



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 04:42 AM UTC

PDB ID : 7RQ8 / pdb_00007rq8
Title : Crystal structure of the wild-type *Thermus thermophilus* 70S ribosome in complex with iboxamycin, mRNA, deacylated A- and E-site tRNAs, and aminoacylated P-site tRNA at 2.50Å resolution
Authors : Mitcheltree, M.J.; Pisipati, A.; Syroegin, E.A.; Silvestre, K.J.; Klepacki, D.; Mason, J.D.; Terwilliger, D.W.; Testolin, G.; Pote, A.R.; Wu, K.J.Y.; Ladley, R.P.; Chatman, K.; Mankin, A.S.; Polikanov, Y.S.; Myers, A.G.
Deposited on : 2021-08-06
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)

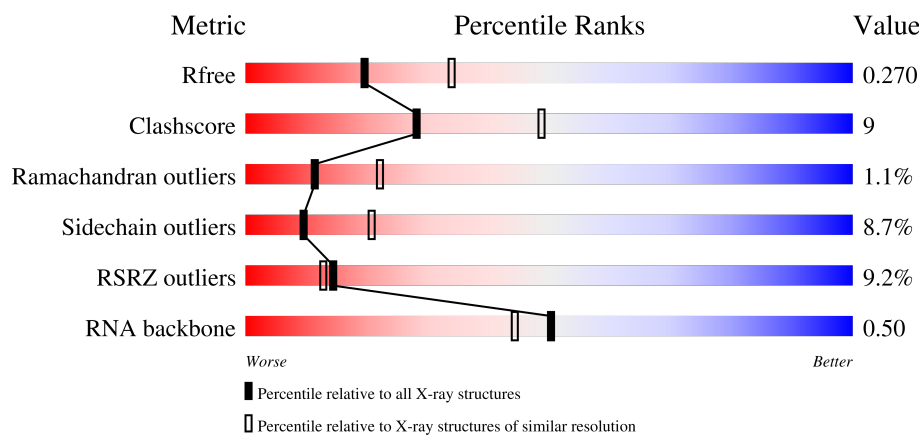
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)
RNA backbone	3983	1003 (2.78-2.22)

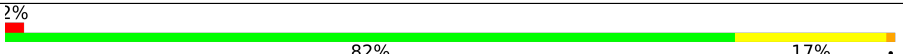
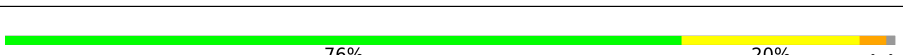
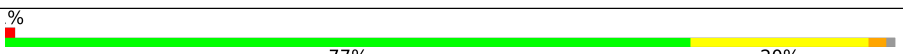
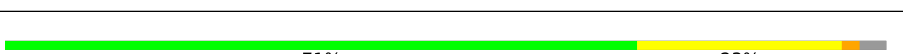
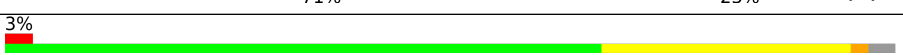
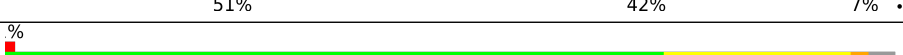
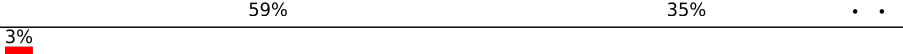
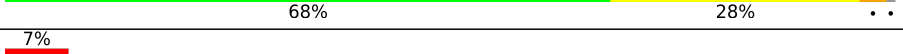
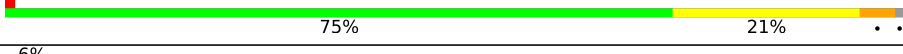
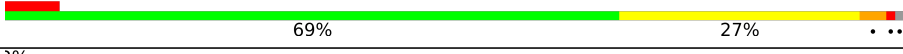
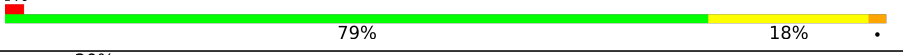
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	4% 67% 25% 6%
1	2A	2915	4% 59% 31% 7%

Continued on next page...

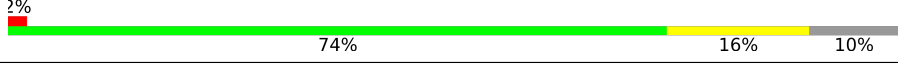
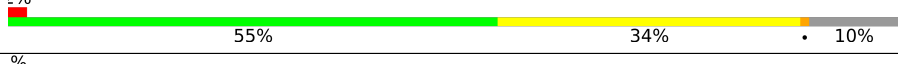
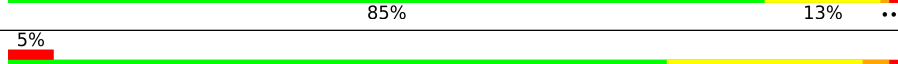
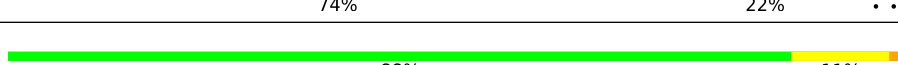
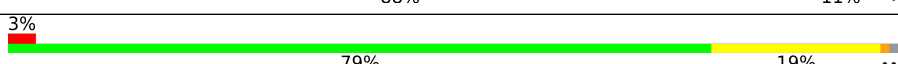
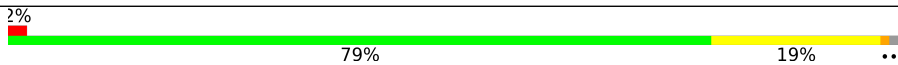
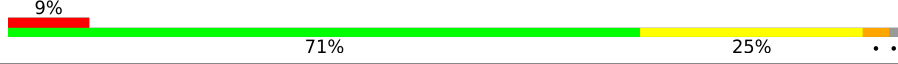
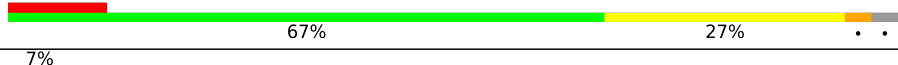
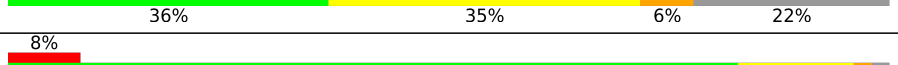
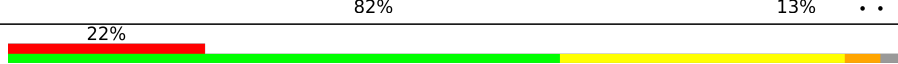
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	1B	121	
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	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
14	2S	112	
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	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
27	15	60	
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	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
39	2h	138	
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	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
52	1u	27	
52	2u	27	
53	1v	24	
53	2v	24	
54	1w	76	
54	2w	76	
55	1x	77	
55	2x	77	
56	1y	76	
56	2y	76	

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
56	PSU	2y	55	-	-	X	-
57	MG	1A	3436	-	-	-	X
57	MG	2a	1646	-	-	-	X
57	MG	2a	1739	-	-	-	X

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 299504 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	203	Total	C	N	O	S	0	0	1
			1584	1009	298	275	2			
5	2F	203	Total	C	N	O	S	0	0	1
			1580	1007	297	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 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 tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	1w	71	Total	C	N	O	P	S	0	0
			1530	685	274	498	71	2		
54	2w	69	Total	C	N	O	P	S	0	0
			1482	662	267	482	69	2		

- Molecule 55 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	1x	76	Total	C	N	O	P	S	0	0
			1635	731	296	530	76	2		
55	2x	76	Total	C	N	O	P	S	0	0
			1635	731	296	530	76	2		

- Molecule 56 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	1y	74	Total	C	N	O	P	S	0	0
			1585	707	285	518	74	1		
56	2y	73	Total	C	N	O	P	S	0	0
			1565	698	283	510	73	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1A	1108	Total	Mg	0	0
			1108	1108		
57	1B	36	Total	Mg	0	0
			36	36		
57	1D	12	Total	Mg	0	0
			12	12		
57	1E	16	Total	Mg	0	0
			16	16		
57	1F	12	Total	Mg	0	0
			12	12		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1G	5	Total 5	Mg 5	0	0
57	1I	1	Total 1	Mg 1	0	0
57	1N	6	Total 6	Mg 6	0	0
57	1O	6	Total 6	Mg 6	0	0
57	1P	6	Total 6	Mg 6	0	0
57	1Q	6	Total 6	Mg 6	0	0
57	1R	4	Total 4	Mg 4	0	0
57	1S	3	Total 3	Mg 3	0	0
57	1T	2	Total 2	Mg 2	0	0
57	1U	9	Total 9	Mg 9	0	0
57	1V	6	Total 6	Mg 6	0	0
57	1W	6	Total 6	Mg 6	0	0
57	1X	5	Total 5	Mg 5	0	0
57	1Y	4	Total 4	Mg 4	0	0
57	1Z	3	Total 3	Mg 3	0	0
57	10	8	Total 8	Mg 8	0	0
57	11	5	Total 5	Mg 5	0	0
57	12	2	Total 2	Mg 2	0	0
57	13	4	Total 4	Mg 4	0	0
57	14	1	Total 1	Mg 1	0	0
57	15	9	Total 9	Mg 9	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	16	1	Total 1	Mg 1	0	0
57	17	6	Total 6	Mg 6	0	0
57	18	6	Total 6	Mg 6	0	0
57	19	1	Total 1	Mg 1	0	0
57	1a	229	Total 229	Mg 229	0	0
57	1b	2	Total 2	Mg 2	0	0
57	1d	1	Total 1	Mg 1	0	0
57	1e	2	Total 2	Mg 2	0	0
57	1f	1	Total 1	Mg 1	0	0
57	1l	3	Total 3	Mg 3	0	0
57	1m	1	Total 1	Mg 1	0	0
57	1n	2	Total 2	Mg 2	0	0
57	1r	1	Total 1	Mg 1	0	0
57	1t	1	Total 1	Mg 1	0	0
57	1v	1	Total 1	Mg 1	0	0
57	1w	5	Total 5	Mg 5	0	0
57	1x	15	Total 15	Mg 15	0	0
57	1y	4	Total 4	Mg 4	0	0
57	2A	729	Total 729	Mg 729	0	0
57	2B	18	Total 18	Mg 18	0	0
57	2D	6	Total 6	Mg 6	0	0

Continued on next page...

Continued from previous page...

