67
48	YT	120/127 (94%)	118 (98%)	2 (2%)	56	75
49	RU	93/94 (99%)	93 (100%)	0	100	100
49	YU	93/94 (99%)	91 (98%)	2 (2%)	47	70
50	RV	82/82 (100%)	82 (100%)	0	100	100
50	YV	82/82 (100%)	80 (98%)	2 (2%)	44	68
51	RW	92/92 (100%)	91 (99%)	1 (1%)	70	83
51	YW	92/92 (100%)	92 (100%)	0	100	100
52	RX	74/78 (95%)	71 (96%)	3 (4%)	26	55
52	YX	74/78 (95%)	72 (97%)	2 (3%)	40	65
53	RY	88/91 (97%)	88 (100%)	0	100	100
53	YY	88/91 (97%)	87 (99%)	1 (1%)	70	83
54	RZ	162/179 (90%)	162 (100%)	0	100	100
54	YZ	167/179 (93%)	165 (99%)	2 (1%)	67	82
All	All	9648/10066 (96%)	9536 (99%)	112 (1%)	67	82

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	QB	36	ARG
2	QB	149	LEU
2	QB	217	ARG
3	QC	38	ARG
3	QC	127	ARG
4	QD	18	LYS
8	QH	59	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	QI	64	THR
9	QI	85	LEU
11	QK	41	THR
14	QN	43	CYS
15	QO	22	THR
15	QO	87	ILE
20	QT	73	HIS
21	QU	6	ARG
24	R0	14	ARG
25	R1	73	LEU
25	R1	92	LYS
29	R5	36	CYS
30	R6	13	CYS
30	R6	23	THR
30	R6	53	LYS
36	RD	242	ARG
36	RD	268	ARG
37	RE	107	THR
37	RE	144	ARG
37	RE	154	LYS
37	RE	176	ILE
38	RF	89	VAL
38	RF	144	LYS
38	RF	195	ASP
40	RH	17	VAL
40	RH	69	ARG
40	RH	123	PHE
40	RH	125	VAL
40	RH	127	GLU
40	RH	129	THR
40	RH	130	ARG
40	RH	131	VAL
42	RN	34	LEU
44	RP	16	ARG
46	RR	10	LEU
46	RR	12	ARG
48	RT	85	LYS
48	RT	111	ARG
48	RT	129	ARG
51	RW	52	GLU
52	RX	16	LYS
52	RX	27	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
52	RX	76	ARG
2	XB	21	ARG
3	XC	12	LEU
3	XC	162	GLN
4	XD	135	LEU
4	XD	191	ARG
5	XE	12	LEU
6	XF	80	ARG
9	XI	25	LYS
9	XI	27	THR
11	XK	117	ASN
12	XL	8	ASN
12	XL	41	ARG
12	XL	89	ARG
12	XL	105	TYR
14	XN	12	ARG
14	XN	27	CYS
14	XN	56	VAL
17	XQ	50	LYS
17	XQ	74	LEU
25	Y1	50	ARG
26	Y2	47	ASN
28	Y4	5	ILE
28	Y4	16	CYS
29	Y5	37	LYS
29	Y5	40	LYS
29	Y5	45	VAL
29	Y5	49	CYS
30	Y6	13	CYS
30	Y6	43	CYS
33	Y9	13	LYS
33	Y9	27	CYS
37	YE	12	THR
37	YE	107	THR
37	YE	184	VAL
39	YG	118	ARG
40	YH	11	VAL
40	YH	67	LEU
40	YH	69	ARG
41	YI	56	LYS
41	YI	86	THR
41	YI	93	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	YI	118	LYS
42	YN	96	GLU
42	YN	115	ARG
43	YO	24	VAL
43	YO	34	THR
43	YO	49	ARG
45	YQ	133	ARG
46	YR	2	ARG
47	YS	4	LEU
47	YS	110	LEU
48	YT	105	LEU
48	YT	129	ARG
49	YU	92	ARG
49	YU	94	ASN
50	YV	46	VAL
50	YV	78	LYS
52	YX	49	VAL
52	YX	66	LEU
53	YY	79	CYS
54	YZ	63	ASP
54	YZ	165	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
7	QG	37	ASN
7	QG	64	GLN
24	R0	12	ASN
32	R8	35	GLN
36	RD	253	GLN
39	RG	79	ASN
46	RR	16	HIS
47	RS	38	GLN
50	RV	11	GLN
4	XD	119	GLN
11	XK	117	ASN
37	YE	132	HIS
39	YG	132	ASN
50	YV	11	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1509/1521 (99%)	309 (20%)	9 (0%)
1	XA	1514/1521 (99%)	322 (21%)	10 (0%)
22	QV	76/77 (98%)	17 (22%)	2 (2%)
22	XV	76/77 (98%)	21 (27%)	1 (1%)
23	QX	18/19 (94%)	4 (22%)	1 (5%)
23	XX	18/19 (94%)	5 (27%)	0
34	RA	2878/2915 (98%)	617 (21%)	40 (1%)
34	YA	2880/2915 (98%)	634 (22%)	44 (1%)
35	RB	119/122 (97%)	21 (17%)	1 (0%)
35	YB	119/122 (97%)	25 (21%)	1 (0%)
All	All	9207/9308 (98%)	1975 (21%)	109 (1%)

All (1975) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	9	G
1	QA	32	A
1	QA	38	G
1	QA	39	G
1	QA	48	C
1	QA	50	A
1	QA	51	A
1	QA	59	A
1	QA	64	G
1	QA	65	U
1	QA	66	G
1	QA	78	G
1	QA	79	G
1	QA	80	G
1	QA	82	U
1	QA	95	G
1	QA	101	A
1	QA	116	A
1	QA	121	C
1	QA	129(B)	G
1	QA	131	C
1	QA	134	A
1	QA	144	G
1	QA	151	A
1	QA	163	C
1	QA	169	C
1	QA	170	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	QA	182	U
1	QA	186(F)	C
1	QA	186(I)	U
1	QA	186(J)	U
1	QA	186(K)	G
1	QA	186(L)	G
1	QA	195	A
1	QA	197	A
1	QA	199	G
1	QA	201(C)	U
1	QA	201(D)	U
1	QA	216	G
1	QA	247	G
1	QA	251	G
1	QA	267	C
1	QA	274	A
1	QA	275	G
1	QA	279	A
1	QA	280	C
1	QA	281	G
1	QA	283	C
1	QA	289	G
1	QA	301	G
1	QA	306	G
1	QA	316	G
1	QA	321	A
1	QA	328	C
1	QA	329	A
1	QA	332	G
1	QA	344	A
1	QA	345	C
1	QA	347	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	384	G
1	QA	388	G
1	QA	389	A
1	QA	390	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	QA	392	G
1	QA	397	A
1	QA	398	C
1	QA	412	A
1	QA	413	G
1	QA	414	A
1	QA	422	C
1	QA	423	G
1	QA	424	G
1	QA	429	U
1	QA	440	A
1	QA	452	A
1	QA	453	A
1	QA	458(C)	A
1	QA	481	G
1	QA	484	G
1	QA	485	G
1	QA	486	U
1	QA	497	A
1	QA	498	U
1	QA	501	C
1	QA	505	G
1	QA	509	A
1	QA	510	A
1	QA	511	C
1	QA	514	C
1	QA	518	C
1	QA	521	G
1	QA	524	G
1	QA	527	G
1	QA	531	U
1	QA	532	A
1	QA	533	A
1	QA	536	C
1	QA	547	A
1	QA	559	A
1	QA	562	C
1	QA	568	G
1	QA	572	A
1	QA	573	A
1	QA	576	G
1	QA	577	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	QA	578	C
1	QA	590	C
1	QA	596	C
1	QA	607	A
1	QA	653	A
1	QA	687	A
1	QA	688	G
1	QA	695	A
1	QA	702	A
1	QA	717	C
1	QA	721	G
1	QA	723	U
1	QA	741	G
1	QA	749	C
1	QA	753	A
1	QA	755	G
1	QA	777	A
1	QA	793	U
1	QA	794	A
1	QA	811	C
1	QA	816	A
1	QA	817	C
1	QA	818	G
1	QA	819	A
1	QA	820	U
1	QA	821	G
1	QA	828	A
1	QA	838(B)	U
1	QA	838(C)	C
1	QA	838(D)	U
1	QA	848	C
1	QA	859	A
1	QA	867	G
1	QA	870	U
1	QA	872	A
1	QA	873	A
1	QA	876	G
1	QA	889	A
1	QA	914	A
1	QA	923	A
1	QA	926	G
1	QA	927	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	QA	934	C
1	QA	935	A
1	QA	960	U
1	QA	961	U
1	QA	966	G
1	QA	967	C
1	QA	969	A
1	QA	971	G
1	QA	974	A
1	QA	975	A
1	QA	976	G
1	QA	977	A
1	QA	981	U
1	QA	992	U
1	QA	993	G
1	QA	994	A
1	QA	1002	G
1	QA	1004	A
1	QA	1006	C
1	QA	1015	A
1	QA	1024	G
1	QA	1025	U
1	QA	1026	G
1	QA	1028(D)	G
1	QA	1037	C
1	QA	1039	C
1	QA	1046	A
1	QA	1053	G
1	QA	1054	C
1	QA	1055	A
1	QA	1060	C
1	QA	1064	G
1	QA	1065	U
1	QA	1066	C
1	QA	1081	G
1	QA	1094	G
1	QA	1095	U
1	QA	1101	A
1	QA	1108	G
1	QA	1117	G
1	QA	1118	C
1	QA	1124	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	QA	1125	U
1	QA	1126	U
1	QA	1130	A
1	QA	1131	G
1	QA	1135	U
1	QA	1137	C
1	QA	1138	G
1	QA	1139	G
1	QA	1145	C
1	QA	1146	A
1	QA	1147	C
1	QA	1157	A
1	QA	1158	C
1	QA	1159	U
1	QA	1160	G
1	QA	1178	G
1	QA	1181	G
1	QA	1182	G
1	QA	1183	A
1	QA	1186	G
1	QA	1190	G
1	QA	1196	U
1	QA	1197	G
1	QA	1200	C
1	QA	1201	A
1	QA	1202	G
1	QA	1212	U
1	QA	1213	A
1	QA	1221	G
1	QA	1222	G
1	QA	1224	G
1	QA	1225	A
1	QA	1226	C
1	QA	1227	A
1	QA	1228	C
1	QA	1240	U
1	QA	1241	G
1	QA	1248	A
1	QA	1256	A
1	QA	1257	U
1	QA	1258	G
1	QA	1274	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	QA	1280	A
1	QA	1281	U
1	QA	1282	C
1	QA	1285	A
1	QA	1286	A
1	QA	1287	A
1	QA	1290	G
1	QA	1297	C
1	QA	1299	A
1	QA	1300	G
1	QA	1303	C
1	QA	1305	G
1	QA	1319	A
1	QA	1321	C
1	QA	1322	C
1	QA	1323	G
1	QA	1325	C
1	QA	1327	C
1	QA	1328	C
1	QA	1329	A
1	QA	1330	U
1	QA	1331	G
1	QA	1335	C
1	QA	1336	C
1	QA	1340	A
1	QA	1346	A
1	QA	1347	G
1	QA	1359	C
1	QA	1362(B)	C
1	QA	1363	A
1	QA	1364	U
1	QA	1365	G
1	QA	1370	G
1	QA	1378	C
1	QA	1381	U
1	QA	1382	C
1	QA	1394	A
1	QA	1397	C
1	QA	1398	A
1	QA	1413	A
1	QA	1419	G
1	QA	1422	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	QA	1440(C)	G
1	QA	1440(D)	G
1	QA	1440(E)	A
1	QA	1440(K)	C
1	QA	1440(L)	G
1	QA	1475	G
1	QA	1492	A
1	QA	1493	A
1	QA	1494	G
1	QA	1497	G
1	QA	1499	A
1	QA	1502	A
1	QA	1503	A
1	QA	1504	G
1	QA	1505	G
1	QA	1506	U
1	QA	1507	A
1	QA	1508	G
1	QA	1517	G
1	QA	1520	G
1	QA	1528	U
1	QA	1529	G
1	QA	1530	G
1	QA	1533	C
1	QA	1534	A
1	QA	1535	C
1	QA	1538	C
1	QA	1539	C
1	QA	1541	U
22	QV	8	U
22	QV	10	G
22	QV	11	C
22	QV	15	G
22	QV	17	C
22	QV	18	U
22	QV	19	G
22	QV	21(B)	A
22	QV	31	G
22	QV	34	C
22	QV	36	G
22	QV	47	U
22	QV	48	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	QV	59	A
22	QV	61	C
22	QV	67	U
22	QV	73	A
23	QX	10	G
23	QX	12	A
23	QX	13	A
23	QX	18	C
34	RA	10	G
34	RA	15	G
34	RA	27	G
34	RA	34	C
34	RA	35	G
34	RA	36	G
34	RA	46	C
34	RA	51	G
34	RA	55	G
34	RA	61	G
34	RA	73	A
34	RA	74	A
34	RA	75	G
34	RA	90	U
34	RA	101	G
34	RA	102	G
34	RA	103	A
34	RA	118	A
34	RA	119	A
34	RA	120	U
34	RA	125	G
34	RA	131	G
34	RA	140	A
34	RA	161	U
34	RA	177	G
34	RA	181	A
34	RA	196	A
34	RA	199	A
34	RA	201	C
34	RA	204	A
34	RA	216	A
34	RA	221	A
34	RA	222	A
34	RA	223	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	RA	229	A
34	RA	230	U
34	RA	232	G
34	RA	233	A
34	RA	241	A
34	RA	242	G
34	RA	243	U
34	RA	248	G
34	RA	249	C
34	RA	252	G
34	RA	265	A
34	RA	266	G
34	RA	267	C
34	RA	270(M)	U
34	RA	270(N)	U
34	RA	270(O)	G
34	RA	270(Q)	C
34	RA	270(Z)	G
34	RA	271(D)	U
34	RA	275	G
34	RA	276	A
34	RA	277	C
34	RA	278	A
34	RA	299	A
34	RA	311	A
34	RA	323	G
34	RA	324	A
34	RA	329	G
34	RA	330	A
34	RA	332	A
34	RA	342	G
34	RA	346	A
34	RA	352	G
34	RA	362	U
34	RA	364	C
34	RA	371	A
34	RA	372	G
34	RA	386	G
34	RA	387	U
34	RA	404	C
34	RA	405	U
34	RA	411	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	RA	412	A
34	RA	423	A
34	RA	428	A
34	RA	435	C
34	RA	444	C
34	RA	448	U
34	RA	453	C
34	RA	454	A
34	RA	456	C
34	RA	457	A
34	RA	458	G
34	RA	467	G
34	RA	470	A
34	RA	481	G
34	RA	494	G
34	RA	501	A
34	RA	504	U
34	RA	505	A
34	RA	508	G
34	RA	509	C
34	RA	510	C
34	RA	512	G
34	RA	513	A
34	RA	529	A
34	RA	531	C
34	RA	532	A
34	RA	533	G
34	RA	537	C
34	RA	539	G
34	RA	540	G
34	RA	546	C
34	RA	547	A
34	RA	556	G
34	RA	563	G
34	RA	568	U
34	RA	573	G
34	RA	575	A
34	RA	603	A
34	RA	604	G
34	RA	607	U
34	RA	614	U
34	RA	615	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	RA	616	A
34	RA	617	G
34	RA	618(A)	G
34	RA	621	A
34	RA	622	G
34	RA	626	U
34	RA	627	A
34	RA	631	A
34	RA	634	C
34	RA	637	A
34	RA	638	G
34	RA	645	C
34	RA	646	A
34	RA	651	G
34	RA	652	C
34	RA	654(A)	A
34	RA	654(B)	G
34	RA	657	U
34	RA	668	G
34	RA	669	G
34	RA	670	A
34	RA	686	G
34	RA	702	G
34	RA	717	G
34	RA	722	A
34	RA	726	G
34	RA	730	C
34	RA	747	U
34	RA	748	G
34	RA	753	C
34	RA	762	U
34	RA	764	A
34	RA	765	G
34	RA	776	G
34	RA	782	A
34	RA	784	A
34	RA	785	G
34	RA	790	C
34	RA	792	G
34	RA	800	A
34	RA	805	G
34	RA	810	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	RA	812	C
34	RA	819	A
34	RA	826	U
34	RA	827	U
34	RA	828	U
34	RA	830	G
34	RA	845	G
34	RA	847	U
34	RA	856	C
34	RA	857	C
34	RA	859	G
34	RA	860	U
34	RA	877	U
34	RA	887	A
34	RA	889	C
34	RA	890	A
34	RA	896	A
34	RA	907	U
34	RA	910	A
34	RA	914	C
34	RA	915	C
34	RA	917	A
34	RA	918	A
34	RA	932	G
34	RA	941	A
34	RA	945	A
34	RA	946	G
34	RA	959	A
34	RA	961	C
34	RA	973	A
34	RA	974(A)	G
34	RA	974(B)	C
34	RA	975	G
34	RA	981	A
34	RA	983	A
34	RA	996	A
34	RA	1003	G
34	RA	1005	C
34	RA	1008	C
34	RA	1011	G
34	RA	1012	U
34	RA	1013	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	RA	1015	G
34	RA	1020	A
34	RA	1022	G
34	RA	1023	U
34	RA	1024	G
34	RA	1025	G
34	RA	1026	U
34	RA	1027	A
34	RA	1033	U
34	RA	1044	G
34	RA	1045	A
34	RA	1046	A
34	RA	1050	A
34	RA	1052	C
34	RA	1062	G
34	RA	1065	U
34	RA	1067	A
34	RA	1070	A
34	RA	1071	G
34	RA	1072	C
34	RA	1073	A
34	RA	1075	C
34	RA	1076	C
34	RA	1082	U
34	RA	1083	U
34	RA	1087	G
34	RA	1088	A
34	RA	1090	U
34	RA	1091	G
34	RA	1097	U
34	RA	1102	C
34	RA	1103	A
34	RA	1104	C
34	RA	1110	G
34	RA	1112	G
34	RA	1126	A
34	RA	1129	A
34	RA	1130	U
34	RA	1131	G
34	RA	1135	C
34	RA	1136	G
34	RA	1139	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	RA	1141	U
34	RA	1142(A)	U
34	RA	1142(B)	A
34	RA	1155	A
34	RA	1170	G
34	RA	1173	G
34	RA	1174	A
34	RA	1175	U
34	RA	1176	G
34	RA	1179	C
34	RA	1181	C
34	RA	1195	G
34	RA	1204	A
34	RA	1205	U
34	RA	1206	G
34	RA	1210	A
34	RA	1212	G
34	RA	1220	A
34	RA	1238	G
34	RA	1248	G
34	RA	1250	G
34	RA	1252	G
34	RA	1253	A
34	RA	1256	G
34	RA	1265	A
34	RA	1272	A
34	RA	1273	U
34	RA	1286	A
34	RA	1300	U
34	RA	1301	A
34	RA	1308	A
34	RA	1313	U
34	RA	1314	C
34	RA	1325	G
34	RA	1329	U
34	RA	1341	U
34	RA	1349	A
34	RA	1352	U
34	RA	1365	A
34	RA	1368	G
34	RA	1370	C
34	RA	1378	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	RA	1379	A
34	RA	1384	A
34	RA	1385	G
34	RA	1395	A
34	RA	1407	C
34	RA	1411	C
34	RA	1416	G
34	RA	1419	A
34	RA	1420	U
34	RA	1421	G
34	RA	1427	A
34	RA	1428	C
34	RA	1444(B)	A
34	RA	1449(A)	A
34	RA	1449(B)	G
34	RA	1455	G
34	RA	1461	G
34	RA	1467	C
34	RA	1471	A
34	RA	1474	C
34	RA	1480	G
34	RA	1482	U
34	RA	1483	G
34	RA	1485	G
34	RA	1493	C
34	RA	1494	A
34	RA	1495	A
34	RA	1496	A
34	RA	1497	U
34	RA	1504	C
34	RA	1506	C
34	RA	1507	A
34	RA	1508	A
34	RA	1510	A
34	RA	1533	C
34	RA	1534	G
34	RA	1535	U
34	RA	1536	A
34	RA	1537	C
34	RA	1538	G
34	RA	1543	A
34	RA	1544	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	RA	1545(A)	A
34	RA	1547	C
34	RA	1558	A
34	RA	1559	G
34	RA	1566	A
34	RA	1569	A
34	RA	1578	U
34	RA	1579	A
34	RA	1586	A
34	RA	1598	C
34	RA	1602	U
34	RA	1603	A
34	RA	1607	C
34	RA	1608	A
34	RA	1609	A
34	RA	1610	A
34	RA	1617	C
34	RA	1618	A
34	RA	1622	G
34	RA	1634	A
34	RA	1640	C
34	RA	1646	C
34	RA	1648	C
34	RA	1653	G
34	RA	1654	A
34	RA	1667	G
34	RA	1668	A
34	RA	1672	C
34	RA	1674	G
34	RA	1688	U
34	RA	1695	G
34	RA	1698	A
34	RA	1725	G
34	RA	1729	A
34	RA	1731	G
34	RA	1742	C
34	RA	1743	G
34	RA	1756	G
34	RA	1762	A
34	RA	1763	G
34	RA	1764	G
34	RA	1773	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	RA	1780	A
34	RA	1781	C
34	RA	1784	A
34	RA	1791	A
34	RA	1799	G
34	RA	1800	C
34	RA	1801	G
34	RA	1811	G
34	RA	1816	G
34	RA	1820	U
34	RA	1829	A
34	RA	1835	G
34	RA	1847	A
34	RA	1848	A
34	RA	1858	G
34	RA	1869	G
34	RA	1870	C
34	RA	1872	A
34	RA	1878	G
