



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 10:47 PM EDT

PDB ID : 8UVS / pdb_00008uvs
Title : Crystal structure of the wild-type *Thermus thermophilus* 70S ribosome in complex with spectinomycin derivative 2694, mRNA, deacylated A- and E-site tRNA^{phe}, and deacylated P-site tRNA^{met} at 2.75Å resolution
Authors : Killam, B.Y.; Phelps, G.A.; Lee, R.E.; Polikanov, Y.S.
Deposited on : 2023-11-03
Resolution : 2.75 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

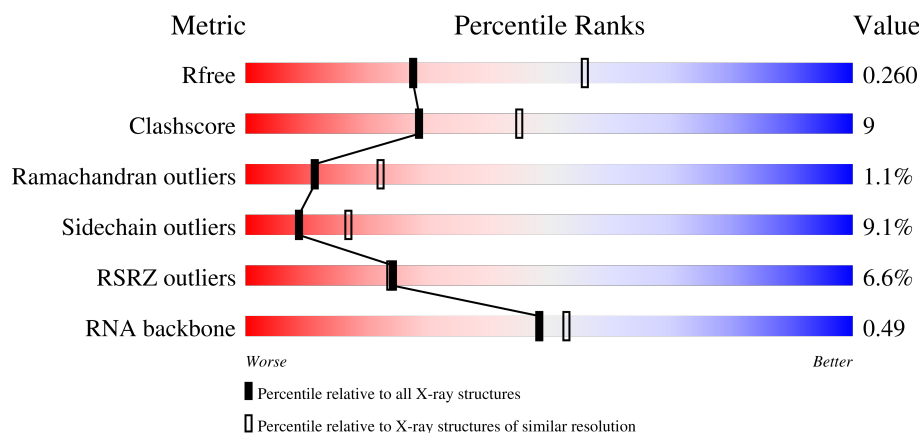
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)
RNA backbone	3983	1179 (3.00-2.52)

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	1A	2915	2% 64% 28% 6%
1	2A	2915	3% 57% 33% 7%
2	1B	121	72% 26%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	2B	121	
3	1D	276	
3	2D	276	
4	1E	206	
4	2E	206	
5	1F	210	
5	2F	210	
6	1G	182	
6	2G	182	
7	1H	180	
7	2H	180	
8	1I	148	
8	2I	148	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	150	
11	2P	150	
12	1Q	141	
12	2Q	141	
13	1R	118	
13	2R	118	
14	1S	112	
14	2S	112	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	1T	146	
15	2T	146	
16	1U	118	
16	2U	118	
17	1V	101	
17	2V	101	
18	1W	113	
18	2W	113	
19	1X	96	
19	2X	96	
20	1Y	110	
20	2Y	110	
21	1Z	206	
21	2Z	206	
22	10	85	
22	20	85	
23	11	98	
23	21	98	
24	12	72	
24	22	72	
25	13	60	
25	23	60	
26	14	71	
26	24	71	
27	15	60	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
27	25	60	
28	16	54	
28	26	54	
29	17	49	
29	27	49	
30	18	65	
30	28	65	
31	19	37	
31	29	37	
32	1a	1521	
32	2a	1521	
33	1b	256	
33	2b	256	
34	1c	239	
34	2c	239	
35	1d	209	
35	2d	209	
36	1e	162	
36	2e	162	
37	1f	101	
37	2f	101	
38	1g	156	
38	2g	156	
39	1h	138	
39	2h	138	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
40	1i	128	
40	2i	128	
41	1j	105	
41	2j	105	
42	1k	129	
42	2k	129	
43	1l	132	
43	2l	132	
44	1m	126	
44	2m	126	
45	1n	61	
45	2n	61	
46	1o	89	
46	2o	89	
47	1p	88	
47	2p	88	
48	1q	105	
48	2q	105	
49	1r	88	
49	2r	88	
50	1s	93	
50	2s	93	
51	1t	106	
51	2t	106	
52	1u	27	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
52	2u	27	
53	1v	24	
53	2v	24	
54	1w	76	
54	1y	76	
54	2w	76	
54	2y	76	
55	1x	77	
55	2x	77	

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
54	PSU	2y	55	-	-	X	-
56	MG	1a	1789	-	-	-	X
56	MG	2a	1822	-	-	-	X

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 300806 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1A	2871	Total	C	N	O	P	0	0	0
			61852	27531	11572	19878	2871			
1	2A	2800	Total	C	N	O	P	0	0	0
			60322	26848	11284	19390	2800			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1B	120	Total	C	N	O	P	0	0	0
			2577	1146	476	835	120			
2	2B	120	Total	C	N	O	P	0	0	0
			2575	1146	476	833	120			

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	1D	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			
3	2D	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	1E	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			
4	2E	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	1F	202	Total	C	N	O	S	0	0	0
			1583	1009	297	275	2			
5	2F	202	Total	C	N	O	S	0	0	0
			1579	1007	296	274	2			

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	1G	181	Total	C	N	O	S	0	0	0
			1423	913	253	253	4			
6	2G	181	Total	C	N	O	S	0	0	0
			1428	913	258	253	4			

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	1H	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			
7	2H	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	1I	146	Total	C	N	O	S	0	0	0
			1097	701	191	204	1			
8	2I	146	Total	C	N	O	S	0	0	0
			1064	681	186	196	1			

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	1N	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			
9	2N	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	1O	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	2O	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	1P	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			
11	2P	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	1Q	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
12	2Q	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	1R	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
13	2R	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	1S	110	Total	C	N	O	0	0	0
			873	550	174	149			
14	2S	110	Total	C	N	O	0	0	0
			870	549	173	148			

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	1T	131	Total	C	N	O	S	0	0	0
			1091	680	225	185	1			
15	2T	131	Total	C	N	O	S	0	0	0
			1083	675	224	183	1			

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	1U	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			
16	2U	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	1V	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			
17	2V	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	1W	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			
18	2W	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	1X	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			
19	2X	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	1Y	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			
20	2Y	107	Total	C	N	O	S	0	0	0
			806	517	152	131	6			

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	1Z	154	Total	C	N	O	S	0	0	0
			1240	795	222	220	3			
21	2Z	160	Total	C	N	O	S	0	0	0
			1271	814	228	227	2			

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			
22	20	83	Total	C	N	O	S	0	0	0
			653	404	139	109	1			

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	11	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			
23	21	97	Total	C	N	O	S	0	0	0
			755	475	148	131	1			

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	12	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			
24	22	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	13	59	Total	C	N	O	0	0	0
			469	298	90	81			
25	23	59	Total	C	N	O	0	0	0
			464	296	90	78			

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	14	69	Total	C	N	O	S	0	0	0
			552	349	99	99	5			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	24	69	Total	C	N	O	S	0	0	0
			532	339	97	91	5			

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	15	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			
27	25	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	16	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			
28	26	53	Total	C	N	O	S	0	0	0
			449	279	91	75	4			

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	17	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
29	27	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	18	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			
30	28	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	19	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
31	29	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 32 is a RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	1a	1500	Total	C	N	O	P	0	0	0
			32246	14358	5975	10413	1500			
32	2a	1503	Total	C	N	O	P	0	0	0
			32327	14396	5990	10438	1503			

- Molecule 33 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	1b	231	Total	C	N	O	S	0	0	0
			1846	1179	331	331	5			
33	2b	231	Total	C	N	O	S	0	0	0
			1825	1167	326	327	5			

- Molecule 34 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	1c	206	Total	C	N	O	S	0	0	0
			1548	973	301	273	1			
34	2c	206	Total	C	N	O	S	0	0	0
			1542	968	300	273	1			

- Molecule 35 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	1d	208	Total	C	N	O	S	0	0	0
			1655	1038	326	284	7			
35	2d	208	Total	C	N	O	S	0	0	0
			1674	1050	333	284	7			

- Molecule 36 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	1e	148	Total	C	N	O	S	0	0	0
			1129	714	213	198	4			
36	2e	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			

- Molecule 37 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	1f	100	Total	C	N	O	S	0	0	0
			810	514	144	149	3			
37	2f	100	Total	C	N	O	S	0	0	0
			816	516	146	151	3			

- Molecule 38 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	1g	155	Total	C	N	O	S	0	0	0
			1231	766	243	216	6			
38	2g	155	Total	C	N	O	S	0	0	0
			1235	769	244	216	6			

- Molecule 39 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	1h	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			
39	2h	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			

- Molecule 40 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	1i	127	Total	C	N	O	0	0	0
			983	623	193	167			
40	2i	127	Total	C	N	O	0	0	0
			978	619	190	169			

- Molecule 41 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	1j	97	Total	C	N	O	0	0	0
			709	440	138	131			
41	2j	96	Total	C	N	O	0	0	0
			714	445	138	131			

- Molecule 42 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	1k	114	Total	C	N	O	S	0	0	0
			829	516	155	155	3			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	2k	114	Total	C	N	O	S	0	0	0
			833	519	156	155	3			

- Molecule 43 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	1l	122	Total	C	N	O	S	0	0	0
			932	586	185	159	2			
43	2l	122	Total	C	N	O	S	0	0	0
			932	586	185	159	2			

- Molecule 44 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	1m	123	Total	C	N	O	S	0	0	0
			958	592	198	166	2			
44	2m	122	Total	C	N	O	S	0	0	0
			950	586	197	165	2			

- Molecule 45 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	1n	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
45	2n	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 46 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	1o	88	Total	C	N	O	S	0	0	0
			728	456	144	126	2			
46	2o	88	Total	C	N	O	S	0	0	0
			728	456	144	126	2			

- Molecule 47 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	1p	82	Total	C	N	O	S	0	0	0
			681	433	134	113	1			
47	2p	82	Total	C	N	O	S	0	0	0
			677	430	133	113	1			

- Molecule 48 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	1q	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
48	2q	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 49 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	1r	68	Total	C	N	O		0	0	0
			555	355	108	92				
49	2r	68	Total	C	N	O		0	0	0
			555	355	108	92				

- Molecule 50 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	1s	83	Total	C	N	O	S	0	0	0
			652	417	120	113	2			
50	2s	83	Total	C	N	O	S	0	0	0
			646	412	119	113	2			

- Molecule 51 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	1t	96	Total	C	N	O	S	0	0	0
			728	446	156	124	2			
51	2t	96	Total	C	N	O	S	0	0	0
			727	446	155	124	2			

- Molecule 52 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
52	1u	23	Total	C	N	O	0	0	0
			199	122	48	29			
52	2u	23	Total	C	N	O	0	0	0
			199	122	48	29			

- Molecule 53 is a RNA chain called MF-mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1v	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			
53	2v	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			

- Molecule 54 is a RNA chain called A-site and E-site Deacylated tRNAphe.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1w	74	Total	C	N	O	P	S	0	0	0
			1592	713	285	518	74	2			
54	1y	74	Total	C	N	O	P	S	0	0	0
			1585	707	285	518	74	1			
54	2w	72	Total	C	N	O	P	S	0	0	0
			1544	690	278	502	72	2			
54	2y	73	Total	C	N	O	P	S	0	0	0
			1565	698	283	510	73	1			

- Molecule 55 is a RNA chain called P-site Deacylated tRNAmet.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
55	1x	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			
55	2x	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1A	1139	Total	Mg	0	0
			1139	1139		
56	1B	37	Total	Mg	0	0
			37	37		
56	1D	13	Total	Mg	0	0
			13	13		
56	1E	14	Total	Mg	0	0
			14	14		
56	1F	13	Total	Mg	0	0
			13	13		
56	1G	5	Total	Mg	0	0
			5	5		
56	1I	1	Total	Mg	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	1N	6	Total Mg 6 6	0	0
56	1O	6	Total Mg 6 6	0	0
56	1P	5	Total Mg 5 5	0	0
56	1Q	7	Total Mg 7 7	0	0
56	1R	3	Total Mg 3 3	0	0
56	1S	3	Total Mg 3 3	0	0
56	1T	4	Total Mg 4 4	0	0
56	1U	10	Total Mg 10 10	0	0
56	1V	7	Total Mg 7 7	0	0
56	1W	7	Total Mg 7 7	0	0
56	1X	5	Total Mg 5 5	0	0
56	1Y	4	Total Mg 4 4	0	0
56	1Z	3	Total Mg 3 3	0	0
56	10	8	Total Mg 8 8	0	0
56	11	4	Total Mg 4 4	0	0
56	12	2	Total Mg 2 2	0	0
56	13	6	Total Mg 6 6	0	0
56	15	4	Total Mg 4 4	0	0
56	16	2	Total Mg 2 2	0	0
56	17	4	Total Mg 4 4	0	0
56	18	7	Total Mg 7 7	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	19	1	Total 1	Mg 1	0	0
56	1a	241	Total 241	Mg 241	0	0
56	1b	2	Total 2	Mg 2	0	0
56	1e	2	Total 2	Mg 2	0	0
56	1f	2	Total 2	Mg 2	0	0
56	1h	1	Total 1	Mg 1	0	0
56	1l	2	Total 2	Mg 2	0	0
56	1m	1	Total 1	Mg 1	0	0
56	1n	1	Total 1	Mg 1	0	0
56	1s	1	Total 1	Mg 1	0	0
56	1t	1	Total 1	Mg 1	0	0
56	1v	2	Total 2	Mg 2	0	0
56	1w	9	Total 9	Mg 9	0	0
56	1x	14	Total 14	Mg 14	0	0
56	1y	2	Total 2	Mg 2	0	0
56	2A	884	Total 884	Mg 884	0	0
56	2B	20	Total 20	Mg 20	0	0
56	2D	7	Total 7	Mg 7	0	0
56	2E	6	Total 6	Mg 6	0	0
56	2F	6	Total 6	Mg 6	0	0
56	2G	1	Total 1	Mg 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	2N	1	Total 1 Mg 1	0	0
56	2O	2	Total 2 Mg 2	0	0
56	2P	2	Total 2 Mg 2	0	0
56	2Q	3	Total 3 Mg 3	0	0
56	2R	3	Total 3 Mg 3	0	0
56	2T	3	Total 3 Mg 3	0	0
56	2U	2	Total 2 Mg 2	0	0
56	2V	2	Total 2 Mg 2	0	0
56	2W	2	Total 2 Mg 2	0	0
56	2X	3	Total 3 Mg 3	0	0
56	2Y	1	Total 1 Mg 1	0	0
56	2Z	1	Total 1 Mg 1	0	0
56	20	3	Total 3 Mg 3	0	0
56	21	2	Total 2 Mg 2	0	0
56	23	2	Total 2 Mg 2	0	0
56	25	5	Total 5 Mg 5	0	0
56	26	1	Total 1 Mg 1	0	0
56	27	4	Total 4 Mg 4	0	0
56	28	3	Total 3 Mg 3	0	0
56	2a	240	Total 240 Mg 240	0	0
56	2d	2	Total 2 Mg 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2e	1	Total	Mg	0	0
			1	1		
56	2f	1	Total	Mg	0	0
			1	1		
56	2g	1	Total	Mg	0	0
			1	1		
56	2j	1	Total	Mg	0	0
			1	1		
56	2k	1	Total	Mg	0	0
			1	1		
56	2l	4	Total	Mg	0	0
			4	4		
56	2m	1	Total	Mg	0	0
			1	1		
56	2p	1	Total	Mg	0	0
			1	1		
56	2q	2	Total	Mg	0	0
			2	2		
56	2r	1	Total	Mg	0	0
			1	1		
56	2t	1	Total	Mg	0	0
			1	1		
56	2v	1	Total	Mg	0	0
			1	1		
56	2w	9	Total	Mg	0	0
			9	9		
56	2x	7	Total	Mg	0	0
			7	7		
56	2y	7	Total	Mg	0	0
			7	7		

- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

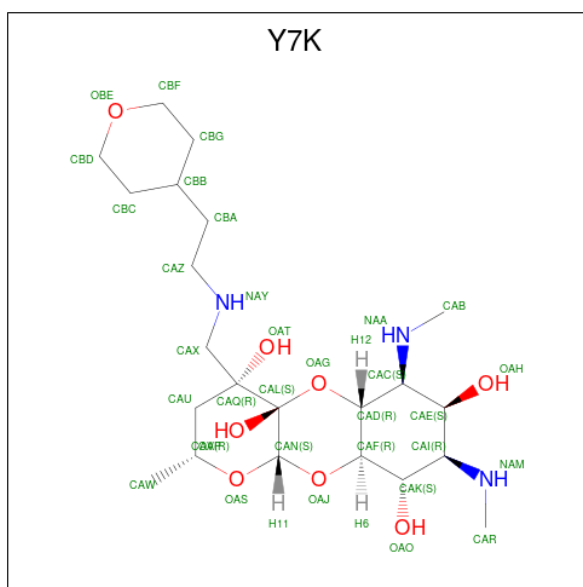
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1Y	1	Total	Zn	0	0
			1	1		
57	14	1	Total	Zn	0	0
			1	1		
57	15	1	Total	Zn	0	0
			1	1		
57	16	1	Total	Zn	0	0
			1	1		

Continued on next page...

Continued from previous page...

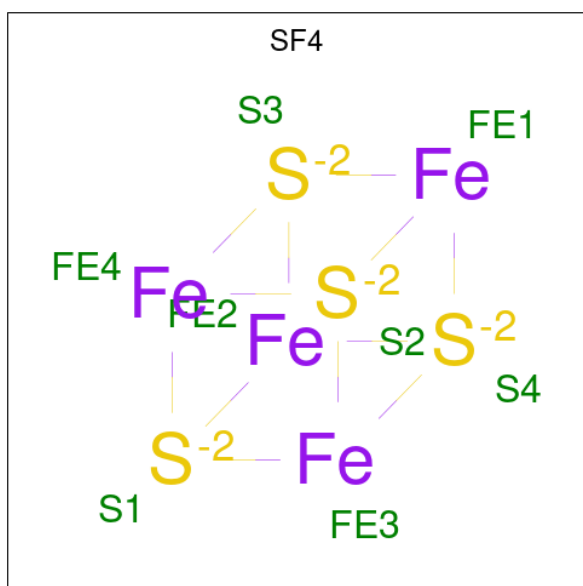
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	19	1	Total	Zn	0	0
			1	1		
57	1n	1	Total	Zn	0	0
			1	1		
57	2Y	1	Total	Zn	0	0
			1	1		
57	24	1	Total	Zn	0	0
			1	1		
57	25	1	Total	Zn	0	0
			1	1		
57	26	1	Total	Zn	0	0
			1	1		
57	29	1	Total	Zn	0	0
			1	1		
57	2n	1	Total	Zn	0	0
			1	1		

- Molecule 58 is (2R,4R,4aS,5aR,6S,7S,8R,9S,9aR,10aS)-2-methyl-6,8-bis(methylamino)-4-({[2-(oxan-4-yl)ethyl]amino}methyl)octahydro-2H-pyrano[2,3-b][1,4]benzodioxine-4,4a,7,9(10aH)-tetrol (CCD ID: Y7K) (formula: C₂₂H₄₁N₃O₈) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
58	1a	1	Total	C	N	O	0	0
			33	22	3	8		
58	2a	1	Total	C	N	O	0	0
			33	22	3	8		

- Molecule 59 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
59	1d	1	Total	Fe	S	0	0
			8	4	4		
59	2d	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 60 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1x	1	Total	K	0	0
			1	1		
60	2A	1	Total	K	0	0
			1	1		

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	2188	Total	O	0	0
			2188	2188		
61	1B	68	Total	O	0	0
			68	68		
61	1D	33	Total	O	0	0
			33	33		
61	1E	30	Total	O	0	0
			30	30		
61	1F	18	Total	O	0	0
			18	18		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1G	3	Total 3	O 3	0	0
61	1H	2	Total 2	O 2	0	0
61	1I	1	Total 1	O 1	0	0
61	1N	8	Total 8	O 8	0	0
61	1O	4	Total 4	O 4	0	0
61	1P	20	Total 20	O 20	0	0
61	1Q	10	Total 10	O 10	0	0
61	1R	12	Total 12	O 12	0	0
61	1S	6	Total 6	O 6	0	0
61	1T	8	Total 8	O 8	0	0
61	1U	17	Total 17	O 17	0	0
61	1V	11	Total 11	O 11	0	0
61	1W	8	Total 8	O 8	0	0
61	1X	7	Total 7	O 7	0	0
61	1Y	2	Total 2	O 2	0	0
61	1Z	1	Total 1	O 1	0	0
61	10	13	Total 13	O 13	0	0
61	11	11	Total 11	O 11	0	0
61	12	4	Total 4	O 4	0	0
61	13	3	Total 3	O 3	0	0
61	14	2	Total 2	O 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	15	8	Total 8	O 8	0	0
61	16	1	Total 1	O 1	0	0
61	17	9	Total 9	O 9	0	0
61	18	11	Total 11	O 11	0	0
61	1a	498	Total 498	O 498	0	0
61	1c	2	Total 2	O 2	0	0
61	1d	1	Total 1	O 1	0	0
61	1e	4	Total 4	O 4	0	0
61	1f	1	Total 1	O 1	0	0
61	1g	3	Total 3	O 3	0	0
61	1i	1	Total 1	O 1	0	0
61	1j	1	Total 1	O 1	0	0
61	1l	8	Total 8	O 8	0	0
61	1m	1	Total 1	O 1	0	0
61	1n	1	Total 1	O 1	0	0
61	1o	1	Total 1	O 1	0	0
61	1p	1	Total 1	O 1	0	0
61	1q	3	Total 3	O 3	0	0
61	1u	1	Total 1	O 1	0	0
61	1v	7	Total 7	O 7	0	0
61	1w	14	Total 14	O 14	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1x	19	Total 19	O 19	0	0
61	1y	1	Total 1	O 1	0	0
61	2A	1294	Total 1294	O 1294	0	0
61	2B	27	Total 27	O 27	0	0
61	2D	24	Total 24	O 24	0	0
61	2E	15	Total 15	O 15	0	0
61	2F	13	Total 13	O 13	0	0
61	2I	3	Total 3	O 3	0	0
61	2N	1	Total 1	O 1	0	0
61	2O	2	Total 2	O 2	0	0
61	2P	16	Total 16	O 16	0	0
61	2Q	2	Total 2	O 2	0	0
61	2R	3	Total 3	O 3	0	0
61	2T	6	Total 6	O 6	0	0
61	2U	4	Total 4	O 4	0	0
61	2W	3	Total 3	O 3	0	0
61	2X	2	Total 2	O 2	0	0
61	2Y	1	Total 1	O 1	0	0
61	2Z	1	Total 1	O 1	0	0
61	20	3	Total 3	O 3	0	0
61	21	8	Total 8	O 8	0	0

Continued on next page...

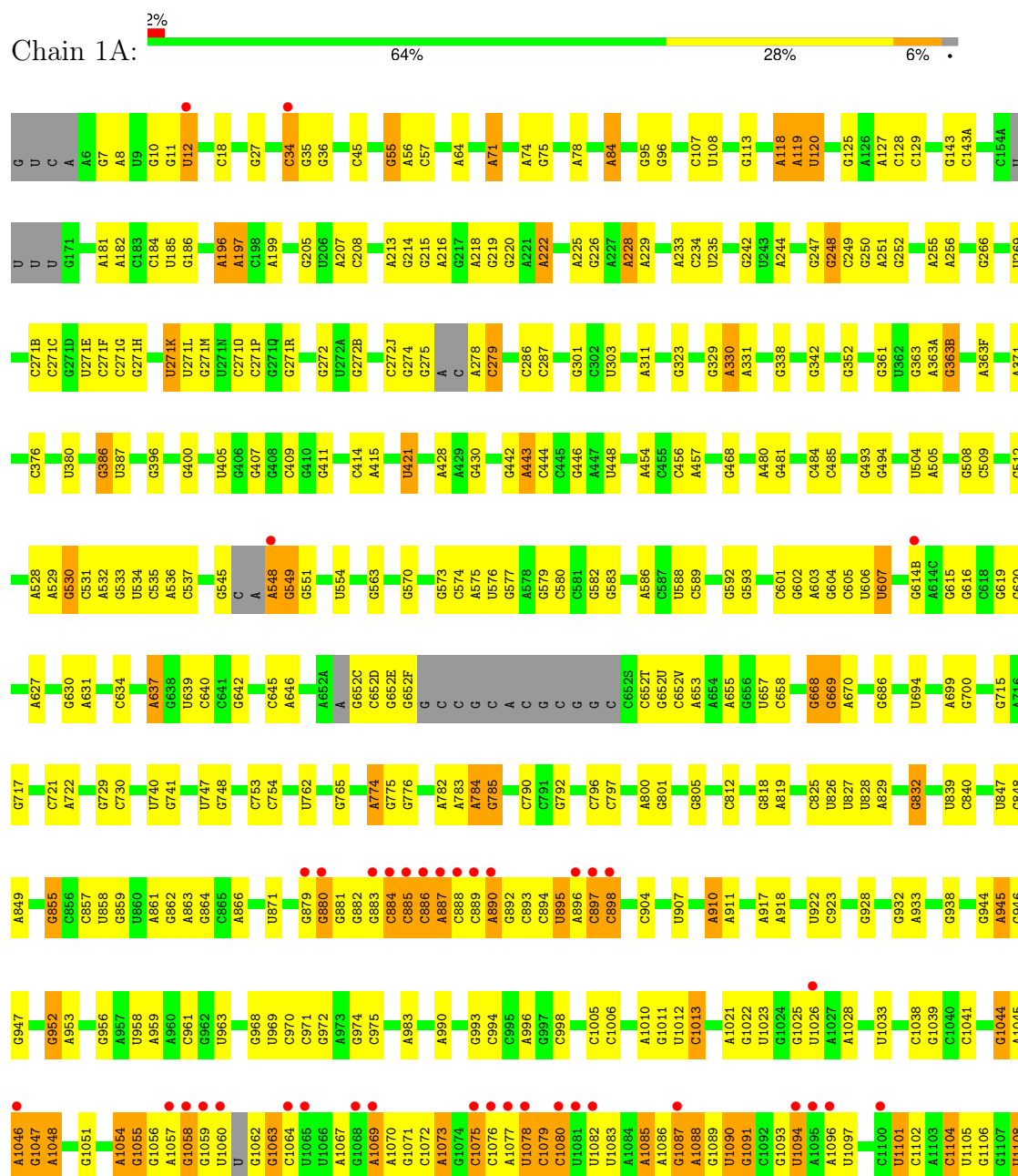
Continued from previous page...

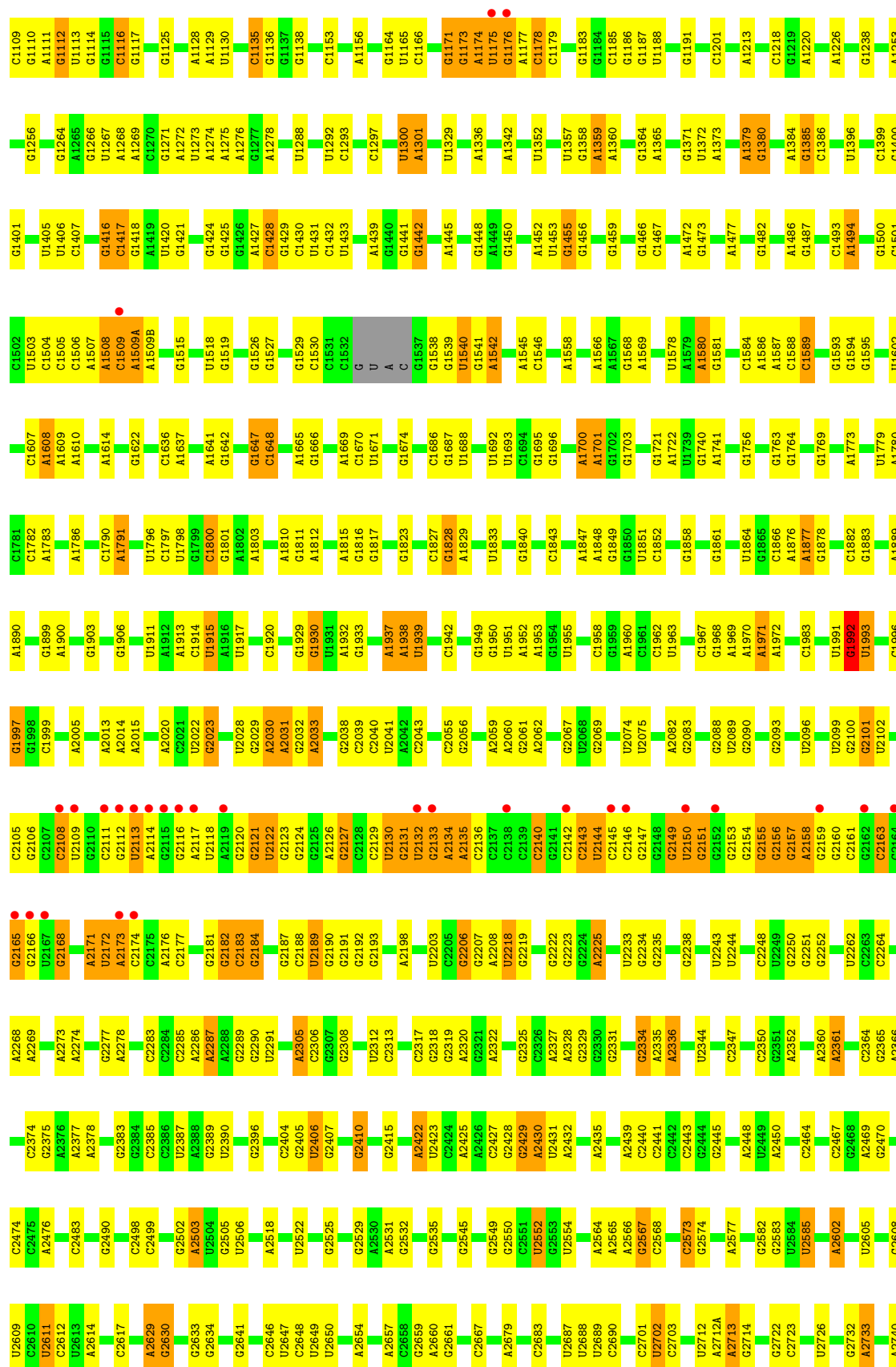
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	23	3	Total 3	O 3	0	0
61	25	1	Total 1	O 1	0	0
61	26	1	Total 1	O 1	0	0
61	27	3	Total 3	O 3	0	0
61	28	3	Total 3	O 3	0	0
61	29	1	Total 1	O 1	0	0
61	2a	296	Total 296	O 296	0	0
61	2c	1	Total 1	O 1	0	0
61	2d	2	Total 2	O 2	0	0
61	2e	1	Total 1	O 1	0	0
61	2f	1	Total 1	O 1	0	0
61	2j	3	Total 3	O 3	0	0
61	2l	4	Total 4	O 4	0	0
61	2n	1	Total 1	O 1	0	0
61	2p	2	Total 2	O 2	0	0
61	2r	1	Total 1	O 1	0	0
61	2t	2	Total 2	O 2	0	0
61	2v	1	Total 1	O 1	0	0
61	2w	4	Total 4	O 4	0	0
61	2x	5	Total 5	O 5	0	0
61	2y	15	Total 15	O 15	0	0

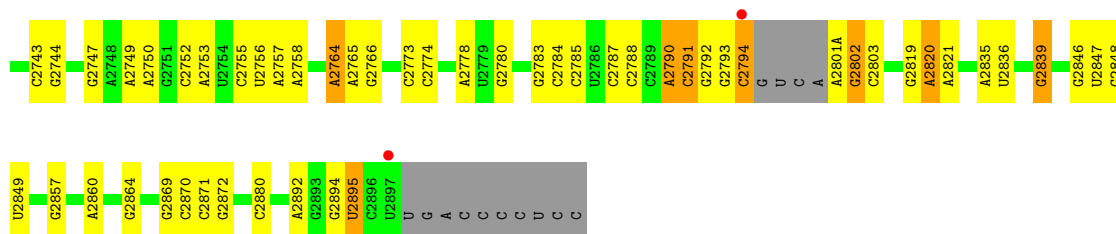
3 Residue-property plots

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.

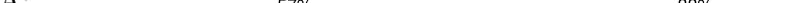
• Molecule 1: 23S Ribosomal RNA

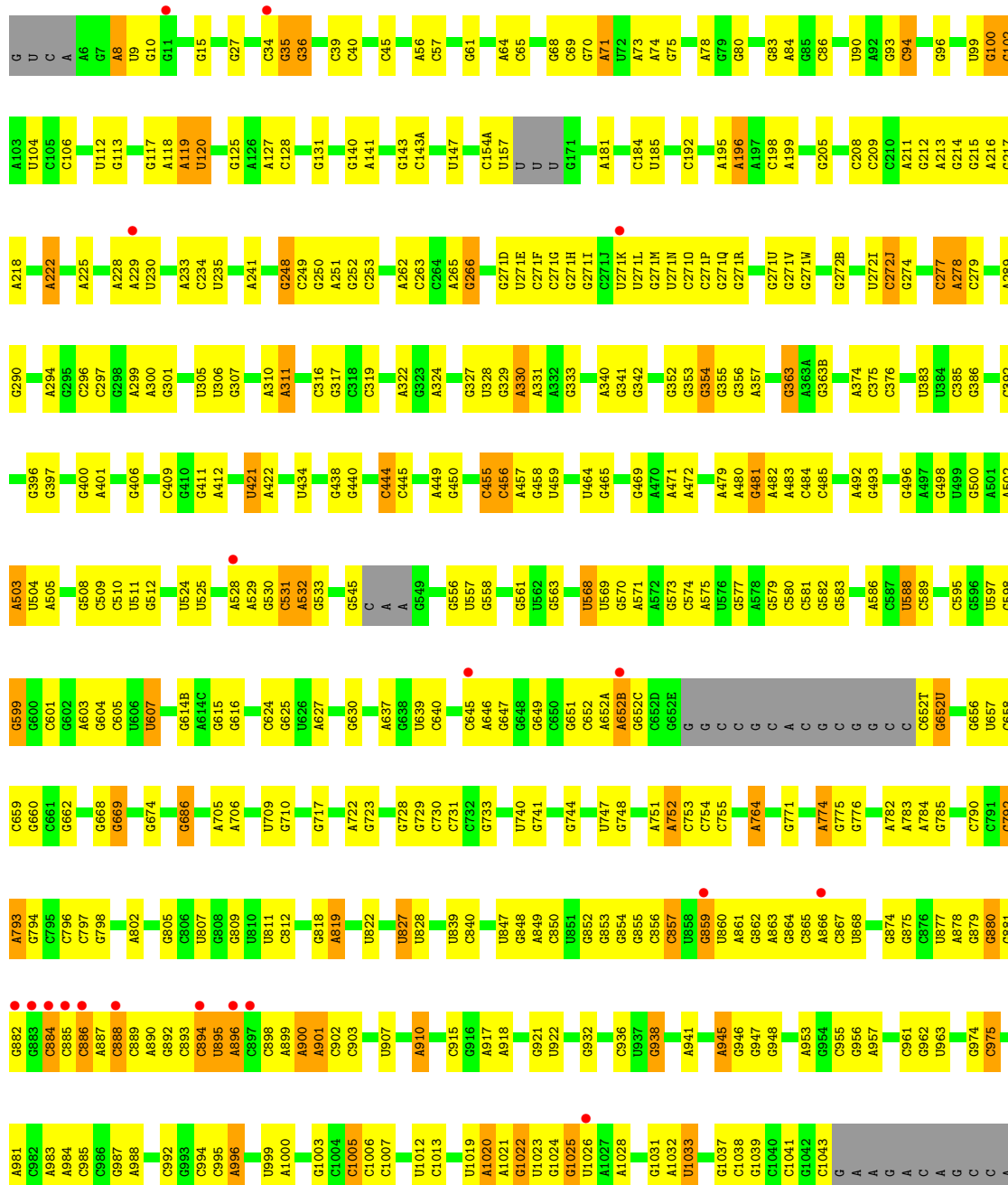




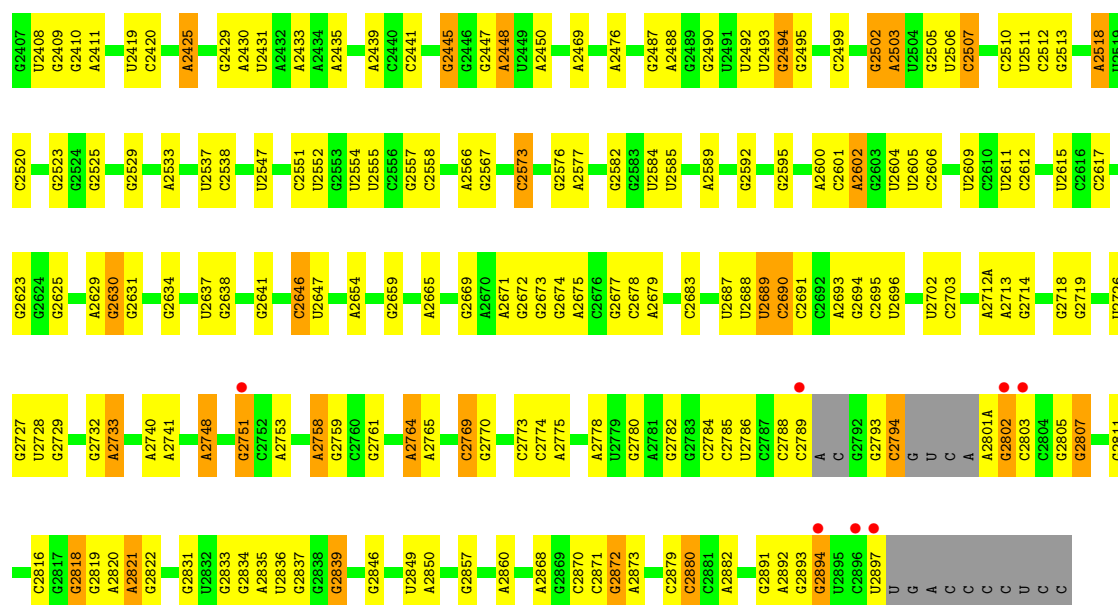


- Molecule 1: 23S Ribosomal RNA

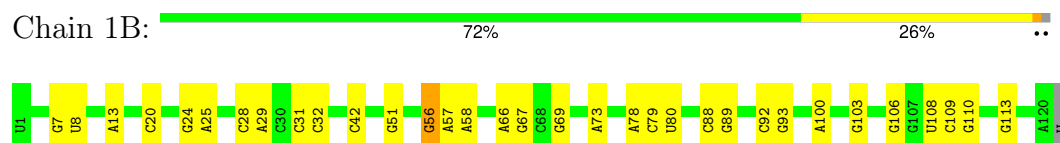
Chain 2A: 



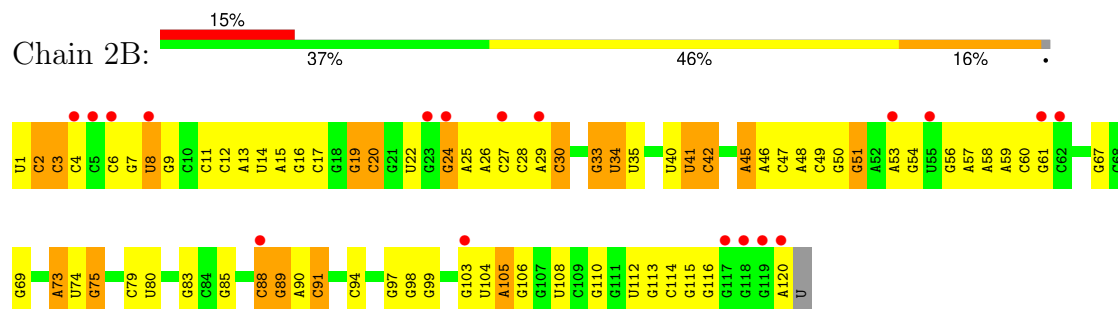
G2330	G2331	G2332	G2333	G2334	G2335	G2336	G2337	G2340	G2341	G2345	G2346	G2347	G2348	G2349	G2350	G2355	G2359	G2360	G2363	G2365	G2366	G2367	G2368	G2369	G2370	G2371	G2375	G2376	G2377	G2378	G2379	G2380	G2381	G2382	G2383	G2384	G2385	A2388	G2389	U2390	G2391	A2392	A2393	G2394	G2395	G2396	G2400	U2401	G2402	G2403	G2404	G2405				
G2238	G2239	G2242	G2251	G2261	G2264	G2268	G2273	G2274	G2275	G2278	G2283	G2284	G2285	G2286	G2287	G2288	G2289	G2290	G2291	G2292	U2296	G2297	G2298	G2299	G2303	G2304	G2305	G2306	G2307	G2308	G2309	G2310	G2314	G2315	G2316	G2317	G2318	G2319	G2320	G2321	G2322	G2323	G2324	G2400	U2401	G2402	G2403	G2404	G2405							
C2145	C2146	G2147	G2148	G2149	G2150	G2151	G2152	G2153	G2154	G2155	G2156	G2157	G2158	G2159	G2160	G2161	G2165	G2166	G2167	G2168	G2169	A2170	A2171	A2172	A2173	A2174	A2175	A2176	A2177	A2178	A2179	G2180	G2181	G2182	G2183	G2184	G2185	G2186	U2189	G2190	G2191	G2192	A2198	G2206	G2207	G2208	U2218	G2223	G2224	G2225	U2227	G2228	U2229			
G2072	G2073	U2074	U2075	U2079	U2086	U2087	U2090	U2091	U2092	U2093	U2096	U2097	U2098	U2099	U2100	G2104	G2105	G2106	G2107	G2108	U2109	G2110	G2111	G2112	U2113	A2114	G2115	G2116	G2117	G2118	G2119	G2120	G2121	G2122	G2123	G2124	G2125	G2126	G2127	G2128	G2129	G2130	G2131	U2132	G2133	A2134	A2135	G2136	G2137	G2138	G2139	G2140	G2141	G2142	G2143	U2144
C1962	U1963	G1967	G1968	A1969	A1970	A1971	A1972	A1973	G1984	U1989	U1991	U1992	U1993	U1996	U1997	G2002	A2001	G2002	G2003	C2006	U2009	U2010	G2011	G2012	A2014	A2019	A2020	A2021	U2022	G2023	A2031	G2032	A2033	G2034	G2035	G2036	U2039	U2040	G2043	G2044	G2045	G2046	G2047	G2048	G2049	G2050	G2051	G2052	G2053	G2054	G2055	G2056	G2057	G2058		
G1857	G1858	U1864	A1877	G1878	G1882	G1883	G1884	G1885	A1889	A1890	G1891	G1896	G1899	A1900	A1901	C1902	G1906	G1907	C1908	U1911	A1912	A1913	C1914	U1915	G1916	U1917	C1924	A1927	A1928	G1929	G1930	G1931	A1932	G1933	A1936	A1937	A1938	U1939	C1942	U1946	G1947	G1948	G1949	G1950	A1952	U1955	C1958	G1959	G1960							
G1769	G1772	A1773	U1778	U1779	A1780	G1781	A1782	A1783	A1789	C1790	A1791	G1792	U1793	U1794	G1795	U1796	C1797	C1798	U1798	G1799	C1800	G1801	A1802	A1803	G1804	U1805	G1811	A1812	G1815	G1816	U1820	A1821	G1822	G1826	G1827	G1828	A1829	C1830	U1833	U1834	G1835	U1846	G1847	G1848	G1849	U1850	G1851	G1852	G1853	G1854	G1855					
C1640	G1645	C1647	C1648	G1651	A1652	G1653	A1654	C1660	G1661	A1665	G1666	G1667	A1668	A1669	G1670	A1671	G1674	U1678	A1679	A1688	A1689	G1696	G1697	G1698	A1700	A1701	G1702	G1703	G1711	G1712	U1713	G1714	G1721	A1722	U1739	G1740	A1741	G1742	G1746	G1756	U1757	G1758	A1760	G1761	G1762	G1763	G1764	G1765	G1766	G1767	G1768					
U1518	G1519	G1529	C1530	C1531	C1532	G1533	U	C1536	C1546	C1547	A1558	G1559	G1560	A1566	A1567	C1568	A1569	U1578	A1579	A1583	C15																																			



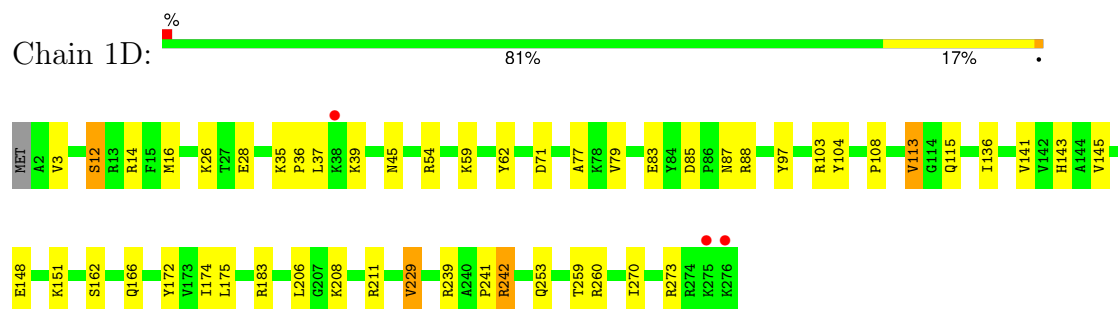
• Molecule 2: 5S Ribosomal RNA



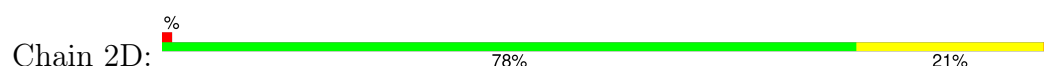
• Molecule 2: 5S Ribosomal RNA

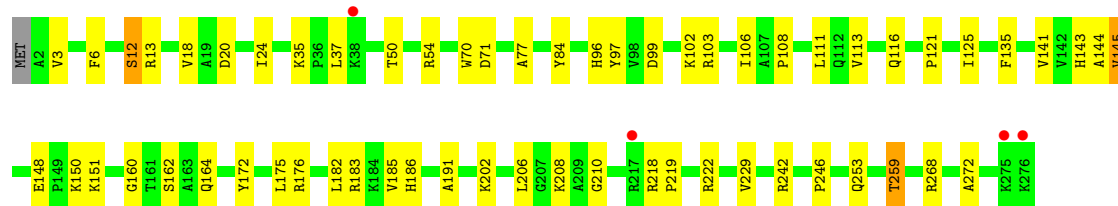


• Molecule 3: 50S ribosomal protein L2



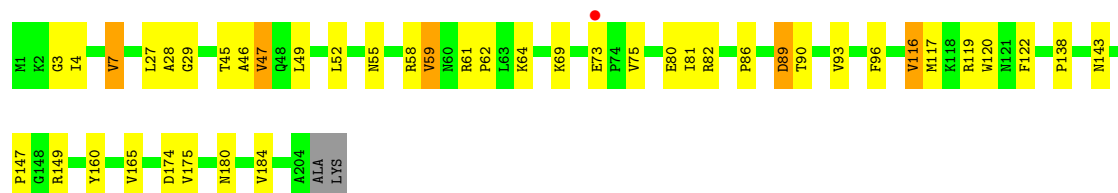
• Molecule 3: 50S ribosomal protein L2





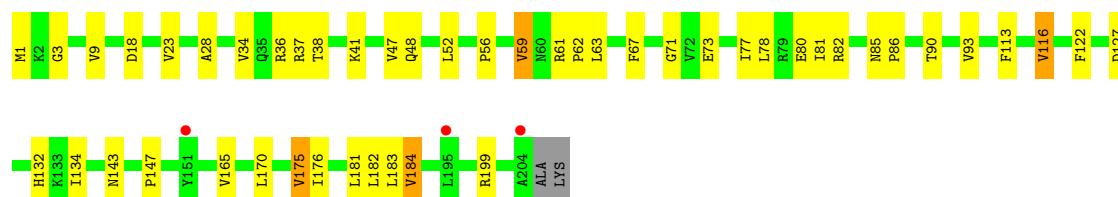
• Molecule 4: 50S ribosomal protein L3

Chain 1E: 78% 18% ..



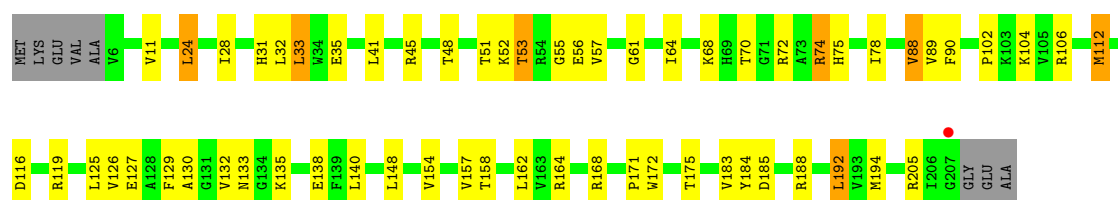
• Molecule 4: 50S ribosomal protein L3

Chain 2E: 76% 21% ..



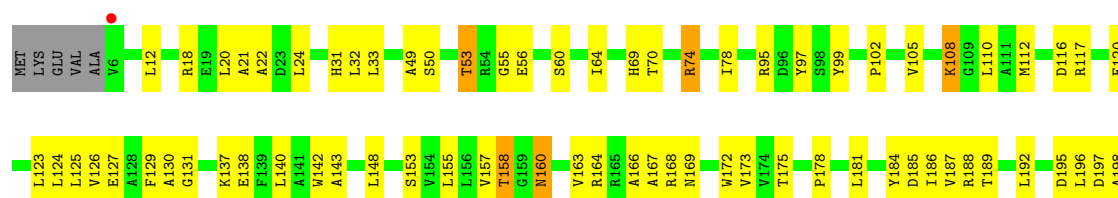
• Molecule 5: 50S ribosomal protein L4

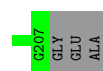
Chain 1F: 68% 25% ..



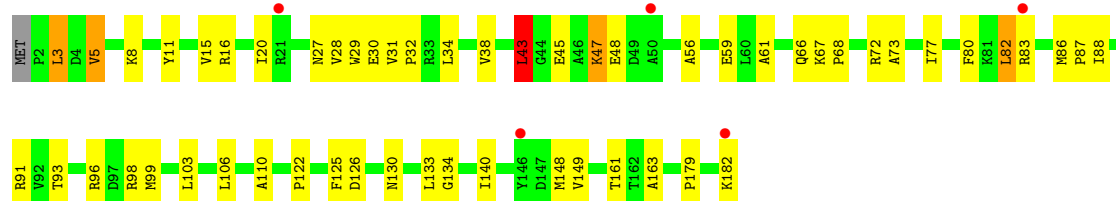
• Molecule 5: 50S ribosomal protein L4

Chain 2F: 62% 32% ..

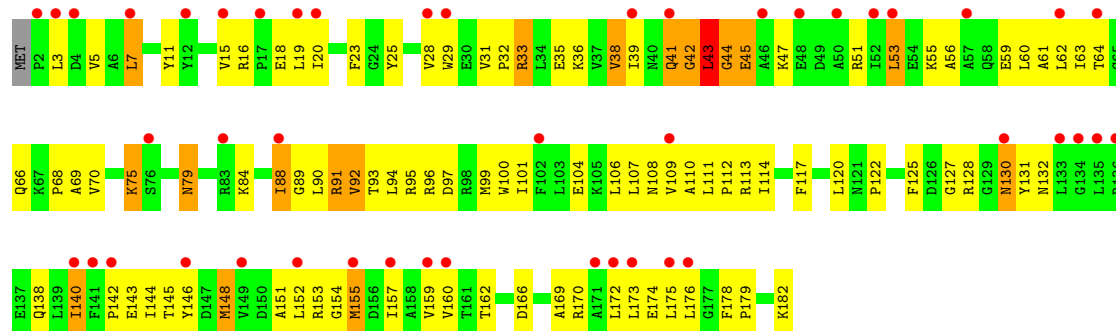
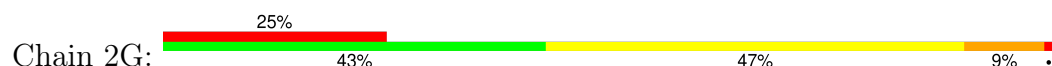




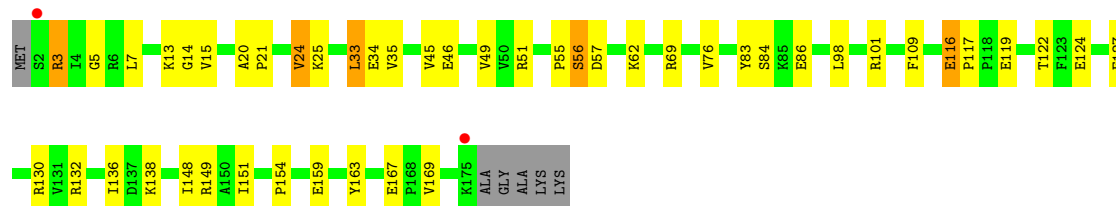
- Molecule 6: 50S ribosomal protein L5



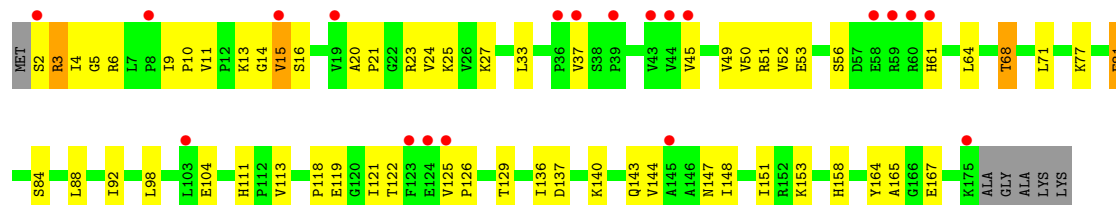
- Molecule 6: 50S ribosomal protein L5



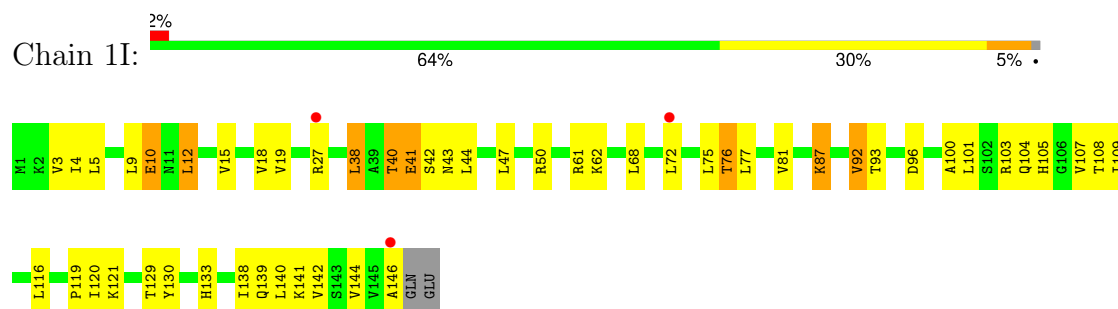
- Molecule 7: 50S ribosomal protein L6



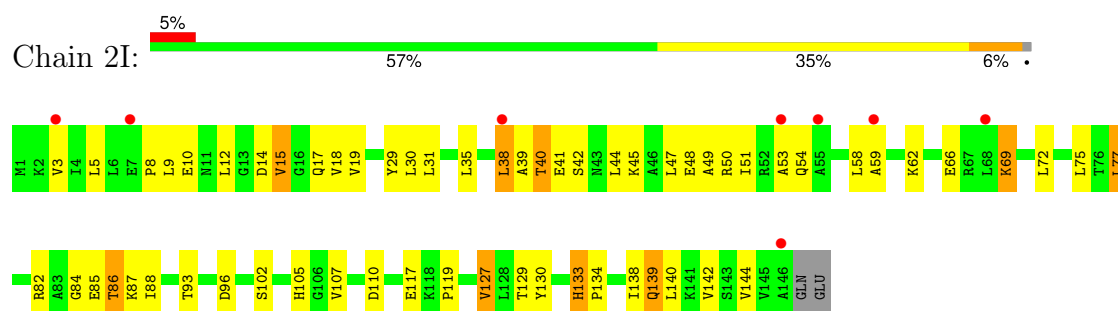
- Molecule 7: 50S ribosomal protein L6



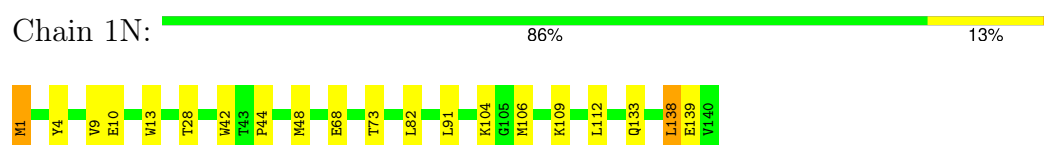
- Molecule 8: 50S ribosomal protein L9



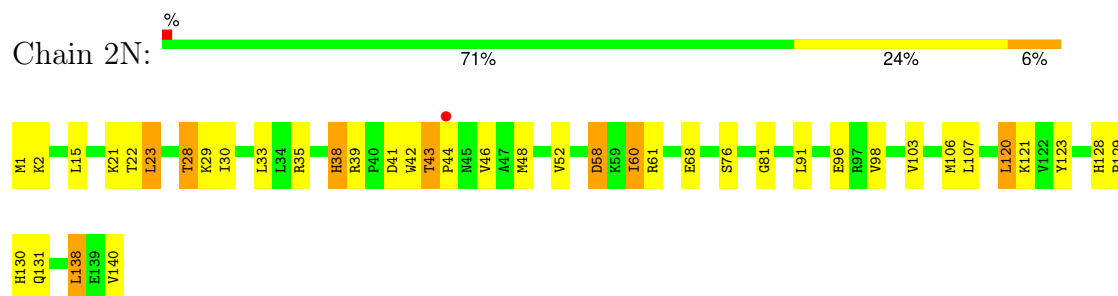
- Molecule 8: 50S ribosomal protein L9



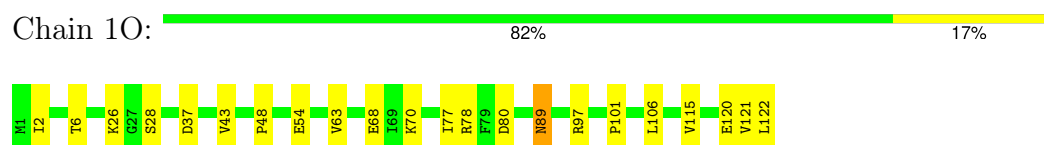
- Molecule 9: 50S ribosomal protein L13



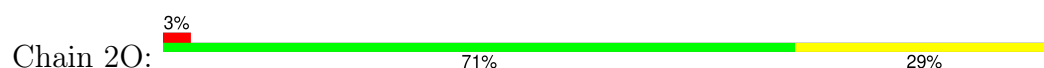
- Molecule 9: 50S ribosomal protein L13

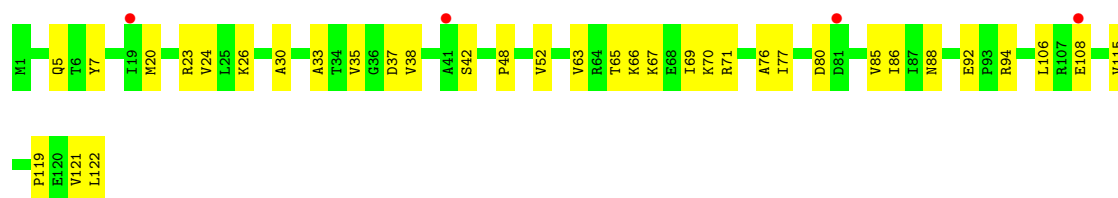


- Molecule 10: 50S ribosomal protein L14



- Molecule 10: 50S ribosomal protein L14





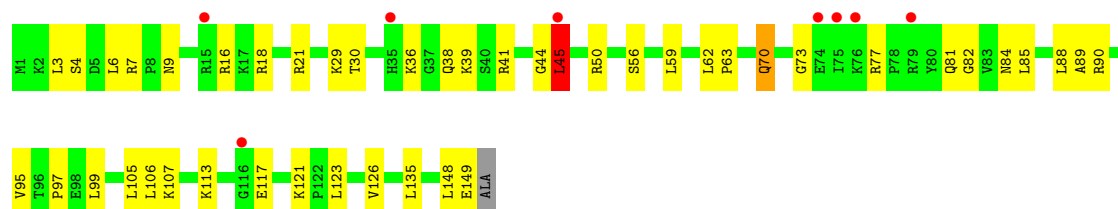
- Molecule 11: 50S ribosomal protein L15

Chain 1P: 68% 27%



- Molecule 11: 50S ribosomal protein L15

Chain 2P: 5% 69% 29%



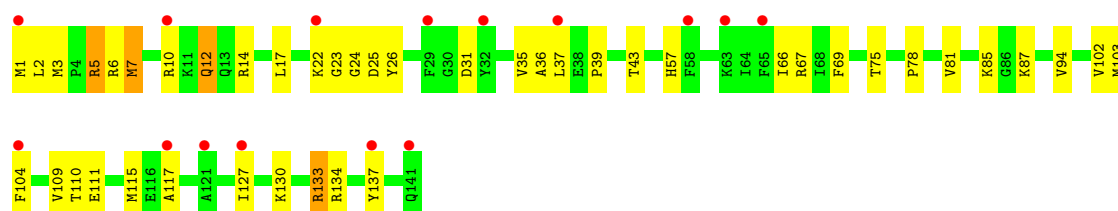
- Molecule 12: 50S ribosomal protein L16

Chain 1Q: 81% 19%



- Molecule 12: 50S ribosomal protein L16

Chain 2Q: 11% 69% 28%

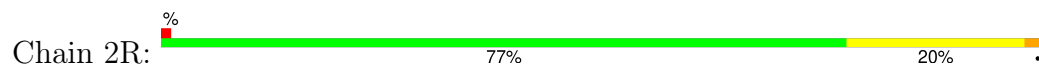


- Molecule 13: 50S ribosomal protein L17

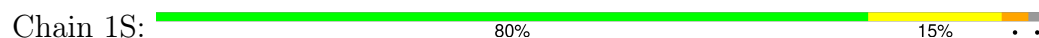
Chain 1R: 81% 17%



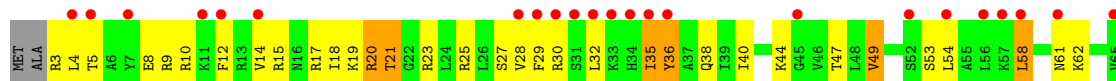
- Molecule 13: 50S ribosomal protein L17



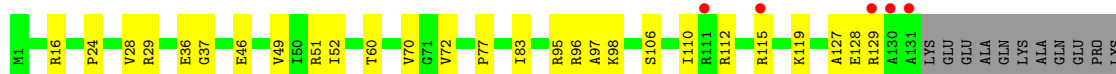
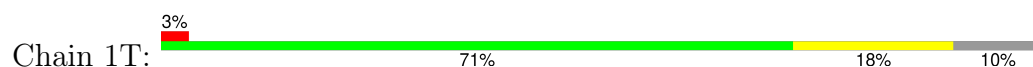
- Molecule 14: 50S ribosomal protein L18



- Molecule 14: 50S ribosomal protein L18



- Molecule 15: 50S ribosomal protein L19

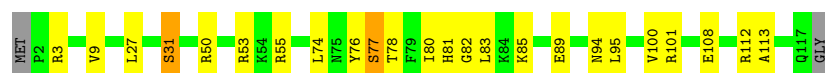


- Molecule 15: 50S ribosomal protein L19



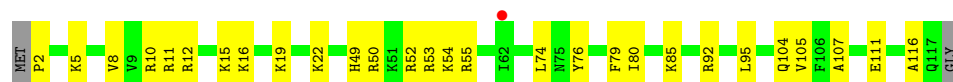
- Molecule 16: 50S ribosomal protein L20

Chain 1U:  78% 19% ..



- Molecule 16: 50S ribosomal protein L20

Chain 2U:  75% 24% .



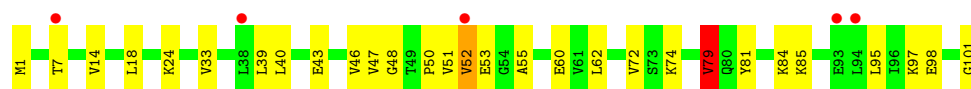
- Molecule 17: 50S ribosomal protein L21

Chain 1V:  84% 15% .



- Molecule 17: 50S ribosomal protein L21

Chain 2V:  71% 27% ..



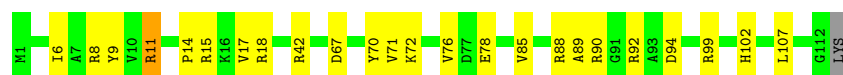
- Molecule 18: 50S ribosomal protein L22

Chain 1W:  81% 16% ..



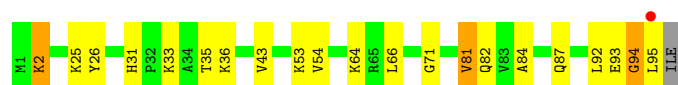
- Molecule 18: 50S ribosomal protein L22

Chain 2W:  78% 20% ..



- Molecule 19: 50S ribosomal protein L23

Chain 1X:  77% 19% ..



- Molecule 19: 50S ribosomal protein L23



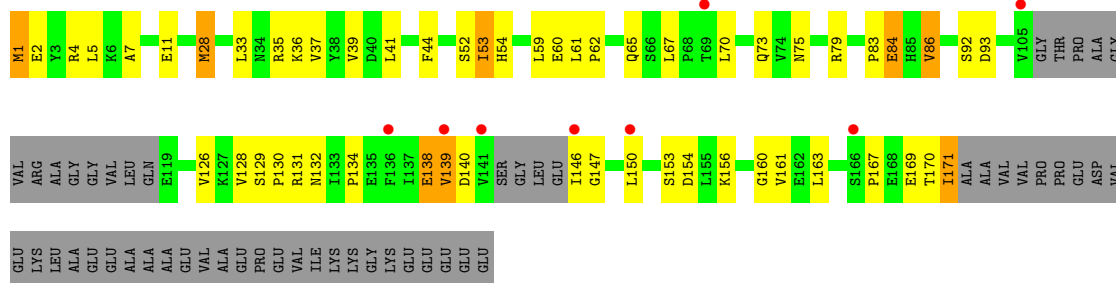
- Molecule 20: 50S ribosomal protein L24



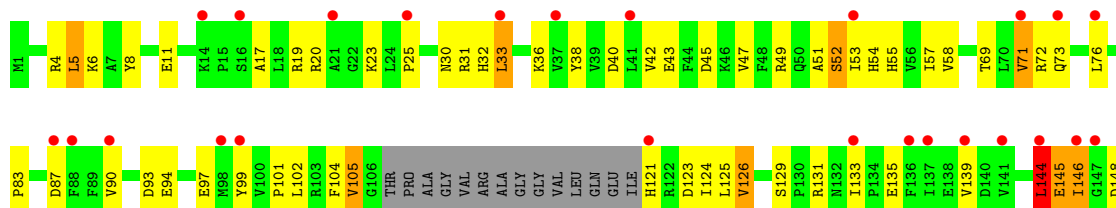
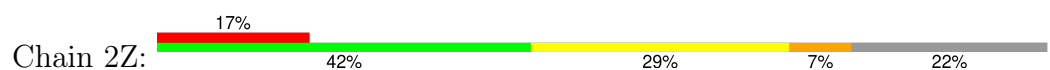
- Molecule 20: 50S ribosomal protein L24

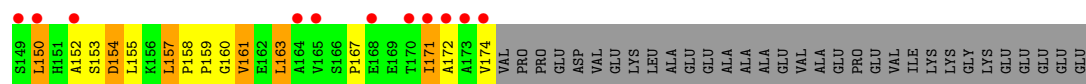


- Molecule 21: 50S ribosomal protein L25

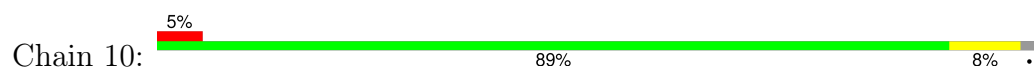


- Molecule 21: 50S ribosomal protein L25

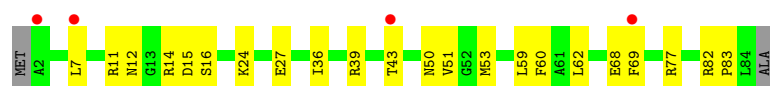
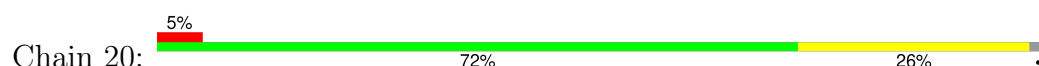




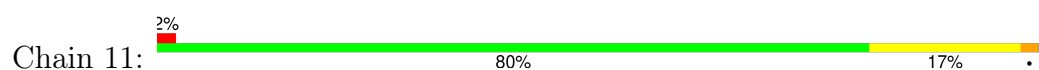
- Molecule 22: 50S ribosomal protein L27



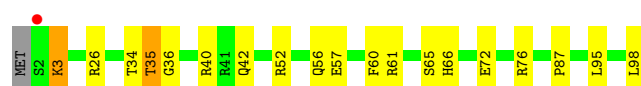
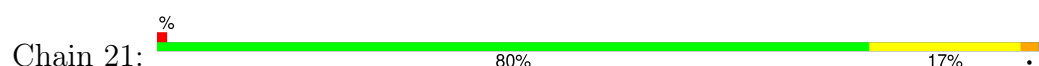
- Molecule 22: 50S ribosomal protein L27



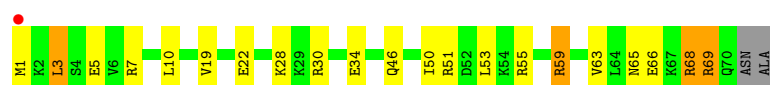
- Molecule 23: 50S ribosomal protein L28



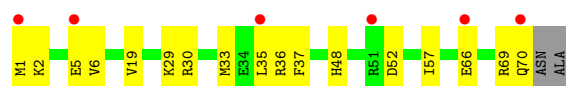
- Molecule 23: 50S ribosomal protein L28



- Molecule 24: 50S ribosomal protein L29

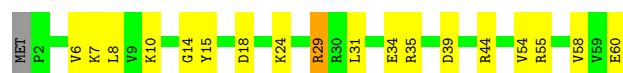


- Molecule 24: 50S ribosomal protein L29



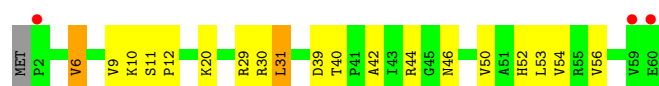
- Molecule 25: 50S ribosomal protein L30

Chain 13:  68% 28% ..



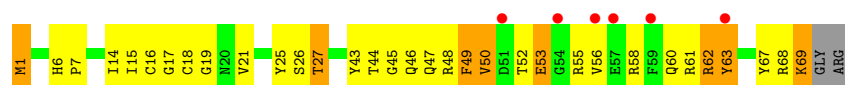
- Molecule 25: 50S ribosomal protein L30

Chain 23:  5% 67% 28% ..



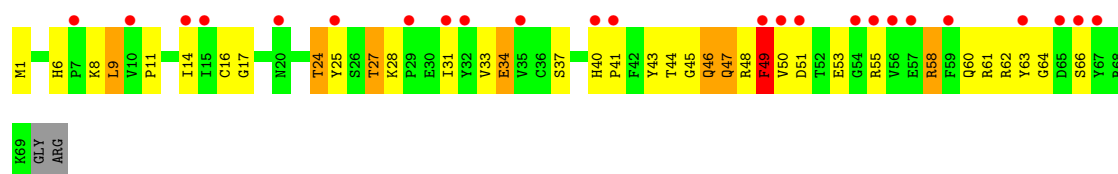
- Molecule 26: 50S ribosomal protein L31

Chain 14:  8% 51% 35% 11% .



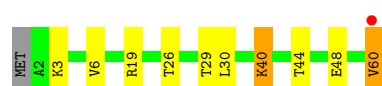
- Molecule 26: 50S ribosomal protein L31

Chain 24:  34% 46% 39% 10% ..



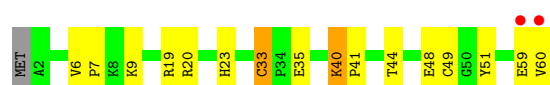
- Molecule 27: 50S ribosomal protein L32

Chain 15:  2% 82% 13% ..



- Molecule 27: 50S ribosomal protein L32

Chain 25:  3% 72% 23% ..

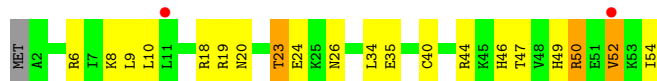


- Molecule 28: 50S ribosomal protein L33

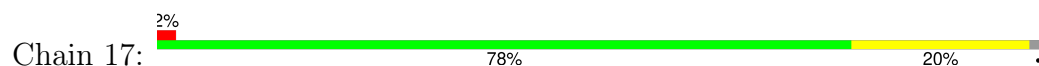
Chain 16:  74% 24% .



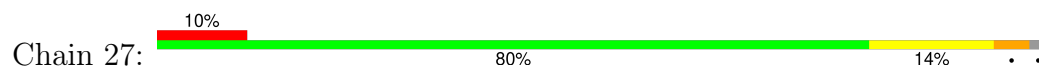
- Molecule 28: 50S ribosomal protein L33



- Molecule 29: 50S ribosomal protein L34



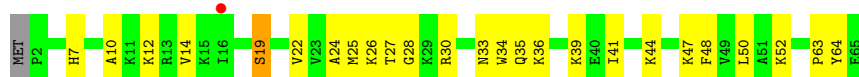
- Molecule 29: 50S ribosomal protein L34



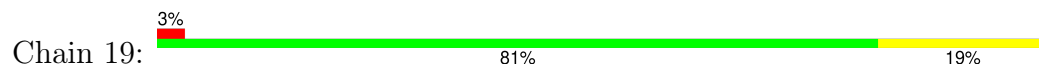
- Molecule 30: 50S ribosomal protein L35



- Molecule 30: 50S ribosomal protein L35



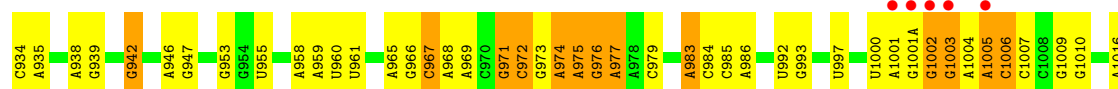
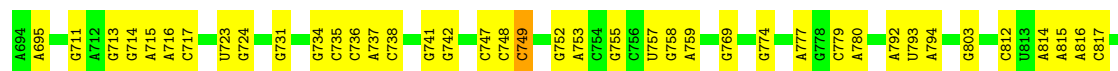
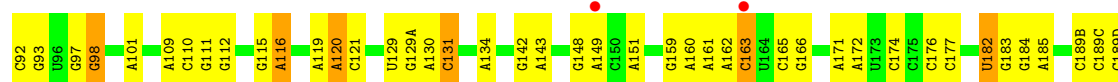
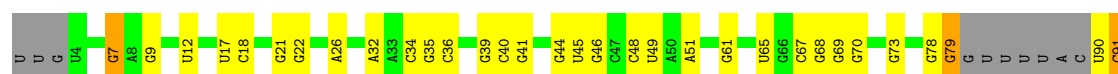
- Molecule 31: 50S ribosomal protein L36

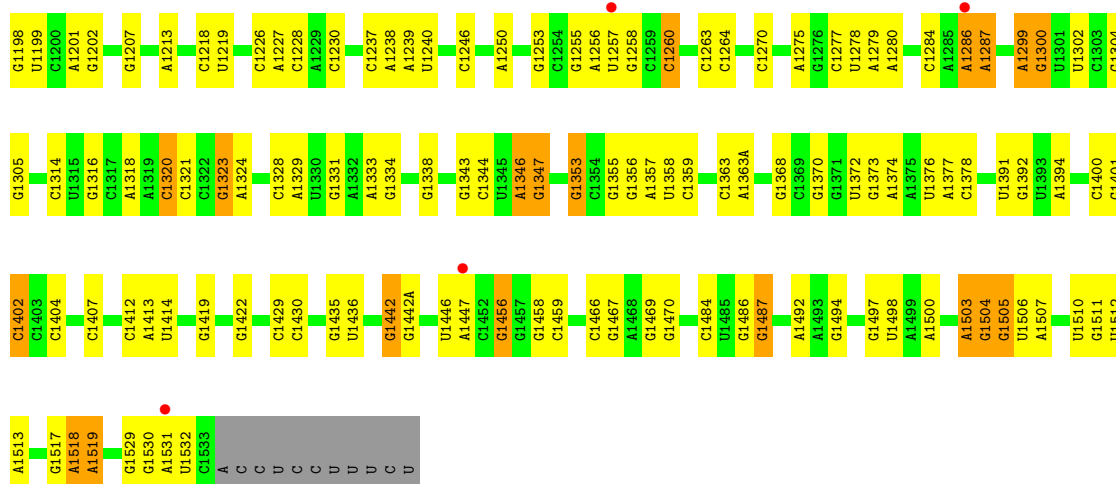


- Molecule 31: 50S ribosomal protein L36

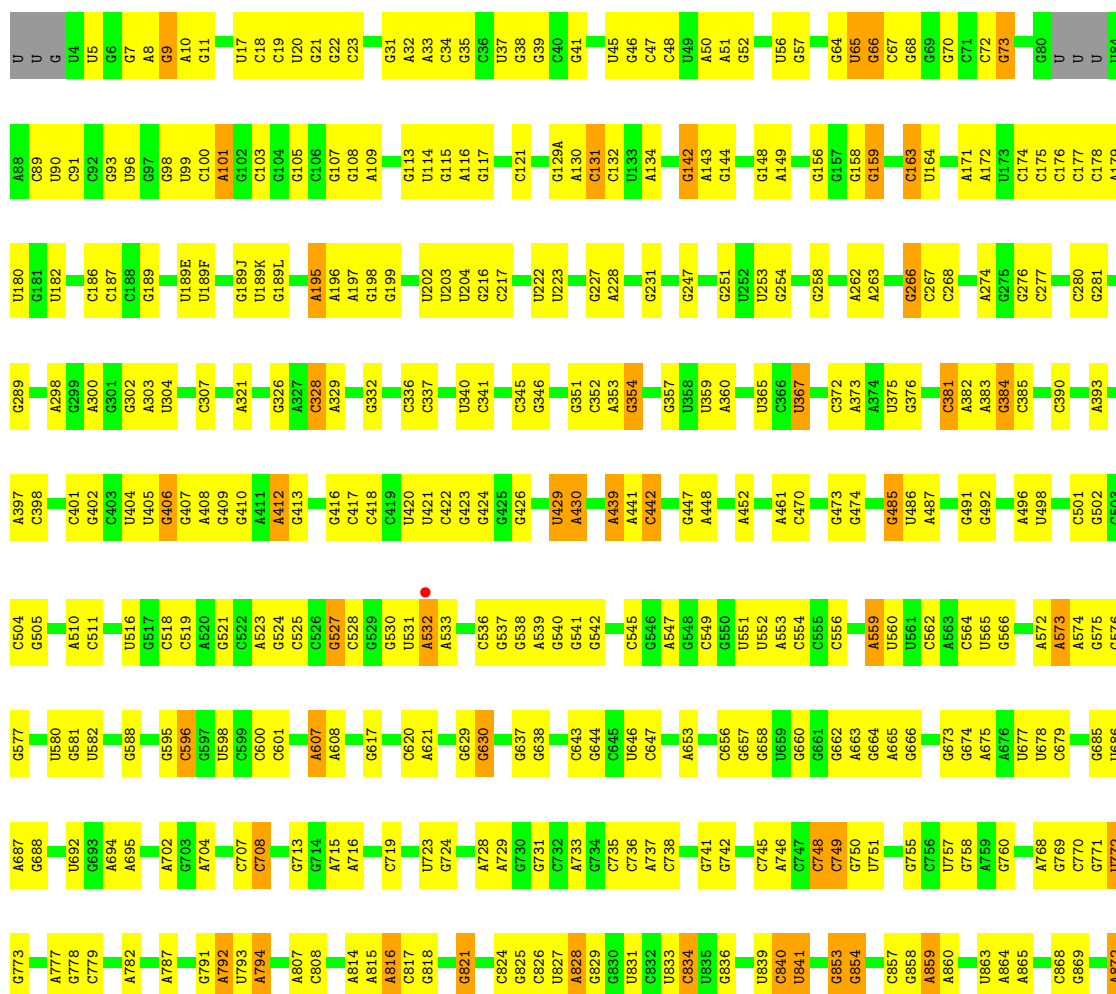


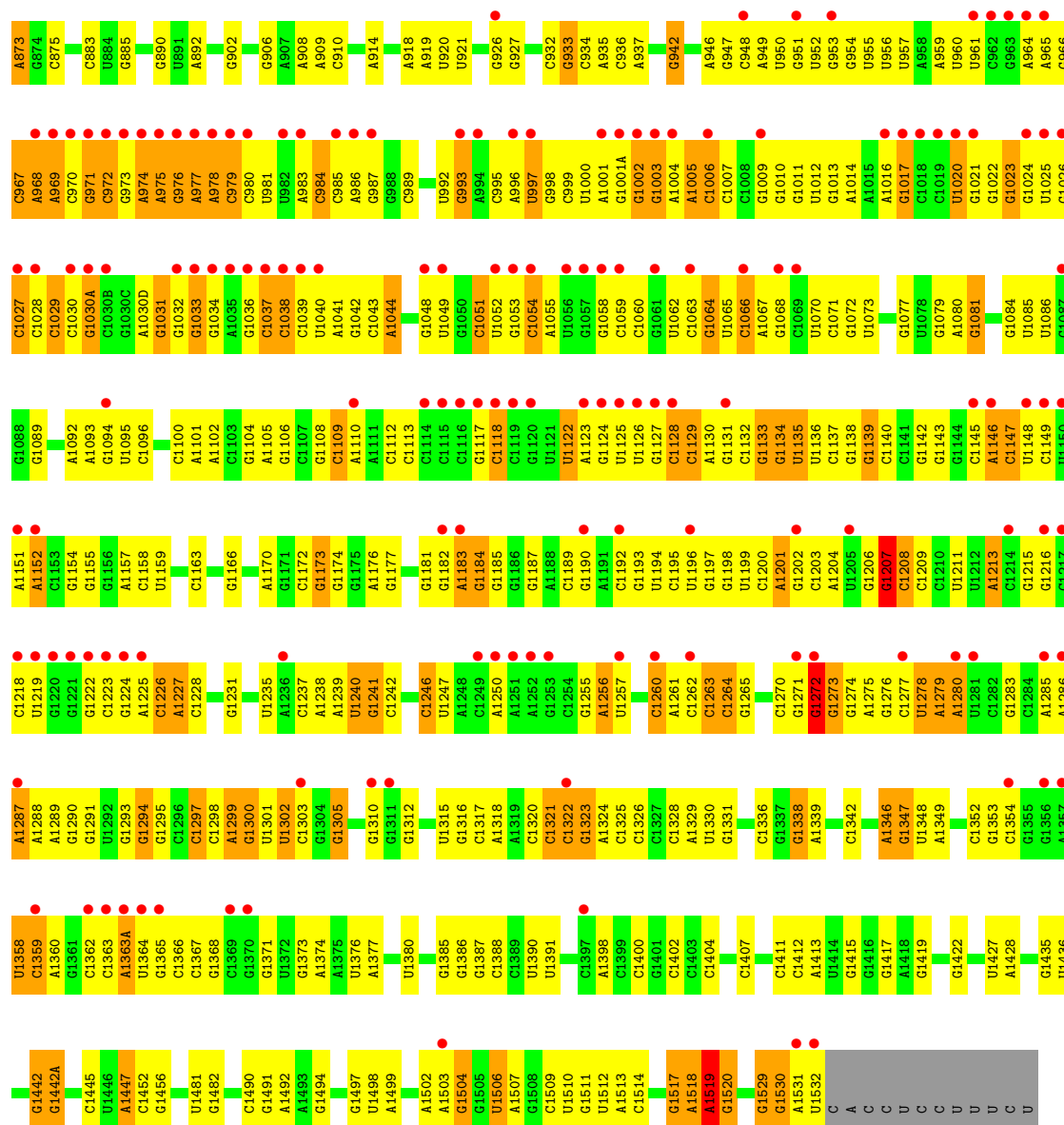
• Molecule 32: 16S Ribosomal RNA



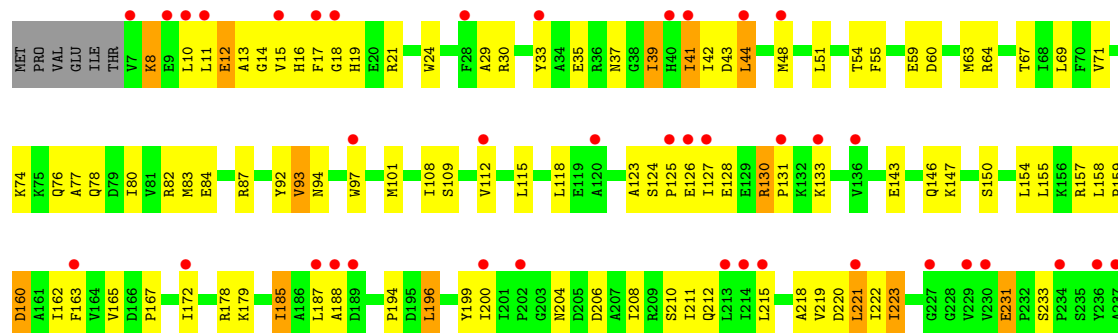


• Molecule 32: 16S Ribosomal RNA



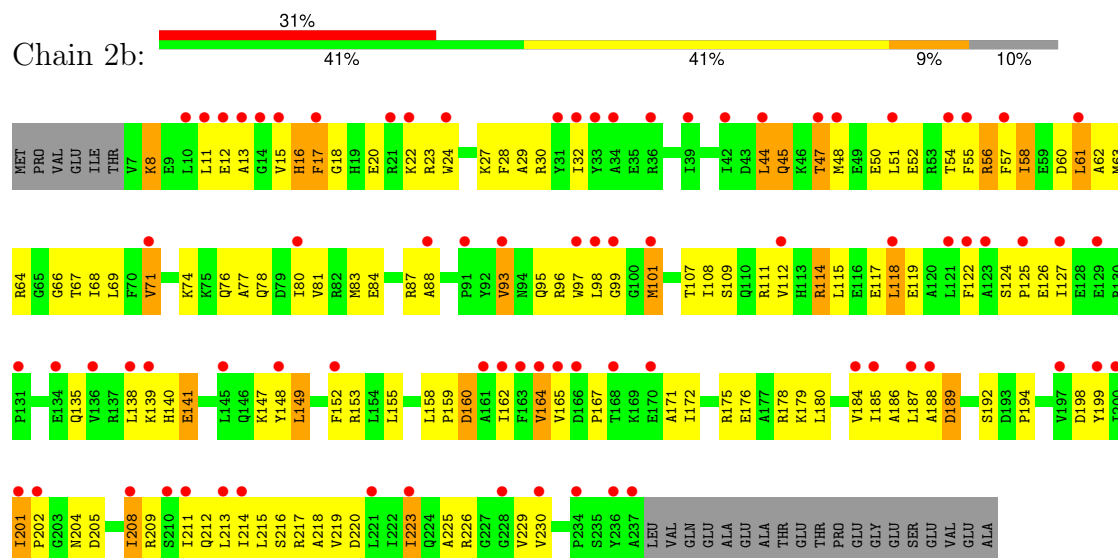


• Molecule 33: 30S ribosomal protein S2

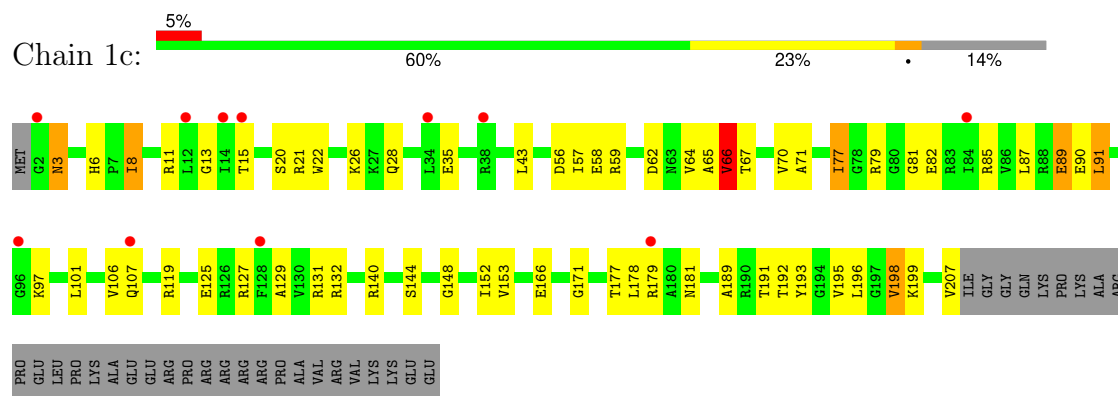


LEU VAL
PRO GLN
GLU GLY
ALA ILE
GLU THR
ALA THR
GLU THR
PRO THR
GLY GLY
GLU GLY
SER SER
GLU VAL
GLU VAL
ALA ALA

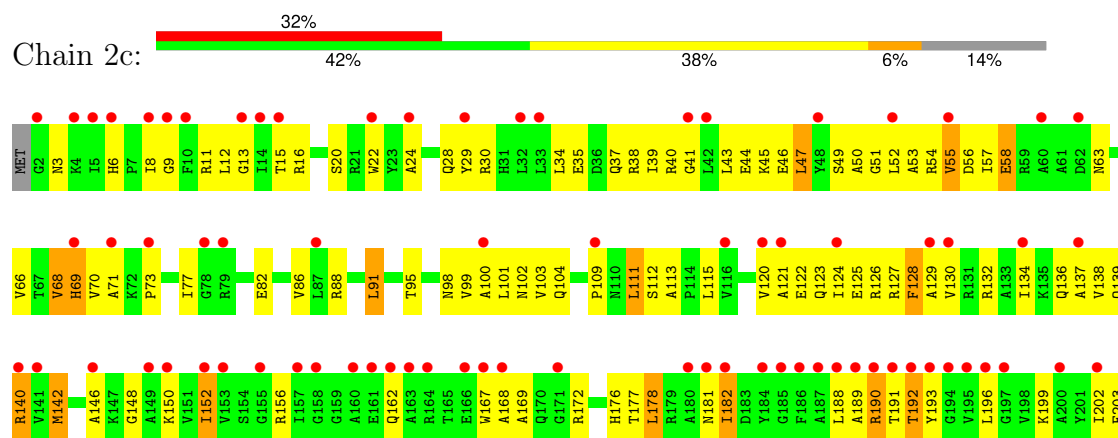
• Molecule 33: 30S ribosomal protein S2

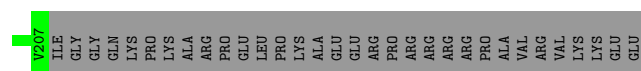


• Molecule 34: 30S ribosomal protein S3

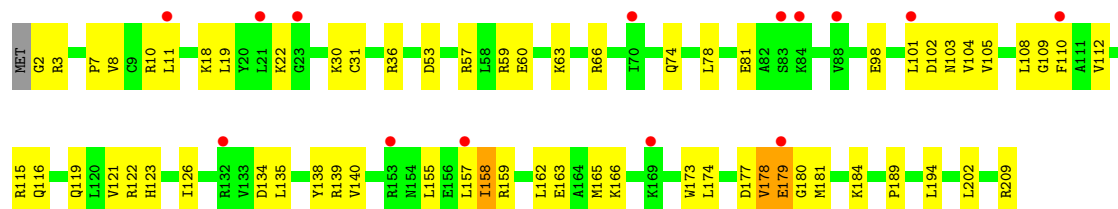


• Molecule 34: 30S ribosomal protein S3

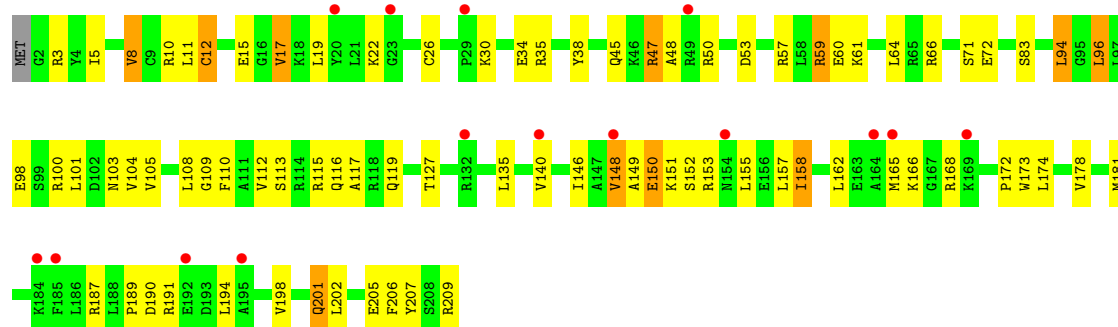




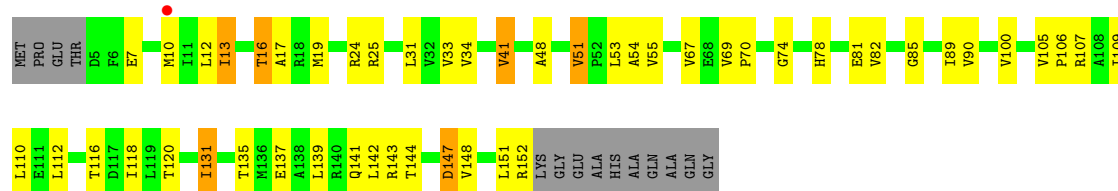
• Molecule 35: 30S ribosomal protein S4



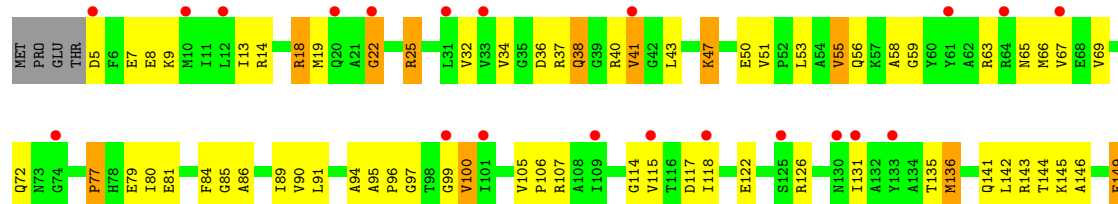
• Molecule 35: 30S ribosomal protein S4

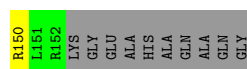


• Molecule 36: 30S ribosomal protein S5



• Molecule 36: 30S ribosomal protein S5





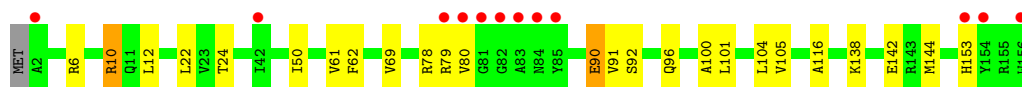
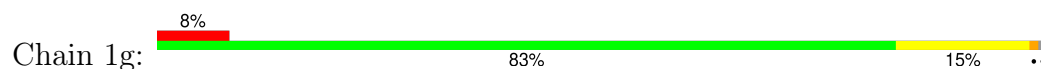
- Molecule 37: 30S ribosomal protein S6



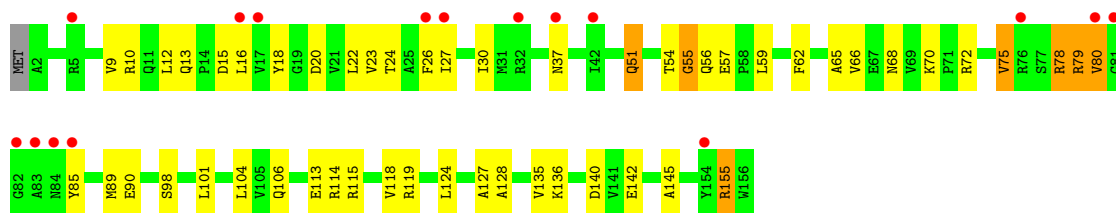
- Molecule 37: 30S ribosomal protein S6



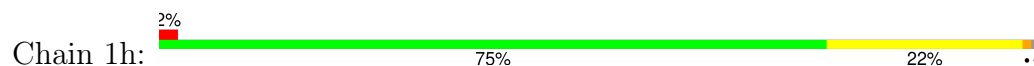
- Molecule 38: 30S ribosomal protein S7



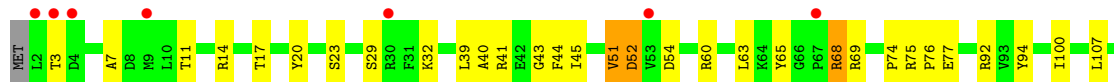
- Molecule 38: 30S ribosomal protein S7



- Molecule 39: 30S ribosomal protein S8

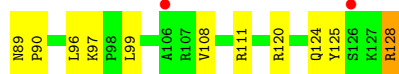
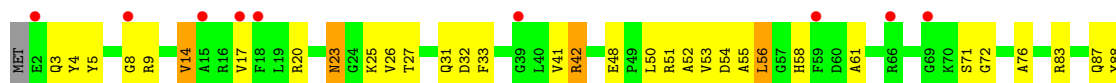


- Molecule 39: 30S ribosomal protein S8

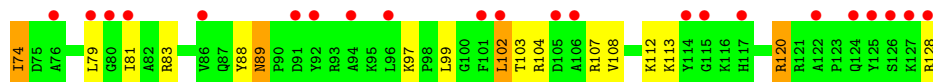
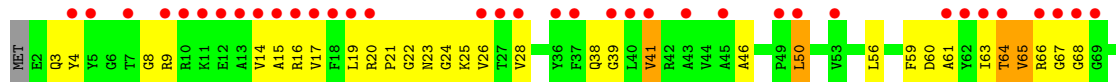




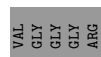
- Molecule 40: 30S ribosomal protein S9



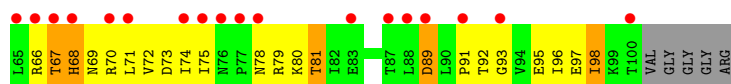
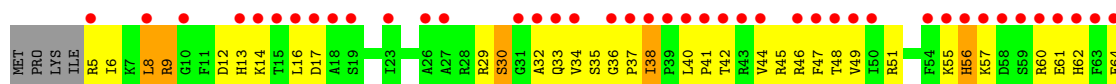
- Molecule 40: 30S ribosomal protein S9



- Molecule 41: 30S ribosomal protein S10



- Molecule 41: 30S ribosomal protein S10

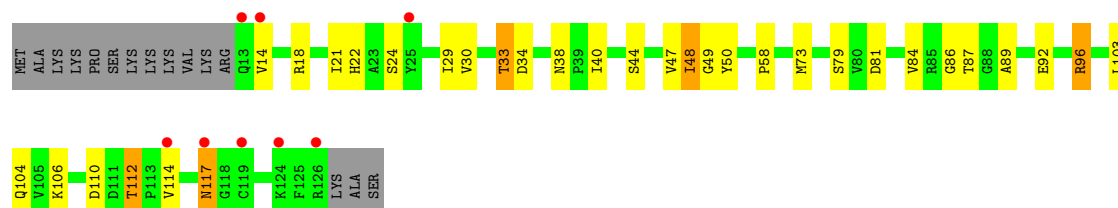


- Molecule 42: 30S ribosomal protein S11

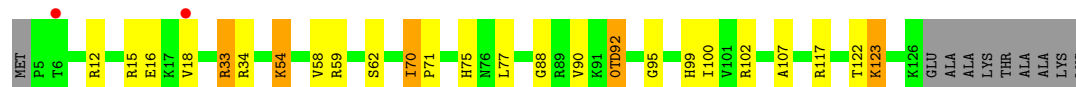
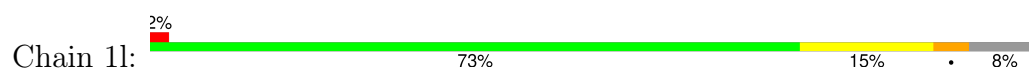




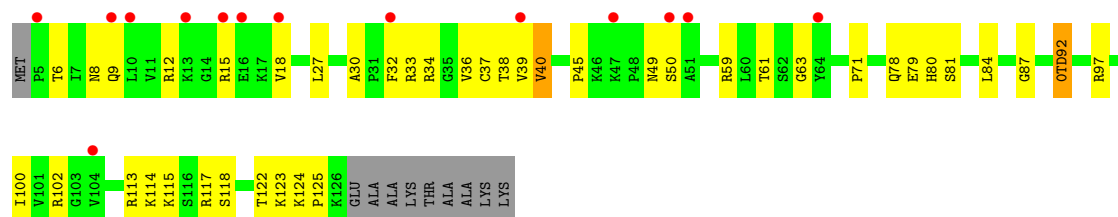
- Molecule 42: 30S ribosomal protein S11



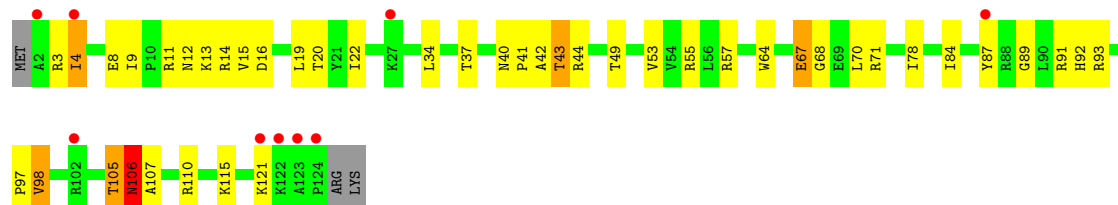
- Molecule 43: 30S ribosomal protein S12



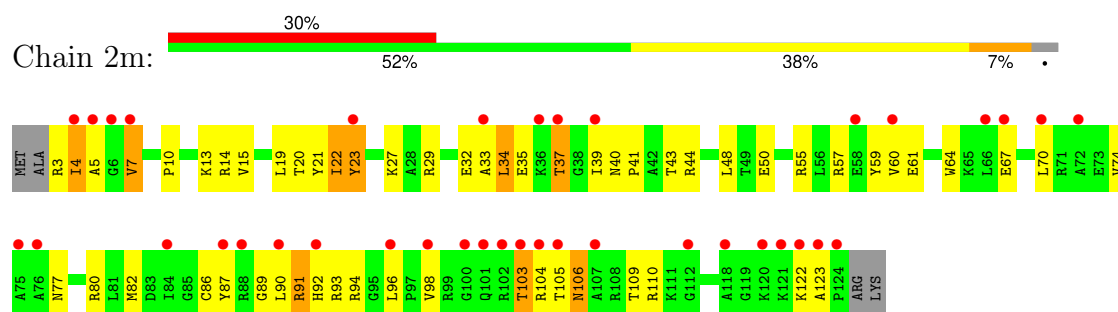
- Molecule 43: 30S ribosomal protein S12



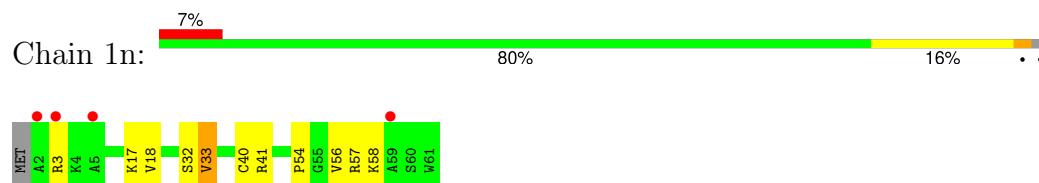
- Molecule 44: 30S ribosomal protein S13



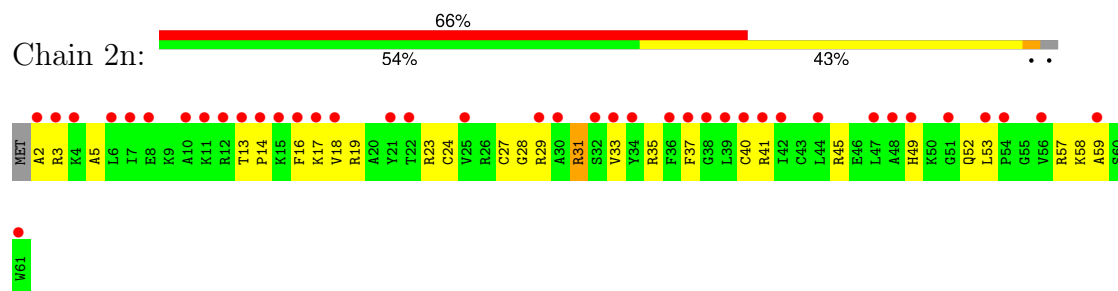
- Molecule 44: 30S ribosomal protein S13



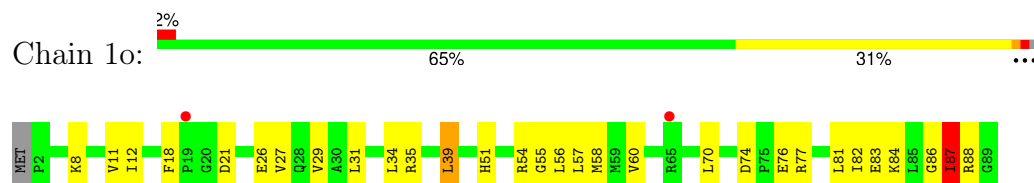
- Molecule 45: 30S ribosomal protein S14 type Z



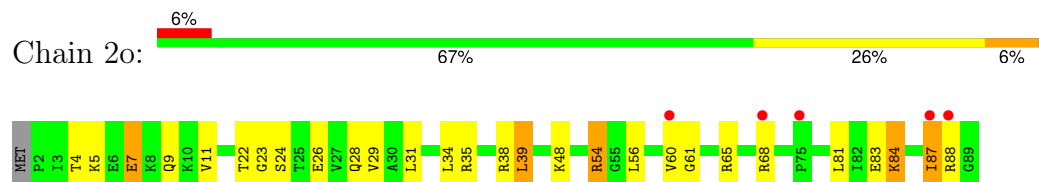
- Molecule 45: 30S ribosomal protein S14 type Z



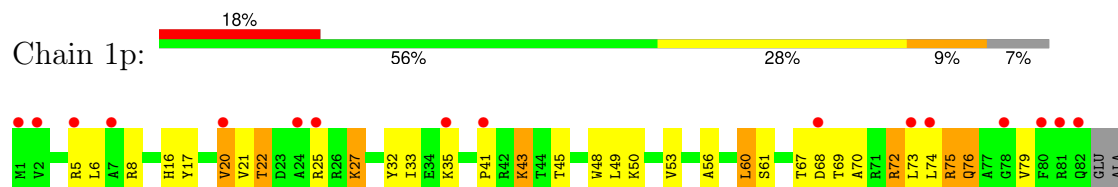
- Molecule 46: 30S ribosomal protein S15



- Molecule 46: 30S ribosomal protein S15

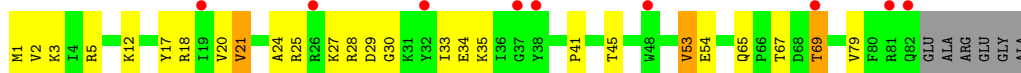


- Molecule 47: 30S ribosomal protein S16

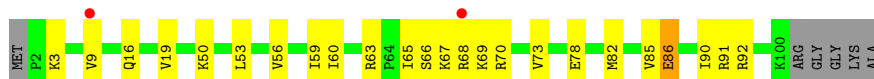


ARG
GLU
GLY
ALA

• Molecule 47: 30S ribosomal protein S16



• Molecule 48: 30S ribosomal protein S17



• Molecule 48: 30S ribosomal protein S17

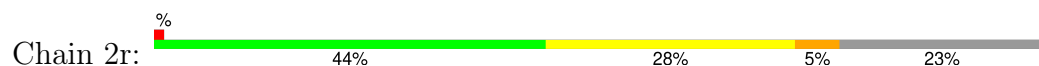


GLY
LYS
ALA

• Molecule 49: 30S ribosomal protein S18



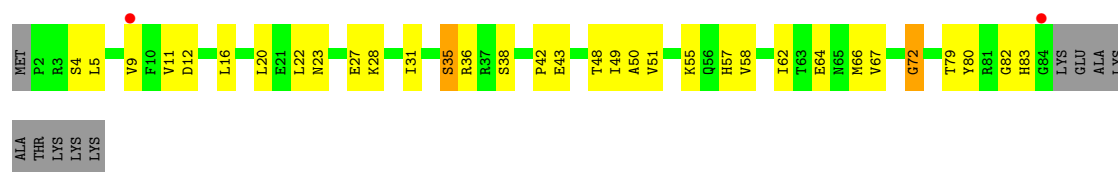
• Molecule 49: 30S ribosomal protein S18



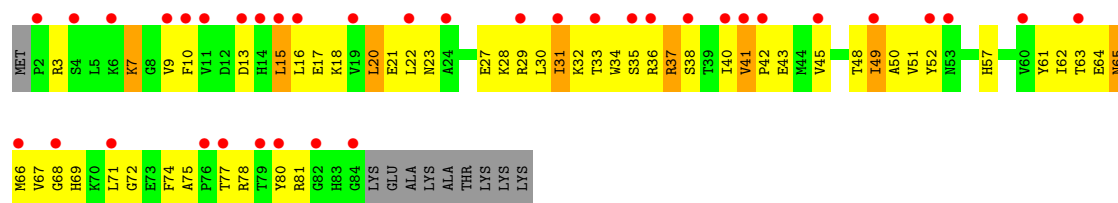
L78
R84
L85
W86
R87
LYS

• Molecule 50: 30S ribosomal protein S19

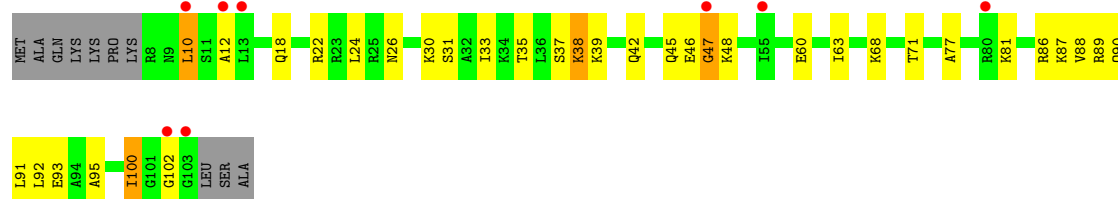




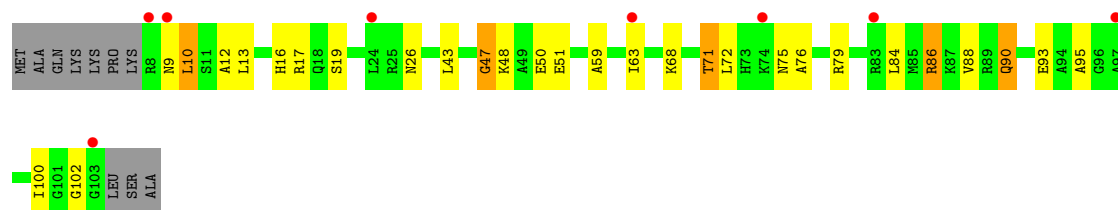
- Molecule 50: 30S ribosomal protein S19



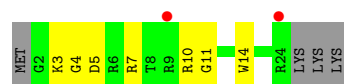
- Molecule 51: 30S ribosomal protein S20



- Molecule 51: 30S ribosomal protein S20

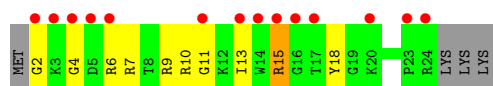


- Molecule 52: 30S ribosomal protein Thx



- Molecule 52: 30S ribosomal protein Thx

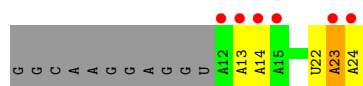
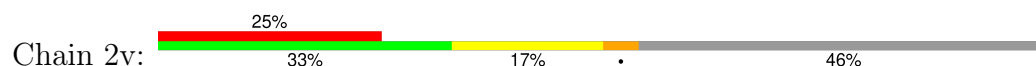




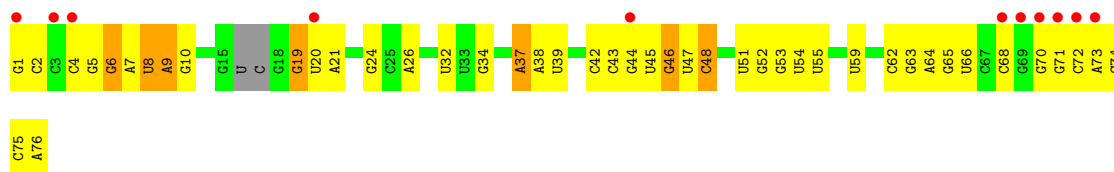
• Molecule 53: MF-mRNA



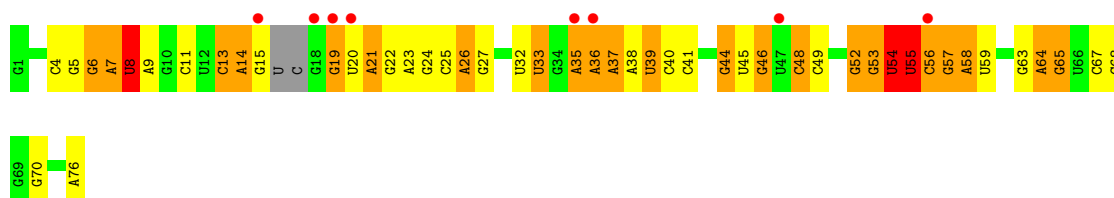
• Molecule 53: MF-mRNA



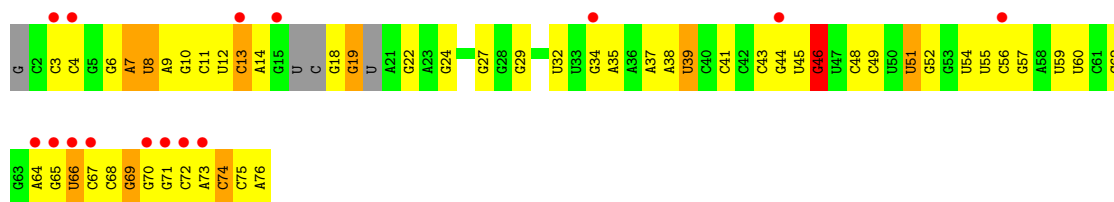
• Molecule 54: A-site and E-site Deacylated tRNAphe



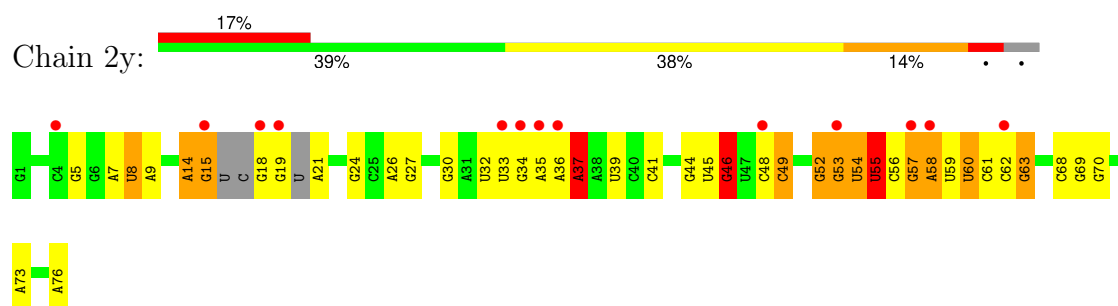
• Molecule 54: A-site and E-site Deacylated tRNAphe



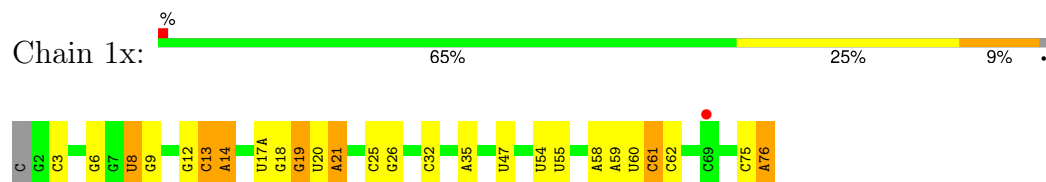
• Molecule 54: A-site and E-site Deacylated tRNAphe



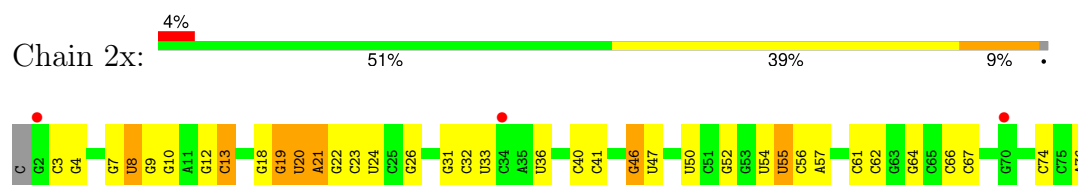
• Molecule 54: A-site and E-site Deacylated tRNAphe



- Molecule 55: P-site Deacylated tRNAmet



- Molecule 55: P-site Deacylated tRNAmet



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.73Å 449.08Å 621.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	121.84 – 2.75 121.84 – 2.75	Depositor EDS
% Data completeness (in resolution range)	98.9 (121.84-2.75) 98.9 (121.84-2.75)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.213 , 0.261 0.213 , 0.260	Depositor DCC
R_{free} test set	74514 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	59.1	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 52.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	300806	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.53% 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: OMU, M2G, 5MU, MIA, SF4, 2MA, K, UR3, MG, 4OC, 0TD, 4SU, PSU, ZN, Y7K, OMC, MA6, OMG, 2MG, G7M, 5MC