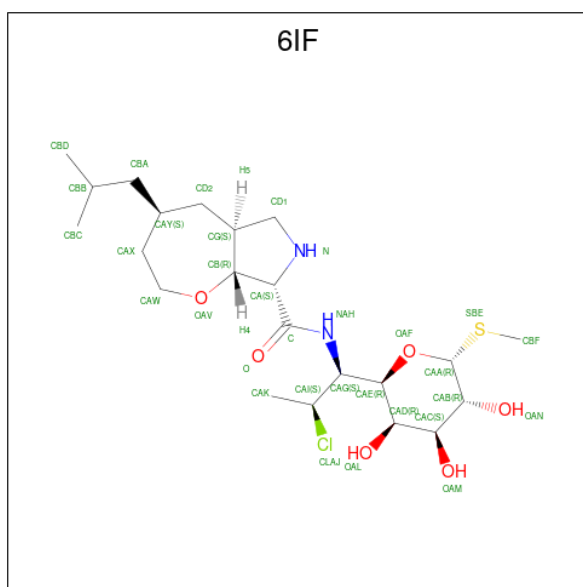
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	2E	7	Total 7	Mg 7	0	0
57	2F	6	Total 6	Mg 6	0	0
57	2G	1	Total 1	Mg 1	0	0
57	2N	1	Total 1	Mg 1	0	0
57	2O	1	Total 1	Mg 1	0	0
57	2Q	1	Total 1	Mg 1	0	0
57	2R	1	Total 1	Mg 1	0	0
57	2T	3	Total 3	Mg 3	0	0
57	2W	1	Total 1	Mg 1	0	0
57	2X	1	Total 1	Mg 1	0	0
57	2Y	1	Total 1	Mg 1	0	0
57	2Z	1	Total 1	Mg 1	0	0
57	20	3	Total 3	Mg 3	0	0
57	21	1	Total 1	Mg 1	0	0
57	23	2	Total 2	Mg 2	0	0
57	25	3	Total 3	Mg 3	0	0
57	26	1	Total 1	Mg 1	0	0
57	27	3	Total 3	Mg 3	0	0
57	28	3	Total 3	Mg 3	0	0
57	2a	186	Total 186	Mg 186	0	0
57	2d	1	Total 1	Mg 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	2e	1	Total	Mg	0	0
			1	1		
57	2f	2	Total	Mg	0	0
			2	2		
57	2l	3	Total	Mg	0	0
			3	3		
57	2q	3	Total	Mg	0	0
			3	3		
57	2r	1	Total	Mg	0	0
			1	1		
57	2t	1	Total	Mg	0	0
			1	1		
57	2v	1	Total	Mg	0	0
			1	1		
57	2w	1	Total	Mg	0	0
			1	1		
57	2x	5	Total	Mg	0	0
			5	5		
57	2y	3	Total	Mg	0	0
			3	3		

- Molecule 58 is methyl 7-chloro-6,7,8-trideoxy-6-{[(4S,5aS,8S,8aR)-4-(2-methylpropyl)octahydro-2H-oxepino[2,3-c]pyrrole-8-carbonyl]amino}-1-thio-L-threo- α -D-galacto-octopyranoside (CCD ID: 6IF) (formula: C₂₂H₃₉ClN₂O₆S).

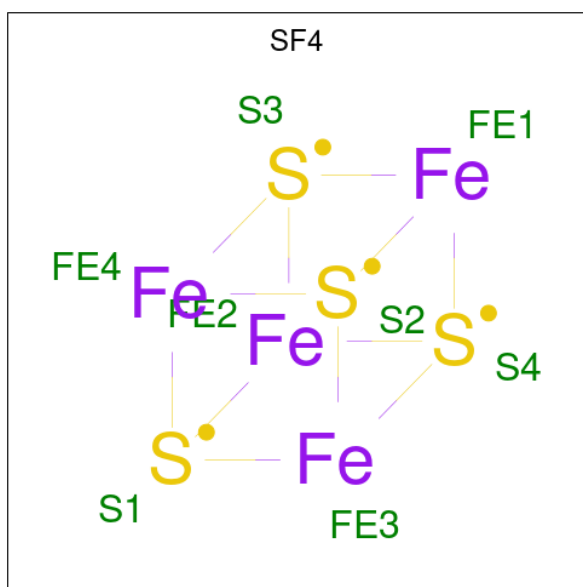


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
58	1A	1	Total	C	Cl	N	O	S	0	0
			32	22	1	2	6	1		
58	2A	1	Total	C	Cl	N	O	S	0	0
			32	22	1	2	6	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1Y	1	Total	Zn	0	0
			1	1		
59	14	1	Total	Zn	0	0
			1	1		
59	15	1	Total	Zn	0	0
			1	1		
59	16	1	Total	Zn	0	0
			1	1		
59	19	1	Total	Zn	0	0
			1	1		
59	1n	1	Total	Zn	0	0
			1	1		
59	2Y	1	Total	Zn	0	0
			1	1		
59	24	1	Total	Zn	0	0
			1	1		
59	25	1	Total	Zn	0	0
			1	1		
59	26	1	Total	Zn	0	0
			1	1		
59	29	1	Total	Zn	0	0
			1	1		
59	2n	1	Total	Zn	0	0
			1	1		

- Molecule 60 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
60	1d	1	Total	Fe	S	0	0
			8	4	4		
60	2d	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 61 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2A	1	Total	K	0	0
			1	1		

- Molecule 62 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	1A	2122	Total	O	0	0
			2122	2122		
62	1B	69	Total	O	0	0
			69	69		
62	1D	24	Total	O	0	0
			24	24		
62	1E	27	Total	O	0	0
			27	27		
62	1F	18	Total	O	0	0
			18	18		
62	1G	7	Total	O	0	0
			7	7		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	1H	2	Total	O	0	0
			2	2		
62	1N	4	Total	O	0	0
			4	4		
62	1O	7	Total	O	0	0
			7	7		
62	1P	20	Total	O	0	0
			20	20		
62	1Q	8	Total	O	0	0
			8	8		
62	1R	10	Total	O	0	0
			10	10		
62	1S	4	Total	O	0	0
			4	4		
62	1T	8	Total	O	0	0
			8	8		
62	1U	10	Total	O	0	0
			10	10		
62	1V	9	Total	O	0	0
			9	9		
62	1W	7	Total	O	0	0
			7	7		
62	1X	7	Total	O	0	0
			7	7		
62	1Y	3	Total	O	0	0
			3	3		
62	1Z	1	Total	O	0	0
			1	1		
62	10	10	Total	O	0	0
			10	10		
62	11	12	Total	O	0	0
			12	12		
62	12	4	Total	O	0	0
			4	4		
62	13	5	Total	O	0	0
			5	5		
62	15	7	Total	O	0	0
			7	7		
62	16	1	Total	O	0	0
			1	1		
62	17	8	Total	O	0	0
			8	8		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	18	10	Total O 10 10	0	0
62	1a	361	Total O 361 361	0	0
62	1b	1	Total O 1 1	0	0
62	1d	1	Total O 1 1	0	0
62	1e	1	Total O 1 1	0	0
62	1g	1	Total O 1 1	0	0
62	1l	4	Total O 4 4	0	0
62	1m	2	Total O 2 2	0	0
62	1q	4	Total O 4 4	0	0
62	1u	1	Total O 1 1	0	0
62	1v	5	Total O 5 5	0	0
62	1w	6	Total O 6 6	0	0
62	1x	16	Total O 16 16	0	0
62	1y	2	Total O 2 2	0	0
62	2A	968	Total O 968 968	0	0
62	2B	15	Total O 15 15	0	0
62	2D	16	Total O 16 16	0	0
62	2E	9	Total O 9 9	0	0
62	2F	9	Total O 9 9	0	0
62	2I	1	Total O 1 1	0	0
62	2N	1	Total O 1 1	0	0

Continued on next page...

Continued from previous page...

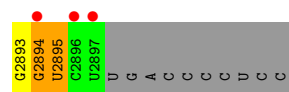
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	2O	2	Total	O	0	0
			2	2		
62	2P	10	Total	O	0	0
			10	10		
62	2Q	1	Total	O	0	0
			1	1		
62	2R	3	Total	O	0	0
			3	3		
62	2T	2	Total	O	0	0
			2	2		
62	2W	1	Total	O	0	0
			1	1		
62	2X	3	Total	O	0	0
			3	3		
62	2Y	1	Total	O	0	0
			1	1		
62	20	2	Total	O	0	0
			2	2		
62	21	3	Total	O	0	0
			3	3		
62	23	2	Total	O	0	0
			2	2		
62	25	2	Total	O	0	0
			2	2		
62	26	1	Total	O	0	0
			1	1		
62	27	2	Total	O	0	0
			2	2		
62	28	6	Total	O	0	0
			6	6		
62	29	1	Total	O	0	0
			1	1		
62	2a	51	Total	O	0	0
			51	51		
62	2d	1	Total	O	0	0
			1	1		
62	2i	1	Total	O	0	0
			1	1		
62	2j	1	Total	O	0	0
			1	1		
62	2l	3	Total	O	0	0
			3	3		

Continued on next page...

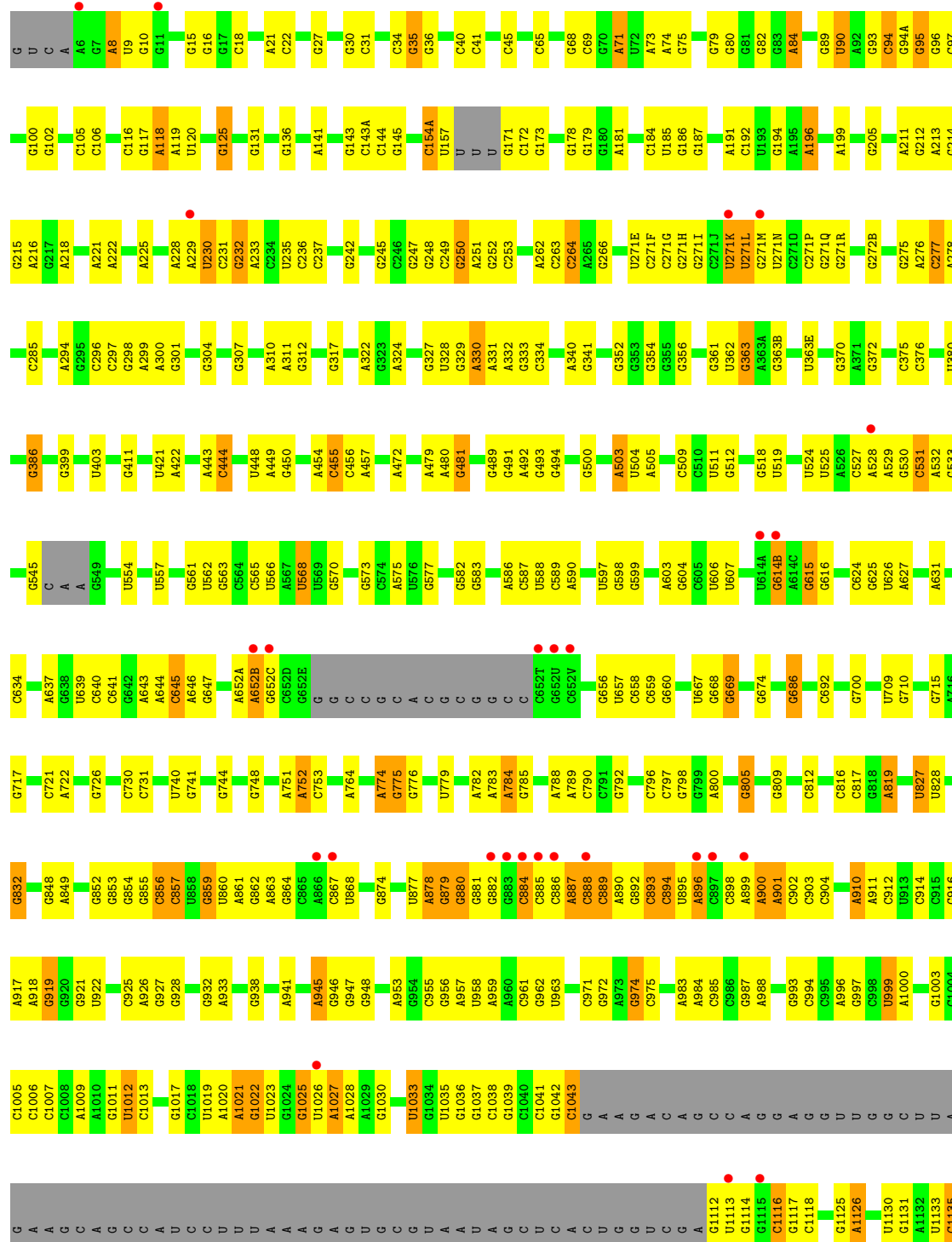
Continued from previous page...