34	RA	1882	C
34	RA	1888	G
34	RA	1889	A
34	RA	1896	G
34	RA	1905	C
34	RA	1906	G
34	RA	1919	A
34	RA	1930	G
34	RA	1931	U
34	RA	1936	A
34	RA	1937	A
34	RA	1938	A
34	RA	1939	U
34	RA	1955	U
34	RA	1963	U
34	RA	1965	C
34	RA	1966	A
34	RA	1967	C
34	RA	1969	A
34	RA	1970	A
34	RA	1971	A
34	RA	1972	A
34	RA	1981	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	RA	1982	C
34	RA	1991	U
34	RA	1992	G
34	RA	1993	U
34	RA	1994	C
34	RA	2021	C
34	RA	2023	G
34	RA	2030	A
34	RA	2031	A
34	RA	2032	G
34	RA	2033	A
34	RA	2043	C
34	RA	2055	C
34	RA	2056	G
34	RA	2059	A
34	RA	2060	A
34	RA	2061	G
34	RA	2062	A
34	RA	2069	G
34	RA	2077	A
34	RA	2080	G
34	RA	2089	U
34	RA	2092	U
34	RA	2093	G
34	RA	2094	G
34	RA	2095	C
34	RA	2096	U
34	RA	2097	C
34	RA	2099	U
34	RA	2100	G
34	RA	2111	C
34	RA	2113	U
34	RA	2114	A
34	RA	2115	G
34	RA	2116	G
34	RA	2118	U
34	RA	2119	A
34	RA	2120	G
34	RA	2126	A
34	RA	2127	G
34	RA	2128	C
34	RA	2131	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	RA	2132	U
34	RA	2133	G
34	RA	2137	C
34	RA	2145	C
34	RA	2146	C
34	RA	2147	G
34	RA	2148	G
34	RA	2158	A
34	RA	2164	C
34	RA	2166	G
34	RA	2167	U
34	RA	2169	A
34	RA	2172	U
34	RA	2173	A
34	RA	2176	A
34	RA	2190	G
34	RA	2191	G
34	RA	2194	G
34	RA	2195	C
34	RA	2198	A
34	RA	2210	G
34	RA	2211	G
34	RA	2212	A
34	RA	2215	G
34	RA	2225	A
34	RA	2238	G
34	RA	2239	G
34	RA	2243	U
34	RA	2245	U
34	RA	2266	A
34	RA	2275	C
34	RA	2280	G
34	RA	2283	C
34	RA	2287	A
34	RA	2288	A
34	RA	2297	C
34	RA	2304	G
34	RA	2305	A
34	RA	2307	G
34	RA	2308	G
34	RA	2310	A
34	RA	2311	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	RA	2319	G
34	RA	2320	A
34	RA	2322	A
34	RA	2325	G
34	RA	2334	G
34	RA	2335	A
34	RA	2342	C
34	RA	2345	G
34	RA	2346	A
34	RA	2347	C
34	RA	2350	C
34	RA	2372	G
34	RA	2383	G
34	RA	2385	C
34	RA	2388	A
34	RA	2391	G
34	RA	2392	A
34	RA	2394	C
34	RA	2402	C
34	RA	2403	C
34	RA	2406	U
34	RA	2410	G
34	RA	2423	U
34	RA	2425	A
34	RA	2428	G
34	RA	2429	G
34	RA	2430	A
34	RA	2431	U
34	RA	2435	A
34	RA	2439	A
34	RA	2440	C
34	RA	2441	C
34	RA	2448	A
34	RA	2460	U
34	RA	2469	A
34	RA	2470	G
34	RA	2478	A
34	RA	2482	G
34	RA	2494	G
34	RA	2502	G
34	RA	2503	A
34	RA	2504	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	RA	2505	G
34	RA	2506	U
34	RA	2518	A
34	RA	2520	C
34	RA	2542	A
34	RA	2543	G
34	RA	2553	G
34	RA	2554	U
34	RA	2562	U
34	RA	2567	G
34	RA	2569	G
34	RA	2572	A
34	RA	2577	A
34	RA	2580	U
34	RA	2602	A
34	RA	2609	U
34	RA	2610	C
34	RA	2611	U
34	RA	2612	C
34	RA	2614	A
34	RA	2629	A
34	RA	2646	C
34	RA	2654	A
34	RA	2655	G
34	RA	2665	A
34	RA	2673	G
34	RA	2686	G
34	RA	2689	U
34	RA	2690	C
34	RA	2691	C
34	RA	2702	U
34	RA	2707	G
34	RA	2711	A
34	RA	2712(A)	U
34	RA	2712(B)	A
34	RA	2713	A
34	RA	2714	G
34	RA	2726	U
34	RA	2733	A
34	RA	2739	U
34	RA	2744	G
34	RA	2748	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	RA	2750	A
34	RA	2757	A
34	RA	2761	G
34	RA	2764	A
34	RA	2765	A
34	RA	2766	G
34	RA	2777	G
34	RA	2778	A
34	RA	2779	U
34	RA	2780	G
34	RA	2789	C
34	RA	2790	A
34	RA	2791	C
34	RA	2792	G
34	RA	2793	G
34	RA	2794	C
34	RA	2797	U
34	RA	2798	C
34	RA	2807	G
34	RA	2808	U
34	RA	2818	G
34	RA	2820	A
34	RA	2821	A
34	RA	2822	G
34	RA	2825	C
34	RA	2830	G
34	RA	2833	G
34	RA	2834	G
34	RA	2849	U
34	RA	2867	G
34	RA	2872	G
34	RA	2880	C
34	RA	2883	A
34	RA	2885	C
34	RA	2892	A
34	RA	2894	G
34	RA	2895	U
35	RB	8	U
35	RB	9	G
35	RB	12	C
35	RB	13	A
35	RB	14	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	RB	15	A
35	RB	22	U
35	RB	25	A
35	RB	32	C
35	RB	41	U
35	RB	42	C
35	RB	44	G
35	RB	45	A
35	RB	53	A
35	RB	56	G
35	RB	67	G
35	RB	73	A
35	RB	77	U
35	RB	81	G
35	RB	96	G
35	RB	109	G
1	XA	6	G
1	XA	9	G
1	XA	31	G
1	XA	32	A
1	XA	39	G
1	XA	47	C
1	XA	48	C
1	XA	51	A
1	XA	54	C
1	XA	65	U
1	XA	66	G
1	XA	68(E)	C
1	XA	68(F)	G
1	XA	68(I)	G
1	XA	68(K)	G
1	XA	68(M)	U
1	XA	68(N)	U
1	XA	68(P)	A
1	XA	68(Q)	C
1	XA	68(R)	U
1	XA	68(S)	C
1	XA	68(W)	G
1	XA	101	A
1	XA	108	G
1	XA	109	A
1	XA	116	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	XA	117	G
1	XA	121	C
1	XA	131	C
1	XA	134	A
1	XA	142	G
1	XA	144	G
1	XA	151	A
1	XA	160	A
1	XA	163	C
1	XA	169	C
1	XA	173	U
1	XA	182	U
1	XA	183	G
1	XA	186(J)	U
1	XA	186(K)	G
1	XA	186(L)	G
1	XA	186(N)	G
1	XA	194	C
1	XA	195	A
1	XA	197	A
1	XA	201(B)	U
1	XA	201(C)	U
1	XA	201(D)	U
1	XA	216	G
1	XA	247	G
1	XA	251	G
1	XA	254	G
1	XA	262	A
1	XA	266	G
1	XA	267	C
1	XA	281	G
1	XA	289	G
1	XA	306	G
1	XA	315	A
1	XA	328	C
1	XA	329	A
1	XA	330	C
1	XA	332	G
1	XA	344	A
1	XA	345	C
1	XA	346	G
1	XA	347	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	XA	348	G
1	XA	352	C
1	XA	353	A
1	XA	354	G
1	XA	356	A
1	XA	366	C
1	XA	368	U
1	XA	372	C
1	XA	373	A
1	XA	384	G
1	XA	388	G
1	XA	389	A
1	XA	392	G
1	XA	397	A
1	XA	398	C
1	XA	406	G
1	XA	412	A
1	XA	413	G
1	XA	414	A
1	XA	422	C
1	XA	424	G
1	XA	428	G
1	XA	429	U
1	XA	440	A
1	XA	441	A
1	XA	452	A
1	XA	453	A
1	XA	458(C)	A
1	XA	458(D)	C
1	XA	481	G
1	XA	484	G
1	XA	485	G
1	XA	495	A
1	XA	497	A
1	XA	498	U
1	XA	508	C
1	XA	509	A
1	XA	511	C
1	XA	518	C
1	XA	521	G
1	XA	524	G
1	XA	527	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	XA	531	U
1	XA	532	A
1	XA	533	A
1	XA	536	C
1	XA	547	A
1	XA	559	A
1	XA	562	C
1	XA	572	A
1	XA	573	A
1	XA	576	G
1	XA	577	G
1	XA	578	C
1	XA	588	G
1	XA	596	C
1	XA	605	U
1	XA	607	A
1	XA	618	C
1	XA	629	G
1	XA	653	A
1	XA	660	G
1	XA	661	G
1	XA	665	A
1	XA	666	G
1	XA	671	G
1	XA	687	A
1	XA	695	A
1	XA	702	A
1	XA	720	C
1	XA	721	G
1	XA	722	A
1	XA	723	U
1	XA	724	G
1	XA	749	C
1	XA	753	A
1	XA	755	G
1	XA	760	G
1	XA	777	A
1	XA	781	A
1	XA	793	U
1	XA	794	A
1	XA	811	C
1	XA	816	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	XA	817	C
1	XA	818	G
1	XA	819	A
1	XA	820	U
1	XA	821	G
1	XA	828	A
1	XA	838(B)	U
1	XA	838(C)	C
1	XA	838(D)	U
1	XA	848	C
1	XA	853	G
1	XA	859	A
1	XA	867	G
1	XA	872	A
1	XA	873	A
1	XA	885	G
1	XA	889	A
1	XA	890	G
1	XA	914	A
1	XA	923	A
1	XA	926	G
1	XA	927	G
1	XA	934	C
1	XA	935	A
1	XA	960	U
1	XA	961	U
1	XA	966	G
1	XA	967	C
1	XA	968	A
1	XA	969	A
1	XA	974	A
1	XA	976	G
1	XA	977	A
1	XA	980	C
1	XA	981	U
1	XA	982	U
1	XA	991	U
1	XA	992	U
1	XA	993	G
1	XA	1004	A
1	XA	1006	C
1	XA	1011	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	XA	1024	G
1	XA	1025	U
1	XA	1026	G
1	XA	1027	C
1	XA	1028(A)	C
1	XA	1028(C)	C
1	XA	1028(G)	A
1	XA	1036	G
1	XA	1045	C
1	XA	1053	G
1	XA	1054	C
1	XA	1055	A
1	XA	1056	U
1	XA	1064	G
1	XA	1065	U
1	XA	1066	C
1	XA	1075	C
1	XA	1081	G
1	XA	1094	G
1	XA	1095	U
1	XA	1101	A
1	XA	1117	G
1	XA	1118	C
1	XA	1125	U
1	XA	1126	U
1	XA	1129	C
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	1146	A
1	XA	1157	A
1	XA	1159	U
1	XA	1160	G
1	XA	1171	G
1	XA	1178	G
1	XA	1181	G
1	XA	1183	A
1	XA	1191	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	XA	1196	U
1	XA	1197	G
1	XA	1200	C
1	XA	1201	A
1	XA	1211	U
1	XA	1212	U
1	XA	1213	A
1	XA	1214	C
1	XA	1224	G
1	XA	1225	A
1	XA	1226	C
1	XA	1227	A
1	XA	1228	C
1	XA	1238	A
1	XA	1240	U
1	XA	1241	G
1	XA	1256	A
1	XA	1257	U
1	XA	1258	G
1	XA	1260	C
1	XA	1263	C
1	XA	1272	G
1	XA	1273	G
1	XA	1280	A
1	XA	1281	U
1	XA	1282	C
1	XA	1286	A
1	XA	1287	A
1	XA	1296	C
1	XA	1299	A
1	XA	1300	G
1	XA	1303	C
1	XA	1305	G
1	XA	1306	A
1	XA	1318	A
1	XA	1321	C
1	XA	1322	C
1	XA	1323	G
1	XA	1331	G
1	XA	1335	C
1	XA	1336	C
1	XA	1340	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	XA	1346	A
1	XA	1347	G
1	XA	1352	C
1	XA	1353	G
1	XA	1359	C
1	XA	1362(B)	C
1	XA	1363	A
1	XA	1364	U
1	XA	1370	G
1	XA	1374	A
1	XA	1378	C
1	XA	1379	G
1	XA	1381	U
1	XA	1394	A
1	XA	1397	C
1	XA	1413	A
1	XA	1419	G
1	XA	1440(C)	G
1	XA	1440(E)	A
1	XA	1440(J)	A
1	XA	1440(K)	C
1	XA	1440(L)	G
1	XA	1469	G
1	XA	1487	G
1	XA	1492	A
1	XA	1493	A
1	XA	1494	G
1	XA	1497	G
1	XA	1503	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	1528	U
1	XA	1529	G
1	XA	1530	G
1	XA	1533	C
1	XA	1534	A
1	XA	1538	C
1	XA	1539	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	XA	1541	U
1	XA	1542	U
22	XV	8	U
22	XV	11	C
22	XV	17	C
22	XV	18	U
22	XV	19	G
22	XV	21(A)	U
22	XV	21(B)	A
22	XV	34	C
22	XV	37	1MG
22	XV	38	A
22	XV	40	G
22	XV	42	A
22	XV	43	G
22	XV	46	G
22	XV	47	U
22	XV	48	C
22	XV	58	A
22	XV	61	C
22	XV	69	A
22	XV	72	G
22	XV	73	A
23	XX	9	G
23	XX	10	G
23	XX	12	A
23	XX	13	A
23	XX	15	A
34	YA	9	U
34	YA	23	G
34	YA	27	G
34	YA	28	A
34	YA	34	C
34	YA	35	G
34	YA	46	C
34	YA	51	G
34	YA	55	G
34	YA	61	G
34	YA	64	A
34	YA	70	G
34	YA	72	U
34	YA	73	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	YA	74	A
34	YA	75	G
34	YA	78	A
34	YA	90	U
34	YA	101	G
34	YA	102	G
34	YA	103	A
34	YA	118	A
34	YA	119	A
34	YA	120	U
34	YA	125	G
34	YA	131	G
34	YA	138	G
34	YA	161	U
34	YA	162	U
34	YA	193	U
34	YA	196	A
34	YA	199	A
34	YA	201	C
34	YA	204	A
34	YA	216	A
34	YA	221	A
34	YA	222	A
34	YA	223	A
34	YA	226	G
34	YA	228	A
34	YA	229	A
34	YA	230	U
34	YA	232	G
34	YA	233	A
34	YA	241	A
34	YA	242	G
34	YA	243	U
34	YA	248	G
34	YA	249	C
34	YA	252	G
34	YA	265	A
34	YA	266	G
34	YA	267	C
34	YA	269	U
34	YA	270(L)	C
34	YA	270(M)	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	YA	270(N)	U
34	YA	270(Q)	C
34	YA	271(D)	U
34	YA	271(E)	G
34	YA	274	G
34	YA	277	C
34	YA	278	A
34	YA	279	C
34	YA	299	A
34	YA	300	A
34	YA	309	G
34	YA	311	A
34	YA	317	G
34	YA	323	G
34	YA	324	A
34	YA	329	G
34	YA	330	A
34	YA	332	A
34	YA	342	G
34	YA	352	G
34	YA	363(A)	G
34	YA	364	C
34	YA	370	G
34	YA	371	A
34	YA	372	G
34	YA	386	G
34	YA	387	U
34	YA	395	U
34	YA	405	U
34	YA	407	G
34	YA	411	G
34	YA	412	A
34	YA	421	U
34	YA	428	A
34	YA	442	G
34	YA	444	C
34	YA	448	U
34	YA	454	A
34	YA	457	A
34	YA	464	U
34	YA	467	G
34	YA	470	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	YA	473	G
34	YA	481	G
34	YA	504	U
34	YA	505	A
34	YA	508	G
34	YA	509	C
34	YA	518	G
34	YA	527	C
34	YA	528	A
34	YA	529	A
34	YA	531	C
34	YA	532	A
34	YA	533	G
34	YA	537	C
34	YA	539	G
34	YA	540	G
34	YA	546	C
34	YA	547	A
34	YA	549	G
34	YA	554	U
34	YA	563	G
34	YA	568	U
34	YA	570	G
34	YA	573	G
34	YA	575	A
34	YA	603	A
34	YA	607	U
34	YA	614	U
34	YA	615	G
34	YA	617	G
34	YA	618(A)	G
34	YA	622	G
34	YA	627	A
34	YA	629	G
34	YA	634	C
34	YA	637	A
34	YA	638	G
34	YA	645	C
34	YA	646	A
34	YA	654(A)	A
34	YA	654(B)	G
34	YA	670	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	YA	686	G
34	YA	701	G
34	YA	704	G
34	YA	717	G
34	YA	722	A
34	YA	726	G
34	YA	730	C
34	YA	748	G
34	YA	753	C
34	YA	762	U
34	YA	782	A
34	YA	783	A
34	YA	784	A
34	YA	785	G
34	YA	790	C
34	YA	800	A
34	YA	805	G
34	YA	812	C
34	YA	819	A
34	YA	827	U
34	YA	828	U
34	YA	830	G
34	YA	847	U
34	YA	854	G
34	YA	856	C
34	YA	857	C
34	YA	860	U
34	YA	866	A
34	YA	870	A
34	YA	878	A
34	YA	889	C
34	YA	890	A
34	YA	896	A
34	YA	897	C
34	YA	899	A
34	YA	901	A
34	YA	907	U
34	YA	910	A
34	YA	914	C
34	YA	915	C
34	YA	917	A
34	YA	918	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	YA	932	G
34	YA	941	A
34	YA	945	A
34	YA	946	G
34	YA	953	A
34	YA	957	A
34	YA	959	A
34	YA	961	C
34	YA	972	G
34	YA	973	A
34	YA	974(A)	G
34	YA	974(B)	C
34	YA	975	G
34	YA	983	A
34	YA	989	G
34	YA	990	A
34	YA	996	A
34	YA	997	G
34	YA	1003	G
34	YA	1005	C
34	YA	1011	G
34	YA	1012	U
34	YA	1013	C
34	YA	1015	G
34	YA	1022	G
34	YA	1023	U
34	YA	1024	G
34	YA	1025	G
34	YA	1026	U
34	YA	1027	A
34	YA	1030	G
34	YA	1033	U
34	YA	1037	G
34	YA	1045	A
34	YA	1046	A
34	YA	1050	A
34	YA	1057	A
34	YA	1059	G
34	YA	1060	U
34	YA	1061	U
34	YA	1062	G
34	YA	1065	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	YA	1067	A
34	YA	1068	G
34	YA	1071	G
34	YA	1073	A
34	YA	1074	G
34	YA	1076	C
34	YA	1077	A
34	YA	1078	U
34	YA	1082	U
34	YA	1083	U
34	YA	1084	A
34	YA	1085	A
34	YA	1086	A
34	YA	1088	A
34	YA	1089	G
34	YA	1093	G
34	YA	1095	A
34	YA	1096	A
34	YA	1097	U
34	YA	1099	G
34	YA	1103	A
34	YA	1104	C
34	YA	1110	G
34	YA	1111	A
34	YA	1112	G
34	YA	1122	G
34	YA	1126	A
34	YA	1131	G
34	YA	1135	C
34	YA	1136	G
34	YA	1139	G
34	YA	1142(A)	U
34	YA	1142(B)	A
34	YA	1173	G
34	YA	1174	A
34	YA	1175	U
34	YA	1176	G
34	YA	1177	A
34	YA	1179	C
34	YA	1180	C
34	YA	1195	G
34	YA	1204	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	YA	1205	U
34	YA	1206	G
34	YA	1210	A
34	YA	1218	C
34	YA	1220	A
34	YA	1225	C
34	YA	1236	G
34	YA	1238	G
34	YA	1244	G
34	YA	1250	G
34	YA	1252	G
34	YA	1253	A
34	YA	1256	G
34	YA	1265	A
34	YA	1271	G
34	YA	1272	A
34	YA	1273	U
34	YA	1275	A
34	YA	1289	C
34	YA	1300	U
34	YA	1301	A
34	YA	1313	U
34	YA	1325	G
34	YA	1326	U
34	YA	1329	U
34	YA	1330	C
34	YA	1341	U
34	YA	1349	A
34	YA	1352	U
34	YA	1365	A
34	YA	1368	G
34	YA	1370	C
34	YA	1378	A
34	YA	1379	A
34	YA	1384	A
34	YA	1385	G
34	YA	1395	A
34	YA	1403	C
34	YA	1404	C
34	YA	1407	C
34	YA	1410	G
34	YA	1416	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	YA	1417	C
34	YA	1419	A
34	YA	1420	U
34	YA	1421	G
34	YA	1427	A
34	YA	1428	C
34	YA	1433	U
34	YA	1444(B)	A
34	YA	1449(A)	A
34	YA	1449(B)	G
34	YA	1455	G
34	YA	1461	G
34	YA	1467	C
34	YA	1471	A
34	YA	1482	U
34	YA	1483	G
34	YA	1485	G
34	YA	1490	A
34	YA	1493	C
34	YA	1497	U
34	YA	1506	C
34	YA	1507	A
34	YA	1508	A
34	YA	1509	C
34	YA	1510	A
34	YA	1511	A
34	YA	1512	G
34	YA	1533	C
34	YA	1534	G
34	YA	1535	U