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	1A	0.29	0/69011	0.46	1/107720 (0.0%)
1	2A	0.21	0/67295	0.39	1/105042 (0.0%)
2	1B	0.23	0/2882	0.40	0/4494
2	2B	0.20	0/2879	0.37	0/4487
3	1D	0.27	0/2186	0.50	0/2944
3	2D	0.22	0/2186	0.46	0/2944
4	1E	0.28	0/1592	0.50	0/2149
4	2E	0.21	0/1592	0.44	0/2149
5	1F	0.28	0/1618	0.49	0/2191
5	2F	0.22	0/1614	0.46	0/2186
6	1G	0.21	0/1448	0.42	0/1957
6	2G	0.20	0/1453	0.50	1/1963 (0.1%)
7	1H	0.23	0/1356	0.44	0/1834
7	2H	0.18	0/1356	0.38	0/1834
8	1I	0.20	0/1112	0.43	0/1514
8	2I	0.19	0/1079	0.42	0/1475
9	1N	0.26	0/1144	0.45	0/1543
9	2N	0.19	0/1144	0.39	0/1543
10	1O	0.28	0/943	0.49	0/1269
10	2O	0.19	0/943	0.46	0/1269
11	1P	0.27	0/1152	0.54	1/1533 (0.1%)
11	2P	0.22	0/1152	0.52	0/1533
12	1Q	0.29	0/1143	0.47	0/1527
12	2Q	0.20	0/1143	0.46	0/1527
13	1R	0.29	0/982	0.49	0/1312
13	2R	0.21	0/982	0.46	0/1312
14	1S	0.23	0/883	0.49	0/1176
14	2S	0.21	0/880	0.46	0/1172
15	1T	0.25	0/1105	0.52	0/1477
15	2T	0.19	0/1097	0.41	0/1468
16	1U	0.29	0/977	0.47	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.20	0/977	0.38	0/1301
17	1V	0.27	0/782	0.48	0/1049
17	2V	0.18	0/782	0.43	0/1049
18	1W	0.30	0/897	0.46	0/1205
18	2W	0.21	0/897	0.40	0/1205
19	1X	0.26	0/764	0.52	2/1025 (0.2%)
19	2X	0.20	0/764	0.46	0/1025
20	1Y	0.24	0/819	0.52	0/1095
20	2Y	0.20	0/819	0.43	0/1095
21	1Z	0.22	0/1267	0.46	0/1717
21	2Z	0.23	0/1299	0.49	1/1763 (0.1%)
22	10	0.27	0/662	0.53	0/881
22	20	0.20	0/662	0.44	0/881
23	11	0.26	0/762	0.42	0/1014
23	21	0.22	0/762	0.41	0/1014
24	12	0.24	0/590	0.43	0/781
24	22	0.18	0/590	0.34	0/781
25	13	0.28	0/474	0.46	0/635
25	23	0.23	0/469	0.41	0/630
26	14	0.24	0/565	0.57	0/761
26	24	0.24	0/545	0.48	0/737
27	15	0.29	0/469	0.49	0/635
27	25	0.26	0/469	0.43	0/635
28	16	0.28	0/460	0.50	0/613
28	26	0.22	0/456	0.46	0/608
29	17	0.30	0/426	0.54	0/561
29	27	0.24	0/426	0.51	0/561
30	18	0.27	0/525	0.47	0/691
30	28	0.20	0/525	0.39	0/691
31	19	0.26	0/310	0.47	0/407
31	29	0.19	0/310	0.40	0/407
32	1a	0.20	0/35795	0.38	0/55864
32	2a	0.20	0/35886	0.37	2/56005 (0.0%)
33	1b	0.22	0/1881	0.49	0/2542
33	2b	0.24	0/1860	0.54	1/2518 (0.0%)
34	1c	0.19	0/1572	0.41	0/2126
34	2c	0.24	0/1566	0.47	0/2119
35	1d	0.19	0/1685	0.44	0/2262
35	2d	0.20	0/1704	0.43	0/2284
36	1e	0.21	0/1145	0.47	0/1543
36	2e	0.21	0/1149	0.48	0/1548
37	1f	0.20	0/823	0.43	0/1115
37	2f	0.20	0/829	0.41	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.19	0/1250	0.39	0/1679
38	2g	0.20	0/1254	0.42	0/1683
39	1h	0.20	0/1108	0.42	0/1494
39	2h	0.17	0/1108	0.40	0/1494
40	1i	0.19	0/1002	0.48	0/1346
40	2i	0.24	0/997	0.50	0/1343
41	1j	0.20	0/722	0.44	0/982
41	2j	0.27	0/727	0.47	0/988
42	1k	0.19	0/844	0.44	0/1145
42	2k	0.19	0/848	0.37	0/1149
43	1l	0.22	0/937	0.41	0/1260
43	2l	0.19	0/937	0.47	1/1260 (0.1%)
44	1m	0.20	0/969	0.49	0/1302
44	2m	0.21	0/961	0.48	0/1291
45	1n	0.19	0/501	0.45	0/664
45	2n	0.21	0/501	0.47	0/664
46	1o	0.20	0/739	0.39	0/985
46	2o	0.17	0/739	0.38	0/985
47	1p	0.22	0/697	0.49	0/939
47	2p	0.21	0/693	0.47	0/935
48	1q	0.19	0/836	0.42	0/1117
48	2q	0.20	0/836	0.48	0/1117
49	1r	0.19	0/560	0.43	0/746
49	2r	0.20	0/560	0.45	0/746
50	1s	0.22	0/667	0.48	0/900
50	2s	0.29	0/661	0.62	0/893
51	1t	0.19	0/730	0.46	0/965
51	2t	0.19	0/729	0.43	0/965
52	1u	0.19	0/203	0.46	0/266
52	2u	0.18	0/203	0.45	0/266
53	1v	0.22	0/310	0.32	0/480
53	2v	0.22	0/310	0.35	0/480
54	1w	0.29	2/1606 (0.1%)	0.38	0/2497
54	1y	0.30	2/1606 (0.1%)	0.43	0/2497
54	2w	0.31	2/1556 (0.1%)	0.39	0/2418
54	2y	0.30	2/1583 (0.1%)	0.39	0/2459
55	1x	0.26	0/1725	0.41	0/2689
55	2x	0.25	0/1725	0.37	0/2689
All	All	0.24	8/316688 (0.0%)	0.42	11/474125 (0.0%)

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
33	1b	0	1
40	2i	0	1
All	All	0	2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	46	G7M	O3'-P	5.78	1.62	1.56
54	2y	46	G7M	O3'-P	5.46	1.61	1.56
54	2w	46	G7M	O3'-P	5.42	1.61	1.56
54	1y	46	G7M	O3'-P	5.15	1.61	1.56
54	1w	8	4SU	O3'-P	5.15	1.61	1.56
54	2y	8	4SU	O3'-P	5.09	1.61	1.56
54	2w	8	4SU	O3'-P	5.08	1.61	1.56
54	1y	8	4SU	O3'-P	5.06	1.61	1.56

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	2G	44	GLY	N-CA-C	-8.42	104.73	115.42
11	1P	116	GLY	N-CA-C	6.46	122.02	113.37
33	2b	114	ARG	N-CA-C	-6.17	107.59	114.62
1	1A	1992	G	C2'-C3'-O3'	5.91	118.36	109.50
1	2A	1992	G	C2'-C3'-O3'	5.67	118.00	109.50
43	2l	63	GLY	N-CA-C	-5.29	108.78	115.08
32	2a	1263	C	N1-C2-O2	5.18	134.43	118.90
19	1X	94	GLY	CA-C-N	5.06	130.81	121.70
19	1X	94	GLY	C-N-CA	5.06	130.81	121.70
21	2Z	105	VAL	N-CA-C	5.04	111.60	106.21
32	2a	1272	G	N1-C2-N2	-5.00	101.20	116.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
33	1b	123	ALA	Peptide
40	2i	38	GLN	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61852	0	31195	574	0
1	2A	60322	0	30424	688	0
2	1B	2577	0	1305	22	0
2	2B	2575	0	1303	57	0
3	1D	2136	0	2218	41	0
3	2D	2136	0	2218	46	0
4	1E	1559	0	1618	29	0
4	2E	1559	0	1618	36	0
5	1F	1583	0	1625	36	0
5	2F	1579	0	1619	43	0
6	1G	1423	0	1436	39	0
6	2G	1428	0	1438	81	0
7	1H	1330	0	1407	24	0
7	2H	1330	0	1407	30	0
8	1I	1097	0	1140	31	0
8	2I	1064	0	1082	41	0
9	1N	1117	0	1184	9	0
9	2N	1117	0	1184	28	0
10	1O	933	0	996	13	0
10	2O	933	0	996	21	0
11	1P	1135	0	1212	34	0
11	2P	1135	0	1212	32	0
12	1Q	1122	0	1179	19	0
12	2Q	1122	0	1179	26	0
13	1R	968	0	1033	15	0
13	2R	968	0	1033	20	0
14	1S	873	0	927	15	0
14	2S	870	0	923	43	0
15	1T	1091	0	1151	14	0
15	2T	1083	0	1136	26	0
16	1U	959	0	1019	14	0
16	2U	959	0	1018	18	0
17	1V	771	0	830	10	0
17	2V	771	0	830	17	0
18	1W	886	0	940	10	0
18	2W	886	0	940	16	0
19	1X	750	0	814	16	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	2X	750	0	814	19	0
20	1Y	806	0	881	13	0
20	2Y	806	0	881	16	0
21	1Z	1240	0	1240	30	0
21	2Z	1271	0	1273	50	0
22	10	653	0	674	6	0
22	20	653	0	674	16	0
23	11	755	0	826	12	0
23	21	755	0	826	18	0
24	12	588	0	643	10	0
24	22	588	0	643	10	0
25	13	469	0	518	9	0
25	23	464	0	514	11	0
26	14	552	0	533	22	0
26	24	532	0	503	39	0
27	15	455	0	465	6	0
27	25	455	0	465	10	0
28	16	453	0	473	6	0
28	26	449	0	469	13	0
29	17	418	0	467	5	0
29	27	418	0	467	6	0
30	18	517	0	582	14	0
30	28	517	0	582	22	0
31	19	307	0	335	5	0
31	29	307	0	335	9	0
32	1a	32246	0	16294	379	0
32	2a	32327	0	16338	551	0
33	1b	1846	0	1867	65	0
33	2b	1825	0	1828	95	0
34	1c	1548	0	1535	36	0
34	2c	1542	0	1517	84	0
35	1d	1655	0	1672	45	0
35	2d	1674	0	1714	61	0
36	1e	1129	0	1185	31	0
36	2e	1133	0	1191	46	0
37	1f	810	0	804	14	0
37	2f	816	0	808	24	0
38	1g	1231	0	1238	12	0
38	2g	1235	0	1249	34	0
39	1h	1088	0	1126	22	0
39	2h	1088	0	1126	34	0
40	1i	983	0	986	28	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	2i	978	0	966	48	0
41	1j	709	0	650	18	0
41	2j	714	0	672	49	0
42	1k	829	0	825	13	0
42	2k	833	0	836	16	0
43	1l	932	0	981	16	0
43	2l	932	0	980	24	0
44	1m	958	0	1002	28	0
44	2m	950	0	988	45	0
45	1n	492	0	529	12	0
45	2n	492	0	529	26	0
46	1o	728	0	760	19	0
46	2o	728	0	760	20	0
47	1p	681	0	697	29	0
47	2p	677	0	686	16	0
48	1q	823	0	891	16	0
48	2q	823	0	891	16	0
49	1r	555	0	618	13	0
49	2r	555	0	618	22	0
50	1s	652	0	662	22	0
50	2s	646	0	644	53	0
51	1t	728	0	798	21	0
51	2t	727	0	796	16	0
52	1u	199	0	208	5	0
52	2u	199	0	208	8	0
53	1v	277	0	140	1	0
53	2v	277	0	140	4	0
54	1w	1592	0	818	15	0
54	1y	1585	0	803	35	0
54	2w	1544	0	787	26	0
54	2y	1565	0	794	24	0
55	1x	1625	0	829	16	0
55	2x	1625	0	829	22	0
56	10	8	0	0	0	0
56	11	4	0	0	0	0
56	12	2	0	0	0	0
56	13	6	0	0	0	0
56	15	4	0	0	0	0
56	16	2	0	0	0	0
56	17	4	0	0	0	0
56	18	7	0	0	0	0
56	19	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	1A	1139	0	0	0	0
56	1B	37	0	0	0	0
56	1D	13	0	0	0	0
56	1E	14	0	0	0	0
56	1F	13	0	0	0	0
56	1G	5	0	0	0	0
56	1I	1	0	0	0	0
56	1N	6	0	0	0	0
56	1O	6	0	0	0	0
56	1P	5	0	0	0	0
56	1Q	7	0	0	0	0
56	1R	3	0	0	0	0
56	1S	3	0	0	0	0
56	1T	4	0	0	0	0
56	1U	10	0	0	0	0
56	1V	7	0	0	0	0
56	1W	7	0	0	0	0
56	1X	5	0	0	0	0
56	1Y	4	0	0	0	0
56	1Z	3	0	0	0	0
56	1a	241	0	0	0	0
56	1b	2	0	0	0	0
56	1e	2	0	0	0	0
56	1f	2	0	0	0	0
56	1h	1	0	0	0	0
56	1l	2	0	0	0	0
56	1m	1	0	0	0	0
56	1n	1	0	0	0	0
56	1s	1	0	0	0	0
56	1t	1	0	0	0	0
56	1v	2	0	0	0	0
56	1w	9	0	0	0	0
56	1x	14	0	0	0	0
56	1y	2	0	0	0	0
56	20	3	0	0	0	0
56	21	2	0	0	0	0
56	23	2	0	0	0	0
56	25	5	0	0	0	0
56	26	1	0	0	0	0
56	27	4	0	0	0	0
56	28	3	0	0	0	0
56	2A	884	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	2B	20	0	0	0	0
56	2D	7	0	0	0	0
56	2E	6	0	0	0	0
56	2F	6	0	0	0	0
56	2G	1	0	0	0	0
56	2N	1	0	0	0	0
56	2O	2	0	0	0	0
56	2P	2	0	0	0	0
56	2Q	3	0	0	0	0
56	2R	3	0	0	0	0
56	2T	3	0	0	0	0
56	2U	2	0	0	0	0
56	2V	2	0	0	0	0
56	2W	2	0	0	0	0
56	2X	3	0	0	0	0
56	2Y	1	0	0	0	0
56	2Z	1	0	0	0	0
56	2a	240	0	0	0	0
56	2d	2	0	0	0	0
56	2e	1	0	0	0	0
56	2f	1	0	0	0	0
56	2g	1	0	0	0	0
56	2j	1	0	0	0	0
56	2k	1	0	0	0	0
56	2l	4	0	0	0	0
56	2m	1	0	0	0	0
56	2p	1	0	0	0	0
56	2q	2	0	0	0	0
56	2r	1	0	0	0	0
56	2t	1	0	0	0	0
56	2v	1	0	0	0	0
56	2w	9	0	0	0	0
56	2x	7	0	0	0	0
56	2y	7	0	0	0	0
57	14	1	0	0	0	0
57	15	1	0	0	0	0
57	16	1	0	0	0	0
57	19	1	0	0	0	0
57	1Y	1	0	0	0	0
57	1n	1	0	0	0	0
57	24	1	0	0	0	0
57	25	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	26	1	0	0	0	0
57	29	1	0	0	0	0
57	2Y	1	0	0	0	0
57	2n	1	0	0	0	0
58	1a	33	0	0	0	0
58	2a	33	0	0	0	0
59	1d	8	0	0	0	0
59	2d	8	0	0	0	0
60	1x	1	0	0	0	0
60	2A	1	0	0	0	0
61	10	13	0	0	1	0
61	11	11	0	0	0	0
61	12	4	0	0	0	0
61	13	3	0	0	0	0
61	14	2	0	0	0	0
61	15	8	0	0	0	0
61	16	1	0	0	0	0
61	17	9	0	0	1	0
61	18	11	0	0	0	0
61	1A	2188	0	0	82	0
61	1B	68	0	0	1	0
61	1D	33	0	0	2	0
61	1E	30	0	0	4	0
61	1F	18	0	0	1	0
61	1G	3	0	0	2	0
61	1H	2	0	0	0	0
61	1I	1	0	0	0	0
61	1N	8	0	0	1	0
61	1O	4	0	0	0	0
61	1P	20	0	0	1	0
61	1Q	10	0	0	0	0
61	1R	12	0	0	0	0
61	1S	6	0	0	0	0
61	1T	8	0	0	0	0
61	1U	17	0	0	1	0
61	1V	11	0	0	0	0
61	1W	8	0	0	0	0
61	1X	7	0	0	0	0
61	1Y	2	0	0	0	0
61	1Z	1	0	0	0	0
61	1a	498	0	0	27	0
61	1c	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6l	1d	1	0	0	0	0
6l	1e	4	0	0	0	0
6l	1f	1	0	0	0	0
6l	1g	3	0	0	0	0
6l	1i	1	0	0	0	0
6l	1j	1	0	0	0	0
6l	1l	8	0	0	0	0
6l	1m	1	0	0	0	0
6l	1n	1	0	0	0	0
6l	1o	1	0	0	0	0
6l	1p	1	0	0	0	0
6l	1q	3	0	0	0	0
6l	1u	1	0	0	0	0
6l	1v	7	0	0	0	0
6l	1w	14	0	0	0	0
6l	1x	19	0	0	3	0
6l	1y	1	0	0	0	0
6l	20	3	0	0	0	0
6l	21	8	0	0	0	0
6l	23	3	0	0	0	0
6l	25	1	0	0	0	0
6l	26	1	0	0	0	0
6l	27	3	0	0	0	0
6l	28	3	0	0	1	0
6l	29	1	0	0	0	0
6l	2A	1294	0	0	98	0
6l	2B	27	0	0	0	0
6l	2D	24	0	0	0	0
6l	2E	15	0	0	1	0
6l	2F	13	0	0	0	0
6l	2I	3	0	0	0	0
6l	2N	1	0	0	0	0
6l	2O	2	0	0	0	0
6l	2P	16	0	0	0	0
6l	2Q	2	0	0	0	0
6l	2R	3	0	0	0	0
6l	2T	6	0	0	0	0
6l	2U	4	0	0	0	0
6l	2W	3	0	0	1	0
6l	2X	2	0	0	0	0
6l	2Y	1	0	0	0	0
6l	2Z	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	2a	296	0	0	17	0
61	2c	1	0	0	0	0
61	2d	2	0	0	0	0
61	2e	1	0	0	0	0
61	2f	1	0	0	0	0
61	2j	3	0	0	1	0
61	2l	4	0	0	0	0
61	2n	1	0	0	0	0
61	2p	2	0	0	1	0
61	2r	1	0	0	0	0
61	2t	2	0	0	0	0
61	2v	1	0	0	0	0
61	2w	4	0	0	0	0
61	2x	5	0	0	1	0
61	2y	15	0	0	0	0
All	All	300806	0	196685	4225	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 9.