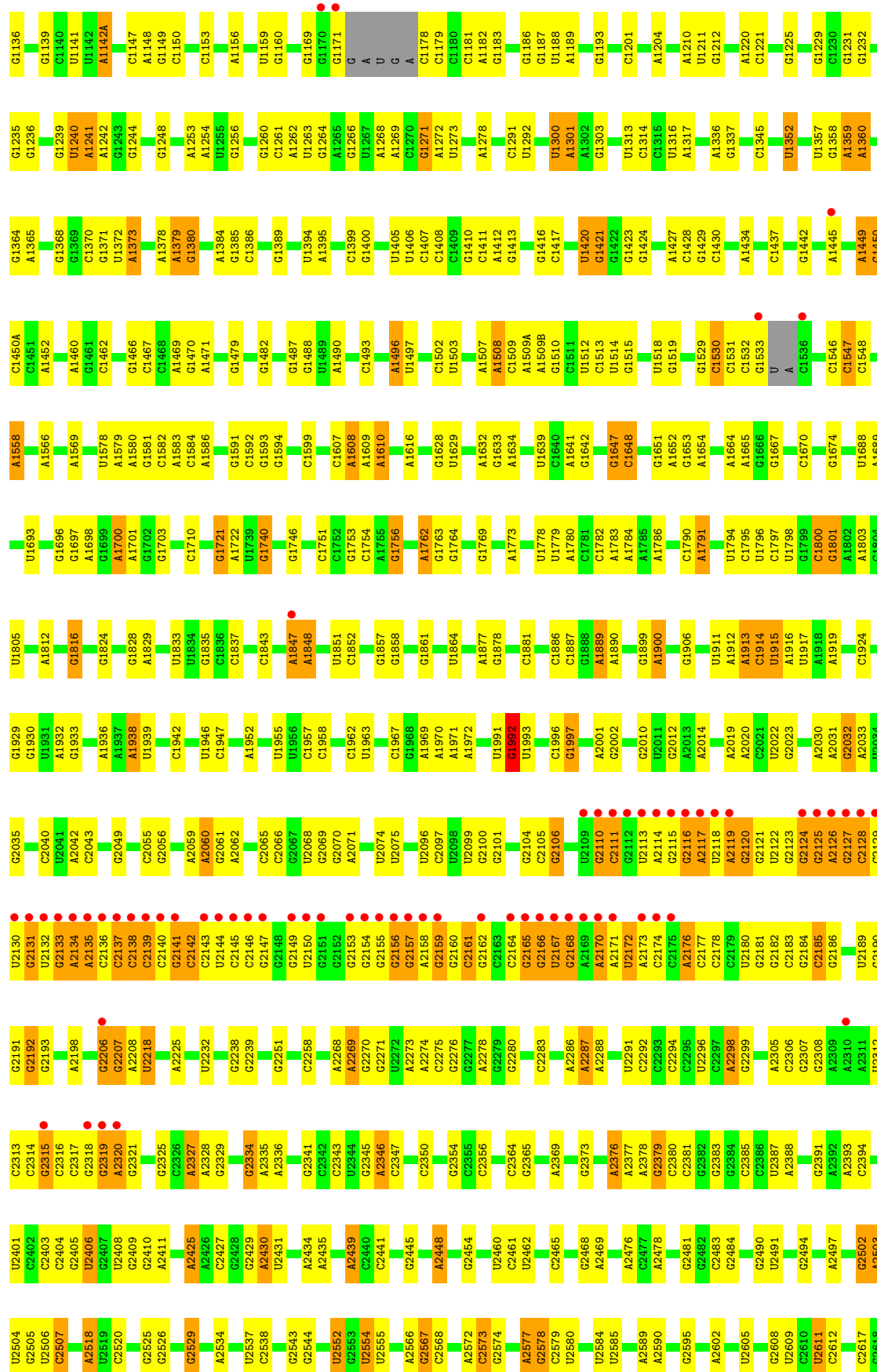
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	2p	1	Total	O	0	0
			1	1		
62	2t	2	Total	O	0	0
			2	2		
62	2x	3	Total	O	0	0
			3	3		
62	2y	8	Total	O	0	0
			8	8		

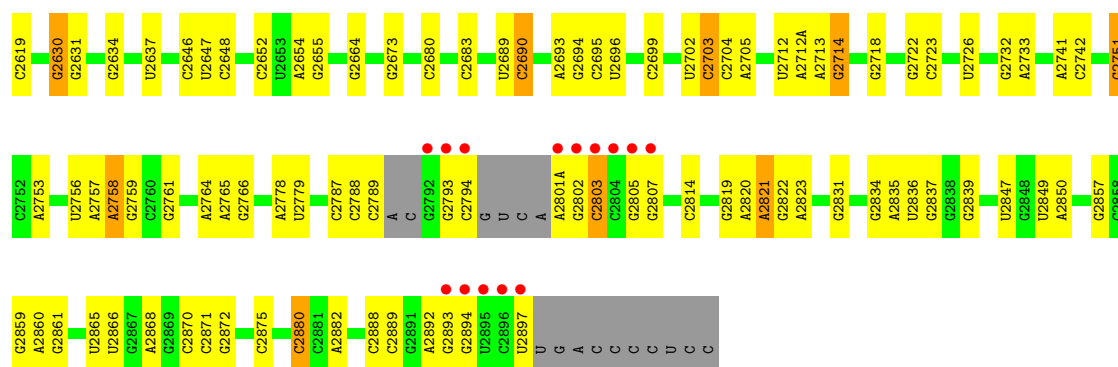
A2778	G2631	A2478	C2359	U2244	G2153	U2086	U1955	A1810	G1674	G1519	C1407	G1286	G1110
U2779	C2646	C2483	A2360	U2245	G2154	G2087	U1956	G1811	G1674	C1532	G1416	G1266	A1111
G2780	C2647	C2483	A2361	G2251	G2155	G2093	C1958	G1814	C1686	G	C1417	G1267	G1112
A2781	C2648	C2499	A2362	G2251	G2156	G2093	C1958	A1815	C1687	U	C1418	U1267	U1113
C2784	C2649	G2502	C2367	C2264	A2157	U2096	C1962	G1816	U1688	C	A1419	C1270	G1114
G2785	C2654	A2503	C2368	C2268	A2159	C2097	U1963	G1823	U1693	G1537	G1421	C1271	G1115
C2787	U2504	G2503	A2377	A2269	G2160	U2098	C1967	G1823	U1693	G1537	G1421	C1271	C1116
G2788	C2661	G2505	A2378	A2269	G2161	U2099	C1967	C1827	A1700	U1540	A1427	G1125	G1125
C2789	A2662	G2506	A2379	U2272	G2162	G2100	A1970	G1828	A1701	C1541	U1273	U1273	A1128
A2790	C2667	A2518	C2380	A2273	G2163	G2101	A1971	G1828	G1702	A1542	C1430	A1278	A1129
C2791	G2668	C2536	C2381	G2277	G2164	U2102	A1972	G1840	G1703	C1543	C1430	U1278	U1130
G2792	C2668	U2528	G2382	G2277	G2166	G2106	U1991	A1847	U1709	C1547	U1431	U1282	U1300
C2793	A2679	G2529	G2383	C2283	U2167	C2107	U1992	A1847	C1710	C1548	C1432	U1292	C1135
G2794	U	G2535	G2384	C2283	G2168	G2108	U1993	U1851	C1710	C1548	C1432	U1292	C1136
U	C2683	G2536	C2385	C2285	A2169	U2109	U1993	U1852	C1712	A1554	G1442	C1297	G1137
C2797	U	G2537	C2386	C2286	A2170	G2110	C1996	G1861	U1713	A1558	A1445	U1300	G1138
C2798	C2687	C2538	A2404	A2287	A2171	C2111	G1997	G1861	G1721	A1566	A1445	U1301	A1142A
A2801A	U2688	C2538	G2405	A2287	U2172	U2112	A2001	C1866	A1722	A1567	G1450	A1301	A1143
G2802	U2689	G2550	U2406	A2288	A2173	U2113	G2002	C1866	A1722	G1568	G1450	G1303	A1156
C2803	C2690	C2551	G2407	G2289	C2174	A2114	G2002	A1876	U1739	C1568	U1453	C1315	G1164
G2804	U2408	U2552	U2408	G2290	C2175	G2115	G2002	A1876	U1739	C1568	U1453	C1315	U1165
C2805	G2409	G2553	G2409	U2291	A2176	G2116	G2012	A1877	G1746	A1569	G1455	C1315	C1166
G2805	C2417	U2554	C2417	C2292	C2177	A2117	A2013	G1878	G1746	A1570	G1455	C1315	G1171
A2810	A2422	A2564	A2422	A2305	G2181	U2118	A2014	A1889	G1750	A1571	G1461	G1332	G1172
G2811	U2423	A2565	U2423	C2306	G2182	G2120	A2014	A1890	G1750	A1571	G1461	G1332	G1173
A2820	C2424	A2566	C2424	C2307	C2183	G2121	A2020	A1890	G1756	A1578	C1467	A1342	G1174
G2821	A2425	G2567	A2425	G2308	C2184	U2122	A2020	G1939	A1762	C1579	C1468	C1345	A1175
U2702	A2426	C2568	A2426	U2312	C2185	G2123	U2022	A1900	G1763	C1581	U1473	U1382	G1176
C2703	C2427	C2568	C2427	C2313	G2186	G2124	A2033	G1906	G1764	C1589	G1473	U1382	G1177
G2710	G2428	C2573	G2428	G2319	U2189	A2126	G2029	U1911	A1773	C1584	A1477	G1356	C1178
A2712A	G2429	G2574	G2429	A2320	C2190	C2127	A2030	A1912	C1774	A1586	A1477	U1357	G1179
G2713	U2430	C2575	A2430	A2320	G2191	G2128	A2031	A1913	C1774	A1587	A1490	G1358	A1188
C2714	U2431	G2578	U2431	G2325	G2192	U2130	A2033	C1914	U1778	C1588	G1365	A1385	G1189
G2723	A2435	A2590	A2435	C2326	G2193	U2131	A2033	U1915	U1779	C1589	A1371	U1372	G1190
C2723	G2436	C2591	G2436	A2327	U2194	U2132	G2038	A1915	A1780	G1594	G1371	U1372	C1201
U2726	A2439	G2592	A2439	A2328	G2195	G2133	C2043	U1917	C1782	G1595	A1490	U1372	G1202
G2727	C2440	A2602	C2440	G2330	G2207	A2134	G2049	A1919	A1783	A1508	C1493	G1371	G1203
C2732	C2441	U2605	C2441	G2331	A2208	C2136	C2050	C1920	A1784	A1509	A1494	U1372	C1201
G2732	G2445	U2606	G2445	G2334	A2208	C2137	C2050	G1929	A1785	A1610	C1498	U1372	G1202
C2733	G2446	G2608	G2446	A2335	G2219	C2138	G2052	U1930	A1786	A1610	C1498	U1372	G1203
G2747	A2447	G2610	A2447	A2336	G2222	C2140	C2055	U1932	A1791	C1640	U1503	A1379	A1220
A2748	C2464	C2611	C2464	G2345	A2225	G2141	C2056	U1933	U1794	C1642	C1505	G1380	C1230
C2749	C2467	G2612	C2467	A2346	U2233	C2142	G2060	G1933	C1795	G1647	C1506	A1384	G1231
C2755	U2468	C2617	U2468	U2347	U2233	U2144	G2061	A1937	U1796	C1647	C1507	A1385	G1231
G2758	A2469	C2617	A2469	G2349	G2234	C2145	A2062	C1938	C1797	C1648	A1508	C1386	A1237
C2758	C2474	C2626	C2474	C2350	G2235	G2147	C2065	U1939	U1798	G1649	A1509	U1396	U1240
A2764	C2475	G2627	C2475	G2354	G2238	G2148	C2066	C1942	G1799	A1664	A1509A	U1396	U1240
C2765	A2476	C2628	A2476	C2355	G2239	U2149	C2066	G1801	G1801	A1668	U1514	C1399	G1243
G2777	C2477	G2630	C2477	C2355	U2243	U2150	G2069	A1952	A1802	A1668	G1515	U1405	G1252
A2892	C2477	C2630	C2477	C2355	U2243	G2152	G2069	A1953	A1803	C1670	U1518	U1406	A1253



