



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 08:29 PM UTC

PDB ID : 6OXI / pdb_00006oxi
Title : Dimeric E.coli YoeB bound to Thermus thermophilus 70S post-cleavage (UAA)
Authors : Pavelich, I.J.; Hoffer, E.D.; Maehigashi, T.; Dunham, C.M.
Deposited on : 2019-05-13
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

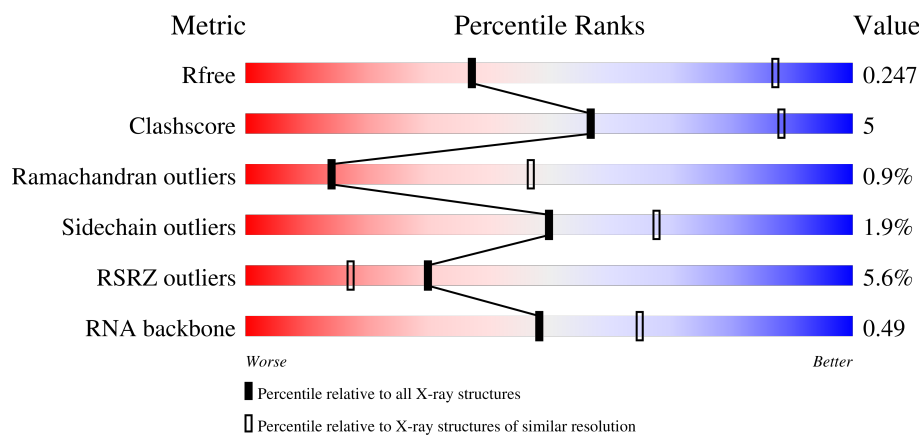
1 Overall quality at a glance

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}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)
RNA backbone	3983	1010 (3.98-3.02)

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	2% 62% 32% 5%
1	XA	1521	2% 64% 30% 5%
2	QB	256	2% 67% 18% 5% 8%
2	XB	256	5% 72% 16% 8%

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	20	
23	XX	20	
24	QY	84	
24	QZ	84	
24	XY	84	
24	XZ	84	
25	R0	85	
25	Y0	85	
26	R1	98	
26	Y1	98	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
27	R2	72	
27	Y2	72	
28	R3	60	
28	Y3	60	
29	R4	71	
29	Y4	71	
30	R5	60	
30	Y5	60	
31	R6	54	
31	Y6	54	
32	R7	49	
32	Y7	49	
33	R8	65	
33	Y8	65	
34	R9	37	
34	Y9	37	
35	RA	2915	
35	YA	2915	
36	RB	124	
36	YB	124	
37	RD	276	
37	YD	276	
38	RE	206	
38	YE	206	
39	RF	210	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
39	YF	210	4% 75% 20% • •
40	RG	182	5% 75% 21% • • •
40	YG	182	8% 75% 23% • • •
41	RH	180	17% 73% 18% • • •
41	YH	180	12% 81% 15% • •
42	RI	148	15% 68% 22% 5% • •
42	YI	148	6% 81% 14% • •
43	RN	140	16% 76% 19% • •
43	YN	140	8% 79% 17% • •
44	RO	122	• 74% 26%
44	YO	122	3% 79% 21%
45	RP	150	11% 69% 27% • •
45	YP	150	7% 77% 22% • •
46	RQ	141	9% 70% 26% • •
46	YQ	141	4% 79% 21%
47	RR	118	3% 79% 19% • •
47	YR	118	9% 77% 20% • • •
48	RS	112	14% 74% 24% • •
48	YS	112	12% 76% 21% • •
49	RT	146	8% 66% 25% • 6%
49	YT	146	8% 71% 19% • 6%
50	RU	118	5% 77% 19% • • •
50	YU	118	11% 81% 15% • • •
51	RV	101	3% 69% 25% • •
51	YV	101	16% 70% 25% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
52	RW	113	
52	YW	113	
53	RX	96	
53	YX	96	
54	RY	110	
54	YY	110	
55	RZ	206	
55	YZ	206	
56	ZA	3	
56	ZB	3	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	QY	101	-	-	-	X
57	MG	RA	3302	-	-	-	X
57	MG	XA	1651	-	-	-	X

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 295153 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	QO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
15	XO	87	Total	C	N	O	S	0	0	0
			729	457	146	124	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	QP	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			
16	XP	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	QQ	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			
17	XQ	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	QS	83	Total	C	N	O	S	0	0	0
			665	424	124	115	2			
19	XS	83	Total	C	N	O	S	0	0	0
			656	418	123	113	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 P-site tRNA-fMet.

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

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QX	18	Total	C	N	O	P	0	0	0
			394	176	79	121	18			
23	XX	18	Total	C	N	O	P	0	0	0
			394	176	79	121	18			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	R1	94	Total	C	N	O	S	0	0	0
			737	463	146	127	1			
26	Y1	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	RB	120	Total	C	N	O	P	0	0	0
			2576	1146	476	834	120			
36	YB	120	Total	C	N	O	P	0	0	0
			2576	1146	476	834	120			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	RE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			
38	YE	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	RH	174	Total	C	N	O	S	0	0	0
			1336	848	251	236	1			
41	YH	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	RP	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			
45	YP	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 56 is a RNA chain called CCPuro.

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

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QA	93	Total	Mg	0	0
			93	93		
57	QD	1	Total	Mg	0	0
			1	1		
57	QE	1	Total	Mg	0	0
			1	1		
57	QV	3	Total	Mg	0	0
			3	3		

Continued on next page...

Continued from previous page...

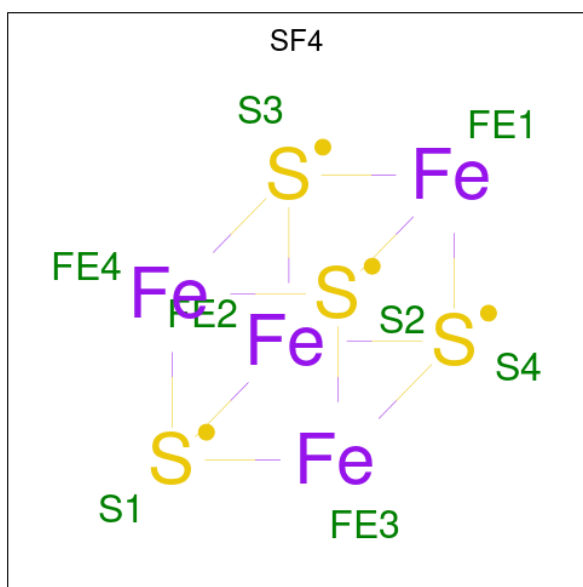
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	QY	1	Total 1	Mg 1	0	0
57	R0	2	Total 2	Mg 2	0	0
57	R3	1	Total 1	Mg 1	0	0
57	RA	302	Total 302	Mg 302	0	0
57	RB	3	Total 3	Mg 3	0	0
57	RD	2	Total 2	Mg 2	0	0
57	RE	1	Total 1	Mg 1	0	0
57	RN	1	Total 1	Mg 1	0	0
57	RO	1	Total 1	Mg 1	0	0
57	RP	1	Total 1	Mg 1	0	0
57	RQ	4	Total 4	Mg 4	0	0
57	RR	1	Total 1	Mg 1	0	0
57	RY	1	Total 1	Mg 1	0	0
57	XA	99	Total 99	Mg 99	0	0
57	XE	1	Total 1	Mg 1	0	0
57	XF	1	Total 1	Mg 1	0	0
57	XL	1	Total 1	Mg 1	0	0
57	XM	1	Total 1	Mg 1	0	0
57	XV	4	Total 4	Mg 4	0	0
57	Y0	2	Total 2	Mg 2	0	0
57	Y1	1	Total 1	Mg 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	Y3	1	Total 1	Mg 1	0	0
57	Y5	1	Total 1	Mg 1	0	0
57	Y9	1	Total 1	Mg 1	0	0
57	YA	335	Total 335	Mg 335	0	0
57	YB	3	Total 3	Mg 3	0	0
57	YD	4	Total 4	Mg 4	0	0
57	YE	5	Total 5	Mg 5	0	0
57	YF	1	Total 1	Mg 1	0	0
57	YG	1	Total 1	Mg 1	0	0
57	YO	1	Total 1	Mg 1	0	0
57	YP	1	Total 1	Mg 1	0	0
57	YQ	5	Total 5	Mg 5	0	0
57	YR	1	Total 1	Mg 1	0	0
57	YV	1	Total 1	Mg 1	0	0

- Molecule 58 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



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

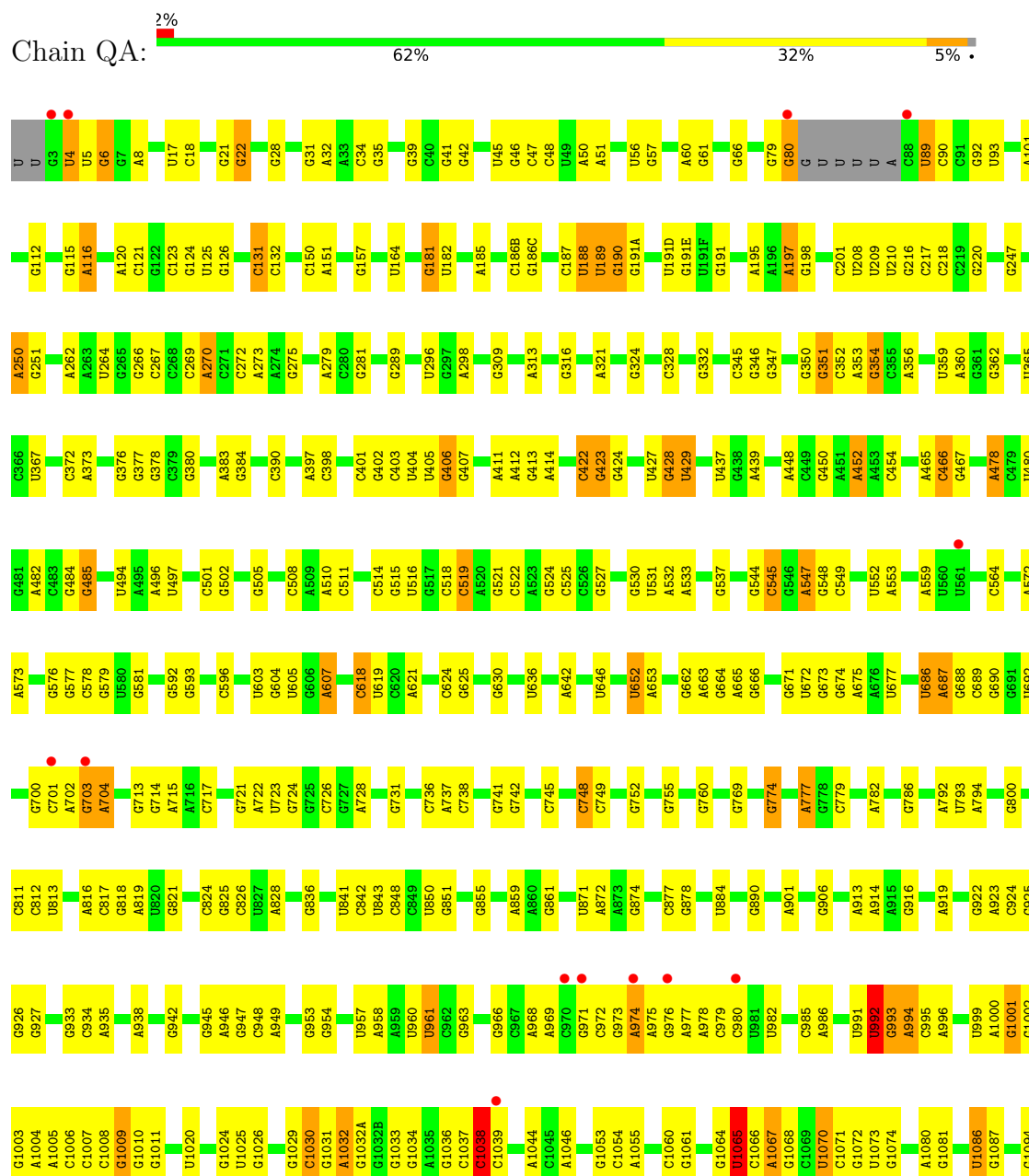
- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

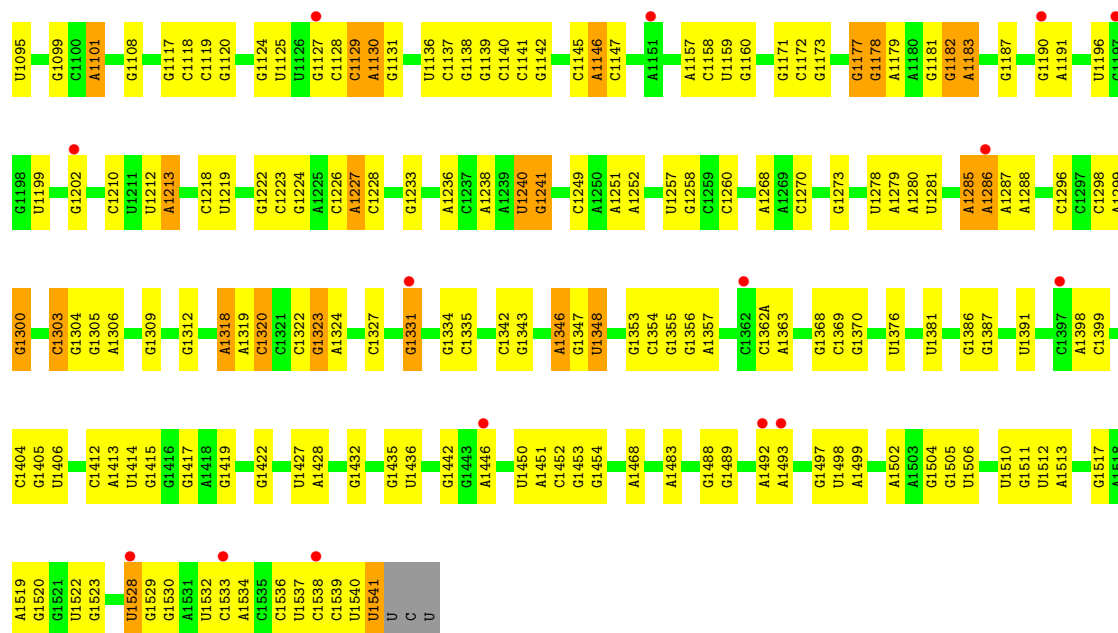
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	QN	1	Total	Zn	0	0
			1	1		
59	R4	1	Total	Zn	0	0
			1	1		
59	R5	1	Total	Zn	0	0
			1	1		
59	R6	1	Total	Zn	0	0
			1	1		
59	R9	1	Total	Zn	0	0
			1	1		
59	XN	1	Total	Zn	0	0
			1	1		
59	Y4	1	Total	Zn	0	0
			1	1		
59	Y6	1	Total	Zn	0	0
			1	1		

3 Residue-property plots

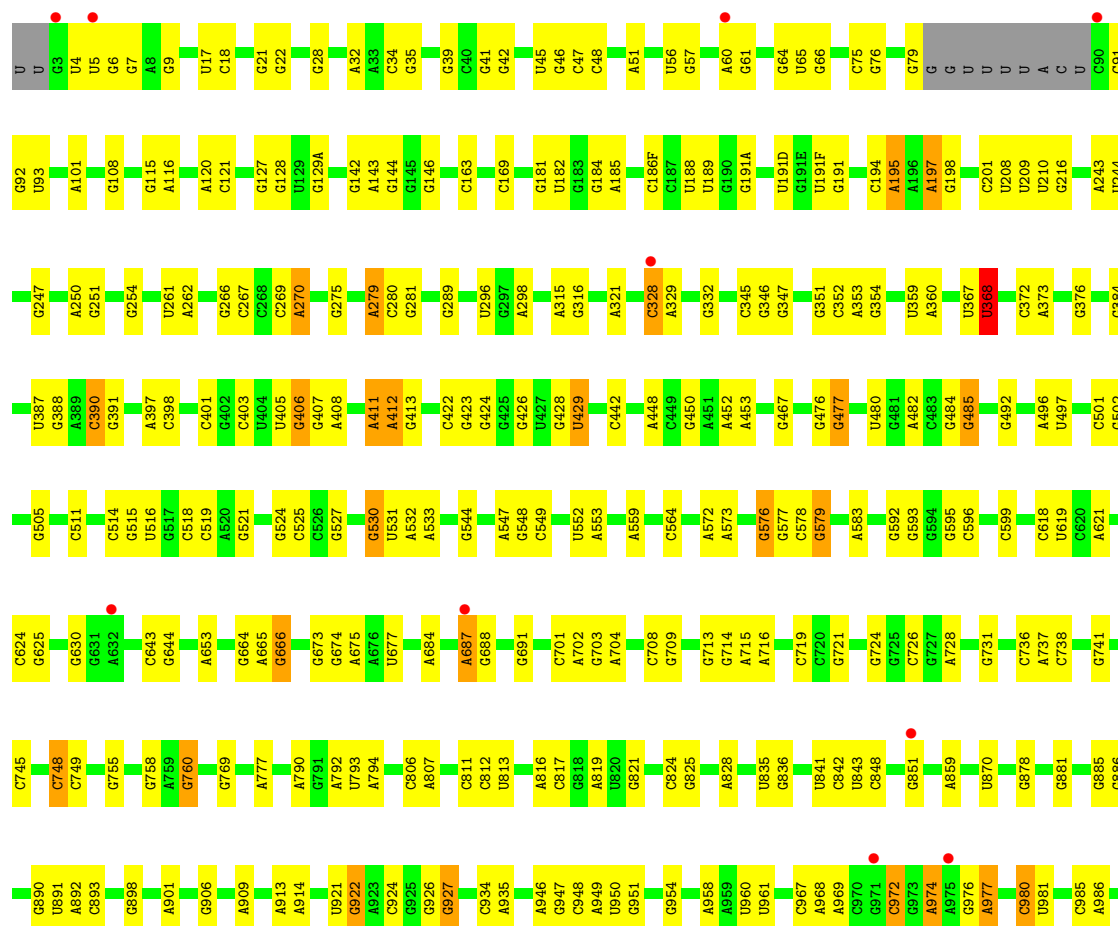
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

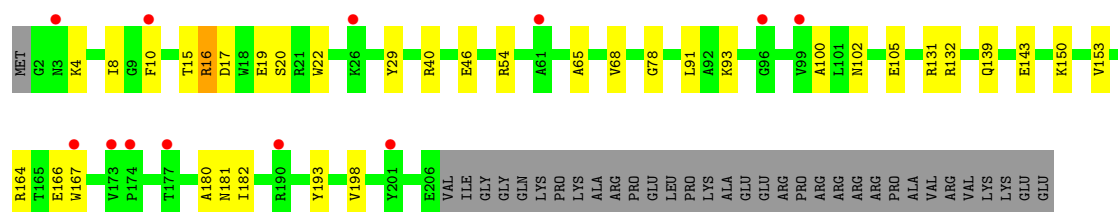
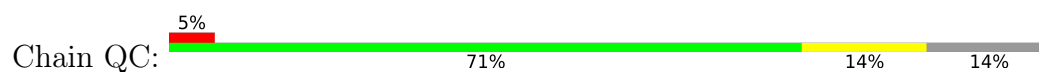
• Molecule 1: 16S rRNA



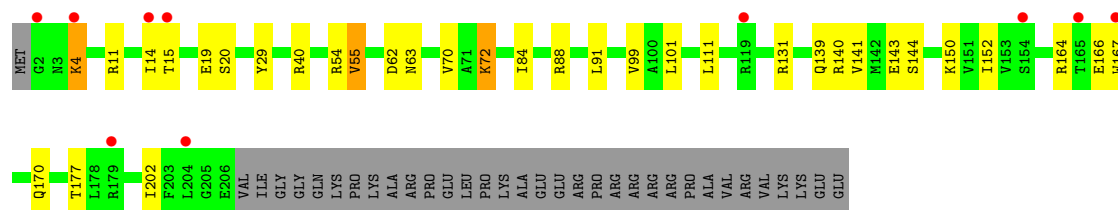
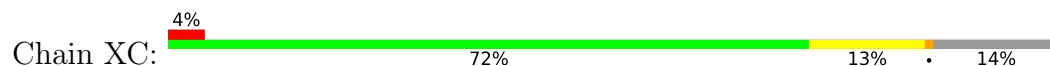


• Molecule 1: 16S rRNA

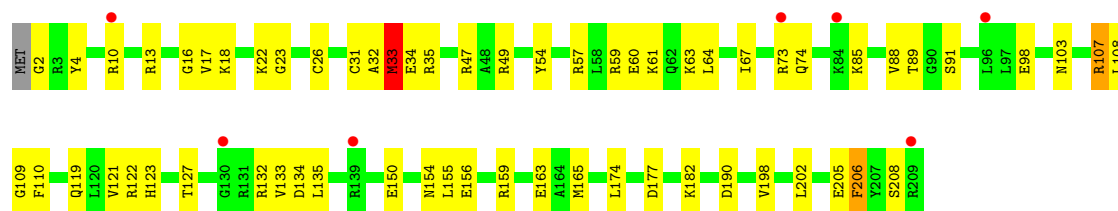
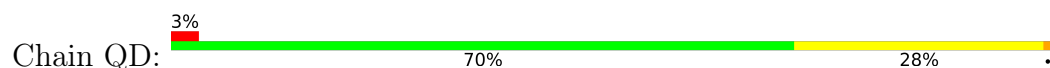




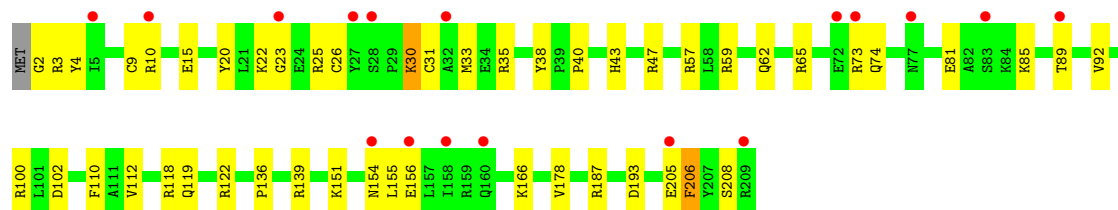
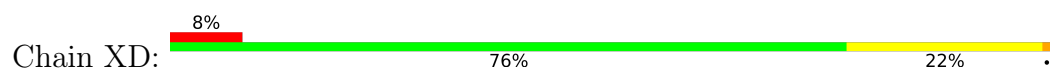
• Molecule 3: 30S ribosomal protein S3



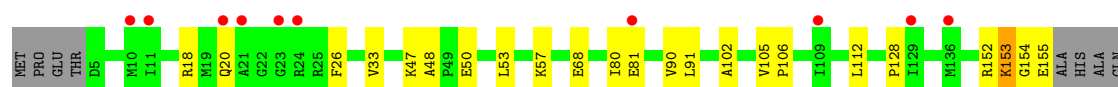
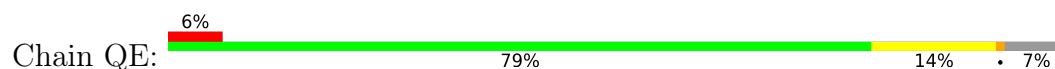
• Molecule 4: 30S ribosomal protein S4



• Molecule 4: 30S ribosomal protein S4



• Molecule 5: 30S ribosomal protein S5



ALA
GLN
GLY

- Molecule 5: 30S ribosomal protein S5

Chain XE:  5% 77% 15% 7%

MET PRO GLU THR D5 M10 I11 M19 Q20 A21 G22 G23 R24 R25 F26 V51 P52 L53 Q56 R63 M66 V69 I80 E81 G85 V90 L91 A102 V105 P106 R107 E111 T120 G124 P128 T135 G154 E155 ALA HIS ALA GLN

ALA
GLN
GLY

- Molecule 6: 30S ribosomal protein S6

Chain QF:  3% 79% 21%

M1 R2 R3 V6 V9 L10 N13 L14 D15 Q16 S17 R46 K54 Y59 F60 L61 W62 Q64 Y65 E66 E69 A76 L79 R80 R87 V88 M89 V90 S93 A101

- Molecule 6: 30S ribosomal protein S6

Chain XF:  83% 16%

M1 R2 V9 L10 E22 L30 V37 L45 R46 Y59 F60 L61 V65 V72 L75 R82 R87 E95 N100 A101

- Molecule 7: 30S ribosomal protein S7

Chain QG:  5% 81% 17%

MET A2 R3 R4 E8 V9 R10 D15 L16 V17 Y18 G19 D20 V23 N28 F29 I30 M31 D45 L59 F60 V61 F62 V75 R78 R79 V80 Y85 Q86 V87 P88 R94 R119 L124 A150 Y151 A152 H153 Y154 W156

- Molecule 7: 30S ribosomal protein S7

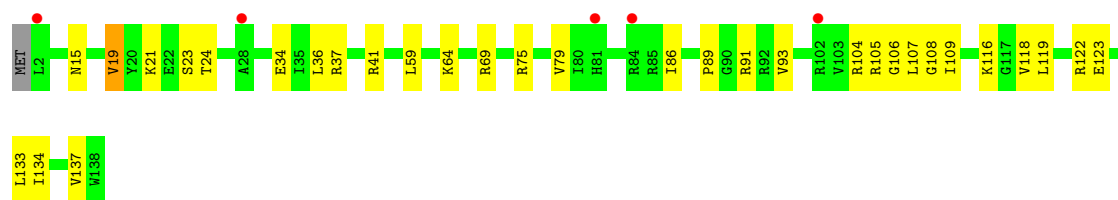
Chain XG:  10% 81% 16%

MET A2 R3 R4 Q13 P14 D15 L16 G19 D20 V23 F26 K29 R32 D33 N37 T42 F43 Y44 E57 R76 S77 R78 R79 V80 G81 G82 A83 N84 V87 R94 S98 L101 R113 R114 R119 M125 D126 A150 Y151 A152

H153 Y154 R155 W156

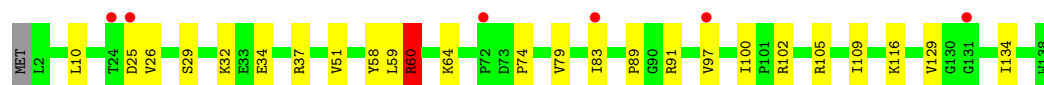
- Molecule 8: 30S ribosomal protein S8

Chain QH:  4% 76% 22%



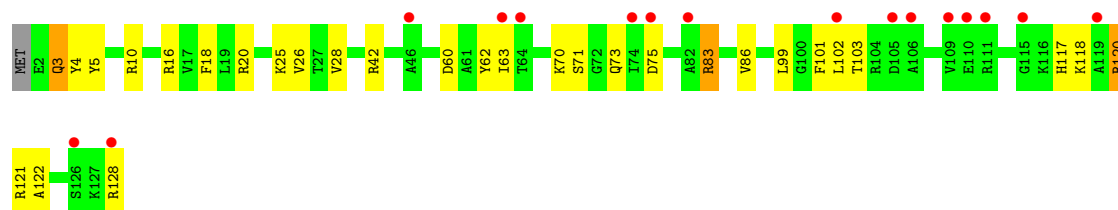
- Molecule 8: 30S ribosomal protein S8

Chain XH: 4% 81% 17% ..



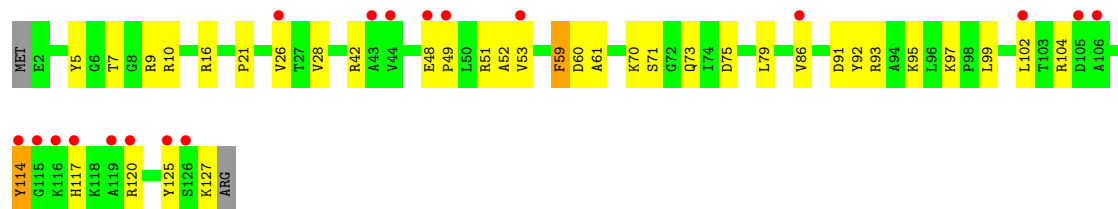
- Molecule 9: 30S ribosomal protein S9

Chain QI: 12% 76% 21% ..



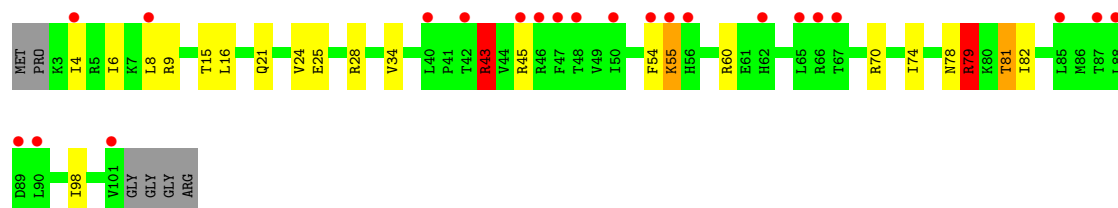
- Molecule 9: 30S ribosomal protein S9

Chain XI: 14% 70% 27% ..



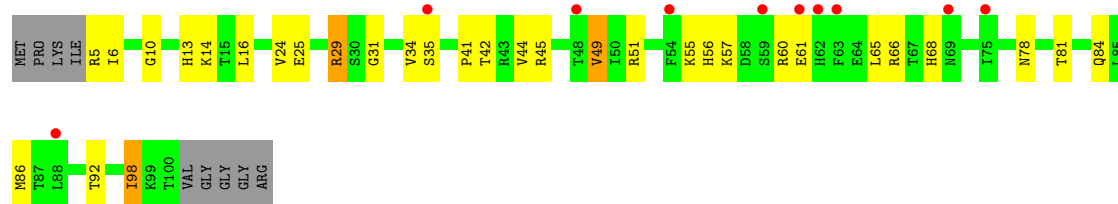
- Molecule 10: 30S ribosomal protein S10

Chain QJ: 21% 72% 18% 6%

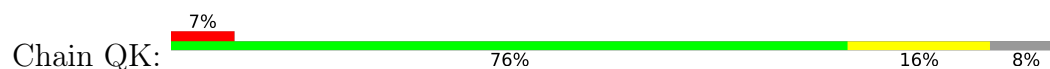


- Molecule 10: 30S ribosomal protein S10

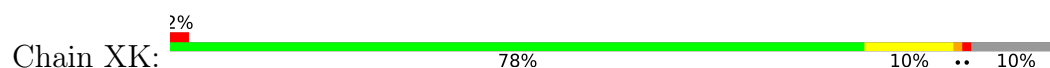
Chain XJ: 10% 61% 28% 9%



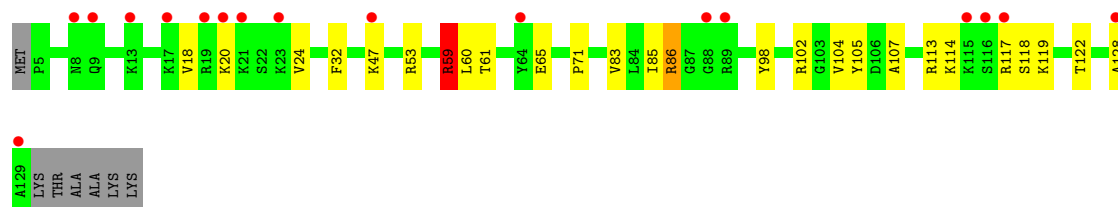
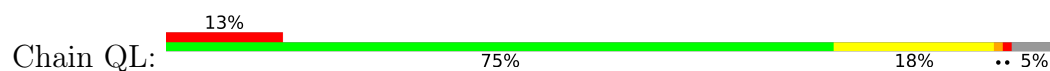
- Molecule 11: 30S ribosomal protein S11



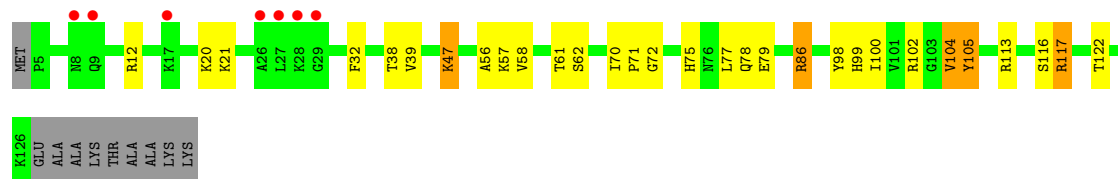
- Molecule 11: 30S ribosomal protein S11



- Molecule 12: 30S ribosomal protein S12



- Molecule 12: 30S ribosomal protein S12

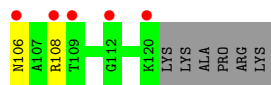
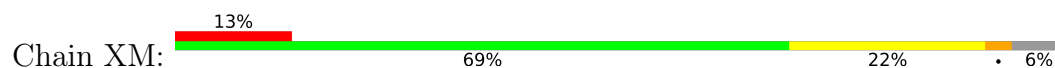


- Molecule 13: 30S ribosomal protein S13

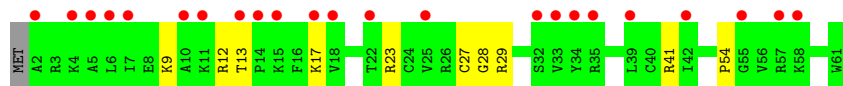
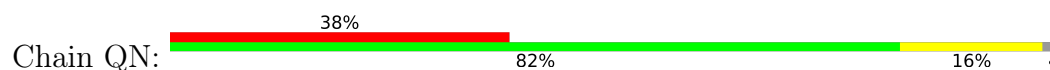




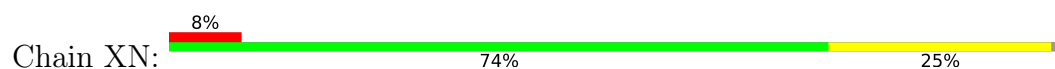
- Molecule 13: 30S ribosomal protein S13



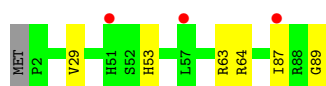
- Molecule 14: 30S ribosomal protein S14 type Z



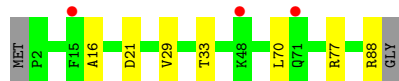
- Molecule 14: 30S ribosomal protein S14 type Z



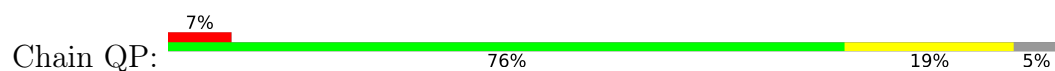
- Molecule 15: 30S ribosomal protein S15

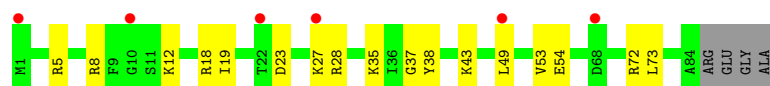


- Molecule 15: 30S ribosomal protein S15

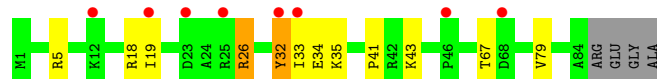
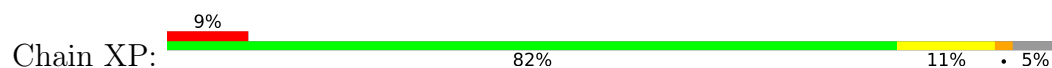


- Molecule 16: 30S ribosomal protein S16

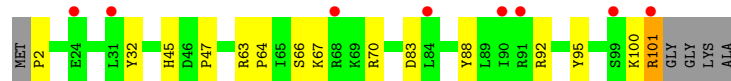
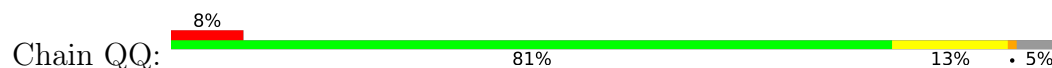




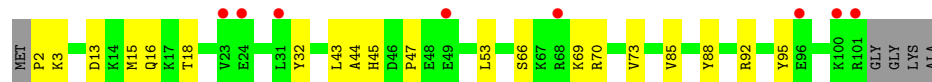
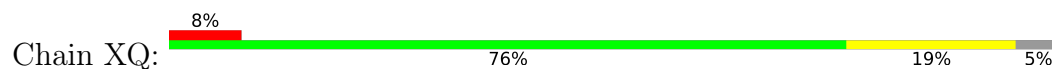
- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17



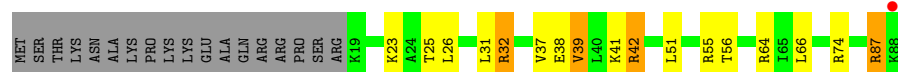
- Molecule 17: 30S ribosomal protein S17



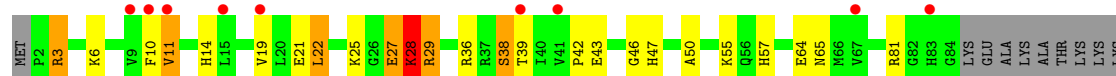
- Molecule 18: 30S ribosomal protein S18



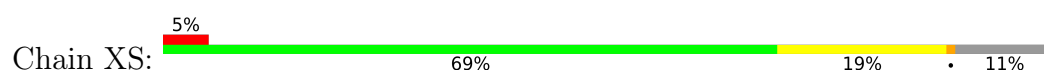
- Molecule 18: 30S ribosomal protein S18



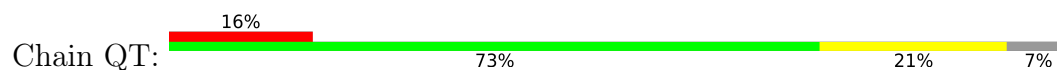
- Molecule 19: 30S ribosomal protein S19



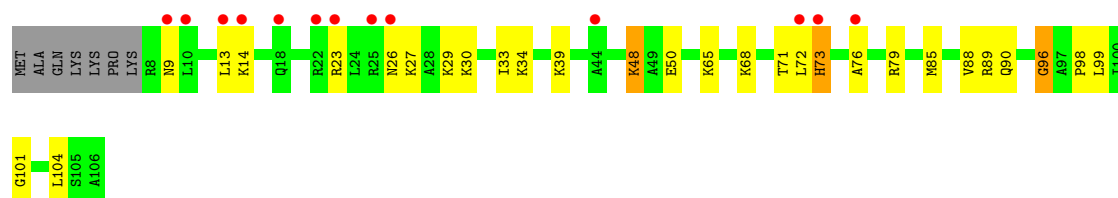
- Molecule 19: 30S ribosomal protein S19



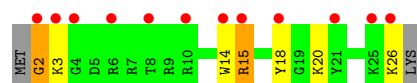
- Molecule 20: 30S ribosomal protein S20



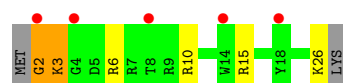
- Molecule 20: 30S ribosomal protein S20



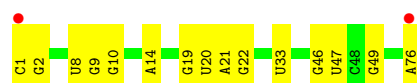
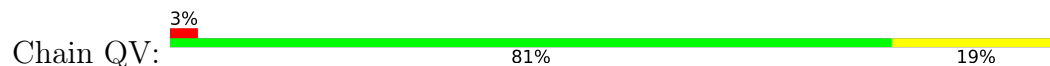
- Molecule 21: 30S ribosomal protein Thx



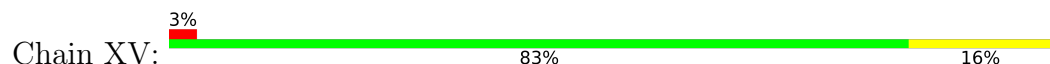
- Molecule 21: 30S ribosomal protein Thx

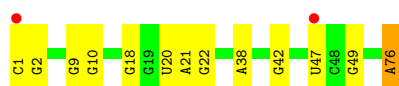


- Molecule 22: P-site tRNA-fMet

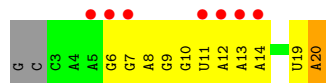


- Molecule 22: P-site tRNA-fMet





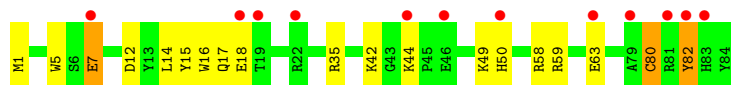
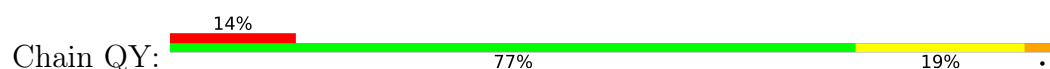
- Molecule 23: mRNA



- Molecule 23: mRNA



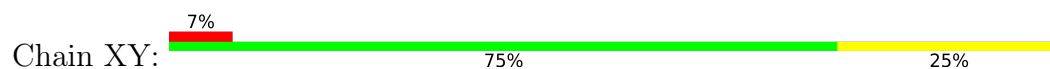
- Molecule 24: Addiction module toxin, Txe/YoeB family



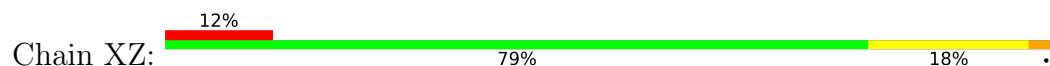
- Molecule 24: Addiction module toxin, Txe/YoeB family



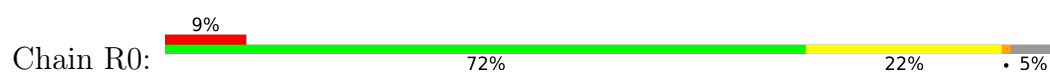
- Molecule 24: Addiction module toxin, Txe/YoeB family



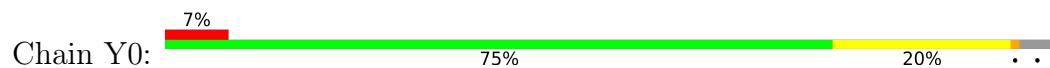
- Molecule 24: Addiction module toxin, Txe/YoeB family



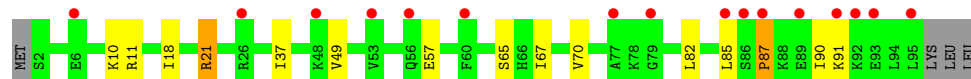
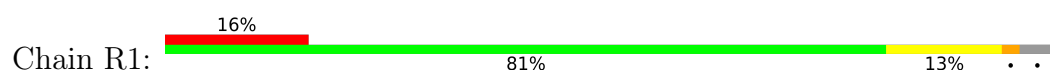
- Molecule 25: 50S ribosomal protein L27



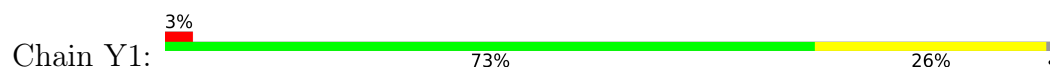
- Molecule 25: 50S ribosomal protein L27



- Molecule 26: 50S ribosomal protein L28



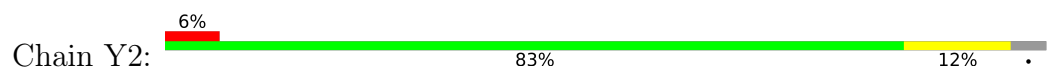
- Molecule 26: 50S ribosomal protein L28



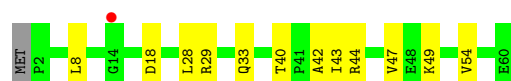
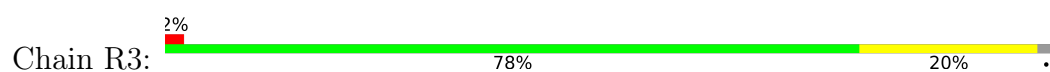
- Molecule 27: 50S ribosomal protein L29



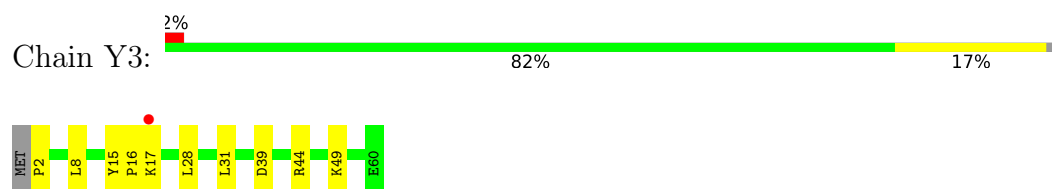
- Molecule 27: 50S ribosomal protein L29



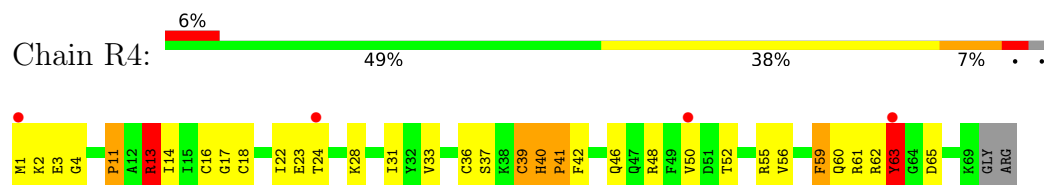
- Molecule 28: 50S ribosomal protein L30



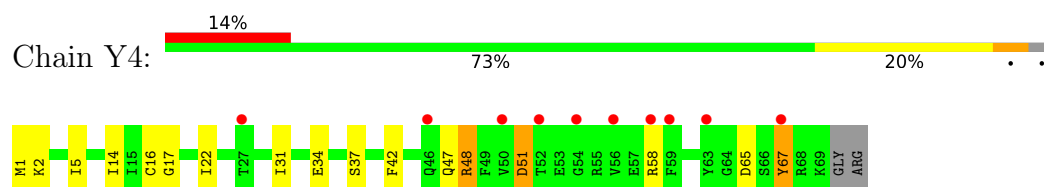
- Molecule 28: 50S ribosomal protein L30



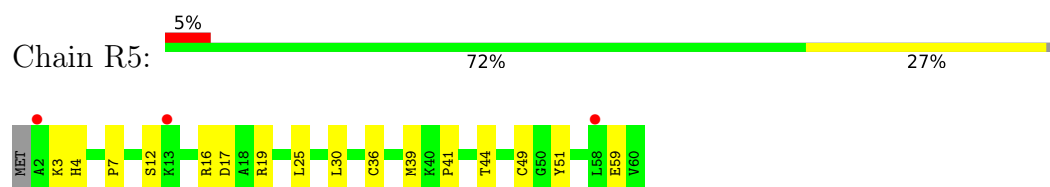
- Molecule 29: 50S ribosomal protein L31



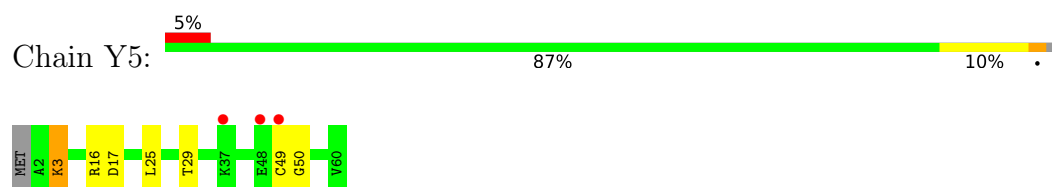
- Molecule 29: 50S ribosomal protein L31



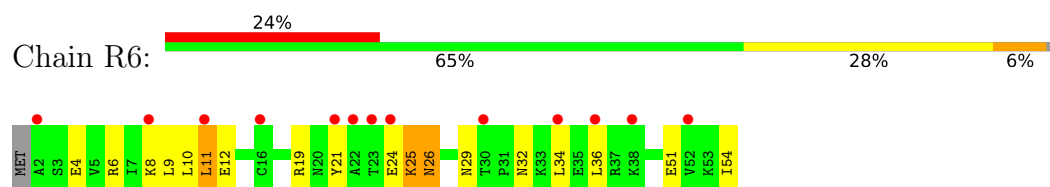
- Molecule 30: 50S ribosomal protein L32



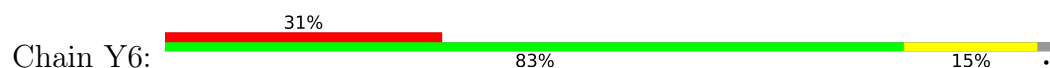
- Molecule 30: 50S ribosomal protein L32

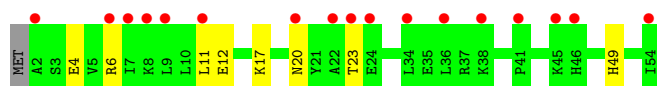


- Molecule 31: 50S ribosomal protein L33

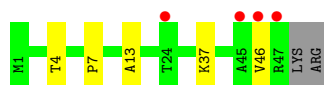
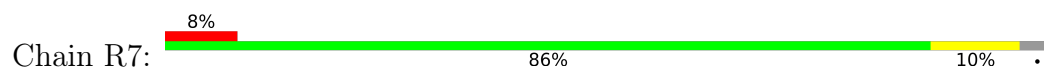


- Molecule 31: 50S ribosomal protein L33

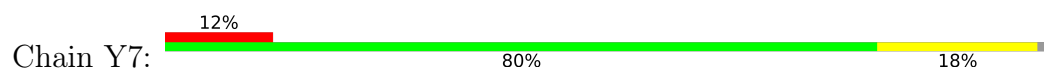




- Molecule 32: 50S ribosomal protein L34



- Molecule 32: 50S ribosomal protein L34



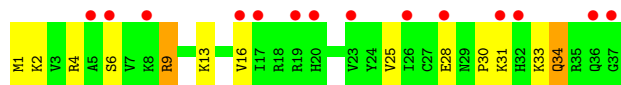
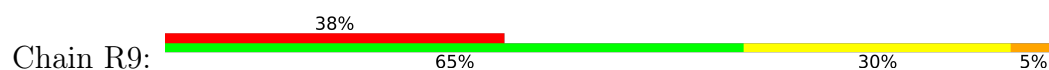
- Molecule 33: 50S ribosomal protein L35



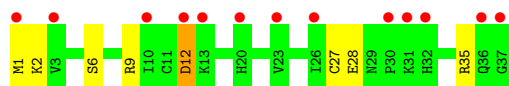
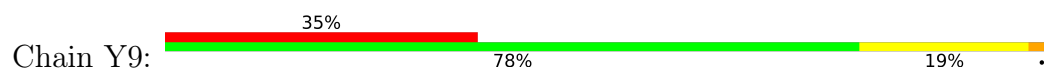
- Molecule 33: 50S ribosomal protein L35



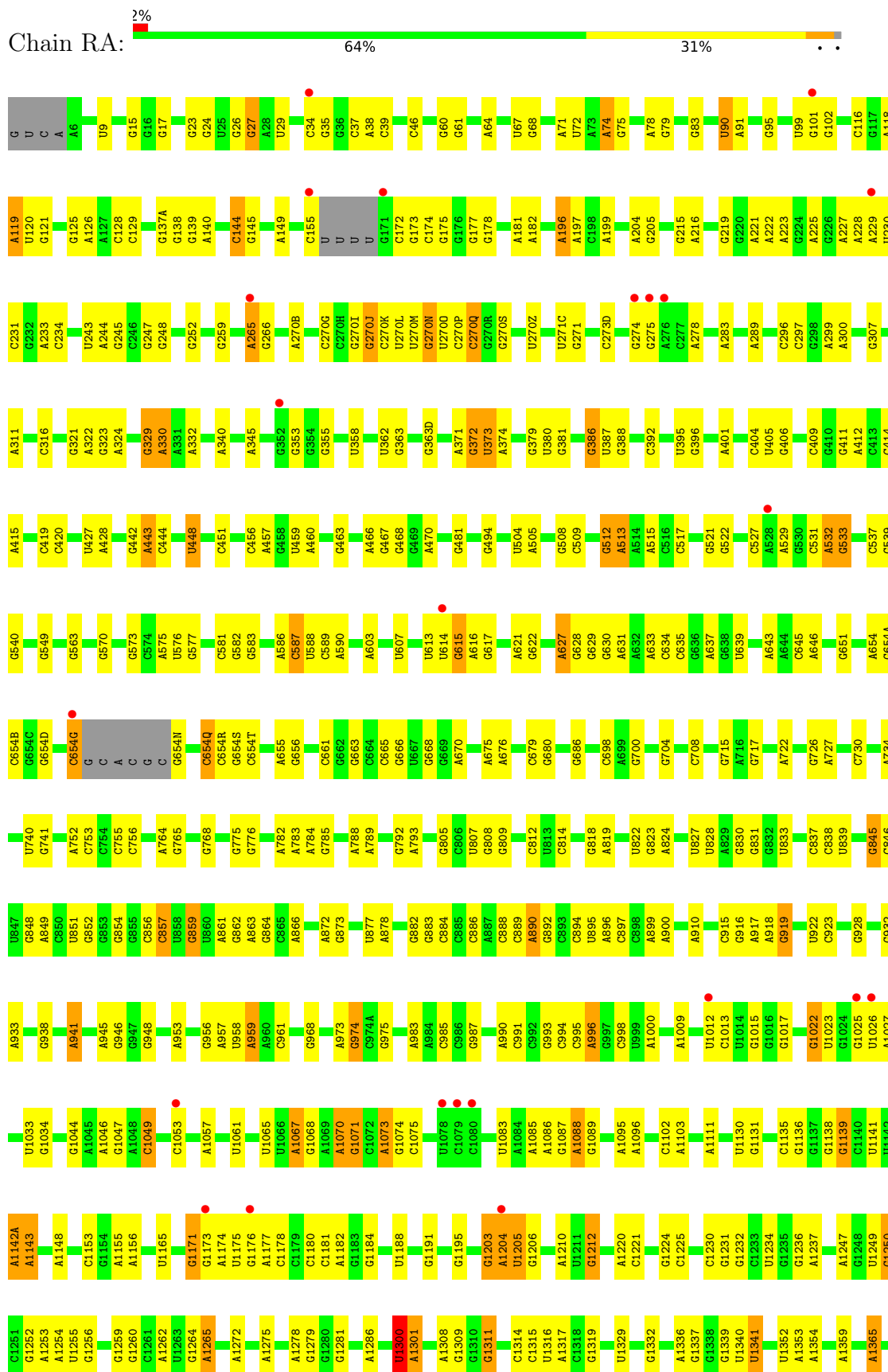
- Molecule 34: 50S ribosomal protein L36



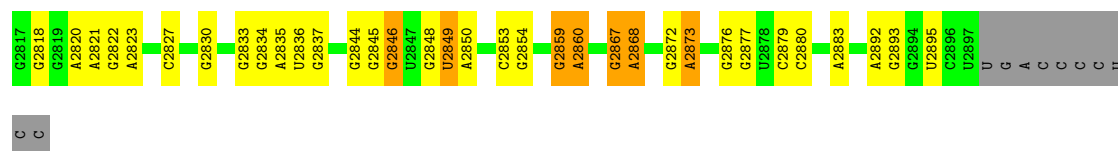
- Molecule 34: 50S ribosomal protein L36



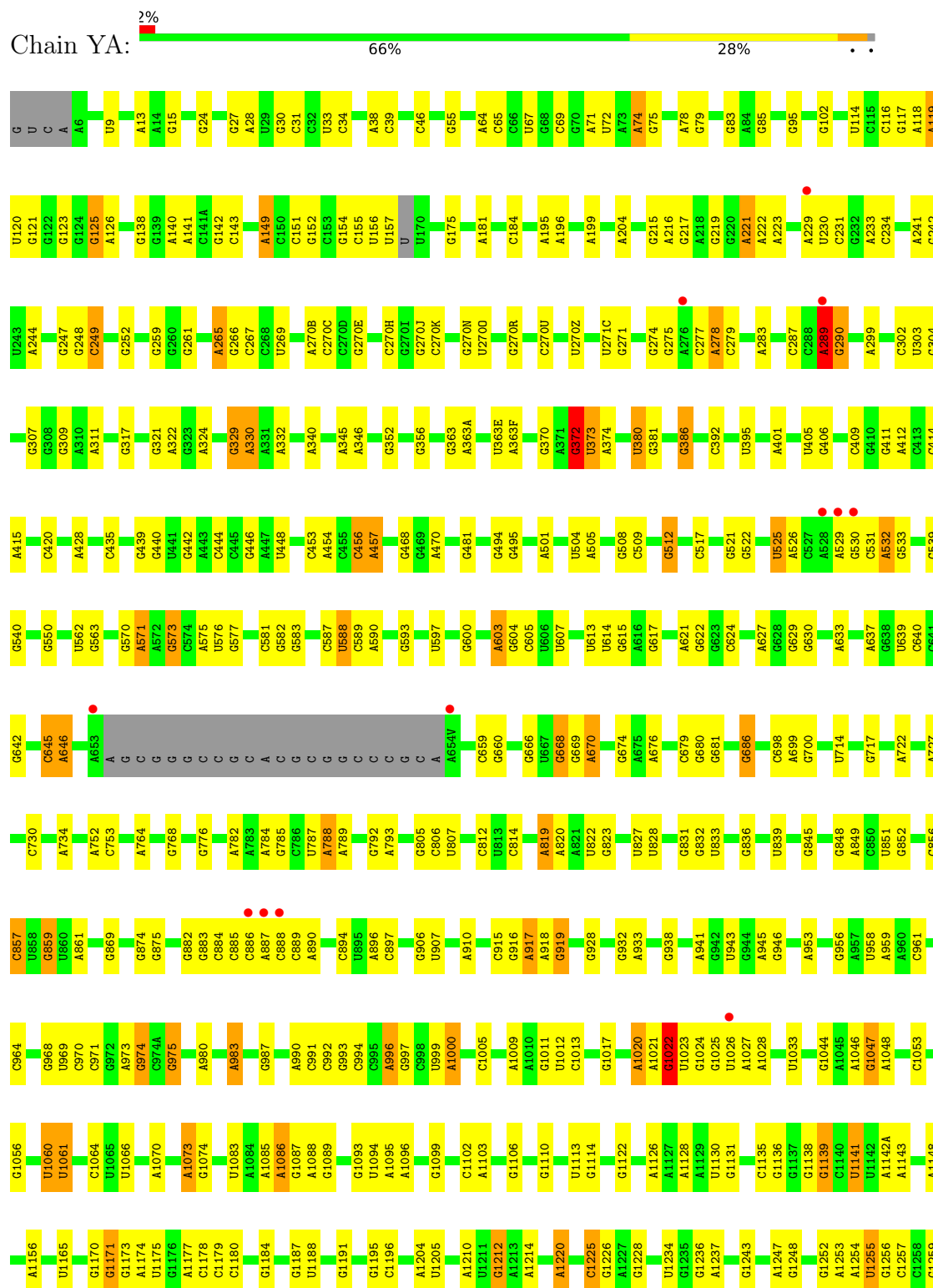
- Molecule 35: 23S rRNA



G2724	A2725	G2726	G2727	U2728	G2729	G2732	A2733	G2743	G2744	G2747	A2748	A2749	A2750	G2751	G2752	A2757	A2758	G2761	G2762	A2765	G2766	G2773	A2776	G2777	A2778	U2779	G2780	A2781	G2784	G2787	G2788	G2789	A2790	G2793	U2797	G2798	A2801	G2802	G2803	G2804	G2805	G2807	U2808	A2809	G2816										
G2588	G2591	G2592	G2597	A2598	A2602	U2609	G2610	G2611	G2612	U2615	G2618	G2629	G2630	G2638	G2646	A2654	G2655	G2665	G2673	G2680	G2681	U2682	U2689	G2690	G2691	G2692	A2693	U2696	G2697	G2701	U2702	G2703	U2712	A2712A	A2713	G2714	G2715	U2716	U2720	G2723															
G2470	G2471	G2472	G2473	G2474	G2475	A2476	G2477	G2481	G2482	U2491	G2502	A2503	U2504	G2505	G2515	G2516	G2517	A2518	U2519	G2524	G2527	U2528	G2529	G2535	G2540	G2541	A2542	G2543	G2544	U2547	U2554	G2560	A2566	G2567	G2568	G2569	A2572	G2573	G2574	G2578	U2584	U2585	G2586	A2587											
G2358	G2369	G2372	G2373	G2374	G2382	G2383	G2384	G2385	A2392	A2393	G2394	G2402	G2403	G2404	G2405	U2406	G2410	A2411	A2412	C2416	A2422	U2423	G2424	G2425	A2426	G2427	G2428	G2429	A2430	A2435	U2438	A2439	G2440	C2441	G2445	G2446	G2447	A2448	U2449	A2450	U2457	G2466	G2467	G2468	A2469										
G2147	G2148	G2149	U2150	G2153	G2161	G2165	G2166	U2167	G2168	A2169	A2170	A2171	U2172	A2173	G2174	G2177	G2178	G2179	U2180	G2181	G2182	G2183	G2184	G2185	G2186	G2187	G2188	U2189	A2190	G2191	G2192	A2198	G2210	G2211	G2212	U2213	G2215	G2225	G2226	G2230	U2233	G2238	G2239	U2243	U2244	U2245	G2246	G2247							
G2056	A2059	A2060	G2061	A2062	G2063	G2069	U2074	U2075	U2079	G2080	G2081	A2082	U2086	U2089	U2092	G2093	U2102	G2103	G2104	G2111	G2112	U2113	G2116	A2117	U2118	A2119	G2120	G2124	G2127	G2128	G2129	U2130	G2131	U2132	G2133	A2134	U2135	G2136	G2139	G2140	G2141	G2142	G2143	U2144	G2145	G2146									
A1819	U1820	G1824	G1827	G1828	G1829	A1830	G1831	G1832	A1837	A1853	G1857	G1858	G1863	G1869	A1872	G1878	C1881	G1882	G1883	A1884	A1885	G1888	A1889	A1890	U1900	G1903	G1906	A1913	G1914	A1927	A1928	G1929	U1930	U1931	G1935	A1936	A1937	A1938	C1941	G1948															
A1554	G1461	G1466	G1467	G1470	A1384	G1385	G1388	G1475	A1476	U1477	G1478	A1392	A1393	U1394	A1395	U1396	C1399	G1400	A1386	A1490	G1402	G1403	U1497	C1407	C1408	A1409	C1505	G1509	A1510	C1518	U1519	U1520	G1521	G1522	U1523	G1524	G1525	G1526	A1529	G1530	U1535	A1536	G1537	G1538	G1539	U1540	U1541	G1542	A1543	G1545	C1544	A1545	C1547	G1550	C1559
G1687	A1688	A1689	G1694	G1695	G1696	G1697	A1698	G1699	A1700	A1701	G1725	G1728	U1729	G1731	G1732	G1733	G1743	C1754	G1756	C1759	C1762	G1763	G1764	G1769	G1770	G1771	G1772	A1773	G1776	U1779	A1780	G1781	G1782	A1783	A1784	A1785	G1651	G1652	G1653	A1654	C1657	G1667	G1674	G1678	C1681	G1816	G1817	U1818							



• Molecule 35: 23S rRNA



G1260	C1261	A1262	U1396	C1493	G1622	U1779	G1910	A2031	A2134	A2225	G2334	A2450	C2573	G1260
C1261	A1262	A1265	G1400	C1509	A1632	U1780	A1913	G2032	A2135	C2226	A2335	A2451	A2577	C1261
A1265	C1402	A1266	G1401	A1510	G1633	C1781	C1914	A2033	C2138	U2232	A2336	U2457	G2578	A1262
A1272	C1403	A1278	C1406	G1511	G1634	C1782	G1929	G2035	C2139	U2233	C2343	C2456	U2584	A1265
A1278	C1407	G1279	U1406	G1512	C1636	A1783	G1930	G2037	C2140	G2238	U2344	A2469	C2591	A1266
G1279	C1408	G1280	C1407	U1523	A1637	A1784	A1936	G2038	C2141	G2239	G2345	G2470	G2592	A1272
G1281	C1411	G1281	C1408	G1524	C1640	A1791	A1937	C2043	C2142	U2245	C2347	C2471	A2602	A1278
U1284	A1412	U1284	U1407	G1525	C1648	G1792	A1938	G2052	C2143	G2246	C2350	U2472	C2609	A1278
U1300	G1416	U1300	C1407	U1535	A1652	G1792	A1948	C2055	C2144	A2247	G2354	C2474	C2610	A1278
A1301	A1419	A1301	C1408	A1536	A1654	G1799	U1955	G2056	C2145	G2247	C2355	C2475	G2612	A1278
A1308	U1420	A1308	U1523	C1537	C1657	C1800	G1968	A2059	C2146	U2247	G2358	A2476	U2609	A1278
G1309	G1421	G1309	G1538	G1539	C1658	G1801	U1965	A2060	C2147	U2247	G2358	A2477	C2618	A1278
G1310	G1422	G1310	G1540	C1540	G1667	G1802	U1966	A2061	C2148	G2251	G2364	C2478	C2618	A1278
G1311	G1424	G1311	A1543	C1544	A1669	G1809	A1967	G2062	C2149	U2251	C2364	C2478	C2618	A1278
C1314	G1427	C1314	A1545	A1545	G1674	A1819	G1968	A2069	C2150	A2251	C2364	C2478	C2618	A1278
C1315	C1428	C1315	C1547	C1547	G1681	U1820	A1969	G2074	C2151	U2251	C2364	C2478	C2618	A1278
U1316	U1431	U1316	A1554	A1554	G1681	U1824	A1970	U2075	C2152	U2251	C2364	C2478	C2618	A1278
A1317	C1432	A1317	A1554	A1554	G1681	U1824	A1971	U2075	C2153	U2251	C2364	C2478	C2618	A1278
U1329	A1434	U1329	A1554	A1554	G1681	U1824	A1971	U2075	C2154	U2251	C2364	C2478	C2618	A1278
C1330	A1434	C1330	A1554	A1554	G1681	U1824	A1971	U2075	C2155	U2251	C2364	C2478	C2618	A1278
U1341	C1437	U1341	A1554	A1554	G1681	U1824	A1971	U2075	C2156	U2251	C2364	C2478	C2618	A1278
A1342	A1444	A1342	A1554	A1554	G1681	U1824	A1971	U2075	C2157	U2251	C2364	C2478	C2618	A1278
U1352	C1445	U1352	A1554	A1554	G1681	U1824	A1971	U2075	C2158	U2251	C2364	C2478	C2618	A1278
A1353	A1449	A1353	A1554	A1554	G1681	U1824	A1971	U2075	C2159	U2251	C2364	C2478	C2618	A1278
A1354	G1449A	A1354	A1554	A1554	G1681	U1824	A1971	U2075	C2160	U2251	C2364	C2478	C2618	A1278
A1359	G1455	A1359	A1554	A1554	G1681	U1824	A1971	U2075	C2161	U2251	C2364	C2478	C2618	A1278
C1363	G1459	C1363	A1554	A1554	G1681	U1824	A1971	U2075	C2162	U2251	C2364	C2478	C2618	A1278
G1368	G1460	G1368	A1554	A1554	G1681	U1824	A1971	U2075	C2163	U2251	C2364	C2478	C2618	A1278
G1369	C1461	G1369	A1554	A1554	G1681	U1824	A1971	U2075	C2164	U2251	C2364	C2478	C2618	A1278
C1370	C1462	C1370	A1554	A1554	G1681	U1824	A1971	U2075	C2165	U2251	C2364	C2478	C2618	A1278
C1378	C1467	C1378	A1554	A1554	G1681	U1824	A1971	U2075	C2166	U2251	C2364	C2478	C2618	A1278
A1379	A1471	A1379	A1554	A1554	G1681	U1824	A1971	U2075	C2167	U2251	C2364	C2478	C2618	A1278
G1380	G1475	G1380	A1554	A1554	G1681	U1824	A1971	U2075	C2168	U2251	C2364	C2478	C2618	A1278
A1394	G1480	A1394	A1554	A1554	G1681	U1824	A1971	U2075	C2169	U2251	C2364	C2478	C2618	A1278
G1385	U1482	G1385	A1554	A1554	G1681	U1824	A1971	U2075	C2170	U2251	C2364	C2478	C2618	A1278
G1388	G1483	G1388	A1554	A1554	G1681	U1824	A1971	U2075	C2171	U2251	C2364	C2478	C2618	A1278
U1391	G1488	U1391	A1554	A1554	G1681	U1824	A1971	U2075	C2172	U2251	C2364	C2478	C2618	A1278
U1394	U1489	U1394	A1554	A1554	G1681	U1824	A1971	U2075	C2173	U2251	C2364	C2478	C2618	A1278
A1395	A1618	A1395	A1554	A1554	G1681	U1824	A1971	U2075	C2174	U2251	C2364	C2478	C2618	A1278
U1396	C1774	U1396	A1554	A1554	G1681	U1824	A1971	U2075	C2175	U2251	C2364	C2478	C2618	A1278
C1493	A1607	C1493	A1554	A1554	G1681	U1824	A1971	U2075	C2176	U2251	C2364	C2478	C2618	A1278
G1622	G1762	G1622	A1554	A1554	G1681	U1824	A1971	U2075	C2177	U2251	C2364	C2478	C2618	A1278
U1779	G1764	U1779	A1554	A1554	G1681	U1824	A1971	U2075	C2178	U2251	C2364	C2478	C2618	A1278
G1910	G1769	G1910	A1554	A1554	G1681	U1824	A1971	U2075	C2179	U2251	C2364	C2478	C2618	A1278
A2031	U2028	A2031	A1554	A1554	G1681	U1824	A1971	U2075	C2180	U2251	C2364	C2478	C2618	A1278
A2134	U2029	A2134	A1554	A1554	G1681	U1824	A1971	U2075	C2181	U2251	C2364	C2478	C2618	A1278
A2225	U2030	A2225	A1554	A1554	G1681	U1824	A1971	U2075	C2182	U2251	C2364	C2478	C2618	A1278
G2334	U2031	G2334	A1554	A1554	G1681	U1824	A1971	U2075	C2183	U2251	C2364	C2478	C2618	A1278
A2450	U2032	A2450	A1554	A1554	G1681	U1824	A1971	U2075	C2184	U2251	C2364	C2478	C2618	A1278
C2573	U2033	C2573	A1554	A1554	G1681	U1824	A1971	U2075	C2185	U2251	C2364	C2478	C2618	A1278
G1260	U2034	G1260	A1554	A1554	G1681	U1824	A1971	U2075	C2186	U2251	C2364	C2478	C2618	A1278
C1261	U2035	C1261	A1554	A1554	G1681	U1824	A1971	U2075	C2187	U2251	C2364	C2478	C2618	A1278
A1262	U2036	A1262	A1554	A1554	G1681	U1824	A1971	U2075	C2188	U2251	C2364	C2478	C2618	A1278
A1265	U2037	A1265	A1554	A1554	G1681	U1824	A1971	U2075	C2189	U2251	C2364	C2478	C2618	A1278
A1272	U2038	A1272	A1554	A1554	G1681	U1824	A1971	U2075	C2190	U2251	C2364	C2478	C2618	A1278
A1278	U2039	A1278	A1554	A1554	G1681	U1824	A1971	U2075	C2191	U2251	C2364	C2478	C2618	A1278
G1279	U2040	G1279	A1554	A1554	G1681	U1824	A1971	U2075	C2192	U2251	C2364	C2478	C2618	A1278
G1280	U2041	G1280	A1554	A1554	G1681	U1824	A1971	U2075	C2193	U2251	C2364	C2478	C2618	A1278
G1281	U2042	G1281	A1554	A1554	G1681	U1824	A1971	U2075	C2194	U2251	C2364	C2478	C2618	A1278
U1284	U2043	U1284	A1554	A1554	G1681	U1824	A1971	U2075	C2195	U2251	C2364	C2478	C2618	A1278
U1300	U2044	U1300	A1554	A1554	G1681	U1824	A1971	U2075	C2196	U2251	C2364	C2478	C2618	A1278
A1301	U2045	A1301	A1554	A1554	G1681	U1824	A1971	U2075	C2197	U2251	C2364	C2478	C2618	A1278
A1308	U2046	A1308	A1554	A1554	G1681	U1824	A1971	U2075	C2198	U2251	C2364	C2478	C2618	A1278
G1309	U2047	G1309	A1554	A1554	G1681	U1824	A1971	U2075	C2199	U2251	C2364	C2478	C2618	A1278
G1310	U2048	G1310	A1554	A1554	G1681	U1824	A1971	U2075	C2200	U2251	C2364	C2478	C2618	A1278
G1311	U2049	G1311	A1554	A1554	G1681	U1824	A1971	U2075	C2201	U2251	C2364	C2478	C2618	A1278
C1314	U2050	C1314	A1554	A1554	G1681	U1824	A1971	U2075	C2202	U2251	C2364	C2478	C2618	A1278
C1315	U2051	C1315	A1554	A1554	G1681	U1824	A1971	U2075	C2203	U2251	C2364	C2478	C2618	A1278
U1316	U2052	U1316	A1554	A1554	G1681	U1824	A1971	U2075	C2204	U2251	C2364	C2478	C2618	A1278
A1317	U2053	A1317	A1554	A1554	G1681	U1824	A1971	U2075	C2205	U2251	C2364	C2478	C2618	A1278
U1329	U2054	U1329	A1554	A1554	G1681	U1824	A1971	U2075	C2206	U2251	C2364	C2478	C2618	A1278
C1330	U2055	C1330	A1554	A1554	G1681	U1824	A1971	U2075	C2207	U2251	C2364	C2478	C2618	A1278
U1341	U2056	U1341	A1554	A1554	G1681	U1824	A1971	U2075	C2208	U2251	C2364	C2478	C2618	A1278
A1342	U2057	A1342	A1554	A1554	G1681	U1824	A1971	U2075	C2209	U2251	C2364	C2478	C2618	A1278
U1352	U2058	U1352	A1554	A1554	G1681	U1824	A1971	U2075	C2210	U2251	C2364	C2478	C2618	A1278
A1353	U2059	A1353	A1554	A1554	G1681	U1824	A1971	U2075	C2211	U2251	C2364	C2478	C2618	A1278
A1354	U2060	A1354	A1554	A1554	G1681	U1824	A1971	U2075	C2212	U2251	C2364	C2478	C2618	A1278
A1359	U2061	A1359	A1554	A1554	G1681	U1824	A1971	U2075	C2213	U2251	C2364	C2478	C2618	A1278
C1363	U2062	C1363	A1554	A1554	G1681	U1824	A1971	U2075	C2214	U2251	C2364	C2478	C2618	A1278
G1368	U2063	G1368	A1554	A1554	G1681	U1824	A1971	U2075	C2215	U2251	C2364	C2478	C2618	A1278
G1369	U2064	G1369	A1554	A1554	G1681	U1824	A1971	U2075	C2216	U2251	C2364	C2478	C2618	A1278
C1370	U2065	C1370	A1554	A1554	G1681	U1824	A1971	U2075	C2217	U2251	C2364	C2478	C2618	A1278
C1378	U2066	C1378	A1554	A1554	G1681	U1824	A1971	U2075	C2218	U2251	C2364	C2478	C2618	A1278
A1379	U2067	A1379	A1554	A1554	G1681	U1824	A1971	U2075	C2219	U2251	C2364	C2478	C2618	A1278
G1380	U2068	G1380	A1554	A1554	G1681	U1824	A1971	U2075	C2220	U2251	C2364	C2478	C2618	A1278
A1394	U2069	A1394	A1554	A1554	G1681	U1824	A1971	U2075	C2221	U2251	C2364	C2478	C2618	