All (4225) 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)
1:1A:1082:U:H3	1:1A:1086:A:N6	1.29	1.29
10:2O:48:PRO:HB3	32:2a:1422:G:H5''	1.41	1.02
32:1a:1002:G:H3'	32:1a:1003:G:H4'	1.49	0.94
1:1A:1082:U:O4	1:1A:1086:A:N1	2.03	0.92
38:2g:78:ARG:HD3	38:2g:79:ARG:H	1.34	0.92
54:2y:55:PSU:HN1	54:2y:57:G:H5''	1.34	0.91
1:1A:2427:C:OP1	61:1A:4209:HOH:O	1.88	0.91
1:1A:2683:C:O2	10:1O:70:LYS:NZ	2.04	0.90
2:2B:7:G:H21	14:2S:38:GLN:HE22	1.17	0.90
1:1A:1062:G:H1	1:1A:1077:A:H61	1.19	0.88
54:2y:18:G:N2	54:2y:55:PSU:N3	2.22	0.88
37:1f:94:GLN:HG2	49:1r:32:ARG:HD3	1.55	0.87
32:2a:1002:G:H1	32:2a:1038:C:H42	1.21	0.86
32:1a:1027:C:C2	32:1a:1034:G:N2	2.44	0.85
42:1k:99:GLN:HG2	42:1k:105:VAL:HG11	1.60	0.84
32:2a:978:A:O2'	32:2a:1321:C:N4	2.09	0.84
54:1y:19:G:N2	54:1y:56:C:N3	2.27	0.83
1:2A:1204:A:H2	1:2A:1241:A:H62	1.25	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2406:U:OP1	61:2A:3904:HOH:O	1.97	0.82
1:2A:783:A:OP2	61:2A:3905:HOH:O	1.97	0.82
17:1V:55:ALA:HA	17:1V:101:GLY:HA2	1.61	0.81
1:1A:2499:C:OP1	61:1A:4210:HOH:O	1.99	0.81
1:2A:1772:G:OP1	61:2A:3906:HOH:O	1.98	0.81
1:1A:2028:U:O4	61:1A:4211:HOH:O	1.99	0.81
1:2A:2807:G:N1	1:2A:2893:G:O6	2.11	0.81
49:2r:25:THR:O	49:2r:42:ARG:NH1	2.15	0.80
1:1A:826:U:OP1	61:1A:4209:HOH:O	1.99	0.80
36:1e:69:VAL:HG12	36:1e:139:LEU:HB3	1.62	0.80
19:2X:35:THR:HG22	19:2X:38:GLU:H	1.46	0.80
4:1E:119:ARG:HD2	4:1E:160:TYR:HB2	1.64	0.80
1:2A:1264:G:OP1	27:25:19:ARG:NH2	2.15	0.79
11:1P:125:VAL:HG21	11:1P:138:LEU:HD21	1.63	0.79
32:2a:559:A:OP1	36:2e:126:ARG:NH2	2.16	0.79
11:1P:42:SER:O	61:1P:301:HOH:O	2.00	0.79
32:2a:772:U:O5'	61:2a:1903:HOH:O	2.00	0.79
6:2G:127:GLY:N	6:2G:166:ASP:OD1	2.11	0.79
32:2a:617:G:OP2	61:2a:1904:HOH:O	2.00	0.79
32:2a:1106:G:H5''	34:2c:172:ARG:HB3	1.63	0.79
41:2j:35:SER:HB3	41:2j:73:ASP:HB2	1.65	0.79
5:2F:21:ALA:HB3	5:2F:22:ALA:HA	1.65	0.78
33:1b:69:LEU:HB3	33:1b:162:ILE:HG22	1.65	0.78
1:2A:731:C:OP1	61:2A:3907:HOH:O	2.01	0.78
1:2A:1798:U:H5'	3:2D:259:THR:HG22	1.65	0.78
1:1A:1185:C:OP2	61:1A:4212:HOH:O	2.01	0.78
11:2P:126:VAL:HG12	11:2P:148:LEU:HD22	1.65	0.78
54:2y:18:G:H22	54:2y:55:PSU:HN3	1.30	0.78
40:1i:48:GLU:HA	40:1i:51:ARG:HD3	1.66	0.77
1:2A:1689:A:H62	1:2A:1698:A:H2	1.33	0.77
50:2s:28:LYS:HB3	50:2s:29:ARG:HA	1.64	0.77
41:1j:5:ARG:NH2	41:1j:73:ASP:OD2	2.18	0.77
1:2A:1019:U:H3	1:2A:1142(A):A:H62	1.32	0.77
3:2D:106:ILE:HD11	3:2D:144:ALA:HB2	1.66	0.77
41:2j:49:VAL:HG23	45:2n:41:ARG:HB2	1.67	0.77
32:2a:1271:G:N2	32:2a:1272:G:N7	2.32	0.77
41:2j:98:ILE:O	61:2j:302:HOH:O	2.02	0.77
40:2i:46:ALA:HB2	40:2i:74:ILE:HG23	1.67	0.77
53:2v:23:A:H4'	53:2v:24:A:H5'	1.67	0.77
1:1A:1452:A:OP2	61:1A:4213:HOH:O	2.01	0.77
33:2b:52:GLU:HG2	33:2b:56:ARG:HH12	1.49	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:981:A:OP1	61:2A:3908:HOH:O	2.02	0.76
1:1A:2100:G:H1	1:1A:2189:U:H3	1.33	0.76
4:1E:28:ALA:HB3	4:1E:93:VAL:HG12	1.67	0.76
1:1A:1890:A:OP2	61:1A:4214:HOH:O	2.03	0.76
1:1A:2163:C:OP1	1:1A:2165:G:N2	2.18	0.76
1:1A:2206:G:H3'	1:1A:2207:G:C8	2.21	0.76
1:2A:962:G:OP1	61:2A:3909:HOH:O	2.04	0.76
7:2H:3:ARG:HD3	7:2H:6:ARG:HH21	1.51	0.76
43:2l:32:PHE:HB3	43:2l:84:LEU:HD11	1.68	0.76
43:1l:71:PRO:O	43:1l:102:ARG:NH1	2.17	0.76
6:2G:29:TRP:O	6:2G:33:ARG:NH2	2.19	0.76
1:1A:2749:A:H5''	7:1H:3:ARG:HH12	1.50	0.76
1:2A:948:G:OP1	61:2A:3909:HOH:O	2.03	0.76
33:1b:87:ARG:NH2	33:1b:220:ASP:OD1	2.19	0.75
55:1x:58:A:OP2	61:1x:201:HOH:O	2.03	0.75
1:2A:583:G:N7	61:2A:3960:HOH:O	2.18	0.75
14:2S:38:GLN:NE2	14:2S:47:THR:OG1	2.19	0.75
19:2X:8:ILE:O	24:22:36:ARG:NH2	2.18	0.75
21:2Z:55:HIS:HE1	21:2Z:135:GLU:HB2	1.51	0.75
1:1A:256:A:OP2	61:1A:4216:HOH:O	2.04	0.75
32:1a:1314:C:OP2	50:1s:4:SER:OG	2.05	0.75
44:1m:12:ASN:O	44:1m:44:ARG:NH1	2.20	0.75
1:2A:938:G:OP2	30:28:52:LYS:NZ	2.16	0.75
54:1y:19:G:N1	54:1y:56:C:N4	2.34	0.75
7:2H:51:ARG:NH1	7:2H:53:GLU:OE2	2.19	0.75
32:2a:673:G:H2'	32:2a:674:G:C8	2.21	0.75
32:2a:1278:U:H5'	32:2a:1279:A:H5'	1.69	0.75
1:1A:1082:U:N3	1:1A:1086:A:N6	2.05	0.75
1:1A:1602:U:O4	61:1A:4217:HOH:O	2.05	0.75
1:1A:1670:C:OP2	61:1A:4215:HOH:O	2.04	0.75
54:2y:5:G:H1	54:2y:68:C:H42	1.34	0.75
17:2V:55:ALA:HA	17:2V:101:GLY:HA2	1.68	0.74
1:1A:880:G:H2'	1:1A:881:G:H8	1.50	0.74
1:2A:2589:A:OP1	61:2A:3905:HOH:O	2.05	0.74
26:24:48:ARG:NH1	26:24:51:ASP:O	2.21	0.74
32:1a:1025:U:O2	32:1a:1036:G:O6	2.06	0.74
40:1i:26:VAL:HG13	40:1i:61:ALA:HB3	1.69	0.74
4:2E:127:ASP:OD2	61:2E:401:HOH:O	2.05	0.74
5:2F:53:THR:HG23	5:2F:55:GLY:H	1.52	0.74
32:2a:1187:G:OP1	40:2i:113:LYS:NZ	2.21	0.74
26:24:34:GLU:HB3	44:2m:57:ARG:HH21	1.51	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1840:G:N7	61:1A:4260:HOH:O	2.20	0.74
1:2A:988:A:N7	61:2A:3971:HOH:O	2.21	0.74
33:2b:178:ARG:HH12	39:2h:68:ARG:HH22	1.34	0.74
2:2B:75:G:N2	21:2Z:87:ASP:OD1	2.21	0.74
41:2j:89:ASP:OD1	41:2j:89:ASP:N	2.19	0.74
1:2A:1434:A:H61	1:2A:1558:A:H62	1.34	0.73
1:2A:963:U:OP2	61:2A:3909:HOH:O	2.07	0.73
1:2A:1783:A:OP1	61:2A:3914:HOH:O	2.07	0.73
32:1a:557:G:OP1	61:1a:1902:HOH:O	2.06	0.73
1:2A:1253:A:OP1	61:2A:3910:HOH:O	2.05	0.73
1:2A:2748:A:H5'	7:2H:4:ILE:HD12	1.68	0.73
54:2w:19:G:H1	54:2w:56:C:H42	1.37	0.73
8:2I:50:ARG:O	8:2I:54:GLN:N	2.20	0.73
32:2a:1104:G:H4'	33:2b:111:ARG:HH21	1.54	0.73
1:1A:2550:G:OP1	61:1A:4215:HOH:O	2.05	0.73
1:1A:2629:A:O2'	1:1A:2630:G:OP2	2.04	0.73
1:2A:1335:U:O4	61:2A:3916:HOH:O	2.07	0.73
6:1G:3:LEU:O	6:1G:8:LYS:NZ	2.22	0.73
36:1e:78:HIS:HE1	36:1e:143:ARG:H	1.37	0.73
32:2a:975:A:H4'	32:2a:976:G:H5''	1.69	0.73
1:2A:1890:A:OP2	61:2A:3912:HOH:O	2.06	0.73
1:2A:2677:G:N3	61:2A:3982:HOH:O	2.22	0.73
26:24:58:ARG:HD3	50:2s:68:GLY:H	1.53	0.73
14:1S:25:ARG:NH1	14:1S:42:ASP:OD1	2.21	0.72
1:2A:994:C:OP1	16:2U:53:ARG:NH2	2.21	0.72
32:2a:1226:C:OP2	44:2m:91:ARG:NH1	2.20	0.72
35:2d:15:GLU:OE2	35:2d:66:ARG:NH1	2.22	0.72
34:2c:120:VAL:HG11	34:2c:137:ALA:HB2	1.70	0.72
1:2A:2206:G:H3'	1:2A:2207:G:C8	2.25	0.72
1:1A:602:G:O2'	1:1A:655:A:N6	2.22	0.72
3:1D:242:ARG:O	61:1D:401:HOH:O	2.07	0.72
1:2A:975:C:OP1	61:2A:3911:HOH:O	2.06	0.72
34:2c:41:GLY:O	34:2c:45:LYS:NZ	2.22	0.72
32:1a:116:A:OP1	61:1a:1904:HOH:O	2.07	0.72
34:1c:58:GLU:HB3	41:1j:92:THR:HG21	1.70	0.72
12:2Q:85:LYS:HG2	22:20:7:LEU:HB3	1.69	0.72
40:2i:16:ARG:HB2	40:2i:64:THR:HG22	1.72	0.72
1:1A:2723:C:OP1	13:1R:3:HIS:ND1	2.19	0.72
1:2A:1670:C:OP1	61:2A:3913:HOH:O	2.06	0.72
1:2A:2499:C:OP2	61:2A:3915:HOH:O	2.07	0.72
1:2A:1648:C:OP1	61:2A:3919:HOH:O	2.08	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:29:25:VAL:HB	31:29:34:GLN:HB2	1.71	0.72
32:2a:664:G:H22	32:2a:741:G:H1	1.38	0.72
1:1A:2014:A:OP2	61:1A:4218:HOH:O	2.07	0.72
3:2D:108:PRO:HD2	3:2D:111:LEU:HD22	1.72	0.72
4:2E:47:VAL:HG11	4:2E:86:PRO:HD2	1.72	0.72
1:2A:1647:G:OP1	61:2A:3919:HOH:O	2.08	0.71
32:2a:953:G:H5'	32:2a:965:A:H61	1.53	0.71
32:1a:1230:C:OP2	61:1a:1903:HOH:O	2.06	0.71
32:1a:1505:G:OP2	61:1a:1907:HOH:O	2.08	0.71
1:2A:2285:C:OP2	28:26:6:ARG:NH1	2.23	0.71
1:2A:2595:G:N7	61:2A:3984:HOH:O	2.23	0.71
1:1A:956:G:O6	61:1A:4219:HOH:O	2.08	0.71
1:2A:450:G:O6	61:2A:3920:HOH:O	2.08	0.71
1:2A:2110:G:H3'	1:2A:2111:C:H5'	1.71	0.71
7:2H:11:VAL:HG13	7:2H:15:VAL:HG22	1.72	0.71
32:2a:117:G:OP2	61:2a:1905:HOH:O	2.09	0.71
1:2A:2576:G:OP1	61:2A:3921:HOH:O	2.08	0.71
32:2a:1347:G:H5''	40:2i:107:ARG:HB3	1.71	0.71
1:1A:2702:U:OP2	61:1A:4221:HOH:O	2.08	0.71
34:1c:6:HIS:HD2	34:1c:8:ILE:H	1.38	0.71
1:1A:2531:A:OP1	61:1A:4220:HOH:O	2.08	0.71
32:1a:693:G:OP2	61:1a:1906:HOH:O	2.08	0.71
32:1a:1255:G:N7	41:1j:43:ARG:NH2	2.39	0.71
1:2A:822:U:OP2	61:2A:3918:HOH:O	2.07	0.71
1:2A:2625:G:O6	61:2A:3923:HOH:O	2.09	0.71
35:2d:173:TRP:CD2	35:2d:189:PRO:HB3	2.26	0.71
2:1B:103:G:H21	21:1Z:73:GLN:HE22	1.39	0.71
32:1a:711:G:OP1	37:1f:54:LYS:NZ	2.24	0.71
32:1a:892:A:OP2	61:1a:1905:HOH:O	2.08	0.71
12:1Q:111:GLU:OE2	12:1Q:133:ARG:NH2	2.23	0.71
36:1e:110:LEU:HD13	36:1e:118:ILE:HG21	1.72	0.71
1:2A:2785:C:OP1	4:2E:41:LYS:NZ	2.23	0.71
32:2a:1029:C:N3	32:2a:1032:G:N2	2.39	0.71
43:2l:71:PRO:O	43:2l:102:ARG:NH1	2.24	0.71
32:1a:353:A:N7	61:1a:1927:HOH:O	2.24	0.71
32:1a:812:C:N3	61:1a:1925:HOH:O	2.23	0.71
32:1a:975:A:H4'	32:1a:976:G:H5''	1.72	0.71
32:2a:1272:G:N2	32:2a:1273:G:N7	2.39	0.71
35:2d:153:ARG:HE	35:2d:181:MET:HG3	1.56	0.71
20:1Y:87:LYS:HG3	20:1Y:95:LYS:HD3	1.73	0.71
1:2A:1568:G:N7	61:2A:3983:HOH:O	2.22	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1603:A:OP1	61:2A:3917:HOH:O	2.07	0.71
1:2A:1671:U:OP2	61:2A:3913:HOH:O	2.09	0.71
32:2a:11:G:H1	32:2a:23:C:H42	1.39	0.71
1:1A:387:U:O4	61:1A:4225:HOH:O	2.09	0.70
10:1O:48:PRO:HB3	32:1a:1422:G:H5''	1.73	0.70
39:1h:34:GLU:OE1	39:1h:37:ARG:NH1	2.24	0.70
1:2A:1271:G:OP2	61:2A:3919:HOH:O	2.08	0.70
1:2A:2637:U:OP1	4:2E:82:ARG:NH1	2.24	0.70
26:14:55:ARG:N	26:14:56:VAL:HA	2.06	0.70
26:24:8:LYS:NZ	26:24:9:LEU:O	2.22	0.70
1:2A:1604:C:OP1	61:2A:3922:HOH:O	2.08	0.70
32:2a:1295:G:O2'	44:2m:14:ARG:NH1	2.24	0.70
1:1A:1300:U:H4'	1:1A:1301:A:H5''	1.73	0.70
32:1a:953:G:H5'	32:1a:965:A:H61	1.56	0.70
11:2P:50:ARG:HD3	30:28:7:HIS:CD2	2.25	0.70
1:2A:955:C:OP1	12:2Q:87:LYS:NZ	2.22	0.70
25:13:39:ASP:OD1	25:13:44:ARG:NH1	2.24	0.70
1:2A:2431:U:OP1	61:2A:3926:HOH:O	2.10	0.70
6:1G:45:GLU:OE2	61:1G:301:HOH:O	2.08	0.70
33:1b:185:ILE:HG22	33:1b:199:TYR:HB2	1.74	0.70
34:2c:88:ARG:HA	34:2c:91:LEU:HD13	1.74	0.70
1:1A:1622:G:OP2	61:1A:4223:HOH:O	2.08	0.70
1:1A:2322:A:OP2	61:1A:4222:HOH:O	2.08	0.70
20:1Y:102:CYS:SG	20:1Y:103:GLY:N	2.63	0.70
32:1a:664:G:H22	32:1a:741:G:H1	1.38	0.70
1:2A:331:A:N3	61:2A:3998:HOH:O	2.25	0.70
1:2A:1356:G:OP1	61:2A:3928:HOH:O	2.10	0.70
1:2A:1420:U:O2'	1:2A:1421:G:OP1	2.09	0.70
3:2D:12:SER:HB3	3:2D:208:LYS:HB3	1.73	0.70
1:1A:120:U:OP2	61:1A:4224:HOH:O	2.09	0.70
1:2A:2602:A:N6	54:2w:76:A:OP2	2.24	0.70
32:1a:542:G:OP1	35:1d:10:ARG:NH2	2.24	0.69
1:2A:2206:G:H3'	1:2A:2207:G:H8	1.57	0.69
32:2a:1216:G:H5''	45:2n:5:ALA:HB2	1.74	0.69
33:2b:69:LEU:HB3	33:2b:162:ILE:HG22	1.73	0.69
41:2j:44:VAL:HG22	41:2j:66:ARG:HG2	1.72	0.69
8:1I:93:THR:H	8:1I:96:ASP:HB2	1.56	0.69
21:1Z:132:ASN:HD22	21:1Z:160:GLY:HA3	1.57	0.69
32:1a:1086:U:H3	32:1a:1099:G:H22	1.40	0.69
1:2A:1024:G:OP2	61:2A:3924:HOH:O	2.09	0.69
1:2A:1973:G:OP1	61:2A:3925:HOH:O	2.09	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1H:124:GLU:HB2	7:1H:132:ARG:HB3	1.73	0.69
33:2b:27:LYS:HB2	33:2b:194:PRO:HD2	1.74	0.69
32:1a:505:G:N7	61:1a:1932:HOH:O	2.26	0.69
37:1f:10:LEU:HD23	37:1f:61:LEU:HD13	1.75	0.69
1:2A:1622:G:OP2	61:2A:3927:HOH:O	2.10	0.69
1:1A:998:C:OP1	61:1A:4226:HOH:O	2.10	0.69
26:24:24:THR:OG1	26:24:25:TYR:N	2.25	0.69
33:2b:165:VAL:HA	33:2b:187:LEU:HB3	1.75	0.69
48:2q:66:SER:HB3	48:2q:69:LYS:HB2	1.74	0.69
32:1a:1228:C:OP1	44:1m:115:LYS:NZ	2.25	0.69
32:1a:1356:G:H2'	32:1a:1357:A:C8	2.27	0.69
32:1a:1500:A:OP2	61:1a:1908:HOH:O	2.10	0.69
1:2A:740:U:OP2	61:2A:3914:HOH:O	2.10	0.69
1:2A:1226:A:OP1	17:2V:84:LYS:NZ	2.19	0.69
8:2I:3:VAL:HG12	8:2I:38:LEU:HA	1.73	0.69
32:2a:113:G:H1'	32:2a:354:G:H5'	1.74	0.69
32:2a:1002:G:H1	32:2a:1038:C:N4	1.91	0.69
1:1A:272(J):C:H2'	1:1A:274:G:H8	1.58	0.69
3:1D:37:LEU:HD12	3:1D:62:TYR:HB2	1.75	0.69
8:1I:129:THR:HG22	8:1I:139:GLN:HE22	1.58	0.69
1:2A:2010:G:H5''	18:2W:42:ARG:HB2	1.73	0.69
1:2A:2206:G:H5''	1:2A:2207:G:N7	2.08	0.69
44:2m:80:ARG:HH22	50:2s:69:HIS:HE1	1.41	0.69
46:2o:29:VAL:HG21	46:2o:81:LEU:HD21	1.73	0.69
1:1A:1647:G:OP1	61:1A:4229:HOH:O	2.11	0.69
24:12:65:ASN:OD1	24:12:69:ARG:NH1	2.25	0.69
44:1m:3:ARG:HD2	44:1m:9:ILE:HG12	1.74	0.69
34:2c:6:HIS:CE1	34:2c:8:ILE:HB	2.28	0.69
1:1A:884:C:H42	1:1A:892:G:H1	1.40	0.68
1:2A:568:U:O4	61:2A:3929:HOH:O	2.10	0.68
1:2A:2183:C:H2'	1:2A:2184:G:H8	1.57	0.68
32:2a:407:G:OP1	35:2d:115:ARG:NH2	2.26	0.68
32:2a:770:C:OP1	61:2a:1906:HOH:O	2.11	0.68
32:1a:613:C:H2'	32:1a:614:A:H8	1.57	0.68
32:2a:737:A:H1'	37:2f:73:ASN:HD21	1.57	0.68
1:2A:2292:C:OP1	14:2S:17:ARG:NH2	2.26	0.68
1:2A:2365:G:N7	30:28:39:LYS:NZ	2.41	0.68
33:2b:88:ALA:HB2	33:2b:219:VAL:HG13	1.75	0.68
1:1A:1991:U:H2'	1:1A:1992:G:H5''	1.75	0.68
8:2I:130:TYR:HB3	8:2I:138:ILE:HB	1.75	0.68
1:1A:588:U:OP2	61:1A:4227:HOH:O	2.10	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:23:6:VAL:HG13	25:23:56:VAL:HG22	1.74	0.68
46:1o:54:ARG:HG2	46:1o:58:MET:HE2	1.76	0.68
1:2A:449:A:OP2	61:2A:3935:HOH:O	2.12	0.68
1:2A:2782:G:OP2	61:2A:3931:HOH:O	2.11	0.68
24:22:1:MET:HE3	24:22:6:VAL:HG22	1.75	0.68
1:1A:1811:G:N7	61:1A:4295:HOH:O	2.27	0.68
1:1A:2552:OMU:OP2	61:1A:4234:HOH:O	2.12	0.68
1:2A:2606:C:O2'	61:2A:3930:HOH:O	2.11	0.68
32:2a:266:G:H5''	32:2a:268:C:H41	1.58	0.68
32:2a:663:A:O3'	49:2r:64:ARG:NH2	2.24	0.68
1:1A:947:G:OP2	61:1A:4228:HOH:O	2.10	0.68
1:1A:1105:U:H2'	1:1A:1106:G:C8	2.29	0.68
54:1y:8:4SU:O2'	54:1y:21:A:N1	2.26	0.68
1:2A:1812:A:OP2	61:2A:3933:HOH:O	2.11	0.68
1:2A:2218:U:O2	23:21:52:ARG:NH1	2.27	0.68
24:22:1:MET:N	24:22:52:ASP:OD1	2.23	0.68
32:2a:1128:C:H1'	32:2a:1147:C:H42	1.58	0.68
5:1F:157:VAL:HB	5:1F:194:MET:HG2	1.76	0.68
1:2A:2166:G:H3'	1:2A:2167:U:H5''	1.74	0.68
1:2A:2345:G:H4'	1:2A:2346:A:H5''	1.76	0.68
34:2c:6:HIS:ND1	45:2n:49:HIS:HB3	2.09	0.68
39:2h:116:LYS:HD3	39:2h:127:LEU:HD13	1.76	0.68
32:1a:972:C:O2'	41:1j:55:LYS:O	2.11	0.67
33:1b:80:ILE:HD13	33:1b:211:ILE:HG22	1.76	0.67
36:1e:81:GLU:HG2	36:1e:90:VAL:HG22	1.77	0.67
1:2A:297:C:OP2	61:2A:3934:HOH:O	2.11	0.67
1:2A:1593:G:H2'	1:2A:1594:G:C8	2.29	0.67
35:2d:149:ALA:HB3	35:2d:152:SER:HB2	1.76	0.67
32:1a:1198:G:OP1	61:1a:1909:HOH:O	2.13	0.67
42:1k:48:ILE:HD12	42:1k:63:LEU:HB2	1.75	0.67
32:2a:562:C:H1'	43:2l:15:ARG:HB3	1.75	0.67
40:1i:9:ARG:HG3	40:1i:14:VAL:HG13	1.76	0.67
1:2A:2502:G:N7	61:2A:4013:HOH:O	2.27	0.67
21:2Z:53:ILE:HG22	21:2Z:71:VAL:HB	1.75	0.67
32:2a:950:U:H3	32:2a:1231:G:H1	1.40	0.67
33:2b:189:ASP:OD1	33:2b:189:ASP:N	2.24	0.67
41:2j:51:ARG:O	45:2n:45:ARG:NH1	2.26	0.67
42:2k:22:HIS:HB3	42:2k:29:ILE:HB	1.75	0.67
1:1A:1269:A:OP2	61:1A:4230:HOH:O	2.11	0.67
1:1A:1418:G:OP2	61:1A:4232:HOH:O	2.12	0.67
32:1a:184:G:H2'	32:1a:185:A:H8	1.59	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:249:C:O2	30:28:12:LYS:NZ	2.23	0.67
1:2A:1344:G:N7	61:2A:4015:HOH:O	2.27	0.67
1:2A:1607:C:N4	1:2A:1622:G:OP2	2.27	0.67
32:2a:656:C:O2'	46:2o:28:GLN:OE1	2.10	0.67
3:1D:12:SER:HB3	3:1D:208:LYS:HB3	1.77	0.67
32:1a:642:A:N3	39:1h:113:SER:OG	2.26	0.67
49:1r:38:GLU:HA	49:1r:41:LYS:HE2	1.76	0.67
1:2A:599:G:N7	61:2A:4016:HOH:O	2.27	0.67
1:1A:1077:A:H2'	1:1A:1078:U:H4'	1.76	0.67
9:1N:73:THR:HB	9:1N:82:LEU:HD11	1.75	0.67
1:2A:1780:A:OP1	61:2A:3938:HOH:O	2.13	0.67
1:1A:855:G:N7	61:1A:4305:HOH:O	2.28	0.67
1:1A:1013:C:OP2	61:1A:4233:HOH:O	2.12	0.67
1:2A:852:G:H2'	1:2A:853:G:H8	1.60	0.67
1:2A:2064:C:OP2	61:2A:3936:HOH:O	2.12	0.67
11:2P:121:LYS:HB3	11:2P:123:LEU:HD13	1.77	0.67
1:1A:1669:A:OP2	61:1A:4215:HOH:O	2.12	0.66
32:1a:92:C:H2'	32:1a:93:G:C8	2.30	0.66
55:1x:12:G:OP2	61:1x:202:HOH:O	2.12	0.66
54:1y:7:A:O2'	54:1y:49:C:OP2	2.11	0.66
36:2e:89:ILE:HG12	36:2e:135:THR:HG22	1.77	0.66
32:1a:1139:G:H4'	32:1a:1140:C:H5'	1.77	0.66
32:2a:974:A:OP2	45:2n:29:ARG:NH2	2.27	0.66
48:2q:66:SER:O	48:2q:70:ARG:NH1	2.29	0.66
34:1c:153:VAL:HG22	34:1c:198:VAL:HG13	1.77	0.66
32:2a:21:G:OP1	61:2a:1907:HOH:O	2.12	0.66
1:2A:574:C:OP1	61:2A:3937:HOH:O	2.12	0.66
7:2H:9:ILE:HB	7:2H:50:VAL:HB	1.78	0.66
2:1B:8:U:O3'	14:1S:25:ARG:NH2	2.28	0.66
1:2A:120:U:OP2	61:2A:3947:HOH:O	2.14	0.66
1:2A:1653:G:H3'	13:2R:2:ARG:HD3	1.78	0.66
7:2H:3:ARG:NH2	7:2H:5:GLY:H	1.94	0.66
41:2j:38:ILE:HG13	41:2j:71:LEU:HB3	1.77	0.66
33:1b:77:ALA:HB2	33:1b:211:ILE:HD13	1.77	0.66
35:1d:7:PRO:HB2	35:1d:10:ARG:HD2	1.77	0.66
41:1j:35:SER:HB3	41:1j:73:ASP:HB2	1.77	0.66
43:1l:117:ARG:HB3	43:1l:122:THR:HB	1.78	0.66
34:2c:37:GLN:NE2	45:2n:52:GLN:OE1	2.20	0.66
1:1A:2067:G:N7	61:1A:4304:HOH:O	2.28	0.66
1:1A:2430:A:OP1	61:1A:4237:HOH:O	2.13	0.66
11:1P:91:PHE:O	11:1P:121:LYS:NZ	2.28	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:376:G:H5''	47:1p:5:ARG:HG2	1.78	0.66
34:2c:125:GLU:O	34:2c:190:ARG:NH2	2.29	0.66
1:1A:2819:G:OP1	61:1A:4241:HOH:O	2.14	0.66
8:1I:92:VAL:HG11	8:1I:144:VAL:HG11	1.78	0.66
46:1o:29:VAL:HG21	46:1o:81:LEU:HD21	1.78	0.66
1:2A:744:G:OP1	61:2A:3941:HOH:O	2.13	0.66
1:2A:2404:C:O3'	11:2P:77:ARG:NH2	2.29	0.66
26:24:16:CYS:SG	26:24:17:GLY:N	2.68	0.66
32:2a:977:A:O2'	32:2a:981:U:N3	2.28	0.66
1:2A:2062:A:OP1	61:2A:3940:HOH:O	2.13	0.66
2:2B:24:G:N3	2:2B:26:A:N6	2.44	0.66
40:2i:128:ARG:NH2	55:2x:33:U:OP2	2.28	0.66
32:1a:803:G:OP1	61:1a:1912:HOH:O	2.14	0.65
1:2A:397:G:N7	61:2A:4020:HOH:O	2.28	0.65
15:2T:92:GLY:O	15:2T:120:ARG:NH2	2.28	0.65
32:2a:1029:C:N4	32:2a:1032:G:N1	2.44	0.65
42:2k:34:ASP:HB3	42:2k:40:ILE:HD11	1.78	0.65
32:1a:567:G:N3	61:1a:1935:HOH:O	2.28	0.65
46:1o:39:LEU:HD13	46:1o:56:LEU:HB2	1.78	0.65
1:2A:1784:A:OP2	61:2A:3914:HOH:O	2.14	0.65
21:2Z:33:LEU:HD21	21:2Z:90:VAL:HG21	1.77	0.65
35:2d:148:VAL:HG11	35:2d:181:MET:HE3	1.77	0.65
6:1G:122:PRO:HG3	6:1G:182:LYS:H	1.58	0.65
1:2A:827:U:OP1	61:2A:3945:HOH:O	2.14	0.65
1:2A:1830:C:OP2	61:2A:3943:HOH:O	2.14	0.65
1:2A:2224:G:OP1	3:2D:268:ARG:NE	2.30	0.65
1:2A:2396:G:O2'	61:2A:3953:HOH:O	2.15	0.65
3:2D:71:ASP:HB2	3:2D:103:ARG:HH12	1.60	0.65
8:2I:69:LYS:HZ3	8:2I:138:ILE:HG12	1.61	0.65
32:2a:393:A:OP1	61:2a:1908:HOH:O	2.14	0.65
32:2a:1029:C:C4	32:2a:1032:G:N1	2.64	0.65
1:1A:248:G:OP1	61:1A:4236:HOH:O	2.13	0.65
32:1a:836:G:OP1	49:1r:61:LYS:NZ	2.21	0.65
32:1a:1054:C:OP1	61:1a:1913:HOH:O	2.14	0.65
32:1a:1435:G:H2'	32:1a:1436:U:C6	2.31	0.65
34:1c:71:ALA:HA	34:1c:106:VAL:HG21	1.77	0.65
47:1p:22:THR:HA	47:1p:33:ILE:HD12	1.78	0.65
9:2N:123:TYR:OH	9:2N:130:HIS:NE2	2.29	0.65
28:26:23:THR:OG1	28:26:24:GLU:N	2.24	0.65
1:1A:2090:G:N7	61:1A:4313:HOH:O	2.30	0.65
1:2A:854:G:H2'	1:2A:855:G:H8	1.60	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:2T:117:ASP:OD2	15:2T:120:ARG:NE	2.26	0.65
34:1c:66:VAL:HG23	34:1c:101:LEU:HA	1.77	0.65
54:1w:51:U:H2'	54:1w:52:G:C8	2.32	0.65
1:2A:994:C:O2'	1:2A:996:A:OP1	2.14	0.65
1:2A:2592:G:OP1	61:2A:3939:HOH:O	2.13	0.65
5:2F:167:ALA:HB1	5:2F:173:VAL:HG11	1.79	0.65
17:2V:62:LEU:HD11	17:2V:95:LEU:HB2	1.78	0.65
26:24:61:ARG:HG2	50:2s:42:PRO:HG3	1.78	0.65
32:2a:1194:U:H4'	36:2e:22:GLY:HA3	1.77	0.65
1:1A:2290:G:OP2	61:1A:4239:HOH:O	2.14	0.65
32:1a:1118:C:OP1	40:1i:9:ARG:NH1	2.29	0.65
32:1a:1500:A:OP1	61:1a:1910:HOH:O	2.14	0.65
50:1s:43:GLU:OE1	50:1s:43:GLU:N	2.29	0.65
1:2A:1973:G:OP2	61:2A:3950:HOH:O	2.14	0.65
1:2A:2273:A:H2'	1:2A:2274:A:C8	2.31	0.65
2:2B:7:G:H21	14:2S:38:GLN:NE2	1.94	0.65
5:1F:185:ASP:HA	5:1F:188:ARG:HD3	1.78	0.65
50:1s:49:ILE:HG13	50:1s:62:ILE:HD11	1.78	0.65
32:2a:1239:A:H62	32:2a:1299:A:H62	1.44	0.65
32:2a:1317:C:O2	50:2s:37:ARG:NH2	2.29	0.65
54:2w:7:A:O2'	54:2w:49:C:O4'	2.14	0.65
1:1A:1023:U:OP2	61:1A:4240:HOH:O	2.14	0.65
1:1A:1800:C:OP1	3:1D:260:ARG:NH2	2.30	0.65
32:2a:501:C:H2'	32:2a:502:G:H8	1.62	0.65
1:1A:376:C:OP1	61:1A:4243:HOH:O	2.15	0.64
17:1V:14:VAL:HB	17:1V:96:ILE:HG13	1.78	0.64
1:2A:400:G:N7	61:2A:4035:HOH:O	2.29	0.64
1:2A:2099:U:H3	1:2A:2190:G:H1	1.45	0.64
1:2A:2577:A:OP1	61:2A:3921:HOH:O	2.14	0.64
33:2b:58:ILE:HA	33:2b:61:LEU:HB3	1.79	0.64
33:2b:80:ILE:HD13	33:2b:211:ILE:HG23	1.79	0.64
33:1b:30:ARG:HH21	33:1b:194:PRO:HB2	1.61	0.64
1:2A:131:G:OP1	61:2A:3952:HOH:O	2.15	0.64
1:2A:1316:U:H2'	1:2A:1317:A:H8	1.62	0.64
24:22:29:LYS:HG2	24:22:57:ILE:HD13	1.79	0.64
32:1a:310:G:OP2	47:1p:27:LYS:NZ	2.30	0.64
32:1a:376:G:O3'	47:1p:5:ARG:NH1	2.30	0.64
1:2A:2319:G:H22	14:2S:3:ARG:HH11	1.46	0.64
1:1A:303:U:O4	61:1A:4235:HOH:O	2.13	0.64
1:1A:2140:C:N3	1:1A:2151:G:O6	2.31	0.64
7:1H:33:LEU:HD21	7:1H:136:ILE:HG13	1.78	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2551:C:OP1	61:2A:3951:HOH:O	2.14	0.64
2:2B:3:C:H2'	2:2B:4:C:C6	2.32	0.64
39:2h:119:LEU:HB3	39:2h:123:GLU:HB2	1.80	0.64
1:1A:184:C:H2'	1:1A:185:U:C6	2.32	0.64
35:1d:101:LEU:HB2	35:1d:138:TYR:HB3	1.78	0.64
46:1o:11:VAL:HG21	46:1o:34:LEU:HD22	1.78	0.64
1:2A:1254:A:OP2	61:2A:3946:HOH:O	2.14	0.64
35:2d:105:VAL:HG23	35:2d:117:ALA:HB1	1.79	0.64
1:1A:2577:A:H5'	27:15:3:LYS:HD2	1.80	0.64
3:1D:71:ASP:HB2	3:1D:103:ARG:HH12	1.63	0.64
3:1D:148:GLU:HB2	3:1D:151:LYS:HD2	1.79	0.64
8:2I:93:THR:HG22	8:2I:119:PRO:HB3	1.79	0.64
11:2P:39:LYS:HG3	11:2P:45:LEU:HD22	1.79	0.64
11:2P:84:ASN:HD22	11:2P:117:GLU:HB3	1.61	0.64
33:2b:16:HIS:HB2	33:2b:204:ASN:HB3	1.79	0.64
38:2g:79:ARG:HH21	38:2g:80:VAL:HA	1.62	0.64
50:2s:38:SER:HB3	50:2s:71:LEU:HD22	1.79	0.64
5:2F:143:ALA:HB1	5:2F:148:LEU:HB2	1.80	0.64
6:2G:38:VAL:HG12	6:2G:93:THR:HG23	1.79	0.64
27:25:41:PRO:O	27:25:44:THR:OG1	2.15	0.64
32:2a:1273:G:H3'	32:2a:1274:G:H8	1.63	0.64
34:2c:11:ARG:NH2	34:2c:177:THR:O	2.29	0.64
32:2a:750:G:N3	46:2o:23:GLY:HA3	2.13	0.64
32:2a:1062:U:H2'	32:2a:1063:C:C6	2.33	0.64
1:2A:1816:G:O6	3:2D:35:LYS:NZ	2.26	0.64
34:2c:20:SER:HB3	34:2c:22:TRP:HE1	1.62	0.64
50:2s:33:THR:HG21	50:2s:71:LEU:HD21	1.79	0.64
8:1I:101:LEU:HG	8:1I:107:VAL:HB	1.80	0.64
32:1a:405:U:O4	35:1d:2:GLY:N	2.31	0.64
1:2A:465:G:O6	61:2A:3932:HOH:O	2.11	0.64
1:2A:1300:U:H4'	1:2A:1301:A:H5''	1.79	0.64
39:1h:51:VAL:HG12	39:1h:52:ASP:H	1.62	0.63
41:1j:40:LEU:HB2	41:1j:69:ASN:HB2	1.79	0.63
1:2A:253:C:O2'	61:2A:3955:HOH:O	2.15	0.63
26:24:53:GLU:HG2	26:24:55:ARG:H	1.63	0.63
32:2a:64:G:H4'	32:2a:65:U:H3'	1.77	0.63
1:1A:2312:U:H5'	6:1G:88:ILE:HD11	1.79	0.63
32:1a:79:G:O6	32:1a:90:U:C2	2.52	0.63
32:1a:562:C:H1'	43:1l:15:ARG:HB3	1.80	0.63
40:1i:23:ASN:HB2	40:1i:25:LYS:HE2	1.80	0.63
48:1q:66:SER:O	48:1q:70:ARG:NH1	2.31	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:2c:44:GLU:HA	34:2c:52:LEU:HD13	1.79	0.63
40:2i:112:LYS:NZ	40:2i:113:LYS:O	2.31	0.63
33:1b:60:ASP:OD2	33:1b:64:ARG:NH2	2.31	0.63
33:1b:178:ARG:NH1	33:1b:196:LEU:O	2.31	0.63
1:2A:2296:U:OP2	14:2S:9:ARG:NH2	2.28	0.63
32:2a:1026:G:O6	32:2a:1036:G:N2	2.31	0.63
32:2a:1271:G:C2	32:2a:1272:G:N7	2.66	0.63
32:1a:26:A:O2'	35:1d:209:ARG:NH2	2.31	0.63
2:2B:22:U:H3	2:2B:61:G:H22	1.46	0.63
5:2F:12:LEU:HD12	5:2F:124:LEU:HD21	1.80	0.63
2:1B:113:G:N2	14:1S:45:GLY:O	2.25	0.63
10:1O:2:ILE:HD12	10:1O:6:THR:HG21	1.80	0.63
14:1S:39:ILE:HB	14:1S:49:VAL:HG13	1.81	0.63
33:1b:48:MET:HA	33:1b:51:LEU:HB2	1.80	0.63
1:2A:2306:C:N4	6:2G:42:GLY:O	2.32	0.63
7:2H:24:VAL:HG13	7:2H:37:VAL:HG21	1.80	0.63
32:2a:35:G:O2'	43:2l:118:SER:O	2.13	0.63
32:2a:1240:U:N3	38:2g:30:ILE:O	2.23	0.63
37:2f:61:LEU:HB3	37:2f:63:TYR:HE2	1.63	0.63
50:2s:41:VAL:HG22	50:2s:42:PRO:HD2	1.79	0.63
50:2s:50:ALA:HB1	50:2s:57:HIS:HB3	1.81	0.63
54:1w:51:U:H2'	54:1w:52:G:H8	1.63	0.63
2:2B:2:C:H2'	2:2B:3:C:H6	1.63	0.63
43:2l:117:ARG:HB3	43:2l:122:THR:HB	1.81	0.63
32:1a:742:G:OP2	46:1o:35:ARG:NH2	2.26	0.63
1:2A:2318:G:H21	14:2S:3:ARG:NE	1.95	0.63
5:2F:137:LYS:HA	5:2F:140:LEU:HD12	1.79	0.63
8:1I:40:THR:O	8:1I:44:LEU:HB2	1.99	0.63
1:2A:2690:C:OP1	13:2R:17:ARG:NH2	2.32	0.63
32:2a:539:A:OP2	43:2l:115:LYS:NZ	2.28	0.63
33:2b:74:LYS:NZ	33:2b:205:ASP:O	2.31	0.63
54:2w:29:G:H1	54:2w:41:C:H42	1.47	0.63
5:1F:53:THR:HG23	5:1F:55:GLY:H	1.64	0.62
8:1I:3:VAL:HG12	8:1I:38:LEU:HA	1.81	0.62
32:2a:1052:U:O2'	32:2a:1055:A:OP2	2.13	0.62
32:2a:1118:C:OP1	40:2i:104:ARG:NH1	2.32	0.62
2:2B:48:A:H4'	14:2S:95:HIS:HD2	1.62	0.62
6:2G:35:GLU:HG2	6:2G:36:LYS:HG2	1.79	0.62
50:2s:41:VAL:HG13	50:2s:43:GLU:H	1.64	0.62
54:1y:48:C:C2	54:1y:59:U:H1'	2.34	0.62
6:2G:42:GLY:HA2	6:2G:89:GLY:HA3	1.80	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:2Q:31:ASP:OD1	12:2Q:134:ARG:NH1	2.31	0.62
32:2a:1225:A:OP1	44:2m:103:THR:OG1	2.15	0.62
34:2c:182:ILE:HG22	34:2c:203:PHE:HA	1.81	0.62
1:1A:2305:A:H5''	6:1G:134:GLY:HA3	1.82	0.62
32:2a:426:G:OP1	35:2d:38:TYR:OH	2.16	0.62
32:2a:1412:C:H2'	32:2a:1413:A:C8	2.35	0.62
36:2e:122:GLU:O	36:2e:126:ARG:NH1	2.32	0.62
10:1O:97:ARG:NH1	32:1a:339:C:OP2	2.30	0.62
21:1Z:93:ASP:HB2	21:1Z:131:ARG:HH12	1.64	0.62
33:2b:15:VAL:HG12	33:2b:16:HIS:HB3	1.80	0.62
1:1A:2038:G:O6	61:1A:4238:HOH:O	2.14	0.62
1:1A:2659:G:O6	61:1A:4231:HOH:O	2.11	0.62
39:1h:121:ASP:HB2	39:1h:125:ARG:HH21	1.65	0.62
1:2A:483:A:O2'	20:2Y:49:VAL:O	2.13	0.62
33:2b:95:GLN:HB3	33:2b:148:TYR:CD1	2.35	0.62
7:1H:56:SER:OG	7:1H:57:ASP:N	2.29	0.62
26:14:55:ARG:H	26:14:56:VAL:HA	1.63	0.62
32:1a:584:G:O6	61:1a:1911:HOH:O	2.14	0.62
12:2Q:57:HIS:HD2	12:2Q:117:ALA:HB2	1.64	0.62
33:2b:217:ARG:HA	33:2b:220:ASP:HB2	1.82	0.62
1:1A:1094:U:N3	1:1A:1097:U:OP2	2.33	0.62
2:1B:20:C:N4	61:1B:303:HOH:O	2.32	0.62
1:2A:2638:G:OP1	4:2E:82:ARG:NH2	2.33	0.62
32:2a:406:G:H21	35:2d:119:GLN:HE22	1.47	0.62
1:1A:1453:U:OP1	13:1R:77:ARG:NH1	2.26	0.62
5:1F:185:ASP:OD1	5:1F:188:ARG:NH1	2.32	0.62
1:2A:1891:G:O6	61:2A:3944:HOH:O	2.14	0.62
2:2B:42:C:O2	6:2G:66:GLN:NE2	2.32	0.62
32:2a:1060:C:HO2'	41:2j:56:HIS:HD1	1.46	0.62
32:2a:1133:G:H2'	32:2a:1134:G:H8	1.64	0.62
32:2a:1263:C:N3	32:2a:1272:G:O6	2.32	0.62
11:1P:50:ARG:HD3	30:18:7:HIS:CD2	2.35	0.62
50:1s:22:LEU:HB3	50:1s:27:GLU:HB3	1.82	0.62
6:2G:114:ILE:HB	6:2G:117:PHE:HD1	1.65	0.62
40:2i:9:ARG:H	40:2i:79:LEU:HD23	1.65	0.62
32:1a:976:G:H5'	32:1a:1358:U:O2'	1.99	0.61
33:1b:82:ARG:NH1	33:1b:92:TYR:OH	2.33	0.61
32:2a:1338:G:H21	55:2x:41:C:H1'	1.65	0.61
34:2c:101:LEU:HD22	34:2c:102:ASN:H	1.65	0.61
55:2x:23:C:H2'	55:2x:24:U:C6	2.35	0.61
1:1A:2646:C:OP2	1:1A:2732:G:O2'	2.18	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1I:116:LEU:HD21	8:1I:119:PRO:HA	1.82	0.61
40:1i:53:VAL:O	40:1i:55:ALA:N	2.32	0.61
1:2A:852:G:H2'	1:2A:853:G:C8	2.34	0.61
1:2A:2816:C:O3'	13:2R:99:LYS:NZ	2.33	0.61
6:2G:7:LEU:HD13	6:2G:104:GLU:HA	1.81	0.61
9:2N:38:HIS:CE1	9:2N:39:ARG:HG3	2.35	0.61
14:2S:10:ARG:HH21	14:2S:91:PRO:HB2	1.65	0.61
32:2a:1145:C:H4'	32:2a:1146:A:H5'	1.81	0.61
1:2A:481:G:O5'	20:2Y:47:LYS:NZ	2.28	0.61
13:2R:28:LEU:HD23	13:2R:48:VAL:HG21	1.82	0.61
32:2a:1226:C:H6	44:2m:103:THR:HB	1.65	0.61
44:2m:37:THR:HB	44:2m:39:ILE:HD12	1.83	0.61
1:1A:493:G:O6	61:1A:4246:HOH:O	2.16	0.61
54:1y:36:A:H2'	54:1y:37:MIA:O4'	1.99	0.61
1:2A:1153:C:OP1	16:2U:92:ARG:NH2	2.33	0.61
32:2a:1250:A:OP1	40:2i:67:GLY:N	2.31	0.61
50:2s:33:THR:HG22	50:2s:35:SER:H	1.65	0.61
1:1A:530:G:N1	1:1A:2023:G:OP1	2.25	0.61
1:1A:1055:G:H1	1:1A:1104:C:H42	1.49	0.61
8:1I:87:LYS:HD3	8:1I:87:LYS:H	1.65	0.61
32:1a:67:C:H2'	32:1a:68:G:C8	2.35	0.61
1:2A:2303:G:O2'	6:2G:132:ASN:ND2	2.33	0.61
4:2E:183:LEU:HD21	15:2T:10:VAL:HG11	1.82	0.61
32:2a:134:A:H61	47:2p:25:ARG:NH1	1.98	0.61
1:1A:1183:G:O3'	25:13:29:ARG:NH1	2.33	0.61
1:1A:1359:A:H2	1:1A:1372:U:O4	1.84	0.61
1:1A:2787:C:H1'	4:1E:62:PRO:HG3	1.83	0.61
32:1a:977:A:OP2	61:1a:1915:HOH:O	2.15	0.61
1:2A:625:G:N7	11:2P:107:LYS:NZ	2.44	0.61
32:2a:1060:C:H5'	45:2n:45:ARG:HH12	1.66	0.61
33:2b:15:VAL:HG13	33:2b:209:ARG:HB3	1.81	0.61
40:2i:26:VAL:HG13	40:2i:61:ALA:HB3	1.81	0.61
50:2s:28:LYS:CB	50:2s:29:ARG:HA	2.30	0.61
1:1A:1385:G:O2'	1:1A:1396:U:O2	2.16	0.61
34:1c:152:ILE:HB	34:1c:199:LYS:HB2	1.83	0.61
6:2G:32:PRO:HB2	6:2G:172:LEU:HD13	1.82	0.61
32:2a:951:G:N3	32:2a:970:C:O2'	2.32	0.61
32:2a:1081:G:OP1	36:2e:18:ARG:HG2	2.00	0.61
44:2m:80:ARG:HH22	50:2s:69:HIS:CE1	2.19	0.61
32:1a:36:C:OP1	43:1l:123:LYS:NZ	2.30	0.61
1:1A:1993:U:OP2	61:1A:4244:HOH:O	2.15	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:353:A:OP1	61:1a:1916:HOH:O	2.16	0.61
1:2A:271(H):G:H2'	1:2A:271(I):G:H8	1.65	0.61
1:2A:322:A:OP2	5:2F:169:ASN:HB2	2.01	0.61
6:2G:179:PRO:HB3	26:24:43:TYR:HE2	1.65	0.61
21:2Z:72:ARG:NH2	21:2Z:97:GLU:O	2.34	0.61
32:2a:772:U:OP2	61:2a:1911:HOH:O	2.16	0.61
39:1h:36:LEU:HD23	39:1h:39:LEU:HD23	1.83	0.61
32:2a:794:A:OP1	61:2a:1909:HOH:O	2.16	0.61
35:1d:178:VAL:C	35:1d:180:GLY:H	2.07	0.60
2:2B:54:G:H21	6:2G:29:TRP:HE1	1.48	0.60
2:2B:114:C:H2'	2:2B:115:G:C8	2.36	0.60
6:2G:15:VAL:HG13	6:2G:175:LEU:HD13	1.83	0.60
32:2a:501:C:H2'	32:2a:502:G:C8	2.36	0.60
1:1A:1174:A:H4'	1:1A:1175:U:OP1	2.00	0.60
32:1a:677:U:H3	32:1a:713:G:H22	1.48	0.60
1:2A:2805:G:H2'	1:2A:2807:G:C8	2.36	0.60
7:2H:143:GLN:NE2	7:2H:147:ASN:OD1	2.34	0.60
25:23:40:THR:HG22	25:23:42:ALA:H	1.66	0.60
32:2a:560:U:H5'	32:2a:566:G:N2	2.16	0.60
32:2a:1129:C:O2	32:2a:1130:A:N6	2.31	0.60
1:1A:2336:A:H61	22:10:43:THR:CG2	2.15	0.60
7:1H:3:ARG:HH21	7:1H:5:GLY:H	1.48	0.60
21:1Z:153:SER:HB3	21:1Z:167:PRO:HB3	1.82	0.60
1:2A:2327:A:H2'	1:2A:2328:A:C8	2.36	0.60
34:2c:35:GLU:HA	34:2c:38:ARG:HB3	1.84	0.60
1:1A:2450:A:O2'	55:1x:76:A:N6	2.34	0.60
32:1a:814:A:OP2	61:1a:1917:HOH:O	2.16	0.60
9:2N:23:LEU:HD13	9:2N:98:VAL:HG12	1.83	0.60
32:2a:1348:U:H4'	40:2i:120:ARG:HG3	1.81	0.60
35:2d:104:VAL:HG21	35:2d:140:VAL:HG21	1.84	0.60
44:2m:13:LYS:HA	44:2m:44:ARG:HH11	1.67	0.60
32:2a:1012:U:H2'	32:2a:1013:G:C8	2.36	0.60
1:1A:430:G:OP2	61:1A:4247:HOH:O	2.16	0.60
5:1F:11:VAL:HG22	5:1F:125:LEU:HB2	1.83	0.60
32:1a:134:A:H61	47:1p:25:ARG:HH12	1.50	0.60
32:2a:412:A:O4'	35:2d:35:ARG:NH2	2.34	0.60
33:2b:60:ASP:O	33:2b:64:ARG:HG2	2.02	0.60
33:2b:208:ILE:HA	33:2b:211:ILE:HG22	1.83	0.60
1:1A:1105:U:H2'	1:1A:1106:G:H8	1.66	0.60
1:1A:2218:U:O4'	23:11:52:ARG:NH2	2.35	0.60
32:1a:328:C:H4'	32:1a:329:A:H5'	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2223:G:OP1	3:2D:172:TYR:OH	2.18	0.60
14:2S:35:ILE:HD11	14:2S:101:LEU:HD12	1.83	0.60
35:2d:61:LYS:NZ	35:2d:72:GLU:OE1	2.27	0.60
1:1A:668:G:H5'	1:1A:669:G:OP2	2.02	0.60
1:2A:855:G:H1	1:2A:922:U:H3	1.50	0.60
1:2A:2104:G:H1	1:2A:2185:C:H42	1.48	0.60
1:2A:2143:C:H2'	1:2A:2144:U:O4'	2.01	0.60
1:2A:2727:G:O2'	10:2O:70:LYS:NZ	2.34	0.60
17:2V:40:LEU:HB2	17:2V:46:VAL:HB	1.84	0.60
30:28:26:LYS:HD3	30:28:48:PHE:HB3	1.84	0.60
32:2a:1200:C:OP1	32:2a:1201:A:O2'	2.19	0.60
32:2a:1264:C:N4	32:2a:1265:G:O6	2.34	0.60
50:2s:77:THR:HG23	50:2s:78:ARG:HG3	1.82	0.60
1:1A:249:C:O2	30:18:12:LYS:NZ	2.32	0.60
32:1a:829:G:O6	61:1a:1914:HOH:O	2.14	0.60
1:2A:1938:A:OP2	61:2A:3956:HOH:O	2.16	0.60
2:2B:7:G:N2	14:2S:38:GLN:HE22	1.94	0.60
8:2I:40:THR:OG1	8:2I:41:GLU:N	2.31	0.60
8:2I:45:LYS:O	8:2I:49:ALA:N	2.32	0.60
18:2W:88:ARG:NH1	18:2W:94:ASP:OD2	2.35	0.60
34:2c:8:ILE:HG23	34:2c:16:ARG:HG2	1.81	0.60
1:1A:409:C:OP1	61:1A:4250:HOH:O	2.17	0.60
1:1A:1342:A:OP2	61:1A:4217:HOH:O	2.15	0.60
35:1d:155:LEU:HB3	35:1d:158:ILE:HD11	1.84	0.60
1:2A:2074:U:H2'	1:2A:2075:U:C6	2.37	0.60
26:24:46:GLN:C	26:24:48:ARG:H	2.10	0.60
34:2c:69:HIS:CD2	34:2c:104:GLN:HG2	2.37	0.60
32:1a:1305:G:O6	61:1a:1918:HOH:O	2.17	0.59
55:1x:61:C:H2'	55:1x:62:C:H6	1.67	0.59
32:2a:1385:G:H2'	32:2a:1386:G:C8	2.37	0.59
36:1e:33:VAL:HG21	36:1e:109:ILE:HA	1.85	0.59
1:2A:2839:G:H5'	13:2R:46:GLY:HA2	1.83	0.59
6:2G:106:LEU:HA	6:2G:110:ALA:HB3	1.84	0.59
1:1A:1494:A:OP1	61:1A:4248:HOH:O	2.16	0.59
32:1a:1145:C:H4'	32:1a:1146:A:H5'	1.84	0.59
34:1c:59:ARG:HG2	34:1c:64:VAL:HB	1.84	0.59
6:2G:69:ALA:HB3	6:2G:91:ARG:HH21	1.66	0.59
32:2a:839:U:H3'	32:2a:840:C:H5'	1.83	0.59
39:2h:51:VAL:HG11	39:2h:60:ARG:HH22	1.67	0.59
1:1A:993:G:OP1	16:1U:50:ARG:NH2	2.35	0.59
1:2A:1278:A:OP1	13:2R:36:THR:HG23	2.03	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:2I:9:LEU:HD21	8:2I:35:LEU:HD23	1.85	0.59
32:2a:1315:U:OP2	50:2s:7:LYS:NZ	2.33	0.59
33:2b:95:GLN:HB3	33:2b:148:TYR:HD1	1.68	0.59
35:2d:53:ASP:O	35:2d:57:ARG:HG2	2.02	0.59
50:2s:49:ILE:HG22	50:2s:62:ILE:HD11	1.83	0.59
1:1A:2160:G:O6	1:1A:2161:C:N4	2.35	0.59
32:1a:190:U:H2'	32:1a:191:G:H8	1.67	0.59
54:1y:19:G:H1	54:1y:56:C:N4	1.99	0.59
1:2A:1031:G:H5''	31:29:8:LYS:HE3	1.83	0.59
1:2A:2130:U:O2	1:2A:2134:A:O2'	2.16	0.59
34:1c:11:ARG:NH2	34:1c:177:THR:O	2.35	0.59
36:1e:78:HIS:CD2	39:1h:104:ARG:HD2	2.37	0.59
6:2G:112:PRO:HG3	26:24:43:TYR:HE1	1.67	0.59
8:2I:59:ALA:HA	8:2I:62:LYS:HG2	1.83	0.59
32:2a:1208:C:H2'	32:2a:1209:C:C6	2.38	0.59
40:2i:4:TYR:HB2	40:2i:19:LEU:HB2	1.85	0.59
1:1A:880:G:H2'	1:1A:881:G:C8	2.35	0.59
1:1A:1828:G:H8	1:1A:1828:G:OP2	1.86	0.59
1:1A:2336:A:H61	22:10:43:THR:HG22	1.67	0.59
33:1b:87:ARG:NH1	33:1b:233:SER:OG	2.34	0.59
36:1e:78:HIS:HD2	39:1h:104:ARG:HD2	1.68	0.59
2:2B:90:A:C5	2:2B:91:C:H1'	2.38	0.59
6:2G:64:THR:HB	6:2G:94:LEU:HD21	1.85	0.59
38:2g:22:LEU:HG	38:2g:62:PHE:HE2	1.67	0.59
54:2w:9:A:O2'	54:2w:10:G:N7	2.34	0.59
1:1A:2753:A:N3	31:19:15:LYS:NZ	2.49	0.59
6:2G:64:THR:HG22	6:2G:94:LEU:HD11	1.85	0.59
8:2I:77:LEU:HB3	8:2I:142:VAL:HG13	1.84	0.59
32:2a:1219:U:O2'	50:2s:34:TRP:HB3	2.02	0.59
35:2d:17:VAL:HG12	35:2d:19:LEU:HD12	1.83	0.59
38:2g:24:THR:HA	38:2g:27:ILE:HD12	1.85	0.59
32:1a:618:C:H5'	32:1a:619:U:H5''	1.85	0.59
1:2A:1593:G:H2'	1:2A:1594:G:H8	1.68	0.59
1:2A:2299:G:N1	1:2A:2318:G:N7	2.51	0.59
1:2A:2340:G:H2'	1:2A:2341:G:H8	1.68	0.59
32:2a:1189:C:OP1	41:2j:51:ARG:NH2	2.36	0.59
1:1A:2156:G:H2'	1:1A:2157:G:C2	2.37	0.59
7:1H:3:ARG:NH2	7:1H:5:GLY:H	2.00	0.59
21:1Z:52:SER:O	21:1Z:54:HIS:N	2.36	0.59
32:1a:276:G:O3'	48:1q:68:ARG:NH1	2.35	0.59
34:1c:3:ASN:OD1	34:1c:3:ASN:N	2.35	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1347:G:N2	32:2a:1373:G:H2'	2.16	0.59
41:2j:16:LEU:HB3	41:2j:70:ARG:HG3	1.85	0.59
44:2m:94:ARG:HB3	44:2m:96:LEU:HG	1.85	0.59
47:2p:53:VAL:HG22	47:2p:79:VAL:HG22	1.84	0.59
1:1A:911:A:H2'	12:1Q:9:TYR:OH	2.03	0.58
1:1A:2629:A:HO2'	1:1A:2630:G:P	2.24	0.58
32:1a:79:G:C6	32:1a:90:U:O2	2.56	0.58
51:1t:60:GLU:HG3	51:1t:81:LYS:HD2	1.84	0.58
1:2A:1203:G:O6	61:2A:3954:HOH:O	2.15	0.58
32:2a:967:5MC:H2'	32:2a:968:A:C8	2.38	0.58
3:1D:166:GLN:HB2	3:1D:174:ILE:HG22	1.85	0.58
33:1b:19:HIS:NE2	33:1b:206:ASP:OD2	2.35	0.58
50:1s:31:ILE:HB	50:1s:49:ILE:HG23	1.84	0.58
6:2G:128:ARG:HB2	6:2G:130:ASN:HD21	1.68	0.58
37:2f:37:VAL:HA	37:2f:65:VAL:HG12	1.85	0.58
37:2f:100:ASN:HD21	49:2r:23:LYS:HG2	1.67	0.58
1:1A:338:G:OP2	61:1A:4245:HOH:O	2.16	0.58
17:1V:76:LYS:HB2	17:1V:81:TYR:HB3	1.83	0.58
32:1a:221:C:H2'	32:1a:222:U:H6	1.68	0.58
32:1a:1029:C:H41	32:1a:1030(A):G:H21	1.49	0.58
1:2A:1796:U:H2'	1:2A:1797:C:C6	2.39	0.58
3:2D:148:GLU:HB2	3:2D:151:LYS:HD2	1.85	0.58
5:2F:184:TYR:CE2	5:2F:188:ARG:HD2	2.38	0.58
18:2W:11:ARG:NH1	18:2W:99:ARG:O	2.36	0.58
34:2c:53:ALA:HB2	34:2c:115:LEU:HD13	1.85	0.58
41:2j:62:HIS:HB3	45:2n:59:ALA:HB3	1.85	0.58
1:1A:1028:A:N6	1:1A:1125:G:H2'	2.18	0.58
1:1A:1815:A:OP2	3:1D:54:ARG:NH2	2.35	0.58
32:2a:34:C:H2'	32:2a:35:G:H8	1.67	0.58
32:2a:1316:G:H5''	45:2n:17:LYS:HD3	1.84	0.58
33:2b:187:LEU:HD12	33:2b:214:ILE:HG21	1.85	0.58
32:1a:262:A:H2'	32:1a:263:A:C8	2.39	0.58
44:1m:67:GLU:HG3	44:1m:71:ARG:HH22	1.68	0.58
1:2A:271(H):G:H2'	1:2A:271(I):G:C8	2.38	0.58
4:2E:48:GLN:HA	4:2E:80:GLU:HA	1.86	0.58
7:2H:113:VAL:HG11	7:2H:151:ILE:HD13	1.86	0.58
10:2O:88:ASN:HD21	10:2O:92:GLU:HB2	1.67	0.58
33:2b:69:LEU:HB2	33:2b:159:PRO:HG2	1.85	0.58
36:1e:78:HIS:CE1	36:1e:143:ARG:H	2.21	0.58
1:2A:1019:U:H2'	1:2A:1020:A:H8	1.69	0.58
1:2A:2518:A:OP2	61:2A:3958:HOH:O	2.17	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:542:G:OP1	35:2d:10:ARG:NH2	2.29	0.58
32:2a:1124:G:N2	32:2a:1125:U:O4	2.36	0.58
40:2i:28:VAL:HG22	40:2i:63:ILE:HB	1.85	0.58
32:1a:1036:G:H3'	32:1a:1037:C:H6	1.67	0.58
1:2A:1259:G:N7	61:2A:4047:HOH:O	2.32	0.58
1:2A:2375:G:N2	1:2A:2378:A:OP2	2.30	0.58
26:24:45:GLY:C	26:24:47:GLN:H	2.12	0.58
32:2a:376:G:H5''	47:2p:5:ARG:HB2	1.84	0.58
32:2a:620:C:OP1	61:2a:1910:HOH:O	2.16	0.58
1:1A:1085:A:O2'	1:1A:1104:C:O2'	2.21	0.58
15:1T:127:ALA:C	15:1T:129:ARG:H	2.10	0.58
32:1a:757:U:H2'	32:1a:758:G:O4'	2.04	0.58
44:1m:3:ARG:HG2	44:1m:8:GLU:HA	1.86	0.58
1:2A:733:G:OP2	61:2A:3957:HOH:O	2.17	0.58
1:2A:2751:G:H8	7:2H:2:SER:HA	1.68	0.58
37:2f:25:ILE:HD13	37:2f:82:ARG:HD3	1.86	0.58
5:1F:70:THR:HG23	5:1F:72:ARG:H	1.68	0.58
32:1a:584:G:H5'	48:1q:91:ARG:HH12	1.69	0.58
32:1a:1021:G:O2'	32:1a:1022:G:O5'	2.22	0.58
33:1b:18:GLY:HA3	33:1b:42:ILE:HG13	1.85	0.58
54:1w:4:C:H2'	54:1w:5:G:C8	2.39	0.58
1:2A:861:A:N3	2:2B:79:C:O2'	2.35	0.58
1:2A:947:G:H2'	1:2A:948:G:C8	2.39	0.58
1:2A:2880:C:O3'	13:2R:90:ARG:NH1	2.37	0.58
32:2a:307:C:OP1	61:2a:1912:HOH:O	2.17	0.58
32:2a:985:C:H2'	32:2a:986:A:C8	2.39	0.58
32:2a:1250:A:H4'	40:2i:68:GLY:H	1.68	0.58
4:1E:116:VAL:HG13	4:1E:122:PHE:HB2	1.85	0.58
32:1a:448:A:OP2	32:1a:485:G:N1	2.27	0.58
1:2A:2379:G:HO2'	14:2S:17:ARG:HH12	1.49	0.58
6:2G:44:GLY:N	6:2G:88:ILE:O	2.37	0.58
32:2a:977:A:N6	32:2a:1224:G:OP1	2.37	0.58
32:2a:1122:U:N3	32:2a:1123:A:N7	2.51	0.58
32:2a:1385:G:H2'	32:2a:1386:G:H8	1.69	0.58
34:2c:123:GLN:O	34:2c:128:PHE:HB2	2.04	0.58
21:1Z:139:VAL:HG11	21:1Z:171:ILE:HD11	1.85	0.57
41:1j:38:ILE:HG13	41:1j:71:LEU:HB3	1.86	0.57
1:2A:646:A:H2'	1:2A:647:G:O4'	2.04	0.57
1:2A:1183:G:H5''	25:23:30:ARG:NH2	2.19	0.57
1:2A:2131:G:H4'	1:2A:2132:U:H3'	1.86	0.57
3:2D:108:PRO:HB3	3:2D:143:HIS:CE1	2.39	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:276:G:O3'	48:2q:68:ARG:NH1	2.36	0.57
32:2a:674:G:H2'	32:2a:675:A:H8	1.69	0.57
32:2a:1190:G:H5'	34:2c:176:HIS:CE1	2.38	0.57
32:2a:1346:A:H61	32:2a:1374:A:H3'	1.69	0.57
32:2a:1376:U:H2'	32:2a:1377:A:H8	1.69	0.57
33:2b:63:MET:HG3	33:2b:225:ALA:HB1	1.86	0.57
34:2c:44:GLU:HG3	34:2c:52:LEU:HD22	1.86	0.57
1:1A:1506:C:H2'	1:1A:1507:A:H8	1.69	0.57
32:1a:171:A:H2'	32:1a:172:A:C8	2.38	0.57
26:24:1:MET:HB3	26:24:6:HIS:CD2	2.38	0.57
32:2a:677:U:H3	32:2a:713:G:H22	1.52	0.57
32:2a:972:C:O2'	41:2j:55:LYS:O	2.21	0.57
32:2a:975:A:N1	41:2j:48:THR:HB	2.18	0.57
1:1A:762:U:OP1	61:1A:4249:HOH:O	2.17	0.57
1:1A:2243:U:H2'	1:1A:2244:U:C6	2.39	0.57
4:1E:89:ASP:OD1	4:1E:89:ASP:N	2.37	0.57
13:1R:67:LEU:HD13	13:1R:76:VAL:HG21	1.85	0.57
32:1a:401:C:H2'	32:1a:402:G:C8	2.39	0.57
1:2A:1939:5MU:OP1	1:2A:2604:U:O2'	2.22	0.57
12:2Q:36:ALA:HB2	12:2Q:103:MET:SD	2.45	0.57
33:2b:149:LEU:HD23	33:2b:152:PHE:HD2	1.69	0.57
21:1Z:52:SER:C	21:1Z:54:HIS:H	2.12	0.57
1:2A:896:A:H1'	54:2w:56:C:H5'	1.86	0.57
32:2a:1387:G:H2'	32:2a:1388:C:C6	2.40	0.57
46:2o:87:ILE:HG22	46:2o:88:ARG:H	1.69	0.57
46:1o:55:GLY:HA2	46:1o:58:MET:HE3	1.86	0.57
1:2A:1266:G:O5'	18:2W:15:ARG:NH2	2.37	0.57
1:2A:2788:C:OP1	4:2E:61:ARG:NH2	2.37	0.57
32:2a:983:A:N1	32:2a:1222:G:N2	2.52	0.57
32:2a:1219:U:OP1	45:2n:19:ARG:NH1	2.23	0.57
33:2b:126:GLU:CD	33:2b:126:GLU:H	2.11	0.57
32:1a:410:G:OP1	35:1d:30:LYS:NZ	2.24	0.57
32:1a:1198:G:OP2	61:1a:1913:HOH:O	2.17	0.57
34:1c:148:GLY:HA2	34:1c:171:GLY:HA3	1.86	0.57
1:2A:796:C:H2'	1:2A:797:C:C6	2.40	0.57
16:2U:74:LEU:HD13	16:2U:79:PHE:HB2	1.87	0.57
32:2a:1030(A):G:N1	32:2a:1030(D):A:OP2	2.35	0.57
34:2c:47:LEU:HG	34:2c:50:ALA:HB3	1.86	0.57
1:1A:2344:U:OP1	28:16:37:ARG:NH1	2.38	0.57
4:1E:29:GLY:HA3	61:1E:401:HOH:O	2.03	0.57
32:1a:421:U:O4	34:1c:127:ARG:NH2	2.37	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1456:G:O3'	51:1t:39:LYS:NZ	2.37	0.57
41:1j:49:VAL:HG23	45:1n:41:ARG:HB2	1.86	0.57
13:2R:97:VAL:HG22	13:2R:114:VAL:HG13	1.86	0.57
15:2T:118:ARG:HG2	32:2a:1442(A):G:C8	2.40	0.57
21:2Z:171:ILE:HD12	21:2Z:172:ALA:H	1.69	0.57
32:2a:537:G:H5'	43:2l:113:ARG:HH12	1.69	0.57
49:2r:31:LEU:HD23	49:2r:31:LEU:H	1.70	0.57
1:2A:752:A:H3'	29:27:1:MET:HE1	1.86	0.57
3:2D:108:PRO:HB3	3:2D:143:HIS:HE1	1.69	0.57
18:2W:15:ARG:NH1	61:2W:301:HOH:O	2.37	0.57
35:2d:150:GLU:OE1	35:2d:151:LYS:N	2.38	0.57
44:2m:15:VAL:HG22	44:2m:48:LEU:HD11	1.87	0.57
48:2q:4:LYS:HE3	48:2q:6:LEU:HD21	1.87	0.57
1:1A:1641:A:H2'	1:1A:1642:G:O4'	2.05	0.57
1:1A:1827:C:C2'	1:1A:1828:G:H5'	2.35	0.57
1:1A:2250:G:OP1	12:1Q:85:LYS:NZ	2.33	0.57
11:1P:95:VAL:HG22	11:1P:125:VAL:HG12	1.87	0.57
32:1a:278:G:OP2	48:1q:92:ARG:NH2	2.37	0.57
1:2A:1800:C:OP2	3:2D:183:ARG:NH2	2.38	0.57
1:2A:2183:C:H2'	1:2A:2184:G:C8	2.39	0.57
1:2A:2818:G:OP2	13:2R:42:LYS:NZ	2.38	0.57
2:2B:3:C:H2'	2:2B:4:C:H6	1.69	0.57
32:2a:976:G:H5'	32:2a:1358:U:O2'	2.05	0.57
32:2a:978:A:HO2'	32:2a:1321:C:N4	2.03	0.57
32:2a:1004:A:N6	32:2a:1037:C:O2	2.25	0.57
1:1A:271(K):U:H1'	8:1I:50:ARG:HD3	1.85	0.57
1:1A:484:C:H2'	1:1A:485:C:C6	2.40	0.57
1:1A:922:U:H2'	1:1A:923:C:C6	2.40	0.57
32:1a:1144:G:N2	32:1a:1146:A:H62	2.03	0.57
36:1e:144:THR:H	36:1e:147:ASP:HB2	1.69	0.57
44:1m:20:THR:C	44:1m:22:ILE:H	2.13	0.57
1:2A:300:A:P	20:2Y:86:ARG:HH22	2.28	0.57
1:2A:301:G:OP2	20:2Y:84:ARG:NH2	2.36	0.57
6:2G:125:PHE:HB3	6:2G:166:ASP:CG	2.30	0.57
28:26:6:ARG:NH1	28:26:26:ASN:HB2	2.19	0.57
32:1a:17:U:H2'	32:1a:18:C:C6	2.40	0.56
32:1a:92:C:H2'	32:1a:93:G:H8	1.70	0.56
45:1n:33:VAL:HA	45:1n:40:CYS:HA	1.86	0.56
46:1o:26:GLU:HG3	46:1o:81:LEU:HD22	1.87	0.56
1:2A:658:C:H2'	1:2A:659:C:C6	2.39	0.56
32:2a:107:G:H2'	32:2a:108:G:O4'	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:909:A:N3	32:2a:1413:A:O2'	2.35	0.56
32:2a:1329:A:OP2	52:2u:7:ARG:NH1	2.35	0.56
37:2f:95:GLU:O	49:2r:32:ARG:NH1	2.38	0.56
4:1E:49:LEU:HD22	4:1E:81:ILE:HD12	1.86	0.56
1:2A:918:A:N3	2:2B:80:U:O2'	2.35	0.56
1:2A:1028:A:N6	1:2A:1125:G:H2'	2.19	0.56
12:2Q:26:TYR:O	12:2Q:67:ARG:NH1	2.36	0.56
32:2a:974:A:OP1	45:2n:31:ARG:HD3	2.05	0.56
38:2g:113:GLU:HG2	38:2g:119:ARG:HG2	1.87	0.56
1:1A:11:G:H2'	1:1A:12:U:H5''	1.86	0.56
1:1A:2153:G:H2'	1:1A:2154:G:C8	2.41	0.56
17:1V:43:GLU:OE1	17:1V:43:GLU:N	2.38	0.56
32:1a:1029:C:H41	32:1a:1030(A):G:N2	2.03	0.56
33:1b:127:ILE:HG21	33:1b:130:ARG:HD3	1.86	0.56
37:1f:89:MET:HE1	49:1r:72:ARG:HB3	1.87	0.56
1:2A:307:G:N1	1:2A:310:A:OP2	2.38	0.56
1:2A:878:A:N6	1:2A:899:A:O2'	2.38	0.56
6:2G:43:LEU:C	6:2G:45:GLU:H	2.13	0.56
9:2N:128:HIS:O	9:2N:131:GLN:NE2	2.38	0.56
19:2X:50:LYS:HB3	19:2X:87:GLN:HE22	1.70	0.56
32:2a:1218:C:H2'	32:2a:1219:U:C6	2.40	0.56
32:2a:1435:G:H2'	32:2a:1436:U:C6	2.41	0.56
38:2g:15:ASP:HB3	38:2g:24:THR:HG23	1.88	0.56
42:2k:73:MET:HG2	42:2k:103:LEU:HD21	1.86	0.56
51:2t:43:LEU:HD13	51:2t:51:GLU:HB3	1.86	0.56
54:2y:14:A:O2'	54:2y:15:G:OP1	2.22	0.56
1:1A:279:C:H42	1:1A:361:G:H1	1.53	0.56
1:1A:323:G:C8	5:1F:171:PRO:HG3	2.40	0.56
1:1A:2614:A:OP1	61:1A:4251:HOH:O	2.18	0.56
32:1a:45:U:H2'	32:1a:46:G:C8	2.40	0.56
32:1a:407:G:OP1	35:1d:115:ARG:NH2	2.39	0.56
8:2I:50:ARG:HA	8:2I:53:ALA:HB3	1.87	0.56
9:2N:42:TRP:HA	9:2N:48:MET:SD	2.46	0.56
32:2a:1134:G:C2	32:2a:1135:U:H1'	2.41	0.56
52:2u:6:ARG:HA	52:2u:11:GLY:HA3	1.88	0.56
32:1a:1510:U:H2'	32:1a:1511:G:C8	2.41	0.56
47:1p:5:ARG:HE	47:1p:22:THR:HG23	1.70	0.56
1:2A:2138:C:H42	1:2A:2153:G:H1	1.53	0.56
6:2G:112:PRO:HG3	26:24:43:TYR:CE1	2.41	0.56
21:2Z:51:ALA:O	21:2Z:52:SER:HB3	2.05	0.56
32:2a:662:G:O2'	32:2a:836:G:OP1	2.23	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1031:G:H2'	32:2a:1032:G:C8	2.40	0.56
40:2i:21:PRO:HA	40:2i:59:PHE:HA	1.86	0.56
42:2k:110:ASP:HB3	49:2r:85:LEU:HB3	1.88	0.56
1:2A:10:G:O2'	1:2A:2801(A):A:N7	2.28	0.56
32:2a:1203:C:OP1	45:2n:3:ARG:HD2	2.05	0.56
32:2a:1263:C:C4	32:2a:1272:G:O6	2.58	0.56
35:2d:64:LEU:HB2	35:2d:198:VAL:HG11	1.88	0.56
54:2y:18:G:N2	54:2y:55:PSU:C4	2.70	0.56
3:1D:183:ARG:HG3	3:1D:270:ILE:HD13	1.88	0.56
51:1t:10:LEU:HB3	51:1t:12:ALA:H	1.70	0.56
55:1x:13:C:H2'	55:1x:14:A:H5''	1.86	0.56
54:1y:52:G:H2'	54:1y:53:G:C8	2.40	0.56
1:2A:143:G:H4'	19:2X:35:THR:HG21	1.86	0.56
1:2A:299:A:N1	1:2A:322:A:O2'	2.36	0.56
1:2A:1507:A:O2'	1:2A:1508:A:O5'	2.23	0.56
6:2G:108:ASN:HA	26:24:37:SER:HB3	1.87	0.56
32:2a:45:U:H2'	32:2a:46:G:C8	2.41	0.56
32:2a:1346:A:N1	32:2a:1374:A:H5''	2.21	0.56
41:2j:8:LEU:HB3	41:2j:96:ILE:HG23	1.88	0.56
1:1A:1264:G:OP1	27:15:19:ARG:NH2	2.32	0.56
4:1E:180:ASN:OD1	61:1E:401:HOH:O	2.18	0.56
23:11:77:ALA:HA	23:11:80:LEU:HD12	1.87	0.56
46:1o:87:ILE:HG22	46:1o:88:ARG:H	1.70	0.56
1:2A:918:A:O2'	2:2B:97:G:N2	2.37	0.56
12:2Q:111:GLU:O	12:2Q:115:MET:HG2	2.05	0.56
19:2X:53:LYS:HB3	19:2X:82:GLN:HB3	1.87	0.56
21:2Z:5:LEU:HB2	21:2Z:47:VAL:HG21	1.86	0.56
41:2j:30:SER:O	41:2j:81:THR:OG1	2.18	0.56
1:1A:2788:C:OP1	4:1E:61:ARG:NH2	2.39	0.56
32:1a:78:G:O6	32:1a:92:C:N4	2.39	0.56
1:2A:2176:A:H2'	1:2A:2177:C:C6	2.41	0.56
32:2a:8:A:N6	35:2d:209:ARG:HB2	2.21	0.56
43:2l:27:LEU:HA	43:2l:33:ARG:HG3	1.88	0.56
6:1G:27:ASN:HB3	6:1G:30:GLU:HG3	1.88	0.56
7:1H:116:GLU:HG3	7:1H:117:PRO:HD2	1.86	0.56
25:13:7:LYS:HB2	25:13:34:GLU:HG2	1.88	0.56
50:1s:11:VAL:HG11	50:1s:16:LEU:HB2	1.86	0.56
1:2A:1316:U:H2'	1:2A:1317:A:C8	2.40	0.56
32:2a:1239:A:H62	32:2a:1299:A:N6	2.04	0.56
33:2b:74:LYS:O	33:2b:78:GLN:HG2	2.06	0.56
33:2b:187:LEU:HD23	33:2b:188:ALA:N	2.21	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:2b:188:ALA:HB1	33:2b:192:SER:HB2	1.87	0.56
43:2l:45:PRO:HB2	43:2l:92:OTD:SB	2.46	0.56
44:2m:92:HIS:CD2	44:2m:98:VAL:HG11	2.41	0.56
13:1R:118:GLU:H	13:1R:118:GLU:CD	2.14	0.55
18:1W:71:VAL:HA	18:1W:107:LEU:HD23	1.88	0.55
38:1g:153:HIS:HE1	42:1k:57:THR:HG22	1.71	0.55
48:1q:53:LEU:HD23	48:1q:82:MET:HE1	1.88	0.55
50:1s:27:GLU:HB2	50:1s:28:LYS:HB3	1.88	0.55
1:2A:1169:G:H1	1:2A:1180:C:H42	1.54	0.55
1:2A:2394:C:N3	54:2y:76:A:O2'	2.38	0.55
21:2Z:52:SER:OG	21:2Z:53:ILE:N	2.37	0.55
34:2c:129:ALA:HB3	34:2c:132:ARG:HB3	1.88	0.55
1:1A:1937:A:H1'	1:1A:1939:5MU:H72	1.88	0.55
1:2A:272(J):C:H42	1:2A:363:G:H1	1.54	0.55
1:2A:1514:U:H2'	1:2A:1515:G:C8	2.42	0.55
1:2A:1514:U:H2'	1:2A:1515:G:H8	1.71	0.55
1:2A:1833:U:O2'	1:2A:1969:A:N1	2.34	0.55
8:2I:110:ASP:N	8:2I:130:TYR:OH	2.39	0.55
26:24:14:ILE:HD12	26:24:31:ILE:HB	1.88	0.55
32:2a:736:C:H2'	32:2a:737:A:C8	2.42	0.55
35:2d:112:VAL:H	35:2d:116:GLN:NE2	2.04	0.55
1:1A:1364:G:OP2	23:11:3:LYS:HG3	2.06	0.55
1:1A:1971:A:OP2	3:1D:242:ARG:NH2	2.38	0.55
1:2A:740:U:H2'	1:2A:741:G:C8	2.42	0.55
1:2A:1378:A:O2'	1:2A:1380:G:N7	2.36	0.55
1:2A:2646:C:OP2	1:2A:2732:G:O2'	2.24	0.55
15:2T:41:ARG:NH2	32:2a:346:G:OP1	2.39	0.55
39:2h:20:TYR:HA	39:2h:65:TYR:CZ	2.41	0.55
54:2w:68:C:H2'	54:2w:69:G:H8	1.72	0.55
1:1A:1156:A:OP1	16:1U:55:ARG:NH1	2.40	0.55
1:1A:2430:A:N3	1:1A:2430:A:H2'	2.22	0.55
7:1H:24:VAL:HG22	7:1H:35:VAL:HB	1.88	0.55
8:1I:75:LEU:HD22	8:1I:105:HIS:CG	2.42	0.55
32:1a:110:C:O2'	47:1p:25:ARG:O	2.22	0.55
32:1a:352:C:O2'	32:1a:354:G:OP1	2.25	0.55
1:2A:2683:C:OP1	15:2T:53:ARG:NH2	2.39	0.55
15:2T:109:GLU:HG3	15:2T:112:ARG:HH21	1.70	0.55
32:2a:406:G:H5'	35:2d:5:ILE:HD11	1.87	0.55
32:2a:646:U:H2'	32:2a:647:C:C6	2.41	0.55
32:2a:1000:U:H2'	32:2a:1001:A:C8	2.40	0.55
36:2e:143:ARG:NE	39:2h:77:GLU:OE2	2.37	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1823:G:OP1	3:1D:54:ARG:NH1	2.40	0.55
1:1A:2791:C:H2'	1:1A:2792:G:C8	2.42	0.55
31:19:8:LYS:O	31:19:34:GLN:NE2	2.26	0.55
32:1a:148:G:H2'	32:1a:149:A:H8	1.72	0.55
32:1a:1112:C:H1'	34:1c:179:ARG:HH11	1.72	0.55
34:1c:87:LEU:O	34:1c:91:LEU:HB2	2.07	0.55
39:1h:112:LEU:HA	39:1h:134:ILE:HG12	1.88	0.55
1:2A:2328:A:H2'	1:2A:2329:G:C8	2.41	0.55
12:2Q:78:PRO:HG2	12:2Q:81:VAL:HG11	1.89	0.55
26:24:37:SER:HA	26:24:43:TYR:CD1	2.42	0.55
26:24:46:GLN:HG3	26:24:48:ARG:H	1.71	0.55
34:2c:122:GLU:O	34:2c:125:GLU:HG2	2.07	0.55
1:1A:443:A:N6	5:1F:41:LEU:O	2.38	0.55
54:1y:49:C:H42	54:1y:65:G:H1	1.55	0.55
1:2A:2836:U:H2'	1:2A:2837:G:C8	2.41	0.55
30:28:33:ASN:HA	30:28:36:LYS:HD2	1.88	0.55
32:2a:664:G:P	49:2r:64:ARG:HH21	2.29	0.55
32:2a:1131:G:H2'	32:2a:1132:C:C6	2.42	0.55
33:2b:138:LEU:HA	33:2b:141:GLU:HB2	1.87	0.55
36:2e:18:ARG:HG3	36:2e:25:ARG:O	2.07	0.55
38:2g:140:ASP:OD1	54:2y:41:C:O2'	2.25	0.55
1:1A:2327:A:H2'	1:1A:2328:A:C8	2.42	0.55
3:1D:206:LEU:HD22	3:1D:211:ARG:HG2	1.87	0.55
6:1G:83:ARG:O	6:1G:86:MET:HG3	2.05	0.55
32:1a:1027:C:C4	32:1a:1034:G:N1	2.74	0.55
32:1a:1355:G:OP1	61:1a:1919:HOH:O	2.18	0.55
34:1c:56:ASP:HB2	34:1c:67:THR:HB	1.87	0.55
46:1o:56:LEU:O	46:1o:60:VAL:HG23	2.06	0.55
54:1y:13:C:H2'	54:1y:14:A:H5''	1.87	0.55
1:2A:2022:U:O2'	1:2A:2617:C:H5'	2.07	0.55
1:2A:2547:U:O2	10:2O:23:ARG:NH2	2.39	0.55
21:2Z:157:LEU:HB3	21:2Z:161:VAL:HG13	1.87	0.55
32:2a:1149:C:O2'	32:2a:1280:A:N1	2.32	0.55
36:2e:7:GLU:OE1	36:2e:37:ARG:NH2	2.30	0.55
1:1A:2577:A:O4'	27:15:3:LYS:HB2	2.07	0.55
32:1a:341:C:H2'	32:1a:342:C:C6	2.42	0.55
1:2A:500:G:N1	1:2A:503:A:OP2	2.40	0.55
4:2E:116:VAL:HG13	4:2E:122:PHE:HB2	1.89	0.55
6:2G:7:LEU:HD11	6:2G:107:LEU:HD12	1.88	0.55
21:2Z:19:ARG:HG3	21:2Z:25:PRO:HD3	1.89	0.55
21:2Z:45:ASP:OD1	21:2Z:49:ARG:NE	2.39	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:890:G:O2'	32:2a:906:G:O6	2.20	0.55
32:2a:948:C:H2'	32:2a:949:A:H8	1.72	0.55
51:2t:10:LEU:HG	51:2t:12:ALA:H	1.71	0.55
1:1A:1405:U:H2'	1:1A:1406:U:C6	2.42	0.55
1:1A:1671:U:O4	61:1A:4215:HOH:O	2.17	0.55
1:1A:1783:A:H5'	1:1A:2608:G:H4'	1.89	0.55
24:12:63:VAL:HA	24:12:66:GLU:HB2	1.87	0.55
32:1a:576:G:O6	32:1a:880:C:O2'	2.25	0.55
32:1a:1305:G:N2	32:1a:1331:G:H1'	2.22	0.55
32:1a:1346:A:N1	32:1a:1374:A:H5''	2.22	0.55
1:1A:363(A):A:H2'	1:1A:363(B):G:C8	2.42	0.55
1:1A:1796:U:H2'	1:1A:1797:C:C6	2.42	0.55
35:1d:112:VAL:H	35:1d:116:GLN:NE2	2.05	0.55
48:1q:66:SER:HB3	48:1q:69:LYS:HB2	1.89	0.55
1:2A:1239:G:H2'	1:2A:1240:U:O4'	2.06	0.55
8:2I:130:TYR:HD2	8:2I:138:ILE:HD12	1.70	0.55
36:2e:84:PHE:O	36:2e:86:ALA:N	2.39	0.55
42:2k:48:ILE:O	42:2k:50:TYR:N	2.30	0.55
1:1A:446:G:OP1	16:1U:3:ARG:NH1	2.40	0.54
1:1A:740:U:OP2	61:1A:4252:HOH:O	2.18	0.54
1:1A:1188:U:H4'	17:1V:79:VAL:HG22	1.88	0.54
1:1A:1406:U:H2'	1:1A:1407:C:C6	2.42	0.54
1:1A:2134:A:O2'	1:1A:2135:A:OP1	2.21	0.54
1:1A:2467:C:H4'	12:1Q:123:HIS:CD2	2.42	0.54
12:1Q:54:MET:HG2	12:1Q:117:ALA:HB1	1.88	0.54
35:1d:98:GLU:OE1	35:1d:103:ASN:ND2	2.40	0.54
35:1d:173:TRP:CD1	35:1d:173:TRP:H	2.23	0.54
50:1s:50:ALA:HB1	50:1s:57:HIS:HB3	1.89	0.54
9:2N:103:VAL:HG11	9:2N:120:LEU:HD22	1.89	0.54
32:2a:1305:G:N2	32:2a:1331:G:H1'	2.22	0.54
32:2a:1347:G:H22	32:2a:1373:G:H2'	1.70	0.54
35:2d:189:PRO:HB2	35:2d:194:LEU:HD21	1.89	0.54
19:1X:94:GLY:H	19:1X:95:LEU:HB2	1.72	0.54
32:1a:1459:C:OP1	51:1t:31:SER:OG	2.25	0.54
36:1e:89:ILE:HG12	36:1e:135:THR:HG22	1.89	0.54
50:1s:12:ASP:OD2	50:1s:35:SER:OG	2.25	0.54
31:29:16:VAL:HG22	31:29:25:VAL:HG22	1.89	0.54
37:2f:69:GLU:CD	37:2f:69:GLU:H	2.15	0.54
1:1A:1518:U:H2'	1:1A:1519:G:O4'	2.08	0.54
4:1E:55:ASN:HB3	4:1E:58:ARG:HG3	1.88	0.54
6:2G:44:GLY:HA2	6:2G:88:ILE:HG22	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:2V:43:GLU:OE1	17:2V:43:GLU:N	2.40	0.54
32:2a:148:G:H2'	32:2a:149:A:C8	2.42	0.54
32:2a:1066:C:H2'	32:2a:1067:A:C8	2.43	0.54
33:2b:17:PHE:HA	33:2b:44:LEU:HD11	1.89	0.54
33:2b:178:ARG:HH12	39:2h:68:ARG:NH2	2.04	0.54
33:2b:223:ILE:HA	33:2b:226:ARG:HG2	1.89	0.54
1:1A:1025:G:C4	1:1A:1135:C:H1'	2.41	0.54
22:20:15:ASP:OD1	22:20:16:SER:N	2.39	0.54
32:2a:19:C:H5''	36:2e:86:ALA:HB1	1.90	0.54
1:1A:897:C:H2'	1:1A:898:C:C6	2.42	0.54
1:1A:2319:G:N1	14:1S:3:ARG:HA	2.22	0.54
32:1a:683:G:H2'	32:1a:684:A:C8	2.43	0.54
32:1a:1036:G:H3'	32:1a:1037:C:C6	2.42	0.54
37:1f:99:ALA:O	49:1r:28:GLU:HA	2.07	0.54
15:2T:26:ASP:OD1	15:2T:120:ARG:NH2	2.34	0.54
30:28:14:VAL:HG22	30:28:24:ALA:HB2	1.89	0.54
32:2a:328:C:H4'	32:2a:329:A:H5'	1.89	0.54
44:2m:40:ASN:HB3	44:2m:43:THR:HG23	1.89	0.54
54:2w:68:C:H2'	54:2w:69:G:C8	2.42	0.54
15:1T:29:ARG:HG3	15:1T:46:GLU:HB2	1.89	0.54
18:1W:68:ARG:NH1	18:1W:112:GLY:H	2.06	0.54
32:1a:1277:C:O2'	32:1a:1279:A:H1'	2.07	0.54
41:1j:61:GLU:OE2	45:1n:58:LYS:NZ	2.35	0.54
54:1y:63:G:H2'	54:1y:64:A:O4'	2.08	0.54
1:2A:296:C:O3'	20:2Y:95:LYS:NZ	2.40	0.54
1:2A:1405:U:H2'	1:2A:1406:U:C6	2.42	0.54
1:2A:1924:C:H4'	55:2x:13:C:O2'	2.08	0.54
11:2P:85:LEU:HA	11:2P:88:LEU:HD12	1.89	0.54
32:2a:692:U:O2'	32:2a:694:A:N7	2.38	0.54
32:2a:936:C:H2'	32:2a:937:A:O4'	2.06	0.54
32:2a:1241:G:H2'	32:2a:1242:C:C6	2.42	0.54
32:2a:1298:C:OP2	38:2g:114:ARG:NH2	2.20	0.54
32:2a:1506:U:OP1	61:2a:1915:HOH:O	2.18	0.54
1:1A:1379:A:H4'	1:1A:1380:G:OP2	2.08	0.54
32:1a:405:U:OP2	35:1d:3:ARG:NH1	2.40	0.54
1:2A:857:C:OP2	22:20:77:ARG:NH2	2.40	0.54
6:2G:19:LEU:HD23	6:2G:32:PRO:HD2	1.89	0.54
32:2a:1051:C:H2'	32:2a:1052:U:H6	1.72	0.54
39:2h:51:VAL:HG12	39:2h:52:ASP:H	1.71	0.54
41:2j:55:LYS:O	41:2j:57:LYS:N	2.41	0.54
1:1A:301:G:OP2	20:1Y:84:ARG:NH2	2.40	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1456:G:OP2	61:1A:4253:HOH:O	2.18	0.54
26:14:46:GLN:O	26:14:48:ARG:N	2.40	0.54
28:16:13:CYS:SG	28:16:47:THR:HG21	2.48	0.54
32:1a:79:G:N2	32:1a:90:U:O2'	2.41	0.54
32:1a:1218:C:H2'	32:1a:1219:U:C6	2.42	0.54
1:2A:1149:G:H2'	1:2A:1150:C:C6	2.42	0.54
1:2A:2870:C:H2'	1:2A:2871:C:O4'	2.08	0.54
32:2a:17:U:H2'	32:2a:18:C:C6	2.42	0.54
32:2a:952:U:H2'	32:2a:953:G:C8	2.43	0.54
32:2a:979:C:OP1	32:2a:1223:C:N4	2.41	0.54
32:2a:1132:C:H42	32:2a:1142:G:H1	1.56	0.54
32:2a:1352:C:H2'	32:2a:1353:G:C8	2.42	0.54
1:1A:1588:C:H2'	1:1A:1589:C:H6	1.73	0.54
24:12:22:GLU:OE2	24:12:68:ARG:NH2	2.36	0.54
32:1a:560:U:O2'	32:1a:561:U:OP2	2.21	0.54
32:1a:613:C:H2'	32:1a:614:A:C8	2.41	0.54
32:1a:1036:G:H5''	32:1a:1037:C:C5	2.43	0.54
33:1b:16:HIS:HB2	33:1b:204:ASN:HB3	1.90	0.54
1:2A:630:G:OP1	30:28:47:LYS:NZ	2.41	0.54
1:2A:729:G:O5'	3:2D:208:LYS:NZ	2.41	0.54
1:2A:1803:A:O2'	3:2D:259:THR:HG21	2.08	0.54
8:2I:31:LEU:HD21	8:2I:38:LEU:HG	1.89	0.54
11:2P:50:ARG:HD3	30:28:7:HIS:HD2	1.72	0.54
19:2X:4:ALA:HB1	19:2X:42:ALA:HA	1.90	0.54
32:2a:407:G:H5''	35:2d:115:ARG:HB3	1.89	0.54
32:2a:1166:G:N2	32:2a:1170:A:OP2	2.34	0.54
7:1H:148:ILE:HA	7:1H:151:ILE:HD12	1.90	0.54
32:1a:674:G:H2'	32:1a:675:A:H8	1.72	0.54
2:2B:2:C:H2'	2:2B:3:C:C6	2.43	0.54
10:2O:76:ALA:HB3	15:2T:75:ILE:HB	1.90	0.54
12:2Q:2:LEU:HB3	12:2Q:69:PHE:CE1	2.43	0.54
21:2Z:145:GLU:HB3	21:2Z:148:ASP:HB2	1.90	0.54
32:2a:1318:A:H1'	50:2s:37:ARG:HH21	1.72	0.54
40:2i:64:THR:OG1	40:2i:66:ARG:NH1	2.41	0.54
21:1Z:93:ASP:HB3	21:1Z:131:ARG:HH22	1.73	0.53
32:1a:250:A:H4'	32:1a:251:G:O5'	2.08	0.53
33:2b:12:GLU:HB2	33:2b:213:LEU:HD21	1.90	0.53
33:2b:84:GLU:HA	33:2b:87:ARG:HB3	1.90	0.53
35:2d:10:ARG:HG3	35:2d:11:LEU:HD12	1.90	0.53
36:2e:41:VAL:O	36:2e:66:MET:HA	2.08	0.53
39:2h:69:ARG:HG3	39:2h:76:PRO:HA	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1794:U:H2'	1:2A:1795:C:C6	2.43	0.53
1:2A:1889:A:H2'	1:2A:1890:A:C8	2.42	0.53
5:2F:178:PRO:HB3	5:2F:198:ALA:HA	1.89	0.53
21:2Z:150:LEU:H	21:2Z:171:ILE:HD11	1.72	0.53
32:2a:8:A:N6	35:2d:205:GLU:O	2.41	0.53
36:2e:100:VAL:HG12	36:2e:118:ILE:HG22	1.90	0.53
37:2f:97:PHE:HE2	49:2r:62:GLU:HG2	1.74	0.53
47:2p:28:ARG:NH1	47:2p:29:ASP:OD1	2.41	0.53
54:2w:56:C:H2'	54:2w:57:G:O4'	2.09	0.53
38:1g:22:LEU:HG	38:1g:62:PHE:HE2	1.73	0.53
44:1m:84:ILE:HB	50:1s:66:MET:HE2	1.90	0.53
1:2A:2127:G:H2'	1:2A:2128:C:C6	2.43	0.53
1:2A:2377:A:H2'	1:2A:2378:A:C8	2.44	0.53
5:2F:155:LEU:HB2	5:2F:189:THR:HG21	1.91	0.53
10:2O:115:VAL:HG13	10:2O:121:VAL:HG21	1.89	0.53
17:2V:60:GLU:HB2	17:2V:97:LYS:HE2	1.90	0.53
21:2Z:102:LEU:HB2	21:2Z:104:PHE:HE2	1.73	0.53
32:2a:600:C:H2'	32:2a:601:C:C6	2.43	0.53
32:2a:1246:C:H2'	32:2a:1247:U:H6	1.73	0.53
33:2b:185:ILE:HB	33:2b:199:TYR:HB2	1.90	0.53
34:2c:9:GLY:HA2	34:2c:12:LEU:HG	1.89	0.53
1:1A:96:G:OP1	24:12:46:GLN:NE2	2.41	0.53
1:1A:1580:A:OP2	1:1A:1580:A:H8	1.91	0.53
1:1A:2483:C:N3	12:1Q:124:LYS:NZ	2.53	0.53
21:1Z:41:LEU:HD11	21:1Z:83:PRO:HG2	1.90	0.53
32:1a:1531:A:H8	32:1a:1531:A:O5'	1.90	0.53
35:1d:108:LEU:HD21	35:1d:174:LEU:HD22	1.89	0.53
1:2A:271(P):C:O3'	8:2I:42:SER:OG	2.26	0.53
7:2H:88:LEU:HD12	7:2H:165:ALA:HA	1.91	0.53
9:2N:96:GLU:CD	9:2N:96:GLU:H	2.16	0.53
32:2a:957:U:H2'	32:2a:959:A:OP2	2.08	0.53
33:2b:45:GLN:HG2	33:2b:48:MET:HE2	1.89	0.53
34:2c:121:ALA:HB1	34:2c:188:LEU:O	2.08	0.53
34:2c:189:ALA:HB3	34:2c:196:LEU:HB2	1.91	0.53
1:1A:1588:C:H2'	1:1A:1589:C:C6	2.44	0.53
1:2A:1007:C:OP1	9:2N:35:ARG:NH1	2.39	0.53
1:2A:1629:U:O4	61:2A:3948:HOH:O	2.14	0.53
1:2A:1645:G:H5''	1:2A:1646:C:H5'	1.90	0.53
19:2X:57:LEU:HD11	19:2X:78:LYS:HE2	1.90	0.53
32:2a:1255:G:OP1	41:2j:45:ARG:NH2	2.40	0.53
1:1A:1587:A:H2'	1:1A:1588:C:C6	2.44	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:373:A:H2'	32:1a:374:A:H8	1.72	0.53
32:1a:1239:A:H62	32:1a:1299:A:N6	2.07	0.53
1:2A:2136:C:O2'	1:2A:2137:C:O5'	2.27	0.53
32:2a:1042:G:H2'	32:2a:1043:C:O4'	2.09	0.53
32:2a:1142:G:H3'	32:2a:1143:G:H8	1.73	0.53
32:2a:1208:C:H2'	32:2a:1209:C:H6	1.72	0.53
32:2a:1286:A:C8	32:2a:1287:A:H4'	2.43	0.53
32:2a:1417:G:O6	61:2a:1913:HOH:O	2.17	0.53
54:2y:5:G:H1	54:2y:68:C:N4	2.03	0.53
54:2y:61:C:H2'	54:2y:62:C:C6	2.44	0.53
1:1A:631:A:OP1	11:1P:65:ARG:NE	2.35	0.53
1:1A:1062:G:P	1:1A:1070:A:H1'	2.48	0.53
32:1a:1442:G:H2'	32:1a:1442:G:N3	2.23	0.53
54:1y:40:C:H2'	54:1y:41:C:H6	1.74	0.53
20:2Y:8:LYS:HD3	20:2Y:97:ARG:NH1	2.24	0.53
21:2Z:152:ALA:HB1	21:2Z:163:LEU:HD11	1.90	0.53
32:2a:263:A:OP1	51:2t:79:ARG:NH1	2.42	0.53
32:2a:1049:U:C6	32:2a:1201:A:H5'	2.43	0.53
1:1A:729:G:C6	3:1D:208:LYS:HB2	2.43	0.53
1:1A:832:G:N3	11:1P:53:GLY:HA3	2.24	0.53
20:1Y:43:ASN:HB3	20:1Y:65:ALA:HB3	1.91	0.53
21:1Z:75:ASN:O	21:1Z:84:GLU:HG3	2.08	0.53
44:1m:67:GLU:HG3	44:1m:71:ARG:NH2	2.24	0.53
1:2A:1696:G:N7	61:2A:4054:HOH:O	2.34	0.53
1:2A:2167:U:H3'	1:2A:2168:G:H21	1.73	0.53
21:2Z:40:ASP:OD2	21:2Z:43:GLU:N	2.33	0.53
33:2b:69:LEU:HD13	33:2b:155:LEU:HD22	1.91	0.53
34:2c:136:GLN:HA	34:2c:139:GLN:HB3	1.90	0.53
54:2w:19:G:N2	54:2w:56:C:N3	2.55	0.53
1:1A:2235:G:N7	61:1A:4337:HOH:O	2.34	0.53
39:1h:124:ALA:O	39:1h:128:GLY:N	2.34	0.53
55:1x:8:4SU:O5'	55:1x:8:4SU:H6	2.09	0.53
1:2A:586:A:N1	1:2A:809:G:O2'	2.35	0.53
4:2E:9:VAL:HG13	15:2T:3:ARG:HG2	1.89	0.53
6:2G:15:VAL:HG22	6:2G:175:LEU:HB3	1.91	0.53
28:26:47:THR:HB	28:26:49:HIS:HE1	1.73	0.53
32:2a:130:A:O2'	32:2a:131:C:O5'	2.26	0.53
34:2c:68:VAL:HG23	34:2c:101:LEU:HD21	1.91	0.53
54:2y:7:A:O2'	54:2y:49:C:O4'	2.25	0.53
1:1A:2687:U:H2'	1:1A:2688:U:O4'	2.09	0.53
32:1a:1074:G:O2'	32:1a:1101:A:N1	2.41	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:531:C:H4'	1:2A:532:A:H5''	1.91	0.53
21:2Z:31:ARG:HG3	21:2Z:32:HIS:CD2	2.44	0.53
32:2a:545:C:O2'	32:2a:549:C:OP1	2.22	0.53
32:2a:768:A:OP2	61:2a:1916:HOH:O	2.19	0.53
32:2a:1129:C:H2'	32:2a:1139:G:N7	2.24	0.53
38:2g:115:ARG:HB2	38:2g:118:VAL:HG23	1.89	0.53
6:1G:66:GLN:HG3	26:14:1:MET:HE1	1.91	0.52
32:1a:848:C:H2'	32:1a:849:C:C6	2.44	0.52
35:1d:178:VAL:O	35:1d:180:GLY:N	2.38	0.52
1:2A:27:G:N2	1:2A:512:G:H1'	2.24	0.52
1:2A:455:C:N3	1:2A:472:A:H2'	2.25	0.52
1:2A:1188:U:H4'	17:2V:79:VAL:HG22	1.89	0.52
15:2T:60:THR:HG22	15:2T:77:PRO:HA	1.91	0.52
21:2Z:4:ARG:HG2	21:2Z:58:VAL:HB	1.90	0.52
32:2a:1002:G:C2	32:2a:1003:G:H1'	2.44	0.52
32:2a:1376:U:H2'	32:2a:1377:A:C8	2.44	0.52
35:2d:98:GLU:OE1	35:2d:103:ASN:ND2	2.41	0.52
48:2q:58:GLU:OE2	48:2q:75:ARG:NH2	2.42	0.52
1:1A:994:C:OP1	16:1U:53:ARG:NH2	2.43	0.52
1:1A:2131:G:H5'	1:1A:2133:G:C8	2.44	0.52
6:1G:34:LEU:HD23	6:1G:161:THR:HG22	1.91	0.52
33:1b:12:GLU:O	33:1b:15:VAL:HG22	2.09	0.52
1:2A:2693:A:H2'	1:2A:2694:G:H8	1.74	0.52
32:2a:1054:C:C5	54:2w:34:G:H1'	2.44	0.52
33:2b:97:TRP:CH2	33:2b:101:MET:HB2	2.45	0.52
1:1A:1165:U:H2'	1:1A:1166:C:C6	2.44	0.52
2:1B:103:G:H21	21:1Z:73:GLN:NE2	2.05	0.52
12:1Q:85:LYS:HG2	22:10:7:LEU:HB3	1.90	0.52
26:14:15:ILE:HG13	26:14:21:VAL:HG22	1.91	0.52
32:1a:598:U:H4'	39:1h:94:TYR:CD2	2.44	0.52
32:1a:674:G:H2'	32:1a:675:A:C8	2.45	0.52
32:1a:1027:C:N1	32:1a:1034:G:N2	2.57	0.52
33:1b:163:PHE:HA	33:1b:185:ILE:HG12	1.90	0.52
39:1h:53:VAL:HB	39:1h:58:TYR:CD2	2.45	0.52
1:2A:143:G:H2'	1:2A:143(A):C:C6	2.44	0.52
32:2a:109:A:C6	32:2a:326:G:C6	2.97	0.52
32:2a:987:G:H1	32:2a:1218:C:H42	1.57	0.52
33:2b:50:GLU:O	33:2b:54:THR:OG1	2.24	0.52
34:2c:58:GLU:HB3	41:2j:92:THR:HG21	1.90	0.52
41:2j:68:HIS:CD2	41:2j:68:HIS:H	2.27	0.52
1:1A:484:C:H2'	1:1A:485:C:H6	1.74	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:588:U:H2'	1:1A:589:C:C6	2.44	0.52
1:1A:1693:U:H1'	3:1D:14:ARG:NH1	2.23	0.52
11:1P:89:ALA:HA	11:1P:121:LYS:HD3	1.92	0.52
32:1a:1166:G:N2	32:1a:1170:A:OP2	2.43	0.52
34:1c:21:ARG:NH2	34:1c:56:ASP:OD2	2.33	0.52
55:1x:75:C:OP1	61:1x:203:HOH:O	2.19	0.52
1:2A:792:G:O6	61:2A:3942:HOH:O	2.13	0.52
1:2A:2419:U:H2'	1:2A:2420:C:C6	2.45	0.52
9:2N:43:THR:HG22	9:2N:44:PRO:HD2	1.91	0.52
32:2a:707:C:H2'	32:2a:708:C:C6	2.44	0.52
32:2a:1279:A:H5''	32:2a:1280:A:OP1	2.10	0.52
37:2f:61:LEU:HB3	37:2f:63:TYR:CE2	2.44	0.52
51:2t:9:ASN:O	51:2t:10:LEU:HB2	2.10	0.52
32:1a:129:U:H5'	48:1q:3:LYS:NZ	2.24	0.52
32:1a:160:A:H1'	32:1a:344:A:C5	2.44	0.52
32:1a:1391:U:H2'	32:1a:1392:G:C8	2.45	0.52
46:1o:74:ASP:HB3	46:1o:77:ARG:HB2	1.92	0.52
1:2A:2079:U:O3'	23:21:35:THR:OG1	2.25	0.52
1:2A:2128:C:H2'	1:2A:2129:C:O4'	2.10	0.52
1:2A:2557:G:H2'	1:2A:2558:C:H6	1.75	0.52
2:2B:6:C:H2'	2:2B:7:G:C8	2.44	0.52
6:2G:16:ARG:O	6:2G:20:ILE:HG13	2.08	0.52
14:2S:25:ARG:HB3	14:2S:40:ILE:HB	1.92	0.52
33:2b:149:LEU:HA	33:2b:152:PHE:HB3	1.91	0.52
37:2f:67:MET:HE1	37:2f:75:LEU:HD22	1.90	0.52
1:1A:2331:G:O2'	1:1A:2336:A:N1	2.38	0.52
1:1A:2794:C:H42	1:1A:2802:G:H22	1.57	0.52
32:1a:165:C:H2'	32:1a:166:G:H8	1.75	0.52
33:1b:12:GLU:C	33:1b:14:GLY:H	2.18	0.52
1:2A:774:A:H2'	1:2A:774:A:N3	2.24	0.52
16:2U:85:LYS:HB3	16:2U:116:ALA:HB1	1.91	0.52
32:2a:148:G:H2'	32:2a:149:A:H8	1.75	0.52
32:2a:660:G:H1	32:2a:745:C:H42	1.58	0.52
36:2e:18:ARG:NH2	36:2e:25:ARG:HD2	2.25	0.52
39:2h:41:ARG:NH2	39:2h:123:GLU:OE2	2.43	0.52
41:2j:78:ASN:O	41:2j:80:LYS:N	2.42	0.52
1:1A:271(E):U:H2'	1:1A:271(F):C:C6	2.44	0.52
1:1A:1011:G:OP1	16:1U:77:SER:OG	2.26	0.52
1:1A:1213:A:N3	1:1A:1238:G:O2'	2.41	0.52
11:1P:98:GLU:O	11:1P:101:VAL:HG12	2.10	0.52
32:1a:1118:C:H1'	32:1a:1179:A:C4	2.45	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1c:125:GLU:HG3	34:1c:189:ALA:HB1	1.92	0.52
1:2A:300:A:OP1	20:2Y:86:ARG:NH2	2.37	0.52
1:2A:1790:C:H5''	1:2A:1791:A:OP1	2.09	0.52
1:2A:2846:G:N7	61:2A:4058:HOH:O	2.34	0.52
32:2a:56:U:H2'	32:2a:57:G:C8	2.45	0.52
32:2a:1445:C:O2'	32:2a:1447:A:N6	2.43	0.52
33:2b:47:THR:HG23	33:2b:202:PRO:HD2	1.92	0.52
33:2b:58:ILE:O	33:2b:62:ALA:N	2.37	0.52
34:2c:137:ALA:HA	34:2c:140:ARG:HH12	1.73	0.52
38:2g:23:VAL:O	38:2g:27:ILE:HG13	2.09	0.52
54:2y:9:A:H5'	54:2y:46:G7M:N3	2.24	0.52
1:1A:1187:G:H5''	17:1V:81:TYR:CE1	2.45	0.52
1:1A:1359:A:C2	1:1A:1372:U:O4	2.63	0.52
1:1A:2564:A:C2	1:1A:2647:U:H4'	2.44	0.52
32:1a:359:U:H2'	32:1a:360:A:C8	2.44	0.52
32:1a:715:A:H2'	32:1a:716:A:C8	2.44	0.52
51:1t:47:GLY:N	51:1t:48:LYS:HB2	2.25	0.52
1:2A:652(T):C:H2'	1:2A:652(U):G:C8	2.45	0.52
1:2A:1364:G:P	23:21:3:LYS:HG3	2.50	0.52
1:2A:2794:C:N4	1:2A:2802:G:O6	2.43	0.52
18:2W:18:ARG:HG2	18:2W:76:VAL:HB	1.91	0.52
32:2a:1010:G:N2	32:2a:1020:U:O2'	2.43	0.52
39:2h:51:VAL:HG11	39:2h:60:ARG:NH2	2.24	0.52
6:1G:3:LEU:HD12	6:1G:5:VAL:HG12	1.92	0.52
41:1j:8:LEU:HD22	41:1j:96:ILE:HG22	1.91	0.52
5:2F:129:PHE:CD2	5:2F:163:VAL:HG21	2.45	0.52
14:2S:49:VAL:HG23	14:2S:80:LEU:HD12	1.92	0.52
32:2a:280:C:N4	48:2q:39:SER:OG	2.39	0.52
32:2a:473:G:H2'	32:2a:474:G:H8	1.75	0.52
32:2a:1014:A:OP2	50:2s:18:LYS:NZ	2.29	0.52
32:2a:1048:G:OP1	45:2n:3:ARG:HB3	2.10	0.52
44:2m:33:ALA:HB1	44:2m:59:TYR:HE2	1.74	0.52
50:2s:30:LEU:HD22	50:2s:31:ILE:H	1.74	0.52
1:1A:1371:G:N7	61:1A:4336:HOH:O	2.34	0.52
5:1F:53:THR:CG2	5:1F:55:GLY:H	2.23	0.52
11:1P:125:VAL:HG23	11:1P:145:PRO:HA	1.91	0.52
27:15:40:LYS:NZ	27:15:44:THR:O	2.42	0.52
32:1a:189(B):C:H2'	32:1a:189(C):C:C6	2.46	0.52
32:1a:195:A:OP1	51:1t:68:LYS:NZ	2.40	0.52
33:1b:33:TYR:HB2	33:1b:43:ASP:HB2	1.92	0.52
33:1b:67:THR:N	33:1b:160:ASP:OD1	2.43	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2D:125:ILE:HB	37:2f:81:ILE:HD11	1.92	0.52
32:2a:340:U:H2'	32:2a:341:C:C6	2.45	0.52
51:2t:47:GLY:HA2	51:2t:48:LYS:C	2.35	0.52
1:1A:1176:G:N2	1:1A:1178:C:O5'	2.44	0.51
32:1a:920:U:H2'	32:1a:921:U:C6	2.45	0.51
32:1a:1518:MA6:H93	32:1a:1519:MA6:H92	1.92	0.51
54:1y:8:4SU:H4'	54:1y:48:C:H4'	1.92	0.51
1:2A:2171:A:H1'	1:2A:2172:U:C6	2.45	0.51
26:24:46:GLN:HE21	26:24:48:ARG:HB2	1.76	0.51
32:2a:171:A:H2'	32:2a:172:A:C8	2.45	0.51
48:2q:95:TYR:HA	48:2q:98:LEU:HG	1.92	0.51
50:2s:3:ARG:NH1	50:2s:7:LYS:HB2	2.25	0.51
1:1A:721:C:H2'	1:1A:722:A:C8	2.45	0.51
1:1A:918:A:N3	2:1B:80:U:O2'	2.36	0.51
5:1F:184:TYR:CE2	5:1F:188:ARG:HD2	2.45	0.51
9:1N:13:TRP:CE2	9:1N:133:GLN:HG2	2.45	0.51
32:1a:79:G:O6	32:1a:90:U:O2	2.28	0.51
32:1a:1316:G:H5''	45:1n:17:LYS:HE3	1.92	0.51
44:1m:11:ARG:C	44:1m:13:LYS:H	2.18	0.51
1:2A:854:G:H2'	1:2A:855:G:C8	2.44	0.51
1:2A:1187:G:H5'	17:2V:81:TYR:CE1	2.46	0.51
1:2A:2138:C:H2'	1:2A:2139:C:O4'	2.10	0.51
5:2F:64:ILE:HG21	5:2F:78:ILE:HG23	1.91	0.51
10:2O:35:VAL:HG13	10:2O:65:THR:HG23	1.92	0.51
12:2Q:37:LEU:HD21	12:2Q:130:LYS:HE2	1.91	0.51
32:2a:222:U:H2'	32:2a:223:U:C6	2.46	0.51
32:2a:447:G:O6	32:2a:485:G:O2'	2.23	0.51
32:2a:814:A:H2'	32:2a:816:A:H5''	1.93	0.51
32:2a:959:A:O2'	32:2a:984:C:O2'	2.26	0.51
33:2b:16:HIS:CG	33:2b:17:PHE:N	2.78	0.51
48:2q:44:ALA:HB1	48:2q:73:VAL:HG23	1.91	0.51
52:2u:6:ARG:HD3	52:2u:15:ARG:HD2	1.91	0.51
1:1A:882:G:H4'	54:1w:19:G:O6	2.11	0.51
1:1A:1427:A:H4'	1:1A:1428:C:O4'	2.10	0.51
1:1A:1783:A:N7	61:1A:4340:HOH:O	2.34	0.51
1:1A:2102:U:H3	1:1A:2187:G:H1	1.59	0.51
1:1A:2206:G:H5''	1:1A:2207:G:C5	2.45	0.51
32:1a:1125:U:H4'	41:1j:5:ARG:HH22	1.75	0.51
35:1d:105:VAL:HG13	35:1d:110:PHE:HB2	1.92	0.51
35:1d:173:TRP:CZ3	35:1d:174:LEU:HG	2.45	0.51
50:1s:51:VAL:O	50:1s:58:VAL:N	2.39	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:24:40:HIS:HB3	26:24:43:TYR:HB2	1.93	0.51
32:2a:504:C:OP1	61:2a:1918:HOH:O	2.19	0.51
35:2d:12:CYS:HB3	35:2d:19:LEU:H	1.75	0.51
50:2s:20:LEU:HA	50:2s:23:ASN:HB2	1.91	0.51
1:1A:1364:G:N7	23:11:3:LYS:HD2	2.25	0.51
12:1Q:103:MET:HE1	12:1Q:125:LEU:HD13	1.92	0.51
28:16:47:THR:HG22	28:16:48:VAL:O	2.10	0.51
32:1a:985:C:H2'	32:1a:986:A:H8	1.75	0.51
1:2A:271(O):C:H4'	8:2I:49:ALA:HB1	1.93	0.51
1:2A:1794:U:H2'	1:2A:1795:C:H6	1.76	0.51
1:2A:2638:G:P	4:2E:82:ARG:HH22	2.34	0.51
6:2G:173:LEU:HB3	6:2G:178:PHE:CD1	2.45	0.51
32:2a:1256:A:N1	32:2a:1278:U:H1'	2.26	0.51
36:2e:8:GLU:HG2	36:2e:34:VAL:HG12	1.92	0.51
36:2e:146:ALA:O	36:2e:150:ARG:HG2	2.11	0.51
38:2g:75:VAL:HG13	38:2g:145:ALA:HA	1.93	0.51
41:2j:8:LEU:HA	41:2j:96:ILE:HA	1.92	0.51
1:1A:34:C:H5''	1:1A:35:G:OP2	2.10	0.51
1:1A:1113:U:H2'	1:1A:1114:G:C8	2.46	0.51
2:1B:31:C:H4'	6:1G:29:TRP:CH2	2.46	0.51
10:1O:68:GLU:OE1	10:1O:78:ARG:NH1	2.44	0.51
32:1a:432:A:H3'	32:1a:433:C:H6	1.76	0.51
32:1a:438:G:H4'	35:1d:123:HIS:CE1	2.46	0.51
39:1h:83:ILE:HG13	39:1h:137:VAL:HG22	1.91	0.51
40:1i:8:GLY:HA3	40:1i:76:ALA:O	2.11	0.51
1:2A:2136:C:H42	1:2A:2155:G:H1	1.58	0.51
5:2F:110:LEU:HD11	5:2F:181:LEU:HD23	1.92	0.51
32:2a:1321:C:H4'	44:2m:87:TYR:CE2	2.46	0.51
38:2g:72:ARG:NH2	38:2g:142:GLU:OE2	2.43	0.51
1:1A:251:A:C5	1:1A:252:G:H1'	2.45	0.51
1:1A:1416:G:O2'	1:1A:1417:C:OP2	2.26	0.51
1:1A:1889:A:H2'	1:1A:1890:A:C8	2.46	0.51
1:1A:2182:G:H2'	1:1A:2183:C:C6	2.46	0.51
32:1a:626:U:H2'	32:1a:627:G:C8	2.46	0.51
32:1a:741:G:H2'	32:1a:742:G:O4'	2.11	0.51
1:2A:1171:G:H1	1:2A:1178:C:H42	1.58	0.51
3:2D:182:LEU:HB2	3:2D:272:ALA:HB3	1.93	0.51
14:2S:66:ALA:O	14:2S:69:VAL:HG12	2.11	0.51
23:21:72:GLU:O	23:21:76:ARG:HG2	2.11	0.51
32:2a:1246:C:H2'	32:2a:1247:U:C6	2.46	0.51
33:2b:52:GLU:O	33:2b:56:ARG:HB3	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:2o:26:GLU:N	46:2o:26:GLU:OE1	2.44	0.51
1:1A:1077:A:C5	1:1A:1078:U:H1'	2.45	0.51
1:1A:2849:U:OP2	15:1T:95:ARG:NH1	2.44	0.51
32:1a:974:A:H8	32:1a:974:A:OP1	1.94	0.51
34:1c:13:GLY:HA3	45:1n:57:ARG:NH1	2.26	0.51
1:2A:1022:G:N2	1:2A:1023:U:O4	2.42	0.51
1:2A:1916:A:H2'	1:2A:1917:PSU:O4'	2.10	0.51
32:2a:1005:A:N6	32:2a:1024:G:H1'	2.26	0.51
32:2a:1014:A:H1'	50:2s:34:TRP:HB2	1.92	0.51
32:2a:1263:C:N4	32:2a:1271:G:O6	2.44	0.51
32:2a:1513:A:H2'	32:2a:1514:C:C6	2.46	0.51
1:2A:1032:A:H2	1:2A:1122:G:H22	1.58	0.51
1:2A:1336:A:H2'	1:2A:1337:G:C8	2.46	0.51
1:2A:1742:G:O6	61:2A:3959:HOH:O	2.18	0.51
1:2A:2340:G:H2'	1:2A:2341:G:C8	2.45	0.51
6:2G:39:ILE:HB	6:2G:92:VAL:HG13	1.91	0.51
14:2S:14:VAL:O	14:2S:18:ILE:HG12	2.10	0.51
32:2a:176:C:H2'	32:2a:177:C:H6	1.74	0.51
32:2a:1216:G:OP1	45:2n:2:ALA:HA	2.11	0.51
35:2d:57:ARG:HB3	35:2d:206:PHE:HB2	1.93	0.51
54:2y:18:G:N1	54:2y:55:PSU:C4	2.73	0.51
1:1A:528:A:O2'	1:1A:529:A:H5'	2.11	0.51
1:1A:593:G:H4'	30:18:4:MET:HE2	1.92	0.51
1:1A:1827:C:H2'	1:1A:1828:G:H5'	1.93	0.51
1:1A:2445:G:OP1	5:1F:74:ARG:NH2	2.41	0.51
32:1a:524:G:H2'	32:1a:525:C:C6	2.45	0.51
32:1a:1144:G:H21	32:1a:1146:A:H62	1.59	0.51
33:1b:16:HIS:HD2	33:1b:204:ASN:H	1.59	0.51
33:1b:55:PHE:CD1	33:1b:221:LEU:HD22	2.46	0.51
1:2A:113:G:OP1	61:2A:3962:HOH:O	2.20	0.51
1:2A:582:G:H2'	1:2A:583:G:C8	2.46	0.51
1:2A:1827:C:OP2	3:2D:222:ARG:NH1	2.44	0.51
1:2A:2408:U:H2'	1:2A:2409:G:C8	2.46	0.51
1:2A:2857:G:N2	1:2A:2860:A:OP2	2.42	0.51
21:2Z:99:TYR:HA	21:2Z:124:ILE:O	2.11	0.51
32:2a:984:C:H2'	32:2a:985:C:H6	1.74	0.51
1:1A:801:G:O6	5:1F:53:THR:OG1	2.28	0.51
1:1A:1466:G:HO2'	1:1A:1546:C:HO2'	1.54	0.51
1:1A:1648:C:OP1	61:1A:4229:HOH:O	2.19	0.51
1:1A:1899:G:N3	1:1A:1899:G:H2'	2.26	0.51
1:1A:1913:A:H4'	1:1A:1914:C:H5''	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2602:A:C5	55:1x:76:A:O3'	2.64	0.51
1:1A:2611:U:H5'	1:1A:2611:U:H6	1.76	0.51
32:1a:1025:U:C2	32:1a:1036:G:O6	2.64	0.51
43:1l:88:GLY:O	43:1l:99:HIS:HD2	1.94	0.51
46:1o:82:ILE:O	46:1o:86:GLY:N	2.44	0.51
49:1r:32:ARG:HA	49:1r:69:THR:HG21	1.92	0.51
1:2A:1171:G:H1	1:2A:1178:C:N4	2.08	0.51
1:2A:1178:C:H2'	1:2A:1179:C:C6	2.46	0.51
1:2A:2128:C:H4'	1:2A:2174:C:H4'	1.93	0.51
14:2S:94:TYR:CE2	14:2S:99:LYS:HG3	2.46	0.51
20:2Y:13:VAL:HG12	20:2Y:74:PRO:HA	1.92	0.51
32:2a:588:G:OP2	61:2a:1917:HOH:O	2.19	0.51
33:2b:96:ARG:O	33:2b:98:LEU:HD12	2.10	0.51
34:2c:162:GLN:NE2	53:2v:24:A:O3'	2.36	0.51
47:2p:27:LYS:HG3	47:2p:30:GLY:HA3	1.93	0.51
54:2w:18:G:H4'	54:2w:60:U:C5	2.46	0.51
55:2x:8:4SU:O5'	55:2x:8:4SU:H6	2.11	0.51
1:1A:443:A:H1'	1:1A:1201:C:O4'	2.11	0.50
1:1A:1058:G:N2	1:1A:1080:C:N3	2.57	0.50
1:1A:1266:G:O5'	18:1W:15:ARG:NH2	2.44	0.50
8:1I:72:LEU:HD21	8:1I:101:LEU:HD21	1.93	0.50
46:1o:84:LYS:O	46:1o:84:LYS:HD3	2.09	0.50
51:1t:42:GLN:NE2	51:1t:46:GLU:OE2	2.44	0.50
1:2A:277:C:H4'	1:2A:278:A:H8	1.76	0.50
1:2A:2448:A:OP1	61:2A:3949:HOH:O	2.20	0.50
8:2I:69:LYS:NZ	8:2I:138:ILE:HA	2.26	0.50
16:2U:8:VAL:O	16:2U:12:ARG:HG3	2.10	0.50
21:2Z:153:SER:HB3	21:2Z:167:PRO:HB3	1.92	0.50
22:20:27:GLU:HB2	22:20:69:PHE:HD1	1.77	0.50
31:29:2:LYS:NZ	31:29:31:LYS:O	2.36	0.50
32:2a:1286:A:H2'	32:2a:1287:A:H4'	1.92	0.50
34:2c:39:ILE:HG22	34:2c:43:LEU:HD11	1.92	0.50
1:1A:222:A:H5''	1:1A:421:U:OP1	2.11	0.50
1:1A:1028:A:H61	1:1A:1125:G:H2'	1.76	0.50
1:1A:2278:A:OP2	22:10:12:ASN:ND2	2.42	0.50
10:1O:63:VAL:HG12	10:1O:106:LEU:HD11	1.93	0.50
33:1b:84:GLU:HB3	33:1b:219:VAL:HG21	1.93	0.50
36:1e:12:LEU:HB3	36:1e:31:LEU:HB2	1.92	0.50
37:1f:76:ALA:O	37:1f:80:ARG:HG3	2.11	0.50
1:2A:96:G:H4'	24:22:48:HIS:CD2	2.45	0.50
2:2B:7:G:H5'	14:2S:29:PHE:CD2	2.45	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2G:39:ILE:HG12	6:2G:157:ILE:HG12	1.94	0.50
16:2U:19:LYS:HG3	16:2U:22:LYS:HE2	1.93	0.50
32:2a:448:A:P	32:2a:485:G:H22	2.34	0.50
35:2d:22:LYS:HB2	35:2d:26:CYS:SG	2.51	0.50
40:2i:8:GLY:O	40:2i:15:ALA:N	2.42	0.50
1:1A:2105:C:H2'	1:1A:2106:G:C8	2.45	0.50
18:1W:68:ARG:HH12	18:1W:112:GLY:H	1.60	0.50
31:19:16:VAL:HG22	31:19:25:VAL:HG22	1.93	0.50
32:1a:1346:A:O2'	38:1g:10:ARG:NH2	2.43	0.50
37:1f:65:VAL:HG21	37:1f:67:MET:HE3	1.92	0.50
48:1q:67:LYS:O	48:1q:68:ARG:HB2	2.12	0.50
54:1w:1:G:H2'	54:1w:2:C:C6	2.47	0.50
1:2A:2180:U:H2'	1:2A:2181:G:O4'	2.10	0.50
28:26:35:GLU:HG2	28:26:50:ARG:HD3	1.93	0.50
34:2c:152:ILE:HG22	34:2c:167:TRP:HB3	1.93	0.50
35:2d:108:LEU:HD21	35:2d:174:LEU:HB3	1.93	0.50
41:2j:89:ASP:O	41:2j:91:PRO:HD3	2.11	0.50
1:1A:642:G:OP1	61:1A:4256:HOH:O	2.20	0.50
1:1A:969:U:H2'	1:1A:970:C:C6	2.46	0.50
8:1I:40:THR:OG1	8:1I:41:GLU:N	2.43	0.50
19:1X:26:TYR:CD1	19:1X:92:LEU:HD12	2.46	0.50
32:1a:429:U:O2'	35:1d:22:LYS:NZ	2.35	0.50
32:1a:544:G:OP1	35:1d:59:ARG:NH2	2.42	0.50
37:1f:69:GLU:H	37:1f:69:GLU:CD	2.20	0.50
47:1p:74:LEU:HB3	47:1p:79:VAL:HG21	1.94	0.50
49:1r:52:PRO:O	49:1r:56:THR:HG23	2.11	0.50
1:2A:1406:U:H2'	1:2A:1407:C:C6	2.47	0.50
1:2A:1697:G:OP2	1:2A:1698:A:O2'	2.19	0.50
4:2E:48:GLN:HE21	4:2E:78:LEU:HD22	1.76	0.50
8:2I:3:VAL:HA	8:2I:39:ALA:H	1.75	0.50
11:2P:63:PRO:HG2	30:28:25:MET:HB2	1.94	0.50
14:2S:28:VAL:HG11	14:2S:98:VAL:HG12	1.94	0.50
20:2Y:5:MET:HE2	20:2Y:30:VAL:HG13	1.94	0.50
32:2a:719:C:O2'	49:2r:49:LYS:HB3	2.10	0.50
32:2a:1273:G:H5'	32:2a:1274:G:OP2	2.11	0.50
33:2b:119:GLU:OE2	33:2b:153:ARG:NH1	2.39	0.50
35:2d:166:LYS:HA	35:2d:178:VAL:HG11	1.93	0.50
54:2w:8:4SU:S4	54:2w:13:C:O2'	2.58	0.50
1:1A:592:G:O6	61:1A:4254:HOH:O	2.19	0.50
1:1A:2029:G:H2'	1:1A:2031:A:OP1	2.11	0.50
4:1E:149:ARG:O	61:1E:402:HOH:O	2.19	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1c:119:ARG:HE	34:1c:140:ARG:NH2	2.10	0.50
48:1q:53:LEU:HB3	48:1q:82:MET:HE1	1.92	0.50
1:2A:2001:A:H2'	1:2A:2002:G:C8	2.47	0.50
11:2P:59:LEU:HD11	30:28:10:ALA:HA	1.94	0.50
32:2a:920:U:H2'	32:2a:921:U:C6	2.46	0.50
34:2c:22:TRP:HA	41:2j:93:GLY:HA2	1.92	0.50
42:2k:18:ARG:HB2	42:2k:33:THR:HG23	1.93	0.50
48:2q:19:VAL:HG23	48:2q:44:ALA:HB3	1.93	0.50
51:2t:16:HIS:O	51:2t:19:SER:OG	2.27	0.50
1:1A:910:A:N1	1:1A:2277:G:H1'	2.26	0.50
1:1A:2870:C:H2'	1:1A:2871:C:O4'	2.12	0.50
7:1H:159:GLU:HG3	7:1H:169:VAL:HG11	1.93	0.50
14:1S:106:ARG:HE	14:1S:112:PHE:C	2.20	0.50
32:1a:431:A:H2'	32:1a:432:A:O4'	2.12	0.50
1:2A:117:G:OP2	1:2A:119:A:O2'	2.26	0.50
1:2A:471:A:H2'	1:2A:472:A:O4'	2.11	0.50
1:2A:2273:A:H2'	1:2A:2274:A:H8	1.77	0.50
32:2a:114:U:O2'	32:2a:115:G:H5'	2.11	0.50
32:2a:979:C:O2	45:2n:19:ARG:HG2	2.12	0.50
32:2a:985:C:H2'	32:2a:986:A:H8	1.75	0.50
54:2w:18:G:O2'	54:2w:57:G:N2	2.27	0.50
1:1A:2131:G:H5''	1:1A:2132:U:H3'	1.93	0.50
3:1D:77:ALA:HB2	3:1D:97:TYR:CD1	2.46	0.50
5:1F:64:ILE:HD11	5:1F:75:HIS:HB2	1.94	0.50
6:1G:77:ILE:HD13	6:1G:82:LEU:HD12	1.93	0.50
11:1P:90:ARG:HH11	11:1P:105:LEU:HD11	1.77	0.50
32:1a:967:5MC:H4'	40:1i:125:TYR:HE1	1.76	0.50
33:1b:115:LEU:O	33:1b:118:LEU:N	2.41	0.50
34:1c:64:VAL:HG22	34:1c:65:ALA:O	2.12	0.50
54:1w:5:G:H2'	54:1w:6:G:C8	2.47	0.50
1:2A:807:U:OP2	11:2P:41:ARG:NH2	2.44	0.50
1:2A:2615:U:C2	27:25:7:PRO:HA	2.47	0.50
1:2A:2833:G:H4'	1:2A:2834:G:OP2	2.12	0.50
17:2V:14:VAL:HA	17:2V:18:LEU:HD23	1.94	0.50
23:21:35:THR:OG1	23:21:35:THR:O	2.28	0.50
34:2c:150:LYS:HG3	34:2c:169:ALA:HB2	1.92	0.50
1:1A:606:U:H4'	1:1A:658:C:H4'	1.93	0.50
1:1A:862:G:H2'	1:1A:863:A:O4'	2.12	0.50
1:1A:2820:A:C5	13:1R:4:LEU:HD11	2.47	0.50
3:1D:108:PRO:HB3	3:1D:143:HIS:CE1	2.46	0.50
25:13:8:LEU:HG	25:13:31:LEU:HD23	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:14:61:ARG:HD3	50:1s:67:VAL:HG12	1.94	0.50
33:1b:16:HIS:CG	33:1b:17:PHE:N	2.80	0.50
35:1d:74:GLN:O	35:1d:78:LEU:HG	2.11	0.50
44:1m:87:TYR:O	44:1m:91:ARG:HG2	2.12	0.50
52:1u:3:LYS:HB3	52:1u:14:TRP:CD1	2.47	0.50
1:2A:764:A:H5''	3:2D:210:GLY:CA	2.42	0.50
1:2A:1412:A:H2'	1:2A:1413:G:C8	2.47	0.50
1:2A:1486:A:H2'	1:2A:1487:G:H8	1.76	0.50
2:2B:27:C:H5''	14:2S:54:LEU:HD21	1.94	0.50
2:2B:56:G:H4'	2:2B:57:A:C8	2.47	0.50
6:2G:55:LYS:O	6:2G:59:GLU:N	2.28	0.50
6:2G:63:ILE:HD11	6:2G:144:ILE:HG13	1.93	0.50
33:2b:74:LYS:HB2	33:2b:77:ALA:HB3	1.93	0.50
35:2d:60:GLU:HG2	35:2d:202:LEU:HB2	1.93	0.50
50:2s:64:GLU:OE1	50:2s:64:GLU:N	2.35	0.50
1:1A:55:G:O2'	1:1A:127:A:N1	2.40	0.50
1:1A:197:A:N6	1:1A:2430:A:O2'	2.43	0.50
1:1A:1686:C:H2'	1:1A:1687:G:O4'	2.12	0.50
4:1E:59:VAL:HG22	4:1E:64:LYS:HG3	1.94	0.50
4:1E:116:VAL:HG21	4:1E:138:PRO:HB3	1.94	0.50
32:1a:667:G:H4'	46:1o:51:HIS:ND1	2.27	0.50
1:2A:127:A:H5''	1:2A:128:C:O4'	2.11	0.50
1:2A:880:G:H2'	1:2A:881:G:H8	1.77	0.50
1:2A:1902:C:H5'	3:2D:246:PRO:HD3	1.93	0.50
5:2F:95:ARG:HD3	5:2F:97:TYR:CZ	2.47	0.50
26:24:37:SER:HA	26:24:43:TYR:HD1	1.77	0.50
32:2a:1060:C:O2'	41:2j:56:HIS:ND1	2.38	0.50
32:2a:1133:G:H2'	32:2a:1134:G:C8	2.44	0.50
1:1A:639:U:H2'	1:1A:640:C:C6	2.47	0.49
1:1A:952:G:OP1	12:1Q:16:ARG:NH2	2.45	0.49
6:1G:32:PRO:HB3	6:1G:163:ALA:HB2	1.93	0.49
15:1T:60:THR:HG22	15:1T:77:PRO:HA	1.93	0.49
32:1a:1305:G:H5''	52:1u:4:GLY:HA3	1.93	0.49
32:1a:1458:G:OP1	51:1t:35:THR:OG1	2.24	0.49
1:2A:662:G:H5''	11:2P:16:ARG:HG2	1.93	0.49
4:2E:59:VAL:HG23	4:2E:63:LEU:HB2	1.94	0.49
5:2F:102:PRO:HB2	5:2F:105:VAL:HG23	1.93	0.49
5:2F:127:GLU:HG2	5:2F:196:LEU:HD11	1.93	0.49
9:2N:138:LEU:HD22	9:2N:140:VAL:HG13	1.94	0.49
32:2a:530:G:N3	54:2w:35:A:O2'	2.41	0.49
32:2a:840:C:H4'	32:2a:841:U:OP1	2.10	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1005:A:H5''	32:2a:1006:C:C5	2.47	0.49
33:2b:118:LEU:O	33:2b:122:PHE:HB3	2.12	0.49
49:2r:35:ARG:O	49:2r:37:VAL:N	2.44	0.49
1:1A:871:U:OP1	12:1Q:5:ARG:HG3	2.12	0.49
1:1A:1364:G:P	23:11:3:LYS:HG3	2.52	0.49
1:1A:1508:A:O2'	1:1A:1509:C:H5''	2.13	0.49
7:1H:20:ALA:HB1	7:1H:21:PRO:HD2	1.94	0.49
9:1N:109:LYS:HE2	61:1N:301:HOH:O	2.12	0.49
19:1X:53:LYS:HB3	19:1X:82:GLN:HB3	1.94	0.49
32:1a:1368:G:OP1	40:1i:111:ARG:NH2	2.45	0.49
34:1c:131:ARG:HH11	34:1c:166:GLU:HG3	1.76	0.49
37:1f:8:ILE:HD11	37:1f:79:LEU:HD13	1.94	0.49
48:1q:59:ILE:HG22	48:1q:73:VAL:HA	1.95	0.49
1:2A:890:A:H2'	1:2A:892:G:H8	1.77	0.49
1:2A:900:A:O2'	1:2A:901:A:OP1	2.28	0.49
1:2A:956:G:H2'	1:2A:957:A:H2'	1.94	0.49
1:2A:994:C:H3'	16:2U:54:LYS:HE3	1.93	0.49
3:2D:70:TRP:CE2	3:2D:150:LYS:HD3	2.47	0.49
7:2H:137:ASP:HB3	7:2H:140:LYS:HB3	1.93	0.49
10:2O:80:ASP:OD2	15:2T:64:ARG:NH2	2.45	0.49
32:2a:163:C:H2'	32:2a:164:U:C6	2.48	0.49
32:2a:448:A:OP2	32:2a:485:G:N1	2.38	0.49
32:2a:523:A:H61	43:2l:92:OTD:CG	2.25	0.49
32:2a:575:G:O2'	32:2a:821:G:H5'	2.13	0.49
32:2a:1072:G:H2'	32:2a:1073:U:C6	2.48	0.49
44:2m:10:PRO:HB2	44:2m:13:LYS:HD2	1.94	0.49
54:2y:62:C:H2'	54:2y:63:G:H8	1.77	0.49
1:1A:1876:A:H2'	1:1A:1877:A:C8	2.48	0.49
1:1A:2112:G:C2	1:1A:2113:U:H1'	2.47	0.49
32:1a:429:U:OP2	35:1d:36:ARG:NH2	2.45	0.49
32:1a:916:G:N7	61:1a:1955:HOH:O	2.35	0.49
34:1c:62:ASP:HA	34:1c:97:LYS:HD3	1.93	0.49
42:1k:85:ARG:HD3	42:1k:113:PRO:HD3	1.94	0.49
1:2A:531:C:OP1	1:2A:561:G:N1	2.43	0.49
1:2A:1667:G:O2'	1:2A:1991:U:O4	2.21	0.49
7:2H:3:ARG:HH21	7:2H:5:GLY:H	1.57	0.49
8:2I:93:THR:OG1	8:2I:96:ASP:OD1	2.20	0.49
8:2I:127:VAL:HG23	8:2I:139:GLN:HG3	1.95	0.49
33:2b:47:THR:O	33:2b:51:LEU:HG	2.12	0.49
33:2b:178:ARG:NH1	39:2h:74:PRO:HG3	2.27	0.49
1:1A:1054:A:H61	1:1A:1105:U:H3	1.60	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1056:G:H5''	1:1A:1057:A:O4'	2.12	0.49
44:1m:16:ASP:OD1	44:1m:16:ASP:N	2.44	0.49
54:1y:58:A:H4'	54:1y:59:U:OP1	2.12	0.49
1:2A:125:G:O2'	29:27:48:LYS:HD3	2.13	0.49
1:2A:1125:G:H5'	31:29:37:GLY:HA2	1.94	0.49
1:2A:2363:C:O2	22:20:39:ARG:NH2	2.45	0.49
5:2F:158:THR:HB	5:2F:195:ASP:HB2	1.95	0.49
6:2G:170:ARG:NH1	6:2G:174:GLU:OE2	2.44	0.49
21:2Z:93:ASP:HA	21:2Z:131:ARG:HH22	1.77	0.49
32:2a:473:G:H2'	32:2a:474:G:C8	2.47	0.49
32:2a:1226:C:C6	44:2m:103:THR:HB	2.47	0.49
34:2c:127:ARG:NH2	34:2c:192:THR:OG1	2.45	0.49
36:2e:43:LEU:H	36:2e:65:ASN:HB3	1.78	0.49
1:1A:1996:C:H4'	1:1A:1997:G:OP1	2.11	0.49
1:1A:2183:C:H2'	1:1A:2184:G:H8	1.77	0.49
32:1a:1240:U:OP2	38:1g:116:ALA:N	2.45	0.49
34:1c:15:THR:HG21	34:1c:181:ASN:HA	1.94	0.49
1:2A:1292:U:H2'	1:2A:1293:C:C6	2.47	0.49
1:2A:2811:G:N2	1:2A:2891:G:H1'	2.28	0.49
6:2G:79:ASN:OD1	6:2G:79:ASN:N	2.43	0.49
11:2P:38:GLN:HG2	11:2P:45:LEU:H	1.78	0.49
17:2V:72:VAL:HB	17:2V:85:LYS:HB3	1.94	0.49
18:2W:71:VAL:HA	18:2W:107:LEU:HD23	1.93	0.49
32:2a:67:C:H2'	32:2a:68:G:C8	2.47	0.49
32:2a:769:G:H4'	32:2a:1513:A:H4'	1.95	0.49
32:2a:1004:A:C6	32:2a:1037:C:H1'	2.47	0.49
32:2a:1290:G:O2'	38:2g:37:ASN:ND2	2.44	0.49
33:2b:67:THR:HB	33:2b:159:PRO:HA	1.93	0.49
37:2f:3:ARG:HD3	37:2f:64:GLN:NE2	2.28	0.49
1:1A:829:A:N7	1:1A:2248:C:H5'	2.28	0.49
1:1A:847:U:OP2	61:1A:4258:HOH:O	2.20	0.49
1:1A:1278:A:OP1	13:1R:36:THR:HG23	2.13	0.49
6:1G:56:ALA:O	6:1G:59:GLU:HG2	2.12	0.49
8:1I:40:THR:HG23	8:1I:43:ASN:OD1	2.13	0.49
14:1S:3:ARG:HD3	14:1S:4:LEU:N	2.27	0.49
15:1T:112:ARG:HG3	15:1T:115:ARG:NH2	2.28	0.49
32:1a:580:U:H2'	32:1a:581:G:O4'	2.13	0.49
49:1r:61:LYS:O	49:1r:65:ILE:HD12	2.13	0.49
54:1y:67:C:H2'	54:1y:68:C:C6	2.47	0.49
1:2A:1802:A:N1	1:2A:1822:G:H1'	2.27	0.49
1:2A:2674:G:H2'	1:2A:2675:A:C8	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:2I:48:GLU:HA	8:2I:51:ILE:HG22	1.94	0.49
32:2a:1005:A:H3'	32:2a:1006:C:C6	2.48	0.49
33:2b:155:LEU:HD11	33:2b:159:PRO:HG3	1.94	0.49
39:2h:112:LEU:HD11	39:2h:124:ALA:HB2	1.95	0.49
45:2n:23:ARG:HG2	45:2n:28:GLY:HA2	1.95	0.49
50:2s:49:ILE:HD13	50:2s:71:LEU:HD11	1.94	0.49
1:1A:630:G:OP2	30:18:15:LYS:NZ	2.32	0.49
30:18:4:MET:HE3	30:18:63:PRO:HG3	1.95	0.49
32:1a:1030(A):G:H1'	32:1a:1031:G:H1	1.77	0.49
35:1d:53:ASP:HB3	35:1d:57:ARG:NH1	2.28	0.49
40:1i:55:ALA:HA	40:1i:58:HIS:CD2	2.48	0.49
1:2A:2537:U:H2'	1:2A:2538:C:C6	2.47	0.49
2:2B:22:U:H3	2:2B:61:G:H1	1.61	0.49
8:2I:29:TYR:HD2	8:2I:30:LEU:HD23	1.78	0.49
32:2a:782:A:OP1	61:2a:1909:HOH:O	2.20	0.49
32:2a:984:C:H2'	32:2a:985:C:C6	2.48	0.49
32:2a:1256:A:H61	32:2a:1278:U:H1'	1.78	0.49
32:2a:1320:C:H2'	32:2a:1321:C:O4'	2.13	0.49
33:2b:212:GLN:O	33:2b:216:SER:N	2.40	0.49
54:2y:52:G:H5'	54:2y:53:G:OP2	2.13	0.49
1:1A:1267:U:OP1	61:1A:4257:HOH:O	2.20	0.49
1:1A:2099:U:H3	1:1A:2190:G:H1	1.60	0.49
1:1A:2130:U:H2'	1:1A:2158:A:C2	2.48	0.49
10:1O:26:LYS:HE2	10:1O:37:ASP:OD2	2.13	0.49
40:1i:50:LEU:HD13	40:1i:56:LEU:HA	1.95	0.49
5:2F:32:LEU:HD22	5:2F:112:MET:HE2	1.93	0.49
10:2O:24:VAL:HG13	10:2O:33:ALA:HB2	1.95	0.49
14:2S:5:THR:OG1	14:2S:8:GLU:HG3	2.13	0.49
32:2a:1348:U:H4'	40:2i:120:ARG:HE	1.78	0.49
1:1A:2123:G:H2'	1:1A:2124:G:O4'	2.13	0.49
11:1P:106:LEU:HD22	11:1P:112:LEU:HD13	1.95	0.49
23:11:23:LYS:HB3	23:11:29:GLY:HA3	1.95	0.49
32:1a:69:G:H2'	32:1a:70:G:C8	2.47	0.49
32:1a:881:G:P	43:1l:12:ARG:HH22	2.36	0.49
32:1a:1414:U:O4	61:1a:1920:HOH:O	2.19	0.49
34:1c:13:GLY:HA3	45:1n:57:ARG:HH12	1.76	0.49
34:1c:193:TYR:HE1	34:1c:196:LEU:HD11	1.78	0.49
1:2A:271(E):U:H2'	1:2A:271(F):C:C6	2.48	0.49
1:2A:568:U:H5'	1:2A:945:A:N1	2.28	0.49
2:2B:51:G:N7	14:2S:62:LYS:NZ	2.43	0.49
14:2S:23:ARG:NH2	14:2S:84:GLN:HG2	2.27	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2S:67:ARG:NH2	14:2S:103:GLU:OE1	2.45	0.49
32:2a:176:C:H2'	32:2a:177:C:C6	2.48	0.49
32:2a:745:C:H2'	32:2a:746:A:C8	2.47	0.49
32:2a:1272:G:N2	32:2a:1273:G:C5	2.81	0.49
36:2e:53:LEU:HA	36:2e:56:GLN:HB2	1.95	0.49
50:2s:31:ILE:HG22	50:2s:49:ILE:HG13	1.94	0.49
1:1A:184:C:H2'	1:1A:185:U:H6	1.77	0.49
1:1A:620:G:N3	1:1A:620:G:H5'	2.27	0.49
1:1A:2105:C:H2'	1:1A:2106:G:H8	1.77	0.49
1:1A:2801(A):A:H1'	1:1A:2895:U:H1'	1.95	0.49
8:1I:4:ILE:HG12	8:1I:18:VAL:HG12	1.95	0.49
10:1O:89:ASN:H	10:1O:89:ASN:ND2	2.11	0.49
32:1a:1328:C:H2'	32:1a:1329:A:O4'	2.13	0.49
54:1y:26:A:N1	54:1y:44:G:N2	2.61	0.49
1:2A:375:C:H2'	1:2A:376:C:C6	2.48	0.49
1:2A:1218:C:H42	1:2A:1231:G:H1	1.60	0.49
1:2A:1651:G:H2'	1:2A:1652:A:O4'	2.13	0.49
1:2A:2879:C:OP2	61:2A:3966:HOH:O	2.20	0.49
9:2N:58:ASP:OD1	9:2N:58:ASP:N	2.36	0.49
12:2Q:57:HIS:CD2	12:2Q:117:ALA:HB2	2.48	0.49
16:2U:49:HIS:HA	16:2U:52:ARG:HB2	1.94	0.49
32:2a:56:U:H2'	32:2a:57:G:H8	1.77	0.49
32:2a:643:C:H2'	32:2a:644:G:H8	1.78	0.49
32:2a:1033:G:H2'	32:2a:1034:G:C8	2.48	0.49
50:2s:15:LEU:HD12	50:2s:18:LYS:HD2	1.95	0.49
1:1A:185:U:H2'	1:1A:186:G:H8	1.78	0.48
1:1A:740:U:H2'	1:1A:741:G:C8	2.48	0.48
1:1A:2149:G:C2	1:1A:2150:U:H1'	2.48	0.48
1:1A:2375:G:O2'	1:1A:2377:A:N7	2.37	0.48
3:1D:85:ASP:OD2	3:1D:88:ARG:NH1	2.39	0.48
5:1F:53:THR:HG22	5:1F:56:GLU:HG3	1.95	0.48
32:1a:390:C:H2'	32:1a:391:G:C8	2.48	0.48
32:1a:652:U:O4	32:1a:752:G:O2'	2.27	0.48
32:1a:1075:C:OP1	33:1b:179:LYS:NZ	2.32	0.48
33:1b:93:VAL:HG11	33:1b:97:TRP:CD1	2.48	0.48
43:1l:33:ARG:HD2	43:1l:62:SER:HB3	1.95	0.48
1:2A:1579:A:H2'	1:2A:1580:A:C8	2.48	0.48
1:2A:1721:G:H8	1:2A:1741:A:H62	1.59	0.48
1:2A:2242:G:OP1	61:2A:3965:HOH:O	2.20	0.48
1:2A:2370:G:C6	1:2A:2371:G:C6	3.01	0.48
7:2H:13:LYS:HA	7:2H:14:GLY:HA2	1.54	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2Z:126:VAL:HG13	21:2Z:161:VAL:HG23	1.95	0.48
21:2Z:159:PRO:HA	21:2Z:160:GLY:HA2	1.48	0.48
32:2a:195:A:N3	32:2a:222:U:O2'	2.42	0.48
32:2a:977:A:O3'	32:2a:980:C:N4	2.46	0.48
32:2a:1321:C:H4'	44:2m:87:TYR:HE2	1.78	0.48
1:1A:592:G:N7	61:1A:4338:HOH:O	2.34	0.48
1:1A:1087:G:H2'	1:1A:1089:G:C8	2.48	0.48
1:1A:1138:G:N3	9:1N:106:MET:HE2	2.28	0.48
2:1B:88:C:H2'	2:1B:89:G:O4'	2.13	0.48
32:1a:1063:C:H2'	32:1a:1064:G:C8	2.49	0.48
32:1a:1376:U:H2'	32:1a:1377:A:C8	2.48	0.48
1:2A:1652:A:C2'	1:2A:1653:G:H5'	2.42	0.48
1:2A:2630:G:H2'	1:2A:2631:G:C8	2.48	0.48
1:2A:2646:C:H2'	1:2A:2647:U:O4'	2.13	0.48
1:2A:2872:G:O2'	1:2A:2873:A:H5'	2.13	0.48
15:2T:88:ILE:HG21	15:2T:91:ARG:NE	2.29	0.48
32:2a:947:G:O3'	44:2m:109:THR:OG1	2.30	0.48
32:2a:1148:U:H2'	32:2a:1149:C:O4'	2.13	0.48
32:2a:1289:A:OP1	52:2u:10:ARG:NH2	2.47	0.48
34:2c:40:ARG:HA	34:2c:43:LEU:HD12	1.93	0.48
37:2f:91:VAL:HG11	49:2r:72:ARG:NH1	2.28	0.48
41:2j:36:GLY:O	41:2j:38:ILE:HG12	2.13	0.48
54:2w:19:G:H1	54:2w:56:C:N4	2.07	0.48
1:1A:1538:G:H2'	1:1A:1539:G:C8	2.49	0.48
1:1A:1538:G:H2'	1:1A:1539:G:H8	1.78	0.48
1:1A:1607:C:H4'	1:1A:1608:A:O5'	2.12	0.48
7:1H:149:ARG:NH1	7:1H:167:GLU:OE2	2.47	0.48
8:1I:77:LEU:HD21	8:1I:100:ALA:HB3	1.96	0.48
32:1a:78:G:C6	32:1a:91:C:N4	2.80	0.48
32:1a:946:A:H2'	32:1a:947:G:C8	2.48	0.48
1:2A:184:C:H2'	1:2A:185:U:C6	2.49	0.48
1:2A:2059:A:O2'	5:2F:69:HIS:HD2	1.96	0.48
1:2A:2155:G:C5	1:2A:2156:G:H1'	2.48	0.48
22:20:36:ILE:HD13	22:20:60:PHE:HB3	1.95	0.48
32:2a:390:C:O3'	47:2p:28:ARG:NH2	2.47	0.48
32:2a:921:U:O2	36:2e:19:MET:HB2	2.12	0.48
41:2j:5:ARG:HA	41:2j:73:ASP:OD1	2.13	0.48
43:2l:8:ASN:O	43:2l:12:ARG:HG3	2.14	0.48
47:2p:21:VAL:HG22	47:2p:33:ILE:HB	1.96	0.48
50:2s:66:MET:HB2	50:2s:74:PHE:CZ	2.48	0.48
1:1A:484:C:OP1	20:1Y:51:VAL:HG22	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1045:A:O2'	1:1A:1047:G:C4	2.65	0.48
1:1A:1058:G:H1	1:1A:1080:C:N4	2.12	0.48
32:1a:691:G:H2'	32:1a:692:U:C6	2.49	0.48
32:1a:1124:G:N7	32:1a:1145:C:O2'	2.46	0.48
32:1a:1260:C:O5'	32:1a:1284:C:H4'	2.13	0.48
1:2A:2321:G:H22	1:2A:2333:A:N6	2.11	0.48
1:2A:2758:A:C2	1:2A:2759:G:H1'	2.49	0.48
2:2B:33:G:C6	2:2B:34:U:C4	3.02	0.48
11:2P:90:ARG:NH1	11:2P:105:LEU:HD11	2.29	0.48
17:2V:46:VAL:HG12	17:2V:52:VAL:HG11	1.93	0.48
32:2a:1134:G:N1	32:2a:1135:U:H1'	2.28	0.48
35:2d:110:PHE:CE2	35:2d:148:VAL:HG23	2.49	0.48
35:2d:148:VAL:HB	35:2d:181:MET:HB3	1.95	0.48
50:2s:48:THR:HG22	50:2s:61:TYR:HA	1.94	0.48
1:1A:818:G:H5'	1:1A:839:U:OP1	2.14	0.48
1:1A:884:C:C5	1:1A:885:C:H1'	2.48	0.48
32:1a:461:A:O2'	32:1a:471:G:N7	2.46	0.48
42:1k:34:ASP:OD1	42:1k:38:ASN:N	2.46	0.48
1:2A:218:A:OP2	61:2A:3961:HOH:O	2.19	0.48
1:2A:984:A:H5''	1:2A:985:C:H5	1.78	0.48
21:2Z:31:ARG:HD2	21:2Z:94:GLU:OE2	2.14	0.48
32:2a:828:A:H2'	32:2a:829:G:O4'	2.14	0.48
34:2c:112:SER:HB3	34:2c:115:LEU:HB2	1.95	0.48
39:2h:121:ASP:O	39:2h:125:ARG:NE	2.46	0.48
1:1A:1430:C:H2'	1:1A:1431:U:C6	2.47	0.48
1:1A:1568:G:H4'	3:1D:59:LYS:HG2	1.94	0.48
1:1A:1688:U:O2	1:1A:1700:A:H5'	2.14	0.48
32:1a:1372:U:OP1	40:1i:72:GLY:N	2.44	0.48
40:1i:50:LEU:HA	40:1i:53:VAL:HG23	1.95	0.48
54:1y:38:A:H2'	54:1y:39:PSU:O4'	2.14	0.48
1:2A:444:C:H4'	5:2F:49:ALA:HB2	1.95	0.48
1:2A:479:A:N3	1:2A:481:G:H5''	2.29	0.48
1:2A:751:A:H5'	18:2W:90:ARG:HA	1.95	0.48
1:2A:2133:G:O2'	1:2A:2157:G:N2	2.46	0.48
1:2A:2317:C:N4	1:2A:2318:G:O6	2.46	0.48
13:2R:42:LYS:HB3	13:2R:45:ARG:HH21	1.79	0.48
32:2a:416:G:C5	32:2a:417:C:C4	3.01	0.48
32:2a:771:G:H3'	61:2a:1926:HOH:O	2.12	0.48
33:2b:12:GLU:CB	33:2b:213:LEU:HD21	2.44	0.48
34:2c:148:GLY:HA3	34:2c:203:PHE:HB3	1.95	0.48
36:2e:55:VAL:O	36:2e:59:GLY:N	2.42	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:2i:19:LEU:HD22	40:2i:59:PHE:HB3	1.94	0.48
51:2t:86:ARG:O	51:2t:90:GLN:HB2	2.13	0.48
54:2y:55:PSU:HN1	54:2y:57:G:C5'	2.16	0.48
1:1A:1336:A:OP2	19:1X:64:LYS:NZ	2.40	0.48
1:1A:1817:G:OP1	3:1D:88:ARG:NH2	2.45	0.48
3:1D:242:ARG:N	3:1D:242:ARG:HD3	2.28	0.48
10:1O:122:LEU:HD13	15:1T:72:VAL:HG11	1.96	0.48
32:1a:34:C:H2'	32:1a:35:G:C8	2.48	0.48
32:1a:555:C:H2'	32:1a:556:C:C6	2.49	0.48
32:1a:672:U:O2'	32:1a:673:G:O5'	2.30	0.48
32:1a:971:G:N1	32:1a:1363(A):A:OP2	2.45	0.48
1:2A:277:C:H4'	1:2A:278:A:C8	2.48	0.48
1:2A:839:U:H2'	1:2A:840:C:C6	2.48	0.48
8:2I:129:THR:HA	8:2I:138:ILE:O	2.14	0.48
20:2Y:1:MET:HG2	20:2Y:2:ARG:N	2.28	0.48
27:25:49:CYS:SG	27:25:51:TYR:HB2	2.54	0.48
30:28:26:LYS:HB2	30:28:44:LYS:O	2.13	0.48
32:2a:417:C:H2'	32:2a:418:C:C6	2.48	0.48
32:2a:973:G:H3'	32:2a:974:A:H5''	1.96	0.48
32:2a:1002:G:N3	32:2a:1003:G:H1'	2.28	0.48
32:2a:1291:G:H4'	40:2i:39:GLY:HA3	1.96	0.48
32:2a:1490:C:H2'	32:2a:1491:G:O4'	2.13	0.48
33:2b:24:TRP:CD1	33:2b:24:TRP:H	2.32	0.48
1:1A:242:G:C8	30:18:5:LYS:HG2	2.49	0.48
1:1A:2583:G:OP2	61:1A:4255:HOH:O	2.19	0.48
21:1Z:146:ILE:HA	21:1Z:147:GLY:HA2	1.61	0.48
32:1a:277:C:P	48:1q:68:ARG:HH12	2.35	0.48
1:2A:902:C:H2'	1:2A:903:C:C6	2.48	0.48
1:2A:2238:G:H2'	1:2A:2238:G:N3	2.29	0.48
6:2G:145:THR:OG1	6:2G:146:TYR:N	2.46	0.48
27:25:40:LYS:NZ	27:25:44:THR:O	2.46	0.48
32:2a:859:A:H2'	32:2a:860:A:O4'	2.13	0.48
32:2a:1128:C:O2'	32:2a:1147:C:N3	2.40	0.48
32:2a:1310:G:H5'	44:2m:77:ASN:HD21	1.77	0.48
33:2b:55:PHE:CE1	33:2b:218:ALA:HA	2.48	0.48
1:1A:1292:U:H2'	1:1A:1293:C:C6	2.48	0.48
1:1A:1740:G:H2'	1:1A:1741:A:C8	2.49	0.48
1:1A:2111:C:N4	1:1A:2144:U:O2'	2.47	0.48
1:1A:2573:C:H3'	61:1A:4294:HOH:O	2.13	0.48
2:1B:66:A:H61	2:1B:108:U:H2'	1.79	0.48
6:1G:61:ALA:HB1	26:14:7:PRO:HG3	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1G:126:ASP:HB2	6:1G:130:ASN:H	1.79	0.48
21:1Z:138:GLU:H	21:1Z:156:LYS:NZ	2.12	0.48
26:14:58:ARG:O	26:14:61:ARG:N	2.47	0.48
32:1a:453:A:O2'	47:1p:68:ASP:O	2.31	0.48
32:1a:658:G:OP1	46:1o:8:LYS:NZ	2.46	0.48
32:1a:942:G:H21	40:1i:124:GLN:NE2	2.11	0.48
32:1a:1124:G:H4'	41:1j:38:ILE:HD13	1.96	0.48
33:1b:80:ILE:HD11	33:1b:212:GLN:HA	1.96	0.48
44:1m:37:THR:O	44:1m:55:ARG:NH1	2.45	0.48
51:1t:47:GLY:HA2	51:1t:48:LYS:C	2.39	0.48
55:1x:75:C:H2'	55:1x:76:A:C8	2.48	0.48
1:2A:652(A):A:H3'	1:2A:652(B):A:H5''	1.95	0.48
1:2A:1434:A:N6	1:2A:1558:A:H62	2.08	0.48
1:2A:1518:U:H2'	1:2A:1519:G:O4'	2.14	0.48
1:2A:2447:G:N2	1:2A:2450:A:OP2	2.47	0.48
1:2A:2850:A:N7	1:2A:2868:A:O2'	2.42	0.48
6:2G:173:LEU:HA	6:2G:176:LEU:HB2	1.96	0.48
8:2I:5:LEU:H	8:2I:5:LEU:HD12	1.79	0.48
9:2N:28:THR:HG22	9:2N:29:LYS:N	2.29	0.48
9:2N:30:ILE:HG21	9:2N:120:LEU:HD13	1.95	0.48
12:2Q:111:GLU:OE2	12:2Q:133:ARG:NH2	2.47	0.48
32:2a:932:C:H2'	32:2a:933:G:H8	1.78	0.48
1:1A:1054:A:N6	1:1A:1105:U:H3	2.12	0.48
1:1A:2273:A:H2'	1:1A:2274:A:C8	2.48	0.48
1:1A:2785:C:O3'	4:1E:69:LYS:HE2	2.14	0.48
2:1B:57:A:H1'	6:1G:29:TRP:HB2	1.96	0.48
9:1N:4:TYR:HB2	16:1U:101:ARG:NH1	2.28	0.48
32:1a:129:U:H5'	48:1q:3:LYS:HZ1	1.79	0.48
32:1a:189(K):U:H2'	32:1a:189(L):G:C8	2.49	0.48
32:1a:537:G:OP2	61:1a:1922:HOH:O	2.20	0.48
1:2A:271(U):G:H2'	1:2A:271(V):G:H8	1.78	0.48
1:2A:880:G:N2	1:2A:898:C:O2	2.46	0.48
1:2A:1462:C:H4'	1:2A:2703:C:H5'	1.94	0.48
1:2A:2320:A:H1'	1:2A:2321:G:C2	2.49	0.48
1:2A:2683:C:O2	10:2O:70:LYS:NZ	2.27	0.48
6:2G:127:GLY:C	6:2G:128:ARG:HD2	2.39	0.48
26:24:60:GLN:O	26:24:62:ARG:NH1	2.46	0.48
32:2a:266:G:H2'	32:2a:266:G:N3	2.29	0.48
32:2a:978:A:H4'	32:2a:1322:C:N3	2.29	0.48
32:2a:1051:C:H2'	32:2a:1052:U:C6	2.49	0.48
32:2a:1276:G:H2'	32:2a:1277:C:C6	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:2d:158:ILE:O	35:2d:162:LEU:HG	2.14	0.48
36:2e:9:LYS:HD2	36:2e:9:LYS:HA	1.67	0.48
38:2g:26:PHE:CE2	38:2g:30:ILE:HD11	2.49	0.48
1:1A:2313:C:H4'	6:1G:91:ARG:HG3	1.95	0.47
13:1R:2:ARG:HA	13:1R:5:LYS:HD2	1.96	0.47
21:1Z:126:VAL:HG12	21:1Z:128:VAL:HB	1.95	0.47
32:1a:1125:U:H4'	41:1j:5:ARG:NH2	2.28	0.47
32:1a:1182:G:H4'	32:1a:1183:A:H5''	1.95	0.47
1:2A:484:C:H2'	1:2A:485:C:C6	2.49	0.47
1:2A:581:C:H2'	1:2A:582:G:C8	2.49	0.47
1:2A:674:G:O2'	5:2F:74:ARG:HD3	2.14	0.47
1:2A:1769:G:O2'	1:2A:1958:C:OP1	2.32	0.47
1:2A:1840:G:OP2	61:2A:3967:HOH:O	2.20	0.47
1:2A:2165:G:H2'	1:2A:2166:G:O4'	2.14	0.47
8:2I:75:LEU:HD13	8:2I:105:HIS:NE2	2.29	0.47
32:2a:993:G:N7	32:2a:1213:A:N6	2.62	0.47
32:2a:1325:C:H2'	32:2a:1326:C:H6	1.79	0.47
41:2j:67:THR:O	41:2j:67:THR:OG1	2.31	0.47
44:2m:3:ARG:N	44:2m:7:VAL:O	2.47	0.47
1:1A:1695:G:N7	3:1D:14:ARG:NH2	2.62	0.47
1:1A:2252:G:N7	61:10:201:HOH:O	2.35	0.47
32:1a:7:G:H5''	32:1a:298:A:O4'	2.12	0.47
32:1a:1033:G:H2'	32:1a:1034:G:H8	1.78	0.47
1:2A:878:A:H61	1:2A:899:A:H1'	1.78	0.47
1:2A:2121:G:H1	1:2A:2177:C:H42	1.61	0.47
1:2A:2512:C:H2'	1:2A:2513:G:O4'	2.13	0.47
3:2D:20:ASP:OD1	3:2D:20:ASP:N	2.38	0.47
8:2I:72:LEU:HD21	8:2I:107:VAL:HG11	1.95	0.47
15:2T:90:GLN:HG3	15:2T:91:ARG:N	2.28	0.47
21:2Z:154:ASP:OD1	21:2Z:154:ASP:N	2.43	0.47
32:2a:519:C:OP2	43:2I:50:SER:OG	2.25	0.47
50:2s:13:ASP:HA	50:2s:16:LEU:HB3	1.96	0.47
55:2x:33:U:N3	55:2x:36:U:OP2	2.44	0.47
11:1P:63:PRO:HD3	30:18:27:THR:HG22	1.95	0.47
12:1Q:78:PRO:HG2	12:1Q:81:VAL:HG11	1.96	0.47
32:1a:324:G:P	51:1t:22:ARG:HE	2.36	0.47
32:1a:601:C:H2'	32:1a:602:A:H8	1.78	0.47
32:1a:1031:G:H2'	32:1a:1032:G:C8	2.49	0.47
33:1b:24:TRP:CD1	33:1b:24:TRP:H	2.32	0.47
1:2A:2125:G:N1	1:2A:2172:U:OP1	2.33	0.47
2:2B:11:C:H3'	2:2B:12:C:C6	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2U:11:ARG:O	16:2U:15:LYS:HG3	2.14	0.47
16:2U:104:GLN:NE2	16:2U:105:VAL:HG23	2.29	0.47
28:26:6:ARG:NE	28:26:24:GLU:OE2	2.28	0.47
30:28:34:TRP:CG	30:28:35:GLN:N	2.82	0.47
32:2a:737:A:H2'	32:2a:738:C:C6	2.49	0.47
32:2a:1265:G:C2	32:2a:1271:G:C2	3.03	0.47
32:2a:1510:U:H2'	32:2a:1511:G:C8	2.49	0.47
38:2g:101:LEU:HA	38:2g:104:LEU:HD12	1.96	0.47
39:2h:39:LEU:HB3	39:2h:45:ILE:HG12	1.95	0.47
45:2n:57:ARG:HG2	45:2n:58:LYS:H	1.79	0.47
54:2y:34:G:H2'	54:2y:35:A:C8	2.50	0.47
1:1A:84:A:H5'	20:1Y:8:LYS:HG2	1.96	0.47
1:1A:1113:U:H2'	1:1A:1114:G:H8	1.79	0.47
1:1A:1740:G:H2'	1:1A:1741:A:H8	1.79	0.47
1:1A:2328:A:H2'	1:1A:2329:G:C8	2.48	0.47
6:1G:125:PHE:O	61:1G:302:HOH:O	2.20	0.47
20:1Y:6:HIS:HE1	20:1Y:72:VAL:O	1.96	0.47
28:16:6:ARG:NH1	28:16:26:ASN:HB2	2.30	0.47
32:1a:21:G:H2'	32:1a:22:G:C8	2.50	0.47
51:1t:45:GLN:HB2	51:1t:91:LEU:HD13	1.96	0.47
1:2A:2314:C:H5'	6:2G:38:VAL:HG21	1.96	0.47
11:2P:63:PRO:HD3	30:28:27:THR:HG22	1.95	0.47
32:2a:539:A:H2'	32:2a:540:G:C8	2.49	0.47
32:2a:1275:A:H3'	32:2a:1276:G:H8	1.79	0.47
33:2b:149:LEU:HD23	33:2b:152:PHE:CD2	2.49	0.47
34:2c:152:ILE:HG13	34:2c:199:LYS:HB2	1.95	0.47
36:2e:43:LEU:HB3	36:2e:65:ASN:HD22	1.79	0.47
37:2f:41:GLU:OE1	49:2r:35:ARG:NH2	2.48	0.47
37:2f:82:ARG:HE	37:2f:82:ARG:HB3	1.41	0.47
49:2r:70:ILE:O	49:2r:74:ARG:HG3	2.15	0.47
1:1A:839:U:H1'	1:1A:1191:G:H1'	1.97	0.47
1:1A:857:C:N4	1:1A:858:U:O4	2.48	0.47
5:1F:51:THR:HB	5:1F:88:VAL:HG11	1.97	0.47
47:1p:5:ARG:HE	47:1p:22:THR:CG2	2.27	0.47
49:1r:47:THR:O	49:1r:83:GLU:N	2.46	0.47
1:2A:383:U:H2'	1:2A:385:C:H5	1.78	0.47
1:2A:918:A:C2	2:2B:80:U:H4'	2.49	0.47
2:2B:48:A:H4'	14:2S:95:HIS:CD2	2.47	0.47
12:2Q:85:LYS:HD3	22:20:7:LEU:HD13	1.97	0.47
18:2W:6:ILE:HG22	18:2W:8:ARG:HG3	1.96	0.47
25:23:11:SER:HA	25:23:31:LEU:HD11	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:376:G:H4'	47:2p:5:ARG:HH21	1.79	0.47
32:2a:417:C:H2'	32:2a:418:C:H6	1.79	0.47
34:2c:35:GLU:O	34:2c:39:ILE:HG13	2.14	0.47
50:2s:17:GLU:O	50:2s:21:GLU:HB2	2.14	0.47
1:1A:971:C:H2'	1:1A:972:G:O4'	2.14	0.47
1:1A:1059:G:OP2	1:1A:1060:U:H3'	2.15	0.47
1:1A:1226:A:OP1	17:1V:84:LYS:HE2	2.15	0.47
1:1A:1999:C:H4'	1:1A:2723:C:O2	2.14	0.47
1:1A:2022:U:O2'	1:1A:2617:C:H5'	2.14	0.47
1:1A:2023:G:H5'	1:1A:2617:C:H4'	1.97	0.47
8:1I:27:ARG:HD3	23:1I:71:TYR:CE2	2.49	0.47
21:1Z:1:MET:HA	21:1Z:2:GLU:HA	1.66	0.47
21:1Z:65:GLN:HE21	21:1Z:67:LEU:HD21	1.80	0.47
32:1a:840:C:H4'	32:1a:841:U:OP1	2.14	0.47
32:1a:1039:C:H2'	32:1a:1040:U:C6	2.50	0.47
32:1a:1062:U:H2'	32:1a:1063:C:C6	2.50	0.47
34:1c:6:HIS:CD2	34:1c:8:ILE:H	2.26	0.47
34:1c:57:ILE:HG12	34:1c:66:VAL:HG12	1.96	0.47
1:2A:208:C:H2'	1:2A:209:C:C6	2.50	0.47
1:2A:1590:U:H2'	1:2A:1591:G:C8	2.50	0.47
1:2A:1591:G:H2'	1:2A:1592:C:C6	2.50	0.47
5:2F:172:TRP:H	5:2F:172:TRP:CD1	2.31	0.47
6:2G:114:ILE:HG13	6:2G:140:ILE:HG12	1.96	0.47
32:2a:1089:G:H1	32:2a:1096:C:H42	1.62	0.47
33:2b:178:ARG:NH1	39:2h:68:ARG:HH22	2.09	0.47
38:2g:66:VAL:O	38:2g:70:LYS:HG3	2.13	0.47
40:2i:50:LEU:H	40:2i:50:LEU:HG	1.52	0.47
1:1A:652(U):G:H2'	1:1A:652(V):C:C6	2.50	0.47
1:1A:894:C:H2'	1:1A:895:U:O4'	2.14	0.47
1:1A:1997:G:H5''	4:1E:117:MET:HE3	1.96	0.47
1:1A:2127:G:H21	1:1A:2173:A:H1'	1.80	0.47
1:1A:2839:G:H5'	13:1R:46:GLY:HA2	1.96	0.47
3:1D:145:VAL:HG11	3:1D:175:LEU:HD11	1.95	0.47
4:1E:7:VAL:HG13	4:1E:27:LEU:HB3	1.97	0.47
8:1I:38:LEU:HG	8:1I:40:THR:HG22	1.96	0.47
8:1I:38:LEU:HD23	8:1I:38:LEU:H	1.79	0.47
15:1T:127:ALA:C	15:1T:129:ARG:N	2.72	0.47
26:14:16:CYS:SG	26:14:17:GLY:N	2.86	0.47
29:17:12:ARG:NH2	29:17:44:PRO:HB3	2.30	0.47
32:1a:134:A:H61	47:1p:25:ARG:NH1	2.10	0.47
32:1a:222:U:H2'	32:1a:223:U:C6	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:456:C:H2'	32:1a:457:C:C6	2.49	0.47
32:1a:600:C:H2'	32:1a:601:C:C6	2.50	0.47
33:1b:10:LEU:HD12	33:1b:48:MET:HE1	1.96	0.47
35:1d:121:VAL:HG22	35:1d:126:ILE:HG13	1.96	0.47
1:2A:71:A:H5''	1:2A:73:A:C8	2.49	0.47
1:2A:218:A:C2	1:2A:235:U:H4'	2.50	0.47
1:2A:818:G:OP2	61:2A:3964:HOH:O	2.20	0.47
1:2A:2139:C:H42	1:2A:2152:G:H1	1.62	0.47
1:2A:2291:U:H2'	1:2A:2292:C:C6	2.50	0.47
2:2B:7:G:H5'	14:2S:29:PHE:CE2	2.50	0.47
2:2B:11:C:H3'	2:2B:12:C:H6	1.78	0.47
2:2B:42:C:H1'	6:2G:68:PRO:HA	1.96	0.47
7:2H:164:TYR:O	7:2H:167:GLU:HB2	2.15	0.47
8:2I:69:LYS:HZ1	8:2I:138:ILE:HA	1.78	0.47
10:2O:26:LYS:HE2	10:2O:37:ASP:OD2	2.15	0.47
11:2P:18:ARG:HH21	11:2P:21:ARG:HG3	1.80	0.47
21:2Z:99:TYR:HB3	21:2Z:123:ASP:HB2	1.96	0.47
26:24:45:GLY:O	26:24:47:GLN:N	2.46	0.47
32:2a:662:G:H2'	32:2a:663:A:C8	2.50	0.47
32:2a:685:G:C2	32:2a:686:U:C4	3.02	0.47
32:2a:748:C:H4'	32:2a:749:C:O5'	2.15	0.47
32:2a:757:U:H2'	32:2a:758:G:O4'	2.15	0.47
32:2a:768:A:N3	32:2a:1512:U:O2'	2.45	0.47
32:2a:932:C:H2'	32:2a:933:G:C8	2.49	0.47
32:2a:1151:A:O2'	32:2a:1152:A:O5'	2.26	0.47
32:2a:1411:C:H2'	32:2a:1412:C:C6	2.49	0.47
33:2b:13:ALA:C	33:2b:15:VAL:H	2.23	0.47
35:2d:8:VAL:HA	35:2d:11:LEU:HD13	1.96	0.47
38:2g:20:ASP:HB3	38:2g:23:VAL:HB	1.96	0.47
39:2h:17:THR:HG22	39:2h:63:LEU:HD23	1.96	0.47