34	YA	1536	A
34	YA	1537	C
34	YA	1538	G
34	YA	1543	A
34	YA	1544	C
34	YA	1545(A)	A
34	YA	1554	A
34	YA	1558	A
34	YA	1559	G
34	YA	1566	A
34	YA	1567	A
34	YA	1569	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	YA	1578	U
34	YA	1585	C
34	YA	1586	A
34	YA	1598	C
34	YA	1608	A
34	YA	1610	A
34	YA	1616	A
34	YA	1617	C
34	YA	1618	A
34	YA	1640	C
34	YA	1646	C
34	YA	1647	G
34	YA	1648	C
34	YA	1651	G
34	YA	1654	A
34	YA	1665	A
34	YA	1671	U
34	YA	1672	C
34	YA	1674	G
34	YA	1695	G
34	YA	1700	A
34	YA	1725	G
34	YA	1729	A
34	YA	1730	U
34	YA	1731	G
34	YA	1742	C
34	YA	1743	G
34	YA	1750	G
34	YA	1753	G
34	YA	1754	C
34	YA	1756	G
34	YA	1763	G
34	YA	1764	G
34	YA	1769	G
34	YA	1773	A
34	YA	1774	C
34	YA	1776	G
34	YA	1780	A
34	YA	1781	C
34	YA	1783	A
34	YA	1784	A
34	YA	1787	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	YA	1791	A
34	YA	1799	G
34	YA	1800	C
34	YA	1801	G
34	YA	1802	A
34	YA	1815	A
34	YA	1816	G
34	YA	1820	U
34	YA	1828	G
34	YA	1829	A
34	YA	1847	A
34	YA	1858	G
34	YA	1864	U
34	YA	1869	G
34	YA	1870	C
34	YA	1872	A
34	YA	1878	G
34	YA	1882	C
34	YA	1888	G
34	YA	1889	A
34	YA	1905	C
34	YA	1906	G
34	YA	1913	A
34	YA	1929	G
34	YA	1930	G
34	YA	1931	U
34	YA	1936	A
34	YA	1938	A
34	YA	1939	U
34	YA	1955	U
34	YA	1963	U
34	YA	1965	C
34	YA	1966	A
34	YA	1967	C
34	YA	1969	A
34	YA	1970	A
34	YA	1971	A
34	YA	1972	A
34	YA	1982	C
34	YA	1992	G
34	YA	1993	U
34	YA	2023	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	YA	2030	A
34	YA	2031	A
34	YA	2033	A
34	YA	2039	C
34	YA	2043	C
34	YA	2049	G
34	YA	2052	G
34	YA	2055	C
34	YA	2056	G
34	YA	2059	A
34	YA	2060	A
34	YA	2061	G
34	YA	2062	A
34	YA	2069	G
34	YA	2093	G
34	YA	2094	G
34	YA	2099	U
34	YA	2111	C
34	YA	2112	G
34	YA	2113	U
34	YA	2114	A
34	YA	2115	G
34	YA	2116	G
34	YA	2117	A
34	YA	2118	U
34	YA	2119	A
34	YA	2120	G
34	YA	2126	A
34	YA	2127	G
34	YA	2128	C
34	YA	2131	G
34	YA	2132	U
34	YA	2133	G
34	YA	2134	A
34	YA	2135	A
34	YA	2136	C
34	YA	2145	C
34	YA	2148	G
34	YA	2158	A
34	YA	2159	G
34	YA	2161	C
34	YA	2164	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	YA	2165	G
34	YA	2166	G
34	YA	2168	G
34	YA	2169	A
34	YA	2172	U
34	YA	2173	A
34	YA	2176	A
34	YA	2190	G
34	YA	2191	G
34	YA	2198	A
34	YA	2199	A
34	YA	2210	G
34	YA	2211	G
34	YA	2212	A
34	YA	2213	U
34	YA	2215	G
34	YA	2225	A
34	YA	2234	G
34	YA	2238	G
34	YA	2239	G
34	YA	2243	U
34	YA	2246	G
34	YA	2249	U
34	YA	2266	A
34	YA	2267	A
34	YA	2275	C
34	YA	2278	A
34	YA	2280	G
34	YA	2283	C
34	YA	2287	A
34	YA	2288	A
34	YA	2307	G
34	YA	2308	G
34	YA	2311	A
34	YA	2318	G
34	YA	2319	G
34	YA	2320	A
34	YA	2325	G
34	YA	2327	A
34	YA	2328	A
34	YA	2329	G
34	YA	2334	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	YA	2335	A
34	YA	2340	G
34	YA	2343	C
34	YA	2345	G
34	YA	2346	A
34	YA	2347	C
34	YA	2350	C
34	YA	2354	G
34	YA	2358	G
34	YA	2383	G
34	YA	2384	G
34	YA	2385	C
34	YA	2392	A
34	YA	2394	C
34	YA	2402	C
34	YA	2403	C
34	YA	2405	G
34	YA	2406	U
34	YA	2410	G
34	YA	2423	U
34	YA	2425	A
34	YA	2426	A
34	YA	2427	C
34	YA	2428	G
34	YA	2429	G
34	YA	2430	A
34	YA	2435	A
34	YA	2439	A
34	YA	2440	C
34	YA	2441	C
34	YA	2448	A
34	YA	2469	A
34	YA	2475	C
34	YA	2476	A
34	YA	2480	C
34	YA	2494	G
34	YA	2502	G
34	YA	2505	G
34	YA	2513	G
34	YA	2518	A
34	YA	2520	C
34	YA	2524	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	YA	2529	G
34	YA	2542	A
34	YA	2543	G
34	YA	2554	U
34	YA	2556	C
34	YA	2562	U
34	YA	2567	G
34	YA	2569	G
34	YA	2572	A
34	YA	2573	C
34	YA	2577	A
34	YA	2578	G
34	YA	2586	C
34	YA	2602	A
34	YA	2609	U
34	YA	2611	U
34	YA	2612	C
34	YA	2615	U
34	YA	2629	A
34	YA	2646	C
34	YA	2655	G
34	YA	2660	A
34	YA	2665	A
34	YA	2673	G
34	YA	2682	U
34	YA	2689	U
34	YA	2690	C
34	YA	2691	C
34	YA	2702	U
34	YA	2703	C
34	YA	2707	G
34	YA	2712(A)	U
34	YA	2712(B)	A
34	YA	2713	A
34	YA	2714	G
34	YA	2718	G
34	YA	2726	U
34	YA	2733	A
34	YA	2734	A
34	YA	2739	U
34	YA	2744	G
34	YA	2750	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	YA	2751	G
34	YA	2761	G
34	YA	2764	A
34	YA	2765	A
34	YA	2766	G
34	YA	2777	G
34	YA	2778	A
34	YA	2779	U
34	YA	2780	G
34	YA	2790	A
34	YA	2791	C
34	YA	2792	G
34	YA	2795	G
34	YA	2797	U
34	YA	2798	C
34	YA	2807	G
34	YA	2818	G
34	YA	2820	A
34	YA	2821	A
34	YA	2833	G
34	YA	2834	G
34	YA	2835	A
34	YA	2846	G
34	YA	2867	G
34	YA	2872	G
34	YA	2879	C
34	YA	2880	C
34	YA	2891	G
34	YA	2892	A
34	YA	2893	G
34	YA	2894	G
34	YA	2895	U
35	YB	7	G
35	YB	8	U
35	YB	9	G
35	YB	13	A
35	YB	15	A
35	YB	16	G
35	YB	19	G
35	YB	21	G
35	YB	22	U
35	YB	25	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	YB	35	U
35	YB	40	U
35	YB	41	U
35	YB	42	C
35	YB	44	G
35	YB	45	A
35	YB	47	C
35	YB	52	A
35	YB	53	A
35	YB	56	G
35	YB	67	G
35	YB	73	A
35	YB	81	G
35	YB	82	G
35	YB	109	G

All (109) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	QA	64	G
1	QA	266	G
1	QA	328	C
1	QA	687	A
1	QA	748	C
1	QA	819	A
1	QA	992	U
1	QA	1285	A
1	QA	1538	C
22	QV	10	G
22	QV	36	G
23	QX	17	C
34	RA	99	U
34	RA	102	G
34	RA	221	A
34	RA	222	A
34	RA	229	A
34	RA	242	G
34	RA	271(C)	G
34	RA	404	C
34	RA	503	A
34	RA	512	G
34	RA	637	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	RA	752	A
34	RA	790	C
34	RA	846	C
34	RA	856	C
34	RA	974(B)	C
34	RA	1022	G
34	RA	1026	U
34	RA	1045	A
34	RA	1130	U
34	RA	1178	C
34	RA	1312	U
34	RA	1427	A
34	RA	1558	A
34	RA	1653	G
34	RA	1694	C
34	RA	1799	G
34	RA	1819	A
34	RA	1930	G
34	RA	1992	G
34	RA	2022	U
34	RA	2060	A
34	RA	2126	A
34	RA	2439	A
34	RA	2566	A
34	RA	2610	C
34	RA	2689	U
34	RA	2712(A)	U
34	RA	2776	A
34	RA	2832	U
35	RB	66	A
1	XA	115	G
1	XA	266	G
1	XA	328	C
1	XA	367	U
1	XA	748	C
1	XA	992	U
1	XA	1064	G
1	XA	1285	A
1	XA	1504	G
1	XA	1537	U
22	XV	10	G
34	YA	99	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	YA	102	G
34	YA	195	A
34	YA	221	A
34	YA	229	A
34	YA	242	G
34	YA	271(C)	G
34	YA	278	A
34	YA	404	C
34	YA	503	A
34	YA	637	A
34	YA	653	A
34	YA	752	A
34	YA	846	C
34	YA	856	C
34	YA	859	G
34	YA	974(A)	G
34	YA	974(B)	C
34	YA	1012	U
34	YA	1022	G
34	YA	1026	U
34	YA	1045	A
34	YA	1085	A
34	YA	1178	C
34	YA	1427	A
34	YA	1508	A
34	YA	1558	A
34	YA	1653	G
34	YA	1694	C
34	YA	1799	G
34	YA	1819	A
34	YA	1930	G
34	YA	1992	G
34	YA	2126	A
34	YA	2319	G
34	YA	2402	C
34	YA	2439	A
34	YA	2566	A
34	YA	2610	C
34	YA	2611	U
34	YA	2681	C
34	YA	2689	U
34	YA	2712(A)	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	YA	2776	A
35	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$
22	1MG	QV	37	22	19,26,27	1.71	4 (21%)	18,39,42	1.38	4 (22%)
22	1MG	XV	37	22	19,26,27	0.91	1 (5%)	18,39,42	1.64	6 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	1MG	QV	37	22	-	2/3/25/26	0/3/3/3
22	1MG	XV	37	22	-	2/3/25/26	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	QV	37	1MG	C2-N1	3.89	1.44	1.37
22	QV	37	1MG	C5-C4	3.29	1.51	1.43
22	QV	37	1MG	C2-N3	3.13	1.38	1.33
22	XV	37	1MG	C2-N1	2.40	1.41	1.37
22	QV	37	1MG	O6-C6	2.31	1.27	1.22

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	XV	37	1MG	CM1-N1-C6	3.19	121.87	117.54
22	XV	37	1MG	C8-N7-C5	2.84	107.38	102.55
22	QV	37	1MG	C5-C6-N1	2.81	118.02	113.96
22	XV	37	1MG	N2-C2-N1	2.59	120.87	118.79
22	XV	37	1MG	C5-C6-N1	2.59	117.71	113.96
22	QV	37	1MG	C8-N7-C5	2.47	106.75	102.55
22	QV	37	1MG	CM1-N1-C2	2.46	123.25	120.70
22	QV	37	1MG	C2-N1-C6	-2.40	118.99	120.99
22	XV	37	1MG	O6-C6-C5	-2.20	120.56	124.18
22	XV	37	1MG	CM1-N1-C2	-2.20	118.43	120.70

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	XV	37	1MG	O4'-C4'-C5'-O5'
22	XV	37	1MG	C3'-C4'-C5'-O5'
22	QV	37	1MG	C3'-C4'-C5'-O5'
22	QV	37	1MG	O4'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	QV	37	1MG	6	0
22	XV	37	1MG	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1110 ligands modelled in this entry, 1108 are monoatomic - leaving 2 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	$\# Z > 2$
56	SF4	QD	301	4	0,12,12	-	-	-		
56	SF4	XD	301	4	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	SF4	QD	301	4	-	-	0/6/5/5
56	SF4	XD	301	4	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	QD	301	SF4	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
41	RI	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	RI	82:ARG	C	83:ALA	N	1.18

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	QA	1511/1521 (99%)	0.43	56 (3%) 45 30	96, 139, 274, 366	0
1	XA	1515/1521 (99%)	0.25	19 (1%) 74 56	72, 129, 225, 307	0
2	QB	235/256 (91%)	0.30	5 (2%) 63 44	128, 165, 188, 207	0
2	XB	236/256 (92%)	0.04	1 (0%) 89 79	106, 138, 172, 188	0
3	QC	205/239 (85%)	0.27	5 (2%) 59 41	140, 169, 191, 211	0
3	XC	205/239 (85%)	0.26	6 (2%) 54 36	127, 152, 176, 192	0
4	QD	208/209 (99%)	0.56	8 (3%) 44 30	95, 130, 151, 168	0
4	XD	208/209 (99%)	0.44	10 (4%) 36 26	91, 134, 156, 172	0
5	QE	151/162 (93%)	0.22	3 (1%) 64 45	111, 132, 161, 167	0
5	XE	151/162 (93%)	-0.05	1 (0%) 84 69	89, 109, 139, 182	0
6	QF	101/101 (100%)	-0.07	2 (1%) 64 45	80, 124, 146, 170	0
6	XF	101/101 (100%)	-0.00	0 100 100	87, 117, 142, 159	0
7	QG	155/156 (99%)	0.18	7 (4%) 39 27	158, 186, 212, 249	0
7	XG	155/156 (99%)	0.05	5 (3%) 50 34	141, 168, 194, 274	0
8	QH	137/138 (99%)	0.56	8 (5%) 30 22	100, 125, 147, 182	0
8	XH	137/138 (99%)	0.41	8 (5%) 30 22	89, 119, 146, 157	0
9	QI	127/128 (99%)	1.01	25 (19%) 3 3	148, 190, 219, 230	0
9	XI	126/128 (98%)	0.74	14 (11%) 12 9	126, 173, 193, 218	0
10	QJ	99/105 (94%)	1.31	20 (20%) 3 3	152, 196, 212, 227	0
10	XJ	96/105 (91%)	0.80	10 (10%) 13 10	134, 169, 192, 207	0
11	QK	119/129 (92%)	0.44	7 (5%) 29 22	100, 125, 158, 177	0
11	XK	116/129 (89%)	0.16	3 (2%) 57 39	72, 115, 142, 153	0
12	QL	125/132 (94%)	0.74	13 (10%) 13 10	99, 118, 143, 181	0
12	XL	122/132 (92%)	0.60	8 (6%) 26 19	84, 102, 125, 137	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
13	QM	120/126 (95%)	0.49	7 (5%)	30	22	150, 184, 210, 224	0
13	XM	114/126 (90%)	0.52	2 (1%)	67	48	121, 175, 195, 213	0
14	QN	60/61 (98%)	1.17	9 (15%)	6	6	124, 163, 182, 191	0
14	XN	60/61 (98%)	0.96	5 (8%)	19	14	123, 150, 185, 200	0
15	QO	88/89 (98%)	0.23	1 (1%)	77	59	92, 112, 135, 150	0
15	XO	87/89 (97%)	0.14	0	100	100	83, 101, 132, 146	0
16	QP	84/88 (95%)	0.74	8 (9%)	15	12	89, 124, 149, 169	0
16	XP	84/88 (95%)	0.38	2 (2%)	59	41	102, 132, 153, 197	0
17	QQ	100/105 (95%)	0.61	5 (5%)	35	25	103, 119, 132, 135	0
17	XQ	100/105 (95%)	0.45	2 (2%)	64	45	84, 104, 127, 141	0
18	QR	70/88 (79%)	-0.04	0	100	100	83, 121, 148, 165	0
18	XR	70/88 (79%)	0.00	0	100	100	96, 116, 144, 160	0
19	QS	83/93 (89%)	1.29	20 (24%)	2	2	171, 204, 229, 245	0
19	XS	84/93 (90%)	0.77	4 (4%)	36	26	126, 167, 200, 228	0
20	QT	99/106 (93%)	0.88	14 (14%)	7	6	86, 118, 165, 176	0
20	XT	99/106 (93%)	0.91	17 (17%)	5	5	88, 116, 160, 173	0
21	QU	25/27 (92%)	2.31	12 (48%)	0	0	153, 183, 204, 213	0
21	XU	25/27 (92%)	2.09	10 (40%)	1	1	145, 158, 182, 187	0
22	QV	76/77 (98%)	0.34	3 (3%)	44	30	119, 205, 269, 284	0
22	XV	76/77 (98%)	0.23	3 (3%)	44	30	74, 177, 222, 267	0
23	QX	19/19 (100%)	1.75	7 (36%)	1	1	143, 241, 287, 290	0
23	XX	19/19 (100%)	1.75	8 (42%)	1	1	126, 234, 286, 304	0
24	R0	81/85 (95%)	0.75	9 (11%)	12	9	84, 104, 169, 198	0
24	Y0	82/85 (96%)	0.40	5 (6%)	28	21	44, 65, 146, 190	0
25	R1	95/98 (96%)	0.63	5 (5%)	33	24	70, 91, 121, 136	0
25	Y1	93/98 (94%)	0.55	5 (5%)	32	23	46, 70, 96, 115	0
26	R2	69/72 (95%)	0.36	2 (2%)	54	36	81, 98, 134, 156	0
26	Y2	68/72 (94%)	0.43	2 (2%)	54	36	44, 73, 104, 125	0
27	R3	59/60 (98%)	0.46	4 (6%)	25	19	80, 106, 135, 187	0
27	Y3	59/60 (98%)	-0.05	0	100	100	27, 53, 96, 147	0
28	R4	45/71 (63%)	0.01	0	100	100	121, 174, 203, 225	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	Y4	46/71 (64%)	0.09	0 100 100	105, 153, 169, 188	0
29	R5	59/60 (98%)	0.25	2 (3%) 48 32	66, 91, 113, 148	0
29	Y5	59/60 (98%)	-0.07	0 100 100	29, 47, 77, 134	0
30	R6	53/54 (98%)	0.06	0 100 100	90, 101, 119, 126	0
30	Y6	53/54 (98%)	-0.00	1 (1%) 66 46	49, 69, 97, 104	0
31	R7	47/49 (95%)	0.52	1 (2%) 63 44	58, 72, 93, 96	0
31	Y7	48/49 (97%)	0.39	3 (6%) 27 20	32, 45, 85, 106	0
32	R8	64/65 (98%)	1.30	11 (17%) 5 5	80, 98, 125, 183	0
32	Y8	64/65 (98%)	0.88	10 (15%) 6 6	48, 58, 82, 143	0
33	R9	37/37 (100%)	0.82	2 (5%) 32 23	86, 110, 136, 145	0
33	Y9	37/37 (100%)	0.67	3 (8%) 19 15	53, 66, 84, 98	0
34	RA	2882/2915 (98%)	0.20	48 (1%) 69 49	55, 100, 221, 404	0
34	YA	2883/2915 (98%)	-0.01	29 (1%) 79 61	28, 58, 166, 367	0
35	RB	120/122 (98%)	0.14	0 100 100	111, 144, 166, 214	0
35	YB	120/122 (98%)	-0.18	0 100 100	55, 83, 103, 128	0
36	RD	272/276 (98%)	0.49	12 (4%) 39 27	62, 86, 105, 141	0
36	YD	272/276 (98%)	0.23	10 (3%) 45 30	41, 60, 83, 116	0
37	RE	205/206 (99%)	0.46	12 (5%) 29 22	72, 101, 130, 153	0
37	YE	205/206 (99%)	0.22	5 (2%) 59 41	37, 59, 101, 127	0
38	RF	202/210 (96%)	0.33	7 (3%) 47 32	69, 101, 135, 161	0
38	YF	202/210 (96%)	0.01	2 (0%) 79 61	28, 64, 102, 125	0
39	RG	181/182 (99%)	0.50	5 (2%) 55 37	121, 153, 191, 218	0
39	YG	181/182 (99%)	0.11	1 (0%) 85 72	71, 117, 157, 187	0
40	RH	174/180 (96%)	0.48	3 (1%) 69 49	112, 154, 176, 195	0
40	YH	174/180 (96%)	0.22	4 (2%) 61 42	42, 77, 103, 147	0