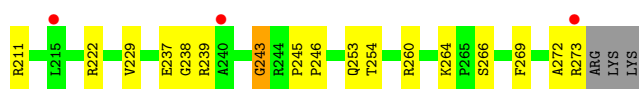
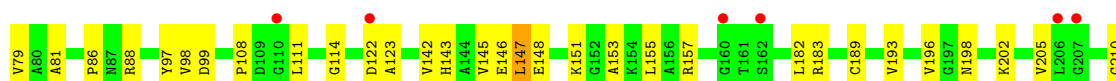
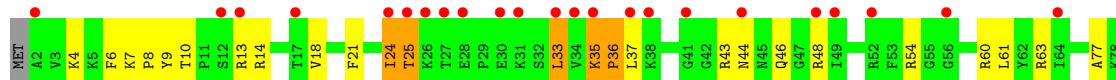
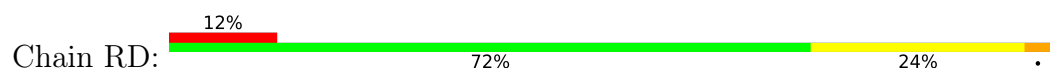
• Molecule 36: 5S rRNA



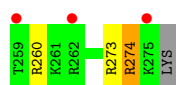
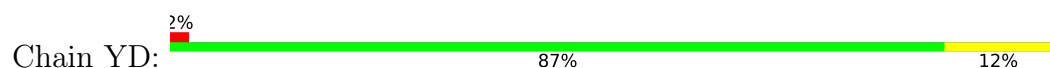
• Molecule 36: 5S rRNA



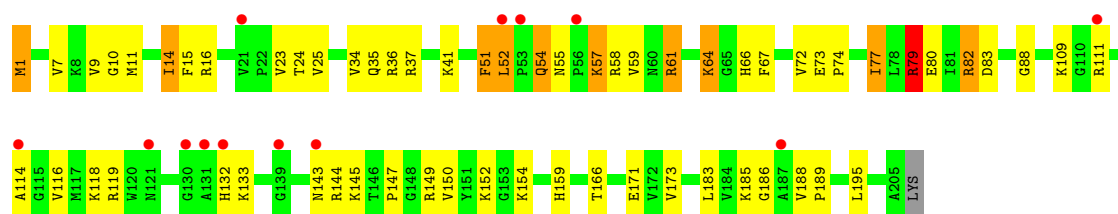
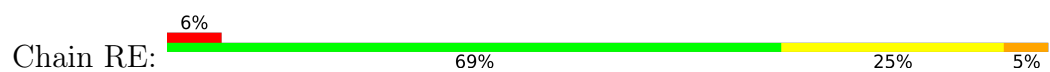
• Molecule 37: 50S ribosomal protein L2



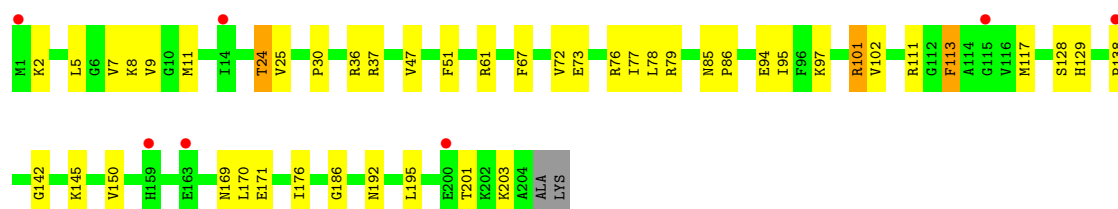
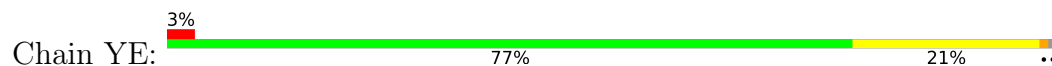
• Molecule 37: 50S ribosomal protein L2



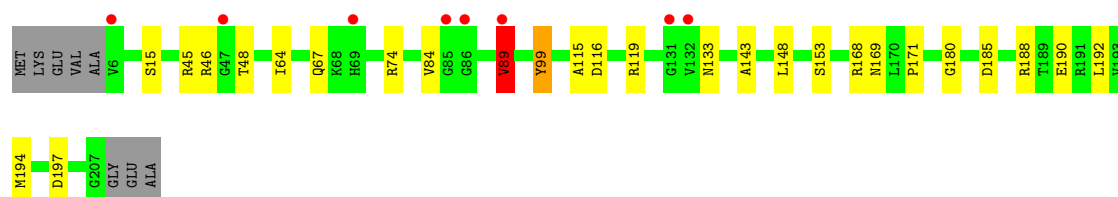
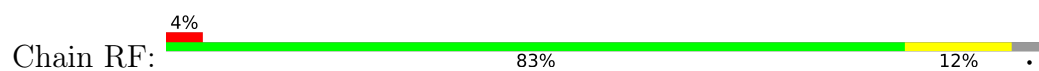
• Molecule 38: 50S ribosomal protein L3



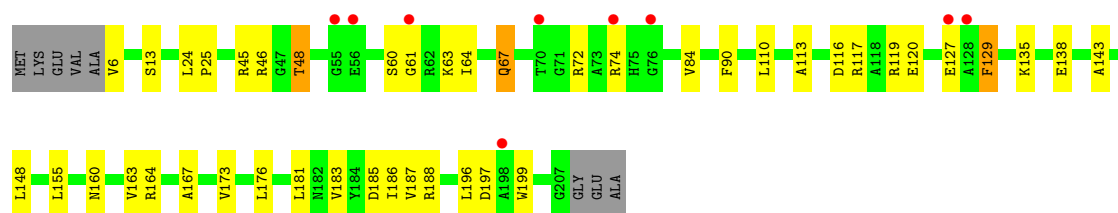
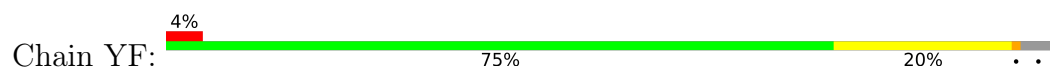
• Molecule 38: 50S ribosomal protein L3



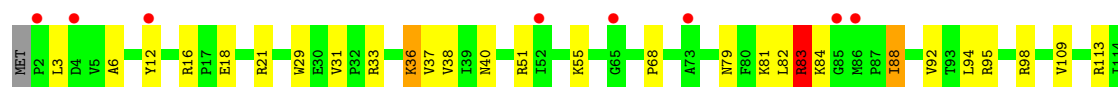
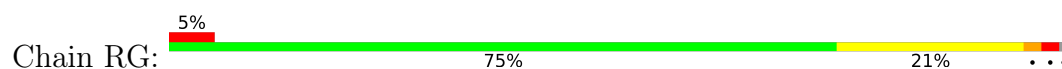
• Molecule 39: 50S ribosomal protein L4

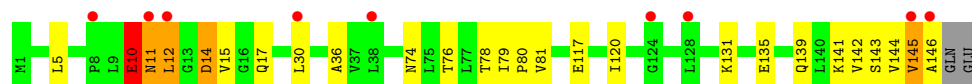


• Molecule 39: 50S ribosomal protein L4

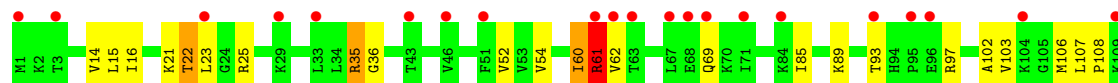
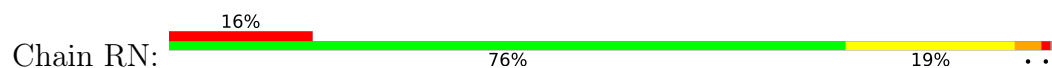


• Molecule 40: 50S ribosomal protein L5

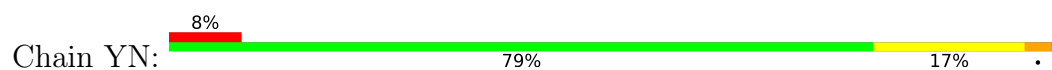




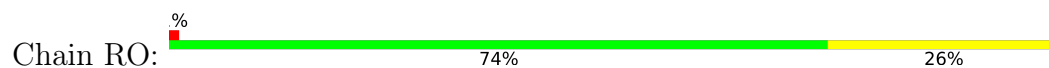
- Molecule 43: 50S ribosomal protein L13



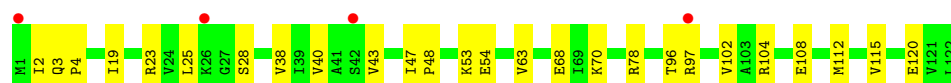
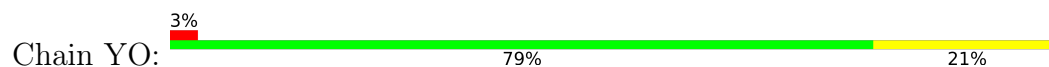
- Molecule 43: 50S ribosomal protein L13



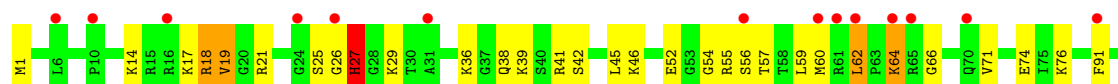
- Molecule 44: 50S ribosomal protein L14



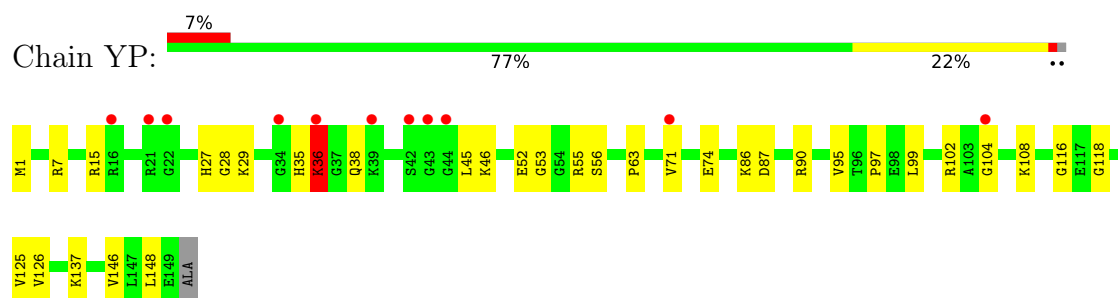
- Molecule 44: 50S ribosomal protein L14



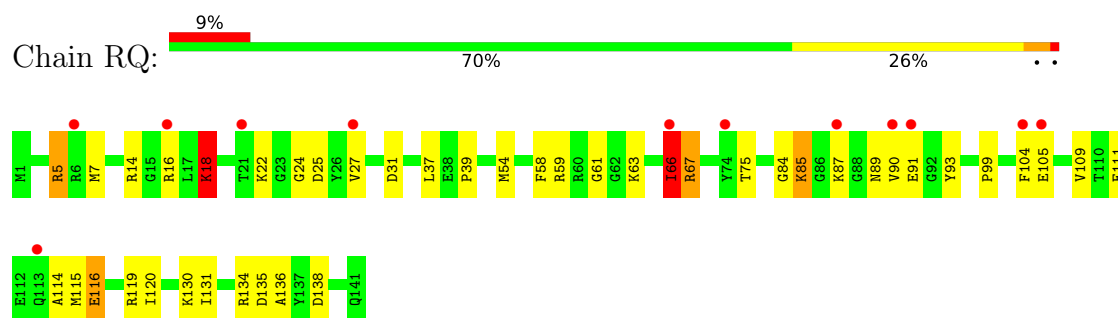
- Molecule 45: 50S ribosomal protein L15



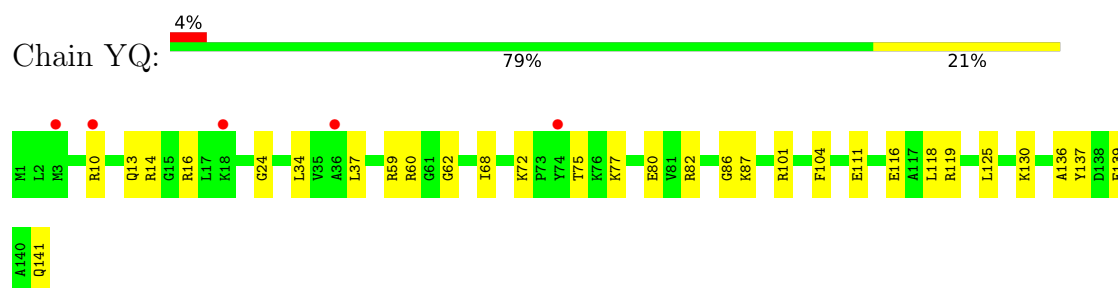
- Molecule 45: 50S ribosomal protein L15



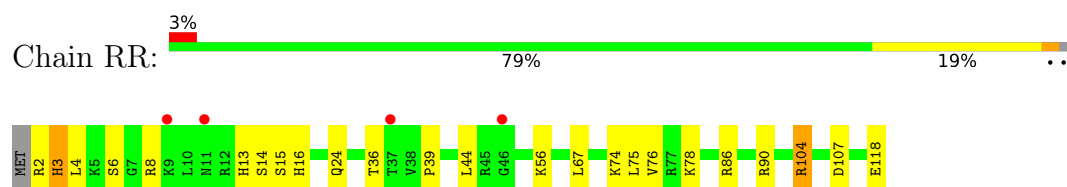
- Molecule 46: 50S ribosomal protein L16



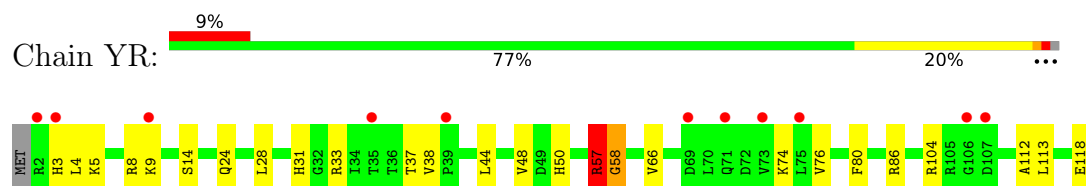
- Molecule 46: 50S ribosomal protein L16



- Molecule 47: 50S ribosomal protein L17

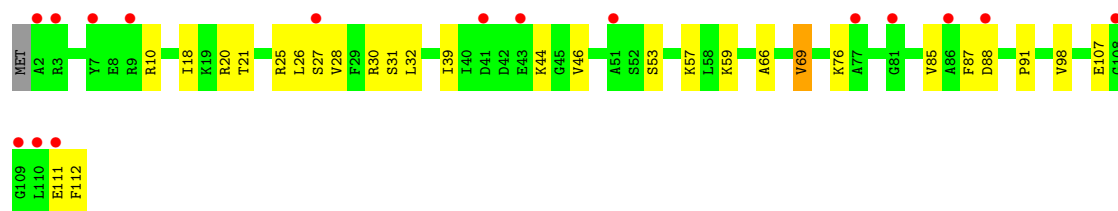


- Molecule 47: 50S ribosomal protein L17

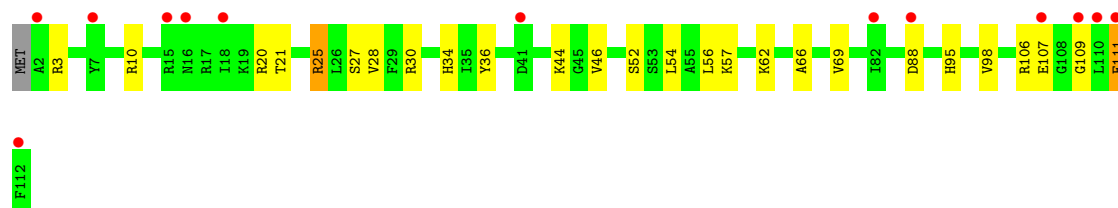
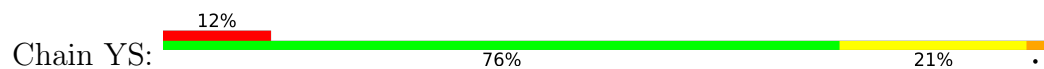


- Molecule 48: 50S ribosomal protein L18

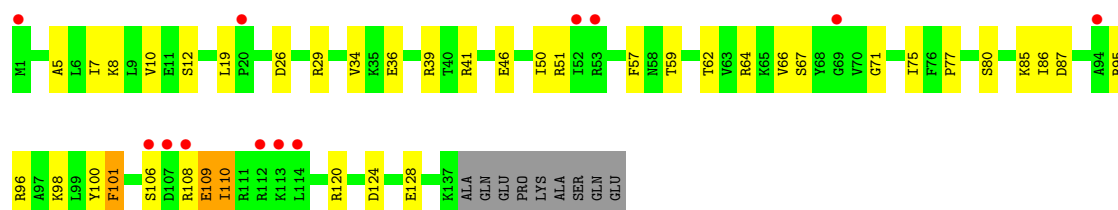




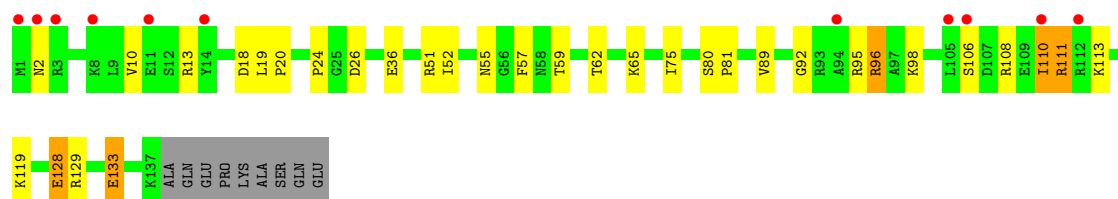
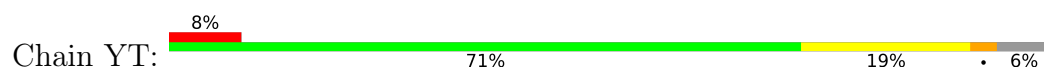
- Molecule 48: 50S ribosomal protein L18



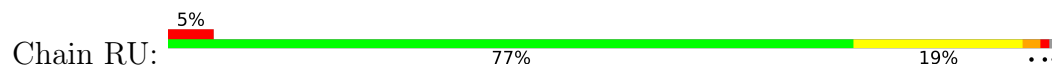
- Molecule 49: 50S ribosomal protein L19



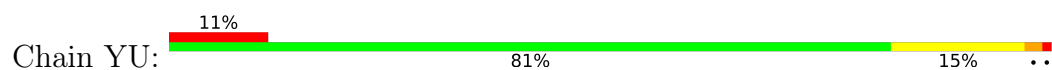
- Molecule 49: 50S ribosomal protein L19

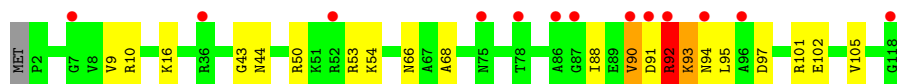


- Molecule 50: 50S ribosomal protein L20

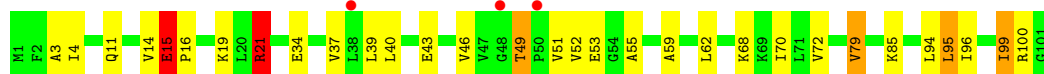


- Molecule 50: 50S ribosomal protein L20

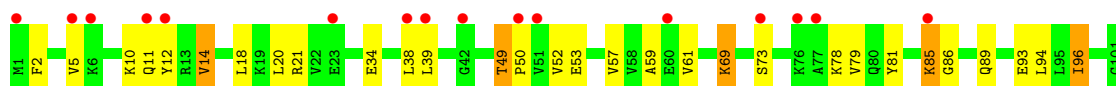
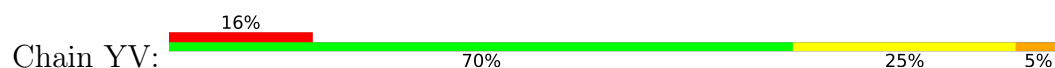




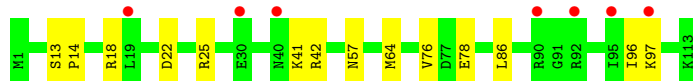
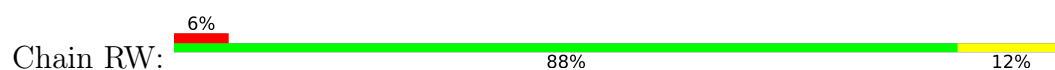
- Molecule 51: 50S ribosomal protein L21



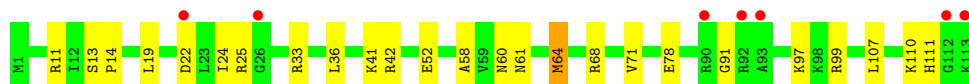
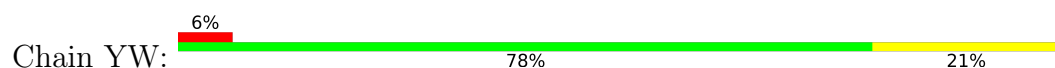
- Molecule 51: 50S ribosomal protein L21



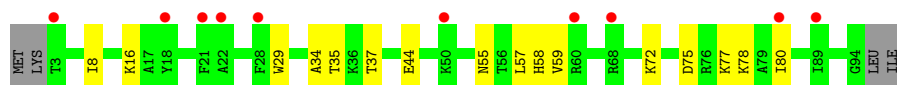
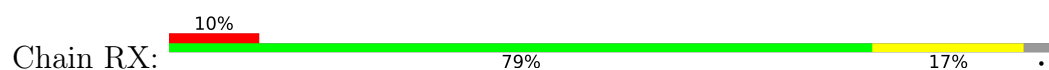
- Molecule 52: 50S ribosomal protein L22



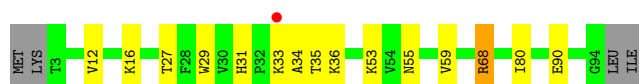
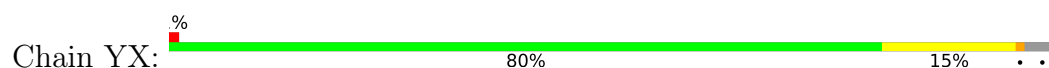
- Molecule 52: 50S ribosomal protein L22



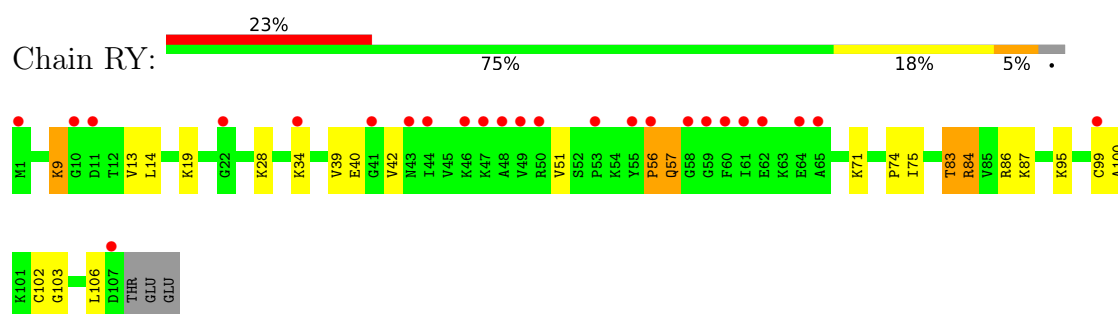
- Molecule 53: 50S ribosomal protein L23



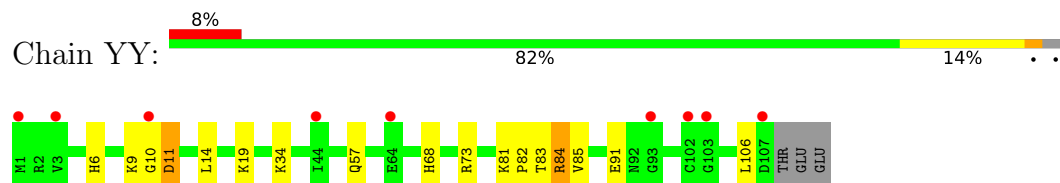
- Molecule 53: 50S ribosomal protein L23



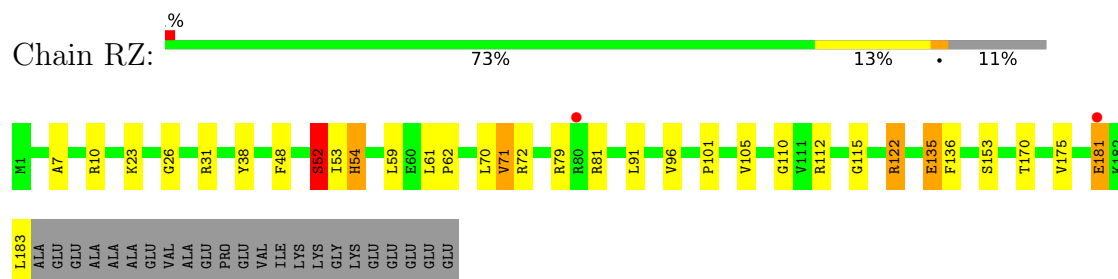
- Molecule 54: 50S ribosomal protein L24



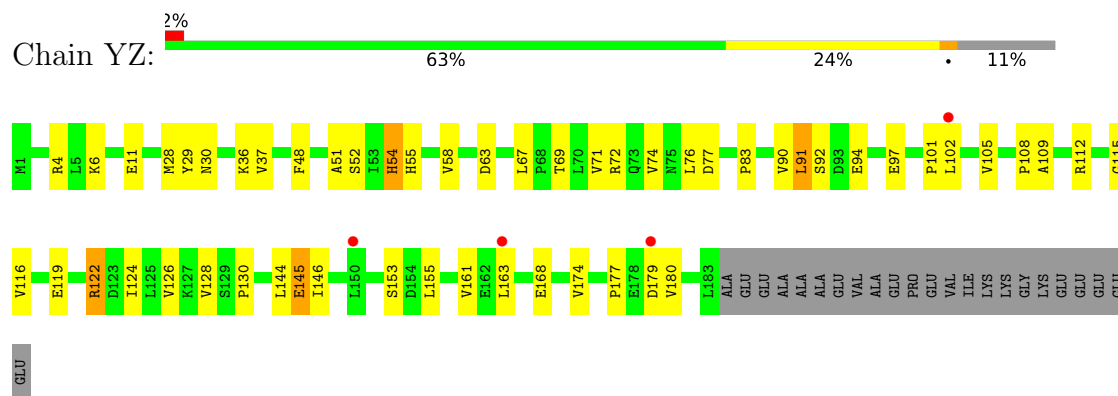
- Molecule 54: 50S ribosomal protein L24



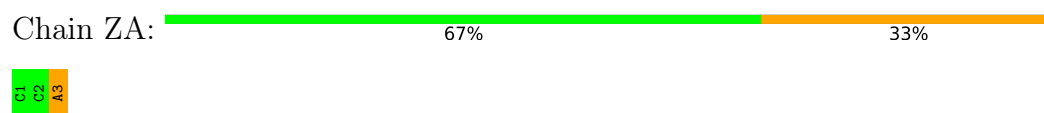
- Molecule 55: 50S ribosomal protein L25



- Molecule 55: 50S ribosomal protein L25



- Molecule 56: CCPuro



- Molecule 56: CCPuro





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	214.68Å 453.51Å 609.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	146.72 – 3.50 146.72 – 3.50	Depositor EDS
% Data completeness (in resolution range)	98.0 (146.72-3.50) 98.0 (146.72-3.50)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 3.49Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.216 , 0.246 0.218 , 0.247	Depositor DCC
R_{free} test set	33274 reflections (4.56%)	wwPDB-VP
Wilson B-factor (Å ²)	89.9	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 86.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	295153	wwPDB-VP
Average B, all atoms (Å ²)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, A3P, PPU, SF4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	QA	0.20	0/36324	0.43	11/56690 (0.0%)
1	XA	0.57	6/36254 (0.0%)	0.44	11/56581 (0.0%)
2	QB	0.63	6/1942 (0.3%)	1.15	21/2619 (0.8%)
2	XB	0.34	0/1950	1.07	18/2630 (0.7%)
3	QC	0.33	0/1629	1.05	12/2195 (0.5%)
3	XC	0.33	0/1629	0.97	5/2195 (0.2%)
4	QD	0.32	0/1733	1.03	13/2318 (0.6%)
4	XD	0.33	0/1733	1.12	19/2318 (0.8%)
5	QE	0.33	0/1171	0.94	3/1576 (0.2%)
5	XE	0.27	0/1171	0.88	3/1576 (0.2%)
6	QF	0.25	0/856	0.83	1/1154 (0.1%)
6	XF	0.27	0/856	0.87	2/1154 (0.2%)
7	QG	0.36	0/1276	1.10	12/1709 (0.7%)
7	XG	0.33	0/1276	0.93	5/1709 (0.3%)
8	QH	0.27	0/1128	0.99	4/1517 (0.3%)
8	XH	0.25	0/1128	0.92	6/1517 (0.4%)
9	QI	0.45	0/1029	1.20	9/1379 (0.7%)
9	XI	0.32	0/1017	1.11	12/1365 (0.9%)
10	QJ	0.42	0/814	1.12	8/1095 (0.7%)
10	XJ	0.35	0/790	1.13	9/1063 (0.8%)
11	QK	0.32	0/900	0.97	4/1213 (0.3%)
11	XK	0.32	0/879	0.98	4/1187 (0.3%)
12	QL	0.30	0/991	1.15	11/1327 (0.8%)
12	XL	0.37	0/972	1.18	15/1301 (1.2%)
13	QM	0.41	0/965	1.29	10/1292 (0.8%)
13	XM	0.35	0/956	1.17	11/1281 (0.9%)
14	QN	0.35	0/501	1.19	3/664 (0.5%)
14	XN	0.26	0/501	0.91	1/664 (0.2%)
15	QO	0.28	0/745	0.85	1/992 (0.1%)
15	XO	0.25	0/740	0.72	0/987
16	QP	0.31	0/721	1.09	6/970 (0.6%)
16	XP	0.28	0/721	1.00	4/970 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	QQ	0.30	0/847	1.04	5/1131 (0.4%)
17	XQ	0.28	0/847	0.84	1/1131 (0.1%)
18	QR	0.34	0/579	1.16	4/768 (0.5%)
18	XR	0.34	0/579	1.08	6/768 (0.8%)
19	QS	0.42	0/680	1.27	15/915 (1.6%)
19	XS	0.30	0/671	1.19	7/904 (0.8%)
20	QT	0.36	0/765	1.27	9/1007 (0.9%)
20	XT	0.35	0/765	1.16	8/1007 (0.8%)
21	QU	0.39	0/221	1.11	3/288 (1.0%)
21	XU	0.26	0/221	1.04	2/288 (0.7%)
22	QV	0.19	0/1832	0.40	0/2855
22	XV	0.19	0/1832	0.39	0/2855
23	QX	0.22	0/414	0.58	0/645
23	XX	0.19	0/414	0.48	0/645
24	QY	0.41	0/743	1.09	7/1002 (0.7%)
24	QZ	0.60	2/743 (0.3%)	1.39	11/1002 (1.1%)
24	XY	0.31	0/743	1.07	5/1002 (0.5%)
24	XZ	0.38	0/743	1.25	11/1002 (1.1%)
25	R0	0.37	0/652	1.17	5/867 (0.6%)
25	Y0	0.28	0/657	0.99	1/874 (0.1%)
26	R1	0.40	0/744	1.07	8/989 (0.8%)
26	Y1	0.36	0/770	1.01	2/1022 (0.2%)
27	R2	0.41	0/583	1.33	11/771 (1.4%)
27	Y2	0.30	0/583	0.93	0/771
28	R3	0.28	0/474	0.96	2/635 (0.3%)
28	Y3	0.31	0/474	1.02	3/635 (0.5%)
29	R4	0.59	0/578	1.59	15/776 (1.9%)
29	Y4	0.37	0/578	1.29	6/776 (0.8%)
30	R5	0.32	0/473	0.92	2/639 (0.3%)
30	Y5	0.39	0/473	1.02	1/639 (0.2%)
31	R6	0.32	0/460	1.18	5/613 (0.8%)
31	Y6	0.33	0/460	0.99	1/613 (0.2%)
32	R7	0.27	0/417	0.84	1/550 (0.2%)
32	Y7	0.29	0/426	0.88	2/561 (0.4%)
33	R8	0.48	0/525	1.28	8/691 (1.2%)
33	Y8	0.50	0/525	1.11	6/691 (0.9%)
34	R9	0.41	0/310	1.10	3/407 (0.7%)
34	Y9	0.32	0/310	1.15	2/407 (0.5%)
35	RA	0.21	0/69739	0.44	8/108870 (0.0%)
35	YA	0.21	0/69419	0.44	9/108369 (0.0%)
36	RB	0.23	0/2881	0.45	1/4494 (0.0%)
36	YB	0.28	0/2881	0.47	1/4494 (0.0%)
37	RD	0.35	0/2165	1.27	25/2919 (0.9%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	YD	0.29	0/2185	1.01	11/2944 (0.4%)
38	RE	0.45	0/1601	1.24	20/2160 (0.9%)
38	YE	0.35	0/1592	1.16	14/2149 (0.7%)
39	RF	0.27	0/1620	0.94	9/2194 (0.4%)
39	YF	0.31	0/1620	1.06	9/2194 (0.4%)
40	RG	0.35	0/1499	1.21	21/2016 (1.0%)
40	YG	0.48	3/1499 (0.2%)	1.13	13/2016 (0.6%)
41	RH	0.44	0/1362	1.48	40/1841 (2.2%)
41	YH	0.35	0/1356	0.96	5/1834 (0.3%)
42	RI	2.65	3/1146 (0.3%)	1.65	31/1551 (2.0%)
42	YI	0.44	0/1151	1.26	20/1558 (1.3%)
43	RN	0.41	0/1131	1.17	10/1525 (0.7%)
43	YN	0.28	0/1131	1.05	10/1525 (0.7%)
44	RO	0.26	0/943	0.96	6/1269 (0.5%)
44	YO	0.29	0/943	0.96	3/1269 (0.2%)
45	RP	0.43	0/1162	1.34	20/1544 (1.3%)
45	YP	0.31	0/1152	1.13	12/1533 (0.8%)
46	RQ	0.46	0/1143	1.19	11/1527 (0.7%)
46	YQ	0.27	0/1143	1.04	6/1527 (0.4%)
47	RR	0.30	0/974	1.20	6/1302 (0.5%)
47	YR	0.35	0/974	1.09	13/1302 (1.0%)
48	RS	0.36	0/892	1.21	7/1187 (0.6%)
48	YS	0.40	0/892	1.21	9/1187 (0.8%)
49	RT	0.41	0/1155	1.16	6/1542 (0.4%)
49	YT	0.41	0/1155	1.16	14/1542 (0.9%)
50	RU	0.34	0/982	1.08	9/1306 (0.7%)
50	YU	0.33	0/982	0.96	5/1306 (0.4%)
51	RV	0.59	1/790 (0.1%)	1.24	6/1057 (0.6%)
51	YV	1.29	6/790 (0.8%)	1.34	10/1057 (0.9%)
52	RW	0.28	0/911	0.96	2/1220 (0.2%)
52	YW	0.28	0/911	0.91	2/1220 (0.2%)
53	RX	0.27	0/739	0.94	2/993 (0.2%)
53	YX	0.31	0/739	0.92	2/993 (0.2%)
54	RY	0.33	0/831	1.10	11/1108 (1.0%)
54	YY	0.29	0/831	1.11	12/1108 (1.1%)
55	RZ	0.37	0/1493	1.15	17/2026 (0.8%)
55	YZ	0.30	0/1493	1.08	13/2026 (0.6%)
56	ZA	0.28	0/40	0.52	0/60
56	ZB	0.27	0/40	0.47	0/60
All	All	0.36	27/319487 (0.0%)	0.69	893/477274 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	QB	0	1
7	XG	0	1
8	XH	0	1
10	QJ	0	1
11	XK	0	1
24	QZ	0	1
37	RD	0	2
37	YD	0	1
38	RE	0	1
40	RG	0	2
40	YG	0	1
41	RH	0	2
41	YH	0	1
42	RI	0	4
47	RR	0	1
47	YR	0	1
51	RV	0	1
All	All	0	23

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	RI	82	ARG	CZ-NH1	87.21	2.54	1.32
1	XA	368	U	N3-C4	47.56	2.33	1.38
1	XA	368	U	C2-N3	46.00	2.29	1.37
1	XA	368	U	N1-C2	41.62	2.21	1.38
1	XA	368	U	N1-C6	40.83	2.19	1.38
1	XA	368	U	C4-C5	37.75	2.19	1.43
1	XA	368	U	C5-C6	35.56	2.05	1.34
51	YV	85	LYS	CD-CE	19.21	2.10	1.52
51	YV	85	LYS	CE-NZ	12.77	1.87	1.49
51	YV	85	LYS	CG-CD	11.22	1.86	1.52
2	QB	8	LYS	C-N	10.16	1.48	1.33
51	YV	85	LYS	CB-CG	10.10	1.82	1.52
2	QB	8	LYS	N-CA	9.70	1.57	1.46
42	RI	82	ARG	NE-CZ	9.25	1.43	1.33
40	YG	72	ARG	CD-NE	9.07	1.58	1.46
24	QZ	22	ARG	CZ-NH1	8.46	1.44	1.32
51	YV	69	LYS	CD-CE	-6.92	1.31	1.52
2	QB	7	VAL	C-N	6.92	1.42	1.33
2	QB	132	LYS	CD-CE	6.86	1.73	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	YG	72	ARG	CG-CD	6.37	1.71	1.52
40	YG	72	ARG	CB-CG	5.30	1.68	1.52
2	QB	7	VAL	CA-C	5.19	1.59	1.52
42	RI	87	LYS	CG-CD	-5.15	1.36	1.52
51	YV	49	THR	CB-CG2	-5.12	1.35	1.52
51	RV	51	VAL	CB-CG2	-5.05	1.35	1.52
2	QB	8	LYS	CA-CB	5.05	1.61	1.53
24	QZ	22	ARG	CZ-NH2	5.04	1.40	1.33