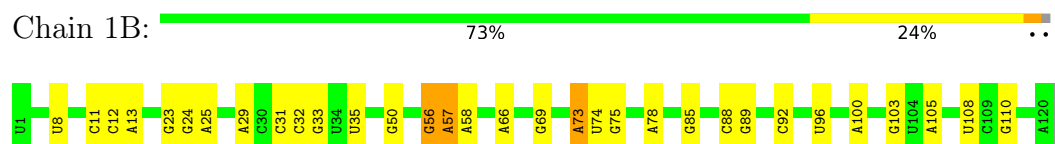
• Molecule 1: 23S Ribosomal RNA



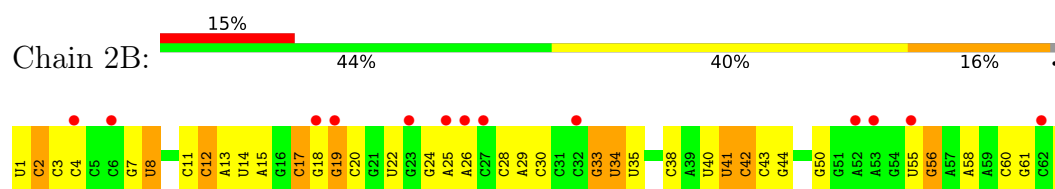




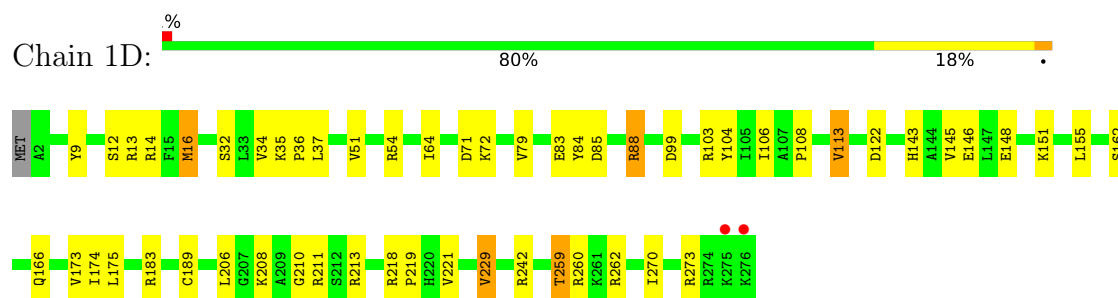
• Molecule 2: 5S Ribosomal RNA



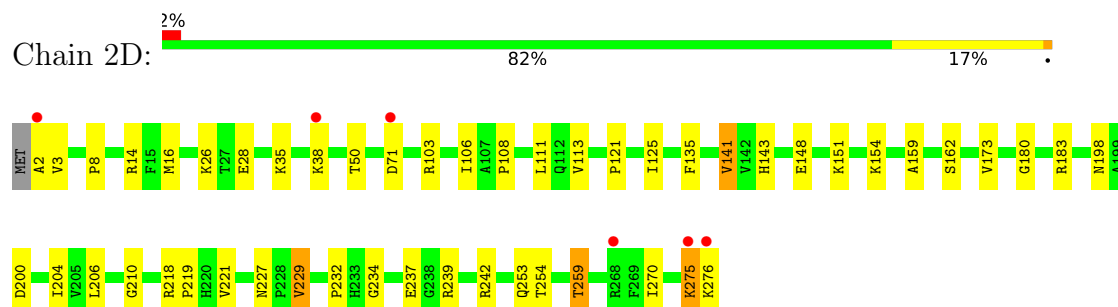
• Molecule 2: 5S Ribosomal RNA



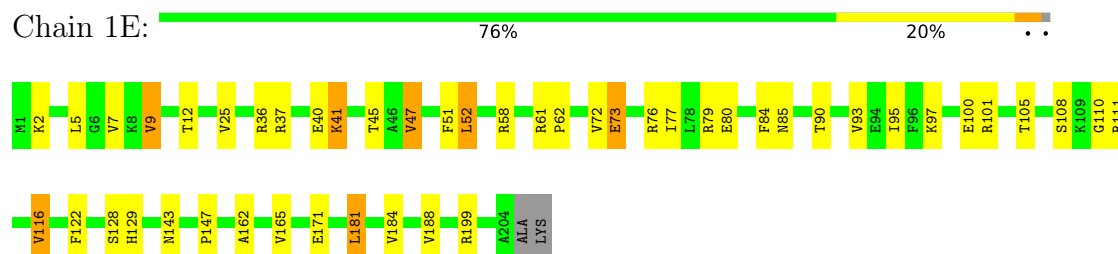
• Molecule 3: 50S ribosomal protein L2



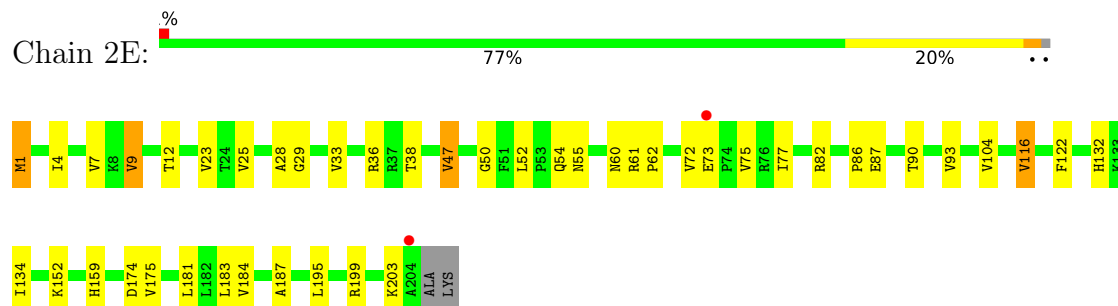
• Molecule 3: 50S ribosomal protein L2



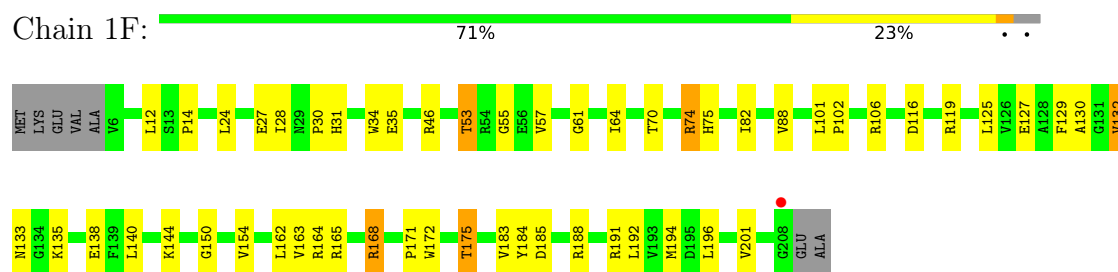
- Molecule 4: 50S ribosomal protein L3



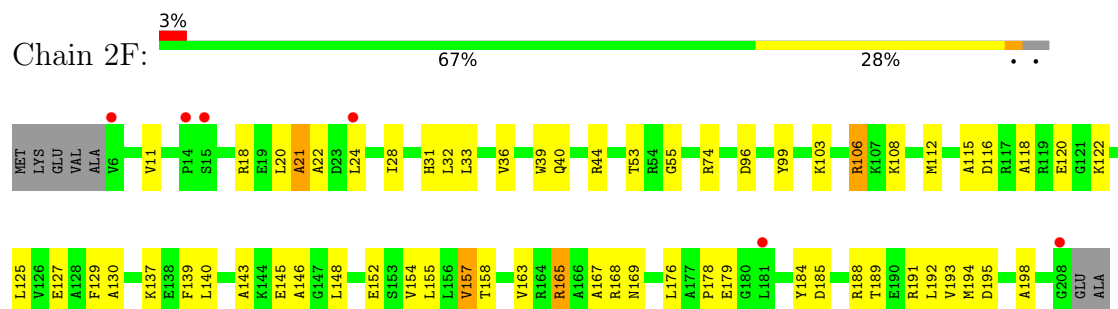
- Molecule 4: 50S ribosomal protein L3



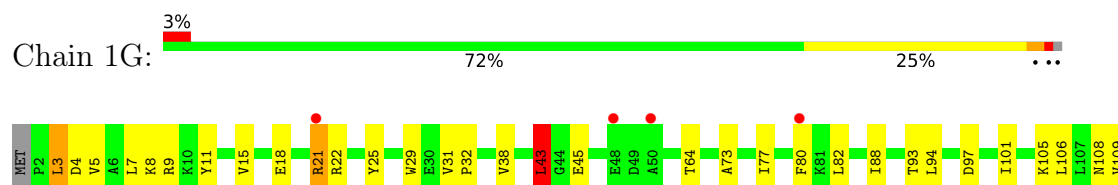
- Molecule 5: 50S ribosomal protein L4

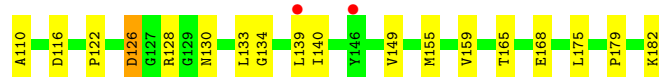


- Molecule 5: 50S ribosomal protein L4

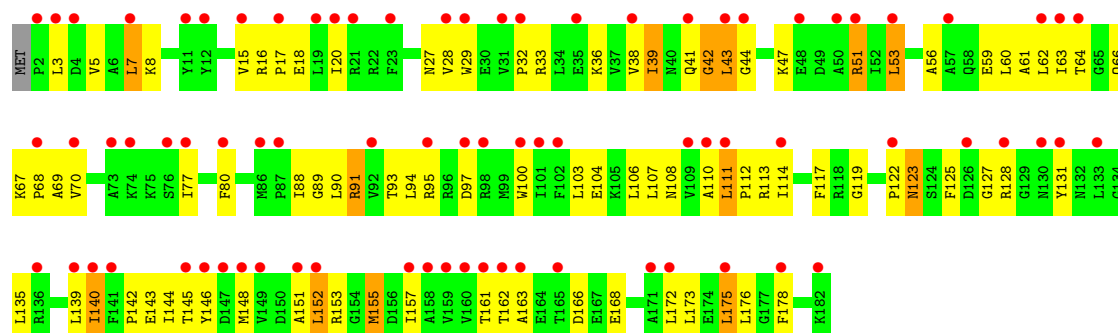
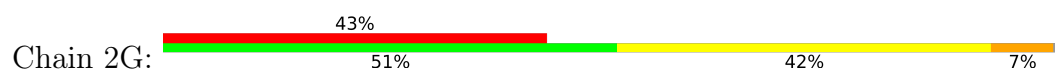


- Molecule 6: 50S ribosomal protein L5

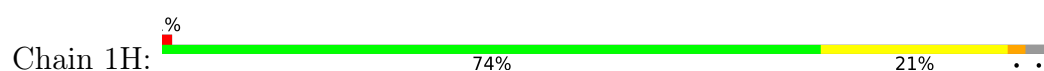




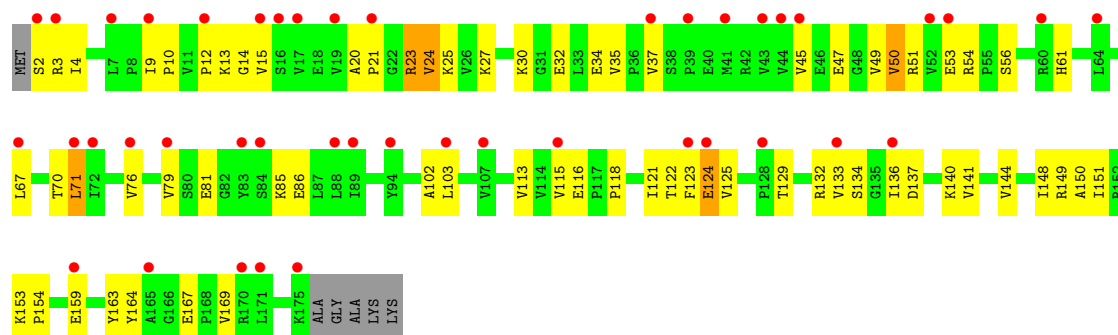
• Molecule 6: 50S ribosomal protein L5



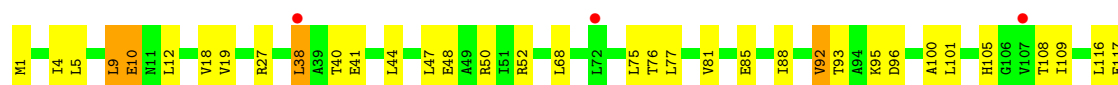
• Molecule 7: 50S ribosomal protein L6



• Molecule 7: 50S ribosomal protein L6

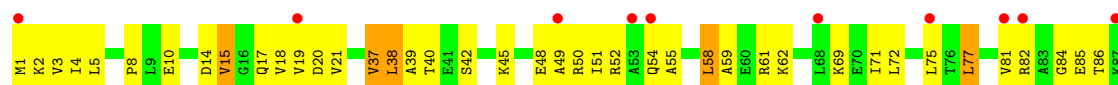