41	RI	146/148 (98%)	0.14	1 (0%) 84 69	94, 126, 156, 193	0
41	YI	146/148 (98%)	0.10	2 (1%) 73 53	69, 117, 137, 144	0
42	RN	138/140 (98%)	0.38	5 (3%) 46 31	62, 103, 138, 161	0
42	YN	138/140 (98%)	0.19	0 100 100	32, 54, 96, 115	0
43	RO	122/122 (100%)	0.25	0 100 100	65, 100, 123, 133	0
43	YO	122/122 (100%)	-0.07	0 100 100	36, 63, 90, 101	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	RP	150/150 (100%)	0.85	22 (14%) 7 6	74, 114, 142, 182	0
44	YP	147/150 (98%)	0.64	10 (6%) 25 19	41, 76, 105, 120	0
45	RQ	141/141 (100%)	0.77	14 (9%) 14 11	87, 116, 143, 165	0
45	YQ	141/141 (100%)	0.45	7 (4%) 35 25	34, 68, 104, 144	0
46	RR	117/118 (99%)	0.51	8 (6%) 25 19	64, 87, 111, 134	0
46	YR	117/118 (99%)	0.34	3 (2%) 57 39	41, 57, 83, 141	0
47	RS	111/112 (99%)	0.64	8 (7%) 23 18	83, 132, 187, 218	0
47	YS	111/112 (99%)	0.29	7 (6%) 27 20	58, 83, 123, 190	0
48	RT	137/146 (93%)	0.41	9 (6%) 26 19	76, 114, 153, 183	0
48	YT	137/146 (93%)	0.28	4 (2%) 54 36	53, 76, 141, 171	0
49	RU	117/118 (99%)	0.59	4 (3%) 48 32	75, 109, 146, 173	0
49	YU	117/118 (99%)	0.29	3 (2%) 57 39	33, 44, 88, 121	0
50	RV	101/101 (100%)	0.15	1 (0%) 79 61	71, 114, 151, 194	0
50	YV	101/101 (100%)	0.08	4 (3%) 43 29	30, 60, 111, 172	0
51	RW	113/113 (100%)	0.34	4 (3%) 47 32	59, 74, 106, 167	0
51	YW	113/113 (100%)	-0.05	1 (0%) 81 64	31, 43, 80, 148	0
52	RX	92/96 (95%)	0.37	5 (5%) 32 23	59, 80, 109, 136	0
52	YX	92/96 (95%)	0.11	0 100 100	38, 55, 81, 100	0
53	RY	107/110 (97%)	0.41	6 (5%) 31 23	68, 104, 134, 175	0
53	YY	107/110 (97%)	0.08	2 (1%) 66 46	39, 66, 91, 130	0
54	RZ	183/206 (88%)	0.29	7 (3%) 44 30	108, 142, 172, 208	0
54	YZ	193/206 (93%)	0.23	4 (2%) 63 44	57, 93, 129, 169	0
All	All	20831/21436 (97%)	0.30	727 (3%) 47 32	27, 108, 200, 404	0

All (727) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	QK	129	SER	13.2
21	QU	16	GLY	10.2
9	QI	123	PRO	7.5
21	XU	16	GLY	6.8
25	Y1	92	LYS	6.5
1	XA	966	G	6.5
24	Y0	2	ALA	6.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	QD	77	ASN	6.4
34	YA	2602	A	6.4
36	RD	36	PRO	6.4
21	QU	14	TRP	6.0
53	RY	1	MET	5.5
10	QJ	62	HIS	5.5
21	XU	2	GLY	5.3
12	QL	6	THR	5.3
48	RT	106	SER	5.2
8	XH	23	SER	5.1
1	QA	966	G	5.1
45	YQ	91	GLU	5.0
34	RA	2319	G	5.0
48	RT	1	MET	4.9
36	YD	36	PRO	4.8
11	QK	49	GLY	4.8
32	R8	31	HIS	4.7
10	QJ	65	LEU	4.6
34	YA	1536	A	4.6
12	XL	28	LYS	4.6
10	QJ	58	ASP	4.6
32	R8	50	LEU	4.5
24	Y0	3	HIS	4.5
32	R8	30	ARG	4.5
37	RE	79	ARG	4.5
32	R8	54	GLU	4.5
34	RA	614	U	4.5
20	XT	73	HIS	4.4
1	QA	135	C	4.4
24	R0	76	GLY	4.4
34	YA	2319	G	4.4
34	YA	2803	C	4.4
34	RA	2602	A	4.3
34	RA	2799	A	4.3
19	QS	35	SER	4.3
47	RS	2	ALA	4.3
10	QJ	57	LYS	4.3
34	RA	1536	A	4.3
8	QH	112	LEU	4.2
34	RA	2797	U	4.2
36	YD	38	LYS	4.2
40	RH	150	ALA	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
21	QU	3	LYS	4.1
36	YD	35	LYS	4.1
10	QJ	63	PHE	4.1
7	XG	2	ALA	4.1
10	QJ	18	ALA	4.1
24	R0	3	HIS	4.0
32	Y8	54	GLU	4.0
10	QJ	59	SER	4.0
16	QP	1	MET	4.0
19	QS	11	VAL	4.0
24	Y0	4	LYS	4.0
9	QI	112	LYS	4.0
9	QI	74	ILE	3.9
47	YS	3	ARG	3.9
34	RA	1087	G	3.9
10	QJ	46	ARG	3.9
53	YY	1	MET	3.9
47	YS	20	ARG	3.8
24	Y0	5	LYS	3.8
44	YP	13	ASN	3.8
1	XA	967	C	3.8
3	XC	201	TYR	3.8
48	RT	69	GLY	3.8
14	QN	57	ARG	3.8
44	RP	65	ARG	3.8
36	YD	240	ALA	3.8
37	YE	79	ARG	3.8
20	QT	73	HIS	3.8
21	XU	11	GLY	3.8
40	YH	3	ARG	3.7
50	YV	45	THR	3.7
34	YA	2794	C	3.7
4	XD	73	ARG	3.7
34	YA	2795	G	3.7
14	XN	59	ALA	3.7
1	XA	1542	U	3.7
34	RA	2801	A	3.7
46	YR	11	ASN	3.7
10	QJ	101	VAL	3.7
19	QS	51	VAL	3.7
36	RD	240	ALA	3.7
19	QS	33	THR	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
44	RP	61	ARG	3.6
33	Y9	37	GLY	3.6
10	QJ	64	GLU	3.6
49	RU	91	ASP	3.6
25	R1	95	LEU	3.6
12	XL	23	LYS	3.6
47	YS	109	GLY	3.6
3	XC	130	VAL	3.6
11	QK	128	ALA	3.5
23	XX	5	A	3.5
21	XU	14	TRP	3.5
34	RA	615	G	3.5
34	RA	2798	C	3.5
44	RP	13	ASN	3.5
1	QA	1286	A	3.5
8	QH	133	LEU	3.5
23	XX	6	G	3.5
21	XU	15	ARG	3.5
52	RX	68	ARG	3.5
23	QX	7	G	3.5
23	XX	7	G	3.5
1	QA	1362(B)	C	3.5
4	XD	5	ILE	3.5
1	QA	134	A	3.5
34	RA	2320	A	3.5
8	QH	72	PRO	3.5
19	QS	76	PRO	3.5
10	XJ	59	SER	3.4
34	RA	2804	C	3.4
10	XJ	62	HIS	3.4
44	RP	64	LYS	3.4
46	YR	2	ARG	3.4
12	QL	129	ALA	3.4
10	QJ	50	ILE	3.4
1	QA	136	C	3.4
10	XJ	64	GLU	3.4
17	QQ	35	VAL	3.4
23	QX	6	G	3.4
8	QH	4	ASP	3.4
49	YU	91	ASP	3.4
9	QI	118	LYS	3.4
34	YA	2804	C	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
9	XI	64	THR	3.4
21	QU	25	LYS	3.4
1	QA	967	C	3.3
1	XA	1538	C	3.3
45	YQ	90	VAL	3.3
32	R8	65	GLU	3.3
29	R5	10	LYS	3.3
9	QI	122	ALA	3.3
44	RP	31	ALA	3.3
42	RN	41	ASP	3.3
40	RH	105	LEU	3.3
49	RU	95	LEU	3.3
1	QA	950	U	3.3
46	RR	71	GLN	3.3
31	Y7	45	ALA	3.3
9	QI	115	GLY	3.3
47	RS	27	SER	3.3
14	XN	56	VAL	3.3
19	XS	76	PRO	3.3
34	RA	2795	G	3.3
25	R1	47	GLN	3.3
4	XD	24	GLU	3.2
20	XT	14	LYS	3.2
34	YA	1177	A	3.2
36	YD	30	GLU	3.2
40	YH	125	VAL	3.2
20	QT	27	LYS	3.2
20	XT	49	ALA	3.2
16	QP	25	ARG	3.2
20	XT	80	ARG	3.2
25	R1	46	LEU	3.2
17	QQ	24	GLU	3.2
37	RE	128	SER	3.2
20	XT	18	GLN	3.2
44	RP	74	GLU	3.2
1	QA	970	C	3.2
34	YA	2798	C	3.2
7	QG	9	VAL	3.2
21	QU	10	ARG	3.2
1	QA	82	U	3.1
3	QC	130	VAL	3.1
1	QA	1368	G	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	RA	2802	G	3.1
34	YA	615	G	3.1
51	YW	92	ARG	3.1
10	QJ	48	THR	3.1
22	XV	21(A)	U	3.1
44	YP	66	GLY	3.1
7	QG	8	GLU	3.1
53	RY	19	LYS	3.1
6	QF	90	VAL	3.1
34	RA	2807	G	3.1
41	YI	1	MET	3.1
36	YD	37	LEU	3.1
49	YU	90	VAL	3.1
2	QB	109	SER	3.1
20	XT	11	SER	3.1
1	QA	60	A	3.1
12	XL	5	PRO	3.1
13	QM	105	THR	3.1
44	RP	50	ARG	3.1
41	YI	20	ASP	3.1
45	RQ	91	GLU	3.1
9	QI	119	ALA	3.1
36	YD	44	ASN	3.1
16	QP	63	GLY	3.0
34	RA	2611	U	3.0
8	QH	87	SER	3.0
20	QT	11	SER	3.0
38	RF	70	THR	3.0
1	QA	972	C	3.0
22	QV	16	C	3.0
19	QS	12	ASP	3.0
23	QX	5	A	3.0
7	QG	27	ILE	3.0
21	XU	6	ARG	3.0
8	QH	15	ASN	3.0
45	YQ	21	THR	3.0
20	QT	22	ARG	3.0
1	QA	968	A	3.0
1	QA	1440(J)	A	3.0
12	QL	5	PRO	3.0
50	YV	36	PRO	3.0
10	XJ	63	PHE	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
36	RD	44	ASN	3.0
8	QH	2	LEU	3.0
37	YE	159	HIS	3.0
1	QA	1364	U	3.0
34	YA	1535	U	3.0
38	RF	67	GLN	3.0
37	YE	204	ALA	3.0
49	YU	89	GLU	3.0
9	QI	37	PHE	3.0
34	YA	34	C	3.0
34	YA	2799	A	3.0
9	XI	122	ALA	3.0
1	XA	723	U	3.0
7	QG	23	VAL	3.0
9	XI	65	VAL	3.0
9	XI	109	VAL	3.0
36	RD	230	ASP	3.0
21	QU	4	GLY	3.0
44	RP	18	ARG	3.0
47	RS	20	ARG	3.0
51	RW	90	ARG	3.0
32	R8	28	GLY	2.9
54	RZ	79	ARG	2.9
44	YP	65	ARG	2.9
1	XA	1353	G	2.9
34	RA	2333	A	2.9
34	YA	2112	G	2.9
1	QA	723	U	2.9
12	XL	18	VAL	2.9
47	RS	3	ARG	2.9
16	XP	1	MET	2.9
25	Y1	91	LYS	2.9
19	QS	15	LEU	2.9
10	QJ	60	ARG	2.9
34	RA	2585	U	2.9
34	YA	2793	G	2.9
14	XN	58	LYS	2.9
3	QC	133	ALA	2.9
4	XD	135	LEU	2.9
10	XJ	74	ILE	2.9
16	QP	21	VAL	2.9
34	RA	34	C	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	RA	1653	G	2.9
51	RW	78	GLU	2.9
36	RD	243	GLY	2.8
14	QN	56	VAL	2.8
44	RP	40	SER	2.8
21	XU	8	THR	2.8
1	QA	824	C	2.8
20	QT	63	ILE	2.8
20	QT	72	LEU	2.8
10	XJ	58	ASP	2.8
26	Y2	20	GLU	2.8
19	QS	71	LEU	2.8
3	XC	168	ALA	2.8
12	QL	95	GLY	2.8
13	QM	118	ALA	2.8
1	QA	1066	C	2.8
1	QA	1320	C	2.8
12	XL	29	GLY	2.8
45	YQ	23	GLY	2.8
54	YZ	152	ALA	2.8
31	R7	47	ARG	2.8
24	R0	4	LYS	2.8
32	Y8	64	TYR	2.8
44	RP	6	LEU	2.8
52	RX	66	LEU	2.8
20	XT	52	ALA	2.8
32	Y8	51	ALA	2.8
9	QI	108	VAL	2.8
11	QK	126	ARG	2.8
34	RA	2805	G	2.8
17	QQ	7	THR	2.8
25	Y1	2	SER	2.8
36	RD	259	THR	2.8
23	XX	11	U	2.8
34	RA	2402	C	2.7
9	QI	33	PHE	2.7
19	QS	56	GLN	2.7
46	RR	2	ARG	2.7
11	QK	127	LYS	2.7
34	RA	1083	U	2.7
19	QS	40	ILE	2.7
14	QN	36	PHE	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
21	QU	8	THR	2.7
38	RF	72	ARG	2.7
27	R3	9	VAL	2.7
8	XH	131	GLY	2.7
11	XK	49	GLY	2.7
51	RW	92	ARG	2.7
1	QA	324	G	2.7
9	XI	110	GLU	2.7
32	Y8	65	GLU	2.7
45	RQ	141	GLN	2.7
34	RA	214	G	2.7
44	YP	24	GLY	2.7
34	RA	2896	C	2.7
37	RE	76	ARG	2.7
16	QP	2	VAL	2.7
54	YZ	184	ALA	2.7
38	YF	70	THR	2.7
39	RG	2	PRO	2.7
1	QA	1065	U	2.7
47	RS	7	TYR	2.7
48	RT	104	ASN	2.7
1	QA	1531	A	2.7
3	XC	10	PHE	2.7
13	XM	99	ARG	2.7
40	YH	152	ARG	2.7
1	QA	971	G	2.7
45	RQ	38	GLU	2.6
46	RR	7	GLY	2.6
46	RR	49	ASP	2.6
1	QA	377	G	2.6
1	QA	1186	G	2.6
9	QI	70	LYS	2.6
10	XJ	46	ARG	2.6
29	R5	19	ARG	2.6
53	RY	105	ALA	2.6
14	QN	13	THR	2.6
21	XU	3	LYS	2.6
32	R8	29	LYS	2.6
40	YH	153	LYS	2.6
9	QI	14	VAL	2.6
13	XM	107	ALA	2.6
48	RT	5	ALA	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	XE	81	GLU	2.6
34	RA	232	G	2.6
36	RD	184	LYS	2.6
1	QA	1440(K)	C	2.6
4	XD	77	ASN	2.6
7	QG	2	ALA	2.6
9	QI	15	ALA	2.6
34	YA	1096	A	2.6
33	R9	37	GLY	2.6
44	RP	44	GLY	2.6
10	QJ	47	PHE	2.6
44	RP	52	GLU	2.6
1	QA	330	C	2.6
9	QI	126	SER	2.6
34	RA	2803	C	2.6
23	QX	9	G	2.6
44	RP	62	LEU	2.6
47	YS	2	ALA	2.6
14	QN	58	LYS	2.6
20	XT	25	ARG	2.6
25	R1	22	GLY	2.6
1	XA	1286	A	2.6
23	XX	8	A	2.6
34	YA	896	A	2.6
4	XD	137	SER	2.6
12	XL	30	ALA	2.6
20	QT	12	ALA	2.6
31	Y7	47	ARG	2.6
50	RV	45	THR	2.5
1	XA	108	G	2.5
9	QI	109	VAL	2.5
10	QJ	72	VAL	2.5
53	RY	24	VAL	2.5
36	YD	31	LYS	2.5
47	YS	110	LEU	2.5
2	QB	108	ILE	2.5
9	XI	106	ALA	2.5
45	YQ	20	ALA	2.5
23	QX	4	A	2.5
4	QD	109	GLY	2.5
48	YT	4	GLY	2.5
53	YY	62	GLU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
12	QL	104	VAL	2.5
24	Y0	7	LEU	2.5
4	QD	3	ARG	2.5
1	QA	1367	C	2.5
20	XT	12	ALA	2.5
45	RQ	36	ALA	2.5
20	XT	9	ASN	2.5
38	RF	131	GLY	2.5
12	QL	16	GLU	2.5
12	QL	19	ARG	2.5
20	XT	23	ARG	2.5
33	R9	32	HIS	2.5
19	XS	71	LEU	2.5
45	RQ	21	THR	2.5
49	RU	96	ALA	2.5
1	QA	1117	G	2.5
34	RA	2112	G	2.5
37	RE	182	LEU	2.5
37	YE	78	LEU	2.5
38	RF	133	ASN	2.5
46	RR	68	ARG	2.5
12	QL	32	PHE	2.5
1	XA	1366	C	2.5
34	RA	2143	C	2.5
34	YA	2178	C	2.5
45	RQ	19	GLY	2.5
12	QL	105	TYR	2.5
1	QA	325	A	2.5
19	XS	31	ILE	2.5
23	XX	14	A	2.5
34	YA	2801	A	2.5
1	QA	332	G	2.4
32	R8	48	PHE	2.4
20	XT	74	LYS	2.4
9	XI	66	ARG	2.4
45	RQ	103	MET	2.4
1	QA	1325	C	2.4
14	XN	60	SER	2.4
36	RD	247	ALA	2.4
44	YP	58	THR	2.4
34	RA	229	A	2.4
44	RP	16	ARG	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
44	RP	43	GLY	2.4
45	RQ	92	GLY	2.4
1	QA	1196	U	2.4
50	YV	26	ASP	2.4
36	YD	15	PHE	2.4
9	QI	113	LYS	2.4
9	QI	116	LYS	2.4
21	QU	26	LYS	2.4
13	QM	116	THR	2.4
1	QA	795	C	2.4
1	XA	328	C	2.4
20	XT	15	ARG	2.4
21	QU	15	ARG	2.4
36	RD	262	ARG	2.4
44	RP	28	GLY	2.4
44	YP	67	MET	2.4
12	QL	64	TYR	2.4
39	RG	13	GLU	2.4
38	RF	98	SER	2.4
52	RX	50	LYS	2.4
11	XK	126	ARG	2.4
34	YA	11	G	2.4
19	QS	67	VAL	2.4
45	YQ	7	MET	2.4
27	R3	15	TYR	2.4
30	Y6	21	TYR	2.4
52	RX	69	TYR	2.4
1	QA	1352	C	2.4
3	QC	129	ALA	2.4
4	QD	147	ALA	2.4
7	XG	7	ALA	2.4
48	YT	124	ASP	2.4
4	QD	139	ARG	2.4
42	RN	46	VAL	2.4
12	QL	13	LYS	2.4
19	QS	2	PRO	2.4
32	Y8	63	PRO	2.4
10	QJ	61	GLU	2.4
10	XJ	61	GLU	2.4
39	YG	13	GLU	2.4
48	RT	21	GLU	2.4
4	QD	73	ARG	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	Y8	50	LEU	2.4
32	Y8	62	LEU	2.4
8	XH	73	ASP	2.4
48	YT	106	SER	2.4
1	QA	1354	C	2.4
24	R0	10	THR	2.3
42	RN	73	THR	2.3
20	QT	68	LYS	2.3
1	XA	60	A	2.3
38	RF	34	TRP	2.3
2	XB	26	PRO	2.3
21	QU	23	PRO	2.3
54	RZ	113	ALA	2.3
1	QA	1542	U	2.3
34	RA	362	U	2.3
48	YT	12	SER	2.3
7	XG	37	ASN	2.3
16	QP	31	LYS	2.3
45	RQ	84	GLY	2.3
1	QA	664	G	2.3
20	QT	23	ARG	2.3
1	XA	1354	C	2.3
47	YS	4	LEU	2.3
8	QH	136	GLU	2.3
1	QA	1183	A	2.3
23	QX	14	A	2.3
24	R0	53	MET	2.3
7	XG	80	VAL	2.3
11	QK	117	ASN	2.3
13	QM	85	GLY	2.3
32	Y8	48	PHE	2.3
45	YQ	19	GLY	2.3
48	RT	100	TYR	2.3
9	QI	94	ALA	2.3
25	R1	15	ALA	2.3
54	YZ	60	GLU	2.3
16	QP	20	VAL	2.3
54	RZ	74	VAL	2.3
3	XC	2	GLY	2.3
34	YA	2805	G	2.3
44	RP	26	GLY	2.3
1	QA	1324	A	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
9	XI	121	ARG	2.3
4	QD	29	PRO	2.3
34	RA	2296	U	2.3
34	RA	2897	U	2.3
8	XH	132	GLU	2.3
45	RQ	112	GLU	2.3
45	RQ	139	GLU	2.3
54	RZ	121	HIS	2.3
5	QE	130	ASN	2.3
11	XK	117	ASN	2.3
37	RE	151	TYR	2.3
15	QO	58	MET	2.3
22	XV	16	C	2.3
22	XV	17	C	2.3
34	YA	277	C	2.3
1	QA	108	G	2.3
1	QA	687	A	2.3
9	XI	26	VAL	2.3
23	XX	9	G	2.3
23	XX	12	A	2.3
19	QS	57	HIS	2.3
44	YP	70	GLN	2.3
25	Y1	40	ARG	2.3
2	QB	190	THR	2.3
6	QF	89	MET	2.2
36	RD	35	LYS	2.2
14	QN	42	ILE	2.2
10	XJ	47	PHE	2.2
1	QA	1515	C	2.2
46	RR	106	GLY	2.2
46	RR	108	GLY	2.2
1	XA	1493	A	2.2
34	RA	2712(B)	A	2.2
1	XA	323	U	2.2
20	QT	9	ASN	2.2
20	QT	70	SER	2.2
21	QU	17	THR	2.2
34	RA	568	U	2.2
34	YA	1534	G	2.2
34	YA	2894	G	2.2
10	QJ	23	ILE	2.2
47	RS	35	ILE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
44	RP	71	VAL	2.2
12	XL	89	ARG	2.2
27	R3	34	GLU	2.2
44	YP	61	ARG	2.2
21	XU	4	GLY	2.2
16	QP	12	LYS	2.2
52	RX	3	THR	2.2
3	QC	5	ILE	2.2
21	QU	13	ILE	2.2
37	RE	77	ILE	2.2
2	QB	183	PRO	2.2
1	QA	1357	A	2.2
20	XT	22	ARG	2.2
24	R0	41	ARG	2.2
5	QE	137	GLU	2.2
12	QL	29	GLY	2.2
34	YA	1176	G	2.2
44	RP	66	GLY	2.2
46	RR	9	LYS	2.2
14	QN	27	CYS	2.2
36	RD	16	MET	2.2
42	RN	1	MET	2.2
20	XT	71	THR	2.2
7	XG	33	ASP	2.2
45	RQ	99	PRO	2.2
53	RY	107	ASP	2.2
54	RZ	177	PRO	2.2
17	XQ	101	ARG	2.2
21	XU	9	ARG	2.2
45	RQ	48	GLU	2.2
37	RE	190	GLY	2.2
49	RU	7	GLY	2.2
34	RA	265	A	2.2
34	YA	1026	U	2.2
10	QJ	100	THR	2.2
26	Y2	69	ARG	2.2
19	QS	59	PRO	2.2
4	QD	102	ASP	2.2
4	XD	144	ASP	2.2
8	XH	25	ASP	2.2
48	RT	2	ASN	2.2
26	R2	20	GLU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
20	QT	29	LYS	2.2
32	R8	15	LYS	2.2