50:2s:40:ILE:HB	50:2s:67:VAL:O	2.15	0.47
1:1A:64:A:C5	19:1X:66:LEU:HD13	2.50	0.47
1:1A:400:G:O6	61:1A:4261:HOH:O	2.20	0.47
1:1A:1164:G:H2'	1:1A:1165:U:C6	2.50	0.47
1:1A:2120:G:O2'	1:1A:2121:G:H5'	2.15	0.47
1:1A:2155:G:H2'	1:1A:2155:G:N3	2.30	0.47
4:1E:143:ASN:HB2	4:1E:147:PRO:HD2	1.97	0.47
5:1F:61:GLY:O	61:1F:401:HOH:O	2.20	0.47
5:1F:116:ASP:OD2	11:1P:1:MET:N	2.40	0.47
32:1a:1237:C:O2'	32:1a:1300:G:N2	2.41	0.47
32:1a:1320:C:H2'	32:1a:1321:C:O4'	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1353:G:OP1	52:1u:10:ARG:NH1	2.48	0.47
47:1p:49:LEU:HD12	47:1p:50:LYS:N	2.30	0.47
1:2A:99:U:H4'	1:2A:100:G:H5'	1.96	0.47
1:2A:867:C:H2'	1:2A:868:U:H6	1.80	0.47
1:2A:2136:C:N4	1:2A:2155:G:H1	2.13	0.47
1:2A:2494:G:C4	1:2A:2495:G:C8	3.03	0.47
4:2E:28:ALA:HB3	4:2E:93:VAL:HG12	1.96	0.47
4:2E:56:PRO:HA	4:2E:59:VAL:HG12	1.96	0.47
5:2F:21:ALA:CB	5:2F:22:ALA:HA	2.42	0.47
6:2G:33:ARG:CZ	6:2G:33:ARG:HB2	2.43	0.47
6:2G:41:GLN:O	6:2G:43:LEU:N	2.47	0.47
10:2O:77:ILE:HB	15:2T:74:ARG:HH11	1.79	0.47
14:2S:77:ALA:HB1	14:2S:82:ILE:HB	1.97	0.47
19:2X:12:VAL:HG22	19:2X:29:TRP:CE2	2.50	0.47
32:2a:11:G:H1	32:2a:23:C:N4	2.08	0.47
32:2a:1318:A:OP1	50:2s:3:ARG:NH2	2.43	0.47
32:2a:1427:U:H2'	32:2a:1428:A:C8	2.50	0.47
33:2b:55:PHE:HE1	33:2b:218:ALA:HA	1.79	0.47
39:2h:29:SER:HB3	39:2h:32:LYS:HG3	1.96	0.47
55:2x:7:G:H5''	55:2x:8:4SU:H5	1.96	0.47
55:2x:74:C:OP2	61:2x:201:HOH:O	2.20	0.47
1:1A:1054:A:C6	1:1A:1055:G:C6	3.02	0.47
1:1A:1268:A:C2	1:1A:2013:A:C4	3.03	0.47
8:1I:12:LEU:HD22	8:1I:19:VAL:HG21	1.97	0.47
32:1a:1033:G:H2'	32:1a:1034:G:C8	2.50	0.47
40:1i:128:ARG:NH1	55:1x:35:A:OP1	2.48	0.47
54:1y:54:5MU:OP2	54:1y:54:5MU:H71	2.15	0.47
1:2A:250:G:C6	1:2A:251:A:C6	3.03	0.47
1:2A:862:G:H2'	1:2A:863:A:O4'	2.15	0.47
1:2A:1429:G:H2'	1:2A:1430:C:C6	2.50	0.47
1:2A:1713:U:H2'	1:2A:1714:G:H8	1.80	0.47
1:2A:2533:A:OP1	1:2A:2665:A:O2'	2.21	0.47
6:2G:107:LEU:HD21	6:2G:178:PHE:CZ	2.49	0.47
9:2N:123:TYR:CZ	9:2N:129:PRO:HD2	2.50	0.47
32:2a:551:U:H2'	32:2a:552:U:C6	2.48	0.47
32:2a:1183:A:O2'	32:2a:1185:G:OP2	2.33	0.47
32:2a:1519:MA6:H5''	32:2a:1520:G:OP2	2.14	0.47
42:2k:87:THR:O	42:2k:87:THR:OG1	2.28	0.47
1:1A:7:G:H2'	1:1A:8:A:C8	2.50	0.47
1:1A:234:C:H2'	1:1A:235:U:H6	1.80	0.47
1:1A:1593:G:H2'	1:1A:1594:G:C8	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1769:G:O2'	1:1A:1958:C:OP1	2.32	0.47
1:1A:2285:C:OP2	28:16:6:ARG:NH1	2.48	0.47
3:1D:35:LYS:HB2	3:1D:36:PRO:HD2	1.97	0.47
30:18:62:LEU:HB3	30:18:65:GLU:HG2	1.96	0.47
32:1a:1304:G:C6	32:1a:1305:G:N1	2.83	0.47
33:1b:13:ALA:HB2	33:1b:44:LEU:HD13	1.97	0.47
1:2A:271(G):C:H2'	1:2A:271(H):G:H8	1.79	0.47
1:2A:1394:U:OP1	61:2A:3922:HOH:O	2.20	0.47
1:2A:1786:A:H1'	1:2A:1938:A:N6	2.29	0.47
1:2A:2831:G:OP1	1:2A:2834:G:H4'	2.15	0.47
2:2B:24:G:O2'	2:2B:56:G:N7	2.42	0.47
2:2B:88:C:H2'	2:2B:89:G:O4'	2.15	0.47
3:2D:242:ARG:HD3	3:2D:242:ARG:N	2.30	0.47
8:2I:77:LEU:HD12	8:2I:140:LEU:HD21	1.97	0.47
32:2a:9:G:H2'	32:2a:10:A:H8	1.80	0.47
32:2a:537:G:H2'	32:2a:538:G:H8	1.80	0.47
32:2a:997:U:H3	32:2a:1044:A:H61	1.63	0.47
32:2a:1237:C:HO2'	32:2a:1300:G:H1	1.61	0.47
34:2c:125:GLU:HB2	34:2c:190:ARG:O	2.15	0.47
44:2m:37:THR:O	44:2m:55:ARG:NH1	2.35	0.47
44:2m:122:LYS:HG3	44:2m:123:ALA:H	1.79	0.47
1:1A:1636:C:H2'	1:1A:1637:A:C8	2.50	0.46
1:1A:1864:U:OP1	1:1A:2410:G:O2'	2.30	0.46
1:1A:2117:A:O2'	1:1A:2118:U:H5''	2.16	0.46
16:1U:76:TYR:CZ	16:1U:80:ILE:HG13	2.50	0.46
32:1a:270:A:H2'	32:1a:271:C:C6	2.50	0.46
32:1a:1090:U:H2'	32:1a:1091:U:C6	2.50	0.46
34:1c:65:ALA:O	34:1c:66:VAL:HG13	2.15	0.46
34:1c:82:GLU:OE2	34:1c:85:ARG:NH1	2.48	0.46
40:1i:32:ASP:OD1	40:1i:33:PHE:N	2.48	0.46
1:2A:140:G:N2	1:2A:1596:A:H4'	2.30	0.46
1:2A:2134:A:H2'	1:2A:2134:A:N3	2.30	0.46
1:2A:2557:G:H2'	1:2A:2558:C:C6	2.50	0.46
7:2H:64:LEU:O	7:2H:68:THR:OG1	2.33	0.46
8:2I:12:LEU:HD22	8:2I:19:VAL:HG21	1.97	0.46
28:26:47:THR:HB	28:26:49:HIS:CE1	2.48	0.46
30:28:30:ARG:NH1	61:28:202:HOH:O	2.45	0.46
32:2a:66:G:H8	32:2a:66:G:OP1	1.98	0.46
32:2a:524:G:H2'	32:2a:525:C:C6	2.49	0.46
32:2a:841:U:H6	32:2a:841:U:P	2.38	0.46
32:2a:1006:C:H2'	32:2a:1007:C:C6	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1029:C:H5'	32:2a:1030:C:OP2	2.14	0.46
32:2a:1184:G:H2'	32:2a:1185:G:H8	1.80	0.46
32:2a:1250:A:H4'	40:2i:68:GLY:N	2.30	0.46
32:2a:1294:G:H2'	32:2a:1295:G:H8	1.80	0.46
34:2c:24:ALA:HB3	34:2c:29:TYR:HD1	1.80	0.46
36:2e:36:ASP:C	36:2e:38:GLN:H	2.23	0.46
46:2o:56:LEU:O	46:2o:60:VAL:HG23	2.15	0.46
1:1A:272:G:N7	1:1A:421:U:H2'	2.30	0.46
1:1A:848:G:H2'	1:1A:849:A:C8	2.50	0.46
1:1A:1079:C:H2'	1:1A:1080:C:O4'	2.16	0.46
1:1A:1903:G:OP1	3:1D:241:PRO:HB2	2.15	0.46
1:1A:2364:C:H2'	1:1A:2365:G:O4'	2.16	0.46
1:1A:2377:A:H2'	1:1A:2378:A:C8	2.50	0.46
5:1F:126:VAL:HG21	5:1F:129:PHE:CZ	2.50	0.46
32:1a:690:G:C6	32:1a:691:G:C6	3.03	0.46
32:1a:1068:G:H8	32:1a:1068:G:OP2	1.98	0.46
32:1a:1101:A:H4'	32:1a:1102:A:O5'	2.15	0.46
47:1p:72:ARG:HA	47:1p:75:ARG:HB3	1.96	0.46
1:2A:1665:A:H4'	10:2O:67:LYS:HB2	1.96	0.46
1:2A:2166:G:H3'	1:2A:2167:U:C5'	2.44	0.46
1:2A:2275:C:H6	1:2A:2275:C:H5'	1.80	0.46
1:2A:2671:A:H2'	1:2A:2672:G:O4'	2.15	0.46
18:2W:70:TYR:OH	18:2W:72:LYS:HG3	2.15	0.46
32:2a:336:C:H2'	32:2a:337:C:C6	2.50	0.46
32:2a:486:U:H2'	32:2a:487:A:C8	2.49	0.46
32:2a:1109:C:H2'	32:2a:1110:A:O4'	2.16	0.46
35:2d:22:LYS:O	35:2d:113:SER:HB3	2.16	0.46
42:2k:92:GLU:O	42:2k:96:ARG:HG2	2.16	0.46
44:2m:91:ARG:HD2	44:2m:96:LEU:HB2	1.97	0.46
1:1A:218:A:C2	1:1A:235:U:H4'	2.49	0.46
1:1A:1058:G:N1	1:1A:1080:C:N4	2.62	0.46
1:1A:1069:A:H2'	1:1A:1073:A:N7	2.30	0.46
1:1A:1069:A:H1'	1:1A:1096:A:H4'	1.97	0.46
4:1E:174:ASP:OD1	4:1E:175:VAL:N	2.49	0.46
20:1Y:68:HIS:ND1	20:1Y:70:SER:HB3	2.29	0.46
32:1a:890:G:O2'	32:1a:906:G:O6	2.22	0.46
33:1b:16:HIS:HB2	33:1b:204:ASN:CB	2.45	0.46
44:1m:15:VAL:HG23	44:1m:43:THR:O	2.14	0.46
54:1y:33:U:O2'	54:1y:35:A:N7	2.45	0.46
1:2A:80:G:O2'	1:2A:294:A:N1	2.41	0.46
1:2A:1946:U:H2'	1:2A:1947:C:C6	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2100:G:H1	1:2A:2189:U:H3	1.62	0.46
2:2B:19:G:H2'	2:2B:20:C:O4'	2.15	0.46
7:2H:3:ARG:HD3	7:2H:6:ARG:NH2	2.23	0.46
7:2H:143:GLN:NE2	7:2H:143:GLN:O	2.48	0.46
10:2O:63:VAL:HG12	10:2O:106:LEU:HD11	1.97	0.46
12:2Q:12:GLN:HE21	12:2Q:12:GLN:HB3	1.55	0.46
15:2T:94:ALA:HB1	15:2T:99:LEU:HD21	1.96	0.46
21:2Z:157:LEU:HD11	21:2Z:163:LEU:HB2	1.98	0.46
23:21:34:THR:HG22	23:21:36:GLY:H	1.80	0.46
23:21:40:ARG:NH2	23:21:42:GLN:HG2	2.30	0.46
32:2a:129(A):G:C6	32:2a:189(E):U:H4'	2.50	0.46
32:2a:1288:A:H2'	32:2a:1289:A:C8	2.49	0.46
32:2a:1323:G:H2'	32:2a:1324:A:C8	2.51	0.46
32:2a:1481:U:H2'	32:2a:1482:G:C8	2.50	0.46
46:2o:4:THR:OG1	46:2o:7:GLU:HG3	2.16	0.46
1:1A:747:U:O2	1:1A:2014:A:H1'	2.15	0.46
1:1A:1060:U:H3	1:1A:1088:A:H8	1.61	0.46
1:1A:2188:C:H2'	1:1A:2189:U:O4'	2.15	0.46
1:1A:2567:G:H2'	1:1A:2568:C:C6	2.51	0.46
1:1A:2750:A:OP2	7:1H:62:LYS:NZ	2.40	0.46
5:1F:31:HIS:NE2	5:1F:35:GLU:OE2	2.49	0.46
21:1Z:4:ARG:NE	21:1Z:60:GLU:OE2	2.43	0.46
32:1a:160:A:H2'	32:1a:161:A:O4'	2.16	0.46
32:1a:345:C:H5'	32:1a:346:G:C4	2.51	0.46
1:2A:1847:A:H3'	1:2A:1848:A:H5'	1.96	0.46
32:2a:1002:G:C6	32:2a:1003:G:H8	2.32	0.46
32:2a:1184:G:H2'	32:2a:1185:G:C8	2.49	0.46
34:2c:63:ASN:HB2	34:2c:98:ASN:HB2	1.97	0.46
35:2d:172:PRO:HB2	35:2d:187:ARG:HH21	1.80	0.46
41:2j:49:VAL:HG12	41:2j:61:GLU:O	2.16	0.46
50:2s:51:VAL:HB	50:2s:75:ALA:HB2	1.97	0.46
1:1A:861:A:C2	1:1A:917:A:C4	3.04	0.46
1:1A:990:A:OP2	61:1A:4263:HOH:O	2.21	0.46
1:1A:2233:U:H2'	1:1A:2234:G:C8	2.51	0.46
7:1H:25:LYS:HG3	7:1H:34:GLU:HG2	1.97	0.46
11:1P:107:LYS:O	11:1P:110:TYR:HB2	2.15	0.46
20:1Y:8:LYS:HD3	20:1Y:97:ARG:NH1	2.31	0.46
32:1a:262:A:C6	32:1a:263:A:C6	3.04	0.46
32:1a:1004:A:C5'	32:1a:1024:G:H22	2.28	0.46
1:2A:888:C:OP2	44:2m:93:ARG:NE	2.48	0.46
1:2A:1410:G:H2'	1:2A:1411:C:H6	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1908:C:O2	55:2x:12:G:H4'	2.16	0.46
7:2H:144:VAL:O	7:2H:148:ILE:HG13	2.16	0.46
14:2S:27:SER:HA	14:2S:88:ASP:HB3	1.97	0.46
32:2a:745:C:H2'	32:2a:746:A:H8	1.81	0.46
32:2a:1058:G:H2'	32:2a:1059:C:O4'	2.16	0.46
35:2d:189:PRO:HB2	35:2d:194:LEU:CD2	2.46	0.46
46:2o:11:VAL:HG21	46:2o:34:LEU:HD22	1.97	0.46
50:2s:32:LYS:HB3	50:2s:57:HIS:CE1	2.50	0.46
51:2t:84:LEU:O	51:2t:88:VAL:HG23	2.16	0.46
1:1A:442:G:N3	5:1F:48:THR:OG1	2.41	0.46
1:1A:1364:G:C8	23:11:3:LYS:HD2	2.51	0.46
1:1A:2014:A:H2'	1:1A:2015:A:C8	2.50	0.46
1:1A:2096:U:H3	1:1A:2193:G:H1	1.63	0.46
1:1A:2869:G:H2'	1:1A:2870:C:O4'	2.15	0.46
6:1G:11:TYR:HA	6:1G:15:VAL:HB	1.97	0.46
12:1Q:16:ARG:HG2	12:1Q:18:LYS:HE2	1.96	0.46
21:1Z:11:GLU:O	21:1Z:36:LYS:NZ	2.40	0.46
32:1a:148:G:H2'	32:1a:149:A:C8	2.50	0.46
32:1a:435:C:H2'	32:1a:436:C:H6	1.80	0.46
33:1b:78:GLN:O	33:1b:94:ASN:ND2	2.49	0.46
50:1s:20:LEU:HD23	50:1s:23:ASN:HD22	1.81	0.46
1:2A:557:U:H2'	1:2A:558:G:C8	2.51	0.46
1:2A:2086:U:H2'	1:2A:2087:G:C8	2.50	0.46
1:2A:2127:G:H2'	1:2A:2128:C:C5	2.50	0.46
2:2B:30:C:OP2	14:2S:32:LEU:HD11	2.15	0.46
3:2D:108:PRO:HG2	3:2D:111:LEU:HB2	1.98	0.46
6:2G:101:ILE:HG21	26:24:9:LEU:HD23	1.97	0.46
8:2I:87:LYS:NZ	8:2I:88:ILE:O	2.49	0.46
14:2S:36:TYR:CD2	14:2S:36:TYR:N	2.83	0.46
15:2T:30:VAL:HG22	15:2T:86:ILE:HG12	1.96	0.46
20:2Y:52:SER:OG	20:2Y:55:TYR:HB2	2.15	0.46
48:2q:29:HIS:CG	48:2q:30:PRO:HD2	2.51	0.46
49:2r:48:GLY:O	49:2r:74:ARG:NH2	2.49	0.46
1:1A:601:C:O2'	1:1A:605:C:H5''	2.16	0.46
1:1A:1048:A:N1	1:1A:1112:G:O2'	2.38	0.46
1:1A:1357:U:H2'	1:1A:1358:G:O4'	2.16	0.46
1:1A:2157:G:H4'	1:1A:2158:A:OP1	2.15	0.46
1:1A:2286:A:H4'	1:1A:2287:A:O4'	2.16	0.46
33:1b:84:GLU:HA	33:1b:87:ARG:HD3	1.97	0.46
44:1m:105:THR:OG1	44:1m:106:ASN:N	2.45	0.46
49:1r:59:SER:H	49:1r:62:GLU:HB2	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1364:G:C8	23:21:3:LYS:HD2	2.51	0.46
1:2A:1791:A:H5'	3:2D:206:LEU:HD12	1.98	0.46
5:2F:108:LYS:O	5:2F:112:MET:HG3	2.15	0.46
6:2G:35:GLU:OE2	6:2G:36:LYS:HE2	2.16	0.46
13:2R:72:ASP:HB3	13:2R:75:LEU:HB3	1.97	0.46
32:2a:1330:U:H4'	44:2m:23:TYR:CE1	2.50	0.46
34:2c:63:ASN:HB3	34:2c:98:ASN:ND2	2.30	0.46
40:2i:3:GLN:HE21	40:2i:20:ARG:NE	2.14	0.46
42:2k:117:ASN:HD22	42:2k:117:ASN:N	2.13	0.46
1:1A:694:U:OP1	3:1D:59:LYS:NZ	2.48	0.46
1:1A:1173:G:OP2	1:1A:1173:G:H2'	2.16	0.46
1:1A:1798:U:H5'	3:1D:259:THR:CG2	2.45	0.46
1:1A:2106:G:H1	1:1A:2183:C:H42	1.62	0.46
7:1H:7:LEU:HD23	7:1H:69:ARG:NH2	2.31	0.46
15:1T:51:ARG:HG3	15:1T:98:LYS:HD2	1.98	0.46
32:1a:432:A:H3'	32:1a:433:C:C6	2.51	0.46
41:1j:65:LEU:HD13	45:1n:56:VAL:HG22	1.96	0.46
1:2A:867:C:H2'	1:2A:868:U:C6	2.50	0.46
1:2A:1155:A:H5''	16:2U:55:ARG:NE	2.31	0.46
1:2A:1590:U:H2'	1:2A:1591:G:H8	1.81	0.46
2:2B:1:U:O2'	2:2B:2:C:O5'	2.27	0.46
2:2B:41:U:O4	6:2G:70:VAL:HG23	2.15	0.46
17:2V:24:LYS:HE2	17:2V:24:LYS:HB3	1.73	0.46
32:2a:72:C:H2'	32:2a:73:G:C8	2.50	0.46
32:2a:1004:A:N3	32:2a:1038:C:C2	2.84	0.46
32:2a:1122:U:C2	32:2a:1123:A:C8	3.04	0.46
32:2a:1289:A:OP1	52:2u:9:ARG:NH1	2.39	0.46
33:2b:192:SER:O	33:2b:194:PRO:HD3	2.16	0.46
34:2c:30:ARG:O	34:2c:34:LEU:HB2	2.16	0.46
44:2m:70:LEU:O	44:2m:74:VAL:HG23	2.15	0.46
54:2y:59:U:H3'	54:2y:60:U:O2	2.15	0.46
1:1A:910:A:N3	1:1A:2264:C:O2'	2.47	0.46
1:1A:1075:C:H2'	1:1A:1076:C:H2'	1.98	0.46
1:1A:1090:U:C2	1:1A:1102:C:H1'	2.51	0.46
1:1A:1700:A:H2'	1:1A:1701:A:H5'	1.97	0.46
2:1B:7:G:H5'	14:1S:29:PHE:CE2	2.50	0.46
32:1a:473:G:H2'	32:1a:474:G:H8	1.81	0.46
32:1a:1030(D):A:H2'	32:1a:1031:G:H4'	1.98	0.46
33:1b:109:SER:O	33:1b:112:VAL:HG22	2.15	0.46
33:1b:167:PRO:HG3	33:1b:188:ALA:HB2	1.98	0.46
34:1c:35:GLU:HB3	34:1c:59:ARG:NH2	2.31	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:577:G:O2'	1:2A:1254:A:OP1	2.26	0.46
1:2A:1430:C:H2'	1:2A:1431:U:C6	2.50	0.46
1:2A:1826:G:H4'	3:2D:242:ARG:CZ	2.46	0.46
1:2A:1864:U:OP1	1:2A:2410:G:O2'	2.28	0.46
1:2A:1915:5MU:H2'	1:2A:1916:A:O4'	2.15	0.46
1:2A:2307:G:H8	1:2A:2307:G:OP1	1.99	0.46
1:2A:2322:A:H2'	1:2A:2323:G:O4'	2.16	0.46
3:2D:218:ARG:HB3	3:2D:219:PRO:HD2	1.98	0.46
9:2N:76:SER:HB3	9:2N:81:GLY:HA3	1.98	0.46
16:2U:76:TYR:CZ	16:2U:80:ILE:HG13	2.51	0.46
20:2Y:44:ILE:HA	20:2Y:63:LYS:O	2.15	0.46
26:24:49:PHE:O	26:24:51:ASP:N	2.49	0.46
35:2d:190:ASP:O	35:2d:194:LEU:HD23	2.16	0.46
44:2m:20:THR:C	44:2m:22:ILE:H	2.24	0.46
55:2x:19:G:H4'	55:2x:20:U:OP2	2.15	0.46
1:1A:271(K):U:O2	8:1I:50:ARG:NE	2.49	0.46
1:1A:371:A:OP1	61:1A:4262:HOH:O	2.20	0.46
4:1E:119:ARG:HG2	4:1E:120:TRP:NE1	2.31	0.46
6:1G:16:ARG:O	6:1G:20:ILE:HG13	2.17	0.46
6:1G:179:PRO:HG3	26:14:43:TYR:OH	2.16	0.46
32:1a:295:C:H2'	32:1a:296:U:O4'	2.16	0.46
32:1a:562:C:O2	43:1l:16:GLU:N	2.35	0.46
32:1a:1006:C:H42	32:1a:1023:G:H1	1.64	0.46
38:1g:144:MET:HE2	38:1g:144:MET:HB3	1.81	0.46
42:1k:86:GLY:H	42:1k:112:THR:HG1	1.61	0.46
1:2A:1913:A:H4'	1:2A:1914:C:O5'	2.14	0.46
2:2B:83:G:H1	2:2B:94:C:H42	1.62	0.46
3:2D:164:GLN:OE1	3:2D:176:ARG:NH1	2.48	0.46
4:2E:143:ASN:HD22	4:2E:147:PRO:HD3	1.80	0.46
6:2G:3:LEU:HD23	26:24:25:TYR:CZ	2.51	0.46
6:2G:122:PRO:HG3	6:2G:182:LYS:C	2.41	0.46
11:2P:89:ALA:HA	11:2P:121:LYS:HD3	1.98	0.46
32:2a:90:U:H2'	32:2a:91:C:C6	2.51	0.46
32:2a:1123:A:H1'	41:2j:37:PRO:O	2.16	0.46
32:2a:1301:U:O2'	32:2a:1302:U:H5'	2.16	0.46
32:2a:1338:G:C2	32:2a:1339:A:C4	3.04	0.46
32:2a:1376:U:OP1	38:2g:98:SER:OG	2.25	0.46
36:2e:18:ARG:HH21	36:2e:25:ARG:HH11	1.63	0.46
50:2s:37:ARG:H	50:2s:37:ARG:HG3	1.55	0.46
55:2x:21:A:H61	55:2x:46:G:H2'	1.81	0.46
55:2x:61:C:H2'	55:2x:62:C:C6	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:185:U:H4'	1:1A:218:A:H4'	1.98	0.45
1:1A:1047:G:H2'	1:1A:1110:G:H22	1.82	0.45
1:1A:2317:C:H2'	1:1A:2318:G:O4'	2.15	0.45
1:1A:2790:A:H3'	1:1A:2790:A:N3	2.30	0.45
3:1D:77:ALA:HA	3:1D:97:TYR:HA	1.98	0.45
5:1F:74:ARG:H	5:1F:74:ARG:HG3	1.42	0.45
6:1G:98:ARG:CZ	26:14:1:MET:HE3	2.47	0.45
32:1a:190:U:H2'	32:1a:191:G:C8	2.50	0.45
32:1a:401:C:H2'	32:1a:402:G:H8	1.81	0.45
32:1a:418:C:H1'	32:1a:540:G:O2'	2.15	0.45
32:1a:625:G:H4'	47:1p:16:HIS:CD2	2.51	0.45
32:1a:977:A:O2'	32:1a:979:C:OP2	2.32	0.45
32:1a:1025:U:O2	32:1a:1036:G:C6	2.69	0.45
1:2A:747:U:H1'	18:2W:92:ARG:NH2	2.31	0.45
1:2A:2238:G:H5''	61:2A:4715:HOH:O	2.15	0.45
6:2G:138:GLN:HB3	6:2G:153:ARG:O	2.16	0.45
19:2X:94:GLY:CA	19:2X:95:LEU:HB2	2.46	0.45
19:2X:94:GLY:HA3	19:2X:95:LEU:HB2	1.98	0.45
32:2a:908:A:H2'	32:2a:909:A:C8	2.51	0.45
32:2a:1055:A:N3	34:2c:156:ARG:NH1	2.64	0.45
32:2a:1213:A:C2	32:2a:1215:G:H1'	2.50	0.45
32:2a:1263:C:H1'	32:2a:1273:G:N2	2.31	0.45
38:2g:65:ALA:HB1	38:2g:127:ALA:HB3	1.98	0.45
54:2w:18:G:HO2'	54:2w:57:G:H22	1.56	0.45
1:1A:330:A:HO2'	1:1A:331:A:H8	1.62	0.45
1:1A:534:U:H2'	1:1A:535:C:C6	2.51	0.45
1:1A:1542:A:H8	1:1A:1542:A:OP1	1.98	0.45
1:1A:1798:U:H5'	3:1D:259:THR:HG22	1.97	0.45
1:1A:2396:G:OP1	23:11:25:LYS:NZ	2.30	0.45
1:1A:2404:C:O3'	11:1P:77:ARG:NH2	2.49	0.45
2:1B:28:C:OP1	14:1S:36:TYR:OH	2.23	0.45
5:1F:148:LEU:HD22	5:1F:154:VAL:HG21	1.97	0.45
6:1G:28:VAL:HG23	6:1G:29:TRP:CD1	2.51	0.45
21:1Z:5:LEU:O	21:1Z:59:LEU:HA	2.17	0.45
32:1a:664:G:P	49:1r:64:ARG:HH21	2.39	0.45
36:1e:31:LEU:HD23	36:1e:31:LEU:HA	1.73	0.45
42:1k:15:ALA:O	42:1k:77:MET:HA	2.16	0.45
42:1k:72:ALA:HB1	42:1k:77:MET:HG2	1.97	0.45
55:1x:19:G:H4'	55:1x:20:U:OP2	2.15	0.45
1:2A:479:A:H4'	1:2A:480:A:OP1	2.16	0.45
1:2A:1464:C:H2'	1:2A:1465:G:C8	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1820:U:C4	3:2D:160:GLY:HA3	2.51	0.45
1:2A:2154:G:N7	1:2A:2156:G:N2	2.63	0.45
1:2A:2310:A:O2'	6:2G:75:LYS:NZ	2.49	0.45
1:2A:2695:C:H2'	1:2A:2696:U:C6	2.52	0.45
1:2A:2740:A:H2'	1:2A:2741:A:C8	2.52	0.45
4:2E:176:ILE:HB	4:2E:181:LEU:HB2	1.98	0.45
6:2G:36:LYS:HD3	6:2G:95:ARG:NH2	2.31	0.45
8:2I:69:LYS:NZ	8:2I:69:LYS:HB2	2.30	0.45
12:2Q:31:ASP:O	12:2Q:134:ARG:N	2.49	0.45
16:2U:16:LYS:HB3	16:2U:16:LYS:HE2	1.79	0.45
18:2W:9:TYR:H	18:2W:102:HIS:CE1	2.34	0.45
24:22:2:LYS:O	24:22:6:VAL:HG23	2.16	0.45
32:2a:538:G:H5''	43:2l:114:LYS:HB2	1.98	0.45
32:2a:644:G:H4'	39:2h:92:ARG:HH21	1.82	0.45
32:2a:975:A:H5''	32:2a:1363(A):A:H62	1.81	0.45
32:2a:1239:A:H4'	32:2a:1240:U:H5'	1.98	0.45
32:2a:1339:A:H2	55:2x:31:G:H4'	1.81	0.45
34:2c:111:LEU:HD23	34:2c:202:ILE:HG21	1.98	0.45
35:2d:38:TYR:CE1	35:2d:45:GLN:HG3	2.50	0.45
42:2k:21:ILE:HD12	42:2k:84:VAL:HG12	1.98	0.45
1:1A:1790:C:H2'	1:1A:1791:A:C5	2.51	0.45
1:1A:1951:U:O2	1:1A:1953:A:H8	1.99	0.45
1:1A:2360:A:H2'	1:1A:2361:A:O4'	2.16	0.45
1:1A:2633:G:H2'	1:1A:2634:G:O4'	2.17	0.45
7:1H:154:PRO:HB3	7:1H:163:TYR:CZ	2.51	0.45
12:1Q:18:LYS:O	12:1Q:98:LYS:NZ	2.25	0.45
21:1Z:28:MET:HE2	21:1Z:35:ARG:HB2	1.98	0.45
32:1a:46:G:O2'	32:1a:365:U:H1'	2.16	0.45
33:1b:55:PHE:HD1	33:1b:221:LEU:HD22	1.81	0.45
47:1p:6:LEU:HB3	47:1p:17:TYR:CD1	2.51	0.45
51:1t:26:ASN:CG	51:1t:71:THR:HG22	2.41	0.45
1:2A:211:A:H2'	1:2A:212:G:O4'	2.16	0.45
1:2A:885:C:H2'	1:2A:886:C:O4'	2.16	0.45
1:2A:1495:A:H2'	1:2A:1496:A:C8	2.50	0.45
1:2A:1899:G:H2'	1:2A:1899:G:N3	2.32	0.45
1:2A:2693:A:H2'	1:2A:2694:G:C8	2.51	0.45
5:2F:123:LEU:HD12	5:2F:124:LEU:H	1.82	0.45
7:2H:77:LYS:HG3	7:2H:81:GLU:CD	2.41	0.45
8:2I:59:ALA:HA	8:2I:62:LYS:HE2	1.98	0.45
9:2N:38:HIS:ND1	9:2N:39:ARG:HG3	2.30	0.45
32:2a:536:C:N4	32:2a:537:G:O6	2.49	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1129:C:OP2	40:2i:66:ARG:NH1	2.49	0.45
32:2a:1305:G:H5'	52:2u:4:GLY:HA3	1.99	0.45
45:2n:57:ARG:HG2	45:2n:58:LYS:N	2.31	0.45
48:2q:58:GLU:OE1	48:2q:75:ARG:NE	2.50	0.45
1:1A:128:C:H2'	1:1A:129:C:H6	1.82	0.45
1:1A:1441:G:H2'	1:1A:1442:G:H8	1.82	0.45
15:1T:127:ALA:O	15:1T:129:ARG:N	2.47	0.45
28:16:10:LEU:HG	28:16:54:ILE:HG13	1.99	0.45
1:2A:147:U:O4	61:2A:3970:HOH:O	2.21	0.45
1:2A:524:U:H2'	1:2A:525:U:C6	2.52	0.45
1:2A:597:U:H2'	1:2A:598:G:H8	1.82	0.45
1:2A:668:G:H5'	1:2A:669:G:OP2	2.17	0.45
1:2A:955:C:OP2	12:2Q:14:ARG:HG3	2.16	0.45
1:2A:1509(B):A:H2'	1:2A:1510:G:C8	2.51	0.45
32:2a:189(K):U:H2'	32:2a:189(L):G:C8	2.51	0.45
32:2a:707:C:H2'	32:2a:708:C:H6	1.81	0.45
32:2a:735:C:H2'	32:2a:736:C:H6	1.82	0.45
32:2a:875:C:O2'	39:2h:14:ARG:HD2	2.16	0.45
32:2a:892:A:O2'	32:2a:1415:G:H4'	2.17	0.45
32:2a:1235:U:O2'	32:2a:1305:G:O5'	2.33	0.45
34:2c:101:LEU:HD22	34:2c:102:ASN:N	2.32	0.45
50:2s:30:LEU:HD13	50:2s:31:ILE:N	2.31	0.45
1:1A:244:A:C2	1:1A:255:A:C4	3.04	0.45
1:1A:576:U:H2'	1:1A:577:G:C8	2.52	0.45
1:1A:1039:G:H1	1:1A:1116:C:H42	1.64	0.45
1:1A:1952:A:C6	1:1A:1953:A:N1	2.85	0.45
1:1A:2415:G:OP1	61:1A:4259:HOH:O	2.20	0.45
6:1G:3:LEU:HD13	26:14:25:TYR:CZ	2.52	0.45
6:1G:77:ILE:HG22	6:1G:80:PHE:H	1.81	0.45
10:1O:43:VAL:HG12	10:1O:54:GLU:HA	1.98	0.45
20:1Y:20:TYR:CG	20:1Y:42:VAL:HG13	2.51	0.45
24:12:51:ARG:HD3	24:12:55:ARG:NH1	2.32	0.45
32:1a:116:A:H61	32:1a:313:A:H1'	1.82	0.45
32:1a:601:C:H2'	32:1a:602:A:C8	2.52	0.45
39:1h:27:PRO:O	39:1h:32:LYS:NZ	2.36	0.45
40:1i:4:TYR:CZ	40:1i:88:TYR:HD1	2.35	0.45
44:1m:3:ARG:HG3	44:1m:4:ILE:N	2.31	0.45
45:1n:32:SER:HB3	45:1n:41:ARG:HB3	1.98	0.45
51:1t:86:ARG:O	51:1t:90:GLN:NE2	2.49	0.45
1:2A:195:A:H61	1:2A:198:C:H3'	1.82	0.45
1:2A:1025:G:C4	1:2A:1135:C:H1'	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1927:A:H2'	1:2A:1928:A:C8	2.51	0.45
1:2A:2882:A:OP1	13:2R:96:ARG:NE	2.45	0.45
2:2B:28:C:H2'	2:2B:29:A:O4'	2.16	0.45
6:2G:97:ASP:HA	6:2G:100:TRP:HD1	1.80	0.45
21:2Z:144:LEU:HD23	21:2Z:174:VAL:HG22	1.99	0.45
32:2a:7:G:H5'	32:2a:298:A:O4'	2.17	0.45
32:2a:868:C:H2'	32:2a:869:G:O4'	2.16	0.45
32:2a:1203:C:H2'	32:2a:1204:A:C8	2.52	0.45
34:2c:134:ILE:HG22	34:2c:168:ALA:HB3	1.99	0.45
38:2g:79:ARG:NH2	38:2g:80:VAL:HA	2.29	0.45
41:2j:9:ARG:HH22	41:2j:69:ASN:HD21	1.63	0.45
44:2m:86:CYS:SG	44:2m:89:GLY:N	2.85	0.45
47:2p:18:ARG:HD3	47:2p:35:LYS:HD2	1.97	0.45
54:2w:43:C:H2'	54:2w:44:G:C8	2.51	0.45
1:1A:1044:G:H5'	1:1A:1045:A:OP2	2.17	0.45
1:1A:2031:A:C6	1:1A:2498:C:H1'	2.52	0.45
1:1A:2176:A:H2'	1:1A:2177:C:C6	2.51	0.45
21:1Z:139:VAL:HG12	21:1Z:140:ASP:H	1.81	0.45
26:14:26:SER:OG	26:14:27:THR:N	2.50	0.45
33:1b:16:HIS:HB3	33:1b:210:SER:HB2	1.99	0.45
33:1b:24:TRP:HZ3	33:1b:29:ALA:HB2	1.80	0.45
38:1g:92:SER:O	38:1g:96:GLN:HG3	2.17	0.45
51:1t:63:ILE:HG22	51:1t:77:ALA:HB1	1.97	0.45
54:1y:56:C:C4	54:1y:57:G:C8	3.05	0.45
1:2A:212:G:H2'	1:2A:213:A:O4'	2.16	0.45
1:2A:307:G:H21	1:2A:330:A:H62	1.63	0.45
1:2A:340:A:H2'	1:2A:341:G:O4'	2.17	0.45
1:2A:1199:U:H2'	1:2A:1200:C:C6	2.51	0.45
1:2A:1297:C:OP2	61:2A:3968:HOH:O	2.21	0.45
3:2D:96:HIS:CD2	3:2D:102:LYS:HG2	2.51	0.45
5:2F:53:THR:HG23	5:2F:55:GLY:N	2.25	0.45
27:25:20:ARG:HG2	27:25:23:HIS:ND1	2.32	0.45
28:26:10:LEU:HB2	28:26:52:VAL:HG12	1.97	0.45
32:2a:384:G:H2'	32:2a:385:C:C6	2.52	0.45
32:2a:442:C:H42	32:2a:492:G:H1	1.65	0.45
32:2a:537:G:H2'	32:2a:538:G:C8	2.51	0.45
32:2a:580:U:H2'	32:2a:581:G:O4'	2.16	0.45
32:2a:658:G:O4'	46:2o:22:THR:HB	2.16	0.45
32:2a:674:G:H2'	32:2a:675:A:C8	2.49	0.45
32:2a:833:U:H2'	32:2a:834:C:C6	2.52	0.45
32:2a:942:G:C2	32:2a:1342:C:C2	3.04	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:2c:63:ASN:HB3	34:2c:98:ASN:HD22	1.82	0.45
34:2c:162:GLN:NE2	53:2v:24:A:O2'	2.49	0.45
36:2e:80:ILE:HG22	36:2e:91:LEU:HB2	1.98	0.45
37:2f:96:PRO:HB3	49:2r:30:ASP:CG	2.41	0.45
38:2g:51:GLN:O	38:2g:55:GLY:HA2	2.16	0.45
41:2j:47:PHE:CZ	45:2n:37:PHE:HE2	2.35	0.45
50:2s:63:THR:HG23	50:2s:66:MET:HE3	1.99	0.45
1:1A:607:U:OP1	5:1F:102:PRO:HA	2.16	0.45
1:1A:2033:A:OP1	61:1A:4211:HOH:O	2.21	0.45
1:1A:2108:C:H2'	1:1A:2109:U:H6	1.82	0.45
3:1D:26:LYS:HE2	3:1D:28:GLU:O	2.16	0.45
32:1a:540:G:H2'	32:1a:541:G:O4'	2.16	0.45
32:1a:769:G:H4'	32:1a:1513:A:H4'	1.98	0.45
32:1a:864:A:H2'	32:1a:865:A:C8	2.52	0.45
32:1a:971:G:H22	32:1a:1363(A):A:P	2.39	0.45
33:1b:41:ILE:HD13	33:1b:41:ILE:HA	1.77	0.45
35:1d:102:ASP:OD1	35:1d:103:ASN:N	2.49	0.45
39:1h:121:ASP:OD1	39:1h:121:ASP:N	2.50	0.45
1:2A:271(D):G:H2'	1:2A:271(E):U:C6	2.50	0.45
1:2A:484:C:H2'	1:2A:485:C:H6	1.81	0.45
1:2A:571:A:N6	1:2A:2499:C:O3'	2.49	0.45
1:2A:764:A:H5''	3:2D:210:GLY:HA3	1.99	0.45
1:2A:848:G:H2'	1:2A:849:A:C8	2.52	0.45
1:2A:987:G:O2'	1:2A:1000:A:N3	2.47	0.45
7:2H:9:ILE:N	7:2H:50:VAL:O	2.44	0.45
8:2I:84:GLY:C	8:2I:86:THR:H	2.24	0.45
14:2S:19:LYS:O	14:2S:21:THR:N	2.50	0.45
14:2S:30:ARG:HD3	14:2S:98:VAL:HG13	1.98	0.45
22:20:53:MET:HG3	22:20:59:LEU:HD23	1.98	0.45
32:2a:728:A:H2'	32:2a:729:A:C8	2.52	0.45
32:2a:1129:C:P	40:2i:16:ARG:HH12	2.39	0.45
32:2a:1348:U:H2'	32:2a:1349:A:H8	1.81	0.45
1:1A:1594:G:H2'	1:1A:1595:G:O4'	2.17	0.45
11:1P:121:LYS:HB3	11:1P:123:LEU:HD13	1.98	0.45
12:1Q:43:THR:HG22	12:1Q:94:VAL:HG12	1.98	0.45
16:1U:81:HIS:CE1	16:1U:85:LYS:HD2	2.52	0.45
19:1X:43:VAL:HG21	19:1X:81:VAL:HG11	1.99	0.45
21:1Z:92:SER:O	21:1Z:130:PRO:HG2	2.16	0.45
32:1a:142:G:H2'	32:1a:143:A:H8	1.82	0.45
32:1a:266:G:H2'	32:1a:266:G:N3	2.31	0.45
32:1a:297:G:H4'	32:1a:557:G:H4'	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1343:G:H2'	32:1a:1344:C:C6	2.52	0.45
34:1c:79:ARG:C	34:1c:81:GLY:H	2.24	0.45
36:1e:139:LEU:HA	36:1e:142:LEU:HD12	1.99	0.45
39:1h:43:GLY:O	39:1h:64:LYS:NZ	2.30	0.45
44:1m:92:HIS:CE1	44:1m:98:VAL:HG11	2.52	0.45
54:1y:23:A:H2'	54:1y:24:G:C8	2.52	0.45
1:2A:458:G:O2'	1:2A:469:G:O6	2.34	0.45
1:2A:729:G:C6	3:2D:208:LYS:HB2	2.52	0.45
1:2A:1113:U:H2'	1:2A:1114:G:C8	2.52	0.45
1:2A:1486:A:H2'	1:2A:1487:G:C8	2.52	0.45
1:2A:1847:A:H4'	1:2A:1848:A:OP2	2.17	0.45
1:2A:2185:C:H2'	1:2A:2186:G:O4'	2.17	0.45
1:2A:2355:C:H4'	22:20:24:LYS:HG3	1.98	0.45
3:2D:175:LEU:HD12	3:2D:185:VAL:HG21	1.99	0.45
4:2E:77:ILE:HA	4:2E:77:ILE:HD13	1.83	0.45
5:2F:131:GLY:O	5:2F:138:GLU:HB3	2.17	0.45
14:2S:15:ARG:HG2	14:2S:19:LYS:NZ	2.32	0.45
32:2a:1330:U:H4'	44:2m:23:TYR:CZ	2.52	0.45
32:2a:1346:A:H5''	40:2i:120:ARG:NH2	2.30	0.45
32:2a:1366:C:H2'	32:2a:1367:C:C6	2.51	0.45
35:2d:101:LEU:HA	35:2d:104:VAL:HG22	1.97	0.45
1:1A:113:G:H5'	61:1A:4774:HOH:O	2.16	0.45
1:1A:579:G:H2'	1:1A:580:C:C6	2.52	0.45
1:1A:774:A:N3	1:1A:774:A:H2'	2.31	0.45
1:1A:2093:G:C6	1:1A:2225:A:C8	3.05	0.45
2:1B:24:G:N7	2:1B:56:G:H2'	2.32	0.45
11:1P:8:PRO:HB2	11:1P:12:ALA:HB3	1.99	0.45
11:1P:97:PRO:HD3	11:1P:126:VAL:O	2.16	0.45
32:1a:523:A:H61	43:1l:92:OTD:CG	2.29	0.45
35:1d:159:ARG:O	35:1d:163:GLU:HG3	2.17	0.45
37:1f:22:GLU:OE1	37:1f:84:ASN:HB2	2.16	0.45
38:1g:79:ARG:HD2	38:1g:80:VAL:N	2.32	0.45
1:2A:445:C:OP1	16:2U:2:PRO:HA	2.17	0.45
1:2A:900:A:HO2'	1:2A:901:A:P	2.40	0.45
1:2A:921:G:C6	1:2A:922:U:C4	3.05	0.45
1:2A:2268:A:OP1	61:2A:3972:HOH:O	2.21	0.45
1:2A:2393:A:H5''	11:2P:63:PRO:HB3	1.99	0.45
1:2A:2821:A:H2'	1:2A:2822:G:C8	2.52	0.45
2:2B:14:U:O3'	2:2B:108:U:O2'	2.35	0.45
11:2P:82:GLY:HA2	11:2P:113:LYS:O	2.16	0.45
32:2a:103:C:P	51:2t:17:ARG:HH21	2.40	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:401:C:O2'	32:2a:621:A:N3	2.45	0.45
33:2b:112:VAL:C	33:2b:114:ARG:H	2.24	0.45
36:2e:105:VAL:HB	36:2e:106:PRO:HD3	1.99	0.45
46:2o:84:LYS:O	46:2o:84:LYS:HD3	2.17	0.45
51:2t:59:ALA:O	51:2t:63:ILE:HG13	2.17	0.45
1:1A:414:C:H2'	1:1A:415:A:C8	2.52	0.45
1:1A:796:C:H2'	1:1A:797:C:C6	2.52	0.45
1:1A:832:G:H5'	11:1P:45:LEU:HD11	1.99	0.45
1:1A:1399:C:OP1	19:1X:25:LYS:NZ	2.50	0.45
1:1A:2679:A:H4'	4:1E:165:VAL:HG11	1.99	0.45
16:1U:82:GLY:HA3	16:1U:113:ALA:HB1	1.99	0.45
26:14:62:ARG:HB2	26:14:63:TYR:CE1	2.52	0.45
32:1a:392:G:OP1	47:1p:8:ARG:NH2	2.50	0.45
32:1a:955:U:O2'	50:1s:83:HIS:HD2	2.00	0.45
32:1a:1004:A:H5''	32:1a:1024:G:H22	1.82	0.45
32:1a:1466:C:H2'	32:1a:1467:G:O4'	2.17	0.45
33:1b:24:TRP:H	33:1b:24:TRP:HD1	1.63	0.45
36:1e:41:VAL:HG23	36:1e:67:VAL:HG13	1.99	0.45
44:1m:4:ILE:HD12	44:1m:57:ARG:HA	1.99	0.45
50:1s:64:GLU:O	50:1s:67:VAL:HG23	2.17	0.45
55:1x:8:4SU:O2	55:1x:21:A:H2	2.00	0.45
1:2A:1952:A:OP1	10:2O:42:SER:OG	2.30	0.45
1:2A:2687:U:H2'	1:2A:2688:U:O4'	2.17	0.45
20:2Y:7:VAL:CG1	20:2Y:27:VAL:HG21	2.47	0.45
32:2a:158:G:H2'	32:2a:159:G:C8	2.52	0.45
32:2a:382:A:H2'	32:2a:383:A:C8	2.52	0.45
32:2a:999:C:H2'	32:2a:1000:U:C6	2.52	0.45
32:2a:1260:C:O2	32:2a:1274:G:N2	2.50	0.45
33:2b:114:ARG:HA	33:2b:117:GLU:HB2	1.98	0.45
39:2h:39:LEU:HD12	39:2h:44:PHE:HB2	1.99	0.45
41:2j:46:ARG:HA	41:2j:64:GLU:HA	1.99	0.45
42:2k:44:SER:OG	42:2k:47:VAL:HG23	2.17	0.45
1:1A:783:A:O2'	1:1A:785:G:OP1	2.31	0.44
1:1A:904:C:O2'	21:1Z:169:GLU:OE2	2.29	0.44
1:1A:1059:G:H2'	1:1A:1060:U:C5	2.52	0.44
1:1A:1500:G:H2'	1:1A:1501:C:C6	2.51	0.44
1:1A:1509(A):A:H3'	1:1A:1509(B):A:H8	1.82	0.44
1:1A:2389:G:H5''	1:1A:2390:U:O4'	2.16	0.44
1:1A:2429:G:OP1	61:1A:4209:HOH:O	2.20	0.44
2:1B:78:A:C2	2:1B:100:A:C4	3.05	0.44
7:1H:5:GLY:HA2	7:1H:69:ARG:HB2	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:1W:58:ALA:HB1	18:1W:64:MET:HB2	1.99	0.44
26:14:50:VAL:HG21	44:1m:64:TRP:C	2.42	0.44
32:1a:130:A:O2'	32:1a:131:C:O5'	2.32	0.44
32:1a:269:C:H2'	32:1a:270:A:C8	2.53	0.44
32:1a:865:A:H2	32:1a:918:A:H4'	1.81	0.44
32:1a:958:A:C6	32:1a:959:A:N1	2.85	0.44
33:1b:157:ARG:HG2	33:1b:158:LEU:N	2.32	0.44
36:1e:78:HIS:HB3	39:1h:107:LEU:HD12	1.98	0.44
36:1e:148:VAL:O	36:1e:152:ARG:HG3	2.17	0.44
1:2A:65:C:O2'	1:2A:456:C:N3	2.44	0.44
1:2A:744:G:OP1	4:2E:132:HIS:ND1	2.49	0.44
1:2A:2689:U:P	1:2A:2719:G:H22	2.40	0.44
2:2B:40:U:H1'	2:2B:45:A:H61	1.82	0.44
2:2B:49:C:H2'	2:2B:50:G:C8	2.52	0.44
5:2F:53:THR:HG22	5:2F:56:GLU:HG3	1.99	0.44
8:2I:38:LEU:H	8:2I:38:LEU:HD12	1.83	0.44
32:2a:107:G:C2	32:2a:108:G:H1'	2.53	0.44
32:2a:1190:G:O2'	34:2c:3:ASN:HB2	2.17	0.44
32:2a:1241:G:H2'	32:2a:1242:C:H6	1.82	0.44
32:2a:1305:G:H22	32:2a:1331:G:H1'	1.82	0.44
34:2c:24:ALA:HB3	34:2c:29:TYR:CD1	2.52	0.44
35:2d:109:GLY:HA3	35:2d:165:MET:HG3	1.99	0.44
55:2x:55:PSU:O2'	55:2x:57:A:N7	2.39	0.44
55:2x:66:C:H2'	55:2x:67:C:O4'	2.16	0.44
1:1A:1866:C:H2'	1:1A:1876:A:O4'	2.17	0.44
1:1A:2406:U:H2'	1:1A:2406:U:OP2	2.17	0.44
23:11:64:ALA:HA	23:11:67:ILE:HG13	1.99	0.44
24:12:1:MET:HB3	24:12:5:GLU:OE1	2.16	0.44
32:1a:438:G:H4'	35:1d:123:HIS:ND1	2.32	0.44
32:1a:458:C:H2'	32:1a:460:G:O4'	2.17	0.44
32:1a:1179:A:H2'	32:1a:1180:A:O4'	2.17	0.44
36:1e:48:ALA:HB3	36:1e:54:ALA:HB2	1.99	0.44
41:1j:55:LYS:O	41:1j:57:LYS:N	2.51	0.44
44:1m:4:ILE:HB	44:1m:57:ARG:HG3	1.98	0.44
50:1s:80:TYR:CZ	50:1s:82:GLY:HA2	2.53	0.44
1:2A:68:G:H2'	1:2A:69:C:O4'	2.17	0.44
1:2A:1839:G:C8	1:2A:1927:A:H1'	2.52	0.44
1:2A:2065:C:H2'	1:2A:2066:C:C6	2.52	0.44
1:2A:2232:U:P	23:21:40:ARG:HH12	2.40	0.44
1:2A:2502:G:OP1	61:2A:3973:HOH:O	2.21	0.44
1:2A:2728:U:H2'	1:2A:2729:G:C8	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2B:1:U:H2'	2:2B:2:C:C6	2.52	0.44
32:2a:20:U:H2'	32:2a:21:G:O4'	2.18	0.44
32:2a:1004:A:N6	32:2a:1037:C:H1'	2.33	0.44
32:2a:1010:G:N1	32:2a:1020:U:H1'	2.31	0.44
34:2c:128:PHE:HD1	34:2c:128:PHE:HA	1.71	0.44
38:2g:18:TYR:CG	38:2g:59:LEU:HD13	2.52	0.44
54:2w:11:C:H42	54:2w:24:G:H1	1.65	0.44
55:2x:61:C:H2'	55:2x:62:C:H6	1.82	0.44
1:1A:1045:A:OP1	1:1A:1046:A:H3'	2.18	0.44
1:1A:1268:A:H2'	1:1A:1269:A:O4'	2.17	0.44
1:1A:1274:A:N3	1:1A:1297:C:H1'	2.31	0.44
1:1A:1665:A:H2'	1:1A:1666:G:O4'	2.18	0.44
1:1A:1930:G:O2'	1:1A:1968:G:O6	2.26	0.44
7:1H:83:TYR:CE1	7:1H:138:LYS:HD2	2.52	0.44
12:1Q:16:ARG:HG3	12:1Q:17:LEU:H	1.81	0.44
12:1Q:20:ALA:HB2	21:1Z:79:ARG:HG3	2.00	0.44
32:1a:973:G:H3'	32:1a:974:A:H5''	1.99	0.44
32:1a:1086:U:H3	32:1a:1099:G:N2	2.11	0.44
35:1d:173:TRP:CD2	35:1d:189:PRO:HG3	2.52	0.44
1:2A:1301:A:H2	1:2A:1626:G:N3	2.15	0.44
7:2H:25:LYS:HD2	7:2H:27:LYS:HE3	1.99	0.44
32:2a:1226:C:H4'	50:2s:80:TYR:CZ	2.51	0.44
32:2a:1272:G:C2	32:2a:1273:G:C8	3.05	0.44
35:2d:153:ARG:HB3	35:2d:181:MET:HE2	1.98	0.44
36:2e:145:LYS:O	36:2e:149:GLU:HB2	2.16	0.44
41:2j:51:ARG:HG2	45:2n:45:ARG:NH2	2.32	0.44
1:1A:1506:C:H2'	1:1A:1507:A:C8	2.50	0.44
1:1A:2660:A:H2'	1:1A:2661:G:O4'	2.17	0.44
1:1A:2743:C:OP1	31:19:33:LYS:NZ	2.50	0.44
1:1A:2846:G:H2'	1:1A:2847:U:O4'	2.17	0.44
5:1F:89:VAL:HG12	5:1F:90:PHE:CD2	2.53	0.44
6:1G:47:LYS:HG3	6:1G:48:GLU:H	1.81	0.44
7:1H:101:ARG:NH2	7:1H:122:THR:HG22	2.33	0.44
8:1I:75:LEU:HD22	8:1I:105:HIS:CD2	2.52	0.44
11:1P:65:ARG:HD2	30:18:25:MET:SD	2.58	0.44
12:1Q:18:LYS:HB2	12:1Q:18:LYS:HE3	1.61	0.44
24:12:3:LEU:O	24:12:7:ARG:HG3	2.16	0.44
32:1a:110:C:H2'	32:1a:111:G:O4'	2.16	0.44
32:1a:382:A:H2'	32:1a:383:A:C8	2.53	0.44
32:1a:455:C:H42	32:1a:476:G:H1	1.66	0.44
32:1a:1084:G:C5	32:1a:1085:U:C4	3.06	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:1l:90:VAL:O	43:1l:92:0TD:N	2.51	0.44
54:1w:37:MIA:H121	54:1w:37:MIA:H162	1.77	0.44
1:2A:1266:G:O4'	18:2W:15:ARG:NH2	2.51	0.44
1:2A:1971:A:OP2	3:2D:242:ARG:NH2	2.51	0.44
1:2A:2364:C:H2'	1:2A:2365:G:O4'	2.17	0.44
1:2A:2371:G:O2'	28:26:46:HIS:ND1	2.43	0.44
1:2A:2401:U:OP1	28:26:18:ARG:NH2	2.51	0.44
1:2A:2784:C:H1'	4:2E:37:ARG:HH12	1.83	0.44
5:2F:31:HIS:HB2	11:2P:9:ASN:OD1	2.17	0.44
5:2F:160:ASN:HB3	5:2F:163:VAL:HB	1.99	0.44
6:2G:96:ARG:O	6:2G:99:MET:HB3	2.16	0.44
6:2G:120:LEU:HD12	6:2G:131:TYR:OH	2.18	0.44
10:2O:86:ILE:HG22	10:2O:94:ARG:HD3	1.98	0.44
21:2Z:69:THR:HG22	21:2Z:90:VAL:HG22	1.99	0.44
26:24:46:GLN:O	26:24:48:ARG:N	2.50	0.44
32:2a:1154:G:H2'	32:2a:1155:G:H8	1.82	0.44
33:2b:28:PHE:CD1	33:2b:194:PRO:HG3	2.52	0.44
40:2i:14:VAL:O	40:2i:65:VAL:HA	2.17	0.44
45:2n:37:PHE:HE1	45:2n:53:LEU:HD22	1.82	0.44
47:2p:12:LYS:NZ	61:2p:201:HOH:O	2.50	0.44
51:2t:72:LEU:HG	51:2t:76:ALA:HB3	2.00	0.44
54:2y:36:A:H2'	54:2y:37:MIA:O4'	2.18	0.44
1:1A:800:A:H8	1:1A:800:A:OP1	1.99	0.44
1:1A:1833:U:O2'	1:1A:1969:A:N1	2.45	0.44
1:1A:2143:C:H2'	1:1A:2144:U:O4'	2.18	0.44
1:1A:2649:U:H2'	1:1A:2650:U:C6	2.52	0.44
1:1A:2712:U:O2'	1:1A:2713:A:H5'	2.17	0.44
2:1B:92:C:H2'	2:1B:93:G:H8	1.83	0.44
3:1D:16:MET:HE3	3:1D:16:MET:HB2	1.91	0.44
8:1I:92:VAL:HG13	8:1I:120:ILE:HB	1.99	0.44
25:13:31:LEU:HD23	25:13:31:LEU:HA	1.87	0.44
32:1a:40:C:H2'	32:1a:41:G:H8	1.82	0.44
32:1a:161:A:H2'	32:1a:162:A:C8	2.53	0.44
32:1a:359:U:H2'	32:1a:360:A:H8	1.82	0.44
32:1a:820:U:H4'	32:1a:821:G:OP2	2.17	0.44
32:1a:976:G:OP1	45:1n:32:SER:N	2.47	0.44
33:1b:155:LEU:HD21	33:1b:159:PRO:HD3	1.99	0.44
37:1f:2:ARG:HD2	37:1f:69:GLU:HB3	1.99	0.44
38:1g:91:VAL:HB	38:1g:96:GLN:HG2	1.98	0.44
40:1i:89:ASN:HA	40:1i:90:PRO:HD3	1.90	0.44
44:1m:87:TYR:CZ	44:1m:91:ARG:HD3	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:1w:48:C:C2	54:1w:59:U:H1'	2.53	0.44
1:2A:1037:G:H1	1:2A:1118:C:H42	1.66	0.44
21:2Z:6:LYS:HE3	21:2Z:8:TYR:HE2	1.82	0.44
25:23:6:VAL:HG12	25:23:54:VAL:HB	2.00	0.44
32:2a:70:G:H1	32:2a:99:U:H3	1.65	0.44
32:2a:109:A:H2'	32:2a:326:G:N2	2.32	0.44
32:2a:707:C:O2'	32:2a:708:C:H5'	2.17	0.44
32:2a:1129:C:H42	32:2a:1143:G:H1	1.64	0.44
32:2a:1518:MA6:H93	32:2a:1519:MA6:H92	1.99	0.44
38:2g:54:THR:O	38:2g:56:GLN:N	2.50	0.44
39:2h:17:THR:HA	39:2h:65:TYR:HE1	1.81	0.44
40:2i:8:GLY:HA2	40:2i:79:LEU:HD23	2.00	0.44
46:2o:5:LYS:O	46:2o:9:GLN:HG2	2.17	0.44
1:1A:630:G:OP1	30:18:47:LYS:NZ	2.46	0.44
1:1A:1790:C:H5''	1:1A:1791:A:OP1	2.18	0.44
5:1F:192:LEU:HD13	5:1F:194:MET:HE2	1.99	0.44
9:1N:91:LEU:HD23	9:1N:91:LEU:HA	1.85	0.44
11:1P:101:VAL:HG23	11:1P:106:LEU:O	2.17	0.44
32:1a:1226:C:H4'	50:1s:80:TYR:CZ	2.53	0.44
54:1w:26:A:H61	54:1w:44:G:H1	1.64	0.44
55:1x:61:C:H2'	55:1x:62:C:C6	2.49	0.44
1:2A:579:G:H2'	1:2A:580:C:C6	2.53	0.44
1:2A:894:C:O2'	1:2A:895:U:H5''	2.17	0.44
1:2A:1410:G:H2'	1:2A:1411:C:C6	2.53	0.44
26:24:61:ARG:HH22	50:2s:9:VAL:HG21	1.83	0.44
32:2a:976:G:N7	32:2a:1359:C:H1'	2.32	0.44
33:2b:162:ILE:HD11	33:2b:184:VAL:HG22	1.99	0.44
33:2b:186:ALA:O	33:2b:201:ILE:HG13	2.16	0.44
33:2b:211:ILE:O	33:2b:215:LEU:HB2	2.17	0.44
37:2f:2:ARG:HE	37:2f:69:GLU:HG2	1.83	0.44
37:2f:80:ARG:NH1	37:2f:88:VAL:O	2.50	0.44
38:2g:10:ARG:O	38:2g:12:LEU:HD12	2.18	0.44
55:2x:3:C:H2'	55:2x:4:G:C8	2.53	0.44
55:2x:40:C:H2'	55:2x:41:C:H6	1.82	0.44
1:1A:570:G:H2'	1:1A:2030:A:N7	2.33	0.44
1:1A:839:U:H2'	1:1A:840:C:C6	2.53	0.44
1:1A:968:G:O6	61:1A:4242:HOH:O	2.14	0.44
1:1A:2464:C:H1'	61:1A:4464:HOH:O	2.17	0.44
3:1D:71:ASP:HB3	3:1D:103:ARG:HH22	1.83	0.44
4:1E:143:ASN:HD22	4:1E:147:PRO:HD3	1.83	0.44
20:1Y:86:ARG:HB2	20:1Y:98:VAL:HG23	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:12:10:LEU:HD21	24:12:59:ARG:HG2	1.99	0.44
26:14:61:ARG:NH1	50:1s:42:PRO:HD3	2.32	0.44
32:1a:1070:U:OP1	36:1e:25:ARG:NH2	2.51	0.44
35:1d:81:GLU:CD	35:1d:139:ARG:HH22	2.25	0.44
54:1w:4:C:H2'	54:1w:5:G:H8	1.82	0.44
55:1x:19:G:H5''	55:1x:60:U:O4	2.18	0.44
1:2A:56:A:H2'	1:2A:57:C:O4'	2.18	0.44
1:2A:353:G:H2'	1:2A:354:G:C8	2.53	0.44
1:2A:464:U:H2'	1:2A:465:G:O4'	2.18	0.44
1:2A:639:U:H2'	1:2A:640:C:C6	2.52	0.44
1:2A:1711:C:H2'	1:2A:1712:C:C6	2.52	0.44
1:2A:1721:G:H2'	1:2A:1740:G:O6	2.18	0.44
1:2A:1857:G:C6	1:2A:1858:G:C6	3.05	0.44
1:2A:2019:A:N7	27:25:9:LYS:HE2	2.33	0.44
1:2A:2376:A:N3	14:2S:106:ARG:NH2	2.62	0.44
2:2B:54:G:N2	6:2G:29:TRP:HE1	2.15	0.44
21:2Z:23:LYS:HB3	21:2Z:38:TYR:CD1	2.53	0.44
26:24:44:THR:O	26:24:46:GLN:N	2.41	0.44
28:26:8:LYS:HD3	30:28:34:TRP:CD2	2.52	0.44
28:26:40:CYS:O	28:26:44:ARG:N	2.48	0.44
32:2a:1032:G:H2'	32:2a:1033:G:C8	2.53	0.44
32:2a:1154:G:H2'	32:2a:1155:G:C8	2.52	0.44
32:2a:1265:G:C4	32:2a:1271:G:N2	2.85	0.44
36:2e:43:LEU:HB2	36:2e:136:MET:HE1	2.00	0.44
39:2h:116:LYS:HE3	39:2h:127:LEU:HD22	2.00	0.44
40:2i:3:GLN:HG3	40:2i:20:ARG:HD2	1.99	0.44
43:2l:34:ARG:O	43:2l:61:THR:HG23	2.18	0.44
44:2m:105:THR:HB	44:2m:106:ASN:H	1.62	0.44
46:2o:39:LEU:HD13	46:2o:56:LEU:HB2	1.98	0.44
1:1A:226:G:N2	1:1A:228:A:H62	2.16	0.44
1:1A:1796:U:H2'	1:1A:1797:C:H6	1.82	0.44
4:1E:96:PHE:O	4:1E:175:VAL:HG21	2.18	0.44
14:1S:110:LEU:HD12	14:1S:110:LEU:HA	1.88	0.44
18:1W:5:ALA:C	18:1W:6:ILE:HG13	2.42	0.44
32:1a:40:C:H2'	32:1a:41:G:C8	2.53	0.44
32:1a:625:G:H2'	32:1a:626:U:C6	2.53	0.44
32:1a:958:A:C2	50:1s:55:LYS:HB2	2.53	0.44
33:1b:185:ILE:HG12	33:1b:185:ILE:O	2.17	0.44
36:1e:90:VAL:O	36:1e:120:THR:HA	2.17	0.44
38:1g:90:GLU:H	38:1g:90:GLU:HG2	1.63	0.44
44:1m:67:GLU:HB3	44:1m:68:GLY:H	1.67	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:1n:3:ARG:HA	45:1n:3:ARG:HE	1.83	0.44
1:2A:709:U:H2'	1:2A:710:G:C8	2.53	0.44
1:2A:722:A:H2'	1:2A:723:G:C8	2.53	0.44
1:2A:884:C:H3'	1:2A:885:C:H6	1.83	0.44
1:2A:1116:C:H2'	1:2A:1117:G:C8	2.53	0.44
1:2A:1358:G:O2'	1:2A:1373:A:N6	2.50	0.44
9:2N:91:LEU:HG	9:2N:98:VAL:HG21	1.99	0.44
10:2O:63:VAL:HG11	10:2O:85:VAL:HG23	2.00	0.44
32:2a:595:G:H1'	32:2a:596:C:H5	1.82	0.44
32:2a:955:U:H2'	32:2a:956:U:O4'	2.17	0.44
32:2a:1163:C:H42	32:2a:1173:G:H1	1.66	0.44
33:2b:99:GLY:HA2	33:2b:176:GLU:OE2	2.18	0.44
37:2f:97:PHE:O	49:2r:31:LEU:HD23	2.17	0.44
38:2g:136:LYS:HA	38:2g:136:LYS:HD3	1.85	0.44
41:2j:9:ARG:C	41:2j:16:LEU:HD11	2.42	0.44
41:2j:64:GLU:OE2	41:2j:66:ARG:NH1	2.49	0.44
1:1A:548:A:H4'	1:1A:549:G:OP2	2.18	0.44
1:1A:825:C:O2	11:1P:55:ARG:NH1	2.49	0.44
1:1A:1721:G:H1'	1:1A:1741:A:H61	1.83	0.44
6:1G:67:LYS:H	26:14:6:HIS:CE1	2.36	0.44
6:1G:67:LYS:HG2	6:1G:68:PRO:HD2	2.00	0.44
9:1N:1:MET:HE1	16:1U:94:ASN:ND2	2.33	0.44
13:1R:95:THR:HG22	13:1R:116:LEU:HD23	1.99	0.44
32:1a:67:C:H2'	32:1a:68:G:H8	1.81	0.44
35:1d:166:LYS:NZ	35:1d:179:GLU:HG3	2.33	0.44
35:1d:178:VAL:C	35:1d:180:GLY:N	2.73	0.44
36:1e:16:THR:OG1	36:1e:17:ALA:N	2.51	0.44
41:1j:46:ARG:HB2	41:1j:46:ARG:HH11	1.83	0.44
47:1p:6:LEU:HD11	47:1p:73:LEU:HD12	1.99	0.44
1:2A:208:C:H2'	1:2A:209:C:H6	1.83	0.44
1:2A:884:C:H3'	1:2A:885:C:C6	2.53	0.44
1:2A:1820:U:C2	3:2D:202:LYS:HD2	2.52	0.44
1:2A:2641:G:O3'	9:2N:76:SER:OG	2.34	0.44
2:2B:28:C:H42	2:2B:56:G:H1	1.65	0.44
3:2D:6:PHE:HE2	3:2D:18:VAL:HG13	1.82	0.44
5:2F:181:LEU:HG	5:2F:186:ILE:HD11	1.99	0.44
7:2H:33:LEU:HD21	7:2H:136:ILE:HG13	1.99	0.44
13:2R:29:LEU:HD22	13:2R:79:LEU:HD13	2.00	0.44
13:2R:95:THR:HG22	13:2R:116:LEU:HD23	2.00	0.44
19:2X:60:ARG:HH22	29:27:47:ARG:HH12	1.64	0.44
21:2Z:40:ASP:HB3	21:2Z:43:GLU:HB2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:25:33:CYS:HB2	27:25:40:LYS:HD3	1.99	0.44
32:2a:815:A:N7	32:2a:1509:C:O2'	2.46	0.44
32:2a:1104:G:H4'	33:2b:111:ARG:NH2	2.29	0.44
32:2a:1294:G:H2'	32:2a:1295:G:C8	2.53	0.44
32:2a:1318:A:H5'	50:2s:10:PHE:CD1	2.53	0.44
35:2d:47:ARG:NH2	35:2d:48:ALA:O	2.51	0.44
36:2e:77:PRO:HD2	36:2e:142:LEU:HD13	2.00	0.44
39:2h:40:ALA:O	39:2h:43:GLY:N	2.50	0.44
43:2l:37:CYS:SG	43:2l:81:SER:HB2	2.57	0.44
1:1A:185:U:H2'	1:1A:186:G:C8	2.53	0.43
1:1A:1021:A:H3'	1:1A:1021:A:N3	2.33	0.43
1:1A:1960:A:O2'	32:1a:1484:C:O2'	2.22	0.43
2:1B:92:C:OP1	21:1Z:79:ARG:NH1	2.51	0.43
8:1I:121:LYS:HE3	8:1I:121:LYS:HB3	1.82	0.43
18:1W:6:ILE:HA	18:1W:103:ILE:O	2.17	0.43
22:10:30:VAL:HG22	22:10:66:VAL:HG22	2.00	0.43
32:1a:430:A:OP2	35:1d:8:VAL:HG12	2.18	0.43
32:1a:868:C:H2'	32:1a:869:G:O4'	2.18	0.43
1:2A:234:C:H2'	1:2A:235:U:C6	2.53	0.43
1:2A:1270:C:O2'	1:2A:1648:C:OP2	2.29	0.43
1:2A:1688:U:O2	1:2A:1700:A:H5'	2.18	0.43
1:2A:2600:A:H2'	1:2A:2601:C:C6	2.53	0.43
4:2E:3:GLY:HA3	4:2E:81:ILE:HD13	2.00	0.43
32:2a:405:U:OP2	35:2d:3:ARG:NH2	2.50	0.43
32:2a:582:U:OP1	46:2o:68:ARG:NH2	2.50	0.43
32:2a:1530:G:OP1	32:2a:1530:G:H4'	2.17	0.43
35:2d:100:ARG:O	35:2d:104:VAL:HG13	2.18	0.43
40:2i:17:VAL:HG11	40:2i:81:ILE:HA	2.00	0.43
41:2j:32:ALA:HA	41:2j:33:GLN:HA	1.69	0.43
55:2x:10:G:N2	55:2x:26:G:H1'	2.33	0.43
1:1A:657:U:H2'	1:1A:658:C:C6	2.53	0.43
1:1A:1186:G:OP2	61:1A:4263:HOH:O	2.21	0.43
5:1F:133:ASN:N	5:1F:138:GLU:OE1	2.42	0.43
11:1P:2:LYS:HG2	11:1P:3:LEU:H	1.82	0.43
11:1P:82:GLY:HA2	11:1P:113:LYS:O	2.18	0.43
15:1T:106:SER:O	15:1T:110:ILE:HG13	2.18	0.43
21:1Z:7:ALA:O	21:1Z:62:PRO:HD3	2.18	0.43
32:1a:1016:A:H2'	32:1a:1017:G:O4'	2.18	0.43
32:1a:1316:G:N2	32:1a:1318:A:H3'	2.33	0.43
33:1b:12:GLU:C	33:1b:14:GLY:N	2.76	0.43
35:1d:122:ARG:HD2	35:1d:122:ARG:HA	1.70	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:1e:105:VAL:HB	36:1e:106:PRO:HD3	1.99	0.43
48:1q:86:GLU:O	48:1q:90:ILE:HG12	2.18	0.43
54:1y:24:G:H2'	54:1y:25:C:C6	2.53	0.43
1:2A:850:C:OP1	61:2A:3969:HOH:O	2.21	0.43
1:2A:1608:A:H1'	1:2A:1610:A:OP2	2.19	0.43
1:2A:2137:C:H42	1:2A:2154:G:H1	1.66	0.43
1:2A:2287:A:C8	1:2A:2289:G:C8	3.06	0.43
14:2S:10:ARG:NH2	14:2S:91:PRO:HB2	2.31	0.43
15:2T:26:ASP:HA	15:2T:92:GLY:H	1.82	0.43
24:22:66:GLU:HA	24:22:69:ARG:NH1	2.33	0.43
32:2a:1026:G:H5'	32:2a:1027:C:O5'	2.18	0.43
32:2a:1328:C:H2'	32:2a:1329:A:O4'	2.18	0.43
32:2a:1346:A:H5''	40:2i:120:ARG:HH21	1.83	0.43
33:2b:178:ARG:HH12	39:2h:74:PRO:HG3	1.83	0.43
36:2e:32:VAL:HG21	36:2e:59:GLY:HA2	1.99	0.43
42:2k:79:SER:HA	42:2k:104:GLN:HB3	2.00	0.43
1:1A:143:G:H2'	1:1A:143(A):C:C6	2.53	0.43
1:1A:887:A:H1'	1:1A:889:C:OP2	2.17	0.43
1:1A:1178:C:H2'	1:1A:1179:C:C6	2.54	0.43
1:1A:1848:A:H2'	1:1A:1849:G:O4'	2.18	0.43
1:1A:2156:G:OP2	1:1A:2156:G:H8	2.00	0.43
1:1A:2334:G:H4'	1:1A:2335:A:OP2	2.18	0.43
23:11:59:THR:O	23:11:91:LYS:NZ	2.33	0.43
27:15:48:GLU:O	27:15:60:VAL:HG11	2.18	0.43
32:1a:182:U:C4	32:1a:183:G:H1'	2.53	0.43
32:1a:255:G:H2'	32:1a:256:U:C6	2.54	0.43
32:1a:1005:A:H1'	32:1a:1036:G:O6	2.17	0.43
32:1a:1133:G:H2'	32:1a:1134:G:C8	2.53	0.43
32:1a:1136:U:H5''	32:1a:1137:C:C4	2.53	0.43
36:1e:131:ILE:O	36:1e:135:THR:HG23	2.18	0.43
1:2A:262:A:H2'	1:2A:263:C:O4'	2.17	0.43
1:2A:747:U:O2	1:2A:2014:A:H1'	2.18	0.43
1:2A:2251:OMG:HM23	1:2A:2251:OMG:H1'	1.72	0.43
6:2G:142:PRO:HG2	6:2G:143:GLU:OE2	2.18	0.43
10:2O:26:LYS:O	10:2O:30:ALA:HB2	2.18	0.43
13:2R:57:ARG:HH22	13:2R:61:HIS:HD2	1.66	0.43
14:2S:99:LYS:HD3	14:2S:103:GLU:OE2	2.18	0.43
19:2X:47:PHE:O	19:2X:49:VAL:HG13	2.18	0.43
26:24:64:GLY:C	26:24:66:SER:H	2.27	0.43
32:2a:142:G:H2'	32:2a:143:A:C8	2.53	0.43
32:2a:277:C:P	48:2q:68:ARG:HH12	2.40	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:553:A:H2'	32:2a:554:C:C6	2.53	0.43
32:2a:1029:C:N4	32:2a:1032:G:C6	2.86	0.43
32:2a:1310:G:H5'	44:2m:77:ASN:ND2	2.33	0.43
33:2b:30:ARG:HH21	33:2b:194:PRO:HB2	1.83	0.43
34:2c:99:VAL:O	34:2c:101:LEU:N	2.48	0.43
36:2e:94:ALA:HB3	36:2e:117:ASP:HB3	2.00	0.43
37:2f:70:ASP:OD1	37:2f:71:ARG:HG3	2.17	0.43
40:2i:28:VAL:HA	40:2i:63:ILE:O	2.19	0.43
1:1A:1999:C:H5''	1:1A:2723:C:O2'	2.19	0.43
1:1A:2405:G:OP1	11:1P:77:ARG:NH2	2.51	0.43
4:1E:4:ILE:HD11	4:1E:29:GLY:HA2	2.01	0.43
7:1H:86:GLU:OE1	7:1H:130:ARG:NH1	2.51	0.43
20:1Y:9:LYS:HA	20:1Y:10:GLY:HA2	1.67	0.43
21:1Z:7:ALA:HB2	21:1Z:59:LEU:HD22	2.00	0.43
32:1a:44:G:C2	32:1a:45:U:H1'	2.53	0.43
32:1a:452:A:H4'	47:1p:72:ARG:CZ	2.48	0.43
32:1a:938:A:C6	32:1a:939:G:C5	3.06	0.43
1:2A:250:G:H2'	1:2A:251:A:C8	2.54	0.43
1:2A:500:G:N2	1:2A:502:A:H3'	2.33	0.43
1:2A:1636:C:H2'	1:2A:1637:A:C8	2.54	0.43
1:2A:1877:A:H5'	1:2A:1878:G:OP2	2.19	0.43
1:2A:2182:G:C6	1:2A:2183:C:C4	3.07	0.43
1:2A:2345:G:N3	1:2A:2381:C:H2'	2.33	0.43
1:2A:2659:G:P	7:2H:158:HIS:HE2	2.41	0.43
3:2D:24:ILE:HD13	3:2D:84:TYR:HB2	2.00	0.43
3:2D:121:PRO:HB3	3:2D:135:PHE:CD2	2.54	0.43
14:2S:3:ARG:NH1	14:2S:4:LEU:H	2.16	0.43
23:21:52:ARG:HA	23:21:56:GLN:O	2.18	0.43
32:2a:131:C:H2'	32:2a:132:C:C6	2.53	0.43
32:2a:532:A:N1	34:2c:156:ARG:NH2	2.62	0.43
32:2a:1442:G:H2'	32:2a:1442:G:N3	2.32	0.43
33:2b:71:VAL:HG22	33:2b:93:VAL:HG23	2.00	0.43
33:2b:101:MET:HA	33:2b:108:ILE:HD11	1.99	0.43
34:2c:73:PRO:HB3	34:2c:103:VAL:HG21	1.99	0.43
41:2j:12:ASP:OD1	41:2j:13:HIS:N	2.52	0.43
41:2j:42:THR:HG23	41:2j:68:HIS:HA	2.01	0.43
50:2s:49:ILE:HG12	50:2s:50:ALA:N	2.34	0.43
1:1A:1453:U:O2'	1:1A:1455:G:N7	2.46	0.43
1:1A:1486:A:H2'	1:1A:1487:G:C8	2.54	0.43
1:1A:1810:A:H2'	1:1A:1811:G:O4'	2.19	0.43
1:1A:2552:OMU:O5'	1:1A:2552:OMU:H6	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1F:135:LYS:HB2	5:1F:138:GLU:CD	2.44	0.43
10:1O:101:PRO:HA	10:1O:120:GLU:O	2.18	0.43
32:1a:1346:A:OP1	40:1i:120:ARG:NH1	2.43	0.43
33:1b:37:ASN:C	33:1b:39:ILE:H	2.27	0.43
33:1b:74:LYS:NZ	33:1b:206:ASP:OD1	2.50	0.43
36:1e:10:MET:HE3	36:1e:10:MET:HB2	1.88	0.43
36:1e:69:VAL:O	36:1e:69:VAL:HG23	2.18	0.43
40:1i:42:ARG:NH1	40:1i:71:SER:OG	2.48	0.43
44:1m:15:VAL:HG12	44:1m:19:LEU:HD11	2.01	0.43
50:1s:36:ARG:NH2	50:1s:72:GLY:O	2.51	0.43
1:2A:80:G:H1	1:2A:106:C:H42	1.66	0.43
1:2A:196:A:N3	1:2A:196:A:H2'	2.33	0.43
1:2A:222:A:H5''	1:2A:421:U:OP1	2.18	0.43
1:2A:511:U:O4	1:2A:512:G:N1	2.51	0.43
1:2A:583:G:OP2	16:2U:10:ARG:NH1	2.50	0.43
1:2A:754:C:H2'	1:2A:755:C:C6	2.53	0.43
1:2A:992:C:OP1	17:2V:74:LYS:NZ	2.36	0.43
1:2A:1033:U:OP1	31:29:9:ARG:NH2	2.41	0.43
1:2A:1449:A:O2'	1:2A:1529:G:N2	2.32	0.43
1:2A:1805:U:O2	3:2D:50:THR:HB	2.18	0.43
1:2A:2637:U:H5''	4:2E:82:ARG:NH1	2.32	0.43
6:2G:35:GLU:HB3	6:2G:160:VAL:O	2.18	0.43
6:2G:166:ASP:HA	6:2G:169:ALA:HB3	1.99	0.43
13:2R:36:THR:HG22	13:2R:37:THR:H	1.83	0.43
19:2X:61:GLY:HA3	19:2X:73:ARG:O	2.19	0.43
32:2a:1084:G:H5'	32:2a:1102:A:OP2	2.19	0.43
32:2a:1105:A:H2'	32:2a:1106:G:H8	1.84	0.43
32:2a:1517:G:N7	32:2a:1518:MA6:H103	2.34	0.43
33:2b:114:ARG:HA	33:2b:117:GLU:CB	2.48	0.43
34:2c:124:ILE:HG21	34:2c:130:VAL:HG13	1.99	0.43
34:2c:136:GLN:O	34:2c:140:ARG:NH1	2.51	0.43
38:2g:113:GLU:HG3	38:2g:118:VAL:HG12	2.00	0.43
40:2i:79:LEU:O	40:2i:83:ARG:HG3	2.19	0.43
46:2o:61:GLY:O	46:2o:65:ARG:HG3	2.19	0.43
50:2s:72:GLY:C	50:2s:74:PHE:H	2.27	0.43
1:1A:2082:A:H2'	1:1A:2083:G:O4'	2.18	0.43
1:1A:2203:U:O4'	3:1D:151:LYS:HE2	2.18	0.43
1:1A:2375:G:N2	1:1A:2378:A:OP2	2.48	0.43
14:1S:27:SER:HA	14:1S:88:ASP:HB3	2.00	0.43
32:1a:221:C:H2'	32:1a:222:U:C6	2.50	0.43
32:1a:909:A:H2'	32:1a:910:C:O4'	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1c:89:GLU:OE1	34:1c:90:GLU:N	2.52	0.43
35:1d:112:VAL:HG22	35:1d:116:GLN:NE2	2.33	0.43
36:1e:7:GLU:O	36:1e:34:VAL:HA	2.19	0.43
36:1e:51:VAL:O	36:1e:55:VAL:HG23	2.19	0.43
37:1f:86:ARG:O	37:1f:87:ARG:HG2	2.17	0.43
43:1l:77:LEU:HD21	43:1l:107:ALA:HA	2.00	0.43
1:2A:93:G:H2'	1:2A:94:C:C6	2.52	0.43
1:2A:1270:C:H5''	1:2A:1271:G:O5'	2.19	0.43
1:2A:2154:G:N1	1:2A:2155:G:O6	2.51	0.43
1:2A:2492:U:H2'	1:2A:2493:U:C6	2.54	0.43
2:2B:51:G:OP2	14:2S:61:ASN:HA	2.19	0.43
14:2S:58:LEU:H	14:2S:58:LEU:HG	1.69	0.43
19:2X:11:PRO:HD3	24:22:37:PHE:CD2	2.53	0.43
26:24:41:PRO:HG3	26:24:49:PHE:CZ	2.53	0.43
32:2a:375:U:OP1	47:2p:69:THR:HG21	2.18	0.43
33:2b:95:GLN:HG2	33:2b:147:LYS:HE3	1.99	0.43
34:2c:15:THR:OG1	34:2c:178:LEU:O	2.29	0.43
34:2c:40:ARG:NH2	34:2c:55:VAL:O	2.49	0.43
1:1A:107:C:H2'	1:1A:108:U:H6	1.82	0.43
1:1A:885:C:H5'	1:1A:886:C:OP2	2.19	0.43
1:1A:1063:G:H2'	1:1A:1064:C:C5	2.54	0.43
1:1A:1803:A:O2'	3:1D:259:THR:HG21	2.19	0.43
1:1A:2305:A:H2'	1:1A:2306:C:O4'	2.19	0.43
5:1F:28:ILE:HD12	5:1F:119:ARG:HH21	1.84	0.43
11:1P:71:VAL:HG22	11:1P:72:PRO:HA	2.01	0.43
16:1U:9:VAL:HA	61:1U:312:HOH:O	2.18	0.43
26:14:17:GLY:C	26:14:19:GLY:H	2.26	0.43
32:1a:560:U:HO2'	32:1a:561:U:P	2.39	0.43
32:1a:872:A:C8	32:1a:874:G:C8	3.06	0.43
33:1b:71:VAL:HG13	33:1b:93:VAL:HG13	2.00	0.43
35:1d:173:TRP:CE3	35:1d:174:LEU:HG	2.54	0.43
40:1i:3:GLN:HE21	40:1i:20:ARG:CZ	2.32	0.43
42:1k:27:ASN:OD1	42:1k:28:THR:N	2.51	0.43
43:1l:54:LYS:HG2	43:1l:75:HIS:CD2	2.53	0.43
49:1r:33:ASP:OD2	49:1r:36:ASN:HB2	2.19	0.43
55:1x:75:C:H5''	55:1x:76:A:OP2	2.19	0.43
54:1y:40:C:H2'	54:1y:41:C:C6	2.53	0.43
1:2A:305:U:H2'	1:2A:306:U:C6	2.53	0.43
1:2A:1469:A:H2'	1:2A:1470:G:O4'	2.19	0.43
1:2A:2839:G:H5'	13:2R:46:GLY:CA	2.48	0.43
15:2T:105:LEU:HD22	15:2T:109:GLU:HB3	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:408:A:H2'	32:2a:409:G:O4'	2.18	0.43
32:2a:814:A:N7	32:2a:816:A:C4	2.86	0.43
32:2a:1316:G:N2	32:2a:1318:A:H3'	2.33	0.43
34:2c:47:LEU:HB3	34:2c:52:LEU:HB2	2.00	0.43
43:2l:6:THR:HG23	43:2l:9:GLN:OE1	2.19	0.43
44:2m:91:ARG:HB2	44:2m:98:VAL:HG12	2.00	0.43
54:2w:11:C:N4	54:2w:24:G:H1	2.16	0.43
54:2y:58:A:H4'	54:2y:59:U:OP1	2.18	0.43
54:2y:62:C:O2'	54:2y:63:G:H5'	2.17	0.43
1:1A:71:A:N7	19:1X:31:HIS:HE1	2.17	0.43
1:1A:207:A:H2'	1:1A:208:C:O4'	2.17	0.43
1:1A:536:A:H2'	1:1A:537:C:C6	2.54	0.43
1:1A:1400:G:H2'	1:1A:1401:G:C8	2.53	0.43
1:1A:1540:U:H2'	1:1A:1541:G:O4'	2.19	0.43
1:1A:2101:G:H2'	1:1A:2102:U:C6	2.54	0.43
26:14:53:GLU:HB2	26:14:55:ARG:O	2.19	0.43
32:1a:271:C:H2'	32:1a:272:C:H6	1.84	0.43
34:1c:6:HIS:HD2	34:1c:8:ILE:N	2.12	0.43
36:1e:100:VAL:HG11	36:1e:107:ARG:HG3	2.01	0.43
1:2A:1467:C:C5	1:2A:1546:C:H2'	2.54	0.43
1:2A:2523:G:N2	1:2A:2764:A:N3	2.62	0.43
1:2A:2802:G:H2'	1:2A:2803:C:O4'	2.17	0.43
2:2B:73:A:C4	2:2B:105:A:C2	3.06	0.43
6:2G:61:ALA:HA	6:2G:66:GLN:O	2.18	0.43
18:2W:11:ARG:HD2	18:2W:11:ARG:HA	1.77	0.43
26:24:27:THR:OG1	26:24:28:LYS:N	2.51	0.43
32:2a:1041:A:C6	32:2a:1042:G:C6	3.07	0.43
32:2a:1305:G:OP1	52:2u:2:GLY:HA3	2.19	0.43
33:2b:98:LEU:H	33:2b:101:MET:HE2	1.84	0.43
35:2d:153:ARG:HH21	35:2d:181:MET:CG	2.32	0.43
40:2i:3:GLN:HE21	40:2i:20:ARG:HE	1.65	0.43
43:2l:40:VAL:HG21	43:2l:78:GLN:HA	2.01	0.43
43:2l:79:GLU:HG2	43:2l:80:HIS:CD2	2.54	0.43
43:2l:124:LYS:HA	43:2l:125:PRO:HD3	1.90	0.43
49:2r:22:VAL:O	49:2r:26:LEU:HD12	2.19	0.43
1:1A:196:A:H2'	1:1A:196:A:N3	2.34	0.43
1:1A:213:A:H2'	1:1A:214:G:O4'	2.19	0.43
1:1A:1541:G:H3'	1:1A:1542:A:H2'	2.01	0.43
1:1A:2121:G:H2'	1:1A:2122:U:C6	2.54	0.43
6:1G:72:ARG:HH12	6:1G:87:PRO:HG3	1.83	0.43
29:17:19:ARG:O	29:17:23:ARG:HG3	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1057:G:H2'	32:1a:1058:G:O4'	2.18	0.43
32:1a:1120:G:H1	32:1a:1153:C:H42	1.67	0.43
32:1a:1347:G:O2'	32:1a:1373:G:O6	2.33	0.43
35:1d:109:GLY:HA3	35:1d:165:MET:SD	2.59	0.43
35:1d:202:LEU:HD23	35:1d:202:LEU:HA	1.88	0.43
1:2A:64:A:O3'	19:2X:71:GLY:HA3	2.18	0.43
1:2A:656:G:H2'	1:2A:657:U:O4'	2.18	0.43
1:2A:705:A:H2'	1:2A:706:A:O4'	2.19	0.43
1:2A:900:A:H2'	1:2A:901:A:H8	1.84	0.43
1:2A:1131:G:O6	1:2A:2040:C:H1'	2.19	0.43
1:2A:1188:U:C4'	17:2V:79:VAL:HG22	2.49	0.43
1:2A:1260:G:C6	1:2A:1261:C:C4	3.07	0.43
1:2A:2513:G:N2	4:2E:143:ASN:OD1	2.52	0.43
4:2E:1:MET:HE3	4:2E:199:ARG:HD2	2.01	0.43
6:2G:108:ASN:O	26:24:37:SER:N	2.52	0.43
8:2I:8:PRO:HD3	8:2I:15:VAL:HB	2.01	0.43
9:2N:123:TYR:CE2	9:2N:129:PRO:HD2	2.53	0.43
21:2Z:6:LYS:NZ	21:2Z:43:GLU:OE2	2.37	0.43
30:28:28:GLY:O	30:28:36:LYS:NZ	2.44	0.43
32:2a:735:C:H2'	32:2a:736:C:C6	2.53	0.43
32:2a:818:G:N2	32:2a:873:A:OP1	2.51	0.43
32:2a:853:G:C2	32:2a:854:G:C8	3.07	0.43
32:2a:949:A:H1'	32:2a:1364:U:H3	1.83	0.43
32:2a:1278:U:H5'	32:2a:1279:A:C5'	2.46	0.43
32:2a:1502:A:H5'	32:2a:1504:G:N7	2.34	0.43
36:2e:100:VAL:O	36:2e:107:ARG:NH1	2.52	0.43
40:2i:4:TYR:CE1	40:2i:88:TYR:HB2	2.54	0.43
40:2i:15:ALA:HB2	40:2i:65:VAL:HG23	2.01	0.43
41:2j:6:ILE:HG12	41:2j:98:ILE:HG12	2.01	0.43
42:2k:58:PRO:HG3	42:2k:89:ALA:O	2.19	0.43
44:2m:23:TYR:HE2	44:2m:70:LEU:HD22	1.83	0.43
44:2m:57:ARG:C	44:2m:59:TYR:H	2.26	0.43
1:1A:271(G):C:H2'	1:1A:271(H):G:C8	2.54	0.43
1:1A:1504:C:H2'	1:1A:1505:C:C6	2.54	0.43
1:1A:2133:G:N2	1:1A:2157:G:H1'	2.34	0.43
1:1A:2352:A:N6	1:1A:2365:G:O2'	2.51	0.43
1:1A:2366:A:OP1	61:1A:4266:HOH:O	2.22	0.43
1:1A:2469:A:C2	1:1A:2470:G:H1'	2.54	0.43
2:1B:29:A:O2'	2:1B:58:A:N1	2.47	0.43
3:1D:83:GLU:OE1	3:1D:104:TYR:OH	2.28	0.43
10:1O:115:VAL:HG13	10:1O:121:VAL:HG21	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:1P:138:LEU:C	11:1P:140:ALA:H	2.27	0.43
19:1X:36:LYS:HG2	19:1X:54:VAL:HG12	2.01	0.43
20:1Y:15:VAL:HG21	20:1Y:42:VAL:HG11	2.01	0.43
26:14:44:THR:O	26:14:46:GLN:N	2.52	0.43
32:1a:162:A:N7	32:1a:163:C:H1'	2.33	0.43
32:1a:339:C:H2'	32:1a:340:U:C6	2.54	0.43
32:1a:1054:C:C4	32:1a:1196:U:H5	2.37	0.43
33:1b:59:GLU:HB2	33:1b:221:LEU:HD21	2.00	0.43
39:1h:9:MET:HG3	39:1h:26:VAL:HG21	2.00	0.43
44:1m:40:ASN:HD21	44:1m:42:ALA:HB3	1.84	0.43
54:1y:26:A:N6	54:1y:44:G:N1	2.64	0.43
1:2A:86:C:H4'	1:2A:104:U:H1'	2.00	0.43
1:2A:185:U:H4'	1:2A:218:A:H4'	2.01	0.43
1:2A:322:A:P	5:2F:169:ASN:HB2	2.59	0.43
1:2A:1591:G:H2'	1:2A:1592:C:H6	1.84	0.43
1:2A:1609:A:OP2	61:2A:3976:HOH:O	2.21	0.43
1:2A:2819:G:H2'	1:2A:2821:A:N7	2.34	0.43
2:2B:98:G:H3'	2:2B:99:G:H8	1.84	0.43
4:2E:175:VAL:HG13	4:2E:182:LEU:HD12	2.00	0.43
5:2F:117:ARG:NH2	5:2F:187:VAL:HA	2.34	0.43
12:2Q:3:MET:HE3	12:2Q:3:MET:HB2	1.81	0.43
32:2a:1286:A:H2	52:2u:18:TYR:OH	2.01	0.43
32:2a:1297:C:OP1	44:2m:44:ARG:NH1	2.51	0.43
32:2a:1328:C:O3'	44:2m:29:ARG:HG3	2.19	0.43
32:2a:1360:A:OP2	45:2n:35:ARG:NH2	2.52	0.43
33:2b:124:SER:HB3	33:2b:125:PRO:HD3	2.01	0.43
34:2c:152:ILE:HD11	34:2c:199:LYS:NZ	2.34	0.43
38:2g:78:ARG:HD3	38:2g:79:ARG:N	2.17	0.43
40:2i:3:GLN:HG2	40:2i:4:TYR:H	1.83	0.43
41:2j:78:ASN:C	41:2j:80:LYS:N	2.77	0.43
43:2l:30:ALA:HB2	43:2l:33:ARG:HH21	1.84	0.43
50:2s:3:ARG:CZ	50:2s:7:LYS:HB2	2.49	0.43
50:2s:7:LYS:H	50:2s:7:LYS:HG2	1.61	0.43
54:2w:9:A:H5'	54:2w:46:G7M:H1'	2.00	0.43
1:1A:27:G:N2	1:1A:512:G:H1'	2.33	0.42
1:1A:1171:G:OP2	1:1A:1174:A:N6	2.52	0.42
1:1A:1529:G:H2'	1:1A:1530:C:O4'	2.18	0.42
1:1A:2005:A:H5''	61:1A:4230:HOH:O	2.18	0.42
1:1A:2312:U:OP1	6:1G:73:ALA:HA	2.19	0.42
1:1A:2722:G:H5'	13:1R:4:LEU:HD12	2.01	0.42
32:1a:625:G:H2'	32:1a:626:U:H6	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:922:G:C6	32:1a:923:A:C6	3.07	0.42
32:1a:1131:G:OP1	40:1i:20:ARG:NH2	2.42	0.42
34:1c:129:ALA:HB3	34:1c:132:ARG:HB2	1.99	0.42
36:1e:74:GLY:HA3	36:1e:116:THR:HG22	2.00	0.42
52:1u:5:ASP:O	52:1u:11:GLY:HA3	2.18	0.42
1:2A:811:U:H2'	11:2P:21:ARG:HA	2.01	0.42
1:2A:819:A:C4	1:2A:1189:A:C2	3.07	0.42
1:2A:864:G:C6	1:2A:865:C:N4	2.87	0.42
4:2E:67:PHE:O	4:2E:71:GLY:N	2.52	0.42
8:2I:14:ASP:O	8:2I:17:GLN:HB2	2.19	0.42
23:21:56:GLN:HE21	23:21:87:PRO:HG3	1.84	0.42
31:29:27:CYS:SG	31:29:28:GLU:N	2.92	0.42
32:2a:178:C:H2'	32:2a:179:A:O4'	2.19	0.42
32:2a:300:A:H1'	32:2a:565:U:O2	2.18	0.42
32:2a:1117:G:H5'	40:2i:104:ARG:HH12	1.84	0.42
33:2b:16:HIS:O	33:2b:18:GLY:N	2.52	0.42
37:2f:14:LEU:HD22	37:2f:18:GLN:HB3	2.01	0.42
41:2j:78:ASN:C	41:2j:80:LYS:H	2.27	0.42
42:2k:34:ASP:OD2	42:2k:38:ASN:HB2	2.19	0.42
48:2q:50:LYS:HG3	48:2q:51:TYR:CE2	2.55	0.42
1:1A:582:G:H2'	1:1A:583:G:C8	2.54	0.42
1:1A:721:C:H2'	1:1A:722:A:H8	1.82	0.42
1:1A:882:G:H1	1:1A:894:C:H42	1.66	0.42
2:1B:79:C:H2'	2:1B:80:U:O4'	2.19	0.42
24:12:30:ARG:O	24:12:34:GLU:HG3	2.19	0.42
32:1a:176:C:H2'	32:1a:177:C:H6	1.84	0.42
32:1a:567:G:H2'	32:1a:568:G:O4'	2.19	0.42
32:1a:779:C:H2'	32:1a:780:A:O4'	2.19	0.42
32:1a:839:U:H3'	32:1a:840:C:H5'	2.01	0.42
33:1b:146:GLN:O	33:1b:150:SER:HB3	2.19	0.42
36:1e:78:HIS:CE1	36:1e:142:LEU:HD23	2.53	0.42
41:1j:39:PRO:HA	41:1j:70:ARG:HD3	2.01	0.42
48:1q:56:VAL:HB	48:1q:78:GLU:HB3	2.01	0.42
54:1y:8:4SU:H2'	54:1y:13:C:N4	2.34	0.42
1:2A:1364:G:OP2	23:21:3:LYS:HG3	2.18	0.42
1:2A:1857:G:C6	1:2A:1858:G:N1	2.87	0.42
1:2A:2114:A:N6	1:2A:2115:G:H21	2.17	0.42
8:2I:133:HIS:HD2	8:2I:134:PRO:HD2	1.83	0.42
8:2I:133:HIS:CD2	8:2I:134:PRO:HD2	2.54	0.42
9:2N:41:ASP:O	9:2N:48:MET:HE1	2.19	0.42
10:2O:71:ARG:HH22	10:2O:122:LEU:C	2.28	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:2P:70:GLN:O	11:2P:73:GLY:N	2.43	0.42
11:2P:81:GLN:HB3	11:2P:106:LEU:HD12	2.00	0.42
11:2P:97:PRO:HD3	11:2P:126:VAL:O	2.20	0.42
25:23:12:PRO:HB2	25:23:20:LYS:HG2	2.00	0.42
32:2a:607:A:H2'	32:2a:608:A:O4'	2.19	0.42
32:2a:1261:A:N6	32:2a:1273:G:H1	2.17	0.42
32:2a:1318:A:O2'	50:2s:37:ARG:NE	2.50	0.42
36:2e:37:ARG:HB3	36:2e:114:GLY:HA2	2.01	0.42
36:2e:95:ALA:O	36:2e:97:GLY:N	2.52	0.42
38:2g:124:LEU:HD23	38:2g:124:LEU:HA	1.94	0.42
41:2j:12:ASP:OD1	41:2j:14:LYS:N	2.43	0.42
42:2k:86:GLY:N	42:2k:112:THR:OG1	2.48	0.42
46:2o:26:GLU:HG3	46:2o:81:LEU:HD22	2.01	0.42
1:1A:226:G:H21	1:1A:228:A:H62	1.67	0.42
1:1A:969:U:H4'	25:13:14:GLY:O	2.19	0.42
1:1A:2648:C:H2'	1:1A:2649:U:C6	2.54	0.42
1:1A:2701:C:H2'	1:1A:2702:U:H2'	2.02	0.42
3:1D:37:LEU:HD13	3:1D:87:ASN:ND2	2.34	0.42
8:1I:81:VAL:O	8:1I:146:ALA:HA	2.19	0.42
32:1a:406:G:H21	35:1d:119:GLN:HE22	1.67	0.42
32:1a:583:A:H2'	32:1a:584:G:O4'	2.19	0.42
32:1a:1503:A:C2	53:1v:12:A:H2	2.37	0.42
33:1b:80:ILE:O	33:1b:84:GLU:HG2	2.18	0.42
34:1c:22:TRP:CH2	45:1n:54:PRO:HG2	2.54	0.42
35:1d:11:LEU:HD13	35:1d:66:ARG:HG2	2.01	0.42
37:1f:35:ALA:HB2	37:1f:67:MET:HE2	2.01	0.42
1:2A:748:G:C8	18:2W:89:ALA:HB1	2.55	0.42
1:2A:2167:U:H3'	1:2A:2168:G:N2	2.34	0.42
2:2B:46:A:H2'	2:2B:47:C:C6	2.54	0.42
6:2G:39:ILE:HG23	6:2G:155:MET:HG3	2.01	0.42
12:2Q:35:VAL:HG22	12:2Q:102:VAL:HG22	2.02	0.42
22:20:11:ARG:O	22:20:14:ARG:NH2	2.52	0.42
32:2a:34:C:H2'	32:2a:35:G:C8	2.50	0.42
32:2a:302:G:O2'	32:2a:556:C:H5''	2.19	0.42
32:2a:376:G:O2'	47:2p:5:ARG:NH2	2.52	0.42
32:2a:532:A:H2'	32:2a:532:A:N3	2.34	0.42
34:2c:71:ALA:HB3	34:2c:109:PRO:HB3	2.02	0.42
34:2c:113:ALA:HB2	34:2c:202:ILE:HG13	2.01	0.42
35:2d:47:ARG:CZ	35:2d:47:ARG:HB2	2.49	0.42
35:2d:61:LYS:HD2	35:2d:207:TYR:OH	2.19	0.42
40:2i:14:VAL:HB	40:2i:66:ARG:HG3	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:286:C:H2'	1:1A:287:C:C6	2.54	0.42
1:1A:933:A:OP1	25:13:24:LYS:NZ	2.53	0.42
1:1A:1508:A:O2'	1:1A:1509:C:OP1	2.21	0.42
1:1A:2262:U:OP1	1:1A:2387:U:O2'	2.32	0.42
1:1A:2732:G:H3'	1:1A:2733:A:O4'	2.19	0.42
1:1A:2747:G:O6	1:1A:2755:C:H5''	2.20	0.42
6:1G:106:LEU:HA	6:1G:110:ALA:HB3	2.01	0.42
16:1U:108:GLU:O	16:1U:112:ARG:HG2	2.20	0.42
24:12:53:LEU:HD23	24:12:53:LEU:HA	1.87	0.42
32:1a:198:G:C5	32:1a:220:G:C2	3.07	0.42
32:1a:255:G:H1'	48:1q:16:GLN:OE1	2.19	0.42
32:1a:1263:C:H2'	32:1a:1264:C:C6	2.54	0.42
40:1i:52:ALA:HB2	40:1i:99:LEU:HD12	2.02	0.42
42:1k:20:TYR:HA	42:1k:83:ILE:O	2.19	0.42
1:2A:251:A:C5	1:2A:252:G:H1'	2.54	0.42
1:2A:289:A:H2'	1:2A:290:G:O4'	2.19	0.42
1:2A:624:C:OP1	61:2A:3979:HOH:O	2.22	0.42
1:2A:651:G:OP1	30:28:19:SER:HB3	2.19	0.42
1:2A:1021:A:H62	1:2A:1141:U:H3	1.68	0.42
1:2A:1379:A:H4'	1:2A:1380:G:OP2	2.19	0.42
1:2A:1586:A:H8	1:2A:1586:A:O5'	2.03	0.42
1:2A:2166:G:N7	1:2A:2167:U:H2'	2.34	0.42
1:2A:2420:C:H5'	28:26:54:ILE:HD11	2.00	0.42
3:2D:145:VAL:HG13	3:2D:191:ALA:HB2	2.01	0.42
4:2E:36:ARG:HG2	4:2E:47:VAL:HG12	2.00	0.42
5:2F:184:TYR:CZ	5:2F:188:ARG:HD2	2.54	0.42
6:2G:7:LEU:CB	6:2G:104:GLU:HB3	2.49	0.42
14:2S:67:ARG:HH22	14:2S:103:GLU:HB2	1.84	0.42
21:2Z:121:HIS:N	21:2Z:171:ILE:O	2.52	0.42
32:2a:540:G:H2'	32:2a:541:G:O4'	2.19	0.42
33:2b:78:GLN:NE2	33:2b:95:GLN:OE1	2.52	0.42
34:2c:142:MET:HE3	34:2c:142:MET:HB3	1.94	0.42
38:2g:89:MET:SD	38:2g:155:ARG:HB2	2.59	0.42
1:1A:468:G:N7	29:17:39:ARG:NH2	2.67	0.42
1:1A:1932:A:H2'	1:1A:1933:G:O4'	2.20	0.42
5:1F:32:LEU:HB3	5:1F:112:MET:HE1	2.01	0.42
30:18:32:LEU:O	30:18:36:LYS:HE3	2.19	0.42
32:1a:1002:G:N7	32:1a:1003:G:H1'	2.34	0.42
33:1b:16:HIS:HD2	33:1b:204:ASN:N	2.17	0.42
50:1s:35:SER:HB3	50:1s:38:SER:HB2	2.01	0.42
54:1w:9:A:O2'	54:1w:10:G:N7	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:234:C:H2'	1:2A:235:U:H6	1.85	0.42
1:2A:241:A:H8	1:2A:241:A:OP1	2.03	0.42
1:2A:607:U:OP1	5:2F:102:PRO:HA	2.19	0.42
1:2A:1209:G:O2'	1:2A:1237:A:N1	2.43	0.42
1:2A:1508:A:H4'	1:2A:1509(A):A:C5	2.55	0.42
1:2A:1932:A:H2'	1:2A:1933:G:O4'	2.20	0.42
4:2E:1:MET:HE3	4:2E:199:ARG:HB3	2.00	0.42
4:2E:23:VAL:HG21	4:2E:183:LEU:HD23	2.00	0.42
13:2R:1:MET:HE3	13:2R:1:MET:HB2	1.92	0.42
15:2T:6:LEU:O	15:2T:10:VAL:HG23	2.20	0.42
32:2a:8:A:C6	35:2d:209:ARG:HB2	2.55	0.42
32:2a:93:G:C6	32:2a:96:U:C4	3.07	0.42
32:2a:552:U:O3'	43:2l:87:GLY:HA3	2.20	0.42
32:2a:971:G:H22	32:2a:1363(A):A:H5'	1.84	0.42
32:2a:993:G:N3	32:2a:993:G:H2'	2.35	0.42
32:2a:1173:G:H2'	32:2a:1174:G:C8	2.55	0.42
33:2b:135:GLN:O	33:2b:139:LYS:HB2	2.20	0.42
33:2b:167:PRO:O	33:2b:171:ALA:N	2.52	0.42
35:2d:15:GLU:OE2	35:2d:59:ARG:NH1	2.52	0.42
35:2d:201:GLN:NE2	36:2e:99:GLY:HA2	2.34	0.42
36:2e:43:LEU:HB2	36:2e:136:MET:CE	2.49	0.42
36:2e:131:ILE:HD13	36:2e:131:ILE:HA	1.81	0.42
36:2e:136:MET:HB2	36:2e:136:MET:HE3	1.62	0.42
39:2h:121:ASP:OD1	39:2h:121:ASP:N	2.52	0.42
47:2p:17:TYR:HE2	47:2p:41:PRO:HG3	1.85	0.42
54:2w:66:U:O4	54:2w:67:C:N4	2.52	0.42
1:1A:2171:A:O2'	1:1A:2172:U:H5''	2.20	0.42
1:1A:2783:G:H2'	1:1A:2784:C:C6	2.53	0.42
32:1a:519:C:H2'	32:1a:520:A:C8	2.54	0.42
33:1b:163:PHE:CD1	33:1b:185:ILE:HG13	2.54	0.42
35:1d:18:LYS:HE2	35:1d:31:CYS:SG	2.60	0.42
1:2A:1207:C:H2'	1:2A:1208:C:H6	1.84	0.42
1:2A:2138:C:N4	1:2A:2153:G:H1	2.15	0.42
1:2A:2315:G:H2'	1:2A:2316:C:C6	2.55	0.42
1:2A:2849:U:H4'	1:2A:2868:A:C2	2.55	0.42
9:2N:33:LEU:HD23	9:2N:38:HIS:CD2	2.55	0.42
29:27:12:ARG:NH2	29:27:44:PRO:HB3	2.34	0.42
32:2a:9:G:H2'	32:2a:10:A:C8	2.54	0.42
32:2a:186:C:H2'	32:2a:187:C:C6	2.54	0.42
32:2a:410:G:H5''	35:2d:30:LYS:NZ	2.35	0.42
32:2a:491:G:H2'	32:2a:492:G:O4'	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:573:A:N3	32:2a:883:C:O2'	2.47	0.42
32:2a:751:U:H4'	46:2o:24:SER:HA	2.01	0.42
34:2c:53:ALA:HB2	34:2c:115:LEU:CD1	2.49	0.42
34:2c:82:GLU:O	34:2c:86:VAL:N	2.36	0.42
34:2c:111:LEU:HD21	34:2c:146:ALA:HB2	2.02	0.42
35:2d:140:VAL:HG11	35:2d:146:ILE:HD11	2.01	0.42
36:2e:89:ILE:HD12	36:2e:89:ILE:HA	1.93	0.42
51:2t:50:GLU:HG3	51:2t:100:ILE:HG21	2.02	0.42
55:2x:21:A:N6	55:2x:46:G:H2'	2.33	0.42
1:1A:1692:U:O2'	1:1A:1693:U:H2'	2.20	0.42
2:1B:28:C:H2'	2:1B:29:A:O4'	2.20	0.42
5:1F:24:LEU:HD12	5:1F:24:LEU:HA	1.84	0.42
21:1Z:132:ASN:O	21:1Z:134:PRO:HD3	2.20	0.42
32:1a:420:U:H2'	32:1a:422:C:C5	2.54	0.42
32:1a:673:G:H2'	32:1a:674:G:C8	2.54	0.42
32:1a:748:C:H4'	32:1a:749:C:O5'	2.20	0.42
32:1a:926:G:H5''	32:1a:927:G:O5'	2.20	0.42
32:1a:1469:G:H2'	32:1a:1470:G:C8	2.55	0.42
32:1a:1504:G:OP1	32:1a:1507:A:H4'	2.19	0.42
33:1b:130:ARG:O	33:1b:131:PRO:C	2.61	0.42
42:1k:98:LEU:O	42:1k:101:SER:OG	2.23	0.42
47:1p:56:ALA:O	47:1p:60:LEU:HB2	2.19	0.42
54:1y:55:PSU:N3	54:1y:57:G:H5'	2.35	0.42
54:1y:56:C:C2	54:1y:57:G:H1'	2.55	0.42
1:2A:271(Q):G:H2'	1:2A:271(R):G:C8	2.54	0.42
1:2A:271(V):G:H2'	1:2A:271(W):G:O4'	2.19	0.42
1:2A:438:G:H2'	1:2A:440:G:C8	2.55	0.42
1:2A:1452:A:OP2	61:2A:3975:HOH:O	2.21	0.42
1:2A:1628:G:H2'	1:2A:1629:U:C6	2.55	0.42
1:2A:2320:A:N3	1:2A:2320:A:H2'	2.35	0.42
1:2A:2347:C:H2'	1:2A:2348:U:C6	2.55	0.42
3:2D:77:ALA:HA	3:2D:97:TYR:HA	2.02	0.42
12:2Q:6:ARG:HG2	12:2Q:7:MET:N	2.35	0.42
20:2Y:68:HIS:CE1	20:2Y:70:SER:HB3	2.54	0.42
21:2Z:121:HIS:N	21:2Z:172:ALA:HB2	2.35	0.42
32:2a:629:G:H2'	32:2a:630:G:O4'	2.20	0.42
32:2a:826:C:H2'	32:2a:827:U:C6	2.54	0.42
32:2a:918:A:H2'	32:2a:919:A:C8	2.53	0.42
32:2a:971:G:N2	32:2a:1363(A):A:H5'	2.34	0.42
33:2b:185:ILE:HG22	33:2b:198:ASP:HB2	2.01	0.42
38:2g:16:LEU:HD12	40:2i:41:VAL:O	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:2h:121:ASP:O	39:2h:125:ARG:HG3	2.19	0.42
42:2k:38:ASN:H	42:2k:38:ASN:ND2	2.18	0.42
55:2x:50:U:H3	55:2x:64:G:H1	1.67	0.42
1:1A:128:C:H2'	1:1A:129:C:C6	2.55	0.42
1:1A:234:C:H2'	1:1A:235:U:C6	2.54	0.42
1:1A:699:A:H2'	1:1A:700:G:O4'	2.20	0.42
1:1A:1288:U:O4	13:1R:106:GLY:HA3	2.19	0.42
7:1H:46:GLU:OE2	7:1H:51:ARG:NE	2.53	0.42
9:1N:42:TRP:CH2	9:1N:44:PRO:HB3	2.55	0.42
27:15:29:THR:O	27:15:30:LEU:HD23	2.20	0.42
32:1a:421:U:H3'	32:1a:422:C:H6	1.85	0.42
32:1a:713:G:H2'	32:1a:714:G:C8	2.54	0.42
32:1a:1152:A:H5'	41:1j:13:HIS:ND1	2.35	0.42
32:1a:1412:C:H2'	32:1a:1413:A:C8	2.54	0.42
35:1d:60:GLU:OE2	35:1d:63:LYS:NZ	2.42	0.42
39:1h:28:ALA:HB3	39:1h:57:PRO:HB2	2.00	0.42
39:1h:121:ASP:HB2	39:1h:125:ARG:NH2	2.34	0.42
40:1i:97:LYS:HB3	40:1i:97:LYS:HE2	1.65	0.42
47:1p:67:THR:H	47:1p:70:ALA:HB3	1.84	0.42
55:1x:25:C:H2'	55:1x:26:G:O4'	2.20	0.42
54:1y:4:C:H2'	54:1y:5:G:O4'	2.20	0.42
1:2A:83:G:O2'	1:2A:102:G:N2	2.52	0.42
1:2A:192:C:O2'	1:2A:802:A:N3	2.51	0.42
1:2A:272(J):C:N4	1:2A:363:G:H1	2.15	0.42
1:2A:947:G:H2'	1:2A:948:G:H8	1.84	0.42
1:2A:2142:C:H2'	1:2A:2143:C:C6	2.54	0.42
1:2A:2330:G:H2'	1:2A:2331:G:O4'	2.20	0.42
1:2A:2375:G:O2'	1:2A:2377:A:N7	2.45	0.42
1:2A:2584:U:H2'	1:2A:2585:U:H2'	2.02	0.42
2:2B:8:U:H3	2:2B:113:G:H1	1.66	0.42
6:2G:122:PRO:O	6:2G:125:PHE:HD2	2.03	0.42
7:2H:16:SER:OG	7:2H:27:LYS:HB2	2.19	0.42
7:2H:118:PRO:O	7:2H:121:ILE:HB	2.20	0.42
11:2P:6:LEU:HD23	11:2P:6:LEU:HA	1.91	0.42
14:2S:19:LYS:C	14:2S:21:THR:H	2.27	0.42
15:2T:119:LYS:HB2	32:2a:1442(A):G:N2	2.35	0.42
16:2U:50:ARG:HH22	17:2V:72:VAL:HG22	1.84	0.42
21:2Z:30:ASN:OD1	21:2Z:33:LEU:HD23	2.20	0.42
24:22:33:MET:HG3	24:22:36:ARG:NH2	2.34	0.42
25:23:39:ASP:OD1	25:23:44:ARG:HD2	2.20	0.42
32:2a:439:A:C5	32:2a:441:A:H1'	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:741:G:H2'	32:2a:742:G:O4'	2.19	0.42
32:2a:1033:G:H2'	32:2a:1034:G:H8	1.83	0.42
32:2a:1079:G:O3'	36:2e:14:ARG:NH2	2.53	0.42
32:2a:1123:A:H4'	41:2j:37:PRO:HD2	2.01	0.42
32:2a:1206:G:C6	32:2a:1207:2MG:C5	3.08	0.42
32:2a:1273:G:H3'	32:2a:1274:G:C8	2.48	0.42
39:2h:114:THR:HG22	39:2h:131:GLY:HA3	2.02	0.42
40:2i:22:GLY:HA3	40:2i:60:ASP:OD1	2.20	0.42
40:2i:102:LEU:HD12	40:2i:103:THR:H	1.85	0.42
50:2s:64:GLU:OE2	50:2s:65:ASN:ND2	2.53	0.42
54:2y:18:G:N2	54:2y:58:A:C5	2.87	0.42
1:1A:593:G:C4'	30:18:4:MET:HE2	2.49	0.42
1:1A:715:G:C2	46:1o:56:LEU:HD21	2.55	0.42
1:1A:848:G:O6	1:1A:928:G:H2'	2.19	0.42
1:1A:1914:C:H2'	1:1A:1915:5MU:O4'	2.19	0.42
1:1A:2127:G:N2	1:1A:2173:A:H1'	2.34	0.42
1:1A:2291:U:O2'	1:1A:2374:C:O2'	2.36	0.42
1:1A:2319:G:H1	14:1S:3:ARG:HA	1.84	0.42
1:1A:2334:G:H5'	14:1S:9:ARG:HG2	2.02	0.42
1:1A:2443:C:OP1	5:1F:68:LYS:HD3	2.20	0.42
1:1A:2545:G:O2'	1:1A:2565:A:N1	2.50	0.42
8:1I:100:ALA:HA	8:1I:103:ARG:NH1	2.35	0.42
17:1V:71:LEU:HD23	17:1V:71:LEU:HA	1.73	0.42
32:1a:544:G:P	35:1d:59:ARG:HH22	2.42	0.42
32:1a:735:C:H2'	32:1a:736:C:H6	1.83	0.42
32:1a:911:U:OP1	43:1l:95:GLY:HA2	2.20	0.42
32:1a:1077:G:N2	32:1a:1080:A:OP2	2.52	0.42
36:1e:12:LEU:O	36:1e:13:ILE:HD12	2.19	0.42
38:1g:101:LEU:O	38:1g:105:VAL:HG23	2.20	0.42
39:1h:77:GLU:HG2	39:1h:78:GLN:H	1.85	0.42
42:1k:48:ILE:O	42:1k:50:TYR:N	2.49	0.42
54:1y:37:MIA:H2'	54:1y:38:A:O4'	2.20	0.42
1:2A:1364:G:N7	23:21:3:LYS:HD2	2.35	0.42
1:2A:1778:U:OP1	61:2A:3978:HOH:O	2.22	0.42
1:2A:2510:C:C4	1:2A:2511:U:C4	3.07	0.42
1:2A:2728:U:H2'	1:2A:2729:G:H8	1.85	0.42
2:2B:59:A:H2'	2:2B:60:C:O4'	2.19	0.42
5:2F:129:PHE:HA	5:2F:142:TRP:NE1	2.35	0.42
23:21:52:ARG:NH2	23:21:57:GLU:HB2	2.34	0.42
27:25:35:GLU:HG2	27:25:51:TYR:CD1	2.54	0.42
32:2a:100:C:H2'	32:2a:101:A:C8	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:303:A:H2'	32:2a:304:U:O4'	2.19	0.42
32:2a:976:G:C8	32:2a:1362:C:N4	2.88	0.42
33:2b:15:VAL:O	33:2b:17:PHE:N	2.49	0.42
54:2w:74:C:C4	54:2w:75:C:C2	3.08	0.42
1:1A:863:A:H2'	1:1A:864:G:C8	2.55	0.42
1:1A:944:G:H5''	1:1A:945:A:O5'	2.20	0.42
1:1A:1843:C:H5'	3:1D:253:GLN:OE1	2.20	0.42
1:1A:1969:A:OP2	61:1A:4267:HOH:O	2.22	0.42
2:1B:42:C:OP1	6:1G:67:LYS:NZ	2.53	0.42
6:1G:38:VAL:HG22	6:1G:93:THR:HG23	2.02	0.42
8:1I:10:GLU:H	8:1I:10:GLU:HG3	1.42	0.42
21:1Z:44:PHE:CE1	21:1Z:86:VAL:HG11	2.54	0.42
32:1a:1333:A:H2'	32:1a:1334:G:O4'	2.20	0.42
33:1b:76:GLN:HG2	33:1b:206:ASP:O	2.20	0.42
33:1b:155:LEU:HD11	33:1b:159:PRO:HG3	2.01	0.42
35:1d:112:VAL:H	35:1d:116:GLN:HE21	1.68	0.42
37:1f:29:ALA:O	37:1f:33:TYR:HD2	2.02	0.42
46:1o:18:PHE:CE2	46:1o:21:ASP:HB2	2.54	0.42
47:1p:43:LYS:HA	47:1p:48:TRP:HB3	2.02	0.42
1:2A:8:A:H2'	1:2A:9:U:C6	2.55	0.42
1:2A:141:A:H8	1:2A:1408:C:HO2'	1.67	0.42
1:2A:1019:U:H2'	1:2A:1020:A:C8	2.50	0.42
1:2A:1142:U:O2'	61:2A:3963:HOH:O	2.20	0.42
1:2A:2678:C:H2'	1:2A:2679:A:O4'	2.20	0.42
2:2B:15:A:OP2	2:2B:69:G:N2	2.53	0.42
10:2O:119:PRO:HB2	15:2T:68:TYR:CZ	2.55	0.42
12:2Q:43:THR:HG22	12:2Q:94:VAL:HG12	2.02	0.42
16:2U:107:ALA:O	16:2U:111:GLU:HG2	2.20	0.42
18:2W:14:PRO:HG2	18:2W:78:GLU:HB2	2.02	0.42
21:2Z:158:PRO:O	21:2Z:161:VAL:HG12	2.20	0.42
32:2a:37:U:H2'	32:2a:38:G:O4'	2.19	0.42
32:2a:302:G:N3	32:2a:556:C:H4'	2.35	0.42
32:2a:357:G:OP1	32:2a:367:U:H5''	2.19	0.42
32:2a:401:C:H2'	32:2a:402:G:C8	2.55	0.42
32:2a:537:G:H5''	43:2I:113:ARG:NH1	2.35	0.42
32:2a:857:C:H2'	32:2a:858:G:O4'	2.20	0.42
32:2a:1017:G:H8	32:2a:1017:G:OP2	2.03	0.42
32:2a:1417:G:C6	32:2a:1482:G:C6	3.08	0.42
33:2b:29:ALA:HA	33:2b:32:ILE:HD12	2.01	0.42
35:2d:96:LEU:HD13	35:2d:96:LEU:HA	1.65	0.42
48:2q:45:HIS:NE2	48:2q:47:PRO:HG3	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:2r:84:LYS:H	49:2r:84:LYS:HG2	1.53	0.42
1:1A:443:A:C6	5:1F:45:ARG:HD2	2.55	0.41
6:1G:72:ARG:NH1	6:1G:87:PRO:HG3	2.35	0.41
12:1Q:60:ARG:HH21	54:1w:53:G:P	2.43	0.41
13:1R:16:HIS:HD2	13:1R:16:HIS:O	2.03	0.41
14:1S:6:ALA:O	14:1S:10:ARG:HB2	2.19	0.41
19:1X:26:TYR:HD1	19:1X:92:LEU:HD12	1.84	0.41
29:17:33:ARG:NH2	61:17:202:HOH:O	2.51	0.41
32:1a:381:C:H2'	32:1a:382:A:O4'	2.20	0.41
33:1b:218:ALA:O	33:1b:222:ILE:HG13	2.19	0.41
35:1d:162:LEU:HD13	35:1d:181:MET:HG2	2.02	0.41
48:1q:50:LYS:H	48:1q:50:LYS:HG2	1.61	0.41
54:1w:75:C:H2'	54:1w:76:A:C8	2.55	0.41
1:2A:764:A:N1	1:2A:1789:A:O2'	2.51	0.41
1:2A:1005:C:H2'	1:2A:1006:C:C6	2.55	0.41
1:2A:2096:U:H2'	1:2A:2097:C:C6	2.55	0.41
1:2A:2320:A:H1'	1:2A:2321:G:N1	2.35	0.41
1:2A:2732:G:H3'	1:2A:2733:A:O4'	2.19	0.41
6:2G:125:PHE:HB3	6:2G:166:ASP:OD1	2.19	0.41
13:2R:100:LEU:HD12	13:2R:100:LEU:HA	1.85	0.41
22:20:50:ASN:C	22:20:62:LEU:HD12	2.45	0.41
27:25:48:GLU:O	27:25:60:VAL:HG11	2.20	0.41
32:2a:872:A:O2'	32:2a:873:A:H5''	2.20	0.41
32:2a:1122:U:H2'	32:2a:1123:A:H8	1.85	0.41
32:2a:1347:G:C8	40:2i:107:ARG:HB2	2.55	0.41
32:2a:1363(A):A:C8	32:2a:1365:G:C5	3.08	0.41
32:2a:1376:U:C2	32:2a:1377:A:N7	2.88	0.41
33:2b:188:ALA:HB1	33:2b:192:SER:CB	2.50	0.41
34:2c:39:ILE:O	34:2c:43:LEU:HG	2.20	0.41
34:2c:138:VAL:O	34:2c:142:MET:N	2.51	0.41
35:2d:172:PRO:HD2	35:2d:173:TRP:CZ3	2.55	0.41
39:2h:69:ARG:NE	39:2h:75:ARG:O	2.51	0.41
1:1A:271(P):C:O3'	8:1I:42:SER:HB2	2.20	0.41
1:1A:1201:C:N4	61:1A:4586:HOH:O	2.54	0.41
1:1A:1372:U:H2'	1:1A:1373:A:O4'	2.20	0.41
1:1A:1786:A:H1'	1:1A:1938:A:N6	2.35	0.41
4:1E:45:THR:N	61:1E:403:HOH:O	2.32	0.41
4:1E:46:ALA:HB2	4:1E:82:ARG:HA	2.02	0.41
11:1P:101:VAL:HA	11:1P:106:LEU:O	2.20	0.41
32:1a:176:C:H2'	32:1a:177:C:C6	2.56	0.41
32:1a:324:G:OP1	51:1t:22:ARG:NE	2.49	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:473:G:H2'	32:1a:474:G:C8	2.55	0.41
32:1a:684:A:O2'	42:1k:39:PRO:O	2.38	0.41
33:1b:223:ILE:H	33:1b:223:ILE:HG12	1.61	0.41
34:1c:91:LEU:HD12	34:1c:91:LEU:HA	1.89	0.41
39:1h:28:ALA:HA	39:1h:59:LEU:HG	2.02	0.41
44:1m:44:ARG:HD3	44:1m:44:ARG:HA	1.69	0.41
51:1t:87:LYS:O	51:1t:91:LEU:HG	2.20	0.41
54:1y:6:G:O6	54:1y:7:A:N6	2.53	0.41
1:2A:945:A:C4	1:2A:2448:A:C2	3.08	0.41
1:2A:1242:A:N1	11:2P:4:SER:OG	2.49	0.41
1:2A:2507:C:H5''	1:2A:2573:C:N4	2.35	0.41
1:2A:2679:A:H4'	4:2E:165:VAL:HG11	2.02	0.41
2:2B:56:G:H4'	2:2B:57:A:H8	1.84	0.41
3:2D:97:TYR:C	3:2D:99:ASP:N	2.76	0.41
7:2H:98:LEU:HD11	7:2H:125:VAL:H	1.84	0.41
14:2S:87:PHE:CZ	14:2S:102:ALA:HB2	2.55	0.41
16:2U:76:TYR:CE2	16:2U:80:ILE:HG13	2.54	0.41
21:2Z:104:PHE:HA	21:2Z:139:VAL:HB	2.02	0.41
23:21:3:LYS:HB2	23:21:61:ARG:HH12	1.85	0.41
32:2a:262:A:H4'	51:2t:75:ASN:HB2	2.02	0.41
32:2a:833:U:H3	32:2a:853:G:H1	1.68	0.41
32:2a:1338:G:H2'	32:2a:1339:A:C8	2.55	0.41
33:2b:8:LYS:HD2	33:2b:217:ARG:HD2	2.02	0.41
33:2b:119:GLU:CD	33:2b:153:ARG:HH12	2.28	0.41
46:2o:31:LEU:O	46:2o:35:ARG:HG3	2.20	0.41
50:2s:22:LEU:O	50:2s:27:GLU:HG2	2.21	0.41
1:1A:588:U:O4	1:1A:670:A:H1'	2.20	0.41
1:1A:784:A:C5	3:1D:229:VAL:HG21	2.55	0.41
1:1A:880:G:H1	1:1A:898:C:H42	1.66	0.41
1:1A:1913:A:C6	54:1w:38:A:H5'	2.56	0.41
1:1A:1949:G:C6	1:1A:1950:G:C6	3.08	0.41
1:1A:2059:A:H2'	1:1A:2503:2MA:HM23	2.01	0.41
1:1A:2099:U:H2'	1:1A:2100:G:C8	2.55	0.41
1:1A:2667:C:H1'	7:1H:109:PHE:CD1	2.55	0.41
1:1A:2864:G:OP1	15:1T:119:LYS:HD2	2.20	0.41
12:1Q:130:LYS:HB3	12:1Q:130:LYS:HE2	1.85	0.41
19:1X:92:LEU:O	19:1X:94:GLY:N	2.54	0.41
32:1a:115:G:H4'	32:1a:116:A:O5'	2.20	0.41
32:1a:159:G:H2'	32:1a:161:A:OP2	2.19	0.41
1:2A:510:C:H2'	1:2A:511:U:O4'	2.21	0.41
1:2A:1243:G:H2'	1:2A:1244:G:O4'	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1423:G:H2'	1:2A:1424:G:H8	1.85	0.41
1:2A:1792:G:H2'	1:2A:1793:C:C6	2.55	0.41
1:2A:2104:G:H1	1:2A:2185:C:N4	2.14	0.41
1:2A:2119:A:N1	1:2A:2170:A:H2'	2.35	0.41
1:2A:2160:G:H2'	1:2A:2160:G:N3	2.35	0.41
6:2G:11:TYR:CZ	6:2G:16:ARG:HD3	2.54	0.41
8:2I:69:LYS:HZ3	8:2I:69:LYS:HB2	1.85	0.41
9:2N:121:LYS:HD3	9:2N:130:HIS:CE1	2.54	0.41
21:2Z:36:LYS:HE3	21:2Z:36:LYS:HB2	1.77	0.41
23:21:65:SER:OG	23:21:66:HIS:ND1	2.47	0.41
31:29:14:CYS:HA	31:29:27:CYS:HB2	2.01	0.41
32:2a:420:U:H2'	32:2a:422:C:C5	2.54	0.41
32:2a:863:U:O2'	32:2a:865:A:N7	2.47	0.41
33:2b:57:PHE:HD2	33:2b:58:ILE:HG12	1.84	0.41
33:2b:66:GLY:HA3	33:2b:160:ASP:OD2	2.20	0.41
34:2c:120:VAL:HG12	34:2c:123:GLN:CD	2.45	0.41
35:2d:150:GLU:HA	35:2d:153:ARG:HG3	2.02	0.41
38:2g:13:GLN:O	38:2g:24:THR:HG21	2.19	0.41
40:2i:23:ASN:ND2	40:2i:25:LYS:HD3	2.35	0.41
40:2i:24:GLY:HA2	40:2i:59:PHE:O	2.20	0.41
47:2p:21:VAL:HG13	47:2p:34:GLU:HB3	2.03	0.41
49:2r:22:VAL:HB	49:2r:56:THR:HA	2.03	0.41
1:1A:1448:G:H4'	1:1A:1542:A:OP1	2.20	0.41
1:1A:2183:C:HO2'	1:1A:2184:G:P	2.43	0.41
2:1B:13:A:N1	2:1B:69:G:O2'	2.48	0.41
8:1I:68:LEU:HD23	8:1I:109:ILE:HD11	2.02	0.41
17:1V:39:LEU:HD13	17:1V:40:LEU:N	2.36	0.41
32:1a:486:U:H2'	32:1a:487:A:H8	1.85	0.41
32:1a:1511:G:H2'	32:1a:1512:U:O4'	2.20	0.41
1:2A:35:G:H2'	1:2A:36:G:O4'	2.20	0.41
1:2A:797:C:H2'	1:2A:798:G:O4'	2.20	0.41
1:2A:1003:G:N2	1:2A:1153:C:C2	2.88	0.41
1:2A:1005:C:O2'	9:2N:28:THR:HG21	2.20	0.41
1:2A:1331:A:H2'	1:2A:1333:C:C5	2.55	0.41
1:2A:1815:A:OP2	3:2D:54:ARG:NH2	2.53	0.41
1:2A:2261:C:H1'	1:2A:2388:A:N3	2.36	0.41
2:2B:15:A:H3'	2:2B:16:G:H8	1.84	0.41
6:2G:41:GLN:HG2	6:2G:154:GLY:O	2.20	0.41
6:2G:62:LEU:HB3	26:24:27:THR:HG21	2.02	0.41
12:2Q:23:GLY:O	12:2Q:25:ASP:N	2.53	0.41
30:28:14:VAL:HG13	30:28:22:VAL:HG13	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:64:G:H4'	32:2a:65:U:C3'	2.49	0.41
32:2a:964:A:N3	32:2a:969:A:O2'	2.48	0.41
32:2a:997:U:H2'	32:2a:998:G:C8	2.55	0.41
32:2a:1027:C:O2'	32:2a:1034:G:N2	2.52	0.41
34:2c:11:ARG:CZ	34:2c:182:ILE:HD11	2.50	0.41
36:2e:95:ALA:C	36:2e:97:GLY:H	2.28	0.41
51:2t:26:ASN:HA	51:2t:71:THR:HG23	2.01	0.41
1:1A:890:A:H2'	1:1A:892:G:O4'	2.21	0.41
1:1A:2168:G:N1	1:1A:2171:A:C8	2.88	0.41
5:1F:52:LYS:HA	5:1F:56:GLU:OE1	2.20	0.41
7:1H:13:LYS:HA	7:1H:14:GLY:HA2	1.61	0.41
32:1a:22:G:H4'	32:1a:885:G:C8	2.55	0.41
32:1a:439:A:C8	32:1a:496:A:C6	3.09	0.41
32:1a:520:A:N1	32:1a:536:C:H1'	2.35	0.41
32:1a:971:G:N2	32:1a:1363(A):A:OP2	2.50	0.41
32:1a:1286:A:H2'	32:1a:1287:A:H4'	2.01	0.41
32:1a:1429:C:H2'	32:1a:1430:C:C6	2.56	0.41
32:1a:1486:G:H2'	32:1a:1487:G:O4'	2.20	0.41
47:1p:20:VAL:HG21	47:1p:32:TYR:CD2	2.56	0.41
1:2A:274:G:C2	1:2A:363:G:C6	3.08	0.41
1:2A:601:C:O2	1:2A:605:C:H4'	2.20	0.41
1:2A:2419:U:H2'	1:2A:2420:C:H6	1.84	0.41
1:2A:2753:A:N3	31:29:15:LYS:NZ	2.59	0.41
4:2E:34:VAL:HG21	4:2E:78:LEU:HD21	2.01	0.41
7:2H:56:SER:HB2	7:2H:61:HIS:ND1	2.34	0.41
32:2a:33:A:N3	43:2l:32:PHE:HE2	2.18	0.41
32:2a:114:U:H2'	32:2a:115:G:C8	2.56	0.41
32:2a:198:G:H2'	32:2a:199:G:H8	1.85	0.41
32:2a:853:G:N3	32:2a:854:G:C8	2.88	0.41
32:2a:1227:A:OP1	50:2s:80:TYR:OH	2.31	0.41
32:2a:1386:G:C2	32:2a:1387:G:C8	3.09	0.41
33:2b:24:TRP:H	33:2b:24:TRP:HD1	1.66	0.41
35:2d:11:LEU:HD23	35:2d:66:ARG:HB3	2.01	0.41
36:2e:43:LEU:HB2	36:2e:136:MET:SD	2.60	0.41
36:2e:53:LEU:HD12	36:2e:53:LEU:H	1.83	0.41
45:2n:14:PRO:HG2	45:2n:16:PHE:O	2.20	0.41
54:2w:29:G:H1	54:2w:41:C:N4	2.13	0.41
54:2w:38:A:H2'	54:2w:39:PSU:O4'	2.20	0.41
1:1A:1108:U:H2'	1:1A:1109:C:O4'	2.19	0.41
1:1A:2773:C:H2'	1:1A:2774:C:H6	1.84	0.41
4:1E:3:GLY:C	4:1E:81:ILE:HD13	2.45	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:1X:84:ALA:HB3	19:1X:87:GLN:CD	2.46	0.41
32:1a:848:C:H2'	32:1a:849:C:H6	1.85	0.41
32:1a:1034:G:N3	32:1a:1034:G:H2'	2.34	0.41
32:1a:1356:G:H2'	32:1a:1357:A:H8	1.82	0.41
32:1a:1429:C:H2'	32:1a:1430:C:H6	1.85	0.41
51:1t:18:GLN:O	51:1t:22:ARG:HG3	2.20	0.41
1:2A:569:U:C4	1:2A:570:G:C6	3.08	0.41
1:2A:686:G:H8	29:27:6:GLN:O	2.04	0.41
1:2A:1607:C:H5''	1:2A:1608:A:H5'	2.02	0.41
1:2A:2336:A:H61	22:20:43:THR:HG22	1.85	0.41
1:2A:2400:G:H2'	1:2A:2401:U:H6	1.85	0.41
1:2A:2773:C:H2'	1:2A:2774:C:H6	1.86	0.41
1:2A:2786:U:O2'	4:2E:62:PRO:O	2.37	0.41
6:2G:114:ILE:HA	6:2G:140:ILE:HD11	2.02	0.41
9:2N:22:THR:HA	9:2N:61:ARG:O	2.20	0.41
9:2N:30:ILE:HG23	9:2N:52:VAL:HG11	2.02	0.41
9:2N:103:VAL:O	9:2N:107:LEU:HG	2.20	0.41
12:2Q:66:ILE:HG12	12:2Q:104:PHE:CD1	2.55	0.41
22:20:24:LYS:HA	22:20:24:LYS:HD3	1.78	0.41
25:23:46:ASN:O	25:23:50:VAL:HG22	2.20	0.41
26:24:40:HIS:CD2	26:24:41:PRO:HD2	2.55	0.41
32:2a:174:C:H2'	32:2a:175:C:H6	1.85	0.41
32:2a:685:G:N1	32:2a:704:A:OP2	2.49	0.41
32:2a:778:G:H2'	32:2a:779:C:O4'	2.21	0.41
32:2a:1063:C:H3'	32:2a:1064:G:H2'	2.03	0.41
32:2a:1100:C:H2'	32:2a:1102:A:O5'	2.21	0.41
32:2a:1151:A:O2'	32:2a:1152:A:H8	2.03	0.41
32:2a:1226:C:N4	44:2m:104:ARG:HG3	2.36	0.41
32:2a:1367:C:H4'	41:2j:48:THR:HG21	2.03	0.41
34:2c:182:ILE:HD12	34:2c:182:ILE:O	2.20	0.41
35:2d:173:TRP:CE2	35:2d:189:PRO:HB3	2.56	0.41
41:2j:40:LEU:HD12	41:2j:69:ASN:HD22	1.84	0.41
44:2m:29:ARG:HD3	44:2m:64:TRP:CD2	2.56	0.41
46:2o:7:GLU:HG3	46:2o:7:GLU:H	1.61	0.41
1:1A:1062:G:O5'	1:1A:1070:A:O2'	2.34	0.41
1:1A:1091:G:C6	1:1A:1101:U:C2	3.08	0.41
1:1A:2222:G:O6	61:1A:4268:HOH:O	2.22	0.41
1:1A:2422:A:O4'	54:1y:76:A:N6	2.53	0.41
1:1A:2749:A:H5''	7:1H:3:ARG:NH1	2.28	0.41
1:1A:2857:G:N2	1:1A:2860:A:OP2	2.45	0.41
5:1F:33:LEU:HB3	11:1P:6:LEU:HD21	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1I:130:TYR:O	8:1I:138:ILE:N	2.51	0.41
22:10:43:THR:OG1	22:10:46:LYS:HG2	2.21	0.41
26:14:61:ARG:NH2	50:1s:9:VAL:HG21	2.35	0.41
32:1a:34:C:H2'	32:1a:35:G:H8	1.86	0.41
32:1a:1358:U:OP2	32:1a:1359:C:N4	2.48	0.41
33:1b:101:MET:HA	33:1b:108:ILE:HD12	2.01	0.41
46:1o:8:LYS:O	46:1o:12:ILE:HG13	2.20	0.41
1:2A:252:G:OP1	11:2P:50:ARG:NH1	2.46	0.41
1:2A:839:U:H2'	1:2A:840:C:H6	1.86	0.41
1:2A:863:A:H2'	1:2A:864:G:H8	1.85	0.41
1:2A:1180:C:H2'	1:2A:1181:C:C6	2.55	0.41
1:2A:1502:C:H2'	1:2A:1503:U:C6	2.55	0.41
1:2A:1815:A:P	3:2D:54:ARG:HH22	2.44	0.41
1:2A:2278:A:OP2	22:20:12:ASN:ND2	2.52	0.41
2:2B:103:G:H21	21:2Z:73:GLN:HE22	1.69	0.41
20:2Y:43:ASN:ND2	20:2Y:65:ALA:HB3	2.36	0.41
25:23:10:LYS:HB3	25:23:53:LEU:HA	2.02	0.41
32:2a:528:C:H41	43:2l:49:ASN:ND2	2.18	0.41
32:2a:807:A:H2'	32:2a:808:C:C6	2.56	0.41
32:2a:824:C:H2'	32:2a:825:G:C8	2.56	0.41
32:2a:831:U:OP1	33:2b:22:LYS:HD3	2.20	0.41
32:2a:953:G:C5	32:2a:954:G:C8	3.09	0.41
32:2a:1176:A:H2'	32:2a:1177:G:O4'	2.20	0.41
32:2a:1299:A:N3	32:2a:1299:A:H2'	2.35	0.41
33:2b:52:GLU:O	33:2b:56:ARG:NH1	2.53	0.41
40:2i:97:LYS:C	40:2i:99:LEU:H	2.29	0.41
41:2j:9:ARG:O	41:2j:16:LEU:HD21	2.20	0.41
44:2m:39:ILE:HG13	44:2m:55:ARG:NH1	2.35	0.41
47:2p:3:LYS:HA	47:2p:65:GLN:O	2.21	0.41
1:1A:1006:C:C2	1:1A:1138:G:N2	2.89	0.41
1:1A:1858:G:N2	1:1A:1883:G:H2'	2.36	0.41
1:1A:2120:G:C2'	1:1A:2121:G:H5'	2.51	0.41
1:1A:2190:G:H2'	1:1A:2191:G:O4'	2.21	0.41
1:1A:2432:A:H5''	61:1A:6042:HOH:O	2.21	0.41
4:1E:59:VAL:CG2	4:1E:64:LYS:HG3	2.51	0.41
11:1P:3:LEU:HD23	11:1P:3:LEU:HA	1.72	0.41
19:1X:94:GLY:N	19:1X:95:LEU:HB2	2.35	0.41
21:1Z:52:SER:C	21:1Z:54:HIS:N	2.75	0.41
25:13:18:ASP:OD1	25:13:18:ASP:N	2.53	0.41
32:1a:619:U:N3	35:1d:134:ASP:OD1	2.50	0.41
43:1l:70:ILE:HG12	43:1l:100:ILE:HD12	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:1m:34:LEU:HD13	44:1m:41:PRO:HB3	2.02	0.41
47:1p:53:VAL:HG13	47:1p:79:VAL:HG12	2.03	0.41
1:2A:272(I):U:H2'	1:2A:272(J):C:O4'	2.21	0.41
1:2A:322:A:H5'	1:2A:340:A:H1'	2.03	0.41
1:2A:1180:C:H2'	1:2A:1181:C:H6	1.86	0.41
1:2A:1394:U:C4	1:2A:1395:A:C5	3.08	0.41
1:2A:2788:C:N4	1:2A:2789:C:H41	2.18	0.41
2:2B:104:U:H2'	2:2B:105:A:O4'	2.20	0.41
32:2a:1112:C:N3	34:2c:178:LEU:HD12	2.36	0.41
34:2c:51:GLY:C	34:2c:70:VAL:HG12	2.46	0.41
44:2m:4:ILE:HG23	44:2m:5:ALA:H	1.86	0.41
54:2w:51:U:H2'	54:2w:52:G:C8	2.55	0.41
54:2y:26:A:N1	54:2y:44:G:C6	2.89	0.41
1:1A:56:A:H2'	1:1A:57:C:O4'	2.21	0.41
1:1A:893:C:H2'	1:1A:894:C:C6	2.56	0.41
1:1A:1477:A:C2	1:1A:1515:G:C2	3.09	0.41
1:1A:1503:U:H2'	1:1A:1504:C:C6	2.55	0.41
1:1A:1614:A:P	1:1A:1614:A:H8	2.44	0.41
1:1A:1779:U:H2'	61:1A:4340:HOH:O	2.21	0.41
1:1A:1882:C:H2'	1:1A:1883:G:O4'	2.21	0.41
1:1A:2223:G:OP1	3:1D:172:TYR:OH	2.30	0.41
1:1A:2506:U:C2	1:1A:2585:U:O4	2.74	0.41
2:1B:32:C:C2	2:1B:51:G:N2	2.89	0.41
6:1G:82:LEU:HD23	6:1G:82:LEU:HA	1.83	0.41
6:1G:96:ARG:N	6:1G:99:MET:HE2	2.36	0.41
8:1I:44:LEU:HD12	8:1I:44:LEU:HA	1.85	0.41
10:1O:48:PRO:CB	32:1a:1422:G:H5''	2.48	0.41
13:1R:78:LYS:O	13:1R:83:ILE:HG13	2.20	0.41
14:1S:89:ARG:HD2	14:1S:92:TYR:O	2.21	0.41
18:1W:29:LEU:HD13	18:1W:51:LEU:HD11	2.02	0.41
18:1W:86:LEU:HD22	18:1W:96:ILE:HD11	2.02	0.41
19:1X:31:HIS:CD2	19:1X:33:LYS:H	2.39	0.41
32:1a:12:U:H4'	32:1a:526:C:H4'	2.03	0.41
32:1a:375:U:OP1	47:1p:69:THR:OG1	2.24	0.41
32:1a:649:G:H2'	32:1a:650:G:H8	1.86	0.41
32:1a:983:A:H5''	32:1a:984:C:OP2	2.21	0.41
32:1a:1002:G:N2	32:1a:1004:A:H1'	2.35	0.41
32:1a:1148:U:O3'	40:1i:14:VAL:HG11	2.21	0.41
32:1a:1355:G:H2'	32:1a:1356:G:C8	2.55	0.41
61:1a:2278:HOH:O	45:1n:3:ARG:HG2	2.20	0.41
33:1b:8:LYS:HB3	33:1b:48:MET:HE3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:1i:5:TYR:N	40:1i:87:GLN:OE1	2.53	0.41
40:1i:27:THR:OG1	40:1i:31:GLN:O	2.35	0.41
43:1l:34:ARG:HE	43:1l:34:ARG:HB3	1.69	0.41
47:1p:41:PRO:O	47:1p:43:LYS:HE2	2.21	0.41
54:1y:14:A:C2	54:1y:15:G:H1'	2.56	0.41
1:2A:311:A:C6	1:2A:328:U:C4	3.09	0.41
1:2A:319:C:C2	1:2A:333:G:N2	2.89	0.41
1:2A:355:G:H2'	1:2A:356:G:O4'	2.21	0.41
1:2A:392:C:H5''	1:2A:409:C:H5''	2.02	0.41
1:2A:459:U:H5''	29:27:40:TRP:CD2	2.56	0.41
1:2A:492:A:H2'	1:2A:493:G:O4'	2.20	0.41
1:2A:674:G:H1'	5:2F:74:ARG:HD3	2.02	0.41
1:2A:764:A:H5''	3:2D:210:GLY:HA2	2.02	0.41
1:2A:859:G:H5'	1:2A:2268:A:O2'	2.21	0.41
1:2A:910:A:H2	1:2A:2264:C:O2	2.04	0.41
1:2A:2067:G:O2'	1:2A:2069:G:H5'	2.20	0.41
1:2A:2431:U:O2'	1:2A:2433:A:N7	2.45	0.41
1:2A:2769:C:H2'	1:2A:2770:G:O4'	2.21	0.41
4:2E:18:ASP:HB3	15:2T:82:LEU:HD21	2.03	0.41
5:2F:116:ASP:O	5:2F:120:GLU:HG2	2.21	0.41
6:2G:43:LEU:C	6:2G:45:GLU:N	2.77	0.41
6:2G:128:ARG:HB2	6:2G:130:ASN:ND2	2.33	0.41
6:2G:151:ALA:HB3	6:2G:153:ARG:NH1	2.35	0.41
7:2H:10:PRO:HA	7:2H:49:VAL:HG23	2.03	0.41
12:2Q:17:LEU:HB3	12:2Q:39:PRO:HB2	2.03	0.41
17:2V:39:LEU:HD22	17:2V:47:VAL:HA	2.02	0.41
21:2Z:146:ILE:HA	21:2Z:174:VAL:O	2.20	0.41
23:21:52:ARG:HH22	23:21:57:GLU:HB2	1.85	0.41
23:21:60:PHE:HE1	23:21:95:LEU:HD21	1.86	0.41
26:24:46:GLN:C	26:24:48:ARG:N	2.76	0.41
26:24:46:GLN:NE2	26:24:48:ARG:HD3	2.36	0.41
32:2a:46:G:O2'	32:2a:365:U:H1'	2.21	0.41
32:2a:130:A:H5'	48:2q:63:ARG:HE	1.86	0.41
32:2a:253:U:H2'	32:2a:254:G:H8	1.85	0.41
32:2a:429:U:H1'	32:2a:430:A:H5''	2.03	0.41
32:2a:646:U:H2'	32:2a:647:C:H6	1.85	0.41
32:2a:678:U:H2'	32:2a:679:C:C6	2.56	0.41
32:2a:728:A:N7	46:2o:54:ARG:HD3	2.36	0.41
32:2a:908:A:H2'	32:2a:909:A:H8	1.85	0.41
32:2a:980:C:H3'	32:2a:981:U:C6	2.56	0.41
32:2a:986:A:N3	50:2s:52:TYR:OH	2.41	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1320:C:N3	50:2s:36:ARG:NH2	2.69	0.41
32:2a:1390:U:H2'	32:2a:1391:U:C6	2.56	0.41
33:2b:158:LEU:HA	33:2b:159:PRO:HD3	1.94	0.41
35:2d:94:LEU:HD12	35:2d:94:LEU:HA	1.76	0.41
35:2d:191:ARG:O	35:2d:191:ARG:NH1	2.54	0.41
36:2e:40:ARG:HD3	36:2e:67:VAL:O	2.20	0.41
37:2f:15:ASP:OD1	37:2f:18:GLN:N	2.42	0.41
37:2f:49:ALA:HB2	49:2r:78:LEU:O	2.21	0.41
39:2h:100:ILE:H	39:2h:100:ILE:HG13	1.75	0.41
44:2m:57:ARG:O	44:2m:61:GLU:HB2	2.20	0.41
45:2n:24:CYS:HB2	45:2n:40:CYS:HB3	2.03	0.41
45:2n:37:PHE:CE1	45:2n:53:LEU:HD22	2.55	0.41
49:2r:33:ASP:CG	49:2r:36:ASN:HB2	2.46	0.41
49:2r:58:LEU:HD22	49:2r:62:GLU:HB3	2.03	0.41
55:2x:3:C:H2'	55:2x:4:G:H8	1.84	0.41
1:1A:7:G:H2'	1:1A:8:A:H8	1.86	0.41
1:1A:637:A:OP1	11:1P:133:SER:OG	2.27	0.41
1:1A:753:C:H2'	1:1A:754:C:H6	1.86	0.41
1:1A:1424:G:H2'	1:1A:1425:G:O4'	2.20	0.41
1:1A:1429:G:H2'	1:1A:1430:C:C6	2.56	0.41
1:1A:1812:A:O2'	3:1D:45:ASN:N	2.47	0.41
1:1A:2646:C:H2'	1:1A:2647:U:O4'	2.21	0.41
1:1A:2740:A:C6	1:1A:2764:A:C8	3.09	0.41
1:1A:2848:G:C8	15:1T:97:ALA:HB2	2.56	0.41
5:1F:172:TRP:CD1	5:1F:172:TRP:H	2.39	0.41
15:1T:24:PRO:HD3	15:1T:52:ILE:HD12	2.03	0.41
16:1U:27:LEU:HB3	16:1U:31:SER:HB3	2.03	0.41
26:14:68:ARG:HD3	26:14:69:LYS:N	2.36	0.41
30:18:26:LYS:HB2	30:18:44:LYS:O	2.21	0.41
32:1a:194:C:H2'	32:1a:195:A:H5''	2.03	0.41
32:1a:232:G:H1'	32:1a:262:A:N1	2.36	0.41
32:1a:1148:U:H2'	32:1a:1149:C:O4'	2.20	0.41
43:1l:33:ARG:HH11	43:1l:62:SER:HB3	1.86	0.41
1:2A:271(D):G:C2	1:2A:271(E):U:C2	3.09	0.41
1:2A:1221(A):C:C2	1:2A:1229:G:C2	3.09	0.41
1:2A:1502:C:H2'	1:2A:1503:U:H6	1.86	0.41
1:2A:1996:C:H4'	1:2A:1997:G:OP1	2.21	0.41
1:2A:2359:C:H2'	1:2A:2360:A:O4'	2.20	0.41
1:2A:2391:G:O6	1:2A:2425:A:H8	2.04	0.41
1:2A:2893:G:H5''	1:2A:2894:G:O4'	2.21	0.41
5:2F:185:ASP:OD1	5:2F:188:ARG:NH1	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2G:11:TYR:OH	6:2G:16:ARG:NH1	2.47	0.41
6:2G:23:PHE:HB2	6:2G:25:TYR:CE2	2.56	0.41
6:2G:109:VAL:O	6:2G:113:ARG:HG3	2.21	0.41
7:2H:20:ALA:HB1	7:2H:21:PRO:HD2	2.02	0.41
9:2N:21:LYS:O	9:2N:60:ILE:HG13	2.21	0.41
11:2P:29:LYS:HG2	11:2P:30:THR:N	2.35	0.41
20:2Y:55:TYR:N	20:2Y:56:PRO:HD3	2.36	0.41
25:23:52:HIS:CD2	25:23:53:LEU:HG	2.56	0.41
32:2a:90:U:H2'	32:2a:91:C:H6	1.86	0.41
32:2a:359:U:H2'	32:2a:360:A:H8	1.85	0.41
32:2a:404:U:H2'	32:2a:405:U:C6	2.56	0.41
32:2a:1198:G:H2'	32:2a:1199:U:C6	2.56	0.41
32:2a:1322:C:P	50:2s:78:ARG:HH12	2.44	0.41
34:2c:188:LEU:HD12	34:2c:188:LEU:HA	1.79	0.41
37:2f:9:VAL:HA	37:2f:59:TYR:O	2.21	0.41
39:2h:134:ILE:HD13	39:2h:134:ILE:HA	1.93	0.41
40:2i:88:TYR:CD2	40:2i:89:ASN:HB2	2.56	0.41
44:2m:29:ARG:HB3	44:2m:64:TRP:CZ3	2.56	0.41
51:2t:13:LEU:O	51:2t:17:ARG:HG3	2.21	0.41
1:1A:27:G:C2	1:1A:512:G:N3	2.88	0.40
1:1A:247:G:H4'	1:1A:386:G:C5	2.56	0.40
1:1A:1076:C:O2'	1:1A:1077:A:N7	2.53	0.40
1:1A:1178:C:H2'	1:1A:1179:C:H6	1.86	0.40
1:1A:2040:C:H2'	1:1A:2041:U:O4'	2.21	0.40
1:1A:2074:U:H2'	1:1A:2075:U:C6	2.56	0.40
1:1A:2791:C:H2'	1:1A:2792:G:H8	1.85	0.40
9:1N:138:LEU:HD23	9:1N:139:GLU:N	2.35	0.40
13:1R:36:THR:HG22	13:1R:37:THR:H	1.86	0.40
13:1R:72:ASP:O	13:1R:76:VAL:HG23	2.21	0.40
19:1X:26:TYR:HB3	19:1X:92:LEU:HD12	2.02	0.40
31:19:32:HIS:O	31:19:34:GLN:HG3	2.22	0.40
32:1a:736:C:H2'	32:1a:737:A:C8	2.57	0.40
32:1a:985:C:H2'	32:1a:986:A:C8	2.54	0.40
32:1a:1149:C:H2'	32:1a:1150:U:C6	2.55	0.40
32:1a:1323:G:H2'	32:1a:1324:A:C8	2.56	0.40
33:1b:63:MET:HE2	33:1b:63:MET:HB3	1.97	0.40
33:1b:219:VAL:HA	33:1b:222:ILE:HD12	2.02	0.40
38:1g:69:VAL:HG12	38:1g:100:ALA:HA	2.01	0.40
1:2A:793:A:OP2	1:2A:2072:G:H5'	2.22	0.40
1:2A:860:U:H1'	1:2A:2268:A:H5'	2.02	0.40
1:2A:1138:G:N3	9:2N:106:MET:HE2	2.36	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1153:C:H2'	1:2A:1154:G:O4'	2.21	0.40
1:2A:1479:G:H5''	1:2A:1560:G:H4'	2.02	0.40
1:2A:1503:U:H2'	1:2A:1504:C:C6	2.57	0.40
1:2A:2319:G:N2	14:2S:3:ARG:HD2	2.37	0.40
1:2A:2774:C:H2'	1:2A:2775:A:O4'	2.21	0.40
2:2B:90:A:N7	2:2B:91:C:H1'	2.36	0.40
3:2D:172:TYR:CD1	3:2D:186:HIS:HA	2.56	0.40
6:2G:38:VAL:HA	6:2G:93:THR:HA	2.03	0.40
8:2I:3:VAL:O	8:2I:18:VAL:HA	2.21	0.40
19:2X:5:TYR:CE2	24:22:30:ARG:HB2	2.56	0.40
21:2Z:54:HIS:ND1	21:2Z:101:PRO:HG3	2.36	0.40
26:24:61:ARG:NH2	50:2s:9:VAL:HG21	2.35	0.40
32:2a:598:U:H4'	39:2h:94:TYR:CD2	2.56	0.40
32:2a:715:A:H2'	32:2a:716:A:C8	2.56	0.40
32:2a:791:G:C6	32:2a:792:A:N7	2.89	0.40
32:2a:946:A:H2'	32:2a:947:G:C8	2.56	0.40
32:2a:1023:G:H3'	32:2a:1024:G:H8	1.85	0.40
32:2a:1070:U:H2'	32:2a:1071:C:H6	1.87	0.40
32:2a:1192:C:N4	32:2a:1193:G:C4	2.89	0.40
32:2a:1529:G:H4'	32:2a:1530:G:OP2	2.21	0.40
34:2c:54:ARG:HB2	34:2c:69:HIS:CG	2.56	0.40
34:2c:123:GLN:HA	34:2c:126:ARG:HD2	2.04	0.40
38:2g:68:ASN:HD22	38:2g:128:ALA:HA	1.86	0.40
40:2i:50:LEU:HD13	40:2i:56:LEU:HA	2.03	0.40
44:2m:4:ILE:CD1	44:2m:19:LEU:HD23	2.51	0.40
46:2o:48:LYS:HA	46:2o:48:LYS:HD3	1.77	0.40
1:1A:64:A:O3'	19:1X:71:GLY:HA3	2.21	0.40
1:1A:118:A:C8	1:1A:119:A:C8	3.09	0.40
1:1A:271(G):C:H2'	1:1A:271(H):G:H8	1.86	0.40
1:1A:1051:G:H4'	1:1A:2752:C:H4'	2.03	0.40
1:1A:2522:U:O2'	1:1A:2647:U:OP1	2.31	0.40
1:1A:2532:G:O2'	1:1A:2657:A:N1	2.53	0.40
3:1D:79:VAL:HG12	3:1D:113:VAL:HA	2.03	0.40
6:1G:103:LEU:HD23	6:1G:103:LEU:HA	1.88	0.40
8:1I:76:THR:HG22	8:1I:141:LYS:HE2	2.03	0.40
15:1T:16:ARG:NH1	15:1T:83:ILE:O	2.40	0.40
32:1a:119:A:H4'	32:1a:120:A:C8	2.56	0.40
32:1a:256:U:H2'	32:1a:257:G:O4'	2.20	0.40
32:1a:737:A:H2'	32:1a:738:C:C6	2.56	0.40
32:1a:1030(A):G:O2'	32:1a:1031:G:N2	2.54	0.40
32:1a:1198:G:H2'	32:1a:1199:U:C6	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:1e:137:GLU:HG3	36:1e:141:GLN:HE21	1.86	0.40
49:1r:58:LEU:HD22	49:1r:62:GLU:HB3	2.03	0.40
51:1t:38:LYS:HE2	51:1t:38:LYS:HB3	1.88	0.40
1:2A:39:C:H2'	1:2A:40:C:C6	2.56	0.40
1:2A:353:G:H2'	1:2A:354:G:H8	1.85	0.40
1:2A:374:A:C2	1:2A:401:A:C4	3.10	0.40
1:2A:1183:G:O3'	25:23:29:ARG:NH1	2.54	0.40
1:2A:1504:C:H2'	1:2A:1505:C:C6	2.56	0.40
1:2A:1637:A:H5'	1:2A:1760:A:O2'	2.21	0.40
1:2A:1660:C:H2'	1:2A:1661:G:H8	1.86	0.40
1:2A:2335:A:C8	1:2A:2337:G:C5	3.09	0.40
1:2A:2390:U:P	30:28:35:GLN:HE22	2.44	0.40
1:2A:2410:G:H2'	1:2A:2411:A:O4'	2.20	0.40
6:2G:53:LEU:HD22	6:2G:53:LEU:HA	1.89	0.40
8:2I:3:VAL:HA	8:2I:39:ALA:N	2.36	0.40
10:2O:7:TYR:CE2	10:2O:20:MET:HB2	2.56	0.40
11:2P:62:LEU:HD11	30:28:50:LEU:HD11	2.03	0.40
11:2P:70:GLN:HE21	11:2P:70:GLN:N	2.19	0.40
12:2Q:5:ARG:H	12:2Q:5:ARG:HG3	1.65	0.40
17:2V:48:GLY:HA2	17:2V:52:VAL:HG13	2.02	0.40
21:2Z:54:HIS:CG	21:2Z:101:PRO:HG3	2.57	0.40
21:2Z:105:VAL:N	21:2Z:139:VAL:O	2.51	0.40
21:2Z:152:ALA:O	21:2Z:155:LEU:HG	2.21	0.40
26:24:8:LYS:HA	26:24:8:LYS:HD2	1.89	0.40
30:28:63:PRO:HG2	30:28:64:TYR:CE2	2.56	0.40
32:2a:909:A:H2'	32:2a:910:C:O4'	2.20	0.40
32:2a:977:A:C2	32:2a:1224:G:C5	3.09	0.40
32:2a:1288:A:N1	32:2a:1371:G:H1'	2.36	0.40
34:2c:13:GLY:HA3	45:2n:57:ARG:NH2	2.36	0.40
34:2c:20:SER:HA	34:2c:57:ILE:HB	2.03	0.40
36:2e:55:VAL:HA	36:2e:58:ALA:HB3	2.03	0.40
39:2h:7:ALA:O	39:2h:11:THR:OG1	2.20	0.40
39:2h:92:ARG:HB3	39:2h:94:TYR:CZ	2.56	0.40
53:2v:22:U:H2'	53:2v:23:A:C8	2.56	0.40
54:2y:18:G:N2	54:2y:55:PSU:HN3	2.02	0.40
1:1A:219:G:H2'	1:1A:220:G:C8	2.57	0.40
1:1A:652(C):G:N2	1:1A:653:A:H1'	2.37	0.40
1:1A:1851:U:H2'	1:1A:1852:C:O4'	2.21	0.40
1:1A:2088:G:C6	1:1A:2089:U:C4	3.10	0.40
23:11:53:VAL:HG22	23:11:74:VAL:HG22	2.03	0.40
29:17:18:PHE:CE2	29:17:22:MET:HG3	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:97:G:H2'	32:1a:98:G:O4'	2.22	0.40
32:1a:1239:A:H62	32:1a:1299:A:H62	1.69	0.40
33:1b:87:ARG:HE	33:1b:87:ARG:HB3	1.67	0.40
34:1c:77:ILE:H	34:1c:77:ILE:HG12	1.68	0.40
54:1w:42:C:H2'	54:1w:43:C:H6	1.87	0.40
54:1y:8:4SU:H4'	54:1y:48:C:C4'	2.51	0.40
54:1y:19:G:C6	54:1y:56:C:N4	2.85	0.40
1:2A:248:G:C2	1:2A:2431:U:H4'	2.56	0.40
1:2A:265:A:H1'	1:2A:266:G:O4'	2.22	0.40
1:2A:652:C:C2'	1:2A:652(A):A:H5'	2.52	0.40
1:2A:1882:C:H2'	1:2A:1883:G:O4'	2.21	0.40
1:2A:2006:C:H6	1:2A:2006:C:O5'	2.04	0.40
5:2F:164:ARG:O	5:2F:168:ARG:HB2	2.21	0.40
6:2G:56:ALA:HA	6:2G:59:GLU:HG2	2.02	0.40
15:2T:29:ARG:HG3	15:2T:46:GLU:HB2	2.02	0.40
32:2a:1203:C:H2'	32:2a:1204:A:H8	1.86	0.40
38:2g:78:ARG:HD3	38:2g:79:ARG:HG3	2.02	0.40
44:2m:34:LEU:HG	44:2m:41:PRO:HB3	2.03	0.40
48:2q:76:LEU:HD12	48:2q:77:VAL:H	1.87	0.40
1:1A:748:G:C8	18:1W:89:ALA:HB1	2.56	0.40
1:1A:1010:A:N3	1:1A:1153:C:H1'	2.36	0.40
1:1A:1045:A:H1'	1:1A:1047:G:N3	2.36	0.40
1:1A:1358:G:N2	1:1A:1372:U:C5	2.89	0.40
5:1F:158:THR:O	5:1F:164:ARG:NH1	2.46	0.40
25:13:10:LYS:NZ	25:13:15:TYR:OH	2.42	0.40
32:1a:49:U:C2	32:1a:361:G:N2	2.89	0.40
32:1a:109:A:C6	32:1a:326:G:C6	3.09	0.40
32:1a:112:G:OP2	47:1p:27:LYS:HD2	2.21	0.40
32:1a:165:C:H2'	32:1a:166:G:C8	2.56	0.40
32:1a:233:C:H2'	32:1a:234:C:H6	1.87	0.40
32:1a:836:G:C6	32:1a:851:G:C6	3.10	0.40
32:1a:1329:A:N7	52:1u:7:ARG:NH2	2.67	0.40
33:1b:17:PHE:HD1	33:1b:41:ILE:HD12	1.86	0.40
38:1g:138:LYS:HE2	38:1g:142:GLU:CD	2.46	0.40
39:1h:51:VAL:HG11	39:1h:60:ARG:HH12	1.87	0.40
40:1i:96:LEU:HD23	40:1i:96:LEU:HA	1.88	0.40
44:1m:89:GLY:O	44:1m:93:ARG:HG3	2.20	0.40
44:1m:97:PRO:N	44:1m:110:ARG:HG2	2.37	0.40
44:1m:106:ASN:HB2	44:1m:107:ALA:H	1.50	0.40
46:1o:8:LYS:HE2	46:1o:31:LEU:HD22	2.03	0.40
47:1p:20:VAL:HG21	47:1p:32:TYR:CE2	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:1p:20:VAL:HG23	47:1p:35:LYS:HA	2.04	0.40
51:1t:88:VAL:O	51:1t:92:LEU:HG	2.21	0.40
51:1t:90:GLN:HA	51:1t:93:GLU:HG2	2.04	0.40
1:2A:70:G:H5''	1:2A:112:U:O2	2.22	0.40
1:2A:217:G:OP2	61:2A:3977:HOH:O	2.22	0.40
1:2A:482:A:H1'	1:2A:498:G:N2	2.36	0.40
1:2A:660:G:H5'	5:2F:99:TYR:CE1	2.57	0.40
1:2A:2061:G:H5''	1:2A:2503:2MA:C2	2.51	0.40
1:2A:2487:G:H2'	1:2A:2488:A:C8	2.56	0.40
4:2E:36:ARG:NH1	4:2E:85:ASN:OD1	2.54	0.40
4:2E:170:LEU:HD23	4:2E:170:LEU:HA	1.93	0.40
5:2F:24:LEU:HD23	5:2F:24:LEU:HA	1.87	0.40
11:2P:121:LYS:O	11:2P:123:LEU:N	2.54	0.40
12:2Q:137:TYR:CE1	21:2Z:83:PRO:HG3	2.57	0.40
15:2T:22:PHE:CE1	15:2T:52:ILE:HD11	2.56	0.40
19:2X:50:LYS:HB3	19:2X:87:GLN:NE2	2.35	0.40
21:2Z:17:ALA:HA	21:2Z:20:ARG:HH11	1.86	0.40
22:20:51:VAL:N	22:20:62:LEU:HD12	2.37	0.40
22:20:82:ARG:HA	22:20:83:PRO:HD3	1.95	0.40
32:2a:227:G:H2'	32:2a:228:A:C8	2.57	0.40
32:2a:381:C:H2'	32:2a:382:A:O4'	2.21	0.40
32:2a:637:G:H2'	32:2a:638:G:H8	1.86	0.40
32:2a:975:A:H62	41:2j:60:ARG:HH22	1.69	0.40
32:2a:975:A:N6	41:2j:60:ARG:HH22	2.18	0.40
33:2b:164:VAL:HG23	33:2b:186:ALA:HB2	2.03	0.40
34:2c:152:ILE:HG22	34:2c:167:TRP:CB	2.51	0.40
36:2e:5:ASP:OD1	36:2e:5:ASP:N	2.53	0.40
41:2j:17:ASP:CG	41:2j:70:ARG:HH21	2.29	0.40
47:2p:1:MET:O	47:2p:24:ALA:N	2.44	0.40
1:1A:18:C:O2'	1:1A:554:U:OP1	2.39	0.40
1:1A:1432:C:H2'	1:1A:1433:U:O4'	2.22	0.40
1:1A:1526:G:C6	1:1A:1527:G:C2	3.09	0.40
3:1D:239:ARG:NE	61:1D:407:HOH:O	2.54	0.40
4:1E:47:VAL:O	4:1E:80:GLU:HA	2.21	0.40
4:1E:47:VAL:HG11	4:1E:86:PRO:HD2	2.02	0.40
6:1G:43:LEU:C	6:1G:45:GLU:H	2.29	0.40
11:1P:50:ARG:HD3	30:18:7:HIS:HD2	1.85	0.40
11:1P:77:ARG:HB2	11:1P:78:PRO:HD2	2.03	0.40
16:1U:89:GLU:HG3	17:1V:50:PRO:HB3	2.04	0.40
32:1a:258:G:H2'	32:1a:259:G:H8	1.87	0.40
32:1a:1401:G:C2	32:1a:1402:4OC:H1'	2.57	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1469:G:H2'	32:1a:1470:G:H8	1.87	0.40
33:1b:143:GLU:O	33:1b:147:LYS:N	2.49	0.40
46:1o:57:LEU:HD23	46:1o:57:LEU:HA	1.81	0.40
47:1p:60:LEU:HD12	47:1p:60:LEU:HA	1.94	0.40
51:1t:33:ILE:O	51:1t:37:SER:OG	2.27	0.40
54:1y:57:G:N3	54:1y:57:G:H2'	2.35	0.40
1:2A:588:U:H2'	1:2A:589:C:C6	2.56	0.40
1:2A:728:G:H5''	3:2D:13:ARG:NH2	2.37	0.40
1:2A:956:G:OP2	12:2Q:14:ARG:NH1	2.53	0.40
1:2A:2445:G:OP1	5:2F:74:ARG:NH2	2.41	0.40
4:2E:170:LEU:HD13	4:2E:184:VAL:HG11	2.03	0.40
6:2G:145:THR:H	6:2G:148:MET:HE1	1.86	0.40
13:2R:54:LEU:HD23	13:2R:54:LEU:HA	1.92	0.40
15:2T:61:PHE:CZ	15:2T:76:PHE:HB2	2.57	0.40
19:2X:50:LYS:O	19:2X:84:ALA:N	2.55	0.40
19:2X:55:ASN:O	19:2X:80:ILE:N	2.42	0.40
21:2Z:6:LYS:HE3	21:2Z:8:TYR:CE2	2.56	0.40
21:2Z:97:GLU:HB3	21:2Z:125:LEU:HD11	2.03	0.40
32:2a:196:A:OP1	51:2t:68:LYS:NZ	2.48	0.40
32:2a:660:G:H1	32:2a:745:C:N4	2.20	0.40
32:2a:977:A:H2	32:2a:1224:G:C5	2.39	0.40
32:2a:1080:A:OP1	36:2e:47:LYS:HD2	2.22	0.40
33:2b:165:VAL:HG23	33:2b:187:LEU:HD13	2.03	0.40
33:2b:179:LYS:HE3	33:2b:179:LYS:HB2	1.88	0.40
34:2c:57:ILE:HD12	34:2c:66:VAL:HG12	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	256 (94%)	17 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	2D	273/276 (99%)	252 (92%)	21 (8%)	0	100	100
4	1E	202/206 (98%)	191 (95%)	10 (5%)	1 (0%)	24	43
4	2E	202/206 (98%)	189 (94%)	11 (5%)	2 (1%)	12	24
5	1F	200/210 (95%)	195 (98%)	4 (2%)	1 (0%)	24	43
5	2F	200/210 (95%)	190 (95%)	7 (4%)	3 (2%)	8	15
6	1G	179/182 (98%)	166 (93%)	11 (6%)	2 (1%)	11	22
6	2G	179/182 (98%)	156 (87%)	18 (10%)	5 (3%)	4	6
7	1H	172/180 (96%)	163 (95%)	8 (5%)	1 (1%)	21	38
7	2H	172/180 (96%)	155 (90%)	16 (9%)	1 (1%)	21	38
8	1I	144/148 (97%)	130 (90%)	13 (9%)	1 (1%)	18	34
8	2I	144/148 (97%)	124 (86%)	18 (12%)	2 (1%)	9	17
9	1N	138/140 (99%)	130 (94%)	8 (6%)	0	100	100
9	2N	138/140 (99%)	130 (94%)	7 (5%)	1 (1%)	18	34
10	1O	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
10	2O	120/122 (98%)	114 (95%)	5 (4%)	1 (1%)	16	30
11	1P	147/150 (98%)	135 (92%)	10 (7%)	2 (1%)	9	17
11	2P	147/150 (98%)	127 (86%)	17 (12%)	3 (2%)	6	11
12	1Q	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
12	2Q	139/141 (99%)	125 (90%)	13 (9%)	1 (1%)	18	34
13	1R	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
13	2R	116/118 (98%)	110 (95%)	5 (4%)	1 (1%)	14	28
14	1S	108/112 (96%)	101 (94%)	7 (6%)	0	100	100
14	2S	108/112 (96%)	93 (86%)	11 (10%)	4 (4%)	2	4
15	1T	129/146 (88%)	118 (92%)	10 (8%)	1 (1%)	16	30
15	2T	129/146 (88%)	120 (93%)	8 (6%)	1 (1%)	16	30
16	1U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
16	2U	114/118 (97%)	108 (95%)	6 (5%)	0	100	100
17	1V	99/101 (98%)	91 (92%)	7 (7%)	1 (1%)	12	24
17	2V	99/101 (98%)	91 (92%)	6 (6%)	2 (2%)	6	11
18	1W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
18	2W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	1X	93/96 (97%)	89 (96%)	2 (2%)	2 (2%)	5	10
19	2X	93/96 (97%)	86 (92%)	7 (8%)	0	100	100
20	1Y	105/110 (96%)	96 (91%)	7 (7%)	2 (2%)	6	12
20	2Y	105/110 (96%)	96 (91%)	9 (9%)	0	100	100
21	1Z	148/206 (72%)	132 (89%)	15 (10%)	1 (1%)	18	34
21	2Z	156/206 (76%)	123 (79%)	28 (18%)	5 (3%)	3	5
22	10	81/85 (95%)	78 (96%)	3 (4%)	0	100	100
22	20	81/85 (95%)	74 (91%)	7 (9%)	0	100	100
23	11	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	11	22
23	21	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	11	22
24	12	68/72 (94%)	66 (97%)	1 (2%)	1 (2%)	8	15
24	22	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
25	13	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
25	23	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
26	14	67/71 (94%)	53 (79%)	9 (13%)	5 (8%)	1	1
26	24	67/71 (94%)	52 (78%)	10 (15%)	5 (8%)	1	1
27	15	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
27	25	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
28	16	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
28	26	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
29	17	46/49 (94%)	46 (100%)	0	0	100	100
29	27	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
31	19	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
31	29	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
33	1b	229/256 (90%)	190 (83%)	33 (14%)	6 (3%)	4	7
33	2b	229/256 (90%)	183 (80%)	44 (19%)	2 (1%)	14	28
34	1c	204/239 (85%)	185 (91%)	17 (8%)	2 (1%)	12	24
34	2c	204/239 (85%)	170 (83%)	30 (15%)	4 (2%)	6	11
35	1d	206/209 (99%)	187 (91%)	18 (9%)	1 (0%)	24	43