• Molecule 8: 50S ribosomal protein L9

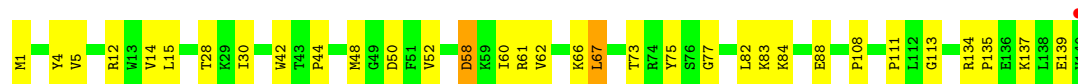
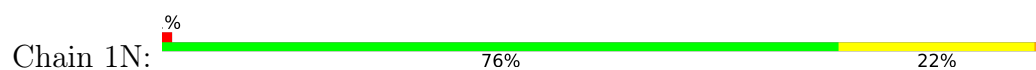




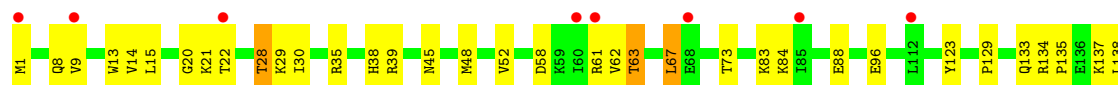
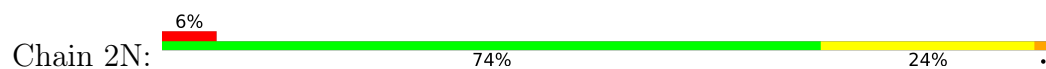
• Molecule 8: 50S ribosomal protein L9



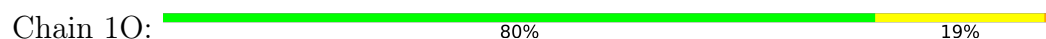
• Molecule 9: 50S ribosomal protein L13



• Molecule 9: 50S ribosomal protein L13



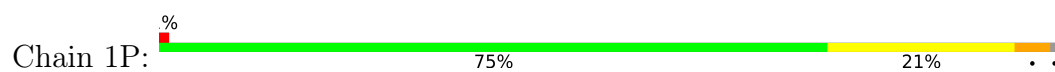
• Molecule 10: 50S ribosomal protein L14



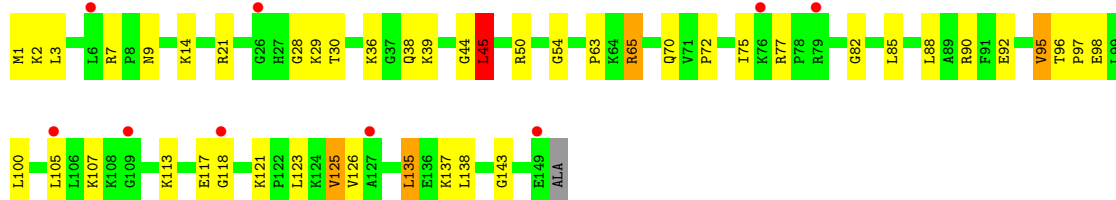
• Molecule 10: 50S ribosomal protein L14



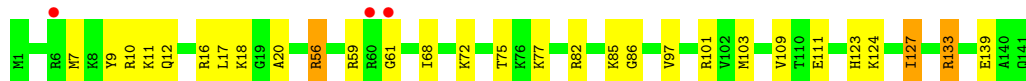
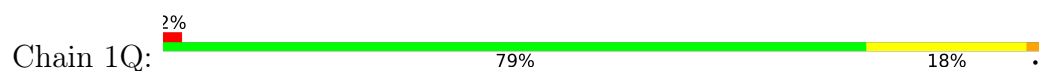
• Molecule 11: 50S ribosomal protein L15



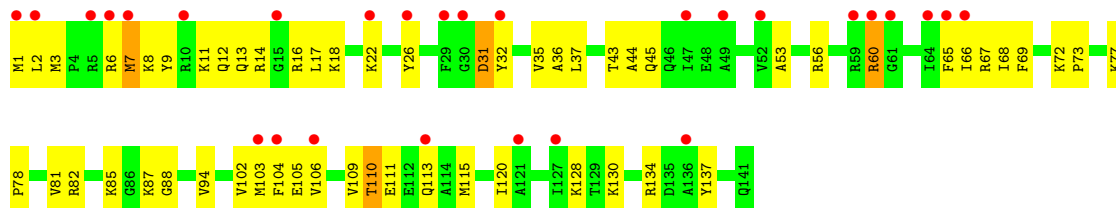
- Molecule 11: 50S ribosomal protein L15



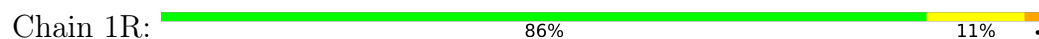
- Molecule 12: 50S ribosomal protein L16



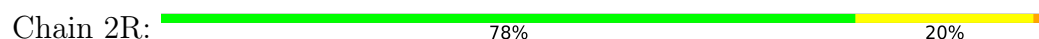
- Molecule 12: 50S ribosomal protein L16



- Molecule 13: 50S ribosomal protein L17



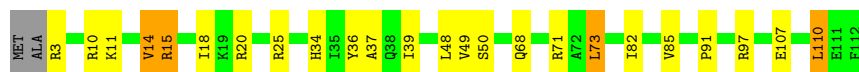
- Molecule 13: 50S ribosomal protein L17





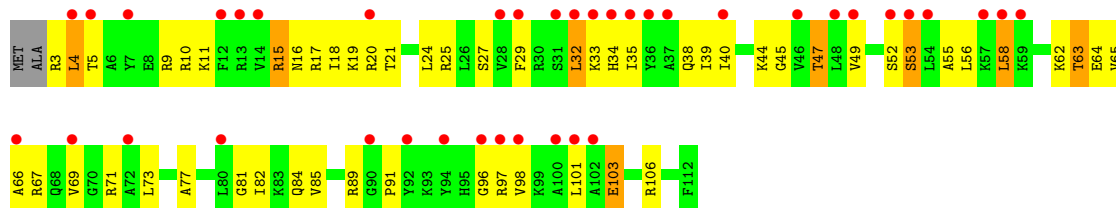
- Molecule 14: 50S ribosomal protein L18

Chain 1S: 77% 18% . .