All (893) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	RR	76	VAL	N-CA-C	-19.67	93.29	112.96
37	RD	35	LYS	N-CA-C	-17.68	92.31	108.22
42	RI	11	ASN	CA-C-N	15.29	149.12	122.67
42	RI	11	ASN	C-N-CA	15.29	149.12	122.67
48	RS	107	GLU	N-CA-C	-15.26	92.38	112.68
42	RI	82	ARG	CD-NE-CZ	15.05	145.47	124.40
24	QZ	50	HIS	CA-C-N	14.80	149.81	121.54
24	QZ	50	HIS	C-N-CA	14.80	149.81	121.54
37	RD	33	LEU	CA-C-N	14.76	148.54	121.97
37	RD	33	LEU	C-N-CA	14.76	148.54	121.97
4	XD	33	MET	N-CA-C	-14.17	98.47	114.62
42	RI	82	ARG	NE-CZ-NH2	-13.93	106.66	119.20
42	RI	143	SER	CA-C-N	13.22	145.76	121.97
42	RI	143	SER	C-N-CA	13.22	145.76	121.97
39	YF	199	TRP	N-CA-C	-12.44	96.56	112.23
46	YQ	139	GLU	N-CA-C	-12.13	98.61	113.41
27	R2	44	LEU	N-CA-C	-12.02	100.92	114.62
14	QN	9	LYS	N-CA-C	-11.63	99.23	113.41
37	YD	20	ASP	N-CA-C	11.37	123.67	111.28
50	RU	97	ASP	N-CA-C	-11.36	98.98	111.36
48	YS	44	LYS	N-CA-C	-11.34	101.69	114.62
20	QT	13	LEU	N-CA-C	-11.29	99.49	113.38
38	YE	101	ARG	CA-CB-CG	11.20	136.50	114.10
51	YV	85	LYS	CD-CE-NZ	11.04	147.22	111.90
49	YT	110	ILE	N-CA-C	-11.04	100.12	110.82
4	QD	34	GLU	N-CA-C	-10.95	100.06	113.41
42	RI	120	ILE	N-CA-C	10.90	127.00	109.78
41	RH	151	ILE	N-CA-C	-10.63	91.92	107.98
37	RD	237	GLU	N-CA-C	-10.57	92.42	109.76
18	XR	56	THR	N-CA-C	-10.51	100.30	113.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	XI	86	VAL	N-CA-C	-10.42	100.53	111.58
40	YG	52	ILE	N-CA-C	-10.42	100.94	111.77
8	QH	79	VAL	N-CA-C	-10.27	101.41	113.42
19	XS	25	LYS	N-CA-C	-10.17	97.28	111.52
17	QQ	100	LYS	CA-C-N	10.14	139.96	121.70
17	QQ	100	LYS	C-N-CA	10.14	139.96	121.70
13	XM	108	ARG	N-CA-C	10.11	125.48	112.34
39	RF	133	ASN	N-CA-C	-10.09	92.72	109.46
43	RN	97	ARG	N-CA-C	-9.95	99.87	112.90
9	QI	120	ARG	N-CA-C	-9.92	103.31	114.62
39	YF	197	ASP	N-CA-C	-9.92	94.53	110.20
41	RH	153	LYS	N-CA-C	9.83	131.54	109.81
49	YT	13	ARG	N-CA-C	-9.82	101.30	113.38
14	QN	13	THR	N-CA-C	9.81	125.50	112.35
42	YI	145	VAL	N-CA-C	9.67	129.45	109.34
41	RH	141	VAL	N-CA-C	-9.66	102.49	111.67
19	QS	29	ARG	CG-CD-NE	-9.61	90.85	112.00
24	QZ	60	ILE	N-CA-C	-9.60	101.50	110.82
37	RD	13	ARG	N-CA-C	-9.55	102.71	114.75
47	RR	3	HIS	CA-C-N	9.55	139.78	121.54
47	RR	3	HIS	C-N-CA	9.55	139.78	121.54
49	RT	110	ILE	N-CA-C	-9.54	101.45	110.42
18	QR	39	VAL	N-CA-C	-9.38	102.66	111.48
40	RG	116	ASP	CA-C-N	9.31	139.32	121.54
40	RG	116	ASP	C-N-CA	9.31	139.32	121.54
43	RN	114	ARG	N-CA-C	-9.29	95.52	110.20
48	YS	21	THR	N-CA-C	-9.27	100.29	111.69
54	YY	57	GLN	N-CA-C	-9.26	102.11	113.41
4	XD	89	THR	N-CA-C	9.25	122.52	111.33
7	XG	4	ARG	N-CA-C	9.21	121.09	111.14
33	R8	36	LYS	N-CA-C	-9.19	94.53	109.96
27	R2	71	ASN	CA-C-N	9.18	138.22	121.70
27	R2	71	ASN	C-N-CA	9.18	138.22	121.70
45	RP	56	SER	CA-C-N	9.17	139.05	121.54
45	RP	56	SER	C-N-CA	9.17	139.05	121.54
37	RD	198	ASN	N-CA-C	-9.11	98.77	111.52
25	R0	9	SER	N-CA-C	9.05	120.18	108.24
19	XS	14	HIS	N-CA-C	-9.03	101.69	112.89
42	RI	82	ARG	NE-CZ-NH1	8.92	130.42	121.50
13	XM	8	GLU	N-CA-C	-8.88	96.20	110.32
26	Y1	90	ILE	N-CA-C	-8.88	102.19	110.53
42	RI	142	VAL	CA-C-N	8.85	138.44	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	RI	142	VAL	C-N-CA	8.85	138.44	121.54
49	RT	59	THR	N-CA-C	-8.84	94.79	109.46
37	RD	35	LYS	CA-C-N	8.80	130.84	119.84
37	RD	35	LYS	C-N-CA	8.80	130.84	119.84
4	QD	89	THR	N-CA-C	8.75	120.43	111.07
24	XZ	83	HIS	CA-C-N	8.73	137.42	121.70
24	XZ	83	HIS	C-N-CA	8.73	137.42	121.70
48	YS	109	GLY	CA-C-N	8.72	138.19	121.54
48	YS	109	GLY	C-N-CA	8.72	138.19	121.54
30	Y5	3	LYS	N-CA-C	8.69	124.33	111.81
50	YU	97	ASP	N-CA-C	-8.68	101.90	111.36
29	R4	65	ASP	N-CA-C	-8.68	101.90	111.36
40	RG	51	ARG	N-CA-C	-8.65	101.79	111.82
2	QB	8	LYS	CA-C-O	8.64	129.40	120.24
42	YI	120	ILE	N-CA-C	8.63	121.85	109.51
29	Y4	42	PHE	N-CA-C	-8.62	103.28	113.88
38	YE	101	ARG	CD-NE-CZ	-8.62	112.33	124.40
41	RH	101	ARG	CG-CD-NE	-8.61	93.07	112.00
13	QM	11	ARG	N-CA-C	-8.60	97.18	110.17
48	RS	59	LYS	N-CA-C	8.58	122.75	110.14
37	YD	274	ARG	CA-C-N	8.58	137.14	121.70
37	YD	274	ARG	C-N-CA	8.58	137.14	121.70
34	R9	31	LYS	N-CA-C	-8.57	101.88	111.14
50	RU	9	VAL	N-CA-C	8.56	118.58	110.53
41	RH	9	ILE	N-CA-C	8.56	122.62	112.35
13	QM	114	ARG	CG-CD-NE	-8.55	93.20	112.00
3	XC	63	ASN	N-CA-C	-8.49	97.02	108.74
41	RH	157	TYR	N-CA-C	-8.48	102.95	113.38
51	YV	52	VAL	N-CA-C	-8.46	97.71	109.21
29	R4	22	ILE	N-CA-C	8.44	121.12	108.80
38	RE	80	GLU	N-CA-C	8.39	123.67	110.32
55	RZ	62	PRO	CA-C-N	8.39	137.56	121.54
55	RZ	62	PRO	C-N-CA	8.39	137.56	121.54
54	RY	57	GLN	N-CA-C	-8.38	100.80	112.45
7	XG	3	ARG	N-CA-C	8.37	120.18	111.14
43	YN	114	ARG	N-CA-C	-8.37	95.90	109.96
42	RI	144	VAL	N-CA-C	-8.36	91.95	109.34
45	YP	71	VAL	N-CA-C	8.36	126.93	108.88
46	YQ	111	GLU	N-CA-C	8.36	121.21	111.02
7	QG	153	HIS	N-CA-C	-8.34	102.12	112.88
20	XT	14	LYS	N-CA-C	-8.31	102.30	111.36
42	RI	114	LEU	N-CA-C	-8.31	102.17	113.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	RI	91	SER	N-CA-C	8.26	121.27	108.96
2	QB	16	HIS	N-CA-C	8.25	122.13	112.72
13	QM	62	ASN	N-CA-C	-8.23	104.37	114.75
16	QP	23	ASP	N-CA-C	-8.23	97.23	110.32
13	QM	8	GLU	CA-C-N	8.23	137.35	122.13
13	QM	8	GLU	C-N-CA	8.23	137.35	122.13
25	R0	51	VAL	N-CA-C	-8.23	95.68	108.44
12	QL	18	VAL	N-CA-C	8.18	123.49	112.04
52	RW	64	MET	N-CA-C	8.17	123.42	112.88
8	XH	79	VAL	N-CA-C	-8.14	100.87	112.35
2	XB	235	SER	CA-C-N	8.14	137.09	121.54
2	XB	235	SER	C-N-CA	8.14	137.09	121.54
43	YN	35	ARG	N-CA-C	-8.14	95.47	108.73
29	Y4	65	ASP	N-CA-C	-8.13	101.37	112.03
40	RG	84	LYS	N-CA-C	8.13	120.87	111.11
43	YN	97	ARG	N-CA-C	-8.12	102.81	112.89
41	RH	9	ILE	CA-C-N	8.12	129.99	119.84
41	RH	9	ILE	C-N-CA	8.12	129.99	119.84
2	XB	124	SER	N-CA-C	8.07	115.48	108.22
18	XR	32	ARG	N-CA-C	-8.06	103.47	113.38
39	RF	89	VAL	N-CA-C	8.06	117.99	110.42
4	XD	118	ARG	CG-CD-NE	8.05	129.72	112.00
55	RZ	112	ARG	CG-CD-NE	-8.04	94.30	112.00
43	YN	116	LEU	N-CA-C	-8.05	103.59	113.41
42	YI	117	GLU	N-CA-C	-8.04	97.96	110.42
26	R1	90	ILE	N-CA-C	8.04	118.05	110.74
39	YF	45	ARG	N-CA-C	8.03	120.68	110.24
20	XT	9	ASN	N-CA-C	8.02	121.26	110.35
38	YE	102	VAL	N-CA-C	8.02	120.35	108.96
24	QY	17	GLN	N-CA-C	-8.02	98.61	110.48
24	QZ	50	HIS	N-CA-C	8.01	122.41	112.47
33	R8	33	ASN	N-CA-C	7.99	121.60	112.57
2	QB	153	ARG	N-CA-C	-7.96	103.57	113.28
43	RN	61	ARG	CG-CD-NE	-7.95	94.51	112.00
52	RW	57	ASN	N-CA-C	-7.95	102.49	112.90
39	RF	64	ILE	N-CA-C	7.95	118.74	110.72
51	RV	15	GLU	CB-CA-C	7.94	122.02	109.55
13	XM	17	VAL	N-CA-C	-7.93	105.46	113.47
42	YI	144	VAL	CA-C-N	7.93	136.24	121.97
42	YI	144	VAL	C-N-CA	7.93	136.24	121.97
4	XD	31	CYS	N-CA-C	7.90	120.99	111.82
55	YZ	122	ARG	N-CA-C	-7.88	102.74	113.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	QB	155	LEU	N-CA-C	7.88	120.87	111.02
4	QD	208	SER	N-CA-C	-7.86	93.62	108.17
48	RS	21	THR	N-CA-C	-7.86	103.67	113.18
37	YD	88	ARG	CD-NE-CZ	7.86	135.40	124.40
55	RZ	59	LEU	N-CA-C	7.85	120.83	111.02
51	YV	85	LYS	CG-CD-CE	7.84	129.33	111.30
27	R2	5	GLU	N-CA-C	-7.83	103.75	113.38
24	XY	17	GLN	N-CA-C	-7.83	98.89	110.48
17	QQ	101	ARG	CA-CB-CG	-7.80	98.50	114.10
14	XN	13	THR	N-CA-C	7.79	127.03	109.81
20	XT	13	LEU	N-CA-C	-7.78	103.79	113.28
40	RG	79	ASN	N-CA-C	-7.77	103.80	113.28
38	YE	101	ARG	CG-CD-NE	7.75	129.06	112.00
43	RN	107	LEU	N-CA-C	-7.73	98.96	110.24
55	RZ	54	HIS	N-CA-C	7.72	119.69	111.28
41	RH	138	LYS	N-CA-C	-7.71	103.71	113.43
48	YS	3	ARG	N-CA-C	-7.71	99.08	110.48
38	RE	132	HIS	N-CA-C	7.70	120.64	111.02
46	RQ	22	LYS	N-CA-C	7.69	121.12	110.35
45	RP	26	GLY	N-CA-C	-7.68	98.26	111.47
45	RP	59	LEU	N-CA-C	-7.67	97.90	109.94
4	XD	47	ARG	CA-CB-CG	-7.67	98.76	114.10
4	XD	151	LYS	N-CA-C	-7.66	102.27	111.69
41	RH	9	ILE	CB-CA-C	-7.65	103.97	114.00
10	XJ	35	SER	N-CA-C	-7.63	96.79	109.07
55	YZ	63	ASP	N-CA-C	-7.63	104.02	112.72
19	XS	9	VAL	N-CA-C	-7.63	98.82	108.89
54	RY	51	VAL	N-CA-C	-7.60	98.86	108.89
41	RH	92	ILE	N-CA-C	7.58	121.62	111.17
44	RO	66	LYS	N-CA-C	-7.58	104.06	113.38
47	RR	104	ARG	N-CA-C	7.57	120.92	110.24
38	YE	101	ARG	N-CA-CB	-7.57	98.43	110.77
54	YY	11	ASP	N-CA-C	7.55	121.78	109.85
10	QJ	43	ARG	CD-NE-CZ	-7.54	113.84	124.40
45	RP	116	GLY	N-CA-C	7.50	125.97	112.02
43	YN	127	ASP	N-CA-C	7.50	119.69	110.91
38	RE	185	LYS	N-CA-C	7.49	121.86	112.87
40	RG	136	ARG	N-CA-C	-7.46	98.95	109.69
49	RT	57	PHE	N-CA-C	-7.45	100.49	110.55
2	QB	152	PHE	N-CA-C	7.45	121.21	112.72
3	QC	91	LEU	N-CA-C	-7.42	102.56	111.69
7	QG	59	LEU	N-CA-C	-7.42	104.36	113.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	QT	9	ASN	N-CA-C	7.41	121.34	110.59
41	RH	127	GLU	N-CA-C	-7.39	100.45	110.36
10	XJ	92	THR	N-CA-C	-7.37	102.66	114.09
45	RP	97	PRO	CA-C-N	7.37	139.49	126.45
45	RP	97	PRO	C-N-CA	7.37	139.49	126.45
40	YG	136	ARG	N-CA-C	-7.37	98.38	109.94
9	QI	62	TYR	N-CA-C	-7.36	96.90	108.90
47	YR	76	VAL	N-CA-C	-7.36	101.97	112.35
19	QS	22	LEU	N-CA-C	7.36	119.30	111.28
2	QB	124	SER	N-CA-C	7.36	117.60	108.11
37	YD	71	ASP	N-CA-C	-7.33	103.22	111.14
4	XD	73	ARG	CA-CB-CG	7.33	128.76	114.10
47	YR	31	HIS	N-CA-C	7.32	120.32	111.40
42	RI	131	LYS	N-CA-C	7.30	122.58	108.85
25	R0	4	LYS	N-CA-C	-7.29	97.80	109.76
16	QP	54	GLU	N-CA-CB	-7.29	98.74	109.82
26	R1	91	LYS	N-CA-C	7.28	119.90	111.02
7	QG	17	VAL	N-CA-C	-7.25	106.83	113.71
40	RG	36	LYS	N-CA-C	7.23	120.05	111.02
55	RZ	181	GLU	N-CA-C	7.23	119.05	111.03
40	YG	114	ILE	N-CA-C	-7.21	102.19	110.05
9	QI	86	VAL	N-CA-C	-7.21	102.18	112.35
24	XY	49	LYS	CA-C-N	7.21	135.30	121.54
24	XY	49	LYS	C-N-CA	7.21	135.30	121.54
5	XE	26	PHE	N-CA-C	7.20	121.18	110.52
12	QL	118	SER	N-CA-C	-7.19	103.37	111.14
50	YU	93	LYS	N-CA-C	-7.19	104.46	113.23
47	YR	58	GLY	N-CA-C	7.18	130.21	113.18
41	RH	11	VAL	N-CA-C	7.18	124.39	108.88
45	RP	99	LEU	N-CA-C	-7.18	103.53	111.36
38	RE	54	GLN	CA-C-N	7.18	139.31	121.80
38	RE	54	GLN	C-N-CA	7.18	139.31	121.80
12	XL	20	LYS	N-CA-C	7.16	119.54	110.24
9	QI	83	ARG	CA-CB-CG	-7.12	99.86	114.10
40	RG	145	THR	N-CA-C	7.11	121.91	112.25
50	RU	6	THR	N-CA-C	-7.10	103.15	111.03
49	YT	59	THR	N-CA-C	-7.09	98.48	109.76
29	R4	22	ILE	CA-C-N	7.09	135.07	121.54
29	R4	22	ILE	C-N-CA	7.09	135.07	121.54
55	YZ	54	HIS	N-CA-C	7.08	120.03	111.82
40	YG	150	ASP	N-CA-C	-7.07	106.56	114.62
2	XB	178	ARG	CA-CB-CG	7.07	128.23	114.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	QT	14	LYS	N-CA-C	-7.07	103.62	111.82
40	YG	53	LEU	N-CA-C	-7.05	103.30	112.68
42	RI	74	ASN	N-CA-C	-7.05	104.31	113.12
4	QD	150	GLU	N-CA-C	7.03	119.83	111.33
24	QY	80	CYS	N-CA-C	-7.02	102.30	111.71
31	R6	26	ASN	N-CA-C	-7.01	97.12	108.41
10	XJ	98	ILE	N-CA-C	7.01	117.00	106.42
41	YH	3	ARG	CD-NE-CZ	6.98	134.17	124.40
40	RG	150	ASP	N-CA-C	-6.97	106.68	114.62
43	RN	35	ARG	N-CA-C	-6.95	97.22	108.41
39	YF	129	PHE	N-CA-C	6.95	125.60	110.80
52	YW	64	MET	N-CA-C	6.94	121.06	112.59
4	XD	154	ASN	CA-C-N	6.92	134.75	121.54
4	XD	154	ASN	C-N-CA	6.92	134.75	121.54
6	XF	46	ARG	CG-CD-NE	-6.90	96.82	112.00
10	XJ	86	MET	N-CA-C	-6.88	105.16	113.97
18	XR	39	VAL	N-CA-C	-6.88	106.33	111.90
10	QJ	15	THR	N-CA-C	-6.88	103.78	112.93
2	QB	20	GLU	N-CA-C	6.87	120.65	110.48
16	XP	19	ILE	N-CA-C	-6.87	98.92	108.12
12	QL	119	LYS	N-CA-C	-6.86	100.33	110.48
29	R4	22	ILE	N-CA-CB	-6.85	102.93	112.52
37	RD	44	ASN	N-CA-C	6.85	120.13	109.52
24	XZ	6	SER	N-CA-C	-6.85	100.39	110.52
29	Y4	67	TYR	N-CA-C	-6.84	96.23	110.80
4	XD	30	LYS	N-CA-C	-6.84	102.95	112.25
20	QT	93	GLU	N-CA-C	-6.82	104.94	112.72
42	RI	117	GLU	N-CA-C	-6.81	100.44	110.52
45	YP	15	ARG	CG-CD-NE	6.81	126.98	112.00
29	Y4	67	TYR	CB-CA-C	6.80	123.95	110.42
55	YZ	30	ASN	N-CA-C	-6.80	99.43	108.34
27	R2	46	GLN	CA-C-N	6.79	134.52	121.54
27	R2	46	GLN	C-N-CA	6.79	134.52	121.54
33	Y8	48	PHE	CA-CB-CG	6.78	120.58	113.80
42	YI	131	LYS	N-CA-C	6.78	123.31	108.66
38	YE	72	VAL	N-CA-C	6.78	119.18	108.87
41	RH	88	LEU	N-CA-C	-6.78	100.45	110.48
40	YG	166	ASP	N-CA-C	6.77	119.68	111.82
41	RH	151	ILE	CA-C-N	6.77	134.48	121.54
41	RH	151	ILE	C-N-CA	6.77	134.48	121.54
41	RH	19	VAL	N-CA-C	6.77	117.64	108.17
12	XL	104	VAL	CA-C-N	6.77	134.46	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	XL	104	VAL	C-N-CA	6.77	134.46	121.54
14	QN	13	THR	CB-CA-C	-6.75	102.03	113.04
12	QL	61	THR	N-CA-C	6.75	120.97	112.87
24	QY	63	GLU	CB-CA-C	-6.74	99.49	110.08
16	XP	67	THR	N-CA-C	-6.73	100.83	110.59
9	QI	3	GLN	N-CA-C	6.71	120.01	110.14
9	XI	28	VAL	N-CA-C	6.71	117.55	107.75
5	QE	26	PHE	N-CA-C	6.71	119.19	110.53
29	R4	63	TYR	CA-CB-CG	6.71	125.98	113.90
9	XI	99	LEU	N-CA-C	-6.71	104.11	112.90
19	XS	23	ASN	N-CA-C	-6.71	103.58	111.03
46	RQ	84	GLY	CA-C-N	6.70	134.34	121.54
46	RQ	84	GLY	C-N-CA	6.70	134.34	121.54
7	QG	87	VAL	N-CA-C	6.70	115.19	107.89
19	QS	21	GLU	N-CA-C	-6.70	102.39	112.04
2	XB	226	ARG	N-CA-C	-6.68	104.14	112.90
25	Y0	44	ARG	N-CA-C	-6.68	104.07	111.82
39	RF	15	SER	N-CA-C	-6.68	103.92	111.14
38	RE	79	ARG	NE-CZ-NH1	-6.68	114.82	121.50
37	YD	98	VAL	N-CA-C	-6.67	103.94	113.07
42	YI	142	VAL	N-CA-C	-6.67	98.78	108.11
26	R1	21	ARG	CG-CD-NE	6.65	126.62	112.00
31	Y6	20	ASN	N-CA-C	6.64	121.02	112.12
11	XK	87	THR	N-CA-C	-6.63	100.66	110.48
15	QO	89	GLY	N-CA-C	-6.63	94.06	113.30
2	QB	200	ILE	N-CA-C	6.63	118.58	108.71
40	YG	30	GLU	N-CA-C	-6.62	105.23	113.38
40	YG	181	ARG	N-CA-C	6.62	120.07	108.56
51	YV	14	VAL	N-CA-C	6.62	118.12	108.53
37	YD	106	ILE	N-CA-C	-6.61	101.05	109.58
13	XM	9	ILE	N-CA-C	6.60	123.14	108.88
9	XI	59	PHE	N-CA-C	6.60	120.16	109.40
39	YF	84	VAL	N-CA-C	-6.59	100.19	108.89
41	YH	46	GLU	N-CA-C	-6.59	101.03	110.59
42	RI	72	LEU	N-CA-C	6.58	118.25	111.14
20	QT	27	LYS	N-CA-C	-6.58	104.89	113.12
46	YQ	59	ARG	CA-C-N	6.57	134.81	123.91
46	YQ	59	ARG	C-N-CA	6.57	134.81	123.91
9	QI	101	PHE	N-CA-C	-6.57	104.30	112.90
54	RY	83	THR	N-CA-C	6.55	116.92	108.34
12	XL	62	SER	N-CA-C	-6.55	104.91	113.17
50	YU	9	VAL	N-CA-C	6.55	116.71	110.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	YY	84	ARG	N-CA-C	-6.55	100.27	110.42
42	RI	84	GLY	CA-C-N	6.54	134.02	121.54
42	RI	84	GLY	C-N-CA	6.54	134.02	121.54
40	RG	146	TYR	CA-CB-CG	6.53	125.66	113.90
37	YD	274	ARG	N-CA-C	6.53	118.95	110.53
38	YE	142	GLY	CA-C-N	6.53	134.01	121.54
38	YE	142	GLY	C-N-CA	6.53	134.01	121.54
3	QC	15	THR	CA-C-N	6.53	134.01	121.54
3	QC	15	THR	C-N-CA	6.53	134.01	121.54
11	XK	75	TYR	N-CA-C	-6.53	105.45	113.41
18	XR	87	ARG	N-CA-C	6.52	118.54	110.91
16	QP	53	VAL	CA-C-N	6.52	129.85	120.79
16	QP	53	VAL	C-N-CA	6.52	129.85	120.79
20	QT	94	ALA	N-CA-C	-6.51	99.67	109.96
42	RI	82	ARG	CG-CD-NE	6.51	126.31	112.00
2	QB	226	ARG	CG-CD-NE	6.49	126.28	112.00
45	RP	25	SER	N-CA-C	-6.49	103.97	112.41
9	XI	70	LYS	N-CA-C	6.49	118.02	111.07
49	YT	55	ASN	N-CA-C	-6.49	102.74	112.54
55	RZ	71	VAL	N-CA-C	6.48	113.15	106.21
12	XL	38	THR	N-CA-C	-6.48	106.58	114.75
9	XI	60	ASP	N-CA-C	-6.48	101.80	110.55
44	RO	40	VAL	N-CA-C	-6.47	99.15	108.53
48	RS	44	LYS	N-CA-C	-6.46	104.58	113.18
42	RI	89	TYR	N-CA-C	-6.45	104.25	111.28
17	QQ	67	LYS	N-CA-C	-6.43	101.87	110.55
37	RD	35	LYS	CB-CA-C	6.43	118.71	110.22
24	XY	71	THR	N-CA-C	-6.42	101.26	111.02
5	QE	153	LYS	N-CA-C	-6.42	105.27	113.23
18	XR	42	ARG	CG-CD-NE	-6.41	97.90	112.00
1	QA	1038	C	C2'-C3'-O3'	6.40	119.10	109.50
19	QS	27	GLU	N-CA-C	6.40	120.38	111.74
4	XD	206	PHE	N-CA-C	-6.40	102.99	111.24
19	XS	11	VAL	N-CA-C	-6.39	99.28	108.48
34	Y9	12	ASP	N-CA-C	6.39	119.05	111.71
39	YF	13	SER	N-CA-C	-6.38	100.68	110.32
16	XP	79	VAL	N-CA-C	-6.38	106.73	111.90
3	QC	17	ASP	N-CA-C	-6.37	101.35	110.59
51	YV	50	PRO	CA-N-CD	-6.36	103.10	112.00
42	YI	120	ILE	CA-C-N	6.36	133.68	121.54
42	YI	120	ILE	C-N-CA	6.36	133.68	121.54
2	XB	231	GLU	N-CA-C	6.35	120.94	109.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	YE	76	ARG	N-CA-C	6.35	119.43	111.24
3	XC	62	ASP	N-CA-C	6.33	119.82	111.28
29	Y4	51	ASP	N-CA-C	6.32	117.86	110.97
55	RZ	105	VAL	N-CA-C	6.32	115.72	106.55
42	YI	74	ASN	N-CA-C	-6.31	106.22	114.04
19	QS	38	SER	N-CA-C	6.30	120.55	109.96
37	RD	98	VAL	N-CA-C	-6.30	103.74	112.50
50	RU	96	ALA	N-CA-C	-6.30	105.54	112.72
31	R6	11	LEU	N-CA-C	-6.30	101.46	110.59
54	YY	19	LYS	N-CA-C	-6.29	104.31	112.23
45	RP	62	LEU	N-CA-C	6.28	123.69	109.81
53	YX	90	GLU	N-CA-C	6.27	117.78	111.07
19	QS	11	VAL	CA-C-N	6.27	133.52	121.54
19	QS	11	VAL	C-N-CA	6.27	133.52	121.54
4	QD	206	PHE	N-CA-C	-6.27	103.75	111.40
38	YE	176	ILE	N-CA-C	-6.27	101.94	108.15
40	YG	147	ASP	N-CA-C	-6.27	104.90	113.30
44	RO	97	ARG	N-CA-C	6.26	118.85	111.02
55	YZ	92	SER	N-CA-C	-6.26	100.72	110.17
10	QJ	79	ARG	CD-NE-CZ	6.25	133.16	124.40
9	XI	92	TYR	N-CA-C	-6.25	105.30	113.17
33	R8	46	ARG	CG-CD-NE	-6.24	98.26	112.00
37	RD	122	ASP	CA-C-N	6.24	137.02	121.80
37	RD	122	ASP	C-N-CA	6.24	137.02	121.80
21	QU	15	ARG	CG-CD-NE	-6.23	98.29	112.00
27	R2	72	ALA	N-CA-C	6.23	128.44	111.00
20	QT	34	LYS	N-CA-C	6.23	118.07	111.28
29	R4	63	TYR	N-CA-C	-6.22	105.63	113.72
46	RQ	90	VAL	N-CA-C	6.22	116.91	111.56
18	XR	25	THR	N-CA-C	-6.21	103.09	112.04
49	YT	133	GLU	CB-CA-C	-6.21	97.51	110.17
44	RO	96	THR	N-CA-C	-6.20	100.76	109.69
11	XK	96	ARG	CD-NE-CZ	6.20	133.07	124.40
50	YU	101	ARG	N-CA-C	6.19	117.83	111.14
35	YA	1225	C	C4'-C3'-C2'	6.19	108.79	102.60
49	YT	89	VAL	N-CA-C	-6.19	107.83	113.71
8	QH	134	ILE	N-CA-C	6.18	116.30	110.30
45	RP	19	VAL	N-CA-C	6.18	118.94	108.86
39	RF	99	TYR	CA-CB-CG	6.18	125.02	113.90
43	YN	112	LEU	N-CA-C	-6.18	105.40	113.12
4	XD	3	ARG	N-CA-C	-6.18	100.85	110.42
29	R4	55	ARG	N-CA-C	6.17	118.81	111.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	YV	89	GLN	N-CA-C	6.16	117.80	109.24
50	RU	92	ARG	CA-C-N	6.16	137.35	126.45
50	RU	92	ARG	C-N-CA	6.16	137.35	126.45
55	YZ	112	ARG	N-CA-C	-6.16	104.47	112.23
47	YR	57	ARG	NE-CZ-NH1	-6.16	115.34	121.50
10	XJ	49	VAL	N-CA-C	6.15	117.15	108.36
43	RN	93	THR	N-CA-C	6.14	119.97	112.23
41	YH	50	VAL	N-CA-C	-6.14	99.62	108.53
47	YR	14	SER	N-CA-C	6.14	117.67	110.97
51	RV	53	GLU	N-CA-C	6.13	117.63	111.07
41	YH	56	SER	N-CA-C	6.12	118.50	109.69
12	QL	47	LYS	N-CA-C	6.11	123.32	109.81
27	R2	21	LEU	N-CA-C	-6.11	104.69	111.36
3	QC	102	ASN	N-CA-C	-6.11	99.74	109.76
49	YT	113	LYS	N-CA-C	-6.11	103.76	112.13
32	Y7	4	THR	N-CA-C	6.11	118.01	111.36
25	R0	44	ARG	N-CA-C	-6.10	104.54	112.23
7	QG	15	ASP	N-CA-C	6.09	118.64	110.35
41	RH	86	GLU	CA-C-N	6.09	133.18	121.54
41	RH	86	GLU	C-N-CA	6.09	133.18	121.54
24	QZ	82	TYR	N-CA-C	6.09	119.31	110.42
54	YY	91	GLU	N-CA-C	-6.09	105.34	112.89
46	RQ	18	LYS	N-CA-C	6.09	121.41	111.37
38	RE	23	VAL	N-CA-C	6.08	118.99	108.95
3	XC	144	SER	N-CA-C	-6.08	100.85	109.96
11	XK	96	ARG	CB-CG-CD	-6.08	97.33	111.30
24	XY	48	LEU	N-CA-C	6.08	119.61	109.95
47	YR	57	ARG	N-CA-C	-6.08	105.36	112.89
41	YH	34	GLU	N-CA-C	-6.07	100.00	109.72
31	R6	4	GLU	N-CA-C	-6.07	105.53	113.12
33	Y8	29	LYS	CA-C-N	6.07	133.13	121.54
33	Y8	29	LYS	C-N-CA	6.07	133.13	121.54
43	YN	71	ILE	N-CA-C	6.07	116.66	108.17
8	XH	134	ILE	N-CA-C	6.06	116.18	110.30
13	XM	84	ILE	N-CA-C	-6.06	107.96	113.71
47	YR	74	LYS	N-CA-C	-6.05	102.38	110.55
13	XM	13	LYS	N-CA-C	6.05	123.69	110.80
51	YV	34	GLU	N-CA-C	6.05	119.51	109.46
13	QM	104	ARG	N-CA-C	-6.05	104.61	112.23
45	RP	147	LEU	N-CA-C	6.03	118.24	108.41
13	QM	11	ARG	CB-CA-C	6.03	123.65	111.60
48	RS	69	VAL	N-CA-C	-6.02	104.53	113.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	RY	56	PRO	CA-C-N	6.02	134.47	121.64
54	RY	56	PRO	C-N-CA	6.02	134.47	121.64
9	XI	120	ARG	N-CA-C	-6.02	107.75	114.62
51	RV	21	ARG	NE-CZ-NH1	6.02	127.52	121.50
9	QI	99	LEU	N-CA-C	-6.01	105.43	112.89
12	XL	79	GLU	N-CA-C	6.00	121.28	111.37
41	RH	10	PRO	CA-C-N	5.99	133.21	122.13
41	RH	10	PRO	C-N-CA	5.99	133.21	122.13
2	XB	16	HIS	N-CA-C	5.98	118.27	110.43
55	YZ	145	GLU	N-CA-C	-5.98	100.40	109.85
55	RZ	122	ARG	N-CA-C	-5.98	105.47	112.89
55	YZ	91	LEU	N-CA-C	5.98	118.47	108.96
39	RF	197	ASP	N-CA-C	-5.97	104.34	111.69
8	XH	97	VAL	N-CA-C	5.97	118.51	111.05
37	RD	269	PHE	N-CA-C	-5.97	105.18	112.88
41	RH	85	LYS	N-CA-C	5.96	118.54	109.95
49	RT	124	ASP	N-CA-C	5.96	119.81	112.54
26	R1	82	LEU	N-CA-C	-5.96	101.37	109.95
16	QP	12	LYS	N-CA-C	-5.95	100.30	109.76
7	QG	45	ASP	N-CA-C	-5.95	104.37	111.69
41	RH	152	ARG	N-CA-C	5.95	123.47	110.80
12	QL	20	LYS	N-CA-C	5.93	117.96	110.24
43	RN	60	ILE	N-CA-C	-5.93	103.58	110.05
2	XB	44	LEU	N-CA-C	5.93	117.83	111.36
33	R8	46	ARG	N-CA-CB	-5.93	101.31	110.56
45	RP	71	VAL	N-CA-C	5.93	121.69	108.88
4	QD	121	VAL	N-CA-C	-5.92	105.08	110.82
46	RQ	7	MET	N-CA-C	-5.92	100.85	110.20
20	XT	72	LEU	CA-C-N	5.91	132.83	121.54
20	XT	72	LEU	C-N-CA	5.91	132.83	121.54
44	YO	96	THR	N-CA-C	-5.91	100.77	109.81
40	RG	176	LEU	N-CA-C	-5.91	105.90	113.23
2	QB	230	VAL	CA-C-N	5.90	136.20	121.80
2	QB	230	VAL	C-N-CA	5.90	136.20	121.80
41	RH	14	GLY	CA-C-N	5.90	132.59	121.97
41	RH	14	GLY	C-N-CA	5.90	132.59	121.97
32	R7	4	THR	N-CA-C	5.90	117.79	111.36
40	RG	115	ARG	N-CA-C	5.90	118.81	109.96
45	YP	35	HIS	CA-C-N	5.90	132.81	121.54
45	YP	35	HIS	C-N-CA	5.90	132.81	121.54
4	QD	49	ARG	N-CA-C	-5.89	102.19	110.50
24	XZ	84	TYR	N-CA-C	-5.89	94.50	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	R8	35	GLN	N-CA-CB	5.88	119.84	111.25
41	RH	83	TYR	N-CA-C	5.88	123.33	110.80
11	QK	11	LYS	CA-C-N	5.88	132.76	121.54
11	QK	11	LYS	C-N-CA	5.88	132.76	121.54
50	RU	100	VAL	N-CA-C	-5.88	107.77	113.53
12	XL	117	ARG	N-CA-C	5.88	120.31	113.20
27	R2	47	ASN	N-CA-C	5.88	123.31	110.80
4	XD	20	TYR	N-CA-C	5.88	118.36	111.02
52	YW	111	HIS	N-CA-C	5.87	123.31	110.80
19	QS	47	HIS	N-CA-C	5.86	119.61	110.17
16	XP	32	TYR	CA-CB-CG	5.86	124.45	113.90
49	YT	57	PHE	N-CA-C	-5.86	102.64	110.55
54	YY	106	LEU	CA-C-N	5.86	132.25	121.70
54	YY	106	LEU	C-N-CA	5.86	132.25	121.70
54	RY	71	LYS	N-CA-C	-5.85	105.91	113.16
41	RH	167	GLU	N-CA-C	-5.85	101.11	109.24
8	XH	100	ILE	N-CA-C	-5.85	103.22	108.95
37	YD	10	THR	N-CA-C	-5.84	101.16	110.10
21	QU	2	GLY	CA-C-N	5.84	132.70	121.54
21	QU	2	GLY	C-N-CA	5.84	132.70	121.54
39	YF	196	LEU	N-CA-C	-5.84	105.92	113.16
31	R6	32	ASN	N-CA-C	-5.84	102.27	110.50
41	RH	101	ARG	N-CA-C	-5.83	105.93	114.39
43	RN	21	LYS	N-CA-C	-5.83	100.76	109.15
9	XI	117	HIS	N-CA-C	5.83	117.50	111.03
40	YG	72	ARG	NE-CZ-NH1	-5.82	115.68	121.50
36	YB	116	G	C1'-O4'-C4'	-5.82	104.08	109.90
29	R4	61	ARG	N-CA-C	-5.81	106.04	114.12
54	YY	34	LYS	N-CA-C	-5.80	106.18	113.72
44	YO	2	ILE	N-CA-C	5.79	116.27	108.17
1	QA	1038	C	P-O3'-C3'	5.78	128.87	120.20
44	YO	40	VAL	N-CA-C	-5.78	100.15	108.53
25	R0	48	GLY	N-CA-C	5.77	126.86	113.18
55	RZ	96	VAL	N-CA-C	-5.76	99.82	108.12
24	QZ	80	CYS	N-CA-C	-5.76	103.99	111.71
38	RE	51	PHE	N-CA-C	5.76	120.02	112.13
2	QB	132	LYS	CD-CE-NZ	5.76	130.32	111.90
45	YP	148	LEU	CA-C-N	5.75	132.06	121.70
45	YP	148	LEU	C-N-CA	5.75	132.06	121.70
38	RE	52	LEU	N-CA-C	5.75	117.23	109.24
38	YE	101	ARG	CB-CA-C	5.75	118.99	110.14
49	YT	18	ASP	N-CA-C	5.75	119.47	112.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	QC	68	VAL	N-CA-C	5.74	116.47	108.89
24	XZ	82	TYR	N-CA-C	5.74	118.38	110.35
9	XI	91	ASP	N-CA-C	-5.73	106.10	112.57
38	RE	79	ARG	N-CA-C	5.73	117.89	109.24
49	RT	12	SER	N-CA-C	5.72	120.00	113.19
29	R4	52	THR	CA-C-N	5.72	131.86	121.97
29	R4	52	THR	C-N-CA	5.72	131.86	121.97
41	RH	154	PRO	N-CA-C	5.72	124.25	112.47
5	XE	69	VAL	N-CA-C	5.71	114.17	107.77
24	QZ	83	HIS	CA-C-N	5.71	131.98	121.70
24	QZ	83	HIS	C-N-CA	5.71	131.98	121.70
24	XZ	66	LEU	N-CA-C	-5.71	99.22	108.52
45	YP	27	HIS	N-CA-C	-5.71	98.65	110.80
1	XA	197	A	P-O3'-C3'	5.70	128.76	120.20
2	XB	236	TYR	N-CA-CB	-5.70	100.85	110.49
47	YR	104	ARG	N-CA-C	5.70	117.65	110.24
17	XQ	13	ASP	N-CA-C	-5.70	104.90	112.94
45	RP	42	SER	N-CA-C	5.70	117.49	111.28
2	XB	122	PHE	CA-CB-CG	5.69	119.49	113.80
4	QD	163	GLU	N-CA-C	-5.68	105.07	112.23
45	RP	54	GLY	N-CA-C	-5.68	106.82	115.00
1	QA	197	A	P-O3'-C3'	5.68	128.72	120.20
10	XJ	31	GLY	N-CA-C	5.68	126.63	113.18
51	RV	43	GLU	CA-CB-CG	-5.67	102.75	114.10
42	RI	143	SER	N-CA-C	-5.67	98.73	110.80
55	RZ	52	SER	CA-C-N	5.67	132.17	121.97
55	RZ	52	SER	C-N-CA	5.67	132.17	121.97
37	RD	48	ARG	N-CA-C	5.67	117.21	110.19
4	QD	190	ASP	N-CA-C	-5.66	102.91	110.55
37	RD	147	LEU	N-CA-C	-5.66	105.16	112.68
31	R6	21	TYR	N-CA-C	5.65	118.71	110.17
24	XZ	49	LYS	CA-C-N	5.65	132.34	121.54
24	XZ	49	LYS	C-N-CA	5.65	132.34	121.54
4	XD	110	PHE	N-CA-C	-5.65	105.11	112.23
6	XF	72	VAL	N-CA-C	5.65	116.42	110.72
12	QL	104	VAL	CA-C-N	5.64	132.31	121.54
12	QL	104	VAL	C-N-CA	5.64	132.31	121.54
43	YN	26	LEU	N-CA-C	-5.64	106.07	113.12
3	XC	55	VAL	N-CA-C	-5.64	100.11	108.45
2	XB	20	GLU	N-CA-C	5.63	119.23	110.17
12	QL	86	ARG	N-CA-C	5.62	120.16	112.68
8	QH	116	LYS	N-CA-C	-5.62	106.31	112.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	QE	68	GLU	N-CA-C	-5.62	101.39	110.32
41	RH	10	PRO	N-CA-C	5.62	124.05	112.47
19	QS	64	GLU	N-CA-C	5.61	122.76	110.80
3	QC	78	GLY	N-CA-C	5.61	126.48	113.18
40	RG	146	TYR	N-CA-CB	-5.61	101.02	110.49
46	RQ	5	ARG	N-CA-C	-5.61	101.14	110.17
55	YZ	153	SER	N-CA-C	-5.60	105.94	112.89
2	QB	207	ALA	CA-C-N	5.60	132.06	121.97
2	QB	207	ALA	C-N-CA	5.60	132.06	121.97
24	QY	49	LYS	CA-C-N	5.60	132.24	121.54
24	QY	49	LYS	C-N-CA	5.60	132.24	121.54
17	QQ	101	ARG	N-CA-C	-5.60	95.32	111.00
38	RE	82	ARG	CA-C-N	5.59	132.23	121.54
38	RE	82	ARG	C-N-CA	5.59	132.23	121.54
10	XJ	84	GLN	N-CA-C	-5.59	105.56	112.72
45	RP	19	VAL	N-CA-CB	-5.59	101.59	111.93
20	XT	73	HIS	N-CA-C	5.59	122.71	110.80
40	RG	16	ARG	N-CA-C	5.59	120.35	112.75
4	XD	43	HIS	N-CA-C	5.59	118.89	112.97
40	RG	88	ILE	N-CA-C	5.58	117.80	111.88
38	YE	61	ARG	N-CA-C	5.58	121.09	113.16
37	YD	260	ARG	N-CA-C	-5.58	102.22	110.48
42	RI	14	ASP	CA-C-N	5.58	132.01	121.97
42	RI	14	ASP	C-N-CA	5.58	132.01	121.97
42	RI	14	ASP	N-CA-C	5.58	118.35	109.65
3	QC	181	ASN	N-CA-C	-5.57	103.76	111.28
3	QC	8	ILE	N-CA-C	-5.57	105.42	110.82
10	QJ	54	PHE	N-CA-C	5.57	122.66	110.80
37	RD	196	VAL	N-CA-C	5.57	116.22	110.82
29	R4	59	PHE	N-CA-C	5.56	117.34	111.28
51	YV	96	ILE	N-CA-C	5.56	116.18	108.84
42	YI	14	ASP	CA-CB-CG	5.55	118.15	112.60
29	R4	13	ARG	CG-CD-NE	5.55	124.21	112.00
49	YT	111	ARG	N-CA-C	-5.55	102.68	110.50
55	RZ	112	ARG	CB-CA-C	5.54	121.68	110.38
3	QC	93	LYS	N-CA-C	-5.54	104.88	111.69
45	YP	104	GLY	N-CA-C	5.54	126.30	113.18
35	YA	603	A	P-O3'-C3'	5.53	128.49	120.20
9	QI	83	ARG	CB-CG-CD	5.53	124.02	111.30
55	RZ	79	ARG	N-CA-C	5.53	117.17	111.03
55	YZ	105	VAL	N-CA-C	5.53	116.55	108.53
47	YR	37	THR	N-CA-C	-5.52	103.10	110.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	R3	49	LYS	N-CA-C	-5.51	105.28	112.23
33	Y8	33	ASN	N-CA-C	5.51	119.75	112.25
40	YG	12	TYR	N-CA-C	5.51	119.10	112.38
27	R2	46	GLN	N-CA-C	-5.51	98.78	108.20
16	QP	54	GLU	CB-CA-C	5.51	119.68	110.92
40	YG	148	MET	N-CA-C	-5.51	106.61	113.38
54	RY	84	ARG	N-CA-C	-5.50	101.15	109.85
12	XL	61	THR	N-CA-C	-5.50	106.57	113.28
42	YI	10	GLU	CA-CB-CG	5.49	125.08	114.10
7	QG	85	TYR	N-CA-C	-5.49	101.32	109.94
38	RE	61	ARG	N-CA-C	5.49	120.96	113.16
29	Y4	67	TYR	CA-CB-CG	5.49	123.78	113.90
41	RH	17	VAL	CA-C-N	5.49	132.03	121.54
41	RH	17	VAL	C-N-CA	5.49	132.03	121.54
37	RD	229	VAL	N-CA-C	-5.48	105.50	110.82
4	XD	208	SER	N-CA-C	-5.48	101.40	109.62
10	QJ	16	LEU	N-CA-C	5.48	116.93	111.07
41	RH	149	ARG	N-CA-C	-5.47	106.11	112.89
54	YY	68	HIS	N-CA-C	-5.47	102.39	110.48
9	XI	114	TYR	CB-CA-C	5.47	118.77	109.53
37	RD	37	LEU	N-CA-C	-5.46	102.68	110.59
7	XG	154	TYR	N-CA-C	-5.46	106.20	112.92
13	QM	114	ARG	N-CA-CB	5.46	118.55	109.60
12	QL	98	TYR	N-CA-C	5.45	115.48	108.34
35	YA	372	G	P-O3'-C3'	5.45	128.38	120.20
29	R4	63	TYR	CB-CA-C	5.45	118.70	109.55
45	YP	102	ARG	N-CA-C	-5.45	102.46	110.52
10	QJ	81	THR	N-CA-C	-5.45	104.88	112.45
26	R1	21	ARG	CB-CG-CD	-5.44	98.79	111.30
46	RQ	116	GLU	N-CA-C	-5.44	104.89	112.45
5	XE	51	VAL	N-CA-C	5.43	120.61	108.88
21	XU	2	GLY	CA-C-N	5.43	131.91	121.54
21	XU	2	GLY	C-N-CA	5.43	131.91	121.54
51	RV	37	VAL	N-CA-C	5.42	115.67	107.75
37	RD	6	PHE	N-CA-C	5.42	117.92	109.52
2	QB	193	ASP	N-CA-C	-5.42	102.14	110.32
53	RX	29	TRP	N-CA-C	-5.42	100.35	109.07
35	YA	1558	A	P-O3'-C3'	5.41	128.32	120.20
18	QR	70	ILE	N-CA-C	-5.41	105.58	110.82
35	RA	1558	A	P-O3'-C3'	5.41	128.31	120.20
2	QB	185	ILE	N-CA-C	-5.40	100.55	108.11
53	RX	59	VAL	N-CA-C	-5.40	100.61	108.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	RZ	153	SER	N-CA-C	-5.39	106.38	113.12
19	QS	43	GLU	N-CA-C	-5.39	106.65	113.18
42	RI	33	ARG	N-CA-C	-5.39	105.49	111.36
44	RO	57	VAL	N-CA-C	-5.39	102.57	109.30
18	QR	83	GLU	CB-CA-C	5.38	119.55	109.86
24	QZ	35	ARG	N-CA-C	-5.38	104.97	112.45
45	YP	36	LYS	N-CA-C	5.38	122.25	110.80
49	YT	96	ARG	CA-CB-CG	5.38	124.86	114.10
48	YS	111	GLU	N-CA-C	5.38	118.61	111.30
3	XC	143	GLU	N-CA-C	-5.37	105.50	111.36
24	QY	82	TYR	N-CA-C	5.37	122.24	110.80
37	YD	53	PHE	N-CA-C	5.36	118.79	111.39
54	YY	9	LYS	N-CA-C	-5.36	103.90	110.65
55	RZ	170	THR	N-CA-C	5.36	118.00	109.96
1	QA	1065	U	P-O3'-C3'	5.36	128.23	120.20
13	XM	37	THR	N-CA-C	-5.36	105.48	112.23
40	RG	98	ARG	N-CA-C	-5.35	107.30	113.88
10	XJ	14	LYS	N-CA-C	-5.35	105.36	111.14
55	YZ	116	VAL	N-CA-C	5.35	118.12	110.09
54	RY	40	GLU	N-CA-C	5.35	118.32	110.30
42	RI	6	LEU	N-CA-C	-5.34	107.13	113.97
20	XT	96	GLY	CA-C-N	5.34	134.82	121.80
20	XT	96	GLY	C-N-CA	5.34	134.82	121.80
7	QG	30	ILE	N-CA-C	-5.34	105.18	111.00
13	QM	114	ARG	CB-CA-C	-5.33	102.56	110.67
4	QD	47	ARG	N-CA-C	5.33	117.96	110.23
50	YU	92	ARG	N-CA-C	5.33	122.15	110.80
54	YY	85	VAL	N-CA-C	5.33	116.65	108.71
48	RS	53	SER	N-CA-C	-5.32	105.93	112.90
46	RQ	66	ILE	N-CA-C	5.32	120.40	109.34
42	YI	145	VAL	CA-C-N	5.31	131.25	121.70
42	YI	145	VAL	C-N-CA	5.31	131.25	121.70
37	RD	260	ARG	N-CA-C	-5.30	101.82	110.20
19	QS	27	GLU	CA-C-N	5.30	131.66	121.54
19	QS	27	GLU	C-N-CA	5.30	131.66	121.54
54	RY	9	LYS	N-CA-C	-5.29	105.05	112.25
35	RA	1300	U	P-O3'-C3'	5.29	128.14	120.20
40	YG	128	ARG	N-CA-C	-5.29	105.10	112.30
1	XA	328	C	P-O3'-C3'	5.29	128.13	120.20
10	QJ	28	ARG	CG-CD-NE	5.29	123.64	112.00
33	Y8	31	HIS	N-CA-C	5.29	122.06	110.80
38	RE	15	PHE	N-CA-C	5.29	116.92	108.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	RP	27	HIS	N-CA-C	5.29	122.06	110.80
48	RS	111	GLU	N-CA-C	5.29	122.06	110.80
1	XA	1038	C	C2'-C3'-O3'	5.28	117.42	109.50
48	YS	25	ARG	N-CA-C	5.28	117.34	108.73
33	Y8	32	LEU	N-CA-C	5.28	116.78	109.54
47	YR	9	LYS	N-CA-C	-5.28	99.91	108.52
12	XL	47	LYS	N-CA-C	5.28	121.47	109.81
19	QS	14	HIS	N-CA-C	5.28	116.72	110.97
30	R5	51	TYR	CA-CB-CG	5.27	123.39	113.90
34	R9	34	GLN	N-CA-C	5.27	116.67	109.18
7	QG	4	ARG	N-CA-C	5.26	118.03	111.24
18	QR	32	ARG	N-CA-C	-5.26	107.03	113.50
2	QB	12	GLU	CG-CD-OE1	-5.26	106.31	118.40
41	RH	40	GLU	N-CA-C	-5.26	101.69	109.94
40	RG	12	TYR	N-CA-C	5.25	117.09	111.36
48	YS	46	VAL	N-CA-C	5.25	115.46	108.11
24	QZ	58	ARG	N-CA-C	-5.25	101.43	109.41
39	RF	99	TYR	CB-CA-C	5.25	119.76	110.16
24	XZ	8	GLU	CB-CG-CD	5.24	121.51	112.60
36	RB	118	G	C1'-C2'-O2'	5.24	116.26	108.40
41	RH	85	LYS	CA-C-N	5.24	131.54	121.54
41	RH	85	LYS	C-N-CA	5.24	131.54	121.54
28	Y3	2	PRO	CA-C-N	5.24	131.54	121.54
28	Y3	2	PRO	C-N-CA	5.24	131.54	121.54
27	R2	20	GLU	N-CA-C	-5.24	106.28	113.30
49	RT	39	ARG	N-CA-C	-5.24	101.33	108.24
45	YP	28	GLY	CA-C-N	5.23	131.54	121.54
45	YP	28	GLY	C-N-CA	5.23	131.54	121.54
43	RN	128	HIS	N-CA-C	-5.23	102.55	110.39
20	QT	91	LEU	N-CA-C	-5.23	107.07	113.50
47	YR	74	LYS	CA-C-N	5.23	131.52	121.54
47	YR	74	LYS	C-N-CA	5.23	131.52	121.54
19	QS	25	LYS	N-CA-C	-5.22	105.19	112.45
39	RF	168	ARG	N-CA-C	5.22	117.88	111.82
35	YA	1022	G	C2'-C3'-O3'	5.22	117.33	109.50
24	XZ	68	TYR	N-CA-C	5.22	115.02	108.45
29	R4	28	LYS	N-CA-C	5.21	118.19	110.32
7	XG	13	GLN	N-CA-C	5.21	116.45	109.83
37	RD	33	LEU	O-C-N	-5.21	115.66	122.59
1	QA	250	A	P-O3'-C3'	5.21	128.02	120.20
40	RG	3	LEU	N-CA-C	5.21	117.86	110.10
55	RZ	31	ARG	N-CA-C	-5.21	106.77	113.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	YQ	62	GLY	N-CA-C	5.21	125.53	113.18
12	XL	86	ARG	N-CA-C	5.21	119.26	112.13
42	YI	14	ASP	CA-C-N	5.21	131.34	121.97
42	YI	14	ASP	C-N-CA	5.21	131.34	121.97
40	RG	83	ARG	CG-CD-NE	5.20	123.44	112.00
26	R1	85	LEU	CA-C-N	5.20	134.49	121.80
26	R1	85	LEU	C-N-CA	5.20	134.49	121.80
12	QL	59	ARG	N-CA-CB	5.20	118.90	110.43
35	YA	1022	G	P-O3'-C3'	5.20	128.00	120.20
4	QD	110	PHE	N-CA-C	-5.20	106.45	112.89
42	RI	11	ASN	N-CA-C	-5.19	104.14	111.56
4	QD	33	MET	N-CA-C	-5.19	106.75	114.64
38	RE	73	GLU	CA-C-N	5.19	126.33	119.84
38	RE	73	GLU	C-N-CA	5.19	126.33	119.84
1	QA	1528	U	P-O3'-C3'	5.19	127.98	120.20
42	YI	143	SER	N-CA-C	5.18	116.17	108.86
35	RA	90	U	P-O3'-C3'	5.18	127.97	120.20
1	XA	1065	U	P-O3'-C3'	5.18	127.97	120.20
1	XA	1038	C	P-O3'-C3'	5.18	127.97	120.20
8	QH	19	VAL	N-CA-C	-5.17	108.08	113.10
20	QT	105	SER	N-CA-C	5.17	117.17	108.96
38	RE	144	ARG	CA-C-N	5.17	131.41	121.54
38	RE	144	ARG	C-N-CA	5.17	131.41	121.54
55	YZ	67	LEU	N-CA-C	5.17	117.11	109.62
37	RD	239	ARG	N-CA-C	5.17	116.95	110.91
49	YT	10	VAL	N-CA-C	-5.16	105.37	111.00
33	R8	51	ALA	CA-C-N	5.16	129.72	121.62
33	R8	51	ALA	C-N-CA	5.16	129.72	121.62
41	RH	68	THR	N-CA-C	5.16	116.90	111.28
41	RH	116	GLU	N-CA-C	-5.16	102.14	109.62
47	YR	57	ARG	CB-CA-C	5.15	120.76	109.99
1	XA	1054	C	P-O3'-C3'	5.15	127.92	120.20
41	RH	130	ARG	CB-CG-CD	5.15	123.14	111.30
9	QI	117	HIS	N-CA-C	5.15	116.70	111.14
46	RQ	5	ARG	CG-CD-NE	5.15	123.32	112.00
42	YI	10	GLU	CB-CG-CD	5.15	121.35	112.60
11	QK	59	TYR	N-CA-C	-5.14	105.36	111.69
35	RA	1022	G	P-O3'-C3'	5.14	127.91	120.20
1	QA	992	U	P-O3'-C3'	5.14	127.91	120.20
24	QZ	71	THR	N-CA-C	-5.14	101.49	109.14
1	XA	1067	A	P-O3'-C3'	5.14	127.91	120.20
19	XS	12	ASP	CA-C-N	5.14	131.35	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	XS	12	ASP	C-N-CA	5.14	131.35	121.54
42	YI	145	VAL	CB-CA-C	-5.13	102.87	111.29
6	QF	64	GLN	N-CA-C	-5.13	100.80	108.96
2	XB	172	ILE	N-CA-C	-5.13	105.54	110.72
10	QJ	82	ILE	N-CA-C	5.13	115.24	110.42
34	Y9	2	LYS	N-CA-C	5.13	117.43	111.02
2	QB	233	SER	N-CA-C	5.12	121.12	109.81
39	RF	84	VAL	N-CA-C	-5.12	102.48	109.55
9	XI	53	VAL	N-CA-C	-5.12	107.72	112.43
1	QA	687	A	P-O3'-C3'	5.12	127.88	120.20
2	QB	131	PRO	CA-C-N	5.12	127.65	120.28
2	QB	131	PRO	C-N-CA	5.12	127.65	120.28
48	YS	57	LYS	N-CA-C	5.12	117.42	111.02
38	RE	116	VAL	CA-C-N	5.12	135.22	126.32
38	RE	116	VAL	C-N-CA	5.12	135.22	126.32
40	RG	115	ARG	CA-C-N	5.11	131.31	121.54
40	RG	115	ARG	C-N-CA	5.11	131.31	121.54
1	QA	1067	A	P-O3'-C3'	5.11	127.86	120.20
35	RA	1171	G	P-O3'-C3'	5.11	127.86	120.20
2	XB	122	PHE	CB-CA-C	5.11	119.53	110.85
38	YE	113	PHE	N-CA-C	-5.11	101.80	109.15
32	Y7	18	PHE	N-CA-C	5.10	116.84	111.28
51	YV	85	LYS	CB-CG-CD	5.10	123.04	111.30
41	RH	151	ILE	CB-CA-C	5.10	116.74	111.23
54	RY	106	LEU	N-CA-C	-5.10	107.09	113.72
13	QM	109	THR	N-CA-C	-5.10	105.80	111.36
3	QC	46	GLU	N-CA-C	5.10	119.35	113.18
43	RN	69	GLN	N-CA-C	5.10	120.13	112.94
1	XA	1000	A	P-O3'-C3'	5.09	127.84	120.20
3	QC	10	PHE	N-CA-C	-5.09	106.92	113.23
44	RO	116	SER	N-CA-C	-5.09	105.37	112.45
35	YA	1559	G	C4'-C3'-O3'	5.09	117.04	109.40
19	QS	29	ARG	CB-CA-C	-5.09	100.92	109.83
12	XL	21	LYS	N-CA-C	5.09	117.85	109.76
54	RY	34	LYS	N-CA-C	-5.09	107.12	113.38
2	XB	211	ILE	N-CA-C	-5.09	105.43	110.62
2	QB	7	VAL	N-CA-CB	-5.08	105.03	111.64
42	YI	135	GLU	N-CA-C	5.08	117.41	110.55
37	RD	243	GLY	N-CA-C	5.08	125.22	113.18
2	XB	86	GLU	N-CA-C	-5.08	106.34	112.54
12	XL	78	GLN	CA-C-N	5.08	128.44	120.82
12	XL	78	GLN	C-N-CA	5.08	128.44	120.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	XD	9	CYS	N-CA-C	-5.08	105.93	111.82
2	XB	27	LYS	N-CA-C	-5.07	107.04	113.18
35	YA	289	A	O5'-P-OP1	-5.07	92.78	108.00
49	YT	128	GLU	N-CA-C	-5.07	106.18	112.93
1	QA	181	G	P-O3'-C3'	5.07	127.81	120.20
7	QG	94	ARG	N-CA-C	-5.07	105.83	111.36
45	RP	64	LYS	N-CA-C	-5.07	106.60	112.89
55	YZ	77	ASP	N-CA-C	-5.07	101.70	109.76
50	RU	71	GLN	N-CA-C	-5.07	105.85	112.23
1	XA	687	A	P-O3'-C3'	5.07	127.80	120.20
43	YN	114	ARG	CA-C-N	5.06	134.81	126.86
43	YN	114	ARG	C-N-CA	5.06	134.81	126.86
49	YT	2	ASN	N-CA-C	5.06	117.72	110.68
46	RQ	111	GLU	N-CA-C	5.06	118.55	112.38
34	R9	9	ARG	N-CA-C	-5.06	100.48	108.73
53	YX	36	LYS	N-CA-C	5.06	116.79	111.28
42	RI	9	LEU	N-CA-C	5.06	121.57	110.80
42	RI	58	LEU	N-CA-C	-5.06	105.23	111.40
33	R8	35	GLN	CB-CA-C	-5.05	102.64	111.23
24	XZ	8	GLU	CB-CA-C	5.05	119.44	110.85
24	QY	14	LEU	N-CA-C	-5.05	106.63	112.89
42	RI	144	VAL	CB-CA-C	5.05	119.57	111.29
8	XH	109	ILE	N-CA-C	5.05	115.18	108.11
8	XH	102	ARG	N-CA-C	-5.05	101.17	109.40
1	XA	748	C	P-O3'-C3'	5.04	127.77	120.20
35	YA	1171	G	P-O3'-C3'	5.04	127.77	120.20
2	XB	133	LYS	N-CA-C	-5.04	104.73	111.24
12	XL	58	VAL	N-CA-C	5.04	115.17	108.11
51	YV	53	GLU	N-CA-C	5.04	116.47	110.97
4	XD	30	LYS	CA-C-N	5.04	127.97	120.31
4	XD	30	LYS	C-N-CA	5.04	127.97	120.31
1	QA	748	C	P-O3'-C3'	5.04	127.75	120.20
7	QG	61	VAL	N-CA-C	-5.04	105.25	112.35
35	RA	119	A	P-O3'-C3'	5.04	127.75	120.20
45	RP	18	ARG	CB-CG-CD	-5.04	99.72	111.30
47	RR	74	LYS	N-CA-C	-5.04	103.29	110.59
4	QD	54	TYR	N-CA-C	-5.03	105.45	112.45
11	QK	75	TYR	N-CA-C	-5.03	106.99	113.23
12	XL	72	GLY	N-CA-C	5.03	120.37	111.01
26	R1	87	PRO	CA-N-CD	-5.03	104.96	112.00
10	XJ	81	THR	N-CA-C	-5.03	107.09	113.43
38	YE	24	THR	N-CA-C	-5.03	101.20	109.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	YF	48	THR	N-CA-C	5.03	118.95	112.41
7	XG	87	VAL	N-CA-C	5.03	114.44	108.96
26	Y1	72	GLU	N-CA-C	-5.03	105.51	111.69
54	YY	6	HIS	N-CA-C	-5.03	106.56	113.30
30	R5	59	GLU	N-CA-C	5.03	117.09	108.90
2	XB	200	ILE	N-CA-C	5.03	116.53	108.89
13	XM	67	GLU	N-CA-C	5.02	121.50	110.80
39	YF	164	ARG	N-CA-C	-5.02	105.89	111.36
28	R3	54	VAL	N-CA-C	5.02	115.14	108.11
1	XA	992	U	P-O3'-C3'	5.02	127.73	120.20
13	XM	81	LEU	N-CA-C	-5.02	106.00	111.82
28	Y3	31	LEU	N-CA-C	-5.02	103.09	110.52
7	QG	8	GLU	N-CA-C	5.02	121.48	110.80
37	RD	237	GLU	CB-CA-C	5.01	117.91	109.48
46	YQ	10	ARG	N-CA-C	5.01	116.83	111.36
35	RA	2439	A	C2'-C3'-O3'	5.01	117.02	109.50
47	RR	67	LEU	N-CA-C	-5.01	107.12	113.18
51	RV	49	THR	CB-CA-C	5.01	120.03	110.17
13	XM	66	LEU	CA-C-N	5.01	131.11	121.54
13	XM	66	LEU	C-N-CA	5.01	131.11	121.54
35	RA	2447	G	P-O3'-C3'	5.00	127.71	120.20
50	RU	93	LYS	N-CA-C	-5.00	105.42	113.28
45	RP	38	GLN	N-CA-C	5.00	117.38	111.33