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	2d	206/209 (99%)	180 (87%)	26 (13%)	0	100	100
36	1e	146/162 (90%)	129 (88%)	15 (10%)	2 (1%)	9	17
36	2e	146/162 (90%)	127 (87%)	13 (9%)	6 (4%)	2	3
37	1f	98/101 (97%)	93 (95%)	5 (5%)	0	100	100
37	2f	98/101 (97%)	93 (95%)	5 (5%)	0	100	100
38	1g	153/156 (98%)	144 (94%)	9 (6%)	0	100	100
38	2g	153/156 (98%)	135 (88%)	16 (10%)	2 (1%)	9	18
39	1h	135/138 (98%)	128 (95%)	7 (5%)	0	100	100
39	2h	135/138 (98%)	121 (90%)	13 (10%)	1 (1%)	18	34
40	1i	125/128 (98%)	109 (87%)	15 (12%)	1 (1%)	16	30
40	2i	125/128 (98%)	108 (86%)	17 (14%)	0	100	100
41	1j	95/105 (90%)	76 (80%)	14 (15%)	5 (5%)	1	2
41	2j	94/105 (90%)	72 (77%)	18 (19%)	4 (4%)	2	3
42	1k	112/129 (87%)	105 (94%)	5 (4%)	2 (2%)	6	13
42	2k	112/129 (87%)	96 (86%)	14 (12%)	2 (2%)	6	13
43	1l	119/132 (90%)	114 (96%)	5 (4%)	0	100	100
43	2l	119/132 (90%)	109 (92%)	10 (8%)	0	100	100
44	1m	121/126 (96%)	111 (92%)	8 (7%)	2 (2%)	7	14
44	2m	120/126 (95%)	97 (81%)	19 (16%)	4 (3%)	3	5
45	1n	58/61 (95%)	54 (93%)	4 (7%)	0	100	100
45	2n	58/61 (95%)	51 (88%)	6 (10%)	1 (2%)	7	14
46	1o	86/89 (97%)	80 (93%)	5 (6%)	1 (1%)	10	20
46	2o	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
47	1p	80/88 (91%)	72 (90%)	6 (8%)	2 (2%)	4	8
47	2p	80/88 (91%)	72 (90%)	8 (10%)	0	100	100
48	1q	97/105 (92%)	86 (89%)	11 (11%)	0	100	100
48	2q	97/105 (92%)	92 (95%)	4 (4%)	1 (1%)	12	24
49	1r	66/88 (75%)	61 (92%)	5 (8%)	0	100	100
49	2r	66/88 (75%)	56 (85%)	9 (14%)	1 (2%)	8	15
50	1s	81/93 (87%)	70 (86%)	10 (12%)	1 (1%)	10	20
50	2s	81/93 (87%)	58 (72%)	23 (28%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	1t	94/106 (89%)	85 (90%)	5 (5%)	4 (4%)	2	3
51	2t	94/106 (89%)	85 (90%)	5 (5%)	4 (4%)	2	3
52	1u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
52	2u	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
All	All	11368/12128 (94%)	10346 (91%)	901 (8%)	121 (1%)	11	22