- Molecule 14: 50S ribosomal protein L18

Chain 2S: 35% 49% 42% 7% .



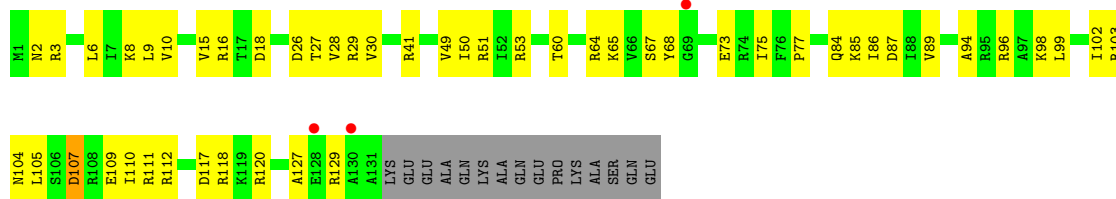
- Molecule 15: 50S ribosomal protein L19

Chain 1T: 2% 74% 16% 10%



- Molecule 15: 50S ribosomal protein L19

Chain 2T: 2% 55% 34% 10%



- Molecule 16: 50S ribosomal protein L20

Chain 1U: 79% 17% . .

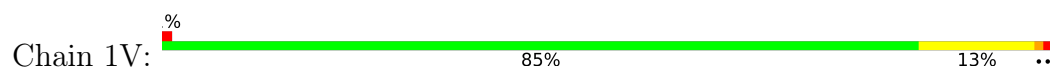


- Molecule 16: 50S ribosomal protein L20

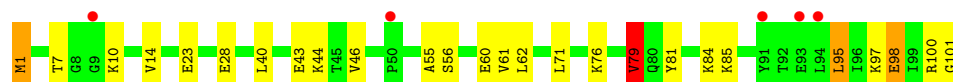
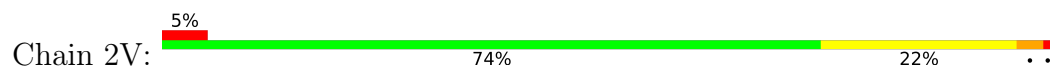
Chain 2U: 75% 23% .



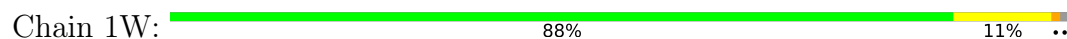
- Molecule 17: 50S ribosomal protein L21



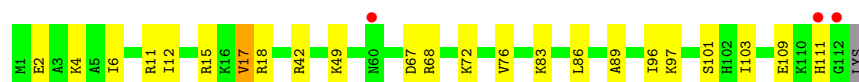
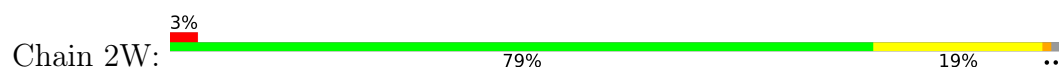
- Molecule 17: 50S ribosomal protein L21



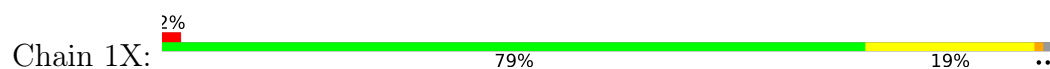
- Molecule 18: 50S ribosomal protein L22



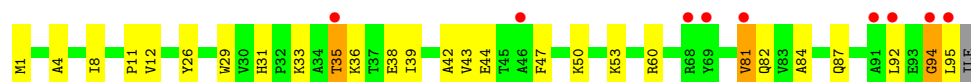
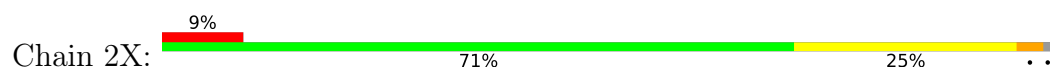
- Molecule 18: 50S ribosomal protein L22



- Molecule 19: 50S ribosomal protein L23



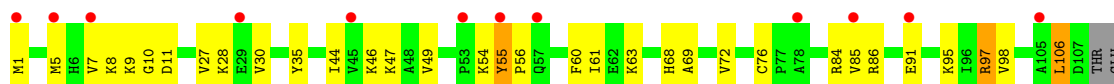
- Molecule 19: 50S ribosomal protein L23



- Molecule 20: 50S ribosomal protein L24

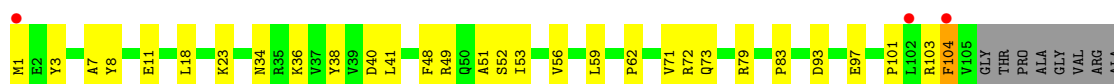


• Molecule 20: 50S ribosomal protein L24



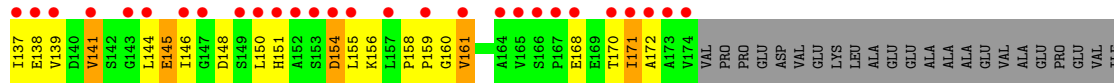
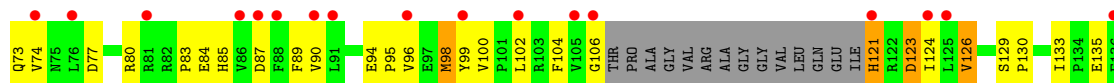
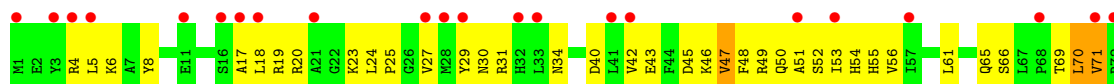
GLU

• Molecule 21: 50S ribosomal protein L25



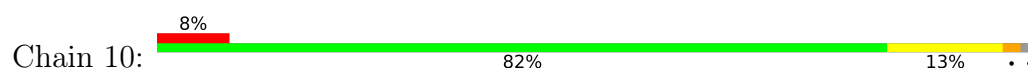
LEU, ALA, GLU, ALA, ALA, GLU, VAL, PRO, GLU, VAL, ILE, LYS, LYS, GLU, GLU, GLU, GLU

• Molecule 21: 50S ribosomal protein L25



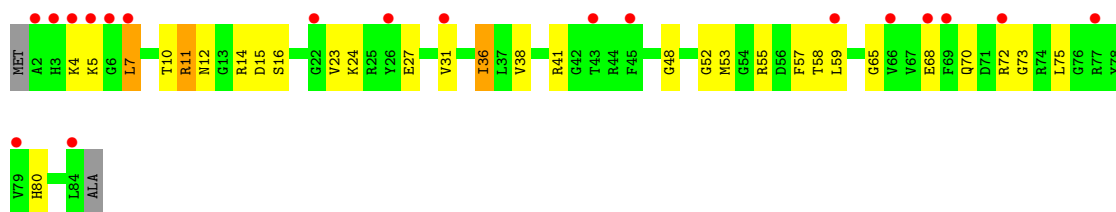
LYS, LYS, GLY, LYS, GLU, GLU, GLU, GLU

• Molecule 22: 50S ribosomal protein L27

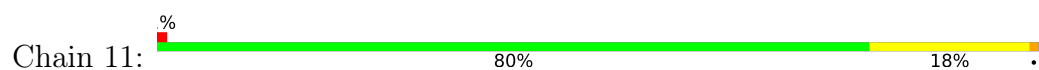




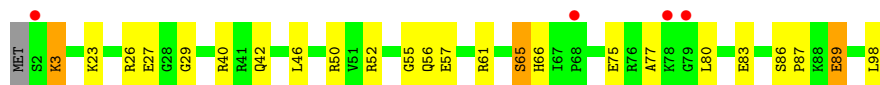
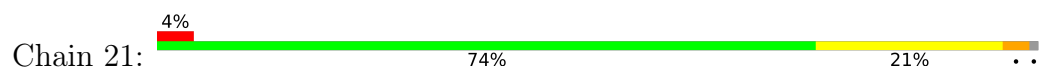
- Molecule 22: 50S ribosomal protein L27



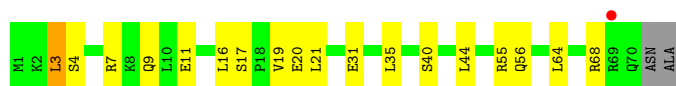
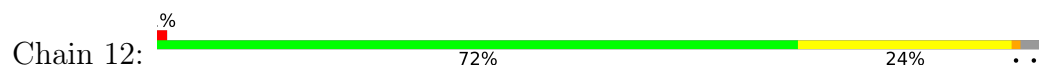
- Molecule 23: 50S ribosomal protein L28



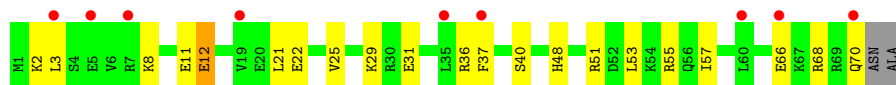
- Molecule 23: 50S ribosomal protein L28



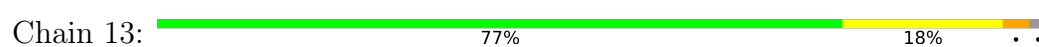
- Molecule 24: 50S ribosomal protein L29



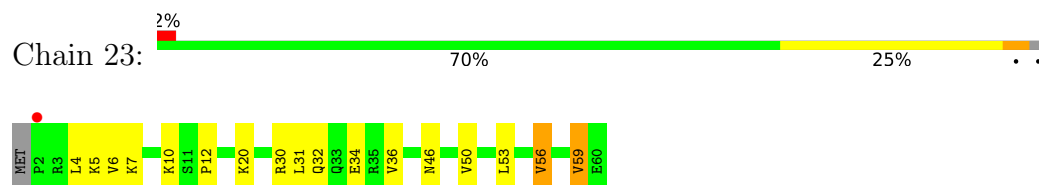
- Molecule 24: 50S ribosomal protein L29



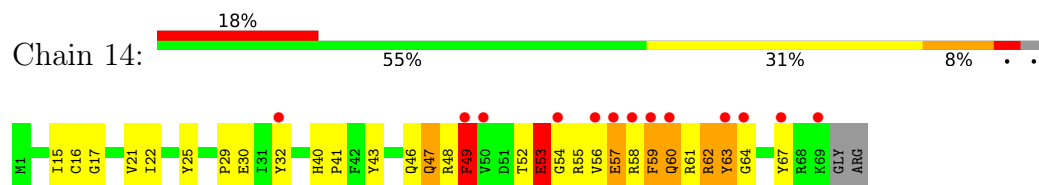
- Molecule 25: 50S ribosomal protein L30