37	YE	130	GLY	2.2
48	RT	4	GLY	2.2
54	YZ	113	ALA	2.2
19	QS	9	VAL	2.2
1	QA	622	A	2.2
1	QA	1234	C	2.2
1	XA	1248	A	2.2
7	QG	38	LEU	2.2
14	XN	61	TRP	2.2
20	QT	98	PRO	2.2
22	QV	17	C	2.2
32	R8	32	LEU	2.2
39	RG	34	LEU	2.2
24	R0	5	LYS	2.1
44	YP	87	ASP	2.2
51	RW	77	ASP	2.2
38	YF	207	GLY	2.1
19	QS	75	ALA	2.1
10	QJ	49	VAL	2.1
19	QS	60	VAL	2.1
31	Y7	46	VAL	2.1
34	RA	1089	G	2.1
34	RA	1090	U	2.1
53	RY	41	GLY	2.1
9	XI	15	ALA	2.1
37	RE	204	ALA	2.1
54	RZ	80	ARG	2.1
44	RP	70	GLN	2.1
44	RP	19	VAL	2.1
4	XD	21	LEU	2.1
5	QE	77	PRO	2.1
19	XS	55	LYS	2.1
37	RE	74	PRO	2.1
39	RG	162	THR	2.1
40	RH	106	THR	2.1
36	YD	32	SER	2.1
37	RE	121	ASN	2.1
45	RQ	115	MET	2.1
8	XH	128	GLY	2.1
9	QI	72	GLY	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	QA	1365	G	2.1
9	QI	82	ALA	2.1
12	QL	30	ALA	2.1
34	RA	11	G	2.1
34	YA	274	G	2.1
7	QG	80	VAL	2.1
13	QM	96	LEU	2.1
27	R3	47	VAL	2.1
34	RA	1026	U	2.1
34	YA	2797	U	2.1
9	QI	11	LYS	2.1
14	QN	17	LYS	2.1
1	QA	1103	C	2.1
1	QA	1249	C	2.1
34	RA	2145	C	2.1
34	YA	884	C	2.1
37	RE	107	THR	2.1
42	RN	43	THR	2.1
9	QI	12	GLU	2.1
9	QI	71	SER	2.1
9	XI	115	GLY	2.1
10	QJ	38	ILE	2.1
16	XP	25	ARG	2.1
32	Y8	45	GLY	2.1
47	RS	13	ARG	2.1
46	YR	72	ASP	2.1
19	QS	10	PHE	2.1
36	RD	15	PHE	2.1
37	RE	162	ALA	2.1
8	XH	2	LEU	2.1
54	RZ	183	LEU	2.1
9	XI	118	LYS	2.1
33	Y9	34	GLN	2.1
44	YP	68	GLN	2.1
2	QB	101	MET	2.1
1	QA	1516	G	2.1
1	XA	1537	U	2.1
13	QM	93	ARG	2.1
24	R0	44	ARG	2.1
34	RA	2334	G	2.1
44	RP	79	ARG	2.1
1	QA	1289	A	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	XD	149	ALA	2.1
19	QS	38	SER	2.1
34	RA	1084	A	2.1
1	QA	1533	C	2.1
3	XC	195	VAL	2.1
4	XD	11	LEU	2.1
12	XL	13	LYS	2.1
17	XQ	30	PRO	2.1
9	QI	77	ILE	2.1
10	XJ	67	THR	2.1
19	QS	39	THR	2.1
26	R2	50	ILE	2.1
47	YS	5	THR	2.1
33	Y9	21	GLY	2.1
39	RG	35	GLU	2.1
20	XT	68	LYS	2.1
9	QI	65	VAL	2.1
1	QA	81	G	2.0
1	XA	331	G	2.0
34	RA	1022	G	2.0
41	RI	1	MET	2.0
1	QA	877	C	2.0
34	RA	2723	C	2.0
3	QC	177	THR	2.0
24	R0	43	THR	2.0
9	XI	112	LYS	2.0
20	XT	10	LEU	2.0
25	Y1	27	GLU	2.0
9	XI	105	ASP	2.0
47	RS	88	ASP	2.0
17	QQ	82	MET	2.0
34	RA	2144	U	2.0
34	RA	2332	U	2.0
17	QQ	37	LYS	2.0
32	R8	36	LYS	2.0
1	QA	969	A	2.0
11	QK	46	GLY	2.0
14	QN	48	ALA	2.0
23	QX	15	A	2.0
32	Y8	40	GLU	2.0
34	RA	226	G	2.0
1	XA	979	C	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	XA	1367	C	2.0
22	QV	1	C	2.0
8	XH	87	SER	2.0
13	QM	97	PRO	2.0
50	YV	50	PRO	2.0
20	QT	24	LEU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
22	1MG	QV	37	24/25	0.72	0.13	187,197,202,203	0
22	1MG	XV	37	24/25	0.73	0.13	183,186,189,189	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
55	MG	YA	3323	1/1	0.14	0.22	208,208,208,208	0
55	MG	RA	3288	1/1	0.40	0.24	110,110,110,110	0
55	MG	QA	1615	1/1	0.42	0.11	79,79,79,79	0
55	MG	RA	3221	1/1	0.43	0.14	74,74,74,74	0
55	MG	YA	3216	1/1	0.48	0.17	53,53,53,53	0
55	MG	RA	3166	1/1	0.49	0.13	70,70,70,70	0
55	MG	YA	3015	1/1	0.51	0.45	76,76,76,76	0
55	MG	YA	3016	1/1	0.51	0.38	39,39,39,39	0
55	MG	XA	1660	1/1	0.52	0.15	62,62,62,62	0
55	MG	YA	3044	1/1	0.53	0.11	90,90,90,90	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	YA	3289	1/1	0.53	0.07	11,11,11,11	0
55	MG	YA	3075	1/1	0.53	0.29	56,56,56,56	0
55	MG	RA	3185	1/1	0.55	0.12	56,56,56,56	0
55	MG	YA	3384	1/1	0.55	0.14	66,66,66,66	0
55	MG	YA	3291	1/1	0.58	0.38	64,64,64,64	0
55	MG	YA	3045	1/1	0.60	0.16	53,53,53,53	0
55	MG	YA	3175	1/1	0.61	0.16	54,54,54,54	0
55	MG	YA	3062	1/1	0.61	0.27	63,63,63,63	0
55	MG	RA	3214	1/1	0.61	0.21	43,43,43,43	0
55	MG	RA	3371	1/1	0.63	0.12	74,74,74,74	0
55	MG	YA	3220	1/1	0.63	0.26	47,47,47,47	0
55	MG	Y2	101	1/1	0.64	0.13	79,79,79,79	0
55	MG	YA	3195	1/1	0.64	0.20	46,46,46,46	0
55	MG	YA	3383	1/1	0.65	0.14	47,47,47,47	0
55	MG	XA	1674	1/1	0.66	0.14	34,34,34,34	0
55	MG	XA	1688	1/1	0.66	0.16	67,67,67,67	0
55	MG	RB	209	1/1	0.67	0.11	51,51,51,51	0
55	MG	YA	3316	1/1	0.68	0.11	44,44,44,44	0
55	MG	XA	1627	1/1	0.69	0.16	55,55,55,55	0
55	MG	RA	3001	1/1	0.69	0.17	50,50,50,50	0
55	MG	XA	1623	1/1	0.69	0.08	102,102,102,102	0
55	MG	YA	3422	1/1	0.69	0.10	52,52,52,52	0
55	MG	RA	3186	1/1	0.70	0.19	63,63,63,63	0
55	MG	YA	3419	1/1	0.71	0.10	35,35,35,35	0
55	MG	YA	3025	1/1	0.71	0.29	50,50,50,50	0
55	MG	YA	3055	1/1	0.72	0.20	35,35,35,35	0
55	MG	XA	1679	1/1	0.72	0.14	62,62,62,62	0
55	MG	RB	207	1/1	0.72	0.26	56,56,56,56	0
55	MG	RA	3294	1/1	0.72	0.10	52,52,52,52	0
55	MG	RA	3178	1/1	0.72	0.26	48,48,48,48	0
55	MG	YA	3425	1/1	0.72	0.23	11,11,11,11	0
55	MG	RA	3202	1/1	0.73	0.20	38,38,38,38	0
55	MG	XA	1643	1/1	0.73	0.15	52,52,52,52	0
55	MG	QA	1647	1/1	0.73	0.14	64,64,64,64	0
55	MG	RA	3424	1/1	0.73	0.21	40,40,40,40	0
55	MG	RA	3416	1/1	0.74	0.14	49,49,49,49	0
55	MG	RA	3068	1/1	0.74	0.12	41,41,41,41	0
55	MG	RA	3133	1/1	0.74	0.11	76,76,76,76	0
55	MG	RA	3042	1/1	0.74	0.09	52,52,52,52	0
55	MG	YA	3368	1/1	0.74	0.21	24,24,24,24	0
55	MG	RA	3265	1/1	0.75	0.09	66,66,66,66	0
55	MG	RA	3122	1/1	0.75	0.14	37,37,37,37	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	RA	3048	1/1	0.75	0.11	52,52,52,52	0
55	MG	RA	3345	1/1	0.75	0.19	64,64,64,64	0
55	MG	YA	3330	1/1	0.75	0.14	50,50,50,50	0
55	MG	RB	210	1/1	0.75	0.08	44,44,44,44	0
55	MG	RA	3365	1/1	0.75	0.12	65,65,65,65	0
55	MG	RA	3015	1/1	0.75	0.15	62,62,62,62	0
55	MG	YA	3397	1/1	0.75	0.14	42,42,42,42	0
55	MG	RA	3400	1/1	0.75	0.27	43,43,43,43	0
55	MG	YA	3040	1/1	0.75	0.15	23,23,23,23	0
55	MG	YA	3268	1/1	0.75	0.18	45,45,45,45	0
55	MG	RA	3299	1/1	0.76	0.20	46,46,46,46	0
55	MG	RA	3387	1/1	0.76	0.10	67,67,67,67	0
55	MG	RA	3330	1/1	0.76	0.29	47,47,47,47	0
55	MG	QA	1601	1/1	0.76	0.10	50,50,50,50	0
55	MG	RA	3010	1/1	0.76	0.17	76,76,76,76	0
55	MG	RB	202	1/1	0.76	0.10	53,53,53,53	0
55	MG	YA	3317	1/1	0.76	0.17	31,31,31,31	0
55	MG	RA	3370	1/1	0.76	0.12	52,52,52,52	0
55	MG	RA	3024	1/1	0.77	0.09	77,77,77,77	0
55	MG	QA	1621	1/1	0.77	0.17	65,65,65,65	0
55	MG	RA	3002	1/1	0.77	0.12	50,50,50,50	0
55	MG	QA	1660	1/1	0.77	0.09	59,59,59,59	0
55	MG	RA	3084	1/1	0.77	0.09	61,61,61,61	0
55	MG	QA	1679	1/1	0.77	0.07	48,48,48,48	0
55	MG	YA	3245	1/1	0.78	0.43	62,62,62,62	0
55	MG	QA	1614	1/1	0.78	0.07	45,45,45,45	0
55	MG	YA	3276	1/1	0.78	0.13	41,41,41,41	0
55	MG	RA	3135	1/1	0.78	0.10	108,108,108,108	0
55	MG	RA	3255	1/1	0.78	0.09	57,57,57,57	0
55	MG	RA	3097	1/1	0.78	0.09	54,54,54,54	0
55	MG	RA	3379	1/1	0.78	0.17	66,66,66,66	0
55	MG	RA	3274	1/1	0.78	0.10	55,55,55,55	0
55	MG	RA	3098	1/1	0.78	0.15	50,50,50,50	0
55	MG	RA	3119	1/1	0.78	0.12	48,48,48,48	0
55	MG	RA	3421	1/1	0.78	0.22	14,14,14,14	0
55	MG	RA	3423	1/1	0.78	0.36	52,52,52,52	0
55	MG	QA	1685	1/1	0.78	0.10	56,56,56,56	0
55	MG	RA	3127	1/1	0.78	0.13	49,49,49,49	0
55	MG	YA	3224	1/1	0.78	0.21	59,59,59,59	0
55	MG	YA	3227	1/1	0.78	0.09	51,51,51,51	0
55	MG	RA	3417	1/1	0.79	0.18	55,55,55,55	0
55	MG	RA	3368	1/1	0.79	0.12	45,45,45,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	RA	3160	1/1	0.79	0.13	65,65,65,65	0
55	MG	RA	3089	1/1	0.79	0.31	65,65,65,65	0
55	MG	RA	3167	1/1	0.79	0.11	48,48,48,48	0
55	MG	RA	3049	1/1	0.79	0.11	57,57,57,57	0
55	MG	QH	201	1/1	0.79	0.10	57,57,57,57	0
55	MG	XA	1689	1/1	0.79	0.18	51,51,51,51	0
55	MG	YA	3068	1/1	0.79	0.16	45,45,45,45	0
55	MG	QA	1645	1/1	0.79	0.16	49,49,49,49	0
55	MG	YA	3126	1/1	0.79	0.13	51,51,51,51	0
55	MG	YB	206	1/1	0.79	0.10	51,51,51,51	0
55	MG	RA	3254	1/1	0.80	0.20	68,68,68,68	0
55	MG	YA	3031	1/1	0.80	0.08	48,48,48,48	0
55	MG	RA	3207	1/1	0.80	0.10	52,52,52,52	0
55	MG	YA	3217	1/1	0.80	0.16	50,50,50,50	0
55	MG	QA	1607	1/1	0.80	0.07	58,58,58,58	0
55	MG	RA	3168	1/1	0.80	0.13	49,49,49,49	0
55	MG	RA	3252	1/1	0.81	0.14	60,60,60,60	0
55	MG	RA	3304	1/1	0.81	0.09	37,37,37,37	0
55	MG	YA	3271	1/1	0.81	0.10	15,15,15,15	0
55	MG	RA	3060	1/1	0.81	0.07	62,62,62,62	0
55	MG	RA	3103	1/1	0.81	0.20	64,64,64,64	0
55	MG	QA	1646	1/1	0.81	0.08	63,63,63,63	0
55	MG	QA	1676	1/1	0.81	0.07	50,50,50,50	0
55	MG	RA	3025	1/1	0.81	0.07	49,49,49,49	0
55	MG	RA	3055	1/1	0.81	0.10	53,53,53,53	0
55	MG	RA	3121	1/1	0.82	0.25	40,40,40,40	0
55	MG	YA	3120	1/1	0.82	0.26	27,27,27,27	0
55	MG	RA	3354	1/1	0.82	0.10	54,54,54,54	0
55	MG	QA	1686	1/1	0.82	0.11	49,49,49,49	0
55	MG	RA	3096	1/1	0.82	0.11	66,66,66,66	0
55	MG	QA	1634	1/1	0.82	0.12	30,30,30,30	0
55	MG	YA	3357	1/1	0.82	0.16	37,37,37,37	0
55	MG	RA	3285	1/1	0.82	0.07	48,48,48,48	0
55	MG	RO	201	1/1	0.82	0.11	69,69,69,69	0
55	MG	RA	3032	1/1	0.82	0.24	76,76,76,76	0
55	MG	RA	3158	1/1	0.82	0.19	42,42,42,42	0
55	MG	QA	1677	1/1	0.82	0.21	50,50,50,50	0
55	MG	RA	3118	1/1	0.82	0.22	35,35,35,35	0
55	MG	RA	3316	1/1	0.82	0.10	41,41,41,41	0
55	MG	RA	3021	1/1	0.82	0.13	62,62,62,62	0
55	MG	RA	3262	1/1	0.83	0.14	56,56,56,56	0
55	MG	QA	1612	1/1	0.83	0.12	71,71,71,71	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	YA	3233	1/1	0.83	0.15	62,62,62,62	0
55	MG	QA	1648	1/1	0.83	0.17	44,44,44,44	0
55	MG	YA	3043	1/1	0.83	0.10	33,33,33,33	0
55	MG	RA	3276	1/1	0.83	0.09	48,48,48,48	0
55	MG	XA	1612	1/1	0.83	0.18	61,61,61,61	0
55	MG	YA	3048	1/1	0.83	0.16	36,36,36,36	0
55	MG	YA	3051	1/1	0.83	0.19	36,36,36,36	0
55	MG	RA	3211	1/1	0.83	0.15	37,37,37,37	0
55	MG	QA	1613	1/1	0.83	0.14	69,69,69,69	0
55	MG	RA	3384	1/1	0.83	0.13	27,27,27,27	0
55	MG	R0	102	1/1	0.83	0.06	40,40,40,40	0
55	MG	YA	3333	1/1	0.83	0.18	44,44,44,44	0
55	MG	YA	3087	1/1	0.83	0.16	35,35,35,35	0
55	MG	RA	3222	1/1	0.83	0.17	68,68,68,68	0
55	MG	RA	3303	1/1	0.83	0.19	47,47,47,47	0
55	MG	RA	3250	1/1	0.83	0.11	51,51,51,51	0
55	MG	YA	3394	1/1	0.83	0.13	34,34,34,34	0
55	MG	RA	3312	1/1	0.83	0.12	64,64,64,64	0
55	MG	YA	3214	1/1	0.83	0.09	49,49,49,49	0
55	MG	RA	3120	1/1	0.83	0.14	40,40,40,40	0
55	MG	RA	3033	1/1	0.83	0.13	59,59,59,59	0
55	MG	RA	3187	1/1	0.83	0.06	81,81,81,81	0
55	MG	RB	211	1/1	0.84	0.07	62,62,62,62	0
55	MG	YA	3278	1/1	0.84	0.15	34,34,34,34	0
55	MG	YA	3107	1/1	0.84	0.09	27,27,27,27	0
55	MG	RA	3009	1/1	0.84	0.14	59,59,59,59	0
55	MG	RP	201	1/1	0.84	0.28	48,48,48,48	0
55	MG	RA	3248	1/1	0.84	0.09	45,45,45,45	0
55	MG	YA	3417	1/1	0.84	0.12	39,39,39,39	0
55	MG	RA	3401	1/1	0.84	0.10	83,83,83,83	0
55	MG	RA	3094	1/1	0.84	0.12	54,54,54,54	0
55	MG	XA	1642	1/1	0.84	0.10	43,43,43,43	0
55	MG	YA	3438	1/1	0.84	0.07	13,13,13,13	0
55	MG	YA	3352	1/1	0.84	0.13	15,15,15,15	0
57	ZN	R9	101	1/1	0.84	0.13	110,110,110,110	0
55	MG	RA	3203	1/1	0.85	0.20	44,44,44,44	0
55	MG	RA	3023	1/1	0.85	0.07	28,28,28,28	0
55	MG	RA	3005	1/1	0.85	0.09	39,39,39,39	0
55	MG	QA	1617	1/1	0.85	0.18	54,54,54,54	0
55	MG	XA	1629	1/1	0.85	0.16	41,41,41,41	0
55	MG	RA	3219	1/1	0.85	0.15	55,55,55,55	0
55	MG	RA	3289	1/1	0.85	0.17	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	XA	1648	1/1	0.85	0.09	46,46,46,46	0
55	MG	QA	1637	1/1	0.85	0.08	46,46,46,46	0
55	MG	YA	3088	1/1	0.85	0.10	34,34,34,34	0
55	MG	RA	3169	1/1	0.85	0.07	44,44,44,44	0
55	MG	YA	3349	1/1	0.85	0.07	48,48,48,48	0
55	MG	RA	3226	1/1	0.85	0.11	37,37,37,37	0
55	MG	XA	1687	1/1	0.85	0.15	47,47,47,47	0
55	MG	YA	3364	1/1	0.85	0.12	16,16,16,16	0
55	MG	RA	3131	1/1	0.85	0.10	57,57,57,57	0
55	MG	YA	3188	1/1	0.85	0.11	52,52,52,52	0
55	MG	RA	3305	1/1	0.85	0.17	48,48,48,48	0
55	MG	RA	3184	1/1	0.85	0.10	44,44,44,44	0
55	MG	Y5	102	1/1	0.85	0.12	18,18,18,18	0
55	MG	QA	1663	1/1	0.85	0.14	51,51,51,51	0
55	MG	QA	1642	1/1	0.85	0.08	62,62,62,62	0
55	MG	RA	3143	1/1	0.85	0.18	52,52,52,52	0
55	MG	RA	3258	1/1	0.85	0.07	49,49,49,49	0
55	MG	RA	3261	1/1	0.85	0.10	32,32,32,32	0
55	MG	YA	3242	1/1	0.85	0.23	27,27,27,27	0
55	MG	RA	3043	1/1	0.85	0.08	57,57,57,57	0
55	MG	QA	1659	1/1	0.86	0.14	49,49,49,49	0
55	MG	RA	3378	1/1	0.86	0.12	53,53,53,53	0
55	MG	QA	1630	1/1	0.86	0.12	43,43,43,43	0
55	MG	RA	3070	1/1	0.86	0.26	51,51,51,51	0
55	MG	XA	1632	1/1	0.86	0.13	40,40,40,40	0
55	MG	YA	3060	1/1	0.86	0.14	38,38,38,38	0
55	MG	RA	3220	1/1	0.86	0.17	72,72,72,72	0
55	MG	RA	3388	1/1	0.86	0.12	41,41,41,41	0
55	MG	RA	3080	1/1	0.86	0.10	33,33,33,33	0
55	MG	XA	1651	1/1	0.86	0.08	25,25,25,25	0
55	MG	RA	3175	1/1	0.86	0.12	51,51,51,51	0
55	MG	QA	1627	1/1	0.86	0.15	41,41,41,41	0
55	MG	RA	3231	1/1	0.86	0.15	50,50,50,50	0
55	MG	RA	3181	1/1	0.86	0.15	55,55,55,55	0
55	MG	YA	3143	1/1	0.86	0.08	9,9,9,9	0
55	MG	YA	3145	1/1	0.86	0.12	38,38,38,38	0
55	MG	RA	3040	1/1	0.86	0.27	53,53,53,53	0
55	MG	YA	3180	1/1	0.86	0.17	14,14,14,14	0
55	MG	YA	3183	1/1	0.86	0.09	47,47,47,47	0
55	MG	QA	1687	1/1	0.86	0.08	70,70,70,70	0
55	MG	YA	3387	1/1	0.86	0.23	47,47,47,47	0
55	MG	YA	3391	1/1	0.86	0.21	44,44,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	QA	1674	1/1	0.86	0.09	41,41,41,41	0
55	MG	YA	3201	1/1	0.86	0.21	40,40,40,40	0
55	MG	RB	206	1/1	0.86	0.11	24,24,24,24	0
55	MG	QH	202	1/1	0.86	0.20	45,45,45,45	0
55	MG	RA	3195	1/1	0.86	0.23	32,32,32,32	0
55	MG	QA	1655	1/1	0.86	0.07	44,44,44,44	0
55	MG	QA	1658	1/1	0.86	0.18	49,49,49,49	0
55	MG	RA	3110	1/1	0.86	0.09	45,45,45,45	0
55	MG	RA	3269	1/1	0.86	0.17	52,52,52,52	0
55	MG	RA	3429	1/1	0.87	0.12	40,40,40,40	0
55	MG	YA	3177	1/1	0.87	0.19	41,41,41,41	0
55	MG	YA	3034	1/1	0.87	0.22	15,15,15,15	0