All (121) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
21	1Z	53	ILE
26	14	49	PHE
26	14	62	ARG
33	1b	125	PRO
33	1b	126	GLU
40	1i	54	ASP
44	1m	67	GLU
44	1m	106	ASN
5	2F	130	ALA
8	2I	10	GLU
11	2P	36	LYS
17	2V	79	VAL
33	2b	17	PHE
38	2g	55	GLY
38	2g	80	VAL
44	2m	67	GLU
48	2q	68	ARG
6	1G	43	LEU
6	1G	47	LYS
15	1T	37	GLY
19	1X	93	GLU
20	1Y	54	LYS
23	1I	3	LYS
26	14	47	GLN
34	1c	66	VAL
36	1e	85	GLY
41	1j	30	SER
41	1j	75	ILE
42	1k	77	MET
6	2G	42	GLY
6	2G	47	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	2G	51	ARG
6	2G	84	LYS
8	2I	40	THR
10	2O	5	GLN
12	2Q	24	GLY
14	2S	96	GLY
21	2Z	52	SER
21	2Z	144	LEU
21	2Z	163	LEU
34	2c	91	LEU
34	2c	95	THR
36	2e	85	GLY
39	2h	68	ARG
41	2j	75	ILE
41	2j	79	ARG
24	12	69	ARG
26	14	45	GLY
35	1d	179	GLU
41	1j	77	PRO
41	1j	79	ARG
47	1p	76	GLN
51	1t	102	GLY
4	2E	52	LEU
5	2F	166	ALA
6	2G	43	LEU
14	2S	84	GLN
23	2I	3	LYS
33	2b	20	GLU
34	2c	100	ALA
34	2c	181	ASN
41	2j	56	HIS
42	2k	106	LYS
44	2m	23	TYR
49	2r	36	ASN
51	2t	95	ALA
4	1E	52	LEU
8	1I	104	GLN
26	14	18	CYS
34	1c	107	GLN
51	1t	95	ALA
5	2F	18	ARG
7	2H	126	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	2N	2	LYS
11	2P	45	LEU
13	2R	2	ARG
14	2S	20	ARG
21	2Z	157	LEU
26	24	46	GLN
42	2k	49	GLY
45	2n	27	CYS
11	1P	29	LYS
17	1V	79	VAL
19	1X	2	LYS
33	1b	8	LYS
33	1b	124	SER
33	1b	231	GLU
41	1j	78	ASN
47	1p	75	ARG
51	1t	47	GLY
51	1t	100	ILE
4	2E	113	PHE
15	2T	55	ASN
21	2Z	146	ILE
26	24	11	PRO
26	24	47	GLN
26	24	49	PHE
36	2e	77	PRO
44	2m	21	TYR
51	2t	10	LEU
51	2t	47	GLY
11	1P	93	GLY
33	1b	165	VAL
36	1e	70	PRO
26	24	50	VAL
36	2e	63	ARG
51	2t	102	GLY
36	2e	69	VAL
7	1H	55	PRO
20	1Y	103	GLY
11	2P	44	GLY
42	1k	105	VAL
44	2m	7	VAL
46	1o	87	ILE
14	2S	35	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	2e	96	PRO
41	2j	41	PRO
50	1s	72	GLY
36	2e	22	GLY
17	2V	50	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	215/218 (99%)	204 (95%)	11 (5%)	21	40
3	2D	215/218 (99%)	204 (95%)	11 (5%)	21	40
4	1E	164/166 (99%)	155 (94%)	9 (6%)	19	37
4	2E	164/166 (99%)	156 (95%)	8 (5%)	22	43
5	1F	160/166 (96%)	141 (88%)	19 (12%)	5	8
5	2F	159/166 (96%)	142 (89%)	17 (11%)	6	12
6	1G	143/156 (92%)	134 (94%)	9 (6%)	16	30
6	2G	143/156 (92%)	117 (82%)	26 (18%)	2	3
7	1H	144/148 (97%)	131 (91%)	13 (9%)	9	17
7	2H	144/148 (97%)	128 (89%)	16 (11%)	6	11
8	1I	113/124 (91%)	95 (84%)	18 (16%)	2	4
8	2I	105/124 (85%)	88 (84%)	17 (16%)	2	3
9	1N	118/119 (99%)	109 (92%)	9 (8%)	12	23
9	2N	118/119 (99%)	106 (90%)	12 (10%)	7	14
10	1O	100/100 (100%)	96 (96%)	4 (4%)	28	50
10	2O	100/100 (100%)	95 (95%)	5 (5%)	22	42
11	1P	115/116 (99%)	104 (90%)	11 (10%)	8	15
11	2P	115/116 (99%)	106 (92%)	9 (8%)	11	21
12	1Q	111/111 (100%)	106 (96%)	5 (4%)	24	46
12	2Q	111/111 (100%)	100 (90%)	11 (10%)	7	15

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	1R	101/101 (100%)	95 (94%)	6 (6%)	18	33
13	2R	101/101 (100%)	97 (96%)	4 (4%)	28	50
14	1S	86/88 (98%)	82 (95%)	4 (5%)	23	45
14	2S	85/88 (97%)	72 (85%)	13 (15%)	3	4
15	1T	115/127 (91%)	109 (95%)	6 (5%)	21	39
15	2T	113/127 (89%)	105 (93%)	8 (7%)	13	25
16	1U	93/94 (99%)	86 (92%)	7 (8%)	12	24
16	2U	93/94 (99%)	91 (98%)	2 (2%)	45	67
17	1V	80/82 (98%)	76 (95%)	4 (5%)	22	42
17	2V	80/82 (98%)	72 (90%)	8 (10%)	7	14
18	1W	90/92 (98%)	83 (92%)	7 (8%)	11	21
18	2W	90/92 (98%)	86 (96%)	4 (4%)	25	47
19	1X	77/78 (99%)	74 (96%)	3 (4%)	28	51
19	2X	77/78 (99%)	74 (96%)	3 (4%)	28	51
20	1Y	85/91 (93%)	73 (86%)	12 (14%)	3	6
20	2Y	85/91 (93%)	73 (86%)	12 (14%)	3	6
21	1Z	135/179 (75%)	116 (86%)	19 (14%)	3	6
21	2Z	137/179 (76%)	121 (88%)	16 (12%)	5	9
22	10	65/67 (97%)	64 (98%)	1 (2%)	57	74
22	20	65/67 (97%)	64 (98%)	1 (2%)	57	74
23	11	80/83 (96%)	74 (92%)	6 (8%)	12	24
23	21	80/83 (96%)	77 (96%)	3 (4%)	29	52
24	12	65/67 (97%)	59 (91%)	6 (9%)	8	17
24	22	65/67 (97%)	61 (94%)	4 (6%)	16	31
25	13	51/52 (98%)	44 (86%)	7 (14%)	3	6
25	23	50/52 (96%)	47 (94%)	3 (6%)	17	32
26	14	59/63 (94%)	48 (81%)	11 (19%)	1	3
26	24	53/63 (84%)	45 (85%)	8 (15%)	3	4
27	15	50/52 (96%)	46 (92%)	4 (8%)	11	20
27	25	50/52 (96%)	46 (92%)	4 (8%)	11	20
28	16	51/52 (98%)	46 (90%)	5 (10%)	7	15

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	26	50/52 (96%)	43 (86%)	7 (14%)	3	6
29	17	41/42 (98%)	39 (95%)	2 (5%)	22	43
29	27	41/42 (98%)	37 (90%)	4 (10%)	7	15
30	18	54/55 (98%)	53 (98%)	1 (2%)	50	70
30	28	54/55 (98%)	52 (96%)	2 (4%)	30	54
31	19	34/34 (100%)	34 (100%)	0	100	100
31	29	34/34 (100%)	33 (97%)	1 (3%)	37	61
33	1b	192/220 (87%)	167 (87%)	25 (13%)	4	7
33	2b	187/220 (85%)	151 (81%)	36 (19%)	1	2
34	1c	142/188 (76%)	124 (87%)	18 (13%)	4	8
34	2c	140/188 (74%)	119 (85%)	21 (15%)	3	5
35	1d	169/181 (93%)	159 (94%)	10 (6%)	18	33
35	2d	173/181 (96%)	153 (88%)	20 (12%)	5	10
36	1e	113/123 (92%)	101 (89%)	12 (11%)	6	13
36	2e	114/123 (93%)	95 (83%)	19 (17%)	2	3
37	1f	84/90 (93%)	78 (93%)	6 (7%)	13	25
37	2f	85/90 (94%)	79 (93%)	6 (7%)	13	25
38	1g	119/127 (94%)	110 (92%)	9 (8%)	12	23
38	2g	120/127 (94%)	109 (91%)	11 (9%)	8	17
39	1h	114/119 (96%)	111 (97%)	3 (3%)	40	63
39	2h	114/119 (96%)	107 (94%)	7 (6%)	17	31
40	1i	90/99 (91%)	81 (90%)	9 (10%)	7	14
40	2i	89/99 (90%)	80 (90%)	9 (10%)	7	14
41	1j	66/92 (72%)	58 (88%)	8 (12%)	5	8
41	2j	69/92 (75%)	54 (78%)	15 (22%)	1	1
42	1k	82/99 (83%)	74 (90%)	8 (10%)	7	15
42	2k	83/99 (84%)	73 (88%)	10 (12%)	5	8
43	1l	96/108 (89%)	89 (93%)	7 (7%)	13	24
43	2l	96/108 (89%)	87 (91%)	9 (9%)	8	16
44	1m	93/101 (92%)	82 (88%)	11 (12%)	5	9
44	2m	92/101 (91%)	77 (84%)	15 (16%)	2	3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	1n	49/50 (98%)	47 (96%)	2 (4%)	27	49
45	2n	49/50 (98%)	45 (92%)	4 (8%)	10	20
46	1o	78/80 (98%)	72 (92%)	6 (8%)	12	22
46	2o	78/80 (98%)	71 (91%)	7 (9%)	9	17
47	1p	69/74 (93%)	59 (86%)	10 (14%)	3	5
47	2p	68/74 (92%)	60 (88%)	8 (12%)	5	9
48	1q	94/97 (97%)	87 (93%)	7 (7%)	13	24
48	2q	94/97 (97%)	86 (92%)	8 (8%)	10	18
49	1r	59/77 (77%)	56 (95%)	3 (5%)	21	40
49	2r	59/77 (77%)	51 (86%)	8 (14%)	3	6
50	1s	69/80 (86%)	65 (94%)	4 (6%)	18	34
50	2s	67/80 (84%)	57 (85%)	10 (15%)	3	5
51	1t	70/82 (85%)	64 (91%)	6 (9%)	10	18
51	2t	70/82 (85%)	66 (94%)	4 (6%)	18	35
52	1u	18/22 (82%)	18 (100%)	0	100	100
52	2u	18/22 (82%)	16 (89%)	2 (11%)	6	11
All	All	9303/10064 (92%)	8452 (91%)	851 (9%)	9	17

All (851) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	3	VAL
3	1D	12	SER
3	1D	39	LYS
3	1D	113	VAL
3	1D	115	GLN
3	1D	136	ILE
3	1D	141	VAL
3	1D	162	SER
3	1D	229	VAL
3	1D	242	ARG
3	1D	273	ARG
4	1E	7	VAL
4	1E	47	VAL
4	1E	59	VAL
4	1E	73	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	1E	75	VAL
4	1E	89	ASP
4	1E	90	THR
4	1E	116	VAL
4	1E	184	VAL
5	1F	24	LEU
5	1F	33	LEU
5	1F	53	THR
5	1F	57	VAL
5	1F	74	ARG
5	1F	78	ILE
5	1F	88	VAL
5	1F	104	LYS
5	1F	106	ARG
5	1F	112	MET
5	1F	127	GLU
5	1F	132	VAL
5	1F	140	LEU
5	1F	162	LEU
5	1F	168	ARG
5	1F	175	THR
5	1F	183	VAL
5	1F	192	LEU
5	1F	205	ARG
6	1G	3	LEU
6	1G	5	VAL
6	1G	31	VAL
6	1G	43	LEU
6	1G	82	LEU
6	1G	133	LEU
6	1G	140	ILE
6	1G	148	MET
6	1G	149	VAL
7	1H	3	ARG
7	1H	15	VAL
7	1H	24	VAL
7	1H	33	LEU
7	1H	45	VAL
7	1H	49	VAL
7	1H	56	SER
7	1H	76	VAL
7	1H	84	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	1H	98	LEU
7	1H	116	GLU
7	1H	119	GLU
7	1H	127	GLU
8	1I	5	LEU
8	1I	9	LEU
8	1I	10	GLU
8	1I	12	LEU
8	1I	15	VAL
8	1I	38	LEU
8	1I	40	THR
8	1I	41	GLU
8	1I	47	LEU
8	1I	61	ARG
8	1I	62	LYS
8	1I	76	THR
8	1I	87	LYS
8	1I	92	VAL
8	1I	108	THR
8	1I	133	HIS
8	1I	140	LEU
8	1I	142	VAL
9	1N	1	MET
9	1N	9	VAL
9	1N	10	GLU
9	1N	28	THR
9	1N	48	MET
9	1N	68	GLU
9	1N	104	LYS
9	1N	112	LEU
9	1N	138	LEU
10	1O	28	SER
10	1O	77	ILE
10	1O	80	ASP
10	1O	89	ASN
11	1P	1	MET
11	1P	4	SER
11	1P	7	ARG
11	1P	42	SER
11	1P	45	LEU
11	1P	95	VAL
11	1P	126	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	1P	138	LEU
11	1P	147	LEU
11	1P	148	LEU
11	1P	149	GLU
12	1Q	1	MET
12	1Q	7	MET
12	1Q	56	ARG
12	1Q	75	THR
12	1Q	109	VAL
13	1R	6	SER
13	1R	36	THR
13	1R	67	LEU
13	1R	100	LEU
13	1R	102	GLU
13	1R	114	VAL
14	1S	36	TYR
14	1S	49	VAL
14	1S	69	VAL
14	1S	110	LEU
15	1T	28	VAL
15	1T	36	GLU
15	1T	49	VAL
15	1T	70	VAL
15	1T	96	ARG
15	1T	128	GLU
16	1U	31	SER
16	1U	74	LEU
16	1U	77	SER
16	1U	78	THR
16	1U	83	LEU
16	1U	95	LEU
16	1U	100	VAL
17	1V	7	THR
17	1V	73	SER
17	1V	79	VAL
17	1V	85	LYS
18	1W	4	LYS
18	1W	6	ILE
18	1W	11	ARG
18	1W	15	ARG
18	1W	17	VAL
18	1W	19	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	1W	63	ASP
19	1X	2	LYS
19	1X	35	THR
19	1X	81	VAL
20	1Y	1	MET
20	1Y	7	VAL
20	1Y	24	VAL
20	1Y	43	ASN
20	1Y	61	ILE
20	1Y	64	GLU
20	1Y	67	LEU
20	1Y	70	SER
20	1Y	72	VAL
20	1Y	91	GLU
20	1Y	99	CYS
20	1Y	106	LEU
21	1Z	1	MET
21	1Z	28	MET
21	1Z	33	LEU
21	1Z	37	VAL
21	1Z	39	VAL
21	1Z	53	ILE
21	1Z	61	LEU
21	1Z	70	LEU
21	1Z	84	GLU
21	1Z	86	VAL
21	1Z	129	SER
21	1Z	138	GLU
21	1Z	139	VAL
21	1Z	150	LEU
21	1Z	154	ASP
21	1Z	161	VAL
21	1Z	163	LEU
21	1Z	170	THR
21	1Z	171	ILE
22	10	49	LYS
23	11	30	VAL
23	11	35	THR
23	11	38	SER
23	11	80	LEU
23	11	83	GLU
23	11	92	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	12	3	LEU
24	12	19	VAL
24	12	28	LYS
24	12	50	ILE
24	12	59	ARG
24	12	68	ARG
25	13	6	VAL
25	13	29	ARG
25	13	35	ARG
25	13	54	VAL
25	13	55	ARG
25	13	58	VAL
25	13	60	GLU
26	14	1	MET
26	14	14	ILE
26	14	27	THR
26	14	49	PHE
26	14	50	VAL
26	14	52	THR
26	14	53	GLU
26	14	60	GLN
26	14	63	TYR
26	14	67	TYR
26	14	69	LYS
27	15	6	VAL
27	15	26	THR
27	15	40	LYS
27	15	60	VAL
28	16	4	GLU
28	16	5	VAL
28	16	9	LEU
28	16	19	ARG
28	16	44	ARG
29	17	1	MET
29	17	43	THR
30	18	14	VAL
33	1b	11	LEU
33	1b	12	GLU
33	1b	21	ARG
33	1b	35	GLU
33	1b	39	ILE
33	1b	41	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	1b	44	LEU
33	1b	54	THR
33	1b	83	MET
33	1b	93	VAL
33	1b	128	GLU
33	1b	130	ARG
33	1b	133	LYS
33	1b	154	LEU
33	1b	160	ASP
33	1b	172	ILE
33	1b	185	ILE
33	1b	187	LEU
33	1b	196	LEU
33	1b	200	ILE
33	1b	208	ILE
33	1b	215	LEU
33	1b	221	LEU
33	1b	223	ILE
33	1b	231	GLU
34	1c	3	ASN
34	1c	8	ILE
34	1c	20	SER
34	1c	26	LYS
34	1c	28	GLN
34	1c	43	LEU
34	1c	66	VAL
34	1c	70	VAL
34	1c	77	ILE
34	1c	89	GLU
34	1c	91	LEU
34	1c	144	SER
34	1c	178	LEU
34	1c	191	THR
34	1c	192	THR
34	1c	195	VAL
34	1c	198	VAL
34	1c	207	VAL
35	1d	19	LEU
35	1d	104	VAL
35	1d	135	LEU
35	1d	140	VAL
35	1d	157	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	1d	158	ILE
35	1d	177	ASP
35	1d	178	VAL
35	1d	184	LYS
35	1d	194	LEU
36	1e	13	ILE
36	1e	16	THR
36	1e	19	MET
36	1e	24	ARG
36	1e	41	VAL
36	1e	51	VAL
36	1e	53	LEU
36	1e	82	VAL
36	1e	112	LEU
36	1e	131	ILE
36	1e	147	ASP
36	1e	151	LEU
37	1f	17	SER
37	1f	19	LEU
37	1f	36	ARG
37	1f	55	ASP
37	1f	75	LEU
37	1f	98	LEU
38	1g	6	ARG
38	1g	10	ARG
38	1g	12	LEU
38	1g	24	THR
38	1g	50	ILE
38	1g	61	VAL
38	1g	78	ARG
38	1g	90	GLU
38	1g	104	LEU
39	1h	39	LEU
39	1h	52	ASP
39	1h	122	ARG
40	1i	14	VAL
40	1i	17	VAL
40	1i	23	ASN
40	1i	41	VAL
40	1i	42	ARG
40	1i	56	LEU
40	1i	83	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	1i	108	VAL
40	1i	128	ARG
41	1j	8	LEU
41	1j	19	SER
41	1j	38	ILE
41	1j	66	ARG
41	1j	67	THR
41	1j	81	THR
41	1j	92	THR
41	1j	95	GLU
42	1k	31	THR
42	1k	33	THR
42	1k	48	ILE
42	1k	84	VAL
42	1k	87	THR
42	1k	109	VAL
42	1k	112	THR
42	1k	114	VAL
43	1l	18	VAL
43	1l	33	ARG
43	1l	54	LYS
43	1l	58	VAL
43	1l	59	ARG
43	1l	70	ILE
43	1l	123	LYS
44	1m	4	ILE
44	1m	14	ARG
44	1m	43	THR
44	1m	49	THR
44	1m	53	VAL
44	1m	70	LEU
44	1m	78	ILE
44	1m	98	VAL
44	1m	105	THR
44	1m	106	ASN
44	1m	121	LYS
45	1n	18	VAL
45	1n	33	VAL
46	1o	27	VAL
46	1o	39	LEU
46	1o	70	LEU
46	1o	76	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
46	1o	83	GLU
46	1o	87	ILE
47	1p	20	VAL
47	1p	21	VAL
47	1p	22	THR
47	1p	27	LYS
47	1p	43	LYS
47	1p	45	THR
47	1p	60	LEU
47	1p	61	SER
47	1p	72	ARG
47	1p	76	GLN
48	1q	9	VAL
48	1q	19	VAL
48	1q	60	ILE
48	1q	63	ARG
48	1q	65	ILE
48	1q	85	VAL
48	1q	86	GLU
49	1r	46	GLU
49	1r	61	LYS
49	1r	63	GLN
50	1s	5	LEU
50	1s	35	SER
50	1s	48	THR
50	1s	79	THR
51	1t	10	LEU
51	1t	24	LEU
51	1t	30	LYS
51	1t	38	LYS
51	1t	89	ARG
51	1t	100	ILE
3	2D	3	VAL
3	2D	12	SER
3	2D	37	LEU
3	2D	113	VAL
3	2D	116	GLN
3	2D	141	VAL
3	2D	145	VAL
3	2D	162	SER
3	2D	229	VAL
3	2D	253	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	2D	259	THR
4	2E	38	THR
4	2E	59	VAL
4	2E	73	GLU
4	2E	90	THR
4	2E	116	VAL
4	2E	134	ILE
4	2E	175	VAL
4	2E	184	VAL
5	2F	20	LEU
5	2F	33	LEU
5	2F	50	SER
5	2F	53	THR
5	2F	60	SER
5	2F	70	THR
5	2F	74	ARG
5	2F	108	LYS
5	2F	125	LEU
5	2F	126	VAL
5	2F	153	SER
5	2F	157	VAL
5	2F	158	THR
5	2F	160	ASN
5	2F	175	THR
5	2F	192	LEU
5	2F	197	ASP
6	2G	5	VAL
6	2G	7	LEU
6	2G	18	GLU
6	2G	28	VAL
6	2G	31	VAL
6	2G	33	ARG
6	2G	38	VAL
6	2G	41	GLN
6	2G	43	LEU
6	2G	45	GLU
6	2G	53	LEU
6	2G	60	LEU
6	2G	75	LYS
6	2G	79	ASN
6	2G	88	ILE
6	2G	90	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	2G	91	ARG
6	2G	92	VAL
6	2G	111	LEU
6	2G	130	ASN
6	2G	140	ILE
6	2G	148	MET
6	2G	152	LEU
6	2G	155	MET
6	2G	159	VAL
6	2G	162	THR
7	2H	3	ARG
7	2H	15	VAL
7	2H	23	ARG
7	2H	45	VAL
7	2H	52	VAL
7	2H	68	THR
7	2H	71	LEU
7	2H	81	GLU
7	2H	84	SER
7	2H	92	ILE
7	2H	104	GLU
7	2H	111	HIS
7	2H	119	GLU
7	2H	122	THR
7	2H	129	THR
7	2H	153	LYS
8	2I	15	VAL
8	2I	38	LEU
8	2I	44	LEU
8	2I	47	LEU
8	2I	58	LEU
8	2I	66	GLU
8	2I	69	LYS
8	2I	77	LEU
8	2I	82	ARG
8	2I	85	GLU
8	2I	86	THR
8	2I	102	SER
8	2I	117	GLU
8	2I	127	VAL
8	2I	133	HIS
8	2I	139	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	2I	144	VAL
9	2N	1	MET
9	2N	15	LEU
9	2N	23	LEU
9	2N	28	THR
9	2N	38	HIS
9	2N	43	THR
9	2N	46	VAL
9	2N	58	ASP
9	2N	60	ILE
9	2N	68	GLU
9	2N	120	LEU
9	2N	138	LEU
10	2O	38	VAL
10	2O	52	VAL
10	2O	66	LYS
10	2O	69	ILE
10	2O	108	GLU
11	2P	3	LEU
11	2P	7	ARG
11	2P	45	LEU
11	2P	56	SER
11	2P	70	GLN
11	2P	95	VAL
11	2P	99	LEU
11	2P	135	LEU
11	2P	149	GLU
12	2Q	1	MET
12	2Q	5	ARG
12	2Q	7	MET
12	2Q	10	ARG
12	2Q	12	GLN
12	2Q	22	LYS
12	2Q	75	THR
12	2Q	109	VAL
12	2Q	110	THR
12	2Q	127	ILE
12	2Q	133	ARG
13	2R	6	SER
13	2R	24	GLN
13	2R	100	LEU
13	2R	114	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	2S	12	PHE
14	2S	20	ARG
14	2S	21	THR
14	2S	36	TYR
14	2S	44	LYS
14	2S	49	VAL
14	2S	53	SER
14	2S	58	LEU
14	2S	71	ARG
14	2S	98	VAL
14	2S	101	LEU
14	2S	107	GLU
14	2S	110	LEU
15	2T	15	VAL
15	2T	17	THR
15	2T	31	SER
15	2T	63	VAL
15	2T	72	VAL
15	2T	83	ILE
15	2T	89	VAL
15	2T	96	ARG
16	2U	5	LYS
16	2U	95	LEU
17	2V	1	MET
17	2V	7	THR
17	2V	33	VAL
17	2V	51	VAL
17	2V	52	VAL
17	2V	53	GLU
17	2V	79	VAL
17	2V	98	GLU
18	2W	11	ARG
18	2W	17	VAL
18	2W	67	ASP
18	2W	85	VAL
19	2X	2	LYS
19	2X	35	THR
19	2X	81	VAL
20	2Y	1	MET
20	2Y	14	LEU
20	2Y	38	ILE
20	2Y	39	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	2Y	42	VAL
20	2Y	49	VAL
20	2Y	61	ILE
20	2Y	70	SER
20	2Y	72	VAL
20	2Y	85	VAL
20	2Y	99	CYS
20	2Y	107	ASP
21	2Z	5	LEU
21	2Z	11	GLU
21	2Z	33	LEU
21	2Z	42	VAL
21	2Z	57	ILE
21	2Z	71	VAL
21	2Z	76	LEU
21	2Z	126	VAL
21	2Z	129	SER
21	2Z	133	ILE
21	2Z	144	LEU
21	2Z	145	GLU
21	2Z	150	LEU
21	2Z	154	ASP
21	2Z	161	VAL
21	2Z	171	ILE
22	20	68	GLU
23	21	26	ARG
23	21	35	THR
23	21	98	LEU
24	22	5	GLU
24	22	19	VAL
24	22	35	LEU
24	22	70	GLN
25	23	6	VAL
25	23	9	VAL
25	23	31	LEU
26	24	9	LEU
26	24	24	THR
26	24	27	THR
26	24	33	VAL
26	24	34	GLU
26	24	49	PHE
26	24	58	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	24	63	TYR
27	25	6	VAL
27	25	33	CYS
27	25	40	LYS
27	25	59	GLU
28	26	9	LEU
28	26	19	ARG
28	26	20	ASN
28	26	23	THR
28	26	34	LEU
28	26	50	ARG
28	26	52	VAL
29	27	1	MET
29	27	4	THR
29	27	43	THR
29	27	47	ARG
30	28	19	SER
30	28	41	ILE
31	29	28	GLU
33	2b	8	LYS
33	2b	11	LEU
33	2b	16	HIS
33	2b	23	ARG
33	2b	44	LEU
33	2b	45	GLN
33	2b	47	THR
33	2b	56	ARG
33	2b	58	ILE
33	2b	61	LEU
33	2b	68	ILE
33	2b	71	VAL
33	2b	76	GLN
33	2b	81	VAL
33	2b	83	MET
33	2b	93	VAL
33	2b	101	MET
33	2b	107	THR
33	2b	109	SER
33	2b	115	LEU
33	2b	118	LEU
33	2b	127	ILE
33	2b	140	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	2b	141	GLU
33	2b	149	LEU
33	2b	160	ASP
33	2b	164	VAL
33	2b	172	ILE
33	2b	175	ARG
33	2b	180	LEU
33	2b	189	ASP
33	2b	201	ILE
33	2b	208	ILE
33	2b	223	ILE
33	2b	229	VAL
33	2b	230	VAL
34	2c	28	GLN
34	2c	46	GLU
34	2c	47	LEU
34	2c	49	SER
34	2c	55	VAL
34	2c	56	ASP
34	2c	58	GLU
34	2c	68	VAL
34	2c	69	HIS
34	2c	77	ILE
34	2c	111	LEU
34	2c	128	PHE
34	2c	140	ARG
34	2c	142	MET
34	2c	152	ILE
34	2c	178	LEU
34	2c	182	ILE
34	2c	190	ARG
34	2c	191	THR
34	2c	192	THR
34	2c	193	TYR
35	2d	8	VAL
35	2d	12	CYS
35	2d	17	VAL
35	2d	34	GLU
35	2d	47	ARG
35	2d	50	ARG
35	2d	59	ARG
35	2d	71	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	2d	83	SER
35	2d	94	LEU
35	2d	96	LEU
35	2d	127	THR
35	2d	135	LEU
35	2d	148	VAL
35	2d	150	GLU
35	2d	155	LEU
35	2d	157	LEU
35	2d	158	ILE
35	2d	168	ARG
35	2d	201	GLN
36	2e	13	ILE
36	2e	18	ARG
36	2e	25	ARG
36	2e	38	GLN
36	2e	41	VAL
36	2e	47	LYS
36	2e	50	GLU
36	2e	51	VAL
36	2e	55	VAL
36	2e	72	GLN
36	2e	79	GLU
36	2e	81	GLU
36	2e	90	VAL
36	2e	100	VAL
36	2e	115	VAL
36	2e	136	MET
36	2e	141	GLN
36	2e	144	THR
36	2e	149	GLU
37	2f	21	LEU
37	2f	36	ARG
37	2f	45	LEU
37	2f	69	GLU
37	2f	75	LEU
37	2f	81	ILE
38	2g	9	VAL
38	2g	51	GLN
38	2g	57	GLU
38	2g	75	VAL
38	2g	78	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	2g	79	ARG
38	2g	85	TYR
38	2g	90	GLU
38	2g	106	GLN
38	2g	135	VAL
38	2g	155	ARG
39	2h	3	THR
39	2h	23	SER
39	2h	51	VAL
39	2h	52	ASP
39	2h	54	ASP
39	2h	107	LEU
39	2h	112	LEU
40	2i	41	VAL
40	2i	50	LEU
40	2i	64	THR
40	2i	65	VAL
40	2i	74	ILE
40	2i	89	ASN
40	2i	102	LEU
40	2i	108	VAL
40	2i	120	ARG
41	2j	8	LEU
41	2j	9	ARG
41	2j	29	ARG
41	2j	30	SER
41	2j	34	VAL
41	2j	38	ILE
41	2j	67	THR
41	2j	68	HIS
41	2j	72	VAL
41	2j	74	ILE
41	2j	81	THR
41	2j	89	ASP
41	2j	95	GLU
41	2j	97	GLU
41	2j	98	ILE
42	2k	14	VAL
42	2k	24	SER
42	2k	30	VAL
42	2k	33	THR
42	2k	48	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
42	2k	81	ASP
42	2k	96	ARG
42	2k	112	THR
42	2k	114	VAL
42	2k	117	ASN
43	2l	18	VAL
43	2l	36	VAL
43	2l	38	THR
43	2l	39	VAL
43	2l	40	VAL
43	2l	59	ARG
43	2l	97	ARG
43	2l	100	ILE
43	2l	123	LYS
44	2m	4	ILE
44	2m	22	ILE
44	2m	27	LYS
44	2m	32	GLU
44	2m	34	LEU
44	2m	35	GLU
44	2m	37	THR
44	2m	50	GLU
44	2m	60	VAL
44	2m	82	MET
44	2m	90	LEU
44	2m	91	ARG
44	2m	103	THR
44	2m	106	ASN
44	2m	110	ARG
45	2n	13	THR
45	2n	18	VAL
45	2n	31	ARG
45	2n	33	VAL
46	2o	7	GLU
46	2o	38	ARG
46	2o	39	LEU
46	2o	54	ARG
46	2o	83	GLU
46	2o	84	LYS
46	2o	87	ILE
47	2p	2	VAL
47	2p	20	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
47	2p	21	VAL
47	2p	45	THR
47	2p	53	VAL
47	2p	54	GLU
47	2p	67	THR
47	2p	69	THR
48	2q	5	VAL
48	2q	9	VAL
48	2q	19	VAL
48	2q	56	VAL
48	2q	60	ILE
48	2q	63	ARG
48	2q	85	VAL
48	2q	99	SER
49	2r	21	LYS
49	2r	31	LEU
49	2r	37	VAL
49	2r	53	ARG
49	2r	54	ARG
49	2r	84	LYS
49	2r	86	VAL
49	2r	87	ARG
50	2s	7	LYS
50	2s	15	LEU
50	2s	20	LEU
50	2s	31	ILE
50	2s	37	ARG
50	2s	41	VAL
50	2s	45	VAL
50	2s	49	ILE
50	2s	65	ASN
50	2s	81	ARG
51	2t	71	THR
51	2t	86	ARG
51	2t	90	GLN
51	2t	93	GLU
52	2u	13	ILE
52	2u	15	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (164) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	87	ASN
3	1D	116	GLN
4	1E	48	GLN
5	1F	69	HIS
5	1F	160	ASN
5	1F	203	GLN
6	1G	26	GLN
9	1N	94	HIS
10	1O	3	GLN
10	1O	89	ASN
12	1Q	123	HIS
13	1R	71	GLN
13	1R	91	GLN
14	1S	68	GLN
15	1T	58	ASN
15	1T	90	GLN
16	1U	72	HIS
16	1U	81	HIS
16	1U	94	ASN
19	1X	31	HIS
19	1X	82	GLN
20	1Y	6	HIS
20	1Y	43	ASN
21	1Z	34	ASN
21	1Z	54	HIS
21	1Z	65	GLN
21	1Z	73	GLN
21	1Z	132	ASN
21	1Z	151	HIS
23	11	56	GLN
25	13	32	GLN
26	14	47	GLN
31	19	20	HIS
33	1b	40	HIS
33	1b	113	HIS
33	1b	135	GLN
33	1b	146	GLN
33	1b	212	GLN
34	1c	6	HIS
34	1c	37	GLN
34	1c	69	HIS
34	1c	98	ASN
34	1c	118	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	1c	162	GLN
35	1d	43	HIS
35	1d	77	ASN
35	1d	116	GLN
35	1d	119	GLN
35	1d	123	HIS
36	1e	78	HIS
37	1f	73	ASN
37	1f	100	ASN
38	1g	13	GLN
38	1g	28	ASN
38	1g	148	ASN
38	1g	153	HIS
40	1i	31	GLN
40	1i	34	ASN
40	1i	38	GLN
40	1i	58	HIS
40	1i	124	GLN
41	1j	56	HIS
43	1l	80	HIS
43	1l	99	HIS
44	1m	40	ASN
44	1m	77	ASN
44	1m	92	HIS
46	1o	13	GLN
47	1p	13	HIS
47	1p	14	ASN
47	1p	76	GLN
48	1q	26	GLN
49	1r	63	GLN
50	1s	23	ASN
50	1s	47	HIS
50	1s	56	GLN
50	1s	83	HIS
51	1t	26	ASN
51	1t	73	HIS
51	1t	90	GLN
3	2D	115	GLN
3	2D	166	GLN
4	2E	48	GLN
5	2F	40	GLN
5	2F	69	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	2F	160	ASN
5	2F	204	ASN
6	2G	108	ASN
6	2G	130	ASN
6	2G	132	ASN
7	2H	111	HIS
8	2I	133	HIS
9	2N	101	HIS
9	2N	131	GLN
11	2P	70	GLN
12	2Q	12	GLN
12	2Q	113	GLN
12	2Q	123	HIS
13	2R	13	HIS
13	2R	71	GLN
14	2S	38	GLN
14	2S	68	GLN
15	2T	58	ASN
15	2T	123	GLN
16	2U	94	ASN
18	2W	60	ASN
21	2Z	32	HIS
21	2Z	55	HIS
21	2Z	73	GLN
21	2Z	151	HIS
22	20	12	ASN
22	20	35	ASN
22	20	70	GLN
23	21	56	GLN
24	22	70	GLN
26	24	40	HIS
26	24	46	GLN
26	24	60	GLN
30	28	35	GLN
33	2b	40	HIS
33	2b	135	GLN
34	2c	98	ASN
34	2c	102	ASN
34	2c	108	ASN
34	2c	162	GLN
35	2d	42	GLN
35	2d	77	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	2d	116	GLN
35	2d	119	GLN
35	2d	125	HIS
35	2d	201	GLN
36	2e	20	GLN
36	2e	38	GLN
36	2e	65	ASN
36	2e	72	GLN
37	2f	73	ASN
37	2f	94	GLN
37	2f	100	ASN
38	2g	11	GLN
38	2g	28	ASN
38	2g	37	ASN
38	2g	68	ASN
38	2g	148	ASN
39	2h	82	HIS
40	2i	3	GLN
40	2i	34	ASN
40	2i	58	HIS
40	2i	89	ASN
41	2j	62	HIS
42	2k	38	ASN
42	2k	104	GLN
42	2k	117	ASN
43	2l	80	HIS
43	2l	99	HIS
44	2m	77	ASN
46	2o	9	GLN
46	2o	13	GLN
47	2p	13	HIS
48	2q	94	ASN
49	2r	63	GLN
50	2s	56	GLN
50	2s	69	HIS
51	2t	16	HIS
51	2t	90	GLN

5.3.3 RNA ⓘ

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	447 (15%)	29 (1%)
1	2A	2791/2915 (95%)	469 (16%)	19 (0%)
2	1B	119/121 (98%)	7 (5%)	0
2	2B	118/121 (97%)	34 (28%)	0
32	1a	1497/1521 (98%)	251 (16%)	0
32	2a	1501/1521 (98%)	309 (20%)	0
53	1v	12/24 (50%)	1 (8%)	0
53	2v	12/24 (50%)	3 (25%)	0
54	1w	72/76 (94%)	24 (33%)	0
54	1y	72/76 (94%)	30 (41%)	0
54	2w	69/76 (90%)	25 (36%)	0
54	2y	71/76 (93%)	26 (36%)	0
55	1x	75/77 (97%)	13 (17%)	0
55	2x	75/77 (97%)	12 (16%)	0
All	All	9348/9620 (97%)	1651 (17%)	48 (0%)

All (1651) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	10	G
1	1A	12	U
1	1A	34	C
1	1A	36	G
1	1A	45	C
1	1A	55	G
1	1A	71	A
1	1A	74	A
1	1A	75	G
1	1A	78	A
1	1A	84	A
1	1A	95	G
1	1A	118	A
1	1A	119	A
1	1A	120	U
1	1A	125	G
1	1A	181	A
1	1A	182	A
1	1A	196	A
1	1A	197	A
1	1A	199	A
1	1A	205	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	215	G
1	1A	216	A
1	1A	222	A
1	1A	225	A
1	1A	228	A
1	1A	229	A
1	1A	233	A
1	1A	248	G
1	1A	250	G
1	1A	269	U
1	1A	271(B)	C
1	1A	271(C)	C
1	1A	271(K)	U
1	1A	271(L)	U
1	1A	271(M)	G
1	1A	271(O)	C
1	1A	271(R)	G
1	1A	272(B)	G
1	1A	275	G
1	1A	279	C
1	1A	311	A
1	1A	329	G
1	1A	330	A
1	1A	342	G
1	1A	352	G
1	1A	363	G
1	1A	363(B)	G
1	1A	363(F)	A
1	1A	380	U
1	1A	386	G
1	1A	396	G
1	1A	405	U
1	1A	407	G
1	1A	411	G
1	1A	421	U
1	1A	428	A
1	1A	443	A
1	1A	444	C
1	1A	448	U
1	1A	454	A
1	1A	456	C
1	1A	457	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	480	A
1	1A	481	G
1	1A	494	G
1	1A	504	U
1	1A	505	A
1	1A	508	G
1	1A	509	C
1	1A	530	G
1	1A	531	C
1	1A	532	A
1	1A	533	G
1	1A	545	G
1	1A	549	G
1	1A	551	G
1	1A	563	G
1	1A	573	G
1	1A	574	C
1	1A	575	A
1	1A	586	A
1	1A	603	A
1	1A	604	G
1	1A	607	U
1	1A	614(B)	G
1	1A	615	G
1	1A	616	G
1	1A	619	G
1	1A	627	A
1	1A	634	C
1	1A	637	A
1	1A	645	C
1	1A	646	A
1	1A	652(D)	C
1	1A	652(E)	G
1	1A	652(F)	G
1	1A	652(T)	C
1	1A	668	G
1	1A	669	G
1	1A	686	G
1	1A	717	G
1	1A	730	C
1	1A	765	G
1	1A	775	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	776	G
1	1A	782	A
1	1A	784	A
1	1A	785	G
1	1A	790	C
1	1A	792	G
1	1A	805	G
1	1A	812	C
1	1A	819	A
1	1A	827	U
1	1A	828	U
1	1A	832	G
1	1A	855	G
1	1A	859	G
1	1A	866	A
1	1A	879	G
1	1A	880	G
1	1A	883	G
1	1A	884	C
1	1A	885	C
1	1A	886	C
1	1A	887	A
1	1A	888	C
1	1A	890	A
1	1A	895	U
1	1A	896	A
1	1A	897	C
1	1A	898	C
1	1A	907	U
1	1A	910	A
1	1A	932	G
1	1A	938	G
1	1A	945	A
1	1A	946	G
1	1A	952	G
1	1A	953	A
1	1A	958	U
1	1A	959	A
1	1A	961	C
1	1A	963	U
1	1A	974	G
1	1A	975	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	983	A
1	1A	996	A
1	1A	1005	C
1	1A	1012	U
1	1A	1013	C
1	1A	1022	G
1	1A	1026	U
1	1A	1033	U
1	1A	1038	C
1	1A	1041	C
1	1A	1044	G
1	1A	1046	A
1	1A	1047	G
1	1A	1048	A
1	1A	1054	A
1	1A	1055	G
1	1A	1058	G
1	1A	1063	G
1	1A	1067	A
1	1A	1069	A
1	1A	1071	G
1	1A	1072	C
1	1A	1073	A
1	1A	1075	C
1	1A	1078	U
1	1A	1079	C
1	1A	1080	C
1	1A	1083	U
1	1A	1085	A
1	1A	1087	G
1	1A	1088	A
1	1A	1090	U
1	1A	1091	G
1	1A	1093	G
1	1A	1094	U
1	1A	1101	U
1	1A	1104	C
1	1A	1108	U
1	1A	1111	A
1	1A	1112	G
1	1A	1116	C
1	1A	1117	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1128	A
1	1A	1129	A
1	1A	1130	U
1	1A	1135	C
1	1A	1136	G
1	1A	1171	G
1	1A	1173	G
1	1A	1174	A
1	1A	1175	U
1	1A	1176	G
1	1A	1177	A
1	1A	1178	C
1	1A	1218	C
1	1A	1220	A
1	1A	1253	A
1	1A	1256	G
1	1A	1271	G
1	1A	1272	A
1	1A	1273	U
1	1A	1276	A
1	1A	1300	U
1	1A	1301	A
1	1A	1329	U
1	1A	1352	U
1	1A	1359	A
1	1A	1360	A
1	1A	1365	A
1	1A	1380	G
1	1A	1384	A
1	1A	1385	G
1	1A	1386	C
1	1A	1416	G
1	1A	1417	C
1	1A	1420	U
1	1A	1421	G
1	1A	1428	C
1	1A	1439	A
1	1A	1445	A
1	1A	1450	G
1	1A	1455	G
1	1A	1459	G
1	1A	1467	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1472	A
1	1A	1473	G
1	1A	1482	G
1	1A	1493	C
1	1A	1494	A
1	1A	1509	C
1	1A	1509(A)	A
1	1A	1540	U
1	1A	1542	A
1	1A	1545	A
1	1A	1558	A
1	1A	1566	A
1	1A	1569	A
1	1A	1578	U
1	1A	1580	A
1	1A	1581	G
1	1A	1584	C
1	1A	1586	A
1	1A	1589	C
1	1A	1608	A
1	1A	1609	A
1	1A	1610	A
1	1A	1647	G
1	1A	1648	C
1	1A	1674	G
1	1A	1696	G
1	1A	1700	A
1	1A	1701	A
1	1A	1703	G
1	1A	1722	A
1	1A	1756	G
1	1A	1763	G
1	1A	1764	G
1	1A	1773	A
1	1A	1780	A
1	1A	1782	C
1	1A	1791	A
1	1A	1800	C
1	1A	1801	G
1	1A	1816	G
1	1A	1828	G
1	1A	1829	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1847	A
1	1A	1861	G
1	1A	1877	A
1	1A	1878	G
1	1A	1900	A
1	1A	1906	G
1	1A	1929	G
1	1A	1930	G
1	1A	1937	A
1	1A	1938	A
1	1A	1955	U
1	1A	1963	U
1	1A	1967	C
1	1A	1970	A
1	1A	1971	A
1	1A	1972	A
1	1A	1983	C
1	1A	1992	G
1	1A	1993	U
1	1A	1997	G
1	1A	2020	A
1	1A	2023	G
1	1A	2030	A
1	1A	2031	A
1	1A	2032	G
1	1A	2033	A
1	1A	2039	C
1	1A	2043	C
1	1A	2055	C
1	1A	2056	G
1	1A	2060	A
1	1A	2061	G
1	1A	2062	A
1	1A	2069	G
1	1A	2101	G
1	1A	2108	C
1	1A	2113	U
1	1A	2114	A
1	1A	2116	G
1	1A	2121	G
1	1A	2122	U
1	1A	2127	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2129	C
1	1A	2130	U
1	1A	2131	G
1	1A	2132	U
1	1A	2133	G
1	1A	2134	A
1	1A	2135	A
1	1A	2136	C
1	1A	2140	C
1	1A	2142	C
1	1A	2143	C
1	1A	2144	U
1	1A	2145	C
1	1A	2146	C
1	1A	2147	G
1	1A	2149	G
1	1A	2150	U
1	1A	2151	G
1	1A	2155	G
1	1A	2156	G
1	1A	2157	G
1	1A	2158	A
1	1A	2159	G
1	1A	2163	C
1	1A	2165	G
1	1A	2166	G
1	1A	2168	G
1	1A	2171	A
1	1A	2172	U
1	1A	2173	A
1	1A	2174	C
1	1A	2182	G
1	1A	2184	G
1	1A	2189	U
1	1A	2192	G
1	1A	2198	A
1	1A	2206	G
1	1A	2208	A
1	1A	2218	U
1	1A	2219	G
1	1A	2225	A
1	1A	2238	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2268	A
1	1A	2269	A
1	1A	2283	C
1	1A	2287	A
1	1A	2289	G
1	1A	2305	A
1	1A	2308	G
1	1A	2320	A
1	1A	2325	G
1	1A	2334	G
1	1A	2336	A
1	1A	2347	C
1	1A	2350	C
1	1A	2361	A
1	1A	2383	G
1	1A	2385	C
1	1A	2406	U
1	1A	2407	G
1	1A	2410	G
1	1A	2422	A
1	1A	2423	U
1	1A	2425	A
1	1A	2428	G
1	1A	2429	G
1	1A	2430	A
1	1A	2431	U
1	1A	2435	A
1	1A	2439	A
1	1A	2440	C
1	1A	2441	C
1	1A	2448	A
1	1A	2474	C
1	1A	2476	A
1	1A	2490	G
1	1A	2502	G
1	1A	2505	G
1	1A	2518	A
1	1A	2525	G
1	1A	2529	G
1	1A	2535	G
1	1A	2549	G
1	1A	2554	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2566	A
1	1A	2567	G
1	1A	2573	C
1	1A	2574	G
1	1A	2582	G
1	1A	2585	U
1	1A	2602	A
1	1A	2609	U
1	1A	2611	U
1	1A	2612	C
1	1A	2629	A
1	1A	2630	G
1	1A	2641	G
1	1A	2654	A
1	1A	2689	U
1	1A	2690	C
1	1A	2702	U
1	1A	2703	C
1	1A	2712(A)	A
1	1A	2713	A
1	1A	2714	G
1	1A	2726	U
1	1A	2733	A
1	1A	2744	G
1	1A	2757	A
1	1A	2758	A
1	1A	2764	A
1	1A	2765	A
1	1A	2766	G
1	1A	2778	A
1	1A	2780	G
1	1A	2790	A
1	1A	2791	C
1	1A	2793	G
1	1A	2794	C
1	1A	2802	G
1	1A	2803	C
1	1A	2820	A
1	1A	2821	A
1	1A	2835	A
1	1A	2836	U
1	1A	2839	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2872	G
1	1A	2880	C
1	1A	2892	A
1	1A	2894	G
1	1A	2895	U
2	1B	25	A
2	1B	56	G
2	1B	67	G
2	1B	73	A
2	1B	106	G
2	1B	109	C
2	1B	110	G
32	1a	7	G
32	1a	9	G
32	1a	32	A
32	1a	39	G
32	1a	48	C
32	1a	51	A
32	1a	61	G
32	1a	65	U
32	1a	73	G
32	1a	79	G
32	1a	91	C
32	1a	98	G
32	1a	101	A
32	1a	116	A
32	1a	120	A
32	1a	121	C
32	1a	129(A)	G
32	1a	131	C
32	1a	151	A
32	1a	163	C
32	1a	174	C
32	1a	182	U
32	1a	189(D)	C
32	1a	189(H)	G
32	1a	189(J)	G
32	1a	195	A
32	1a	197	A
32	1a	203	U
32	1a	204	U
32	1a	216	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	219	C
32	1a	222	U
32	1a	247	G
32	1a	251	G
32	1a	258	G
32	1a	266	G
32	1a	267	C
32	1a	289	G
32	1a	301	G
32	1a	317	G
32	1a	318	G
32	1a	321	A
32	1a	328	C
32	1a	332	G
32	1a	342	C
32	1a	344	A
32	1a	345	C
32	1a	348	G
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	384	G
32	1a	397	A
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	413	G
32	1a	422	C
32	1a	423	G
32	1a	424	G
32	1a	429	U
32	1a	439	A
32	1a	442	C
32	1a	452	A
32	1a	458	C
32	1a	461	A
32	1a	470	C
32	1a	483	C
32	1a	485	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	496	A
32	1a	498	U
32	1a	509	A
32	1a	510	A
32	1a	511	C
32	1a	518	C
32	1a	524	G
32	1a	527	G7M
32	1a	531	U
32	1a	532	A
32	1a	547	A
32	1a	559	A
32	1a	561	U
32	1a	568	G
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	577	G
32	1a	596	C
32	1a	630	G
32	1a	639	G
32	1a	653	A
32	1a	661	G
32	1a	665	A
32	1a	666	G
32	1a	671	G
32	1a	672	U
32	1a	673	G
32	1a	687	A
32	1a	688	G
32	1a	693	G
32	1a	695	A
32	1a	717	C
32	1a	723	U
32	1a	724	G
32	1a	731	G
32	1a	734	G
32	1a	747	C
32	1a	749	C
32	1a	753	A
32	1a	755	G
32	1a	759	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	774	G
32	1a	777	A
32	1a	792	A
32	1a	793	U
32	1a	794	A
32	1a	815	A
32	1a	816	A
32	1a	817	C
32	1a	828	A
32	1a	840	C
32	1a	841	U
32	1a	851	G
32	1a	872	A
32	1a	876	G
32	1a	902	G
32	1a	913	A
32	1a	914	A
32	1a	916	G
32	1a	926	G
32	1a	927	G
32	1a	934	C
32	1a	935	A
32	1a	942	G
32	1a	960	U
32	1a	961	U
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	972	C
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	983	A
32	1a	992	U
32	1a	993	G
32	1a	997	U
32	1a	1000	U
32	1a	1001	A
32	1a	1001(A)	G
32	1a	1002	G
32	1a	1003	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	1005	A
32	1a	1006	C
32	1a	1007	C
32	1a	1009	G
32	1a	1010	G
32	1a	1020	U
32	1a	1022	G
32	1a	1023	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C
32	1a	1028	C
32	1a	1029	C
32	1a	1030	C
32	1a	1030(A)	G
32	1a	1030(C)	G
32	1a	1031	G
32	1a	1033	G
32	1a	1041	A
32	1a	1042	G
32	1a	1043	C
32	1a	1044	A
32	1a	1046	A
32	1a	1063	C
32	1a	1068	G
32	1a	1081	G
32	1a	1086	U
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1123	A
32	1a	1124	G
32	1a	1125	U
32	1a	1134	G
32	1a	1137	C
32	1a	1138	G
32	1a	1139	G
32	1a	1141	C
32	1a	1146	A
32	1a	1152	A
32	1a	1159	U
32	1a	1183	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	1184	G
32	1a	1193	G
32	1a	1196	U
32	1a	1197	G
32	1a	1201	A
32	1a	1202	G
32	1a	1213	A
32	1a	1227	A
32	1a	1238	A
32	1a	1246	C
32	1a	1250	A
32	1a	1253	G
32	1a	1256	A
32	1a	1257	U
32	1a	1258	G
32	1a	1260	C
32	1a	1270	C
32	1a	1275	A
32	1a	1278	U
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1320	C
32	1a	1323	G
32	1a	1338	G
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1370	G
32	1a	1378	C
32	1a	1394	A
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1446	U
32	1a	1447	A
32	1a	1456	G
32	1a	1487	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	1492	A
32	1a	1494	G
32	1a	1497	G
32	1a	1503	A
32	1a	1504	G
32	1a	1505	G
32	1a	1506	U
32	1a	1517	G
32	1a	1529	G
32	1a	1530	G
32	1a	1532	U
53	1v	13	A
54	1w	6	G
54	1w	7	A
54	1w	8	4SU
54	1w	9	A
54	1w	19	G
54	1w	20	U
54	1w	21	A
54	1w	24	G
54	1w	34	G
54	1w	45	U
54	1w	46	G7M
54	1w	47	U
54	1w	48	C
54	1w	62	C
54	1w	63	G
54	1w	64	A
54	1w	65	G
54	1w	66	U
54	1w	68	C
54	1w	70	G
54	1w	71	G
54	1w	72	C
54	1w	73	A
54	1w	74	C
55	1x	3	C
55	1x	6	G
55	1x	9	G
55	1x	13	C
55	1x	14	A
55	1x	17(A)	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
55	1x	18	G
55	1x	19	G
55	1x	21	A
55	1x	47	U
55	1x	59	A
55	1x	61	C
55	1x	76	A
54	1y	6	G
54	1y	7	A
54	1y	8	4SU
54	1y	9	A
54	1y	11	C
54	1y	13	C
54	1y	14	A
54	1y	19	G
54	1y	20	U
54	1y	21	A
54	1y	22	G
54	1y	26	A
54	1y	27	G
54	1y	33	U
54	1y	35	A
54	1y	36	A
54	1y	44	G
54	1y	45	U
54	1y	46	G7M
54	1y	48	C
54	1y	52	G
54	1y	53	G
54	1y	54	5MU
54	1y	55	PSU
54	1y	56	C
54	1y	57	G
54	1y	58	A
54	1y	64	A
54	1y	65	G
54	1y	70	G
1	2A	8	A
1	2A	15	G
1	2A	34	C
1	2A	35	G
1	2A	36	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	45	C
1	2A	61	G
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	78	A
1	2A	84	A
1	2A	90	U
1	2A	94	C
1	2A	100	G
1	2A	102	G
1	2A	118	A
1	2A	119	A
1	2A	120	U
1	2A	154(A)	C
1	2A	157	U
1	2A	181	A
1	2A	196	A
1	2A	199	A
1	2A	205	G
1	2A	214	G
1	2A	215	G
1	2A	216	A
1	2A	222	A
1	2A	225	A
1	2A	228	A
1	2A	229	A
1	2A	230	U
1	2A	233	A
1	2A	248	G
1	2A	266	G
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	272(B)	G
1	2A	272(J)	C
1	2A	277	C
1	2A	278	A
1	2A	279	C
1	2A	311	A
1	2A	316	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	317	G
1	2A	324	A
1	2A	327	G
1	2A	329	G
1	2A	330	A
1	2A	342	G
1	2A	352	G
1	2A	354	G
1	2A	357	A
1	2A	363	G
1	2A	363(B)	G
1	2A	386	G
1	2A	396	G
1	2A	406	G
1	2A	411	G
1	2A	412	A
1	2A	421	U
1	2A	422	A
1	2A	434	U
1	2A	444	C
1	2A	455	C
1	2A	456	C
1	2A	457	A
1	2A	481	G
1	2A	496	G
1	2A	503	A
1	2A	504	U
1	2A	505	A
1	2A	508	G
1	2A	509	C
1	2A	529	A
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	545	G
1	2A	556	G
1	2A	563	G
1	2A	568	U
1	2A	573	G
1	2A	575	A
1	2A	588	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	595	C
1	2A	599	G
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	614(B)	G
1	2A	615	G
1	2A	616	G
1	2A	627	A
1	2A	637	A
1	2A	645	C
1	2A	649	G
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	652(U)	G
1	2A	669	G
1	2A	686	G
1	2A	717	G
1	2A	730	C
1	2A	752	A
1	2A	753	C
1	2A	764	A
1	2A	771	G
1	2A	774	A
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	790	C
1	2A	792	G
1	2A	793	A
1	2A	794	G
1	2A	805	G
1	2A	812	C
1	2A	819	A
1	2A	827	U
1	2A	828	U
1	2A	847	U
1	2A	857	C
1	2A	859	G
1	2A	866	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	874	G
1	2A	875	G
1	2A	877	U
1	2A	879	G
1	2A	880	G
1	2A	882	G
1	2A	884	C
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	893	C
1	2A	894	C
1	2A	895	U
1	2A	896	A
1	2A	900	A
1	2A	901	A
1	2A	907	U
1	2A	910	A
1	2A	915	C
1	2A	917	A
1	2A	932	G
1	2A	936	C
1	2A	938	G
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	953	A
1	2A	961	C
1	2A	974	G
1	2A	975	C
1	2A	983	A
1	2A	995	C
1	2A	996	A
1	2A	999	U
1	2A	1005	C
1	2A	1012	U
1	2A	1013	C
1	2A	1020	A
1	2A	1022	G
1	2A	1025	G
1	2A	1026	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1033	U
1	2A	1038	C
1	2A	1039	G
1	2A	1041	C
1	2A	1043	C
1	2A	1114	G
1	2A	1116	C
1	2A	1126	A
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1139	G
1	2A	1142(A)	A
1	2A	1169	G
1	2A	1171	G
1	2A	1195	G
1	2A	1204	A
1	2A	1205	U
1	2A	1210	A
1	2A	1211	U
1	2A	1212	G
1	2A	1220	A
1	2A	1244	G
1	2A	1250	G
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1273	U
1	2A	1300	U
1	2A	1301	A
1	2A	1303	G
1	2A	1314	C
1	2A	1352	U
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1368	G
1	2A	1370	C
1	2A	1373	A
1	2A	1379	A
1	2A	1384	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1385	G
1	2A	1386	C
1	2A	1395	A
1	2A	1412	A
1	2A	1416	G
1	2A	1417	C
1	2A	1421	G
1	2A	1428	C
1	2A	1436	G
1	2A	1437	C
1	2A	1445	A
1	2A	1449	A
1	2A	1450	G
1	2A	1460	A
1	2A	1461	G
1	2A	1467	C
1	2A	1471	A
1	2A	1482	G
1	2A	1490	A
1	2A	1493	C
1	2A	1496	A
1	2A	1497	U
1	2A	1506	C
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1531	C
1	2A	1532	C
1	2A	1547	C
1	2A	1558	A
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1583	A
1	2A	1584	C
1	2A	1608	A
1	2A	1609	A
1	2A	1610	A
1	2A	1616	A
1	2A	1640	C
1	2A	1648	C
1	2A	1653	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1654	A
1	2A	1664	A
1	2A	1674	G
1	2A	1696	G
1	2A	1700	A
1	2A	1701	A
1	2A	1703	G
1	2A	1721	G
1	2A	1722	A
1	2A	1740	G
1	2A	1746	G
1	2A	1756	G
1	2A	1758	G
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A
1	2A	1780	A
1	2A	1782	C
1	2A	1786	A
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1811	G
1	2A	1812	A
1	2A	1816	G
1	2A	1828	G
1	2A	1829	A
1	2A	1835	G
1	2A	1847	A
1	2A	1848	A
1	2A	1877	A
1	2A	1878	G
1	2A	1896	G
1	2A	1900	A
1	2A	1906	G
1	2A	1913	A
1	2A	1914	C
1	2A	1927	A
1	2A	1929	G
1	2A	1930	G
1	2A	1936	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1938	A
1	2A	1955	U
1	2A	1963	U
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1984	G
1	2A	1992	G
1	2A	1993	U
1	2A	1997	G
1	2A	2020	A
1	2A	2023	G
1	2A	2031	A
1	2A	2032	G
1	2A	2033	A
1	2A	2035	G
1	2A	2036	C
1	2A	2043	C
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2063	C
1	2A	2069	G
1	2A	2093	G
1	2A	2106	G
1	2A	2108	C
1	2A	2109	U
1	2A	2111	C
1	2A	2112	G
1	2A	2116	G
1	2A	2119	A
1	2A	2120	G
1	2A	2122	U
1	2A	2124	G
1	2A	2125	G
1	2A	2126	A
1	2A	2127	G
1	2A	2128	C
1	2A	2130	U
1	2A	2131	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2132	U
1	2A	2134	A
1	2A	2135	A
1	2A	2136	C
1	2A	2137	C
1	2A	2138	C
1	2A	2139	C
1	2A	2140	C
1	2A	2143	C
1	2A	2146	C
1	2A	2148	G
1	2A	2150	U
1	2A	2155	G
1	2A	2156	G
1	2A	2157	G
1	2A	2158	A
1	2A	2161	C
1	2A	2165	G
1	2A	2166	G
1	2A	2167	U
1	2A	2168	G
1	2A	2172	U
1	2A	2174	C
1	2A	2176	A
1	2A	2178	C
1	2A	2181	G
1	2A	2182	G
1	2A	2185	C
1	2A	2189	U
1	2A	2190	G
1	2A	2192	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2218	U
1	2A	2225	A
1	2A	2239	G
1	2A	2275	C
1	2A	2278	A
1	2A	2283	C
1	2A	2287	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2305	A
1	2A	2308	G
1	2A	2319	G
1	2A	2320	A
1	2A	2325	G
1	2A	2334	G
1	2A	2336	A
1	2A	2346	A
1	2A	2347	C
1	2A	2350	C
1	2A	2376	A
1	2A	2383	G
1	2A	2385	C
1	2A	2403	C
1	2A	2406	U
1	2A	2425	A
1	2A	2429	G
1	2A	2430	A
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2445	G
1	2A	2448	A
1	2A	2469	A
1	2A	2476	A
1	2A	2490	G
1	2A	2494	G
1	2A	2502	G
1	2A	2505	G
1	2A	2506	U
1	2A	2507	C
1	2A	2518	A
1	2A	2520	C
1	2A	2525	G
1	2A	2529	G
1	2A	2554	U
1	2A	2555	U
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2582	G
1	2A	2602	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2609	U
1	2A	2611	U
1	2A	2612	C
1	2A	2623	G
1	2A	2629	A
1	2A	2630	G
1	2A	2634	G
1	2A	2646	C
1	2A	2654	A
1	2A	2669	G
1	2A	2673	G
1	2A	2689	U
1	2A	2690	C
1	2A	2691	C
1	2A	2702	U
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2718	G
1	2A	2726	U
1	2A	2733	A
1	2A	2748	A
1	2A	2751	G
1	2A	2758	A
1	2A	2761	G
1	2A	2764	A
1	2A	2765	A
1	2A	2769	C
1	2A	2778	A
1	2A	2780	G
1	2A	2793	G
1	2A	2794	C
1	2A	2802	G
1	2A	2807	G
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2835	A
1	2A	2839	G
1	2A	2872	G
1	2A	2880	C
1	2A	2892	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2894	G
1	2A	2897	U
2	2B	2	C
2	2B	3	C
2	2B	8	U
2	2B	9	G
2	2B	13	A
2	2B	17	C
2	2B	19	G
2	2B	20	C
2	2B	24	G
2	2B	25	A
2	2B	30	C
2	2B	33	G
2	2B	34	U
2	2B	35	U
2	2B	41	U
2	2B	42	C
2	2B	45	A
2	2B	51	G
2	2B	53	A
2	2B	58	A
2	2B	67	G
2	2B	73	A
2	2B	74	U
2	2B	75	G
2	2B	85	G
2	2B	88	C
2	2B	89	G
2	2B	91	C
2	2B	105	A
2	2B	106	G
2	2B	110	G
2	2B	112	U
2	2B	116	G
2	2B	120	A
32	2a	5	U
32	2a	9	G
32	2a	22	G
32	2a	31	G
32	2a	32	A
32	2a	39	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	41	G
32	2a	47	C
32	2a	48	C
32	2a	50	A
32	2a	51	A
32	2a	52	G
32	2a	65	U
32	2a	66	G
32	2a	73	G
32	2a	89	C
32	2a	98	G
32	2a	101	A
32	2a	105	G
32	2a	116	A
32	2a	121	C
32	2a	131	C
32	2a	142	G
32	2a	144	G
32	2a	156	G
32	2a	159	G
32	2a	163	C
32	2a	180	U
32	2a	182	U
32	2a	189	G
32	2a	189(F)	U
32	2a	189(J)	G
32	2a	195	A
32	2a	197	A
32	2a	202	U
32	2a	203	U
32	2a	204	U
32	2a	216	G
32	2a	217	C
32	2a	231	G
32	2a	247	G
32	2a	251	G
32	2a	258	G
32	2a	266	G
32	2a	267	C
32	2a	274	A
32	2a	281	G
32	2a	289	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	345	C
32	2a	351	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	367	U
32	2a	372	C
32	2a	373	A
32	2a	381	C
32	2a	384	G
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	412	A
32	2a	413	G
32	2a	421	U
32	2a	423	G
32	2a	424	G
32	2a	429	U
32	2a	430	A
32	2a	439	A
32	2a	442	C
32	2a	452	A
32	2a	461	A
32	2a	470	C
32	2a	485	G
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	510	A
32	2a	511	C
32	2a	518	C
32	2a	521	G
32	2a	527	G7M
32	2a	531	U
32	2a	532	A
32	2a	533	A
32	2a	547	A
32	2a	559	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	564	C
32	2a	572	A
32	2a	573	A
32	2a	574	A
32	2a	576	G
32	2a	577	G
32	2a	596	C
32	2a	607	A
32	2a	630	G
32	2a	653	A
32	2a	657	G
32	2a	665	A
32	2a	666	G
32	2a	687	A
32	2a	688	G
32	2a	695	A
32	2a	702	A
32	2a	708	C
32	2a	723	U
32	2a	724	G
32	2a	731	G
32	2a	733	A
32	2a	748	C
32	2a	749	C
32	2a	755	G
32	2a	760	G
32	2a	772	U
32	2a	773	G
32	2a	777	A
32	2a	787	A
32	2a	792	A
32	2a	793	U
32	2a	794	A
32	2a	816	A
32	2a	817	C
32	2a	821	G
32	2a	828	A
32	2a	834	C
32	2a	840	C
32	2a	841	U
32	2a	853	G
32	2a	854	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	859	A
32	2a	864	A
32	2a	872	A
32	2a	873	A
32	2a	885	G
32	2a	902	G
32	2a	914	A
32	2a	926	G
32	2a	927	G
32	2a	933	G
32	2a	934	C
32	2a	935	A
32	2a	942	G
32	2a	960	U
32	2a	961	U
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	972	C
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	978	A
32	2a	979	C
32	2a	984	C
32	2a	989	C
32	2a	992	U
32	2a	993	G
32	2a	995	C
32	2a	996	A
32	2a	997	U
32	2a	1001(A)	G
32	2a	1002	G
32	2a	1003	G
32	2a	1005	A
32	2a	1006	C
32	2a	1009	G
32	2a	1011	G
32	2a	1016	A
32	2a	1017	G
32	2a	1020	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1021	G
32	2a	1022	G
32	2a	1023	G
32	2a	1025	U
32	2a	1027	C
32	2a	1028	C
32	2a	1029	C
32	2a	1030(A)	G
32	2a	1031	G
32	2a	1033	G
32	2a	1037	C
32	2a	1038	C
32	2a	1039	C
32	2a	1040	U
32	2a	1044	A
32	2a	1051	C
32	2a	1053	G
32	2a	1054	C
32	2a	1064	G
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1077	G
32	2a	1081	G
32	2a	1085	U
32	2a	1086	U
32	2a	1092	A
32	2a	1093	A
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A
32	2a	1108	G
32	2a	1109	C
32	2a	1113	C
32	2a	1118	C
32	2a	1122	U
32	2a	1126	U
32	2a	1127	G
32	2a	1128	C
32	2a	1129	C
32	2a	1133	G
32	2a	1134	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1135	U
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1140	C
32	2a	1146	A
32	2a	1147	C
32	2a	1152	A
32	2a	1157	A
32	2a	1158	C
32	2a	1159	U
32	2a	1172	C
32	2a	1173	G
32	2a	1181	G
32	2a	1182	G
32	2a	1183	A
32	2a	1184	G
32	2a	1195	C
32	2a	1196	U
32	2a	1197	G
32	2a	1201	A
32	2a	1202	G
32	2a	1207	2MG
32	2a	1208	C
32	2a	1211	U
32	2a	1213	A
32	2a	1226	C
32	2a	1227	A
32	2a	1228	C
32	2a	1238	A
32	2a	1240	U
32	2a	1241	G
32	2a	1246	C
32	2a	1256	A
32	2a	1257	U
32	2a	1260	C
32	2a	1262	C
32	2a	1264	C
32	2a	1270	C
32	2a	1272	G
32	2a	1273	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1278	U
32	2a	1279	A
32	2a	1280	A
32	2a	1283	G
32	2a	1285	A
32	2a	1287	A
32	2a	1293	G
32	2a	1294	G
32	2a	1297	C
32	2a	1299	A
32	2a	1300	G
32	2a	1302	U
32	2a	1303	C
32	2a	1305	G
32	2a	1312	G
32	2a	1321	C
32	2a	1322	C
32	2a	1323	G
32	2a	1336	C
32	2a	1338	G
32	2a	1346	A
32	2a	1347	G
32	2a	1354	C
32	2a	1358	U
32	2a	1359	C
32	2a	1363	C
32	2a	1363(A)	A
32	2a	1368	G
32	2a	1380	U
32	2a	1398	A
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1447	A
32	2a	1452	C
32	2a	1456	G
32	2a	1492	A
32	2a	1494	G
32	2a	1497	G
32	2a	1499	A
32	2a	1503	A
32	2a	1504	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1506	U
32	2a	1507	A
32	2a	1517	G
32	2a	1519	MA6
32	2a	1520	G
32	2a	1529	G
32	2a	1530	G
32	2a	1531	A
32	2a	1532	U
53	2v	13	A
53	2v	14	A
53	2v	23	A
54	2w	3	C
54	2w	4	C
54	2w	6	G
54	2w	7	A
54	2w	12	U
54	2w	13	C
54	2w	14	A
54	2w	19	G
54	2w	22	G
54	2w	27	G
54	2w	45	U
54	2w	46	G7M
54	2w	48	C
54	2w	51	U
54	2w	59	U
54	2w	62	C
54	2w	64	A
54	2w	65	G
54	2w	66	U
54	2w	69	G
54	2w	70	G
54	2w	71	G
54	2w	72	C
54	2w	73	A
54	2w	74	C
55	2x	9	G
55	2x	13	C
55	2x	18	G
55	2x	19	G
55	2x	20	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
55	2x	21	A
55	2x	22	G
55	2x	46	G
55	2x	47	U
55	2x	52	G
55	2x	56	C
55	2x	76	A
54	2y	8	4SU
54	2y	14	A
54	2y	15	G
54	2y	19	G
54	2y	21	A
54	2y	24	G
54	2y	27	G
54	2y	30	G
54	2y	33	U
54	2y	37	MIA
54	2y	45	U
54	2y	46	G7M
54	2y	48	C
54	2y	49	C
54	2y	52	G
54	2y	53	G
54	2y	54	5MU
54	2y	55	PSU
54	2y	56	C
54	2y	57	G
54	2y	58	A
54	2y	60	U
54	2y	63	G
54	2y	69	G
54	2y	70	G
54	2y	73	A

All (48) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	196	A
1	1A	266	G
1	1A	271(K)	U
1	1A	278	A
1	1A	548	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	774	A
1	1A	827	U
1	1A	974	G
1	1A	1047	G
1	1A	1067	A
1	1A	1174	A
1	1A	1176	G
1	1A	1275	A
1	1A	1379	A
1	1A	1442	G
1	1A	1508	A
1	1A	1608	A
1	1A	1992	G
1	1A	2126	A
1	1A	2134	A
1	1A	2181	G
1	1A	2183	C
1	1A	2406	U
1	1A	2422	A
1	1A	2430	A
1	1A	2439	A
1	1A	2629	A
1	1A	2689	U
1	1A	2756	U
1	2A	196	A
1	2A	228	A
1	2A	266	G
1	2A	271(M)	G
1	2A	277	C
1	2A	528	A
1	2A	752	A
1	2A	774	A
1	2A	856	C
1	2A	900	A
1	2A	1210	A
1	2A	1420	U
1	2A	1530	C
1	2A	1653	G
1	2A	1913	A
1	2A	1992	G
1	2A	2119	A
1	2A	2126	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2689	U

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

84 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
55	4SU	2x	8	56,55	18,21,22	2.02	5 (27%)	25,30,33	1.31	4 (16%)
54	5MU	1y	54	54	19,22,23	1.47	5 (26%)	27,32,35	1.60	5 (18%)
54	PSU	2w	39	54	18,21,22	1.48	2 (11%)	21,30,33	1.59	5 (23%)
1	PSU	2A	1917	1	18,21,22	1.37	2 (11%)	21,30,33	2.03	4 (19%)
54	5MU	2w	54	54	19,22,23	1.42	4 (21%)	27,32,35	1.62	5 (18%)
32	PSU	1a	516	32,56	18,21,22	1.39	3 (16%)	21,30,33	2.01	4 (19%)
54	G7M	1w	46	54	23,26,27	1.55	3 (13%)	34,39,42	1.60	4 (11%)
32	MA6	2a	1518	32	23,26,27	0.42	0	33,38,41	2.01	9 (27%)
32	UR3	1a	1498	32	19,22,23	1.09	1 (5%)	26,32,35	1.71	3 (11%)
54	PSU	2w	55	54	18,21,22	1.38	2 (11%)	21,30,33	2.06	3 (14%)
54	PSU	1w	32	56,54	18,21,22	1.34	2 (11%)	21,30,33	1.80	3 (14%)
32	2MG	2a	1207	32,56	23,26,27	1.27	3 (13%)	33,38,41	2.07	7 (21%)
1	OMU	2A	2552	1,56	19,22,23	1.20	3 (15%)	25,31,34	1.78	5 (20%)
54	5MU	2y	54	54	19,22,23	1.52	4 (21%)	27,32,35	1.95	9 (33%)
32	M2G	1a	966	32	24,27,28	1.33	4 (16%)	33,40,43	1.89	5 (15%)
1	5MU	1A	1915	1	19,22,23	1.40	5 (26%)	27,32,35	2.14	7 (25%)
32	PSU	2a	516	32	18,21,22	1.35	2 (11%)	21,30,33	1.87	4 (19%)
1	5MC	2A	1962	1,56	19,22,23	1.65	3 (15%)	26,32,35	1.19	2 (7%)
54	4SU	1w	8	54	18,21,22	1.77	5 (27%)	25,30,33	1.95	5 (20%)
54	PSU	1w	39	54	18,21,22	1.33	2 (11%)	21,30,33	2.17	4 (19%)
1	PSU	2A	1911	1	18,21,22	1.40	2 (11%)	21,30,33	1.89	4 (19%)
54	4SU	2w	8	54	18,21,22	1.69	6 (33%)	25,30,33	2.07	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMC	2A	1920	1	19,22,23	0.76	0	25,31,34	0.84	0
54	PSU	2y	39	54	18,21,22	1.42	2 (11%)	21,30,33	1.67	3 (14%)
32	M2G	2a	966	32	24,27,28	1.31	4 (16%)	33,40,43	1.84	6 (18%)
32	5MC	2a	1400	32	19,22,23	1.77	3 (15%)	26,32,35	1.19	3 (11%)
54	PSU	2y	32	54	18,21,22	1.38	2 (11%)	21,30,33	1.91	3 (14%)
54	MIA	2y	37	54	21,24,32	1.69	3 (14%)	30,35,47	1.97	8 (26%)
1	OMG	1A	2251	1,56,55	23,26,27	1.21	3 (13%)	32,38,41	2.09	7 (21%)
32	5MC	2a	1404	32	19,22,23	1.64	3 (15%)	26,32,35	1.10	2 (7%)
1	5MU	2A	1939	1,56	19,22,23	1.42	5 (26%)	27,32,35	2.32	6 (22%)
54	G7M	1y	46	54	23,26,27	1.58	3 (13%)	34,39,42	1.77	4 (11%)
32	5MC	1a	967	32	19,22,23	1.64	3 (15%)	26,32,35	1.10	2 (7%)
1	5MU	2A	1915	1,56	19,22,23	1.43	6 (31%)	27,32,35	2.21	6 (22%)
43	0TD	1l	92	43	8,9,10	4.55	1 (12%)	6,11,13	4.88	2 (33%)
32	MA6	1a	1519	32	23,26,27	0.45	0	33,38,41	2.13	9 (27%)
43	0TD	2l	92	43	8,9,10	4.67	2 (25%)	6,11,13	9.21	1 (16%)
54	PSU	2y	55	54	18,21,22	1.31	2 (11%)	21,30,33	1.95	4 (19%)
1	PSU	1A	1911	1	18,21,22	1.42	2 (11%)	21,30,33	2.01	4 (19%)
1	OMG	2A	2251	1,56,55	23,26,27	1.20	3 (13%)	32,38,41	1.97	6 (18%)
32	G7M	2a	527	32,56	23,26,27	1.47	4 (17%)	34,39,42	1.68	5 (14%)
54	MIA	1y	37	54	21,24,32	1.67	3 (14%)	30,35,47	2.01	8 (26%)
1	PSU	1A	1917	1	18,21,22	1.42	3 (16%)	21,30,33	2.06	3 (14%)
32	MA6	2a	1519	32	23,26,27	0.44	0	33,38,41	2.07	10 (30%)
54	MIA	2w	37	54	24,27,32	2.10	5 (20%)	32,39,47	2.40	10 (31%)
54	PSU	2w	32	54	18,21,22	1.35	2 (11%)	21,30,33	1.98	4 (19%)
54	4SU	2y	8	54	18,21,22	1.73	4 (22%)	25,30,33	2.09	4 (16%)
55	PSU	2x	55	55	18,21,22	1.33	2 (11%)	21,30,33	2.11	4 (19%)
1	5MC	1A	1962	1,56	19,22,23	1.73	3 (15%)	26,32,35	1.13	2 (7%)
32	4OC	2a	1402	32,56	20,23,24	0.79	0	25,32,35	1.10	3 (12%)
1	PSU	2A	2605	1	18,21,22	1.34	3 (16%)	21,30,33	2.00	5 (23%)
1	5MC	1A	1942	1,56	19,22,23	1.40	3 (15%)	26,32,35	1.12	2 (7%)
54	PSU	1y	32	54	18,21,22	1.38	2 (11%)	21,30,33	1.90	3 (14%)
54	G7M	2w	46	54	23,26,27	1.43	4 (17%)	34,39,42	1.70	5 (14%)
1	5MU	1A	1939	1,56	19,22,23	1.42	4 (21%)	27,32,35	2.30	6 (22%)
54	5MU	1w	54	54	19,22,23	1.41	6 (31%)	27,32,35	1.95	7 (25%)
32	5MC	1a	1404	32	19,22,23	1.83	3 (15%)	26,32,35	1.23	4 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	2MA	1A	2503	1,56	22,25,26	1.43	3 (13%)	32,37,40	2.44	10 (31%)
1	OMC	1A	1920	1	19,22,23	0.85	0	25,31,34	1.08	1 (4%)
54	4SU	1y	8	54	18,21,22	1.83	6 (33%)	25,30,33	1.75	4 (16%)
55	PSU	1x	55	55	18,21,22	1.37	2 (11%)	21,30,33	2.05	3 (14%)
1	PSU	1A	2605	1,56	18,21,22	1.39	4 (22%)	21,30,33	2.01	4 (19%)
55	5MC	2x	32	55	19,22,23	1.60	3 (15%)	26,32,35	1.19	3 (11%)
55	5MU	2x	54	55	19,22,23	1.39	5 (26%)	27,32,35	2.08	6 (22%)
55	5MU	1x	54	55	19,22,23	1.40	6 (31%)	27,32,35	2.13	6 (22%)
54	PSU	1y	39	54	18,21,22	1.41	2 (11%)	21,30,33	1.96	5 (23%)
32	5MC	2a	967	32	19,22,23	1.73	3 (15%)	26,32,35	1.13	3 (11%)
54	G7M	2y	46	54	23,26,27	1.62	3 (13%)	34,39,42	1.90	3 (8%)
32	UR3	2a	1498	32	19,22,23	1.05	2 (10%)	26,32,35	1.71	2 (7%)
32	2MG	1a	1207	32	23,26,27	1.22	3 (13%)	33,38,41	2.35	9 (27%)
32	4OC	1a	1402	32,56	20,23,24	0.73	0	25,32,35	0.93	1 (4%)
55	5MC	1x	32	55	19,22,23	1.69	3 (15%)	26,32,35	1.21	3 (11%)
54	PSU	1y	55	54	18,21,22	1.37	2 (11%)	21,30,33	2.05	5 (23%)
1	OMU	1A	2552	1	19,22,23	1.11	3 (15%)	25,31,34	2.07	5 (20%)
54	MIA	1w	37	54	28,31,32	2.32	6 (21%)	38,44,47	2.77	12 (31%)
32	G7M	1a	527	32,56	23,26,27	1.54	4 (17%)	34,39,42	1.64	4 (11%)
1	5MC	2A	1942	1	19,22,23	1.54	3 (15%)	26,32,35	1.11	2 (7%)
32	5MC	1a	1400	32	19,22,23	1.63	3 (15%)	26,32,35	1.15	3 (11%)
32	5MC	1a	1407	32	19,22,23	1.56	3 (15%)	26,32,35	1.13	3 (11%)
54	PSU	1w	55	54	18,21,22	1.41	2 (11%)	21,30,33	1.97	4 (19%)
55	4SU	1x	8	55	18,21,22	2.11	5 (27%)	25,30,33	1.45	5 (20%)
32	MA6	1a	1518	32	23,26,27	0.42	0	33,38,41	2.00	9 (27%)
32	5MC	2a	1407	32	19,22,23	1.65	3 (15%)	26,32,35	1.21	3 (11%)
1	2MA	2A	2503	1,56	22,25,26	1.41	5 (22%)	32,37,40	2.30	9 (28%)

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
55	4SU	2x	8	56,55	-	0/7/25/26	0/2/2/2
54	5MU	1y	54	54	-	2/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	32,56	-	0/7/25/26	0/2/2/2
54	G7M	1w	46	54	-	1/7/25/26	0/3/3/3
32	MA6	2a	1518	32	-	0/11/29/30	0/3/3/3
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
54	PSU	1w	32	56,54	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32,56	-	2/9/27/28	0/3/3/3
1	OMU	2A	2552	1,56	-	0/9/27/28	0/2/2/2
54	5MU	2y	54	54	-	3/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
1	5MU	1A	1915	1	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	1,56	-	0/7/25/26	0/2/2/2
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
54	PSU	2y	39	54	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
54	PSU	2y	32	54	-	0/7/25/26	0/2/2/2
54	MIA	2y	37	54	-	3/7/25/34	0/3/3/3
1	OMG	1A	2251	1,56,55	-	0/9/27/28	0/3/3/3
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	1,56	-	0/7/25/26	0/2/2/2
54	G7M	1y	46	54	-	3/7/25/26	0/3/3/3
32	5MC	1a	967	32	-	1/7/25/26	0/2/2/2
1	5MU	2A	1915	1,56	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	3/7/12/14	-
32	MA6	1a	1519	32	-	2/11/29/30	0/3/3/3
43	0TD	2l	92	43	-	3/7/12/14	-
54	PSU	2y	55	54	-	4/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	1,56,55	-	2/9/27/28	0/3/3/3
32	G7M	2a	527	32,56	-	2/7/25/26	0/3/3/3
54	MIA	1y	37	54	-	0/7/25/34	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	3/11/29/30	0/3/3/3
54	MIA	2w	37	54	-	2/11/29/34	0/3/3/3
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
54	4SU	2y	8	54	-	2/7/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	1,56	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32,56	-	2/9/29/30	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
1	5MC	1A	1942	1,56	-	0/7/25/26	0/2/2/2
54	PSU	1y	32	54	-	0/7/25/26	0/2/2/2
54	G7M	2w	46	54	-	1/7/25/26	0/3/3/3
1	5MU	1A	1939	1,56	-	0/7/25/26	0/2/2/2
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
1	2MA	1A	2503	1,56	-	2/7/25/26	0/3/3/3
1	OMC	1A	1920	1	-	0/9/27/28	0/2/2/2
54	4SU	1y	8	54	-	3/7/25/26	0/2/2/2
55	PSU	1x	55	55	-	2/7/25/26	0/2/2/2
1	PSU	1A	2605	1,56	-	0/7/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
55	5MU	1x	54	55	-	0/7/25/26	0/2/2/2
54	PSU	1y	39	54	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
54	G7M	2y	46	54	-	2/7/25/26	0/3/3/3
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/9/27/28	0/3/3/3
32	4OC	1a	1402	32,56	-	1/9/29/30	0/2/2/2
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
54	PSU	1y	55	54	-	2/7/25/26	0/2/2/2
1	OMU	1A	2552	1	-	0/9/27/28	0/2/2/2
54	MIA	1w	37	54	-	1/15/33/34	0/3/3/3
32	G7M	1a	527	32,56	-	3/7/25/26	0/3/3/3
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	2/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	1,56	-	0/7/25/26	0/3/3/3