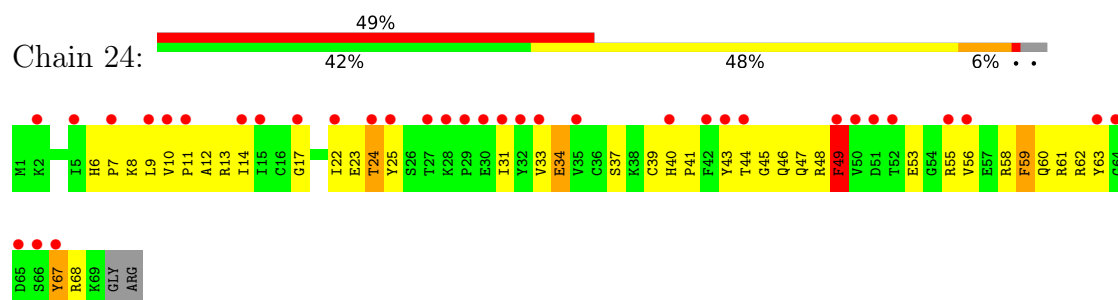
- Molecule 25: 50S ribosomal protein L30



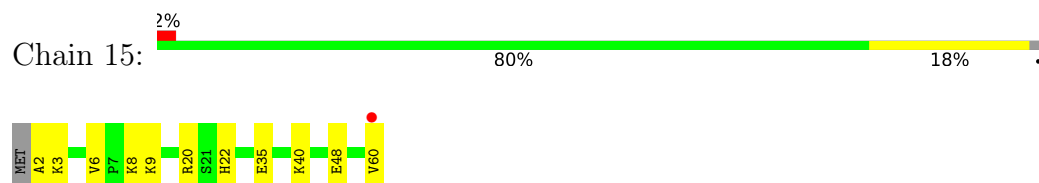
- Molecule 26: 50S ribosomal protein L31



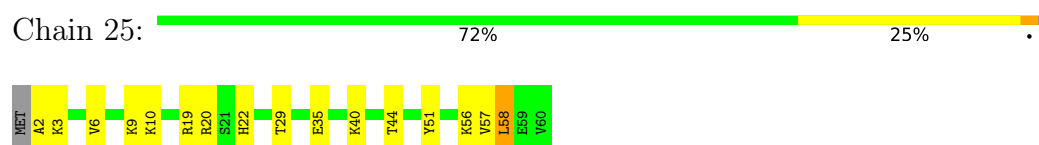
- Molecule 26: 50S ribosomal protein L31



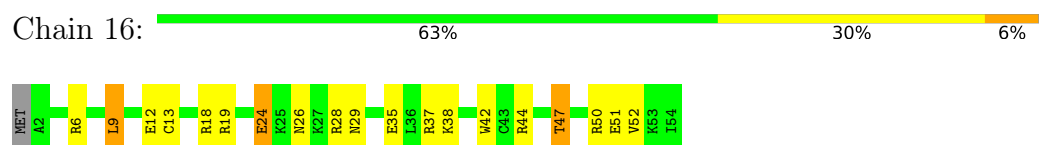
- Molecule 27: 50S ribosomal protein L32



- Molecule 27: 50S ribosomal protein L32

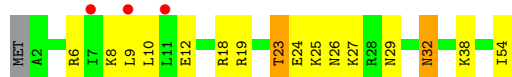


- Molecule 28: 50S ribosomal protein L33

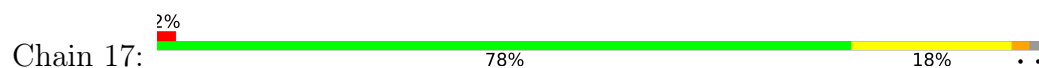


- Molecule 28: 50S ribosomal protein L33

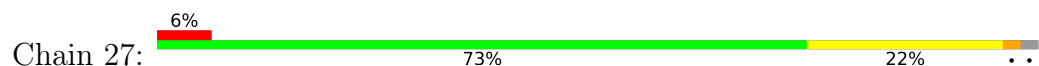




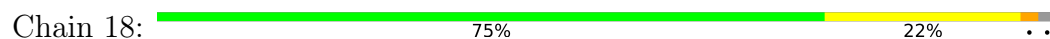
- Molecule 29: 50S ribosomal protein L34



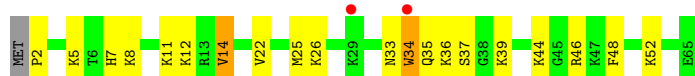
- Molecule 29: 50S ribosomal protein L34



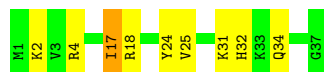
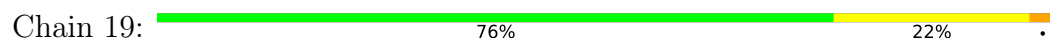
- Molecule 30: 50S ribosomal protein L35



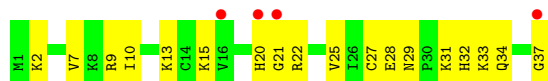
- Molecule 30: 50S ribosomal protein L35



- Molecule 31: 50S ribosomal protein L36



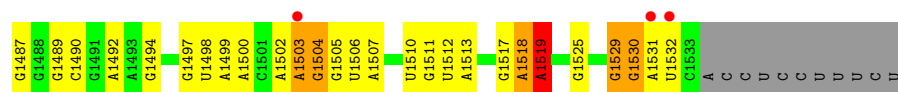
- Molecule 31: 50S ribosomal protein L36