55	MG	RA	3190	1/1	0.87	0.18	61,61,61,61	0
55	MG	RA	3030	1/1	0.87	0.23	57,57,57,57	0
55	MG	YA	3341	1/1	0.87	0.12	32,32,32,32	0
55	MG	YA	3348	1/1	0.87	0.09	27,27,27,27	0
55	MG	RA	3266	1/1	0.87	0.09	59,59,59,59	0
55	MG	XA	1658	1/1	0.87	0.17	31,31,31,31	0
55	MG	QA	1669	1/1	0.87	0.30	47,47,47,47	0
55	MG	XA	1669	1/1	0.87	0.07	45,45,45,45	0
55	MG	QA	1609	1/1	0.87	0.06	46,46,46,46	0
55	MG	YA	3377	1/1	0.87	0.11	47,47,47,47	0
55	MG	RA	3395	1/1	0.87	0.07	54,54,54,54	0
55	MG	RA	3035	1/1	0.87	0.15	40,40,40,40	0
55	MG	RA	3279	1/1	0.87	0.14	28,28,28,28	0
55	MG	YA	3390	1/1	0.87	0.24	39,39,39,39	0
55	MG	QA	1623	1/1	0.87	0.12	49,49,49,49	0
55	MG	YA	3234	1/1	0.87	0.20	27,27,27,27	0
55	MG	XE	201	1/1	0.87	0.08	53,53,53,53	0
55	MG	QA	1605	1/1	0.87	0.16	45,45,45,45	0
55	MG	XA	1626	1/1	0.87	0.11	54,54,54,54	0
55	MG	QA	1628	1/1	0.87	0.10	40,40,40,40	0
55	MG	QA	1662	1/1	0.87	0.16	45,45,45,45	0
55	MG	QA	1654	1/1	0.87	0.18	36,36,36,36	0
55	MG	YA	3028	1/1	0.87	0.22	1,1,1,1	0
55	MG	YA	3147	1/1	0.87	0.16	39,39,39,39	0
55	MG	RA	3209	1/1	0.88	0.06	53,53,53,53	0
55	MG	RA	3327	1/1	0.88	0.10	47,47,47,47	0
55	MG	RA	3069	1/1	0.88	0.16	22,22,22,22	0
55	MG	QA	1673	1/1	0.88	0.10	51,51,51,51	0
55	MG	RA	3346	1/1	0.88	0.12	61,61,61,61	0
55	MG	YA	3036	1/1	0.88	0.26	18,18,18,18	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	RA	3351	1/1	0.88	0.10	22,22,22,22	0
55	MG	RA	3216	1/1	0.88	0.13	59,59,59,59	0
55	MG	XA	1601	1/1	0.88	0.10	69,69,69,69	0
55	MG	XA	1604	1/1	0.88	0.08	61,61,61,61	0
55	MG	XA	1609	1/1	0.88	0.11	53,53,53,53	0
55	MG	RA	3268	1/1	0.88	0.09	62,62,62,62	0
55	MG	YA	3304	1/1	0.88	0.16	37,37,37,37	0
55	MG	YA	3053	1/1	0.88	0.11	25,25,25,25	0
55	MG	RA	3218	1/1	0.88	0.19	34,34,34,34	0
55	MG	RA	3018	1/1	0.88	0.24	48,48,48,48	0
55	MG	RA	3020	1/1	0.88	0.18	38,38,38,38	0
55	MG	RA	3278	1/1	0.88	0.07	47,47,47,47	0
55	MG	YA	3336	1/1	0.88	0.14	56,56,56,56	0
55	MG	YA	3338	1/1	0.88	0.22	49,49,49,49	0
55	MG	XA	1630	1/1	0.88	0.09	53,53,53,53	0
55	MG	QA	1618	1/1	0.88	0.14	60,60,60,60	0
55	MG	RA	3383	1/1	0.88	0.10	31,31,31,31	0
55	MG	YA	3092	1/1	0.88	0.17	38,38,38,38	0
55	MG	RA	3284	1/1	0.88	0.11	30,30,30,30	0
55	MG	QA	1622	1/1	0.88	0.09	43,43,43,43	0
55	MG	QA	1620	1/1	0.88	0.14	50,50,50,50	0
55	MG	RA	3134	1/1	0.88	0.07	83,83,83,83	0
55	MG	XA	1659	1/1	0.88	0.10	29,29,29,29	0
55	MG	RA	3008	1/1	0.88	0.13	45,45,45,45	0
55	MG	RA	3296	1/1	0.88	0.16	65,65,65,65	0
55	MG	YA	3388	1/1	0.88	0.11	20,20,20,20	0
55	MG	QA	1670	1/1	0.88	0.07	40,40,40,40	0
55	MG	XA	1677	1/1	0.88	0.11	42,42,42,42	0
55	MG	RA	3099	1/1	0.88	0.08	32,32,32,32	0
55	MG	RA	3420	1/1	0.88	0.12	40,40,40,40	0
55	MG	YA	3416	1/1	0.88	0.15	41,41,41,41	0
55	MG	RA	3031	1/1	0.88	0.10	17,17,17,17	0
55	MG	RA	3061	1/1	0.88	0.15	25,25,25,25	0
55	MG	RA	3306	1/1	0.88	0.07	55,55,55,55	0
55	MG	YA	3215	1/1	0.88	0.10	60,60,60,60	0
55	MG	YA	3430	1/1	0.88	0.11	27,27,27,27	0
55	MG	YA	3431	1/1	0.88	0.10	31,31,31,31	0
55	MG	RA	3427	1/1	0.88	0.10	47,47,47,47	0
55	MG	RA	3311	1/1	0.88	0.17	58,58,58,58	0
55	MG	R0	101	1/1	0.88	0.12	69,69,69,69	0
55	MG	YA	3281	1/1	0.89	0.10	51,51,51,51	0
55	MG	RA	3286	1/1	0.89	0.16	35,35,35,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	RA	3189	1/1	0.89	0.10	35,35,35,35	0
55	MG	YA	3298	1/1	0.89	0.12	28,28,28,28	0
55	MG	YA	3091	1/1	0.89	0.06	24,24,24,24	0
55	MG	XA	1619	1/1	0.89	0.09	39,39,39,39	0
55	MG	YA	3095	1/1	0.89	0.09	21,21,21,21	0
55	MG	YA	3318	1/1	0.89	0.17	40,40,40,40	0
55	MG	XA	1620	1/1	0.89	0.19	54,54,54,54	0
55	MG	QA	1638	1/1	0.89	0.09	58,58,58,58	0
55	MG	XA	1625	1/1	0.89	0.07	56,56,56,56	0
55	MG	YA	3136	1/1	0.89	0.08	29,29,29,29	0
55	MG	RA	3147	1/1	0.89	0.07	34,34,34,34	0
55	MG	RA	3362	1/1	0.89	0.15	67,67,67,67	0
55	MG	RA	3198	1/1	0.89	0.09	41,41,41,41	0
55	MG	RA	3150	1/1	0.89	0.10	47,47,47,47	0
55	MG	RA	3152	1/1	0.89	0.12	44,44,44,44	0
55	MG	QA	1668	1/1	0.89	0.11	53,53,53,53	0
55	MG	YA	3361	1/1	0.89	0.14	16,16,16,16	0
55	MG	YA	3032	1/1	0.89	0.05	60,60,60,60	0
55	MG	RA	3237	1/1	0.89	0.06	39,39,39,39	0
55	MG	XA	1646	1/1	0.89	0.06	69,69,69,69	0
55	MG	YA	3196	1/1	0.89	0.15	33,33,33,33	0
55	MG	YA	3199	1/1	0.89	0.11	58,58,58,58	0
55	MG	RA	3093	1/1	0.89	0.07	20,20,20,20	0
55	MG	XA	1649	1/1	0.89	0.14	46,46,46,46	0
55	MG	RA	3310	1/1	0.89	0.06	57,57,57,57	0
55	MG	RA	3249	1/1	0.89	0.08	58,58,58,58	0
55	MG	YA	3047	1/1	0.89	0.17	48,48,48,48	0
55	MG	RA	3163	1/1	0.89	0.05	28,28,28,28	0
55	MG	YA	3403	1/1	0.89	0.09	26,26,26,26	0
55	MG	RA	3014	1/1	0.89	0.10	55,55,55,55	0
55	MG	XA	1668	1/1	0.89	0.15	73,73,73,73	0
55	MG	YA	3054	1/1	0.89	0.17	36,36,36,36	0
55	MG	RA	3253	1/1	0.89	0.09	28,28,28,28	0
55	MG	XA	1670	1/1	0.89	0.06	56,56,56,56	0
55	MG	RA	3137	1/1	0.89	0.20	52,52,52,52	0
55	MG	YA	3067	1/1	0.89	0.18	43,43,43,43	0
55	MG	RA	3341	1/1	0.89	0.10	52,52,52,52	0
55	MG	XA	1678	1/1	0.89	0.17	40,40,40,40	0
55	MG	YF	301	1/1	0.89	0.09	26,26,26,26	0
55	MG	YA	3080	1/1	0.89	0.19	52,52,52,52	0
55	MG	XA	1667	1/1	0.90	0.11	48,48,48,48	0
55	MG	YA	3275	1/1	0.90	0.14	45,45,45,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	YA	3071	1/1	0.90	0.08	38,38,38,38	0
55	MG	RA	3291	1/1	0.90	0.14	46,46,46,46	0
55	MG	YA	3079	1/1	0.90	0.19	18,18,18,18	0
55	MG	RB	208	1/1	0.90	0.17	57,57,57,57	0
55	MG	RA	3293	1/1	0.90	0.09	27,27,27,27	0
55	MG	RA	3138	1/1	0.90	0.10	45,45,45,45	0
55	MG	YA	3089	1/1	0.90	0.07	19,19,19,19	0
55	MG	RA	3045	1/1	0.90	0.07	41,41,41,41	0
55	MG	RD	301	1/1	0.90	0.22	38,38,38,38	0
55	MG	YA	3094	1/1	0.90	0.27	40,40,40,40	0
55	MG	RF	302	1/1	0.90	0.12	46,46,46,46	0
55	MG	YA	3325	1/1	0.90	0.13	61,61,61,61	0
55	MG	YA	3100	1/1	0.90	0.14	28,28,28,28	0
55	MG	RN	201	1/1	0.90	0.06	48,48,48,48	0
55	MG	RA	3027	1/1	0.90	0.12	44,44,44,44	0
55	MG	RA	3091	1/1	0.90	0.10	36,36,36,36	0
55	MG	QA	1682	1/1	0.90	0.08	38,38,38,38	0
55	MG	QA	1640	1/1	0.90	0.10	49,49,49,49	0
55	MG	RA	3126	1/1	0.90	0.07	46,46,46,46	0
55	MG	RA	3224	1/1	0.90	0.15	44,44,44,44	0
55	MG	YA	3170	1/1	0.90	0.17	17,17,17,17	0
55	MG	YA	3360	1/1	0.90	0.24	6,6,6,6	0
55	MG	RA	3394	1/1	0.90	0.08	44,44,44,44	0
55	MG	YA	3176	1/1	0.90	0.16	26,26,26,26	0
55	MG	RA	3270	1/1	0.90	0.08	53,53,53,53	0
55	MG	YA	3369	1/1	0.90	0.13	39,39,39,39	0
55	MG	RA	3399	1/1	0.90	0.06	45,45,45,45	0
55	MG	YA	3380	1/1	0.90	0.16	34,34,34,34	0
55	MG	RA	3161	1/1	0.90	0.08	39,39,39,39	0
55	MG	RA	3162	1/1	0.90	0.15	47,47,47,47	0
55	MG	RA	3410	1/1	0.90	0.14	36,36,36,36	0
55	MG	RA	3415	1/1	0.90	0.11	35,35,35,35	0
55	MG	QA	1661	1/1	0.90	0.10	50,50,50,50	0
55	MG	QA	1635	1/1	0.90	0.18	50,50,50,50	0
55	MG	XA	1638	1/1	0.90	0.12	49,49,49,49	0
55	MG	YA	3395	1/1	0.90	0.08	31,31,31,31	0
55	MG	RA	3418	1/1	0.90	0.21	43,43,43,43	0
55	MG	YA	3401	1/1	0.90	0.12	17,17,17,17	0
55	MG	RA	3283	1/1	0.90	0.06	49,49,49,49	0
55	MG	YA	3412	1/1	0.90	0.11	31,31,31,31	0
55	MG	QA	1606	1/1	0.90	0.26	40,40,40,40	0
55	MG	QA	1629	1/1	0.90	0.07	41,41,41,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	QA	1639	1/1	0.90	0.06	41,41,41,41	0
55	MG	YA	3420	1/1	0.90	0.07	35,35,35,35	0
55	MG	XA	1650	1/1	0.90	0.07	43,43,43,43	0
55	MG	YA	3423	1/1	0.90	0.18	52,52,52,52	0
55	MG	RA	3013	1/1	0.90	0.15	66,66,66,66	0
55	MG	RA	3356	1/1	0.90	0.07	47,47,47,47	0
55	MG	YA	3238	1/1	0.90	0.14	37,37,37,37	0
55	MG	YA	3436	1/1	0.90	0.08	23,23,23,23	0
55	MG	RA	3213	1/1	0.90	0.11	56,56,56,56	0
55	MG	YB	201	1/1	0.90	0.08	17,17,17,17	0
55	MG	YB	202	1/1	0.90	0.09	26,26,26,26	0
55	MG	YA	3244	1/1	0.90	0.13	43,43,43,43	0
55	MG	YD	301	1/1	0.90	0.13	28,28,28,28	0
55	MG	YA	3066	1/1	0.90	0.23	35,35,35,35	0
55	MG	YR	201	1/1	0.90	0.16	25,25,25,25	0
57	ZN	QN	101	1/1	0.90	0.08	158,158,158,158	0
55	MG	RA	3364	1/1	0.90	0.08	36,36,36,36	0
55	MG	XA	1647	1/1	0.91	0.05	49,49,49,49	0
55	MG	RA	3376	1/1	0.91	0.12	59,59,59,59	0
55	MG	QL	201	1/1	0.91	0.06	55,55,55,55	0
55	MG	YA	3342	1/1	0.91	0.07	59,59,59,59	0
55	MG	YA	3345	1/1	0.91	0.12	43,43,43,43	0
55	MG	YA	3182	1/1	0.91	0.08	49,49,49,49	0
55	MG	RA	3086	1/1	0.91	0.06	30,30,30,30	0
55	MG	QA	1650	1/1	0.91	0.16	36,36,36,36	0
55	MG	YA	3353	1/1	0.91	0.11	34,34,34,34	0
55	MG	QA	1672	1/1	0.91	0.10	40,40,40,40	0
55	MG	RA	3272	1/1	0.91	0.07	53,53,53,53	0
55	MG	RE	301	1/1	0.91	0.11	36,36,36,36	0
55	MG	QA	1678	1/1	0.91	0.09	41,41,41,41	0
55	MG	YA	3367	1/1	0.91	0.16	31,31,31,31	0
55	MG	YA	3206	1/1	0.91	0.22	9,9,9,9	0
55	MG	RA	3314	1/1	0.91	0.12	37,37,37,37	0
55	MG	YA	3370	1/1	0.91	0.07	19,19,19,19	0
55	MG	QA	1653	1/1	0.91	0.08	49,49,49,49	0
55	MG	RA	3236	1/1	0.91	0.19	57,57,57,57	0
55	MG	RA	3062	1/1	0.91	0.26	44,44,44,44	0
55	MG	XA	1603	1/1	0.91	0.07	44,44,44,44	0
55	MG	RA	3165	1/1	0.91	0.16	50,50,50,50	0
55	MG	RA	3402	1/1	0.91	0.06	67,67,67,67	0
55	MG	XA	1686	1/1	0.91	0.15	41,41,41,41	0
55	MG	RA	3406	1/1	0.91	0.07	28,28,28,28	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	RA	3066	1/1	0.91	0.21	43,43,43,43	0
55	MG	RA	3067	1/1	0.91	0.10	28,28,28,28	0
55	MG	QA	1633	1/1	0.91	0.23	43,43,43,43	0
55	MG	RA	3101	1/1	0.91	0.08	43,43,43,43	0
55	MG	YA	3258	1/1	0.91	0.13	56,56,56,56	0
55	MG	YA	3404	1/1	0.91	0.09	26,26,26,26	0
55	MG	YA	3405	1/1	0.91	0.09	22,22,22,22	0
55	MG	YA	3409	1/1	0.91	0.28	43,43,43,43	0
55	MG	YA	3261	1/1	0.91	0.08	19,19,19,19	0
55	MG	YA	3413	1/1	0.91	0.25	62,62,62,62	0
55	MG	YA	3414	1/1	0.91	0.07	41,41,41,41	0
55	MG	RA	3029	1/1	0.91	0.15	42,42,42,42	0
55	MG	YA	3002	1/1	0.91	0.12	29,29,29,29	0
55	MG	YA	3272	1/1	0.91	0.19	48,48,48,48	0
55	MG	YA	3274	1/1	0.91	0.20	38,38,38,38	0
55	MG	YA	3421	1/1	0.91	0.08	44,44,44,44	0
55	MG	YA	3003	1/1	0.91	0.09	21,21,21,21	0
55	MG	YA	3004	1/1	0.91	0.18	33,33,33,33	0
55	MG	YA	3103	1/1	0.91	0.06	22,22,22,22	0
55	MG	RA	3177	1/1	0.91	0.09	42,42,42,42	0
55	MG	YA	3109	1/1	0.91	0.06	36,36,36,36	0
55	MG	YA	3115	1/1	0.91	0.18	3,3,3,3	0
55	MG	RA	3257	1/1	0.91	0.11	47,47,47,47	0
55	MG	RA	3139	1/1	0.91	0.05	58,58,58,58	0
55	MG	RA	3217	1/1	0.91	0.08	52,52,52,52	0
55	MG	YA	3139	1/1	0.91	0.15	41,41,41,41	0
55	MG	XA	1633	1/1	0.91	0.09	47,47,47,47	0
55	MG	RA	3006	1/1	0.91	0.10	30,30,30,30	0
55	MG	RA	3046	1/1	0.91	0.08	56,56,56,56	0
55	MG	YX	101	1/1	0.91	0.09	37,37,37,37	0
55	MG	RA	3374	1/1	0.91	0.10	37,37,37,37	0
55	MG	RA	3375	1/1	0.91	0.07	46,46,46,46	0
55	MG	YA	3312	1/1	0.92	0.17	12,12,12,12	0
55	MG	YA	3315	1/1	0.92	0.04	47,47,47,47	0
55	MG	XA	1672	1/1	0.92	0.07	47,47,47,47	0
55	MG	QA	1608	1/1	0.92	0.07	44,44,44,44	0
55	MG	QA	1649	1/1	0.92	0.09	40,40,40,40	0
55	MG	QA	1641	1/1	0.92	0.16	41,41,41,41	0
55	MG	YA	3101	1/1	0.92	0.07	22,22,22,22	0
55	MG	YA	3327	1/1	0.92	0.10	26,26,26,26	0
55	MG	RA	3238	1/1	0.92	0.16	23,23,23,23	0
55	MG	XA	1682	1/1	0.92	0.06	33,33,33,33	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	XA	1685	1/1	0.92	0.19	41,41,41,41	0
55	MG	RA	3372	1/1	0.92	0.06	59,59,59,59	0
55	MG	RA	3242	1/1	0.92	0.17	25,25,25,25	0
55	MG	QA	1651	1/1	0.92	0.16	36,36,36,36	0
55	MG	RA	3193	1/1	0.92	0.09	52,52,52,52	0
55	MG	RA	3295	1/1	0.92	0.09	38,38,38,38	0
55	MG	YA	3141	1/1	0.92	0.12	20,20,20,20	0
55	MG	RA	3016	1/1	0.92	0.18	51,51,51,51	0
55	MG	RA	3038	1/1	0.92	0.12	25,25,25,25	0
55	MG	RA	3300	1/1	0.92	0.20	13,13,13,13	0
55	MG	YA	3148	1/1	0.92	0.12	32,32,32,32	0
55	MG	YA	3149	1/1	0.92	0.15	1,1,1,1	0
55	MG	YA	3155	1/1	0.92	0.11	42,42,42,42	0
55	MG	XA	1606	1/1	0.92	0.16	51,51,51,51	0
55	MG	YA	3171	1/1	0.92	0.15	43,43,43,43	0
55	MG	QA	1616	1/1	0.92	0.07	64,64,64,64	0
55	MG	YA	3013	1/1	0.92	0.15	15,15,15,15	0
55	MG	YA	3375	1/1	0.92	0.09	22,22,22,22	0
55	MG	R8	101	1/1	0.92	0.14	35,35,35,35	0
55	MG	XA	1613	1/1	0.92	0.08	32,32,32,32	0
55	MG	YA	3024	1/1	0.92	0.09	35,35,35,35	0
55	MG	RA	3389	1/1	0.92	0.09	46,46,46,46	0
55	MG	YA	3385	1/1	0.92	0.11	32,32,32,32	0
55	MG	RA	3392	1/1	0.92	0.10	51,51,51,51	0
55	MG	RA	3204	1/1	0.92	0.18	42,42,42,42	0
55	MG	RA	3072	1/1	0.92	0.07	24,24,24,24	0
55	MG	RA	3309	1/1	0.92	0.07	96,96,96,96	0
55	MG	RA	3208	1/1	0.92	0.12	27,27,27,27	0
55	MG	RA	3079	1/1	0.92	0.06	40,40,40,40	0
55	MG	QA	1681	1/1	0.92	0.06	52,52,52,52	0
55	MG	QA	1643	1/1	0.92	0.16	38,38,38,38	0
55	MG	RA	3407	1/1	0.92	0.13	44,44,44,44	0
55	MG	XA	1634	1/1	0.92	0.07	46,46,46,46	0
55	MG	XA	1635	1/1	0.92	0.07	69,69,69,69	0
55	MG	QA	1683	1/1	0.92	0.07	51,51,51,51	0
55	MG	RA	3319	1/1	0.92	0.14	16,16,16,16	0
55	MG	RA	3132	1/1	0.92	0.10	40,40,40,40	0
55	MG	XA	1645	1/1	0.92	0.06	49,49,49,49	0
55	MG	YA	3057	1/1	0.92	0.11	12,12,12,12	0
55	MG	YA	3059	1/1	0.92	0.16	26,26,26,26	0
55	MG	RA	3171	1/1	0.92	0.19	38,38,38,38	0
55	MG	RA	3333	1/1	0.92	0.16	22,22,22,22	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	YA	3063	1/1	0.92	0.24	36,36,36,36	0
55	MG	RA	3337	1/1	0.92	0.17	25,25,25,25	0
55	MG	QA	1602	1/1	0.92	0.12	49,49,49,49	0
55	MG	RA	3176	1/1	0.92	0.07	33,33,33,33	0
55	MG	YA	3070	1/1	0.92	0.13	57,57,57,57	0
55	MG	QA	1610	1/1	0.92	0.13	54,54,54,54	0
55	MG	YA	3073	1/1	0.92	0.27	42,42,42,42	0
55	MG	QA	1624	1/1	0.92	0.16	55,55,55,55	0
55	MG	YA	3439	1/1	0.92	0.12	42,42,42,42	0