All (250) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-12.51	1.69	1.82
43	2l	92	0TD	CB-SB	-12.43	1.69	1.82
54	2w	37	MIA	C2-S10	-6.82	1.70	1.75
32	1a	1404	5MC	C5-C4	6.79	1.49	1.44
54	1w	37	MIA	C13-C14	6.76	1.52	1.32
54	1w	37	MIA	C2-S10	-6.71	1.70	1.75
32	2a	1400	5MC	C5-C4	6.59	1.49	1.44
1	1A	1962	5MC	C5-C4	6.41	1.49	1.44
32	2a	967	5MC	C5-C4	6.31	1.48	1.44
55	1x	32	5MC	C5-C4	6.05	1.48	1.44
32	1a	967	5MC	C5-C4	5.94	1.48	1.44
32	2a	1404	5MC	C5-C4	5.93	1.48	1.44
1	2A	1962	5MC	C5-C4	5.92	1.48	1.44
32	1a	1400	5MC	C5-C4	5.80	1.48	1.44
32	2a	1407	5MC	C5-C4	5.79	1.48	1.44
55	2x	32	5MC	C5-C4	5.69	1.48	1.44
32	1a	1407	5MC	C5-C4	5.61	1.48	1.44
1	2A	1942	5MC	C5-C4	5.38	1.48	1.44
54	1y	37	MIA	C5-C4	5.36	1.48	1.39
54	2y	37	MIA	C5-C4	5.33	1.48	1.39
54	2w	37	MIA	C5-C4	5.03	1.48	1.39
54	1w	37	MIA	C5-C4	4.90	1.47	1.39
55	2x	8	4SU	C4-N3	-4.79	1.32	1.37
54	2y	8	4SU	C4-S4	-4.73	1.60	1.68
55	1x	8	4SU	C4-N3	-4.72	1.32	1.37
54	1y	8	4SU	C4-S4	-4.69	1.60	1.68
1	1A	1942	5MC	C5-C4	4.69	1.47	1.44
54	1w	46	G7M	C5-N7	-4.67	1.33	1.39
54	1w	8	4SU	C4-S4	-4.67	1.60	1.68
54	2y	46	G7M	C5-N7	-4.64	1.33	1.39
32	1a	527	G7M	C5-N7	-4.59	1.33	1.39
55	1x	8	4SU	C4-S4	-4.55	1.60	1.68
54	1y	46	G7M	C5-N7	-4.50	1.34	1.39
54	2w	8	4SU	C4-S4	-4.47	1.60	1.68
55	2x	8	4SU	C4-S4	-4.29	1.61	1.68
54	2w	46	G7M	C5-N7	-4.16	1.34	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2w	39	PSU	C6-C5	4.12	1.39	1.35
54	1y	39	PSU	C6-C5	4.12	1.39	1.35
1	1A	2503	2MA	C5-C4	4.06	1.46	1.39
32	2a	527	G7M	C5-N7	-4.06	1.34	1.39
1	2A	2503	2MA	C5-C4	4.02	1.46	1.39
54	1w	55	PSU	C6-C5	4.00	1.39	1.35
54	2y	32	PSU	C6-C5	3.94	1.39	1.35
54	2w	55	PSU	C6-C5	3.92	1.39	1.35
54	2y	39	PSU	C6-C5	3.91	1.39	1.35
1	1A	1911	PSU	C6-C5	3.88	1.39	1.35
54	1y	32	PSU	C6-C5	3.87	1.39	1.35
54	1y	55	PSU	C6-C5	3.87	1.39	1.35
54	2y	46	G7M	C5-C4	3.79	1.47	1.38
1	1A	1917	PSU	C6-C5	3.77	1.39	1.35
55	1x	8	4SU	C2-N3	-3.73	1.31	1.38
54	1y	46	G7M	C5-C4	3.64	1.47	1.38
1	2A	1911	PSU	C6-C5	3.64	1.39	1.35
32	2a	516	PSU	C6-C5	3.62	1.39	1.35
54	2w	32	PSU	C6-C5	3.57	1.39	1.35
43	2l	92	0TD	CB-CA	3.55	1.55	1.54
54	1y	8	4SU	C4-N3	-3.54	1.34	1.37
32	1a	516	PSU	C6-C5	3.52	1.39	1.35
55	2x	55	PSU	C6-C5	3.52	1.39	1.35
1	2A	1917	PSU	C6-C5	3.47	1.39	1.35
54	1w	46	G7M	C5-C4	3.42	1.46	1.38
32	1a	527	G7M	C5-C4	3.41	1.46	1.38
32	2a	966	M2G	C5-C4	3.38	1.48	1.38
32	2a	527	G7M	C5-C4	3.38	1.46	1.38
32	2a	1207	2MG	C5-C4	3.32	1.47	1.38
54	1w	32	PSU	C6-C5	3.29	1.38	1.35
1	2A	2605	PSU	C6-C5	3.27	1.38	1.35
55	1x	8	4SU	C5-C4	-3.26	1.38	1.42
54	2y	54	5MU	C2-N1	3.22	1.43	1.38
55	1x	55	PSU	C6-C5	3.21	1.38	1.35
32	1a	966	M2G	C5-C4	3.19	1.47	1.38
54	1w	39	PSU	C6-C5	3.19	1.38	1.35
1	2A	2251	OMG	C5-C4	3.17	1.47	1.38
54	2w	46	G7M	C5-C4	3.17	1.46	1.38
54	1y	37	MIA	C5-C6	3.14	1.49	1.41
54	1y	54	5MU	C6-C5	3.12	1.39	1.34
54	1w	8	4SU	C4-N3	-3.11	1.34	1.37
1	1A	1939	5MU	C4-N3	-3.10	1.33	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	2x	8	4SU	C5-C4	-3.08	1.38	1.42
54	2y	55	PSU	C6-C5	3.08	1.38	1.35
55	1x	32	5MC	C6-C5	3.07	1.39	1.34
1	1A	2251	OMG	C5-C4	3.07	1.47	1.38
54	2y	37	MIA	C5-C6	3.06	1.49	1.41
54	2y	54	5MU	C6-C5	3.01	1.39	1.34
32	1a	966	M2G	C2-N2	2.99	1.40	1.35
54	2w	54	5MU	C6-C5	2.98	1.39	1.34
54	1y	54	5MU	C4-N3	-2.97	1.33	1.38
1	2A	1942	5MC	C6-C5	2.94	1.39	1.34
55	2x	8	4SU	C2-N3	-2.94	1.32	1.38
54	2w	37	MIA	C5-C6	2.93	1.49	1.41
54	2w	8	4SU	C4-N3	-2.93	1.34	1.37
32	1a	1207	2MG	C5-C4	2.93	1.46	1.38
55	2x	54	5MU	C6-C5	2.92	1.39	1.34
1	1A	2605	PSU	C4-N3	-2.90	1.33	1.38
55	2x	32	5MC	C6-C5	2.88	1.39	1.34
32	2a	1404	5MC	C6-C5	2.87	1.39	1.34
32	2a	967	5MC	C6-C5	2.87	1.39	1.34
54	2w	39	PSU	C4-N3	-2.87	1.33	1.38
32	1a	1400	5MC	C6-C5	2.86	1.39	1.34
54	2y	8	4SU	C4-N3	-2.86	1.34	1.37
32	2a	966	M2G	C2-N2	2.83	1.40	1.35
32	2a	1407	5MC	C6-C5	2.80	1.39	1.34
1	2A	1939	5MU	C6-C5	2.77	1.39	1.34
54	1w	37	MIA	C5-C6	2.76	1.48	1.41
1	1A	1939	5MU	C6-C5	2.72	1.39	1.34
1	2A	1939	5MU	C4-N3	-2.71	1.33	1.38
54	1w	54	5MU	C4-N3	-2.71	1.33	1.38
55	1x	54	5MU	C6-C5	2.70	1.39	1.34
1	2A	1911	PSU	C4-N3	-2.70	1.33	1.38
32	1a	967	5MC	C6-C5	2.69	1.39	1.34
1	1A	2605	PSU	C6-C5	2.68	1.38	1.35
1	1A	1915	5MU	C6-C5	2.67	1.39	1.34
32	1a	1498	UR3	C2-N1	2.65	1.42	1.38
54	1w	39	PSU	C4-N3	-2.65	1.33	1.38
55	1x	54	5MU	C4-N3	-2.65	1.33	1.38
1	2A	2552	OMU	C4-N3	-2.64	1.34	1.38
1	2A	2605	PSU	C4-N3	-2.64	1.33	1.38
54	1w	32	PSU	C4-N3	-2.63	1.33	1.38
1	2A	1915	5MU	C6-C5	2.63	1.38	1.34
1	1A	1917	PSU	C4-N3	-2.63	1.33	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1a	1407	5MC	C6-C5	2.62	1.38	1.34
1	2A	1915	5MU	C4-C5	2.61	1.49	1.44
32	1a	1404	5MC	C6-C5	2.61	1.38	1.34
54	2y	54	5MU	C4-C5	2.60	1.49	1.44
54	1w	54	5MU	C6-C5	2.59	1.38	1.34
1	1A	1915	5MU	C2-N1	2.59	1.42	1.38
54	2y	8	4SU	C5-C4	-2.59	1.39	1.42
1	1A	1915	5MU	C4-N3	-2.59	1.34	1.38
54	2y	37	MIA	C8-N7	2.59	1.36	1.31
54	2y	39	PSU	C4-N3	-2.59	1.34	1.38
1	2A	1939	5MU	C4-C5	2.59	1.49	1.44
32	1a	966	M2G	C6-N1	-2.57	1.34	1.38
1	1A	2552	OMU	C4-N3	-2.57	1.34	1.38
32	1a	1404	5MC	C6-N1	-2.56	1.33	1.38
32	2a	1400	5MC	C6-C5	2.55	1.38	1.34
54	2y	46	G7M	C6-N1	-2.55	1.34	1.38
1	1A	2251	OMG	C6-N1	-2.54	1.34	1.38
1	2A	1962	5MC	C6-C5	2.54	1.38	1.34
54	1w	8	4SU	C5-C4	-2.54	1.39	1.42
1	1A	1911	PSU	C4-N3	-2.53	1.34	1.38
1	1A	1962	5MC	C6-C5	2.53	1.38	1.34
1	1A	1942	5MC	C6-C5	2.52	1.38	1.34
1	2A	1917	PSU	C4-N3	-2.52	1.34	1.38
1	2A	1915	5MU	C2-N1	2.51	1.42	1.38
54	1y	39	PSU	C4-N3	-2.51	1.34	1.38
54	2w	54	5MU	C2-N1	2.50	1.42	1.38
1	2A	1915	5MU	C4-N3	-2.50	1.34	1.38
54	1y	8	4SU	C5-C4	-2.49	1.39	1.42
54	1w	54	5MU	C4-C5	2.48	1.48	1.44
55	2x	54	5MU	C4-C5	2.48	1.48	1.44
54	2y	54	5MU	C4-N3	-2.47	1.34	1.38
32	1a	1207	2MG	C6-N1	-2.47	1.34	1.38
54	2y	55	PSU	C4-N3	-2.46	1.34	1.38
32	1a	516	PSU	C4-N3	-2.46	1.34	1.38
54	1w	55	PSU	C4-N3	-2.46	1.34	1.38
54	1w	37	MIA	C5-N7	-2.46	1.34	1.39
54	2w	54	5MU	C4-N3	-2.46	1.34	1.38
1	1A	1939	5MU	C2-N3	-2.46	1.33	1.38
55	1x	54	5MU	C4-C5	2.45	1.48	1.44
54	1y	37	MIA	C8-N7	2.45	1.36	1.31
1	2A	1962	5MC	C6-N1	-2.45	1.33	1.38
55	2x	55	PSU	C4-N3	-2.45	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1939	5MU	C6-N1	-2.44	1.33	1.38
1	1A	1942	5MC	C6-N1	-2.43	1.33	1.38
54	1y	46	G7M	C6-N1	-2.43	1.34	1.38
54	1y	32	PSU	C4-N3	-2.41	1.34	1.38
1	2A	2503	2MA	C5-N7	-2.41	1.34	1.39
55	2x	54	5MU	C4-N3	-2.41	1.34	1.38
1	1A	2503	2MA	C5-N7	-2.41	1.34	1.39
32	1a	527	G7M	C6-N1	-2.40	1.34	1.38
54	2y	32	PSU	C4-N3	-2.39	1.34	1.38
54	1w	37	MIA	C8-N7	2.39	1.36	1.31
54	1y	55	PSU	C4-N3	-2.38	1.34	1.38
1	1A	2552	OMU	C2-N3	-2.37	1.33	1.38
1	2A	1939	5MU	C6-N1	-2.37	1.34	1.38
32	2a	1207	2MG	C6-N1	-2.37	1.34	1.38
32	2a	1498	UR3	C2-N1	2.36	1.41	1.38
1	2A	2251	OMG	C6-N1	-2.35	1.34	1.38
32	2a	1400	5MC	C6-N1	-2.35	1.34	1.38
55	1x	55	PSU	C4-N3	-2.35	1.34	1.38
54	2w	37	MIA	C8-N7	2.34	1.36	1.31
32	2a	516	PSU	C4-N3	-2.34	1.34	1.38
55	2x	8	4SU	O2-C2	2.34	1.27	1.23
1	1A	1962	5MC	C6-N1	-2.33	1.34	1.38
54	2w	55	PSU	C4-N3	-2.33	1.34	1.38
1	1A	1915	5MU	C4-C5	2.32	1.48	1.44
32	1a	967	5MC	C6-N1	-2.32	1.34	1.38
1	2A	2605	PSU	C2-N3	-2.31	1.33	1.37
1	1A	2503	2MA	C5-C6	2.31	1.47	1.41
54	1w	46	G7M	C6-N1	-2.29	1.34	1.38
1	2A	2503	2MA	C5-C6	2.28	1.47	1.41
32	2a	527	G7M	C6-N1	-2.28	1.34	1.38
54	1y	54	5MU	C2-N1	2.27	1.42	1.38
54	2w	54	5MU	C4-C5	2.26	1.48	1.44
54	1w	54	5MU	C2-N3	-2.26	1.34	1.38
55	1x	32	5MC	C6-N1	-2.26	1.34	1.38
54	2w	32	PSU	C4-N3	-2.25	1.34	1.38
1	2A	2503	2MA	C4-N9	-2.25	1.33	1.37
32	2a	1404	5MC	C6-N1	-2.24	1.34	1.38
1	1A	2605	PSU	C2-N3	-2.23	1.33	1.37
55	2x	54	5MU	C2-N1	2.23	1.42	1.38
54	2w	8	4SU	C5-C4	-2.23	1.39	1.42
1	2A	2503	2MA	C8-N7	2.22	1.36	1.31
54	1w	8	4SU	C2-N1	2.22	1.41	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1x	54	5MU	C6-N1	-2.20	1.34	1.38
1	1A	2251	OMG	C5-N7	-2.19	1.34	1.39
32	1a	1400	5MC	C6-N1	-2.18	1.34	1.38
32	2a	1407	5MC	C6-N1	-2.18	1.34	1.38
54	2w	8	4SU	C2-N1	2.18	1.41	1.38
32	2a	966	M2G	C6-N1	-2.18	1.34	1.38
1	2A	1915	5MU	C6-N1	-2.17	1.34	1.38
32	2a	1498	UR3	C6-C5	2.16	1.40	1.35
32	1a	1407	5MC	C6-N1	-2.16	1.34	1.38
54	1y	8	4SU	C2-N3	-2.15	1.34	1.38
54	2w	46	G7M	C4-N9	-2.14	1.32	1.38
54	2w	37	MIA	C5-N7	-2.14	1.35	1.39
54	1y	8	4SU	C2-N1	2.13	1.41	1.38
32	2a	527	G7M	C5-C6	2.13	1.49	1.43
55	1x	54	5MU	C2-N1	2.13	1.41	1.38
1	1A	2605	PSU	C2-N1	-2.12	1.33	1.36
1	2A	1942	5MC	C6-N1	-2.11	1.34	1.38
32	2a	967	5MC	C6-N1	-2.11	1.34	1.38
1	2A	2251	OMG	C5-N7	-2.11	1.34	1.39
55	1x	54	5MU	C2-N3	-2.11	1.34	1.38
54	2y	8	4SU	C2-N1	2.10	1.41	1.38
1	2A	1915	5MU	C2-N3	-2.10	1.34	1.38
54	1y	54	5MU	O2-C2	2.10	1.26	1.23
32	2a	1207	2MG	C5-N7	-2.10	1.34	1.39
1	1A	1917	PSU	C2-N3	-2.09	1.34	1.37
54	2w	8	4SU	C6-C5	2.09	1.39	1.35
1	2A	2552	OMU	C2-N3	-2.09	1.34	1.38
54	1w	54	5MU	C2-N1	2.08	1.41	1.38
1	1A	1915	5MU	C6-N1	-2.08	1.34	1.38
54	1w	8	4SU	C2-N3	-2.07	1.34	1.38
54	2w	46	G7M	C5-C6	2.06	1.48	1.43
32	1a	527	G7M	C4-N9	-2.06	1.32	1.38
32	1a	1207	2MG	C4-N9	-2.06	1.32	1.38
32	1a	516	PSU	C2-N3	-2.06	1.34	1.37
1	2A	1939	5MU	C2-N3	-2.05	1.34	1.38
55	1x	8	4SU	C6-C5	2.05	1.39	1.35
32	2a	966	M2G	C5-N7	-2.05	1.35	1.39
54	1w	54	5MU	C6-N1	-2.04	1.34	1.38
54	1y	54	5MU	C4-C5	2.04	1.48	1.44
54	1y	8	4SU	C6-C5	2.03	1.39	1.35
32	1a	966	M2G	C5-N7	-2.03	1.35	1.39
54	2w	8	4SU	C2-N3	-2.02	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	2552	OMU	C5-C4	-2.02	1.39	1.43
55	2x	32	5MC	C6-N1	-2.01	1.34	1.38
55	2x	54	5MU	C6-N1	-2.00	1.34	1.38
1	1A	2552	OMU	C6-C5	2.00	1.39	1.35

All (394) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	2l	92	0TD	CSB-SB-CB	-22.41	62.09	102.36
43	1l	92	0TD	CSB-SB-CB	-11.49	81.70	102.36
54	1w	37	MIA	C12-C13-C14	-9.19	110.52	127.01
54	2w	37	MIA	C5-C4-N3	-8.33	118.41	127.18
54	1w	37	MIA	C5-C4-N3	-8.30	118.44	127.18
1	2A	2503	2MA	C5-C4-N3	-7.92	118.84	127.18
1	1A	2503	2MA	C5-C4-N3	-7.82	118.95	127.18
32	1a	1207	2MG	C2-N3-C4	7.05	120.82	112.00
1	1A	2503	2MA	N3-C4-N9	6.97	135.83	126.99
32	2a	1498	UR3	C4-N3-C2	-6.79	119.12	124.58
54	1w	39	PSU	N1-C2-N3	6.73	122.27	115.17
32	2a	1207	2MG	C2-N3-C4	6.69	120.37	112.00
32	1a	1498	UR3	C4-N3-C2	-6.56	119.30	124.58
1	1A	1917	PSU	N1-C2-N3	6.55	122.08	115.17
1	1A	2251	OMG	C5-C4-N3	-6.53	118.00	128.39
55	2x	55	PSU	N1-C2-N3	6.53	122.06	115.17
54	2w	37	MIA	N3-C4-N9	6.53	135.27	126.99
54	1w	37	MIA	N3-C4-N9	6.41	135.13	126.99
54	2y	46	G7M	N9-C4-N3	6.41	138.76	125.95
54	1y	55	PSU	N1-C2-N3	6.35	121.87	115.17
1	2A	1917	PSU	N1-C2-N3	6.35	121.86	115.17
55	1x	55	PSU	N1-C2-N3	6.33	121.85	115.17
32	1a	966	M2G	C5-C4-N3	-6.30	118.36	128.39
54	2w	8	4SU	C4-N3-C2	-6.27	121.31	127.31
1	1A	2605	PSU	N1-C2-N3	6.26	121.77	115.17
32	1a	516	PSU	N1-C2-N3	6.22	121.73	115.17
54	2w	55	PSU	N1-C2-N3	6.21	121.72	115.17
54	1y	39	PSU	N1-C2-N3	6.21	121.72	115.17
54	2w	32	PSU	N1-C2-N3	6.12	121.62	115.17
32	2a	966	M2G	C5-C4-N3	-6.11	118.67	128.39
54	2y	8	4SU	C4-N3-C2	-6.07	121.50	127.31
1	2A	2251	OMG	C5-C4-N3	-6.05	118.76	128.39
1	1A	1911	PSU	N1-C2-N3	6.03	121.53	115.17
1	2A	2503	2MA	N3-C4-N9	6.00	134.60	126.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2y	32	PSU	N1-C2-N3	5.96	121.45	115.17
54	1w	55	PSU	N1-C2-N3	5.94	121.44	115.17
54	1y	37	MIA	C5-C4-N3	-5.94	118.54	126.72
54	1y	46	G7M	N9-C4-N3	5.92	137.78	125.95
54	1y	32	PSU	N1-C2-N3	5.85	121.34	115.17
1	2A	1911	PSU	N1-C2-N3	5.82	121.31	115.17
32	2a	516	PSU	N1-C2-N3	5.80	121.29	115.17
1	2A	1939	5MU	C4-N3-C2	-5.79	119.75	127.34
32	2a	1207	2MG	C5-C4-N3	-5.76	119.22	128.39
1	2A	2605	PSU	N1-C2-N3	5.76	121.25	115.17
54	2y	55	PSU	N1-C2-N3	5.71	121.19	115.17
54	2y	46	G7M	C5-C4-N3	-5.68	117.41	128.15
54	1w	8	4SU	C4-N3-C2	-5.67	121.88	127.31
32	1a	1207	2MG	C5-C4-N3	-5.63	119.42	128.39
1	1A	1939	5MU	C4-N3-C2	-5.60	119.99	127.34
54	1w	32	PSU	N1-C2-N3	5.58	121.06	115.17
54	2y	37	MIA	C5-C4-N3	-5.57	119.05	126.72
1	2A	1915	5MU	C4-N3-C2	-5.47	120.16	127.34
54	1y	46	G7M	C5-C4-N3	-5.47	117.81	128.15
1	1A	2552	OMU	C4-N3-C2	-5.43	119.87	126.61
1	1A	2251	OMG	C2-N3-C4	5.42	121.64	112.30
32	2a	527	G7M	N9-C4-N3	5.36	136.68	125.95
55	1x	54	5MU	N3-C2-N1	5.33	121.83	114.89
55	2x	54	5MU	N3-C2-N1	5.32	121.82	114.89
54	2y	8	4SU	C5-C4-N3	5.32	119.70	114.75
1	1A	1939	5MU	C5-C4-N3	5.30	119.93	115.32
54	2y	39	PSU	N1-C2-N3	5.28	120.74	115.17
54	1w	46	G7M	N9-C4-N3	5.22	136.39	125.95
55	1x	54	5MU	C4-N3-C2	-5.18	120.55	127.34
1	1A	1915	5MU	N3-C2-N1	5.16	121.61	114.89
1	2A	1939	5MU	C5-C4-N3	5.15	119.80	115.32
1	2A	1915	5MU	C5-C4-N3	5.13	119.78	115.32
32	1a	527	G7M	N9-C4-N3	5.13	136.21	125.95
32	1a	1519	MA6	N1-C2-N3	-5.11	120.84	128.58
32	2a	527	G7M	C5-C4-N3	-5.10	118.50	128.15
1	1A	1915	5MU	C4-N3-C2	-5.09	120.67	127.34
32	1a	527	G7M	C5-C4-N3	-5.08	118.55	128.15
1	2A	1939	5MU	N3-C2-N1	5.07	121.49	114.89
32	1a	1518	MA6	N1-C2-N3	-5.06	120.92	128.58
54	1w	8	4SU	C5-C4-N3	5.06	119.46	114.75
1	1A	2251	OMG	N9-C4-N3	5.06	136.06	125.95
1	1A	2552	OMU	N3-C2-N1	5.05	121.46	114.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	2x	54	5MU	C4-N3-C2	-5.02	120.75	127.34
54	2y	46	G7M	C2-N3-C4	5.02	120.95	112.30
54	2w	39	PSU	N1-C2-N3	4.98	120.42	115.17
54	2w	8	4SU	C5-C4-N3	4.97	119.38	114.75
1	1A	1939	5MU	N3-C2-N1	4.97	121.36	114.89
54	1y	8	4SU	C4-N3-C2	-4.97	122.55	127.31
1	2A	1915	5MU	N3-C2-N1	4.87	121.23	114.89
1	2A	2251	OMG	C2-N3-C4	4.87	120.69	112.30
32	2a	1518	MA6	N1-C2-N3	-4.87	121.22	128.58
54	2w	46	G7M	N9-C4-N3	4.86	135.68	125.95
54	1y	46	G7M	C2-N3-C4	4.79	120.54	112.30
54	2w	46	G7M	C5-C4-N3	-4.77	119.13	128.15
32	1a	1519	MA6	C5-C4-N3	-4.77	120.15	126.72
54	1w	46	G7M	C5-C4-N3	-4.76	119.15	128.15
54	1y	8	4SU	C5-C4-N3	4.71	119.13	114.75
32	2a	1519	MA6	N1-C2-N3	-4.71	121.45	128.58
32	2a	966	M2G	N9-C4-N3	4.68	135.30	125.95
1	1A	1939	5MU	C5-C6-N1	-4.68	118.23	123.31
54	1w	54	5MU	N3-C2-N1	4.66	120.95	114.89
32	1a	966	M2G	C2-N3-C4	4.64	121.09	112.51
1	2A	2552	OMU	C4-N3-C2	-4.63	120.86	126.61
32	1a	966	M2G	N9-C4-N3	4.63	135.21	125.95
32	2a	1519	MA6	C5-C4-N3	-4.63	120.34	126.72
54	1w	54	5MU	C4-N3-C2	-4.59	121.32	127.34
1	2A	2251	OMG	N9-C4-N3	4.59	135.14	125.95
32	2a	527	G7M	C2-N3-C4	4.58	120.19	112.30
54	1y	37	MIA	N3-C4-N9	4.57	134.94	127.17
1	2A	1939	5MU	C5-C6-N1	-4.55	118.37	123.31
1	1A	1939	5MU	O4-C4-C5	-4.53	119.73	124.92
54	2w	46	G7M	C2-N3-C4	4.50	120.05	112.30
32	1a	527	G7M	C2-N3-C4	4.49	120.04	112.30
54	1w	39	PSU	C4-N3-C2	-4.48	120.20	126.37
1	1A	1915	5MU	C5-C4-N3	4.48	119.21	115.32
32	2a	1518	MA6	C5-C4-N3	-4.45	120.59	126.72
55	2x	55	PSU	C4-N3-C2	-4.42	120.28	126.37
54	2y	54	5MU	N3-C2-N1	4.41	120.63	114.89
54	2y	37	MIA	N3-C4-N9	4.38	134.62	127.17
32	1a	1518	MA6	C2-N1-C6	4.36	122.48	111.83
1	2A	2552	OMU	N3-C2-N1	4.35	120.56	114.89
1	2A	2605	PSU	C4-N3-C2	-4.34	120.39	126.37
54	2w	8	4SU	N3-C2-N1	4.32	120.51	114.89
54	2y	54	5MU	C4-N3-C2	-4.30	121.70	127.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2552	OMU	O2-C2-N1	-4.29	117.21	122.80
32	2a	966	M2G	C2-N3-C4	4.29	120.44	112.51
32	1a	1207	2MG	C6-C5-N7	4.22	137.97	130.29
54	2w	55	PSU	C4-N3-C2	-4.20	120.59	126.37
54	1w	54	5MU	C5-C4-N3	4.20	118.97	115.32
54	2y	55	PSU	C4-N3-C2	-4.18	120.61	126.37
55	1x	54	5MU	C5-C4-N3	4.16	118.94	115.32
54	1w	46	G7M	C2-N3-C4	4.16	119.46	112.30
54	1y	55	PSU	C4-N3-C2	-4.14	120.67	126.37
54	2y	54	5MU	C5-C4-N3	4.11	118.90	115.32
1	1A	2605	PSU	C4-N3-C2	-4.11	120.71	126.37
32	1a	1207	2MG	N1-C2-N2	4.11	120.75	116.56
1	1A	2552	OMU	C5-C4-N3	4.10	120.55	114.80
32	2a	1519	MA6	C4-C5-N7	-4.10	105.89	110.58
1	2A	1915	5MU	O4-C4-C5	-4.10	120.23	124.92
32	2a	1207	2MG	N9-C4-N3	4.06	134.08	125.95
32	2a	1518	MA6	C2-N1-C6	4.06	121.75	111.83
55	1x	55	PSU	O2-C2-N1	-4.06	118.61	122.79
1	1A	1911	PSU	C4-N3-C2	-4.04	120.81	126.37
1	2A	1917	PSU	C4-N3-C2	-4.04	120.81	126.37
32	1a	1519	MA6	C2-N1-C6	4.03	121.67	111.83
1	1A	1915	5MU	O4-C4-C5	-4.01	120.33	124.92
54	1y	39	PSU	C4-N3-C2	-4.00	120.86	126.37
54	1w	37	MIA	C15-C14-C13	-3.99	110.68	122.66
1	1A	1917	PSU	C4-N3-C2	-3.97	120.90	126.37
1	2A	1939	5MU	O4-C4-C5	-3.97	120.38	124.92
54	1w	37	MIA	C16-C14-C13	-3.96	110.77	122.66
54	2y	8	4SU	C5-C4-S4	-3.96	119.78	124.31
32	1a	516	PSU	C4-N3-C2	-3.95	120.93	126.37
55	1x	54	5MU	O4-C4-C5	-3.94	120.41	124.92
55	2x	54	5MU	O4-C4-C5	-3.93	120.42	124.92
55	2x	54	5MU	C5-C4-N3	3.93	118.74	115.32
54	2w	32	PSU	C4-N3-C2	-3.91	120.98	126.37
32	2a	1519	MA6	C5-N7-C8	3.91	109.59	103.45
32	2a	1519	MA6	C2-N1-C6	3.89	121.32	111.83
54	1w	39	PSU	O2-C2-N1	-3.87	118.80	122.79
32	1a	1519	MA6	C5-N7-C8	3.85	109.50	103.45
1	1A	2503	2MA	C4-N9-C8	3.83	109.75	105.74
32	1a	1518	MA6	C5-N7-C8	3.83	109.46	103.45
54	2y	8	4SU	N3-C2-N1	3.80	119.84	114.89
55	1x	32	5MC	C5-C6-N1	-3.80	119.19	123.31
32	1a	1519	MA6	C4-C5-N7	-3.80	106.24	110.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	1x	55	PSU	C4-N3-C2	-3.80	121.14	126.37
54	1y	32	PSU	C4-N3-C2	-3.80	121.14	126.37
54	1y	37	MIA	C4-C5-N7	-3.77	106.27	110.58
1	2A	1915	5MU	C5-C6-N1	-3.75	119.24	123.31
32	2a	516	PSU	C4-N3-C2	-3.74	121.21	126.37
54	2w	32	PSU	O2-C2-N1	-3.72	118.95	122.79
54	2y	32	PSU	C4-N3-C2	-3.71	121.26	126.37
54	1y	54	5MU	C5-C4-N3	3.70	118.54	115.32
55	1x	8	4SU	C6-C5-C4	-3.69	116.75	119.95
54	1y	54	5MU	N3-C2-N1	3.69	119.69	114.89
32	1a	1518	MA6	C5-C4-N3	-3.69	121.64	126.72
54	1w	8	4SU	N3-C2-N1	3.68	119.69	114.89
1	2A	2503	2MA	C4-C5-N7	-3.68	106.37	110.58
54	1y	37	MIA	C2-N3-C4	3.67	120.80	111.83
54	1w	55	PSU	C4-N3-C2	-3.67	121.31	126.37
32	2a	1400	5MC	C5-C6-N1	-3.67	119.33	123.31
32	1a	1519	MA6	C2-N3-C4	3.64	120.72	111.83
54	2w	54	5MU	N3-C2-N1	3.64	119.62	114.89
1	2A	1911	PSU	C4-N3-C2	-3.64	121.36	126.37
32	2a	1518	MA6	C5-N7-C8	3.63	109.16	103.45
1	1A	1942	5MC	C5-C6-N1	-3.61	119.39	123.31
55	2x	55	PSU	O2-C2-N1	-3.60	119.07	122.79
32	1a	1518	MA6	N9-C8-N7	-3.59	108.84	113.94
1	2A	1917	PSU	O2-C2-N1	-3.58	119.09	122.79
54	2y	37	MIA	C2-N3-C4	3.58	120.58	111.83
54	2w	54	5MU	O4-C4-C5	-3.58	120.82	124.92
54	2y	37	MIA	C4-C5-N7	-3.57	106.50	110.58
54	2w	55	PSU	O2-C2-N1	-3.55	119.13	122.79
54	2w	54	5MU	C5-C4-N3	3.51	118.38	115.32
54	1w	32	PSU	C4-N3-C2	-3.51	121.54	126.37
32	2a	1518	MA6	C4-C5-N7	-3.50	106.58	110.58
54	1w	37	MIA	C2-N3-C4	3.49	121.44	112.29
32	1a	1518	MA6	C4-C5-N7	-3.49	106.59	110.58
32	1a	1207	2MG	N9-C4-N3	3.48	132.91	125.95
54	2w	37	MIA	C2-N3-C4	3.47	121.37	112.29
1	1A	1911	PSU	O2-C2-N1	-3.47	119.21	122.79
54	1y	54	5MU	C4-N3-C2	-3.46	122.80	127.34
55	1x	54	5MU	C5-C6-N1	-3.46	119.55	123.31
54	2w	54	5MU	C4-N3-C2	-3.45	122.81	127.34
32	2a	1519	MA6	C2-N3-C4	3.45	120.27	111.83
54	2y	55	PSU	O2-C2-N1	-3.45	119.23	122.79
54	1y	54	5MU	O4-C4-C5	-3.44	120.98	124.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	967	5MC	C5-C6-N1	-3.44	119.58	123.31
32	2a	1404	5MC	C5-C6-N1	-3.44	119.58	123.31
1	1A	2503	2MA	N6-C6-N1	3.44	121.66	117.03
54	2y	54	5MU	O4-C4-C5	-3.43	121.00	124.92
54	2y	37	MIA	N3-C2-N1	-3.41	123.42	128.58
1	2A	2552	OMU	C5-C4-N3	3.41	119.57	114.80
32	2a	1518	MA6	C2-N3-C4	3.40	120.14	111.83
54	1y	8	4SU	N3-C2-N1	3.40	119.32	114.89
32	1a	1207	2MG	N2-C2-N3	-3.40	116.18	120.51
32	1a	1207	2MG	C4-C5-N7	-3.40	105.28	110.67
54	1y	55	PSU	O2-C2-N1	-3.39	119.29	122.79
54	2w	37	MIA	C4-C5-N7	-3.38	106.72	110.58
32	1a	1519	MA6	N9-C8-N7	-3.38	109.14	113.94
1	2A	1939	5MU	O2-C2-N1	-3.38	118.40	122.80
54	1w	55	PSU	O2-C2-N1	-3.36	119.32	122.79
32	2a	1207	2MG	C6-C5-N7	3.35	136.38	130.29
32	1a	516	PSU	O2-C2-N1	-3.33	119.35	122.79
54	1y	37	MIA	N3-C2-N1	-3.31	123.58	128.58
1	1A	1962	5MC	C5-C6-N1	-3.30	119.72	123.31
1	2A	1942	5MC	C5-C6-N1	-3.29	119.74	123.31
54	1w	8	4SU	C5-C4-S4	-3.28	120.56	124.31
32	1a	1498	UR3	C5-C4-N3	3.27	119.34	115.04
32	1a	1400	5MC	C5-C6-N1	-3.26	119.77	123.31
54	1w	37	MIA	C4-C5-N7	-3.26	106.86	110.58
32	2a	1519	MA6	N9-C8-N7	-3.24	109.34	113.94
1	2A	1962	5MC	C5-C6-N1	-3.24	119.80	123.31
32	1a	967	5MC	C5-C6-N1	-3.22	119.81	123.31
55	1x	8	4SU	C5-C4-N3	3.22	117.75	114.75
32	2a	1518	MA6	N9-C8-N7	-3.21	109.38	113.94
54	1w	54	5MU	O4-C4-C5	-3.21	121.25	124.92
55	2x	54	5MU	C5-C6-N1	-3.20	119.84	123.31
1	1A	1917	PSU	O2-C2-N1	-3.20	119.49	122.79
54	1w	54	5MU	C5-C6-N1	-3.19	119.85	123.31
1	2A	2552	OMU	O2-C2-N1	-3.19	118.65	122.80
54	2y	32	PSU	O2-C2-N1	-3.18	119.50	122.79
1	2A	2251	OMG	C6-C5-N7	3.18	136.08	130.29
54	2w	8	4SU	C5-C4-S4	-3.17	120.69	124.31
32	1a	1518	MA6	C2-N3-C4	3.13	119.47	111.83
1	1A	2251	OMG	C6-C5-N7	3.12	135.97	130.29
55	2x	8	4SU	C6-C5-C4	-3.12	117.25	119.95
32	1a	966	M2G	C6-C5-N7	3.11	135.94	130.29
1	1A	2605	PSU	O2-C2-N1	-3.10	119.59	122.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1498	UR3	C5-C4-N3	3.10	119.12	115.04
32	1a	1407	5MC	C5-C4-N3	-3.10	118.58	121.75
32	1a	1404	5MC	C5-C6-N1	-3.09	119.95	123.31
1	2A	1911	PSU	O2-C2-N1	-3.08	119.61	122.79
54	1y	54	5MU	C5-C6-N1	-3.06	119.99	123.31
32	2a	1407	5MC	C5-C4-N3	-3.05	118.63	121.75
55	1x	32	5MC	C5-C4-N3	-3.04	118.64	121.75
54	2y	39	PSU	C4-N3-C2	-3.04	122.19	126.37
55	2x	8	4SU	C1'-N1-C2	3.03	123.04	117.59
1	2A	2503	2MA	C4-N9-C8	3.00	108.89	105.74
54	2w	37	MIA	C6-C5-N7	2.97	135.67	132.43
1	1A	2503	2MA	C4-C5-N7	-2.96	107.19	110.58
54	2y	54	5MU	C5-C6-N1	-2.96	120.10	123.31
32	1a	1519	MA6	N3-C4-N9	2.95	132.19	127.17
55	1x	8	4SU	O2-C2-N1	2.95	126.63	122.80
54	1w	32	PSU	O2-C2-N1	-2.92	119.78	122.79
54	1w	37	MIA	C6-C5-N7	2.91	135.60	132.43
32	2a	516	PSU	O2-C2-N1	-2.91	119.79	122.79
1	2A	2503	2MA	N6-C6-N1	2.89	120.93	117.03
1	1A	2503	2MA	C2-N1-C6	2.89	122.54	118.10
32	2a	1407	5MC	C5-C6-N1	-2.89	120.18	123.31
1	1A	1915	5MU	C5-C6-N1	-2.85	120.22	123.31
55	2x	32	5MC	C5-C6-N1	-2.85	120.22	123.31
54	2w	37	MIA	C12-N6-C6	-2.84	120.21	122.85
32	1a	1404	5MC	C5-C4-N3	-2.84	118.85	121.75
32	2a	1518	MA6	N3-C4-N9	2.83	131.99	127.17
32	1a	1400	5MC	C5-C4-N3	-2.82	118.86	121.75
1	1A	1962	5MC	C5-C4-N3	-2.82	118.86	121.75
1	1A	1939	5MU	O2-C2-N1	-2.80	119.15	122.80
55	1x	54	5MU	O2-C2-N1	-2.80	119.16	122.80
55	2x	8	4SU	C5-C4-N3	2.79	117.34	114.75
54	2w	46	G7M	O6-C6-C5	-2.78	121.80	128.01
54	1y	32	PSU	O2-C2-N1	-2.77	119.93	122.79
55	2x	54	5MU	O2-C2-N1	-2.77	119.20	122.80
1	2A	2503	2MA	C5-N7-C8	2.76	107.79	103.45
32	2a	966	M2G	C6-C5-N7	2.75	135.30	130.29
32	1a	1407	5MC	C5-C6-N1	-2.73	120.35	123.31
54	1y	37	MIA	C5-N7-C8	2.70	107.69	103.45
32	2a	1207	2MG	C4-C5-N7	-2.69	106.41	110.67
1	2A	1942	5MC	C5-C4-N3	-2.69	119.00	121.75
1	2A	1962	5MC	C5-C4-N3	-2.68	119.00	121.75
32	2a	1407	5MC	O2-C2-N3	-2.67	118.12	122.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	967	5MC	C5-C4-N3	-2.67	119.02	121.75
1	1A	1920	OMC	O2-C2-N3	-2.66	118.14	122.33
32	1a	967	5MC	C5-C4-N3	-2.65	119.04	121.75
55	2x	32	5MC	C5-C4-N3	-2.65	119.04	121.75
32	2a	1404	5MC	C5-C4-N3	-2.64	119.05	121.75
54	1y	39	PSU	O2-C2-N1	-2.63	120.08	122.79
1	1A	1942	5MC	C5-C4-N3	-2.62	119.07	121.75
1	1A	2503	2MA	C5-N7-C8	2.61	107.55	103.45
1	2A	2552	OMU	O4-C4-C5	-2.59	120.70	125.16
1	1A	2552	OMU	O4-C4-C5	-2.58	120.71	125.16
1	1A	2503	2MA	N9-C8-N7	-2.57	110.28	113.94
54	2y	54	5MU	C1'-N1-C2	2.55	122.18	117.59
32	1a	1404	5MC	CM5-C5-C6	-2.55	119.40	122.85
32	2a	1519	MA6	N3-C4-N9	2.55	131.50	127.17
32	1a	966	M2G	C4-C5-N7	-2.53	106.66	110.67
54	2y	37	MIA	C4-N9-C8	2.52	108.39	105.74
32	1a	1519	MA6	C4-C5-C6	2.52	118.52	115.91
54	1w	54	5MU	C5M-C5-C4	2.52	121.47	118.78
32	2a	1518	MA6	C4-C5-C6	2.51	118.51	115.91
1	2A	2503	2MA	N9-C8-N7	-2.51	110.38	113.94
32	2a	1400	5MC	C5-C4-N3	-2.50	119.20	121.75
1	2A	2251	OMG	C4-C5-N7	-2.49	106.73	110.67
54	2w	54	5MU	C5-C6-N1	-2.49	120.61	123.31
55	2x	32	5MC	O2-C2-N3	-2.48	118.41	122.33
54	2w	39	PSU	C4-N3-C2	-2.48	122.95	126.37
32	2a	1519	MA6	C4-C5-C6	2.48	118.47	115.91
54	2y	37	MIA	C5-N7-C8	2.48	107.34	103.45
43	1l	92	0TD	OD2-CG-CB	2.46	118.47	113.15
55	2x	55	PSU	C5-C6-N1	-2.45	118.74	122.14
1	2A	2605	PSU	C5-C6-N1	-2.43	118.76	122.14
54	2w	37	MIA	C5-N7-C8	2.43	107.27	103.45
54	1w	37	MIA	N3-C2-N1	-2.40	122.61	127.00
32	1a	1518	MA6	N3-C4-N9	2.40	131.25	127.17
1	1A	2251	OMG	C4-C5-N7	-2.40	106.87	110.67
1	2A	2503	2MA	C2-N1-C6	2.40	121.79	118.10
32	1a	1207	2MG	CM2-N2-C2	-2.39	118.51	123.65
1	1A	2251	OMG	O6-C6-C5	-2.38	120.25	126.53
54	1y	8	4SU	C5-C4-S4	-2.38	121.59	124.31
55	1x	8	4SU	C1'-N1-C2	2.37	121.84	117.59
1	1A	1911	PSU	C6-C5-C4	-2.33	116.60	118.17
54	1w	46	G7M	O6-C6-C5	-2.32	122.83	128.01
32	2a	966	M2G	C4-C5-N7	-2.32	106.99	110.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1915	5MU	C5M-C5-C4	2.32	121.25	118.78
54	1w	37	MIA	C2-N1-C6	2.31	121.93	117.54
1	2A	2251	OMG	O6-C6-C5	-2.31	120.45	126.53
1	1A	1915	5MU	C5M-C5-C4	2.30	121.24	118.78
32	2a	1402	4OC	O2-C2-N3	-2.29	118.71	122.33
54	2y	54	5MU	O2-C2-N3	-2.29	117.27	121.49
1	2A	2503	2MA	C6-C5-N7	2.29	136.50	132.09
32	2a	527	G7M	O6-C6-C5	-2.29	122.91	128.01
54	2w	37	MIA	N3-C2-N1	-2.28	122.83	127.00
32	2a	1402	4OC	C6-C5-C4	2.28	119.75	117.00
54	2w	46	G7M	C5-C6-N1	2.27	116.53	111.84
32	2a	527	G7M	C5-C6-N1	2.27	116.52	111.84
54	2w	37	MIA	C2-N1-C6	2.26	121.83	117.54
54	1w	37	MIA	C5-N7-C8	2.25	106.99	103.45
32	1a	1498	UR3	C1'-N1-C2	2.25	120.72	117.04
32	2a	1207	2MG	N1-C2-N2	2.24	118.85	116.56
54	1w	55	PSU	C6-C5-C4	-2.24	116.67	118.17
32	2a	966	M2G	O6-C6-C5	-2.23	120.64	126.53
54	2y	54	5MU	C1'-N1-C6	-2.23	117.48	121.15
1	2A	2605	PSU	O2-C2-N1	-2.22	120.50	122.79
54	1w	54	5MU	O2-C2-N1	-2.22	119.91	122.80
32	2a	1400	5MC	CM5-C5-C6	-2.22	119.85	122.85
32	1a	527	G7M	O6-C6-C5	-2.21	123.07	128.01
32	1a	1207	2MG	C8-N7-C5	2.21	108.20	104.26
1	1A	2605	PSU	C5-C6-N1	-2.20	119.08	122.14
32	1a	1402	4OC	C6-C5-C4	2.20	119.65	117.00
54	1w	39	PSU	C5-C6-N1	-2.20	119.09	122.14
54	1y	55	PSU	O4'-C1'-C2'	2.20	108.19	105.15
1	1A	2251	OMG	C5-C6-N1	2.19	118.83	113.25
54	2w	8	4SU	O2-C2-N1	-2.19	119.95	122.80
32	1a	1404	5MC	O2-C2-N3	-2.18	118.89	122.33
54	2w	37	MIA	C4-N9-C8	2.17	108.02	105.74
32	2a	516	PSU	O4'-C1'-C2'	2.17	108.15	105.15
32	1a	1518	MA6	C4-N9-C8	2.16	108.00	105.74
32	2a	1519	MA6	C5-C4-N9	2.15	108.16	105.81
54	1y	37	MIA	C4-N9-C8	2.14	107.99	105.74
1	1A	2503	2MA	N3-C2-N1	-2.14	121.98	125.77
54	2y	39	PSU	O2-C2-N3	-2.13	118.07	121.86
54	1y	46	G7M	O6-C6-C5	-2.13	123.26	128.01
54	2y	55	PSU	C5-C6-N1	-2.12	119.19	122.14
54	1y	37	MIA	C6-C5-N7	2.12	136.18	132.09
32	1a	1407	5MC	CM5-C5-C6	-2.12	119.98	122.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1y	55	PSU	C5-C6-N1	-2.11	119.22	122.14
1	2A	1917	PSU	C5-C6-N1	-2.10	119.23	122.14
54	2y	54	5MU	C5M-C5-C4	2.09	121.02	118.78
32	1a	1400	5MC	O2-C2-N3	-2.09	119.03	122.33
54	2w	32	PSU	O4'-C1'-C2'	2.09	108.04	105.15
54	2y	37	MIA	C6-C5-N7	2.08	136.10	132.09
1	1A	1915	5MU	O2-C2-N1	-2.08	120.09	122.80
54	1w	8	4SU	C1'-N1-C2	2.07	121.30	117.59
54	1w	37	MIA	C4-N9-C8	2.06	107.90	105.74
54	1y	39	PSU	O2-C2-N3	-2.06	118.20	121.86
55	1x	8	4SU	O2-C2-N3	-2.06	117.69	121.49
32	2a	1207	2MG	N2-C2-N3	-2.06	117.89	120.51
54	2w	39	PSU	O2-C2-N3	-2.06	118.21	121.86
1	1A	2503	2MA	C6-C5-N7	2.05	136.05	132.09
54	1y	39	PSU	C5-C6-N1	-2.05	119.29	122.14
1	2A	1911	PSU	C6-C5-C4	-2.03	116.80	118.17
32	1a	516	PSU	O4'-C1'-C2'	2.03	107.96	105.15
1	2A	2605	PSU	O2-C2-N3	-2.03	118.26	121.86
32	2a	967	5MC	O2-C2-N3	-2.02	119.14	122.33
55	1x	32	5MC	O2-C2-N3	-2.02	119.14	122.33
32	2a	1402	4OC	CM4-N4-C4	-2.02	118.51	122.45
54	2w	39	PSU	C6-C5-C4	-2.01	116.82	118.17
55	2x	8	4SU	O2-C2-N1	2.01	125.41	122.80
54	2w	39	PSU	O4'-C1'-C2'	2.01	107.93	105.15

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	1l	92	0TD	O-C-CA-CB
54	1w	37	MIA	C12-C13-C14-C16
54	1y	8	4SU	O4'-C4'-C5'-O5'
54	1y	46	G7M	C4'-C5'-O5'-P
54	1y	54	5MU	O4'-C4'-C5'-O5'
54	1y	55	PSU	C3'-C4'-C5'-O5'
54	1y	55	PSU	O4'-C4'-C5'-O5'
32	2a	1519	MA6	O4'-C4'-C5'-O5'
43	2l	92	0TD	CA-CB-SB-CSB
43	2l	92	0TD	CG-CB-SB-CSB
54	2w	37	MIA	N1-C2-S10-C11
54	2w	37	MIA	N3-C2-S10-C11
54	2y	8	4SU	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
54	2y	54	5MU	O4'-C4'-C5'-O5'
54	2y	55	PSU	O4'-C1'-C5-C6
54	2y	55	PSU	O4'-C4'-C5'-O5'
32	1a	527	G7M	C3'-C4'-C5'-O5'
32	1a	1519	MA6	O4'-C4'-C5'-O5'
54	1y	8	4SU	C3'-C4'-C5'-O5'
32	2a	1207	2MG	O4'-C4'-C5'-O5'
32	2a	1207	2MG	C3'-C4'-C5'-O5'
54	2y	37	MIA	C3'-C4'-C5'-O5'
54	2y	54	5MU	C3'-C4'-C5'-O5'
54	2y	55	PSU	C3'-C4'-C5'-O5'
54	1y	46	G7M	C3'-C4'-C5'-O5'
32	2a	1402	4OC	O4'-C4'-C5'-O5'
54	2y	8	4SU	C3'-C4'-C5'-O5'
54	2y	37	MIA	O4'-C4'-C5'-O5'
54	1y	54	5MU	C3'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
32	1a	527	G7M	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
55	1x	55	PSU	O4'-C4'-C5'-O5'
32	2a	1402	4OC	C3'-C4'-C5'-O5'
32	1a	1400	5MC	O4'-C4'-C5'-O5'
43	1l	92	0TD	SB-CB-CG-OD1
43	2l	92	0TD	SB-CB-CG-OD1
32	2a	527	G7M	C4'-C5'-O5'-P
54	2w	46	G7M	C4'-C5'-O5'-P
54	1y	46	G7M	O4'-C4'-C5'-O5'
54	2y	37	MIA	C4'-C5'-O5'-P
32	2a	527	G7M	C3'-C4'-C5'-O5'
54	1w	46	G7M	C4'-C5'-O5'-P
32	1a	967	5MC	O4'-C4'-C5'-O5'
54	1y	8	4SU	C4'-C5'-O5'-P
1	2A	2251	OMG	C1'-C2'-O2'-CM2
54	2y	46	G7M	C2'-C1'-N9-C8
32	1a	1402	4OC	O4'-C4'-C5'-O5'
43	1l	92	0TD	CG-CB-SB-CSB
54	2y	55	PSU	C2'-C1'-C5-C6
1	1A	2503	2MA	C4'-C5'-O5'-P
1	2A	2251	OMG	C4'-C5'-O5'-P
55	1x	55	PSU	C3'-C4'-C5'-O5'
54	2y	54	5MU	C2'-C1'-N1-C2
32	1a	527	G7M	C4'-C5'-O5'-P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	2a	1519	MA6	C4'-C5'-O5'-P
54	2y	46	G7M	C2'-C1'-N9-C4
1	1A	2503	2MA	O4'-C4'-C5'-O5'
32	1a	1400	5MC	C3'-C4'-C5'-O5'

There are no ring outliers.

34 monomers are involved in 49 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	2x	8	4SU	2	0
54	1y	54	5MU	1	0
54	2w	39	PSU	1	0
1	2A	1917	PSU	1	0
32	2a	1518	MA6	2	0
32	2a	1207	2MG	1	0
1	1A	1915	5MU	1	0
54	2w	8	4SU	1	0
54	2y	37	MIA	1	0
1	2A	1939	5MU	1	0
32	1a	967	5MC	1	0
1	2A	1915	5MU	1	0
43	1l	92	0TD	2	0
32	1a	1519	MA6	1	0
43	2l	92	0TD	2	0
54	2y	55	PSU	7	0
1	2A	2251	OMG	1	0
54	1y	37	MIA	2	0
32	2a	1519	MA6	2	0
55	2x	55	PSU	1	0
54	2w	46	G7M	1	0
1	1A	1939	5MU	1	0
1	1A	2503	2MA	1	0
54	1y	8	4SU	4	0
54	1y	39	PSU	1	0
32	2a	967	5MC	1	0
54	2y	46	G7M	1	0
32	1a	1402	4OC	1	0
54	1y	55	PSU	1	0
1	1A	2552	OMU	2	0
54	1w	37	MIA	1	0
55	1x	8	4SU	2	0
32	1a	1518	MA6	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2A	2503	2MA	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2879 ligands modelled in this entry, 2875 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
59	SF4	2d	303	35	0,12,12	-	-	-		
58	Y7K	1a	1842	-	33,36,36	0.83	1 (3%)	37,54,54	1.55	5 (13%)
58	Y7K	2a	1841	-	33,36,36	0.70	1 (3%)	37,54,54	1.25	3 (8%)
59	SF4	1d	501	35	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
59	SF4	2d	303	35	-	-	0/6/5/5
58	Y7K	1a	1842	-	-	1/11/77/77	0/4/4/4
58	Y7K	2a	1841	-	-	4/11/77/77	0/4/4/4
59	SF4	1d	501	35	-	-	0/6/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	1a	1842	Y7K	OAP-CAL	2.69	1.44	1.39
58	2a	1841	Y7K	OAP-CAL	2.43	1.43	1.39

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	1a	1842	Y7K	OAS-CAN-OAJ	-6.10	102.52	107.40
58	2a	1841	Y7K	CAR-NAM-CAI	-4.10	108.93	114.23
58	1a	1842	Y7K	CAR-NAM-CAI	-3.94	109.15	114.23
58	2a	1841	Y7K	CAU-CAQ-CAL	-3.17	108.16	110.33
58	2a	1841	Y7K	CAB-NAA-CAC	2.85	117.91	114.23
58	1a	1842	Y7K	CAU-CAQ-CAL	-2.79	108.42	110.33
58	1a	1842	Y7K	CAB-NAA-CAC	-2.52	110.98	114.23
58	1a	1842	Y7K	CAZ-NAY-CAX	-2.44	108.41	113.35

There are no chirality outliers.

All (5) torsion outliers are listed below:

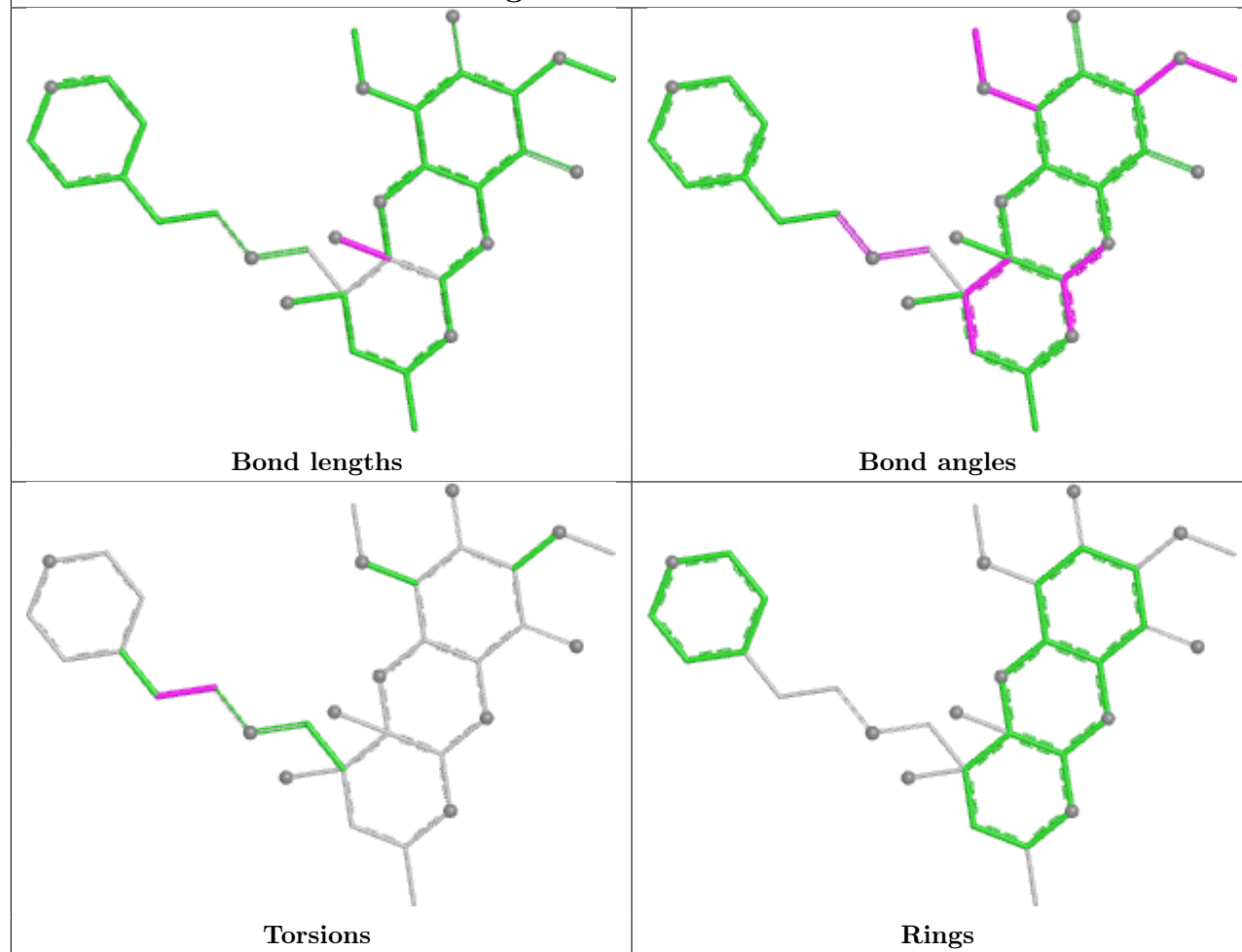
Mol	Chain	Res	Type	Atoms
58	1a	1842	Y7K	NAY-CAZ-CBA-CBB
58	2a	1841	Y7K	NAY-CAZ-CBA-CBB
58	2a	1841	Y7K	CAZ-CBA-CBB-CBC
58	2a	1841	Y7K	CAZ-CBA-CBB-CBG
58	2a	1841	Y7K	CBA-CAZ-NAY-CAX

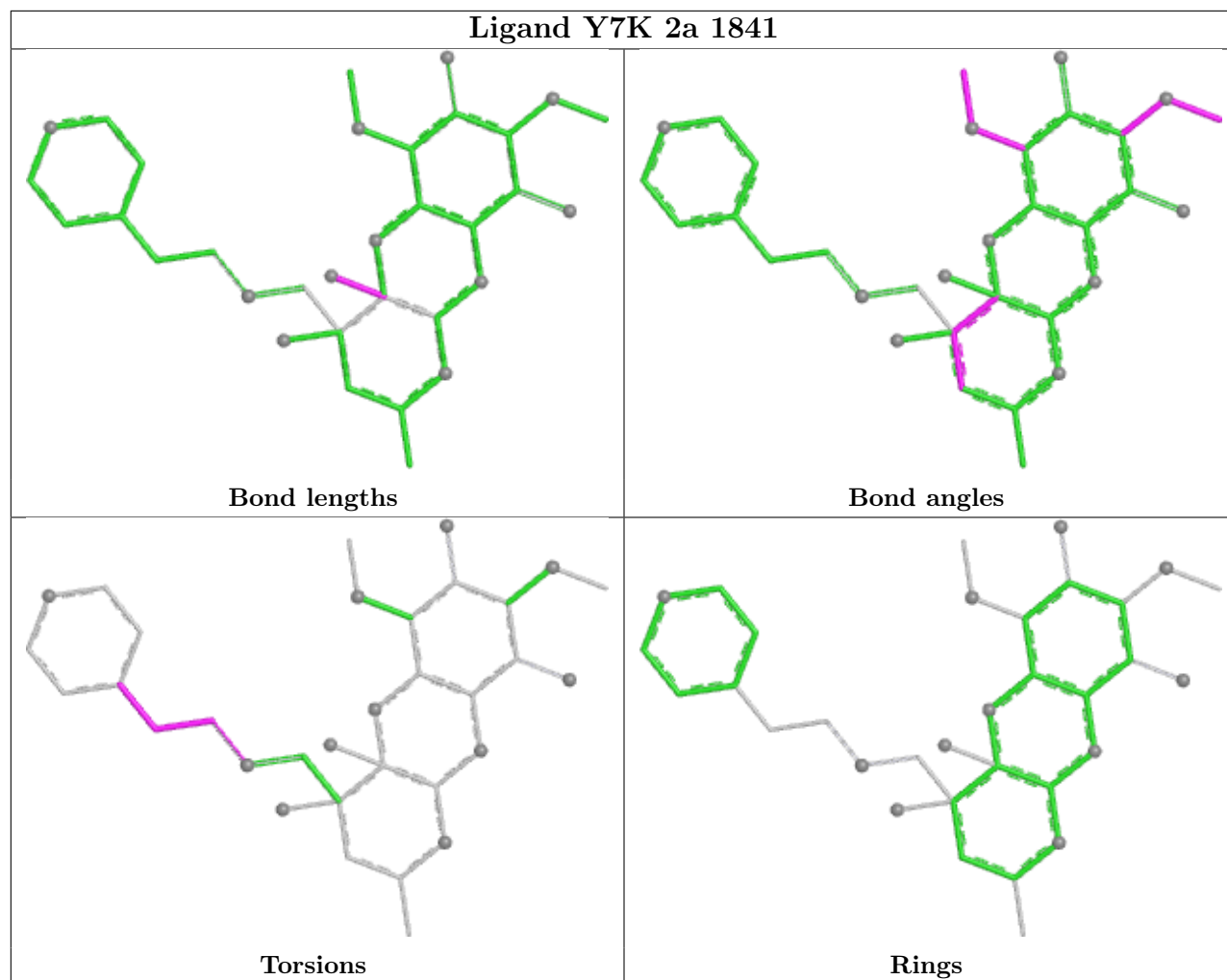
There are no ring outliers.

No monomer is involved in short contacts.

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

Ligand Y7K 1a 1842





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	1A	2860/2915 (98%)	-0.60	70 (2%) 59 57	17, 35, 94, 110	0
1	2A	2789/2915 (95%)	-0.02	81 (2%) 53 52	33, 60, 95, 109	0
2	1B	120/121 (99%)	-0.54	0 100 100	26, 48, 60, 87	0
2	2B	120/121 (99%)	1.20	18 (15%) 5 5	65, 87, 96, 98	0
3	1D	275/276 (99%)	-0.23	3 (1%) 78 77	21, 36, 51, 80	0
3	2D	275/276 (99%)	0.23	4 (1%) 72 71	32, 52, 66, 85	0
4	1E	204/206 (99%)	-0.25	1 (0%) 87 87	19, 38, 59, 74	0
4	2E	204/206 (99%)	0.33	3 (1%) 72 71	36, 61, 73, 85	0
5	1F	202/210 (96%)	-0.18	1 (0%) 87 87	20, 40, 67, 86	0
5	2F	202/210 (96%)	0.46	1 (0%) 87 87	38, 70, 83, 88	0
6	1G	181/182 (99%)	0.36	5 (2%) 55 53	40, 59, 72, 90	0
6	2G	181/182 (99%)	1.49	46 (25%) 1 1	74, 85, 90, 96	0
7	1H	174/180 (96%)	0.05	2 (1%) 78 77	39, 53, 66, 70	0
7	2H	174/180 (96%)	1.13	20 (11%) 9 8	70, 86, 93, 98	0
8	1I	146/148 (98%)	0.60	3 (2%) 63 61	45, 73, 83, 86	0
8	2I	146/148 (98%)	0.91	8 (5%) 30 30	56, 75, 85, 88	0
9	1N	140/140 (100%)	-0.21	0 100 100	25, 37, 60, 73	0
9	2N	140/140 (100%)	0.48	1 (0%) 84 84	49, 66, 79, 88	0
10	1O	122/122 (100%)	-0.16	0 100 100	24, 39, 57, 65	0
10	2O	122/122 (100%)	0.45	4 (3%) 49 47	48, 61, 72, 78	0
11	1P	149/150 (99%)	-0.00	0 100 100	17, 42, 68, 75	0
11	2P	149/150 (99%)	0.59	8 (5%) 31 31	37, 70, 85, 88	0
12	1Q	141/141 (100%)	-0.17	0 100 100	27, 39, 57, 73	0
12	2Q	141/141 (100%)	1.06	15 (10%) 11 10	47, 70, 80, 85	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	-0.37	0 100 100	25, 33, 50, 60	0
13	2R	118/118 (100%)	0.12	1 (0%) 82 82	43, 54, 64, 73	0
14	1S	110/112 (98%)	0.00	0 100 100	37, 48, 60, 65	0
14	2S	110/112 (98%)	1.47	27 (24%) 2 1	69, 80, 86, 90	0
15	1T	131/146 (89%)	0.04	5 (3%) 44 41	33, 43, 66, 75	0
15	2T	131/146 (89%)	0.54	2 (1%) 72 71	52, 64, 78, 85	0
16	1U	116/118 (98%)	-0.38	0 100 100	20, 30, 46, 61	0
16	2U	116/118 (98%)	0.50	1 (0%) 81 81	45, 63, 78, 85	0
17	1V	101/101 (100%)	-0.41	0 100 100	22, 38, 58, 70	0
17	2V	101/101 (100%)	0.79	5 (4%) 34 34	46, 74, 84, 87	0
18	1W	112/113 (99%)	-0.30	0 100 100	23, 32, 47, 76	0
18	2W	112/113 (99%)	0.14	0 100 100	39, 51, 67, 90	0
19	1X	95/96 (98%)	-0.25	1 (1%) 78 77	23, 38, 59, 75	0
19	2X	95/96 (98%)	0.54	1 (1%) 78 77	45, 62, 76, 79	0
20	1Y	107/110 (97%)	0.18	1 (0%) 81 81	36, 49, 69, 77	0
20	2Y	107/110 (97%)	0.95	9 (8%) 17 17	62, 74, 82, 88	0
21	1Z	154/206 (74%)	0.56	8 (5%) 33 32	38, 63, 82, 93	0
21	2Z	160/206 (77%)	1.58	36 (22%) 2 2	71, 84, 92, 97	0
22	10	83/85 (97%)	0.10	4 (4%) 35 35	28, 37, 60, 77	0
22	20	83/85 (97%)	1.08	4 (4%) 35 35	45, 68, 78, 83	0
23	11	97/98 (98%)	0.12	2 (2%) 63 61	24, 42, 69, 74	0
23	21	97/98 (98%)	0.52	1 (1%) 79 79	40, 58, 78, 84	0
24	12	70/72 (97%)	0.09	1 (1%) 73 73	34, 47, 60, 74	0
24	22	70/72 (97%)	0.77	6 (8%) 16 16	59, 73, 80, 82	0
25	13	59/60 (98%)	-0.25	0 100 100	23, 34, 58, 80	0
25	23	59/60 (98%)	0.57	3 (5%) 33 33	55, 67, 79, 88	0
26	14	69/71 (97%)	0.73	6 (8%) 16 16	48, 73, 88, 92	0
26	24	69/71 (97%)	1.71	24 (34%) 1 0	79, 90, 95, 101	0
27	15	59/60 (98%)	-0.33	1 (1%) 69 67	19, 32, 47, 62	0
27	25	59/60 (98%)	0.16	2 (3%) 48 46	40, 52, 66, 81	0
28	16	53/54 (98%)	-0.27	0 100 100	30, 42, 56, 61	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.67	2 (3%) 44 41	54, 64, 71, 75	0
29	17	48/49 (97%)	-0.24	1 (2%) 63 61	21, 27, 55, 63	0
29	27	48/49 (97%)	0.26	5 (10%) 11 11	32, 43, 63, 78	0
30	18	64/65 (98%)	-0.19	0 100 100	26, 33, 43, 55	0
30	28	64/65 (98%)	0.60	1 (1%) 70 69	48, 58, 67, 75	0
31	19	37/37 (100%)	-0.16	1 (2%) 56 54	29, 40, 59, 63	0
31	29	37/37 (100%)	0.84	3 (8%) 18 18	62, 71, 80, 85	0
32	1a	1488/1521 (97%)	0.14	27 (1%) 67 65	37, 67, 93, 110	0
32	2a	1491/1521 (98%)	0.73	154 (10%) 12 11	53, 81, 99, 109	0
33	1b	231/256 (90%)	1.24	39 (16%) 4 4	66, 81, 89, 94	0
33	2b	231/256 (90%)	1.75	79 (34%) 1 0	75, 88, 94, 96	0
34	1c	206/239 (86%)	0.76	11 (5%) 32 31	62, 72, 84, 89	0
34	2c	206/239 (86%)	1.71	76 (36%) 1 0	76, 87, 92, 95	0
35	1d	208/209 (99%)	0.77	14 (6%) 24 23	58, 71, 80, 83	0
35	2d	208/209 (99%)	0.97	15 (7%) 21 21	63, 74, 82, 89	0
36	1e	148/162 (91%)	0.47	1 (0%) 84 84	54, 65, 74, 90	0
36	2e	148/162 (91%)	1.17	21 (14%) 6 5	68, 79, 85, 90	0
37	1f	100/101 (99%)	0.48	2 (2%) 65 63	53, 66, 76, 78	0
37	2f	100/101 (99%)	0.42	1 (1%) 79 79	61, 72, 79, 83	0
38	1g	155/156 (99%)	0.69	12 (7%) 19 19	53, 70, 87, 96	0
38	2g	155/156 (99%)	0.92	16 (10%) 12 11	68, 80, 89, 98	0
39	1h	137/138 (99%)	0.54	3 (2%) 62 60	54, 67, 74, 79	0
39	2h	137/138 (99%)	1.05	9 (6%) 24 24	71, 80, 85, 90	0
40	1i	127/128 (99%)	0.90	11 (8%) 16 16	54, 75, 84, 88	0
40	2i	127/128 (99%)	1.96	58 (45%) 0 0	75, 86, 93, 97	0
41	1j	97/105 (92%)	1.06	10 (10%) 12 11	60, 78, 87, 90	0
41	2j	96/105 (91%)	2.35	60 (62%) 0 0	78, 88, 93, 96	0
42	1k	114/129 (88%)	0.56	2 (1%) 67 65	45, 66, 77, 83	0
42	2k	114/129 (88%)	0.84	8 (7%) 22 22	59, 74, 82, 85	0
43	1l	121/132 (91%)	0.18	2 (1%) 69 67	45, 55, 67, 76	0
43	2l	121/132 (91%)	1.07	14 (11%) 9 8	60, 72, 80, 86	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	1m	123/126 (97%)	0.69	9 (7%) 21 21	57, 69, 78, 82	0
44	2m	122/126 (96%)	1.75	38 (31%) 1 1	75, 87, 92, 94	0
45	1n	60/61 (98%)	0.88	4 (6%) 24 23	59, 67, 73, 75	0
45	2n	60/61 (98%)	2.52	40 (66%) 0 0	81, 88, 93, 98	0
46	1o	88/89 (98%)	0.54	2 (2%) 61 59	51, 66, 75, 79	0
46	2o	88/89 (98%)	0.86	5 (5%) 29 29	66, 75, 83, 86	0
47	1p	82/88 (93%)	1.38	16 (19%) 3 2	55, 69, 78, 87	0
47	2p	82/88 (93%)	1.10	9 (10%) 10 9	61, 71, 81, 89	0
48	1q	99/105 (94%)	0.70	2 (2%) 65 63	56, 68, 78, 80	0
48	2q	99/105 (94%)	0.92	6 (6%) 27 27	65, 75, 85, 88	0
49	1r	68/88 (77%)	0.23	2 (2%) 53 52	56, 66, 77, 80	0
49	2r	68/88 (77%)	0.56	1 (1%) 72 71	63, 73, 82, 85	0
50	1s	83/93 (89%)	0.47	2 (2%) 59 57	62, 72, 80, 87	0
50	2s	83/93 (89%)	1.88	37 (44%) 0 0	82, 91, 97, 101	0
51	1t	96/106 (90%)	0.97	8 (8%) 17 18	60, 69, 81, 88	0
51	2t	96/106 (90%)	0.79	8 (8%) 17 18	62, 73, 83, 85	0
52	1u	23/27 (85%)	1.03	2 (8%) 16 16	60, 67, 73, 76	0
52	2u	23/27 (85%)	2.43	14 (60%) 0 0	79, 83, 88, 89	0
53	1v	13/24 (54%)	0.66	3 (23%) 2 1	48, 62, 93, 100	0
53	2v	13/24 (54%)	1.94	6 (46%) 0 0	74, 89, 100, 104	0
54	1w	67/76 (88%)	0.98	11 (16%) 4 4	55, 91, 102, 107	0
54	1y	67/76 (88%)	0.93	8 (11%) 9 7	37, 95, 102, 106	0
54	2w	65/76 (85%)	1.51	15 (23%) 2 1	77, 101, 107, 109	0
54	2y	66/76 (86%)	1.43	13 (19%) 3 2	57, 101, 105, 106	0
55	1x	72/77 (93%)	0.25	1 (1%) 73 73	39, 68, 85, 93	0
55	2x	72/77 (93%)	0.83	3 (4%) 40 39	58, 85, 94, 104	0
All	All	20873/21748 (95%)	0.35	1368 (6%) 24 24	17, 65, 92, 110	0