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	QB	12	GLU	Sidechain
10	QJ	79	ARG	Sidechain
24	QZ	50	HIS	Peptide
37	RD	33	LEU	Peptide
37	RD	35	LYS	Peptide
38	RE	79	ARG	Sidechain
40	RG	116	ASP	Peptide
40	RG	83	ARG	Sidechain
41	RH	116	GLU	Sidechain
41	RH	9	ILE	Peptide
42	RI	11	ASN	Peptide
42	RI	142	VAL	Peptide
42	RI	143	SER	Peptide
42	RI	82	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
47	RR	3	HIS	Peptide
51	RV	15	GLU	Sidechain
7	XG	111	ARG	Sidechain
8	XH	60	ARG	Sidechain
11	XK	96	ARG	Sidechain
37	YD	88	ARG	Sidechain
40	YG	72	ARG	Sidechain
41	YH	3	ARG	Sidechain
47	YR	57	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	32452	0	16383	245	0
1	XA	32389	0	16350	221	0
2	QB	1907	0	1958	31	0
2	XB	1915	0	1969	27	0
3	QC	1605	0	1668	13	0
3	XC	1605	0	1668	17	0
4	QD	1703	0	1767	32	0
4	XD	1703	0	1767	24	0
5	QE	1155	0	1213	12	0
5	XE	1155	0	1213	15	0
6	QF	843	0	857	13	0
6	XF	843	0	857	10	0
7	QG	1257	0	1296	10	0
7	XG	1257	0	1296	17	0
8	QH	1108	0	1165	21	0
8	XH	1108	0	1165	13	0
9	QI	1010	0	1037	17	0
9	XI	998	0	1024	20	0
10	QJ	801	0	849	11	0
10	XJ	777	0	816	18	0
11	QK	885	0	904	12	0
11	XK	864	0	881	9	0
12	QL	975	0	1062	11	0
12	XL	956	0	1046	13	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	QM	955	0	1021	27	0
13	XM	946	0	1008	16	0
14	QN	492	0	529	5	0
14	XN	492	0	529	12	0
15	QO	734	0	771	4	0
15	XO	729	0	768	4	0
16	QP	705	0	725	12	0
16	XP	705	0	725	6	0
17	QQ	834	0	904	9	0
17	XQ	834	0	904	12	0
18	QR	574	0	644	9	0
18	XR	574	0	644	12	0
19	QS	665	0	686	15	0
19	XS	656	0	666	9	0
20	QT	763	0	861	9	0
20	XT	763	0	861	15	0
21	QU	217	0	234	5	0
21	XU	217	0	234	7	0
22	QV	1640	0	837	4	0
22	XV	1640	0	837	3	0
23	QX	394	0	196	2	0
23	XX	394	0	196	4	0
24	QY	723	0	713	11	0
24	QZ	723	0	713	11	0
24	XY	723	0	713	9	0
24	XZ	723	0	713	7	0
25	R0	643	0	667	13	0
25	Y0	648	0	672	15	0
26	R1	737	0	813	6	0
26	Y1	763	0	848	18	0
27	R2	581	0	629	8	0
27	Y2	581	0	629	4	0
28	R3	469	0	518	5	0
28	Y3	469	0	518	5	0
29	R4	565	0	561	26	0
29	Y4	565	0	559	10	0
30	R5	459	0	476	11	0
30	Y5	459	0	480	6	0
31	R6	453	0	474	10	0
31	Y6	453	0	474	4	0
32	R7	409	0	454	3	0
32	Y7	418	0	467	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	R8	517	0	582	11	0
33	Y8	517	0	582	12	0
34	R9	307	0	337	10	0
34	Y9	307	0	336	5	0
35	RA	62266	0	31392	354	0
35	YA	61981	0	31243	341	0
36	RB	2576	0	1303	28	0
36	YB	2576	0	1305	19	0
37	RD	2115	0	2195	39	0
37	YD	2135	0	2221	19	0
38	RE	1568	0	1634	38	0
38	YE	1559	0	1617	25	0
39	RF	1585	0	1632	15	0
39	YF	1585	0	1632	25	0
40	RG	1474	0	1535	23	0
40	YG	1474	0	1535	20	0
41	RH	1336	0	1418	12	0
41	YH	1330	0	1407	18	0
42	RI	1131	0	1218	16	0
42	YI	1136	0	1223	9	0
43	RN	1104	0	1180	17	0
43	YN	1104	0	1180	15	0
44	RO	933	0	996	17	0
44	YO	933	0	996	16	0
45	RP	1145	0	1228	29	0
45	YP	1135	0	1212	17	0
46	RQ	1122	0	1179	27	0
46	YQ	1122	0	1179	20	0
47	RR	960	0	1021	12	0
47	YR	960	0	1021	11	0
48	RS	882	0	943	14	0
48	YS	882	0	943	15	0
49	RT	1141	0	1202	21	0
49	YT	1141	0	1202	14	0
50	RU	964	0	1022	19	0
50	YU	964	0	1022	22	0
51	RV	779	0	852	16	0
51	YV	779	0	852	26	0
52	RW	900	0	964	8	0
52	YW	900	0	964	16	0
53	RX	725	0	778	11	0
53	YX	725	0	778	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	RY	818	0	913	12	0
54	YY	818	0	913	5	0
55	RZ	1461	0	1493	17	0
55	YZ	1461	0	1493	27	0
56	ZA	74	0	51	2	0
56	ZB	74	0	51	7	0
57	QA	93	0	0	0	0
57	QD	1	0	0	0	0
57	QE	1	0	0	0	0
57	QV	3	0	0	0	0
57	QY	1	0	0	0	0
57	R0	2	0	0	0	0
57	R3	1	0	0	0	0
57	RA	302	0	0	0	0
57	RB	3	0	0	0	0
57	RD	2	0	0	0	0
57	RE	1	0	0	0	0
57	RN	1	0	0	0	0
57	RO	1	0	0	0	0
57	RP	1	0	0	0	0
57	RQ	4	0	0	0	0
57	RR	1	0	0	0	0
57	RY	1	0	0	0	0
57	XA	99	0	0	0	0
57	XE	1	0	0	0	0
57	XF	1	0	0	0	0
57	XL	1	0	0	0	0
57	XM	1	0	0	0	0
57	XV	4	0	0	0	0
57	Y0	2	0	0	0	0
57	Y1	1	0	0	0	0
57	Y3	1	0	0	0	0
57	Y5	1	0	0	0	0
57	Y9	1	0	0	0	0
57	YA	335	0	0	0	0
57	YB	3	0	0	0	0
57	YD	4	0	0	0	0
57	YE	5	0	0	0	0
57	YF	1	0	0	0	0
57	YG	1	0	0	0	0
57	YO	1	0	0	0	0
57	YP	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	YQ	5	0	0	0	0
57	YR	1	0	0	0	0
57	YV	1	0	0	0	0
58	QD	8	0	0	0	0
58	XD	8	0	0	0	0
59	QN	1	0	0	0	0
59	R4	1	0	0	0	0
59	R5	1	0	0	0	0
59	R6	1	0	0	0	0
59	R9	1	0	0	0	0
59	XN	1	0	0	0	0
59	Y4	1	0	0	0	0
59	Y6	1	0	0	0	0
All	All	295153	0	201057	2224	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (2224) 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)
51:YV:85:LYS:CG	51:YV:85:LYS:CD	1.86	1.53
51:YV:85:LYS:CG	51:YV:85:LYS:CB	1.82	1.50
1:XA:368:U:C5	1:XA:368:U:C6	2.05	1.45
51:YV:85:LYS:NZ	51:YV:85:LYS:CE	1.87	1.36
51:YV:85:LYS:CD	51:YV:85:LYS:CE	2.10	1.30
1:XA:368:U:C5	1:XA:368:U:C4	2.19	1.29
23:QX:20:A3P:C1'	23:QX:20:A3P:O4'	1.67	1.27
29:R4:39:CYS:C	29:R4:41:PRO:HD3	1.58	1.26
23:XX:20:A3P:C1'	23:XX:20:A3P:O4'	1.66	1.15
1:XA:368:U:C6	1:XA:368:U:N1	2.19	1.10
1:XA:368:U:N1	1:XA:368:U:C2	2.21	1.08
29:R4:39:CYS:O	29:R4:41:PRO:HD3	1.54	1.04
35:RA:1311:G:N2	35:RA:1603:A:H62	1.57	1.03
1:XA:368:U:C2	1:XA:368:U:N3	2.29	1.00
35:RA:1311:G:H21	35:RA:1603:A:N6	1.61	0.98
1:XA:368:U:C4	1:XA:368:U:N3	2.33	0.95
29:R4:18:CYS:HB3	29:R4:39:CYS:SG	2.07	0.94
29:R4:39:CYS:O	29:R4:39:CYS:SG	2.28	0.91
29:R4:39:CYS:O	29:R4:41:PRO:CD	2.18	0.90
35:YA:2141:G:H1	35:YA:2150:U:H3	1.20	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:1311:G:H21	35:RA:1603:A:H62	0.87	0.84
35:YA:2808:U:H3	35:YA:2892:A:H62	1.22	0.83
6:XF:46:ARG:HH22	18:XR:37:VAL:HG11	1.43	0.83
29:R4:39:CYS:C	29:R4:41:PRO:CD	2.50	0.81
29:R4:36:CYS:HB3	29:R4:39:CYS:HB3	1.63	0.80
29:R4:18:CYS:CB	29:R4:39:CYS:SG	2.71	0.78
51:RV:16:PRO:HD3	51:RV:99:ILE:HD11	1.64	0.78
35:RA:676:A:H8	35:RA:2069:G:H21	1.31	0.77
33:Y8:26:LYS:HG2	33:Y8:48:PHE:HD2	1.52	0.74
51:RV:40:LEU:HB2	51:RV:46:VAL:HG12	1.70	0.73
35:YA:676:A:H8	35:YA:2069:G:H21	1.35	0.73
1:QA:663:A:H61	1:QA:742:G:H1	1.37	0.73
35:RA:2141:G:H1	35:RA:2150:U:H3	1.35	0.73
51:RV:15:GLU:HG3	51:RV:16:PRO:HD2	1.72	0.70
35:RA:2584:U:H5'	56:ZA:3:PPU:H103	1.73	0.70
24:QY:7:GLU:OE1	24:QY:7:GLU:N	2.18	0.70
35:RA:1857:G:H21	35:RA:1885:A:H62	1.39	0.70
13:XM:94:ARG:HH12	35:YA:887:A:H5'	1.57	0.69
42:RI:82:ARG:CZ	42:RI:82:ARG:NH1	2.54	0.69
1:XA:1357:A:H61	1:XA:1365:G:H1	1.38	0.69
56:ZA:3:PPU:H93	56:ZA:3:PPU:N7	2.06	0.69
24:QY:7:GLU:H	24:QY:7:GLU:CD	2.01	0.69
29:R4:36:CYS:HB3	29:R4:39:CYS:CB	2.23	0.69
32:Y7:11:LYS:HE2	35:YA:686:G:H5''	1.73	0.69
56:ZB:3:PPU:H93	56:ZB:3:PPU:N7	2.07	0.69
46:RQ:24:GLY:HA2	46:RQ:67:ARG:HH21	1.58	0.69
46:RQ:75:THR:HA	46:RQ:89:ASN:HA	1.75	0.68
33:R8:25:MET:HG3	45:RP:64:LYS:HB3	1.75	0.68
1:XA:1086:U:H3	1:XA:1099:G:H22	1.39	0.68
38:RE:9:VAL:HB	38:RE:25:VAL:HG23	1.75	0.68
35:YA:67:U:H3	35:YA:74:A:H2	1.42	0.68
46:RQ:66:ILE:HA	46:RQ:104:PHE:HA	1.74	0.68
36:RB:118:G:HO2'	36:RB:119:A:C4'	2.07	0.68
49:RT:36:GLU:HG3	49:RT:41:ARG:HE	1.58	0.68
3:QC:150:LYS:HE3	3:QC:167:TRP:HE1	1.57	0.67
4:QD:154:ASN:HA	4:QD:159:ARG:HH21	1.59	0.67
1:XA:452:A:H62	1:XA:480:U:H3	1.42	0.67
9:QI:25:LYS:N	9:QI:60:ASP:OD1	2.28	0.67
36:RB:3:C:N4	36:RB:118:G:H1	1.93	0.67
35:YA:1053:C:H42	35:YA:1106:G:H1	1.40	0.67
29:Y4:16:CYS:SG	29:Y4:17:GLY:N	2.66	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:259:G:H21	35:RA:621:A:H8	1.41	0.67
38:RE:11:MET:HG2	38:RE:24:THR:HG22	1.76	0.67
1:XA:677:U:H3	1:XA:713:G:H22	1.42	0.67
13:XM:99:ARG:HB2	13:XM:101:GLN:HE22	1.60	0.67
36:YB:22:U:H3	36:YB:61:G:H1	1.42	0.66
3:XC:70:VAL:HG12	3:XC:72:LYS:H	1.61	0.66
6:XF:9:VAL:HB	6:XF:87:ARG:HB2	1.78	0.66
33:Y8:6:THR:HG22	33:Y8:63:PRO:HD2	1.77	0.66
4:QD:18:LYS:NZ	4:QD:31:CYS:SG	2.60	0.65
45:YP:126:VAL:HG12	45:YP:146:VAL:HB	1.75	0.65
35:YA:845:G:H21	35:YA:933:A:H61	1.43	0.65
38:YE:9:VAL:HB	38:YE:25:VAL:HG23	1.78	0.65
35:RA:68:G:H21	35:RA:74:A:H5'	1.62	0.65
38:RE:25:VAL:HG12	38:RE:183:LEU:HD22	1.77	0.65
43:RN:22:THR:OG1	43:RN:23:LEU:N	2.30	0.65
35:YA:994:C:O2	51:YV:10:LYS:NZ	2.30	0.65
35:RA:845:G:H21	35:RA:933:A:H61	1.44	0.65
8:XH:10:LEU:HD22	8:XH:83:ILE:HD11	1.79	0.65
2:QB:9:GLU:HA	2:QB:12:GLU:HG2	1.79	0.65
1:XA:1157:A:C2	1:XA:1178:G:N2	2.64	0.65
41:YH:4:ILE:HG22	41:YH:69:ARG:HD2	1.78	0.65
41:YH:54:ARG:HH21	41:YH:57:ASP:HA	1.62	0.64
1:XA:1030:C:N4	1:XA:1032:A:N7	2.46	0.64
4:XD:62:GLN:HE22	4:XD:65:ARG:HH21	1.45	0.64
14:QN:23:ARG:NH1	14:QN:28:GLY:O	2.30	0.64
20:QT:30:LYS:HZ3	20:QT:72:LEU:HD21	1.63	0.64
34:R9:13:LYS:HE3	34:R9:28:GLU:HG2	1.79	0.64
55:YZ:91:LEU:HD23	55:YZ:130:PRO:HB3	1.78	0.64
1:XA:991:U:H3	1:XA:1213:A:H62	1.45	0.64
1:XA:1238:A:H62	1:XA:1301:U:H3	1.46	0.64
45:YP:86:LYS:HB3	45:YP:118:GLY:HA3	1.77	0.64
35:RA:2777:G:H5''	35:RA:2778:A:H5'	1.80	0.64
5:QE:81:GLU:HG3	5:QE:90:VAL:HG12	1.80	0.64
35:YA:1899:G:H21	35:YA:1902:C:H41	1.46	0.64
35:RA:2303:G:N3	40:RG:132:ASN:ND2	2.46	0.64
50:YU:92:ARG:HD2	51:YV:11:GLN:HB2	1.79	0.64
1:QA:782:A:H62	1:QA:800:G:H21	1.46	0.64
38:RE:16:ARG:NH2	38:RE:171:GLU:OE2	2.31	0.64
1:QA:1422:G:H5''	44:RO:48:PRO:HB3	1.80	0.63
36:RB:3:C:C4	36:RB:118:G:N1	2.57	0.63
2:QB:84:GLU:HB3	2:QB:219:VAL:HG21	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:RE:24:THR:HG23	38:RE:186:GLY:HA2	1.79	0.63
44:YO:104:ARG:NH1	49:YT:36:GLU:OE1	2.32	0.63
35:RA:2245:U:H5'	35:RA:2246:G:H5'	1.79	0.63
33:Y8:30:ARG:HH21	45:YP:63:PRO:HB2	1.64	0.63
35:YA:974:G:O2'	35:YA:975:G:N7	2.29	0.63
35:YA:1009:A:OP2	43:YN:37:LYS:NZ	2.30	0.63
38:YE:201:THR:HG22	38:YE:203:LYS:H	1.64	0.63
50:YU:92:ARG:NH1	51:YV:11:GLN:O	2.32	0.63
41:RH:101:ARG:NH2	41:RH:121:ILE:O	2.30	0.63
13:QM:23:TYR:HB3	13:QM:67:GLU:HG2	1.81	0.63
2:XB:87:ARG:HH21	2:XB:219:VAL:HB	1.63	0.62
4:XD:166:LYS:HB2	4:XD:178:VAL:HG11	1.81	0.62
1:QA:4:U:O2	8:QH:105:ARG:NH1	2.31	0.62
35:RA:993:G:OP1	50:RU:50:ARG:NH2	2.32	0.62
24:QY:5:TRP:HB2	24:QZ:3:LEU:HB2	1.81	0.62
36:RB:30:C:H1'	36:RB:57:A:H61	1.64	0.62
36:RB:118:G:O2'	36:RB:119:A:O4'	2.18	0.62
46:YQ:136:ALA:HB1	55:YZ:52:SER:HB3	1.80	0.62
1:QA:692:U:OP2	11:QK:26:ASN:ND2	2.33	0.62
17:QQ:66:SER:O	17:QQ:70:ARG:NH1	2.32	0.62
26:R1:49:VAL:HG11	26:R1:70:VAL:HG11	1.82	0.62
51:RV:62:LEU:HD11	51:RV:95:LEU:HB2	1.82	0.62
2:XB:231:GLU:HG3	2:XB:233:SER:H	1.65	0.62
35:RA:17:G:H4'	50:RU:25:TRP:HE1	1.65	0.62
29:Y4:1:MET:SD	40:YG:98:ARG:NH1	2.72	0.62
39:RF:153:SER:HB2	39:RF:190:GLU:H	1.65	0.62
49:RT:51:ARG:HG2	49:RT:98:LYS:HD2	1.81	0.62
35:YA:345:A:O2'	35:YA:346:A:N7	2.33	0.62
26:R1:21:ARG:NH2	35:RA:2079:U:OP1	2.33	0.62
55:RZ:52:SER:O	55:RZ:54:HIS:N	2.31	0.62
7:XG:79:ARG:HE	7:XG:84:ASN:HB2	1.64	0.62
35:YA:727:A:OP1	35:YA:1431:U:O2'	2.18	0.62
12:QL:114:LYS:O	12:QL:117:ARG:NH1	2.33	0.61
1:QA:1306:A:N6	1:QA:1331:G:O2'	2.33	0.61
42:RI:88:ILE:HG22	42:RI:90:GLY:H	1.64	0.61
1:XA:674:G:H2'	1:XA:675:A:H8	1.65	0.61
35:RA:67:U:H3	35:RA:74:A:H2	1.47	0.61
31:R6:25:LYS:NZ	31:R6:51:GLU:OE2	2.34	0.61
35:RA:956:G:OP2	46:RQ:14:ARG:NH2	2.33	0.61
19:XS:41:VAL:HG12	19:XS:43:GLU:H	1.66	0.61
35:YA:2304:G:H22	35:YA:2312:U:H3	1.47	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:QB:16:HIS:HE1	2:QB:209:ARG:HG2	1.65	0.61
35:RA:2618:G:H21	38:RE:150:VAL:HG21	1.65	0.61
54:RY:102:CYS:SG	54:RY:103:GLY:N	2.74	0.61
47:YR:38:VAL:HG12	47:YR:112:ALA:HB2	1.83	0.61
25:Y0:55:ARG:NH1	35:YA:2364:C:OP1	2.34	0.61
35:YA:2010:G:H5''	52:YW:42:ARG:HB2	1.83	0.61
38:YE:2:LYS:HB2	38:YE:95:ILE:HD12	1.83	0.61
13:XM:6:GLY:O	40:YG:115:ARG:NH1	2.34	0.61
1:QA:1130:A:O2'	9:QI:3:GLN:NE2	2.34	0.60
44:RO:104:ARG:HH21	49:RT:34:VAL:HG11	1.66	0.60
50:RU:92:ARG:HD2	51:RV:11:GLN:HB2	1.82	0.60
12:XL:117:ARG:HB2	12:XL:122:THR:HB	1.82	0.60
11:QK:124:LYS:O	11:QK:127:LYS:NZ	2.34	0.60
55:RZ:135:GLU:HG2	55:RZ:136:PHE:HD1	1.66	0.60
4:XD:187:ARG:NH2	4:XD:193:ASP:OD2	2.35	0.60
40:YG:37:VAL:HG22	40:YG:159:VAL:HG12	1.84	0.60
55:YZ:119:GLU:O	55:YZ:122:ARG:NH1	2.34	0.60
18:QR:31:LEU:HD12	18:QR:66:LEU:HB2	1.82	0.60
29:R4:59:PHE:HA	29:R4:62:ARG:HG2	1.82	0.60
35:RA:1451:C:O2'	35:RA:1457:A:N6	2.34	0.60
9:QI:28:VAL:HB	9:QI:63:ILE:HG13	1.84	0.60
10:XJ:10:GLY:HA3	10:XJ:16:LEU:HD21	1.84	0.60
1:QA:217:C:O2'	1:QA:466:C:N4	2.34	0.60
35:RA:1139:G:O2'	35:RA:1143:A:N6	2.32	0.60
33:Y8:11:LYS:NZ	33:Y8:65:GLU:OE2	2.33	0.60
35:YA:1992:G:N2	35:YA:1996:C:O2'	2.35	0.60
41:RH:164:TYR:HB2	41:RH:167:GLU:HB2	1.82	0.60
1:QA:1252:A:H61	1:QA:1285:A:H61	1.48	0.60
6:QF:10:LEU:HB2	6:QF:59:TYR:HB3	1.84	0.60
40:RG:29:TRP:O	40:RG:33:ARG:NH1	2.35	0.60
39:YF:120:GLU:OE2	45:YP:1:MET:N	2.34	0.60
35:RA:265:A:N6	35:RA:427:U:O2'	2.34	0.60
35:RA:2393:A:H4'	45:RP:62:LEU:H	1.67	0.60
49:RT:19:LEU:HD22	49:RT:86:ILE:HG22	1.84	0.60
3:XC:84:ILE:HG12	3:XC:88:ARG:HE	1.67	0.60
9:XI:48:GLU:OE1	9:XI:51:ARG:NH2	2.35	0.60
1:QA:674:G:H2'	1:QA:675:A:H8	1.67	0.60
30:R5:19:ARG:NH2	35:RA:1264:G:OP1	2.35	0.60
36:RB:118:G:H2'	36:RB:119:A:O4'	2.02	0.60
35:YA:1482:U:H3	35:YA:1512:G:H1	1.48	0.60
35:YA:2135:A:H62	35:YA:2156:G:H21	1.50	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:YD:17:THR:HB	37:YD:205:VAL:H	1.66	0.60
35:RA:959:A:N3	35:RA:2457:U:O2'	2.33	0.59
22:XV:76:A:O3'	35:YA:2602:A:N6	2.35	0.59
35:RA:587:C:OP2	45:RP:21:ARG:NH1	2.32	0.59
35:RA:1265:A:H61	35:RA:2013:A:H5''	1.67	0.59
50:RU:95:LEU:HD13	51:RV:4:ILE:HD13	1.82	0.59
24:XY:16:TRP:NE1	24:XY:80:CYS:O	2.34	0.59
35:RA:1900:A:H1'	35:RA:1970:A:H2'	1.83	0.59
12:XL:39:VAL:HB	12:XL:57:LYS:HB3	1.83	0.59
35:YA:2305:A:H5''	40:YG:134:GLY:HA3	1.84	0.59
1:QA:1086:U:H3	1:QA:1099:G:H22	1.51	0.59
3:QC:153:VAL:HG22	3:QC:198:VAL:HG12	1.85	0.59
35:RA:2010:G:H5''	52:RW:42:ARG:HB2	1.84	0.59
37:RD:25:THR:HG21	37:RD:81:ALA:HA	1.84	0.59
54:RY:83:THR:OG1	54:RY:84:ARG:N	2.35	0.59
7:XG:111:ARG:NH2	7:XG:126:ASP:OD2	2.36	0.59
15:XO:16:ALA:HB1	15:XO:21:ASP:HB3	1.83	0.59
48:YS:106:ARG:NH1	48:YS:107:GLU:OE2	2.35	0.59
36:RB:118:G:O2'	36:RB:119:A:C4'	2.51	0.59
1:QA:422:C:O2'	1:QA:423:G:N2	2.35	0.59
1:QA:664:G:H22	1:QA:741:G:H1	1.50	0.59
35:RA:768:G:O2'	35:RA:1379:A:N6	2.33	0.59
1:XA:452:A:OP1	16:XP:43:LYS:NZ	2.36	0.59
19:XS:50:ALA:HB1	19:XS:57:HIS:HB3	1.85	0.59
35:YA:2789:C:O2'	35:YA:2893:G:N2	2.33	0.59
31:R6:26:ASN:ND2	31:R6:29:ASN:OD1	2.34	0.59
35:RA:1138:G:H21	43:RN:106:MET:HE3	1.68	0.59
38:RE:14:ILE:HG21	38:RE:173:VAL:HG11	1.84	0.59
46:RQ:75:THR:HG22	46:RQ:89:ASN:HB2	1.83	0.59
43:YN:73:THR:HB	43:YN:82:LEU:HD11	1.84	0.59
50:YU:92:ARG:HD3	50:YU:94:ASN:HB3	1.85	0.59
5:QE:80:ILE:HG22	5:QE:91:LEU:HB2	1.85	0.58
1:XA:413:G:N2	1:XA:429:U:OP2	2.35	0.58
10:XJ:49:VAL:HG23	14:XN:41:ARG:HB2	1.84	0.58
26:Y1:73:LEU:HD21	26:Y1:98:LEU:HD23	1.83	0.58
35:YA:495:G:N3	52:YW:61:ASN:ND2	2.51	0.58
51:YV:69:LYS:HE2	51:YV:86:GLY:HA3	1.85	0.58
1:XA:1191:A:OP1	3:XC:4:LYS:NZ	2.37	0.58
1:XA:1454:G:OP1	20:XT:39:LYS:NZ	2.34	0.58
1:XA:1540:U:O2'	18:XR:55:ARG:NH2	2.36	0.58
27:Y2:65:ASN:ND2	35:YA:72:U:O4	2.36	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YA:1689:A:H62	35:YA:1698:A:H2	1.52	0.58
35:YA:2134:A:N7	35:YA:2157:G:O2'	2.37	0.58
2:QB:185:ILE:HG22	2:QB:199:TYR:HB2	1.86	0.58
35:RA:2032:G:H22	35:RA:2572:A:H5'	1.68	0.58
1:XA:1178:G:OP2	9:XI:93:ARG:NH2	2.36	0.58
4:XD:23:GLY:N	4:XD:26:CYS:SG	2.76	0.58
35:YA:1138:G:H21	43:YN:106:MET:HE3	1.68	0.58
35:YA:1824:G:N3	37:YD:254:THR:OG1	2.36	0.58
40:YG:118:ARG:HG3	40:YG:181:ARG:HD3	1.84	0.58
1:QA:1191:A:H5''	3:QC:4:LYS:HE3	1.84	0.58
1:QA:1318:A:H4'	19:QS:11:VAL:HG11	1.85	0.58
25:R0:48:GLY:O	25:R0:80:HIS:ND1	2.37	0.58
43:RN:54:VAL:HB	43:RN:122:VAL:HG12	1.85	0.58
45:RP:19:VAL:HG23	45:RP:27:HIS:HB3	1.86	0.58
35:RA:1812:A:H4'	37:RD:46:GLN:HE22	1.67	0.58
37:RD:43:ARG:HB2	37:RD:54:ARG:HB2	1.85	0.58
25:R0:23:VAL:HG21	35:RA:857:C:H4'	1.85	0.58
2:XB:118:LEU:HB3	2:XB:142:LEU:HD13	1.86	0.58
17:XQ:88:TYR:OH	17:XQ:92:ARG:NH1	2.36	0.58
35:YA:1667:G:O2'	35:YA:1669:A:N6	2.36	0.58
55:YZ:109:ALA:HB3	55:YZ:145:GLU:HG2	1.86	0.58
17:XQ:15:MET:HE1	17:XQ:43:LEU:HD22	1.85	0.58
24:XY:4:ILE:HB	24:XY:76:LEU:HA	1.85	0.58
35:YA:1980:G:O2'	35:YA:1982:C:OP2	2.22	0.58
39:YF:143:ALA:HB1	39:YF:148:LEU:HB2	1.86	0.58
1:QA:958:A:OP1	24:QZ:36:ARG:NH1	2.37	0.57
29:R4:16:CYS:SG	29:R4:36:CYS:HB2	2.44	0.57
6:QF:9:VAL:HB	6:QF:87:ARG:HB2	1.84	0.57
31:R6:6:ARG:NH2	35:RA:2285:C:OP2	2.37	0.57
35:RA:586:A:H5'	39:RF:89:VAL:HG11	1.86	0.57
36:YB:30:C:H1'	36:YB:57:A:H61	1.69	0.57
1:QA:316:G:OP2	1:QA:351:G:O2'	2.22	0.57
17:QQ:88:TYR:OH	17:QQ:92:ARG:NH2	2.37	0.57
35:YA:583:G:OP2	50:YU:10:ARG:NH1	2.37	0.57
53:YX:53:LYS:NZ	53:YX:55:ASN:OD1	2.36	0.57
1:QA:861:G:HO2'	1:QA:874:G:HO2'	1.51	0.57
11:QK:58:PRO:HB2	11:QK:93:GLN:HG3	1.86	0.57
29:R4:23:GLU:OE2	40:RG:6:ALA:N	2.32	0.57
49:YT:51:ARG:HG2	49:YT:98:LYS:HD2	1.86	0.57
25:R0:36:ILE:HA	25:R0:60:PHE:HA	1.87	0.57
38:RE:34:VAL:HG12	38:RE:72:VAL:HG21	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:4:U:O2	8:XH:105:ARG:NH1	2.37	0.57
36:YB:50:G:OP2	48:YS:62:LYS:NZ	2.37	0.57
42:YI:80:PRO:HB2	42:YI:146:ALA:HB2	1.87	0.57
1:QA:1030:C:N4	35:YA:2167:U:O2'	2.38	0.57
34:R9:6:SER:HB3	35:RA:2466:C:H5''	1.86	0.57
1:XA:811:C:O2'	1:XA:901:A:N1	2.38	0.57
1:XA:951:G:OP2	13:XM:102:ARG:NH1	2.37	0.57
35:YA:269:U:H3	35:YA:370:G:H1	1.52	0.57
1:QA:878:G:H5'	8:QH:89:PRO:HG2	1.87	0.57
22:QV:19:G:O6	40:RG:83:ARG:NH2	2.37	0.57
31:R6:8:LYS:HG3	31:R6:54:ILE:HD13	1.87	0.57
47:RR:75:LEU:HA	47:RR:78:LYS:HB3	1.86	0.57
1:XA:972:C:H1'	10:XJ:55:LYS:HE2	1.87	0.57
13:XM:3:ARG:NH1	13:XM:8:GLU:OE2	2.37	0.57
38:YE:67:PHE:HZ	38:YE:78:LEU:HD11	1.70	0.57
46:YQ:13:GLN:O	46:YQ:72:LYS:NZ	2.37	0.57
1:QA:974:A:OP2	14:QN:41:ARG:NH1	2.38	0.57
35:RA:727:A:OP1	35:RA:1431:U:O2'	2.21	0.57
35:RA:1992:G:N2	35:RA:1996:C:O2'	2.37	0.57
51:RV:52:VAL:HG21	51:RV:55:ALA:HB3	1.86	0.57
35:YA:987:G:O2'	35:YA:1000:A:N3	2.34	0.57
27:R2:22:GLU:OE2	27:R2:68:ARG:NH2	2.37	0.57
44:RO:2:ILE:HB	44:RO:33:ALA:HB3	1.85	0.57
4:XD:57:ARG:NH2	4:XD:205:GLU:OE2	2.38	0.57
1:QA:1304:G:OP1	21:QU:2:GLY:N	2.38	0.57
34:R9:1:MET:HG2	35:RA:2477:C:H2'	1.86	0.57
35:RA:862:G:OP1	46:RQ:18:LYS:NZ	2.38	0.57
35:RA:995:C:H5''	50:RU:54:LYS:HG2	1.85	0.57
35:RA:2848:G:O2'	35:RA:2867:G:N2	2.34	0.57
36:RB:104:A:OP1	55:RZ:72:ARG:NH2	2.38	0.57
40:RG:82:LEU:HD12	40:RG:88:ILE:HG21	1.86	0.57
35:YA:116:C:O2'	35:YA:126:A:N3	2.36	0.57
1:QA:672:U:H2'	1:QA:673:G:H8	1.69	0.56
4:QD:60:GLU:HG3	4:QD:202:LEU:HD12	1.87	0.56
45:YP:38:GLN:HB3	45:YP:45:LEU:HB3	1.86	0.56
12:XL:47:LYS:O	24:XY:44:LYS:NZ	2.37	0.56
1:QA:774:G:OP1	37:RD:202:LYS:NZ	2.38	0.56
8:XH:51:VAL:HG11	8:XH:60:ARG:HG3	1.87	0.56
30:Y5:49:CYS:SG	30:Y5:50:GLY:N	2.78	0.56
35:YA:184:C:O2'	35:YA:217:G:N3	2.38	0.56
36:YB:37:C:O2	48:YS:95:HIS:NE2	2.38	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:YE:8:LYS:NZ	38:YE:192:ASN:OD1	2.38	0.56
35:RA:1102:C:H2'	35:RA:1103:A:H8	1.70	0.56
35:RA:1138:G:O2'	43:RN:102:ALA:O	2.23	0.56
1:XA:664:G:H22	1:XA:741:G:H1	1.51	0.56
35:YA:674:G:H1'	39:YF:74:ARG:HD3	1.88	0.56
49:YT:106:SER:HA	49:YT:110:ILE:HD11	1.87	0.56
55:YZ:126:VAL:HG12	55:YZ:163:LEU:HA	1.86	0.56
47:RR:86:ARG:NH2	47:RR:118:GLU:OXT	2.39	0.56
52:RW:18:ARG:HD2	52:RW:76:VAL:HB	1.87	0.56
4:XD:10:ARG:HG3	4:XD:40:PRO:HG3	1.86	0.56
5:XE:102:ALA:HB1	5:XE:106:PRO:HG2	1.88	0.56
9:XI:10:ARG:NH1	9:XI:75:ASP:OD2	2.38	0.56
35:YA:15:G:H1	35:YA:525:U:H3	1.53	0.56
35:YA:807:U:O2'	35:YA:2060:A:N1	2.38	0.56
50:YU:90:VAL:HG22	51:YV:38:LEU:HB3	1.85	0.56
13:QM:23:TYR:HD2	13:QM:67:GLU:HA	1.71	0.56
35:RA:2148:G:H2'	35:RA:2149:G:H8	1.69	0.56
1:XA:544:G:OP1	4:XD:59:ARG:NH2	2.38	0.56
26:Y1:91:LYS:O	26:Y1:95:LEU:HG	2.05	0.56
35:YA:996:A:OP2	50:YU:92:ARG:NH2	2.39	0.56
51:YV:85:LYS:CG	51:YV:85:LYS:CA	2.79	0.56
55:YZ:102:LEU:HD21	55:YZ:155:LEU:HD11	1.87	0.56
8:QH:34:GLU:OE1	8:QH:37:ARG:NH2	2.39	0.56
25:R0:19:LYS:NZ	35:RA:2261:C:OP1	2.35	0.56
36:RB:9:G:H1	36:RB:111:U:H3	1.52	0.56
38:RE:119:ARG:NH1	38:RE:159:HIS:O	2.39	0.56
39:YF:116:ASP:OD1	39:YF:119:ARG:NH2	2.38	0.56
52:YW:24:ILE:HD13	52:YW:36:LEU:HD11	1.88	0.56
1:QA:686:U:H1'	11:QK:42:TRP:HE1	1.71	0.56
1:XA:1247:U:H3	1:XA:1290:G:H1	1.53	0.56
10:XJ:45:ARG:HB3	10:XJ:65:LEU:HB3	1.87	0.56
48:YS:27:SER:HA	48:YS:88:ASP:HB3	1.87	0.56
49:YT:128:GLU:HG3	49:YT:129:ARG:HG3	1.88	0.56
1:QA:1236:A:H4'	1:QA:1304:G:H4'	1.86	0.56
1:QA:1320:C:O2	19:QS:36:ARG:NH2	2.39	0.56
35:RA:2445:G:OP1	39:RF:74:ARG:NH1	2.39	0.56
1:XA:405:U:O4	4:XD:2:GLY:N	2.39	0.56
7:XG:78:ARG:NH1	7:XG:154:TYR:O	2.38	0.56
41:YH:9:ILE:HD11	41:YH:69:ARG:HG2	1.88	0.56
24:QZ:57:SER:HB2	24:QZ:67:VAL:HG12	1.88	0.56
35:RA:629:G:N3	35:RA:639:U:O2'	2.39	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:958:U:OP2	46:RQ:14:ARG:NH1	2.39	0.56
35:RA:1782:C:H1'	35:RA:2609:U:H5''	1.87	0.56
35:RA:1817:G:OP1	37:RD:88:ARG:NH2	2.39	0.56
9:XI:26:VAL:HG12	9:XI:61:ALA:HB3	1.87	0.56
35:YA:768:G:O2'	35:YA:1379:A:N6	2.39	0.56
1:QA:811:C:O2'	1:QA:901:A:N1	2.38	0.55
13:QM:58:GLU:O	13:QM:62:ASN:HB2	2.06	0.55
52:RW:86:LEU:HD22	52:RW:96:ILE:HD11	1.87	0.55
33:R8:52:LYS:H	33:R8:52:LYS:HD3	1.70	0.55
35:RA:2751:G:OP1	35:RA:2751:G:N2	2.37	0.55
26:Y1:92:LYS:NZ	26:Y1:96:LYS:NZ	2.55	0.55
32:Y7:35:ARG:HG3	32:Y7:42:LEU:HD21	1.88	0.55
1:QA:403:C:OP2	4:QD:74:GLN:NE2	2.40	0.55
1:QA:957:U:OP1	19:QS:81:ARG:NH2	2.39	0.55
44:RO:80:ASP:OD2	49:RT:64:ARG:NH2	2.40	0.55
55:YZ:108:PRO:HB3	55:YZ:144:LEU:HB2	1.87	0.55
35:RA:987:G:O2'	35:RA:1000:A:N3	2.37	0.55
35:RA:1858:G:O2'	35:RA:1884:A:N6	2.39	0.55
35:RA:2472:G:H5'	35:RA:2473:U:H5''	1.89	0.55
35:YA:964:C:O2'	35:YA:2273:A:N3	2.38	0.55
35:YA:1139:G:O2'	35:YA:1143:A:N6	2.40	0.55
35:YA:2495:G:H5''	46:YQ:82:ARG:HG2	1.88	0.55
52:YW:22:ASP:OD1	52:YW:25:ARG:NH1	2.39	0.55
2:QB:109:SER:O	2:QB:113:HIS:ND1	2.39	0.55
42:RI:4:ILE:HG12	42:RI:18:VAL:HG12	1.88	0.55
1:QA:186(B):C:H2'	1:QA:186(C):G:H8	1.70	0.55
35:RA:521:G:H2'	35:RA:522:G:H8	1.72	0.55
35:RA:1250:G:OP2	45:RP:18:ARG:NH2	2.40	0.55
48:RS:18:ILE:HG13	48:RS:88:ASP:HA	1.88	0.55
26:Y1:93:GLU:O	26:Y1:97:LEU:HD13	2.06	0.55
35:YA:270(E):G:H1	35:YA:270(U):C:H42	1.54	0.55
35:YA:1654:A:O2'	38:YE:113:PHE:O	2.24	0.55
35:RA:1565:C:OP1	37:RD:4:LYS:NZ	2.37	0.55
35:YA:2749:A:H5''	41:YH:3:ARG:HE	1.72	0.55
53:YX:55:ASN:HB2	53:YX:80:ILE:HG23	1.87	0.55
1:QA:112:G:OP2	16:QP:27:LYS:NZ	2.39	0.55
35:RA:665:C:H2'	35:RA:666:G:H8	1.71	0.55
35:RA:1339:G:H5''	53:RX:16:LYS:HD3	1.88	0.55
2:XB:88:ALA:HB2	2:XB:219:VAL:HG13	1.89	0.55
24:XY:73:ASP:OD1	24:XY:73:ASP:N	2.40	0.55
35:YA:2130:U:H3	35:YA:2158:A:H1'	1.71	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:547:A:OP1	4:QD:73:ARG:NH2	2.40	0.55
1:QA:1119:C:H2'	1:QA:1120:G:H8	1.71	0.55
35:RA:39:C:O2	39:RF:46:ARG:NH2	2.40	0.55
35:YA:1102:C:H2'	35:YA:1103:A:H8	1.72	0.55
35:YA:2245:U:H5''	35:YA:2246:G:H5'	1.89	0.55
48:YS:56:LEU:HD12	48:YS:69:VAL:HG23	1.88	0.55
35:RA:2291:U:O2'	35:RA:2374:C:O2	2.25	0.55
35:RA:2816:C:O2	35:RA:2883:A:O2'	2.25	0.55
41:RH:56:SER:OG	41:RH:57:ASP:N	2.39	0.55
20:XT:85:MET:HA	20:XT:88:VAL:HG22	1.89	0.55
25:Y0:51:VAL:HG21	25:Y0:79:VAL:HG23	1.89	0.55
1:QA:405:U:O4	4:QD:2:GLY:N	2.40	0.54
20:QT:89:ARG:HD2	20:QT:104:LEU:HD11	1.89	0.54
19:XS:11:VAL:HG12	19:XS:13:ASP:H	1.72	0.54
35:YA:859:G:N2	35:YA:917:A:OP2	2.40	0.54
1:QA:544:G:OP1	4:QD:59:ARG:NH2	2.38	0.54
44:RO:25:LEU:HB2	44:RO:38:VAL:HG13	1.88	0.54
25:Y0:77:ARG:NH2	35:YA:857:C:OP2	2.40	0.54
29:Y4:48:ARG:NH2	29:Y4:51:ASP:OD2	2.37	0.54
47:YR:28:LEU:HD23	47:YR:48:VAL:HG21	1.88	0.54
30:R5:16:ARG:NH2	35:RA:517:C:OP1	2.40	0.54
35:RA:392:C:H5''	35:RA:409:C:H5''	1.89	0.54
46:RQ:27:VAL:N	46:RQ:138:ASP:OD2	2.40	0.54
1:XA:1357:A:N6	1:XA:1365:G:H1	2.04	0.54
10:XJ:61:GLU:HB2	14:XN:58:LYS:HE2	1.88	0.54
35:YA:1901:A:OP2	37:YD:255:LYS:NZ	2.37	0.54
38:YE:101:ARG:HH21	38:YE:171:GLU:HB2	1.72	0.54
1:QA:552:U:H2'	1:QA:553:A:H8	1.73	0.54
1:QA:963:G:H21	10:QJ:55:LYS:HG2	1.72	0.54
2:QB:16:HIS:CE1	2:QB:209:ARG:HG2	2.42	0.54
6:QF:3:ARG:NH1	6:QF:66:GLU:OE1	2.39	0.54
7:QG:28:ASN:HA	7:QG:31:MET:HE3	1.89	0.54
13:QM:88:ARG:HG2	13:QM:98:VAL:HB	1.89	0.54
26:R1:18:ILE:HG12	26:R1:37:ILE:HG12	1.89	0.54
1:XA:1304:G:OP1	21:XU:2:GLY:N	2.40	0.54
3:XC:20:SER:HB2	3:XC:40:ARG:HH22	1.72	0.54
8:XH:34:GLU:OE1	8:XH:37:ARG:NH2	2.41	0.54
35:YA:2303:G:N3	40:YG:132:ASN:ND2	2.55	0.54
1:QA:452:A:H62	1:QA:480:U:H3	1.55	0.54
1:QA:1119:C:OP1	9:QI:83:ARG:NH2	2.40	0.54
29:R4:56:VAL:O	29:R4:60:GLN:NE2	2.40	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:RD:18:VAL:HA	37:RD:211:ARG:HH22	1.73	0.54
10:XJ:51:ARG:HB2	10:XJ:60:ARG:HA	1.89	0.54
26:Y1:76:ARG:HH22	26:Y1:97:LEU:HB3	1.72	0.54
35:YA:997:G:H5'	50:YU:93:LYS:HD2	1.89	0.54
45:YP:95:VAL:HB	45:YP:125:VAL:HG12	1.89	0.54
1:QA:218:C:H5'	1:QA:466:C:H42	1.73	0.54
1:QA:262:A:H5''	20:QT:76:ALA:HB2	1.88	0.54
8:QH:106:GLY:O	8:QH:122:ARG:NH2	2.40	0.54
34:R9:25:VAL:HB	34:R9:34:GLN:HB2	1.89	0.54
1:XA:1251:A:N3	1:XA:1369:C:O2'	2.37	0.54
35:YA:219:G:N3	35:YA:234:C:O2'	2.40	0.54
1:QA:701:C:O2'	1:QA:703:G:N3	2.41	0.54
1:QA:1240:U:OP1	7:QG:119:ARG:NH2	2.41	0.54
35:RA:2547:U:O2	44:RO:23:ARG:NH2	2.41	0.54
1:XA:1502:A:H2	1:XA:1505:G:H1	1.54	0.54
2:XB:70:PHE:HD1	2:XB:163:PHE:HB3	1.73	0.54
39:YF:135:LYS:HB2	39:YF:138:GLU:HG3	1.90	0.54
41:YH:5:GLY:HA2	41:YH:69:ARG:HG3	1.88	0.54
47:YR:24:GLN:HG3	47:YR:44:LEU:HD13	1.89	0.54
1:QA:380:G:N2	1:QA:383:A:OP2	2.34	0.54
29:R4:16:CYS:SG	29:R4:17:GLY:N	2.80	0.54
35:YA:2680:C:OP2	38:YE:111:ARG:NH2	2.41	0.54
46:YQ:116:GLU:OE2	46:YQ:119:ARG:NH1	2.41	0.54
24:QZ:59:ARG:NH2	24:QZ:62:GLU:OE1	2.41	0.54
30:R5:36:CYS:HB3	30:R5:49:CYS:HB3	1.90	0.54
35:RA:299:A:N1	35:RA:322:A:O2'	2.37	0.54
36:RB:8:U:O2'	48:RS:25:ARG:NH2	2.41	0.54
1:XA:1219:U:OP1	14:XN:19:ARG:NH2	2.41	0.54
1:XA:1297:C:O2'	7:XG:114:ARG:NH1	2.41	0.54
37:YD:69:ARG:NH2	37:YD:128:GLY:O	2.41	0.54
48:YS:28:VAL:HG11	48:YS:98:VAL:HG12	1.89	0.54
1:QA:437:U:O2'	4:QD:123:HIS:ND1	2.39	0.54
5:QE:102:ALA:HB1	5:QE:106:PRO:HG2	1.90	0.54
10:QJ:34:VAL:HG22	10:QJ:74:ILE:HG23	1.90	0.54
40:RG:68:PRO:HB3	40:RG:92:VAL:HB	1.90	0.54
45:RP:101:VAL:HB	45:RP:106:LEU:HB3	1.90	0.54
1:QA:401:C:O2'	1:QA:621:A:N3	2.39	0.53
1:QA:953:G:N7	13:QM:104:ARG:NH2	2.56	0.53
1:QA:992:U:H3	1:QA:1044:A:H62	1.55	0.53
35:RA:974:G:O2'	35:RA:975:G:N7	2.34	0.53
53:RX:72:LYS:NZ	53:RX:75:ASP:OD1	2.38	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:XB:118:LEU:HD11	2:XB:138:LEU:HD12	1.88	0.53
39:YF:167:ALA:HB1	39:YF:173:VAL:HG11	1.89	0.53
46:YQ:137:TYR:HB3	55:YZ:76:LEU:HD21	1.90	0.53
1:QA:1032:A:N6	35:YA:2167:U:O3'	2.42	0.53
20:QT:41:ILE:HD13	20:QT:87:LYS:HD3	1.90	0.53
35:RA:372:G:N2	35:RA:401:A:OP2	2.37	0.53
35:RA:2701:C:H3'	35:RA:2702:U:H5''	1.91	0.53
46:RQ:58:PHE:HD2	46:RQ:61:GLY:HA3	1.72	0.53
49:RT:50:ILE:HD11	49:RT:100:TYR:HA	1.89	0.53
35:YA:700:G:O2'	35:YA:1632:A:N3	2.37	0.53
35:YA:1388:G:HO2'	35:YA:1525:G:HO2'	1.56	0.53
35:YA:1859:A:N6	35:YA:1883:G:O2'	2.41	0.53
15:QO:29:VAL:HG23	15:QO:63:ARG:HG3	1.89	0.53
35:RA:1300:U:H4'	35:RA:1301:A:H5'	1.90	0.53
1:XA:958:A:N3	1:XA:985:C:O2'	2.37	0.53
15:XO:70:LEU:HD11	15:XO:77:ARG:HE	1.73	0.53
35:YA:259:G:H21	35:YA:621:A:H8	1.57	0.53
38:YE:77:ILE:HD13	38:YE:195:LEU:HD13	1.89	0.53
38:YE:101:ARG:NH1	38:YE:169:ASN:O	2.42	0.53
32:R7:37:LYS:NZ	35:RA:468:G:OP2	2.40	0.53
55:RZ:7:ALA:HB3	55:RZ:61:LEU:HB3	1.89	0.53
1:XA:1288:A:O3'	21:XU:10:ARG:NH1	2.39	0.53
35:YA:2748:A:H8	41:YH:63:SER:HB2	1.73	0.53
44:YO:23:ARG:NH2	44:YO:28:SER:O	2.41	0.53
9:QI:42:ARG:NH1	9:QI:71:SER:OG	2.41	0.53
46:RQ:138:ASP:OD1	55:RZ:81:ARG:NH2	2.41	0.53
35:YA:2547:U:O2	44:YO:23:ARG:NH2	2.41	0.53
36:YB:47:C:OP1	48:YS:10:ARG:NH2	2.41	0.53
1:QA:973:G:O6	1:QA:974:A:N6	2.42	0.53
35:RA:1863:G:HO2'	35:RA:2411:A:HO2'	1.56	0.53
25:Y0:2:ALA:N	35:YA:2494:G:OP1	2.41	0.53
35:YA:1433:U:H3	35:YA:1560:G:H1	1.55	0.53
35:YA:2451:A:C2	56:ZB:3:PPU:HD2	2.43	0.53
2:QB:7:VAL:HG12	2:QB:12:GLU:OE1	2.09	0.53
9:QI:128:ARG:NH2	22:QV:33:U:OP2	2.38	0.53
33:R8:29:LYS:O	33:R8:31:HIS:N	2.32	0.53
35:RA:631:A:OP1	45:RP:64:LYS:NZ	2.41	0.53
35:RA:996:A:OP2	50:RU:92:ARG:NH2	2.42	0.53
38:RE:24:THR:HG21	38:RE:188:VAL:HG12	1.90	0.53
1:XA:191:G:O2'	20:XT:101:GLY:O	2.26	0.53
1:XA:1210:C:O2'	1:XA:1213:A:O2'	2.26	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:1522:U:H2'	1:XA:1523:G:H8	1.74	0.53
35:YA:2646:C:OP2	35:YA:2732:G:O2'	2.26	0.53
38:YE:128:SER:OG	38:YE:129:HIS:N	2.40	0.53
43:YN:21:LYS:HB3	43:YN:26:LEU:HB2	1.90	0.53
5:QE:153:LYS:HE2	5:QE:155:GLU:HB3	1.89	0.53
35:RA:1490:A:O2'	37:RD:99:ASP:OD1	2.24	0.53
53:RX:57:LEU:HG	53:RX:78:LYS:HB2	1.89	0.53
1:XA:673:G:H2'	1:XA:674:G:C8	2.44	0.53
35:YA:114:U:O2'	53:YX:33:LYS:NZ	2.41	0.53
35:YA:181:A:H1'	35:YA:435:C:H5'	1.90	0.53
35:YA:392:C:H5''	35:YA:409:C:H5''	1.91	0.53
35:YA:2287:A:H62	35:YA:2344:U:H3	1.56	0.53
44:YO:47:ILE:O	44:YO:53:LYS:NZ	2.42	0.53
42:RI:40:THR:HG23	42:RI:43:ASN:H	1.73	0.53
42:RI:140:LEU:HD12	42:RI:142:VAL:HG12	1.90	0.53
26:Y1:92:LYS:HZ1	26:Y1:96:LYS:NZ	2.07	0.53
35:YA:833:U:O2	45:YP:55:ARG:NH2	2.41	0.53
44:YO:43:VAL:HG23	44:YO:54:GLU:HA	1.89	0.53
1:QA:1286:A:H4'	21:QU:26:LYS:HD2	1.91	0.53
40:RG:37:VAL:HB	40:RG:94:LEU:HB2	1.90	0.53
43:RN:15:LEU:HD22	43:RN:134:ARG:HD3	1.90	0.53
48:RS:27:SER:HA	48:RS:88:ASP:HB3	1.90	0.53
49:RT:66:VAL:HA	49:RT:71:GLY:HA2	1.91	0.53
1:XA:1492:A:H2'	35:YA:1913:A:H61	1.73	0.53
38:YE:94:GLU:O	38:YE:97:LYS:NZ	2.42	0.53
4:QD:57:ARG:NH2	4:QD:205:GLU:OE2	2.35	0.52
35:YA:1196:C:HO2'	35:YA:1228:G:HO2'	1.57	0.52
1:QA:1073:U:O2	2:QB:104:ASN:ND2	2.43	0.52
5:QE:48:ALA:HB2	5:QE:57:LYS:HE3	1.90	0.52
35:RA:998:C:OP2	50:RU:58:ARG:NH1	2.42	0.52
48:RS:26:LEU:HB3	48:RS:87:PHE:HA	1.90	0.52
52:RW:22:ASP:OD1	52:RW:25:ARG:NH1	2.42	0.52
4:XD:15:GLU:OE2	4:XD:59:ARG:NH1	2.41	0.52
35:YA:1543:A:H2'	35:YA:1544:C:H3'	1.92	0.52
35:YA:1728:G:N7	35:YA:1731:G:N2	2.50	0.52
35:YA:2251:G:OP2	46:YQ:82:ARG:NH2	2.41	0.52
1:QA:450:G:OP1	16:QP:43:LYS:NZ	2.35	0.52
2:QB:87:ARG:NH1	2:QB:220:ASP:OD1	2.26	0.52
35:RA:270(J):G:N2	35:RA:270(Q):C:O2	2.42	0.52
1:XA:261:U:OP2	20:XT:79:ARG:NH2	2.42	0.52
35:YA:1889:A:N3	35:YA:2086:U:O2'	2.43	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:YZ:54:HIS:HB3	55:YZ:101:PRO:HD3	1.90	0.52
1:QA:1296:C:O3'	13:QM:13:LYS:NZ	2.42	0.52
2:QB:67:THR:HG21	2:QB:155:LEU:HG	1.91	0.52
38:RE:36:ARG:NH2	38:RE:88:GLY:O	2.42	0.52
1:XA:514:C:H2'	1:XA:515:G:H8	1.74	0.52
2:XB:174:VAL:O	2:XB:178:ARG:HB3	2.09	0.52
5:XE:80:ILE:HG22	5:XE:91:LEU:HB2	1.90	0.52
35:YA:309:G:N3	35:YA:329:G:O2'	2.42	0.52
13:QM:49:THR:HG22	13:QM:51:ALA:H	1.75	0.52
29:R4:14:ILE:HG13	29:R4:31:ILE:HG13	1.92	0.52
35:RA:26:G:H1'	35:RA:515:A:H61	1.73	0.52
39:RF:116:ASP:OD2	45:RP:1:MET:N	2.36	0.52
6:XF:95:GLU:O	18:XR:32:ARG:NH1	2.42	0.52
35:YA:1827:C:OP2	37:YD:222:ARG:NH1	2.43	0.52
39:YF:160:ASN:HB3	39:YF:163:VAL:HG12	1.91	0.52
40:YG:161:THR:HG22	40:YG:163:ALA:H	1.73	0.52
1:QA:501:C:H1'	1:QA:549:C:H1'	1.91	0.52
25:R0:24:LYS:NZ	35:RA:2355:C:O2'	2.42	0.52
35:RA:442:G:H1'	39:RF:48:THR:HG21	1.90	0.52
35:RA:581:C:H2'	35:RA:582:G:H8	1.74	0.52
35:RA:1864:U:H3	35:RA:1878:G:H1	1.56	0.52
35:RA:1980:G:O2'	35:RA:1982:C:OP2	2.24	0.52
35:RA:2725:A:O2'	35:RA:2726:U:O2	2.27	0.52
51:RV:59:ALA:HB1	51:RV:94:LEU:HB3	1.91	0.52
10:XJ:13:HIS:HA	10:XJ:16:LEU:HB2	1.90	0.52
24:XY:67:VAL:HG23	24:XY:78:ALA:HB3	1.92	0.52
35:YA:918:A:N3	36:YB:80:U:O2'	2.41	0.52
39:YF:185:ASP:OD1	39:YF:188:ARG:NH1	2.38	0.52
51:YV:59:ALA:HB2	51:YV:96:ILE:HD13	1.91	0.52
56:ZB:3:PPU:N7	56:ZB:3:PPU:C9	2.73	0.52
1:QA:1128:C:O2	1:QA:1146:A:N6	2.41	0.52
1:QA:1279:A:OP2	10:QJ:9:ARG:NH1	2.42	0.52
3:QC:139:GLN:O	3:QC:143:GLU:HB2	2.10	0.52
35:RA:1952:A:N3	35:RA:2560:C:O2'	2.39	0.52
44:RO:87:ILE:HD12	44:RO:91:LEU:HD13	1.92	0.52
24:XZ:33:ASP:OD1	24:XZ:37:THR:OG1	2.28	0.52
35:YA:2849:U:OP1	49:YT:95:ARG:NH1	2.42	0.52
1:QA:1145:C:H4'	1:QA:1146:A:H8	1.75	0.52
1:QA:1241:G:H1	1:QA:1296:C:H42	1.57	0.52
4:QD:32:ALA:HA	4:QD:35:ARG:HB2	1.92	0.52
35:RA:833:U:O2	45:RP:55:ARG:NH1	2.40	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:XI:93:ARG:HH21	9:XI:97:LYS:HD2	1.75	0.52
35:YA:994:C:OP1	50:YU:53:ARG:NH2	2.43	0.52
35:YA:1798:U:OP2	37:YD:274:ARG:NH2	2.43	0.52
41:YH:54:ARG:HH22	41:YH:62:LYS:HE2	1.74	0.52
1:QA:979:C:OP1	1:QA:1223:C:N4	2.43	0.52
1:QA:1522:U:H2'	1:QA:1523:G:H8	1.74	0.52
35:RA:1689:A:H62	35:RA:1698:A:H2	1.58	0.52
1:XA:406:G:N3	4:XD:119:GLN:NE2	2.54	0.52
33:Y8:29:LYS:O	33:Y8:31:HIS:N	2.32	0.52
35:YA:1011:G:OP2	50:YU:66:ASN:ND2	2.42	0.52
35:YA:1047:G:O2'	35:YA:1110:G:N2	2.43	0.52
38:YE:36:ARG:HG2	38:YE:47:VAL:HG12	1.90	0.52
44:RO:120:GLU:OE1	49:RT:67:SER:OG	2.26	0.52
48:RS:31:SER:OG	48:RS:32:LEU:N	2.42	0.52
49:RT:64:ARG:NH1	49:RT:106:SER:OG	2.41	0.52
35:YA:13:A:O2'	35:YA:15:G:N7	2.41	0.52
35:YA:1131:G:C2	43:YN:75:TYR:HB2	2.45	0.52
36:YB:13:A:N1	36:YB:69:G:O2'	2.41	0.52
1:QA:427:U:OP1	4:QD:13:ARG:NH2	2.42	0.51
1:QA:855:G:OP2	1:QA:871:U:N3	2.43	0.51
4:QD:23:GLY:N	4:QD:26:CYS:SG	2.83	0.51
35:RA:2638:G:OP1	38:RE:82:ARG:NH2	2.43	0.51
36:RB:48:A:OP2	48:RS:30:ARG:NH2	2.43	0.51
37:RD:148:GLU:HB2	37:RD:151:LYS:HD2	1.91	0.51
45:RP:39:LYS:HE2	45:RP:45:LEU:HD11	1.91	0.51
49:RT:29:ARG:NH1	49:RT:46:GLU:OE1	2.44	0.51
1:XA:714:G:H2'	1:XA:715:A:C8	2.45	0.51
1:XA:1356:G:H2'	1:XA:1357:A:H8	1.73	0.51
35:YA:442:G:H1'	39:YF:48:THR:HG21	1.91	0.51
35:YA:2148:G:H2'	35:YA:2149:G:H8	1.75	0.51
35:YA:2795:G:H21	35:YA:2801:A:H62	1.58	0.51
44:YO:3:GLN:HG2	44:YO:4:PRO:HD2	1.92	0.51
1:QA:80:G:N2	1:QA:89:U:O2	2.40	0.51
1:QA:925:G:H1	1:QA:1391:U:H3	1.56	0.51
25:R0:74:ARG:NH1	36:RB:12:C:O2	2.42	0.51
35:RA:116:C:O2'	35:RA:126:A:N3	2.40	0.51
1:XA:673:G:O3'	6:XF:87:ARG:NH2	2.43	0.51
1:XA:1417:G:O2'	1:XA:1483:A:N6	2.42	0.51
35:YA:2115:G:N2	35:YA:2170:A:N7	2.58	0.51
43:YN:133:GLN:HG2	43:YN:135:PRO:HD3	1.92	0.51
46:YQ:34:LEU:HB2	46:YQ:118:LEU:HD22	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:YZ:28:MET:HG3	55:YZ:37:VAL:HG21	1.92	0.51
1:QA:501:C:H2'	1:QA:502:G:H8	1.75	0.51
1:QA:581:G:O3'	15:QO:64:ARG:NH2	2.43	0.51
35:RA:1165:U:H3	35:RA:1184:G:H1	1.58	0.51
35:RA:1454:U:O2'	35:RA:1455:G:N7	2.43	0.51
35:RA:1550:C:H5'	35:RA:1733:G:H22	1.76	0.51
35:RA:1889:A:N3	35:RA:2086:U:O2'	2.43	0.51
48:RS:10:ARG:NH1	48:RS:91:PRO:O	2.44	0.51
2:XB:127:ILE:O	2:XB:135:GLN:NE2	2.43	0.51
32:Y7:37:LYS:NZ	35:YA:468:G:OP2	2.38	0.51
35:YA:289:A:H3'	35:YA:290:G:H8	1.76	0.51
35:YA:1791:A:N6	35:YA:1828:G:O2'	2.40	0.51
33:R8:52:LYS:HD3	33:R8:52:LYS:N	2.25	0.51
35:RA:1142(A):A:O2'	43:RN:25:ARG:NH2	2.43	0.51
35:RA:1385:G:O2'	35:RA:1396:U:O2	2.27	0.51
1:XA:501:C:H1'	1:XA:549:C:H1'	1.93	0.51
33:Y8:29:LYS:HG3	33:Y8:30:ARG:H	1.75	0.51
36:YB:104:A:OP1	55:YZ:72:ARG:NH1	2.43	0.51
46:YQ:104:PHE:HE2	46:YQ:125:LEU:HD11	1.76	0.51
51:YV:14:VAL:HG11	51:YV:57:VAL:HG11	1.93	0.51
16:QP:5:ARG:NH2	16:QP:27:LYS:O	2.43	0.51
31:R6:6:ARG:HH12	35:RA:2285:C:H5	1.58	0.51
34:R9:1:MET:HE3	34:R9:4:ARG:HH21	1.76	0.51
35:RA:1791:A:N6	35:RA:1828:G:O2'	2.43	0.51
40:RG:83:ARG:HH11	40:RG:83:ARG:HG3	1.75	0.51
2:XB:178:ARG:NH2	2:XB:198:ASP:OD1	2.44	0.51
2:XB:185:ILE:HG22	2:XB:199:TYR:HB2	1.92	0.51
24:XZ:67:VAL:HG13	24:XZ:78:ALA:HB3	1.93	0.51
35:YA:2584:U:H5'	56:ZB:3:PPU:H103	1.91	0.51
50:YU:92:ARG:CZ	51:YV:11:GLN:H	2.24	0.51
1:QA:537:G:H5''	12:QL:113:ARG:HH12	1.76	0.51
1:QA:1129:C:N4	1:QA:1142:G:O6	2.44	0.51
27:R2:18:PRO:HA	27:R2:21:LEU:HB2	1.93	0.51
37:RD:146:GLU:HB2	37:RD:189:CYS:HB3	1.92	0.51
1:XA:501:C:H2'	1:XA:502:G:H8	1.76	0.51
1:XA:1125:U:O4	10:XJ:5:ARG:NH1	2.43	0.51
1:XA:1147:C:O2	9:XI:16:ARG:NH1	2.43	0.51
13:XM:45:VAL:HA	13:XM:48:LEU:HD22	1.92	0.51
35:YA:993:G:OP1	50:YU:50:ARG:NH2	2.44	0.51
35:YA:1681:G:O2'	35:YA:1762:A:O2'	2.28	0.51
36:YB:24:G:H1'	36:YB:27:C:H41	1.74	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:34:C:H2'	1:QA:35:G:H8	1.76	0.51
35:RA:2788:C:O2'	35:RA:2809:A:N3	2.44	0.51
44:RO:76:ALA:HB3	49:RT:75:ILE:HD12	1.93	0.51
1:XA:448:A:OP2	1:XA:485:G:N2	2.42	0.51
1:XA:618:C:H5'	1:XA:619:U:H5''	1.92	0.51
1:XA:1139:G:N2	1:XA:1143:G:O6	2.44	0.51
1:XA:1356:G:H2'	1:XA:1357:A:C8	2.45	0.51
41:RH:127:GLU:HG2	41:RH:130:ARG:HE	1.75	0.51
43:RN:14:VAL:HB	43:RN:52:VAL:HG13	1.93	0.51
1:XA:501:C:OP1	12:XL:117:ARG:NH2	2.44	0.51
1:XA:890:G:O2'	1:XA:906:G:O6	2.29	0.51
35:YA:532:A:N1	35:YA:2035:G:N2	2.58	0.51
35:YA:2566:A:N1	44:YO:28:SER:OG	2.43	0.51
19:QS:10:PHE:CE1	19:QS:38:SER:HB2	2.46	0.51
35:RA:1863:G:O2'	35:RA:2411:A:O2'	2.28	0.51
42:RI:81:VAL:HG21	42:RI:88:ILE:HD13	1.91	0.51
50:RU:74:LEU:HD11	50:RU:114:LYS:HE3	1.93	0.51
11:XK:45:GLY:HA2	11:XK:48:ILE:HD12	1.93	0.51
24:QZ:12:ASP:OD1	24:QZ:81:ARG:NH1	2.44	0.51
35:RA:307:G:H21	35:RA:330:A:H62	1.58	0.51
35:RA:2468:G:OP1	46:RQ:119:ARG:NH2	2.38	0.51
1:XA:954:G:H21	1:XA:1227:A:H62	1.58	0.51
9:XI:9:ARG:HB3	9:XI:104:ARG:HE	1.74	0.51
33:Y8:63:PRO:HB2	35:YA:593:G:H4'	1.92	0.51
35:YA:642:G:H21	35:YA:646:A:H2	1.59	0.51
35:YA:1799:G:OP2	37:YD:273:ARG:NH2	2.44	0.51
1:QA:782:A:H62	1:QA:800:G:N2	2.09	0.50
1:QA:1356:G:H2'	1:QA:1357:A:C8	2.46	0.50
13:QM:15:VAL:HG23	13:QM:34:LEU:HD21	1.92	0.50
42:RI:133:HIS:HB3	42:RI:134:PRO:HD3	1.93	0.50
4:XD:4:TYR:OH	4:XD:10:ARG:NH2	2.43	0.50
17:XQ:66:SER:O	17:XQ:70:ARG:NH1	2.44	0.50
35:YA:2099:U:O2	35:YA:2190:G:O6	2.29	0.50
10:QJ:6:ILE:HG22	10:QJ:98:ILE:HG22	1.92	0.50
10:QJ:78:ASN:HB2	10:QJ:81:THR:HG23	1.91	0.50
35:RA:1818:U:H2'	37:RD:157:ARG:HG2	1.93	0.50
44:RO:43:VAL:HG13	44:RO:54:GLU:HA	1.92	0.50
1:XA:578:C:O2'	1:XA:728:A:N3	2.40	0.50
1:XA:891:U:H2'	1:XA:892:A:H8	1.75	0.50
1:XA:1141:C:H2'	1:XA:1142:G:H8	1.76	0.50
1:XA:1375:A:H4'	7:XG:29:LYS:HD3	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:XQ:18:THR:OG1	17:XQ:69:LYS:NZ	2.39	0.50
35:YA:1434:A:H61	35:YA:1558:A:H62	1.59	0.50
35:YA:2515:C:H2'	35:YA:2516:G:H8	1.75	0.50
42:YI:30:LEU:HB3	42:YI:36:ALA:HB3	1.93	0.50
45:YP:97:PRO:HD3	45:YP:126:VAL:HG23	1.93	0.50
1:QA:945:G:N2	1:QA:1334:G:O2'	2.44	0.50
2:QB:6:THR:O	2:QB:217:ARG:NH1	2.44	0.50
7:QG:75:VAL:HA	7:QG:88:PRO:HA	1.94	0.50
35:RA:1681:G:O2'	35:RA:1762:A:O2'	2.29	0.50
37:RD:8:PRO:HB3	37:RD:14:ARG:HB3	1.93	0.50
1:XA:924:C:O2'	1:XA:1502:A:N6	2.41	0.50
26:Y1:92:LYS:NZ	26:Y1:96:LYS:HZ2	2.09	0.50
35:YA:302:C:OP2	54:YY:73:ARG:NH1	2.43	0.50
35:YA:571:A:H5'	35:YA:2030:A:H62	1.76	0.50
35:YA:629:G:N3	35:YA:639:U:O2'	2.43	0.50
35:YA:1188:U:H4'	51:YV:79:VAL:HG22	1.92	0.50
35:YA:1394:U:O2	53:YX:16:LYS:NZ	2.42	0.50
35:YA:2291:U:O2'	35:YA:2374:C:O2	2.28	0.50
35:YA:2618:G:H21	38:YE:150:VAL:HG21	1.76	0.50
38:YE:36:ARG:NH1	38:YE:85:ASN:OD1	2.45	0.50
43:YN:34:LEU:HD11	43:YN:120:LEU:HB2	1.93	0.50
1:QA:1251:A:N3	1:QA:1369:C:O2'	2.39	0.50
54:RY:99:CYS:SG	54:RY:100:ALA:N	2.84	0.50
5:XE:11:ILE:HD12	5:XE:105:VAL:HG13	1.94	0.50
5:XE:81:GLU:HG2	5:XE:90:VAL:HG12	1.92	0.50
35:YA:668:G:H2'	35:YA:670:A:H62	1.76	0.50
35:YA:1462:C:H4'	35:YA:2703:C:H5'	1.93	0.50
35:YA:2808:U:O4	35:YA:2892:A:N7	2.45	0.50
1:QA:978:A:OP2	1:QA:1362(A):C:N4	2.45	0.50
22:QV:8:U:H3	22:QV:14:A:H62	1.59	0.50
35:YA:2298:A:H62	35:YA:2318:G:H8	1.59	0.50
1:QA:995:C:H2'	1:QA:996:A:H8	1.77	0.50
1:QA:1202:G:O4'	14:QN:29:ARG:NH1	2.44	0.50
2:QB:163:PHE:HD1	2:QB:185:ILE:HG13	1.77	0.50
4:QD:98:GLU:HA	4:QD:103:ASN:HD22	1.76	0.50
33:R8:6:THR:HG22	33:R8:63:PRO:HD2	1.92	0.50
35:RA:373:U:H2'	35:RA:374:A:H8	1.77	0.50
35:RA:459:U:H2'	35:RA:460:A:H8	1.77	0.50
35:RA:1657:C:H4'	38:RE:133:LYS:HB3	1.93	0.50
35:RA:2646:C:OP2	35:RA:2732:G:O2'	2.23	0.50
49:RT:62:THR:HG22	49:RT:75:ILE:HG12	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YA:372:G:N2	35:YA:401:A:OP2	2.41	0.50
1:QA:924:C:O2'	1:QA:1502:A:N6	2.44	0.50
35:RA:783:A:H4'	35:RA:2588:G:H4'	1.94	0.50
2:XB:19:HIS:ND1	2:XB:20:GLU:OE2	2.45	0.50
18:XR:38:GLU:OE1	18:XR:41:LYS:NZ	2.44	0.50
20:XT:30:LYS:HG3	20:XT:34:LYS:HE2	1.93	0.50
45:YP:52:GLU:OE1	45:YP:55:ARG:NH1	2.45	0.50
35:RA:2328:A:H2'	35:RA:2329:G:C8	2.47	0.50
36:RB:44:G:H1'	36:RB:47:C:H42	1.77	0.50
49:RT:26:ASP:OD1	49:RT:120:ARG:NH2	2.40	0.50
50:YU:105:VAL:HG11	51:YV:39:LEU:HD21	1.94	0.50
2:QB:113:HIS:HB3	2:QB:114:ARG:HH21	1.76	0.50
12:QL:71:PRO:O	12:QL:102:ARG:NH1	2.38	0.50
34:R9:30:PRO:HB2	35:RA:2527:C:H4'	1.94	0.50
35:RA:1857:G:N2	35:RA:1885:A:H62	2.07	0.50
37:RD:21:PHE:HB3	37:RD:24:ILE:HG12	1.93	0.50
1:XA:835:U:OP1	18:XR:64:ARG:NH2	2.41	0.50
13:XM:91:ARG:HB2	13:XM:98:VAL:HG12	1.93	0.50
35:YA:581:C:H2'	35:YA:582:G:H8	1.76	0.50
35:YA:764:A:H5'	37:YD:210:GLY:HA2	1.94	0.50
55:YZ:115:GLY:HA2	55:YZ:177:PRO:HD3	1.94	0.50
1:QA:1510:U:H2'	1:QA:1511:G:C8	2.47	0.49
35:RA:1340:U:OP2	53:RX:78:LYS:NZ	2.44	0.49
35:RA:1678:G:N2	35:RA:1989:G:H22	2.10	0.49
55:RZ:23:LYS:HD2	55:RZ:38:TYR:HE2	1.76	0.49
1:XA:643:C:H2'	1:XA:644:G:H8	1.76	0.49
1:XA:1073:U:O2	2:XB:104:ASN:ND2	2.45	0.49
5:XE:154:GLY:HA2	8:XH:64:LYS:HD3	1.93	0.49
35:YA:1598:C:O3'	53:YX:35:THR:OG1	2.29	0.49
35:YA:1607:C:N4	35:YA:1622:G:OP2	2.34	0.49
46:YQ:37:LEU:HD11	46:YQ:130:LYS:HB2	1.93	0.49
9:QI:121:ARG:NH1	9:QI:122:ALA:O	2.45	0.49
11:QK:34:ASP:OD1	11:QK:38:ASN:N	2.45	0.49
35:RA:2343:C:O2'	35:RA:2373:G:O2'	2.27	0.49
54:RY:14:LEU:HB2	54:RY:75:ILE:HD11	1.95	0.49
1:XA:34:C:H2'	1:XA:35:G:H8	1.77	0.49
1:XA:715:A:H2'	1:XA:716:A:C8	2.47	0.49
11:XK:18:ARG:HB3	11:XK:33:THR:HG23	1.94	0.49
22:XV:9:G:O2'	22:XV:10:G:N7	2.41	0.49
26:Y1:56:GLN:HG3	26:Y1:87:PRO:HD3	1.95	0.49
31:Y6:23:THR:HG21	35:YA:2286:A:H61	1.76	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YA:1022:G:N7	43:YN:66:LYS:NZ	2.60	0.49
1:QA:191:G:O2'	20:QT:101:GLY:O	2.26	0.49
1:QA:516:U:O2'	1:QA:519:C:N3	2.41	0.49
2:QB:8:LYS:O	2:QB:11:LEU:N	2.34	0.49
2:QB:223:ILE:HD12	2:QB:226:ARG:HG2	1.94	0.49
35:RA:527:C:N4	35:RA:2779:U:OP2	2.46	0.49
39:RF:185:ASP:OD1	39:RF:188:ARG:NH2	2.45	0.49
1:XA:412:A:OP2	4:XD:35:ARG:NH2	2.44	0.49
1:XA:530:G:N7	24:XY:59:ARG:NH1	2.59	0.49
1:XA:1249:C:O2'	9:XI:73:GLN:OE1	2.30	0.49
35:YA:1254:A:H5''	35:YA:1255:U:H5'	1.94	0.49
38:YE:11:MET:HG2	38:YE:24:THR:HG22	1.95	0.49
1:QA:677:U:O2	1:QA:777:A:O2'	2.27	0.49
15:QO:53:HIS:NE2	35:RA:715:G:O6	2.42	0.49
21:QU:14:TRP:HZ3	21:QU:15:ARG:HH21	1.61	0.49
35:RA:679:C:H2'	35:RA:680:G:H8	1.76	0.49
35:RA:814:C:O2'	35:RA:1225:C:N3	2.44	0.49
35:RA:2749:A:H5''	41:RH:4:ILE:HD12	1.95	0.49
46:RQ:54:MET:HE1	46:RQ:104:PHE:HB3	1.93	0.49
1:XA:1119:C:OP2	9:XI:9:ARG:NH2	2.45	0.49
3:XC:14:ILE:HG13	3:XC:15:THR:HG23	1.94	0.49
3:XC:141:VAL:HG11	3:XC:202:ILE:HG12	1.95	0.49
16:XP:33:ILE:HG22	16:XP:34:GLU:HG3	1.94	0.49
34:Y9:9:ARG:HH21	34:Y9:12:ASP:HA	1.78	0.49
35:YA:1228:G:OP2	50:YU:16:LYS:NZ	2.46	0.49
35:YA:2731:G:OP1	38:YE:169:ASN:ND2	2.44	0.49
36:YB:90:C:OP2	46:YQ:16:ARG:NH1	2.45	0.49
40:YG:82:LEU:HD11	40:YG:88:ILE:HD13	1.94	0.49
1:QA:1141:C:H2'	1:QA:1142:G:H8	1.77	0.49
1:QA:1541:U:OP2	18:QR:55:ARG:NH1	2.44	0.49
3:QC:19:GLU:HG2	3:QC:54:ARG:HE	1.77	0.49
11:QK:22:HIS:HB3	11:QK:29:ILE:HG23	1.94	0.49
17:QQ:83:ASP:N	17:QQ:83:ASP:OD1	2.45	0.49
35:RA:994:C:OP1	50:RU:53:ARG:NH2	2.46	0.49
46:RQ:37:LEU:HD11	46:RQ:130:LYS:HB2	1.95	0.49
54:RY:56:PRO:HG2	54:RY:57:GLN:HE22	1.78	0.49
1:XA:824:C:H2'	1:XA:825:G:H8	1.78	0.49
35:YA:659:C:H2'	35:YA:660:G:H8	1.77	0.49
35:YA:1257:C:OP1	39:YF:72:ARG:NH2	2.44	0.49
1:QA:1312:G:OP2	29:R4:62:ARG:NH2	2.45	0.49
2:QB:74:LYS:NZ	2:QB:206:ASP:OD1	2.40	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:QC:20:SER:OG	3:QC:22:TRP:NE1	2.45	0.49
12:QL:117:ARG:HB2	12:QL:122:THR:HB	1.95	0.49
35:RA:1678:G:H21	35:RA:1989:G:H22	1.59	0.49
35:RA:2844:G:H3'	35:RA:2845:G:H8	1.77	0.49
1:XA:1350:A:O2'	7:XG:33:ASP:OD1	2.28	0.49
10:XJ:25:GLU:O	10:XJ:29:ARG:HB3	2.13	0.49
35:YA:1165:U:H3	35:YA:1184:G:H1	1.61	0.49
49:YT:24:PRO:HG3	49:YT:52:ILE:HG22	1.95	0.49
52:YW:58:ALA:HB1	52:YW:64:MET:HB2	1.95	0.49
1:QA:677:U:H3	1:QA:713:G:H22	1.60	0.49
9:QI:118:LYS:H	9:QI:121:ARG:HB3	1.77	0.49
25:R0:7:LEU:HD13	46:RQ:85:LYS:HZ1	1.77	0.49
35:RA:1230:C:H2'	35:RA:1231:G:H8	1.76	0.49
35:RA:2720:U:H3	35:RA:2873:A:H2	1.58	0.49
47:RR:56:LYS:NZ	47:RR:90:ARG:O	2.44	0.49
1:XA:1353:G:OP1	21:XU:10:ARG:NH2	2.43	0.49
2:XB:219:VAL:HA	2:XB:222:ILE:HD12	1.95	0.49
35:YA:2472:G:H5'	35:YA:2473:U:H5''	1.93	0.49
44:YO:25:LEU:HB2	44:YO:38:VAL:HG13	1.94	0.49
45:YP:95:VAL:HA	45:YP:99:LEU:HD23	1.95	0.49
46:YQ:68:ILE:HG22	46:YQ:101:ARG:HE	1.77	0.49
46:YQ:141:GLN:NE2	55:YZ:74:VAL:O	2.45	0.49
51:YV:21:ARG:HA	51:YV:93:GLU:HA	1.95	0.49
1:QA:673:G:H1'	18:QR:75:ILE:HD12	1.95	0.49
35:RA:379:G:H1	35:RA:395:U:H3	1.60	0.49
42:RI:88:ILE:HB	42:RI:121:LYS:HG2	1.93	0.49
46:RQ:115:MET:HG2	46:RQ:131:ILE:HG21	1.95	0.49
46:RQ:134:ARG:HH22	55:RZ:122:ARG:HG3	1.78	0.49
35:YA:2443:C:H2'	35:YA:2444:G:H8	1.77	0.49
41:YH:7:LEU:HD12	41:YH:8:PRO:HD2	1.95	0.49
29:R4:36:CYS:SG	29:R4:37:SER:N	2.84	0.49
32:R7:13:ALA:HB2	32:R7:46:VAL:HG11	1.94	0.49
35:RA:270(N):G:H5''	42:RI:57:ARG:HH12	1.77	0.49
36:RB:39:A:O2'	36:RB:46:A:N1	2.43	0.49
1:XA:583:A:N6	1:XA:758:G:O2'	2.46	0.49
6:XF:100:ASN:ND2	18:XR:23:LYS:O	2.45	0.49
12:XL:71:PRO:HG3	12:XL:99:HIS:HD2	1.78	0.49
39:YF:117:ARG:HH21	39:YF:187:VAL:HA	1.77	0.49
1:QA:593:G:H1	1:QA:646:U:H3	1.61	0.49
1:QA:663:A:N6	1:QA:742:G:H1	2.07	0.49
6:QF:61:LEU:HD23	6:QF:63:TYR:HE2	1.77	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:QH:34:GLU:HB3	8:QH:118:VAL:HG11	1.94	0.49
30:R5:25:LEU:HD11	52:RW:41:LYS:HE2	1.94	0.49
35:RA:698:C:O2'	35:RA:734:A:N6	2.45	0.49
1:XA:1151:A:H5''	10:XJ:42:THR:HG23	1.95	0.49
1:XA:1321:C:H5''	1:XA:1322:C:H2'	1.94	0.49
3:XC:139:GLN:OE1	3:XC:170:GLN:NE2	2.45	0.49
1:QA:429:U:O2'	4:QD:22:LYS:NZ	2.45	0.48
1:QA:923:A:O2'	1:QA:1399:C:OP2	2.27	0.48
35:RA:259:G:O2'	35:RA:621:A:O2'	2.25	0.48
35:RA:2566:A:N1	44:RO:28:SER:OG	2.42	0.48
35:RA:2747:G:N2	35:RA:2748:A:N1	2.61	0.48
53:RX:55:ASN:HB2	53:RX:80:ILE:HB	1.94	0.48
1:XA:666:G:H5'	1:XA:726:C:H1'	1.95	0.48
35:YA:321:G:O2'	35:YA:340:A:N3	2.44	0.48
35:YA:380:U:H2'	35:YA:381:G:H8	1.78	0.48
1:QA:673:G:H2'	1:QA:674:G:C8	2.48	0.48
1:QA:971:G:N2	1:QA:1363:A:OP2	2.43	0.48
2:QB:223:ILE:HG12	2:QB:230:VAL:HG22	1.95	0.48
25:R0:7:LEU:HB3	46:RQ:85:LYS:NZ	2.28	0.48
29:R4:39:CYS:O	29:R4:41:PRO:CG	2.60	0.48
1:XA:191(F):U:H2'	1:XA:191:G:H8	1.78	0.48
4:XD:23:GLY:HA3	4:XD:112:VAL:HG22	1.96	0.48
27:Y2:18:PRO:HA	27:Y2:21:LEU:HB2	1.95	0.48
35:YA:117:G:OP2	35:YA:119:A:O2'	2.30	0.48
36:YB:15:A:OP2	36:YB:107:U:O2'	2.31	0.48
50:YU:50:ARG:O	50:YU:54:LYS:NZ	2.46	0.48
1:QA:713:G:H2'	1:QA:714:G:C8	2.48	0.48
34:R9:16:VAL:HG22	34:R9:25:VAL:HG22	1.95	0.48
40:RG:18:GLU:OE2	40:RG:21:ARG:NH2	2.38	0.48
43:RN:128:HIS:CE1	43:RN:134:ARG:HG3	2.48	0.48
53:RX:34:ALA:O	53:RX:77:LYS:NZ	2.43	0.48
3:XC:131:ARG:NH1	3:XC:167:TRP:O	2.46	0.48
4:XD:57:ARG:HB3	4:XD:206:PHE:HB2	1.95	0.48
35:YA:581:C:H2'	35:YA:582:G:C8	2.48	0.48
45:YP:116:GLY:O	45:YP:137:LYS:NZ	2.42	0.48
4:QD:64:LEU:HB2	4:QD:198:VAL:HG11	1.96	0.48
35:RA:818:G:HO2'	35:RA:838:C:HO2'	1.60	0.48
35:RA:2470:G:OP1	46:RQ:59:ARG:NH2	2.45	0.48
35:RA:2723:C:OP2	38:RE:109:LYS:NZ	2.46	0.48
38:RE:7:VAL:HG13	38:RE:51:PHE:HE2	1.78	0.48
44:RO:8:LEU:HB2	44:RO:19:ILE:HG13	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:XE:105:VAL:HG21	5:XE:128:PRO:HB3	1.94	0.48
12:XL:75:HIS:HA	12:XL:102:ARG:HH22	1.78	0.48
25:Y0:41:ARG:HA	25:Y0:41:ARG:HE	1.77	0.48
35:YA:270(H):C:H42	35:YA:270(R):G:H1	1.60	0.48
35:YA:2816:C:O2	35:YA:2883:A:O2'	2.26	0.48
37:YD:206:LEU:HA	37:YD:211:ARG:HD2	1.94	0.48
51:YV:61:VAL:HA	51:YV:94:LEU:HD23	1.95	0.48
1:QA:501:C:H2'	1:QA:502:G:C8	2.48	0.48
8:QH:119:LEU:HD22	8:QH:123:GLU:HB3	1.96	0.48
27:R2:66:GLU:OE1	27:R2:69:ARG:NH2	2.47	0.48
35:RA:654(G):C:N3	35:RA:654(N):G:N1	2.61	0.48
35:RA:1824:G:N3	37:RD:254:THR:OG1	2.46	0.48
35:RA:2081:C:H2'	35:RA:2082:A:H8	1.79	0.48
38:RE:35:GLN:HB2	38:RE:66:HIS:HE1	1.78	0.48
1:XA:127:G:O2'	17:XQ:2:PRO:O	2.30	0.48
35:YA:307:G:H21	35:YA:330:A:H62	1.60	0.48
35:YA:851:U:H2'	35:YA:852:G:H8	1.79	0.48
30:R5:3:LYS:HG2	35:RA:2611:U:C4	2.49	0.48
35:RA:24:G:O2'	52:RW:78:GLU:O	2.27	0.48
35:RA:270(G):C:H42	35:RA:270(S):G:H1	1.62	0.48
35:RA:296:C:O3'	54:RY:95:LYS:NZ	2.46	0.48
35:RA:521:G:H2'	35:RA:522:G:C8	2.49	0.48
35:RA:2441:C:OP2	35:RA:2586:C:O2'	2.30	0.48
41:RH:88:LEU:HA	41:RH:130:ARG:HA	1.96	0.48
1:XA:691:G:O6	11:XK:55:LYS:NZ	2.47	0.48
13:XM:58:GLU:O	13:XM:62:ASN:HB2	2.14	0.48
45:YP:87:ASP:O	45:YP:90:ARG:NH1	2.47	0.48
1:QA:1414:U:H2'	1:QA:1415:G:H8	1.78	0.48
4:QD:18:LYS:HB3	4:QD:18:LYS:HE3	1.66	0.48
35:RA:1067:A:N6	35:RA:1068:G:O6	2.47	0.48
35:RA:1598:C:O3'	53:RX:35:THR:OG1	2.29	0.48
40:RG:113:ARG:HB2	40:RG:140:ILE:HB	1.96	0.48
1:XA:501:C:H2'	1:XA:502:G:C8	2.48	0.48
1:XA:1308:U:H2'	1:XA:1309:G:H8	1.79	0.48
25:Y0:47:PRO:HB2	48:YS:20:ARG:HH12	1.79	0.48
35:YA:28:A:N6	35:YA:512:G:O2'	2.47	0.48
35:YA:1385:G:O2'	35:YA:1396:U:O2	2.29	0.48
1:QA:126:G:OP1	1:QA:605:U:O2'	2.28	0.48
28:R3:44:ARG:HA	28:R3:47:VAL:HG12	1.96	0.48
35:RA:512:G:OP1	35:RA:1234:U:O2'	2.24	0.48
38:RE:77:ILE:HG21	38:RE:195:LEU:HD22	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:RQ:135:ASP:OD2	55:RZ:81:ARG:NH1	2.43	0.48
2:XB:101:MET:HA	2:XB:108:ILE:HG13	1.95	0.48
35:YA:2685:G:H1'	35:YA:2726:U:H5	1.79	0.48
44:YO:112:MET:HA	44:YO:115:VAL:HG22	1.95	0.48
47:YR:3:HIS:O	47:YR:5:LYS:N	2.46	0.48
1:QA:738:C:H5''	6:QF:69:GLU:HB2	1.96	0.48
35:RA:1652:A:OP1	47:RR:8:ARG:NH1	2.41	0.48
36:RB:44:G:O2'	36:RB:47:C:N4	2.47	0.48
1:XA:1060:C:H2'	1:XA:1061:G:H8	1.79	0.48
12:XL:56:ALA:HB2	12:XL:70:ILE:HD11	1.95	0.48
26:Y1:71:TYR:HA	26:Y1:74:VAL:HG12	1.95	0.48
31:R6:6:ARG:HD2	31:R6:24:GLU:HB2	1.96	0.48
35:RA:577:G:O2'	35:RA:1254:A:OP1	2.32	0.48
35:RA:1842:G:O2'	37:RD:253:GLN:NE2	2.45	0.48
35:RA:2405:G:O2'	35:RA:2412:A:N6	2.47	0.48
37:RD:182:LEU:H	37:RD:272:ALA:HB3	1.79	0.48
46:RQ:63:LYS:HD2	55:RZ:175:VAL:HG21	1.96	0.48
49:RT:106:SER:HA	49:RT:110:ILE:HD11	1.96	0.48
1:XA:769:G:H4'	1:XA:1513:A:H4'	1.96	0.48
1:XA:1175:G:H2'	1:XA:1176:A:C8	2.49	0.48
10:XJ:44:VAL:HG22	10:XJ:66:ARG:HG2	1.96	0.48
13:XM:105:THR:HG22	13:XM:106:ASN:H	1.78	0.48
1:QA:269:C:H2'	1:QA:270:A:C8	2.48	0.47
1:QA:745:C:OP1	1:QA:851:G:O2'	2.31	0.47
2:QB:88:ALA:HB2	2:QB:219:VAL:HG13	1.96	0.47
5:QE:50:GLU:HB3	5:QE:53:LEU:HD13	1.94	0.47
10:QJ:34:VAL:HG13	10:QJ:74:ILE:HG12	1.96	0.47
19:QS:27:GLU:HB3	19:QS:29:ARG:HH21	1.79	0.47
35:RA:27:G:N2	35:RA:513:A:OP2	2.45	0.47
35:RA:581:C:H2'	35:RA:582:G:C8	2.49	0.47
35:RA:851:U:H2'	35:RA:852:G:H8	1.78	0.47
1:XA:21:G:H2'	1:XA:22:G:C8	2.49	0.47
1:XA:1047:G:H5''	14:YN:4:LYS:HD2	1.95	0.47
1:XA:1413:A:H2	1:XA:1487:G:H22	1.60	0.47
12:XL:32:PHE:HE1	12:XL:86:ARG:HG3	1.79	0.47
12:XL:70:ILE:HG12	12:XL:77:LEU:HD12	1.96	0.47
35:YA:577:G:O2'	35:YA:1254:A:OP1	2.32	0.47
35:YA:1769:G:O2'	35:YA:1958:C:OP1	2.32	0.47
35:YA:2747:G:N2	35:YA:2748:A:N1	2.62	0.47
41:YH:89:ILE:O	41:YH:129:THR:OG1	2.33	0.47
1:QA:21:G:H2'	1:QA:22:G:C8	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:624:C:H2'	1:QA:625:G:H8	1.79	0.47
1:QA:1009:G:O6	1:QA:1020:U:O2	2.31	0.47
4:QD:16:GLY:C	4:QD:33:MET:HE1	2.39	0.47
4:QD:57:ARG:HB3	4:QD:206:PHE:HB2	1.95	0.47
8:QH:91:ARG:NH1	17:QQ:32:TYR:O	2.46	0.47
19:QS:3:ARG:HH12	19:QS:11:VAL:HG12	1.78	0.47
35:RA:297:C:OP1	54:RY:87:LYS:NZ	2.43	0.47
35:RA:655:A:H4'	35:RA:656:G:H5'	1.96	0.47
35:RA:1139:G:H21	35:RA:1143:A:H8	1.60	0.47
41:RH:52:VAL:O	41:RH:65:HIS:NE2	2.42	0.47
55:RZ:54:HIS:HB3	55:RZ:101:PRO:HD3	1.96	0.47
1:XA:1355:G:H2'	1:XA:1356:G:H8	1.79	0.47
25:Y0:51:VAL:O	48:YS:20:ARG:NH2	2.48	0.47
37:YD:142:VAL:HG23	37:YD:193:VAL:HA	1.96	0.47
40:YG:67:LYS:HD2	40:YG:68:PRO:HD2	1.96	0.47
50:YU:102:GLU:HG3	51:YV:2:PHE:HE1	1.78	0.47
56:ZB:3:PPU:N	56:ZB:3:PPU:CD1	2.73	0.47
1:QA:545:C:OP1	4:QD:61:LYS:NZ	2.48	0.47
9:QI:25:LYS:NZ	9:QI:60:ASP:OD2	2.39	0.47
37:RD:153:ALA:O	37:RD:157:ARG:NH1	2.47	0.47
43:RN:103:VAL:HG21	43:RN:120:LEU:HD13	1.96	0.47
35:YA:839:U:H1'	35:YA:1191:G:H1'	1.96	0.47
35:YA:2304:G:N2	40:YG:156:ASP:OD2	2.46	0.47
38:YE:170:LEU:HD23	38:YE:186:GLY:HA3	1.96	0.47
49:YT:26:ASP:HB3	49:YT:92:GLY:H	1.79	0.47
10:QJ:21:GLN:HA	10:QJ:24:VAL:HG22	1.96	0.47
18:XR:51:LEU:HD22	18:XR:55:ARG:HD2	1.95	0.47
41:YH:3:ARG:HH21	41:YH:54:ARG:HH12	1.63	0.47
50:YU:102:GLU:HG3	51:YV:2:PHE:CE1	2.49	0.47
1:QA:1210:C:O2'	1:QA:1213:A:O2'	2.30	0.47
1:QA:1323:G:H2'	1:QA:1324:A:C8	2.49	0.47
3:QC:19:GLU:O	3:QC:40:ARG:NH2	2.47	0.47
3:QC:131:ARG:NH1	3:QC:167:TRP:O	2.43	0.47
35:RA:1212:G:O2'	35:RA:1237:A:N6	2.48	0.47
35:RA:2306:C:H5'	35:RA:2307:G:H5''	1.96	0.47
35:RA:2853:C:H2'	35:RA:2854:G:H8	1.79	0.47
47:RR:104:ARG:HG3	47:RR:107:ASP:HB3	1.96	0.47
1:XA:1026:G:H22	1:XA:1035:A:H2	1.61	0.47
3:XC:164:ARG:NH1	3:XC:166:GLU:OE2	2.47	0.47
20:XT:48:LYS:HA	20:XT:48:LYS:HD3	1.56	0.47
29:Y4:31:ILE:HG21	40:YG:142:PRO:HB2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YA:39:C:O2	39:YF:46:ARG:NH2	2.44	0.47
1:QA:56:U:H2'	1:QA:57:G:H8	1.79	0.47
1:QA:187:C:H2'	1:QA:188:U:H4'	1.96	0.47
1:QA:578:C:O2'	1:QA:728:A:N3	2.39	0.47
1:QA:958:A:C5	19:QS:55:LYS:HG3	2.49	0.47
1:QA:961:U:OP2	1:QA:1222:G:O2'	2.33	0.47
1:QA:1071:C:H2'	1:QA:1072:G:H8	1.79	0.47
33:R8:9:GLY:O	33:R8:13:ARG:NE	2.41	0.47
39:RF:143:ALA:HB1	39:RF:148:LEU:HB2	1.95	0.47
3:XC:88:ARG:NH2	3:XC:101:LEU:O	2.48	0.47
10:XJ:6:ILE:HD12	10:XJ:98:ILE:HG22	1.97	0.47
35:YA:1833:U:O2'	35:YA:1969:A:N1	2.45	0.47
35:YA:2144:U:H1'	35:YA:2147:G:H22	1.79	0.47
36:YB:5:C:O2'	36:YB:27:C:O2	2.30	0.47
38:YE:47:VAL:HG11	38:YE:86:PRO:HD2	1.96	0.47
40:YG:119:GLY:HA3	40:YG:181:ARG:HG3	1.97	0.47
55:YZ:4:ARG:HG2	55:YZ:58:VAL:HB	1.97	0.47
1:QA:157:G:H1	1:QA:164:U:H3	1.62	0.47
1:QA:714:G:H2'	1:QA:715:A:C8	2.50	0.47
1:QA:826:C:O2	8:QH:15:ASN:ND2	2.48	0.47
1:QA:1286:A:N1	21:QU:18:TYR:OH	2.37	0.47
1:QA:1417:G:O2'	1:QA:1483:A:N6	2.46	0.47
3:QC:29:TYR:OH	14:QN:54:PRO:O	2.32	0.47
7:QG:15:ASP:HB3	7:QG:19:GLY:H	1.79	0.47
24:QY:1:MET:HB2	24:QY:35:ARG:HG3	1.97	0.47
35:RA:837:C:N3	35:RA:941:A:N6	2.62	0.47
35:RA:1009:A:N3	35:RA:1153:C:O2'	2.46	0.47
35:RA:2822:G:OP1	38:RE:159:HIS:NE2	2.48	0.47
46:RQ:136:ALA:HB1	55:RZ:52:SER:HB2	1.96	0.47
49:RT:85:LYS:NZ	49:RT:87:ASP:OD2	2.46	0.47
1:XA:909:A:N3	1:XA:1413:A:O2'	2.44	0.47
1:XA:1236:A:H4'	1:XA:1304:G:H4'	1.95	0.47
12:XL:113:ARG:NH2	12:XL:116:SER:OG	2.43	0.47
21:XU:6:ARG:HH21	21:XU:15:ARG:HH21	1.61	0.47
28:Y3:39:ASP:OD1	28:Y3:44:ARG:NH2	2.47	0.47
35:YA:956:G:OP2	46:YQ:14:ARG:NH2	2.48	0.47
35:YA:2012:G:OP1	52:YW:11:ARG:NH2	2.47	0.47
37:YD:70:TRP:NE1	37:YD:146:GLU:OE2	2.39	0.47
41:YH:149:ARG:NH2	41:YH:167:GLU:OE2	2.47	0.47
1:QA:131:C:OP1	1:QA:190:G:N2	2.46	0.47
29:R4:40:HIS:N	29:R4:41:PRO:HD3	2.24	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:839:U:H1'	35:RA:1191:G:H1'	1.97	0.47
35:RA:919:G:N2	35:RA:2269:A:OP2	2.44	0.47
37:RD:142:VAL:HG23	37:RD:193:VAL:HA	1.97	0.47
1:XA:45:U:H2'	1:XA:46:G:C8	2.50	0.47
3:XC:19:GLU:HG2	3:XC:54:ARG:HE	1.80	0.47
30:Y5:16:ARG:NH1	30:Y5:17:ASP:OD1	2.47	0.47
35:YA:2844:G:H3'	35:YA:2845:G:H8	1.80	0.47
1:QA:592:G:H2'	1:QA:593:G:H8	1.80	0.47
1:QA:618:C:H5'	1:QA:619:U:H5''	1.96	0.47
2:QB:171:ALA:HA	2:QB:174:VAL:HG22	1.97	0.47
12:QL:83:VAL:HG12	12:QL:107:ALA:HB2	1.95	0.47
36:RB:118:G:C2'	36:RB:119:A:O4'	2.63	0.47
40:RG:139:LEU:HD21	40:RG:149:VAL:HG21	1.96	0.47
46:RQ:39:PRO:HB3	46:RQ:99:PRO:HD3	1.97	0.47
55:RZ:181:GLU:HB2	55:RZ:183:LEU:HG	1.97	0.47
1:XA:624:C:H2'	1:XA:625:G:H8	1.79	0.47
1:XA:1071:C:H2'	1:XA:1072:G:H8	1.79	0.47
4:XD:25:ARG:NE	4:XD:30:LYS:O	2.42	0.47
35:YA:1791:A:H3'	35:YA:1792:G:H8	1.80	0.47
35:YA:2692:C:H2'	35:YA:2693:A:H8	1.80	0.47
38:YE:77:ILE:HD11	38:YE:79:ARG:HH21	1.79	0.47
55:YZ:11:GLU:HA	55:YZ:36:LYS:HE2	1.97	0.47
1:QA:674:G:H2'	1:QA:675:A:C8	2.49	0.47
13:QM:19:LEU:HD11	13:QM:56:LEU:HD21	1.97	0.47
35:RA:2845:G:H2'	35:RA:2846:G:H8	1.80	0.47
37:RD:36:PRO:HG3	37:RD:63:ARG:HG3	1.98	0.47
1:XA:429:U:O2'	4:XD:22:LYS:NZ	2.48	0.47
9:XI:125:TYR:HE1	9:XI:127:LYS:HE3	1.80	0.47
13:XM:47:ASP:OD1	13:XM:47:ASP:N	2.48	0.47
35:YA:699:A:N3	35:YA:1633:G:O2'	2.40	0.47
37:YD:69:ARG:HH11	37:YD:105:ILE:HG21	1.79	0.47
56:ZB:3:PPU:CD1	56:ZB:3:PPU:HN2	2.26	0.47
1:QA:150:C:H2'	1:QA:151:A:H8	1.80	0.46
1:QA:186(B):C:H2'	1:QA:186(C):G:C8	2.49	0.46
1:QA:390:C:O3'	16:QP:28:ARG:NH2	2.49	0.46
1:QA:1342:C:H2'	1:QA:1343:G:C8	2.50	0.46
2:QB:27:LYS:HD2	2:QB:193:ASP:HB2	1.96	0.46
13:QM:11:ARG:NH2	40:RG:146:TYR:OH	2.41	0.46
18:QR:32:ARG:HE	18:QR:65:ILE:HD11	1.79	0.46
35:RA:1049:C:N4	35:RA:2751:G:O6	2.48	0.46
35:RA:1230:C:H2'	35:RA:1231:G:C8	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:RD:9:TYR:HD1	37:RD:10:THR:HG23	1.80	0.46
38:RE:57:LYS:HD3	38:RE:57:LYS:HA	1.37	0.46
45:RP:115:LEU:HA	45:RP:134:ALA:HB2	1.97	0.46
55:RZ:110:GLY:O	55:RZ:115:GLY:N	2.48	0.46
1:XA:576:G:N2	1:XA:760:G:OP2	2.48	0.46
1:XA:1512:U:H2'	1:XA:1513:A:C8	2.50	0.46
35:YA:2030:A:H4'	35:YA:2031:A:H8	1.79	0.46
1:QA:779:C:H5''	11:QK:122:LYS:HG2	1.97	0.46
2:QB:47:THR:HA	2:QB:202:PRO:HG2	1.97	0.46
27:R2:36:ARG:NH2	53:RX:8:ILE:O	2.48	0.46
35:RA:225:A:N6	35:RA:419:C:O2'	2.47	0.46
35:RA:1057:A:N6	35:RA:1088:A:OP2	2.49	0.46
35:RA:1530:G:H1	35:RA:1541:U:H3	1.62	0.46
35:RA:1667:G:O2'	35:RA:1991:U:O4	2.32	0.46
35:RA:1830:C:H2'	35:RA:1831:G:H8	1.80	0.46
37:RD:147:LEU:HD21	37:RD:183:ARG:HH22	1.80	0.46
39:RF:115:ALA:O	39:RF:119:ARG:HB2	2.15	0.46
48:RS:66:ALA:HA	48:RS:69:VAL:HG12	1.98	0.46
49:RT:96:ARG:HD2	49:RT:101:PHE:HE2	1.79	0.46
1:XA:376:G:H1	1:XA:387:U:H3	1.64	0.46
17:XQ:45:HIS:CD2	17:XQ:47:PRO:HG3	2.51	0.46
31:Y6:11:LEU:HG	31:Y6:49:HIS:HB3	1.96	0.46
35:YA:1139:G:HO2'	35:YA:1143:A:H62	1.63	0.46
35:YA:1243:G:O2'	45:YP:7:ARG:NH2	2.49	0.46
52:YW:33:ARG:NE	52:YW:52:GLU:OE2	2.46	0.46
1:QA:1435:G:H2'	1:QA:1436:U:C6	2.50	0.46
24:QY:12:ASP:O	24:QY:15:TYR:N	2.48	0.46
25:R0:50:ASN:HA	25:R0:62:LEU:HD12	1.97	0.46
30:R5:4:HIS:O	35:RA:2056:G:N2	2.48	0.46
35:RA:1434:A:H61	35:RA:1558:A:N6	2.14	0.46
45:RP:148:LEU:HD23	45:RP:148:LEU:HA	1.74	0.46
7:XG:20:ASP:HB3	7:XG:23:VAL:HG23	1.97	0.46
28:Y3:17:LYS:NZ	35:YA:968:G:OP1	2.47	0.46
35:YA:30:G:O2'	35:YA:1214:A:N3	2.42	0.46
35:YA:907:U:OP1	46:YQ:24:GLY:N	2.48	0.46
37:YD:145:VAL:HB	37:YD:155:LEU:HB2	1.97	0.46
46:YQ:75:THR:HG21	46:YQ:87:LYS:HG2	1.96	0.46
1:QA:736:C:O2'	6:QF:90:VAL:O	2.31	0.46
10:QJ:43:ARG:HH11	10:QJ:43:ARG:HD2	1.47	0.46
35:RA:2849:U:H3	35:RA:2867:G:H1'	1.80	0.46
36:RB:47:C:H5'	48:RS:10:ARG:HH12	1.79	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:RD:245:PRO:HA	37:RD:246:PRO:HD3	1.85	0.46
41:RH:24:VAL:HB	41:RH:35:VAL:HG13	1.98	0.46
44:RO:98:VAL:HG11	44:RO:114:ILE:HG23	1.98	0.46
1:XA:1119:C:H2'	1:XA:1120:G:H8	1.79	0.46
1:XA:1126:U:N3	1:XA:1281:U:O4'	2.45	0.46
7:XG:15:ASP:HB3	7:XG:19:GLY:H	1.80	0.46
35:YA:24:G:O2'	52:YW:78:GLU:O	2.32	0.46
35:YA:247:G:OP2	35:YA:249:C:N4	2.49	0.46
35:YA:959:A:N3	35:YA:2457:U:O2'	2.46	0.46
39:YF:60:SER:OG	39:YF:61:GLY:N	2.48	0.46
1:QA:652:U:O4	1:QA:752:G:O2'	2.32	0.46
4:QD:177:ASP:HB3	4:QD:182:LYS:HG2	1.98	0.46
7:QG:78:ARG:HE	7:QG:156:TRP:CD1	2.34	0.46
16:QP:49:LEU:HD11	16:QP:73:LEU:HG	1.98	0.46
35:RA:1954:G:O2'	35:RA:1956:U:O4	2.30	0.46
1:XA:579:G:H5'	1:XA:728:A:H1'	1.98	0.46
1:XA:972:C:OP2	10:XJ:57:LYS:NZ	2.46	0.46
11:XK:106:LYS:O	18:XR:87:ARG:NH1	2.48	0.46
1:QA:824:C:H2'	1:QA:825:G:H8	1.81	0.46
4:QD:133:VAL:HG12	4:QD:135:LEU:H	1.80	0.46
8:QH:104:ARG:HG3	8:QH:107:LEU:HB2	1.98	0.46
13:QM:24:GLY:O	13:QM:29:ARG:NH1	2.49	0.46
30:R5:16:ARG:NH1	30:R5:17:ASP:OD1	2.48	0.46
35:RA:197:A:H62	35:RA:2430:A:H2'	1.79	0.46
35:RA:668:G:H2'	35:RA:670:A:H62	1.81	0.46
35:RA:2037:G:H2'	35:RA:2038:G:C8	2.51	0.46
37:RD:79:VAL:O	37:RD:114:GLY:N	2.46	0.46
50:RU:90:VAL:C	50:RU:92:ARG:H	2.23	0.46
1:XA:376:G:O3'	16:XP:5:ARG:NH1	2.42	0.46
26:Y1:18:ILE:HG12	26:Y1:37:ILE:HG12	1.98	0.46
35:YA:2148:G:H2'	35:YA:2149:G:C8	2.51	0.46
35:YA:2693:A:H2'	35:YA:2694:G:H8	1.80	0.46
30:R5:41:PRO:O	30:R5:44:THR:OG1	2.28	0.46
4:XD:85:LYS:HD2	4:XD:92:VAL:HG11	1.98	0.46
35:YA:971:C:O2'	35:YA:983:A:N3	2.44	0.46
47:YR:33:ARG:HE	47:YR:113:LEU:HD11	1.80	0.46
1:QA:662:G:H2'	1:QA:663:A:C8	2.51	0.46
35:RA:300:A:OP1	54:RY:86:ARG:NH2	2.48	0.46
35:RA:1388:G:O2'	35:RA:1525:G:O2'	2.30	0.46
35:RA:1607:C:N4	35:RA:1622:G:OP2	2.37	0.46
35:RA:2089:U:H3	35:RA:2230:G:H1	1.63	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:2298:A:H62	35:RA:2318:G:H8	1.64	0.46
1:XA:1130:A:H62	1:XA:1144:G:H21	1.63	0.46
24:XY:3:LEU:HB2	24:XY:35:ARG:HH21	1.81	0.46
35:YA:1056:G:H4'	35:YA:1086:A:H1'	1.98	0.46
35:YA:2029:G:N1	35:YA:2033:A:OP1	2.32	0.46
55:YZ:146:ILE:HA	55:YZ:174:VAL:HG23	1.97	0.46
1:QA:28:G:O2'	1:QA:296:U:OP1	2.27	0.46
1:QA:1249:C:O2'	9:QI:73:GLN:NE2	2.48	0.46
16:QP:18:ARG:HA	16:QP:38:TYR:HA	1.98	0.46
18:QR:32:ARG:HA	18:QR:69:THR:HG21	1.98	0.46
19:QS:28:LYS:NZ	19:QS:46:GLY:O	2.31	0.46
26:R1:67:ILE:O	26:R1:70:VAL:HG12	2.15	0.46
35:RA:589:C:H2'	35:RA:590:A:C8	2.51	0.46
35:RA:1853:A:N3	35:RA:2233:U:O2'	2.46	0.46
35:RA:2124:G:H22	35:RA:2174:C:H42	1.64	0.46
40:RG:124:SER:O	40:RG:124:SER:OG	2.34	0.46
40:RG:166:ASP:OD1	40:RG:166:ASP:N	2.49	0.46
1:XA:991:U:O4	1:XA:1212:U:O2'	2.31	0.46
35:YA:831:G:N2	45:YP:53:GLY:O	2.47	0.46
35:YA:1830:C:H2'	35:YA:1831:G:H8	1.79	0.46
1:QA:948:C:H2'	1:QA:949:A:H8	1.80	0.46
1:QA:1346:A:OP1	9:QI:120:ARG:NH1	2.48	0.46
2:QB:53:ARG:HG2	2:QB:56:ARG:HH21	1.80	0.46
2:QB:74:LYS:NZ	2:QB:205:ASP:O	2.44	0.46
4:QD:4:TYR:OH	4:QD:10:ARG:NH2	2.49	0.46
9:QI:10:ARG:NH1	9:QI:75:ASP:OD2	2.49	0.46
35:RA:29:U:H5''	50:RU:7:GLY:HA2	1.98	0.46
35:RA:138:G:N1	53:RX:44:GLU:OE1	2.38	0.46
35:RA:1598:C:H5'	53:RX:37:THR:HG23	1.98	0.46
35:RA:2130:U:O2	35:RA:2133:G:O2'	2.29	0.46
41:RH:130:ARG:HH11	41:RH:132:ARG:HB2	1.81	0.46
48:RS:28:VAL:HG11	48:RS:98:VAL:HG12	1.98	0.46
1:XA:128:G:O2'	17:XQ:3:LYS:NZ	2.49	0.46
1:XA:552:U:H2'	1:XA:553:A:H8	1.81	0.46
1:XA:592:G:H2'	1:XA:593:G:H8	1.81	0.46
1:XA:806:C:H2'	1:XA:807:A:H8	1.80	0.46
1:XA:885:G:H2'	1:XA:886:G:H8	1.81	0.46
1:XA:948:C:H2'	1:XA:949:A:H8	1.81	0.46
1:XA:1510:U:H2'	1:XA:1511:G:C8	2.51	0.46
4:XD:100:ARG:NH2	4:XD:136:PRO:O	2.49	0.46
7:XG:16:LEU:HD13	9:XI:42:ARG:HA	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y0:27:GLU:HG3	25:Y0:68:GLU:HA	1.98	0.46
35:YA:600:G:N2	35:YA:605:C:O3'	2.49	0.46
35:YA:1779:U:OP2	35:YA:1784:A:N6	2.40	0.46
44:YO:19:ILE:HG22	44:YO:43:VAL:HG12	1.96	0.46
1:QA:671:G:O2'	6:QF:80:ARG:NH2	2.44	0.45
1:QA:1354:C:H2'	1:QA:1355:G:H8	1.79	0.45
24:QY:16:TRP:NE1	24:QY:80:CYS:O	2.48	0.45
35:RA:443:A:OP2	35:RA:615:G:N2	2.35	0.45
35:RA:1249:U:H2'	45:RP:18:ARG:HH22	1.81	0.45
43:RN:35:ARG:HH11	43:RN:108:PRO:HG3	1.81	0.45
45:RP:95:VAL:HB	45:RP:125:VAL:HA	1.97	0.45
1:XA:599:C:O2'	8:XH:129:VAL:O	2.25	0.45
1:XA:1312:G:H5'	19:XS:5:LEU:HD11	1.98	0.45
14:XN:26:ARG:HD3	14:XN:43:CYS:HB3	1.98	0.45
35:YA:1262:A:OP1	52:YW:99:ARG:NH1	2.49	0.45
1:QA:1074:G:O2'	1:QA:1101:A:N1	2.49	0.45
10:QJ:43:ARG:HH12	10:QJ:45:ARG:HB2	1.82	0.45
19:QS:6:LYS:HB2	19:QS:6:LYS:HE3	1.74	0.45
28:R3:40:THR:HG22	28:R3:42:ALA:H	1.81	0.45
35:RA:918:A:N3	36:RB:80:U:O2'	2.47	0.45
35:RA:1262:A:OP2	52:RW:97:LYS:NZ	2.48	0.45
35:RA:2186:G:H2'	35:RA:2187:G:H8	1.81	0.45
38:RE:10:GLY:HA3	49:RT:7:ILE:HD11	1.98	0.45
43:RN:23:LEU:HB2	43:RN:62:VAL:HG12	1.98	0.45
1:XA:684:A:O2'	11:XK:39:PRO:O	2.34	0.45
9:XI:5:TYR:HE1	9:XI:16:ARG:HB2	1.81	0.45
32:Y7:28:ARG:NH2	35:YA:1368:G:OP1	2.46	0.45
35:YA:2135:A:N6	35:YA:2156:G:H21	2.14	0.45
35:YA:2784:C:H1'	38:YE:37:ARG:HH12	1.81	0.45
1:QA:553:A:H5''	12:QL:24:VAL:HG21	1.98	0.45
4:QD:109:GLY:HA3	4:QD:165:MET:HG3	1.98	0.45
24:QZ:58:ARG:HG3	24:QZ:68:TYR:HE1	1.81	0.45
29:R4:17:GLY:N	29:R4:33:VAL:O	2.49	0.45
35:RA:704:G:O2'	35:RA:726:G:N2	2.49	0.45
35:RA:1827:C:OP2	37:RD:222:ARG:NH1	2.45	0.45
35:RA:2773:C:OP1	38:RE:166:THR:OG1	2.33	0.45
40:RG:37:VAL:HG22	40:RG:159:VAL:HG12	1.97	0.45
47:RR:2:ARG:HD2	47:RR:2:ARG:HA	1.71	0.45
1:XA:713:G:H2'	1:XA:714:G:C8	2.52	0.45
8:XH:25:ASP:HB3	8:XH:58:TYR:HD2	1.82	0.45
9:XI:21:PRO:HA	9:XI:59:PHE:HA	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YA:2392:A:H2	35:YA:2424:C:H42	1.64	0.45
36:YB:48:A:OP2	48:YS:30:ARG:NH2	2.49	0.45
1:QA:264:U:O2'	17:QQ:64:PRO:O	2.34	0.45
1:QA:1177:G:H2'	1:QA:1178:G:C4	2.52	0.45
35:RA:740:U:H2'	35:RA:741:G:C8	2.51	0.45
35:RA:1636:C:H2'	35:RA:1637:A:C8	2.52	0.45
35:RA:1779:U:OP2	35:RA:1784:A:N6	2.38	0.45
35:RA:2591:C:H2'	35:RA:2592:G:C8	2.51	0.45
2:XB:90:MET:HE2	2:XB:226:ARG:NH2	2.31	0.45
35:YA:814:C:O2'	35:YA:1225:C:N3	2.48	0.45
35:YA:1028:A:N3	35:YA:2486:G:O2'	2.44	0.45
42:YI:76:THR:OG1	42:YI:139:GLN:NE2	2.49	0.45
54:YY:11:ASP:OD1	54:YY:11:ASP:N	2.49	0.45
1:QA:985:C:H2'	1:QA:986:A:H8	1.81	0.45
1:QA:1432:G:O2'	1:QA:1468:A:N6	2.49	0.45
20:QT:51:GLU:HA	20:QT:54:LYS:HG2	1.99	0.45
35:RA:1423:G:H2'	35:RA:1424:G:H8	1.81	0.45
35:RA:2801:A:OP1	35:RA:2895:U:O2'	2.35	0.45
40:RG:109:VAL:HG11	40:RG:142:PRO:HB3	1.98	0.45
50:RU:34:LYS:HA	50:RU:34:LYS:HD2	1.71	0.45
1:XA:17:U:H2'	1:XA:18:C:C6	2.52	0.45
1:XA:452:A:O2'	1:XA:453:A:O4'	2.33	0.45
4:XD:81:GLU:OE1	4:XD:139:ARG:NH2	2.49	0.45
35:YA:277:C:H3'	35:YA:278:A:H8	1.81	0.45
35:YA:2701:C:H3'	35:YA:2702:U:H5''	1.97	0.45
43:YN:22:THR:OG1	43:YN:23:LEU:N	2.46	0.45
50:YU:88:ILE:HG23	50:YU:90:VAL:HG23	1.98	0.45
1:QA:377:G:H2'	1:QA:378:G:H8	1.82	0.45
1:QA:1147:C:O2'	9:QI:5:TYR:OH	2.30	0.45
35:RA:1315:C:O2'	35:RA:1392:A:N3	2.48	0.45
37:RD:79:VAL:HG21	37:RD:111:LEU:HD11	1.98	0.45
38:RE:147:PRO:HB2	38:RE:149:ARG:HG2	1.99	0.45
42:RI:109:ILE:HD11	42:RI:130:TYR:CZ	2.52	0.45
51:RV:3:ALA:HB2	51:RV:40:LEU:HD23	1.99	0.45
1:XA:254:G:O2'	17:XQ:16:GLN:O	2.34	0.45
5:XE:107:ARG:O	5:XE:111:GLU:HB2	2.17	0.45
21:XU:26:LYS:HA	21:XU:26:LYS:HD2	1.78	0.45
35:YA:2246:G:H2'	35:YA:2247:A:H8	1.81	0.45
1:QA:309:G:O2'	1:QA:607:A:N1	2.50	0.45
29:R4:2:LYS:HD3	29:R4:2:LYS:HA	1.60	0.45
32:R7:7:PRO:HB2	35:RA:1309:G:H4'	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:586:A:N1	35:RA:809:G:O2'	2.47	0.45
36:RB:60:C:H2'	36:RB:61:G:H8	1.82	0.45
41:RH:121:ILE:HD11	41:RH:133:VAL:HG22	1.99	0.45
49:RT:77:PRO:HB2	49:RT:80:SER:HB2	1.99	0.45
6:XF:10:LEU:HD13	6:XF:61:LEU:HD13	1.97	0.45
35:YA:1782:C:H1'	35:YA:2609:U:H5''	1.97	0.45
35:YA:2246:G:H2'	35:YA:2247:A:C8	2.51	0.45
42:YI:78:THR:HG22	42:YI:141:LYS:HB2	1.98	0.45
43:YN:1:MET:HG2	51:YV:12:TYR:HD1	1.81	0.45
46:YQ:77:LYS:NZ	46:YQ:86:GLY:O	2.49	0.45
1:QA:359:U:H2'	1:QA:360:A:H8	1.82	0.45
1:QA:1327:C:H5''	21:QU:20:LYS:HE2	1.99	0.45
31:R6:34:LEU:HG	31:R6:36:LEU:HD13	1.97	0.45
35:RA:230:U:H2'	35:RA:231:C:H6	1.82	0.45
51:RV:68:LYS:H	51:RV:68:LYS:HD2	1.82	0.45
54:RY:9:LYS:NZ	54:RY:28:LYS:O	2.34	0.45
1:XA:1469:G:H2'	1:XA:1470:G:H8	1.81	0.45
35:YA:582:G:H2'	35:YA:583:G:H8	1.82	0.45
35:YA:861:A:N3	36:YB:79:C:O2'	2.49	0.45
35:YA:1636:C:H2'	35:YA:1637:A:C8	2.52	0.45
52:YW:71:VAL:HA	52:YW:107:LEU:HD23	1.99	0.45
1:QA:666:G:H5'	1:QA:726:C:H1'	1.99	0.45
2:QB:201:ILE:HG21	2:QB:214:ILE:HG21	1.99	0.45
5:QE:154:GLY:HA2	8:QH:64:LYS:HE3	1.99	0.45
8:QH:104:ARG:HB3	8:QH:108:GLY:H	1.82	0.45
24:QZ:24:VAL:HA	24:QZ:27:ILE:HD12	1.99	0.45
35:RA:1600:C:OP1	53:RX:58:HIS:NE2	2.45	0.45
1:XA:411:A:H62	1:XA:413:G:H21	1.65	0.45
16:XP:18:ARG:HH11	16:XP:35:LYS:HD2	1.82	0.45
26:Y1:40:ARG:NH2	35:YA:2232:U:OP2	2.50	0.45
34:Y9:27:CYS:SG	34:Y9:28:GLU:N	2.89	0.45
35:YA:573:G:OP2	51:YV:78:LYS:NZ	2.48	0.45
44:YO:120:GLU:OE2	49:YT:65:LYS:NZ	2.49	0.45
50:YU:91:ASP:HA	50:YU:95:LEU:HB2	1.97	0.45
1:QA:922:G:H4'	5:QE:20:GLN:HA	1.99	0.45
1:QA:1512:U:H2'	1:QA:1513:A:C8	2.52	0.45
24:QZ:4:ILE:HB	24:QZ:76:LEU:HA	1.99	0.45
35:RA:2777:G:OP2	35:RA:2781:A:O2'	2.26	0.45
35:RA:2867:G:O2'	35:RA:2868:A:O4'	2.35	0.45
45:RP:121:LYS:HB3	45:RP:123:LEU:HD22	1.98	0.45
45:RP:134:ALA:O	45:RP:138:LEU:HB2	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:RV:21:ARG:HG3	51:RV:21:ARG:HH11	1.82	0.45
55:RZ:48:PHE:HE1	55:RZ:71:VAL:HG21	1.82	0.45
2:XB:67:THR:HG21	2:XB:155:LEU:HD11	1.98	0.45
35:YA:78:A:H2'	35:YA:79:G:H8	1.81	0.45
35:YA:521:G:H2'	35:YA:522:G:H8	1.82	0.45
35:YA:848:G:H2'	35:YA:849:A:C8	2.52	0.45
35:YA:919:G:N2	35:YA:2269:A:OP2	2.51	0.45
39:YF:113:ALA:HB2	39:YF:183:VAL:HG23	1.99	0.45
1:QA:112:G:O2'	1:QA:354:G:O2'	2.33	0.44
24:QY:42:LYS:O	24:QY:58:ARG:NH1	2.48	0.44
30:R5:12:SER:OG	35:RA:2021:C:OP1	2.34	0.44
35:RA:2680:C:H5'	38:RE:189:PRO:HA	1.97	0.44
1:XA:401:C:O2'	1:XA:621:A:N3	2.47	0.44
1:XA:407:G:H2'	1:XA:408:A:H8	1.82	0.44
26:Y1:76:ARG:NH2	26:Y1:97:LEU:HB3	2.32	0.44
35:YA:539:G:H2'	35:YA:540:G:H8	1.82	0.44
35:YA:589:C:H2'	35:YA:590:A:H8	1.82	0.44
35:YA:2720:U:H3	35:YA:2873:A:H2	1.65	0.44
7:QG:20:ASP:HB3	7:QG:23:VAL:HG12	2.00	0.44
35:RA:1399:C:H2'	35:RA:1400:G:H8	1.81	0.44
1:XA:426:G:OP1	4:XD:38:TYR:OH	2.30	0.44
1:XA:950:U:H3	1:XA:1231:G:H1	1.66	0.44
1:XA:1128:C:H1'	1:XA:1146:A:H61	1.83	0.44
25:Y0:56:ASP:HA	35:YA:2386:C:H4'	1.98	0.44
38:YE:5:LEU:HD11	38:YE:79:ARG:HB2	1.98	0.44
1:QA:17:U:H2'	1:QA:18:C:C6	2.52	0.44
1:QA:769:G:H4'	1:QA:1513:A:H4'	1.99	0.44
6:QF:6:VAL:HB	6:QF:63:TYR:HB2	1.99	0.44
13:QM:98:VAL:HG23	13:QM:99:ARG:HG3	1.99	0.44
31:R6:9:LEU:HA	31:R6:54:ILE:HB	1.99	0.44
35:RA:1188:U:H4'	51:RV:79:VAL:HG22	1.98	0.44
35:RA:1651:G:H4'	47:RR:39:PRO:HG2	2.00	0.44
3:XC:150:LYS:HE3	3:XC:167:TRP:HE1	1.82	0.44
7:XG:26:PHE:HD1	7:XG:101:LEU:HG	1.82	0.44
9:XI:9:ARG:H	9:XI:79:LEU:HD23	1.82	0.44
25:Y0:48:GLY:O	48:YS:20:ARG:NH1	2.50	0.44
34:Y9:6:SER:HB3	35:YA:2466:C:H5''	2.00	0.44
35:YA:121:G:H4'	35:YA:149:A:H5'	1.99	0.44
35:YA:2208:U:O2'	37:YD:150:LYS:O	2.35	0.44
35:YA:2429:G:N7	45:YP:56:SER:OG	2.48	0.44
43:YN:54:VAL:HB	43:YN:122:VAL:HG12	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:YX:29:TRP:HZ3	53:YX:59:VAL:HG11	1.82	0.44
1:QA:993:G:O2'	1:QA:994:A:N7	2.50	0.44
1:QA:1172:C:H2'	1:QA:1173:G:H8	1.83	0.44
1:QA:1404:C:H2'	1:QA:1405:G:C8	2.53	0.44
35:RA:321:G:O2'	35:RA:340:A:N3	2.47	0.44
35:RA:627:A:H4'	35:RA:628:G:H5'	1.99	0.44
35:RA:995:C:H5'	50:RU:53:ARG:HG2	1.99	0.44
35:RA:1568:G:OP1	37:RD:63:ARG:NH1	2.41	0.44
35:RA:1936:A:N6	35:RA:1963:U:O2	2.49	0.44
35:RA:2246:G:H2'	35:RA:2247:A:C8	2.53	0.44
47:RR:14:SER:OG	47:RR:15:SER:N	2.50	0.44
55:RZ:70:LEU:HG	55:RZ:91:LEU:HD11	1.98	0.44
4:XD:57:ARG:HE	4:XD:205:GLU:HG3	1.82	0.44
9:XI:5:TYR:HH	9:XI:7:THR:HG1	1.62	0.44
11:XK:87:THR:HA	11:XK:91:ARG:HD2	1.97	0.44
35:YA:2451:A:C4	56:ZB:3:PPU:HD2	2.51	0.44
35:YA:2692:C:H2'	35:YA:2693:A:C8	2.52	0.44
41:YH:86:GLU:OE2	41:YH:132:ARG:NH2	2.50	0.44
48:YS:25:ARG:HG2	48:YS:88:ASP:HB2	1.99	0.44
1:QA:6:G:H4'	1:QA:298:A:H4'	1.99	0.44
1:QA:919:A:O2'	1:QA:1080:A:N1	2.43	0.44
1:QA:1179:A:H4'	9:QI:103:THR:HA	1.99	0.44
8:QH:86:ILE:HG22	8:QH:93:VAL:HG11	1.98	0.44
13:QM:13:LYS:HD2	13:QM:13:LYS:HA	1.72	0.44
24:QY:5:TRP:CD1	24:QZ:5:TRP:HD1	2.36	0.44
26:R1:10:LYS:NZ	26:R1:65:SER:OG	2.50	0.44
35:RA:700:G:O2'	35:RA:1632:A:N3	2.49	0.44
35:RA:2052:G:O2'	38:RE:143:ASN:O	2.30	0.44
35:RA:2859:G:H2'	35:RA:2860:A:C8	2.52	0.44
37:RD:145:VAL:O	37:RD:155:LEU:N	2.49	0.44
38:RE:58:ARG:HA	38:RE:58:ARG:HD2	1.50	0.44
40:RG:31:VAL:O	40:RG:33:ARG:NH1	2.48	0.44
45:RP:29:LYS:HE3	45:RP:29:LYS:HB3	1.80	0.44
5:XE:51:VAL:HG23	5:XE:52:PRO:HD3	1.99	0.44
34:Y9:1:MET:HB2	35:YA:2526:G:H1'	1.98	0.44
35:YA:247:G:H4'	35:YA:386:G:C5	2.52	0.44
55:YZ:69:THR:HG22	55:YZ:90:VAL:HG12	1.98	0.44
1:QA:279:A:OP2	17:QQ:95:TYR:OH	2.31	0.44
1:QA:1381:U:O2'	7:QG:79:ARG:O	2.31	0.44
15:QO:87:ILE:HD12	15:QO:87:ILE:HA	1.92	0.44
35:RA:539:G:H2'	35:RA:540:G:H8	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:675:A:H4'	39:RF:67:GLN:HE22	1.83	0.44
35:RA:1571:A:H2'	35:RA:1572:A:C8	2.53	0.44
37:RD:147:LEU:HD11	37:RD:183:ARG:HH12	1.83	0.44
1:XA:450:G:H4'	16:XP:41:PRO:HB2	1.99	0.44
1:XA:745:C:OP1	1:XA:851:G:O2'	2.35	0.44
8:XH:116:LYS:HG2	8:XH:129:VAL:HG11	1.99	0.44
27:Y2:8:LYS:HA	27:Y2:11:GLU:HG2	1.98	0.44
35:YA:630:G:N2	35:YA:633:A:OP2	2.38	0.44
35:YA:2329:G:H2'	35:YA:2330:G:C8	2.53	0.44
35:YA:2511:U:O2'	38:YE:138:PRO:O	2.34	0.44
55:YZ:76:LEU:HA	55:YZ:83:PRO:HA	2.00	0.44
2:QB:80:ILE:HD13	2:QB:211:ILE:HG22	1.98	0.44
34:R9:33:LYS:NZ	35:RA:2743:C:OP1	2.38	0.44
35:RA:873:G:O3'	46:RQ:63:LYS:NZ	2.50	0.44
42:RI:26:ALA:HA	42:RI:30:LEU:HB2	1.98	0.44
50:RU:88:ILE:HG23	50:RU:90:VAL:HG23	2.00	0.44
51:RV:85:LYS:HE2	51:RV:85:LYS:HB2	1.66	0.44
1:XA:1353:G:OP2	21:XU:3:LYS:NZ	2.49	0.44
1:XA:1355:G:H2'	1:XA:1356:G:C8	2.52	0.44
1:XA:1483:A:H1'	35:YA:1948:G:H1'	1.99	0.44
2:XB:19:HIS:ND1	2:XB:205:ASP:OD1	2.50	0.44
8:XH:91:ARG:NE	17:XQ:32:TYR:O	2.51	0.44
32:Y7:7:PRO:HB2	35:YA:1309:G:H4'	1.99	0.44
35:YA:2328:A:H2'	35:YA:2329:G:C8	2.52	0.44
35:YA:2469:A:H2	35:YA:2481:G:H21	1.64	0.44
1:QA:836:G:H1	1:QA:850:U:H3	1.65	0.44
1:QA:1348:U:H4'	9:QI:120:ARG:HD2	1.99	0.44
1:QA:1386:G:H2'	1:QA:1387:G:H8	1.82	0.44
13:QM:91:ARG:HB2	13:QM:98:VAL:HG12	1.97	0.44
25:R0:35:ASN:ND2	35:RA:2353:G:O2'	2.51	0.44
33:R8:57:ARG:NH1	45:RP:52:GLU:OE2	2.48	0.44
35:RA:144:C:H2'	35:RA:145:G:H8	1.82	0.44
35:RA:247:G:H4'	35:RA:386:G:C5	2.53	0.44
35:RA:1204:A:H1'	35:RA:1206:G:C5	2.52	0.44
35:RA:2074:U:H2'	35:RA:2075:U:C6	2.53	0.44
35:RA:2183:C:H2'	35:RA:2184:G:H8	1.82	0.44
38:RE:154:LYS:HA	38:RE:154:LYS:HD2	1.82	0.44
42:RI:128:LEU:O	42:RI:138:ILE:N	2.51	0.44
44:RO:11:ALA:O	44:RO:99:PHE:N	2.40	0.44
54:RY:13:VAL:HG12	54:RY:74:PRO:HA	2.00	0.44
1:XA:1300:G:O2'	1:XA:1303:C:N4	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:XL:70:ILE:HG13	12:XL:100:ILE:HD12	1.98	0.44
24:XZ:37:THR:OG1	24:XZ:37:THR:O	2.35	0.44
28:Y3:49:LYS:HE2	35:YA:851:U:H5'	1.98	0.44
35:YA:819:A:OP2	35:YA:1187:G:N2	2.40	0.44
39:YF:110:LEU:HD11	39:YF:181:LEU:HG	1.99	0.44
48:YS:36:TYR:CD1	48:YS:52:SER:HB2	2.53	0.44
1:QA:552:U:H2'	1:QA:553:A:C8	2.52	0.44
1:QA:877:C:H2'	1:QA:878:G:H8	1.83	0.44
1:QA:938:A:N3	1:QA:1376:U:O2'	2.44	0.44
1:QA:1001:G:H2'	1:QA:1002:G:C8	2.53	0.44
1:QA:1300:G:O2'	1:QA:1303:C:N4	2.44	0.44
2:QB:59:GLU:HG3	2:QB:221:LEU:HD21	1.99	0.44
16:QP:19:ILE:N	16:QP:37:GLY:O	2.45	0.44
31:R6:12:GLU:HB3	31:R6:19:ARG:HG3	2.00	0.44
35:RA:654(D):G:H1	35:RA:654(Q):C:H42	1.65	0.44
35:RA:1181:C:H2'	35:RA:1182:A:C8	2.53	0.44
35:RA:1518:C:H2'	35:RA:1519:G:H8	1.83	0.44
39:RF:192:LEU:HD21	39:RF:194:MET:HE3	2.00	0.44
1:XA:946:A:H2'	1:XA:947:G:C8	2.52	0.44
1:XA:985:C:H2'	1:XA:986:A:C8	2.53	0.44
30:Y5:25:LEU:HD12	52:YW:19:LEU:HB3	1.98	0.44
35:YA:859:G:O2'	35:YA:916:G:O6	2.34	0.44
35:YA:2135:A:H62	35:YA:2156:G:N2	2.16	0.44
1:QA:692:U:OP1	11:QK:124:LYS:NZ	2.39	0.43
1:QA:717:C:O2'	11:QK:116:HIS:O	2.32	0.43
4:QD:103:ASN:O	4:QD:107:ARG:HB2	2.18	0.43
4:QD:127:THR:HA	4:QD:132:ARG:HA	2.00	0.43
19:QS:50:ALA:HB1	19:QS:57:HIS:HB3	1.99	0.43
24:QY:7:GLU:N	24:QY:7:GLU:CD	2.73	0.43
25:R0:77:ARG:NH2	35:RA:857:C:OP2	2.49	0.43
35:RA:1542:G:O6	35:RA:1543:A:N6	2.51	0.43
35:RA:2572:A:OP1	35:RA:2574:G:O2'	2.28	0.43
1:XA:476:G:H2'	1:XA:477:G:C8	2.53	0.43
29:Y4:2:LYS:HB3	29:Y4:5:ILE:HG12	2.00	0.43
29:Y4:51:ASP:OD1	29:Y4:51:ASP:N	2.50	0.43
33:Y8:28:GLY:HA3	33:Y8:44:LYS:HD3	2.00	0.43
35:YA:142:G:H2'	35:YA:143:C:C6	2.53	0.43
35:YA:589:C:H2'	35:YA:590:A:C8	2.53	0.43
35:YA:2443:C:H2'	35:YA:2444:G:C8	2.53	0.43
53:YX:12:VAL:HB	53:YX:27:THR:HG23	1.99	0.43
1:QA:603:U:H2'	1:QA:604:G:H8	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:736:C:H2'	1:QA:737:A:H8	1.83	0.43
1:QA:1172:C:H2'	1:QA:1173:G:C8	2.53	0.43
5:QE:33:VAL:HG13	5:QE:112:LEU:HD12	1.99	0.43
35:RA:1403:C:H5''	35:RA:1471:A:H1'	2.00	0.43
35:RA:2446:G:N2	35:RA:2449:U:O2	2.51	0.43
35:RA:2696:U:H2'	35:RA:2697:G:C8	2.53	0.43
1:XA:403:C:OP2	4:XD:74:GLN:NE2	2.47	0.43
1:XA:991:U:O4	1:XA:1213:A:N7	2.51	0.43
19:XS:11:VAL:HG11	19:XS:16:LEU:HB2	2.00	0.43
35:YA:1259:G:H2'	35:YA:1260:G:C8	2.52	0.43
46:YQ:60:ARG:HA	55:YZ:179:ASP:HA	2.00	0.43
1:QA:985:C:H2'	1:QA:986:A:C8	2.52	0.43
1:QA:1502:A:H2	1:QA:1505:G:H1	1.65	0.43
24:QY:5:TRP:CD1	24:QZ:5:TRP:CD1	3.05	0.43
35:RA:244:A:H4'	45:RP:74:GLU:HB2	2.00	0.43
35:RA:859:G:O2'	35:RA:916:G:O6	2.35	0.43
35:RA:1995:U:O2	44:RO:3:GLN:NE2	2.51	0.43
35:RA:2853:C:H2'	35:RA:2854:G:C8	2.53	0.43
38:RE:25:VAL:HG21	49:RT:7:ILE:HG12	2.00	0.43
50:RU:75:ASN:HB2	50:RU:78:THR:HG23	2.01	0.43
55:RZ:10:ARG:NH1	55:RZ:26:GLY:O	2.51	0.43
1:XA:878:G:H5'	8:XH:89:PRO:HG2	2.00	0.43
1:XA:967:C:HO2'	9:XI:125:TYR:HH	1.53	0.43
1:XA:1323:G:H2'	1:XA:1324:A:C8	2.53	0.43
1:XA:1422:G:H5''	44:YO:48:PRO:HB3	1.98	0.43
30:Y5:16:ARG:NH2	35:YA:517:C:OP1	2.41	0.43
33:Y8:5:LYS:HG2	35:YA:242:G:C8	2.52	0.43
35:YA:570:G:H2'	35:YA:2030:A:C5	2.53	0.43
35:YA:1571:A:H2'	35:YA:1572:A:C8	2.53	0.43
36:YB:24:G:O6	36:YB:56:G:O2'	2.37	0.43
39:YF:113:ALA:HB1	39:YF:186:ILE:HG21	1.99	0.43
39:YF:143:ALA:O	39:YF:148:LEU:N	2.51	0.43
42:YI:5:LEU:HD21	42:YI:12:LEU:HB3	2.01	0.43
1:QA:514:C:H2'	1:QA:515:G:H8	1.84	0.43
1:QA:689:C:H3'	1:QA:690:G:H21	1.84	0.43
4:QD:60:GLU:OE2	4:QD:63:LYS:NZ	2.36	0.43
13:QM:12:ASN:HB3	13:QM:46:LYS:HB3	2.00	0.43
35:RA:1073:A:H2'	35:RA:1074:G:H8	1.82	0.43
35:RA:2119:A:N6	35:RA:2170:A:N7	2.66	0.43
35:RA:2438:U:O3'	35:RA:2439:A:H3'	2.18	0.43
35:RA:2873:A:H8	47:RR:6:SER:H	1.64	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:RD:147:LEU:HD12	37:RD:155:LEU:HD11	1.99	0.43
42:RI:88:ILE:HG13	42:RI:121:LYS:HA	2.00	0.43
1:XA:262:A:H5''	20:XT:76:ALA:HB2	2.00	0.43
42:YI:14:ASP:H	42:YI:17:GLN:HB3	1.84	0.43
44:YO:63:VAL:HB	44:YO:102:VAL:HG12	2.00	0.43
1:QA:390:C:H4'	16:QP:28:ARG:HH21	1.83	0.43
1:QA:452:A:O2'	16:QP:72:ARG:NH1	2.51	0.43
1:QA:1086:U:H2'	1:QA:1087:G:H8	1.84	0.43
1:QA:1309:G:OP1	13:QM:88:ARG:NH2	2.51	0.43
2:QB:102:LEU:HD23	2:QB:182:ILE:HD12	2.01	0.43
2:QB:119:GLU:OE2	2:QB:153:ARG:NH2	2.51	0.43
35:RA:2291:U:H2'	35:RA:2292:C:C6	2.54	0.43
38:RE:52:LEU:HB3	38:RE:54:GLN:OE1	2.18	0.43
44:RO:7:TYR:HE1	44:RO:44:LYS:HG3	1.83	0.43
54:RY:39:VAL:HG13	54:RY:42:VAL:HB	2.00	0.43
1:XA:1127:G:H2'	1:XA:1128:C:C6	2.53	0.43
2:XB:15:VAL:HG11	2:XB:209:ARG:HB2	2.01	0.43
2:XB:55:PHE:HA	2:XB:58:ILE:HB	2.00	0.43
2:XB:168:THR:HB	2:XB:192:SER:HB2	2.00	0.43
35:YA:65:C:O2'	35:YA:456:C:N3	2.49	0.43
35:YA:303:U:H2'	35:YA:304:G:H8	1.83	0.43
35:YA:414:C:H2'	35:YA:415:A:C8	2.54	0.43
35:YA:2291:U:OP1	35:YA:2380:C:O2'	2.36	0.43
43:YN:116:LEU:HD23	43:YN:116:LEU:HA	1.89	0.43
47:YR:86:ARG:NH2	47:YR:118:GLU:OXT	2.44	0.43
55:YZ:128:VAL:HG22	55:YZ:161:VAL:HA	2.01	0.43
1:QA:324:G:OP1	20:QT:70:SER:OG	2.34	0.43
1:QA:736:C:H2'	1:QA:737:A:C8	2.53	0.43
2:QB:48:MET:HA	2:QB:51:LEU:HD12	2.00	0.43
35:RA:380:U:H2'	35:RA:381:G:H8	1.83	0.43
35:RA:755:C:H2'	35:RA:756:C:C6	2.53	0.43
35:RA:1070:A:H5'	35:RA:1071:G:H5''	2.00	0.43
35:RA:1332:G:H8	35:RA:1332:G:H2'	1.74	0.43
35:RA:2845:G:H2'	35:RA:2846:G:C8	2.53	0.43
1:XA:1404:C:H2'	1:XA:1405:G:C8	2.54	0.43
4:XD:122:ARG:HD2	4:XD:122:ARG:HA	1.80	0.43
24:XY:5:TRP:HB2	24:XZ:3:LEU:HB2	2.01	0.43
35:YA:221:A:H61	35:YA:265:A:H8	1.65	0.43
35:YA:874:G:H2'	35:YA:875:G:H8	1.84	0.43
35:YA:1341:U:OP2	35:YA:1394:U:O2'	2.36	0.43
35:YA:2657:A:O3'	41:YH:160:LYS:NZ	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YA:2821:A:O2'	35:YA:2826:A:N1	2.48	0.43
35:YA:2871:C:OP1	47:YR:50:HIS:NE2	2.50	0.43
42:YI:10:GLU:O	42:YI:11:ASN:ND2	2.51	0.43
1:QA:216:G:H2'	1:QA:217:C:C6	2.54	0.43
1:QA:946:A:H2'	1:QA:947:G:C8	2.53	0.43
1:QA:1355:G:H2'	1:QA:1356:G:H8	1.84	0.43
8:QH:23:SER:OG	8:QH:24:THR:N	2.52	0.43
20:QT:71:THR:HG22	20:QT:72:LEU:HG	2.00	0.43
35:RA:2503:A:O2'	35:RA:2505:G:OP2	2.34	0.43
43:RN:15:LEU:HD23	43:RN:136:GLU:HG2	1.99	0.43
45:RP:64:LYS:O	45:RP:66:GLY:N	2.52	0.43
5:XE:63:ARG:HA	5:XE:66:MET:HE3	2.00	0.43
28:Y3:8:LEU:HG	28:Y3:28:LEU:HD13	2.01	0.43
35:YA:221:A:N1	35:YA:265:A:O2'	2.52	0.43
35:YA:1614:A:C6	52:YW:91:GLY:HA2	2.54	0.43
35:YA:2591:C:H2'	35:YA:2592:G:C8	2.54	0.43
1:QA:8:A:N6	4:QD:205:GLU:O	2.51	0.43
1:QA:413:G:O2'	1:QA:428:G:N2	2.52	0.43
4:QD:108:LEU:HD12	4:QD:174:LEU:HD13	2.00	0.43
11:QK:62:GLN:HG3	11:QK:97:ALA:HB2	2.01	0.43
35:RA:589:C:H2'	35:RA:590:A:H8	1.84	0.43
35:RA:630:G:N2	35:RA:633:A:OP2	2.47	0.43
35:RA:661:C:HO2'	45:RP:14:LYS:H	1.62	0.43
35:RA:1203:G:O6	35:RA:1204:A:N6	2.52	0.43
35:RA:1380:G:O2'	35:RA:1569:A:N6	2.52	0.43
35:RA:1792:G:H5'	37:RD:205:VAL:HG13	2.00	0.43
35:RA:1800:C:H42	35:RA:1817:G:N2	2.17	0.43
36:RB:24:G:H1'	36:RB:27:C:H41	1.83	0.43
43:RN:23:LEU:HD13	43:RN:60:ILE:HD12	2.01	0.43
51:RV:14:VAL:HB	51:RV:96:ILE:HG12	2.00	0.43
1:XA:56:U:H2'	1:XA:57:G:H8	1.82	0.43
1:XA:677:U:O2	1:XA:777:A:O2'	2.34	0.43
8:XH:26:VAL:O	8:XH:59:LEU:N	2.46	0.43
25:Y0:68:GLU:HG3	25:Y0:80:HIS:HB2	2.01	0.43
29:Y4:14:ILE:HB	29:Y4:22:ILE:HB	1.99	0.43
35:YA:373:U:H2'	35:YA:374:A:H8	1.84	0.43
35:YA:1073:A:H2'	35:YA:1074:G:C8	2.54	0.43
35:YA:1434:A:H61	35:YA:1558:A:N6	2.16	0.43
41:YH:3:ARG:HA	41:YH:3:ARG:HD3	1.46	0.43
50:YU:43:GLY:HA3	51:YV:73:SER:OG	2.18	0.43
1:QA:376:G:H5''	16:QP:5:ARG:HB2	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:1065:U:O5'	1:QA:1190:G:N2	2.51	0.43
9:QL:5:TYR:HE1	9:QL:16:ARG:HB2	1.84	0.43
12:QL:59:ARG:HA	12:QL:65:GLU:HA	2.01	0.43
35:RA:1568:G:H5''	37:RD:61:LEU:HD23	2.01	0.43
35:RA:2784:C:O2	38:RE:37:ARG:NH2	2.52	0.43
36:RB:90:C:OP2	46:RQ:16:ARG:NH2	2.34	0.43
41:RH:59:ARG:HA	41:RH:62:LYS:HD2	1.99	0.43
46:RQ:109:VAL:HB	46:RQ:114:ALA:HB2	2.01	0.43
1:XA:279:A:OP2	17:XQ:95:TYR:OH	2.28	0.43
1:XA:368:U:C2	1:XA:368:U:C1'	3.02	0.43
1:XA:1202:G:O4'	14:XN:29:ARG:NH1	2.52	0.43
1:XA:1218:C:H2'	1:XA:1219:U:C6	2.54	0.43
6:XF:37:VAL:HA	6:XF:65:VAL:HG12	2.00	0.43
15:XO:88:ARG:NH2	35:YA:714:U:OP2	2.49	0.43
26:Y1:8:SER:HB3	26:Y1:66:HIS:CD2	2.53	0.43
35:YA:244:A:H4'	45:YP:74:GLU:HB2	2.01	0.43
35:YA:822:U:H2'	35:YA:823:G:H8	1.83	0.43
35:YA:1899:G:H21	35:YA:1902:C:N4	2.16	0.43
35:YA:1997:G:H5'	38:YE:117:MET:HE3	2.00	0.43
40:YG:41:GLN:HG2	40:YG:43:LEU:HD21	1.99	0.43
8:QH:109:ILE:HG22	8:QH:137:VAL:HB	2.01	0.43
12:QL:32:PHE:HE1	12:QL:86:ARG:HG3	1.84	0.43
30:R5:7:PRO:O	35:RA:2016:U:O2'	2.32	0.43
33:R8:29:LYS:HG3	33:R8:30:ARG:H	1.83	0.43
35:RA:443:A:C8	39:RF:45:ARG:HG3	2.54	0.43
35:RA:2543:G:H2'	35:RA:2544:G:C8	2.54	0.43
36:RB:113:C:H4'	48:RS:46:VAL:HG22	2.01	0.43
45:RP:97:PRO:O	45:RP:98:GLU:HG3	2.18	0.43
50:RU:92:ARG:NH1	51:RV:11:GLN:O	2.52	0.43
1:XA:974:A:OP2	14:XN:41:ARG:NH1	2.45	0.43
1:XA:1308:U:H2'	1:XA:1309:G:C8	2.54	0.43
35:YA:230:U:H2'	35:YA:231:C:H6	1.84	0.43
35:YA:512:G:OP1	35:YA:1234:U:O2'	2.32	0.43
35:YA:642:G:N2	35:YA:645:C:OP2	2.51	0.43
35:YA:1278:A:H2'	35:YA:1279:G:C8	2.53	0.43
36:YB:14:U:O2'	36:YB:107:U:O2'	2.35	0.43
1:QA:45:U:H2'	1:QA:46:G:C8	2.54	0.42
1:QA:636:U:H5'	17:QQ:2:PRO:HG3	2.00	0.42
1:QA:1224:G:O2'	1:QA:1322:C:OP1	2.31	0.42
7:QG:62:PHE:HD1	7:QG:124:LEU:HD21	1.84	0.42
19:QS:19:VAL:HA	19:QS:22:LEU:HB2	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:1316:U:H2'	35:RA:1317:A:C8	2.54	0.42
37:RD:60:ARG:NH1	37:RD:86:PRO:O	2.52	0.42
38:RE:111:ARG:HA	47:RR:2:ARG:HH12	1.83	0.42
50:RU:34:LYS:NZ	50:RU:37:GLU:OE1	2.39	0.42
1:XA:1326:C:OP2	21:XU:6:ARG:NH1	2.51	0.42
10:XJ:24:VAL:HG13	10:XJ:34:VAL:HG21	2.01	0.42
33:Y8:12:LYS:NZ	35:YA:249:C:O2	2.40	0.42
35:YA:223:A:O2'	35:YA:420:C:O2	2.32	0.42
35:YA:1113:U:H2'	35:YA:1114:G:C8	2.54	0.42
35:YA:1316:U:H2'	35:YA:1317:A:H8	1.82	0.42
36:YB:80:U:H2'	36:YB:81:G:H21	1.82	0.42
1:QA:448:A:OP2	1:QA:485:G:N2	2.39	0.42
1:QA:1412:C:H2'	1:QA:1413:A:C8	2.54	0.42
6:QF:79:LEU:HB3	6:QF:88:VAL:HG21	2.00	0.42
35:RA:704:G:HO2'	35:RA:726:G:H22	1.67	0.42
35:RA:2314:C:H2'	35:RA:2315:G:H8	1.84	0.42
35:RA:2779:U:H6	35:RA:2779:U:H2'	1.73	0.42
36:RB:49:C:OP2	48:RS:30:ARG:NH1	2.52	0.42
37:RD:264:LYS:HD3	37:RD:266:SER:HB3	2.00	0.42
1:XA:516:U:O2'	1:XA:519:C:N3	2.43	0.42
1:XA:1030:C:H42	1:XA:1032:A:H62	1.67	0.42
1:XA:1244:C:H2'	1:XA:1245:A:H8	1.84	0.42
1:XA:1392:G:N2	1:XA:1502:A:H8	2.17	0.42
9:XI:95:LYS:HE2	9:XI:95:LYS:HB2	1.88	0.42
13:XM:25:ILE:HD11	13:XM:64:TRP:HE1	1.84	0.42
25:Y0:36:ILE:HD13	25:Y0:60:PHE:HB3	2.02	0.42
35:YA:820:A:N3	35:YA:943:U:O2'	2.47	0.42
35:YA:1278:A:H2'	35:YA:1279:G:H8	1.84	0.42
35:YA:1342:A:H2	35:YA:1602:U:H3	1.66	0.42
35:YA:2074:U:H2'	35:YA:2075:U:C6	2.54	0.42
40:YG:32:PRO:HB2	40:YG:172:LEU:HD22	2.01	0.42
1:QA:890:G:O2'	1:QA:906:G:O6	2.36	0.42
1:QA:1342:C:H2'	1:QA:1343:G:H8	1.85	0.42
3:QC:180:ALA:HB1	3:QC:182:ILE:HG23	2.01	0.42
12:QL:60:LEU:HD22	12:QL:85:ILE:HG21	2.01	0.42
13:QM:49:THR:HB	13:QM:52:GLU:HG3	2.02	0.42
24:QY:44:LYS:CE	24:QY:59:ARG:HE	2.32	0.42
37:RD:108:PRO:HB3	37:RD:143:HIS:CE1	2.53	0.42
37:RD:108:PRO:HD2	37:RD:111:LEU:HD22	2.02	0.42
1:XA:407:G:H2'	1:XA:408:A:C8	2.54	0.42
1:XA:922:G:OP1	5:XE:20:GLN:NE2	2.48	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:XL:104:VAL:HG12	12:XL:105:TYR:H	1.84	0.42
13:XM:17:VAL:O	13:XM:20:THR:OG1	2.31	0.42
17:XQ:44:ALA:HB1	17:XQ:73:VAL:HG22	2.01	0.42
24:XY:34:THR:OG1	24:XY:58:ARG:NH1	2.51	0.42
24:XZ:19:THR:OG1	24:XZ:20:ASP:N	2.52	0.42
28:Y3:15:TYR:HA	28:Y3:16:PRO:HD3	1.92	0.42
35:YA:1020:A:N1	35:YA:1141:U:H2'	2.34	0.42
35:YA:1353:A:H2'	35:YA:1354:A:C8	2.53	0.42
35:YA:1568:G:H4'	37:YD:59:LYS:HB3	2.01	0.42
35:YA:2438:U:O3'	35:YA:2439:A:H3'	2.19	0.42
35:YA:2693:A:H2'	35:YA:2694:G:C8	2.54	0.42
35:YA:2853:C:H2'	35:YA:2854:G:H8	1.85	0.42
1:QA:508:C:O2	1:QA:510:A:N6	2.52	0.42
1:QA:1218:C:H2'	1:QA:1219:U:C6	2.54	0.42
6:QF:76:ALA:O	6:QF:80:ARG:NE	2.50	0.42
35:RA:1353:A:H2'	35:RA:1354:A:C8	2.55	0.42
1:XA:41:G:H2'	1:XA:42:G:H8	1.84	0.42
1:XA:1129:C:H4'	1:XA:1130:A:H5'	2.01	0.42
1:XA:1539:C:H42	23:XX:7:G:H1	1.65	0.42
2:XB:70:PHE:CD1	2:XB:163:PHE:HB3	2.54	0.42
25:Y0:48:GLY:HA3	25:Y0:80:HIS:CE1	2.54	0.42
26:Y1:21:ARG:HD3	26:Y1:35:THR:HG21	2.01	0.42
26:Y1:92:LYS:HZ1	26:Y1:96:LYS:HZ3	1.67	0.42
35:YA:439:G:H2'	35:YA:440:G:C8	2.55	0.42
43:YN:40:PRO:HB3	50:YU:68:ALA:HB2	2.00	0.42
3:QC:65:ALA:HA	3:QC:100:ALA:HB3	2.01	0.42
18:QR:44:LEU:HD21	18:QR:74:ARG:HH21	1.85	0.42
27:R2:41:ILE:HG21	27:R2:44:LEU:HD22	2.02	0.42
35:RA:23:G:OP1	35:RA:504:U:N3	2.43	0.42
35:RA:2258:C:O2'	35:RA:2427:C:OP2	2.34	0.42
35:RA:2416:C:H5''	45:RP:64:LYS:HE2	2.00	0.42
42:RI:114:LEU:HD12	42:RI:130:TYR:HB2	2.01	0.42
43:RN:85:ILE:HD11	43:RN:89:LYS:HG2	2.01	0.42
1:XA:28:G:O2'	1:XA:296:U:OP1	2.31	0.42
1:XA:1432:G:OP1	49:YT:108:ARG:N	2.53	0.42
2:XB:208:ILE:HA	2:XB:211:ILE:HD12	2.00	0.42
6:XF:22:GLU:OE2	6:XF:82:ARG:NH2	2.45	0.42
11:XK:38:ASN:HA	11:XK:39:PRO:HD3	1.88	0.42
14:XN:12:ARG:HH21	14:XN:14:PRO:HD3	1.85	0.42
26:Y1:73:LEU:HD12	26:Y1:97:LEU:HB2	2.01	0.42
35:YA:2469:A:N6	35:YA:2481:G:O2'	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YA:2683:C:O2	44:YO:70:LYS:NZ	2.43	0.42
35:YA:2791:C:O2	35:YA:2805:G:N2	2.51	0.42
44:YO:68:GLU:HG3	44:YO:78:ARG:HD3	2.01	0.42
48:YS:66:ALA:HA	48:YS:69:VAL:HG12	2.01	0.42
1:QA:522:C:H41	12:QL:53:ARG:NH2	2.18	0.42
8:QH:36:LEU:HD12	8:QH:59:LEU:HD23	2.01	0.42
16:QP:8:ARG:HB3	16:QP:28:ARG:NH1	2.35	0.42
18:QR:60:ALA:O	18:QR:64:ARG:NH1	2.53	0.42
24:QZ:19:THR:OG1	24:QZ:20:ASP:N	2.51	0.42
35:RA:679:C:H2'	35:RA:680:G:C8	2.54	0.42
35:RA:704:G:HO2'	35:RA:726:G:N2	2.17	0.42
35:RA:807:U:OP2	45:RP:41:ARG:NH1	2.53	0.42
35:RA:948:G:N2	35:RA:985:C:OP2	2.51	0.42
35:RA:1858:G:H2'	35:RA:1883:G:H22	1.84	0.42
35:RA:1882:C:H3'	35:RA:1883:G:H8	1.84	0.42
35:RA:2328:A:H2'	35:RA:2329:G:H8	1.85	0.42
35:RA:2515:C:H2'	35:RA:2516:G:H8	1.84	0.42
35:RA:2692:C:H2'	35:RA:2693:A:H8	1.84	0.42
43:RN:137:LYS:HD3	43:RN:137:LYS:HA	1.77	0.42
52:RW:13:SER:HA	52:RW:14:PRO:HD3	1.92	0.42
1:XA:921:U:O2'	5:XE:19:MET:O	2.35	0.42
3:XC:11:ARG:NH2	3:XC:177:THR:O	2.47	0.42
35:YA:1400:G:H2'	35:YA:1401:G:C8	2.55	0.42
35:YA:1568:G:H5''	37:YD:61:LEU:HG	2.01	0.42
35:YA:2745:C:O2	41:YH:139:GLN:NE2	2.42	0.42
36:YB:66:A:H61	36:YB:107:U:H2'	1.85	0.42
44:YO:78:ARG:HH12	49:YT:75:ILE:HD11	1.84	0.42
47:YR:58:GLY:HA2	47:YR:80:PHE:HE2	1.84	0.42
1:QA:123:C:H2'	1:QA:124:G:H8	1.84	0.42
1:QA:406:G:H2'	1:QA:407:G:H8	1.85	0.42
1:QA:522:C:H41	12:QL:53:ARG:HH22	1.68	0.42
13:QM:7:VAL:HB	13:QM:9:ILE:HG12	2.01	0.42
35:RA:1205:U:C4	39:RF:171:PRO:HA	2.55	0.42
35:RA:2392:A:H2	35:RA:2424:C:H42	1.67	0.42
1:XA:985:C:H2'	1:XA:986:A:H8	1.83	0.42
1:XA:1058:G:H1	1:XA:1199:U:H3	1.67	0.42
1:XA:1172:C:H2'	1:XA:1173:G:H8	1.84	0.42
16:XP:26:ARG:HD3	16:XP:26:ARG:HA	1.91	0.42
24:XZ:49:LYS:HA	24:XZ:49:LYS:HD3	1.81	0.42
35:YA:38:A:H2'	35:YA:39:C:C6	2.55	0.42
35:YA:380:U:H2'	35:YA:381:G:C8	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YA:597:U:H3	35:YA:660:G:H1	1.67	0.42
35:YA:2162:G:O2'	35:YA:2173:A:OP2	2.27	0.42
54:YY:83:THR:OG1	54:YY:84:ARG:N	2.52	0.42
1:QA:700:G:H4'	1:QA:704:A:H1'	2.00	0.42
1:QA:1010:G:H2'	1:QA:1011:G:H8	1.84	0.42
1:QA:1298:C:H4'	1:QA:1299:A:C4	2.54	0.42
1:QA:1512:U:H2'	1:QA:1513:A:H8	1.84	0.42
13:QM:13:LYS:HA	13:QM:44:ARG:HH11	1.84	0.42
35:RA:576:U:H2'	35:RA:577:G:C8	2.55	0.42
35:RA:643:A:N1	35:RA:2369:A:O2'	2.48	0.42
35:RA:822:U:H2'	35:RA:823:G:H8	1.84	0.42
35:RA:890:A:H2'	35:RA:892:G:C8	2.55	0.42
35:RA:1259:G:H2'	35:RA:1260:G:C8	2.55	0.42
38:RE:41:LYS:HE2	38:RE:41:LYS:HB3	1.87	0.42
40:RG:109:VAL:O	40:RG:113:ARG:HG2	2.19	0.42
1:XA:1378:C:O2	7:XG:76:ARG:NH2	2.49	0.42
11:XK:80:VAL:HG13	11:XK:103:LEU:HD12	2.01	0.42
13:XM:51:ALA:HA	13:XM:54:VAL:HG12	2.02	0.42
33:Y8:37:SER:HB3	33:Y8:40:GLU:HG3	2.01	0.42
35:YA:958:U:OP2	46:YQ:14:ARG:NH1	2.52	0.42
35:YA:1021:A:OP2	43:YN:65:LYS:NZ	2.42	0.42
35:YA:1225:C:H2'	35:YA:1226:G:C8	2.54	0.42
35:YA:1363:C:O2'	35:YA:1809:A:N3	2.44	0.42
35:YA:1568:G:OP2	37:YD:63:ARG:NH2	2.41	0.42
37:YD:133:LEU:HD23	37:YD:136:ILE:HD12	2.02	0.42
52:YW:110:LYS:HA	52:YW:110:LYS:HD3	1.90	0.42
55:YZ:6:LYS:HD2	55:YZ:6:LYS:HA	1.83	0.42
55:YZ:51:ALA:HB1	55:YZ:55:HIS:HB2	2.02	0.42
1:QA:413:G:N2	1:QA:429:U:OP2	2.44	0.42
1:QA:1356:G:H2'	1:QA:1357:A:H8	1.85	0.42
4:QD:119:GLN:O	4:QD:123:HIS:N	2.49	0.42
35:RA:137(A):G:O2'	35:RA:138:G:N2	2.53	0.42
35:RA:863:A:H2'	35:RA:864:G:C8	2.55	0.42
40:RG:36:LYS:HE2	40:RG:95:ARG:HH12	1.85	0.42
1:XA:1151:A:H5'	10:XJ:41:PRO:HA	2.01	0.42
2:XB:69:LEU:HB3	2:XB:162:ILE:HG22	2.00	0.42
2:XB:208:ILE:H	2:XB:208:ILE:HG13	1.65	0.42
5:XE:53:LEU:HA	5:XE:56:GLN:HG2	2.02	0.42
9:XI:42:ARG:NH1	9:XI:71:SER:OG	2.53	0.42
35:YA:1212:G:O2'	35:YA:1237:A:N6	2.52	0.42
35:YA:1482:U:O4	35:YA:1512:G:O6	2.37	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:YF:63:LYS:HE2	39:YF:67:GLN:HB2	2.02	0.42
39:YF:64:ILE:H	39:YF:64:ILE:HG13	1.71	0.42
54:YY:14:LEU:HD22	54:YY:82:PRO:HG3	2.00	0.42
1:QA:1060:C:H2'	1:QA:1061:G:H8	1.84	0.42
1:QA:1226:C:OP1	13:QM:91:ARG:NH1	2.53	0.42
8:QH:19:VAL:HG13	8:QH:21:LYS:HG3	2.02	0.42
13:QM:47:ASP:N	13:QM:47:ASP:OD1	2.52	0.42
40:RG:82:LEU:HD11	40:RG:88:ILE:HD13	2.01	0.42
45:RP:91:PHE:HE2	45:RP:95:VAL:HG22	1.85	0.42
1:XA:41:G:H2'	1:XA:42:G:C8	2.55	0.42
5:XE:5:ASP:OD1	5:XE:5:ASP:N	2.52	0.42
10:XJ:42:THR:HG22	10:XJ:68:HIS:HA	2.01	0.42
13:XM:94:ARG:NH2	35:YA:887:A:OP1	2.46	0.42
15:XO:29:VAL:O	15:XO:33:THR:OG1	2.37	0.42
20:XT:89:ARG:HG3	20:XT:104:LEU:HD21	2.01	0.42
25:Y0:39:ARG:HH21	35:YA:2355:C:H1'	1.84	0.42
35:YA:78:A:H2'	35:YA:79:G:C8	2.55	0.42
35:YA:151:C:H2'	35:YA:152:G:H8	1.83	0.42
35:YA:530:G:N2	35:YA:2022:U:OP1	2.53	0.42
35:YA:2688:U:OP1	35:YA:2713:A:N6	2.52	0.42
41:YH:94:TYR:OH	41:YH:152:ARG:NH1	2.53	0.42
52:YW:13:SER:HA	52:YW:14:PRO:HD3	1.94	0.42
1:QA:404:U:H2'	1:QA:405:U:H6	1.84	0.41
6:QF:15:ASP:OD2	6:QF:17:SER:OG	2.38	0.41
6:QF:46:ARG:HA	6:QF:46:ARG:HD2	1.88	0.41
11:QK:38:ASN:HA	11:QK:39:PRO:HD3	1.92	0.41
27:R2:28:LYS:HA	27:R2:28:LYS:HD3	1.90	0.41
35:RA:532:A:H4'	35:RA:533:G:C8	2.55	0.41
35:RA:1567:A:H3'	37:RD:86:PRO:HG3	2.02	0.41
35:RA:1569:A:H5'	37:RD:61:LEU:HD21	2.02	0.41
35:RA:1754:C:N3	35:RA:2716:U:O2'	2.48	0.41
1:XA:891:U:H2'	1:XA:892:A:C8	2.54	0.41
1:XA:980:C:H1'	14:YN:19:ARG:HA	2.02	0.41
7:XG:29:LYS:HA	7:XG:29:LYS:HD2	1.90	0.41
11:XK:108:ILE:O	18:XR:87:ARG:N	2.51	0.41
19:XS:2:PRO:HB2	19:XS:3:ARG:H	1.61	0.41
34:Y9:1:MET:HE3	34:Y9:35:ARG:HB2	2.01	0.41
35:YA:299:A:N1	35:YA:322:A:O2'	2.42	0.41
35:YA:414:C:H2'	35:YA:415:A:H8	1.84	0.41
35:YA:820:A:H4'	35:YA:836:G:N2	2.35	0.41
35:YA:1853:A:N3	35:YA:2233:U:O2'	2.44	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YA:2329:G:H2'	35:YA:2330:G:H8	1.84	0.41
40:YG:166:ASP:OD1	40:YG:166:ASP:N	2.53	0.41
49:YT:19:LEU:HA	49:YT:20:PRO:HD3	1.90	0.41
55:YZ:124:ILE:HG22	55:YZ:126:VAL:HG13	2.01	0.41
1:QA:619:U:N3	4:QD:134:ASP:OD1	2.53	0.41
5:QE:105:VAL:HG11	5:QE:128:PRO:HB3	2.01	0.41
5:QE:152:ARG:NH2	8:QH:107:LEU:O	2.53	0.41
35:RA:2591:C:H2'	35:RA:2592:G:H8	1.84	0.41
41:RH:89:ILE:HG23	41:RH:162:ILE:HG22	2.01	0.41
1:XA:56:U:H2'	1:XA:57:G:C8	2.55	0.41
1:XA:194:C:H5''	20:XT:65:LYS:HG3	2.02	0.41
1:XA:977:A:O2'	1:XA:981:U:O4	2.38	0.41
1:XA:1240:U:OP1	7:XG:119:ARG:NH2	2.53	0.41
1:XA:1412:C:H2'	1:XA:1413:A:C8	2.55	0.41
1:XA:1493:A:O2'	23:XX:20:A3P:H8	2.20	0.41
25:Y0:5:LYS:HD3	46:YQ:80:GLU:HG3	2.02	0.41
35:YA:30:G:H2'	35:YA:31:C:C6	2.55	0.41
35:YA:2867:G:OP2	49:YT:119:LYS:NZ	2.44	0.41
39:YF:46:ARG:HA	39:YF:46:ARG:HD2	1.86	0.41
40:YG:72:ARG:HH11	40:YG:72:ARG:HG2	1.85	0.41
55:YZ:179:ASP:OD1	55:YZ:180:VAL:N	2.53	0.41
1:QA:1182:G:H5''	1:QA:1183:A:H5'	2.02	0.41
35:RA:219:G:N3	35:RA:234:C:O2'	2.48	0.41
35:RA:223:A:O2'	35:RA:420:C:O2	2.36	0.41
35:RA:329:G:O6	54:RY:19:LYS:N	2.54	0.41
35:RA:1470:G:O2'	35:RA:1522:G:O6	2.32	0.41
35:RA:2033:A:O2'	35:RA:2035:G:OP2	2.34	0.41
35:RA:2836:U:H2'	35:RA:2837:G:C8	2.55	0.41
51:RV:34:GLU:OE2	51:RV:100:ARG:NH2	2.51	0.41
1:XA:269:C:H2'	1:XA:270:A:C8	2.55	0.41
18:XR:26:LEU:HD11	18:XR:39:VAL:HG13	2.03	0.41
19:XS:27:GLU:HG2	19:XS:29:ARG:NH1	2.35	0.41
24:XZ:81:ARG:HG2	24:XZ:82:TYR:H	1.85	0.41
32:Y7:10:ARG:HD2	35:YA:125:G:C6	2.55	0.41
36:YB:114:G:H2'	36:YB:115:G:H8	1.85	0.41
47:YR:66:VAL:HG21	47:YR:80:PHE:HE1	1.85	0.41
55:YZ:119:GLU:HB2	55:YZ:122:ARG:HH11	1.85	0.41
1:QA:359:U:H2'	1:QA:360:A:C8	2.56	0.41
1:QA:933:G:O6	7:QG:3:ARG:NH2	2.53	0.41
3:QC:16:ARG:HD2	3:QC:16:ARG:HA	1.68	0.41
8:QH:69:ARG:NH2	8:QH:75:ARG:O	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:QJ:4:ILE:HG23	10:QJ:74:ILE:HB	2.01	0.41
31:R6:25:LYS:HB2	31:R6:25:LYS:HE2	1.67	0.41
35:RA:196:A:O5'	45:RP:46:LYS:NZ	2.53	0.41
35:RA:1687:G:O2'	35:RA:1701:A:N6	2.47	0.41
35:RA:2314:C:H5'	40:RG:38:VAL:HG11	2.02	0.41
45:RP:46:LYS:HD2	45:RP:46:LYS:HA	1.96	0.41
47:RR:13:HIS:CE1	47:RR:16:HIS:HB2	2.55	0.41
1:XA:790:A:OP1	22:XV:38:A:O2'	2.34	0.41
1:XA:1096:C:H2'	1:XA:1097:C:H6	1.86	0.41
5:XE:106:PRO:HB3	5:XE:135:THR:HG21	2.01	0.41
7:XG:13:GLN:HA	7:XG:14:PRO:HD3	1.91	0.41
18:XR:31:LEU:HD12	18:XR:66:LEU:HB2	2.03	0.41
20:XT:29:LYS:O	20:XT:33:ILE:HG12	2.21	0.41
33:Y8:10:ALA:HB3	33:Y8:62:LEU:HD21	2.02	0.41
35:YA:2471:C:H3'	35:YA:2472:G:H8	1.84	0.41
48:YS:34:HIS:CD2	48:YS:54:LEU:HD12	2.56	0.41
17:QQ:45:HIS:CD2	17:QQ:47:PRO:HG3	2.55	0.41
18:QR:53:ARG:HH21	18:QR:59:SER:HA	1.86	0.41
35:RA:177:G:H3'	35:RA:178:G:H8	1.84	0.41
35:RA:2788:C:H5'	38:RE:61:ARG:HH12	1.86	0.41
40:RG:40:ASN:HB3	40:RG:156:ASP:HB2	2.02	0.41
49:RT:5:ALA:HA	49:RT:8:LYS:HB3	2.03	0.41
1:XA:390:C:H2'	1:XA:391:G:C8	2.55	0.41
3:XC:40:ARG:HG2	3:XC:55:VAL:HG21	2.01	0.41
8:XH:29:SER:HB3	8:XH:32:LYS:HG3	2.03	0.41
17:XQ:53:LEU:HD23	17:XQ:85:VAL:HG11	2.02	0.41
35:YA:806:C:O2	35:YA:2444:G:O2'	2.36	0.41
35:YA:970:C:H2'	35:YA:971:C:C6	2.56	0.41
35:YA:1187:G:H5''	51:YV:81:TYR:CE1	2.55	0.41
35:YA:1403:C:H5''	35:YA:1471:A:H1'	2.02	0.41
41:YH:54:ARG:NH2	41:YH:57:ASP:OD1	2.54	0.41
49:YT:62:THR:HG22	49:YT:75:ILE:HG12	2.02	0.41
50:YU:92:ARG:NH2	51:YV:11:GLN:H	2.18	0.41
1:QA:454:C:H41	1:QA:478:A:H61	1.68	0.41
1:QA:524:G:H2'	1:QA:525:C:C6	2.56	0.41
1:QA:1354:C:H2'	1:QA:1355:G:C8	2.56	0.41
27:R2:14:ARG:HG2	27:R2:63:VAL:HG21	2.03	0.41
28:R3:8:LEU:HG	28:R3:28:LEU:HD12	2.01	0.41
30:R5:30:LEU:HD12	30:R5:39:MET:HB3	2.02	0.41
33:R8:58:ILE:HA	33:R8:61:LEU:HD12	2.03	0.41
35:RA:414:C:H2'	35:RA:415:A:C8	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:1341:U:OP2	35:RA:1394:U:O2'	2.28	0.41
35:RA:1771:C:H2'	35:RA:1772:G:C8	2.56	0.41
47:RR:24:GLN:HG3	47:RR:44:LEU:HD13	2.02	0.41
1:XA:45:U:H2'	1:XA:46:G:H8	1.85	0.41
1:XA:359:U:H2'	1:XA:360:A:C8	2.56	0.41
1:XA:524:G:H2'	1:XA:525:C:C6	2.55	0.41
1:XA:736:C:H2'	1:XA:737:A:C8	2.55	0.41
1:XA:1251:A:H2'	1:XA:1252:A:C8	2.56	0.41
1:XA:1436:U:OP1	20:XT:23:ARG:NH2	2.53	0.41
9:XI:49:PRO:HA	9:XI:52:ALA:HB3	2.03	0.41
14:YN:37:PHE:HB3	14:YN:39:LEU:HD13	2.03	0.41
26:Y1:60:PHE:HE1	26:Y1:91:LYS:HG3	1.86	0.41
35:YA:2291:U:H2'	35:YA:2292:C:C6	2.55	0.41
8:QH:41:ARG:NH2	8:QH:123:GLU:OE1	2.53	0.41
10:QJ:8:LEU:HB3	10:QJ:70:ARG:HB2	2.02	0.41
13:QM:65:LYS:HZ1	29:R4:50:VAL:HG11	1.86	0.41
35:RA:121:G:H4'	35:RA:149:A:H5'	2.02	0.41
35:RA:570:G:H2'	35:RA:2030:A:C5	2.55	0.41
35:RA:1231:G:H2'	35:RA:1232:G:H8	1.85	0.41
38:RE:1:MET:SD	38:RE:1:MET:N	2.70	0.41
38:RE:64:LYS:HA	38:RE:64:LYS:HD3	1.73	0.41
1:XA:1127:G:H21	1:XA:1147:C:H42	1.67	0.41
1:XA:1182:G:H4'	1:XA:1183:A:H5'	2.03	0.41
3:XC:91:LEU:HB3	3:XC:99:VAL:HG11	2.03	0.41
20:XT:26:ASN:HB2	20:XT:71:THR:HG23	2.03	0.41
30:Y5:3:LYS:H	35:YA:2577:A:H4'	1.85	0.41
35:YA:33:U:O4	35:YA:446:G:O2'	2.33	0.41
35:YA:679:C:H2'	35:YA:680:G:H8	1.86	0.41
35:YA:1423:G:H2'	35:YA:1424:G:H8	1.85	0.41
39:YF:155:LEU:HD11	39:YF:176:LEU:HB2	2.03	0.41
1:QA:116:A:H61	1:QA:313:A:H1'	1.85	0.41
1:QA:362:G:N2	1:QA:365:U:OP2	2.52	0.41
1:QA:377:G:H2'	1:QA:378:G:C8	2.56	0.41
13:QM:23:TYR:CE2	13:QM:71:ARG:HG3	2.55	0.41
29:R4:2:LYS:O	29:R4:4:GLY:N	2.53	0.41
44:RO:22:ILE:HD11	44:RO:42:SER:HB2	2.02	0.41
46:RQ:116:GLU:O	46:RQ:120:ILE:HG12	2.20	0.41
1:XA:142:G:H2'	1:XA:143:A:C8	2.56	0.41
1:XA:195:A:H4'	20:XT:68:LYS:HE3	2.03	0.41
1:XA:898:G:N2	1:XA:901:A:OP2	2.48	0.41
1:XA:1127:G:N2	1:XA:1147:C:H42	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:XJ:66:ARG:HD2	14:XN:57:ARG:HH22	1.85	0.41
23:XX:14:A:H2'	23:XX:15:A:H8	1.86	0.41
35:YA:764:A:H2	37:YD:219:PRO:HG3	1.85	0.41
35:YA:2001:A:H2'	35:YA:2002:G:C8	2.56	0.41
35:YA:2103:C:N4	35:YA:2187:G:O6	2.54	0.41
35:YA:2749:A:O2'	41:YH:59:ARG:NE	2.48	0.41
1:QA:80:G:H1	1:QA:89:U:H3	1.68	0.41
1:QA:132:C:O3'	20:QT:74:LYS:NZ	2.50	0.41
1:QA:189:U:O4	17:QQ:63:ARG:N	2.53	0.41
1:QA:1228:C:H4'	13:QM:116:THR:HA	2.02	0.41
1:QA:1427:U:H2'	1:QA:1428:A:C8	2.56	0.41
7:QG:88:PRO:HG2	7:QG:152:ALA:HB2	2.03	0.41
8:QH:36:LEU:HD23	8:QH:36:LEU:HA	1.92	0.41
8:QH:86:ILE:HD12	8:QH:133:LEU:HD22	2.03	0.41
9:QI:102:LEU:HD23	9:QI:102:LEU:HA	1.81	0.41
13:QM:3:ARG:HA	13:QM:8:GLU:HA	2.03	0.41
13:QM:121:LYS:HD2	13:QM:121:LYS:HA	1.81	0.41
22:QV:9:G:O2'	22:QV:10:G:N7	2.46	0.41
28:R3:29:ARG:N	28:R3:33:GLN:OE1	2.50	0.41
29:R4:13:ARG:HA	29:R4:13:ARG:HD3	1.94	0.41
29:R4:13:ARG:C	29:R4:24:THR:HG21	2.45	0.41
35:RA:824:A:H1'	35:RA:2358:G:N7	2.36	0.41
35:RA:922:U:H2'	35:RA:923:C:C6	2.56	0.41
35:RA:1278:A:H2'	35:RA:1279:G:C8	2.56	0.41
35:RA:1336:A:H2'	35:RA:1337:G:C8	2.56	0.41
35:RA:2186:G:H2'	35:RA:2187:G:C8	2.56	0.41
35:RA:2597:G:H2'	35:RA:2598:A:C8	2.55	0.41
37:RD:77:ALA:HA	37:RD:97:TYR:HA	2.02	0.41
38:RE:25:VAL:HG11	49:RT:10:VAL:HG11	2.03	0.41
42:RI:72:LEU:HG	42:RI:138:ILE:HG13	2.01	0.41
1:XA:708:C:H2'	1:XA:709:G:H8	1.86	0.41
1:XA:806:C:H2'	1:XA:807:A:C8	2.56	0.41
1:XA:892:A:H2'	1:XA:893:C:C6	2.56	0.41
2:XB:15:VAL:HG11	2:XB:210:SER:N	2.35	0.41
3:XC:152:ILE:HG12	3:XC:167:TRP:HD1	1.85	0.41
6:XF:45:LEU:HD12	6:XF:59:TYR:HD1	1.86	0.41
10:XJ:78:ASN:OD1	10:XJ:78:ASN:N	2.50	0.41
27:Y2:48:HIS:ND1	35:YA:95:G:O2'	2.50	0.41
35:YA:195:A:H5''	45:YP:46:LYS:NZ	2.36	0.41
35:YA:453:C:O2	35:YA:457:A:O2'	2.35	0.41
35:YA:1657:C:H2'	35:YA:1658:C:C6	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YA:2853:C:H2'	35:YA:2854:G:C8	2.56	0.41
38:YE:7:VAL:HG13	38:YE:51:PHE:HE2	1.86	0.41
39:YF:24:LEU:HA	39:YF:25:PRO:HD3	1.94	0.41
40:YG:64:THR:HG23	40:YG:66:GLN:H	1.86	0.41
42:YI:14:ASP:H	42:YI:17:GLN:CB	2.34	0.41
1:QA:41:G:H2'	1:QA:42:G:H8	1.85	0.41
1:QA:1119:C:H2'	1:QA:1120:G:C8	2.55	0.41
1:QA:1199:U:O2'	1:QA:1202:G:OP1	2.35	0.41
13:QM:84:ILE:HD13	19:QS:65:ASN:HD21	1.86	0.41
19:QS:42:PRO:HD3	29:R4:63:TYR:OH	2.20	0.41
25:R0:39:ARG:HD3	25:R0:39:ARG:HA	1.88	0.41
35:RA:635:C:O2'	35:RA:639:U:OP1	2.37	0.41
35:RA:861:A:N3	36:RB:79:C:O2'	2.53	0.41
35:RA:1400:G:H2'	35:RA:1401:G:C8	2.55	0.41
36:RB:60:C:H2'	36:RB:61:G:C8	2.56	0.41
38:RE:34:VAL:HG12	38:RE:72:VAL:HG11	2.02	0.41
43:RN:61:ARG:O	43:RN:61:ARG:HG2	2.14	0.41
46:RQ:31:ASP:OD1	55:RZ:122:ARG:NH2	2.47	0.41
50:RU:32:PHE:CZ	50:RU:36:ARG:HD2	2.56	0.41
1:XA:1435:G:H2'	1:XA:1436:U:C6	2.56	0.41
1:XA:1513:A:H2'	1:XA:1514:C:C6	2.55	0.41
35:YA:550:G:O2'	35:YA:1220:A:N3	2.53	0.41
35:YA:680:G:H2'	35:YA:681:G:C8	2.55	0.41
35:YA:992:C:H2'	35:YA:993:G:H8	1.85	0.41
35:YA:1262:A:OP2	52:YW:97:LYS:NZ	2.54	0.41
35:YA:2698:U:H2'	35:YA:2699:C:C6	2.56	0.41
52:YW:68:ARG:NE	52:YW:110:LYS:O	2.48	0.41
1:QA:125:U:H2'	1:QA:126:G:C8	2.55	0.40
1:QA:1032:A:N7	35:YA:2167:U:O2'	2.54	0.40
1:QA:1037:C:H2'	1:QA:1038:C:C6	2.56	0.40
4:QD:122:ARG:HA	4:QD:122:ARG:HD2	1.94	0.40
16:QP:18:ARG:HH11	16:QP:35:LYS:HD2	1.86	0.40
18:QR:40:LEU:HB3	18:QR:79:LEU:HD21	2.02	0.40
26:R1:11:ARG:NH2	35:RA:1365:A:O2'	2.52	0.40
33:R8:8:LYS:NZ	35:RA:243:U:OP2	2.50	0.40
35:RA:463:G:N2	35:RA:466:A:OP2	2.42	0.40
35:RA:764:A:H5'	37:RD:210:GLY:HA2	2.02	0.40
35:RA:1316:U:H2'	35:RA:1317:A:H8	1.86	0.40
35:RA:1399:C:H2'	35:RA:1400:G:C8	2.56	0.40
35:RA:1409:C:H2'	35:RA:1410:G:H8	1.86	0.40
35:RA:1449:A:C4	35:RA:1529:A:H2	2.39	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:1889:A:H2'	35:RA:1890:A:C8	2.56	0.40
48:RS:39:ILE:HD12	48:RS:85:VAL:HG11	2.02	0.40
1:XA:269:C:H2'	1:XA:270:A:H8	1.86	0.40
1:XA:1311:G:OP1	29:Y4:58:ARG:NH2	2.54	0.40
1:XA:1441:G:O2'	1:XA:1446:A:N6	2.49	0.40
3:XC:29:TYR:OH	14:YN:54:PRO:O	2.35	0.40
7:XG:94:ARG:NH1	7:XG:98:SER:OG	2.54	0.40
9:XI:42:ARG:NH2	9:XI:75:ASP:OD1	2.52	0.40
35:YA:141:A:C8	35:YA:1408:C:H1'	2.56	0.40
35:YA:2037:G:H2'	35:YA:2038:G:C8	2.56	0.40
40:YG:29:TRP:O	40:YG:33:ARG:NH1	2.54	0.40
46:YQ:116:GLU:HA	46:YQ:119:ARG:HG2	2.03	0.40
49:YT:80:SER:HA	49:YT:81:PRO:HD3	1.92	0.40
50:YU:90:VAL:HG11	51:YV:39:LEU:HB2	2.04	0.40
54:YY:81:LYS:HD2	54:YY:82:PRO:HD2	2.03	0.40
1:QA:401:C:H2'	1:QA:402:G:H8	1.86	0.40
1:QA:1101:A:N6	2:QB:176:GLU:OE2	2.54	0.40
3:QC:164:ARG:NH1	3:QC:166:GLU:OE2	2.37	0.40
6:QF:3:ARG:HB3	6:QF:93:SER:HB2	2.03	0.40
19:QS:10:PHE:HE1	19:QS:38:SER:HB2	1.85	0.40
25:R0:49:LYS:HB3	25:R0:80:HIS:HD1	1.85	0.40
27:R2:65:ASN:ND2	35:RA:72:U:O4	2.54	0.40
35:RA:582:G:H2'	35:RA:583:G:C8	2.56	0.40
38:RE:114:ALA:HB1	38:RE:118:LYS:HD2	2.02	0.40
45:RP:60:MET:HE3	45:RP:60:MET:HB3	1.93	0.40
1:XA:881:G:OP2	12:XL:12:ARG:NH2	2.54	0.40
1:XA:927:G:H1	1:XA:1390:U:H3	1.68	0.40
1:XA:993:G:O2'	1:XA:994:A:N7	2.54	0.40
1:XA:1159:U:O2'	1:XA:1160:G:N7	2.53	0.40
2:XB:16:HIS:ND1	2:XB:17:PHE:O	2.54	0.40
2:XB:178:ARG:NH1	8:XH:74:PRO:HB3	2.36	0.40
4:XD:102:ASP:N	4:XD:102:ASP:OD1	2.53	0.40
20:XT:27:LYS:HA	20:XT:27:LYS:HD3	1.92	0.40
20:XT:50:GLU:HB3	20:XT:99:LEU:HD21	2.04	0.40
35:YA:698:C:O2'	35:YA:734:A:N6	2.55	0.40
35:YA:969:U:H2'	35:YA:970:C:C6	2.56	0.40
35:YA:1652:A:OP1	47:YR:8:ARG:NH1	2.44	0.40
35:YA:2327:A:H2'	35:YA:2328:A:C8	2.56	0.40
39:YF:155:LEU:HD23	39:YF:186:ILE:HD13	2.02	0.40
42:YI:79:ILE:HG22	42:YI:81:VAL:HG13	2.03	0.40
47:YR:58:GLY:HA2	47:YR:80:PHE:CE2	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:YX:31:HIS:HB3	53:YX:34:ALA:HB2	2.03	0.40
55:YZ:48:PHE:HE1	55:YZ:71:VAL:HG21	1.86	0.40
1:QA:954:G:H21	1:QA:1227:A:N6	2.19	0.40
1:QA:1488:G:H2'	1:QA:1489:G:C8	2.56	0.40
2:QB:133:LYS:HA	2:QB:133:LYS:HD2	1.91	0.40
11:QK:70:LYS:HD3	11:QK:70:LYS:HA	1.87	0.40
23:QX:6:G:H2'	23:QX:7:G:C8	2.57	0.40
33:R8:46:ARG:HD2	33:R8:46:ARG:HA	1.83	0.40
35:RA:270(I):G:H2'	35:RA:270(J):G:C8	2.57	0.40
35:RA:663:G:H5''	45:RP:17:LYS:HD3	2.04	0.40
35:RA:807:U:H2'	35:RA:808:G:H8	1.85	0.40
35:RA:1529:A:H62	35:RA:1542:G:N2	2.19	0.40
35:RA:2728:U:H2'	35:RA:2729:G:C8	2.56	0.40
36:RB:9:G:H5'	48:RS:25:ARG:HH22	1.86	0.40
38:RE:67:PHE:HD1	38:RE:67:PHE:HA	1.75	0.40
43:RN:16:ILE:HB	43:RN:54:VAL:HG22	2.03	0.40
1:XA:7:G:O2'	5:XE:120:THR:O	2.40	0.40
1:XA:1314:C:N4	19:XS:2:PRO:O	2.55	0.40
1:XA:1354:C:H2'	1:XA:1355:G:H8	1.86	0.40
7:XG:15:ASP:OD1	7:XG:44:TYR:OH	2.38	0.40
7:XG:78:ARG:HE	7:XG:80:VAL:HG23	1.87	0.40
13:XM:3:ARG:NH1	29:Y4:34:GLU:OE2	2.54	0.40
26:Y1:73:LEU:HD13	26:Y1:73:LEU:HA	1.82	0.40
31:Y6:6:ARG:NH1	35:YA:2285:C:OP2	2.53	0.40
35:YA:576:U:H2'	35:YA:577:G:C8	2.56	0.40
35:YA:787:U:H5''	35:YA:788:A:H5'	2.04	0.40
35:YA:1411:C:H2'	35:YA:1412:A:H8	1.86	0.40
43:YN:96:GLU:HG3	43:YN:122:VAL:HG23	2.04	0.40
1:QA:603:U:H2'	1:QA:604:G:C8	2.57	0.40
1:QA:1128:C:H1'	1:QA:1146:A:H61	1.86	0.40
4:QD:88:VAL:HG13	4:QD:91:SER:HB2	2.02	0.40
28:R3:18:ASP:OD1	28:R3:18:ASP:N	2.54	0.40
34:R9:6:SER:O	34:R9:6:SER:OG	2.40	0.40
35:RA:37:C:H2'	35:RA:38:A:C8	2.57	0.40
35:RA:78:A:H2'	35:RA:79:G:H8	1.85	0.40
35:RA:323:G:H2'	39:RF:169:ASN:ND2	2.37	0.40
35:RA:616:A:C4	39:RF:180:GLY:HA3	2.56	0.40
35:RA:1935:G:H1'	35:RA:1964:G:N2	2.37	0.40
36:RB:14:U:O2'	36:RB:107:U:O2'	2.38	0.40
36:RB:105:G:H2'	36:RB:106:G:H8	1.85	0.40
40:RG:124:SER:OG	40:RG:132:ASN:O	2.38	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:RI:65:ALA:HB1	42:RI:134:PRO:HD2	2.03	0.40
50:RU:61:TRP:HB3	50:RU:93:LYS:O	2.22	0.40
1:XA:719:C:N3	18:XR:74:ARG:NH1	2.49	0.40
1:XA:1064:G:H1'	1:XA:1066:C:C6	2.56	0.40
1:XA:1064:G:O6	1:XA:1193:G:N1	2.54	0.40
1:XA:1287:A:H2	1:XA:1353:G:H1'	1.86	0.40
19:XS:40:ILE:HG12	19:XS:71:LEU:HG	2.03	0.40
29:Y4:37:SER:HB3	40:YG:108:ASN:HA	2.04	0.40
31:Y6:17:LYS:HA	31:Y6:17:LYS:HD3	1.85	0.40
35:YA:588:U:H1'	39:YF:90:PHE:HB3	2.04	0.40
35:YA:1060:U:H5'	35:YA:1061:U:H5	1.86	0.40
40:YG:59:GLU:OE1	40:YG:153:ARG:NH2	2.55	0.40
51:YV:12:TYR:CD1	51:YV:20:LEU:HD11	2.56	0.40
55:YZ:72:ARG:NH2	55:YZ:97:GLU:O	2.54	0.40
1:QA:272:C:H2'	1:QA:273:A:H8	1.87	0.40
1:QA:411:A:H62	1:QA:413:G:H21	1.70	0.40
1:QA:1070:U:OP1	5:QE:18:ARG:NH2	2.45	0.40
14:QN:27:CYS:SG	14:QN:28:GLY:N	2.94	0.40
19:QS:10:PHE:HB2	19:QS:39:THR:HB	2.02	0.40
34:R9:2:LYS:HE2	34:R9:33:LYS:HG2	2.04	0.40
35:RA:448:U:C4	35:RA:583:G:H1'	2.57	0.40
35:RA:848:G:H2'	35:RA:849:A:C8	2.57	0.40
1:XA:674:G:H2'	1:XA:675:A:C8	2.51	0.40
1:XA:737:A:H2'	1:XA:738:C:C6	2.56	0.40
6:XF:30:LEU:HD23	6:XF:75:LEU:HD11	2.03	0.40
13:XM:15:VAL:HA	13:XM:18:ALA:HB3	2.02	0.40
30:Y5:29:THR:HG21	35:YA:2815:C:H5'	2.03	0.40
35:YA:639:U:H2'	35:YA:640:C:C6	2.57	0.40
35:YA:2006:C:O2'	35:YA:2823:A:N3	2.51	0.40
35:YA:2025:C:H2'	35:YA:2026:C:C6	2.56	0.40
39:YF:6:VAL:HB	39:YF:24:LEU:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	QB	233/256 (91%)	202 (87%)	27 (12%)	4 (2%)	7	35
2	XB	234/256 (91%)	211 (90%)	21 (9%)	2 (1%)	14	47
3	QC	203/239 (85%)	186 (92%)	17 (8%)	0	100	100
3	XC	203/239 (85%)	188 (93%)	14 (7%)	1 (0%)	24	57
4	QD	206/209 (99%)	193 (94%)	11 (5%)	2 (1%)	12	44
4	XD	206/209 (99%)	187 (91%)	17 (8%)	2 (1%)	12	44
5	QE	149/162 (92%)	140 (94%)	9 (6%)	0	100	100
5	XE	149/162 (92%)	142 (95%)	7 (5%)	0	100	100
6	QF	99/101 (98%)	98 (99%)	1 (1%)	0	100	100
6	XF	99/101 (98%)	99 (100%)	0	0	100	100
7	QG	153/156 (98%)	144 (94%)	8 (5%)	1 (1%)	18	51
7	XG	153/156 (98%)	147 (96%)	6 (4%)	0	100	100
8	QH	135/138 (98%)	129 (96%)	6 (4%)	0	100	100
8	XH	135/138 (98%)	129 (96%)	6 (4%)	0	100	100
9	QI	125/128 (98%)	112 (90%)	13 (10%)	0	100	100
9	XI	124/128 (97%)	113 (91%)	11 (9%)	0	100	100
10	QJ	97/105 (92%)	85 (88%)	12 (12%)	0	100	100
10	XJ	94/105 (90%)	80 (85%)	13 (14%)	1 (1%)	11	43
11	QK	117/129 (91%)	107 (92%)	10 (8%)	0	100	100
11	XK	114/129 (88%)	105 (92%)	9 (8%)	0	100	100
12	QL	123/132 (93%)	110 (89%)	11 (9%)	2 (2%)	7	36
12	XL	120/132 (91%)	103 (86%)	16 (13%)	1 (1%)	16	49
13	QM	118/126 (94%)	102 (86%)	13 (11%)	3 (2%)	4	28
13	XM	117/126 (93%)	96 (82%)	21 (18%)	0	100	100
14	QN	58/61 (95%)	53 (91%)	4 (7%)	1 (2%)	7	35
14	XN	58/61 (95%)	54 (93%)	3 (5%)	1 (2%)	7	35
15	QO	86/89 (97%)	80 (93%)	6 (7%)	0	100	100
15	XO	85/89 (96%)	84 (99%)	1 (1%)	0	100	100
16	QP	82/88 (93%)	78 (95%)	4 (5%)	0	100	100
16	XP	82/88 (93%)	78 (95%)	4 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	QQ	98/105 (93%)	93 (95%)	5 (5%)	0	100	100
17	XQ	98/105 (93%)	93 (95%)	5 (5%)	0	100	100
18	QR	68/88 (77%)	64 (94%)	4 (6%)	0	100	100
18	XR	68/88 (77%)	64 (94%)	4 (6%)	0	100	100
19	QS	81/93 (87%)	69 (85%)	11 (14%)	1 (1%)	10	41
19	XS	81/93 (87%)	75 (93%)	6 (7%)	0	100	100
20	QT	97/106 (92%)	90 (93%)	7 (7%)	0	100	100
20	XT	97/106 (92%)	88 (91%)	6 (6%)	3 (3%)	3	25
21	QU	23/27 (85%)	20 (87%)	2 (9%)	1 (4%)	2	18
21	XU	23/27 (85%)	22 (96%)	0	1 (4%)	2	18
24	QY	82/84 (98%)	70 (85%)	10 (12%)	2 (2%)	4	29
24	QZ	82/84 (98%)	72 (88%)	10 (12%)	0	100	100
24	XY	82/84 (98%)	71 (87%)	8 (10%)	3 (4%)	2	21
24	XZ	82/84 (98%)	70 (85%)	11 (13%)	1 (1%)	10	41
25	R0	79/85 (93%)	72 (91%)	6 (8%)	1 (1%)	9	39
25	Y0	80/85 (94%)	72 (90%)	8 (10%)	0	100	100
26	R1	92/98 (94%)	82 (89%)	10 (11%)	0	100	100
26	Y1	95/98 (97%)	91 (96%)	3 (3%)	1 (1%)	11	43
27	R2	67/72 (93%)	61 (91%)	5 (8%)	1 (2%)	8	37
27	Y2	67/72 (93%)	63 (94%)	2 (3%)	2 (3%)	3	25
28	R3	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
28	Y3	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
29	R4	67/71 (94%)	46 (69%)	17 (25%)	4 (6%)	1	12
29	Y4	67/71 (94%)	54 (81%)	12 (18%)	1 (2%)	8	37
30	R5	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
30	Y5	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
31	R6	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
31	Y6	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
32	R7	45/49 (92%)	45 (100%)	0	0	100	100
32	Y7	46/49 (94%)	46 (100%)	0	0	100	100
33	R8	62/65 (95%)	54 (87%)	6 (10%)	2 (3%)	3	24