55	MG	RA	3057	1/1	0.92	0.09	63,63,63,63	0
55	MG	RB	201	1/1	0.92	0.11	61,61,61,61	0
55	MG	YA	3286	1/1	0.92	0.17	9,9,9,9	0
55	MG	RA	3058	1/1	0.92	0.04	63,63,63,63	0
55	MG	RA	3059	1/1	0.92	0.06	58,58,58,58	0
55	MG	YA	3293	1/1	0.92	0.17	31,31,31,31	0
55	MG	RA	3363	1/1	0.92	0.17	37,37,37,37	0
55	MG	YA	3299	1/1	0.92	0.09	11,11,11,11	0
55	MG	RA	3230	1/1	0.92	0.07	43,43,43,43	0
55	MG	RA	3411	1/1	0.93	0.17	36,36,36,36	0
55	MG	RA	3412	1/1	0.93	0.06	39,39,39,39	0
55	MG	RA	3003	1/1	0.93	0.05	42,42,42,42	0
55	MG	QA	1626	1/1	0.93	0.09	50,50,50,50	0
55	MG	QA	1656	1/1	0.93	0.11	46,46,46,46	0
55	MG	RA	3153	1/1	0.93	0.10	33,33,33,33	0
55	MG	QA	1632	1/1	0.93	0.07	33,33,33,33	0
55	MG	QA	1644	1/1	0.93	0.10	40,40,40,40	0
55	MG	RA	3422	1/1	0.93	0.19	37,37,37,37	0
55	MG	QA	1664	1/1	0.93	0.14	32,32,32,32	0
55	MG	RA	3301	1/1	0.93	0.11	46,46,46,46	0
55	MG	YA	3037	1/1	0.93	0.26	8,8,8,8	0
55	MG	YA	3350	1/1	0.93	0.10	35,35,35,35	0
55	MG	RA	3369	1/1	0.93	0.07	41,41,41,41	0
55	MG	XA	1640	1/1	0.93	0.12	54,54,54,54	0
55	MG	RA	3022	1/1	0.93	0.07	48,48,48,48	0
55	MG	RA	3074	1/1	0.93	0.06	24,24,24,24	0
55	MG	RA	3192	1/1	0.93	0.17	48,48,48,48	0
55	MG	YA	3190	1/1	0.93	0.12	32,32,32,32	0
55	MG	RB	203	1/1	0.93	0.11	45,45,45,45	0
55	MG	RB	204	1/1	0.93	0.10	48,48,48,48	0
55	MG	RA	3164	1/1	0.93	0.06	62,62,62,62	0
55	MG	RA	3307	1/1	0.93	0.14	33,33,33,33	0
55	MG	RA	3308	1/1	0.93	0.05	26,26,26,26	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	YA	3207	1/1	0.93	0.13	13,13,13,13	0
55	MG	YA	3378	1/1	0.93	0.13	36,36,36,36	0
55	MG	RA	3229	1/1	0.93	0.06	52,52,52,52	0
55	MG	XA	1653	1/1	0.93	0.11	41,41,41,41	0
55	MG	XA	1657	1/1	0.93	0.11	44,44,44,44	0
55	MG	YA	3061	1/1	0.93	0.07	14,14,14,14	0
55	MG	RA	3011	1/1	0.93	0.05	66,66,66,66	0
55	MG	RA	3039	1/1	0.93	0.15	29,29,29,29	0
55	MG	RA	3012	1/1	0.93	0.08	31,31,31,31	0
55	MG	YA	3230	1/1	0.93	0.17	39,39,39,39	0
55	MG	RA	3313	1/1	0.93	0.13	54,54,54,54	0
55	MG	RA	3116	1/1	0.93	0.19	29,29,29,29	0
55	MG	YA	3235	1/1	0.93	0.16	38,38,38,38	0
55	MG	RA	3085	1/1	0.93	0.04	36,36,36,36	0
55	MG	RA	3239	1/1	0.93	0.10	44,44,44,44	0
55	MG	RA	3324	1/1	0.93	0.08	40,40,40,40	0
55	MG	XA	1673	1/1	0.93	0.04	33,33,33,33	0
55	MG	RQ	201	1/1	0.93	0.07	34,34,34,34	0
55	MG	YA	3410	1/1	0.93	0.17	45,45,45,45	0
55	MG	XA	1675	1/1	0.93	0.21	46,46,46,46	0
55	MG	RA	3325	1/1	0.93	0.08	23,23,23,23	0
55	MG	XA	1602	1/1	0.93	0.09	41,41,41,41	0
55	MG	RA	3280	1/1	0.93	0.13	56,56,56,56	0
55	MG	YA	3273	1/1	0.93	0.19	9,9,9,9	0
55	MG	RA	3170	1/1	0.93	0.07	45,45,45,45	0
55	MG	XA	1684	1/1	0.93	0.09	37,37,37,37	0
55	MG	XA	1605	1/1	0.93	0.09	46,46,46,46	0
55	MG	RA	3244	1/1	0.93	0.20	45,45,45,45	0
55	MG	RA	3247	1/1	0.93	0.10	39,39,39,39	0
55	MG	YA	3284	1/1	0.93	0.15	9,9,9,9	0
55	MG	YA	3427	1/1	0.93	0.12	18,18,18,18	0
55	MG	YA	3428	1/1	0.93	0.17	58,58,58,58	0
55	MG	XA	1611	1/1	0.93	0.09	24,24,24,24	0
55	MG	RA	3140	1/1	0.93	0.14	50,50,50,50	0
55	MG	QA	1666	1/1	0.93	0.23	51,51,51,51	0
55	MG	XA	1615	1/1	0.93	0.06	53,53,53,53	0
55	MG	YA	3111	1/1	0.93	0.17	30,30,30,30	0
55	MG	YA	3114	1/1	0.93	0.21	1,1,1,1	0
55	MG	YA	3303	1/1	0.93	0.13	33,33,33,33	0
55	MG	YB	204	1/1	0.93	0.17	16,16,16,16	0
55	MG	XA	1617	1/1	0.93	0.15	36,36,36,36	0
55	MG	YB	207	1/1	0.93	0.08	42,42,42,42	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	YA	3310	1/1	0.93	0.10	30,30,30,30	0
55	MG	YE	302	1/1	0.93	0.17	51,51,51,51	0
55	MG	Y8	101	1/1	0.93	0.12	5,5,5,5	0
55	MG	XA	1618	1/1	0.93	0.10	42,42,42,42	0
55	MG	YA	3127	1/1	0.93	0.22	12,12,12,12	0
55	MG	RA	3144	1/1	0.93	0.19	25,25,25,25	0
55	MG	YA	3137	1/1	0.93	0.08	26,26,26,26	0
55	MG	RA	3200	1/1	0.94	0.06	30,30,30,30	0
55	MG	YA	3029	1/1	0.94	0.14	17,17,17,17	0
55	MG	YA	3313	1/1	0.94	0.14	50,50,50,50	0
55	MG	YA	3314	1/1	0.94	0.11	30,30,30,30	0
55	MG	YA	3138	1/1	0.94	0.14	20,20,20,20	0
55	MG	RA	3334	1/1	0.94	0.21	19,19,19,19	0
55	MG	RA	3290	1/1	0.94	0.13	47,47,47,47	0
55	MG	RA	3339	1/1	0.94	0.18	12,12,12,12	0
55	MG	RA	3130	1/1	0.94	0.14	57,57,57,57	0
55	MG	RA	3225	1/1	0.94	0.14	34,34,34,34	0
55	MG	QA	1611	1/1	0.94	0.11	58,58,58,58	0
55	MG	YA	3329	1/1	0.94	0.07	25,25,25,25	0
55	MG	YA	3042	1/1	0.94	0.12	9,9,9,9	0
55	MG	YA	3152	1/1	0.94	0.11	17,17,17,17	0
55	MG	XA	1655	1/1	0.94	0.14	20,20,20,20	0
55	MG	YA	3157	1/1	0.94	0.10	25,25,25,25	0
55	MG	YA	3158	1/1	0.94	0.12	8,8,8,8	0
55	MG	YA	3159	1/1	0.94	0.13	6,6,6,6	0
55	MG	YA	3164	1/1	0.94	0.15	5,5,5,5	0
55	MG	YA	3346	1/1	0.94	0.08	41,41,41,41	0
55	MG	YA	3347	1/1	0.94	0.06	26,26,26,26	0
55	MG	XA	1656	1/1	0.94	0.07	43,43,43,43	0
55	MG	RA	3259	1/1	0.94	0.04	30,30,30,30	0
55	MG	YA	3046	1/1	0.94	0.09	18,18,18,18	0
55	MG	RA	3179	1/1	0.94	0.06	44,44,44,44	0
55	MG	RA	3007	1/1	0.94	0.07	34,34,34,34	0
55	MG	YA	3354	1/1	0.94	0.21	15,15,15,15	0
55	MG	YA	3178	1/1	0.94	0.08	26,26,26,26	0
55	MG	YA	3050	1/1	0.94	0.04	19,19,19,19	0
55	MG	RA	3357	1/1	0.94	0.09	25,25,25,25	0
55	MG	YA	3052	1/1	0.94	0.09	14,14,14,14	0
55	MG	YA	3184	1/1	0.94	0.08	42,42,42,42	0
55	MG	YA	3186	1/1	0.94	0.16	28,28,28,28	0
55	MG	XA	1661	1/1	0.94	0.06	48,48,48,48	0
55	MG	XA	1663	1/1	0.94	0.13	41,41,41,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	YA	3193	1/1	0.94	0.15	11,11,11,11	0
55	MG	XA	1608	1/1	0.94	0.17	22,22,22,22	0
55	MG	RA	3263	1/1	0.94	0.17	27,27,27,27	0
55	MG	XA	1610	1/1	0.94	0.15	67,67,67,67	0
55	MG	YA	3381	1/1	0.94	0.06	11,11,11,11	0
55	MG	RA	3075	1/1	0.94	0.13	13,13,13,13	0
55	MG	YA	3205	1/1	0.94	0.10	18,18,18,18	0
55	MG	XA	1671	1/1	0.94	0.11	47,47,47,47	0
55	MG	RA	3234	1/1	0.94	0.08	51,51,51,51	0
55	MG	RA	3148	1/1	0.94	0.15	40,40,40,40	0
55	MG	YA	3065	1/1	0.94	0.17	29,29,29,29	0
55	MG	XA	1614	1/1	0.94	0.06	39,39,39,39	0
55	MG	RA	3419	1/1	0.94	0.13	47,47,47,47	0
55	MG	YA	3218	1/1	0.94	0.10	22,22,22,22	0
55	MG	XA	1616	1/1	0.94	0.15	36,36,36,36	0
55	MG	YA	3398	1/1	0.94	0.08	42,42,42,42	0
55	MG	YA	3399	1/1	0.94	0.14	36,36,36,36	0
55	MG	YA	3400	1/1	0.94	0.17	31,31,31,31	0
55	MG	RA	3210	1/1	0.94	0.09	35,35,35,35	0
55	MG	RA	3149	1/1	0.94	0.12	27,27,27,27	0
55	MG	YA	3229	1/1	0.94	0.15	31,31,31,31	0
55	MG	XA	1680	1/1	0.94	0.08	38,38,38,38	0
55	MG	YA	3408	1/1	0.94	0.19	45,45,45,45	0
55	MG	YA	3074	1/1	0.94	0.14	1,1,1,1	0
55	MG	RA	3051	1/1	0.94	0.12	27,27,27,27	0
55	MG	YA	3411	1/1	0.94	0.14	36,36,36,36	0
55	MG	RA	3240	1/1	0.94	0.06	38,38,38,38	0
55	MG	RA	3275	1/1	0.94	0.13	62,62,62,62	0
55	MG	YA	3240	1/1	0.94	0.12	39,39,39,39	0
55	MG	YA	3081	1/1	0.94	0.22	51,51,51,51	0
55	MG	QA	1667	1/1	0.94	0.15	44,44,44,44	0
55	MG	RA	3215	1/1	0.94	0.08	17,17,17,17	0
55	MG	YA	3249	1/1	0.94	0.22	13,13,13,13	0
55	MG	RA	3125	1/1	0.94	0.14	50,50,50,50	0
55	MG	RA	3155	1/1	0.94	0.08	26,26,26,26	0
55	MG	RA	3281	1/1	0.94	0.17	56,56,56,56	0
55	MG	RA	3380	1/1	0.94	0.04	37,37,37,37	0
55	MG	RA	3382	1/1	0.94	0.08	33,33,33,33	0
55	MG	RA	3156	1/1	0.94	0.09	18,18,18,18	0
55	MG	YA	3001	1/1	0.94	0.06	16,16,16,16	0
55	MG	RA	3081	1/1	0.94	0.18	41,41,41,41	0
55	MG	XA	1637	1/1	0.94	0.05	43,43,43,43	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	RA	3386	1/1	0.94	0.10	41,41,41,41	0
55	MG	YA	3110	1/1	0.94	0.20	29,29,29,29	0
55	MG	YA	3283	1/1	0.94	0.09	3,3,3,3	0
55	MG	RA	3251	1/1	0.94	0.08	41,41,41,41	0
55	MG	RA	3196	1/1	0.94	0.19	16,16,16,16	0
55	MG	RA	3287	1/1	0.94	0.09	38,38,38,38	0
55	MG	YA	3116	1/1	0.94	0.17	32,32,32,32	0
55	MG	YA	3020	1/1	0.94	0.17	7,7,7,7	0
55	MG	YA	3124	1/1	0.94	0.10	10,10,10,10	0
55	MG	XA	1644	1/1	0.94	0.11	32,32,32,32	0
55	MG	YA	3302	1/1	0.94	0.12	20,20,20,20	0
55	MG	RA	3019	1/1	0.94	0.14	57,57,57,57	0
55	MG	YA	3131	1/1	0.94	0.20	2,2,2,2	0
55	MG	YA	3308	1/1	0.94	0.20	15,15,15,15	0
55	MG	YA	3151	1/1	0.95	0.08	21,21,21,21	0
55	MG	YA	3309	1/1	0.95	0.21	33,33,33,33	0
55	MG	R3	3101	1/1	0.95	0.07	42,42,42,42	0
55	MG	RA	3123	1/1	0.95	0.05	30,30,30,30	0
55	MG	QA	1625	1/1	0.95	0.21	39,39,39,39	0
55	MG	RA	3044	1/1	0.95	0.11	35,35,35,35	0
55	MG	QA	1684	1/1	0.95	0.05	42,42,42,42	0
55	MG	YA	3163	1/1	0.95	0.12	15,15,15,15	0
55	MG	YA	3058	1/1	0.95	0.16	25,25,25,25	0
55	MG	YA	3167	1/1	0.95	0.08	15,15,15,15	0
55	MG	YA	3321	1/1	0.95	0.07	21,21,21,21	0
55	MG	RA	3197	1/1	0.95	0.07	66,66,66,66	0
55	MG	RA	3128	1/1	0.95	0.06	54,54,54,54	0
55	MG	RA	3413	1/1	0.95	0.20	30,30,30,30	0
55	MG	RA	3199	1/1	0.95	0.11	30,30,30,30	0
55	MG	RA	3129	1/1	0.95	0.05	58,58,58,58	0
55	MG	YA	3064	1/1	0.95	0.06	42,42,42,42	0
55	MG	YA	3179	1/1	0.95	0.11	18,18,18,18	0
55	MG	QA	1657	1/1	0.95	0.10	37,37,37,37	0
55	MG	YA	3181	1/1	0.95	0.07	22,22,22,22	0
55	MG	RA	3355	1/1	0.95	0.04	29,29,29,29	0
55	MG	YA	3343	1/1	0.95	0.08	39,39,39,39	0
55	MG	XA	1622	1/1	0.95	0.13	41,41,41,41	0
55	MG	XA	1683	1/1	0.95	0.07	31,31,31,31	0
55	MG	RA	3246	1/1	0.95	0.14	44,44,44,44	0
55	MG	XA	1624	1/1	0.95	0.05	58,58,58,58	0
55	MG	RA	3095	1/1	0.95	0.09	64,64,64,64	0
55	MG	RA	3359	1/1	0.95	0.18	36,36,36,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	YA	3194	1/1	0.95	0.12	8,8,8,8	0
55	MG	QA	1665	1/1	0.95	0.07	39,39,39,39	0
55	MG	YA	3076	1/1	0.95	0.10	28,28,28,28	0
55	MG	YA	3078	1/1	0.95	0.27	32,32,32,32	0
55	MG	YA	3359	1/1	0.95	0.18	22,22,22,22	0
55	MG	YA	3200	1/1	0.95	0.09	18,18,18,18	0
55	MG	XA	1628	1/1	0.95	0.10	44,44,44,44	0
55	MG	RA	3206	1/1	0.95	0.11	47,47,47,47	0
55	MG	YA	3365	1/1	0.95	0.07	6,6,6,6	0
55	MG	RA	3004	1/1	0.95	0.08	21,21,21,21	0
55	MG	YA	3084	1/1	0.95	0.23	16,16,16,16	0
55	MG	YA	3213	1/1	0.95	0.09	24,24,24,24	0
55	MG	YA	3086	1/1	0.95	0.22	9,9,9,9	0
55	MG	YA	3372	1/1	0.95	0.25	19,19,19,19	0
55	MG	RA	3050	1/1	0.95	0.14	24,24,24,24	0
55	MG	RA	3428	1/1	0.95	0.07	45,45,45,45	0
55	MG	RA	3367	1/1	0.95	0.06	53,53,53,53	0
55	MG	QA	1619	1/1	0.95	0.09	56,56,56,56	0
55	MG	YA	3219	1/1	0.95	0.09	36,36,36,36	0
55	MG	QA	1652	1/1	0.95	0.17	33,33,33,33	0
55	MG	RA	3077	1/1	0.95	0.05	28,28,28,28	0
55	MG	YA	3012	1/1	0.95	0.12	7,7,7,7	0
55	MG	YA	3386	1/1	0.95	0.08	35,35,35,35	0
55	MG	YA	3096	1/1	0.95	0.18	0,0,0,0	0
55	MG	YA	3097	1/1	0.95	0.17	1,1,1,1	0
55	MG	YA	3231	1/1	0.95	0.13	39,39,39,39	0
55	MG	RA	3212	1/1	0.95	0.09	23,23,23,23	0
55	MG	YA	3393	1/1	0.95	0.12	29,29,29,29	0
55	MG	XA	1641	1/1	0.95	0.12	37,37,37,37	0
55	MG	RA	3256	1/1	0.95	0.13	56,56,56,56	0
55	MG	YA	3236	1/1	0.95	0.08	26,26,26,26	0
55	MG	YA	3237	1/1	0.95	0.20	39,39,39,39	0
55	MG	RA	3104	1/1	0.95	0.09	38,38,38,38	0
55	MG	YA	3023	1/1	0.95	0.10	17,17,17,17	0
55	MG	RA	3106	1/1	0.95	0.09	31,31,31,31	0
55	MG	RA	3107	1/1	0.95	0.07	50,50,50,50	0
55	MG	YA	3112	1/1	0.95	0.05	49,49,49,49	0
55	MG	RA	3260	1/1	0.95	0.09	45,45,45,45	0
55	MG	YA	3407	1/1	0.95	0.05	29,29,29,29	0
55	MG	YA	3256	1/1	0.95	0.10	39,39,39,39	0
55	MG	RA	3056	1/1	0.95	0.09	46,46,46,46	0
55	MG	YA	3260	1/1	0.95	0.09	35,35,35,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	RA	3145	1/1	0.95	0.07	24,24,24,24	0
55	MG	YA	3118	1/1	0.95	0.12	21,21,21,21	0
55	MG	YA	3269	1/1	0.95	0.10	32,32,32,32	0
55	MG	YA	3270	1/1	0.95	0.16	17,17,17,17	0
55	MG	RA	3115	1/1	0.95	0.09	22,22,22,22	0
55	MG	YA	3121	1/1	0.95	0.08	35,35,35,35	0
55	MG	YA	3033	1/1	0.95	0.16	12,12,12,12	0
55	MG	YA	3125	1/1	0.95	0.25	36,36,36,36	0
55	MG	RA	3182	1/1	0.95	0.12	39,39,39,39	0
55	MG	RA	3183	1/1	0.95	0.13	36,36,36,36	0
55	MG	YA	3277	1/1	0.95	0.18	40,40,40,40	0
55	MG	YA	3128	1/1	0.95	0.15	10,10,10,10	0
55	MG	YA	3279	1/1	0.95	0.07	7,7,7,7	0
55	MG	RA	3385	1/1	0.95	0.09	41,41,41,41	0
55	MG	YA	3429	1/1	0.95	0.21	26,26,26,26	0
55	MG	QA	1631	1/1	0.95	0.10	35,35,35,35	0
55	MG	QA	1603	1/1	0.95	0.05	41,41,41,41	0
55	MG	YA	3285	1/1	0.95	0.11	1,1,1,1	0
55	MG	RA	3082	1/1	0.95	0.09	57,57,57,57	0
55	MG	RA	3318	1/1	0.95	0.11	32,32,32,32	0
55	MG	QA	1604	1/1	0.95	0.11	46,46,46,46	0
55	MG	RA	3188	1/1	0.95	0.16	54,54,54,54	0
55	MG	YA	3294	1/1	0.95	0.20	0,0,0,0	0
55	MG	YB	205	1/1	0.95	0.14	41,41,41,41	0
55	MG	YA	3295	1/1	0.95	0.20	8,8,8,8	0
55	MG	YA	3297	1/1	0.95	0.20	26,26,26,26	0
55	MG	RA	3228	1/1	0.95	0.20	39,39,39,39	0
55	MG	YA	3146	1/1	0.95	0.18	33,33,33,33	0
55	MG	YA	3301	1/1	0.95	0.14	12,12,12,12	0
55	MG	XA	1662	1/1	0.95	0.08	26,26,26,26	0
55	MG	YR	202	1/1	0.95	0.13	33,33,33,33	0
55	MG	YU	201	1/1	0.95	0.09	37,37,37,37	0
55	MG	QA	1671	1/1	0.95	0.04	34,34,34,34	0
55	MG	RA	3329	1/1	0.95	0.15	46,46,46,46	0
55	MG	YA	3307	1/1	0.95	0.14	55,55,55,55	0
57	ZN	RY	201	1/1	0.95	0.05	137,137,137,137	0
55	MG	RA	3361	1/1	0.96	0.14	37,37,37,37	0
55	MG	YA	3098	1/1	0.96	0.17	2,2,2,2	0
55	MG	YA	3334	1/1	0.96	0.08	31,31,31,31	0
55	MG	YA	3335	1/1	0.96	0.14	2,2,2,2	0
55	MG	RA	3034	1/1	0.96	0.08	27,27,27,27	0
55	MG	YA	3337	1/1	0.96	0.04	24,24,24,24	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	YA	3030	1/1	0.96	0.13	0,0,0,0	0
55	MG	YA	3340	1/1	0.96	0.12	48,48,48,48	0
55	MG	RA	3408	1/1	0.96	0.14	21,21,21,21	0
55	MG	YA	3105	1/1	0.96	0.10	9,9,9,9	0
55	MG	RA	3282	1/1	0.96	0.04	37,37,37,37	0
55	MG	RA	3071	1/1	0.96	0.07	74,74,74,74	0
55	MG	RA	3173	1/1	0.96	0.18	34,34,34,34	0
55	MG	YA	3035	1/1	0.96	0.22	10,10,10,10	0