All (1368) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
45	1n	2	ALA	7.2
38	2g	82	GLY	7.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
38	2g	83	ALA	6.9
38	2g	84	ASN	6.8
44	1m	124	PRO	6.7
45	2n	2	ALA	6.7
22	10	6	GLY	6.6
44	2m	123	ALA	6.6
44	2m	102	ARG	6.5
33	2b	165	VAL	6.0
41	2j	55	LYS	5.9
23	21	2	SER	5.8
1	1A	885	C	5.8
44	2m	124	PRO	5.5
32	2a	1150	U	5.5
40	2i	14	VAL	5.4
51	1t	103	GLY	5.3
33	2b	161	ALA	5.3
26	24	54	GLY	5.2
41	2j	40	LEU	5.2
22	10	7	LEU	5.1
41	2j	47	PHE	5.1
1	2A	2112	G	5.0
44	1m	122	LYS	4.9
41	2j	65	LEU	4.9
45	2n	25	VAL	4.9
6	2G	20	ILE	4.8
38	1g	80	VAL	4.8
32	2a	1149	C	4.8
40	2i	102	LEU	4.8
40	2i	9	ARG	4.8
41	2j	41	PRO	4.8
21	2Z	21	ALA	4.8
47	1p	82	GLN	4.8
38	2g	80	VAL	4.7
32	2a	1224	G	4.7
44	2m	90	LEU	4.6
34	2c	124	ILE	4.6
40	2i	7	THR	4.6
40	2i	11	LYS	4.5
32	1a	1035	A	4.5
6	2G	28	VAL	4.5
33	2b	185	ILE	4.5
21	2Z	172	ALA	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	2a	1034	G	4.5
52	2u	14	TRP	4.4
12	2Q	104	PHE	4.4
26	14	56	VAL	4.4
1	1A	888	C	4.4
40	2i	18	PHE	4.3
50	2s	9	VAL	4.3
33	2b	187	LEU	4.3
45	2n	33	VAL	4.3
14	2S	54	LEU	4.3
1	2A	2155	G	4.3
32	1a	1023	G	4.3
1	2A	2803	C	4.2
32	2a	1033	G	4.2
40	2i	5	TYR	4.2
1	2A	2113	U	4.2
21	2Z	146	ILE	4.2
38	1g	82	GLY	4.2
21	1Z	141	VAL	4.2
40	2i	128	ARG	4.2
8	2I	146	ALA	4.1
15	1T	130	ALA	4.1
21	2Z	164	ALA	4.1
34	2c	2	GLY	4.1
45	2n	7	ILE	4.1
45	2n	39	LEU	4.1
32	1a	1034	G	4.1
33	2b	200	ILE	4.1
32	2a	1219	U	4.1
14	2S	32	LEU	4.1
40	2i	126	SER	4.1
15	1T	131	ALA	4.0
7	1H	2	SER	4.0
1	2A	2133	G	4.0
33	2b	214	ILE	4.0
44	2m	121	LYS	4.0
41	2j	63	PHE	4.0
33	2b	10	LEU	4.0
52	2u	16	GLY	4.0
26	24	51	ASP	4.0
32	2a	1220	G	3.9
45	2n	30	ALA	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	1094	U	3.9
46	1o	19	PRO	3.9
33	2b	99	GLY	3.9
44	2m	122	LYS	3.9
33	2b	163	PHE	3.9
32	1a	1025	U	3.9
34	2c	5	ILE	3.9
41	2j	38	ILE	3.9
26	24	65	ASP	3.9
21	2Z	174	VAL	3.9
40	2i	10	ARG	3.8
44	2m	70	LEU	3.8
38	1g	81	GLY	3.8
1	1A	886	C	3.8
40	2i	125	TYR	3.8
21	1Z	146	ILE	3.8
44	1m	2	ALA	3.8
32	1a	630	G	3.8
44	2m	104	ARG	3.8
32	2a	1223	C	3.8
14	2S	35	ILE	3.8
1	2A	2802	G	3.8
3	1D	276	LYS	3.8
50	2s	2	PRO	3.8
45	2n	49	HIS	3.8
50	2s	14	HIS	3.8
11	2P	116	GLY	3.8
33	1b	17	PHE	3.8
45	2n	21	TYR	3.7
45	2n	34	TYR	3.7
41	2j	42	THR	3.7
41	2j	32	ALA	3.7
1	2A	1536	C	3.7
50	2s	79	THR	3.7
34	2c	155	GLY	3.7
1	1A	2119	A	3.7
1	2A	2119	A	3.7
33	1b	48	MET	3.7
1	2A	2115	G	3.7
32	1a	1024	G	3.7
32	2a	1038	C	3.7
41	2j	37	PRO	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	2a	1363(A)	A	3.6
33	2b	121	LEU	3.6
52	2u	6	ARG	3.6
54	2w	15	G	3.6
40	2i	13	ALA	3.6
50	2s	63	THR	3.6
1	1A	1081	U	3.6
33	2b	123	ALA	3.6
12	2Q	10	ARG	3.6
50	2s	13	ASP	3.6
53	2v	14	A	3.6
33	2b	57	PHE	3.6
44	2m	66	LEU	3.6
52	2u	24	ARG	3.6
42	2k	117	ASN	3.6
45	2n	6	LEU	3.6
50	2s	76	PRO	3.5
40	2i	17	VAL	3.5
7	2H	2	SER	3.5
41	2j	59	SER	3.5
34	2c	182	ILE	3.5
34	2c	189	ALA	3.5
40	2i	49	PRO	3.5
45	2n	17	LYS	3.5
1	2A	883	G	3.5
2	2B	118	G	3.5
26	24	50	VAL	3.5
32	2a	1036	G	3.5
50	2s	11	VAL	3.5
1	2A	2169	A	3.5
1	2A	2173	A	3.5
1	2A	2128	C	3.5
1	1A	2115	G	3.5
32	2a	1030(A)	G	3.5
33	2b	88	ALA	3.5
40	1i	106	ALA	3.5
21	2Z	76	LEU	3.5
34	2c	14	ILE	3.4
1	1A	1087	G	3.4
33	1b	237	ALA	3.4
35	2d	154	ASN	3.4
41	2j	78	ASN	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
44	2m	72	ALA	3.4
33	1b	221	LEU	3.4
41	2j	8	LEU	3.4
26	14	59	PHE	3.4
1	1A	1057	A	3.4
21	2Z	170	THR	3.4
1	2A	2174	C	3.4
26	14	57	GLU	3.4
33	2b	34	ALA	3.4
40	2i	106	ALA	3.4
52	2u	11	GLY	3.4
2	2B	23	G	3.4
32	2a	1117	G	3.4
14	2S	7	TYR	3.4
6	2G	172	LEU	3.4
40	2i	66	ARG	3.4
6	2G	15	VAL	3.4
42	2k	114	VAL	3.4
33	1b	214	ILE	3.4
41	2j	75	ILE	3.4
1	2A	2154	G	3.4
33	2b	213	LEU	3.4
44	2m	76	ALA	3.4
33	1b	7	VAL	3.4
45	2n	11	LYS	3.3
32	1a	204	U	3.3
45	2n	3	ARG	3.3
32	2a	1251	A	3.3
50	2s	24	ALA	3.3
32	2a	1053	G	3.3
51	1t	55	ILE	3.3
52	2u	3	LYS	3.3
32	1a	1027	C	3.3
33	2b	44	LEU	3.3
38	2g	16	LEU	3.3
34	1c	2	GLY	3.3
33	1b	229	VAL	3.3
34	2c	4	LYS	3.3
39	2h	53	VAL	3.3
1	1A	2117	A	3.3
1	2A	2170	A	3.3
41	2j	43	ARG	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
41	2j	46	ARG	3.3
21	2Z	173	ALA	3.3
1	2A	2111	C	3.3
32	2a	1030	C	3.3
14	2S	12	PHE	3.3
47	1p	68	ASP	3.3
1	2A	896	A	3.3
32	2a	1026	G	3.3
33	2b	202	PRO	3.3
41	2j	71	LEU	3.3
20	1Y	1	MET	3.3
33	2b	148	TYR	3.3
50	2s	80	TYR	3.3
21	2Z	147	GLY	3.3
43	2l	13	LYS	3.3
1	1A	1078	U	3.3
27	15	60	VAL	3.3
33	2b	152	PHE	3.3
34	2c	195	VAL	3.3
41	1j	76	ASN	3.3
41	2j	44	VAL	3.3
1	2A	2145	C	3.2
47	1p	81	ARG	3.2
53	1v	13	A	3.2
52	2u	2	GLY	3.2
41	1j	32	ALA	3.2
14	2S	29	PHE	3.2
32	2a	1002	G	3.2
33	2b	136	VAL	3.2
40	2i	105	ASP	3.2
2	2B	5	C	3.2
8	1I	146	ALA	3.2
34	2c	187	ALA	3.2
40	2i	15	ALA	3.2
53	2v	13	A	3.2
33	2b	122	PHE	3.2
34	2c	134	ILE	3.2
52	2u	17	THR	3.2
31	29	37	GLY	3.2
55	1x	69	C	3.2
33	2b	71	VAL	3.2
41	2j	54	PHE	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	887	A	3.2
53	2v	24	A	3.2
24	22	1	MET	3.2
45	2n	40	CYS	3.2
1	1A	2112	G	3.2
54	1y	20	U	3.2
26	24	63	TYR	3.2
35	1d	169	LYS	3.1
22	10	3	HIS	3.1
33	1b	202	PRO	3.1
44	2m	100	GLY	3.1
32	2a	1126	U	3.1
34	2c	157	ILE	3.1
6	2G	109	VAL	3.1
1	1A	2162	G	3.1
2	2B	119	G	3.1
32	1a	1003	G	3.1
54	1w	1	G	3.1
29	27	48	LYS	3.1
32	2a	1119	C	3.1
1	1A	548	A	3.1
32	2a	965	A	3.1
32	2a	1151	A	3.1
34	2c	163	ALA	3.1
34	2c	167	TRP	3.1
45	2n	37	PHE	3.1
32	1a	1257	U	3.1
33	2b	11	LEU	3.1
45	2n	44	LEU	3.1
51	1t	10	LEU	3.1
32	2a	1124	G	3.1
33	1b	9	GLU	3.1
40	2i	12	GLU	3.1
55	2x	70	G	3.1
33	1b	131	PRO	3.1
47	1p	41	PRO	3.1
32	2a	1054	C	3.1
34	2c	185	GLY	3.1
35	2d	23	GLY	3.1
1	1A	1096	A	3.1
6	1G	21	ARG	3.1
26	24	35	VAL	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
45	2n	29	ARG	3.1
45	2n	56	VAL	3.1
50	2s	38	SER	3.1
1	2A	1026	U	3.1
32	1a	1001(A)	G	3.1
32	1a	1033	G	3.1
50	2s	84	GLY	3.1
54	1w	71	G	3.1
33	2b	39	ILE	3.1
44	1m	121	LYS	3.1
40	2i	16	ARG	3.1
47	1p	25	ARG	3.1
32	2a	1116	C	3.1
34	2c	55	VAL	3.1
43	1l	18	VAL	3.1
43	2l	32	PHE	3.1
21	2Z	144	LEU	3.0
41	2j	68	HIS	3.0
41	2j	76	ASN	3.0
45	2n	4	LYS	3.0
38	2g	81	GLY	3.0
44	2m	6	GLY	3.0
45	2n	38	GLY	3.0
29	27	47	ARG	3.0
33	2b	237	ALA	3.0
35	2d	164	ALA	3.0
44	2m	118	ALA	3.0
6	2G	141	PHE	3.0
45	2n	16	PHE	3.0
32	1a	1002	G	3.0
22	20	7	LEU	3.0
33	1b	213	LEU	3.0
45	2n	53	LEU	3.0
1	1A	1064	C	3.0
25	23	2	PRO	3.0
33	2b	131	PRO	3.0
3	2D	38	LYS	3.0
2	2B	55	U	3.0
44	2m	33	ALA	3.0
34	2c	141	VAL	3.0
34	2c	153	VAL	3.0
45	2n	36	PHE	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
6	2G	12	TYR	3.0
1	1A	1059	G	3.0
1	2A	2166	G	3.0
1	2A	2896	C	3.0
54	1w	4	C	3.0
33	1b	172	ILE	3.0
34	2c	8	ILE	3.0
41	2j	18	ALA	3.0
32	2a	1257	U	3.0
21	2Z	88	PHE	3.0
34	2c	188	LEU	3.0
20	2Y	29	GLU	3.0
34	2c	13	GLY	3.0
1	1A	2166	G	3.0
1	2A	2127	G	3.0
32	2a	1202	G	3.0
1	2A	885	C	3.0
32	2a	1030(B)	C	3.0
34	2c	129	ALA	3.0
32	2a	994	A	3.0
41	2j	34	VAL	3.0
46	2o	60	VAL	3.0
1	1A	2113	U	2.9
12	2Q	22	LYS	2.9
21	2Z	149	SER	2.9
41	2j	39	PRO	2.9
47	2p	82	GLN	2.9
44	2m	87	TYR	2.9
33	1b	189	ASP	2.9
33	2b	201	ILE	2.9
36	2e	101	ILE	2.9
41	2j	36	GLY	2.9
41	2j	67	THR	2.9
8	2I	53	ALA	2.9
33	1b	230	VAL	2.9
33	2b	138	LEU	2.9
1	1A	2174	C	2.9
14	2S	57	LYS	2.9
32	2a	1001(A)	G	2.9
40	2i	127	LYS	2.9
26	24	29	PRO	2.9
21	1Z	166	SER	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
26	24	66	SER	2.9
54	2y	33	U	2.9
12	2Q	1	MET	2.9
38	2g	37	ASN	2.9
38	2g	85	TYR	2.9
40	2i	62	TYR	2.9
48	2q	32	TYR	2.9
26	24	31	ILE	2.9
51	2t	103	GLY	2.9
40	1i	15	ALA	2.9
43	2l	39	VAL	2.9
17	2V	94	LEU	2.9
39	1h	2	LEU	2.9
41	2j	16	LEU	2.9
50	2s	16	LEU	2.9
38	1g	153	HIS	2.9
48	2q	97	SER	2.9
1	2A	2062	A	2.9
32	2a	974	A	2.9
54	2y	36	A	2.9
1	1A	2165	G	2.9
1	2A	2132	U	2.9
32	2a	1032	G	2.9
32	2a	1196	U	2.9
32	2a	1356	G	2.9
32	2a	1532	U	2.9
54	1w	70	G	2.9
54	1y	18	G	2.9
44	2m	4	ILE	2.9
34	2c	15	THR	2.9
47	1p	7	ALA	2.9
47	1p	24	ALA	2.9
33	2b	17	PHE	2.9
35	1d	110	PHE	2.9
35	1d	157	LEU	2.9
45	2n	18	VAL	2.9
34	2c	161	GLU	2.9
52	2u	23	PRO	2.9
47	1p	5	ARG	2.9
36	2e	130	ASN	2.9
1	1A	1080	C	2.9
6	2G	134	GLY	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
12	2Q	32	TYR	2.9
32	2a	1027	C	2.9
32	2a	1250	A	2.9
33	2b	199	TYR	2.9
53	2v	12	A	2.9
54	2w	73	A	2.9
1	1A	1058	G	2.9
1	2A	2318	G	2.9
1	2A	2894	G	2.9
12	2Q	121	ALA	2.9
33	2b	13	ALA	2.9
34	2c	52	LEU	2.9
44	1m	123	ALA	2.9
50	1s	9	VAL	2.9
15	2T	108	ARG	2.8
43	2l	50	SER	2.8
38	1g	84	ASN	2.8
47	2p	19	ILE	2.8
7	2H	175	LYS	2.8
34	2c	158	GLY	2.8
44	2m	103	THR	2.8
6	2G	102	PHE	2.8
32	2a	962	C	2.8
33	2b	12	GLU	2.8
41	2j	61	GLU	2.8
45	2n	14	PRO	2.8
2	2B	117	G	2.8
32	2a	1021	G	2.8
42	2k	13	GLN	2.8
35	1d	23	GLY	2.8
40	2i	61	ALA	2.8
45	1n	5	ALA	2.8
22	20	69	PHE	2.8
35	2d	148	VAL	2.8
35	2d	185	PHE	2.8
40	2i	86	VAL	2.8
1	2A	2118	U	2.8
32	2a	1225	A	2.8
32	2a	972	C	2.8
33	2b	162	ILE	2.8
1	2A	2319	G	2.8
32	2a	1127	G	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	2a	1310	G	2.8
54	2w	65	G	2.8
34	2c	171	GLY	2.8
36	2e	31	LEU	2.8
34	2c	168	ALA	2.8
40	2i	64	THR	2.8
44	2m	5	ALA	2.8
50	2s	77	THR	2.8
33	2b	55	PHE	2.8
40	2i	41	VAL	2.8
6	2G	2	PRO	2.8
52	2u	15	ARG	2.8
32	1a	1531	A	2.8
1	1A	34	C	2.8
40	1i	126	SER	2.8
47	2p	48	TRP	2.8
50	2s	71	LEU	2.8
34	1c	15	THR	2.8
40	2i	122	ALA	2.8
44	2m	75	ALA	2.8
1	2A	2116	G	2.8
32	2a	973	G	2.8
40	2i	36	TYR	2.8
54	2w	71	G	2.8
26	24	41	PRO	2.7
36	2e	109	ILE	2.7
19	2X	92	LEU	2.7
1	1A	2114	A	2.7
41	2j	13	HIS	2.7
33	2b	134	GLU	2.7
34	2c	192	THR	2.7
40	1i	2	GLU	2.7
41	2j	17	ASP	2.7
3	2D	217	ARG	2.7
32	1a	1028	C	2.7
55	2x	34	C	2.7
33	2b	236	TYR	2.7
34	2c	73	PRO	2.7
36	2e	61	TYR	2.7
6	2G	41	GLN	2.7
1	1A	883	G	2.7
1	2A	882	G	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
6	2G	3	LEU	2.7
6	2G	176	LEU	2.7
19	1X	95	LEU	2.7
21	2Z	121	HIS	2.7
34	2c	194	GLY	2.7
51	1t	47	GLY	2.7
51	2t	9	ASN	2.7
32	2a	1357	A	2.7
3	2D	276	LYS	2.7
14	2S	36	TYR	2.7
26	24	32	TYR	2.7
35	2d	169	LYS	2.7
1	1A	2145	C	2.7
1	2A	645	C	2.7
32	2a	1066	C	2.7
34	2c	202	ILE	2.7
6	2G	62	LEU	2.7
33	2b	48	MET	2.7
1	2A	2125	G	2.7
32	1a	306	G	2.7
32	1a	1030(A)	G	2.7
54	2y	18	G	2.7
54	2y	19	G	2.7
6	2G	136	ARG	2.7
7	2H	19	VAL	2.7
7	2H	145	ALA	2.7
12	2Q	117	ALA	2.7
33	2b	15	VAL	2.7
6	2G	4	ASP	2.7
47	1p	80	PHE	2.7
6	2G	17	PRO	2.7
32	2a	1020	U	2.7
41	2j	14	LYS	2.7
34	2c	193	TYR	2.7
1	2A	2114	A	2.7
32	2a	1123	A	2.7
32	2a	1114	C	2.7
21	1Z	150	LEU	2.7
34	2c	32	LEU	2.7
34	2c	33	LEU	2.7
41	2j	31	GLY	2.7
17	2V	93	GLU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
21	2Z	141	VAL	2.7
33	2b	184	VAL	2.7
34	2c	137	ALA	2.7
45	2n	10	ALA	2.7
1	2A	2156	G	2.6
32	1a	1026	G	2.6
40	2i	124	GLN	2.6
54	2y	34	G	2.6
44	2m	23	TYR	2.6
21	2Z	171	ILE	2.6
50	2s	31	ILE	2.6
20	2Y	1	MET	2.6
32	2a	1035	A	2.6
32	2a	1503	A	2.6
1	1A	2111	C	2.6
31	29	8	LYS	2.6
32	2a	1218	C	2.6
50	2s	53	ASN	2.6
7	2H	37	VAL	2.6
12	2Q	65	PHE	2.6
26	24	10	VAL	2.6
33	1b	234	PRO	2.6
14	2S	92	TYR	2.6
34	2c	29	TYR	2.6
42	2k	25	TYR	2.6
44	1m	87	TYR	2.6
1	2A	11	G	2.6
1	2A	2144	U	2.6
32	2a	1024	G	2.6
54	2y	15	G	2.6
50	2s	36	ARG	2.6
33	1b	133	LYS	2.6
44	2m	67	GLU	2.6
32	2a	996	A	2.6
53	1v	12	A	2.6
5	2F	6	VAL	2.6
26	24	56	VAL	2.6
33	1b	15	VAL	2.6
34	2c	71	ALA	2.6
40	2i	43	ALA	2.6
41	2j	49	VAL	2.6
44	2m	105	THR	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	888	C	2.6
1	2A	2175	C	2.6
32	2a	1359	C	2.6
54	2w	4	C	2.6
33	2b	211	ILE	2.6
6	2G	7	LEU	2.6
6	2G	175	LEU	2.6
20	2Y	90	LEU	2.6
33	2b	31	TYR	2.6
33	2b	221	LEU	2.6
40	2i	19	LEU	2.6
44	1m	27	LYS	2.6
22	10	8	GLY	2.6
36	2e	22	GLY	2.6
40	2i	67	GLY	2.6
1	2A	2123	G	2.6
35	2d	195	ALA	2.6
36	2e	67	VAL	2.6
40	2i	28	VAL	2.6
50	2s	41	VAL	2.6
39	2h	3	THR	2.6
1	2A	2117	A	2.6
32	2a	983	A	2.6
32	2a	1531	A	2.6
41	2j	58	ASP	2.6
52	2u	5	ASP	2.6
26	24	14	ILE	2.6
1	1A	1509	C	2.6
8	2I	68	LEU	2.6
32	2a	1018	C	2.6
41	2j	88	LEU	2.6
40	2i	4	TYR	2.6
45	2n	41	ARG	2.6
11	2P	35	HIS	2.6
31	29	15	LYS	2.6
40	2i	69	GLY	2.6
7	2H	43	VAL	2.6
32	2a	982	U	2.6
33	1b	120	ALA	2.6
40	2i	76	ALA	2.6
34	1c	107	GLN	2.6
44	2m	101	GLN	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
6	2G	29	TRP	2.5
33	2b	210	SER	2.5
1	1A	2159	G	2.5
1	2A	2131	G	2.5
1	2A	2168	G	2.5
1	2A	528	A	2.5
14	2S	56	LEU	2.5
32	2a	1286	A	2.5
37	2f	21	LEU	2.5
53	2v	15	A	2.5
41	2j	70	ARG	2.5
20	2Y	55	TYR	2.5
54	1w	3	C	2.5
54	2w	67	C	2.5
5	1F	207	GLY	2.5
41	2j	10	GLY	2.5
7	2H	125	VAL	2.5
9	2N	44	PRO	2.5
20	2Y	7	VAL	2.5
21	2Z	71	VAL	2.5
47	1p	20	VAL	2.5
26	24	49	PHE	2.5
34	2c	60	ALA	2.5
38	1g	83	ALA	2.5
49	2r	60	ALA	2.5
50	2s	33	THR	2.5
1	2A	2897	U	2.5
13	2R	14	SER	2.5
45	2n	42	ILE	2.5
8	1I	27	ARG	2.5
34	2c	42	LEU	2.5
39	2h	30	ARG	2.5
44	2m	88	ARG	2.5
45	2n	12	ARG	2.5
45	2n	47	LEU	2.5
41	2j	62	HIS	2.5
32	2a	971	G	2.5
32	2a	1272	G	2.5
32	2a	1370	G	2.5
1	1A	1046	A	2.5
32	1a	1005	A	2.5
32	2a	1280	A	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	2b	129	GLU	2.5
34	2c	184	TYR	2.5
36	2e	74	GLY	2.5
7	2H	39	PRO	2.5
33	2b	91	PRO	2.5
43	2l	5	PRO	2.5
50	2s	45	VAL	2.5
26	24	59	PHE	2.5
41	2j	27	ALA	2.5
1	1A	884	C	2.5
1	1A	2108	C	2.5
1	1A	2164	C	2.5
1	2A	886	C	2.5
1	2A	2136	C	2.5
2	2B	6	C	2.5
32	2a	980	C	2.5
54	2w	72	C	2.5
33	2b	168	THR	2.5
3	1D	275	LYS	2.5
26	24	15	ILE	2.5
42	1k	51	LYS	2.5
21	2Z	33	LEU	2.5
32	2a	1148	U	2.5
33	2b	118	LEU	2.5
26	24	57	GLU	2.5
34	2c	48	TYR	2.5
47	2p	38	TYR	2.5
7	2H	36	PRO	2.5
1	2A	2126	A	2.5
1	2A	2157	G	2.5
1	2A	2308	G	2.5
21	2Z	98	MET	2.5
32	2a	951	G	2.5
32	2a	1120	G	2.5
32	2a	1216	G	2.5
32	2a	1285	A	2.5
33	2b	164	VAL	2.5
33	2b	188	ALA	2.5
39	2h	9	MET	2.5
43	2l	9	GLN	2.5
50	2s	60	VAL	2.5
44	2m	107	ALA	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	2c	191	THR	2.5
14	2S	52	SER	2.5
21	2Z	16	SER	2.5
33	1b	10	LEU	2.5
33	2b	61	LEU	2.5
34	2c	79	ARG	2.5
34	2c	190	ARG	2.5
36	2e	12	LEU	2.5
40	2i	96	LEU	2.5
43	2l	10	LEU	2.5
48	2q	90	ILE	2.5
50	2s	29	ARG	2.5
50	2s	35	SER	2.5
1	2A	884	C	2.5
26	14	51	ASP	2.5
32	2a	1115	C	2.5
33	2b	24	TRP	2.5
1	2A	2109	U	2.5
6	2G	146	TYR	2.5
33	1b	236	TYR	2.5
38	1g	85	TYR	2.5
40	2i	39	GLY	2.5
40	2i	115	GLY	2.5
48	2q	95	TYR	2.5
24	22	70	GLN	2.5
34	2c	116	VAL	2.5
21	2Z	152	ALA	2.5
40	1i	59	PHE	2.5
45	2n	48	ALA	2.5
14	2S	11	LYS	2.4
41	2j	15	THR	2.4
41	2j	100	THR	2.4
45	2n	13	THR	2.4
32	1a	1447	A	2.4
32	2a	964	A	2.4
33	2b	21	ARG	2.4
36	2e	64	ARG	2.4
47	2p	81	ARG	2.4
52	1u	24	ARG	2.4
54	1y	36	A	2.4
33	2b	51	LEU	2.4
35	1d	11	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
40	2i	63	ILE	2.4
1	1A	614(B)	G	2.4
1	2A	2124	G	2.4
32	2a	953	G	2.4
32	2a	1253	G	2.4
41	2j	19	SER	2.4
1	1A	2146	C	2.4
32	2a	979	C	2.4
32	2a	1063	C	2.4
32	2a	1322	C	2.4
54	1y	56	C	2.4
6	2G	142	PRO	2.4
14	2S	45	GLY	2.4
32	2a	997	U	2.4
26	14	63	TYR	2.4
38	2g	154	TYR	2.4
14	2S	69	VAL	2.4
51	2t	74	LYS	2.4
6	2G	46	ALA	2.4
6	2G	50	ALA	2.4
41	2j	26	ALA	2.4
51	1t	12	ALA	2.4
24	22	51	ARG	2.4
47	2p	69	THR	2.4
34	1c	14	ILE	2.4
34	1c	34	LEU	2.4
41	2j	23	ILE	2.4
51	2t	63	ILE	2.4
14	2S	34	HIS	2.4
1	1A	890	A	2.4
32	2a	532	A	2.4
1	1A	1176	G	2.4
1	2A	1533	G	2.4
2	2B	24	G	2.4
32	2a	1190	G	2.4
54	2y	57	G	2.4
40	1i	8	GLY	2.4
41	2j	91	PRO	2.4
1	1A	889	C	2.4
6	2G	159	VAL	2.4
27	25	60	VAL	2.4
32	2a	1028	C	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	2a	1249	C	2.4
38	1g	154	TYR	2.4
42	1k	14	VAL	2.4
1	1A	2150	U	2.4
1	1A	2897	U	2.4
1	2A	2150	U	2.4
6	2G	57	ALA	2.4
34	2c	149	ALA	2.4
40	1i	66	ARG	2.4
41	1j	79	ARG	2.4
14	2S	5	THR	2.4
14	2S	58	LEU	2.4
21	2Z	150	LEU	2.4
33	1b	127	ILE	2.4
33	2b	32	ILE	2.4
40	2i	81	ILE	2.4
44	1m	4	ILE	2.4
48	2q	43	LEU	2.4
1	1A	896	A	2.4
3	2D	275	LYS	2.4
32	2a	1152	A	2.4
32	2a	1287	A	2.4
33	1b	18	GLY	2.4
33	1b	125	PRO	2.4
41	1j	77	PRO	2.4
14	2S	65	VAL	2.4
1	1A	2116	G	2.4
1	2A	2149	G	2.4
11	2P	79	ARG	2.4
12	2Q	58	PHE	2.4
21	2Z	99	TYR	2.4
32	2a	1048	G	2.4
34	2c	160	ALA	2.4
35	1d	132	ARG	2.4
38	2g	32	ARG	2.4
41	2j	66	ARG	2.4
44	1m	102	ARG	2.4
54	2w	34	G	2.4
1	1A	1060	U	2.4
6	2G	39	ILE	2.4
21	2Z	137	ILE	2.4
34	2c	87	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	2146	C	2.4
41	2j	56	HIS	2.4
7	2H	58	GLU	2.4
36	2e	125	SER	2.4
39	1h	4	ASP	2.4
33	1b	97	TRP	2.4
38	1g	156	TRP	2.4
34	2c	41	GLY	2.4
34	2c	197	GLY	2.4
7	2H	44	VAL	2.4
21	2Z	165	VAL	2.4
36	2e	41	VAL	2.4
32	2a	968	A	2.4
33	1b	163	PHE	2.4
50	2s	10	PHE	2.4
51	2t	97	ALA	2.4
35	1d	21	LEU	2.3
39	2h	2	LEU	2.3
47	1p	74	LEU	2.3
6	2G	140	ILE	2.3
6	2G	157	ILE	2.3
40	2i	117	HIS	2.3
1	1A	880	G	2.3
7	2H	124	GLU	2.3
24	22	5	GLU	2.3
41	2j	64	GLU	2.3
6	2G	155	MET	2.3
1	1A	898	C	2.3
32	2a	1363	C	2.3
42	2k	119	CYS	2.3
33	1b	227	GLY	2.3
15	1T	115	ARG	2.3
35	2d	49	ARG	2.3
14	2S	28	VAL	2.3
21	1Z	139	VAL	2.3
33	2b	230	VAL	2.3
36	2e	115	VAL	2.3
40	2i	53	VAL	2.3
6	2G	133	LEU	2.3
22	20	2	ALA	2.3
40	2i	40	LEU	2.3
33	2b	42	ILE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
44	2m	84	ILE	2.3
32	2a	977	A	2.3
32	2a	1004	A	2.3
32	2a	1110	A	2.3
7	1H	175	LYS	2.3
41	2j	83	GLU	2.3
45	2n	15	LYS	2.3
1	1A	2109	U	2.3
39	2h	4	ASP	2.3
1	1A	1068	G	2.3
1	1A	2133	G	2.3
32	2a	1057	G	2.3
32	2a	1365	G	2.3
33	2b	234	PRO	2.3
39	2h	67	PRO	2.3
41	2j	77	PRO	2.3
54	1y	15	G	2.3
7	2H	60	ARG	2.3
32	2a	1019	C	2.3
32	2a	1145	C	2.3
33	2b	14	GLY	2.3
40	1i	39	GLY	2.3
50	1s	84	GLY	2.3
52	1u	9	ARG	2.3
8	2I	3	VAL	2.3
20	2Y	45	VAL	2.3
21	2Z	139	VAL	2.3
33	2b	93	VAL	2.3
34	2c	130	VAL	2.3
35	2d	140	VAL	2.3
6	2G	171	ALA	2.3
14	2S	4	LEU	2.3
21	1Z	136	PHE	2.3
33	1b	188	ALA	2.3
33	1b	215	LEU	2.3
45	1n	59	ALA	2.3
6	2G	88	ILE	2.3
12	2Q	127	ILE	2.3
35	1d	70	ILE	2.3
40	2i	114	TYR	2.3
41	2j	87	THR	2.3
24	22	66	GLU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
43	2l	47	LYS	2.3
1	2A	866	A	2.3
32	1a	1030(D)	A	2.3
14	2S	31	SER	2.3
21	2Z	87	ASP	2.3
26	24	7	PRO	2.3
29	27	23	ARG	2.3
41	2j	5	ARG	2.3
45	2n	54	PRO	2.3
44	2m	112	GLY	2.3
50	2s	82	GLY	2.3
52	2u	4	GLY	2.3
1	1A	2167	U	2.3
32	2a	1052	U	2.3
32	2a	1281	U	2.3
21	1Z	105	VAL	2.3
33	2b	112	VAL	2.3
21	2Z	41	LEU	2.3
28	26	11	LEU	2.3
35	1d	101	LEU	2.3
8	2I	55	ALA	2.3
16	2U	62	ILE	2.3
1	1A	897	C	2.3
1	1A	2138	C	2.3
1	1A	2142	C	2.3
1	2A	897	C	2.3
1	2A	2164	C	2.3
32	1a	1029	C	2.3
32	2a	926	G	2.3
34	2c	152	ILE	2.3
32	2a	1118	C	2.3
32	2a	1214	C	2.3
6	1G	182	LYS	2.3
6	1G	146	TYR	2.3
14	2S	61	ASN	2.3
15	1T	111	ARG	2.3
15	1T	129	ARG	2.3
26	24	55	ARG	2.3
46	1o	65	ARG	2.3
48	2q	91	ARG	2.3
51	2t	8	ARG	2.3
2	2B	29	A	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	2B	120	A	2.3
34	2c	162	GLN	2.3
40	2i	80	GLY	2.3
54	2y	58	A	2.3
37	1f	90	VAL	2.3
40	2i	26	VAL	2.3
1	1A	12	U	2.2
34	2c	24	ALA	2.2
40	2i	94	ALA	2.2
33	1b	40	HIS	2.2
14	2S	33	LYS	2.2
35	2d	184	LYS	2.2
27	25	59	GLU	2.2
1	1A	2152	G	2.2
32	2a	1094	G	2.2
32	2a	1182	G	2.2
55	2x	2	G	2.2
40	2i	20	ARG	2.2
41	1j	43	ARG	2.2
36	2e	20	GLN	2.2
7	2H	45	VAL	2.2
33	1b	11	LEU	2.2
33	2b	97	TRP	2.2
42	2k	14	VAL	2.2
33	2b	80	ILE	2.2
34	2c	186	PHE	2.2
41	2j	50	ILE	2.2
50	2s	49	ILE	2.2
54	2y	35	A	2.2
35	2d	165	MET	2.2
36	1e	10	MET	2.2
1	1A	1175	U	2.2
6	2G	48	GLU	2.2
22	20	43	THR	2.2
33	1b	126	GLU	2.2
41	1j	83	GLU	2.2
41	2j	48	THR	2.2
26	24	67	TYR	2.2
47	2p	32	TYR	2.2
15	2T	111	ARG	2.2
33	2b	36	ARG	2.2
42	2k	126	ARG	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
21	2Z	25	PRO	2.2
1	1A	1075	C	2.2
1	2A	2297	C	2.2
21	2Z	73	GLN	2.2
32	1a	1030(B)	C	2.2
32	2a	1262	C	2.2
32	2a	1354	C	2.2
32	2a	1397	C	2.2
34	2c	62	ASP	2.2
1	2A	859	G	2.2
2	2B	61	G	2.2
2	2B	103	G	2.2
20	2Y	106	LEU	2.2
32	2a	987	G	2.2
47	1p	78	GLY	2.2
54	2w	44	G	2.2
40	1i	17	VAL	2.2
52	2u	20	LYS	2.2
40	2i	101	PHE	2.2
50	2s	66	MET	2.2
6	1G	50	ALA	2.2
34	2c	121	ALA	2.2
45	2n	59	ALA	2.2
35	1d	179	GLU	2.2
1	1A	1069	A	2.2
1	1A	2173	A	2.2
1	2A	229	A	2.2
1	2A	1445	A	2.2
32	1a	1286	A	2.2
32	2a	978	A	2.2
43	1l	6	THR	2.2
54	1w	73	A	2.2
54	2w	64	A	2.2
1	1A	1026	U	2.2
1	2A	2172	U	2.2
32	2a	1025	U	2.2
33	1b	33	TYR	2.2
46	2o	75	PRO	2.2
50	2s	42	PRO	2.2
4	2E	195	LEU	2.2
6	2G	53	LEU	2.2
6	2G	76	SER	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
17	2V	38	LEU	2.2
33	1b	44	LEU	2.2
33	2b	166	ASP	2.2
41	1j	65	LEU	2.2
42	2k	124	LYS	2.2
44	2m	36	LYS	2.2
51	2t	24	LEU	2.2
20	2Y	5	MET	2.2
35	1d	88	VAL	2.2
41	1j	72	VAL	2.2
43	2l	104	VAL	2.2
1	1A	2794	C	2.2
2	2B	27	C	2.2
32	2a	1037	C	2.2
32	2a	1069	C	2.2
32	2a	1192	C	2.2
33	2b	127	ILE	2.2
34	2c	69	HIS	2.2
54	1w	68	C	2.2
54	1w	72	C	2.2
4	2E	204	ALA	2.2
40	2i	45	ALA	2.2
1	2A	2110	G	2.2
10	2O	108	GLU	2.2
32	2a	963	G	2.2
32	2a	1009	G	2.2
35	2d	192	GLU	2.2
6	2G	64	THR	2.2
33	2b	47	THR	2.2
44	2m	37	THR	2.2
6	1G	83	ARG	2.2
14	2S	30	ARG	2.2
34	2c	164	ARG	2.2
35	2d	132	ARG	2.2
41	1j	46	ARG	2.2
46	2o	88	ARG	2.2
1	1A	1095	A	2.2
1	2A	652(B)	A	2.2
32	2a	986	A	2.2
32	2a	1236	A	2.2
33	2b	125	PRO	2.2
35	2d	20	TYR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
43	2l	64	TYR	2.2
1	2A	271(K)	U	2.2
12	2Q	141	GLN	2.2
29	17	48	LYS	2.2
32	2a	1040	U	2.2
33	2b	139	LYS	2.2
54	2w	66	U	2.2
40	1i	69	GLY	2.2
50	2s	15	LEU	2.2
51	1t	102	GLY	2.2
10	2O	81	ASP	2.2
36	2e	10	MET	2.2
7	2H	15	VAL	2.2
10	2O	19	ILE	2.2
14	2S	14	VAL	2.2
33	1b	41	ILE	2.2
38	2g	27	ILE	2.2
34	2c	166	GLU	2.1
1	1A	1076	C	2.1
1	2A	2789	C	2.1
6	2G	83	ARG	2.1
32	2a	1039	C	2.1
32	2a	1303	C	2.1
38	1g	79	ARG	2.1
38	2g	5	ARG	2.1
54	2w	3	C	2.1
1	2A	2751	G	2.1
32	2a	1017	G	2.1
32	2a	1058	G	2.1
32	2a	1087	G	2.1
32	2a	1131	G	2.1
32	2a	1311	G	2.1
54	2w	70	G	2.1
33	2b	22	LYS	2.1
40	2i	92	TYR	2.1
41	2j	33	GLN	2.1
7	2H	103	LEU	2.1
8	2I	38	LEU	2.1
11	2P	45	LEU	2.1
33	2b	101	MET	2.1
1	2A	2158	A	2.1
1	2A	2305	A	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	2a	1016	A	2.1
32	2a	1146	A	2.1
32	2a	1183	A	2.1
45	2n	51	GLY	2.1
1	1A	1065	U	2.1
21	2Z	133	ILE	2.1
32	2a	1364	U	2.1
20	2Y	17	SER	2.1
33	1b	200	ILE	2.1
33	2b	208	ILE	2.1
33	2b	223	ILE	2.1
34	2c	6	HIS	2.1
36	2e	33	VAL	2.1
36	2e	131	ILE	2.1
38	2g	17	VAL	2.1
41	2j	74	ILE	2.1
41	2j	89	ASP	2.1
50	2s	4	SER	2.1
52	2u	13	ILE	2.1
12	2Q	29	PHE	2.1
11	2P	74	GLU	2.1
23	1l	75	GLU	2.1
34	2c	22	TRP	2.1
44	2m	58	GLU	2.1
7	2H	59	ARG	2.1
34	1c	38	ARG	2.1
34	1c	179	ARG	2.1
35	1d	153	ARG	2.1
38	2g	76	ARG	2.1
17	2V	7	THR	2.1
45	2n	22	THR	2.1
41	2j	57	LYS	2.1
1	2A	894	C	2.1
2	2B	4	C	2.1
32	2a	948	C	2.1
32	2a	970	C	2.1
32	2a	1217	C	2.1
6	2G	130	ASN	2.1
14	2S	110	LEU	2.1
26	24	25	TYR	2.1
33	1b	187	LEU	2.1
34	2c	196	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
40	2i	50	LEU	2.1
26	14	54	GLY	2.1
34	2c	9	GLY	2.1
34	2c	78	GLY	2.1
36	2e	99	GLY	2.1
21	2Z	37	VAL	2.1
21	2Z	53	ILE	2.1
32	2a	993	G	2.1
33	1b	136	VAL	2.1
36	2e	5	ASP	2.1
40	2i	91	ASP	2.1
44	2m	60	VAL	2.1
54	1w	44	G	2.1
54	2y	53	G	2.1
34	1c	128	PHE	2.1
38	2g	26	PHE	2.1
1	1A	1077	A	2.1
1	2A	1847	A	2.1
10	2O	41	ALA	2.1
32	1a	1001	A	2.1
32	2a	969	A	2.1
32	2a	975	A	2.1
32	2a	1252	A	2.1
34	2c	200	ALA	2.1
43	2l	51	ALA	2.1
53	2v	23	A	2.1
4	1E	73	GLU	2.1
43	2l	16	GLU	2.1
41	2j	60	ARG	2.1
43	2l	15	ARG	2.1
11	2P	76	LYS	2.1
12	2Q	63	LYS	2.1
50	2s	6	LYS	2.1
34	2c	109	PRO	2.1
47	1p	1	MET	2.1
12	2Q	37	LEU	2.1
23	11	98	LEU	2.1
33	2b	98	LEU	2.1
44	2m	96	LEU	2.1
47	1p	73	LEU	2.1
49	1r	78	LEU	2.1
51	1t	13	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	2c	181	ASN	2.1
14	2S	96	GLY	2.1
26	24	40	HIS	2.1
41	2j	93	GLY	2.1
44	2m	92	HIS	2.1
1	2A	34	C	2.1
1	2A	2108	C	2.1
2	2B	62	C	2.1
2	2B	88	C	2.1
6	2G	160	VAL	2.1
30	28	16	ILE	2.1
32	2a	1128	C	2.1
33	1b	112	VAL	2.1
34	1c	84	ILE	2.1
39	2h	137	VAL	2.1
44	2m	7	VAL	2.1
48	1q	9	VAL	2.1
50	2s	40	ILE	2.1
54	2w	13	C	2.1
34	2c	146	ALA	2.1
35	1d	83	SER	2.1
38	1g	2	ALA	2.1
45	2n	32	SER	2.1
48	1q	68	ARG	2.1
49	1r	20	ALA	2.1
1	1A	879	G	2.1
32	2a	1061	G	2.1
32	2a	1068	G	2.1
32	2a	1222	G	2.1
45	2n	61	TRP	2.1
34	2c	150	LYS	2.1
35	1d	84	LYS	2.1
54	1w	69	G	2.1
54	1y	19	G	2.1
1	1A	2132	U	2.1
2	2B	8	U	2.1
32	2a	1001	A	2.1
32	2a	1049	U	2.1
24	12	1	MET	2.1
29	27	1	MET	2.1
6	2G	19	LEU	2.1
40	2i	79	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
29	27	27	GLY	2.1
33	2b	228	GLY	2.1
50	2s	68	GLY	2.1
4	2E	151	TYR	2.1
11	2P	75	ILE	2.1
12	2Q	137	TYR	2.1
33	2b	33	TYR	2.1
36	2e	118	ILE	2.1
41	1j	4	ILE	2.1
44	2m	39	ILE	2.1
25	23	59	VAL	2.1
28	26	52	VAL	2.1
34	2c	120	VAL	2.1
21	2Z	136	PHE	2.1
33	1b	28	PHE	2.1
37	1f	83	ASP	2.0
40	2i	37	PHE	2.1
8	2I	7	GLU	2.0
11	2P	15	ARG	2.0
8	2I	59	ALA	2.0
21	2Z	168	GLU	2.0
25	23	60	GLU	2.0
45	1n	3	ARG	2.0
51	1t	80	ARG	2.0
34	2c	100	ALA	2.0
1	1A	1100	C	2.0
1	2A	1509	C	2.0
1	2A	2137	C	2.0
3	1D	38	LYS	2.0
21	2Z	14	LYS	2.0
32	2a	1260	C	2.0
32	2a	1362	C	2.0
32	2a	1369	C	2.0
47	1p	35	LYS	2.0
54	2w	56	C	2.0
54	2y	4	C	2.0
21	1Z	69	THR	2.0
40	2i	27	THR	2.0
6	2G	173	LEU	2.0
8	1I	72	LEU	2.0
32	2a	1056	U	2.0
32	2a	1125	U	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	2a	1205	U	2.0
34	1c	12	LEU	2.0
39	1h	112	LEU	2.0
50	2s	22	LEU	2.0
54	1w	20	U	2.0
54	1y	47	U	2.0
1	2A	2134	A	2.0
1	2A	2153	G	2.0
2	2B	53	A	2.0
32	2a	976	G	2.0
32	2a	1003	G	2.0
32	2a	1221	G	2.0
32	2a	1271	G	2.0
53	1v	24	A	2.0
54	1y	35	A	2.0
26	24	20	ASN	2.0
38	1g	42	ILE	2.0
38	2g	42	ILE	2.0
39	2h	128	GLY	2.0
40	2i	68	GLY	2.0
46	2o	87	ILE	2.0
21	2Z	90	VAL	2.0
33	2b	197	VAL	2.0
36	2e	133	TYR	2.0
47	1p	2	VAL	2.0
50	2s	52	TYR	2.0
7	2H	123	PHE	2.0
33	2b	170	GLU	2.0
34	2c	10	PHE	2.0
40	1i	18	PHE	2.0
51	2t	83	ARG	2.0
31	19	12	ASP	2.0
45	2n	8	GLU	2.0
34	2c	180	ALA	2.0
44	2m	120	LYS	2.0
7	2H	8	PRO	2.0
33	2b	54	THR	2.0
35	2d	29	PRO	2.0
6	2G	135	LEU	2.0
6	2G	152	LEU	2.0
24	22	35	LEU	2.0
32	1a	163	C	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	2a	985	C	2.0
32	2a	1006	C	2.0
32	2a	1059	C	2.0
32	2a	1277	C	2.0
33	2b	145	LEU	2.0
54	2y	48	C	2.0
54	2y	62	C	2.0
7	2H	61	HIS	2.0
1	1A	1082	U	2.0
32	2a	961	U	2.0
6	2G	52	ILE	2.0
34	1c	96	GLY	2.0
47	2p	37	GLY	2.0
6	2G	149	VAL	2.0
17	2V	52	VAL	2.0
32	1a	149	A	2.0
34	2c	140	ARG	2.0
43	2l	18	VAL	2.0
44	2m	98	VAL	2.0
46	2o	68	ARG	2.0
47	2p	26	ARG	2.0
50	2s	19	VAL	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($\text{\AA}^2$)	Q<0.9
54	G7M	2w	46	24/25	0.47	0.15	92,100,108,128	0
54	4SU	2y	8	20/21	0.58	0.15	95,102,115,124	0
54	PSU	2y	55	20/21	0.58	0.16	95,103,112,114	0
54	G7M	2y	46	24/25	0.59	0.16	93,103,108,124	0
54	G7M	1w	46	24/25	0.61	0.14	83,91,108,125	0
54	4SU	2w	8	20/21	0.62	0.14	95,104,113,122	0
54	5MU	2y	54	21/22	0.63	0.17	89,99,108,126	0
54	MIA	2y	37	22/30	0.68	0.15	84,95,103,113	0
54	PSU	1y	55	20/21	0.68	0.14	88,97,106,113	0
54	MIA	1y	37	22/30	0.69	0.14	78,88,99,105	0
54	4SU	1y	8	20/21	0.72	0.12	93,96,106,109	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	G7M	1y	46	24/25	0.72	0.14	91,98,104,115	0
54	PSU	2w	55	20/21	0.74	0.13	83,96,105,108	0
54	5MU	2w	54	21/22	0.76	0.13	76,89,94,97	0
54	PSU	2y	32	20/21	0.76	0.15	86,95,106,107	0
54	5MU	1y	54	21/22	0.76	0.14	83,89,100,115	0
54	PSU	2y	39	20/21	0.77	0.12	87,90,101,107	0
55	4SU	2x	8	20/21	0.78	0.16	84,89,98,98	0
54	4SU	1w	8	20/21	0.79	0.12	83,88,96,99	0
54	PSU	1y	39	20/21	0.82	0.11	78,85,93,95	0
54	PSU	1y	32	20/21	0.82	0.11	82,90,99,99	0
32	2MG	2a	1207	24/25	0.82	0.15	84,90,101,109	0
55	PSU	2x	55	20/21	0.83	0.10	81,84,92,96	0
54	PSU	1w	55	20/21	0.83	0.10	69,81,87,90	0
32	PSU	2a	516	20/21	0.84	0.12	76,82,88,90	0
54	PSU	2w	39	20/21	0.84	0.12	80,90,96,98	0
32	M2G	2a	966	25/26	0.85	0.22	64,73,88,95	0
55	5MU	2x	54	21/22	0.85	0.11	81,85,90,105	0
1	5MU	2A	1915	21/22	0.86	0.14	77,82,91,99	0
54	PSU	2w	32	20/21	0.86	0.13	85,92,99,107	0
54	MIA	2w	37	25/30	0.87	0.14	84,88,95,97	0
32	5MC	2a	967	21/22	0.88	0.18	65,74,83,86	0
43	0TD	1l	92	10/11	0.88	0.14	50,55,58,79	0
55	5MC	2x	32	21/22	0.88	0.15	72,81,83,87	0
32	G7M	2a	527	24/25	0.89	0.15	64,71,78,84	0
55	5MU	1x	54	21/22	0.91	0.10	60,70,76,79	0
1	PSU	2A	1911	20/21	0.91	0.10	63,72,76,81	0
32	5MC	2a	1400	21/22	0.91	0.14	71,77,83,87	0
32	4OC	2a	1402	22/23	0.91	0.14	64,71,77,80	0
32	5MC	2a	1404	21/22	0.91	0.12	61,67,73,73	0
43	0TD	2l	92	10/11	0.91	0.13	71,74,75,87	0
32	2MG	1a	1207	24/25	0.92	0.10	65,71,76,78	0
54	PSU	1w	32	20/21	0.92	0.14	63,69,88,88	0
1	PSU	2A	1917	20/21	0.92	0.10	66,75,81,83	0
32	5MC	2a	1407	21/22	0.93	0.11	58,63,67,75	0
1	5MU	1A	1915	21/22	0.93	0.10	51,58,62,70	0
55	PSU	1x	55	20/21	0.93	0.08	58,65,73,77	0
55	4SU	1x	8	20/21	0.93	0.11	64,70,78,88	0
1	5MC	2A	1962	21/22	0.93	0.10	42,54,61,72	0
32	UR3	2a	1498	21/22	0.94	0.13	60,66,71,76	0
32	MA6	2a	1518	24/25	0.94	0.12	53,68,73,74	0
1	OMC	2A	1920	21/22	0.94	0.10	63,71,74,77	0
32	MA6	2a	1519	24/25	0.95	0.12	50,68,74,78	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	MIA	1w	37	29/30	0.95	0.12	49,59,67,72	0
32	5MC	1a	967	21/22	0.95	0.10	53,59,63,69	0
55	5MC	1x	32	21/22	0.95	0.10	52,55,60,63	0
54	5MU	1w	54	21/22	0.95	0.07	60,71,78,82	0
1	5MU	2A	1939	21/22	0.96	0.08	38,44,50,51	0
1	5MC	2A	1942	21/22	0.96	0.10	55,61,67,68	0
32	MA6	1a	1519	24/25	0.96	0.10	37,43,49,51	0
1	OMG	2A	2251	24/25	0.96	0.09	37,47,52,53	0
1	2MA	2A	2503	23/24	0.96	0.10	32,39,44,48	0
32	PSU	1a	516	20/21	0.96	0.08	55,61,66,68	0
32	G7M	1a	527	24/25	0.96	0.08	36,46,53,59	0
32	M2G	1a	966	25/26	0.96	0.11	51,55,62,65	0
1	PSU	1A	1917	20/21	0.96	0.08	45,53,65,68	0
54	PSU	1w	39	20/21	0.96	0.10	57,66,72,77	0
1	5MC	1A	1942	21/22	0.96	0.09	35,41,46,52	0
32	5MC	1a	1404	21/22	0.96	0.09	39,43,49,54	0
32	5MC	1a	1407	21/22	0.97	0.07	37,40,44,45	0
32	UR3	1a	1498	21/22	0.97	0.07	37,42,47,48	0
1	5MC	1A	1962	21/22	0.97	0.07	28,34,42,44	0
1	PSU	1A	2605	20/21	0.97	0.07	24,28,30,35	0
1	OMC	1A	1920	21/22	0.97	0.08	35,43,46,50	0
32	5MC	1a	1400	21/22	0.97	0.10	43,51,56,67	0
32	4OC	1a	1402	22/23	0.97	0.08	41,46,53,57	0
1	OMU	2A	2552	21/22	0.97	0.08	38,45,48,54	0
1	PSU	2A	2605	20/21	0.97	0.07	35,42,46,46	0
1	PSU	1A	1911	20/21	0.97	0.07	41,46,50,53	0
32	MA6	1a	1518	24/25	0.98	0.08	32,41,45,46	0
1	OMU	1A	2552	21/22	0.98	0.06	23,28,35,36	0
1	5MU	1A	1939	21/22	0.98	0.07	23,26,32,40	0
1	2MA	1A	2503	23/24	0.99	0.05	16,21,24,25	0
1	OMG	1A	2251	24/25	0.99	0.05	18,26,32,37	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
56	MG	2a	1822	1/1	0.31	0.77	94,94,94,94	0
56	MG	1B	229	1/1	0.32	0.20	77,77,77,77	0
56	MG	2A	3581	1/1	0.40	0.29	82,82,82,82	0
56	MG	2A	3763	1/1	0.47	0.30	80,80,80,80	0
56	MG	2A	3878	1/1	0.49	0.23	82,82,82,82	0
56	MG	2A	3521	1/1	0.51	0.29	65,65,65,65	0
56	MG	1v	101	1/1	0.52	0.25	78,78,78,78	0
56	MG	2A	3608	1/1	0.53	0.21	76,76,76,76	0
56	MG	1A	3947	1/1	0.56	0.19	70,70,70,70	0
56	MG	2y	106	1/1	0.56	0.23	89,89,89,89	0
56	MG	2A	3820	1/1	0.58	0.17	79,79,79,79	0
56	MG	2A	3620	1/1	0.58	0.20	72,72,72,72	0
56	MG	1A	3696	1/1	0.59	0.14	60,60,60,60	0
56	MG	1a	1817	1/1	0.59	0.16	84,84,84,84	0
56	MG	1A	3992	1/1	0.59	0.18	88,88,88,88	0
56	MG	1x	113	1/1	0.60	0.20	79,79,79,79	0
56	MG	2A	3787	1/1	0.60	0.33	83,83,83,83	0
56	MG	2a	1780	1/1	0.61	0.25	72,72,72,72	0
56	MG	1a	1801	1/1	0.61	0.17	89,89,89,89	0
56	MG	2y	101	1/1	0.61	0.16	83,83,83,83	0
56	MG	2A	3343	1/1	0.61	0.11	72,72,72,72	0
56	MG	1B	223	1/1	0.62	0.14	72,72,72,72	0
56	MG	2a	1771	1/1	0.62	0.30	84,84,84,84	0
56	MG	2a	1839	1/1	0.63	0.21	93,93,93,93	0
56	MG	2y	105	1/1	0.63	0.27	94,94,94,94	0
56	MG	2j	201	1/1	0.63	0.16	83,83,83,83	0
56	MG	2B	215	1/1	0.64	0.13	84,84,84,84	0
56	MG	2A	3218	1/1	0.64	0.10	82,82,82,82	0
56	MG	2A	3716	1/1	0.64	0.22	81,81,81,81	0
56	MG	2w	103	1/1	0.65	0.18	73,73,73,73	0
56	MG	1y	102	1/1	0.65	0.17	90,90,90,90	0
56	MG	1x	109	1/1	0.65	0.23	85,85,85,85	0
56	MG	1w	107	1/1	0.65	0.18	95,95,95,95	0
56	MG	2A	3498	1/1	0.66	0.18	61,61,61,61	0
56	MG	1A	4090	1/1	0.67	0.19	70,70,70,70	0
56	MG	2A	3719	1/1	0.67	0.16	82,82,82,82	0
56	MG	2a	1837	1/1	0.67	0.19	70,70,70,70	0
56	MG	2G	201	1/1	0.68	0.22	79,79,79,79	0
56	MG	2A	3648	1/1	0.68	0.23	75,75,75,75	0
56	MG	1a	1819	1/1	0.68	0.22	61,61,61,61	0
56	MG	2a	1791	1/1	0.68	0.22	81,81,81,81	0
56	MG	1w	108	1/1	0.68	0.21	82,82,82,82	0
56	MG	2A	3325	1/1	0.68	0.20	70,70,70,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3748	1/1	0.69	0.17	44,44,44,44	0
56	MG	1a	1807	1/1	0.69	0.19	81,81,81,81	0
56	MG	2a	1738	1/1	0.69	0.15	62,62,62,62	0
56	MG	2A	3236	1/1	0.69	0.21	68,68,68,68	0
56	MG	1F	313	1/1	0.69	0.20	63,63,63,63	0
56	MG	2x	103	1/1	0.69	0.27	86,86,86,86	0
56	MG	2a	1787	1/1	0.69	0.24	80,80,80,80	0
56	MG	1A	3925	1/1	0.69	0.17	52,52,52,52	0
56	MG	2a	1819	1/1	0.69	0.25	91,91,91,91	0
56	MG	1A	4065	1/1	0.70	0.24	73,73,73,73	0
56	MG	2A	3856	1/1	0.70	0.18	73,73,73,73	0
56	MG	1A	3539	1/1	0.70	0.12	68,68,68,68	0
56	MG	2A	3230	1/1	0.70	0.13	90,90,90,90	0
56	MG	2A	3234	1/1	0.70	0.24	68,68,68,68	0
56	MG	2a	1630	1/1	0.70	0.23	77,77,77,77	0
56	MG	2A	3520	1/1	0.70	0.38	82,82,82,82	0
56	MG	2A	3798	1/1	0.71	0.15	75,75,75,75	0
56	MG	2A	3799	1/1	0.71	0.19	61,61,61,61	0
56	MG	2a	1638	1/1	0.71	0.10	71,71,71,71	0
56	MG	2A	3091	1/1	0.71	0.26	70,70,70,70	0
56	MG	2a	1751	1/1	0.71	0.13	85,85,85,85	0
56	MG	1A	3989	1/1	0.71	0.23	94,94,94,94	0
56	MG	2A	3867	1/1	0.71	0.22	75,75,75,75	0
56	MG	2A	3678	1/1	0.71	0.21	66,66,66,66	0
56	MG	1a	1788	1/1	0.71	0.28	71,71,71,71	0
56	MG	2a	1808	1/1	0.71	0.24	76,76,76,76	0
56	MG	2A	3729	1/1	0.72	0.14	87,87,87,87	0
56	MG	2A	3604	1/1	0.72	0.22	79,79,79,79	0
56	MG	2q	202	1/1	0.72	0.18	79,79,79,79	0
56	MG	1a	1825	1/1	0.72	0.21	77,77,77,77	0
56	MG	2A	3714	1/1	0.72	0.19	66,66,66,66	0
56	MG	2a	1821	1/1	0.72	0.19	95,95,95,95	0
56	MG	2A	3587	1/1	0.72	0.23	68,68,68,68	0
56	MG	2A	3624	1/1	0.72	0.25	86,86,86,86	0
56	MG	1a	1767	1/1	0.73	0.22	75,75,75,75	0
56	MG	2a	1689	1/1	0.73	0.12	80,80,80,80	0
56	MG	1A	4130	1/1	0.73	0.18	69,69,69,69	0
56	MG	2A	3273	1/1	0.73	0.14	70,70,70,70	0
56	MG	2A	3591	1/1	0.73	0.22	74,74,74,74	0
56	MG	2A	3274	1/1	0.73	0.22	64,64,64,64	0
56	MG	2A	3845	1/1	0.73	0.19	71,71,71,71	0
56	MG	2A	3450	1/1	0.74	0.17	69,69,69,69	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2B	211	1/1	0.74	0.24	77,77,77,77	0
56	MG	1A	3797	1/1	0.74	0.16	56,56,56,56	0
56	MG	2A	3619	1/1	0.74	0.14	75,75,75,75	0
56	MG	2a	1828	1/1	0.74	0.27	80,80,80,80	0
56	MG	2a	1830	1/1	0.74	0.15	87,87,87,87	0
56	MG	2A	3499	1/1	0.74	0.21	78,78,78,78	0
56	MG	2A	3231	1/1	0.74	0.16	70,70,70,70	0
56	MG	1a	1789	1/1	0.74	0.41	82,82,82,82	0
56	MG	2A	3667	1/1	0.74	0.18	54,54,54,54	0
56	MG	1A	3292	1/1	0.74	0.22	78,78,78,78	0
56	MG	2A	3837	1/1	0.74	0.20	73,73,73,73	0
56	MG	2A	3685	1/1	0.74	0.16	49,49,49,49	0
56	MG	2A	3353	1/1	0.74	0.25	78,78,78,78	0
56	MG	2A	3426	1/1	0.74	0.14	52,52,52,52	0
56	MG	2A	3688	1/1	0.75	0.12	63,63,63,63	0
56	MG	2A	3704	1/1	0.75	0.14	70,70,70,70	0
56	MG	2A	3094	1/1	0.75	0.20	79,79,79,79	0
56	MG	2A	3181	1/1	0.75	0.14	69,69,69,69	0
56	MG	1A	3643	1/1	0.75	0.17	57,57,57,57	0
56	MG	1A	3435	1/1	0.75	0.19	85,85,85,85	0
56	MG	2A	3868	1/1	0.75	0.17	68,68,68,68	0
56	MG	1B	224	1/1	0.75	0.18	76,76,76,76	0
56	MG	2A	3081	1/1	0.75	0.23	86,86,86,86	0
56	MG	1A	3991	1/1	0.75	0.15	69,69,69,69	0
56	MG	2B	218	1/1	0.75	0.31	82,82,82,82	0
56	MG	2A	3455	1/1	0.75	0.17	53,53,53,53	0
56	MG	1A	3741	1/1	0.76	0.27	62,62,62,62	0
56	MG	1a	1821	1/1	0.76	0.24	76,76,76,76	0
56	MG	1A	3538	1/1	0.76	0.23	65,65,65,65	0
56	MG	2A	3616	1/1	0.76	0.20	69,69,69,69	0
56	MG	1T	204	1/1	0.76	0.17	41,41,41,41	0
56	MG	2A	3087	1/1	0.76	0.18	71,71,71,71	0
56	MG	15	104	1/1	0.76	0.17	57,57,57,57	0
56	MG	2A	3248	1/1	0.76	0.12	70,70,70,70	0
56	MG	2A	3788	1/1	0.76	0.16	60,60,60,60	0
56	MG	2A	3251	1/1	0.76	0.12	68,68,68,68	0
56	MG	2a	1656	1/1	0.76	0.13	62,62,62,62	0
56	MG	2a	1678	1/1	0.76	0.30	74,74,74,74	0
56	MG	2A	3673	1/1	0.76	0.21	64,64,64,64	0
56	MG	1A	3140	1/1	0.76	0.14	41,41,41,41	0
56	MG	2A	3145	1/1	0.76	0.12	64,64,64,64	0
56	MG	2A	3147	1/1	0.76	0.21	79,79,79,79	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3847	1/1	0.76	0.13	86,86,86,86	0
56	MG	2a	1687	1/1	0.77	0.26	75,75,75,75	0
56	MG	2A	3057	1/1	0.77	0.19	79,79,79,79	0
56	MG	2A	3280	1/1	0.77	0.25	67,67,67,67	0
56	MG	1A	3666	1/1	0.77	0.12	24,24,24,24	0
56	MG	2a	1604	1/1	0.77	0.36	85,85,85,85	0
56	MG	2A	3809	1/1	0.77	0.29	71,71,71,71	0
56	MG	2g	201	1/1	0.77	0.10	84,84,84,84	0
56	MG	2a	1632	1/1	0.77	0.30	77,77,77,77	0
56	MG	2m	201	1/1	0.77	0.19	81,81,81,81	0
56	MG	1A	3704	1/1	0.77	0.19	53,53,53,53	0
56	MG	2a	1795	1/1	0.77	0.15	78,78,78,78	0
56	MG	2w	109	1/1	0.77	0.20	75,75,75,75	0
56	MG	2a	1804	1/1	0.77	0.12	78,78,78,78	0
56	MG	2A	3829	1/1	0.77	0.19	66,66,66,66	0
56	MG	2a	1815	1/1	0.77	0.28	75,75,75,75	0
56	MG	1a	1667	1/1	0.77	0.33	64,64,64,64	0
56	MG	1A	3735	1/1	0.78	0.15	56,56,56,56	0
56	MG	1A	4094	1/1	0.78	0.10	51,51,51,51	0
56	MG	2a	1793	1/1	0.78	0.14	75,75,75,75	0
56	MG	1A	3421	1/1	0.78	0.15	56,56,56,56	0
56	MG	1A	3581	1/1	0.78	0.16	57,57,57,57	0
56	MG	2a	1807	1/1	0.78	0.25	81,81,81,81	0
56	MG	1a	1699	1/1	0.78	0.13	84,84,84,84	0
56	MG	2A	3306	1/1	0.78	0.12	53,53,53,53	0
56	MG	2A	3312	1/1	0.78	0.18	67,67,67,67	0
56	MG	2a	1602	1/1	0.78	0.16	82,82,82,82	0
56	MG	2A	3208	1/1	0.78	0.16	69,69,69,69	0
56	MG	2a	1605	1/1	0.78	0.19	68,68,68,68	0
56	MG	2a	1622	1/1	0.78	0.24	71,71,71,71	0
56	MG	1A	4074	1/1	0.78	0.17	59,59,59,59	0
56	MG	2A	3351	1/1	0.78	0.09	75,75,75,75	0
56	MG	2A	3221	1/1	0.78	0.19	69,69,69,69	0
56	MG	2A	3805	1/1	0.78	0.17	73,73,73,73	0
56	MG	2A	3395	1/1	0.78	0.16	70,70,70,70	0
56	MG	2A	3664	1/1	0.78	0.26	72,72,72,72	0
56	MG	2w	102	1/1	0.78	0.29	80,80,80,80	0
56	MG	2A	3053	1/1	0.78	0.14	58,58,58,58	0
56	MG	2a	1724	1/1	0.78	0.14	86,86,86,86	0
56	MG	1A	4089	1/1	0.78	0.22	58,58,58,58	0
56	MG	1a	1840	1/1	0.78	0.33	75,75,75,75	0
56	MG	1a	1841	1/1	0.78	0.09	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
56	MG	2A	3237	1/1	0.78	0.15	76,76,76,76	0
56	MG	2A	3724	1/1	0.79	0.19	57,57,57,57	0
56	MG	2B	214	1/1	0.79	0.18	70,70,70,70	0
56	MG	1a	1823	1/1	0.79	0.23	69,69,69,69	0
56	MG	1B	225	1/1	0.79	0.14	67,67,67,67	0
56	MG	1a	1834	1/1	0.79	0.27	67,67,67,67	0
56	MG	1a	1787	1/1	0.79	0.33	75,75,75,75	0
56	MG	2a	1809	1/1	0.79	0.30	74,74,74,74	0
56	MG	1A	3921	1/1	0.79	0.12	74,74,74,74	0
56	MG	1A	3347	1/1	0.79	0.23	64,64,64,64	0
56	MG	2a	1617	1/1	0.79	0.29	82,82,82,82	0
56	MG	2A	3634	1/1	0.79	0.12	64,64,64,64	0
56	MG	1A	3995	1/1	0.79	0.14	56,56,56,56	0
56	MG	2A	3249	1/1	0.79	0.11	79,79,79,79	0
56	MG	1A	4057	1/1	0.79	0.14	49,49,49,49	0
56	MG	2a	1641	1/1	0.79	0.37	94,94,94,94	0
56	MG	2A	3149	1/1	0.79	0.22	87,87,87,87	0
56	MG	1a	1620	1/1	0.79	0.22	63,63,63,63	0
56	MG	1A	3474	1/1	0.79	0.14	69,69,69,69	0
56	MG	2A	3522	1/1	0.79	0.23	63,63,63,63	0
56	MG	2A	3217	1/1	0.79	0.17	89,89,89,89	0
56	MG	2A	3857	1/1	0.79	0.14	64,64,64,64	0
56	MG	2A	3311	1/1	0.79	0.12	65,65,65,65	0
56	MG	2a	1760	1/1	0.79	0.24	86,86,86,86	0
56	MG	1A	3423	1/1	0.79	0.23	57,57,57,57	0
56	MG	2y	102	1/1	0.79	0.11	87,87,87,87	0
56	MG	2y	104	1/1	0.79	0.15	79,79,79,79	0
56	MG	2A	3869	1/1	0.79	0.18	76,76,76,76	0
56	MG	2A	3599	1/1	0.79	0.25	85,85,85,85	0
56	MG	2A	3092	1/1	0.80	0.23	72,72,72,72	0
56	MG	1a	1784	1/1	0.80	0.19	72,72,72,72	0
56	MG	2A	3120	1/1	0.80	0.13	55,55,55,55	0
56	MG	1A	4082	1/1	0.80	0.17	50,50,50,50	0
56	MG	2A	3253	1/1	0.80	0.11	64,64,64,64	0
56	MG	1A	3209	1/1	0.80	0.12	73,73,73,73	0
56	MG	1A	3926	1/1	0.80	0.12	45,45,45,45	0
56	MG	2A	3580	1/1	0.80	0.14	85,85,85,85	0
56	MG	2A	3276	1/1	0.80	0.24	69,69,69,69	0
56	MG	1A	4015	1/1	0.80	0.16	65,65,65,65	0
56	MG	2Z	301	1/1	0.80	0.17	85,85,85,85	0
56	MG	1a	1805	1/1	0.80	0.15	71,71,71,71	0
56	MG	2A	3307	1/1	0.80	0.14	70,70,70,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1603	1/1	0.80	0.15	67,67,67,67	0
56	MG	1A	4021	1/1	0.80	0.17	44,44,44,44	0
56	MG	1a	1629	1/1	0.80	0.19	74,74,74,74	0
56	MG	2A	3341	1/1	0.80	0.36	74,74,74,74	0
56	MG	2A	3224	1/1	0.80	0.21	70,70,70,70	0
56	MG	1A	3705	1/1	0.80	0.23	54,54,54,54	0
56	MG	2A	3814	1/1	0.80	0.20	68,68,68,68	0
56	MG	2A	3633	1/1	0.80	0.23	68,68,68,68	0
56	MG	2A	3821	1/1	0.80	0.13	79,79,79,79	0
56	MG	2A	3828	1/1	0.80	0.20	73,73,73,73	0
56	MG	2a	1688	1/1	0.80	0.25	70,70,70,70	0
56	MG	1A	3856	1/1	0.80	0.11	66,66,66,66	0
56	MG	2x	104	1/1	0.80	0.26	79,79,79,79	0
56	MG	1a	1758	1/1	0.80	0.13	81,81,81,81	0
56	MG	2A	3839	1/1	0.80	0.10	77,77,77,77	0
56	MG	2A	3651	1/1	0.80	0.23	67,67,67,67	0
56	MG	2A	3408	1/1	0.80	0.29	66,66,66,66	0
56	MG	1A	3391	1/1	0.80	0.19	55,55,55,55	0
56	MG	2a	1766	1/1	0.81	0.25	73,73,73,73	0
56	MG	1A	3261	1/1	0.81	0.23	60,60,60,60	0
56	MG	2A	3025	1/1	0.81	0.20	70,70,70,70	0
56	MG	1A	3384	1/1	0.81	0.22	77,77,77,77	0
56	MG	2A	3337	1/1	0.81	0.16	56,56,56,56	0
56	MG	1A	3250	1/1	0.81	0.20	60,60,60,60	0
56	MG	1A	4077	1/1	0.81	0.13	64,64,64,64	0
56	MG	28	101	1/1	0.81	0.25	77,77,77,77	0
56	MG	1A	3392	1/1	0.81	0.14	68,68,68,68	0
56	MG	1A	4087	1/1	0.81	0.11	55,55,55,55	0
56	MG	1A	3333	1/1	0.81	0.17	51,51,51,51	0
56	MG	2a	1810	1/1	0.81	0.14	76,76,76,76	0
56	MG	2a	1611	1/1	0.81	0.23	67,67,67,67	0
56	MG	2a	1612	1/1	0.81	0.25	69,69,69,69	0
56	MG	1A	3595	1/1	0.81	0.11	55,55,55,55	0
56	MG	2A	3117	1/1	0.81	0.30	79,79,79,79	0
56	MG	1A	3609	1/1	0.81	0.21	66,66,66,66	0
56	MG	1A	3822	1/1	0.81	0.13	27,27,27,27	0
56	MG	2A	3492	1/1	0.81	0.20	73,73,73,73	0
56	MG	2a	1639	1/1	0.81	0.29	72,72,72,72	0
56	MG	2A	3254	1/1	0.81	0.17	74,74,74,74	0
56	MG	2a	1642	1/1	0.81	0.12	75,75,75,75	0
56	MG	2A	3269	1/1	0.81	0.20	76,76,76,76	0
56	MG	1A	4135	1/1	0.81	0.21	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
56	MG	2a	1681	1/1	0.81	0.27	71,71,71,71	0
56	MG	2a	1682	1/1	0.81	0.42	79,79,79,79	0
56	MG	2A	3855	1/1	0.81	0.17	62,62,62,62	0
56	MG	1A	3838	1/1	0.81	0.12	25,25,25,25	0
56	MG	2A	3162	1/1	0.81	0.12	78,78,78,78	0
56	MG	2a	1715	1/1	0.81	0.17	70,70,70,70	0
56	MG	1A	3335	1/1	0.81	0.23	72,72,72,72	0
56	MG	2A	3300	1/1	0.81	0.09	73,73,73,73	0
56	MG	1A	4036	1/1	0.81	0.16	62,62,62,62	0
56	MG	1A	4038	1/1	0.81	0.18	52,52,52,52	0
56	MG	1A	3780	1/1	0.82	0.13	19,19,19,19	0
56	MG	2a	1699	1/1	0.82	0.25	64,64,64,64	0
56	MG	2A	3381	1/1	0.82	0.14	50,50,50,50	0
56	MG	2A	3250	1/1	0.82	0.26	73,73,73,73	0
56	MG	2A	3662	1/1	0.82	0.13	69,69,69,69	0
56	MG	1A	3864	1/1	0.82	0.12	60,60,60,60	0
56	MG	2a	1752	1/1	0.82	0.14	72,72,72,72	0
56	MG	1A	3878	1/1	0.82	0.14	67,67,67,67	0
56	MG	1B	232	1/1	0.82	0.16	52,52,52,52	0
56	MG	2A	3268	1/1	0.82	0.15	62,62,62,62	0
56	MG	2a	1778	1/1	0.82	0.21	79,79,79,79	0
56	MG	2A	3490	1/1	0.82	0.22	71,71,71,71	0
56	MG	1A	3894	1/1	0.82	0.16	26,26,26,26	0
56	MG	1A	3227	1/1	0.82	0.26	60,60,60,60	0
56	MG	1a	1800	1/1	0.82	0.14	64,64,64,64	0
56	MG	2A	3507	1/1	0.82	0.17	65,65,65,65	0
56	MG	2D	307	1/1	0.82	0.18	74,74,74,74	0
56	MG	1Y	203	1/1	0.82	0.09	69,69,69,69	0
56	MG	1a	1803	1/1	0.82	0.13	66,66,66,66	0
56	MG	25	105	1/1	0.82	0.11	57,57,57,57	0
56	MG	1A	3804	1/1	0.82	0.10	40,40,40,40	0
56	MG	2A	3546	1/1	0.82	0.12	54,54,54,54	0
56	MG	2A	3560	1/1	0.82	0.16	46,46,46,46	0
56	MG	2A	3785	1/1	0.82	0.10	76,76,76,76	0
56	MG	1A	3618	1/1	0.82	0.14	70,70,70,70	0
56	MG	1A	3929	1/1	0.82	0.17	63,63,63,63	0
56	MG	2a	1614	1/1	0.82	0.25	73,73,73,73	0
56	MG	2a	1831	1/1	0.82	0.22	70,70,70,70	0
56	MG	2A	3227	1/1	0.82	0.18	58,58,58,58	0
56	MG	1A	3521	1/1	0.82	0.23	58,58,58,58	0
56	MG	2a	1623	1/1	0.82	0.13	71,71,71,71	0
56	MG	2A	3802	1/1	0.82	0.23	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3324	1/1	0.82	0.23	75,75,75,75	0
56	MG	1a	1666	1/1	0.82	0.24	63,63,63,63	0
56	MG	2A	3811	1/1	0.82	0.19	70,70,70,70	0
56	MG	2A	3332	1/1	0.82	0.21	70,70,70,70	0
56	MG	2A	3612	1/1	0.82	0.10	68,68,68,68	0
56	MG	1B	209	1/1	0.82	0.16	61,61,61,61	0
56	MG	2A	3827	1/1	0.82	0.18	66,66,66,66	0
56	MG	2x	106	1/1	0.82	0.13	72,72,72,72	0
56	MG	2A	3338	1/1	0.82	0.16	55,55,55,55	0
56	MG	1A	3953	1/1	0.82	0.15	55,55,55,55	0
56	MG	2a	1683	1/1	0.82	0.17	60,60,60,60	0
56	MG	1a	1829	1/1	0.82	0.12	63,63,63,63	0
56	MG	2A	3103	1/1	0.82	0.16	62,62,62,62	0
56	MG	2A	3844	1/1	0.83	0.19	82,82,82,82	0
56	MG	2A	3429	1/1	0.83	0.20	74,74,74,74	0
56	MG	2A	3656	1/1	0.83	0.16	72,72,72,72	0
56	MG	1A	3257	1/1	0.83	0.16	57,57,57,57	0
56	MG	1A	3671	1/1	0.83	0.18	64,64,64,64	0
56	MG	2A	3479	1/1	0.83	0.18	51,51,51,51	0
56	MG	2A	3859	1/1	0.83	0.10	67,67,67,67	0
56	MG	2A	3861	1/1	0.83	0.18	65,65,65,65	0
56	MG	2A	3864	1/1	0.83	0.15	67,67,67,67	0
56	MG	1A	3604	1/1	0.83	0.15	43,43,43,43	0
56	MG	2A	3291	1/1	0.83	0.17	73,73,73,73	0
56	MG	2a	1764	1/1	0.83	0.18	81,81,81,81	0
56	MG	2A	3299	1/1	0.83	0.17	69,69,69,69	0
56	MG	1a	1826	1/1	0.83	0.20	66,66,66,66	0
56	MG	2a	1773	1/1	0.83	0.12	78,78,78,78	0
56	MG	2B	209	1/1	0.83	0.26	80,80,80,80	0
56	MG	10	105	1/1	0.83	0.17	74,74,74,74	0
56	MG	2A	3509	1/1	0.83	0.14	63,63,63,63	0
56	MG	1a	1830	1/1	0.83	0.19	63,63,63,63	0
56	MG	2A	3308	1/1	0.83	0.23	64,64,64,64	0
56	MG	2A	3309	1/1	0.83	0.11	70,70,70,70	0
56	MG	2F	306	1/1	0.83	0.14	59,59,59,59	0
56	MG	1A	3176	1/1	0.83	0.16	69,69,69,69	0
56	MG	2N	201	1/1	0.83	0.23	72,72,72,72	0
56	MG	1B	216	1/1	0.83	0.15	51,51,51,51	0
56	MG	2A	3569	1/1	0.83	0.13	54,54,54,54	0
56	MG	2A	3318	1/1	0.83	0.09	74,74,74,74	0
56	MG	1A	3616	1/1	0.83	0.15	45,45,45,45	0
56	MG	1h	201	1/1	0.83	0.11	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3791	1/1	0.83	0.20	69,69,69,69	0
56	MG	2A	3792	1/1	0.83	0.21	62,62,62,62	0
56	MG	1A	3221	1/1	0.83	0.30	73,73,73,73	0
56	MG	2A	3134	1/1	0.83	0.24	67,67,67,67	0
56	MG	1A	3415	1/1	0.83	0.12	66,66,66,66	0
56	MG	2A	3607	1/1	0.83	0.13	55,55,55,55	0
56	MG	1A	4035	1/1	0.83	0.15	71,71,71,71	0
56	MG	1a	1810	1/1	0.83	0.18	65,65,65,65	0
56	MG	2a	1631	1/1	0.83	0.28	64,64,64,64	0
56	MG	1A	3950	1/1	0.83	0.15	53,53,53,53	0
56	MG	2A	3179	1/1	0.83	0.16	64,64,64,64	0
56	MG	2A	3363	1/1	0.83	0.24	58,58,58,58	0
56	MG	2w	108	1/1	0.83	0.10	85,85,85,85	0
56	MG	2A	3825	1/1	0.83	0.12	78,78,78,78	0
56	MG	2A	3263	1/1	0.83	0.15	65,65,65,65	0
56	MG	2a	1645	1/1	0.83	0.13	79,79,79,79	0
56	MG	2a	1655	1/1	0.83	0.18	67,67,67,67	0
56	MG	2A	3632	1/1	0.83	0.12	51,51,51,51	0
56	MG	2a	1669	1/1	0.83	0.31	70,70,70,70	0
56	MG	1D	313	1/1	0.83	0.24	40,40,40,40	0
56	MG	2A	3195	1/1	0.83	0.17	48,48,48,48	0
56	MG	2A	3207	1/1	0.83	0.38	57,57,57,57	0
56	MG	2A	3366	1/1	0.84	0.27	60,60,60,60	0
56	MG	2A	3639	1/1	0.84	0.11	62,62,62,62	0
56	MG	2A	3642	1/1	0.84	0.20	76,76,76,76	0
56	MG	1A	3755	1/1	0.84	0.44	34,34,34,34	0
56	MG	2A	3140	1/1	0.84	0.15	63,63,63,63	0
56	MG	2A	3264	1/1	0.84	0.17	77,77,77,77	0
56	MG	1A	3914	1/1	0.84	0.08	82,82,82,82	0
56	MG	2a	1694	1/1	0.84	0.16	66,66,66,66	0
56	MG	1a	1684	1/1	0.84	0.24	60,60,60,60	0
56	MG	2a	1712	1/1	0.84	0.30	75,75,75,75	0
56	MG	2A	3271	1/1	0.84	0.12	70,70,70,70	0
56	MG	2a	1718	1/1	0.84	0.38	69,69,69,69	0
56	MG	2A	3862	1/1	0.84	0.11	60,60,60,60	0
56	MG	2a	1733	1/1	0.84	0.09	105,105,105,105	0
56	MG	2a	1736	1/1	0.84	0.24	78,78,78,78	0
56	MG	1A	3417	1/1	0.84	0.15	64,64,64,64	0
56	MG	2a	1742	1/1	0.84	0.12	75,75,75,75	0
56	MG	2A	3866	1/1	0.84	0.21	78,78,78,78	0
56	MG	1a	1729	1/1	0.84	0.14	77,77,77,77	0
56	MG	2a	1759	1/1	0.84	0.26	66,66,66,66	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3374	1/1	0.84	0.13	55,55,55,55	0
56	MG	2A	3687	1/1	0.84	0.20	70,70,70,70	0
56	MG	1B	218	1/1	0.84	0.15	60,60,60,60	0
56	MG	2A	3880	1/1	0.84	0.13	74,74,74,74	0
56	MG	2B	201	1/1	0.84	0.18	76,76,76,76	0
56	MG	2A	3283	1/1	0.84	0.14	70,70,70,70	0
56	MG	2A	3711	1/1	0.84	0.17	71,71,71,71	0
56	MG	2a	1783	1/1	0.84	0.25	72,72,72,72	0
56	MG	2a	1784	1/1	0.84	0.21	81,81,81,81	0
56	MG	2a	1785	1/1	0.84	0.25	67,67,67,67	0
56	MG	2B	212	1/1	0.84	0.15	77,77,77,77	0
56	MG	2A	3193	1/1	0.84	0.27	74,74,74,74	0
56	MG	2A	3293	1/1	0.84	0.25	69,69,69,69	0
56	MG	2A	3295	1/1	0.84	0.23	72,72,72,72	0
56	MG	2A	3296	1/1	0.84	0.12	83,83,83,83	0
56	MG	1A	3158	1/1	0.84	0.18	60,60,60,60	0
56	MG	1A	4056	1/1	0.84	0.11	47,47,47,47	0
56	MG	1A	3813	1/1	0.84	0.13	43,43,43,43	0
56	MG	2A	3776	1/1	0.84	0.14	59,59,59,59	0
56	MG	1A	3425	1/1	0.84	0.17	65,65,65,65	0
56	MG	2A	3567	1/1	0.84	0.29	68,68,68,68	0
56	MG	1A	3341	1/1	0.84	0.11	51,51,51,51	0
56	MG	2A	3790	1/1	0.84	0.24	64,64,64,64	0
56	MG	2A	3019	1/1	0.84	0.20	70,70,70,70	0
56	MG	1D	309	1/1	0.84	0.17	41,41,41,41	0
56	MG	2A	3584	1/1	0.84	0.12	53,53,53,53	0
56	MG	1A	3850	1/1	0.84	0.17	68,68,68,68	0
56	MG	1A	4081	1/1	0.84	0.16	60,60,60,60	0
56	MG	1A	3453	1/1	0.84	0.11	66,66,66,66	0
56	MG	1A	3990	1/1	0.84	0.14	62,62,62,62	0
56	MG	2a	1624	1/1	0.84	0.23	71,71,71,71	0
56	MG	1A	3180	1/1	0.84	0.14	50,50,50,50	0
56	MG	1A	3877	1/1	0.84	0.10	58,58,58,58	0
56	MG	2A	3239	1/1	0.84	0.19	72,72,72,72	0
56	MG	1A	3372	1/1	0.84	0.10	51,51,51,51	0
56	MG	2A	3823	1/1	0.84	0.16	54,54,54,54	0
56	MG	1A	4100	1/1	0.84	0.13	53,53,53,53	0
56	MG	2A	3826	1/1	0.84	0.12	58,58,58,58	0
56	MG	2a	1644	1/1	0.84	0.28	80,80,80,80	0
56	MG	2A	3110	1/1	0.84	0.10	67,67,67,67	0
56	MG	1a	1626	1/1	0.84	0.10	47,47,47,47	0
56	MG	2A	3354	1/1	0.84	0.12	71,71,71,71	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	1660	1/1	0.84	0.28	69,69,69,69	0
56	MG	1A	4115	1/1	0.84	0.15	66,66,66,66	0
56	MG	2a	1685	1/1	0.85	0.13	50,50,50,50	0
56	MG	2A	3657	1/1	0.85	0.14	61,61,61,61	0
56	MG	2A	3660	1/1	0.85	0.09	51,51,51,51	0
56	MG	2A	3003	1/1	0.85	0.27	57,57,57,57	0
56	MG	10	102	1/1	0.85	0.16	56,56,56,56	0
56	MG	2a	1695	1/1	0.85	0.21	58,58,58,58	0
56	MG	1A	4029	1/1	0.85	0.26	65,65,65,65	0
56	MG	1A	3839	1/1	0.85	0.12	30,30,30,30	0
56	MG	1a	1602	1/1	0.85	0.23	63,63,63,63	0
56	MG	2A	3059	1/1	0.85	0.20	44,44,44,44	0
56	MG	2a	1720	1/1	0.85	0.11	72,72,72,72	0
56	MG	2A	3502	1/1	0.85	0.21	59,59,59,59	0
56	MG	2A	3067	1/1	0.85	0.20	73,73,73,73	0
56	MG	2A	3695	1/1	0.85	0.13	63,63,63,63	0
56	MG	2A	3701	1/1	0.85	0.14	50,50,50,50	0
56	MG	1A	4109	1/1	0.85	0.15	63,63,63,63	0
56	MG	2A	3710	1/1	0.85	0.14	66,66,66,66	0
56	MG	1A	4078	1/1	0.85	0.17	73,73,73,73	0
56	MG	1a	1838	1/1	0.85	0.20	62,62,62,62	0
56	MG	1A	3178	1/1	0.85	0.13	43,43,43,43	0
56	MG	2B	213	1/1	0.85	0.21	76,76,76,76	0
56	MG	1B	233	1/1	0.85	0.17	67,67,67,67	0
56	MG	2A	3554	1/1	0.85	0.18	53,53,53,53	0
56	MG	1e	201	1/1	0.85	0.12	72,72,72,72	0
56	MG	1A	3988	1/1	0.85	0.12	60,60,60,60	0
56	MG	1A	4013	1/1	0.85	0.13	41,41,41,41	0
56	MG	2A	3764	1/1	0.85	0.21	74,74,74,74	0
56	MG	2A	3579	1/1	0.85	0.20	65,65,65,65	0
56	MG	1v	102	1/1	0.85	0.17	77,77,77,77	0
56	MG	2A	3335	1/1	0.85	0.31	81,81,81,81	0
56	MG	1w	104	1/1	0.85	0.10	83,83,83,83	0
56	MG	1A	3737	1/1	0.85	0.21	49,49,49,49	0
56	MG	2A	3590	1/1	0.85	0.15	58,58,58,58	0
56	MG	2a	1801	1/1	0.85	0.25	77,77,77,77	0
56	MG	2A	3143	1/1	0.85	0.12	51,51,51,51	0
56	MG	2A	3797	1/1	0.85	0.11	89,89,89,89	0
56	MG	2A	3597	1/1	0.85	0.23	63,63,63,63	0
56	MG	2a	1613	1/1	0.85	0.27	67,67,67,67	0
56	MG	1a	1697	1/1	0.85	0.16	64,64,64,64	0
56	MG	2a	1814	1/1	0.85	0.24	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	1616	1/1	0.85	0.21	85,85,85,85	0
56	MG	2a	1817	1/1	0.85	0.16	66,66,66,66	0
56	MG	1x	105	1/1	0.85	0.19	73,73,73,73	0
56	MG	1x	107	1/1	0.85	0.28	82,82,82,82	0
56	MG	2A	3806	1/1	0.85	0.23	67,67,67,67	0
56	MG	2a	1823	1/1	0.85	0.13	81,81,81,81	0
56	MG	2A	3154	1/1	0.85	0.15	72,72,72,72	0
56	MG	2A	3609	1/1	0.85	0.18	44,44,44,44	0
56	MG	2A	3155	1/1	0.85	0.21	65,65,65,65	0
56	MG	2A	3159	1/1	0.85	0.24	66,66,66,66	0
56	MG	2A	3160	1/1	0.85	0.15	65,65,65,65	0
56	MG	2d	302	1/1	0.85	0.19	65,65,65,65	0
56	MG	2A	3389	1/1	0.85	0.10	63,63,63,63	0
56	MG	1A	3923	1/1	0.85	0.12	44,44,44,44	0
56	MG	2k	201	1/1	0.85	0.18	68,68,68,68	0
56	MG	1B	220	1/1	0.85	0.16	68,68,68,68	0
56	MG	2A	3425	1/1	0.85	0.12	58,58,58,58	0
56	MG	2w	101	1/1	0.85	0.13	79,79,79,79	0
56	MG	1a	1738	1/1	0.85	0.16	51,51,51,51	0
56	MG	2a	1649	1/1	0.85	0.14	76,76,76,76	0
56	MG	2A	3427	1/1	0.85	0.17	43,43,43,43	0
56	MG	2A	3830	1/1	0.85	0.10	57,57,57,57	0
56	MG	2A	3188	1/1	0.85	0.11	60,60,60,60	0
56	MG	2a	1665	1/1	0.85	0.23	69,69,69,69	0
56	MG	2A	3647	1/1	0.85	0.12	69,69,69,69	0
56	MG	2a	1677	1/1	0.85	0.21	73,73,73,73	0
56	MG	2A	3843	1/1	0.85	0.10	67,67,67,67	0
56	MG	2A	3439	1/1	0.85	0.23	74,74,74,74	0
56	MG	2A	3442	1/1	0.85	0.12	58,58,58,58	0
56	MG	2A	3192	1/1	0.85	0.12	59,59,59,59	0
56	MG	2A	3544	1/1	0.86	0.27	63,63,63,63	0
56	MG	1A	3826	1/1	0.86	0.10	49,49,49,49	0
56	MG	1A	3640	1/1	0.86	0.10	18,18,18,18	0
56	MG	2A	3135	1/1	0.86	0.18	66,66,66,66	0
56	MG	2A	3281	1/1	0.86	0.24	75,75,75,75	0
56	MG	2a	1668	1/1	0.86	0.37	72,72,72,72	0
56	MG	1A	3276	1/1	0.86	0.12	49,49,49,49	0
56	MG	1A	3443	1/1	0.86	0.12	53,53,53,53	0
56	MG	1A	4097	1/1	0.86	0.10	61,61,61,61	0
56	MG	2A	3817	1/1	0.86	0.15	62,62,62,62	0
56	MG	2A	3818	1/1	0.86	0.16	74,74,74,74	0
56	MG	1A	3154	1/1	0.86	0.12	65,65,65,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3111	1/1	0.86	0.12	41,41,41,41	0
56	MG	2A	3822	1/1	0.86	0.15	73,73,73,73	0
56	MG	1A	3997	1/1	0.86	0.17	64,64,64,64	0
56	MG	2A	3824	1/1	0.86	0.12	64,64,64,64	0
56	MG	2a	1690	1/1	0.86	0.20	77,77,77,77	0
56	MG	1a	1643	1/1	0.86	0.28	65,65,65,65	0
56	MG	2A	3304	1/1	0.86	0.14	69,69,69,69	0
56	MG	1a	1664	1/1	0.86	0.22	61,61,61,61	0
56	MG	1A	4128	1/1	0.86	0.08	65,65,65,65	0
56	MG	2a	1714	1/1	0.86	0.26	77,77,77,77	0
56	MG	1A	3866	1/1	0.86	0.16	60,60,60,60	0
56	MG	2A	3172	1/1	0.86	0.28	57,57,57,57	0
56	MG	2A	3310	1/1	0.86	0.18	67,67,67,67	0
56	MG	2a	1722	1/1	0.86	0.10	89,89,89,89	0
56	MG	1A	3182	1/1	0.86	0.10	50,50,50,50	0
56	MG	1A	3336	1/1	0.86	0.14	61,61,61,61	0
56	MG	1A	3886	1/1	0.86	0.11	28,28,28,28	0
56	MG	2A	3320	1/1	0.86	0.17	61,61,61,61	0
56	MG	1w	105	1/1	0.86	0.18	69,69,69,69	0
56	MG	1a	1700	1/1	0.86	0.15	49,49,49,49	0
56	MG	2A	3327	1/1	0.86	0.25	64,64,64,64	0
56	MG	1A	3889	1/1	0.86	0.10	54,54,54,54	0
56	MG	2A	3205	1/1	0.86	0.18	43,43,43,43	0
56	MG	2A	3638	1/1	0.86	0.14	59,59,59,59	0
56	MG	2a	1765	1/1	0.86	0.21	65,65,65,65	0
56	MG	1x	102	1/1	0.86	0.11	67,67,67,67	0
56	MG	2a	1769	1/1	0.86	0.23	72,72,72,72	0
56	MG	1A	3719	1/1	0.86	0.13	33,33,33,33	0
56	MG	2A	3213	1/1	0.86	0.15	66,66,66,66	0
56	MG	1A	3409	1/1	0.86	0.13	71,71,71,71	0
56	MG	1A	3207	1/1	0.86	0.20	53,53,53,53	0
56	MG	2A	3652	1/1	0.86	0.14	73,73,73,73	0
56	MG	2A	3870	1/1	0.86	0.20	70,70,70,70	0
56	MG	1a	1774	1/1	0.86	0.24	69,69,69,69	0
56	MG	1a	1778	1/1	0.86	0.11	60,60,60,60	0
56	MG	1A	3342	1/1	0.86	0.17	71,71,71,71	0
56	MG	2a	1792	1/1	0.86	0.13	66,66,66,66	0
56	MG	2A	3228	1/1	0.86	0.12	55,55,55,55	0
56	MG	1A	4061	1/1	0.86	0.10	61,61,61,61	0
56	MG	2a	1797	1/1	0.86	0.35	64,64,64,64	0
56	MG	1A	3599	1/1	0.86	0.18	50,50,50,50	0
56	MG	2A	3233	1/1	0.86	0.16	73,73,73,73	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	4071	1/1	0.86	0.10	58,58,58,58	0
56	MG	2A	3235	1/1	0.86	0.14	65,65,65,65	0
56	MG	2B	217	1/1	0.86	0.29	82,82,82,82	0
56	MG	1a	1792	1/1	0.86	0.22	61,61,61,61	0
56	MG	2D	304	1/1	0.86	0.27	51,51,51,51	0
56	MG	2D	306	1/1	0.86	0.19	69,69,69,69	0
56	MG	1a	1799	1/1	0.86	0.20	62,62,62,62	0
56	MG	2A	3692	1/1	0.86	0.13	71,71,71,71	0
56	MG	1A	3056	1/1	0.86	0.28	61,61,61,61	0
56	MG	2A	3700	1/1	0.86	0.10	64,64,64,64	0
56	MG	2A	3242	1/1	0.86	0.11	71,71,71,71	0
56	MG	2A	3072	1/1	0.86	0.22	57,57,57,57	0
56	MG	2A	3078	1/1	0.86	0.13	58,58,58,58	0
56	MG	1A	3362	1/1	0.86	0.10	59,59,59,59	0
56	MG	2a	1833	1/1	0.86	0.19	67,67,67,67	0
56	MG	2a	1836	1/1	0.86	0.25	69,69,69,69	0
56	MG	1E	312	1/1	0.86	0.14	64,64,64,64	0
56	MG	2A	3486	1/1	0.86	0.12	30,30,30,30	0
56	MG	2a	1608	1/1	0.86	0.33	72,72,72,72	0
56	MG	2A	3488	1/1	0.86	0.10	41,41,41,41	0
56	MG	2A	3720	1/1	0.86	0.15	73,73,73,73	0
56	MG	1A	3370	1/1	0.86	0.20	60,60,60,60	0
56	MG	1G	203	1/1	0.86	0.09	67,67,67,67	0
56	MG	2A	3742	1/1	0.86	0.12	73,73,73,73	0
56	MG	2A	3258	1/1	0.86	0.14	79,79,79,79	0
56	MG	2A	3758	1/1	0.86	0.12	57,57,57,57	0
56	MG	2A	3262	1/1	0.86	0.09	64,64,64,64	0
56	MG	1O	201	1/1	0.86	0.08	66,66,66,66	0
56	MG	2A	3102	1/1	0.86	0.12	65,65,65,65	0
56	MG	2A	3782	1/1	0.86	0.19	77,77,77,77	0
56	MG	1a	1814	1/1	0.86	0.12	66,66,66,66	0
56	MG	1A	3434	1/1	0.86	0.16	67,67,67,67	0
56	MG	2A	3116	1/1	0.86	0.11	65,65,65,65	0
56	MG	1A	3637	1/1	0.86	0.11	21,21,21,21	0
56	MG	2A	3523	1/1	0.86	0.14	61,61,61,61	0
56	MG	2A	3533	1/1	0.86	0.12	47,47,47,47	0
56	MG	2A	3540	1/1	0.86	0.21	69,69,69,69	0
58	Y7K	2a	1841	33/33	0.86	0.18	75,81,88,93	0
56	MG	2A	3100	1/1	0.87	0.15	68,68,68,68	0
56	MG	1A	3628	1/1	0.87	0.15	67,67,67,67	0
56	MG	1A	3629	1/1	0.87	0.13	56,56,56,56	0
56	MG	2A	3661	1/1	0.87	0.21	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
56	MG	1a	1655	1/1	0.87	0.37	71,71,71,71	0
56	MG	2a	1698	1/1	0.87	0.21	77,77,77,77	0
56	MG	2A	3860	1/1	0.87	0.24	59,59,59,59	0
56	MG	2a	1701	1/1	0.87	0.24	75,75,75,75	0
56	MG	2a	1704	1/1	0.87	0.12	72,72,72,72	0
56	MG	1A	3483	1/1	0.87	0.24	58,58,58,58	0
56	MG	1A	3489	1/1	0.87	0.09	48,48,48,48	0
56	MG	1A	3020	1/1	0.87	0.18	52,52,52,52	0
56	MG	2A	3124	1/1	0.87	0.25	78,78,78,78	0
56	MG	1A	4059	1/1	0.87	0.17	53,53,53,53	0
56	MG	1A	3836	1/1	0.87	0.14	68,68,68,68	0
56	MG	1b	302	1/1	0.87	0.18	71,71,71,71	0
56	MG	2a	1730	1/1	0.87	0.14	68,68,68,68	0
56	MG	1A	3661	1/1	0.87	0.11	29,29,29,29	0
56	MG	2a	1735	1/1	0.87	0.12	83,83,83,83	0
56	MG	1A	3293	1/1	0.87	0.16	53,53,53,53	0
56	MG	2A	3146	1/1	0.87	0.21	75,75,75,75	0
56	MG	2A	3884	1/1	0.87	0.32	75,75,75,75	0
56	MG	2A	3272	1/1	0.87	0.09	56,56,56,56	0
56	MG	2B	202	1/1	0.87	0.12	63,63,63,63	0
56	MG	2B	203	1/1	0.87	0.14	73,73,73,73	0
56	MG	1A	3955	1/1	0.87	0.12	46,46,46,46	0
56	MG	1a	1732	1/1	0.87	0.10	82,82,82,82	0
56	MG	2A	3153	1/1	0.87	0.18	51,51,51,51	0
56	MG	1a	1733	1/1	0.87	0.14	66,66,66,66	0
56	MG	1A	3975	1/1	0.87	0.12	67,67,67,67	0
56	MG	1A	3977	1/1	0.87	0.14	63,63,63,63	0
56	MG	1a	1766	1/1	0.87	0.16	73,73,73,73	0
56	MG	1A	3978	1/1	0.87	0.10	51,51,51,51	0
56	MG	2B	220	1/1	0.87	0.16	68,68,68,68	0
56	MG	2A	3727	1/1	0.87	0.12	63,63,63,63	0
56	MG	2A	3525	1/1	0.87	0.12	61,61,61,61	0
56	MG	2A	3166	1/1	0.87	0.08	71,71,71,71	0
56	MG	2a	1786	1/1	0.87	0.20	60,60,60,60	0
56	MG	2E	302	1/1	0.87	0.24	47,47,47,47	0
56	MG	2A	3168	1/1	0.87	0.21	67,67,67,67	0
56	MG	1A	3346	1/1	0.87	0.12	59,59,59,59	0
56	MG	2A	3177	1/1	0.87	0.20	78,78,78,78	0
56	MG	2Q	202	1/1	0.87	0.11	66,66,66,66	0
56	MG	1A	3579	1/1	0.87	0.08	40,40,40,40	0
56	MG	2A	3774	1/1	0.87	0.20	63,63,63,63	0
56	MG	1I	201	1/1	0.87	0.12	64,64,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3185	1/1	0.87	0.18	63,63,63,63	0
56	MG	1A	3389	1/1	0.87	0.13	61,61,61,61	0
56	MG	2A	3571	1/1	0.87	0.39	71,71,71,71	0
56	MG	1S	203	1/1	0.87	0.11	69,69,69,69	0
56	MG	1A	3167	1/1	0.87	0.26	52,52,52,52	0
56	MG	2A	3194	1/1	0.87	0.15	77,77,77,77	0
56	MG	2A	3008	1/1	0.87	0.14	55,55,55,55	0
56	MG	2a	1818	1/1	0.87	0.34	79,79,79,79	0
56	MG	1A	3354	1/1	0.87	0.09	50,50,50,50	0
56	MG	2A	3020	1/1	0.87	0.18	67,67,67,67	0
56	MG	2A	3321	1/1	0.87	0.19	74,74,74,74	0
56	MG	2A	3596	1/1	0.87	0.17	74,74,74,74	0
56	MG	1A	3408	1/1	0.87	0.39	45,45,45,45	0
56	MG	2A	3209	1/1	0.87	0.17	68,68,68,68	0
56	MG	2A	3326	1/1	0.87	0.16	62,62,62,62	0
56	MG	2A	3606	1/1	0.87	0.24	69,69,69,69	0
56	MG	2a	1834	1/1	0.87	0.14	63,63,63,63	0
56	MG	2A	3027	1/1	0.87	0.17	58,58,58,58	0
56	MG	2a	1635	1/1	0.87	0.19	65,65,65,65	0
56	MG	2A	3050	1/1	0.87	0.18	61,61,61,61	0
56	MG	2A	3051	1/1	0.87	0.21	61,61,61,61	0
56	MG	1A	3448	1/1	0.87	0.14	64,64,64,64	0
56	MG	1l	102	1/1	0.87	0.17	50,50,50,50	0
56	MG	13	101	1/1	0.87	0.11	46,46,46,46	0
56	MG	1A	4007	1/1	0.87	0.19	48,48,48,48	0
56	MG	2A	3347	1/1	0.87	0.12	75,75,75,75	0
56	MG	2r	101	1/1	0.87	0.15	75,75,75,75	0
56	MG	2A	3626	1/1	0.87	0.17	58,58,58,58	0
56	MG	18	105	1/1	0.87	0.16	46,46,46,46	0
56	MG	1A	3025	1/1	0.87	0.09	54,54,54,54	0
56	MG	1A	3184	1/1	0.87	0.46	49,49,49,49	0
56	MG	1A	3621	1/1	0.87	0.13	76,76,76,76	0
56	MG	1a	1622	1/1	0.87	0.30	62,62,62,62	0
56	MG	2a	1674	1/1	0.87	0.20	83,83,83,83	0
56	MG	2A	3832	1/1	0.87	0.11	63,63,63,63	0
56	MG	2x	107	1/1	0.87	0.22	55,55,55,55	0
56	MG	2A	3835	1/1	0.87	0.15	75,75,75,75	0
56	MG	2A	3370	1/1	0.87	0.21	72,72,72,72	0
56	MG	2y	103	1/1	0.87	0.08	72,72,72,72	0
56	MG	2A	3379	1/1	0.87	0.23	52,52,52,52	0
56	MG	1A	3919	1/1	0.87	0.07	56,56,56,56	0
56	MG	1a	1627	1/1	0.87	0.21	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3097	1/1	0.87	0.35	73,73,73,73	0
56	MG	1A	4052	1/1	0.88	0.10	44,44,44,44	0
56	MG	2A	3691	1/1	0.88	0.21	58,58,58,58	0
56	MG	2a	1621	1/1	0.88	0.20	75,75,75,75	0
56	MG	2A	3173	1/1	0.88	0.14	70,70,70,70	0
56	MG	1a	1836	1/1	0.88	0.09	45,45,45,45	0
56	MG	2A	3178	1/1	0.88	0.18	68,68,68,68	0
56	MG	1A	3881	1/1	0.88	0.15	20,20,20,20	0
56	MG	1A	3251	1/1	0.88	0.25	65,65,65,65	0
56	MG	2A	3709	1/1	0.88	0.09	88,88,88,88	0
56	MG	2A	3356	1/1	0.88	0.23	65,65,65,65	0
56	MG	2A	3359	1/1	0.88	0.27	53,53,53,53	0
56	MG	2A	3183	1/1	0.88	0.20	61,61,61,61	0
56	MG	2A	3184	1/1	0.88	0.29	68,68,68,68	0
56	MG	2A	3368	1/1	0.88	0.26	53,53,53,53	0
56	MG	1A	3887	1/1	0.88	0.16	59,59,59,59	0
56	MG	2A	3721	1/1	0.88	0.12	68,68,68,68	0
56	MG	1A	3725	1/1	0.88	0.22	50,50,50,50	0
56	MG	1A	3733	1/1	0.88	0.11	55,55,55,55	0
56	MG	2A	3386	1/1	0.88	0.10	41,41,41,41	0
56	MG	1A	3895	1/1	0.88	0.11	22,22,22,22	0
56	MG	1t	201	1/1	0.88	0.15	60,60,60,60	0
56	MG	1A	3896	1/1	0.88	0.24	46,46,46,46	0
56	MG	2A	3409	1/1	0.88	0.11	63,63,63,63	0
56	MG	1A	3902	1/1	0.88	0.14	51,51,51,51	0
56	MG	2A	3772	1/1	0.88	0.14	58,58,58,58	0
56	MG	1w	103	1/1	0.88	0.18	68,68,68,68	0
56	MG	1A	3606	1/1	0.88	0.19	60,60,60,60	0
56	MG	1A	4080	1/1	0.88	0.13	36,36,36,36	0
56	MG	1A	3121	1/1	0.88	0.11	45,45,45,45	0
56	MG	2A	3441	1/1	0.88	0.13	64,64,64,64	0
56	MG	1A	3476	1/1	0.88	0.20	56,56,56,56	0
56	MG	1a	1635	1/1	0.88	0.25	65,65,65,65	0
56	MG	1a	1640	1/1	0.88	0.13	47,47,47,47	0
56	MG	2A	3464	1/1	0.88	0.12	49,49,49,49	0
56	MG	2A	3793	1/1	0.88	0.17	71,71,71,71	0
56	MG	2A	3476	1/1	0.88	0.15	43,43,43,43	0
56	MG	1a	1641	1/1	0.88	0.20	57,57,57,57	0
56	MG	1A	4085	1/1	0.88	0.13	72,72,72,72	0
56	MG	1a	1647	1/1	0.88	0.14	66,66,66,66	0
56	MG	2a	1703	1/1	0.88	0.32	70,70,70,70	0
56	MG	1a	1652	1/1	0.88	0.17	63,63,63,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	1705	1/1	0.88	0.28	71,71,71,71	0
56	MG	1A	3298	1/1	0.88	0.09	48,48,48,48	0
56	MG	2a	1713	1/1	0.88	0.26	77,77,77,77	0
56	MG	2A	3493	1/1	0.88	0.14	48,48,48,48	0
56	MG	2A	3232	1/1	0.88	0.14	67,67,67,67	0
56	MG	1A	3760	1/1	0.88	0.11	47,47,47,47	0
56	MG	2A	3013	1/1	0.88	0.18	64,64,64,64	0
56	MG	1A	3763	1/1	0.88	0.12	43,43,43,43	0
56	MG	1A	3764	1/1	0.88	0.10	35,35,35,35	0
56	MG	2A	3511	1/1	0.88	0.23	58,58,58,58	0
56	MG	1A	3765	1/1	0.88	0.15	41,41,41,41	0
56	MG	1a	1691	1/1	0.88	0.11	54,54,54,54	0
56	MG	2A	3039	1/1	0.88	0.23	80,80,80,80	0
56	MG	2A	3245	1/1	0.88	0.20	58,58,58,58	0
56	MG	2a	1741	1/1	0.88	0.08	70,70,70,70	0
56	MG	2A	3046	1/1	0.88	0.17	56,56,56,56	0
56	MG	1A	3948	1/1	0.88	0.15	73,73,73,73	0
56	MG	1A	3773	1/1	0.88	0.23	61,61,61,61	0
56	MG	2A	3543	1/1	0.88	0.32	69,69,69,69	0
56	MG	1A	3484	1/1	0.88	0.15	56,56,56,56	0
56	MG	2A	3252	1/1	0.88	0.25	67,67,67,67	0
56	MG	1a	1715	1/1	0.88	0.14	71,71,71,71	0
56	MG	1a	1724	1/1	0.88	0.09	57,57,57,57	0
56	MG	2A	3060	1/1	0.88	0.20	66,66,66,66	0
56	MG	2A	3842	1/1	0.88	0.09	64,64,64,64	0
56	MG	1A	4124	1/1	0.88	0.17	67,67,67,67	0
56	MG	1A	3954	1/1	0.88	0.12	46,46,46,46	0
56	MG	1A	3790	1/1	0.88	0.09	23,23,23,23	0
56	MG	2A	3265	1/1	0.88	0.28	68,68,68,68	0
56	MG	2A	3852	1/1	0.88	0.19	68,68,68,68	0
56	MG	1A	3961	1/1	0.88	0.09	42,42,42,42	0
56	MG	2A	3085	1/1	0.88	0.12	46,46,46,46	0
56	MG	1A	4136	1/1	0.88	0.16	46,46,46,46	0
56	MG	2a	1789	1/1	0.88	0.15	73,73,73,73	0
56	MG	2A	3089	1/1	0.88	0.13	61,61,61,61	0
56	MG	1A	4138	1/1	0.88	0.24	50,50,50,50	0
56	MG	1A	3794	1/1	0.88	0.15	31,31,31,31	0
56	MG	1A	3376	1/1	0.88	0.13	51,51,51,51	0
56	MG	1A	3802	1/1	0.88	0.32	25,25,25,25	0
56	MG	2A	3601	1/1	0.88	0.14	73,73,73,73	0
56	MG	2A	3602	1/1	0.88	0.12	61,61,61,61	0
56	MG	2A	3098	1/1	0.88	0.17	64,64,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3491	1/1	0.88	0.15	61,61,61,61	0
56	MG	2A	3290	1/1	0.88	0.17	82,82,82,82	0
56	MG	1A	3806	1/1	0.88	0.11	42,42,42,42	0
56	MG	2a	1812	1/1	0.88	0.17	76,76,76,76	0
56	MG	2A	3879	1/1	0.88	0.17	58,58,58,58	0
56	MG	2A	3292	1/1	0.88	0.18	72,72,72,72	0
56	MG	1A	3496	1/1	0.88	0.11	55,55,55,55	0
56	MG	2A	3614	1/1	0.88	0.17	61,61,61,61	0
56	MG	1A	3377	1/1	0.88	0.13	54,54,54,54	0
56	MG	2a	1820	1/1	0.88	0.11	84,84,84,84	0
56	MG	1A	3641	1/1	0.88	0.25	65,65,65,65	0
56	MG	2B	207	1/1	0.88	0.18	59,59,59,59	0
56	MG	2A	3297	1/1	0.88	0.20	81,81,81,81	0
56	MG	1a	1796	1/1	0.88	0.11	64,64,64,64	0
56	MG	2A	3625	1/1	0.88	0.19	60,60,60,60	0
56	MG	1A	3331	1/1	0.88	0.08	40,40,40,40	0
56	MG	2A	3627	1/1	0.88	0.16	73,73,73,73	0
56	MG	1A	3165	1/1	0.88	0.30	36,36,36,36	0
56	MG	2a	1835	1/1	0.88	0.11	64,64,64,64	0
56	MG	1A	3663	1/1	0.88	0.12	37,37,37,37	0
56	MG	1A	4012	1/1	0.88	0.10	45,45,45,45	0
56	MG	2A	3635	1/1	0.88	0.17	62,62,62,62	0
56	MG	1A	3334	1/1	0.88	0.23	59,59,59,59	0
56	MG	1a	1806	1/1	0.88	0.19	53,53,53,53	0
56	MG	1F	311	1/1	0.88	0.12	64,64,64,64	0
56	MG	1A	4014	1/1	0.88	0.18	54,54,54,54	0
56	MG	2I	204	1/1	0.88	0.12	68,68,68,68	0
56	MG	2E	303	1/1	0.88	0.18	57,57,57,57	0
56	MG	2p	101	1/1	0.88	0.18	60,60,60,60	0
56	MG	1A	3437	1/1	0.88	0.07	57,57,57,57	0
56	MG	1a	1815	1/1	0.88	0.11	71,71,71,71	0
56	MG	2A	3150	1/1	0.88	0.22	63,63,63,63	0
56	MG	2A	3151	1/1	0.88	0.11	70,70,70,70	0
56	MG	2A	3323	1/1	0.88	0.22	47,47,47,47	0
56	MG	20	102	1/1	0.88	0.16	68,68,68,68	0
56	MG	1A	3692	1/1	0.88	0.11	22,22,22,22	0
56	MG	1A	3361	1/1	0.88	0.15	62,62,62,62	0
56	MG	28	103	1/1	0.88	0.19	45,45,45,45	0
56	MG	1P	205	1/1	0.88	0.34	47,47,47,47	0
56	MG	1A	3214	1/1	0.88	0.10	59,59,59,59	0
56	MG	1T	203	1/1	0.88	0.20	53,53,53,53	0
56	MG	2A	3334	1/1	0.88	0.12	69,69,69,69	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3675	1/1	0.88	0.25	67,67,67,67	0
56	MG	1A	3601	1/1	0.88	0.13	31,31,31,31	0
56	MG	1Y	202	1/1	0.88	0.28	71,71,71,71	0
56	MG	1A	3879	1/1	0.88	0.10	71,71,71,71	0
56	MG	2a	1615	1/1	0.88	0.29	63,63,63,63	0
56	MG	2a	1653	1/1	0.89	0.37	72,72,72,72	0
56	MG	2A	3561	1/1	0.89	0.12	50,50,50,50	0
56	MG	1A	4027	1/1	0.89	0.13	38,38,38,38	0
56	MG	1a	1665	1/1	0.89	0.16	68,68,68,68	0
56	MG	2a	1664	1/1	0.89	0.18	61,61,61,61	0
56	MG	1f	202	1/1	0.89	0.14	66,66,66,66	0
56	MG	1A	3912	1/1	0.89	0.11	43,43,43,43	0
56	MG	1A	3514	1/1	0.89	0.14	29,29,29,29	0
56	MG	2a	1670	1/1	0.89	0.22	71,71,71,71	0
56	MG	1a	1669	1/1	0.89	0.10	61,61,61,61	0
56	MG	2a	1676	1/1	0.89	0.25	60,60,60,60	0
56	MG	2A	3819	1/1	0.89	0.16	66,66,66,66	0
56	MG	1a	1674	1/1	0.89	0.10	53,53,53,53	0
56	MG	1w	101	1/1	0.89	0.21	74,74,74,74	0
56	MG	1a	1675	1/1	0.89	0.24	52,52,52,52	0
56	MG	2A	3167	1/1	0.89	0.11	64,64,64,64	0
56	MG	1a	1682	1/1	0.89	0.22	54,54,54,54	0
56	MG	1A	3918	1/1	0.89	0.10	60,60,60,60	0
56	MG	1a	1687	1/1	0.89	0.17	65,65,65,65	0
56	MG	1A	3783	1/1	0.89	0.16	34,34,34,34	0
56	MG	1w	109	1/1	0.89	0.09	86,86,86,86	0
56	MG	2a	1691	1/1	0.89	0.16	75,75,75,75	0
56	MG	1A	4039	1/1	0.89	0.13	54,54,54,54	0
56	MG	1A	4047	1/1	0.89	0.08	37,37,37,37	0
56	MG	2a	1696	1/1	0.89	0.16	77,77,77,77	0
56	MG	1A	3375	1/1	0.89	0.16	61,61,61,61	0
56	MG	1a	1713	1/1	0.89	0.09	57,57,57,57	0
56	MG	1x	111	1/1	0.89	0.32	65,65,65,65	0
56	MG	1D	310	1/1	0.89	0.11	53,53,53,53	0
56	MG	1A	3138	1/1	0.89	0.29	58,58,58,58	0
56	MG	1A	3291	1/1	0.89	0.15	51,51,51,51	0
56	MG	2a	1711	1/1	0.89	0.21	64,64,64,64	0
56	MG	1A	3551	1/1	0.89	0.10	52,52,52,52	0
56	MG	1A	3577	1/1	0.89	0.16	52,52,52,52	0
56	MG	2A	3014	1/1	0.89	0.22	52,52,52,52	0
56	MG	1A	3688	1/1	0.89	0.13	53,53,53,53	0
56	MG	2A	3854	1/1	0.89	0.08	72,72,72,72	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1757	1/1	0.89	0.12	69,69,69,69	0
56	MG	1A	3018	1/1	0.89	0.12	29,29,29,29	0
56	MG	1A	3816	1/1	0.89	0.12	37,37,37,37	0
56	MG	2a	1728	1/1	0.89	0.12	82,82,82,82	0
56	MG	2A	3034	1/1	0.89	0.13	38,38,38,38	0
56	MG	2A	3035	1/1	0.89	0.13	62,62,62,62	0
56	MG	2A	3220	1/1	0.89	0.28	73,73,73,73	0
56	MG	1O	204	1/1	0.89	0.11	56,56,56,56	0
56	MG	2A	3223	1/1	0.89	0.12	65,65,65,65	0
56	MG	2A	3365	1/1	0.89	0.37	55,55,55,55	0
56	MG	1a	1769	1/1	0.89	0.14	63,63,63,63	0
56	MG	2A	3047	1/1	0.89	0.23	65,65,65,65	0
56	MG	1A	3236	1/1	0.89	0.28	36,36,36,36	0
56	MG	2A	3378	1/1	0.89	0.16	60,60,60,60	0
56	MG	2A	3874	1/1	0.89	0.15	71,71,71,71	0
56	MG	2A	3876	1/1	0.89	0.08	62,62,62,62	0
56	MG	1S	201	1/1	0.89	0.21	44,44,44,44	0
56	MG	1A	3194	1/1	0.89	0.13	34,34,34,34	0
56	MG	1A	3300	1/1	0.89	0.13	41,41,41,41	0
56	MG	2A	3388	1/1	0.89	0.27	46,46,46,46	0
56	MG	2A	3058	1/1	0.89	0.20	66,66,66,66	0
56	MG	1A	3399	1/1	0.89	0.09	63,63,63,63	0
56	MG	1A	3723	1/1	0.89	0.17	55,55,55,55	0
56	MG	1a	1791	1/1	0.89	0.20	68,68,68,68	0
56	MG	2A	3410	1/1	0.89	0.14	38,38,38,38	0
56	MG	2A	3411	1/1	0.89	0.26	67,67,67,67	0
56	MG	1A	3470	1/1	0.89	0.09	37,37,37,37	0
56	MG	2A	3077	1/1	0.89	0.14	58,58,58,58	0
56	MG	1a	1794	1/1	0.89	0.21	69,69,69,69	0
56	MG	2A	3243	1/1	0.89	0.14	54,54,54,54	0
56	MG	1A	3406	1/1	0.89	0.16	51,51,51,51	0
56	MG	1A	3734	1/1	0.89	0.11	52,52,52,52	0
56	MG	2B	219	1/1	0.89	0.15	77,77,77,77	0
56	MG	1A	3310	1/1	0.89	0.13	47,47,47,47	0
56	MG	2a	1800	1/1	0.89	0.20	65,65,65,65	0
56	MG	1A	3480	1/1	0.89	0.11	42,42,42,42	0
56	MG	1A	3142	1/1	0.89	0.17	56,56,56,56	0
56	MG	1A	4098	1/1	0.89	0.17	60,60,60,60	0
56	MG	2E	301	1/1	0.89	0.28	67,67,67,67	0
56	MG	2A	3466	1/1	0.89	0.11	42,42,42,42	0
56	MG	1A	3619	1/1	0.89	0.16	52,52,52,52	0
56	MG	2E	306	1/1	0.89	0.17	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3252	1/1	0.89	0.12	49,49,49,49	0
56	MG	1a	1605	1/1	0.89	0.11	65,65,65,65	0
56	MG	2A	3717	1/1	0.89	0.14	60,60,60,60	0
56	MG	2P	202	1/1	0.89	0.14	56,56,56,56	0
56	MG	2A	3718	1/1	0.89	0.10	63,63,63,63	0
56	MG	2W	202	1/1	0.89	0.19	56,56,56,56	0
56	MG	2A	3260	1/1	0.89	0.31	66,66,66,66	0
56	MG	2A	3261	1/1	0.89	0.30	71,71,71,71	0
56	MG	25	104	1/1	0.89	0.13	56,56,56,56	0
56	MG	1A	4113	1/1	0.89	0.09	43,43,43,43	0
56	MG	26	101	1/1	0.89	0.14	68,68,68,68	0
56	MG	1A	3078	1/1	0.89	0.13	60,60,60,60	0
56	MG	2A	3494	1/1	0.89	0.13	49,49,49,49	0
56	MG	1A	3998	1/1	0.89	0.19	57,57,57,57	0
56	MG	2A	3736	1/1	0.89	0.13	44,44,44,44	0
56	MG	2A	3740	1/1	0.89	0.10	52,52,52,52	0
56	MG	2a	1607	1/1	0.89	0.38	79,79,79,79	0
56	MG	1A	3419	1/1	0.89	0.10	46,46,46,46	0
56	MG	1A	4009	1/1	0.89	0.17	60,60,60,60	0
56	MG	2e	201	1/1	0.89	0.09	76,76,76,76	0
56	MG	2A	3756	1/1	0.89	0.09	64,64,64,64	0
56	MG	2A	3505	1/1	0.89	0.15	60,60,60,60	0
56	MG	1A	3494	1/1	0.89	0.09	46,46,46,46	0
56	MG	1A	3769	1/1	0.89	0.20	41,41,41,41	0
56	MG	2A	3771	1/1	0.89	0.17	59,59,59,59	0
56	MG	2A	3510	1/1	0.89	0.10	54,54,54,54	0
56	MG	2a	1618	1/1	0.89	0.25	65,65,65,65	0
56	MG	1A	3771	1/1	0.89	0.31	35,35,35,35	0
56	MG	2v	101	1/1	0.89	0.20	64,64,64,64	0
56	MG	2A	3518	1/1	0.89	0.20	75,75,75,75	0
56	MG	2A	3779	1/1	0.89	0.08	66,66,66,66	0
56	MG	2A	3126	1/1	0.89	0.22	63,63,63,63	0
56	MG	2A	3132	1/1	0.89	0.16	61,61,61,61	0
56	MG	1B	207	1/1	0.89	0.27	61,61,61,61	0
56	MG	1a	1646	1/1	0.89	0.12	54,54,54,54	0
56	MG	2a	1634	1/1	0.89	0.15	57,57,57,57	0
56	MG	2x	105	1/1	0.89	0.30	71,71,71,71	0
56	MG	1A	3125	1/1	0.89	0.37	39,39,39,39	0
56	MG	2A	3282	1/1	0.89	0.16	58,58,58,58	0
56	MG	1a	1649	1/1	0.89	0.13	51,51,51,51	0
56	MG	2a	1640	1/1	0.89	0.14	74,74,74,74	0
56	MG	1A	3776	1/1	0.89	0.11	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1839	1/1	0.89	0.12	57,57,57,57	0
56	MG	1A	4023	1/1	0.89	0.12	53,53,53,53	0
56	MG	1a	1663	1/1	0.89	0.30	65,65,65,65	0
56	MG	2A	3294	1/1	0.89	0.25	75,75,75,75	0
56	MG	1B	235	1/1	0.90	0.16	65,65,65,65	0
56	MG	2A	3287	1/1	0.90	0.10	71,71,71,71	0
56	MG	1a	1673	1/1	0.90	0.17	68,68,68,68	0
56	MG	1A	3739	1/1	0.90	0.12	68,68,68,68	0
56	MG	2A	3532	1/1	0.90	0.10	32,32,32,32	0
56	MG	1A	4063	1/1	0.90	0.14	48,48,48,48	0
56	MG	1A	3322	1/1	0.90	0.27	41,41,41,41	0
56	MG	1A	4069	1/1	0.90	0.12	49,49,49,49	0
56	MG	1F	306	1/1	0.90	0.17	25,25,25,25	0
56	MG	1A	4070	1/1	0.90	0.11	52,52,52,52	0
56	MG	2a	1667	1/1	0.90	0.22	67,67,67,67	0
56	MG	2A	3810	1/1	0.90	0.16	63,63,63,63	0
56	MG	1A	3754	1/1	0.90	0.11	49,49,49,49	0
56	MG	1G	202	1/1	0.90	0.15	57,57,57,57	0
56	MG	1A	3853	1/1	0.90	0.15	65,65,65,65	0
56	MG	2a	1675	1/1	0.90	0.20	69,69,69,69	0
56	MG	2A	3562	1/1	0.90	0.11	57,57,57,57	0
56	MG	2A	3565	1/1	0.90	0.14	62,62,62,62	0
56	MG	2A	3302	1/1	0.90	0.19	53,53,53,53	0
56	MG	1x	104	1/1	0.90	0.18	74,74,74,74	0
56	MG	1a	1709	1/1	0.90	0.19	68,68,68,68	0
56	MG	2A	3574	1/1	0.90	0.15	73,73,73,73	0
56	MG	1x	106	1/1	0.90	0.13	71,71,71,71	0
56	MG	1A	3972	1/1	0.90	0.09	46,46,46,46	0
56	MG	2A	3175	1/1	0.90	0.15	66,66,66,66	0
56	MG	1A	3855	1/1	0.90	0.07	39,39,39,39	0
56	MG	1a	1722	1/1	0.90	0.14	64,64,64,64	0
56	MG	2A	3589	1/1	0.90	0.13	73,73,73,73	0
56	MG	1A	3451	1/1	0.90	0.18	63,63,63,63	0
56	MG	2A	3316	1/1	0.90	0.19	77,77,77,77	0
56	MG	2A	3834	1/1	0.90	0.12	47,47,47,47	0
56	MG	2a	1697	1/1	0.90	0.14	86,86,86,86	0
56	MG	2A	3317	1/1	0.90	0.14	59,59,59,59	0
56	MG	1x	115	1/1	0.90	0.15	67,67,67,67	0
56	MG	2A	3319	1/1	0.90	0.28	56,56,56,56	0
56	MG	2A	3182	1/1	0.90	0.12	55,55,55,55	0
56	MG	1A	3343	1/1	0.90	0.12	58,58,58,58	0
56	MG	2A	3322	1/1	0.90	0.14	66,66,66,66	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	1707	1/1	0.90	0.16	60,60,60,60	0
56	MG	2a	1708	1/1	0.90	0.38	80,80,80,80	0
56	MG	2a	1710	1/1	0.90	0.27	55,55,55,55	0
56	MG	2A	3002	1/1	0.90	0.22	59,59,59,59	0
56	MG	2A	3846	1/1	0.90	0.17	70,70,70,70	0
56	MG	1A	3985	1/1	0.90	0.22	52,52,52,52	0
56	MG	2A	3851	1/1	0.90	0.20	54,54,54,54	0
56	MG	1A	3865	1/1	0.90	0.22	50,50,50,50	0
56	MG	2a	1717	1/1	0.90	0.10	60,60,60,60	0
56	MG	2A	3190	1/1	0.90	0.16	63,63,63,63	0
56	MG	1A	3458	1/1	0.90	0.15	39,39,39,39	0
56	MG	2A	3330	1/1	0.90	0.15	50,50,50,50	0
56	MG	2A	3615	1/1	0.90	0.13	48,48,48,48	0
56	MG	2a	1726	1/1	0.90	0.07	80,80,80,80	0
56	MG	1a	1742	1/1	0.90	0.13	48,48,48,48	0
56	MG	2A	3333	1/1	0.90	0.18	71,71,71,71	0
56	MG	1A	3555	1/1	0.90	0.08	27,27,27,27	0
56	MG	1U	210	1/1	0.90	0.37	46,46,46,46	0
56	MG	1A	3469	1/1	0.90	0.48	44,44,44,44	0
56	MG	1A	4093	1/1	0.90	0.09	58,58,58,58	0
56	MG	1A	3325	1/1	0.90	0.12	71,71,71,71	0
56	MG	10	104	1/1	0.90	0.25	43,43,43,43	0
56	MG	2A	3346	1/1	0.90	0.14	74,74,74,74	0
56	MG	1A	3770	1/1	0.90	0.31	47,47,47,47	0
56	MG	2a	1757	1/1	0.90	0.09	65,65,65,65	0
56	MG	2A	3215	1/1	0.90	0.13	76,76,76,76	0
56	MG	2A	3041	1/1	0.90	0.10	57,57,57,57	0
56	MG	2A	3044	1/1	0.90	0.16	55,55,55,55	0
56	MG	1A	3295	1/1	0.90	0.15	55,55,55,55	0
56	MG	11	104	1/1	0.90	0.11	43,43,43,43	0
56	MG	2A	3882	1/1	0.90	0.08	52,52,52,52	0
56	MG	1A	3048	1/1	0.90	0.11	53,53,53,53	0
56	MG	2A	3650	1/1	0.90	0.24	70,70,70,70	0
56	MG	2a	1777	1/1	0.90	0.15	75,75,75,75	0
56	MG	13	102	1/1	0.90	0.26	56,56,56,56	0
56	MG	1A	4000	1/1	0.90	0.16	46,46,46,46	0
56	MG	2B	205	1/1	0.90	0.15	60,60,60,60	0
56	MG	1A	3684	1/1	0.90	0.08	39,39,39,39	0
56	MG	1A	3777	1/1	0.90	0.09	41,41,41,41	0
56	MG	2B	210	1/1	0.90	0.22	72,72,72,72	0
56	MG	2A	3373	1/1	0.90	0.22	55,55,55,55	0
56	MG	1A	4119	1/1	0.90	0.10	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
56	MG	1A	3358	1/1	0.90	0.07	39,39,39,39	0
56	MG	2A	3380	1/1	0.90	0.26	66,66,66,66	0
56	MG	1a	1614	1/1	0.90	0.10	57,57,57,57	0
56	MG	2a	1794	1/1	0.90	0.14	74,74,74,74	0
56	MG	2A	3668	1/1	0.90	0.11	74,74,74,74	0
56	MG	1a	1615	1/1	0.90	0.14	56,56,56,56	0
56	MG	2A	3074	1/1	0.90	0.19	54,54,54,54	0
56	MG	1A	4127	1/1	0.90	0.10	56,56,56,56	0
56	MG	2a	1803	1/1	0.90	0.13	55,55,55,55	0
56	MG	2A	3681	1/1	0.90	0.16	63,63,63,63	0
56	MG	2A	3390	1/1	0.90	0.17	57,57,57,57	0
56	MG	1A	3299	1/1	0.90	0.43	57,57,57,57	0
56	MG	2A	3405	1/1	0.90	0.13	59,59,59,59	0
56	MG	1A	3784	1/1	0.90	0.10	58,58,58,58	0
56	MG	1A	3275	1/1	0.90	0.08	53,53,53,53	0
56	MG	2E	304	1/1	0.90	0.12	34,34,34,34	0
56	MG	1A	3432	1/1	0.90	0.10	44,44,44,44	0
56	MG	2F	301	1/1	0.90	0.15	49,49,49,49	0
56	MG	2A	3244	1/1	0.90	0.12	62,62,62,62	0
56	MG	2A	3417	1/1	0.90	0.10	67,67,67,67	0
56	MG	2A	3088	1/1	0.90	0.13	65,65,65,65	0
56	MG	2A	3708	1/1	0.90	0.15	55,55,55,55	0
56	MG	1a	1630	1/1	0.90	0.12	44,44,44,44	0
56	MG	1A	3490	1/1	0.90	0.13	56,56,56,56	0
56	MG	2a	1824	1/1	0.90	0.16	76,76,76,76	0
56	MG	2a	1826	1/1	0.90	0.26	79,79,79,79	0
56	MG	2a	1827	1/1	0.90	0.17	77,77,77,77	0
56	MG	1a	1638	1/1	0.90	0.22	58,58,58,58	0
56	MG	2A	3713	1/1	0.90	0.17	54,54,54,54	0
56	MG	20	103	1/1	0.90	0.14	60,60,60,60	0
56	MG	2A	3433	1/1	0.90	0.20	63,63,63,63	0
56	MG	2A	3715	1/1	0.90	0.12	70,70,70,70	0
56	MG	1A	3614	1/1	0.90	0.12	41,41,41,41	0
56	MG	1A	3301	1/1	0.90	0.12	46,46,46,46	0
56	MG	1A	3400	1/1	0.90	0.16	53,53,53,53	0
56	MG	1a	1645	1/1	0.90	0.09	64,64,64,64	0
56	MG	2d	301	1/1	0.90	0.14	73,73,73,73	0
56	MG	1A	3809	1/1	0.90	0.44	35,35,35,35	0
56	MG	2A	3259	1/1	0.90	0.12	61,61,61,61	0
56	MG	2a	1606	1/1	0.90	0.19	68,68,68,68	0
56	MG	2A	3465	1/1	0.90	0.07	49,49,49,49	0
56	MG	1a	1827	1/1	0.90	0.19	75,75,75,75	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1B	219	1/1	0.90	0.09	57,57,57,57	0
56	MG	2A	3732	1/1	0.90	0.12	48,48,48,48	0
56	MG	1A	3729	1/1	0.90	0.10	57,57,57,57	0
56	MG	1a	1833	1/1	0.90	0.16	62,62,62,62	0
56	MG	1a	1650	1/1	0.90	0.17	59,59,59,59	0
56	MG	1A	3403	1/1	0.90	0.12	49,49,49,49	0
56	MG	1A	3933	1/1	0.90	0.14	61,61,61,61	0
56	MG	1a	1658	1/1	0.90	0.21	54,54,54,54	0
56	MG	2a	1620	1/1	0.90	0.20	70,70,70,70	0
56	MG	2w	105	1/1	0.90	0.32	90,90,90,90	0
56	MG	2w	107	1/1	0.90	0.12	86,86,86,86	0
56	MG	2A	3759	1/1	0.90	0.10	25,25,25,25	0
56	MG	2A	3270	1/1	0.90	0.13	58,58,58,58	0
56	MG	2A	3133	1/1	0.90	0.09	53,53,53,53	0
56	MG	1a	1659	1/1	0.90	0.20	59,59,59,59	0
56	MG	2a	1625	1/1	0.90	0.08	82,82,82,82	0
56	MG	1A	3934	1/1	0.90	0.09	33,33,33,33	0
56	MG	2A	3137	1/1	0.90	0.13	59,59,59,59	0
56	MG	2A	3275	1/1	0.90	0.26	64,64,64,64	0
56	MG	1B	227	1/1	0.90	0.14	62,62,62,62	0
56	MG	2A	3279	1/1	0.90	0.12	60,60,60,60	0
56	MG	1A	3620	1/1	0.90	0.15	55,55,55,55	0
56	MG	2A	3514	1/1	0.90	0.14	63,63,63,63	0
56	MG	1A	3506	1/1	0.90	0.13	48,48,48,48	0
56	MG	1A	3049	1/1	0.90	0.10	52,52,52,52	0
56	MG	2A	3384	1/1	0.91	0.33	53,53,53,53	0
56	MG	1A	3085	1/1	0.91	0.08	31,31,31,31	0
56	MG	2A	3204	1/1	0.91	0.12	59,59,59,59	0
56	MG	1A	3665	1/1	0.91	0.08	34,34,34,34	0
56	MG	2a	1626	1/1	0.91	0.08	87,87,87,87	0
56	MG	2a	1627	1/1	0.91	0.19	52,52,52,52	0
56	MG	1a	1624	1/1	0.91	0.26	56,56,56,56	0
56	MG	1s	101	1/1	0.91	0.07	74,74,74,74	0
56	MG	2A	3397	1/1	0.91	0.06	47,47,47,47	0
56	MG	1a	1625	1/1	0.91	0.14	51,51,51,51	0
56	MG	2A	3210	1/1	0.91	0.22	64,64,64,64	0
56	MG	2A	3728	1/1	0.91	0.13	61,61,61,61	0
56	MG	2A	3212	1/1	0.91	0.11	79,79,79,79	0
56	MG	1A	3966	1/1	0.91	0.11	15,15,15,15	0
56	MG	1A	4102	1/1	0.91	0.13	57,57,57,57	0
56	MG	2A	3739	1/1	0.91	0.07	45,45,45,45	0
56	MG	2A	3216	1/1	0.91	0.23	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
56	MG	2A	3422	1/1	0.91	0.13	65,65,65,65	0
56	MG	1A	3970	1/1	0.91	0.07	38,38,38,38	0
56	MG	1A	3512	1/1	0.91	0.14	11,11,11,11	0
56	MG	2a	1654	1/1	0.91	0.15	61,61,61,61	0
56	MG	1a	1634	1/1	0.91	0.19	68,68,68,68	0
56	MG	1A	3973	1/1	0.91	0.18	54,54,54,54	0
56	MG	2a	1658	1/1	0.91	0.17	53,53,53,53	0
56	MG	2A	3760	1/1	0.91	0.10	76,76,76,76	0
56	MG	2A	3762	1/1	0.91	0.13	41,41,41,41	0
56	MG	1A	3812	1/1	0.91	0.12	22,22,22,22	0
56	MG	1A	4120	1/1	0.91	0.13	49,49,49,49	0
56	MG	1A	3141	1/1	0.91	0.15	56,56,56,56	0
56	MG	1A	3679	1/1	0.91	0.06	68,68,68,68	0
56	MG	2A	3229	1/1	0.91	0.18	61,61,61,61	0
56	MG	2A	3453	1/1	0.91	0.29	60,60,60,60	0
56	MG	1A	3516	1/1	0.91	0.11	29,29,29,29	0
56	MG	2A	3780	1/1	0.91	0.13	67,67,67,67	0
56	MG	2A	3456	1/1	0.91	0.18	60,60,60,60	0
56	MG	1A	4129	1/1	0.91	0.09	61,61,61,61	0
56	MG	2a	1680	1/1	0.91	0.14	57,57,57,57	0
56	MG	1A	3092	1/1	0.91	0.09	43,43,43,43	0
56	MG	1A	4133	1/1	0.91	0.09	55,55,55,55	0
56	MG	1A	3529	1/1	0.91	0.15	50,50,50,50	0
56	MG	2a	1684	1/1	0.91	0.15	64,64,64,64	0
56	MG	1x	110	1/1	0.91	0.12	71,71,71,71	0
56	MG	1A	3144	1/1	0.91	0.10	38,38,38,38	0
56	MG	1A	4137	1/1	0.91	0.20	37,37,37,37	0
56	MG	2A	3238	1/1	0.91	0.11	61,61,61,61	0
56	MG	1a	1657	1/1	0.91	0.16	65,65,65,65	0
56	MG	1A	3028	1/1	0.91	0.11	44,44,44,44	0
56	MG	1A	4139	1/1	0.91	0.14	60,60,60,60	0
56	MG	2A	3804	1/1	0.91	0.23	66,66,66,66	0
56	MG	2A	3497	1/1	0.91	0.17	50,50,50,50	0
56	MG	1a	1660	1/1	0.91	0.18	64,64,64,64	0
56	MG	1A	3840	1/1	0.91	0.09	56,56,56,56	0
56	MG	1A	3546	1/1	0.91	0.13	55,55,55,55	0
56	MG	1B	212	1/1	0.91	0.09	46,46,46,46	0
56	MG	1A	3371	1/1	0.91	0.12	36,36,36,36	0
56	MG	2A	3815	1/1	0.91	0.20	63,63,63,63	0
56	MG	1A	3311	1/1	0.91	0.18	56,56,56,56	0
56	MG	2a	1706	1/1	0.91	0.21	76,76,76,76	0
56	MG	2A	3022	1/1	0.91	0.16	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3436	1/1	0.91	0.17	79,79,79,79	0
56	MG	1a	1671	1/1	0.91	0.13	67,67,67,67	0
56	MG	2A	3257	1/1	0.91	0.23	74,74,74,74	0
56	MG	1A	3863	1/1	0.91	0.22	25,25,25,25	0
56	MG	1A	3321	1/1	0.91	0.39	42,42,42,42	0
56	MG	1A	3038	1/1	0.91	0.17	57,57,57,57	0
56	MG	1a	1679	1/1	0.91	0.24	58,58,58,58	0
56	MG	2A	3524	1/1	0.91	0.18	64,64,64,64	0
56	MG	1A	3591	1/1	0.91	0.10	31,31,31,31	0
56	MG	1a	1683	1/1	0.91	0.12	48,48,48,48	0
56	MG	2a	1721	1/1	0.91	0.26	57,57,57,57	0
56	MG	1A	3867	1/1	0.91	0.22	55,55,55,55	0
56	MG	2A	3538	1/1	0.91	0.19	71,71,71,71	0
56	MG	2A	3049	1/1	0.91	0.21	69,69,69,69	0
56	MG	1A	3592	1/1	0.91	0.08	20,20,20,20	0
56	MG	1a	1688	1/1	0.91	0.18	53,53,53,53	0
56	MG	1A	3323	1/1	0.91	0.29	41,41,41,41	0
56	MG	2A	3553	1/1	0.91	0.20	40,40,40,40	0
56	MG	1a	1695	1/1	0.91	0.18	53,53,53,53	0
56	MG	2A	3557	1/1	0.91	0.11	39,39,39,39	0
56	MG	1A	3268	1/1	0.91	0.16	50,50,50,50	0
56	MG	1A	3328	1/1	0.91	0.18	41,41,41,41	0
56	MG	1A	3883	1/1	0.91	0.10	33,33,33,33	0
56	MG	1a	1703	1/1	0.91	0.19	66,66,66,66	0
56	MG	2a	1756	1/1	0.91	0.12	65,65,65,65	0
56	MG	1A	4032	1/1	0.91	0.11	61,61,61,61	0
56	MG	1A	4034	1/1	0.91	0.12	56,56,56,56	0
56	MG	1E	302	1/1	0.91	0.20	42,42,42,42	0
56	MG	2a	1762	1/1	0.91	0.16	77,77,77,77	0
56	MG	1a	1721	1/1	0.91	0.11	72,72,72,72	0
56	MG	2A	3080	1/1	0.91	0.10	62,62,62,62	0
56	MG	1A	3742	1/1	0.91	0.10	55,55,55,55	0
56	MG	2a	1767	1/1	0.91	0.23	67,67,67,67	0
56	MG	1A	3743	1/1	0.91	0.14	66,66,66,66	0
56	MG	1F	309	1/1	0.91	0.07	47,47,47,47	0
56	MG	1F	310	1/1	0.91	0.17	38,38,38,38	0
56	MG	1A	4037	1/1	0.91	0.10	39,39,39,39	0
56	MG	1a	1737	1/1	0.91	0.11	68,68,68,68	0
56	MG	1A	3888	1/1	0.91	0.11	47,47,47,47	0
56	MG	2a	1781	1/1	0.91	0.21	71,71,71,71	0
56	MG	2A	3594	1/1	0.91	0.11	63,63,63,63	0
56	MG	1a	1739	1/1	0.91	0.09	61,61,61,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1741	1/1	0.91	0.10	60,60,60,60	0
56	MG	1A	3746	1/1	0.91	0.13	31,31,31,31	0
56	MG	1A	3603	1/1	0.91	0.10	35,35,35,35	0
56	MG	2A	3875	1/1	0.91	0.10	42,42,42,42	0
56	MG	1G	204	1/1	0.91	0.14	46,46,46,46	0
56	MG	1G	205	1/1	0.91	0.24	66,66,66,66	0
56	MG	1A	4050	1/1	0.91	0.10	52,52,52,52	0
56	MG	1A	3272	1/1	0.91	0.15	57,57,57,57	0
56	MG	1a	1772	1/1	0.91	0.13	64,64,64,64	0
56	MG	1a	1773	1/1	0.91	0.11	63,63,63,63	0
56	MG	1A	3759	1/1	0.91	0.13	46,46,46,46	0
56	MG	1O	205	1/1	0.91	0.10	64,64,64,64	0
56	MG	2A	3130	1/1	0.91	0.25	40,40,40,40	0
56	MG	1a	1779	1/1	0.91	0.11	52,52,52,52	0
56	MG	1a	1781	1/1	0.91	0.12	63,63,63,63	0
56	MG	1A	3467	1/1	0.91	0.32	45,45,45,45	0
56	MG	1Q	205	1/1	0.91	0.14	36,36,36,36	0
56	MG	1R	202	1/1	0.91	0.16	38,38,38,38	0
56	MG	2a	1811	1/1	0.91	0.23	75,75,75,75	0
56	MG	1A	3026	1/1	0.91	0.19	72,72,72,72	0
56	MG	1A	3127	1/1	0.91	0.15	35,35,35,35	0
56	MG	1A	3277	1/1	0.91	0.10	48,48,48,48	0
56	MG	1A	4064	1/1	0.91	0.07	54,54,54,54	0
56	MG	1U	204	1/1	0.91	0.21	56,56,56,56	0
56	MG	1A	3282	1/1	0.91	0.40	39,39,39,39	0
56	MG	1V	203	1/1	0.91	0.29	34,34,34,34	0
56	MG	1V	205	1/1	0.91	0.08	51,51,51,51	0
56	MG	2A	3328	1/1	0.91	0.21	69,69,69,69	0
56	MG	1V	206	1/1	0.91	0.10	41,41,41,41	0
56	MG	1W	207	1/1	0.91	0.22	38,38,38,38	0
56	MG	1A	4068	1/1	0.91	0.14	49,49,49,49	0
56	MG	1A	3285	1/1	0.91	0.23	43,43,43,43	0
56	MG	1Z	301	1/1	0.91	0.08	45,45,45,45	0
56	MG	1A	3922	1/1	0.91	0.10	44,44,44,44	0
56	MG	1A	3215	1/1	0.91	0.15	70,70,70,70	0
56	MG	2A	3340	1/1	0.91	0.13	71,71,71,71	0
56	MG	2F	304	1/1	0.91	0.15	50,50,50,50	0
56	MG	1A	3407	1/1	0.91	0.09	54,54,54,54	0
56	MG	1O	107	1/1	0.91	0.13	61,61,61,61	0
56	MG	2A	3344	1/1	0.91	0.17	70,70,70,70	0
56	MG	2O	201	1/1	0.91	0.18	72,72,72,72	0
56	MG	2A	3665	1/1	0.91	0.12	75,75,75,75	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3175	1/1	0.91	0.14	47,47,47,47	0
56	MG	1a	1822	1/1	0.91	0.16	60,60,60,60	0
56	MG	2X	102	1/1	0.91	0.12	68,68,68,68	0
56	MG	2A	3669	1/1	0.91	0.14	60,60,60,60	0
56	MG	20	101	1/1	0.91	0.12	56,56,56,56	0
56	MG	2A	3672	1/1	0.91	0.33	44,44,44,44	0
56	MG	2A	3350	1/1	0.91	0.19	64,64,64,64	0
56	MG	25	102	1/1	0.91	0.18	46,46,46,46	0
56	MG	1A	3084	1/1	0.91	0.20	67,67,67,67	0
56	MG	1A	3228	1/1	0.91	0.13	39,39,39,39	0
56	MG	1A	3353	1/1	0.91	0.07	63,63,63,63	0
56	MG	1A	3937	1/1	0.91	0.07	50,50,50,50	0
56	MG	18	101	1/1	0.91	0.15	64,64,64,64	0
56	MG	2a	1601	1/1	0.91	0.29	74,74,74,74	0
56	MG	2w	104	1/1	0.91	0.13	73,73,73,73	0
56	MG	2A	3362	1/1	0.91	0.31	46,46,46,46	0
56	MG	2w	106	1/1	0.91	0.14	71,71,71,71	0
56	MG	18	103	1/1	0.91	0.09	39,39,39,39	0
56	MG	1A	3495	1/1	0.91	0.15	56,56,56,56	0
56	MG	2A	3694	1/1	0.91	0.07	78,78,78,78	0
56	MG	18	106	1/1	0.91	0.18	43,43,43,43	0
56	MG	1a	1601	1/1	0.91	0.08	52,52,52,52	0
56	MG	2A	3187	1/1	0.91	0.20	48,48,48,48	0
56	MG	2A	3703	1/1	0.91	0.10	83,83,83,83	0
56	MG	2A	3372	1/1	0.91	0.25	48,48,48,48	0
56	MG	1A	3418	1/1	0.91	0.13	59,59,59,59	0
56	MG	1A	3949	1/1	0.91	0.07	17,17,17,17	0
56	MG	1A	3648	1/1	0.91	0.12	31,31,31,31	0
56	MG	1A	3652	1/1	0.91	0.23	52,52,52,52	0
56	MG	2A	3712	1/1	0.91	0.16	56,56,56,56	0
56	MG	1A	3505	1/1	0.91	0.12	32,32,32,32	0
56	MG	2A	3382	1/1	0.91	0.11	51,51,51,51	0
56	MG	2A	3537	1/1	0.92	0.14	53,53,53,53	0
56	MG	1A	4134	1/1	0.92	0.10	48,48,48,48	0
56	MG	2A	3169	1/1	0.92	0.23	64,64,64,64	0
56	MG	2A	3542	1/1	0.92	0.09	33,33,33,33	0
56	MG	2a	1650	1/1	0.92	0.18	52,52,52,52	0
56	MG	2a	1652	1/1	0.92	0.07	62,62,62,62	0
56	MG	1A	3096	1/1	0.92	0.08	44,44,44,44	0
56	MG	2A	3796	1/1	0.92	0.09	59,59,59,59	0
56	MG	1A	4019	1/1	0.92	0.21	44,44,44,44	0
56	MG	2A	3174	1/1	0.92	0.12	57,57,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3245	1/1	0.92	0.23	44,44,44,44	0
56	MG	2a	1659	1/1	0.92	0.09	66,66,66,66	0
56	MG	2A	3800	1/1	0.92	0.15	59,59,59,59	0
56	MG	2A	3176	1/1	0.92	0.09	61,61,61,61	0
56	MG	17	104	1/1	0.92	0.09	55,55,55,55	0
56	MG	2a	1666	1/1	0.92	0.14	72,72,72,72	0
56	MG	1a	1736	1/1	0.92	0.09	70,70,70,70	0
56	MG	1A	3248	1/1	0.92	0.21	60,60,60,60	0
56	MG	2A	3807	1/1	0.92	0.09	59,59,59,59	0
56	MG	1x	114	1/1	0.92	0.11	68,68,68,68	0
56	MG	1A	3212	1/1	0.92	0.27	49,49,49,49	0
56	MG	1A	4028	1/1	0.92	0.28	38,38,38,38	0
56	MG	1A	3424	1/1	0.92	0.13	59,59,59,59	0
56	MG	1A	3901	1/1	0.92	0.06	54,54,54,54	0
56	MG	2A	3572	1/1	0.92	0.25	65,65,65,65	0
56	MG	2A	3186	1/1	0.92	0.13	43,43,43,43	0
56	MG	1B	213	1/1	0.92	0.08	37,37,37,37	0
56	MG	1A	3630	1/1	0.92	0.09	68,68,68,68	0
56	MG	1A	3124	1/1	0.92	0.17	41,41,41,41	0
56	MG	2A	3582	1/1	0.92	0.22	67,67,67,67	0
56	MG	1A	3638	1/1	0.92	0.12	26,26,26,26	0
56	MG	2A	3585	1/1	0.92	0.09	52,52,52,52	0
56	MG	1A	3917	1/1	0.92	0.14	53,53,53,53	0
56	MG	1A	3185	1/1	0.92	0.10	35,35,35,35	0
56	MG	1A	3509	1/1	0.92	0.14	46,46,46,46	0
56	MG	2A	3198	1/1	0.92	0.12	60,60,60,60	0
56	MG	2a	1693	1/1	0.92	0.21	68,68,68,68	0
56	MG	2A	3203	1/1	0.92	0.17	66,66,66,66	0
56	MG	2A	3595	1/1	0.92	0.10	58,58,58,58	0
56	MG	1A	4041	1/1	0.92	0.12	50,50,50,50	0
56	MG	2A	3032	1/1	0.92	0.09	51,51,51,51	0
56	MG	2A	3598	1/1	0.92	0.21	75,75,75,75	0
56	MG	1A	3143	1/1	0.92	0.24	39,39,39,39	0
56	MG	1A	3382	1/1	0.92	0.18	53,53,53,53	0
56	MG	2A	3840	1/1	0.92	0.15	60,60,60,60	0
56	MG	2A	3841	1/1	0.92	0.15	49,49,49,49	0
56	MG	1a	1780	1/1	0.92	0.12	60,60,60,60	0
56	MG	2A	3040	1/1	0.92	0.13	61,61,61,61	0
56	MG	1A	3222	1/1	0.92	0.17	56,56,56,56	0
56	MG	1a	1782	1/1	0.92	0.17	70,70,70,70	0
56	MG	2A	3214	1/1	0.92	0.16	61,61,61,61	0
56	MG	2A	3045	1/1	0.92	0.15	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1783	1/1	0.92	0.22	68,68,68,68	0
56	MG	1A	3654	1/1	0.92	0.09	14,14,14,14	0
56	MG	2A	3853	1/1	0.92	0.12	52,52,52,52	0
56	MG	1A	3519	1/1	0.92	0.10	38,38,38,38	0
56	MG	1A	3263	1/1	0.92	0.20	56,56,56,56	0
56	MG	2A	3360	1/1	0.92	0.19	40,40,40,40	0
56	MG	1A	3793	1/1	0.92	0.07	43,43,43,43	0
56	MG	2A	3622	1/1	0.92	0.09	65,65,65,65	0
56	MG	2A	3222	1/1	0.92	0.17	62,62,62,62	0
56	MG	1D	312	1/1	0.92	0.09	56,56,56,56	0
56	MG	2a	1725	1/1	0.92	0.14	90,90,90,90	0
56	MG	2A	3054	1/1	0.92	0.08	50,50,50,50	0
56	MG	2a	1727	1/1	0.92	0.08	66,66,66,66	0
56	MG	2A	3367	1/1	0.92	0.25	63,63,63,63	0
56	MG	1A	3440	1/1	0.92	0.10	34,34,34,34	0
56	MG	2a	1732	1/1	0.92	0.21	75,75,75,75	0
56	MG	1A	3534	1/1	0.92	0.08	36,36,36,36	0
56	MG	1E	306	1/1	0.92	0.11	61,61,61,61	0
56	MG	1a	1644	1/1	0.92	0.15	54,54,54,54	0
56	MG	1A	3442	1/1	0.92	0.26	42,42,42,42	0
56	MG	1A	3675	1/1	0.92	0.10	39,39,39,39	0
56	MG	1A	3390	1/1	0.92	0.10	66,66,66,66	0
56	MG	2a	1750	1/1	0.92	0.10	67,67,67,67	0
56	MG	2A	3076	1/1	0.92	0.10	55,55,55,55	0
56	MG	1A	3446	1/1	0.92	0.12	55,55,55,55	0
56	MG	2a	1753	1/1	0.92	0.26	62,62,62,62	0
56	MG	1A	3686	1/1	0.92	0.13	74,74,74,74	0
56	MG	1A	3267	1/1	0.92	0.13	53,53,53,53	0
56	MG	1A	3226	1/1	0.92	0.14	62,62,62,62	0
56	MG	2A	3655	1/1	0.92	0.10	61,61,61,61	0
56	MG	2A	3885	1/1	0.92	0.13	65,65,65,65	0
56	MG	2a	1763	1/1	0.92	0.23	62,62,62,62	0
56	MG	2A	3084	1/1	0.92	0.37	57,57,57,57	0
56	MG	2A	3240	1/1	0.92	0.08	50,50,50,50	0
56	MG	2A	3658	1/1	0.92	0.18	63,63,63,63	0
56	MG	2A	3392	1/1	0.92	0.21	66,66,66,66	0
56	MG	2a	1768	1/1	0.92	0.13	67,67,67,67	0
56	MG	1A	3561	1/1	0.92	0.13	23,23,23,23	0
56	MG	1A	4079	1/1	0.92	0.13	57,57,57,57	0
56	MG	2A	3400	1/1	0.92	0.36	48,48,48,48	0
56	MG	2A	3402	1/1	0.92	0.08	62,62,62,62	0
56	MG	1A	3452	1/1	0.92	0.09	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	1779	1/1	0.92	0.20	64,64,64,64	0
56	MG	1A	3344	1/1	0.92	0.15	54,54,54,54	0
56	MG	1a	1820	1/1	0.92	0.17	73,73,73,73	0
56	MG	2A	3670	1/1	0.92	0.09	39,39,39,39	0
56	MG	1a	1662	1/1	0.92	0.24	55,55,55,55	0
56	MG	1A	3708	1/1	0.92	0.09	48,48,48,48	0
56	MG	2A	3414	1/1	0.92	0.22	49,49,49,49	0
56	MG	1A	3718	1/1	0.92	0.08	32,32,32,32	0
56	MG	2a	1788	1/1	0.92	0.28	65,65,65,65	0
56	MG	2A	3419	1/1	0.92	0.16	65,65,65,65	0
56	MG	2D	305	1/1	0.92	0.23	42,42,42,42	0
56	MG	1A	4086	1/1	0.92	0.24	48,48,48,48	0
56	MG	1A	3304	1/1	0.92	0.18	35,35,35,35	0
56	MG	1A	3721	1/1	0.92	0.09	32,32,32,32	0
56	MG	1A	3204	1/1	0.92	0.19	37,37,37,37	0
56	MG	2A	3428	1/1	0.92	0.23	51,51,51,51	0
56	MG	2A	3107	1/1	0.92	0.23	51,51,51,51	0
56	MG	2E	305	1/1	0.92	0.14	60,60,60,60	0
56	MG	1a	1670	1/1	0.92	0.09	57,57,57,57	0
56	MG	2A	3697	1/1	0.92	0.09	64,64,64,64	0
56	MG	2F	303	1/1	0.92	0.09	64,64,64,64	0
56	MG	2A	3699	1/1	0.92	0.07	77,77,77,77	0
56	MG	2A	3436	1/1	0.92	0.11	68,68,68,68	0
56	MG	2A	3437	1/1	0.92	0.17	58,58,58,58	0
56	MG	2A	3112	1/1	0.92	0.17	50,50,50,50	0
56	MG	2A	3114	1/1	0.92	0.14	55,55,55,55	0
56	MG	2O	202	1/1	0.92	0.13	68,68,68,68	0
56	MG	2P	201	1/1	0.92	0.14	50,50,50,50	0
56	MG	1A	3404	1/1	0.92	0.08	51,51,51,51	0
56	MG	2A	3446	1/1	0.92	0.09	46,46,46,46	0
56	MG	1S	202	1/1	0.92	0.17	48,48,48,48	0
56	MG	1A	3274	1/1	0.92	0.17	55,55,55,55	0
56	MG	2Y	201	1/1	0.92	0.17	55,55,55,55	0
56	MG	1A	3312	1/1	0.92	0.17	39,39,39,39	0
56	MG	2A	3267	1/1	0.92	0.20	60,60,60,60	0
56	MG	1a	1677	1/1	0.92	0.20	46,46,46,46	0
56	MG	2A	3127	1/1	0.92	0.12	45,45,45,45	0
56	MG	2I	101	1/1	0.92	0.40	56,56,56,56	0
56	MG	25	101	1/1	0.92	0.28	55,55,55,55	0
56	MG	1A	3315	1/1	0.92	0.08	54,54,54,54	0
56	MG	2A	3473	1/1	0.92	0.13	71,71,71,71	0
56	MG	1A	3478	1/1	0.92	0.13	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
56	MG	1b	301	1/1	0.92	0.09	84,84,84,84	0
56	MG	1A	3039	1/1	0.92	0.11	35,35,35,35	0
56	MG	1A	3994	1/1	0.92	0.21	46,46,46,46	0
56	MG	2A	3723	1/1	0.92	0.10	47,47,47,47	0
56	MG	1f	201	1/1	0.92	0.14	52,52,52,52	0
56	MG	2a	1840	1/1	0.92	0.11	73,73,73,73	0
56	MG	1A	3482	1/1	0.92	0.25	38,38,38,38	0
56	MG	1A	3873	1/1	0.92	0.09	57,57,57,57	0
56	MG	1m	3001	1/1	0.92	0.07	63,63,63,63	0
56	MG	1A	4116	1/1	0.92	0.12	51,51,51,51	0
56	MG	1A	3413	1/1	0.92	0.06	44,44,44,44	0
56	MG	2A	3737	1/1	0.92	0.09	37,37,37,37	0
56	MG	2l	201	1/1	0.92	0.11	77,77,77,77	0
56	MG	1a	1696	1/1	0.92	0.09	71,71,71,71	0
56	MG	2A	3501	1/1	0.92	0.11	67,67,67,67	0
56	MG	2A	3286	1/1	0.92	0.09	55,55,55,55	0
56	MG	2A	3747	1/1	0.92	0.13	68,68,68,68	0
56	MG	1A	3229	1/1	0.92	0.14	49,49,49,49	0
56	MG	2t	201	1/1	0.92	0.14	56,56,56,56	0
56	MG	2A	3752	1/1	0.92	0.14	48,48,48,48	0
56	MG	1a	1698	1/1	0.92	0.07	52,52,52,52	0
56	MG	1A	4002	1/1	0.92	0.08	31,31,31,31	0
56	MG	1A	3615	1/1	0.92	0.11	53,53,53,53	0
56	MG	10	103	1/1	0.92	0.09	53,53,53,53	0
56	MG	2A	3156	1/1	0.92	0.17	59,59,59,59	0
56	MG	2A	3516	1/1	0.92	0.11	59,59,59,59	0
56	MG	1A	3744	1/1	0.92	0.11	45,45,45,45	0
56	MG	2A	3765	1/1	0.92	0.07	38,38,38,38	0
56	MG	2A	3768	1/1	0.92	0.08	46,46,46,46	0
56	MG	2a	1628	1/1	0.92	0.14	63,63,63,63	0
56	MG	2a	1629	1/1	0.92	0.16	75,75,75,75	0
56	MG	1A	3488	1/1	0.92	0.14	53,53,53,53	0
56	MG	1A	3753	1/1	0.92	0.12	34,34,34,34	0
56	MG	2A	3298	1/1	0.92	0.08	55,55,55,55	0
56	MG	2a	1633	1/1	0.92	0.47	67,67,67,67	0
56	MG	2A	3163	1/1	0.92	0.36	67,67,67,67	0
56	MG	2A	3165	1/1	0.92	0.35	68,68,68,68	0
56	MG	1a	1720	1/1	0.92	0.14	46,46,46,46	0
56	MG	2A	3528	1/1	0.92	0.09	55,55,55,55	0
56	MG	2A	3303	1/1	0.92	0.23	60,60,60,60	0
56	MG	1A	3363	1/1	0.92	0.14	54,54,54,54	0
60	K	2A	3393	1/1	0.92	0.10	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1824	1/1	0.93	0.16	63,63,63,63	0
56	MG	1A	3906	1/1	0.93	0.11	28,28,28,28	0
56	MG	1A	3589	1/1	0.93	0.10	21,21,21,21	0
56	MG	2A	3383	1/1	0.93	0.20	57,57,57,57	0
56	MG	18	104	1/1	0.93	0.19	36,36,36,36	0
56	MG	1A	3305	1/1	0.93	0.17	46,46,46,46	0
56	MG	1A	3365	1/1	0.93	0.10	49,49,49,49	0
56	MG	1A	3307	1/1	0.93	0.16	56,56,56,56	0
56	MG	1A	3749	1/1	0.93	0.14	62,62,62,62	0
56	MG	2A	3391	1/1	0.93	0.21	57,57,57,57	0
56	MG	1A	4092	1/1	0.93	0.11	45,45,45,45	0
56	MG	1A	3309	1/1	0.93	0.25	40,40,40,40	0
56	MG	2A	3396	1/1	0.93	0.17	55,55,55,55	0
56	MG	1a	1610	1/1	0.93	0.19	70,70,70,70	0
56	MG	2A	3398	1/1	0.93	0.26	60,60,60,60	0
56	MG	1A	3162	1/1	0.93	0.09	42,42,42,42	0
56	MG	2A	3401	1/1	0.93	0.17	65,65,65,65	0
56	MG	2A	3722	1/1	0.93	0.11	67,67,67,67	0
56	MG	1A	3086	1/1	0.93	0.18	35,35,35,35	0
56	MG	2A	3404	1/1	0.93	0.20	72,72,72,72	0
56	MG	2a	1637	1/1	0.93	0.12	61,61,61,61	0
56	MG	1a	1616	1/1	0.93	0.07	60,60,60,60	0
56	MG	2A	3407	1/1	0.93	0.20	59,59,59,59	0
56	MG	1A	3088	1/1	0.93	0.08	25,25,25,25	0
56	MG	1A	3314	1/1	0.93	0.26	41,41,41,41	0
56	MG	2A	3735	1/1	0.93	0.09	54,54,54,54	0
56	MG	2a	1643	1/1	0.93	0.08	58,58,58,58	0
56	MG	2A	3197	1/1	0.93	0.11	59,59,59,59	0
56	MG	1a	1623	1/1	0.93	0.19	51,51,51,51	0
56	MG	2a	1646	1/1	0.93	0.14	82,82,82,82	0
56	MG	2a	1648	1/1	0.93	0.09	70,70,70,70	0
56	MG	2A	3413	1/1	0.93	0.12	60,60,60,60	0
56	MG	1A	3762	1/1	0.93	0.10	32,32,32,32	0
56	MG	2a	1651	1/1	0.93	0.09	72,72,72,72	0
56	MG	1A	4103	1/1	0.93	0.06	42,42,42,42	0
56	MG	1A	4106	1/1	0.93	0.11	61,61,61,61	0
56	MG	1n	101	1/1	0.93	0.21	53,53,53,53	0
56	MG	1A	4107	1/1	0.93	0.07	63,63,63,63	0
56	MG	1a	1628	1/1	0.93	0.20	51,51,51,51	0
56	MG	1A	4108	1/1	0.93	0.14	34,34,34,34	0
56	MG	1A	3174	1/1	0.93	0.09	34,34,34,34	0
56	MG	1a	1633	1/1	0.93	0.32	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	1661	1/1	0.93	0.18	61,61,61,61	0
56	MG	2a	1662	1/1	0.93	0.16	59,59,59,59	0
56	MG	2A	3431	1/1	0.93	0.20	57,57,57,57	0
56	MG	1A	4111	1/1	0.93	0.08	24,24,24,24	0
56	MG	1A	3316	1/1	0.93	0.06	41,41,41,41	0
56	MG	1a	1637	1/1	0.93	0.20	43,43,43,43	0
56	MG	2A	3766	1/1	0.93	0.07	47,47,47,47	0
56	MG	2A	3438	1/1	0.93	0.16	58,58,58,58	0
56	MG	2A	3770	1/1	0.93	0.08	61,61,61,61	0
56	MG	2a	1672	1/1	0.93	0.15	64,64,64,64	0
56	MG	1A	3318	1/1	0.93	0.18	46,46,46,46	0
56	MG	1a	1639	1/1	0.93	0.11	58,58,58,58	0
56	MG	2A	3219	1/1	0.93	0.09	50,50,50,50	0
56	MG	1A	3938	1/1	0.93	0.08	50,50,50,50	0
56	MG	2A	3777	1/1	0.93	0.06	63,63,63,63	0
56	MG	1A	4117	1/1	0.93	0.11	47,47,47,47	0
56	MG	1A	3944	1/1	0.93	0.09	43,43,43,43	0
56	MG	1A	3945	1/1	0.93	0.05	35,35,35,35	0
56	MG	2A	3783	1/1	0.93	0.19	56,56,56,56	0
56	MG	1A	4122	1/1	0.93	0.11	47,47,47,47	0
56	MG	2A	3457	1/1	0.93	0.11	47,47,47,47	0
56	MG	2A	3461	1/1	0.93	0.10	31,31,31,31	0
56	MG	1A	3767	1/1	0.93	0.14	28,28,28,28	0
56	MG	1A	3768	1/1	0.93	0.07	35,35,35,35	0
56	MG	1A	3217	1/1	0.93	0.08	48,48,48,48	0
56	MG	1A	3218	1/1	0.93	0.10	30,30,30,30	0
56	MG	2A	3474	1/1	0.93	0.09	43,43,43,43	0
56	MG	1A	3070	1/1	0.93	0.16	43,43,43,43	0
56	MG	1A	4132	1/1	0.93	0.07	38,38,38,38	0
56	MG	2A	3481	1/1	0.93	0.08	60,60,60,60	0
56	MG	1A	3772	1/1	0.93	0.25	31,31,31,31	0
56	MG	1A	3324	1/1	0.93	0.08	60,60,60,60	0
56	MG	1A	3396	1/1	0.93	0.20	50,50,50,50	0
56	MG	2a	1700	1/1	0.93	0.28	72,72,72,72	0
56	MG	1A	3962	1/1	0.93	0.10	11,11,11,11	0
56	MG	1A	3398	1/1	0.93	0.24	40,40,40,40	0
56	MG	2A	3012	1/1	0.93	0.13	42,42,42,42	0
56	MG	1A	3779	1/1	0.93	0.24	52,52,52,52	0
56	MG	1A	3033	1/1	0.93	0.21	27,27,27,27	0
56	MG	1B	206	1/1	0.93	0.13	49,49,49,49	0
56	MG	1A	3487	1/1	0.93	0.25	57,57,57,57	0
56	MG	1A	3631	1/1	0.93	0.09	52,52,52,52	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3816	1/1	0.93	0.08	52,52,52,52	0
56	MG	1A	3976	1/1	0.93	0.09	45,45,45,45	0
56	MG	2A	3246	1/1	0.93	0.23	68,68,68,68	0
56	MG	1A	3098	1/1	0.93	0.11	35,35,35,35	0
56	MG	2A	3028	1/1	0.93	0.17	49,49,49,49	0
56	MG	2A	3029	1/1	0.93	0.12	52,52,52,52	0
56	MG	1A	3791	1/1	0.93	0.08	25,25,25,25	0
56	MG	1A	3982	1/1	0.93	0.12	40,40,40,40	0
56	MG	1A	3330	1/1	0.93	0.10	48,48,48,48	0
56	MG	2A	3519	1/1	0.93	0.10	38,38,38,38	0
56	MG	2A	3036	1/1	0.93	0.14	57,57,57,57	0
56	MG	2A	3255	1/1	0.93	0.27	62,62,62,62	0
56	MG	2A	3038	1/1	0.93	0.11	57,57,57,57	0
56	MG	1A	3987	1/1	0.93	0.15	57,57,57,57	0
56	MG	1B	222	1/1	0.93	0.06	38,38,38,38	0
56	MG	2A	3831	1/1	0.93	0.21	57,57,57,57	0
56	MG	1A	3106	1/1	0.93	0.36	32,32,32,32	0
56	MG	2A	3043	1/1	0.93	0.23	64,64,64,64	0
56	MG	1a	1680	1/1	0.93	0.41	56,56,56,56	0
56	MG	1A	3278	1/1	0.93	0.24	52,52,52,52	0
56	MG	2A	3838	1/1	0.93	0.09	60,60,60,60	0
56	MG	1A	3799	1/1	0.93	0.09	42,42,42,42	0
56	MG	1A	3801	1/1	0.93	0.15	34,34,34,34	0
56	MG	2a	1743	1/1	0.93	0.12	58,58,58,58	0
56	MG	2a	1749	1/1	0.93	0.07	77,77,77,77	0
56	MG	1A	3492	1/1	0.93	0.33	42,42,42,42	0
56	MG	1A	3646	1/1	0.93	0.08	52,52,52,52	0
56	MG	1A	3110	1/1	0.93	0.12	77,77,77,77	0
56	MG	1a	1692	1/1	0.93	0.08	43,43,43,43	0
56	MG	2A	3545	1/1	0.93	0.06	40,40,40,40	0
56	MG	1A	3996	1/1	0.93	0.09	60,60,60,60	0
56	MG	2A	3548	1/1	0.93	0.14	55,55,55,55	0
56	MG	2A	3849	1/1	0.93	0.14	44,44,44,44	0
56	MG	2A	3056	1/1	0.93	0.14	74,74,74,74	0
56	MG	1D	307	1/1	0.93	0.13	45,45,45,45	0
56	MG	1A	3283	1/1	0.93	0.14	36,36,36,36	0
56	MG	1A	3080	1/1	0.93	0.09	39,39,39,39	0
56	MG	1A	3655	1/1	0.93	0.14	47,47,47,47	0
56	MG	2A	3063	1/1	0.93	0.12	63,63,63,63	0
56	MG	2A	3564	1/1	0.93	0.08	64,64,64,64	0
56	MG	2A	3858	1/1	0.93	0.08	64,64,64,64	0
56	MG	2a	1770	1/1	0.93	0.21	71,71,71,71	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	4001	1/1	0.93	0.07	33,33,33,33	0
56	MG	2A	3566	1/1	0.93	0.09	49,49,49,49	0
56	MG	2A	3070	1/1	0.93	0.08	48,48,48,48	0
56	MG	1A	3657	1/1	0.93	0.11	17,17,17,17	0
56	MG	1a	1708	1/1	0.93	0.10	57,57,57,57	0
56	MG	2A	3284	1/1	0.93	0.19	66,66,66,66	0
56	MG	2A	3075	1/1	0.93	0.13	53,53,53,53	0
56	MG	2a	1782	1/1	0.93	0.28	59,59,59,59	0
56	MG	1A	3817	1/1	0.93	0.12	67,67,67,67	0
56	MG	2A	3289	1/1	0.93	0.08	57,57,57,57	0
56	MG	1A	3497	1/1	0.93	0.13	39,39,39,39	0
56	MG	2A	3872	1/1	0.93	0.15	63,63,63,63	0
56	MG	1F	302	1/1	0.93	0.26	33,33,33,33	0
56	MG	1a	1719	1/1	0.93	0.11	67,67,67,67	0
56	MG	1A	3337	1/1	0.93	0.24	39,39,39,39	0
56	MG	2a	1790	1/1	0.93	0.07	65,65,65,65	0
56	MG	2A	3082	1/1	0.93	0.07	49,49,49,49	0
56	MG	2A	3083	1/1	0.93	0.10	44,44,44,44	0
56	MG	1A	3338	1/1	0.93	0.16	66,66,66,66	0
56	MG	1A	3416	1/1	0.93	0.07	42,42,42,42	0
56	MG	1A	3287	1/1	0.93	0.23	60,60,60,60	0
56	MG	1a	1726	1/1	0.93	0.08	59,59,59,59	0
56	MG	2a	1798	1/1	0.93	0.19	64,64,64,64	0
56	MG	1A	3029	1/1	0.93	0.20	36,36,36,36	0
56	MG	1A	3844	1/1	0.93	0.07	48,48,48,48	0
56	MG	2a	1802	1/1	0.93	0.18	71,71,71,71	0
56	MG	1A	3515	1/1	0.93	0.15	55,55,55,55	0
56	MG	2B	204	1/1	0.93	0.14	77,77,77,77	0
56	MG	2a	1805	1/1	0.93	0.24	72,72,72,72	0
56	MG	1A	3240	1/1	0.93	0.26	34,34,34,34	0
56	MG	1A	3193	1/1	0.93	0.14	28,28,28,28	0
56	MG	1A	3422	1/1	0.93	0.17	39,39,39,39	0
56	MG	1N	201	1/1	0.93	0.10	55,55,55,55	0
56	MG	1A	3857	1/1	0.93	0.07	24,24,24,24	0
56	MG	1O	203	1/1	0.93	0.26	66,66,66,66	0
56	MG	2A	3104	1/1	0.93	0.18	41,41,41,41	0
56	MG	2A	3105	1/1	0.93	0.11	48,48,48,48	0
56	MG	2A	3313	1/1	0.93	0.17	57,57,57,57	0
56	MG	1a	1743	1/1	0.93	0.10	56,56,56,56	0
56	MG	1A	3860	1/1	0.93	0.10	55,55,55,55	0
56	MG	1A	3689	1/1	0.93	0.10	48,48,48,48	0
56	MG	1O	206	1/1	0.93	0.11	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3246	1/1	0.93	0.14	53,53,53,53	0
56	MG	1A	3533	1/1	0.93	0.11	39,39,39,39	0
56	MG	1A	3297	1/1	0.93	0.10	40,40,40,40	0
56	MG	2a	1825	1/1	0.93	0.13	53,53,53,53	0
56	MG	2A	3121	1/1	0.93	0.23	52,52,52,52	0
56	MG	2A	3123	1/1	0.93	0.19	52,52,52,52	0
56	MG	1R	203	1/1	0.93	0.09	44,44,44,44	0
56	MG	1A	3535	1/1	0.93	0.12	52,52,52,52	0
56	MG	1A	3350	1/1	0.93	0.08	38,38,38,38	0
56	MG	2a	1832	1/1	0.93	0.36	50,50,50,50	0
56	MG	1A	4042	1/1	0.93	0.09	53,53,53,53	0
56	MG	1A	3876	1/1	0.93	0.07	62,62,62,62	0
56	MG	2A	3331	1/1	0.93	0.11	59,59,59,59	0
56	MG	2F	302	1/1	0.93	0.07	61,61,61,61	0
56	MG	1A	3712	1/1	0.93	0.11	45,45,45,45	0
56	MG	1A	3715	1/1	0.93	0.07	39,39,39,39	0
56	MG	1A	4055	1/1	0.93	0.16	52,52,52,52	0
56	MG	1V	202	1/1	0.93	0.33	42,42,42,42	0
56	MG	1A	3430	1/1	0.93	0.07	47,47,47,47	0
56	MG	1A	3541	1/1	0.93	0.08	40,40,40,40	0
56	MG	2A	3339	1/1	0.93	0.10	76,76,76,76	0
56	MG	1A	4058	1/1	0.93	0.15	44,44,44,44	0
56	MG	1W	201	1/1	0.93	0.13	40,40,40,40	0
56	MG	2A	3342	1/1	0.93	0.27	67,67,67,67	0
56	MG	2l	202	1/1	0.93	0.10	70,70,70,70	0
56	MG	2V	202	1/1	0.93	0.12	59,59,59,59	0
56	MG	1W	202	1/1	0.93	0.13	39,39,39,39	0
56	MG	2X	101	1/1	0.93	0.14	72,72,72,72	0
56	MG	2q	201	1/1	0.93	0.07	86,86,86,86	0
56	MG	1A	3155	1/1	0.93	0.12	62,62,62,62	0
56	MG	2A	3345	1/1	0.93	0.16	78,78,78,78	0
56	MG	1A	3884	1/1	0.93	0.09	30,30,30,30	0
56	MG	2A	3663	1/1	0.93	0.13	51,51,51,51	0
56	MG	1a	1797	1/1	0.93	0.09	43,43,43,43	0
56	MG	2A	3348	1/1	0.93	0.17	65,65,65,65	0
56	MG	1A	3249	1/1	0.93	0.23	51,51,51,51	0
56	MG	1A	3355	1/1	0.93	0.08	41,41,41,41	0
56	MG	1Z	302	1/1	0.93	0.09	64,64,64,64	0
56	MG	1A	3198	1/1	0.93	0.09	60,60,60,60	0
56	MG	1A	3563	1/1	0.93	0.05	22,22,22,22	0
56	MG	2A	3357	1/1	0.93	0.23	42,42,42,42	0
56	MG	27	104	1/1	0.93	0.10	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2x	102	1/1	0.93	0.17	62,62,62,62	0
56	MG	1A	3890	1/1	0.93	0.10	55,55,55,55	0
56	MG	1A	3891	1/1	0.93	0.10	48,48,48,48	0
56	MG	1a	1808	1/1	0.93	0.08	65,65,65,65	0
56	MG	1A	3574	1/1	0.93	0.14	48,48,48,48	0
56	MG	1A	3575	1/1	0.93	0.08	46,46,46,46	0
56	MG	1A	3156	1/1	0.93	0.12	40,40,40,40	0
56	MG	1A	3900	1/1	0.93	0.09	75,75,75,75	0
56	MG	1a	1818	1/1	0.93	0.08	53,53,53,53	0
56	MG	1A	3438	1/1	0.93	0.06	62,62,62,62	0
56	MG	15	103	1/1	0.93	0.14	44,44,44,44	0
56	MG	1A	3064	1/1	0.93	0.20	39,39,39,39	0
56	MG	16	101	1/1	0.93	0.12	44,44,44,44	0
56	MG	1A	3904	1/1	0.93	0.07	22,22,22,22	0
56	MG	1Q	203	1/1	0.94	0.08	47,47,47,47	0
56	MG	1A	3545	1/1	0.94	0.08	61,61,61,61	0
56	MG	1Q	206	1/1	0.94	0.08	35,35,35,35	0
56	MG	2A	3037	1/1	0.94	0.14	75,75,75,75	0
56	MG	1a	1705	1/1	0.94	0.10	62,62,62,62	0
56	MG	1A	4075	1/1	0.94	0.09	53,53,53,53	0
56	MG	1A	3668	1/1	0.94	0.09	17,17,17,17	0
56	MG	1A	3454	1/1	0.94	0.39	36,36,36,36	0
56	MG	2A	3730	1/1	0.94	0.14	57,57,57,57	0
56	MG	1A	3457	1/1	0.94	0.25	31,31,31,31	0
56	MG	1A	3940	1/1	0.94	0.13	27,27,27,27	0
56	MG	2a	1636	1/1	0.94	0.19	55,55,55,55	0
56	MG	1A	3676	1/1	0.94	0.08	56,56,56,56	0
56	MG	1A	3552	1/1	0.94	0.13	46,46,46,46	0
56	MG	2A	3449	1/1	0.94	0.12	58,58,58,58	0
56	MG	1A	3554	1/1	0.94	0.07	29,29,29,29	0
56	MG	2A	3451	1/1	0.94	0.09	29,29,29,29	0
56	MG	2A	3746	1/1	0.94	0.08	66,66,66,66	0
56	MG	1U	206	1/1	0.94	0.23	32,32,32,32	0
56	MG	2A	3454	1/1	0.94	0.14	57,57,57,57	0
56	MG	1A	3136	1/1	0.94	0.12	32,32,32,32	0
56	MG	2A	3755	1/1	0.94	0.07	60,60,60,60	0
56	MG	1a	1727	1/1	0.94	0.07	60,60,60,60	0
56	MG	1A	3306	1/1	0.94	0.23	48,48,48,48	0
56	MG	1A	3468	1/1	0.94	0.18	39,39,39,39	0
56	MG	2A	3055	1/1	0.94	0.16	54,54,54,54	0
56	MG	2A	3761	1/1	0.94	0.08	56,56,56,56	0
56	MG	1A	3951	1/1	0.94	0.12	59,59,59,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3952	1/1	0.94	0.14	43,43,43,43	0
56	MG	1V	207	1/1	0.94	0.10	65,65,65,65	0
56	MG	2A	3256	1/1	0.94	0.25	58,58,58,58	0
56	MG	1A	3568	1/1	0.94	0.07	21,21,21,21	0
56	MG	1A	3094	1/1	0.94	0.11	29,29,29,29	0
56	MG	1W	206	1/1	0.94	0.16	25,25,25,25	0
56	MG	2A	3065	1/1	0.94	0.11	60,60,60,60	0
56	MG	1A	4095	1/1	0.94	0.07	67,67,67,67	0
56	MG	2A	3489	1/1	0.94	0.16	53,53,53,53	0
56	MG	2A	3069	1/1	0.94	0.12	46,46,46,46	0
56	MG	2A	3491	1/1	0.94	0.07	38,38,38,38	0
56	MG	1A	3814	1/1	0.94	0.14	34,34,34,34	0
56	MG	1a	1756	1/1	0.94	0.12	75,75,75,75	0
56	MG	2A	3781	1/1	0.94	0.11	67,67,67,67	0
56	MG	2A	3073	1/1	0.94	0.11	55,55,55,55	0
56	MG	2A	3495	1/1	0.94	0.06	36,36,36,36	0
56	MG	2A	3784	1/1	0.94	0.16	39,39,39,39	0
56	MG	2A	3496	1/1	0.94	0.10	43,43,43,43	0
56	MG	1A	3959	1/1	0.94	0.12	52,52,52,52	0
56	MG	1Y	204	1/1	0.94	0.18	48,48,48,48	0
56	MG	1a	1761	1/1	0.94	0.07	51,51,51,51	0
56	MG	1a	1764	1/1	0.94	0.07	60,60,60,60	0
56	MG	1a	1765	1/1	0.94	0.18	58,58,58,58	0
56	MG	1A	3703	1/1	0.94	0.48	30,30,30,30	0
56	MG	1A	3308	1/1	0.94	0.09	48,48,48,48	0
56	MG	10	101	1/1	0.94	0.15	47,47,47,47	0
56	MG	1A	3820	1/1	0.94	0.07	61,61,61,61	0
56	MG	2a	1686	1/1	0.94	0.15	50,50,50,50	0
56	MG	1A	3473	1/1	0.94	0.16	38,38,38,38	0
56	MG	2A	3277	1/1	0.94	0.13	56,56,56,56	0
56	MG	1A	3825	1/1	0.94	0.06	43,43,43,43	0
56	MG	1a	1775	1/1	0.94	0.06	64,64,64,64	0
56	MG	1A	3069	1/1	0.94	0.20	29,29,29,29	0
56	MG	1A	3828	1/1	0.94	0.10	45,45,45,45	0
56	MG	1A	4110	1/1	0.94	0.12	60,60,60,60	0
56	MG	1A	3349	1/1	0.94	0.11	43,43,43,43	0
56	MG	2A	3285	1/1	0.94	0.24	65,65,65,65	0
56	MG	1A	3044	1/1	0.94	0.06	30,30,30,30	0
56	MG	2A	3812	1/1	0.94	0.07	63,63,63,63	0
56	MG	1A	3717	1/1	0.94	0.04	27,27,27,27	0
56	MG	1A	3979	1/1	0.94	0.09	31,31,31,31	0
56	MG	2A	3531	1/1	0.94	0.09	30,30,30,30	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	1702	1/1	0.94	0.20	62,62,62,62	0
56	MG	2A	3099	1/1	0.94	0.15	46,46,46,46	0
56	MG	1a	1786	1/1	0.94	0.14	57,57,57,57	0
56	MG	2A	3534	1/1	0.94	0.10	47,47,47,47	0
56	MG	2A	3101	1/1	0.94	0.32	65,65,65,65	0
56	MG	1A	3351	1/1	0.94	0.16	56,56,56,56	0
56	MG	1A	3352	1/1	0.94	0.19	55,55,55,55	0
56	MG	2a	1709	1/1	0.94	0.21	63,63,63,63	0
56	MG	16	102	1/1	0.94	0.07	54,54,54,54	0
56	MG	1A	3224	1/1	0.94	0.12	42,42,42,42	0
56	MG	1A	3597	1/1	0.94	0.06	20,20,20,20	0
56	MG	1A	3724	1/1	0.94	0.18	44,44,44,44	0
56	MG	1a	1795	1/1	0.94	0.07	79,79,79,79	0
56	MG	2A	3113	1/1	0.94	0.19	70,70,70,70	0
56	MG	1A	3104	1/1	0.94	0.12	51,51,51,51	0
56	MG	2A	3115	1/1	0.94	0.09	52,52,52,52	0
56	MG	2A	3555	1/1	0.94	0.06	30,30,30,30	0
56	MG	1A	3486	1/1	0.94	0.12	33,33,33,33	0
56	MG	1A	3859	1/1	0.94	0.07	48,48,48,48	0
56	MG	19	101	1/1	0.94	0.07	41,41,41,41	0
56	MG	1A	3732	1/1	0.94	0.08	58,58,58,58	0
56	MG	2A	3122	1/1	0.94	0.17	45,45,45,45	0
56	MG	1A	3862	1/1	0.94	0.08	36,36,36,36	0
56	MG	1a	1804	1/1	0.94	0.12	62,62,62,62	0
56	MG	1A	3602	1/1	0.94	0.09	45,45,45,45	0
56	MG	1A	3016	1/1	0.94	0.21	44,44,44,44	0
56	MG	2A	3570	1/1	0.94	0.08	50,50,50,50	0
56	MG	1a	1608	1/1	0.94	0.09	55,55,55,55	0
56	MG	1A	3356	1/1	0.94	0.11	53,53,53,53	0
56	MG	2a	1737	1/1	0.94	0.10	74,74,74,74	0
56	MG	1A	3736	1/1	0.94	0.06	40,40,40,40	0
56	MG	2A	3576	1/1	0.94	0.13	71,71,71,71	0
56	MG	2A	3578	1/1	0.94	0.17	70,70,70,70	0
56	MG	1A	3109	1/1	0.94	0.12	50,50,50,50	0
56	MG	2a	1747	1/1	0.94	0.17	70,70,70,70	0
56	MG	2a	1748	1/1	0.94	0.07	78,78,78,78	0
56	MG	1A	3869	1/1	0.94	0.10	58,58,58,58	0
56	MG	1A	4004	1/1	0.94	0.08	57,57,57,57	0
56	MG	1B	204	1/1	0.94	0.20	60,60,60,60	0
56	MG	2A	3583	1/1	0.94	0.08	39,39,39,39	0
56	MG	1A	4006	1/1	0.94	0.23	55,55,55,55	0
56	MG	2a	1755	1/1	0.94	0.10	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3144	1/1	0.94	0.14	66,66,66,66	0
56	MG	2A	3586	1/1	0.94	0.09	49,49,49,49	0
56	MG	1A	3871	1/1	0.94	0.07	63,63,63,63	0
56	MG	1B	208	1/1	0.94	0.22	71,71,71,71	0
56	MG	1A	3872	1/1	0.94	0.07	35,35,35,35	0
56	MG	2A	3148	1/1	0.94	0.14	70,70,70,70	0
56	MG	2A	3863	1/1	0.94	0.09	74,74,74,74	0
56	MG	2A	3593	1/1	0.94	0.17	33,33,33,33	0
56	MG	1A	3420	1/1	0.94	0.18	45,45,45,45	0
56	MG	1A	3874	1/1	0.94	0.07	69,69,69,69	0
56	MG	1B	215	1/1	0.94	0.12	61,61,61,61	0
56	MG	1A	3613	1/1	0.94	0.09	51,51,51,51	0
56	MG	1A	3024	1/1	0.94	0.12	39,39,39,39	0
56	MG	2A	3871	1/1	0.94	0.11	51,51,51,51	0
56	MG	1A	4016	1/1	0.94	0.10	40,40,40,40	0
56	MG	2a	1776	1/1	0.94	0.20	77,77,77,77	0
56	MG	1A	4017	1/1	0.94	0.08	44,44,44,44	0
56	MG	1a	1636	1/1	0.94	0.09	62,62,62,62	0
56	MG	1A	3234	1/1	0.94	0.09	31,31,31,31	0
56	MG	2A	3877	1/1	0.94	0.12	60,60,60,60	0
56	MG	2A	3605	1/1	0.94	0.11	69,69,69,69	0
56	MG	1A	4020	1/1	0.94	0.08	44,44,44,44	0
56	MG	1A	3493	1/1	0.94	0.17	31,31,31,31	0
56	MG	2A	3164	1/1	0.94	0.07	65,65,65,65	0
56	MG	1A	4022	1/1	0.94	0.10	45,45,45,45	0
56	MG	1B	226	1/1	0.94	0.10	51,51,51,51	0
56	MG	1A	3319	1/1	0.94	0.40	33,33,33,33	0
56	MG	1A	3882	1/1	0.94	0.10	26,26,26,26	0
56	MG	1B	230	1/1	0.94	0.06	39,39,39,39	0
56	MG	2A	3170	1/1	0.94	0.17	67,67,67,67	0
56	MG	1A	3188	1/1	0.94	0.26	65,65,65,65	0
56	MG	1A	3751	1/1	0.94	0.10	21,21,21,21	0
56	MG	2B	208	1/1	0.94	0.08	65,65,65,65	0
56	MG	2A	3623	1/1	0.94	0.08	36,36,36,36	0
56	MG	1a	1648	1/1	0.94	0.16	69,69,69,69	0
56	MG	2a	1796	1/1	0.94	0.12	69,69,69,69	0
56	MG	1A	3752	1/1	0.94	0.13	25,25,25,25	0
56	MG	1B	237	1/1	0.94	0.07	47,47,47,47	0
56	MG	1a	1651	1/1	0.94	0.13	57,57,57,57	0
56	MG	2A	3628	1/1	0.94	0.07	53,53,53,53	0
56	MG	2A	3630	1/1	0.94	0.14	44,44,44,44	0
56	MG	2B	216	1/1	0.94	0.12	66,66,66,66	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3358	1/1	0.94	0.24	55,55,55,55	0
56	MG	1D	305	1/1	0.94	0.15	42,42,42,42	0
56	MG	1a	1654	1/1	0.94	0.23	58,58,58,58	0
56	MG	2A	3361	1/1	0.94	0.17	47,47,47,47	0
56	MG	1A	3368	1/1	0.94	0.18	45,45,45,45	0
56	MG	1A	3238	1/1	0.94	0.09	23,23,23,23	0
56	MG	2A	3640	1/1	0.94	0.10	52,52,52,52	0
56	MG	1A	3503	1/1	0.94	0.08	27,27,27,27	0
56	MG	1A	3190	1/1	0.94	0.10	38,38,38,38	0
56	MG	1A	3050	1/1	0.94	0.09	45,45,45,45	0
56	MG	2A	3649	1/1	0.94	0.14	68,68,68,68	0
56	MG	1a	1661	1/1	0.94	0.06	62,62,62,62	0
56	MG	2A	3369	1/1	0.94	0.35	62,62,62,62	0
56	MG	1E	301	1/1	0.94	0.12	49,49,49,49	0
56	MG	2A	3371	1/1	0.94	0.25	57,57,57,57	0
56	MG	1A	3003	1/1	0.94	0.08	24,24,24,24	0
56	MG	1E	305	1/1	0.94	0.12	39,39,39,39	0
56	MG	2A	3191	1/1	0.94	0.28	55,55,55,55	0
56	MG	1A	3634	1/1	0.94	0.08	48,48,48,48	0
56	MG	1x	103	1/1	0.94	0.24	66,66,66,66	0
56	MG	1E	309	1/1	0.94	0.22	62,62,62,62	0
56	MG	1E	310	1/1	0.94	0.09	30,30,30,30	0
56	MG	2A	3196	1/1	0.94	0.14	60,60,60,60	0
56	MG	1A	3157	1/1	0.94	0.13	38,38,38,38	0
56	MG	2A	3385	1/1	0.94	0.24	53,53,53,53	0
56	MG	1A	4045	1/1	0.94	0.09	49,49,49,49	0
56	MG	2R	202	1/1	0.94	0.18	38,38,38,38	0
56	MG	2U	202	1/1	0.94	0.05	62,62,62,62	0
56	MG	2V	201	1/1	0.94	0.32	50,50,50,50	0
56	MG	2A	3387	1/1	0.94	0.08	61,61,61,61	0
56	MG	2a	1838	1/1	0.94	0.06	67,67,67,67	0
56	MG	2A	3199	1/1	0.94	0.12	49,49,49,49	0
56	MG	2A	3671	1/1	0.94	0.10	56,56,56,56	0
56	MG	1F	304	1/1	0.94	0.12	33,33,33,33	0
56	MG	1a	1672	1/1	0.94	0.18	48,48,48,48	0
56	MG	1A	3294	1/1	0.94	0.06	45,45,45,45	0
56	MG	2f	201	1/1	0.94	0.07	51,51,51,51	0
56	MG	1x	112	1/1	0.94	0.20	62,62,62,62	0
56	MG	2A	3679	1/1	0.94	0.10	57,57,57,57	0
56	MG	2A	3680	1/1	0.94	0.11	55,55,55,55	0
56	MG	1A	3766	1/1	0.94	0.10	41,41,41,41	0
56	MG	23	102	1/1	0.94	0.07	64,64,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3683	1/1	0.94	0.10	44,44,44,44	0
56	MG	1A	3123	1/1	0.94	0.23	31,31,31,31	0
56	MG	2A	3686	1/1	0.94	0.14	61,61,61,61	0
56	MG	1A	3332	1/1	0.94	0.17	50,50,50,50	0
56	MG	1A	3441	1/1	0.94	0.24	34,34,34,34	0
56	MG	27	103	1/1	0.94	0.12	60,60,60,60	0
56	MG	2A	3690	1/1	0.94	0.07	55,55,55,55	0
56	MG	2A	3399	1/1	0.94	0.05	65,65,65,65	0
56	MG	1A	3058	1/1	0.94	0.16	56,56,56,56	0
56	MG	1A	3042	1/1	0.94	0.14	37,37,37,37	0
56	MG	2A	3004	1/1	0.94	0.12	52,52,52,52	0
56	MG	2A	3403	1/1	0.94	0.07	56,56,56,56	0
56	MG	1A	3067	1/1	0.94	0.07	48,48,48,48	0
56	MG	2A	3010	1/1	0.94	0.14	51,51,51,51	0
56	MG	2A	3406	1/1	0.94	0.13	59,59,59,59	0
56	MG	1A	4060	1/1	0.94	0.10	39,39,39,39	0
56	MG	2a	1609	1/1	0.94	0.15	60,60,60,60	0
56	MG	2a	1610	1/1	0.94	0.16	65,65,65,65	0
56	MG	1A	3253	1/1	0.94	0.12	37,37,37,37	0
56	MG	1A	3449	1/1	0.94	0.20	55,55,55,55	0
56	MG	1a	1689	1/1	0.94	0.09	52,52,52,52	0
56	MG	1a	1690	1/1	0.94	0.08	64,64,64,64	0
56	MG	1A	3537	1/1	0.94	0.15	11,11,11,11	0
56	MG	1A	3659	1/1	0.94	0.07	27,27,27,27	0
56	MG	1A	3168	1/1	0.94	0.09	38,38,38,38	0
56	MG	1A	3662	1/1	0.94	0.10	24,24,24,24	0
56	MG	2A	3420	1/1	0.94	0.07	65,65,65,65	0
56	MG	1A	3303	1/1	0.94	0.10	40,40,40,40	0
56	MG	2A	3424	1/1	0.94	0.11	70,70,70,70	0
56	MG	2A	3031	1/1	0.94	0.11	36,36,36,36	0
56	MG	1A	3173	1/1	0.94	0.17	52,52,52,52	0
56	MG	2A	3434	1/1	0.95	0.12	36,36,36,36	0
56	MG	1O	202	1/1	0.95	0.17	53,53,53,53	0
56	MG	1A	3650	1/1	0.95	0.06	42,42,42,42	0
56	MG	1A	4066	1/1	0.95	0.09	54,54,54,54	0
56	MG	1A	4067	1/1	0.95	0.14	51,51,51,51	0
56	MG	2A	3440	1/1	0.95	0.11	45,45,45,45	0
56	MG	1A	3145	1/1	0.95	0.10	39,39,39,39	0
56	MG	1P	202	1/1	0.95	0.17	30,30,30,30	0
56	MG	2A	3443	1/1	0.95	0.08	59,59,59,59	0
56	MG	1A	3147	1/1	0.95	0.30	28,28,28,28	0
56	MG	1Q	201	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
56	MG	1Q	202	1/1	0.95	0.12	56,56,56,56	0
56	MG	1A	3401	1/1	0.95	0.12	44,44,44,44	0
56	MG	1Q	204	1/1	0.95	0.06	42,42,42,42	0
56	MG	1A	3540	1/1	0.95	0.15	26,26,26,26	0
56	MG	1A	3782	1/1	0.95	0.12	33,33,33,33	0
56	MG	1A	3302	1/1	0.95	0.19	49,49,49,49	0
56	MG	1A	3345	1/1	0.95	0.06	45,45,45,45	0
56	MG	2A	3458	1/1	0.95	0.09	49,49,49,49	0
56	MG	2A	3459	1/1	0.95	0.06	63,63,63,63	0
56	MG	1a	1712	1/1	0.95	0.15	55,55,55,55	0
56	MG	1A	3935	1/1	0.95	0.07	33,33,33,33	0
56	MG	2A	3745	1/1	0.95	0.08	45,45,45,45	0
56	MG	1A	3936	1/1	0.95	0.12	42,42,42,42	0
56	MG	1A	3210	1/1	0.95	0.04	43,43,43,43	0
56	MG	2A	3467	1/1	0.95	0.08	45,45,45,45	0
56	MG	2A	3749	1/1	0.95	0.09	49,49,49,49	0
56	MG	2A	3052	1/1	0.95	0.21	53,53,53,53	0
56	MG	1T	201	1/1	0.95	0.07	43,43,43,43	0
56	MG	2A	3475	1/1	0.95	0.14	37,37,37,37	0
56	MG	1T	202	1/1	0.95	0.12	52,52,52,52	0
56	MG	1A	3548	1/1	0.95	0.07	44,44,44,44	0
56	MG	1A	3792	1/1	0.95	0.07	56,56,56,56	0
56	MG	1U	203	1/1	0.95	0.21	33,33,33,33	0
56	MG	1A	4083	1/1	0.95	0.12	56,56,56,56	0
56	MG	1a	1728	1/1	0.95	0.08	80,80,80,80	0
56	MG	2a	1657	1/1	0.95	0.21	51,51,51,51	0
56	MG	1A	4084	1/1	0.95	0.09	47,47,47,47	0
56	MG	2A	3062	1/1	0.95	0.14	45,45,45,45	0
56	MG	1A	3942	1/1	0.95	0.07	41,41,41,41	0
56	MG	2A	3064	1/1	0.95	0.13	55,55,55,55	0
56	MG	1A	3550	1/1	0.95	0.11	42,42,42,42	0
56	MG	2a	1663	1/1	0.95	0.32	73,73,73,73	0
56	MG	2A	3266	1/1	0.95	0.15	61,61,61,61	0
56	MG	1a	1734	1/1	0.95	0.08	55,55,55,55	0
56	MG	2A	3773	1/1	0.95	0.07	56,56,56,56	0
56	MG	2A	3068	1/1	0.95	0.11	51,51,51,51	0
56	MG	1A	3148	1/1	0.95	0.07	30,30,30,30	0
56	MG	1A	3177	1/1	0.95	0.09	40,40,40,40	0
56	MG	1A	3669	1/1	0.95	0.08	16,16,16,16	0
56	MG	2a	1671	1/1	0.95	0.11	55,55,55,55	0
56	MG	1A	3553	1/1	0.95	0.13	29,29,29,29	0
56	MG	2a	1673	1/1	0.95	0.24	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3503	1/1	0.95	0.13	53,53,53,53	0
56	MG	1A	3153	1/1	0.95	0.14	38,38,38,38	0
56	MG	1A	3216	1/1	0.95	0.21	29,29,29,29	0
56	MG	1W	205	1/1	0.95	0.13	36,36,36,36	0
56	MG	1a	1750	1/1	0.95	0.09	63,63,63,63	0
56	MG	1a	1755	1/1	0.95	0.06	84,84,84,84	0
56	MG	1A	3678	1/1	0.95	0.05	18,18,18,18	0
56	MG	2A	3515	1/1	0.95	0.06	51,51,51,51	0
56	MG	1A	4096	1/1	0.95	0.09	55,55,55,55	0
56	MG	1X	101	1/1	0.95	0.45	33,33,33,33	0
56	MG	1A	3807	1/1	0.95	0.09	39,39,39,39	0
56	MG	1A	3808	1/1	0.95	0.10	38,38,38,38	0
56	MG	1A	3556	1/1	0.95	0.07	18,18,18,18	0
56	MG	1A	3681	1/1	0.95	0.05	26,26,26,26	0
56	MG	1A	3557	1/1	0.95	0.07	22,22,22,22	0
56	MG	1A	3477	1/1	0.95	0.07	48,48,48,48	0
56	MG	2A	3801	1/1	0.95	0.18	53,53,53,53	0
56	MG	2A	3288	1/1	0.95	0.23	63,63,63,63	0
56	MG	1A	3963	1/1	0.95	0.06	43,43,43,43	0
56	MG	2A	3529	1/1	0.95	0.16	56,56,56,56	0
56	MG	2A	3530	1/1	0.95	0.07	58,58,58,58	0
56	MG	1A	3414	1/1	0.95	0.15	38,38,38,38	0
56	MG	2A	3093	1/1	0.95	0.11	34,34,34,34	0
56	MG	1A	3967	1/1	0.95	0.07	54,54,54,54	0
56	MG	1A	3565	1/1	0.95	0.06	33,33,33,33	0
56	MG	2A	3535	1/1	0.95	0.12	43,43,43,43	0
56	MG	2A	3813	1/1	0.95	0.19	64,64,64,64	0
56	MG	2A	3536	1/1	0.95	0.12	40,40,40,40	0
56	MG	1a	1777	1/1	0.95	0.21	62,62,62,62	0
56	MG	1A	3818	1/1	0.95	0.15	37,37,37,37	0
56	MG	2A	3539	1/1	0.95	0.09	55,55,55,55	0
56	MG	1A	3052	1/1	0.95	0.30	52,52,52,52	0
56	MG	11	103	1/1	0.95	0.10	58,58,58,58	0
56	MG	1A	3693	1/1	0.95	0.09	18,18,18,18	0
56	MG	1A	3570	1/1	0.95	0.09	17,17,17,17	0
56	MG	1A	3697	1/1	0.95	0.06	36,36,36,36	0
56	MG	2A	3301	1/1	0.95	0.16	57,57,57,57	0
56	MG	13	104	1/1	0.95	0.13	38,38,38,38	0
56	MG	2A	3551	1/1	0.95	0.14	58,58,58,58	0
56	MG	13	105	1/1	0.95	0.13	54,54,54,54	0
56	MG	2a	1716	1/1	0.95	0.17	67,67,67,67	0
56	MG	13	106	1/1	0.95	0.16	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3111	1/1	0.95	0.05	73,73,73,73	0
56	MG	1A	3699	1/1	0.95	0.04	23,23,23,23	0
56	MG	2A	3559	1/1	0.95	0.09	68,68,68,68	0
56	MG	1A	3481	1/1	0.95	0.41	34,34,34,34	0
56	MG	1A	4121	1/1	0.95	0.10	53,53,53,53	0
56	MG	2A	3833	1/1	0.95	0.07	58,58,58,58	0
56	MG	1A	3980	1/1	0.95	0.08	46,46,46,46	0
56	MG	1A	3101	1/1	0.95	0.07	47,47,47,47	0
56	MG	2A	3836	1/1	0.95	0.06	59,59,59,59	0
56	MG	2a	1729	1/1	0.95	0.21	68,68,68,68	0
56	MG	1A	4126	1/1	0.95	0.37	34,34,34,34	0
56	MG	2a	1731	1/1	0.95	0.07	82,82,82,82	0
56	MG	2A	3119	1/1	0.95	0.09	46,46,46,46	0
56	MG	2A	3315	1/1	0.95	0.15	69,69,69,69	0
56	MG	2A	3568	1/1	0.95	0.19	43,43,43,43	0
56	MG	1A	3984	1/1	0.95	0.11	43,43,43,43	0
56	MG	1A	3264	1/1	0.95	0.38	33,33,33,33	0
56	MG	1A	3219	1/1	0.95	0.07	55,55,55,55	0
56	MG	1A	3842	1/1	0.95	0.07	62,62,62,62	0
56	MG	18	107	1/1	0.95	0.13	46,46,46,46	0
56	MG	1a	1802	1/1	0.95	0.08	51,51,51,51	0
56	MG	1A	3485	1/1	0.95	0.10	41,41,41,41	0
56	MG	2A	3848	1/1	0.95	0.06	64,64,64,64	0
56	MG	1A	3588	1/1	0.95	0.09	65,65,65,65	0
56	MG	2A	3850	1/1	0.95	0.07	49,49,49,49	0
56	MG	1A	3103	1/1	0.95	0.17	44,44,44,44	0
56	MG	1A	3854	1/1	0.95	0.05	36,36,36,36	0
56	MG	1a	1604	1/1	0.95	0.14	59,59,59,59	0
56	MG	2a	1754	1/1	0.95	0.10	77,77,77,77	0
56	MG	1A	3993	1/1	0.95	0.08	39,39,39,39	0
56	MG	1a	1607	1/1	0.95	0.21	62,62,62,62	0
56	MG	1A	3001	1/1	0.95	0.07	36,36,36,36	0
56	MG	2A	3141	1/1	0.95	0.08	62,62,62,62	0
56	MG	1a	1609	1/1	0.95	0.24	49,49,49,49	0
56	MG	1A	3223	1/1	0.95	0.08	55,55,55,55	0
56	MG	1A	3593	1/1	0.95	0.11	38,38,38,38	0
56	MG	1B	203	1/1	0.95	0.10	61,61,61,61	0
56	MG	1A	3076	1/1	0.95	0.12	49,49,49,49	0
56	MG	1A	3007	1/1	0.95	0.09	35,35,35,35	0
56	MG	1a	1621	1/1	0.95	0.08	51,51,51,51	0
56	MG	1A	3861	1/1	0.95	0.05	23,23,23,23	0
56	MG	1A	3598	1/1	0.95	0.06	17,17,17,17	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3728	1/1	0.95	0.10	59,59,59,59	0
56	MG	1A	3191	1/1	0.95	0.17	43,43,43,43	0
56	MG	2a	1772	1/1	0.95	0.16	54,54,54,54	0
56	MG	1A	4005	1/1	0.95	0.09	48,48,48,48	0
56	MG	2a	1774	1/1	0.95	0.09	60,60,60,60	0
56	MG	1A	3731	1/1	0.95	0.06	30,30,30,30	0
56	MG	2A	3157	1/1	0.95	0.09	49,49,49,49	0
56	MG	2A	3158	1/1	0.95	0.09	39,39,39,39	0
56	MG	1A	3367	1/1	0.95	0.14	36,36,36,36	0
56	MG	2A	3349	1/1	0.95	0.09	60,60,60,60	0
56	MG	1A	3427	1/1	0.95	0.17	29,29,29,29	0
56	MG	2A	3161	1/1	0.95	0.07	55,55,55,55	0
56	MG	1A	3041	1/1	0.95	0.17	33,33,33,33	0
56	MG	1a	1631	1/1	0.95	0.20	48,48,48,48	0
56	MG	2A	3355	1/1	0.95	0.13	43,43,43,43	0
56	MG	1a	1632	1/1	0.95	0.12	58,58,58,58	0
56	MG	2A	3617	1/1	0.95	0.09	65,65,65,65	0
56	MG	1A	3280	1/1	0.95	0.12	38,38,38,38	0
56	MG	1A	3433	1/1	0.95	0.12	54,54,54,54	0
56	MG	1A	3607	1/1	0.95	0.14	51,51,51,51	0
56	MG	1A	3095	1/1	0.95	0.09	34,34,34,34	0
56	MG	1A	3611	1/1	0.95	0.11	59,59,59,59	0
56	MG	1A	3612	1/1	0.95	0.07	37,37,37,37	0
56	MG	2A	3171	1/1	0.95	0.19	49,49,49,49	0
56	MG	2A	3364	1/1	0.95	0.07	48,48,48,48	0
56	MG	1e	202	1/1	0.95	0.15	61,61,61,61	0
56	MG	1A	3499	1/1	0.95	0.07	28,28,28,28	0
56	MG	2A	3631	1/1	0.95	0.10	42,42,42,42	0
56	MG	1B	228	1/1	0.95	0.06	54,54,54,54	0
56	MG	1A	3501	1/1	0.95	0.10	24,24,24,24	0
56	MG	1a	1642	1/1	0.95	0.14	48,48,48,48	0
56	MG	1A	3230	1/1	0.95	0.16	42,42,42,42	0
56	MG	2A	3636	1/1	0.95	0.09	68,68,68,68	0
56	MG	1A	3504	1/1	0.95	0.07	49,49,49,49	0
56	MG	1A	4026	1/1	0.95	0.08	29,29,29,29	0
56	MG	2A	3180	1/1	0.95	0.07	59,59,59,59	0
56	MG	2A	3641	1/1	0.95	0.10	31,31,31,31	0
56	MG	2A	3374	1/1	0.95	0.08	71,71,71,71	0
56	MG	2A	3645	1/1	0.95	0.08	66,66,66,66	0
56	MG	2A	3376	1/1	0.95	0.13	44,44,44,44	0
56	MG	1A	3750	1/1	0.95	0.10	58,58,58,58	0
56	MG	1B	236	1/1	0.95	0.08	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3284	1/1	0.95	0.07	38,38,38,38	0
56	MG	1w	102	1/1	0.95	0.18	46,46,46,46	0
56	MG	1A	3885	1/1	0.95	0.12	25,25,25,25	0
56	MG	2A	3654	1/1	0.95	0.06	50,50,50,50	0
56	MG	1D	306	1/1	0.95	0.09	48,48,48,48	0
56	MG	1A	4031	1/1	0.95	0.09	21,21,21,21	0
56	MG	1A	3233	1/1	0.95	0.10	42,42,42,42	0
56	MG	2A	3189	1/1	0.95	0.12	52,52,52,52	0
56	MG	2A	3659	1/1	0.95	0.07	81,81,81,81	0
56	MG	1a	1653	1/1	0.95	0.15	61,61,61,61	0
56	MG	1A	4033	1/1	0.95	0.05	52,52,52,52	0
56	MG	1A	3507	1/1	0.95	0.10	35,35,35,35	0
56	MG	1a	1656	1/1	0.95	0.17	50,50,50,50	0
56	MG	1A	3197	1/1	0.95	0.21	42,42,42,42	0
56	MG	1A	3288	1/1	0.95	0.13	55,55,55,55	0
56	MG	1A	3758	1/1	0.95	0.08	46,46,46,46	0
56	MG	1E	303	1/1	0.95	0.07	28,28,28,28	0
56	MG	2T	201	1/1	0.95	0.11	65,65,65,65	0
56	MG	2T	202	1/1	0.95	0.13	53,53,53,53	0
56	MG	1x	108	1/1	0.95	0.13	62,62,62,62	0
56	MG	1A	3009	1/1	0.95	0.06	29,29,29,29	0
56	MG	2A	3200	1/1	0.95	0.13	46,46,46,46	0
56	MG	1A	3201	1/1	0.95	0.11	54,54,54,54	0
56	MG	1A	3761	1/1	0.95	0.07	49,49,49,49	0
56	MG	1A	3388	1/1	0.95	0.08	48,48,48,48	0
56	MG	2X	103	1/1	0.95	0.09	58,58,58,58	0
56	MG	2A	3676	1/1	0.95	0.08	60,60,60,60	0
56	MG	2A	3677	1/1	0.95	0.07	56,56,56,56	0
56	MG	1A	3202	1/1	0.95	0.17	34,34,34,34	0
56	MG	1F	301	1/1	0.95	0.15	37,37,37,37	0
56	MG	1A	3635	1/1	0.95	0.06	43,43,43,43	0
56	MG	1A	4049	1/1	0.95	0.12	43,43,43,43	0
56	MG	23	101	1/1	0.95	0.08	59,59,59,59	0
56	MG	2A	3682	1/1	0.95	0.14	57,57,57,57	0
56	MG	1A	3241	1/1	0.95	0.10	39,39,39,39	0
56	MG	1A	3903	1/1	0.95	0.07	30,30,30,30	0
56	MG	1A	4053	1/1	0.95	0.10	45,45,45,45	0
56	MG	2A	3005	1/1	0.95	0.11	60,60,60,60	0
56	MG	1A	3525	1/1	0.95	0.05	35,35,35,35	0
56	MG	27	101	1/1	0.95	0.20	39,39,39,39	0
56	MG	27	102	1/1	0.95	0.23	55,55,55,55	0
56	MG	2A	3689	1/1	0.95	0.10	61,61,61,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3639	1/1	0.95	0.07	47,47,47,47	0
56	MG	1A	3242	1/1	0.95	0.13	49,49,49,49	0
56	MG	28	102	1/1	0.95	0.14	54,54,54,54	0
56	MG	2A	3416	1/1	0.95	0.11	46,46,46,46	0
56	MG	1A	3913	1/1	0.95	0.06	47,47,47,47	0
56	MG	1A	3531	1/1	0.95	0.08	22,22,22,22	0
56	MG	2A	3018	1/1	0.95	0.18	48,48,48,48	0
56	MG	2x	101	1/1	0.95	0.13	55,55,55,55	0
56	MG	2A	3421	1/1	0.95	0.18	59,59,59,59	0
56	MG	1A	3915	1/1	0.95	0.06	66,66,66,66	0
56	MG	1a	1681	1/1	0.95	0.19	58,58,58,58	0
56	MG	2A	3702	1/1	0.95	0.07	65,65,65,65	0
56	MG	1A	3244	1/1	0.95	0.07	53,53,53,53	0
56	MG	2A	3226	1/1	0.95	0.08	62,62,62,62	0
56	MG	2A	3705	1/1	0.95	0.07	49,49,49,49	0
56	MG	2A	3707	1/1	0.95	0.16	68,68,68,68	0
56	MG	2A	3024	1/1	0.95	0.16	46,46,46,46	0
56	MG	1A	3203	1/1	0.95	0.40	30,30,30,30	0
56	MG	2A	3026	1/1	0.95	0.18	48,48,48,48	0
56	MG	1N	203	1/1	0.95	0.09	42,42,42,42	0
57	ZN	24	501	1/1	0.95	0.10	128,128,128,128	0
58	Y7K	1a	1842	33/33	0.95	0.13	51,58,66,70	0
56	MG	2A	3432	1/1	0.95	0.12	28,28,28,28	0
56	MG	1A	3097	1/1	0.95	0.10	36,36,36,36	0
56	MG	1a	1759	1/1	0.96	0.08	76,76,76,76	0
56	MG	2A	3653	1/1	0.96	0.08	56,56,56,56	0
56	MG	1A	3339	1/1	0.96	0.14	37,37,37,37	0
56	MG	1a	1762	1/1	0.96	0.07	68,68,68,68	0
56	MG	1a	1763	1/1	0.96	0.07	62,62,62,62	0
56	MG	1A	3694	1/1	0.96	0.07	35,35,35,35	0
56	MG	1A	4054	1/1	0.96	0.07	46,46,46,46	0
56	MG	2A	3129	1/1	0.96	0.20	60,60,60,60	0
56	MG	1A	3868	1/1	0.96	0.10	66,66,66,66	0
56	MG	2A	3131	1/1	0.96	0.12	41,41,41,41	0
56	MG	1A	3695	1/1	0.96	0.07	36,36,36,36	0
56	MG	1A	3870	1/1	0.96	0.09	71,71,71,71	0
56	MG	1a	1770	1/1	0.96	0.09	51,51,51,51	0
56	MG	1A	3340	1/1	0.96	0.06	55,55,55,55	0
56	MG	2a	1603	1/1	0.96	0.20	53,53,53,53	0
56	MG	2A	3666	1/1	0.96	0.18	57,57,57,57	0
56	MG	2A	3136	1/1	0.96	0.10	57,57,57,57	0
56	MG	1U	208	1/1	0.96	0.35	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
56	MG	2A	3138	1/1	0.96	0.17	55,55,55,55	0
56	MG	2A	3375	1/1	0.96	0.08	45,45,45,45	0
56	MG	1U	209	1/1	0.96	0.33	38,38,38,38	0
56	MG	2A	3377	1/1	0.96	0.29	48,48,48,48	0
56	MG	1A	3102	1/1	0.96	0.06	42,42,42,42	0
56	MG	1A	3428	1/1	0.96	0.17	42,42,42,42	0
56	MG	1A	3152	1/1	0.96	0.21	46,46,46,46	0
56	MG	1A	4062	1/1	0.96	0.06	39,39,39,39	0
56	MG	1A	3542	1/1	0.96	0.09	39,39,39,39	0
56	MG	1A	3543	1/1	0.96	0.06	31,31,31,31	0
56	MG	1A	3706	1/1	0.96	0.05	33,33,33,33	0
56	MG	1A	3707	1/1	0.96	0.08	46,46,46,46	0
56	MG	2a	1619	1/1	0.96	0.14	56,56,56,56	0
56	MG	1W	204	1/1	0.96	0.09	37,37,37,37	0
56	MG	1A	3431	1/1	0.96	0.18	34,34,34,34	0
56	MG	2A	3152	1/1	0.96	0.12	39,39,39,39	0
56	MG	1A	3710	1/1	0.96	0.11	59,59,59,59	0
56	MG	1A	3211	1/1	0.96	0.08	58,58,58,58	0
56	MG	1A	3075	1/1	0.96	0.10	44,44,44,44	0
56	MG	1a	1790	1/1	0.96	0.06	51,51,51,51	0
56	MG	1X	103	1/1	0.96	0.05	41,41,41,41	0
56	MG	1X	105	1/1	0.96	0.06	56,56,56,56	0
56	MG	1a	1793	1/1	0.96	0.14	45,45,45,45	0
56	MG	1Y	201	1/1	0.96	0.13	45,45,45,45	0
56	MG	1A	3716	1/1	0.96	0.06	26,26,26,26	0
56	MG	1A	4072	1/1	0.96	0.08	44,44,44,44	0
56	MG	1A	3549	1/1	0.96	0.08	40,40,40,40	0
56	MG	1A	3213	1/1	0.96	0.06	39,39,39,39	0
56	MG	1A	3006	1/1	0.96	0.20	54,54,54,54	0
56	MG	1A	3720	1/1	0.96	0.07	31,31,31,31	0
56	MG	1A	3281	1/1	0.96	0.25	45,45,45,45	0
56	MG	1A	3077	1/1	0.96	0.12	19,19,19,19	0
56	MG	1A	3108	1/1	0.96	0.38	36,36,36,36	0
56	MG	1A	3439	1/1	0.96	0.06	45,45,45,45	0
56	MG	1A	3726	1/1	0.96	0.12	56,56,56,56	0
56	MG	1A	3899	1/1	0.96	0.05	60,60,60,60	0
56	MG	1A	3727	1/1	0.96	0.09	43,43,43,43	0
56	MG	2A	3412	1/1	0.96	0.07	60,60,60,60	0
56	MG	1A	3027	1/1	0.96	0.26	24,24,24,24	0
56	MG	1a	1812	1/1	0.96	0.09	81,81,81,81	0
56	MG	2a	1647	1/1	0.96	0.29	58,58,58,58	0
56	MG	1a	1813	1/1	0.96	0.21	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	12	101	1/1	0.96	0.08	44,44,44,44	0
56	MG	2A	3418	1/1	0.96	0.07	67,67,67,67	0
56	MG	12	102	1/1	0.96	0.09	48,48,48,48	0
56	MG	1A	3053	1/1	0.96	0.09	35,35,35,35	0
56	MG	1A	3730	1/1	0.96	0.09	35,35,35,35	0
56	MG	1A	3286	1/1	0.96	0.25	26,26,26,26	0
56	MG	2A	3423	1/1	0.96	0.07	56,56,56,56	0
56	MG	1A	3161	1/1	0.96	0.21	36,36,36,36	0
56	MG	1A	3910	1/1	0.96	0.07	38,38,38,38	0
56	MG	15	101	1/1	0.96	0.15	32,32,32,32	0
56	MG	1A	3220	1/1	0.96	0.18	60,60,60,60	0
56	MG	1A	3447	1/1	0.96	0.21	62,62,62,62	0
56	MG	1A	3569	1/1	0.96	0.06	20,20,20,20	0
56	MG	2A	3430	1/1	0.96	0.08	32,32,32,32	0
56	MG	2A	3731	1/1	0.96	0.06	39,39,39,39	0
56	MG	1A	3290	1/1	0.96	0.11	67,67,67,67	0
56	MG	2A	3733	1/1	0.96	0.11	39,39,39,39	0
56	MG	2A	3734	1/1	0.96	0.06	33,33,33,33	0
56	MG	17	103	1/1	0.96	0.11	39,39,39,39	0
56	MG	1a	1828	1/1	0.96	0.06	54,54,54,54	0
56	MG	1A	3573	1/1	0.96	0.05	27,27,27,27	0
56	MG	2A	3738	1/1	0.96	0.10	60,60,60,60	0
56	MG	1A	4099	1/1	0.96	0.08	35,35,35,35	0
56	MG	1a	1832	1/1	0.96	0.12	58,58,58,58	0
56	MG	18	102	1/1	0.96	0.20	41,41,41,41	0
56	MG	1A	3082	1/1	0.96	0.07	42,42,42,42	0
56	MG	1A	4101	1/1	0.96	0.05	48,48,48,48	0
56	MG	1A	3450	1/1	0.96	0.09	48,48,48,48	0
56	MG	1A	3360	1/1	0.96	0.14	45,45,45,45	0
56	MG	1A	4105	1/1	0.96	0.07	47,47,47,47	0
56	MG	2a	1679	1/1	0.96	0.16	42,42,42,42	0
56	MG	2A	3444	1/1	0.96	0.07	32,32,32,32	0
56	MG	2A	3754	1/1	0.96	0.11	70,70,70,70	0
56	MG	2A	3445	1/1	0.96	0.10	51,51,51,51	0
56	MG	1A	3112	1/1	0.96	0.09	36,36,36,36	0
56	MG	2A	3447	1/1	0.96	0.09	47,47,47,47	0
56	MG	2A	3201	1/1	0.96	0.20	45,45,45,45	0
56	MG	1A	3166	1/1	0.96	0.05	34,34,34,34	0
56	MG	1A	3924	1/1	0.96	0.05	41,41,41,41	0
56	MG	1A	3745	1/1	0.96	0.09	58,58,58,58	0
56	MG	1A	3582	1/1	0.96	0.07	28,28,28,28	0
56	MG	1A	3747	1/1	0.96	0.08	17,17,17,17	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3930	1/1	0.96	0.05	47,47,47,47	0
56	MG	1A	4114	1/1	0.96	0.06	61,61,61,61	0
56	MG	2A	3211	1/1	0.96	0.08	63,63,63,63	0
56	MG	2A	3769	1/1	0.96	0.13	52,52,52,52	0
56	MG	1l	201	1/1	0.96	0.07	68,68,68,68	0
56	MG	1l	202	1/1	0.96	0.08	56,56,56,56	0
56	MG	1A	3932	1/1	0.96	0.07	60,60,60,60	0
56	MG	1A	3585	1/1	0.96	0.14	21,21,21,21	0
56	MG	1a	1612	1/1	0.96	0.07	57,57,57,57	0
56	MG	1A	3586	1/1	0.96	0.09	16,16,16,16	0
56	MG	2A	3472	1/1	0.96	0.14	50,50,50,50	0
56	MG	1A	4118	1/1	0.96	0.20	36,36,36,36	0
56	MG	1A	3587	1/1	0.96	0.05	24,24,24,24	0
56	MG	1a	1617	1/1	0.96	0.07	53,53,53,53	0
56	MG	1a	1618	1/1	0.96	0.15	57,57,57,57	0
56	MG	2A	3478	1/1	0.96	0.07	23,23,23,23	0
56	MG	1A	3115	1/1	0.96	0.17	35,35,35,35	0
56	MG	2A	3480	1/1	0.96	0.09	65,65,65,65	0
56	MG	1A	3116	1/1	0.96	0.06	42,42,42,42	0
56	MG	2A	3483	1/1	0.96	0.12	56,56,56,56	0
56	MG	2A	3484	1/1	0.96	0.09	40,40,40,40	0
56	MG	2A	3485	1/1	0.96	0.09	44,44,44,44	0
56	MG	1A	3366	1/1	0.96	0.14	38,38,38,38	0
56	MG	2A	3225	1/1	0.96	0.17	62,62,62,62	0
56	MG	1w	106	1/1	0.96	0.25	63,63,63,63	0
56	MG	1A	3939	1/1	0.96	0.14	30,30,30,30	0
56	MG	1A	4125	1/1	0.96	0.23	49,49,49,49	0
56	MG	1A	3460	1/1	0.96	0.06	41,41,41,41	0
56	MG	1A	3941	1/1	0.96	0.09	28,28,28,28	0
56	MG	1A	3461	1/1	0.96	0.09	36,36,36,36	0
56	MG	2a	1723	1/1	0.96	0.06	61,61,61,61	0
56	MG	1A	3464	1/1	0.96	0.41	42,42,42,42	0
56	MG	2A	3803	1/1	0.96	0.13	46,46,46,46	0
56	MG	1A	3596	1/1	0.96	0.09	26,26,26,26	0
56	MG	1A	3465	1/1	0.96	0.10	45,45,45,45	0
56	MG	1A	3170	1/1	0.96	0.06	27,27,27,27	0
56	MG	1A	3171	1/1	0.96	0.06	38,38,38,38	0
56	MG	1A	3600	1/1	0.96	0.10	27,27,27,27	0
56	MG	1A	3120	1/1	0.96	0.06	49,49,49,49	0
56	MG	1A	3054	1/1	0.96	0.13	49,49,49,49	0
56	MG	2A	3504	1/1	0.96	0.11	49,49,49,49	0
56	MG	1A	3472	1/1	0.96	0.14	41,41,41,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3231	1/1	0.96	0.06	36,36,36,36	0
56	MG	1B	201	1/1	0.96	0.04	39,39,39,39	0
56	MG	1A	3605	1/1	0.96	0.09	52,52,52,52	0
56	MG	1y	101	1/1	0.96	0.11	42,42,42,42	0
56	MG	1A	3957	1/1	0.96	0.05	26,26,26,26	0
56	MG	1B	205	1/1	0.96	0.06	51,51,51,51	0
56	MG	2a	1745	1/1	0.96	0.08	63,63,63,63	0
56	MG	1A	3012	1/1	0.96	0.05	31,31,31,31	0
56	MG	2A	3517	1/1	0.96	0.13	54,54,54,54	0
56	MG	1A	3475	1/1	0.96	0.14	34,34,34,34	0
56	MG	1A	3057	1/1	0.96	0.07	26,26,26,26	0
56	MG	1A	3235	1/1	0.96	0.15	29,29,29,29	0
56	MG	2A	3009	1/1	0.96	0.07	50,50,50,50	0
56	MG	1B	210	1/1	0.96	0.06	55,55,55,55	0
56	MG	2A	3011	1/1	0.96	0.12	47,47,47,47	0
56	MG	1B	211	1/1	0.96	0.10	40,40,40,40	0
56	MG	1A	3774	1/1	0.96	0.15	37,37,37,37	0
56	MG	1A	3775	1/1	0.96	0.19	36,36,36,36	0
56	MG	2A	3016	1/1	0.96	0.15	54,54,54,54	0
56	MG	1A	3969	1/1	0.96	0.07	43,43,43,43	0
56	MG	2a	1761	1/1	0.96	0.11	66,66,66,66	0
56	MG	1A	3004	1/1	0.96	0.07	30,30,30,30	0
56	MG	1B	217	1/1	0.96	0.16	61,61,61,61	0
56	MG	1A	3479	1/1	0.96	0.15	42,42,42,42	0
56	MG	2A	3023	1/1	0.96	0.07	37,37,37,37	0
56	MG	1A	3380	1/1	0.96	0.21	52,52,52,52	0
56	MG	1A	3381	1/1	0.96	0.26	42,42,42,42	0
56	MG	1A	3089	1/1	0.96	0.20	34,34,34,34	0
56	MG	1A	3239	1/1	0.96	0.28	28,28,28,28	0
56	MG	1A	3385	1/1	0.96	0.15	42,42,42,42	0
56	MG	1A	3787	1/1	0.96	0.10	18,18,18,18	0
56	MG	1A	3387	1/1	0.96	0.07	39,39,39,39	0
56	MG	1A	3128	1/1	0.96	0.14	42,42,42,42	0
56	MG	1A	3983	1/1	0.96	0.15	42,42,42,42	0
56	MG	1A	3623	1/1	0.96	0.17	51,51,51,51	0
56	MG	1A	3181	1/1	0.96	0.13	49,49,49,49	0
56	MG	2A	3547	1/1	0.96	0.11	42,42,42,42	0
56	MG	1A	3131	1/1	0.96	0.17	43,43,43,43	0
56	MG	2A	3549	1/1	0.96	0.09	31,31,31,31	0
56	MG	1A	3132	1/1	0.96	0.21	31,31,31,31	0
56	MG	2A	3552	1/1	0.96	0.08	35,35,35,35	0
56	MG	2A	3278	1/1	0.96	0.09	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3798	1/1	0.96	0.04	47,47,47,47	0
56	MG	1a	1668	1/1	0.96	0.09	39,39,39,39	0
56	MG	1A	3133	1/1	0.96	0.15	37,37,37,37	0
56	MG	2A	3558	1/1	0.96	0.09	58,58,58,58	0
56	MG	2A	3042	1/1	0.96	0.16	30,30,30,30	0
56	MG	1A	3800	1/1	0.96	0.04	32,32,32,32	0
56	MG	1A	3393	1/1	0.96	0.22	45,45,45,45	0
56	MG	1A	3394	1/1	0.96	0.12	43,43,43,43	0
56	MG	2A	3563	1/1	0.96	0.07	50,50,50,50	0
56	MG	1A	3803	1/1	0.96	0.08	47,47,47,47	0
56	MG	1A	3395	1/1	0.96	0.08	46,46,46,46	0
56	MG	1A	3134	1/1	0.96	0.07	42,42,42,42	0
56	MG	1a	1676	1/1	0.96	0.16	45,45,45,45	0
56	MG	1D	311	1/1	0.96	0.08	45,45,45,45	0
56	MG	1A	3397	1/1	0.96	0.08	41,41,41,41	0
56	MG	1A	3189	1/1	0.96	0.10	40,40,40,40	0
56	MG	1A	3135	1/1	0.96	0.07	36,36,36,36	0
56	MG	1A	3091	1/1	0.96	0.16	28,28,28,28	0
56	MG	1A	3645	1/1	0.96	0.06	35,35,35,35	0
56	MG	1E	304	1/1	0.96	0.10	29,29,29,29	0
56	MG	1A	3500	1/1	0.96	0.08	45,45,45,45	0
56	MG	1A	3815	1/1	0.96	0.22	56,56,56,56	0
56	MG	1A	3059	1/1	0.96	0.16	26,26,26,26	0
56	MG	1A	3502	1/1	0.96	0.08	43,43,43,43	0
56	MG	1A	3320	1/1	0.96	0.36	36,36,36,36	0
56	MG	2A	3881	1/1	0.96	0.18	60,60,60,60	0
56	MG	1E	313	1/1	0.96	0.14	38,38,38,38	0
56	MG	1A	4011	1/1	0.96	0.12	29,29,29,29	0
56	MG	2A	3066	1/1	0.96	0.08	52,52,52,52	0
56	MG	1A	3139	1/1	0.96	0.08	40,40,40,40	0
56	MG	1F	303	1/1	0.96	0.06	30,30,30,30	0
56	MG	1A	3195	1/1	0.96	0.08	46,46,46,46	0
56	MG	1A	3060	1/1	0.96	0.11	24,24,24,24	0
56	MG	1F	307	1/1	0.96	0.19	33,33,33,33	0
56	MG	2B	206	1/1	0.96	0.08	69,69,69,69	0
56	MG	1A	3658	1/1	0.96	0.07	18,18,18,18	0
56	MG	1a	1704	1/1	0.96	0.12	61,61,61,61	0
56	MG	1A	3259	1/1	0.96	0.22	55,55,55,55	0
56	MG	2A	3314	1/1	0.96	0.19	67,67,67,67	0
56	MG	1a	1706	1/1	0.96	0.09	55,55,55,55	0
56	MG	1A	3832	1/1	0.96	0.05	40,40,40,40	0
56	MG	1A	3834	1/1	0.96	0.07	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
56	MG	2A	3600	1/1	0.96	0.06	39,39,39,39	0
56	MG	1a	1710	1/1	0.96	0.14	45,45,45,45	0
56	MG	1A	3508	1/1	0.96	0.08	43,43,43,43	0
56	MG	2A	3603	1/1	0.96	0.12	57,57,57,57	0
56	MG	1A	3031	1/1	0.96	0.23	26,26,26,26	0
56	MG	1a	1714	1/1	0.96	0.19	58,58,58,58	0
56	MG	1A	3511	1/1	0.96	0.06	37,37,37,37	0
56	MG	2D	303	1/1	0.96	0.11	37,37,37,37	0
56	MG	1A	3664	1/1	0.96	0.07	32,32,32,32	0
56	MG	2A	3086	1/1	0.96	0.08	39,39,39,39	0
56	MG	1A	4024	1/1	0.96	0.13	35,35,35,35	0
56	MG	2A	3610	1/1	0.96	0.06	76,76,76,76	0
56	MG	2A	3611	1/1	0.96	0.09	35,35,35,35	0
56	MG	1A	3412	1/1	0.96	0.23	34,34,34,34	0
56	MG	1A	3327	1/1	0.96	0.21	40,40,40,40	0
56	MG	2A	3090	1/1	0.96	0.06	47,47,47,47	0
56	MG	2A	3329	1/1	0.96	0.09	50,50,50,50	0
56	MG	1a	1723	1/1	0.96	0.07	48,48,48,48	0
56	MG	2A	3618	1/1	0.96	0.09	71,71,71,71	0
56	MG	2I	203	1/1	0.96	0.07	68,68,68,68	0
56	MG	1A	3846	1/1	0.96	0.06	54,54,54,54	0
56	MG	1a	1725	1/1	0.96	0.10	57,57,57,57	0
56	MG	2A	3621	1/1	0.96	0.07	60,60,60,60	0
56	MG	2F	305	1/1	0.96	0.24	50,50,50,50	0
56	MG	1A	3847	1/1	0.96	0.11	45,45,45,45	0
56	MG	2A	3096	1/1	0.96	0.20	45,45,45,45	0
56	MG	1A	3848	1/1	0.96	0.06	54,54,54,54	0
56	MG	2A	3336	1/1	0.96	0.09	60,60,60,60	0
56	MG	1A	3849	1/1	0.96	0.07	55,55,55,55	0
56	MG	1A	3262	1/1	0.96	0.12	38,38,38,38	0
56	MG	1a	1730	1/1	0.96	0.06	63,63,63,63	0
56	MG	2Q	201	1/1	0.96	0.12	59,59,59,59	0
56	MG	1A	3047	1/1	0.96	0.11	33,33,33,33	0
56	MG	1A	3032	1/1	0.96	0.58	33,33,33,33	0
56	MG	2R	203	1/1	0.96	0.06	43,43,43,43	0
56	MG	1P	204	1/1	0.96	0.35	35,35,35,35	0
56	MG	1A	3520	1/1	0.96	0.09	49,49,49,49	0
56	MG	2T	203	1/1	0.96	0.11	61,61,61,61	0
56	MG	2U	201	1/1	0.96	0.10	55,55,55,55	0
56	MG	1A	3265	1/1	0.96	0.09	58,58,58,58	0
56	MG	1A	3524	1/1	0.96	0.05	33,33,33,33	0
56	MG	2A	3109	1/1	0.96	0.25	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3266	1/1	0.96	0.22	40,40,40,40	0
56	MG	1A	4040	1/1	0.96	0.08	57,57,57,57	0
56	MG	1A	3527	1/1	0.96	0.07	28,28,28,28	0
56	MG	1A	3017	1/1	0.96	0.12	64,64,64,64	0
56	MG	1a	1744	1/1	0.96	0.06	75,75,75,75	0
56	MG	2A	3644	1/1	0.96	0.06	30,30,30,30	0
56	MG	1A	3099	1/1	0.96	0.23	28,28,28,28	0
56	MG	1A	3269	1/1	0.96	0.09	50,50,50,50	0
56	MG	1A	3072	1/1	0.96	0.12	31,31,31,31	0
57	ZN	2n	501	1/1	0.96	0.05	109,109,109,109	0
56	MG	2A	3118	1/1	0.96	0.10	49,49,49,49	0
56	MG	1A	3273	1/1	0.96	0.13	49,49,49,49	0
56	MG	1A	4051	1/1	0.96	0.13	45,45,45,45	0
56	MG	1a	1685	1/1	0.97	0.12	54,54,54,54	0
56	MG	1a	1686	1/1	0.97	0.13	51,51,51,51	0
56	MG	1A	3722	1/1	0.97	0.12	37,37,37,37	0
56	MG	1A	3196	1/1	0.97	0.21	42,42,42,42	0
56	MG	1U	202	1/1	0.97	0.14	28,28,28,28	0
56	MG	1A	3386	1/1	0.97	0.09	48,48,48,48	0
56	MG	1A	3610	1/1	0.97	0.05	17,17,17,17	0
56	MG	1A	3329	1/1	0.97	0.09	41,41,41,41	0
56	MG	1a	1693	1/1	0.97	0.09	39,39,39,39	0
56	MG	1U	207	1/1	0.97	0.13	35,35,35,35	0
56	MG	1A	4112	1/1	0.97	0.06	31,31,31,31	0
56	MG	1A	3046	1/1	0.97	0.13	26,26,26,26	0
56	MG	2A	3001	1/1	0.97	0.30	51,51,51,51	0
56	MG	1A	3079	1/1	0.97	0.17	38,38,38,38	0
56	MG	1V	201	1/1	0.97	0.19	21,21,21,21	0
56	MG	1A	3851	1/1	0.97	0.07	59,59,59,59	0
56	MG	1A	3852	1/1	0.97	0.07	36,36,36,36	0
56	MG	2A	3007	1/1	0.97	0.17	57,57,57,57	0
56	MG	1V	204	1/1	0.97	0.14	31,31,31,31	0
56	MG	1A	3986	1/1	0.97	0.19	52,52,52,52	0
56	MG	1A	3526	1/1	0.97	0.05	15,15,15,15	0
56	MG	1a	1707	1/1	0.97	0.12	51,51,51,51	0
56	MG	1A	3199	1/1	0.97	0.22	26,26,26,26	0
56	MG	1A	3455	1/1	0.97	0.18	31,31,31,31	0
56	MG	2A	3202	1/1	0.97	0.14	37,37,37,37	0
56	MG	1A	3456	1/1	0.97	0.09	31,31,31,31	0
56	MG	1A	3532	1/1	0.97	0.09	49,49,49,49	0
56	MG	1A	4123	1/1	0.97	0.11	59,59,59,59	0
56	MG	2A	3206	1/1	0.97	0.10	66,66,66,66	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3200	1/1	0.97	0.12	25,25,25,25	0
56	MG	1A	3036	1/1	0.97	0.16	32,32,32,32	0
56	MG	1a	1718	1/1	0.97	0.11	49,49,49,49	0
56	MG	1A	3622	1/1	0.97	0.09	46,46,46,46	0
56	MG	1X	102	1/1	0.97	0.10	30,30,30,30	0
56	MG	1A	3459	1/1	0.97	0.24	34,34,34,34	0
56	MG	1X	104	1/1	0.97	0.12	36,36,36,36	0
56	MG	1A	3738	1/1	0.97	0.10	39,39,39,39	0
56	MG	1A	3624	1/1	0.97	0.09	53,53,53,53	0
56	MG	1A	3740	1/1	0.97	0.05	55,55,55,55	0
56	MG	2A	3030	1/1	0.97	0.14	53,53,53,53	0
56	MG	1A	4131	1/1	0.97	0.08	48,48,48,48	0
56	MG	1A	3625	1/1	0.97	0.05	36,36,36,36	0
56	MG	2A	3033	1/1	0.97	0.05	43,43,43,43	0
56	MG	1A	3536	1/1	0.97	0.04	24,24,24,24	0
56	MG	1A	3163	1/1	0.97	0.16	32,32,32,32	0
56	MG	1Z	303	1/1	0.97	0.14	52,52,52,52	0
56	MG	1a	1731	1/1	0.97	0.09	80,80,80,80	0
56	MG	1A	3037	1/1	0.97	0.22	40,40,40,40	0
56	MG	1A	3463	1/1	0.97	0.40	40,40,40,40	0
56	MG	2A	3415	1/1	0.97	0.05	50,50,50,50	0
56	MG	1A	3633	1/1	0.97	0.05	54,54,54,54	0
56	MG	1A	3243	1/1	0.97	0.09	39,39,39,39	0
56	MG	1A	4008	1/1	0.97	0.09	17,17,17,17	0
56	MG	10	106	1/1	0.97	0.10	53,53,53,53	0
56	MG	1A	3748	1/1	0.97	0.20	44,44,44,44	0
56	MG	1a	1740	1/1	0.97	0.07	71,71,71,71	0
56	MG	1B	202	1/1	0.97	0.11	48,48,48,48	0
56	MG	1A	3289	1/1	0.97	0.07	38,38,38,38	0
56	MG	2A	3048	1/1	0.97	0.12	56,56,56,56	0
56	MG	1A	3105	1/1	0.97	0.32	35,35,35,35	0
56	MG	2A	3865	1/1	0.97	0.04	58,58,58,58	0
56	MG	1A	3205	1/1	0.97	0.11	43,43,43,43	0
56	MG	1a	1745	1/1	0.97	0.05	65,65,65,65	0
56	MG	2a	1719	1/1	0.97	0.05	64,64,64,64	0
56	MG	1a	1746	1/1	0.97	0.06	55,55,55,55	0
56	MG	1a	1747	1/1	0.97	0.08	69,69,69,69	0
56	MG	2A	3241	1/1	0.97	0.19	49,49,49,49	0
56	MG	1a	1748	1/1	0.97	0.07	52,52,52,52	0
56	MG	1A	3544	1/1	0.97	0.06	28,28,28,28	0
56	MG	1a	1751	1/1	0.97	0.05	75,75,75,75	0
56	MG	1A	3061	1/1	0.97	0.25	33,33,33,33	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3247	1/1	0.97	0.06	49,49,49,49	0
56	MG	1A	3642	1/1	0.97	0.04	54,54,54,54	0
56	MG	1A	3756	1/1	0.97	0.07	36,36,36,36	0
56	MG	2A	3061	1/1	0.97	0.15	49,49,49,49	0
56	MG	1A	3107	1/1	0.97	0.19	38,38,38,38	0
56	MG	1a	1760	1/1	0.97	0.05	75,75,75,75	0
56	MG	1A	3137	1/1	0.97	0.12	31,31,31,31	0
56	MG	2a	1734	1/1	0.97	0.06	67,67,67,67	0
56	MG	2A	3883	1/1	0.97	0.07	57,57,57,57	0
56	MG	1A	3296	1/1	0.97	0.10	49,49,49,49	0
56	MG	1A	3063	1/1	0.97	0.07	31,31,31,31	0
56	MG	1A	3019	1/1	0.97	0.19	42,42,42,42	0
56	MG	2a	1739	1/1	0.97	0.17	57,57,57,57	0
56	MG	1A	3651	1/1	0.97	0.14	46,46,46,46	0
56	MG	1A	3348	1/1	0.97	0.15	40,40,40,40	0
56	MG	2A	3448	1/1	0.97	0.09	42,42,42,42	0
56	MG	2a	1744	1/1	0.97	0.05	79,79,79,79	0
56	MG	1A	3066	1/1	0.97	0.11	25,25,25,25	0
56	MG	2A	3071	1/1	0.97	0.16	30,30,30,30	0
56	MG	1a	1768	1/1	0.97	0.12	62,62,62,62	0
56	MG	2A	3452	1/1	0.97	0.05	57,57,57,57	0
56	MG	1A	3893	1/1	0.97	0.06	42,42,42,42	0
56	MG	1A	4030	1/1	0.97	0.16	23,23,23,23	0
56	MG	1A	3411	1/1	0.97	0.09	27,27,27,27	0
56	MG	2A	3674	1/1	0.97	0.07	61,61,61,61	0
56	MG	1A	3002	1/1	0.97	0.07	47,47,47,47	0
56	MG	1A	3255	1/1	0.97	0.05	35,35,35,35	0
56	MG	1A	3558	1/1	0.97	0.05	44,44,44,44	0
56	MG	2A	3079	1/1	0.97	0.04	42,42,42,42	0
56	MG	2a	1758	1/1	0.97	0.10	50,50,50,50	0
56	MG	1A	3559	1/1	0.97	0.06	37,37,37,37	0
56	MG	2A	3463	1/1	0.97	0.10	43,43,43,43	0
56	MG	1A	3256	1/1	0.97	0.09	53,53,53,53	0
56	MG	1A	3090	1/1	0.97	0.31	38,38,38,38	0
56	MG	2D	301	1/1	0.97	0.10	55,55,55,55	0
56	MG	2D	302	1/1	0.97	0.15	49,49,49,49	0
56	MG	1A	3258	1/1	0.97	0.06	55,55,55,55	0
56	MG	2A	3684	1/1	0.97	0.06	40,40,40,40	0
56	MG	1A	3567	1/1	0.97	0.07	24,24,24,24	0
56	MG	2A	3468	1/1	0.97	0.07	32,32,32,32	0
56	MG	2A	3470	1/1	0.97	0.07	28,28,28,28	0
56	MG	1A	3905	1/1	0.97	0.05	27,27,27,27	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1B	234	1/1	0.97	0.06	42,42,42,42	0
56	MG	1a	1606	1/1	0.97	0.07	52,52,52,52	0
56	MG	1a	1785	1/1	0.97	0.09	32,32,32,32	0
56	MG	1A	3113	1/1	0.97	0.12	41,41,41,41	0
56	MG	2a	1775	1/1	0.97	0.09	51,51,51,51	0
56	MG	1A	3908	1/1	0.97	0.04	39,39,39,39	0
56	MG	1A	4044	1/1	0.97	0.06	32,32,32,32	0
56	MG	1D	301	1/1	0.97	0.08	40,40,40,40	0
56	MG	2A	3698	1/1	0.97	0.08	63,63,63,63	0
56	MG	1a	1611	1/1	0.97	0.10	28,28,28,28	0
56	MG	2A	3482	1/1	0.97	0.08	36,36,36,36	0
56	MG	1D	303	1/1	0.97	0.05	23,23,23,23	0
56	MG	2A	3095	1/1	0.97	0.14	53,53,53,53	0
56	MG	1a	1613	1/1	0.97	0.08	65,65,65,65	0
56	MG	1D	304	1/1	0.97	0.16	28,28,28,28	0
56	MG	2A	3487	1/1	0.97	0.06	50,50,50,50	0
56	MG	2A	3706	1/1	0.97	0.06	63,63,63,63	0
56	MG	1A	3909	1/1	0.97	0.04	34,34,34,34	0
56	MG	1A	3114	1/1	0.97	0.14	31,31,31,31	0
56	MG	1A	3357	1/1	0.97	0.06	37,37,37,37	0
56	MG	2R	201	1/1	0.97	0.18	64,64,64,64	0
56	MG	1D	308	1/1	0.97	0.21	32,32,32,32	0
56	MG	1a	1798	1/1	0.97	0.06	64,64,64,64	0
56	MG	1A	3670	1/1	0.97	0.04	33,33,33,33	0
56	MG	1A	3572	1/1	0.97	0.07	20,20,20,20	0
56	MG	1A	3672	1/1	0.97	0.05	50,50,50,50	0
56	MG	2A	3106	1/1	0.97	0.14	64,64,64,64	0
56	MG	1A	3674	1/1	0.97	0.08	21,21,21,21	0
56	MG	2a	1799	1/1	0.97	0.18	71,71,71,71	0
56	MG	1A	3179	1/1	0.97	0.28	37,37,37,37	0
56	MG	1A	3785	1/1	0.97	0.09	51,51,51,51	0
56	MG	2W	201	1/1	0.97	0.13	42,42,42,42	0
56	MG	1A	3786	1/1	0.97	0.06	35,35,35,35	0
56	MG	1A	3040	1/1	0.97	0.09	27,27,27,27	0
56	MG	1A	3788	1/1	0.97	0.05	22,22,22,22	0
56	MG	2a	1806	1/1	0.97	0.09	71,71,71,71	0
56	MG	1A	3677	1/1	0.97	0.07	41,41,41,41	0
56	MG	1A	3146	1/1	0.97	0.35	32,32,32,32	0
56	MG	1a	1811	1/1	0.97	0.09	57,57,57,57	0
56	MG	2A	3305	1/1	0.97	0.31	62,62,62,62	0
56	MG	1E	307	1/1	0.97	0.05	44,44,44,44	0
56	MG	1A	3576	1/1	0.97	0.06	25,25,25,25	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3022	1/1	0.97	0.07	32,32,32,32	0
56	MG	2I	102	1/1	0.97	0.11	55,55,55,55	0
56	MG	1E	311	1/1	0.97	0.08	18,18,18,18	0
56	MG	1a	1816	1/1	0.97	0.09	59,59,59,59	0
56	MG	1A	3119	1/1	0.97	0.12	15,15,15,15	0
56	MG	1A	3364	1/1	0.97	0.13	39,39,39,39	0
56	MG	1E	314	1/1	0.97	0.10	56,56,56,56	0
56	MG	1A	3687	1/1	0.97	0.11	58,58,58,58	0
56	MG	1A	3149	1/1	0.97	0.08	18,18,18,18	0
56	MG	1A	3584	1/1	0.97	0.06	31,31,31,31	0
56	MG	1A	3151	1/1	0.97	0.08	35,35,35,35	0
56	MG	1A	3225	1/1	0.97	0.09	37,37,37,37	0
56	MG	1A	3270	1/1	0.97	0.23	51,51,51,51	0
56	MG	1F	308	1/1	0.97	0.05	49,49,49,49	0
56	MG	2a	1829	1/1	0.97	0.11	53,53,53,53	0
56	MG	1A	3498	1/1	0.97	0.07	22,22,22,22	0
56	MG	1A	3369	1/1	0.97	0.16	32,32,32,32	0
56	MG	1A	3590	1/1	0.97	0.13	44,44,44,44	0
56	MG	1A	3317	1/1	0.97	0.07	36,36,36,36	0
56	MG	2A	3750	1/1	0.97	0.07	41,41,41,41	0
56	MG	2A	3751	1/1	0.97	0.07	58,58,58,58	0
56	MG	1a	1831	1/1	0.97	0.09	50,50,50,50	0
56	MG	1G	201	1/1	0.97	0.15	33,33,33,33	0
56	MG	1A	4076	1/1	0.97	0.07	46,46,46,46	0
56	MG	1A	3943	1/1	0.97	0.05	43,43,43,43	0
56	MG	2A	3757	1/1	0.97	0.06	69,69,69,69	0
56	MG	1A	3700	1/1	0.97	0.08	18,18,18,18	0
56	MG	1a	1837	1/1	0.97	0.13	48,48,48,48	0
56	MG	1A	3271	1/1	0.97	0.11	44,44,44,44	0
56	MG	1A	3034	1/1	0.97	0.07	37,37,37,37	0
56	MG	2A	3541	1/1	0.97	0.06	43,43,43,43	0
56	MG	1A	3594	1/1	0.97	0.12	23,23,23,23	0
56	MG	1N	202	1/1	0.97	0.18	46,46,46,46	0
56	MG	1A	3073	1/1	0.97	0.21	29,29,29,29	0
56	MG	1N	204	1/1	0.97	0.18	45,45,45,45	0
56	MG	2A	3767	1/1	0.97	0.14	59,59,59,59	0
56	MG	1N	206	1/1	0.97	0.05	44,44,44,44	0
56	MG	1A	3074	1/1	0.97	0.23	41,41,41,41	0
56	MG	1A	3192	1/1	0.97	0.09	38,38,38,38	0
56	MG	1A	3709	1/1	0.97	0.06	50,50,50,50	0
56	MG	1A	3819	1/1	0.97	0.06	41,41,41,41	0
56	MG	1A	3055	1/1	0.97	0.11	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
56	MG	1A	3711	1/1	0.97	0.06	25,25,25,25	0
56	MG	2A	3775	1/1	0.97	0.10	64,64,64,64	0
56	MG	1A	3824	1/1	0.97	0.08	42,42,42,42	0
56	MG	1P	203	1/1	0.97	0.16	31,31,31,31	0
56	MG	2A	3778	1/1	0.97	0.04	53,53,53,53	0
56	MG	1A	3958	1/1	0.97	0.05	48,48,48,48	0
56	MG	1A	3378	1/1	0.97	0.06	46,46,46,46	0
56	MG	1A	3714	1/1	0.97	0.05	33,33,33,33	0
56	MG	1A	3827	1/1	0.97	0.05	17,17,17,17	0
56	MG	1A	3379	1/1	0.97	0.07	35,35,35,35	0
56	MG	1A	3965	1/1	0.97	0.07	39,39,39,39	0
56	MG	2A	3352	1/1	0.97	0.12	62,62,62,62	0
56	MG	2A	3786	1/1	0.97	0.07	51,51,51,51	0
56	MG	1A	3035	1/1	0.97	0.18	18,18,18,18	0
56	MG	1A	3045	1/1	0.97	0.05	26,26,26,26	0
56	MG	2A	3789	1/1	0.97	0.07	77,77,77,77	0
56	MG	1R	201	1/1	0.97	0.13	45,45,45,45	0
56	MG	1A	3968	1/1	0.97	0.08	38,38,38,38	0
56	MG	1a	1678	1/1	0.97	0.18	36,36,36,36	0
56	MG	1A	3445	1/1	0.97	0.20	41,41,41,41	0
56	MG	2A	3795	1/1	0.97	0.15	62,62,62,62	0
56	MG	1A	3326	1/1	0.97	0.19	33,33,33,33	0
56	MG	1A	3383	1/1	0.97	0.06	27,27,27,27	0
56	MG	1A	4104	1/1	0.97	0.03	17,17,17,17	0
56	MG	2A	3573	1/1	0.97	0.06	59,59,59,59	0
56	MG	1A	3279	1/1	0.97	0.15	42,42,42,42	0
56	MG	2A	3575	1/1	0.97	0.09	49,49,49,49	0
56	MG	1A	3841	1/1	0.97	0.09	58,58,58,58	0
60	K	1x	101	1/1	0.97	0.08	59,59,59,59	0
56	MG	2A	3577	1/1	0.97	0.07	67,67,67,67	0
56	MG	1A	3778	1/1	0.98	0.05	47,47,47,47	0
56	MG	1A	3186	1/1	0.98	0.12	38,38,38,38	0
56	MG	1A	3649	1/1	0.98	0.05	20,20,20,20	0
56	MG	1A	4043	1/1	0.98	0.11	20,20,20,20	0
56	MG	1A	3781	1/1	0.98	0.05	18,18,18,18	0
56	MG	1Q	207	1/1	0.98	0.06	41,41,41,41	0
56	MG	2A	3808	1/1	0.98	0.05	54,54,54,54	0
56	MG	2A	3513	1/1	0.98	0.04	36,36,36,36	0
56	MG	2a	1740	1/1	0.98	0.04	62,62,62,62	0
56	MG	2A	3247	1/1	0.98	0.05	67,67,67,67	0
56	MG	25	103	1/1	0.98	0.11	58,58,58,58	0
56	MG	1a	1753	1/1	0.98	0.07	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3187	1/1	0.98	0.07	41,41,41,41	0
56	MG	1A	3071	1/1	0.98	0.14	40,40,40,40	0
56	MG	2a	1746	1/1	0.98	0.04	77,77,77,77	0
56	MG	1A	4048	1/1	0.98	0.06	28,28,28,28	0
56	MG	1A	3373	1/1	0.98	0.05	42,42,42,42	0
56	MG	1A	3653	1/1	0.98	0.06	42,42,42,42	0
56	MG	1A	3956	1/1	0.98	0.04	35,35,35,35	0
56	MG	1A	3410	1/1	0.98	0.06	38,38,38,38	0
56	MG	2A	3128	1/1	0.98	0.14	45,45,45,45	0
56	MG	1A	3093	1/1	0.98	0.13	36,36,36,36	0
56	MG	1A	3122	1/1	0.98	0.13	26,26,26,26	0
56	MG	2A	3526	1/1	0.98	0.07	70,70,70,70	0
56	MG	2A	3527	1/1	0.98	0.06	49,49,49,49	0
56	MG	1A	3960	1/1	0.98	0.05	43,43,43,43	0
56	MG	2A	3006	1/1	0.98	0.08	42,42,42,42	0
56	MG	1U	201	1/1	0.98	0.17	26,26,26,26	0
56	MG	1A	3789	1/1	0.98	0.04	22,22,22,22	0
56	MG	1B	214	1/1	0.98	0.04	27,27,27,27	0
56	MG	1A	3164	1/1	0.98	0.19	28,28,28,28	0
56	MG	1U	205	1/1	0.98	0.10	29,29,29,29	0
56	MG	2A	3394	1/1	0.98	0.14	28,28,28,28	0
56	MG	1A	3015	1/1	0.98	0.11	26,26,26,26	0
56	MG	2A	3139	1/1	0.98	0.07	34,34,34,34	0
56	MG	1A	3660	1/1	0.98	0.05	35,35,35,35	0
56	MG	1A	3875	1/1	0.98	0.10	52,52,52,52	0
56	MG	2A	3015	1/1	0.98	0.04	33,33,33,33	0
56	MG	1A	3083	1/1	0.98	0.06	41,41,41,41	0
56	MG	2A	3017	1/1	0.98	0.09	34,34,34,34	0
56	MG	1A	3313	1/1	0.98	0.04	19,19,19,19	0
56	MG	1A	3795	1/1	0.98	0.06	45,45,45,45	0
56	MG	1A	3796	1/1	0.98	0.04	25,25,25,25	0
56	MG	2A	3021	1/1	0.98	0.09	51,51,51,51	0
56	MG	1A	3971	1/1	0.98	0.08	32,32,32,32	0
56	MG	2A	3693	1/1	0.98	0.04	57,57,57,57	0
56	MG	1A	3005	1/1	0.98	0.07	41,41,41,41	0
56	MG	1A	3126	1/1	0.98	0.19	31,31,31,31	0
56	MG	2A	3696	1/1	0.98	0.04	58,58,58,58	0
56	MG	2A	3550	1/1	0.98	0.06	47,47,47,47	0
56	MG	1A	3974	1/1	0.98	0.06	51,51,51,51	0
56	MG	1A	3043	1/1	0.98	0.06	42,42,42,42	0
56	MG	1A	3254	1/1	0.98	0.09	34,34,34,34	0
56	MG	1A	3667	1/1	0.98	0.04	47,47,47,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1W	203	1/1	0.98	0.17	35,35,35,35	0
56	MG	1B	231	1/1	0.98	0.07	30,30,30,30	0
56	MG	1A	3065	1/1	0.98	0.12	26,26,26,26	0
56	MG	1A	4073	1/1	0.98	0.09	55,55,55,55	0
56	MG	1A	3608	1/1	0.98	0.06	55,55,55,55	0
56	MG	1A	3172	1/1	0.98	0.07	26,26,26,26	0
56	MG	1A	3981	1/1	0.98	0.11	33,33,33,33	0
56	MG	1A	3129	1/1	0.98	0.06	27,27,27,27	0
56	MG	1A	3130	1/1	0.98	0.16	36,36,36,36	0
56	MG	1D	302	1/1	0.98	0.15	31,31,31,31	0
56	MG	1A	3466	1/1	0.98	0.08	47,47,47,47	0
56	MG	1A	3892	1/1	0.98	0.03	47,47,47,47	0
56	MG	1A	3087	1/1	0.98	0.09	37,37,37,37	0
56	MG	1A	3562	1/1	0.98	0.05	26,26,26,26	0
56	MG	1A	3426	1/1	0.98	0.23	30,30,30,30	0
56	MG	1A	3564	1/1	0.98	0.07	21,21,21,21	0
56	MG	1A	3897	1/1	0.98	0.10	18,18,18,18	0
56	MG	1A	3260	1/1	0.98	0.20	47,47,47,47	0
56	MG	1A	3680	1/1	0.98	0.07	44,44,44,44	0
56	MG	1A	4088	1/1	0.98	0.05	57,57,57,57	0
56	MG	2A	3873	1/1	0.98	0.04	65,65,65,65	0
56	MG	1A	3100	1/1	0.98	0.06	33,33,33,33	0
56	MG	1A	3682	1/1	0.98	0.03	36,36,36,36	0
56	MG	1A	3683	1/1	0.98	0.03	38,38,38,38	0
56	MG	2A	3725	1/1	0.98	0.06	65,65,65,65	0
56	MG	2A	3726	1/1	0.98	0.03	40,40,40,40	0
56	MG	1A	3471	1/1	0.98	0.06	44,44,44,44	0
56	MG	2a	1813	1/1	0.98	0.12	54,54,54,54	0
56	MG	10	108	1/1	0.98	0.07	57,57,57,57	0
56	MG	11	101	1/1	0.98	0.22	27,27,27,27	0
56	MG	2a	1816	1/1	0.98	0.05	68,68,68,68	0
56	MG	1A	3821	1/1	0.98	0.06	40,40,40,40	0
56	MG	1A	3429	1/1	0.98	0.15	31,31,31,31	0
56	MG	1A	3999	1/1	0.98	0.06	36,36,36,36	0
56	MG	1A	3823	1/1	0.98	0.06	30,30,30,30	0
56	MG	1E	308	1/1	0.98	0.05	47,47,47,47	0
56	MG	1A	3517	1/1	0.98	0.09	24,24,24,24	0
56	MG	2A	3588	1/1	0.98	0.07	44,44,44,44	0
56	MG	1A	3021	1/1	0.98	0.03	17,17,17,17	0
56	MG	1A	4003	1/1	0.98	0.06	27,27,27,27	0
56	MG	1a	1694	1/1	0.98	0.10	32,32,32,32	0
56	MG	2A	3592	1/1	0.98	0.09	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3232	1/1	0.98	0.10	44,44,44,44	0
56	MG	1A	3690	1/1	0.98	0.05	16,16,16,16	0
56	MG	1A	3359	1/1	0.98	0.25	45,45,45,45	0
56	MG	15	102	1/1	0.98	0.04	26,26,26,26	0
56	MG	1A	3829	1/1	0.98	0.04	50,50,50,50	0
56	MG	1A	3626	1/1	0.98	0.07	24,24,24,24	0
56	MG	1a	1701	1/1	0.98	0.06	33,33,33,33	0
56	MG	1a	1702	1/1	0.98	0.11	36,36,36,36	0
56	MG	1A	3833	1/1	0.98	0.09	50,50,50,50	0
56	MG	1A	4010	1/1	0.98	0.04	25,25,25,25	0
56	MG	17	101	1/1	0.98	0.04	27,27,27,27	0
56	MG	2A	3460	1/1	0.98	0.06	58,58,58,58	0
56	MG	17	102	1/1	0.98	0.09	29,29,29,29	0
56	MG	1F	305	1/1	0.98	0.03	36,36,36,36	0
56	MG	1a	1835	1/1	0.98	0.07	73,73,73,73	0
56	MG	1A	3757	1/1	0.98	0.11	48,48,48,48	0
56	MG	1A	3920	1/1	0.98	0.04	45,45,45,45	0
56	MG	1A	3835	1/1	0.98	0.03	49,49,49,49	0
56	MG	1A	3051	1/1	0.98	0.05	25,25,25,25	0
56	MG	2a	1692	1/1	0.98	0.05	74,74,74,74	0
56	MG	2A	3469	1/1	0.98	0.05	54,54,54,54	0
56	MG	2A	3613	1/1	0.98	0.04	60,60,60,60	0
56	MG	1A	3010	1/1	0.98	0.07	28,28,28,28	0
56	MG	2A	3471	1/1	0.98	0.12	34,34,34,34	0
56	MG	1A	3117	1/1	0.98	0.15	30,30,30,30	0
56	MG	1F	312	1/1	0.98	0.04	44,44,44,44	0
56	MG	1a	1717	1/1	0.98	0.03	42,42,42,42	0
56	MG	1A	3578	1/1	0.98	0.09	22,22,22,22	0
56	MG	1A	4018	1/1	0.98	0.10	34,34,34,34	0
56	MG	2A	3477	1/1	0.98	0.08	50,50,50,50	0
56	MG	1A	3698	1/1	0.98	0.13	56,56,56,56	0
56	MG	1A	3208	1/1	0.98	0.07	40,40,40,40	0
56	MG	1A	3528	1/1	0.98	0.07	17,17,17,17	0
56	MG	1A	3931	1/1	0.98	0.05	48,48,48,48	0
56	MG	1A	3845	1/1	0.98	0.05	79,79,79,79	0
56	MG	1A	3701	1/1	0.98	0.05	34,34,34,34	0
56	MG	1A	4025	1/1	0.98	0.05	33,33,33,33	0
56	MG	1A	3237	1/1	0.98	0.12	35,35,35,35	0
56	MG	1A	3583	1/1	0.98	0.09	26,26,26,26	0
56	MG	1N	205	1/1	0.98	0.07	32,32,32,32	0
56	MG	1A	3118	1/1	0.98	0.09	31,31,31,31	0
56	MG	2Q	203	1/1	0.98	0.09	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3008	1/1	0.98	0.06	15,15,15,15	0
56	MG	1A	3183	1/1	0.98	0.19	41,41,41,41	0
56	MG	1A	3402	1/1	0.98	0.16	28,28,28,28	0
56	MG	1A	3159	1/1	0.98	0.07	37,37,37,37	0
56	MG	1A	3160	1/1	0.98	0.07	28,28,28,28	0
56	MG	1A	3644	1/1	0.98	0.04	33,33,33,33	0
56	MG	1P	201	1/1	0.98	0.12	28,28,28,28	0
56	MG	1a	1619	1/1	0.98	0.05	50,50,50,50	0
56	MG	2A	3643	1/1	0.98	0.04	33,33,33,33	0
56	MG	2A	3794	1/1	0.98	0.06	52,52,52,52	0
56	MG	1A	3444	1/1	0.98	0.17	38,38,38,38	0
56	MG	2y	107	1/1	0.98	0.05	77,77,77,77	0
57	ZN	14	501	1/1	0.98	0.04	94,94,94,94	0
57	ZN	2Y	202	1/1	0.98	0.05	95,95,95,95	0
56	MG	2A	3108	1/1	0.98	0.18	66,66,66,66	0
56	MG	1A	3713	1/1	0.98	0.31	31,31,31,31	0
56	MG	2A	3500	1/1	0.98	0.12	32,32,32,32	0
56	MG	1A	3858	1/1	0.98	0.04	41,41,41,41	0
56	MG	1A	3946	1/1	0.98	0.06	23,23,23,23	0
56	MG	1A	3405	1/1	0.98	0.05	46,46,46,46	0
56	MG	1B	221	1/1	0.99	0.09	39,39,39,39	0
56	MG	1A	3513	1/1	0.99	0.05	27,27,27,27	0
56	MG	1A	3837	1/1	0.99	0.05	33,33,33,33	0
56	MG	1A	3647	1/1	0.99	0.05	34,34,34,34	0
56	MG	1a	1749	1/1	0.99	0.04	49,49,49,49	0
56	MG	1A	3911	1/1	0.99	0.09	28,28,28,28	0
56	MG	1A	3169	1/1	0.99	0.05	32,32,32,32	0
56	MG	1a	1752	1/1	0.99	0.04	41,41,41,41	0
56	MG	2A	3142	1/1	0.99	0.04	60,60,60,60	0
56	MG	1A	3014	1/1	0.99	0.04	27,27,27,27	0
56	MG	1a	1754	1/1	0.99	0.03	56,56,56,56	0
56	MG	1A	3011	1/1	0.99	0.09	39,39,39,39	0
56	MG	1a	1809	1/1	0.99	0.04	63,63,63,63	0
56	MG	1A	3030	1/1	0.99	0.12	22,22,22,22	0
56	MG	1A	3916	1/1	0.99	0.04	50,50,50,50	0
56	MG	1A	3518	1/1	0.99	0.08	27,27,27,27	0
56	MG	1A	3081	1/1	0.99	0.15	23,23,23,23	0
56	MG	2A	3741	1/1	0.99	0.09	31,31,31,31	0
56	MG	1A	3880	1/1	0.99	0.04	45,45,45,45	0
56	MG	2A	3743	1/1	0.99	0.03	47,47,47,47	0
56	MG	2A	3744	1/1	0.99	0.04	56,56,56,56	0
56	MG	1A	3013	1/1	0.99	0.19	23,23,23,23	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1711	1/1	0.99	0.11	47,47,47,47	0
56	MG	2A	3435	1/1	0.99	0.09	34,34,34,34	0
56	MG	1A	3810	1/1	0.99	0.02	21,21,21,21	0
56	MG	2A	3556	1/1	0.99	0.06	41,41,41,41	0
56	MG	1A	4046	1/1	0.99	0.04	68,68,68,68	0
56	MG	1A	3580	1/1	0.99	0.05	22,22,22,22	0
56	MG	13	103	1/1	0.99	0.11	32,32,32,32	0
56	MG	2A	3753	1/1	0.99	0.03	33,33,33,33	0
56	MG	1a	1716	1/1	0.99	0.06	53,53,53,53	0
56	MG	1A	3685	1/1	0.99	0.09	17,17,17,17	0
56	MG	1A	4091	1/1	0.99	0.11	50,50,50,50	0
56	MG	1A	3656	1/1	0.99	0.07	38,38,38,38	0
56	MG	1a	1771	1/1	0.99	0.04	54,54,54,54	0
56	MG	1A	3068	1/1	0.99	0.07	36,36,36,36	0
56	MG	1A	3522	1/1	0.99	0.06	18,18,18,18	0
56	MG	2A	3629	1/1	0.99	0.05	28,28,28,28	0
56	MG	1A	3927	1/1	0.99	0.02	21,21,21,21	0
56	MG	2A	3506	1/1	0.99	0.05	39,39,39,39	0
56	MG	1A	3928	1/1	0.99	0.03	45,45,45,45	0
56	MG	2A	3508	1/1	0.99	0.05	54,54,54,54	0
56	MG	1a	1776	1/1	0.99	0.09	48,48,48,48	0
56	MG	1A	3560	1/1	0.99	0.03	38,38,38,38	0
56	MG	1A	3632	1/1	0.99	0.05	48,48,48,48	0
56	MG	2A	3512	1/1	0.99	0.05	39,39,39,39	0
56	MG	1A	3691	1/1	0.99	0.06	22,22,22,22	0
56	MG	1A	3523	1/1	0.99	0.03	44,44,44,44	0
56	MG	1A	3206	1/1	0.99	0.20	38,38,38,38	0
56	MG	1A	3062	1/1	0.99	0.04	11,11,11,11	0
56	MG	1A	3636	1/1	0.99	0.08	50,50,50,50	0
56	MG	1A	3023	1/1	0.99	0.03	20,20,20,20	0
56	MG	1A	3510	1/1	0.99	0.06	17,17,17,17	0
56	MG	1A	3566	1/1	0.99	0.02	35,35,35,35	0
56	MG	1A	3898	1/1	0.99	0.04	30,30,30,30	0
56	MG	1a	1735	1/1	0.99	0.02	48,48,48,48	0
56	MG	2A	3462	1/1	0.99	0.05	46,46,46,46	0
56	MG	1A	3462	1/1	0.99	0.13	28,28,28,28	0
56	MG	2A	3125	1/1	0.99	0.16	34,34,34,34	0
57	ZN	1Y	205	1/1	0.99	0.03	63,63,63,63	0
56	MG	1A	3547	1/1	0.99	0.06	28,28,28,28	0
57	ZN	1n	102	1/1	0.99	0.03	69,69,69,69	0
56	MG	1A	3150	1/1	0.99	0.04	33,33,33,33	0
56	MG	1A	3831	1/1	0.99	0.04	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	ZN	25	106	1/1	0.99	0.06	59,59,59,59	0
57	ZN	26	102	1/1	0.99	0.04	73,73,73,73	0
57	ZN	29	501	1/1	0.99	0.04	76,76,76,76	0
56	MG	1A	3530	1/1	0.99	0.12	23,23,23,23	0
56	MG	1A	3617	1/1	0.99	0.06	23,23,23,23	0
56	MG	1A	3673	1/1	0.99	0.04	24,24,24,24	0
59	SF4	1d	501	8/8	0.99	0.05	55,69,72,74	0
59	SF4	2d	303	8/8	0.99	0.04	70,78,89,91	0
56	MG	1A	3571	1/1	0.99	0.05	25,25,25,25	0
56	MG	1A	3907	1/1	0.99	0.04	23,23,23,23	0
56	MG	1A	3964	1/1	1.00	0.05	22,22,22,22	0
56	MG	1A	3805	1/1	1.00	0.08	40,40,40,40	0
56	MG	2A	3637	1/1	1.00	0.02	47,47,47,47	0
56	MG	2A	3646	1/1	1.00	0.03	36,36,36,36	0
56	MG	1A	3627	1/1	1.00	0.05	21,21,21,21	0
56	MG	1A	3830	1/1	1.00	0.06	22,22,22,22	0
56	MG	1A	3702	1/1	1.00	0.07	27,27,27,27	0
56	MG	1A	3811	1/1	1.00	0.02	27,27,27,27	0
57	ZN	15	105	1/1	1.00	0.06	44,44,44,44	0
57	ZN	16	103	1/1	1.00	0.04	46,46,46,46	0
57	ZN	19	102	1/1	1.00	0.04	42,42,42,42	0
56	MG	1A	3843	1/1	1.00	0.04	44,44,44,44	0

6.5 Other polymers ⓘ

There are no such residues in this entry.