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	Y8	62/65 (95%)	56 (90%)	4 (6%)	2 (3%)	3	24
34	R9	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
34	Y9	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
37	RD	270/276 (98%)	244 (90%)	22 (8%)	4 (2%)	8	37
37	YD	272/276 (99%)	263 (97%)	9 (3%)	0	100	100
38	RE	203/206 (98%)	179 (88%)	20 (10%)	4 (2%)	6	32
38	YE	202/206 (98%)	191 (95%)	9 (4%)	2 (1%)	12	44
39	RF	200/210 (95%)	195 (98%)	5 (2%)	0	100	100
39	YF	200/210 (95%)	184 (92%)	14 (7%)	2 (1%)	12	44
40	RG	179/182 (98%)	152 (85%)	24 (13%)	3 (2%)	7	35
40	YG	179/182 (98%)	151 (84%)	26 (14%)	2 (1%)	11	43
41	RH	172/180 (96%)	137 (80%)	29 (17%)	6 (4%)	3	23
41	YH	172/180 (96%)	164 (95%)	8 (5%)	0	100	100
42	RI	143/148 (97%)	117 (82%)	20 (14%)	6 (4%)	2	19
42	YI	144/148 (97%)	123 (85%)	19 (13%)	2 (1%)	9	38
43	RN	136/140 (97%)	117 (86%)	17 (12%)	2 (2%)	8	37
43	YN	136/140 (97%)	118 (87%)	16 (12%)	2 (2%)	8	37
44	RO	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
44	YO	120/122 (98%)	114 (95%)	5 (4%)	1 (1%)	16	49
45	RP	148/150 (99%)	125 (84%)	19 (13%)	4 (3%)	4	27
45	YP	147/150 (98%)	138 (94%)	7 (5%)	2 (1%)	9	38
46	RQ	139/141 (99%)	121 (87%)	13 (9%)	5 (4%)	2	22
46	YQ	139/141 (99%)	131 (94%)	8 (6%)	0	100	100
47	RR	115/118 (98%)	108 (94%)	6 (5%)	1 (1%)	14	47
47	YR	115/118 (98%)	103 (90%)	11 (10%)	1 (1%)	14	47
48	RS	109/112 (97%)	93 (85%)	15 (14%)	1 (1%)	14	47
48	YS	109/112 (97%)	93 (85%)	16 (15%)	0	100	100
49	RT	135/146 (92%)	119 (88%)	15 (11%)	1 (1%)	18	51
49	YT	135/146 (92%)	119 (88%)	16 (12%)	0	100	100
50	RU	115/118 (98%)	106 (92%)	8 (7%)	1 (1%)	14	47
50	YU	115/118 (98%)	107 (93%)	7 (6%)	1 (1%)	14	47