55	MG	RA	3366	1/1	0.96	0.10	29,29,29,29	0
55	MG	RA	3414	1/1	0.96	0.09	41,41,41,41	0
55	MG	YA	3225	1/1	0.96	0.11	30,30,30,30	0
55	MG	YA	3226	1/1	0.96	0.22	45,45,45,45	0
55	MG	YA	3039	1/1	0.96	0.12	1,1,1,1	0
55	MG	YA	3228	1/1	0.96	0.14	20,20,20,20	0
55	MG	RA	3191	1/1	0.96	0.13	28,28,28,28	0
55	MG	YA	3117	1/1	0.96	0.09	26,26,26,26	0
55	MG	YA	3041	1/1	0.96	0.20	12,12,12,12	0
55	MG	YA	3119	1/1	0.96	0.10	36,36,36,36	0
55	MG	RA	3157	1/1	0.96	0.15	24,24,24,24	0
55	MG	RA	3315	1/1	0.96	0.10	31,31,31,31	0
55	MG	YA	3366	1/1	0.96	0.12	25,25,25,25	0
55	MG	YA	3122	1/1	0.96	0.10	12,12,12,12	0
55	MG	QA	1675	1/1	0.96	0.08	46,46,46,46	0
55	MG	RA	3317	1/1	0.96	0.09	20,20,20,20	0
55	MG	RA	3194	1/1	0.96	0.17	42,42,42,42	0
55	MG	YA	3241	1/1	0.96	0.06	14,14,14,14	0
55	MG	YA	3373	1/1	0.96	0.16	19,19,19,19	0
55	MG	RA	3373	1/1	0.96	0.09	25,25,25,25	0
55	MG	YA	3376	1/1	0.96	0.18	9,9,9,9	0
55	MG	RA	3113	1/1	0.96	0.11	14,14,14,14	0
55	MG	YA	3049	1/1	0.96	0.13	18,18,18,18	0
55	MG	YA	3379	1/1	0.96	0.13	29,29,29,29	0
55	MG	YA	3132	1/1	0.96	0.17	1,1,1,1	0
55	MG	YA	3254	1/1	0.96	0.16	49,49,49,49	0
55	MG	YA	3255	1/1	0.96	0.09	18,18,18,18	0
55	MG	YA	3133	1/1	0.96	0.07	6,6,6,6	0
55	MG	XA	1621	1/1	0.96	0.06	45,45,45,45	0
55	MG	YA	3259	1/1	0.96	0.08	31,31,31,31	0
55	MG	RA	3320	1/1	0.96	0.14	30,30,30,30	0
55	MG	XA	1676	1/1	0.96	0.10	29,29,29,29	0
55	MG	YA	3263	1/1	0.96	0.11	4,4,4,4	0
55	MG	YA	3264	1/1	0.96	0.15	41,41,41,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	YA	3392	1/1	0.96	0.12	14,14,14,14	0
55	MG	YA	3266	1/1	0.96	0.06	23,23,23,23	0
55	MG	RA	3083	1/1	0.96	0.04	44,44,44,44	0
55	MG	RA	3264	1/1	0.96	0.10	25,25,25,25	0
55	MG	RA	3292	1/1	0.96	0.06	40,40,40,40	0
55	MG	YA	3056	1/1	0.96	0.16	31,31,31,31	0
55	MG	RA	3037	1/1	0.96	0.15	26,26,26,26	0
55	MG	RA	3180	1/1	0.96	0.14	31,31,31,31	0
55	MG	RA	3245	1/1	0.96	0.13	32,32,32,32	0
55	MG	YA	3402	1/1	0.96	0.22	44,44,44,44	0
55	MG	R1	101	1/1	0.96	0.23	40,40,40,40	0
55	MG	RA	3297	1/1	0.96	0.09	26,26,26,26	0
55	MG	RA	3298	1/1	0.96	0.12	49,49,49,49	0
55	MG	RA	3026	1/1	0.96	0.06	20,20,20,20	0
55	MG	RA	3344	1/1	0.96	0.06	39,39,39,39	0
55	MG	RA	3087	1/1	0.96	0.07	59,59,59,59	0
55	MG	XA	1636	1/1	0.96	0.08	26,26,26,26	0
55	MG	YA	3160	1/1	0.96	0.14	11,11,11,11	0
55	MG	YA	3161	1/1	0.96	0.07	18,18,18,18	0
55	MG	Y1	101	1/1	0.96	0.05	31,31,31,31	0
55	MG	RA	3390	1/1	0.96	0.08	41,41,41,41	0
55	MG	YA	3166	1/1	0.96	0.14	9,9,9,9	0
55	MG	YA	3292	1/1	0.96	0.20	29,29,29,29	0
55	MG	YA	3418	1/1	0.96	0.26	42,42,42,42	0
55	MG	RA	3273	1/1	0.96	0.04	63,63,63,63	0
55	MG	YA	3168	1/1	0.96	0.06	22,22,22,22	0
55	MG	Y7	101	1/1	0.96	0.11	24,24,24,24	0
55	MG	YA	3072	1/1	0.96	0.14	6,6,6,6	0
55	MG	YA	3173	1/1	0.96	0.15	12,12,12,12	0
55	MG	YA	3424	1/1	0.96	0.17	39,39,39,39	0
55	MG	YA	3174	1/1	0.96	0.04	20,20,20,20	0
55	MG	RA	3102	1/1	0.96	0.10	46,46,46,46	0
55	MG	RA	3223	1/1	0.96	0.17	35,35,35,35	0
55	MG	RE	302	1/1	0.96	0.09	25,25,25,25	0
55	MG	RE	303	1/1	0.96	0.16	16,16,16,16	0
55	MG	YA	3305	1/1	0.96	0.13	28,28,28,28	0
55	MG	YA	3434	1/1	0.96	0.07	23,23,23,23	0
55	MG	YA	3306	1/1	0.96	0.21	43,43,43,43	0
55	MG	YA	3437	1/1	0.96	0.07	23,23,23,23	0
55	MG	RE	304	1/1	0.96	0.12	14,14,14,14	0
55	MG	YA	3005	1/1	0.96	0.26	26,26,26,26	0
55	MG	YA	3006	1/1	0.96	0.12	3,3,3,3	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	YA	3011	1/1	0.96	0.21	13,13,13,13	0
55	MG	YA	3311	1/1	0.96	0.13	18,18,18,18	0
55	MG	RA	3397	1/1	0.96	0.12	29,29,29,29	0
55	MG	YA	3085	1/1	0.96	0.07	24,24,24,24	0
55	MG	RA	3398	1/1	0.96	0.09	36,36,36,36	0
55	MG	YA	3014	1/1	0.96	0.14	4,4,4,4	0
55	MG	RA	3078	1/1	0.96	0.15	16,16,16,16	0
55	MG	RA	3205	1/1	0.96	0.09	40,40,40,40	0
55	MG	RA	3052	1/1	0.96	0.13	28,28,28,28	0
55	MG	RA	3154	1/1	0.96	0.15	17,17,17,17	0
55	MG	YA	3093	1/1	0.96	0.17	3,3,3,3	0
55	MG	YA	3324	1/1	0.96	0.04	33,33,33,33	0
55	MG	RA	3403	1/1	0.96	0.04	25,25,25,25	0
55	MG	RA	3404	1/1	0.96	0.18	37,37,37,37	0
55	MG	YA	3026	1/1	0.96	0.07	5,5,5,5	0
55	MG	RA	3352	1/1	0.97	0.05	35,35,35,35	0
55	MG	YA	3363	1/1	0.97	0.07	9,9,9,9	0
55	MG	QF	301	1/1	0.97	0.06	46,46,46,46	0
55	MG	RA	3036	1/1	0.97	0.11	32,32,32,32	0
55	MG	YA	3069	1/1	0.97	0.07	15,15,15,15	0
55	MG	RA	3041	1/1	0.97	0.07	46,46,46,46	0
55	MG	YA	3185	1/1	0.97	0.04	41,41,41,41	0
55	MG	YA	3123	1/1	0.97	0.24	22,22,22,22	0
55	MG	RA	3302	1/1	0.97	0.04	37,37,37,37	0
55	MG	YA	3371	1/1	0.97	0.10	21,21,21,21	0
55	MG	XA	1639	1/1	0.97	0.07	38,38,38,38	0
55	MG	RA	3358	1/1	0.97	0.16	19,19,19,19	0
55	MG	YA	3374	1/1	0.97	0.10	27,27,27,27	0
55	MG	RA	3088	1/1	0.97	0.06	36,36,36,36	0
55	MG	YA	3280	1/1	0.97	0.12	4,4,4,4	0
55	MG	RA	3142	1/1	0.97	0.06	11,11,11,11	0
55	MG	YA	3282	1/1	0.97	0.10	3,3,3,3	0
55	MG	YA	3129	1/1	0.97	0.13	10,10,10,10	0
55	MG	YA	3197	1/1	0.97	0.07	27,27,27,27	0
55	MG	YA	3130	1/1	0.97	0.12	22,22,22,22	0
55	MG	RA	3326	1/1	0.97	0.03	21,21,21,21	0
55	MG	YA	3287	1/1	0.97	0.11	31,31,31,31	0
55	MG	YA	3288	1/1	0.97	0.05	37,37,37,37	0
55	MG	RA	3201	1/1	0.97	0.08	38,38,38,38	0
55	MG	YA	3203	1/1	0.97	0.14	10,10,10,10	0
55	MG	YA	3204	1/1	0.97	0.10	10,10,10,10	0
55	MG	RA	3235	1/1	0.97	0.09	35,35,35,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	YA	3134	1/1	0.97	0.10	28,28,28,28	0
55	MG	RA	3172	1/1	0.97	0.17	36,36,36,36	0
55	MG	YA	3208	1/1	0.97	0.07	20,20,20,20	0
55	MG	YA	3209	1/1	0.97	0.23	21,21,21,21	0
55	MG	YA	3038	1/1	0.97	0.09	7,7,7,7	0
55	MG	RA	3331	1/1	0.97	0.14	36,36,36,36	0
55	MG	RA	3054	1/1	0.97	0.04	21,21,21,21	0
55	MG	YA	3140	1/1	0.97	0.15	10,10,10,10	0
55	MG	RB	205	1/1	0.97	0.08	24,24,24,24	0
55	MG	YA	3142	1/1	0.97	0.25	1,1,1,1	0
55	MG	RA	3090	1/1	0.97	0.27	27,27,27,27	0
55	MG	YA	3144	1/1	0.97	0.06	14,14,14,14	0
55	MG	YA	3223	1/1	0.97	0.12	12,12,12,12	0
55	MG	RA	3335	1/1	0.97	0.07	51,51,51,51	0
55	MG	YA	3406	1/1	0.97	0.21	33,33,33,33	0
55	MG	RA	3336	1/1	0.97	0.12	31,31,31,31	0
55	MG	YA	3090	1/1	0.97	0.04	27,27,27,27	0
55	MG	XA	1654	1/1	0.97	0.16	27,27,27,27	0
55	MG	RA	3047	1/1	0.97	0.11	37,37,37,37	0
55	MG	RA	3405	1/1	0.97	0.14	24,24,24,24	0
55	MG	RA	3338	1/1	0.97	0.12	28,28,28,28	0
55	MG	YA	3153	1/1	0.97	0.11	16,16,16,16	0
55	MG	YA	3232	1/1	0.97	0.16	24,24,24,24	0
55	MG	YA	3154	1/1	0.97	0.06	21,21,21,21	0
55	MG	RA	3073	1/1	0.97	0.06	23,23,23,23	0
55	MG	YA	3322	1/1	0.97	0.14	18,18,18,18	0
55	MG	RA	3277	1/1	0.97	0.04	28,28,28,28	0
55	MG	RA	3343	1/1	0.97	0.12	14,14,14,14	0
55	MG	RA	3017	1/1	0.97	0.12	16,16,16,16	0
55	MG	YA	3326	1/1	0.97	0.06	18,18,18,18	0
55	MG	YA	3099	1/1	0.97	0.14	0,0,0,0	0
55	MG	YA	3328	1/1	0.97	0.09	9,9,9,9	0
55	MG	YA	3239	1/1	0.97	0.09	30,30,30,30	0
55	MG	RA	3377	1/1	0.97	0.10	30,30,30,30	0
55	MG	YA	3331	1/1	0.97	0.08	40,40,40,40	0
55	MG	YA	3332	1/1	0.97	0.07	39,39,39,39	0
55	MG	YA	3162	1/1	0.97	0.11	20,20,20,20	0
55	MG	RA	3028	1/1	0.97	0.05	42,42,42,42	0
55	MG	YA	3432	1/1	0.97	0.08	12,12,12,12	0
55	MG	YA	3243	1/1	0.97	0.18	0,0,0,0	0
55	MG	YA	3102	1/1	0.97	0.06	1,1,1,1	0
55	MG	YA	3008	1/1	0.97	0.09	7,7,7,7	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	YA	3247	1/1	0.97	0.09	2,2,2,2	0
55	MG	XA	1664	1/1	0.97	0.10	28,28,28,28	0
55	MG	YA	3250	1/1	0.97	0.22	30,30,30,30	0
55	MG	YA	3252	1/1	0.97	0.16	1,1,1,1	0
55	MG	YB	203	1/1	0.97	0.10	13,13,13,13	0
55	MG	XA	1665	1/1	0.97	0.18	34,34,34,34	0
55	MG	YA	3108	1/1	0.97	0.11	2,2,2,2	0
55	MG	XA	1666	1/1	0.97	0.04	48,48,48,48	0
55	MG	YA	3257	1/1	0.97	0.04	14,14,14,14	0
55	MG	YA	3172	1/1	0.97	0.12	3,3,3,3	0
55	MG	YE	301	1/1	0.97	0.17	24,24,24,24	0
55	MG	RA	3124	1/1	0.97	0.11	18,18,18,18	0
55	MG	RA	3347	1/1	0.97	0.04	57,57,57,57	0
55	MG	YA	3351	1/1	0.97	0.16	22,22,22,22	0
55	MG	XA	1631	1/1	0.97	0.04	36,36,36,36	0
55	MG	YA	3019	1/1	0.97	0.11	1,1,1,1	0
55	MG	RA	3348	1/1	0.97	0.10	54,54,54,54	0
56	SF4	QD	301	8/8	0.97	0.05	96,109,113,114	0
55	MG	YA	3021	1/1	0.97	0.07	13,13,13,13	0
55	MG	YA	3267	1/1	0.97	0.10	9,9,9,9	0
55	MG	RA	3136	1/1	0.97	0.09	52,52,52,52	0
57	ZN	Y9	101	1/1	0.97	0.05	54,54,54,54	0
55	MG	RA	3076	1/1	0.98	0.04	19,19,19,19	0
55	MG	XA	1681	1/1	0.98	0.14	20,20,20,20	0
55	MG	YA	3265	1/1	0.98	0.11	21,21,21,21	0
55	MG	YA	3027	1/1	0.98	0.12	5,5,5,5	0
55	MG	RA	3340	1/1	0.98	0.07	11,11,11,11	0
55	MG	RA	3141	1/1	0.98	0.06	17,17,17,17	0
55	MG	YA	3396	1/1	0.98	0.11	38,38,38,38	0
55	MG	YA	3210	1/1	0.98	0.23	25,25,25,25	0
55	MG	YA	3211	1/1	0.98	0.17	19,19,19,19	0
55	MG	RA	3342	1/1	0.98	0.05	31,31,31,31	0
55	MG	RA	3117	1/1	0.98	0.07	35,35,35,35	0
55	MG	RA	3105	1/1	0.98	0.03	15,15,15,15	0
55	MG	RA	3064	1/1	0.98	0.08	22,22,22,22	0
55	MG	RA	3100	1/1	0.98	0.06	29,29,29,29	0
55	MG	RA	3146	1/1	0.98	0.19	18,18,18,18	0
55	MG	RA	3323	1/1	0.98	0.07	11,11,11,11	0
55	MG	RA	3349	1/1	0.98	0.05	25,25,25,25	0
55	MG	YA	3339	1/1	0.98	0.04	20,20,20,20	0
55	MG	YA	3221	1/1	0.98	0.10	26,26,26,26	0
55	MG	YA	3222	1/1	0.98	0.17	8,8,8,8	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	YA	3077	1/1	0.98	0.15	12,12,12,12	0
55	MG	RA	3409	1/1	0.98	0.06	24,24,24,24	0
55	MG	YA	3344	1/1	0.98	0.08	11,11,11,11	0
55	MG	RA	3243	1/1	0.98	0.11	17,17,17,17	0
55	MG	RA	3108	1/1	0.98	0.09	10,10,10,10	0
55	MG	YA	3415	1/1	0.98	0.16	38,38,38,38	0
55	MG	RA	3353	1/1	0.98	0.18	36,36,36,36	0
55	MG	YA	3083	1/1	0.98	0.05	11,11,11,11	0
55	MG	RF	301	1/1	0.98	0.10	37,37,37,37	0
55	MG	RA	3381	1/1	0.98	0.04	22,22,22,22	0
55	MG	RA	3109	1/1	0.98	0.07	21,21,21,21	0
55	MG	YA	3290	1/1	0.98	0.10	1,1,1,1	0
55	MG	RA	3065	1/1	0.98	0.07	18,18,18,18	0
55	MG	RA	3328	1/1	0.98	0.16	22,22,22,22	0
55	MG	RA	3111	1/1	0.98	0.05	29,29,29,29	0
55	MG	YA	3358	1/1	0.98	0.07	13,13,13,13	0
55	MG	YA	3007	1/1	0.98	0.11	1,1,1,1	0
55	MG	RA	3151	1/1	0.98	0.20	39,39,39,39	0
55	MG	YA	3296	1/1	0.98	0.12	17,17,17,17	0
55	MG	YA	3362	1/1	0.98	0.10	18,18,18,18	0
55	MG	YA	3009	1/1	0.98	0.15	1,1,1,1	0
55	MG	YA	3010	1/1	0.98	0.10	9,9,9,9	0
55	MG	RA	3267	1/1	0.98	0.08	10,10,10,10	0
55	MG	YA	3435	1/1	0.98	0.04	17,17,17,17	0
55	MG	YA	3300	1/1	0.98	0.09	5,5,5,5	0
55	MG	RA	3360	1/1	0.98	0.13	39,39,39,39	0
55	MG	YA	3187	1/1	0.98	0.04	22,22,22,22	0
55	MG	QA	1636	1/1	0.98	0.03	38,38,38,38	0
55	MG	YA	3189	1/1	0.98	0.14	40,40,40,40	0
55	MG	RA	3114	1/1	0.98	0.13	6,6,6,6	0
55	MG	YA	3191	1/1	0.98	0.03	56,56,56,56	0
55	MG	YA	3246	1/1	0.98	0.07	3,3,3,3	0
55	MG	YA	3192	1/1	0.98	0.25	50,50,50,50	0
55	MG	YA	3248	1/1	0.98	0.05	1,1,1,1	0
55	MG	RA	3232	1/1	0.98	0.11	20,20,20,20	0
55	MG	YB	208	1/1	0.98	0.03	25,25,25,25	0
55	MG	XA	1607	1/1	0.98	0.06	28,28,28,28	0
55	MG	YA	3017	1/1	0.98	0.13	7,7,7,7	0
55	MG	RA	3393	1/1	0.98	0.04	38,38,38,38	0
55	MG	RA	3271	1/1	0.98	0.17	47,47,47,47	0
55	MG	YQ	201	1/1	0.98	0.04	30,30,30,30	0
55	MG	RA	3233	1/1	0.98	0.09	16,16,16,16	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	YA	3382	1/1	0.98	0.12	24,24,24,24	0
55	MG	YA	3104	1/1	0.98	0.03	26,26,26,26	0
55	MG	YA	3150	1/1	0.98	0.12	2,2,2,2	0
55	MG	YA	3202	1/1	0.98	0.04	17,17,17,17	0
55	MG	YA	3319	1/1	0.98	0.03	1,1,1,1	0
55	MG	RA	3396	1/1	0.98	0.03	29,29,29,29	0
55	MG	RA	3092	1/1	0.98	0.03	50,50,50,50	0
57	ZN	XN	101	1/1	0.98	0.05	144,144,144,144	0
57	ZN	Y5	101	1/1	0.98	0.04	66,66,66,66	0
55	MG	YA	3389	1/1	0.98	0.08	15,15,15,15	0
55	MG	YA	3433	1/1	0.99	0.04	18,18,18,18	0
55	MG	YA	3165	1/1	0.99	0.17	13,13,13,13	0
55	MG	RA	3350	1/1	0.99	0.03	29,29,29,29	0
55	MG	YA	3262	1/1	0.99	0.20	5,5,5,5	0
55	MG	YA	3212	1/1	0.99	0.07	22,22,22,22	0
55	MG	RA	3053	1/1	0.99	0.14	23,23,23,23	0
55	MG	RA	3321	1/1	0.99	0.05	23,23,23,23	0
55	MG	YA	3320	1/1	0.99	0.07	42,42,42,42	0
55	MG	YA	3169	1/1	0.99	0.05	15,15,15,15	0
55	MG	RA	3332	1/1	0.99	0.04	4,4,4,4	0
55	MG	RA	3241	1/1	0.99	0.18	5,5,5,5	0
55	MG	XA	1652	1/1	0.99	0.06	26,26,26,26	0
55	MG	RA	3227	1/1	0.99	0.06	20,20,20,20	0
55	MG	RA	3426	1/1	0.99	0.05	34,34,34,34	0
55	MG	YA	3355	1/1	0.99	0.06	5,5,5,5	0
55	MG	YA	3356	1/1	0.99	0.04	0,0,0,0	0
55	MG	QA	1680	1/1	0.99	0.04	32,32,32,32	0
55	MG	YA	3198	1/1	0.99	0.22	5,5,5,5	0
55	MG	YA	3135	1/1	0.99	0.02	32,32,32,32	0
55	MG	RA	3174	1/1	0.99	0.06	8,8,8,8	0
55	MG	YA	3156	1/1	0.99	0.04	6,6,6,6	0
55	MG	YA	3082	1/1	0.99	0.04	10,10,10,10	0
55	MG	YA	3251	1/1	0.99	0.19	5,5,5,5	0
55	MG	YA	3018	1/1	0.99	0.15	1,1,1,1	0
55	MG	YA	3253	1/1	0.99	0.03	1,1,1,1	0
56	SF4	XD	301	8/8	0.99	0.03	95,101,103,103	0
55	MG	RA	3391	1/1	0.99	0.08	25,25,25,25	0
57	ZN	R5	101	1/1	0.99	0.04	84,84,84,84	0
57	ZN	R6	101	1/1	0.99	0.05	70,70,70,70	0
55	MG	RA	3159	1/1	0.99	0.04	31,31,31,31	0
55	MG	RA	3063	1/1	0.99	0.09	17,17,17,17	0
55	MG	YA	3022	1/1	0.99	0.07	8,8,8,8	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
55	MG	RA	3112	1/1	0.99	0.06	26,26,26,26	0
55	MG	YA	3106	1/1	0.99	0.04	18,18,18,18	0
57	ZN	YY	201	1/1	0.99	0.02	69,69,69,69	0
55	MG	RA	3322	1/1	1.00	0.03	33,33,33,33	0
55	MG	YA	3113	1/1	1.00	0.07	10,10,10,10	0
57	ZN	Y6	101	1/1	1.00	0.02	44,44,44,44	0
55	MG	YA	3426	1/1	1.00	0.17	4,4,4,4	0
55	MG	RA	3425	1/1	1.00	0.02	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.