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	RV	99/101 (98%)	90 (91%)	9 (9%)	0	100	100
51	YV	99/101 (98%)	91 (92%)	7 (7%)	1 (1%)	12	44
52	RW	111/113 (98%)	105 (95%)	6 (5%)	0	100	100
52	YW	111/113 (98%)	105 (95%)	6 (5%)	0	100	100
53	RX	90/96 (94%)	86 (96%)	4 (4%)	0	100	100
53	YX	90/96 (94%)	86 (96%)	3 (3%)	1 (1%)	11	43
54	RY	105/110 (96%)	94 (90%)	11 (10%)	0	100	100
54	YY	105/110 (96%)	101 (96%)	3 (3%)	1 (1%)	12	44
55	RZ	181/206 (88%)	166 (92%)	13 (7%)	2 (1%)	11	43
55	YZ	181/206 (88%)	168 (93%)	13 (7%)	0	100	100
All	All	11789/12464 (95%)	10734 (91%)	950 (8%)	105 (1%)	14	47

All (105) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	QB	208	ILE
14	QN	17	LYS
21	QU	3	LYS
24	QY	82	TYR
27	R2	47	ASN
29	R4	40	HIS
33	R8	29	LYS
33	R8	30	ARG
41	RH	152	ARG
42	RI	132	PRO
42	RI	143	SER
42	RI	144	VAL
43	RN	22	THR
45	RP	27	HIS
45	RP	57	THR
45	RP	108	LYS
46	RQ	85	LYS
55	RZ	53	ILE
2	XB	236	TYR
12	XL	105	TYR
14	XN	17	LYS
20	XT	73	HIS
21	XU	3	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	XY	82	TYR
33	Y8	30	ARG
42	YI	145	VAL
43	YN	22	THR
47	YR	4	LEU
51	YV	49	THR
4	QD	155	LEU
12	QL	105	TYR
12	QL	128	ALA
29	R4	3	GLU
29	R4	11	PRO
29	R4	41	PRO
37	RD	238	GLY
37	RD	243	GLY
38	RE	145	LYS
41	RH	10	PRO
41	RH	86	GLU
50	RU	92	ARG
4	XD	155	LEU
24	XZ	50	HIS
26	Y1	83	GLU
27	Y2	71	ASN
33	Y8	29	LYS
39	YF	129	PHE
40	YG	137	GLU
42	YI	15	VAL
45	YP	36	LYS
50	YU	92	ARG
2	QB	9	GLU
4	QD	156	GLU
13	QM	12	ASN
19	QS	28	LYS
24	QY	50	HIS
37	RD	36	PRO
38	RE	55	ASN
38	RE	74	PRO
40	RG	117	PHE
46	RQ	25	ASP
47	RR	4	LEU
55	RZ	52	SER
10	XJ	56	HIS
29	Y4	47	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	YX	68	ARG
25	R0	47	PRO
38	RE	83	ASP
40	RG	81	LYS
40	RG	116	ASP
41	RH	15	VAL
41	RH	87	LEU
42	RI	134	PRO
4	XD	156	GLU
24	XY	50	HIS
24	XY	83	HIS
39	YF	67	GLN
40	YG	81	LYS
7	QG	8	GLU
13	QM	67	GLU
42	RI	10	GLU
42	RI	133	HIS
43	RN	36	GLY
45	RP	36	LYS
46	RQ	105	GLU
27	Y2	70	GLN
38	YE	30	PRO
43	YN	23	LEU
45	YP	29	LYS
2	QB	231	GLU
2	QB	233	SER
13	QM	9	ILE
41	RH	154	PRO
46	RQ	67	ARG
48	RS	57	LYS
49	RT	109	GLU
2	XB	233	SER
3	XC	4	LYS
38	YE	145	LYS
44	YO	97	ARG
46	RQ	66	ILE
54	YY	10	GLY
20	XT	98	PRO
37	RD	123	ALA
20	XT	96	GLY

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%)	196 (97%)	7 (3%)	32	57
2	XB	204/220 (93%)	201 (98%)	3 (2%)	57	71
3	QC	159/188 (85%)	155 (98%)	4 (2%)	42	63
3	XC	159/188 (85%)	156 (98%)	3 (2%)	50	68
4	QD	180/181 (99%)	175 (97%)	5 (3%)	38	61
4	XD	180/181 (99%)	180 (100%)	0	100	100
5	QE	116/123 (94%)	115 (99%)	1 (1%)	70	76
5	XE	116/123 (94%)	115 (99%)	1 (1%)	70	76
6	QF	90/90 (100%)	89 (99%)	1 (1%)	65	74
6	XF	90/90 (100%)	89 (99%)	1 (1%)	65	74
7	QG	126/127 (99%)	123 (98%)	3 (2%)	43	64
7	XG	126/127 (99%)	124 (98%)	2 (2%)	55	70
8	QH	118/119 (99%)	118 (100%)	0	100	100
8	XH	118/119 (99%)	117 (99%)	1 (1%)	73	77
9	QI	98/99 (99%)	93 (95%)	5 (5%)	21	48
9	XI	97/99 (98%)	95 (98%)	2 (2%)	47	66
10	QJ	89/92 (97%)	84 (94%)	5 (6%)	19	46
10	XJ	86/92 (94%)	85 (99%)	1 (1%)	63	73
11	QK	90/99 (91%)	88 (98%)	2 (2%)	45	65
11	XK	88/99 (89%)	87 (99%)	1 (1%)	65	74
12	QL	104/109 (95%)	103 (99%)	1 (1%)	68	75
12	XL	103/109 (94%)	102 (99%)	1 (1%)	68	75
13	QM	96/101 (95%)	95 (99%)	1 (1%)	68	75
13	XM	95/101 (94%)	93 (98%)	2 (2%)	47	66
14	QN	49/50 (98%)	48 (98%)	1 (2%)	48	67
14	XN	49/50 (98%)	49 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	QO	79/80 (99%)	79 (100%)	0	100	100
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%)	70 (97%)	2 (3%)	38	61
17	QQ	95/97 (98%)	94 (99%)	1 (1%)	65	74
17	XQ	95/97 (98%)	95 (100%)	0	100	100
18	QR	61/77 (79%)	58 (95%)	3 (5%)	22	48
18	XR	61/77 (79%)	60 (98%)	1 (2%)	55	70
19	QS	72/80 (90%)	70 (97%)	2 (3%)	38	61
19	XS	69/80 (86%)	69 (100%)	0	100	100
20	QT	76/82 (93%)	76 (100%)	0	100	100
20	XT	76/82 (93%)	74 (97%)	2 (3%)	40	62
21	QU	20/22 (91%)	20 (100%)	0	100	100
21	XU	20/22 (91%)	20 (100%)	0	100	100
24	QY	78/78 (100%)	76 (97%)	2 (3%)	40	62
24	QZ	78/78 (100%)	74 (95%)	4 (5%)	21	48
24	XY	78/78 (100%)	78 (100%)	0	100	100
24	XZ	78/78 (100%)	76 (97%)	2 (3%)	40	62
25	R0	65/67 (97%)	65 (100%)	0	100	100
25	Y0	65/67 (97%)	63 (97%)	2 (3%)	35	59
26	R1	79/83 (95%)	77 (98%)	2 (2%)	42	63
26	Y1	82/83 (99%)	81 (99%)	1 (1%)	63	73
27	R2	64/67 (96%)	62 (97%)	2 (3%)	35	59
27	Y2	64/67 (96%)	63 (98%)	1 (2%)	55	70
28	R3	51/52 (98%)	50 (98%)	1 (2%)	48	67
28	Y3	51/52 (98%)	51 (100%)	0	100	100
29	R4	62/63 (98%)	54 (87%)	8 (13%)	4	21
29	Y4	62/63 (98%)	60 (97%)	2 (3%)	34	59
30	R5	51/52 (98%)	51 (100%)	0	100	100
30	Y5	51/52 (98%)	51 (100%)	0	100	100
31	R6	51/52 (98%)	48 (94%)	3 (6%)	18	44

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	Y6	51/52 (98%)	49 (96%)	2 (4%)	28	54
32	R7	40/42 (95%)	40 (100%)	0	100	100
32	Y7	41/42 (98%)	41 (100%)	0	100	100
33	R8	54/55 (98%)	50 (93%)	4 (7%)	13	37
33	Y8	54/55 (98%)	52 (96%)	2 (4%)	30	56
34	R9	34/34 (100%)	33 (97%)	1 (3%)	37	60
34	Y9	34/34 (100%)	34 (100%)	0	100	100
37	RD	214/218 (98%)	210 (98%)	4 (2%)	50	68
37	YD	216/218 (99%)	215 (100%)	1 (0%)	81	80
38	RE	165/166 (99%)	157 (95%)	8 (5%)	23	49
38	YE	164/166 (99%)	163 (99%)	1 (1%)	78	79
39	RF	161/166 (97%)	159 (99%)	2 (1%)	63	73
39	YF	161/166 (97%)	160 (99%)	1 (1%)	78	79
40	RG	155/156 (99%)	151 (97%)	4 (3%)	40	62
40	YG	155/156 (99%)	153 (99%)	2 (1%)	61	72
41	RH	145/148 (98%)	142 (98%)	3 (2%)	47	66
41	YH	144/148 (97%)	141 (98%)	3 (2%)	47	66
42	RI	122/124 (98%)	116 (95%)	6 (5%)	22	48
42	YI	122/124 (98%)	119 (98%)	3 (2%)	42	63
43	RN	117/119 (98%)	116 (99%)	1 (1%)	70	76
43	YN	117/119 (98%)	116 (99%)	1 (1%)	70	76
44	RO	100/100 (100%)	100 (100%)	0	100	100
44	YO	100/100 (100%)	99 (99%)	1 (1%)	68	75
45	RP	116/116 (100%)	114 (98%)	2 (2%)	53	70
45	YP	115/116 (99%)	113 (98%)	2 (2%)	53	70
46	RQ	111/111 (100%)	106 (96%)	5 (4%)	24	50
46	YQ	111/111 (100%)	111 (100%)	0	100	100
47	RR	100/101 (99%)	99 (99%)	1 (1%)	68	75
47	YR	100/101 (99%)	99 (99%)	1 (1%)	68	75
48	RS	87/88 (99%)	84 (97%)	3 (3%)	32	57
48	YS	87/88 (99%)	86 (99%)	1 (1%)	65	74

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	RT	120/127 (94%)	115 (96%)	5 (4%)	26	52
49	YT	120/127 (94%)	117 (98%)	3 (2%)	42	63
50	RU	93/94 (99%)	92 (99%)	1 (1%)	65	74
50	YU	93/94 (99%)	91 (98%)	2 (2%)	45	65
51	RV	82/82 (100%)	73 (89%)	9 (11%)	6	26
51	YV	82/82 (100%)	80 (98%)	2 (2%)	43	64
52	RW	92/92 (100%)	92 (100%)	0	100	100
52	YW	92/92 (100%)	90 (98%)	2 (2%)	45	65
53	RX	74/78 (95%)	74 (100%)	0	100	100
53	YX	74/78 (95%)	73 (99%)	1 (1%)	59	71
54	RY	88/91 (97%)	88 (100%)	0	100	100
54	YY	88/91 (97%)	88 (100%)	0	100	100
55	RZ	162/179 (90%)	161 (99%)	1 (1%)	78	79
55	YZ	162/179 (90%)	159 (98%)	3 (2%)	50	68
All	All	10001/10378 (96%)	9812 (98%)	189 (2%)	50	68

All (189) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	QB	11	LEU
2	QB	15	VAL
2	QB	114	ARG
2	QB	121	LEU
2	QB	132	LYS
2	QB	209	ARG
2	QB	226	ARG
3	QC	16	ARG
3	QC	105	GLU
3	QC	132	ARG
3	QC	193	TYR
4	QD	17	VAL
4	QD	33	MET
4	QD	67	ILE
4	QD	85	LYS
4	QD	107	ARG
5	QE	47	LYS
6	QF	54	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	QG	10	ARG
7	QG	23	VAL
7	QG	155	ARG
9	QI	4	TYR
9	QI	18	PHE
9	QI	20	ARG
9	QI	26	VAL
9	QI	70	LYS
10	QJ	25	GLU
10	QJ	43	ARG
10	QJ	55	LYS
10	QJ	60	ARG
10	QJ	79	ARG
11	QK	12	ARG
11	QK	92	GLU
12	QL	59	ARG
13	QM	11	ARG
14	QN	12	ARG
17	QQ	101	ARG
18	QR	34	TYR
18	QR	54	ARG
18	QR	83	GLU
19	QS	3	ARG
19	QS	28	LYS
24	QY	7	GLU
24	QY	18	GLU
24	QZ	7	GLU
24	QZ	22	ARG
24	QZ	36	ARG
24	QZ	63	GLU
26	R1	57	GLU
26	R1	87	PRO
27	R2	23	LYS
27	R2	53	LEU
28	R3	43	ILE
29	R4	1	MET
29	R4	11	PRO
29	R4	13	ARG
29	R4	39	CYS
29	R4	42	PHE
29	R4	46	GLN
29	R4	48	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
29	R4	63	TYR
31	R6	10	LEU
31	R6	11	LEU
31	R6	25	LYS
33	R8	35	GLN
33	R8	46	ARG
33	R8	52	LYS
33	R8	65	GLU
34	R9	9	ARG
37	RD	7	LYS
37	RD	24	ILE
37	RD	25	THR
37	RD	273	ARG
38	RE	1	MET
38	RE	14	ILE
38	RE	57	LYS
38	RE	59	VAL
38	RE	64	LYS
38	RE	77	ILE
38	RE	79	ARG
38	RE	152	LYS
39	RF	89	VAL
39	RF	99	TYR
40	RG	55	LYS
40	RG	83	ARG
40	RG	115	ARG
40	RG	146	TYR
41	RH	116	GLU
41	RH	152	ARG
41	RH	154	PRO
42	RI	81	VAL
42	RI	85	GLU
42	RI	86	THR
42	RI	136	VAL
42	RI	138	ILE
42	RI	142	VAL
43	RN	61	ARG
45	RP	76	LYS
45	RP	125	VAL
46	RQ	5	ARG
46	RQ	18	LYS
46	RQ	87	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
46	RQ	91	GLU
46	RQ	93	TYR
47	RR	36	THR
48	RS	20	ARG
48	RS	76	LYS
48	RS	112	PHE
49	RT	95	ARG
49	RT	101	PHE
49	RT	108	ARG
49	RT	109	GLU
49	RT	128	GLU
50	RU	90	VAL
51	RV	19	LYS
51	RV	21	ARG
51	RV	39	LEU
51	RV	49	THR
51	RV	70	ILE
51	RV	72	VAL
51	RV	79	VAL
51	RV	95	LEU
51	RV	99	ILE
55	RZ	135	GLU
2	XB	17	PHE
2	XB	122	PHE
2	XB	236	TYR
3	XC	72	LYS
3	XC	111	LEU
3	XC	140	ARG
5	XE	155	GLU
6	XF	2	ARG
7	XG	57	GLU
7	XG	111	ARG
8	XH	60	ARG
9	XI	102	LEU
9	XI	114	TYR
10	XJ	29	ARG
11	XK	96	ARG
12	XL	98	TYR
13	XM	58	GLU
13	XM	102	ARG
16	XP	26	ARG
16	XP	32	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	XR	42	ARG
20	XT	48	LYS
20	XT	90	GLN
24	XZ	8	GLU
24	XZ	40	GLU
25	Y0	41	ARG
25	Y0	82	ARG
26	Y1	53	VAL
27	Y2	16	LEU
29	Y4	48	ARG
29	Y4	67	TYR
31	Y6	4	GLU
31	Y6	12	GLU
33	Y8	48	PHE
33	Y8	50	LEU
37	YD	88	ARG
38	YE	73	GLU
39	YF	127	GLU
40	YG	18	GLU
40	YG	55	LYS
41	YH	3	ARG
41	YH	13	LYS
41	YH	124	GLU
42	YI	10	GLU
42	YI	11	ASN
42	YI	12	LEU
43	YN	98	VAL
44	YO	108	GLU
45	YP	36	LYS
45	YP	108	LYS
47	YR	57	ARG
48	YS	111	GLU
49	YT	96	ARG
49	YT	111	ARG
49	YT	133	GLU
50	YU	44	ASN
50	YU	90	VAL
51	YV	5	VAL
51	YV	18	LEU
52	YW	41	LYS
52	YW	60	ASN
53	YX	68	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
55	YZ	29	TYR
55	YZ	94	GLU
55	YZ	168	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
3	QC	6	HIS
3	QC	69	HIS
3	QC	108	ASN
4	QD	161	ASN
6	QF	32	ASN
7	QG	68	ASN
7	QG	148	ASN
9	QI	3	GLN
9	QI	34	ASN
9	QI	73	GLN
13	QM	40	ASN
13	QM	77	ASN
13	QM	101	GLN
13	QM	106	ASN
15	QO	37	ASN
15	QO	50	HIS
18	QR	63	GLN
29	R4	46	GLN
34	R9	34	GLN
37	RD	46	GLN
38	RE	137	HIS
39	RF	203	GLN
40	RG	40	ASN
40	RG	41	GLN
43	RN	94	HIS
43	RN	101	HIS
46	RQ	57	HIS
47	RR	71	GLN
48	RS	61	ASN
49	RT	90	GLN
50	RU	75	ASN
52	RW	62	HIS
53	RX	55	ASN
4	XD	77	ASN
4	XD	161	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	XG	109	ASN
7	XG	122	HIS
9	XI	31	GLN
10	XJ	62	HIS
10	XJ	84	GLN
13	XM	101	GLN
16	XP	13	HIS
17	XQ	45	HIS
24	XZ	28	ASN
29	Y4	40	HIS
37	YD	201	HIS
40	YG	132	ASN
42	YI	11	ASN
43	YN	56	ASN
46	YQ	57	HIS
48	YS	34	HIS
52	YW	60	ASN
54	YY	92	ASN
55	YZ	34	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1508/1521 (99%)	293 (19%)	33 (2%)
1	XA	1505/1521 (98%)	302 (20%)	40 (2%)
22	QV	77/77 (100%)	8 (10%)	1 (1%)
22	XV	77/77 (100%)	9 (11%)	1 (1%)
23	QX	16/20 (80%)	7 (43%)	2 (12%)
23	XX	16/20 (80%)	8 (50%)	0
35	RA	2888/2915 (99%)	623 (21%)	37 (1%)
35	YA	2875/2915 (98%)	579 (20%)	28 (0%)
36	RB	119/124 (95%)	24 (20%)	1 (0%)
36	YB	119/124 (95%)	17 (14%)	1 (0%)
56	ZA	1/3 (33%)	0	0
56	ZB	1/3 (33%)	0	0
All	All	9202/9320 (98%)	1870 (20%)	144 (1%)

All (1870) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	4	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	QA	5	U
1	QA	6	G
1	QA	22	G
1	QA	32	A
1	QA	39	G
1	QA	47	C
1	QA	48	C
1	QA	50	A
1	QA	51	A
1	QA	61	G
1	QA	66	G
1	QA	79	G
1	QA	80	G
1	QA	89	U
1	QA	90	C
1	QA	92	G
1	QA	93	U
1	QA	101	A
1	QA	116	A
1	QA	120	A
1	QA	121	C
1	QA	131	C
1	QA	182	U
1	QA	185	A
1	QA	188	U
1	QA	189	U
1	QA	190	G
1	QA	191(A)	G
1	QA	191(D)	U
1	QA	191(E)	G
1	QA	195	A
1	QA	197	A
1	QA	198	G
1	QA	208	U
1	QA	209	U
1	QA	210	U
1	QA	220	G
1	QA	247	G
1	QA	251	G
1	QA	266	G
1	QA	267	C
1	QA	270	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	QA	275	G
1	QA	281	G
1	QA	289	G
1	QA	321	A
1	QA	328	C
1	QA	332	G
1	QA	345	C
1	QA	346	G
1	QA	347	G
1	QA	350	G
1	QA	351	G
1	QA	352	C
1	QA	353	A
1	QA	354	G
1	QA	356	A
1	QA	367	U
1	QA	372	C
1	QA	373	A
1	QA	384	G
1	QA	397	A
1	QA	398	C
1	QA	406	G
1	QA	412	A
1	QA	414	A
1	QA	422	C
1	QA	423	G
1	QA	424	G
1	QA	429	U
1	QA	439	A
1	QA	452	A
1	QA	465	A
1	QA	466	C
1	QA	467	G
1	QA	478	A
1	QA	482	A
1	QA	484	G
1	QA	485	G
1	QA	494	U
1	QA	497	U
1	QA	505	G
1	QA	511	C
1	QA	518	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	QA	519	C
1	QA	521	G
1	QA	527	G
1	QA	530	G
1	QA	531	U
1	QA	532	A
1	QA	533	A
1	QA	545	C
1	QA	547	A
1	QA	548	G
1	QA	559	A
1	QA	564	C
1	QA	572	A
1	QA	573	A
1	QA	576	G
1	QA	577	G
1	QA	579	G
1	QA	596	C
1	QA	607	A
1	QA	618	C
1	QA	630	G
1	QA	642	A
1	QA	652	U
1	QA	653	A
1	QA	665	A
1	QA	686	U
1	QA	688	G
1	QA	702	A
1	QA	703	G
1	QA	704	A
1	QA	721	G
1	QA	722	A
1	QA	723	U
1	QA	724	G
1	QA	731	G
1	QA	749	C
1	QA	755	G
1	QA	760	G
1	QA	774	G
1	QA	777	A
1	QA	786	G
1	QA	793	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	QA	794	A
1	QA	813	U
1	QA	816	A
1	QA	817	C
1	QA	818	G
1	QA	819	A
1	QA	821	G
1	QA	828	A
1	QA	841	U
1	QA	842	C
1	QA	843	U
1	QA	848	C
1	QA	859	A
1	QA	872	A
1	QA	884	U
1	QA	914	A
1	QA	916	G
1	QA	926	G
1	QA	927	G
1	QA	934	C
1	QA	935	A
1	QA	942	G
1	QA	960	U
1	QA	961	U
1	QA	966	G
1	QA	968	A
1	QA	969	A
1	QA	972	C
1	QA	974	A
1	QA	975	A
1	QA	976	G
1	QA	977	A
1	QA	980	C
1	QA	982	U
1	QA	991	U
1	QA	992	U
1	QA	993	G
1	QA	994	A
1	QA	999	U
1	QA	1000	A
1	QA	1001	G
1	QA	1003	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	QA	1004	A
1	QA	1005	A
1	QA	1006	C
1	QA	1007	C
1	QA	1008	C
1	QA	1009	G
1	QA	1024	G
1	QA	1025	U
1	QA	1026	G
1	QA	1029	G
1	QA	1030	C
1	QA	1031	G
1	QA	1032	A
1	QA	1032(A)	G
1	QA	1033	G
1	QA	1034	G
1	QA	1036	G
1	QA	1039	C
1	QA	1046	A
1	QA	1053	G
1	QA	1054	C
1	QA	1055	A
1	QA	1064	G
1	QA	1065	U
1	QA	1066	C
1	QA	1068	G
1	QA	1070	U
1	QA	1081	G
1	QA	1086	U
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
1	QA	1125	U
1	QA	1127	G
1	QA	1129	C
1	QA	1130	A
1	QA	1131	G
1	QA	1136	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	QA	1137	C
1	QA	1138	G
1	QA	1139	G
1	QA	1140	C
1	QA	1146	A
1	QA	1157	A
1	QA	1158	C
1	QA	1159	U
1	QA	1160	G
1	QA	1171	G
1	QA	1177	G
1	QA	1178	G
1	QA	1181	G
1	QA	1182	G
1	QA	1183	A
1	QA	1187	G
1	QA	1196	U
1	QA	1212	U
1	QA	1213	A
1	QA	1227	A
1	QA	1233	G
1	QA	1238	A
1	QA	1240	U
1	QA	1241	G
1	QA	1257	U
1	QA	1258	G
1	QA	1260	C
1	QA	1268	A
1	QA	1270	C
1	QA	1273	G
1	QA	1278	U
1	QA	1280	A
1	QA	1281	U
1	QA	1285	A
1	QA	1286	A
1	QA	1287	A
1	QA	1288	A
1	QA	1300	G
1	QA	1303	C
1	QA	1305	G
1	QA	1318	A
1	QA	1319	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	QA	1320	C
1	QA	1323	G
1	QA	1331	G
1	QA	1335	C
1	QA	1346	A
1	QA	1347	G
1	QA	1348	U
1	QA	1353	G
1	QA	1368	G
1	QA	1370	G
1	QA	1398	A
1	QA	1406	U
1	QA	1419	G
1	QA	1442	G
1	QA	1446	A
1	QA	1450	U
1	QA	1451	A
1	QA	1452	C
1	QA	1453	G
1	QA	1454	G
1	QA	1492	A
1	QA	1493	A
1	QA	1497	G
1	QA	1499	A
1	QA	1504	G
1	QA	1506	U
1	QA	1517	G
1	QA	1519	A
1	QA	1520	G
1	QA	1529	G
1	QA	1530	G
1	QA	1532	U
1	QA	1533	C
1	QA	1534	A
1	QA	1536	C
1	QA	1537	U
1	QA	1538	C
1	QA	1539	C
1	QA	1540	U
1	QA	1541	U
22	QV	2	G
22	QV	20	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	QV	21	A
22	QV	22	G
22	QV	46	G
22	QV	47	U
22	QV	49	G
22	QV	76	A
23	QX	8	A
23	QX	10	G
23	QX	11	U
23	QX	12	A
23	QX	13	A
23	QX	14	A
23	QX	19	U
35	RA	9	U
35	RA	15	G
35	RA	27	G
35	RA	34	C
35	RA	35	G
35	RA	46	C
35	RA	60	G
35	RA	61	G
35	RA	64	A
35	RA	71	A
35	RA	74	A
35	RA	75	G
35	RA	83	G
35	RA	91	A
35	RA	95	G
35	RA	99	U
35	RA	101	G
35	RA	102	G
35	RA	118	A
35	RA	119	A
35	RA	120	U
35	RA	125	G
35	RA	129	C
35	RA	139	G
35	RA	140	A
35	RA	144	C
35	RA	155	C
35	RA	172	C
35	RA	173	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	RA	174	C
35	RA	175	G
35	RA	181	A
35	RA	182	A
35	RA	196	A
35	RA	199	A
35	RA	204	A
35	RA	205	G
35	RA	215	G
35	RA	216	A
35	RA	221	A
35	RA	222	A
35	RA	228	A
35	RA	229	A
35	RA	233	A
35	RA	245	G
35	RA	248	G
35	RA	252	G
35	RA	265	A
35	RA	266	G
35	RA	270(B)	A
35	RA	270(J)	G
35	RA	270(K)	C
35	RA	270(L)	U
35	RA	270(M)	U
35	RA	270(N)	G
35	RA	270(O)	U
35	RA	270(P)	C
35	RA	270(Q)	C
35	RA	270(Z)	U
35	RA	271(C)	U
35	RA	271	G
35	RA	273(D)	C
35	RA	274	G
35	RA	275	G
35	RA	278	A
35	RA	283	A
35	RA	289	A
35	RA	311	A
35	RA	316	C
35	RA	324	A
35	RA	329	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	RA	330	A
35	RA	332	A
35	RA	345	A
35	RA	353	G
35	RA	355	G
35	RA	358	U
35	RA	362	U
35	RA	363	G
35	RA	363(D)	G
35	RA	371	A
35	RA	372	G
35	RA	373	U
35	RA	386	G
35	RA	388	G
35	RA	396	G
35	RA	405	U
35	RA	406	G
35	RA	411	G
35	RA	412	A
35	RA	428	A
35	RA	443	A
35	RA	444	C
35	RA	448	U
35	RA	451	C
35	RA	456	C
35	RA	457	A
35	RA	467	G
35	RA	470	A
35	RA	481	G
35	RA	494	G
35	RA	505	A
35	RA	508	G
35	RA	509	C
35	RA	512	G
35	RA	513	A
35	RA	529	A
35	RA	531	C
35	RA	532	A
35	RA	533	G
35	RA	537	C
35	RA	549	G
35	RA	563	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	RA	573	G
35	RA	575	A
35	RA	587	C
35	RA	588	U
35	RA	603	A
35	RA	607	U
35	RA	613	U
35	RA	614	U
35	RA	615	G
35	RA	617	G
35	RA	622	G
35	RA	627	A
35	RA	634	C
35	RA	637	A
35	RA	645	C
35	RA	646	A
35	RA	651	G
35	RA	654	A
35	RA	654(A)	G
35	RA	654(B)	C
35	RA	654(G)	C
35	RA	654(Q)	C
35	RA	654(R)	C
35	RA	654(S)	G
35	RA	654(T)	C
35	RA	686	G
35	RA	708	C
35	RA	717	G
35	RA	722	A
35	RA	730	C
35	RA	753	C
35	RA	765	G
35	RA	775	G
35	RA	776	G
35	RA	782	A
35	RA	784	A
35	RA	785	G
35	RA	788	A
35	RA	789	A
35	RA	792	G
35	RA	793	A
35	RA	805	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	RA	812	C
35	RA	819	A
35	RA	827	U
35	RA	828	U
35	RA	830	G
35	RA	831	G
35	RA	845	G
35	RA	846	C
35	RA	854	G
35	RA	856	C
35	RA	857	C
35	RA	859	G
35	RA	866	A
35	RA	872	A
35	RA	878	A
35	RA	882	G
35	RA	883	G
35	RA	884	C
35	RA	886	C
35	RA	888	C
35	RA	889	C
35	RA	890	A
35	RA	894	C
35	RA	895	U
35	RA	896	A
35	RA	897	C
35	RA	899	A
35	RA	900	A
35	RA	910	A
35	RA	915	C
35	RA	917	A
35	RA	919	G
35	RA	928	G
35	RA	932	G
35	RA	938	G
35	RA	941	A
35	RA	945	A
35	RA	946	G
35	RA	953	A
35	RA	957	A
35	RA	959	A
35	RA	961	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	RA	968	G
35	RA	973	A
35	RA	974	G
35	RA	983	A
35	RA	990	A
35	RA	991	C
35	RA	996	A
35	RA	1012	U
35	RA	1013	C
35	RA	1015	G
35	RA	1017	G
35	RA	1022	G
35	RA	1023	U
35	RA	1025	G
35	RA	1026	U
35	RA	1027	A
35	RA	1033	U
35	RA	1034	G
35	RA	1044	G
35	RA	1046	A
35	RA	1047	G
35	RA	1049	C
35	RA	1053	C
35	RA	1061	U
35	RA	1065	U
35	RA	1067	A
35	RA	1070	A
35	RA	1071	G
35	RA	1073	A
35	RA	1075	C
35	RA	1083	U
35	RA	1086	A
35	RA	1087	G
35	RA	1088	A
35	RA	1089	G
35	RA	1095	A
35	RA	1096	A
35	RA	1111	A
35	RA	1130	U
35	RA	1131	G
35	RA	1135	C
35	RA	1136	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	RA	1139	G
35	RA	1141	U
35	RA	1142(A)	A
35	RA	1143	A
35	RA	1148	A
35	RA	1155	A
35	RA	1156	A
35	RA	1173	G
35	RA	1174	A
35	RA	1175	U
35	RA	1176	G
35	RA	1177	A
35	RA	1178	C
35	RA	1180	C
35	RA	1195	G
35	RA	1203	G
35	RA	1204	A
35	RA	1205	U
35	RA	1210	A
35	RA	1212	G
35	RA	1220	A
35	RA	1221	C
35	RA	1224	G
35	RA	1236	G
35	RA	1247	A
35	RA	1250	G
35	RA	1252	G
35	RA	1253	A
35	RA	1255	U
35	RA	1256	G
35	RA	1265	A
35	RA	1272	A
35	RA	1275	A
35	RA	1281	G
35	RA	1286	A
35	RA	1300	U
35	RA	1301	A
35	RA	1308	A
35	RA	1311	G
35	RA	1314	C
35	RA	1319	G
35	RA	1329	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	RA	1341	U
35	RA	1352	U
35	RA	1359	A
35	RA	1365	A
35	RA	1368	G
35	RA	1378	A
35	RA	1379	A
35	RA	1380	G
35	RA	1384	A
35	RA	1385	G
35	RA	1391	U
35	RA	1395	A
35	RA	1407	C
35	RA	1408	C
35	RA	1416	G
35	RA	1417	C
35	RA	1419	A
35	RA	1420	U
35	RA	1421	G
35	RA	1428	C
35	RA	1437	C
35	RA	1444(A)	A
35	RA	1449	A
35	RA	1449(A)	G
35	RA	1453	A
35	RA	1455	G
35	RA	1458	C
35	RA	1461	G
35	RA	1466	G
35	RA	1467	C
35	RA	1471	A
35	RA	1475	G
35	RA	1476	C
35	RA	1478	G
35	RA	1482	U
35	RA	1483	G
35	RA	1487	G
35	RA	1488	G
35	RA	1490	A
35	RA	1493	C
35	RA	1497	U
35	RA	1505	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	RA	1509	C
35	RA	1510	A
35	RA	1521	G
35	RA	1523	U
35	RA	1526	G
35	RA	1535	U
35	RA	1536	A
35	RA	1537	C
35	RA	1538	G
35	RA	1540	G
35	RA	1543	A
35	RA	1544	C
35	RA	1545	A
35	RA	1547	C
35	RA	1554	A
35	RA	1558	A
35	RA	1559	G
35	RA	1560	G
35	RA	1566	A
35	RA	1569	A
35	RA	1578	U
35	RA	1580	A
35	RA	1585	C
35	RA	1586	A
35	RA	1587	A
35	RA	1592	C
35	RA	1598	C
35	RA	1603	A
35	RA	1608	A
35	RA	1640	C
35	RA	1648	C
35	RA	1651	G
35	RA	1654	A
35	RA	1674	G
35	RA	1688	U
35	RA	1695	G
35	RA	1696	G
35	RA	1698	A
35	RA	1699	G
35	RA	1700	A
35	RA	1725	G
35	RA	1728	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	RA	1729	A
35	RA	1730	U
35	RA	1731	G
35	RA	1743	G
35	RA	1756	G
35	RA	1762	A
35	RA	1763	G
35	RA	1764	G
35	RA	1769	G
35	RA	1773	A
35	RA	1776	G
35	RA	1780	A
35	RA	1782	C
35	RA	1791	A
35	RA	1800	C
35	RA	1801	G
35	RA	1802	A
35	RA	1811	G
35	RA	1816	G
35	RA	1820	U
35	RA	1828	G
35	RA	1829	A
35	RA	1847	A
35	RA	1853	A
35	RA	1858	G
35	RA	1864	U
35	RA	1869	G
35	RA	1872	A
35	RA	1878	G
35	RA	1881	C
35	RA	1882	C
35	RA	1888	G
35	RA	1889	A
35	RA	1903	G
35	RA	1906	G
35	RA	1913	A
35	RA	1927	A
35	RA	1929	G
35	RA	1930	G
35	RA	1931	U
35	RA	1936	A
35	RA	1938	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	RA	1941	C
35	RA	1948	G
35	RA	1955	U
35	RA	1963	U
35	RA	1965	C
35	RA	1966	A
35	RA	1967	C
35	RA	1970	A
35	RA	1971	A
35	RA	1972	A
35	RA	1980	G
35	RA	1982	C
35	RA	1992	G
35	RA	1993	U
35	RA	1996	C
35	RA	2004	G
35	RA	2020	A
35	RA	2021	C
35	RA	2022	U
35	RA	2023	G
35	RA	2026	C
35	RA	2031	A
35	RA	2032	G
35	RA	2033	A
35	RA	2034	U
35	RA	2043	C
35	RA	2052	G
35	RA	2055	C
35	RA	2056	G
35	RA	2059	A
35	RA	2060	A
35	RA	2061	G
35	RA	2062	A
35	RA	2063	C
35	RA	2069	G
35	RA	2092	U
35	RA	2093	G
35	RA	2111	C
35	RA	2112	G
35	RA	2113	U
35	RA	2116	G
35	RA	2117	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	RA	2119	A
35	RA	2127	G
35	RA	2128	C
35	RA	2130	U
35	RA	2131	G
35	RA	2132	U
35	RA	2134	A
35	RA	2136	C
35	RA	2139	C
35	RA	2145	C
35	RA	2147	G
35	RA	2148	G
35	RA	2153	G
35	RA	2161	C
35	RA	2165	G
35	RA	2167	U
35	RA	2168	G
35	RA	2169	A
35	RA	2170	A
35	RA	2171	A
35	RA	2173	A
35	RA	2178	C
35	RA	2189	U
35	RA	2190	G
35	RA	2192	G
35	RA	2198	A
35	RA	2210	G
35	RA	2212	A
35	RA	2213	U
35	RA	2215	G
35	RA	2225	A
35	RA	2226	C
35	RA	2238	G
35	RA	2239	G
35	RA	2243	U
35	RA	2246	G
35	RA	2275	C
35	RA	2278	A
35	RA	2279	G
35	RA	2280	G
35	RA	2282	G
35	RA	2283	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	RA	2302	G
35	RA	2305	A
35	RA	2306	C
35	RA	2307	G
35	RA	2308	G
35	RA	2309	A
35	RA	2311	A
35	RA	2312	U
35	RA	2319	G
35	RA	2320	A
35	RA	2321	G
35	RA	2325	G
35	RA	2334	G
35	RA	2343	C
35	RA	2347	C
35	RA	2350	C
35	RA	2354	G
35	RA	2358	G
35	RA	2372	G
35	RA	2382	G
35	RA	2383	G
35	RA	2385	C
35	RA	2392	A
35	RA	2394	C
35	RA	2402	C
35	RA	2403	C
35	RA	2406	U
35	RA	2410	G
35	RA	2411	A
35	RA	2422	A
35	RA	2423	U
35	RA	2425	A
35	RA	2428	G
35	RA	2429	G
35	RA	2430	A
35	RA	2435	A
35	RA	2439	A
35	RA	2440	C
35	RA	2441	C
35	RA	2445	G
35	RA	2448	A
35	RA	2450	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	RA	2469	A
35	RA	2471	C
35	RA	2472	G
35	RA	2475	C
35	RA	2476	A
35	RA	2482	G
35	RA	2491	U
35	RA	2502	G
35	RA	2505	G
35	RA	2518	A
35	RA	2519	U
35	RA	2524	G
35	RA	2527	C
35	RA	2529	G
35	RA	2535	G
35	RA	2540	C
35	RA	2542	A
35	RA	2543	G
35	RA	2554	U
35	RA	2566	A
35	RA	2567	G
35	RA	2569	G
35	RA	2572	A
35	RA	2573	C
35	RA	2578	G
35	RA	2585	U
35	RA	2602	A
35	RA	2609	U
35	RA	2610	C
35	RA	2612	C
35	RA	2615	U
35	RA	2629	A
35	RA	2630	G
35	RA	2646	C
35	RA	2654	A
35	RA	2655	G
35	RA	2665	A
35	RA	2673	G
35	RA	2682	U
35	RA	2689	U
35	RA	2690	C
35	RA	2702	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	RA	2703	C
35	RA	2712	U
35	RA	2712(A)	A
35	RA	2713	A
35	RA	2714	G
35	RA	2726	U
35	RA	2733	A
35	RA	2744	G
35	RA	2748	A
35	RA	2752	C
35	RA	2757	A
35	RA	2758	A
35	RA	2761	G
35	RA	2762	G
35	RA	2765	A
35	RA	2766	G
35	RA	2777	G
35	RA	2778	A
35	RA	2779	U
35	RA	2780	G
35	RA	2787	C
35	RA	2790	A
35	RA	2797	U
35	RA	2799	A
35	RA	2807	G
35	RA	2808	U
35	RA	2818	G
35	RA	2820	A
35	RA	2821	A
35	RA	2823	A
35	RA	2827	C
35	RA	2830	G
35	RA	2833	G
35	RA	2834	G
35	RA	2835	A
35	RA	2846	G
35	RA	2850	A
35	RA	2860	A
35	RA	2867	G
35	RA	2868	A
35	RA	2872	G
35	RA	2873	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	RA	2876	G
35	RA	2877	G
35	RA	2879	C
35	RA	2880	C
35	RA	2892	A
35	RA	2893	G
36	RB	2	C
36	RB	8	U
36	RB	13	A
36	RB	15	A
36	RB	19	G
36	RB	25	A
36	RB	27	C
36	RB	40	U
36	RB	41	U
36	RB	42	C
36	RB	45	A
36	RB	47	C
36	RB	53	A
36	RB	67	G
36	RB	73	A
36	RB	81	G
36	RB	88	C
36	RB	89	G
36	RB	92	G
36	RB	105	G
36	RB	108	C
36	RB	109	G
36	RB	117	G
36	RB	119	A
1	XA	5	U
1	XA	6	G
1	XA	9	G
1	XA	32	A
1	XA	39	G
1	XA	47	C
1	XA	48	C
1	XA	51	A
1	XA	61	G
1	XA	64	G
1	XA	65	U
1	XA	66	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	XA	75	C
1	XA	76	G
1	XA	79	G
1	XA	91	C
1	XA	93	U
1	XA	101	A
1	XA	108	G
1	XA	115	G
1	XA	116	A
1	XA	120	A
1	XA	121	C
1	XA	129(A)	G
1	XA	144	G
1	XA	146	G
1	XA	163	C
1	XA	169	C
1	XA	182	U
1	XA	184	G
1	XA	185	A
1	XA	186(F)	C
1	XA	188	U
1	XA	189	U
1	XA	191(A)	G
1	XA	191(D)	U
1	XA	195	A
1	XA	197	A
1	XA	198	G
1	XA	208	U
1	XA	209	U
1	XA	210	U
1	XA	216	G
1	XA	244	U
1	XA	247	G
1	XA	251	G
1	XA	266	G
1	XA	267	C
1	XA	270	A
1	XA	275	G
1	XA	279	A
1	XA	280	C
1	XA	281	G
1	XA	289	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	XA	298	A
1	XA	316	G
1	XA	321	A
1	XA	328	C
1	XA	329	A
1	XA	332	G
1	XA	345	C
1	XA	346	G
1	XA	347	G
1	XA	351	G
1	XA	352	C
1	XA	353	A
1	XA	354	G
1	XA	367	U
1	XA	368	U
1	XA	372	C
1	XA	373	A
1	XA	384	G
1	XA	388	G
1	XA	390	C
1	XA	397	A
1	XA	398	C
1	XA	406	G
1	XA	411	A
1	XA	412	A
1	XA	422	C
1	XA	423	G
1	XA	424	G
1	XA	429	U
1	XA	442	C
1	XA	467	G
1	XA	477	G
1	XA	482	A
1	XA	484	G
1	XA	485	G
1	XA	492	G
1	XA	496	A
1	XA	497	U
1	XA	505	G
1	XA	511	C
1	XA	518	C
1	XA	521	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	XA	527	G
1	XA	530	G
1	XA	531	U
1	XA	532	A
1	XA	533	A
1	XA	547	A
1	XA	548	G
1	XA	559	A
1	XA	564	C
1	XA	572	A
1	XA	573	A
1	XA	576	G
1	XA	577	G
1	XA	579	G
1	XA	595	G
1	XA	596	C
1	XA	630	G
1	XA	653	A
1	XA	665	A
1	XA	666	G
1	XA	688	G
1	XA	701	C
1	XA	702	A
1	XA	703	G
1	XA	704	A
1	XA	721	G
1	XA	724	G
1	XA	731	G
1	XA	749	C
1	XA	755	G
1	XA	760	G
1	XA	792	A
1	XA	793	U
1	XA	794	A
1	XA	812	C
1	XA	813	U
1	XA	816	A
1	XA	817	C
1	XA	819	A
1	XA	821	G
1	XA	828	A
1	XA	836	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	XA	841	U
1	XA	842	C
1	XA	843	U
1	XA	848	C
1	XA	859	A
1	XA	870	U
1	XA	914	A
1	XA	922	G
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	968	A
1	XA	969	A
1	XA	972	C
1	XA	974	A
1	XA	976	G
1	XA	977	A
1	XA	980	C
1	XA	989	C
1	XA	991	U
1	XA	992	U
1	XA	993	G
1	XA	994	A
1	XA	999	U
1	XA	1000	A
1	XA	1001	G
1	XA	1002	G
1	XA	1004	A
1	XA	1005	A
1	XA	1006	C
1	XA	1007	C
1	XA	1008	C
1	XA	1009	G
1	XA	1010	G
1	XA	1020	U
1	XA	1024	G
1	XA	1028(A)	C
1	XA	1029	G
1	XA	1031	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	XA	1032(A)	G
1	XA	1033	G
1	XA	1034	G
1	XA	1036	G
1	XA	1038	C
1	XA	1039	C
1	XA	1042	G
1	XA	1046	A
1	XA	1053	G
1	XA	1054	C
1	XA	1055	A
1	XA	1064	G
1	XA	1065	U
1	XA	1066	C
1	XA	1068	G
1	XA	1070	U
1	XA	1081	G
1	XA	1094	G
1	XA	1101	A
1	XA	1108	G
1	XA	1117	G
1	XA	1118	C
1	XA	1124	G
1	XA	1125	U
1	XA	1127	G
1	XA	1130	A
1	XA	1131	G
1	XA	1136	U
1	XA	1137	C
1	XA	1138	G
1	XA	1139	G
1	XA	1140	C
1	XA	1146	A
1	XA	1147	C
1	XA	1157	A
1	XA	1158	C
1	XA	1159	U
1	XA	1160	G
1	XA	1171	G
1	XA	1176	A
1	XA	1177	G
1	XA	1178	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	XA	1181	G
1	XA	1183	A
1	XA	1184	G
1	XA	1191	A
1	XA	1196	U
1	XA	1212	U
1	XA	1213	A
1	XA	1214	C
1	XA	1225	A
1	XA	1226	C
1	XA	1227	A
1	XA	1238	A
1	XA	1240	U
1	XA	1241	G
1	XA	1255	G
1	XA	1257	U
1	XA	1258	G
1	XA	1260	C
1	XA	1270	C
1	XA	1273	G
1	XA	1278	U
1	XA	1280	A
1	XA	1281	U
1	XA	1285	A
1	XA	1286	A
1	XA	1287	A
1	XA	1288	A
1	XA	1300	G
1	XA	1301	U
1	XA	1303	C
1	XA	1305	G
1	XA	1306	A
1	XA	1319	A
1	XA	1320	C
1	XA	1323	G
1	XA	1331	G
1	XA	1345	U
1	XA	1346	A
1	XA	1347	G
1	XA	1353	G
1	XA	1362(A)	C
1	XA	1363	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	XA	1370	G
1	XA	1381	U
1	XA	1394	A
1	XA	1397	C
1	XA	1398	A
1	XA	1400	C
1	XA	1419	G
1	XA	1442	G
1	XA	1446	A
1	XA	1450	U
1	XA	1451	A
1	XA	1452	C
1	XA	1453	G
1	XA	1454	G
1	XA	1487	G
1	XA	1492	A
1	XA	1493	A
1	XA	1497	G
1	XA	1499	A
1	XA	1504	G
1	XA	1505	G
1	XA	1506	U
1	XA	1507	A
1	XA	1517	G
1	XA	1519	A
1	XA	1520	G
1	XA	1529	G
1	XA	1530	G
1	XA	1531	A
1	XA	1532	U
1	XA	1533	C
1	XA	1534	A
1	XA	1535	C
1	XA	1536	C
1	XA	1537	U
1	XA	1538	C
1	XA	1540	U
1	XA	1541	U
22	XV	2	G
22	XV	18	G
22	XV	20	U
22	XV	21	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	XV	22	G
22	XV	42	G
22	XV	47	U
22	XV	49	G
22	XV	76	A
23	XX	5	A
23	XX	8	A
23	XX	10	G
23	XX	11	U
23	XX	12	A
23	XX	13	A
23	XX	14	A
23	XX	19	U
35	YA	9	U
35	YA	27	G
35	YA	34	C
35	YA	46	C
35	YA	55	G
35	YA	64	A
35	YA	69	C
35	YA	71	A
35	YA	74	A
35	YA	75	G
35	YA	83	G
35	YA	85	G
35	YA	102	G
35	YA	118	A
35	YA	119	A
35	YA	120	U
35	YA	123	G
35	YA	125	G
35	YA	138	G
35	YA	140	A
35	YA	149	A
35	YA	154	G
35	YA	155	C
35	YA	156	U
35	YA	157	U
35	YA	175	G
35	YA	196	A
35	YA	199	A
35	YA	204	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	YA	215	G
35	YA	216	A
35	YA	221	A
35	YA	222	A
35	YA	229	A
35	YA	233	A
35	YA	241	A
35	YA	248	G
35	YA	249	C
35	YA	252	G
35	YA	261	G
35	YA	265	A
35	YA	266	G
35	YA	267	C
35	YA	270(B)	A
35	YA	270(C)	C
35	YA	270(J)	G
35	YA	270(K)	C
35	YA	270(N)	G
35	YA	270(O)	U
35	YA	270(Z)	U
35	YA	271(C)	U
35	YA	271	G
35	YA	274	G
35	YA	275	G
35	YA	278	A
35	YA	279	C
35	YA	283	A
35	YA	287	C
35	YA	289	A
35	YA	290	G
35	YA	311	A
35	YA	317	G
35	YA	324	A
35	YA	329	G
35	YA	330	A
35	YA	332	A
35	YA	352	G
35	YA	356	G
35	YA	363	G
35	YA	363(A)	A
35	YA	363(E)	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	YA	363(F)	A
35	YA	372	G
35	YA	373	U
35	YA	380	U
35	YA	386	G
35	YA	395	U
35	YA	405	U
35	YA	406	G
35	YA	411	G
35	YA	412	A
35	YA	428	A
35	YA	444	C
35	YA	448	U
35	YA	454	A
35	YA	456	C
35	YA	457	A
35	YA	470	A
35	YA	481	G
35	YA	494	G
35	YA	501	A
35	YA	504	U
35	YA	505	A
35	YA	508	G
35	YA	509	C
35	YA	512	G
35	YA	525	U
35	YA	526	A
35	YA	529	A
35	YA	531	C
35	YA	532	A
35	YA	533	G
35	YA	562	U
35	YA	563	G
35	YA	571	A
35	YA	573	G
35	YA	575	A
35	YA	588	U
35	YA	603	A
35	YA	604	G
35	YA	607	U
35	YA	613	U
35	YA	614	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	YA	615	G
35	YA	617	G
35	YA	622	G
35	YA	624	C
35	YA	627	A
35	YA	637	A
35	YA	645	C
35	YA	646	A
35	YA	666	G
35	YA	668	G
35	YA	669	G
35	YA	670	A
35	YA	686	G
35	YA	717	G
35	YA	722	A
35	YA	730	C
35	YA	753	C
35	YA	776	G
35	YA	782	A
35	YA	784	A
35	YA	785	G
35	YA	788	A
35	YA	789	A
35	YA	792	G
35	YA	793	A
35	YA	805	G
35	YA	812	C
35	YA	819	A
35	YA	827	U
35	YA	828	U
35	YA	832	G
35	YA	856	C
35	YA	857	C
35	YA	859	G
35	YA	869	G
35	YA	882	G
35	YA	883	G
35	YA	884	C
35	YA	885	C
35	YA	886	C
35	YA	888	C
35	YA	889	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	YA	890	A
35	YA	894	C
35	YA	896	A
35	YA	897	C
35	YA	906	G
35	YA	910	A
35	YA	915	C
35	YA	917	A
35	YA	919	G
35	YA	928	G
35	YA	932	G
35	YA	938	G
35	YA	941	A
35	YA	945	A
35	YA	946	G
35	YA	953	A
35	YA	961	C
35	YA	973	A
35	YA	974	G
35	YA	975	G
35	YA	980	A
35	YA	983	A
35	YA	990	A
35	YA	991	C
35	YA	996	A
35	YA	999	U
35	YA	1000	A
35	YA	1005	C
35	YA	1012	U
35	YA	1013	C
35	YA	1017	G
35	YA	1020	A
35	YA	1022	G
35	YA	1023	U
35	YA	1024	G
35	YA	1025	G
35	YA	1026	U
35	YA	1027	A
35	YA	1033	U
35	YA	1044	G
35	YA	1046	A
35	YA	1047	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	YA	1048	A
35	YA	1060	U
35	YA	1061	U
35	YA	1064	C
35	YA	1066	U
35	YA	1070	A
35	YA	1073	A
35	YA	1083	U
35	YA	1085	A
35	YA	1086	A
35	YA	1087	G
35	YA	1088	A
35	YA	1089	G
35	YA	1093	G
35	YA	1094	U
35	YA	1095	A
35	YA	1096	A
35	YA	1099	G
35	YA	1122	G
35	YA	1126	A
35	YA	1128	A
35	YA	1130	U
35	YA	1135	C
35	YA	1136	G
35	YA	1139	G
35	YA	1141	U
35	YA	1142(A)	A
35	YA	1148	A
35	YA	1156	A
35	YA	1170	G
35	YA	1173	G
35	YA	1174	A
35	YA	1175	U
35	YA	1177	A
35	YA	1178	C
35	YA	1179	C
35	YA	1180	C
35	YA	1195	G
35	YA	1204	A
35	YA	1205	U
35	YA	1210	A
35	YA	1212	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	YA	1220	A
35	YA	1236	G
35	YA	1247	A
35	YA	1248	G
35	YA	1252	G
35	YA	1253	A
35	YA	1255	U
35	YA	1256	G
35	YA	1265	A
35	YA	1272	A
35	YA	1281	G
35	YA	1294	U
35	YA	1300	U
35	YA	1301	A
35	YA	1308	A
35	YA	1311	G
35	YA	1314	C
35	YA	1329	U
35	YA	1330	C
35	YA	1352	U
35	YA	1359	A
35	YA	1360	A
35	YA	1368	G
35	YA	1370	C
35	YA	1378	A
35	YA	1379	A
35	YA	1380	G
35	YA	1384	A
35	YA	1385	G
35	YA	1391	U
35	YA	1395	A
35	YA	1406	U
35	YA	1416	G
35	YA	1419	A
35	YA	1420	U
35	YA	1421	G
35	YA	1428	C
35	YA	1437	C
35	YA	1444(A)	A
35	YA	1445	C
35	YA	1449	A
35	YA	1449(A)	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	YA	1455	G
35	YA	1459	G
35	YA	1460	A
35	YA	1461	G
35	YA	1467	C
35	YA	1471	A
35	YA	1475	G
35	YA	1480	G
35	YA	1482	U
35	YA	1483	G
35	YA	1488	G
35	YA	1490	A
35	YA	1493	C
35	YA	1509	C
35	YA	1510	A
35	YA	1516	U
35	YA	1522	G
35	YA	1523	U
35	YA	1535	U
35	YA	1536	A
35	YA	1537	C
35	YA	1538	G
35	YA	1540	G
35	YA	1543	A
35	YA	1544	C
35	YA	1545	A
35	YA	1547	C
35	YA	1554	A
35	YA	1558	A
35	YA	1559	G
35	YA	1560	G
35	YA	1566	A
35	YA	1569	A
35	YA	1578	U
35	YA	1580	A
35	YA	1585	C
35	YA	1586	A
35	YA	1598	C
35	YA	1608	A
35	YA	1613	G
35	YA	1618	A
35	YA	1634	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	YA	1640	C
35	YA	1648	C
35	YA	1654	A
35	YA	1667	G
35	YA	1674	G
35	YA	1696	G
35	YA	1700	A
35	YA	1703	G
35	YA	1725	G
35	YA	1728	G
35	YA	1729	A
35	YA	1743	G
35	YA	1753	G
35	YA	1754	C
35	YA	1756	G
35	YA	1762	A
35	YA	1763	G
35	YA	1764	G
35	YA	1773	A
35	YA	1774	C
35	YA	1780	A
35	YA	1782	C
35	YA	1791	A
35	YA	1800	C
35	YA	1801	G
35	YA	1802	A
35	YA	1816	G
35	YA	1820	U
35	YA	1828	G
35	YA	1829	A
35	YA	1835	G
35	YA	1847	A
35	YA	1858	G
35	YA	1872	A
35	YA	1878	G
35	YA	1881	C
35	YA	1882	C
35	YA	1888	G
35	YA	1889	A
35	YA	1903	G
35	YA	1906	G
35	YA	1910	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	YA	1913	A
35	YA	1929	G
35	YA	1930	G
35	YA	1936	A
35	YA	1938	A
35	YA	1955	U
35	YA	1963	U
35	YA	1964	G
35	YA	1966	A
35	YA	1967	C
35	YA	1970	A
35	YA	1971	A
35	YA	1972	A
35	YA	1980	G
35	YA	1982	C
35	YA	1992	G
35	YA	1993	U
35	YA	2020	A
35	YA	2021	C
35	YA	2023	G
35	YA	2027	G
35	YA	2031	A
35	YA	2032	G
35	YA	2033	A
35	YA	2043	C
35	YA	2052	G
35	YA	2055	C
35	YA	2056	G
35	YA	2059	A
35	YA	2060	A
35	YA	2061	G
35	YA	2062	A
35	YA	2069	G
35	YA	2093	G
35	YA	2099	U
35	YA	2111	C
35	YA	2112	G
35	YA	2113	U
35	YA	2114	A
35	YA	2116	G
35	YA	2117	A
35	YA	2119	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	YA	2120	G
35	YA	2123	G
35	YA	2126	A
35	YA	2128	C
35	YA	2130	U
35	YA	2131	G
35	YA	2132	U
35	YA	2134	A
35	YA	2140	C
35	YA	2145	C
35	YA	2147	G
35	YA	2148	G
35	YA	2157	G
35	YA	2161	C
35	YA	2167	U
35	YA	2168	G
35	YA	2169	A
35	YA	2170	A
35	YA	2171	A
35	YA	2173	A
35	YA	2174	C
35	YA	2177	C
35	YA	2189	U
35	YA	2190	G
35	YA	2191	G
35	YA	2192	G
35	YA	2198	A
35	YA	2210	G
35	YA	2211	G
35	YA	2212	A
35	YA	2215	G
35	YA	2225	A
35	YA	2226	C
35	YA	2238	G
35	YA	2239	G
35	YA	2266	A
35	YA	2275	C
35	YA	2278	A
35	YA	2283	C
35	YA	2287	A
35	YA	2288	A
35	YA	2305	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	YA	2306	C
35	YA	2307	G
35	YA	2308	G
35	YA	2309	A
35	YA	2312	U
35	YA	2316	C
35	YA	2318	G
35	YA	2320	A
35	YA	2325	G
35	YA	2334	G
35	YA	2335	A
35	YA	2336	A
35	YA	2343	C
35	YA	2346	A
35	YA	2347	C
35	YA	2350	C
35	YA	2354	G
35	YA	2358	G
35	YA	2383	G
35	YA	2385	C
35	YA	2392	A
35	YA	2402	C
35	YA	2403	C
35	YA	2406	U
35	YA	2410	G
35	YA	2422	A
35	YA	2423	U
35	YA	2424	C
35	YA	2425	A
35	YA	2429	G
35	YA	2430	A
35	YA	2435	A
35	YA	2439	A
35	YA	2440	C
35	YA	2441	C
35	YA	2448	A
35	YA	2450	A
35	YA	2469	A
35	YA	2472	G
35	YA	2474	C
35	YA	2475	C
35	YA	2476	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	YA	2478	A
35	YA	2484	G
35	YA	2491	U
35	YA	2494	G
35	YA	2498	C
35	YA	2502	G
35	YA	2505	G
35	YA	2518	A
35	YA	2529	G
35	YA	2535	G
35	YA	2542	A
35	YA	2543	G
35	YA	2554	U
35	YA	2566	A
35	YA	2567	G
35	YA	2572	A
35	YA	2573	C
35	YA	2578	G
35	YA	2602	A
35	YA	2609	U
35	YA	2611	U
35	YA	2612	C
35	YA	2629	A
35	YA	2630	G
35	YA	2645	G
35	YA	2646	C
35	YA	2655	G
35	YA	2665	A
35	YA	2673	G
35	YA	2682	U
35	YA	2686	G
35	YA	2689	U
35	YA	2690	C
35	YA	2691	C
35	YA	2702	U
35	YA	2703	C
35	YA	2712	U
35	YA	2713	A
35	YA	2714	G
35	YA	2724	C
35	YA	2725	A
35	YA	2726	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	YA	2732	G
35	YA	2733	A
35	YA	2734	A
35	YA	2739	U
35	YA	2744	G
35	YA	2748	A
35	YA	2751	G
35	YA	2752	C
35	YA	2754	U
35	YA	2757	A
35	YA	2762	G
35	YA	2764	A
35	YA	2766	G
35	YA	2777	G
35	YA	2778	A
35	YA	2779	U
35	YA	2780	G
35	YA	2790	A
35	YA	2791	C
35	YA	2792	G
35	YA	2807	G
35	YA	2808	U
35	YA	2811	G
35	YA	2818	G
35	YA	2820	A
35	YA	2821	A
35	YA	2823	A
35	YA	2830	G
35	YA	2832	U
35	YA	2833	G
35	YA	2834	G
35	YA	2835	A
35	YA	2846	G
35	YA	2848	G
35	YA	2849	U
35	YA	2850	A
35	YA	2860	A
35	YA	2872	G
35	YA	2873	A
35	YA	2879	C
35	YA	2880	C
35	YA	2892	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	YA	2893	G
35	YA	2894	G
35	YA	2896	C
35	YA	2897	U
36	YB	8	U
36	YB	13	A
36	YB	14	U
36	YB	15	A
36	YB	16	G
36	YB	25	A
36	YB	42	C
36	YB	44	G
36	YB	45	A
36	YB	57	A
36	YB	67	G
36	YB	73	A
36	YB	81	G
36	YB	88	C
36	YB	109	G
36	YB	112	G
36	YB	119	A

All (144) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	QA	5	U
1	QA	31	G
1	QA	60	A
1	QA	115	G
1	QA	181	G
1	QA	190	G
1	QA	197	A
1	QA	201	C
1	QA	208	U
1	QA	250	A
1	QA	428	G
1	QA	484	G
1	QA	496	A
1	QA	518	C
1	QA	547	A
1	QA	687	A
1	QA	748	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	QA	792	A
1	QA	812	C
1	QA	841	U
1	QA	913	A
1	QA	960	U
1	QA	992	U
1	QA	1038	C
1	QA	1065	U
1	QA	1067	A
1	QA	1137	C
1	QA	1182	G
1	QA	1346	A
1	QA	1347	G
1	QA	1498	U
1	QA	1528	U
1	QA	1532	U
22	QV	1	C
23	QX	9	G
23	QX	11	U
35	RA	90	U
35	RA	119	A
35	RA	128	C
35	RA	227	A
35	RA	372	G
35	RA	387	U
35	RA	404	C
35	RA	587	C
35	RA	752	A
35	RA	845	G
35	RA	856	C
35	RA	877	U
35	RA	1022	G
35	RA	1085	A
35	RA	1171	G
35	RA	1204	A
35	RA	1300	U
35	RA	1427	A
35	RA	1558	A
35	RA	1559	G
35	RA	1653	G
35	RA	1694	C
35	RA	1699	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	RA	1819	A
35	RA	1930	G
35	RA	1992	G
35	RA	2092	U
35	RA	2144	U
35	RA	2191	G
35	RA	2211	G
35	RA	2439	A
35	RA	2447	G
35	RA	2481	G
35	RA	2689	U
35	RA	2776	A
35	RA	2849	U
35	RA	2859	G
36	RB	66	A
1	XA	5	U
1	XA	60	A
1	XA	92	G
1	XA	115	G
1	XA	181	G
1	XA	197	A
1	XA	201	C
1	XA	243	A
1	XA	250	A
1	XA	279	A
1	XA	315	A
1	XA	328	C
1	XA	428	G
1	XA	547	A
1	XA	595	G
1	XA	687	A
1	XA	703	G
1	XA	748	C
1	XA	792	A
1	XA	812	C
1	XA	913	A
1	XA	960	U
1	XA	992	U
1	XA	1000	A
1	XA	1004	A
1	XA	1033	G
1	XA	1038	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	XA	1054	C
1	XA	1065	U
1	XA	1067	A
1	XA	1124	G
1	XA	1137	C
1	XA	1139	G
1	XA	1157	A
1	XA	1182	G
1	XA	1190	G
1	XA	1300	G
1	XA	1305	G
1	XA	1498	U
1	XA	1532	U
22	XV	1	C
35	YA	119	A
35	YA	372	G
35	YA	587	C
35	YA	603	A
35	YA	752	A
35	YA	827	U
35	YA	856	C
35	YA	1022	G
35	YA	1171	G
35	YA	1379	A
35	YA	1427	A
35	YA	1558	A
35	YA	1559	G
35	YA	1653	G
35	YA	1819	A
35	YA	2144	U
35	YA	2166	G
35	YA	2191	G
35	YA	2211	G
35	YA	2225	A
35	YA	2439	A
35	YA	2447	G
35	YA	2610	C
35	YA	2689	U
35	YA	2776	A
35	YA	2848	G
35	YA	2849	U
35	YA	2859	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	YB	66	A

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

4 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
23	A3P	QX	20	23	25,28,29	3.31	9 (36%)	37,42,45	2.18	11 (29%)
56	PPU	ZB	3	35,56	37,40,41	1.24	5 (13%)	47,57,60	2.40	19 (40%)
56	PPU	ZA	3	35,56	37,40,41	1.25	6 (16%)	47,57,60	2.29	14 (29%)
23	A3P	XX	20	23	25,28,29	3.32	8 (32%)	37,42,45	2.12	9 (24%)

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
23	A3P	QX	20	23	-	3/12/30/31	0/3/3/3
56	PPU	ZB	3	35,56	-	13/25/43/44	0/4/4/4
56	PPU	ZA	3	35,56	-	6/25/43/44	0/4/4/4
23	A3P	XX	20	23	-	1/12/30/31	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	QX	20	A3P	O4'-C1'	11.03	1.67	1.42
23	XX	20	A3P	O4'-C1'	10.74	1.66	1.42
23	XX	20	A3P	C2'-C1'	-6.54	1.32	1.53
23	QX	20	A3P	C2'-C1'	-6.40	1.33	1.53
23	XX	20	A3P	O4'-C4'	-5.95	1.31	1.45
23	QX	20	A3P	O4'-C4'	-5.94	1.31	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	QX	20	A3P	P1-O3'	5.03	1.68	1.59
23	XX	20	A3P	C6-N6	4.54	1.45	1.34
23	XX	20	A3P	P1-O3'	4.29	1.67	1.59
56	ZB	3	PPU	C5-C4	4.04	1.46	1.39
23	QX	20	A3P	C6-N6	4.01	1.44	1.34
56	ZA	3	PPU	C5-C4	3.95	1.46	1.39
23	XX	20	A3P	O3'-C3'	-3.67	1.31	1.44
23	QX	20	A3P	O3'-C3'	-3.44	1.32	1.44
56	ZB	3	PPU	C5-N7	-3.02	1.33	1.39
56	ZA	3	PPU	C5-N7	-2.95	1.33	1.39
56	ZB	3	PPU	C8-N9	-2.61	1.33	1.37
56	ZB	3	PPU	C4-N9	-2.44	1.32	1.37
56	ZA	3	PPU	C4-N9	-2.40	1.32	1.37
56	ZA	3	PPU	C5-C6	2.25	1.47	1.41
23	QX	20	A3P	C8-N9	-2.25	1.33	1.37
56	ZB	3	PPU	C5-C6	2.22	1.47	1.41
23	XX	20	A3P	C3'-C4'	2.21	1.58	1.52
56	ZA	3	PPU	C8-N9	-2.16	1.33	1.37
23	XX	20	A3P	C8-N9	-2.15	1.33	1.37
23	QX	20	A3P	C2'-C3'	2.06	1.57	1.53
56	ZA	3	PPU	C8-N7	2.03	1.35	1.31
23	QX	20	A3P	C3'-C4'	2.02	1.58	1.52

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	QX	20	A3P	C5-C4-N3	-6.47	117.81	126.72
56	ZB	3	PPU	C5-C4-N3	-6.28	118.07	126.72
23	XX	20	A3P	C5-C4-N3	-6.07	118.35	126.72
56	ZA	3	PPU	C5-C4-N3	-6.05	118.39	126.72
23	XX	20	A3P	N3-C2-N1	-5.02	120.98	128.58
56	ZB	3	PPU	N3-C4-N9	4.89	135.49	127.17
56	ZA	3	PPU	C9-N6-C6	-4.89	108.08	120.52
56	ZA	3	PPU	N3-C4-N9	4.83	135.38	127.17
56	ZB	3	PPU	C10-N6-C6	-4.55	108.95	120.52
56	ZB	3	PPU	C9-N6-C6	-4.52	109.03	120.52
56	ZB	3	PPU	CG-CB-CA	-4.45	105.02	114.13
23	QX	20	A3P	N3-C4-N9	4.30	134.48	127.17
56	ZA	3	PPU	N1-C6-N6	4.28	122.08	116.86
23	XX	20	A3P	C2-N3-C4	4.24	122.19	111.83
23	QX	20	A3P	N3-C2-N1	-4.14	122.32	128.58
56	ZA	3	PPU	C10-N6-C6	-4.04	110.24	120.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	QX	20	A3P	C2-N3-C4	3.89	121.32	111.83
56	ZA	3	PPU	C3'-N3'-C	-3.88	117.30	123.20
56	ZB	3	PPU	C2-N1-C6	3.86	121.27	111.83
23	XX	20	A3P	C4-C5-N7	-3.76	106.28	110.58
56	ZA	3	PPU	C2-N1-C6	3.75	120.99	111.83
56	ZA	3	PPU	CA-C-N3'	3.74	121.27	116.21
56	ZA	3	PPU	C2-N3-C4	3.73	120.95	111.83
23	XX	20	A3P	N3-C4-N9	3.73	133.50	127.17
56	ZB	3	PPU	C2-N3-C4	3.71	120.89	111.83
56	ZB	3	PPU	C4-C5-N7	-3.61	106.46	110.58
56	ZB	3	PPU	N1-C6-N6	3.58	121.22	116.86
23	QX	20	A3P	C4-C5-N7	-3.58	106.49	110.58
56	ZA	3	PPU	C5-C6-N6	-3.56	119.70	125.33
23	QX	20	A3P	C5-N7-C8	3.30	108.63	103.45
23	XX	20	A3P	C3'-C2'-C1'	3.26	107.07	99.89
56	ZB	3	PPU	C2'-C1'-N9	-3.20	105.35	113.30
23	XX	20	A3P	C5-N7-C8	3.17	108.44	103.45
56	ZA	3	PPU	C4-C5-N7	-3.10	107.04	110.58
56	ZA	3	PPU	N3-C2-N1	-3.08	123.92	128.58
56	ZB	3	PPU	N3-C2-N1	-2.99	124.05	128.58
23	QX	20	A3P	P1-O3'-C3'	-2.87	115.78	123.43
23	XX	20	A3P	N9-C8-N7	-2.86	109.88	113.94
23	QX	20	A3P	N9-C8-N7	-2.80	109.96	113.94
56	ZB	3	PPU	C5-C6-N6	-2.69	121.07	125.33
56	ZB	3	PPU	CA-C-N3'	-2.69	112.57	116.21
23	QX	20	A3P	C3'-C2'-C1'	2.69	105.80	99.89
56	ZA	3	PPU	C4-N9-C8	2.62	108.49	105.74
56	ZB	3	PPU	CB-CA-C	2.61	115.07	108.97
56	ZB	3	PPU	C4-N9-C8	2.60	108.47	105.74
56	ZB	3	PPU	C5-N7-C8	2.46	107.31	103.45
23	QX	20	A3P	C2'-C3'-C4'	2.45	107.53	103.24
56	ZB	3	PPU	C10-N6-C9	-2.38	108.53	116.18
56	ZB	3	PPU	C3'-N3'-C	2.38	126.82	123.20
23	QX	20	A3P	C5-C6-N6	-2.35	117.47	123.29
56	ZA	3	PPU	C5-N7-C8	2.23	106.96	103.45
23	XX	20	A3P	C5-C4-N9	2.14	108.14	105.81
56	ZB	3	PPU	C4-C5-C6	2.03	118.01	115.91

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	ZA	3	PPU	N-CA-CB-CG
56	ZA	3	PPU	C-CA-CB-CG
56	ZB	3	PPU	N3'-C-CA-N
56	ZB	3	PPU	O-C-CA-CB
56	ZB	3	PPU	N3'-C-CA-CB
56	ZB	3	PPU	CA-C-N3'-C3'
56	ZB	3	PPU	C5-C6-N6-C10
56	ZB	3	PPU	O-C-N3'-C3'
56	ZA	3	PPU	CE2-CZ-OC-CM
56	ZB	3	PPU	CE1-CZ-OC-CM
56	ZB	3	PPU	CE2-CZ-OC-CM
56	ZA	3	PPU	CE1-CZ-OC-CM
56	ZB	3	PPU	N1-C6-N6-C10
23	QX	20	A3P	C3'-C4'-C5'-O5'
56	ZA	3	PPU	C5-C6-N6-C9
56	ZB	3	PPU	CA-CB-CG-CD1
56	ZB	3	PPU	CA-CB-CG-CD2
56	ZA	3	PPU	C5-C6-N6-C10
56	ZB	3	PPU	O-C-CA-N
23	QX	20	A3P	O4'-C4'-C5'-O5'
23	XX	20	A3P	C3'-O3'-P1-O1P
56	ZB	3	PPU	C5-C6-N6-C9
23	QX	20	A3P	O4'-C1'-N9-C8

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	QX	20	A3P	1	0
56	ZB	3	PPU	7	0
56	ZA	3	PPU	2	0
23	XX	20	A3P	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 900 ligands modelled in this entry, 898 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	$\# Z > 2$
58	SF4	QD	302	4	0,12,12	-	-	-		
58	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
58	SF4	QD	302	4	-	-	0/6/5/5
58	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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1510/1521 (99%)	0.21	28 (1%) 66 41	49, 98, 212, 355	0
1	XA	1507/1521 (99%)	0.08	25 (1%) 69 43	45, 94, 192, 357	0
2	QB	235/256 (91%)	0.30	4 (1%) 69 43	74, 129, 195, 233	0
2	XB	236/256 (92%)	0.65	14 (5%) 28 16	70, 117, 191, 215	0
3	QC	205/239 (85%)	0.58	12 (5%) 28 16	78, 124, 163, 185	0
3	XC	205/239 (85%)	0.51	10 (4%) 35 19	66, 105, 158, 211	0
4	QD	208/209 (99%)	0.56	7 (3%) 48 27	56, 89, 122, 140	0
4	XD	208/209 (99%)	0.70	17 (8%) 17 11	54, 94, 137, 176	0
5	QE	151/162 (93%)	0.66	10 (6%) 24 15	51, 89, 126, 167	0
5	XE	151/162 (93%)	0.55	8 (5%) 32 18	59, 85, 129, 186	0
6	QF	101/101 (100%)	0.38	3 (2%) 52 30	75, 108, 147, 204	0
6	XF	101/101 (100%)	0.20	0 100 100	52, 85, 118, 164	0
7	QG	155/156 (99%)	0.49	8 (5%) 33 19	88, 127, 172, 241	0
7	XG	155/156 (99%)	0.67	15 (9%) 13 9	75, 113, 160, 233	0
8	QH	137/138 (99%)	0.45	5 (3%) 46 25	58, 91, 125, 158	0
8	XH	137/138 (99%)	0.61	6 (4%) 39 21	60, 90, 128, 156	0
9	QI	127/128 (99%)	1.04	16 (12%) 8 6	86, 142, 179, 263	0
9	XI	126/128 (98%)	0.98	18 (14%) 6 5	66, 121, 162, 174	0
10	QJ	99/105 (94%)	1.21	22 (22%) 2 2	95, 143, 201, 251	0
10	XJ	96/105 (91%)	0.87	10 (10%) 11 8	87, 133, 196, 223	0
11	QK	119/129 (92%)	0.84	9 (7%) 20 13	61, 109, 164, 270	0
11	XK	116/129 (89%)	0.44	2 (1%) 69 43	48, 93, 136, 182	0
12	QL	125/132 (94%)	0.73	17 (13%) 7 5	49, 80, 121, 230	0
12	XL	122/132 (92%)	0.62	7 (5%) 29 17	46, 78, 112, 193	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	QM	120/126 (95%)	0.91	18 (15%) 5 5	74, 129, 179, 206	0
13	XM	119/126 (94%)	0.92	17 (14%) 6 5	75, 113, 158, 172	0
14	QN	60/61 (98%)	1.72	23 (38%) 1 1	81, 121, 159, 212	0
14	XN	60/61 (98%)	0.83	5 (8%) 17 11	75, 102, 144, 214	0
15	QO	88/89 (98%)	0.74	3 (3%) 48 27	59, 96, 131, 139	0
15	XO	87/89 (97%)	0.70	3 (3%) 48 27	52, 88, 118, 147	0
16	QP	84/88 (95%)	0.78	6 (7%) 22 14	58, 87, 127, 181	0
16	XP	84/88 (95%)	0.87	8 (9%) 14 9	64, 100, 143, 184	0
17	QQ	100/105 (95%)	0.70	8 (8%) 18 12	60, 92, 126, 153	0
17	XQ	100/105 (95%)	0.72	8 (8%) 18 12	62, 93, 118, 175	0
18	QR	70/88 (79%)	0.45	0 100 100	70, 110, 153, 155	0
18	XR	70/88 (79%)	0.09	1 (1%) 73 48	48, 85, 130, 156	0
19	QS	83/93 (89%)	0.80	9 (10%) 11 8	91, 135, 185, 224	0
19	XS	83/93 (89%)	0.63	5 (6%) 27 16	84, 116, 169, 214	0
20	QT	99/106 (93%)	0.97	17 (17%) 4 4	68, 104, 173, 248	0
20	XT	99/106 (93%)	0.95	13 (13%) 7 6	72, 115, 173, 205	0
21	QU	25/27 (92%)	1.64	12 (48%) 0 1	97, 124, 152, 161	0
21	XU	25/27 (92%)	1.27	5 (20%) 3 3	92, 120, 141, 153	0
22	QV	77/77 (100%)	-0.05	2 (2%) 57 33	51, 103, 134, 192	0
22	XV	77/77 (100%)	-0.13	2 (2%) 57 33	56, 88, 122, 191	0
23	QX	17/20 (85%)	1.83	7 (41%) 0 1	76, 258, 314, 321	0
23	XX	17/20 (85%)	1.68	6 (35%) 1 1	57, 237, 321, 369	0
24	QY	84/84 (100%)	0.85	12 (14%) 6 5	65, 97, 131, 170	0
24	QZ	84/84 (100%)	0.31	1 (1%) 76 52	94, 149, 209, 227	0
24	XY	84/84 (100%)	0.65	6 (7%) 22 14	58, 91, 129, 154	0
24	XZ	84/84 (100%)	0.97	10 (11%) 9 6	88, 145, 204, 270	0
25	R0	81/85 (95%)	0.81	8 (9%) 13 8	52, 80, 104, 153	0
25	Y0	82/85 (96%)	0.93	6 (7%) 21 13	48, 83, 110, 131	0
26	R1	94/98 (95%)	1.21	16 (17%) 4 4	39, 83, 137, 200	0
26	Y1	97/98 (98%)	0.60	3 (3%) 51 29	34, 72, 113, 185	0
27	R2	69/72 (95%)	0.82	5 (7%) 21 14	54, 95, 135, 193	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
27	Y2	69/72 (95%)	0.57	4 (5%)	29	17	49, 83, 118, 238	0
28	R3	59/60 (98%)	0.45	1 (1%)	69	43	50, 82, 140, 155	0
28	Y3	59/60 (98%)	0.44	1 (1%)	69	43	52, 83, 125, 170	0
29	R4	69/71 (97%)	0.71	4 (5%)	29	17	105, 164, 223, 306	0
29	Y4	69/71 (97%)	0.97	10 (14%)	6	5	95, 131, 211, 285	0
30	R5	59/60 (98%)	0.74	3 (5%)	33	19	46, 81, 150, 183	0
30	Y5	59/60 (98%)	0.76	3 (5%)	33	19	42, 87, 154, 179	0
31	R6	53/54 (98%)	1.44	13 (24%)	2	2	147, 191, 254, 315	0
31	Y6	53/54 (98%)	1.53	17 (32%)	1	1	153, 180, 229, 243	0
32	R7	47/49 (95%)	0.60	4 (8%)	16	11	37, 57, 98, 138	0
32	Y7	48/49 (97%)	0.93	6 (12%)	8	6	38, 57, 88, 136	0
33	R8	64/65 (98%)	1.10	10 (15%)	5	5	42, 75, 121, 168	0
33	Y8	64/65 (98%)	1.02	11 (17%)	4	4	48, 75, 112, 154	0
34	R9	37/37 (100%)	1.61	14 (37%)	1	1	122, 162, 209, 225	0
34	Y9	37/37 (100%)	1.64	13 (35%)	1	1	135, 156, 195, 222	0
35	RA	2891/2915 (99%)	0.02	54 (1%)	66	41	39, 76, 264, 453	0
35	YA	2878/2915 (98%)	-0.06	66 (2%)	61	37	34, 73, 271, 478	0
36	RB	120/124 (96%)	0.18	5 (4%)	40	22	74, 122, 167, 189	0
36	YB	120/124 (96%)	0.11	2 (1%)	69	43	74, 109, 162, 192	0
37	RD	272/276 (98%)	0.91	32 (11%)	9	6	33, 74, 112, 258	0
37	YD	274/276 (99%)	0.32	5 (1%)	67	42	31, 57, 86, 130	0
38	RE	205/206 (99%)	0.74	13 (6%)	26	15	48, 88, 136, 200	0
38	YE	204/206 (99%)	0.60	7 (3%)	48	27	44, 83, 122, 169	0
39	RF	202/210 (96%)	0.42	8 (3%)	42	23	29, 67, 117, 227	0
39	YF	202/210 (96%)	0.56	9 (4%)	38	20	38, 76, 135, 191	0
40	RG	181/182 (99%)	0.61	9 (4%)	34	19	80, 123, 166, 244	0
40	YG	181/182 (99%)	0.86	15 (8%)	17	11	64, 111, 158, 189	0
41	RH	174/180 (96%)	1.15	30 (17%)	4	4	91, 141, 215, 280	0
41	YH	174/180 (96%)	0.69	21 (12%)	8	6	77, 128, 184, 219	0
42	RI	145/148 (97%)	1.03	22 (15%)	5	5	72, 115, 152, 209	0
42	YI	146/148 (98%)	0.58	9 (6%)	26	16	61, 103, 147, 217	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
43	RN	138/140 (98%)	1.07	23 (16%) 4 4	58, 96, 143, 175	0
43	YN	138/140 (98%)	0.90	11 (7%) 18 12	50, 88, 135, 171	0
44	RO	122/122 (100%)	0.48	1 (0%) 82 60	37, 73, 103, 126	0
44	YO	122/122 (100%)	0.64	4 (3%) 49 28	36, 68, 97, 137	0
45	RP	150/150 (100%)	0.91	16 (10%) 11 8	44, 85, 129, 206	0
45	YP	149/150 (99%)	0.60	11 (7%) 20 13	40, 78, 107, 144	0
46	RQ	141/141 (100%)	0.94	12 (8%) 16 11	45, 87, 131, 190	0
46	YQ	141/141 (100%)	0.43	5 (3%) 47 26	53, 82, 113, 137	0
47	RR	117/118 (99%)	0.57	4 (3%) 48 27	50, 79, 110, 218	0
47	YR	117/118 (99%)	0.68	11 (9%) 14 9	47, 77, 114, 162	0
48	RS	111/112 (99%)	1.04	16 (14%) 6 5	79, 116, 157, 259	0
48	YS	111/112 (99%)	0.87	13 (11%) 9 6	72, 100, 145, 293	0
49	RT	137/146 (93%)	0.71	12 (8%) 15 10	57, 89, 152, 199	0
49	YT	137/146 (93%)	0.66	11 (8%) 18 12	52, 86, 169, 273	0
50	RU	117/118 (99%)	0.72	6 (5%) 33 19	41, 74, 125, 172	0
50	YU	117/118 (99%)	0.93	13 (11%) 10 7	51, 82, 124, 170	0
51	RV	101/101 (100%)	0.44	3 (2%) 52 30	46, 87, 139, 175	0
51	YV	101/101 (100%)	1.05	16 (15%) 5 4	53, 96, 137, 220	0
52	RW	113/113 (100%)	0.71	7 (6%) 26 16	47, 71, 121, 195	0
52	YW	113/113 (100%)	0.57	7 (6%) 26 16	44, 73, 126, 229	0
53	RX	92/96 (95%)	0.70	10 (10%) 10 7	54, 84, 118, 167	0
53	YX	92/96 (95%)	0.37	1 (1%) 78 54	39, 72, 106, 140	0
54	RY	107/110 (97%)	1.21	25 (23%) 2 2	54, 93, 163, 279	0
54	YY	107/110 (97%)	0.80	9 (8%) 17 11	57, 98, 152, 179	0
55	RZ	183/206 (88%)	0.49	2 (1%) 78 54	79, 118, 157, 207	0
55	YZ	183/206 (88%)	0.47	4 (2%) 62 37	70, 113, 152, 166	0
56	ZA	2/3 (66%)	-0.43	0 100 100	49, 49, 49, 58	0
56	ZB	2/3 (66%)	-0.30	0 100 100	53, 53, 53, 62	0
All	All	21211/21784 (97%)	0.43	1192 (5%) 30 17	29, 91, 181, 478	0

All (1192) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	QK	129	SER	9.6
12	XL	28	LYS	9.4
14	QN	13	THR	8.2
14	QN	2	ALA	7.6
49	RT	106	SER	7.4
54	RY	10	GLY	7.1
26	R1	92	LYS	6.8
38	RE	130	GLY	6.6
14	XN	2	ALA	6.4
50	YU	91	ASP	6.4
7	QG	2	ALA	6.4
49	YT	106	SER	6.2
20	QT	9	ASN	6.1
24	QY	82	TYR	6.1
37	RD	33	LEU	6.0
45	RP	65	ARG	6.0
37	RD	34	VAL	5.9
13	QM	100	GLY	5.9
13	XM	102	ARG	5.8
20	QT	73	HIS	5.8
37	RD	44	ASN	5.7
1	QA	971	G	5.7
10	QJ	54	PHE	5.6
41	YH	2	SER	5.6
31	Y6	2	ALA	5.6
46	RQ	90	VAL	5.6
35	RA	2402	C	5.4
35	YA	1536	A	5.4
35	YA	2111	C	5.4
12	XL	29	GLY	5.3
35	YA	2114	A	5.3
41	RH	88	LEU	5.2
29	Y4	56	VAL	5.2
10	XJ	54	PHE	5.1
8	XH	25	ASP	5.1
26	R1	91	LYS	5.1
1	XA	1531	A	5.1
38	RE	131	ALA	5.1
35	YA	2112	G	5.1
22	XV	1	C	5.1
23	XX	14	A	5.0
12	QL	129	ALA	5.0
45	RP	56	SER	5.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
9	QI	111	ARG	4.9
33	R8	65	GLU	4.8
31	R6	2	ALA	4.8
24	XY	50	HIS	4.8
9	QI	102	LEU	4.8
40	YG	65	GLY	4.7
35	YA	2143	C	4.7
22	QV	1	C	4.7
32	Y7	48	LYS	4.7
2	QB	19	HIS	4.7
41	RH	165	ALA	4.7
35	YA	2110	G	4.6
37	RD	26	LYS	4.6
7	XG	81	GLY	4.5
32	Y7	46	VAL	4.5
37	RD	240	ALA	4.5
20	XT	73	HIS	4.5
42	RI	10	GLU	4.5
35	YA	653	A	4.5
37	RD	37	LEU	4.4
41	YH	45	VAL	4.4
39	YF	55	GLY	4.4
13	QM	105	THR	4.4
51	YV	76	LYS	4.4
33	R8	35	GLN	4.4
9	QI	126	SER	4.4
48	YS	2	ALA	4.4
43	YN	46	VAL	4.4
48	RS	2	ALA	4.3
32	Y7	1	MET	4.3
48	RS	7	TYR	4.3
9	QI	119	ALA	4.3
41	RH	152	ARG	4.3
17	XQ	101	ARG	4.3
37	RD	25	THR	4.2
41	RH	159	GLU	4.2
48	YS	111	GLU	4.2
19	QS	10	PHE	4.2
35	YA	1537	C	4.2
25	R0	3	HIS	4.1
35	RA	2104	G	4.1
3	QC	3	ASN	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	R5	2	ALA	4.1
54	RY	58	GLY	4.1
15	QO	57	LEU	4.0
10	QJ	55	LYS	4.0
35	RA	2179	C	4.0
5	XE	22	GLY	4.0
11	QK	128	ALA	4.0
23	XX	12	A	4.0
35	RA	1026	U	4.0
14	QN	17	LYS	4.0
9	QI	105	ASP	4.0
24	XZ	76	LEU	4.0
7	XG	4	ARG	3.9
40	RG	2	PRO	3.9
51	RV	50	PRO	3.9
46	RQ	91	GLU	3.9
1	XA	1532	U	3.9
39	RF	6	VAL	3.8
10	QJ	62	HIS	3.8
46	RQ	6	ARG	3.8
7	XG	80	VAL	3.8
21	QU	2	GLY	3.8
42	RI	9	LEU	3.8
32	Y7	47	ARG	3.8
48	RS	110	LEU	3.8
45	RP	150	ALA	3.8
41	YH	53	GLU	3.8
51	YV	12	TYR	3.8
49	RT	112	ARG	3.7
48	YS	110	LEU	3.7
13	XM	109	THR	3.7
35	YA	2109	U	3.7
14	XN	34	TYR	3.7
24	QY	44	LYS	3.7
35	RA	2182	G	3.7
41	RH	125	VAL	3.7
3	XC	2	GLY	3.7
21	QU	4	GLY	3.7
36	RB	88	C	3.7
42	RI	41	GLU	3.7
24	QY	50	HIS	3.7
24	QY	79	ALA	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
19	QS	19	VAL	3.7
43	YN	43	THR	3.7
35	YA	2181	G	3.6
10	XJ	62	HIS	3.6
35	YA	2115	G	3.6
33	R8	34	TRP	3.6
9	XI	120	ARG	3.6
34	Y9	1	MET	3.6
4	XD	89	THR	3.6
43	RN	138	LEU	3.6
47	YR	71	GLN	3.6
51	YV	77	ALA	3.6
4	XD	156	GLU	3.6
49	YT	1	MET	3.6
49	YT	2	ASN	3.6
3	XC	15	THR	3.6
36	RB	89(A)	A	3.5
54	RY	99	CYS	3.5
45	YP	44	GLY	3.5
38	RE	187	ALA	3.5
1	XA	1397	C	3.5
35	YA	2188	C	3.5
24	XZ	38	PRO	3.5
51	YV	1	MET	3.5
34	R9	17	ILE	3.5
14	QN	35	ARG	3.5
23	QX	12	A	3.5
35	YA	2104	G	3.5
45	RP	64	LYS	3.5
39	RF	132	VAL	3.5
33	Y8	31	HIS	3.5
40	YG	137	GLU	3.4
5	XE	21	ALA	3.4
9	XI	119	ALA	3.4
26	R1	85	LEU	3.4
38	YE	159	HIS	3.4
54	RY	44	ILE	3.4
20	QT	21	LYS	3.4
40	YG	80	PHE	3.4
42	YI	12	LEU	3.4
37	RD	2	ALA	3.4
13	QM	106	ASN	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
31	R6	11	LEU	3.4
31	Y6	34	LEU	3.4
9	QI	106	ALA	3.4
10	QJ	47	PHE	3.4
8	QH	84	ARG	3.4
21	QU	15	ARG	3.4
53	RX	89	ILE	3.4
29	Y4	52	THR	3.4
35	YA	2142	C	3.3
35	YA	2180	U	3.3
54	RY	55	TYR	3.3
14	QN	58	LYS	3.3
37	RD	27	THR	3.3
54	RY	56	PRO	3.3
46	RQ	105	GLU	3.3
23	XX	15	A	3.3
31	Y6	38	LYS	3.3
42	YI	146	ALA	3.3
48	YS	88	ASP	3.3
23	XX	11	U	3.3
35	RA	2178	C	3.3
50	RU	90	VAL	3.3
33	Y8	52	LYS	3.3
14	QN	32	SER	3.3
21	XU	2	GLY	3.3
32	R7	45	ALA	3.3
35	YA	2165	G	3.3
42	RI	20	ASP	3.3
1	XA	1534	A	3.3
1	XA	1345	U	3.3
20	XT	23	ARG	3.3
49	YT	112	ARG	3.3
1	XA	1533	C	3.3
42	RI	16	GLY	3.3
42	RI	110	ASP	3.3
31	Y6	36	LEU	3.3
33	Y8	34	TRP	3.3
54	RY	41	GLY	3.3
54	YY	10	GLY	3.3
5	QE	20	GLN	3.2
7	XG	153	HIS	3.2
19	QS	11	VAL	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	XD	32	ALA	3.2
35	RA	352	G	3.2
35	YA	2182	G	3.2
23	QX	14	A	3.2
14	QN	39	LEU	3.2
20	XT	14	LYS	3.2
43	YN	48	MET	3.2
31	R6	22	ALA	3.2
40	RG	73	ALA	3.2
46	YQ	36	ALA	3.2
20	QT	8	ARG	3.2
10	QJ	65	LEU	3.2
29	Y4	67	TYR	3.2
31	R6	36	LEU	3.2
1	QA	1492	A	3.2
35	YA	2168	G	3.2
16	QP	22	THR	3.2
24	XZ	80	CYS	3.2
35	YA	2145	C	3.2
43	RN	3	THR	3.2
50	RU	91	ASP	3.2
31	Y6	24	GLU	3.2
26	Y1	73	LEU	3.2
41	RH	11	VAL	3.2
9	QI	64	THR	3.2
13	QM	43	THR	3.2
25	R0	6	GLY	3.2
41	YH	5	GLY	3.2
31	R6	34	LEU	3.2
37	RD	12	SER	3.2
42	RI	1	MET	3.2
8	XH	131	GLY	3.1
42	RI	122	GLU	3.1
13	XM	106	ASN	3.1
23	QX	7	G	3.1
23	XX	10	G	3.1
5	QE	24	ARG	3.1
33	R8	60	LEU	3.1
37	RD	30	GLU	3.1
35	RA	2144	U	3.1
34	Y9	23	VAL	3.1
1	QA	1493	A	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	QA	1533	C	3.1
35	YA	2023	G	3.1
14	QN	25	VAL	3.1
31	R6	16	CYS	3.1
41	RH	24	VAL	3.1
17	QQ	101	ARG	3.1
19	QS	83	HIS	3.1
43	RN	69	GLN	3.1
48	RS	81	GLY	3.1
12	QL	116	SER	3.1
41	RH	155	SER	3.1
26	R1	93	GLU	3.1
35	RA	155	C	3.1
48	RS	88	ASP	3.1
14	QN	15	LYS	3.1
4	XD	154	ASN	3.1
54	RY	48	ALA	3.1
10	QJ	46	ARG	3.1
13	QM	102	ARG	3.1
5	QE	81	GLU	3.1
13	XM	8	GLU	3.1
24	XY	8	GLU	3.1
54	RY	60	PHE	3.1
1	QA	974	A	3.1
23	QX	5	A	3.1
45	YP	39	LYS	3.1
15	QO	87	ILE	3.1
40	YG	2	PRO	3.1
25	Y0	2	ALA	3.0
54	RY	65	ALA	3.0
42	RI	34	GLY	3.0
48	YS	109	GLY	3.0
31	R6	23	THR	3.0
42	RI	12	LEU	3.0
13	QM	101	GLN	3.0
35	RA	2103	C	3.0
35	YA	2178	C	3.0
39	RF	131	GLY	3.0
45	RP	26	GLY	3.0
3	XC	4	LYS	3.0
29	R4	24	THR	3.0
43	RN	62	VAL	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
49	RT	113	LYS	3.0
9	XI	48	GLU	3.0
37	RD	28	GLU	3.0
38	YE	163	GLU	3.0
1	QA	1528	U	3.0
41	RH	128	PRO	3.0
35	YA	2169	A	3.0
4	XD	158	ILE	3.0
25	R0	21	LEU	3.0
30	R5	58	LEU	3.0
24	XY	82	TYR	3.0
40	YG	116	ASP	3.0
51	YV	85	LYS	3.0
4	XD	23	GLY	3.0
54	YY	93	GLY	3.0
1	QA	80	G	3.0
47	RR	37	THR	3.0
54	YY	1	MET	3.0
2	XB	44	LEU	3.0
35	YA	2179	C	3.0
40	YG	97	ASP	3.0
41	RH	14	GLY	3.0
41	YH	37	VAL	3.0
35	YA	2144	U	3.0
3	XC	14	ILE	3.0
41	YH	7	LEU	2.9
47	YR	75	LEU	2.9
14	QN	14	PRO	2.9
54	RY	62	GLU	2.9
13	QM	75	ALA	2.9
13	XM	120	LYS	2.9
49	YT	94	ALA	2.9
29	Y4	63	TYR	2.9
35	RA	265	A	2.9
14	QN	18	VAL	2.9
40	RG	4	ASP	2.9
45	RP	61	ARG	2.9
46	RQ	21	THR	2.9
9	XI	106	ALA	2.9
41	RH	26	VAL	2.9
43	YN	9	VAL	2.9
21	XU	4	GLY	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
36	RB	89	G	2.9
2	XB	5	ILE	2.9
46	RQ	66	ILE	2.9
13	XM	94	ARG	2.9
20	QT	99	LEU	2.9
24	XZ	66	LEU	2.9
3	QC	174	PRO	2.9
31	R6	24	GLU	2.9
41	RH	168	PRO	2.9
2	XB	97	TRP	2.9
12	XL	26	ALA	2.9
9	XI	53	VAL	2.9
37	RD	13	ARG	2.9
37	RD	215	LEU	2.9
45	RP	60	MET	2.9
54	RY	34	LYS	2.9
35	RA	275	G	2.9
41	RH	115	VAL	2.9
50	YU	90	VAL	2.9
1	XA	90	C	2.9
35	YA	888	C	2.9
35	RA	1012	U	2.9
49	RT	69	GLY	2.9
4	QD	209	ARG	2.9
26	R1	26	ARG	2.9
10	QJ	8	LEU	2.9
43	RN	23	LEU	2.9
54	YY	44	ILE	2.9
19	QS	39	THR	2.9
34	Y9	30	PRO	2.9
41	YH	8	PRO	2.9
41	YH	47	GLU	2.9
43	RN	68	GLU	2.9
3	QC	99	VAL	2.9
13	XM	7	VAL	2.9
33	Y8	45	GLY	2.9
1	XA	1094	G	2.9
9	XI	102	LEU	2.9
20	QT	74	LYS	2.9
35	YA	530	G	2.9
43	RN	43	THR	2.8
24	QY	63	GLU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
14	XN	33	VAL	2.8
50	YU	75	ASN	2.8
10	QJ	88	LEU	2.8
43	RN	51	PHE	2.8
42	RI	130	TYR	2.8
12	QL	9	GLN	2.8
1	XA	60	A	2.8
45	YP	42	SER	2.8
13	XM	105	THR	2.8
1	QA	1397	C	2.8
2	XB	9	GLU	2.8
3	QC	177	THR	2.8
12	QL	19	ARG	2.8
49	YT	3	ARG	2.8
10	QJ	85	LEU	2.8
28	R3	14	GLY	2.8
45	YP	22	GLY	2.8
54	RY	59	GLY	2.8
4	QD	10	ARG	2.8
41	RH	29	PRO	2.8
34	Y9	13	LYS	2.8
49	YT	8	LYS	2.8
49	YT	11	GLU	2.8
35	YA	654(V)	A	2.8
54	RY	107	ASP	2.8
45	RP	24	GLY	2.8
1	QA	88	C	2.8
35	RA	1914	C	2.8
35	YA	886	C	2.8
10	XJ	59	SER	2.8
43	RN	104	LYS	2.8
10	QJ	42	THR	2.8
10	XJ	48	THR	2.8
24	XZ	37	THR	2.8
38	RE	52	LEU	2.8
14	QN	7	ILE	2.8
40	RG	86	MET	2.8
41	RH	162	ILE	2.8
12	XL	8	ASN	2.8
4	XD	27	TYR	2.8
23	XX	13	A	2.8
7	XG	79	ARG	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
38	RE	114	ALA	2.8
41	YH	6	ARG	2.8
34	Y9	31	LYS	2.8
1	QA	3	G	2.8
9	QI	74	ILE	2.8
48	YS	112	PHE	2.7
43	YN	1	MET	2.7
50	RU	118	GLY	2.7
52	RW	40	ASN	2.7
48	YS	7	TYR	2.7
24	QY	83	HIS	2.7
32	R7	47	ARG	2.7
37	YD	262	ARG	2.7
47	YR	2	ARG	2.7
20	QT	12	ALA	2.7
54	YY	102	CYS	2.7
43	YN	138	LEU	2.7
2	XB	12	GLU	2.7
2	XB	17	PHE	2.7
24	QY	7	GLU	2.7
24	QY	19	THR	2.7
30	Y5	48	GLU	2.7
35	YA	2402	C	2.7
36	RB	90	C	2.7
51	YV	60	GLU	2.7
39	YF	61	GLY	2.7
1	QA	1331	G	2.7
34	R9	31	LYS	2.7
40	RG	12	TYR	2.7
46	RQ	87	LYS	2.7
47	YR	9	LYS	2.7
14	QN	5	ALA	2.7
33	Y8	35	GLN	2.7
33	Y8	43	GLN	2.7
35	RA	276	A	2.7
37	RD	41	GLY	2.7
17	QQ	68	ARG	2.7
17	XQ	68	ARG	2.7
21	QU	6	ARG	2.7
13	QM	120	LYS	2.7
54	YY	107	ASP	2.7
16	XP	32	TYR	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
49	YT	14	TYR	2.7
12	QL	8	ASN	2.7
48	RS	77	ALA	2.7
35	YA	2120	G	2.7
35	YA	2166	G	2.7
35	YA	2308	G	2.7
51	YV	11	GLN	2.7
34	Y9	26	ILE	2.7
9	XI	115	GLY	2.7
39	YF	76	GLY	2.7
40	RG	65	GLY	2.7
51	RV	48	GLY	2.7
21	QU	3	LYS	2.7
52	RW	97	LYS	2.7
35	RA	229	A	2.7
35	RA	1204	A	2.7
9	XI	26	VAL	2.7
20	XT	9	ASN	2.7
37	RD	206	LEU	2.7
43	RN	33	LEU	2.7
27	Y2	70	GLN	2.7
35	RA	2145	C	2.7
15	XO	15	PHE	2.7
2	QB	18	GLY	2.7
2	XB	18	GLY	2.7
13	XM	26	GLY	2.7
14	QN	6	LEU	2.7
21	XU	18	TYR	2.7
45	RP	62	LEU	2.7
1	XA	975	A	2.6
3	QC	10	PHE	2.6
40	YG	105	LYS	2.6
43	RN	109	LYS	2.6
5	XE	23	GLY	2.6
17	QQ	24	GLU	2.6
26	R1	89	GLU	2.6
41	YH	48	GLY	2.6
52	YW	112	GLY	2.6
17	QQ	99	SER	2.6
1	XA	971	G	2.6
7	XG	42	ILE	2.6
35	RA	2181	G	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
35	YA	2116	G	2.6
40	RG	52	ILE	2.6
49	RT	108	ARG	2.6
5	XE	124	GLY	2.6
39	RF	86	GLY	2.6
45	YP	43	GLY	2.6
50	YU	7	GLY	2.6
6	QF	101	ALA	2.6
12	XL	27	LEU	2.6
20	XT	13	LEU	2.6
41	RH	15	VAL	2.6
54	RY	49	VAL	2.6
1	QA	980	C	2.6
26	R1	86	SER	2.6
36	YB	88	C	2.6
12	XL	17	LYS	2.6
20	QT	14	LYS	2.6
47	YR	107	ASP	2.6
55	YZ	179	ASP	2.6
13	QM	26	GLY	2.6
41	RH	120	GLY	2.6
41	RH	161	GLY	2.6
40	RG	165	THR	2.6
45	RP	16	ARG	2.6
9	XI	126	SER	2.6
34	R9	32	HIS	2.6
13	XM	101	GLN	2.6
15	XO	71	GLN	2.6
48	RS	108	GLY	2.6
4	QD	96	LEU	2.6
25	Y0	37	LEU	2.6
27	R2	44	LEU	2.6
33	Y8	55	ALA	2.6
47	YR	73	VAL	2.6
51	YV	51	VAL	2.6
24	QY	81	ARG	2.6
35	YA	1535	U	2.6
35	YA	2118	U	2.6
42	RI	52	ARG	2.6
43	RN	84	LYS	2.6
52	RW	92	ARG	2.6
35	RA	1176	G	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
35	YA	528	A	2.6
7	XG	82	GLY	2.6
19	XS	13	ASP	2.6
33	R8	45	GLY	2.6
38	RE	121	ASN	2.6
1	QA	1538	C	2.6
1	XA	1113	C	2.6
12	QL	115	LYS	2.6
21	QU	10	ARG	2.6
38	RE	111	ARG	2.6
44	YO	97	ARG	2.6
10	XJ	75	ILE	2.5
38	YE	1	MET	2.5
2	XB	122	PHE	2.5
10	XJ	63	PHE	2.5
46	RQ	104	PHE	2.5
34	R9	20	HIS	2.5
34	Y9	20	HIS	2.5
4	XD	160	GLN	2.5
49	YT	105	LEU	2.5
51	RV	38	LEU	2.5
9	QI	128	ARG	2.5
9	XI	86	VAL	2.5
16	XP	25	ARG	2.5
27	R2	5	GLU	2.5
32	R7	46	VAL	2.5
34	R9	23	VAL	2.5
35	YA	2148	G	2.5
42	RI	14	ASP	2.5
52	YW	113	LYS	2.5
54	RY	43	ASN	2.5
39	YF	127	GLU	2.5
10	QJ	67	THR	2.5
38	YE	14	ILE	2.5
35	RA	2803	C	2.5
2	XB	16	HIS	2.5
13	QM	10	PRO	2.5
20	QT	98	PRO	2.5
13	XM	112	GLY	2.5
20	QT	72	LEU	2.5
34	R9	37	GLY	2.5
2	XB	175	ARG	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	XC	179	ARG	2.5
7	QG	79	ARG	2.5
13	QM	121	LYS	2.5
34	R9	16	VAL	2.5
16	QP	68	ASP	2.5
43	YN	96	GLU	2.5
50	RU	37	GLU	2.5
1	QA	1151	A	2.5
1	XA	687	A	2.5
35	YA	2062	A	2.5
35	YA	2141	G	2.5
25	Y0	3	HIS	2.5
10	QJ	90	LEU	2.5
18	XR	88	LYS	2.5
30	Y5	37	LYS	2.5
35	RA	654(G)	C	2.5
45	RP	70	GLN	2.5
41	YH	44	VAL	2.5
43	RN	46	VAL	2.5
49	RT	94	ALA	2.5
38	YE	200	GLU	2.5
54	RY	64	GLU	2.5
13	QM	83	ASP	2.5
31	Y6	54	ILE	2.5
37	YD	71	ASP	2.5
42	RI	11	ASN	2.5
29	R4	1	MET	2.5
43	YN	90	MET	2.5
26	R1	60	PHE	2.5
43	RN	93	THR	2.5
8	QH	81	HIS	2.5
12	QL	21	LYS	2.5
14	QN	11	LYS	2.5
31	R6	21	TYR	2.5
54	RY	53	PRO	2.5
43	RN	29	LYS	2.5
43	YN	115	ARG	2.5
45	RP	6	LEU	2.5
53	RX	68	ARG	2.5
35	YA	887	A	2.5
26	R1	53	VAL	2.5
26	R1	56	GLN	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
46	RQ	113	GLN	2.5
35	YA	1667	G	2.5
35	YA	2147	G	2.5
50	YU	86	ALA	2.5
51	YV	73	SER	2.5
35	RA	1053	C	2.5
35	RA	1079	C	2.5
35	YA	2798	C	2.5
55	RZ	181	GLU	2.5
19	XS	12	ASP	2.5
35	RA	614	U	2.5
35	YA	2113	U	2.5
41	RH	129	THR	2.5
12	QL	117	ARG	2.5
20	XT	22	ARG	2.5
34	Y9	32	HIS	2.5
40	YG	146	TYR	2.5
8	XH	83	ILE	2.4
35	YA	276	A	2.4
2	QB	24	TRP	2.4
33	R8	46	ARG	2.4
41	YH	3	ARG	2.4
42	YI	11	ASN	2.4
55	RZ	80	ARG	2.4
1	QA	701	C	2.4
14	XN	39	LEU	2.4
38	RE	132	HIS	2.4
20	QT	101	GLY	2.4
7	QG	152	ALA	2.4
25	R0	17	GLN	2.4
39	YF	198	ALA	2.4
43	RN	96	GLU	2.4
48	RS	111	GLU	2.4
11	QK	123	LYS	2.4
15	XO	48	LYS	2.4
25	Y0	11	ARG	2.4
37	RD	31	LYS	2.4
37	RD	48	ARG	2.4
53	RX	50	LYS	2.4
54	RY	46	LYS	2.4
49	RT	114	LEU	2.4
52	RW	19	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	XC	165	THR	2.4
19	XS	79	THR	2.4
52	YW	22	ASP	2.4
8	XH	72	PRO	2.4
15	QO	51	HIS	2.4
29	Y4	50	VAL	2.4
29	Y4	54	GLY	2.4
42	YI	124	GLY	2.4
1	QA	1362	C	2.4
13	QM	9	ILE	2.4
26	R1	77	ALA	2.4
20	XT	18	GLN	2.4
41	RH	95	ARG	2.4
41	RH	97	ARG	2.4
45	YP	36	LYS	2.4
4	XD	205	GLU	2.4
27	R2	11	GLU	2.4
41	RH	124	GLU	2.4
17	XQ	31	LEU	2.4
31	Y6	9	LEU	2.4
3	QC	167	TRP	2.4
10	QJ	48	THR	2.4
10	QJ	87	THR	2.4
10	QJ	89	ASP	2.4
10	QJ	101	VAL	2.4
48	RS	41	ASP	2.4
7	XG	151	TYR	2.4
12	QL	88	GLY	2.4
40	YG	131	TYR	2.4
1	QA	1446	A	2.4
23	QX	13	A	2.4
34	Y9	10	ILE	2.4
10	QJ	45	ARG	2.4
11	QK	127	LYS	2.4
12	QL	20	LYS	2.4
31	R6	8	LYS	2.4
45	RP	91	PHE	2.4
1	XA	5	U	2.4
1	XA	1126	U	2.4
20	XT	10	LEU	2.4
31	Y6	11	LEU	2.4
41	YH	116	GLU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
51	YV	23	GLU	2.4
23	QX	6	G	2.4
35	RA	1173	G	2.4
35	YA	1816	G	2.4
3	XC	167	TRP	2.4
21	XU	14	TRP	2.4
20	XT	26	ASN	2.4
11	QK	36	ASP	2.4
45	YP	104	GLY	2.4
5	QE	109	ILE	2.4
7	QG	150	ALA	2.4
9	XI	43	ALA	2.4
14	QN	10	ALA	2.4
29	R4	63	TYR	2.4
34	R9	5	ALA	2.4
16	QP	27	LYS	2.4
34	R9	8	LYS	2.4
20	XT	25	ARG	2.4
26	Y1	21	ARG	2.4
31	Y6	6	ARG	2.4
46	YQ	3	MET	2.4
8	QH	2	LEU	2.4
26	R1	6	GLU	2.4
27	Y2	5	GLU	2.4
38	RE	21	VAL	2.4
32	R7	24	THR	2.3
35	YA	2138	C	2.3
47	YR	106	GLY	2.3
24	XY	51	ASN	2.3
31	Y6	45	LYS	2.3
39	RF	69	HIS	2.3
10	QJ	66	ARG	2.3
37	RD	273	ARG	2.3
39	YF	128	ALA	2.3
46	RQ	16	ARG	2.3
46	YQ	74	TYR	2.3
48	YS	15	ARG	2.3
52	YW	93	ALA	2.3
25	R0	53	MET	2.3
1	XA	3	G	2.3
13	XM	90	LEU	2.3
40	YG	82	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
53	RX	28	PHE	2.3
55	YZ	163	LEU	2.3
17	XQ	24	GLU	2.3
1	XA	632	A	2.3
3	XC	154	SER	2.3
45	RP	145	PRO	2.3
5	QE	23	GLY	2.3
12	QL	23	LYS	2.3
35	YA	529	A	2.3
5	QE	129	ILE	2.3
34	R9	19	ARG	2.3
8	QH	28	ALA	2.3
41	RH	89	ILE	2.3
7	QG	85	TYR	2.3
9	XI	114	TYR	2.3
1	XA	328	C	2.3
35	RA	2142	C	2.3
54	RY	11	ASP	2.3
42	YI	128	LEU	2.3
35	RA	171	G	2.3
35	YA	2307	G	2.3
36	RB	86	G	2.3
37	RD	35	LYS	2.3
41	RH	27	LYS	2.3
9	QI	63	ILE	2.3
16	QP	10	GLY	2.3
21	QU	14	TRP	2.3
34	R9	26	ILE	2.3
37	RD	162	SER	2.3
43	RN	71	ILE	2.3
43	YN	36	GLY	2.3
48	RS	86	ALA	2.3
9	XI	117	HIS	2.3
49	RT	1	MET	2.3
19	QS	15	LEU	2.3
31	Y6	20	ASN	2.3
42	RI	77	LEU	2.3
16	XP	68	ASP	2.3
47	YR	69	ASP	2.3
1	QA	4	U	2.3
12	XL	9	GLN	2.3
29	Y4	46	GLN	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
12	QL	47	LYS	2.3
33	R8	47	LYS	2.3
39	RF	89	VAL	2.3
33	Y8	53	PRO	2.3
43	RN	95	PRO	2.3
26	R1	79	GLY	2.3
37	YD	259	THR	2.3
43	RN	63	THR	2.3
31	Y6	46	HIS	2.3
48	RS	27	SER	2.3
3	QC	201	TYR	2.3
21	QU	18	TYR	2.3
33	Y8	64	TYR	2.3
35	RA	2120	G	2.3
35	YA	2159	G	2.3
46	RQ	74	TYR	2.3
47	RR	11	ASN	2.3
25	R0	71	ASP	2.3
37	RD	122	ASP	2.3
4	XD	10	ARG	2.3
7	QG	80	VAL	2.3
14	QN	33	VAL	2.3
17	XQ	49	GLU	2.3
35	YA	229	A	2.3
48	RS	9	ARG	2.3
50	YU	92	ARG	2.3
35	RA	1078	U	2.3
35	YA	2132	U	2.3
5	QE	11	ILE	2.3
13	QM	4	ILE	2.3
49	RT	52	ILE	2.3
54	RY	61	ILE	2.3
35	RA	2143	C	2.3
3	XC	204	LEU	2.3
29	Y4	27	THR	2.3
42	YI	30	LEU	2.3
31	R6	38	LYS	2.3
47	RR	9	LYS	2.3
48	YS	16	ASN	2.3
50	YU	94	ASN	2.3
4	XD	209	ARG	2.3
52	YW	92	ARG	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	QC	173	VAL	2.3
9	QI	75	ASP	2.3
1	QA	976	G	2.2
1	QA	1190	G	2.2
53	RX	80	ILE	2.2
9	XI	49	PRO	2.2
5	QE	10	MET	2.2
38	RE	139	GLY	2.2
45	YP	34	GLY	2.2
1	XA	1492	A	2.2
20	XT	72	LEU	2.2
25	R0	7	LEU	2.2
35	RA	2189	U	2.2
35	YA	1026	U	2.2
35	YA	2726	U	2.2
24	XZ	39	PHE	2.2
31	R6	30	THR	2.2
4	XD	83	SER	2.2
37	RD	38	LYS	2.2
40	YG	36	LYS	2.2
41	YH	16	SER	2.2
46	YQ	18	LYS	2.2
1	QA	1039	C	2.2
3	QC	190	ARG	2.2
5	XE	107	ARG	2.2
24	QY	22	ARG	2.2
37	RD	52	ARG	2.2
17	XQ	23	VAL	2.2
24	XZ	20	ASP	2.2
25	Y0	15	ASP	2.2
31	Y6	7	ILE	2.2
4	QD	130	GLY	2.2
10	QJ	40	LEU	2.2
11	QK	23	ALA	2.2
20	QT	95	ALA	2.2
31	Y6	22	ALA	2.2
45	RP	10	PRO	2.2
50	YU	87	GLY	2.2
50	YU	96	ALA	2.2
55	YZ	102	LEU	2.2
1	QA	703	G	2.2
1	XA	851	G	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
14	QN	22	THR	2.2
16	XP	12	LYS	2.2
17	XQ	100	LYS	2.2
21	QU	25	LYS	2.2
35	RA	101	G	2.2
35	YA	2187	G	2.2
35	YA	2490	G	2.2
51	YV	6	LYS	2.2
4	QD	139	ARG	2.2
5	XE	24	ARG	2.2
22	XV	47	U	2.2
23	QX	11	U	2.2
39	YF	74	ARG	2.2
45	YP	21	ARG	2.2
22	QV	76	A	2.2
19	QS	67	VAL	2.2
41	RH	49	VAL	2.2
7	XG	37	ASN	2.2
24	QY	46	GLU	2.2
33	Y8	56	GLU	2.2
42	RI	79	ILE	2.2
35	RA	2139	C	2.2
35	YA	2108	C	2.2
5	QE	136	MET	2.2
48	YS	41	ASP	2.2
13	XM	10	PRO	2.2
39	RF	47	GLY	2.2
41	YH	21	PRO	2.2
51	YV	42	GLY	2.2
7	XG	3	ARG	2.2
12	QL	89	ARG	2.2
43	RN	115	ARG	2.2
45	YP	16	ARG	2.2
43	YN	22	THR	2.2
50	YU	78	THR	2.2
9	XI	125	TYR	2.2
9	QI	109	VAL	2.2
9	XI	44	VAL	2.2
34	Y9	3	VAL	2.2
37	YD	22	SER	2.2
2	QB	76	GLN	2.2
48	YS	82	ILE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
35	RA	2793	G	2.2
35	YA	1762	A	2.2
41	YH	33	LEU	2.2
42	YI	38	LEU	2.2
9	QI	46	ALA	2.2
44	YO	1	MET	2.2
37	RD	207	GLY	2.2
42	YI	8	PRO	2.2
47	YR	39	PRO	2.2
48	RS	51	ALA	2.2
40	YG	166	ASP	2.2
7	XG	32	ARG	2.2
46	YQ	10	ARG	2.2
50	YU	52	ARG	2.2
35	RA	1080	C	2.2
35	RA	2140	C	2.2
50	RU	25	TRP	2.2
7	QG	153	HIS	2.2
19	QS	41	VAL	2.2
13	QM	25	ILE	2.2
37	RD	64	ILE	2.2
17	QQ	31	LEU	2.2
20	QT	24	LEU	2.2
24	XZ	1	MET	2.2
4	XD	77	ASN	2.2
9	QI	110	GLU	2.2
54	RY	1	MET	2.2
12	QL	13	LYS	2.2
12	QL	17	LYS	2.2
19	XS	65	ASN	2.2
20	XT	44	ALA	2.2
20	XT	76	ALA	2.2
30	R5	13	LYS	2.2
33	R8	39	LYS	2.2
35	RA	2102	U	2.2
37	RD	56	GLY	2.2
38	YE	115	GLY	2.2
52	YW	26	GLY	2.2
54	RY	22	GLY	2.2
4	QD	73	ARG	2.2
8	QH	102	ARG	2.2
20	QT	25	ARG	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	QA	1286	A	2.2
35	RA	1762	A	2.2
35	YA	289	A	2.2
1	QA	1127	G	2.2
35	RA	1025	G	2.2
8	XH	24	THR	2.1
12	QL	64	TYR	2.1
10	QJ	50	ILE	2.1
13	XM	9	ILE	2.1
6	QF	61	LEU	2.1
20	QT	13	LEU	2.1
34	Y9	36	GLN	2.1
7	XG	125	MET	2.1
19	XS	4	SER	2.1
24	XY	74	SER	2.1
26	R1	48	LYS	2.1
28	Y3	17	LYS	2.1
37	YD	275	LYS	2.1
43	RN	1	MET	2.1
44	RO	1	MET	2.1
4	XD	72	GLU	2.1
5	QE	21	ALA	2.1
13	XM	108	ARG	2.1
41	RH	104	GLU	2.1
37	RD	110	GLY	2.1
37	RD	160	GLY	2.1
41	YH	42	ARG	2.1
54	YY	64	GLU	2.1
47	RR	46	GLY	2.1
11	QK	117	ASN	2.1
29	Y4	59	PHE	2.1
35	YA	2189	U	2.1
8	XH	97	VAL	2.1
41	RH	169	VAL	2.1
42	RI	144	VAL	2.1
42	YI	145	VAL	2.1
21	QU	8	THR	2.1
25	Y0	10	THR	2.1
39	YF	70	THR	2.1
47	YR	35	THR	2.1
14	QN	42	ILE	2.1
37	RD	24	ILE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	XB	98	LEU	2.1
14	QN	4	LYS	2.1
26	R1	95	LEU	2.1
26	Y1	92	LYS	2.1
27	R2	15	LYS	2.1
17	QQ	91	ARG	2.1
27	R2	43	GLN	2.1
27	Y2	69	ARG	2.1
32	Y7	36	GLN	2.1
33	R8	43	GLN	2.1
49	RT	53	ARG	2.1
52	RW	90	ARG	2.1
7	QG	8	GLU	2.1
31	Y6	41	PRO	2.1
34	Y9	37	GLY	2.1
35	YA	2146	C	2.1
38	YE	138	PRO	2.1
40	YG	45	GLU	2.1
44	YO	42	SER	2.1
48	RS	43	GLU	2.1
48	YS	107	GLU	2.1
51	YV	50	PRO	2.1
27	Y2	71	ASN	2.1
7	XG	33	ASP	2.1
9	XI	105	ASP	2.1
13	QM	45	VAL	2.1
49	RT	107	ASP	2.1
51	YV	5	VAL	2.1
11	QK	25	TYR	2.1
13	QM	19	LEU	2.1
16	QP	49	LEU	2.1
17	QQ	90	ILE	2.1
33	R8	62	LEU	2.1
48	YS	18	ILE	2.1
41	RH	163	TYR	2.1
52	YW	90	ARG	2.1
12	QL	128	ALA	2.1
45	RP	31	ALA	2.1
53	RX	22	ALA	2.1
3	QC	96	GLY	2.1
14	QN	55	GLY	2.1
24	QY	18	GLU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	R9	28	GLU	2.1
35	RA	1379	A	2.1
39	YF	56	GLU	2.1
40	RG	85	GLY	2.1
34	R9	6	SER	2.1
38	RE	143	ASN	2.1
1	QA	1202	G	2.1
1	XA	1178	G	2.1
2	XB	136	VAL	2.1
31	R6	52	VAL	2.1
35	RA	274	G	2.1
41	YH	24	VAL	2.1
35	RA	1537	C	2.1
35	RA	2804	C	2.1
3	QC	26	LYS	2.1
4	QD	84	LYS	2.1
2	XB	211	ILE	2.1
16	XP	23	ASP	2.1
42	RI	112	LYS	2.1
47	YR	3	HIS	2.1
54	RY	47	LYS	2.1
16	XP	33	ILE	2.1
51	YV	39	LEU	2.1
52	RW	95	ILE	2.1
3	XC	119	ARG	2.1
24	XZ	35	ARG	2.1
37	RD	17	THR	2.1
53	RX	3	THR	2.1
5	XE	10	MET	2.1
9	QI	82	ALA	2.1
35	RA	2712	U	2.1
35	YA	2102	U	2.1
9	QI	115	GLY	2.1
41	YH	22	GLY	2.1
54	YY	103	GLY	2.1
10	XJ	61	GLU	2.1
11	XK	125	PHE	2.1
17	XQ	96	GLU	2.1
42	RI	143	SER	2.1
19	QS	9	VAL	2.1
45	YP	71	VAL	2.1
46	RQ	27	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
54	YY	3	VAL	2.1
1	XA	1446	A	2.1
6	QF	13	ASN	2.1
10	XJ	69	ASN	2.1
24	XY	44	LYS	2.1
35	RA	2335	A	2.1
10	QJ	4	ILE	2.1
37	RD	49	ILE	2.1
48	RS	3	ARG	2.1
51	YV	38	LEU	2.1
14	QN	34	TYR	2.1
21	QU	21	TYR	2.1
1	QA	970	C	2.1
1	XA	1128	C	2.1
1	QA	1197	G	2.1
1	XA	1190	G	2.1
3	QC	61	ALA	2.1
35	RA	2177	C	2.1
35	RA	2319	G	2.1
35	YA	2186	G	2.1
41	RH	145	ALA	2.1
20	QT	18	GLN	2.1
48	RS	109	GLY	2.1
50	RU	7	GLY	2.1
16	XP	46	PRO	2.1
24	QZ	40	GLU	2.1
26	R1	87	PRO	2.1
49	RT	20	PRO	2.1
53	RX	21	PHE	2.1
1	XA	1196	U	2.0
21	QU	26	LYS	2.0
33	Y8	59	LYS	2.0
35	RA	2180	U	2.0
35	RA	2702	U	2.0
41	RH	153	LYS	2.0
41	YH	15	VAL	2.0
44	YO	26	LYS	2.0
10	XJ	35	SER	2.0
2	XB	196	LEU	2.0
10	XJ	88	LEU	2.0
11	XK	83	ILE	2.0
40	YG	52	ILE	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
43	RN	61	ARG	2.0
54	RY	50	ARG	2.0
55	YZ	150	LEU	2.0
10	QJ	56	HIS	2.0
16	QP	1	MET	2.0
7	XG	150	ALA	2.0
7	XG	154	TYR	2.0
13	XM	63	THR	2.0
31	Y6	23	THR	2.0
34	Y9	12	ASP	2.0
35	RA	528	A	2.0
35	RA	2119	A	2.0
42	RI	40	THR	2.0
11	QK	90	GLY	2.0
40	YG	44	GLY	2.0
50	YU	118	GLY	2.0
38	RE	53	PRO	2.0
9	XI	116	LYS	2.0
52	RW	30	GLU	2.0
29	R4	50	VAL	2.0
35	RA	2183	C	2.0
35	YA	2103	C	2.0
25	R0	55	ARG	2.0
29	Y4	58	ARG	2.0
35	YA	2405	G	2.0
43	RN	67	LEU	2.0
53	RX	60	ARG	2.0
4	XD	28	SER	2.0
16	XP	19	ILE	2.0
1	QA	561	U	2.0
42	RI	43	ASN	2.0
13	XM	43	THR	2.0
20	QT	71	THR	2.0
21	XU	8	THR	2.0
53	RX	18	TYR	2.0
24	XZ	72	ASP	2.0
5	XE	85	GLY	2.0
30	Y5	49	CYS	2.0
39	RF	85	GLY	2.0
42	RI	84	GLY	2.0
13	QM	113	PRO	2.0
31	Y6	8	LYS	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	Y7	6	GLN	2.0
34	R9	36	GLN	2.0
38	RE	56	PRO	2.0
53	YX	33	LYS	2.0
36	YB	52	A	2.0
4	XD	73	ARG	2.0
14	QN	57	ARG	2.0
41	YH	69	ARG	2.0
50	YU	36	ARG	2.0
14	XN	44	LEU	2.0
17	QQ	84	LEU	2.0
4	XD	5	ILE	2.0
49	YT	110	ILE	2.0
35	RA	34	C	2.0
35	YA	1914	C	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
23	A3P	QX	20	26/27	0.91	0.13	82,85,97,100	0
23	A3P	XX	20	26/27	0.91	0.11	71,76,82,84	0
56	PPU	ZA	3	37/38	0.91	0.15	41,59,68,71	0
56	PPU	ZB	3	37/38	0.94	0.13	38,56,67,69	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
57	MG	Y9	101	1/1	0.33	0.27	122,122,122,122	0
59	ZN	Y6	101	1/1	0.36	0.25	229,229,229,229	0
57	MG	RA	3174	1/1	0.49	0.21	51,51,51,51	0
57	MG	QA	1673	1/1	0.51	0.26	69,69,69,69	0
57	MG	YA	3081	1/1	0.54	0.29	38,38,38,38	0
57	MG	QA	1645	1/1	0.57	0.17	81,81,81,81	0
57	MG	RA	3155	1/1	0.57	0.21	89,89,89,89	0
57	MG	XA	1651	1/1	0.58	0.69	81,81,81,81	0
57	MG	RA	3295	1/1	0.63	0.20	51,51,51,51	0
57	MG	XA	1636	1/1	0.63	0.22	72,72,72,72	0
57	MG	YA	3235	1/1	0.65	0.19	208,208,208,208	0
59	ZN	R5	101	1/1	0.66	0.20	244,244,244,244	0
57	MG	XA	1676	1/1	0.67	0.32	53,53,53,53	0
57	MG	XA	1699	1/1	0.67	0.19	49,49,49,49	0
57	MG	RA	3164	1/1	0.67	0.24	57,57,57,57	0
57	MG	YA	3060	1/1	0.67	0.34	40,40,40,40	0
57	MG	RA	3012	1/1	0.67	0.17	48,48,48,48	0
57	MG	RA	3081	1/1	0.67	0.34	55,55,55,55	0
57	MG	RA	3112	1/1	0.67	0.23	41,41,41,41	0
57	MG	QA	1646	1/1	0.67	0.13	67,67,67,67	0
57	MG	XA	1644	1/1	0.68	0.11	76,76,76,76	0
57	MG	RQ	202	1/1	0.68	0.18	58,58,58,58	0
57	MG	RA	3058	1/1	0.69	0.35	46,46,46,46	0
57	MG	YA	3103	1/1	0.69	0.31	81,81,81,81	0
57	MG	RA	3190	1/1	0.69	0.11	55,55,55,55	0
57	MG	YA	3321	1/1	0.69	0.12	69,69,69,69	0
57	MG	RA	3242	1/1	0.69	0.26	47,47,47,47	0
57	MG	RA	3134	1/1	0.69	0.16	52,52,52,52	0
57	MG	XA	1674	1/1	0.70	0.12	28,28,28,28	0
57	MG	RA	3086	1/1	0.70	0.21	26,26,26,26	0
57	MG	XA	1685	1/1	0.70	0.20	62,62,62,62	0
57	MG	QA	1657	1/1	0.71	0.32	74,74,74,74	0
57	MG	QY	101	1/1	0.71	0.41	77,77,77,77	0
57	MG	YA	3175	1/1	0.72	0.19	57,57,57,57	0
57	MG	RA	3167	1/1	0.72	0.14	59,59,59,59	0
57	MG	XA	1603	1/1	0.72	0.20	48,48,48,48	0
57	MG	YA	3057	1/1	0.72	0.17	38,38,38,38	0
57	MG	YA	3149	1/1	0.72	0.19	76,76,76,76	0
57	MG	RA	3177	1/1	0.73	0.17	46,46,46,46	0
57	MG	RA	3296	1/1	0.73	0.22	40,40,40,40	0
57	MG	XA	1693	1/1	0.73	0.23	48,48,48,48	0
57	MG	YA	3194	1/1	0.74	0.13	61,61,61,61	0
57	MG	RA	3271	1/1	0.74	0.11	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3305	1/1	0.74	0.20	50,50,50,50	0
57	MG	XA	1687	1/1	0.75	0.17	50,50,50,50	0
57	MG	RA	3189	1/1	0.75	0.21	58,58,58,58	0
57	MG	RA	3294	1/1	0.75	0.28	54,54,54,54	0
57	MG	RA	3248	1/1	0.75	0.18	28,28,28,28	0
57	MG	YA	3287	1/1	0.76	0.13	44,44,44,44	0
57	MG	YA	3168	1/1	0.76	0.15	62,62,62,62	0
57	MG	YA	3222	1/1	0.76	0.18	29,29,29,29	0
57	MG	RA	3301	1/1	0.76	0.24	31,31,31,31	0
57	MG	YA	3246	1/1	0.76	0.14	61,61,61,61	0
57	MG	RA	3302	1/1	0.77	0.49	80,80,80,80	0
57	MG	RA	3143	1/1	0.77	0.22	59,59,59,59	0
57	MG	YA	3265	1/1	0.77	0.11	44,44,44,44	0
57	MG	RA	3133	1/1	0.77	0.20	51,51,51,51	0
57	MG	YA	3011	1/1	0.77	0.33	43,43,43,43	0
57	MG	YA	3019	1/1	0.77	0.29	32,32,32,32	0
57	MG	RA	3061	1/1	0.77	0.22	67,67,67,67	0
57	MG	RA	3165	1/1	0.77	0.12	47,47,47,47	0
57	MG	YA	3257	1/1	0.78	0.18	50,50,50,50	0
57	MG	QA	1628	1/1	0.78	0.08	74,74,74,74	0
57	MG	YA	3279	1/1	0.78	0.17	50,50,50,50	0
57	MG	RA	3283	1/1	0.78	0.32	61,61,61,61	0
57	MG	RA	3147	1/1	0.79	0.14	56,56,56,56	0
57	MG	YA	3066	1/1	0.79	0.12	38,38,38,38	0
57	MG	RA	3014	1/1	0.79	0.23	58,58,58,58	0
57	MG	YA	3091	1/1	0.79	0.17	36,36,36,36	0
57	MG	YA	3055	1/1	0.79	0.14	7,7,7,7	0
59	ZN	R4	101	1/1	0.79	0.20	176,176,176,176	0
57	MG	RA	3107	1/1	0.79	0.20	41,41,41,41	0
59	ZN	R6	101	1/1	0.79	0.28	227,227,227,227	0
57	MG	YA	3161	1/1	0.79	0.10	44,44,44,44	0
57	MG	YA	3273	1/1	0.80	0.12	58,58,58,58	0
57	MG	YA	3277	1/1	0.80	0.10	52,52,52,52	0
57	MG	RA	3182	1/1	0.80	0.15	44,44,44,44	0
57	MG	YA	3107	1/1	0.80	0.24	71,71,71,71	0
57	MG	YA	3288	1/1	0.80	0.10	28,28,28,28	0
57	MG	YA	3110	1/1	0.80	0.20	41,41,41,41	0
57	MG	YA	3117	1/1	0.80	0.11	55,55,55,55	0
57	MG	YE	303	1/1	0.80	0.18	69,69,69,69	0
57	MG	YA	3236	1/1	0.80	0.17	38,38,38,38	0
57	MG	YA	3034	1/1	0.80	0.18	75,75,75,75	0
57	MG	XA	1641	1/1	0.80	0.20	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3072	1/1	0.80	0.24	14,14,14,14	0
57	MG	YA	3184	1/1	0.81	0.19	37,37,37,37	0
57	MG	YA	3143	1/1	0.81	0.09	60,60,60,60	0
57	MG	YA	3219	1/1	0.81	0.25	37,37,37,37	0
57	MG	YG	201	1/1	0.81	0.14	59,59,59,59	0
57	MG	YA	3084	1/1	0.81	0.24	24,24,24,24	0
57	MG	YA	3049	1/1	0.81	0.19	42,42,42,42	0
57	MG	YA	3002	1/1	0.81	0.21	32,32,32,32	0
57	MG	YA	3138	1/1	0.81	0.16	38,38,38,38	0
57	MG	RA	3056	1/1	0.82	0.11	54,54,54,54	0
57	MG	RA	3237	1/1	0.82	0.20	40,40,40,40	0
57	MG	RA	3276	1/1	0.82	0.18	48,48,48,48	0
57	MG	YA	3311	1/1	0.82	0.17	45,45,45,45	0
57	MG	RA	3277	1/1	0.82	0.14	45,45,45,45	0
57	MG	RB	202	1/1	0.82	0.19	27,27,27,27	0
57	MG	YE	305	1/1	0.82	0.11	66,66,66,66	0
57	MG	YA	3261	1/1	0.82	0.15	35,35,35,35	0
57	MG	RA	3241	1/1	0.82	0.12	36,36,36,36	0
57	MG	QA	1617	1/1	0.82	0.13	57,57,57,57	0
57	MG	YA	3141	1/1	0.82	0.16	41,41,41,41	0
57	MG	YA	3220	1/1	0.82	0.14	22,22,22,22	0
57	MG	XA	1677	1/1	0.83	0.18	46,46,46,46	0
57	MG	YA	3281	1/1	0.83	0.18	37,37,37,37	0
57	MG	YA	3183	1/1	0.83	0.14	44,44,44,44	0
57	MG	YB	202	1/1	0.83	0.32	47,47,47,47	0
57	MG	YD	301	1/1	0.83	0.20	24,24,24,24	0
57	MG	RA	3020	1/1	0.83	0.23	39,39,39,39	0
57	MG	YA	3223	1/1	0.84	0.15	31,31,31,31	0
57	MG	RA	3035	1/1	0.84	0.12	34,34,34,34	0
57	MG	RA	3268	1/1	0.84	0.23	56,56,56,56	0
57	MG	QA	1693	1/1	0.84	0.12	50,50,50,50	0
57	MG	YA	3251	1/1	0.84	0.19	68,68,68,68	0
57	MG	RA	3108	1/1	0.84	0.12	43,43,43,43	0
57	MG	XA	1667	1/1	0.84	0.20	26,26,26,26	0
57	MG	XA	1670	1/1	0.84	0.13	46,46,46,46	0
57	MG	YA	3270	1/1	0.84	0.17	44,44,44,44	0
57	MG	XA	1672	1/1	0.84	0.14	30,30,30,30	0
57	MG	QA	1618	1/1	0.84	0.15	55,55,55,55	0
57	MG	XA	1675	1/1	0.84	0.20	35,35,35,35	0
57	MG	YA	3280	1/1	0.84	0.24	42,42,42,42	0
57	MG	RA	3126	1/1	0.84	0.15	60,60,60,60	0
57	MG	YA	3133	1/1	0.84	0.14	32,32,32,32	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3059	1/1	0.84	0.19	27,27,27,27	0
57	MG	RA	3183	1/1	0.84	0.19	56,56,56,56	0
57	MG	QA	1642	1/1	0.84	0.10	64,64,64,64	0
57	MG	YA	3314	1/1	0.84	0.14	50,50,50,50	0
57	MG	YA	3319	1/1	0.84	0.18	57,57,57,57	0
57	MG	QA	1620	1/1	0.84	0.15	75,75,75,75	0
57	MG	RA	3236	1/1	0.84	0.25	47,47,47,47	0
57	MG	RA	3074	1/1	0.84	0.26	23,23,23,23	0
57	MG	RD	301	1/1	0.84	0.13	30,30,30,30	0
57	MG	YE	304	1/1	0.84	0.25	60,60,60,60	0
57	MG	YA	3010	1/1	0.84	0.11	35,35,35,35	0
57	MG	RN	201	1/1	0.84	0.31	72,72,72,72	0
57	MG	YQ	202	1/1	0.84	0.34	70,70,70,70	0
57	MG	RO	201	1/1	0.84	0.24	60,60,60,60	0
57	MG	QA	1682	1/1	0.84	0.08	33,33,33,33	0
57	MG	RQ	204	1/1	0.84	0.14	53,53,53,53	0
57	MG	RA	3160	1/1	0.84	0.26	33,33,33,33	0
57	MG	YA	3097	1/1	0.85	0.10	52,52,52,52	0
57	MG	QA	1649	1/1	0.85	0.11	53,53,53,53	0
57	MG	RA	3258	1/1	0.85	0.27	44,44,44,44	0
57	MG	QA	1664	1/1	0.85	0.24	46,46,46,46	0
57	MG	RA	3270	1/1	0.85	0.14	41,41,41,41	0
57	MG	YA	3127	1/1	0.85	0.26	66,66,66,66	0
57	MG	RA	3090	1/1	0.85	0.13	34,34,34,34	0
57	MG	YA	3135	1/1	0.85	0.12	34,34,34,34	0
57	MG	RA	3106	1/1	0.85	0.18	18,18,18,18	0
57	MG	XA	1613	1/1	0.85	0.33	52,52,52,52	0
57	MG	YA	3283	1/1	0.85	0.20	32,32,32,32	0
57	MG	XA	1617	1/1	0.85	0.10	30,30,30,30	0
57	MG	XA	1619	1/1	0.85	0.14	48,48,48,48	0
57	MG	YA	3290	1/1	0.85	0.19	57,57,57,57	0
57	MG	XA	1635	1/1	0.85	0.15	36,36,36,36	0
57	MG	YA	3309	1/1	0.85	0.16	52,52,52,52	0
57	MG	YA	3012	1/1	0.85	0.14	68,68,68,68	0
57	MG	YA	3312	1/1	0.85	0.09	43,43,43,43	0
57	MG	YA	3171	1/1	0.85	0.13	45,45,45,45	0
57	MG	RA	3188	1/1	0.85	0.15	57,57,57,57	0
57	MG	R0	102	1/1	0.85	0.14	31,31,31,31	0
57	MG	YA	3328	1/1	0.85	0.44	77,77,77,77	0
57	MG	YA	3046	1/1	0.85	0.24	31,31,31,31	0
57	MG	RA	3158	1/1	0.85	0.08	40,40,40,40	0
57	MG	YA	3210	1/1	0.85	0.18	34,34,34,34	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3215	1/1	0.85	0.24	35,35,35,35	0
57	MG	RA	3191	1/1	0.85	0.18	118,118,118,118	0
57	MG	RA	3024	1/1	0.85	0.25	13,13,13,13	0
57	MG	RA	3298	1/1	0.85	0.12	57,57,57,57	0
57	MG	XA	1671	1/1	0.85	0.18	39,39,39,39	0
57	MG	RA	3009	1/1	0.85	0.19	41,41,41,41	0
57	MG	RA	3120	1/1	0.85	0.12	45,45,45,45	0
57	MG	RA	3047	1/1	0.85	0.20	19,19,19,19	0
57	MG	RA	3032	1/1	0.86	0.23	33,33,33,33	0
57	MG	YA	3109	1/1	0.86	0.24	35,35,35,35	0
57	MG	QA	1679	1/1	0.86	0.14	35,35,35,35	0
57	MG	YA	3297	1/1	0.86	0.13	31,31,31,31	0
57	MG	YA	3115	1/1	0.86	0.17	18,18,18,18	0
57	MG	RA	3013	1/1	0.86	0.22	43,43,43,43	0
57	MG	XA	1618	1/1	0.86	0.11	42,42,42,42	0
57	MG	YA	3231	1/1	0.86	0.16	26,26,26,26	0
57	MG	YA	3042	1/1	0.86	0.21	9,9,9,9	0
57	MG	RA	3076	1/1	0.86	0.24	31,31,31,31	0
57	MG	XA	1630	1/1	0.86	0.09	66,66,66,66	0
57	MG	YA	3325	1/1	0.86	0.08	61,61,61,61	0
57	MG	XA	1632	1/1	0.86	0.12	47,47,47,47	0
57	MG	XA	1634	1/1	0.86	0.07	77,77,77,77	0
57	MG	R0	101	1/1	0.86	0.07	9,9,9,9	0
57	MG	QD	301	1/1	0.86	0.09	81,81,81,81	0
57	MG	QV	102	1/1	0.86	0.15	55,55,55,55	0
57	MG	XE	201	1/1	0.86	0.11	32,32,32,32	0
57	MG	RA	3170	1/1	0.86	0.17	74,74,74,74	0
57	MG	RA	3092	1/1	0.86	0.11	38,38,38,38	0
57	MG	YQ	203	1/1	0.86	0.20	64,64,64,64	0
57	MG	YA	3102	1/1	0.86	0.09	52,52,52,52	0
57	MG	RA	3100	1/1	0.86	0.14	39,39,39,39	0
57	MG	YA	3195	1/1	0.86	0.10	38,38,38,38	0
57	MG	YA	3284	1/1	0.86	0.15	36,36,36,36	0
57	MG	YA	3276	1/1	0.87	0.21	49,49,49,49	0
57	MG	QA	1612	1/1	0.87	0.26	33,33,33,33	0
57	MG	XA	1656	1/1	0.87	0.18	34,34,34,34	0
57	MG	YA	3152	1/1	0.87	0.10	44,44,44,44	0
57	MG	QA	1639	1/1	0.87	0.09	59,59,59,59	0
57	MG	RA	3178	1/1	0.87	0.25	63,63,63,63	0
57	MG	RA	3007	1/1	0.87	0.12	25,25,25,25	0
57	MG	RA	3097	1/1	0.87	0.09	36,36,36,36	0
57	MG	YA	3177	1/1	0.87	0.27	68,68,68,68	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3261	1/1	0.87	0.18	44,44,44,44	0
57	MG	YA	3291	1/1	0.87	0.10	39,39,39,39	0
57	MG	RA	3186	1/1	0.87	0.13	36,36,36,36	0
57	MG	YA	3190	1/1	0.87	0.09	44,44,44,44	0
57	MG	QA	1665	1/1	0.87	0.19	31,31,31,31	0
57	MG	QA	1692	1/1	0.87	0.20	42,42,42,42	0
57	MG	YA	3087	1/1	0.87	0.28	22,22,22,22	0
57	MG	YA	3211	1/1	0.87	0.13	26,26,26,26	0
57	MG	RA	3274	1/1	0.87	0.22	53,53,53,53	0
57	MG	RA	3142	1/1	0.87	0.25	28,28,28,28	0
57	MG	RA	3169	1/1	0.87	0.09	63,63,63,63	0
57	MG	RA	3193	1/1	0.87	0.15	57,57,57,57	0
57	MG	RA	3286	1/1	0.87	0.16	51,51,51,51	0
57	MG	XL	201	1/1	0.87	0.08	66,66,66,66	0
57	MG	RA	3207	1/1	0.87	0.17	17,17,17,17	0
57	MG	YA	3112	1/1	0.87	0.17	65,65,65,65	0
57	MG	YA	3239	1/1	0.87	0.09	39,39,39,39	0
57	MG	RA	3210	1/1	0.87	0.14	19,19,19,19	0
57	MG	YA	3006	1/1	0.87	0.12	33,33,33,33	0
57	MG	YA	3009	1/1	0.87	0.15	41,41,41,41	0
57	MG	RA	3211	1/1	0.87	0.22	27,27,27,27	0
57	MG	XA	1638	1/1	0.87	0.12	41,41,41,41	0
57	MG	RA	3232	1/1	0.87	0.31	57,57,57,57	0
59	ZN	R9	101	1/1	0.87	0.34	127,127,127,127	0
57	MG	RA	3082	1/1	0.87	0.17	33,33,33,33	0
57	MG	RA	3041	1/1	0.88	0.19	18,18,18,18	0
57	MG	RA	3029	1/1	0.88	0.10	35,35,35,35	0
57	MG	XA	1673	1/1	0.88	0.17	45,45,45,45	0
57	MG	RA	3166	1/1	0.88	0.24	54,54,54,54	0
57	MG	XA	1606	1/1	0.88	0.21	29,29,29,29	0
57	MG	YA	3286	1/1	0.88	0.10	33,33,33,33	0
57	MG	XA	1609	1/1	0.88	0.22	19,19,19,19	0
57	MG	YA	3185	1/1	0.88	0.17	68,68,68,68	0
57	MG	RA	3131	1/1	0.88	0.14	61,61,61,61	0
57	MG	YA	3191	1/1	0.88	0.10	56,56,56,56	0
57	MG	YA	3294	1/1	0.88	0.16	57,57,57,57	0
57	MG	YA	3085	1/1	0.88	0.15	14,14,14,14	0
57	MG	YA	3301	1/1	0.88	0.14	33,33,33,33	0
57	MG	XA	1679	1/1	0.88	0.14	36,36,36,36	0
57	MG	RA	3208	1/1	0.88	0.11	37,37,37,37	0
57	MG	RA	3066	1/1	0.88	0.15	36,36,36,36	0
57	MG	RA	3103	1/1	0.88	0.12	24,24,24,24	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	XA	1620	1/1	0.88	0.12	42,42,42,42	0
57	MG	YA	3316	1/1	0.88	0.16	66,66,66,66	0
57	MG	RA	3136	1/1	0.88	0.18	52,52,52,52	0
57	MG	RA	3289	1/1	0.88	0.27	56,56,56,56	0
57	MG	RA	3141	1/1	0.88	0.15	32,32,32,32	0
57	MG	RA	3085	1/1	0.88	0.14	15,15,15,15	0
57	MG	YA	3003	1/1	0.88	0.15	36,36,36,36	0
57	MG	YA	3005	1/1	0.88	0.17	34,34,34,34	0
57	MG	R3	101	1/1	0.88	0.22	24,24,24,24	0
57	MG	RA	3088	1/1	0.88	0.14	33,33,33,33	0
57	MG	RA	3245	1/1	0.88	0.23	48,48,48,48	0
57	MG	RA	3111	1/1	0.88	0.17	41,41,41,41	0
57	MG	XA	1648	1/1	0.88	0.07	34,34,34,34	0
57	MG	QA	1689	1/1	0.88	0.16	70,70,70,70	0
57	MG	YV	301	1/1	0.88	0.08	68,68,68,68	0
57	MG	YA	3266	1/1	0.88	0.23	47,47,47,47	0
57	MG	RA	3115	1/1	0.88	0.23	25,25,25,25	0
57	MG	RA	3263	1/1	0.88	0.16	51,51,51,51	0
57	MG	RA	3264	1/1	0.88	0.16	41,41,41,41	0
57	MG	YA	3164	1/1	0.88	0.16	39,39,39,39	0
57	MG	YA	3165	1/1	0.89	0.07	49,49,49,49	0
57	MG	RA	3139	1/1	0.89	0.12	32,32,32,32	0
57	MG	YA	3169	1/1	0.89	0.17	44,44,44,44	0
57	MG	YA	3063	1/1	0.89	0.23	31,31,31,31	0
57	MG	RA	3096	1/1	0.89	0.12	38,38,38,38	0
57	MG	QA	1605	1/1	0.89	0.22	30,30,30,30	0
57	MG	RA	3045	1/1	0.89	0.18	40,40,40,40	0
57	MG	RA	3195	1/1	0.89	0.18	44,44,44,44	0
57	MG	RA	3205	1/1	0.89	0.26	16,16,16,16	0
57	MG	XA	1642	1/1	0.89	0.13	55,55,55,55	0
57	MG	XV	102	1/1	0.89	0.15	32,32,32,32	0
57	MG	YA	3193	1/1	0.89	0.17	38,38,38,38	0
57	MG	XV	103	1/1	0.89	0.18	57,57,57,57	0
57	MG	Y5	101	1/1	0.89	0.14	71,71,71,71	0
57	MG	YA	3302	1/1	0.89	0.22	50,50,50,50	0
57	MG	YA	3205	1/1	0.89	0.15	17,17,17,17	0
57	MG	RA	3173	1/1	0.89	0.13	29,29,29,29	0
57	MG	XA	1645	1/1	0.89	0.09	60,60,60,60	0
57	MG	RA	3025	1/1	0.89	0.18	15,15,15,15	0
57	MG	YA	3313	1/1	0.89	0.14	51,51,51,51	0
57	MG	RA	3209	1/1	0.89	0.20	26,26,26,26	0
57	MG	RA	3154	1/1	0.89	0.13	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3221	1/1	0.89	0.20	27,27,27,27	0
57	MG	XA	1666	1/1	0.89	0.18	40,40,40,40	0
57	MG	YA	3322	1/1	0.89	0.12	71,71,71,71	0
57	MG	YA	3121	1/1	0.89	0.13	34,34,34,34	0
57	MG	YA	3228	1/1	0.89	0.14	34,34,34,34	0
57	MG	YA	3329	1/1	0.89	0.19	36,36,36,36	0
57	MG	XA	1604	1/1	0.89	0.18	21,21,21,21	0
57	MG	RA	3130	1/1	0.89	0.20	38,38,38,38	0
57	MG	RA	3223	1/1	0.89	0.16	38,38,38,38	0
57	MG	QA	1671	1/1	0.89	0.21	34,34,34,34	0
57	MG	YA	3240	1/1	0.89	0.18	36,36,36,36	0
57	MG	YA	3140	1/1	0.89	0.14	27,27,27,27	0
57	MG	RA	3089	1/1	0.89	0.21	25,25,25,25	0
57	MG	RA	3185	1/1	0.89	0.14	33,33,33,33	0
57	MG	RA	3239	1/1	0.89	0.24	57,57,57,57	0
57	MG	YA	3150	1/1	0.89	0.15	58,58,58,58	0
57	MG	QA	1662	1/1	0.89	0.18	63,63,63,63	0
57	MG	YA	3154	1/1	0.89	0.09	56,56,56,56	0
57	MG	QA	1641	1/1	0.89	0.23	55,55,55,55	0
57	MG	XA	1678	1/1	0.89	0.19	35,35,35,35	0
57	MG	RY	201	1/1	0.90	0.13	51,51,51,51	0
57	MG	YA	3014	1/1	0.90	0.17	38,38,38,38	0
57	MG	QA	1651	1/1	0.90	0.09	81,81,81,81	0
57	MG	YA	3030	1/1	0.90	0.10	27,27,27,27	0
57	MG	YA	3275	1/1	0.90	0.19	53,53,53,53	0
57	MG	RA	3280	1/1	0.90	0.11	37,37,37,37	0
57	MG	RA	3282	1/1	0.90	0.29	28,28,28,28	0
57	MG	YA	3163	1/1	0.90	0.14	41,41,41,41	0
57	MG	RA	3161	1/1	0.90	0.10	34,34,34,34	0
57	MG	XA	1612	1/1	0.90	0.15	27,27,27,27	0
57	MG	YA	3052	1/1	0.90	0.09	40,40,40,40	0
57	MG	RA	3033	1/1	0.90	0.19	55,55,55,55	0
57	MG	QA	1684	1/1	0.90	0.26	51,51,51,51	0
57	MG	YA	3059	1/1	0.90	0.22	8,8,8,8	0
57	MG	RA	3293	1/1	0.90	0.21	26,26,26,26	0
57	MG	RA	3037	1/1	0.90	0.14	18,18,18,18	0
57	MG	XA	1680	1/1	0.90	0.10	45,45,45,45	0
57	MG	YA	3071	1/1	0.90	0.18	16,16,16,16	0
57	MG	YA	3187	1/1	0.90	0.11	33,33,33,33	0
57	MG	RA	3039	1/1	0.90	0.13	31,31,31,31	0
57	MG	XA	1686	1/1	0.90	0.13	47,47,47,47	0
57	MG	RA	3110	1/1	0.90	0.15	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	XA	1689	1/1	0.90	0.06	27,27,27,27	0
57	MG	QA	1602	1/1	0.90	0.18	33,33,33,33	0
57	MG	YA	3203	1/1	0.90	0.18	15,15,15,15	0
57	MG	RA	3299	1/1	0.90	0.21	47,47,47,47	0
57	MG	YA	3207	1/1	0.90	0.20	36,36,36,36	0
57	MG	YA	3100	1/1	0.90	0.39	67,67,67,67	0
57	MG	QA	1630	1/1	0.90	0.24	36,36,36,36	0
57	MG	YA	3320	1/1	0.90	0.14	57,57,57,57	0
57	MG	XF	301	1/1	0.90	0.05	35,35,35,35	0
57	MG	YA	3104	1/1	0.90	0.18	22,22,22,22	0
57	MG	YA	3324	1/1	0.90	0.19	47,47,47,47	0
57	MG	QA	1635	1/1	0.90	0.17	57,57,57,57	0
57	MG	YA	3327	1/1	0.90	0.36	71,71,71,71	0
57	MG	RB	201	1/1	0.90	0.08	41,41,41,41	0
57	MG	RA	3116	1/1	0.90	0.15	40,40,40,40	0
57	MG	YA	3331	1/1	0.90	0.11	30,30,30,30	0
57	MG	YA	3334	1/1	0.90	0.10	42,42,42,42	0
57	MG	YA	3335	1/1	0.90	0.28	44,44,44,44	0
57	MG	RB	203	1/1	0.90	0.13	21,21,21,21	0
57	MG	RA	3148	1/1	0.90	0.14	25,25,25,25	0
57	MG	YE	301	1/1	0.90	0.16	25,25,25,25	0
57	MG	YA	3230	1/1	0.90	0.15	34,34,34,34	0
57	MG	RA	3055	1/1	0.90	0.12	24,24,24,24	0
57	MG	RA	3099	1/1	0.90	0.15	37,37,37,37	0
57	MG	YA	3004	1/1	0.90	0.13	52,52,52,52	0
57	MG	XA	1649	1/1	0.90	0.24	55,55,55,55	0
57	MG	RQ	201	1/1	0.90	0.15	42,42,42,42	0
57	MG	YQ	204	1/1	0.90	0.18	86,86,86,86	0
57	MG	YA	3136	1/1	0.90	0.10	41,41,41,41	0
57	MG	RA	3227	1/1	0.90	0.12	31,31,31,31	0
57	MG	YA	3256	1/1	0.90	0.17	34,34,34,34	0
57	MG	RQ	203	1/1	0.90	0.14	32,32,32,32	0
57	MG	RA	3127	1/1	0.90	0.10	35,35,35,35	0
57	MG	YA	3262	1/1	0.90	0.11	55,55,55,55	0
57	MG	YA	3036	1/1	0.91	0.17	19,19,19,19	0
57	MG	XA	1607	1/1	0.91	0.10	51,51,51,51	0
57	MG	RA	3231	1/1	0.91	0.12	26,26,26,26	0
57	MG	YA	3048	1/1	0.91	0.19	9,9,9,9	0
57	MG	QA	1637	1/1	0.91	0.17	43,43,43,43	0
57	MG	YA	3162	1/1	0.91	0.18	42,42,42,42	0
57	MG	RA	3285	1/1	0.91	0.23	18,18,18,18	0
57	MG	RA	3031	1/1	0.91	0.16	29,29,29,29	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3137	1/1	0.91	0.11	41,41,41,41	0
57	MG	YA	3282	1/1	0.91	0.10	24,24,24,24	0
57	MG	YA	3167	1/1	0.91	0.25	25,25,25,25	0
57	MG	RA	3138	1/1	0.91	0.15	46,46,46,46	0
57	MG	RA	3240	1/1	0.91	0.22	41,41,41,41	0
57	MG	YA	3061	1/1	0.91	0.16	23,23,23,23	0
57	MG	XA	1629	1/1	0.91	0.17	26,26,26,26	0
57	MG	QA	1619	1/1	0.91	0.14	55,55,55,55	0
57	MG	YA	3178	1/1	0.91	0.15	41,41,41,41	0
57	MG	QA	1621	1/1	0.91	0.17	41,41,41,41	0
57	MG	XA	1696	1/1	0.91	0.08	55,55,55,55	0
57	MG	YA	3298	1/1	0.91	0.15	36,36,36,36	0
57	MG	YA	3082	1/1	0.91	0.21	21,21,21,21	0
57	MG	XA	1698	1/1	0.91	0.26	49,49,49,49	0
57	MG	RA	3297	1/1	0.91	0.16	45,45,45,45	0
57	MG	RA	3101	1/1	0.91	0.17	40,40,40,40	0
57	MG	YA	3310	1/1	0.91	0.14	27,27,27,27	0
57	MG	RA	3246	1/1	0.91	0.16	43,43,43,43	0
57	MG	YA	3095	1/1	0.91	0.14	22,22,22,22	0
57	MG	YA	3096	1/1	0.91	0.23	23,23,23,23	0
57	MG	RA	3247	1/1	0.91	0.15	31,31,31,31	0
57	MG	XA	1640	1/1	0.91	0.24	59,59,59,59	0
57	MG	RA	3069	1/1	0.91	0.22	20,20,20,20	0
57	MG	YA	3209	1/1	0.91	0.16	30,30,30,30	0
57	MG	RA	3201	1/1	0.91	0.18	14,14,14,14	0
57	MG	RA	3172	1/1	0.91	0.14	60,60,60,60	0
57	MG	QA	1623	1/1	0.91	0.09	41,41,41,41	0
57	MG	RA	3128	1/1	0.91	0.19	16,16,16,16	0
57	MG	RA	3266	1/1	0.91	0.16	37,37,37,37	0
57	MG	YA	3111	1/1	0.91	0.17	33,33,33,33	0
57	MG	RA	3176	1/1	0.91	0.12	26,26,26,26	0
57	MG	RA	3152	1/1	0.91	0.10	75,75,75,75	0
57	MG	YA	3224	1/1	0.91	0.14	24,24,24,24	0
57	MG	XA	1657	1/1	0.91	0.21	28,28,28,28	0
57	MG	YA	3119	1/1	0.91	0.17	50,50,50,50	0
57	MG	QA	1643	1/1	0.91	0.30	69,69,69,69	0
57	MG	YA	3124	1/1	0.91	0.18	40,40,40,40	0
57	MG	RA	3272	1/1	0.91	0.07	38,38,38,38	0
57	MG	RA	3057	1/1	0.91	0.20	15,15,15,15	0
57	MG	YA	3134	1/1	0.91	0.13	54,54,54,54	0
57	MG	RA	3226	1/1	0.91	0.12	32,32,32,32	0
57	MG	YA	3248	1/1	0.91	0.09	39,39,39,39	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3094	1/1	0.91	0.15	24,24,24,24	0
57	MG	YA	3254	1/1	0.91	0.19	39,39,39,39	0
57	MG	YA	3024	1/1	0.91	0.21	23,23,23,23	0
57	MG	YA	3139	1/1	0.91	0.19	32,32,32,32	0
57	MG	YA	3260	1/1	0.91	0.13	28,28,28,28	0
57	MG	RA	3279	1/1	0.91	0.15	44,44,44,44	0
57	MG	YA	3033	1/1	0.91	0.22	25,25,25,25	0
59	ZN	Y4	101	1/1	0.91	0.09	230,230,230,230	0
57	MG	RA	3228	1/1	0.91	0.19	23,23,23,23	0
57	MG	RA	3091	1/1	0.92	0.12	32,32,32,32	0
57	MG	YA	3269	1/1	0.92	0.11	24,24,24,24	0
57	MG	RA	3038	1/1	0.92	0.22	26,26,26,26	0
57	MG	YA	3054	1/1	0.92	0.16	14,14,14,14	0
57	MG	YA	3274	1/1	0.92	0.10	43,43,43,43	0
57	MG	RA	3149	1/1	0.92	0.07	69,69,69,69	0
57	MG	RA	3150	1/1	0.92	0.11	58,58,58,58	0
57	MG	RA	3288	1/1	0.92	0.19	38,38,38,38	0
57	MG	RA	3117	1/1	0.92	0.25	44,44,44,44	0
57	MG	XA	1624	1/1	0.92	0.14	30,30,30,30	0
57	MG	XA	1690	1/1	0.92	0.20	54,54,54,54	0
57	MG	RA	3093	1/1	0.92	0.16	30,30,30,30	0
57	MG	YA	3174	1/1	0.92	0.20	45,45,45,45	0
57	MG	XA	1695	1/1	0.92	0.18	61,61,61,61	0
57	MG	YA	3073	1/1	0.92	0.08	46,46,46,46	0
57	MG	QA	1650	1/1	0.92	0.27	53,53,53,53	0
57	MG	YA	3179	1/1	0.92	0.24	49,49,49,49	0
57	MG	YA	3289	1/1	0.92	0.19	42,42,42,42	0
57	MG	YA	3180	1/1	0.92	0.19	50,50,50,50	0
57	MG	XA	1631	1/1	0.92	0.22	45,45,45,45	0
57	MG	YA	3292	1/1	0.92	0.16	49,49,49,49	0
57	MG	QA	1675	1/1	0.92	0.08	33,33,33,33	0
57	MG	RA	3243	1/1	0.92	0.10	22,22,22,22	0
57	MG	RA	3244	1/1	0.92	0.19	34,34,34,34	0
57	MG	YA	3299	1/1	0.92	0.16	31,31,31,31	0
57	MG	YA	3089	1/1	0.92	0.09	45,45,45,45	0
57	MG	RA	3043	1/1	0.92	0.26	16,16,16,16	0
57	MG	YA	3303	1/1	0.92	0.08	38,38,38,38	0
57	MG	YA	3192	1/1	0.92	0.15	70,70,70,70	0
57	MG	XV	101	1/1	0.92	0.16	8,8,8,8	0
57	MG	QA	1677	1/1	0.92	0.07	22,22,22,22	0
57	MG	XA	1639	1/1	0.92	0.14	33,33,33,33	0
57	MG	XV	104	1/1	0.92	0.10	18,18,18,18	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3101	1/1	0.92	0.12	28,28,28,28	0
57	MG	RA	3077	1/1	0.92	0.17	6,6,6,6	0
57	MG	RA	3197	1/1	0.92	0.23	13,13,13,13	0
57	MG	YA	3317	1/1	0.92	0.10	32,32,32,32	0
57	MG	RA	3250	1/1	0.92	0.11	36,36,36,36	0
57	MG	RA	3255	1/1	0.92	0.10	29,29,29,29	0
57	MG	RA	3198	1/1	0.92	0.21	22,22,22,22	0
57	MG	RA	3079	1/1	0.92	0.16	32,32,32,32	0
57	MG	QA	1626	1/1	0.92	0.23	33,33,33,33	0
57	MG	XA	1650	1/1	0.92	0.07	76,76,76,76	0
57	MG	RA	3105	1/1	0.92	0.16	47,47,47,47	0
57	MG	QA	1613	1/1	0.92	0.18	44,44,44,44	0
57	MG	QA	1614	1/1	0.92	0.06	53,53,53,53	0
57	MG	QA	1686	1/1	0.92	0.21	55,55,55,55	0
57	MG	YA	3229	1/1	0.92	0.12	38,38,38,38	0
57	MG	YA	3015	1/1	0.92	0.24	13,13,13,13	0
57	MG	YA	3018	1/1	0.92	0.13	28,28,28,28	0
57	MG	YA	3232	1/1	0.92	0.10	34,34,34,34	0
57	MG	QA	1611	1/1	0.92	0.18	21,21,21,21	0
57	MG	YA	3020	1/1	0.92	0.09	29,29,29,29	0
57	MG	RA	3212	1/1	0.92	0.17	26,26,26,26	0
57	MG	RA	3219	1/1	0.92	0.13	35,35,35,35	0
57	MG	YA	3137	1/1	0.92	0.12	42,42,42,42	0
57	MG	QA	1610	1/1	0.92	0.13	23,23,23,23	0
57	MG	XA	1605	1/1	0.92	0.18	18,18,18,18	0
57	MG	RA	3175	1/1	0.92	0.14	47,47,47,47	0
57	MG	YA	3037	1/1	0.92	0.21	29,29,29,29	0
57	MG	YA	3142	1/1	0.92	0.28	41,41,41,41	0
57	MG	YA	3258	1/1	0.92	0.10	19,19,19,19	0
57	MG	QA	1625	1/1	0.92	0.12	40,40,40,40	0
57	MG	YA	3044	1/1	0.92	0.22	23,23,23,23	0
57	MG	RA	3146	1/1	0.92	0.15	17,17,17,17	0
57	MG	XA	1610	1/1	0.92	0.24	33,33,33,33	0
57	MG	YA	3072	1/1	0.93	0.09	47,47,47,47	0
57	MG	XA	1602	1/1	0.93	0.10	47,47,47,47	0
57	MG	YA	3272	1/1	0.93	0.23	35,35,35,35	0
57	MG	YA	3077	1/1	0.93	0.25	20,20,20,20	0
57	MG	XA	1652	1/1	0.93	0.18	24,24,24,24	0
57	MG	YA	3001	1/1	0.93	0.15	31,31,31,31	0
57	MG	RA	3050	1/1	0.93	0.16	22,22,22,22	0
57	MG	YA	3173	1/1	0.93	0.07	59,59,59,59	0
57	MG	RA	3053	1/1	0.93	0.14	19,19,19,19	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	XA	1661	1/1	0.93	0.23	38,38,38,38	0
57	MG	YA	3088	1/1	0.93	0.12	20,20,20,20	0
57	MG	RA	3023	1/1	0.93	0.14	25,25,25,25	0
57	MG	QV	101	1/1	0.93	0.20	20,20,20,20	0
57	MG	YA	3092	1/1	0.93	0.14	26,26,26,26	0
57	MG	YA	3008	1/1	0.93	0.20	46,46,46,46	0
57	MG	QA	1634	1/1	0.93	0.16	42,42,42,42	0
57	MG	RA	3179	1/1	0.93	0.12	30,30,30,30	0
57	MG	RA	3234	1/1	0.93	0.19	22,22,22,22	0
57	MG	YA	3189	1/1	0.93	0.16	34,34,34,34	0
57	MG	QA	1652	1/1	0.93	0.14	54,54,54,54	0
57	MG	QA	1656	1/1	0.93	0.17	37,37,37,37	0
57	MG	RA	3119	1/1	0.93	0.12	33,33,33,33	0
57	MG	YA	3295	1/1	0.93	0.13	41,41,41,41	0
57	MG	QA	1615	1/1	0.93	0.12	46,46,46,46	0
57	MG	YA	3105	1/1	0.93	0.20	90,90,90,90	0
57	MG	RA	3124	1/1	0.93	0.15	37,37,37,37	0
57	MG	YA	3196	1/1	0.93	0.21	48,48,48,48	0
57	MG	YA	3198	1/1	0.93	0.19	19,19,19,19	0
57	MG	YA	3108	1/1	0.93	0.15	10,10,10,10	0
57	MG	YA	3304	1/1	0.93	0.08	47,47,47,47	0
57	MG	QA	1624	1/1	0.93	0.08	40,40,40,40	0
57	MG	YA	3021	1/1	0.93	0.17	16,16,16,16	0
57	MG	YA	3023	1/1	0.93	0.16	10,10,10,10	0
57	MG	RA	3156	1/1	0.93	0.14	20,20,20,20	0
57	MG	YA	3113	1/1	0.93	0.15	75,75,75,75	0
57	MG	YA	3114	1/1	0.93	0.21	33,33,33,33	0
57	MG	YA	3029	1/1	0.93	0.18	10,10,10,10	0
57	MG	YA	3315	1/1	0.93	0.09	40,40,40,40	0
57	MG	QA	1607	1/1	0.93	0.05	44,44,44,44	0
57	MG	YA	3031	1/1	0.93	0.20	35,35,35,35	0
57	MG	XA	1683	1/1	0.93	0.07	63,63,63,63	0
57	MG	RA	3192	1/1	0.93	0.10	31,31,31,31	0
57	MG	RA	3071	1/1	0.93	0.11	30,30,30,30	0
57	MG	QA	1688	1/1	0.93	0.09	57,57,57,57	0
57	MG	YA	3323	1/1	0.93	0.18	39,39,39,39	0
57	MG	RA	3162	1/1	0.93	0.13	33,33,33,33	0
57	MG	QA	1648	1/1	0.93	0.10	73,73,73,73	0
57	MG	XA	1692	1/1	0.93	0.12	42,42,42,42	0
57	MG	RA	3254	1/1	0.93	0.15	39,39,39,39	0
57	MG	YA	3233	1/1	0.93	0.21	34,34,34,34	0
57	MG	RA	3132	1/1	0.93	0.17	34,34,34,34	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3332	1/1	0.93	0.14	28,28,28,28	0
57	MG	YA	3051	1/1	0.93	0.11	11,11,11,11	0
57	MG	YA	3237	1/1	0.93	0.12	45,45,45,45	0
57	MG	RA	3203	1/1	0.93	0.16	11,11,11,11	0
57	MG	QA	1640	1/1	0.93	0.18	51,51,51,51	0
57	MG	YD	304	1/1	0.93	0.23	56,56,56,56	0
57	MG	YA	3241	1/1	0.93	0.05	6,6,6,6	0
57	MG	RA	3102	1/1	0.93	0.18	22,22,22,22	0
57	MG	RA	3168	1/1	0.93	0.11	40,40,40,40	0
57	MG	QA	1672	1/1	0.93	0.12	52,52,52,52	0
57	MG	RA	3017	1/1	0.93	0.26	25,25,25,25	0
57	MG	YP	201	1/1	0.93	0.12	9,9,9,9	0
57	MG	YA	3151	1/1	0.93	0.20	25,25,25,25	0
57	MG	XA	1647	1/1	0.93	0.10	42,42,42,42	0
57	MG	RA	3171	1/1	0.93	0.11	45,45,45,45	0
57	MG	YQ	205	1/1	0.93	0.16	59,59,59,59	0
57	MG	YA	3156	1/1	0.93	0.13	36,36,36,36	0
57	MG	YA	3160	1/1	0.93	0.25	24,24,24,24	0
57	MG	QA	1633	1/1	0.93	0.15	49,49,49,49	0
57	MG	YA	3264	1/1	0.93	0.14	34,34,34,34	0
57	MG	YA	3068	1/1	0.93	0.19	16,16,16,16	0
57	MG	RA	3022	1/1	0.93	0.17	17,17,17,17	0
57	MG	YA	3267	1/1	0.93	0.13	51,51,51,51	0
57	MG	RR	201	1/1	0.94	0.20	33,33,33,33	0
57	MG	XA	1659	1/1	0.94	0.11	10,10,10,10	0
57	MG	RA	3224	1/1	0.94	0.16	26,26,26,26	0
57	MG	YA	3093	1/1	0.94	0.10	30,30,30,30	0
57	MG	RA	3028	1/1	0.94	0.13	20,20,20,20	0
57	MG	RA	3157	1/1	0.94	0.23	11,11,11,11	0
57	MG	XA	1668	1/1	0.94	0.18	24,24,24,24	0
57	MG	RA	3273	1/1	0.94	0.25	47,47,47,47	0
57	MG	RA	3129	1/1	0.94	0.17	37,37,37,37	0
57	MG	RA	3052	1/1	0.94	0.13	23,23,23,23	0
57	MG	QA	1608	1/1	0.94	0.12	45,45,45,45	0
57	MG	QA	1622	1/1	0.94	0.20	28,28,28,28	0
57	MG	RA	3235	1/1	0.94	0.05	22,22,22,22	0
57	MG	YA	3022	1/1	0.94	0.16	39,39,39,39	0
57	MG	QA	1616	1/1	0.94	0.12	43,43,43,43	0
57	MG	RA	3084	1/1	0.94	0.15	19,19,19,19	0
57	MG	YA	3025	1/1	0.94	0.09	2,2,2,2	0
57	MG	QA	1681	1/1	0.94	0.10	53,53,53,53	0
57	MG	RA	3194	1/1	0.94	0.23	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	QA	1606	1/1	0.94	0.28	40,40,40,40	0
57	MG	YA	3032	1/1	0.94	0.15	21,21,21,21	0
57	MG	XA	1682	1/1	0.94	0.11	41,41,41,41	0
57	MG	YA	3116	1/1	0.94	0.31	28,28,28,28	0
57	MG	YA	3212	1/1	0.94	0.17	27,27,27,27	0
57	MG	RA	3015	1/1	0.94	0.24	29,29,29,29	0
57	MG	YA	3118	1/1	0.94	0.18	42,42,42,42	0
57	MG	XA	1622	1/1	0.94	0.17	15,15,15,15	0
57	MG	RA	3291	1/1	0.94	0.05	48,48,48,48	0
57	MG	YA	3122	1/1	0.94	0.15	44,44,44,44	0
57	MG	YA	3039	1/1	0.94	0.19	13,13,13,13	0
57	MG	XA	1628	1/1	0.94	0.06	47,47,47,47	0
57	MG	YA	3130	1/1	0.94	0.11	31,31,31,31	0
57	MG	YA	3131	1/1	0.94	0.10	36,36,36,36	0
57	MG	RA	3060	1/1	0.94	0.16	10,10,10,10	0
57	MG	QA	1667	1/1	0.94	0.13	64,64,64,64	0
57	MG	YA	3047	1/1	0.94	0.15	33,33,33,33	0
57	MG	XA	1691	1/1	0.94	0.13	49,49,49,49	0
57	MG	RA	3202	1/1	0.94	0.24	20,20,20,20	0
57	MG	RA	3062	1/1	0.94	0.12	36,36,36,36	0
57	MG	XA	1694	1/1	0.94	0.13	20,20,20,20	0
57	MG	XA	1633	1/1	0.94	0.12	49,49,49,49	0
57	MG	RA	3204	1/1	0.94	0.14	26,26,26,26	0
57	MG	YA	3330	1/1	0.94	0.08	38,38,38,38	0
57	MG	QA	1638	1/1	0.94	0.11	32,32,32,32	0
57	MG	RA	3067	1/1	0.94	0.07	21,21,21,21	0
57	MG	RA	3300	1/1	0.94	0.12	38,38,38,38	0
57	MG	RA	3251	1/1	0.94	0.09	14,14,14,14	0
57	MG	RA	3118	1/1	0.94	0.16	33,33,33,33	0
57	MG	YA	3064	1/1	0.94	0.21	14,14,14,14	0
57	MG	YD	303	1/1	0.94	0.16	25,25,25,25	0
57	MG	QA	1653	1/1	0.94	0.14	38,38,38,38	0
57	MG	YA	3067	1/1	0.94	0.18	31,31,31,31	0
57	MG	YA	3157	1/1	0.94	0.23	4,4,4,4	0
57	MG	QA	1632	1/1	0.94	0.13	40,40,40,40	0
57	MG	RA	3260	1/1	0.94	0.27	46,46,46,46	0
57	MG	RA	3123	1/1	0.94	0.21	50,50,50,50	0
57	MG	Y1	101	1/1	0.94	0.12	44,44,44,44	0
57	MG	YA	3074	1/1	0.94	0.23	22,22,22,22	0
57	MG	RD	302	1/1	0.94	0.06	27,27,27,27	0
57	MG	YA	3166	1/1	0.94	0.13	42,42,42,42	0
57	MG	RA	3262	1/1	0.94	0.12	39,39,39,39	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YR	201	1/1	0.94	0.06	34,34,34,34	0
57	MG	RA	3003	1/1	0.94	0.13	30,30,30,30	0
57	MG	RA	3218	1/1	0.94	0.16	33,33,33,33	0
57	MG	RA	3265	1/1	0.94	0.12	41,41,41,41	0
57	MG	YA	3086	1/1	0.94	0.22	34,34,34,34	0
57	MG	RA	3098	1/1	0.94	0.20	49,49,49,49	0
57	MG	RA	3005	1/1	0.94	0.20	36,36,36,36	0
57	MG	YA	3278	1/1	0.94	0.10	37,37,37,37	0
57	MG	YA	3075	1/1	0.95	0.13	25,25,25,25	0
57	MG	QA	1691	1/1	0.95	0.15	44,44,44,44	0
57	MG	YA	3079	1/1	0.95	0.11	12,12,12,12	0
57	MG	RA	3083	1/1	0.95	0.14	36,36,36,36	0
57	MG	YA	3271	1/1	0.95	0.11	26,26,26,26	0
57	MG	RA	3049	1/1	0.95	0.17	10,10,10,10	0
57	MG	RA	3200	1/1	0.95	0.18	10,10,10,10	0
57	MG	QA	1680	1/1	0.95	0.17	35,35,35,35	0
57	MG	RA	3006	1/1	0.95	0.11	35,35,35,35	0
57	MG	YA	3007	1/1	0.95	0.15	37,37,37,37	0
57	MG	XA	1655	1/1	0.95	0.16	24,24,24,24	0
57	MG	RA	3122	1/1	0.95	0.19	21,21,21,21	0
57	MG	YA	3090	1/1	0.95	0.14	21,21,21,21	0
57	MG	RA	3087	1/1	0.95	0.14	10,10,10,10	0
57	MG	YA	3176	1/1	0.95	0.16	30,30,30,30	0
57	MG	RA	3163	1/1	0.95	0.08	27,27,27,27	0
57	MG	RA	3026	1/1	0.95	0.27	12,12,12,12	0
57	MG	XA	1664	1/1	0.95	0.12	40,40,40,40	0
57	MG	XA	1601	1/1	0.95	0.09	17,17,17,17	0
57	MG	YA	3181	1/1	0.95	0.06	61,61,61,61	0
57	MG	YA	3016	1/1	0.95	0.20	4,4,4,4	0
57	MG	YA	3098	1/1	0.95	0.10	56,56,56,56	0
57	MG	YA	3017	1/1	0.95	0.11	1,1,1,1	0
57	MG	YA	3186	1/1	0.95	0.07	33,33,33,33	0
57	MG	QA	1654	1/1	0.95	0.16	22,22,22,22	0
57	MG	YA	3293	1/1	0.95	0.06	46,46,46,46	0
57	MG	RA	3008	1/1	0.95	0.11	31,31,31,31	0
57	MG	XA	1669	1/1	0.95	0.11	34,34,34,34	0
57	MG	YA	3296	1/1	0.95	0.15	40,40,40,40	0
57	MG	RA	3030	1/1	0.95	0.16	36,36,36,36	0
57	MG	QA	1636	1/1	0.95	0.11	33,33,33,33	0
57	MG	RA	3010	1/1	0.95	0.21	42,42,42,42	0
57	MG	RA	3213	1/1	0.95	0.10	25,25,25,25	0
57	MG	RA	3216	1/1	0.95	0.24	29,29,29,29	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	QA	1683	1/1	0.95	0.25	51,51,51,51	0
57	MG	XA	1611	1/1	0.95	0.24	31,31,31,31	0
57	MG	YA	3199	1/1	0.95	0.18	10,10,10,10	0
57	MG	YA	3201	1/1	0.95	0.21	21,21,21,21	0
57	MG	YA	3202	1/1	0.95	0.24	22,22,22,22	0
57	MG	RA	3034	1/1	0.95	0.13	1,1,1,1	0
57	MG	QA	1603	1/1	0.95	0.05	33,33,33,33	0
57	MG	RA	3065	1/1	0.95	0.13	7,7,7,7	0
57	MG	RA	3225	1/1	0.95	0.13	28,28,28,28	0
57	MG	RA	3135	1/1	0.95	0.08	34,34,34,34	0
57	MG	RA	3036	1/1	0.95	0.21	35,35,35,35	0
57	MG	XA	1621	1/1	0.95	0.12	10,10,10,10	0
57	MG	QA	1676	1/1	0.95	0.08	27,27,27,27	0
57	MG	YA	3120	1/1	0.95	0.11	24,24,24,24	0
57	MG	XA	1623	1/1	0.95	0.06	40,40,40,40	0
57	MG	YA	3045	1/1	0.95	0.09	11,11,11,11	0
57	MG	RA	3229	1/1	0.95	0.20	45,45,45,45	0
57	MG	XA	1626	1/1	0.95	0.07	38,38,38,38	0
57	MG	YA	3128	1/1	0.95	0.20	4,4,4,4	0
57	MG	YA	3326	1/1	0.95	0.15	22,22,22,22	0
57	MG	YA	3225	1/1	0.95	0.10	31,31,31,31	0
57	MG	QA	1687	1/1	0.95	0.06	46,46,46,46	0
57	MG	RA	3016	1/1	0.95	0.10	24,24,24,24	0
57	MG	RA	3140	1/1	0.95	0.10	23,23,23,23	0
57	MG	RA	3181	1/1	0.95	0.19	7,7,7,7	0
57	MG	QA	1660	1/1	0.95	0.10	25,25,25,25	0
57	MG	RA	3073	1/1	0.95	0.06	50,50,50,50	0
57	MG	RA	3184	1/1	0.95	0.16	45,45,45,45	0
57	MG	YA	3058	1/1	0.95	0.23	28,28,28,28	0
57	MG	RA	3042	1/1	0.95	0.12	24,24,24,24	0
57	MG	YD	302	1/1	0.95	0.18	1,1,1,1	0
57	MG	RA	3075	1/1	0.95	0.15	11,11,11,11	0
57	MG	XA	1637	1/1	0.95	0.14	43,43,43,43	0
57	MG	YA	3062	1/1	0.95	0.16	23,23,23,23	0
57	MG	QA	1661	1/1	0.95	0.14	26,26,26,26	0
57	MG	YA	3147	1/1	0.95	0.04	37,37,37,37	0
57	MG	RA	3044	1/1	0.95	0.12	5,5,5,5	0
57	MG	YA	3252	1/1	0.95	0.12	23,23,23,23	0
57	MG	YO	201	1/1	0.95	0.23	57,57,57,57	0
57	MG	YA	3253	1/1	0.95	0.10	23,23,23,23	0
57	MG	RA	3078	1/1	0.95	0.12	52,52,52,52	0
57	MG	YA	3255	1/1	0.95	0.05	35,35,35,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3002	1/1	0.95	0.07	23,23,23,23	0
57	MG	RA	3151	1/1	0.95	0.20	36,36,36,36	0
57	MG	XA	1643	1/1	0.95	0.09	29,29,29,29	0
57	MG	YA	3259	1/1	0.95	0.06	19,19,19,19	0
57	MG	YA	3155	1/1	0.95	0.05	61,61,61,61	0
57	MG	Y3	101	1/1	0.95	0.15	11,11,11,11	0
57	MG	RA	3113	1/1	0.95	0.16	19,19,19,19	0
57	MG	YA	3263	1/1	0.95	0.13	28,28,28,28	0
57	MG	YA	3158	1/1	0.95	0.06	33,33,33,33	0
57	MG	RA	3046	1/1	0.95	0.14	31,31,31,31	0
57	MG	RA	3217	1/1	0.96	0.11	21,21,21,21	0
57	MG	XA	1681	1/1	0.96	0.11	35,35,35,35	0
57	MG	YA	3053	1/1	0.96	0.16	25,25,25,25	0
57	MG	RA	3196	1/1	0.96	0.06	33,33,33,33	0
57	MG	RA	3104	1/1	0.96	0.18	12,12,12,12	0
57	MG	XA	1646	1/1	0.96	0.11	30,30,30,30	0
57	MG	YA	3300	1/1	0.96	0.19	56,56,56,56	0
57	MG	YA	3234	1/1	0.96	0.25	47,47,47,47	0
57	MG	XA	1614	1/1	0.96	0.06	66,66,66,66	0
57	MG	RA	3180	1/1	0.96	0.08	24,24,24,24	0
57	MG	XA	1688	1/1	0.96	0.14	49,49,49,49	0
57	MG	YA	3013	1/1	0.96	0.16	38,38,38,38	0
57	MG	QA	1669	1/1	0.96	0.09	38,38,38,38	0
57	MG	QA	1647	1/1	0.96	0.14	37,37,37,37	0
57	MG	YA	3243	1/1	0.96	0.18	33,33,33,33	0
57	MG	RA	3051	1/1	0.96	0.10	27,27,27,27	0
57	MG	YA	3247	1/1	0.96	0.08	29,29,29,29	0
57	MG	RA	3278	1/1	0.96	0.17	47,47,47,47	0
57	MG	RE	301	1/1	0.96	0.16	21,21,21,21	0
57	MG	QA	1631	1/1	0.96	0.11	64,64,64,64	0
57	MG	YA	3069	1/1	0.96	0.11	19,19,19,19	0
57	MG	RA	3109	1/1	0.96	0.12	35,35,35,35	0
57	MG	XA	1625	1/1	0.96	0.20	24,24,24,24	0
57	MG	YA	3182	1/1	0.96	0.23	19,19,19,19	0
57	MG	XA	1697	1/1	0.96	0.17	22,22,22,22	0
57	MG	QA	1685	1/1	0.96	0.06	34,34,34,34	0
57	MG	XA	1663	1/1	0.96	0.07	16,16,16,16	0
57	MG	YA	3076	1/1	0.96	0.09	21,21,21,21	0
57	MG	RA	3206	1/1	0.96	0.18	25,25,25,25	0
57	MG	YA	3078	1/1	0.96	0.13	31,31,31,31	0
57	MG	YA	3027	1/1	0.96	0.09	12,12,12,12	0
57	MG	RA	3257	1/1	0.96	0.07	36,36,36,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	RA	3125	1/1	0.96	0.09	21,21,21,21	0
57	MG	YA	3083	1/1	0.96	0.07	17,17,17,17	0
57	MG	XM	201	1/1	0.96	0.04	52,52,52,52	0
57	MG	YA	3268	1/1	0.96	0.05	37,37,37,37	0
57	MG	RA	3233	1/1	0.96	0.24	28,28,28,28	0
57	MG	QA	1601	1/1	0.96	0.11	28,28,28,28	0
57	MG	YB	203	1/1	0.96	0.17	28,28,28,28	0
57	MG	QA	1627	1/1	0.96	0.07	34,34,34,34	0
57	MG	RA	3292	1/1	0.96	0.10	29,29,29,29	0
57	MG	Y0	101	1/1	0.96	0.07	9,9,9,9	0
57	MG	YA	3145	1/1	0.96	0.12	14,14,14,14	0
57	MG	YA	3146	1/1	0.96	0.10	21,21,21,21	0
57	MG	YA	3204	1/1	0.96	0.12	18,18,18,18	0
57	MG	RA	3159	1/1	0.96	0.09	32,32,32,32	0
57	MG	YA	3148	1/1	0.96	0.14	23,23,23,23	0
57	MG	YA	3040	1/1	0.96	0.05	16,16,16,16	0
57	MG	YA	3041	1/1	0.96	0.13	20,20,20,20	0
57	MG	RA	3068	1/1	0.96	0.18	12,12,12,12	0
57	MG	RA	3114	1/1	0.96	0.10	29,29,29,29	0
57	MG	YA	3213	1/1	0.96	0.07	16,16,16,16	0
57	MG	YA	3153	1/1	0.96	0.05	30,30,30,30	0
57	MG	YA	3285	1/1	0.96	0.09	36,36,36,36	0
57	MG	RA	3018	1/1	0.96	0.15	10,10,10,10	0
57	MG	RA	3267	1/1	0.96	0.05	32,32,32,32	0
57	MG	XA	1608	1/1	0.96	0.11	28,28,28,28	0
57	MG	QE	201	1/1	0.96	0.21	42,42,42,42	0
57	MG	RA	3269	1/1	0.96	0.12	34,34,34,34	0
57	MG	YA	3159	1/1	0.96	0.10	23,23,23,23	0
57	MG	YA	3050	1/1	0.96	0.16	22,22,22,22	0
57	MG	YA	3226	1/1	0.96	0.16	27,27,27,27	0
57	MG	YA	3245	1/1	0.97	0.20	24,24,24,24	0
57	MG	RA	3249	1/1	0.97	0.11	28,28,28,28	0
57	MG	YA	3144	1/1	0.97	0.07	25,25,25,25	0
57	MG	XA	1658	1/1	0.97	0.18	34,34,34,34	0
57	MG	YA	3250	1/1	0.97	0.12	35,35,35,35	0
57	MG	YA	3306	1/1	0.97	0.14	48,48,48,48	0
57	MG	YA	3307	1/1	0.97	0.05	24,24,24,24	0
57	MG	YA	3308	1/1	0.97	0.11	30,30,30,30	0
57	MG	RA	3199	1/1	0.97	0.17	17,17,17,17	0
57	MG	XA	1660	1/1	0.97	0.06	23,23,23,23	0
57	MG	QA	1609	1/1	0.97	0.08	31,31,31,31	0
57	MG	XA	1662	1/1	0.97	0.06	22,22,22,22	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	XA	1627	1/1	0.97	0.08	37,37,37,37	0
57	MG	YA	3197	1/1	0.97	0.04	42,42,42,42	0
57	MG	YA	3106	1/1	0.97	0.12	25,25,25,25	0
57	MG	RA	3252	1/1	0.97	0.06	29,29,29,29	0
57	MG	YA	3200	1/1	0.97	0.22	23,23,23,23	0
57	MG	YA	3318	1/1	0.97	0.13	41,41,41,41	0
57	MG	RA	3284	1/1	0.97	0.05	16,16,16,16	0
57	MG	RA	3144	1/1	0.97	0.04	27,27,27,27	0
57	MG	RA	3145	1/1	0.97	0.10	54,54,54,54	0
57	MG	YA	3070	1/1	0.97	0.09	25,25,25,25	0
57	MG	RA	3027	1/1	0.97	0.15	23,23,23,23	0
57	MG	QA	1629	1/1	0.97	0.05	33,33,33,33	0
57	MG	RA	3230	1/1	0.97	0.11	33,33,33,33	0
57	MG	RA	3040	1/1	0.97	0.12	10,10,10,10	0
57	MG	RA	3054	1/1	0.97	0.18	14,14,14,14	0
57	MG	RA	3187	1/1	0.97	0.14	5,5,5,5	0
57	MG	QA	1644	1/1	0.97	0.11	43,43,43,43	0
57	MG	RA	3001	1/1	0.97	0.13	8,8,8,8	0
57	MG	YA	3216	1/1	0.97	0.13	14,14,14,14	0
57	MG	YA	3217	1/1	0.97	0.05	37,37,37,37	0
57	MG	YA	3218	1/1	0.97	0.05	10,10,10,10	0
57	MG	RA	3019	1/1	0.97	0.11	13,13,13,13	0
57	MG	YA	3080	1/1	0.97	0.07	37,37,37,37	0
57	MG	QA	1663	1/1	0.97	0.16	36,36,36,36	0
57	MG	YA	3123	1/1	0.97	0.18	17,17,17,17	0
57	MG	RA	3011	1/1	0.97	0.05	30,30,30,30	0
57	MG	YA	3125	1/1	0.97	0.05	36,36,36,36	0
57	MG	YA	3126	1/1	0.97	0.11	15,15,15,15	0
57	MG	YA	3043	1/1	0.97	0.16	13,13,13,13	0
57	MG	YE	302	1/1	0.97	0.09	25,25,25,25	0
57	MG	YA	3227	1/1	0.97	0.20	36,36,36,36	0
57	MG	RA	3121	1/1	0.97	0.20	50,50,50,50	0
57	MG	RA	3214	1/1	0.97	0.17	35,35,35,35	0
57	MG	RA	3215	1/1	0.97	0.15	21,21,21,21	0
57	MG	XA	1615	1/1	0.97	0.11	28,28,28,28	0
57	MG	XA	1616	1/1	0.97	0.10	37,37,37,37	0
57	MG	YQ	201	1/1	0.97	0.12	58,58,58,58	0
57	MG	QA	1678	1/1	0.97	0.05	33,33,33,33	0
57	MG	RA	3004	1/1	0.97	0.10	26,26,26,26	0
57	MG	QA	1659	1/1	0.97	0.14	44,44,44,44	0
57	MG	RA	3275	1/1	0.97	0.23	40,40,40,40	0
57	MG	RA	3064	1/1	0.97	0.13	20,20,20,20	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3238	1/1	0.97	0.16	27,27,27,27	0
57	MG	XA	1653	1/1	0.97	0.16	17,17,17,17	0
57	MG	RA	3220	1/1	0.97	0.13	34,34,34,34	0
57	MG	RA	3095	1/1	0.97	0.18	28,28,28,28	0
57	MG	YA	3242	1/1	0.97	0.14	10,10,10,10	0
59	ZN	XN	101	1/1	0.97	0.05	90,90,90,90	0
57	MG	YA	3188	1/1	0.97	0.17	8,8,8,8	0
57	MG	YA	3244	1/1	0.97	0.30	37,37,37,37	0
57	MG	RA	3070	1/1	0.98	0.12	16,16,16,16	0
57	MG	YA	3035	1/1	0.98	0.17	2,2,2,2	0
57	MG	YA	3333	1/1	0.98	0.12	36,36,36,36	0
57	MG	RA	3259	1/1	0.98	0.15	26,26,26,26	0
57	MG	RA	3290	1/1	0.98	0.07	11,11,11,11	0
57	MG	YB	201	1/1	0.98	0.10	11,11,11,11	0
57	MG	YA	3206	1/1	0.98	0.12	14,14,14,14	0
57	MG	YA	3038	1/1	0.98	0.10	6,6,6,6	0
57	MG	YA	3208	1/1	0.98	0.18	17,17,17,17	0
57	MG	XA	1684	1/1	0.98	0.11	53,53,53,53	0
57	MG	YA	3065	1/1	0.98	0.07	38,38,38,38	0
57	MG	RA	3221	1/1	0.98	0.11	16,16,16,16	0
57	MG	XA	1665	1/1	0.98	0.05	34,34,34,34	0
57	MG	RA	3080	1/1	0.98	0.08	50,50,50,50	0
57	MG	YA	3214	1/1	0.98	0.15	22,22,22,22	0
57	MG	RA	3048	1/1	0.98	0.10	23,23,23,23	0
57	MG	RP	201	1/1	0.98	0.13	33,33,33,33	0
57	MG	YF	301	1/1	0.98	0.04	32,32,32,32	0
57	MG	RA	3063	1/1	0.98	0.22	12,12,12,12	0
57	MG	YA	3099	1/1	0.98	0.11	19,19,19,19	0
57	MG	QA	1674	1/1	0.98	0.15	36,36,36,36	0
57	MG	RA	3238	1/1	0.98	0.14	23,23,23,23	0
57	MG	YA	3129	1/1	0.98	0.09	25,25,25,25	0
57	MG	QA	1658	1/1	0.98	0.15	20,20,20,20	0
57	MG	RA	3281	1/1	0.98	0.18	44,44,44,44	0
57	MG	YA	3132	1/1	0.98	0.14	21,21,21,21	0
57	MG	XA	1654	1/1	0.98	0.15	28,28,28,28	0
57	MG	QA	1666	1/1	0.98	0.07	22,22,22,22	0
58	SF4	QD	302	8/8	0.98	0.07	59,76,106,109	0
58	SF4	XD	301	8/8	0.98	0.07	68,75,103,103	0
57	MG	YA	3028	1/1	0.98	0.05	14,14,14,14	0
57	MG	RA	3021	1/1	0.98	0.10	19,19,19,19	0
57	MG	QV	103	1/1	0.98	0.14	33,33,33,33	0
57	MG	RA	3256	1/1	0.98	0.19	37,37,37,37	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	YA	3056	1/1	0.98	0.14	15,15,15,15	0
57	MG	QA	1670	1/1	0.98	0.12	37,37,37,37	0
57	MG	RA	3287	1/1	0.98	0.07	42,42,42,42	0
57	MG	RA	3253	1/1	0.99	0.06	10,10,10,10	0
57	MG	QA	1690	1/1	0.99	0.05	13,13,13,13	0
57	MG	RA	3153	1/1	0.99	0.04	23,23,23,23	0
57	MG	YA	3026	1/1	0.99	0.19	16,16,16,16	0
57	MG	YA	3170	1/1	0.99	0.03	56,56,56,56	0
57	MG	QA	1604	1/1	0.99	0.06	43,43,43,43	0
59	ZN	QN	101	1/1	0.99	0.05	112,112,112,112	0
57	MG	YA	3172	1/1	0.99	0.09	21,21,21,21	0
57	MG	QA	1655	1/1	0.99	0.11	33,33,33,33	0
57	MG	Y0	102	1/1	0.99	0.18	24,24,24,24	0
57	MG	QA	1668	1/1	0.99	0.06	44,44,44,44	0
57	MG	YA	3094	1/1	0.99	0.09	27,27,27,27	0
57	MG	YA	3249	1/1	0.99	0.05	18,18,18,18	0
57	MG	RA	3222	1/1	0.99	0.09	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.