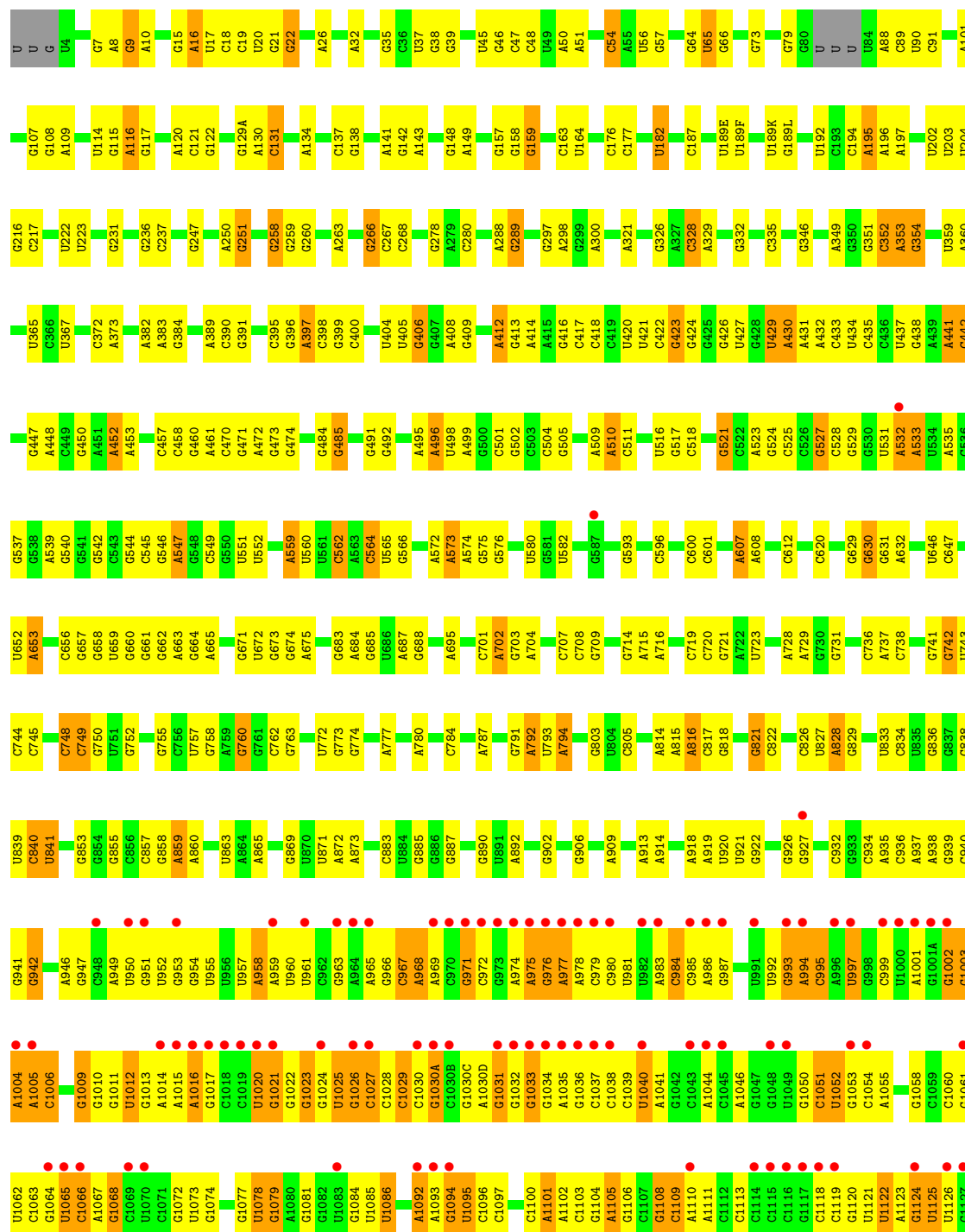
- Molecule 32: 16S Ribosomal RNA

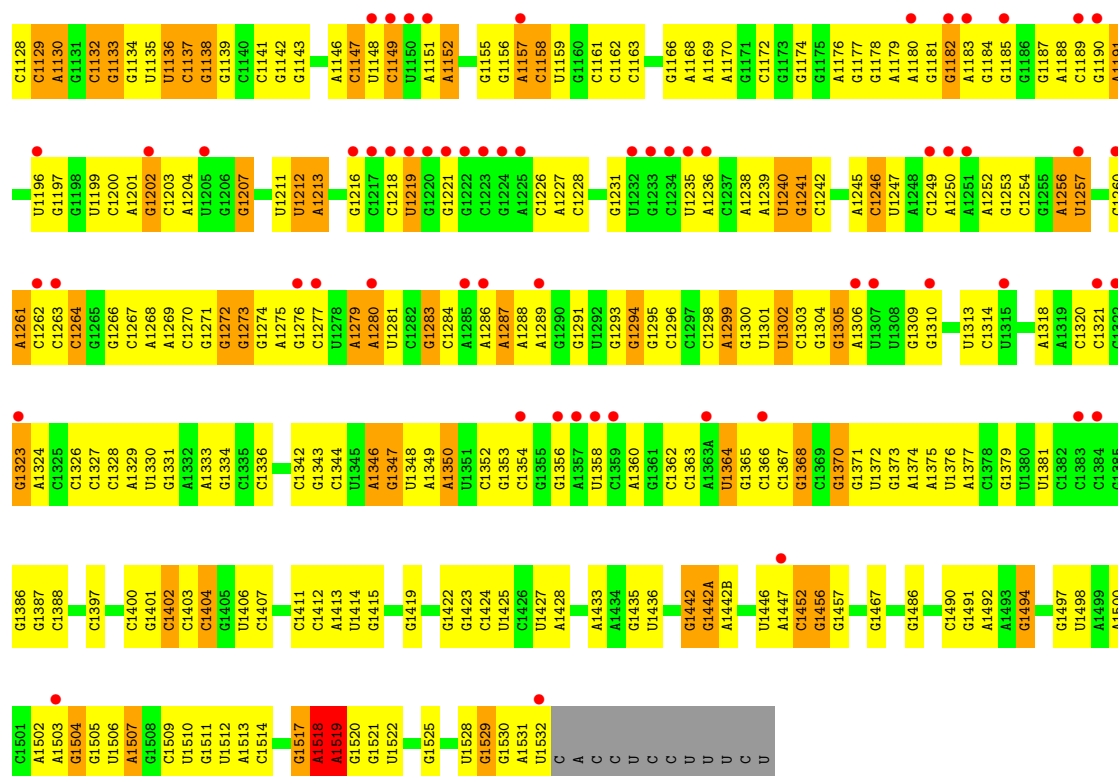


G1356	C1264	C1145	C1038	C972	G627	G505	G399	G289	A185	U
A1357	G1265	A1146	C1039	G973	G628	G506	C400	G289	C186	U
U1358	G1266	C1147	U1040	A974	G629	A509	U404	U294	C187	G
A1359	C1270	U1148	A1044	A975	G630	A510	U405	U295	C188	U4
A1360	C1271	A1152	C1045	A977	G631	C511	G406	U296	G189	
C1363	G1273	C1158	G1053	U981	U636	U516	G410	G297	C189D	G7
A1363A	G1274	U1159	G1053	U982	G637	G517	A411	A298	U189E	A8
G1370	A1275	G1160	C1060	A983	A642	C518	A412	G299	G98	G9
G1371	C1277	A1168	G1061	A986	U646	G524	G413	A300	U189J	A10
U1372	U1278	A1169	U1062	G987	C647	G527	A414	A300	U189K	G11
G1373	A1279	A1176	C1063	A987	A648	A531	C418	C311	G189L	U17
A1374	A1280	A1176	G1068	U992	G649	A532	C419	G316	U190	C18
C1378	C1284	A1179	U1073	U993	A653	A533	C422	G317	G191	C19
U1381	A1285	A1180	G1074	A994	G662	A536	G423	G318	U192	U20
A1381	A1286	A1180	C995	A996	A663	A539	G424	G318	G193	G22
A1287	A1287	A1183	C1075	U997	G664	G540	A431	G324	C194	
A1288	A1288	A1184	C1076	U998	G665	G542	A432	A325	A195	A26
A1289	G1290	C1189	G1077	U999	G667	G547	U429	A327	A197	
G1291	G1291	C1189	U1078	U1000	G673	A559	A430	G328	G198	A32
U1292	U1292	C1194	G1079	U1001	G674	G541	A431	A329	G199	C36
A1299	A1299	C1195	A1080	G1001A	A676	G542	A432	G332	G200	U37
G1300	G1300	C1196	G1081	G1002	A677	A547	U434	U203	C201	U18
U1301	C1301	U1196	U1086	G1003	U677	A559	C435	U204	U202	G38
C1402	U1302	G1197	G1094	G1004	A684	A561	G438	C339	C219	G42
C1403	C1303	C1200	C1095	C1005	G685	A564	A441	U340	G122	C43
C1404	G1304	A1201	U1095	C1006	U686	C564	A442	C341	G123	C44
C1407	G1305	G1202	C1099	C1007	A687	A572	C442	C342	G124	U45
G1410	G1312	G1206	C1100	A1015	U688	A573	G445	C343	A130	C46
C1411	U1313	G1207	A1101	A1016	C689	A576	G446	C344	C131	C47
C1412	C1314	G1207	A1102	G1017	G690	G577	G447	C347	A134	C48
C1413	C1314	G1214	G1106	G1018	G691	G577	G448	G351	G145	A51
U1414	C1320	C1223	C1107	C1019	G692	A577	A452	C352	G146	G52
G1419	C1321	G1224	G1108	U1020	A695	G577	A453	C353	G147	U56
G1422	C1327	A1227	C1112	G1021	G711	G577	C456	C354	G148	G57
U1427	C1328	A1236	C1118	G1022	G712	U582	C457	U367	A159	C58
A1428	A1329	C1237	U1121	G1023	G713	A583	A461	C372	A160	G61
G1435	U1330	A1238	U1122	U952	G714	G584	C470	A373	A161	G66
U1436	G1331	A1239	A1123	G954	A715	G585	G471	U375	A162	C67
G1442	A1338	U1240	G1124	A958	A716	C596	A472	G376	C163	G68
G1442A	A1340	A1250	U1125	U960	G721	G597	G473	G377	C165	G69
U1446	G1343	G1255	C1129	U961	U722	U598	G474	A382	G166	G70
A1447	C1344	U1257	G1134	C962	U723	C599	G475	A383	G167	G73
C1452	A1345	G1258	U1135	G963	G724	G610	G485	G384	C265	C76
G1456	G1346	C1259	U1136	A964	A728	G613	A496	C390	C267	G79
G1457	G1347	C1260	G1137	A965	G730	A614	U498	G391	A270	G
G1458	C1352	A1261	G1138	A966	G731	G615	G502	C396	C271	U
G1466	G1353	C1262	G1139	A969	C735	G617	C503	A397	C272	U
			G1144	C970	C736		C504	C398	U182	U
				C1037					G183	U
									G184	A

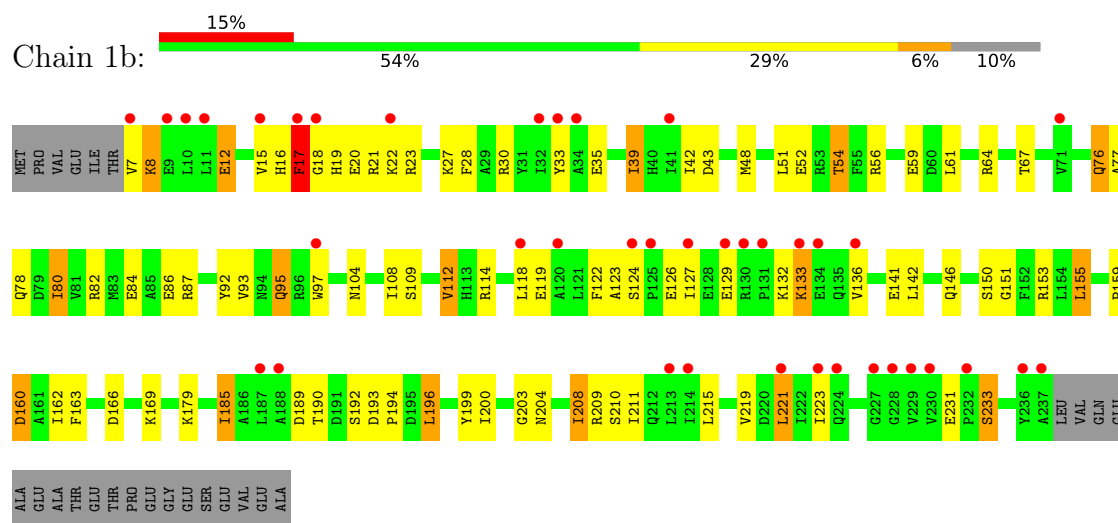


• Molecule 32: 16S Ribosomal RNA

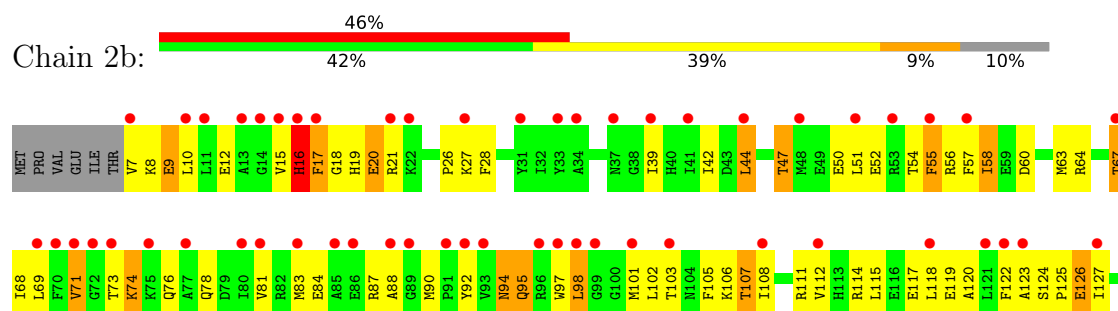


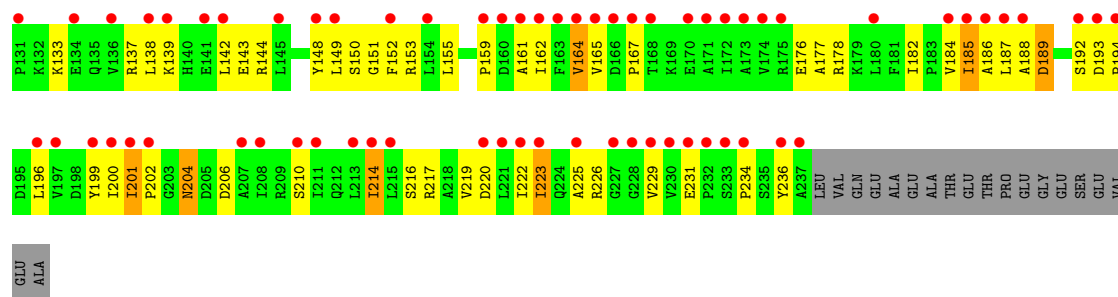


• Molecule 33: 30S ribosomal protein S2

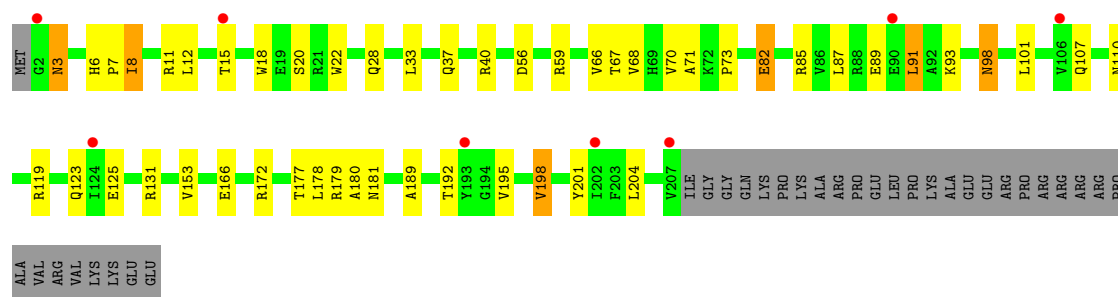


• Molecule 33: 30S ribosomal protein S2

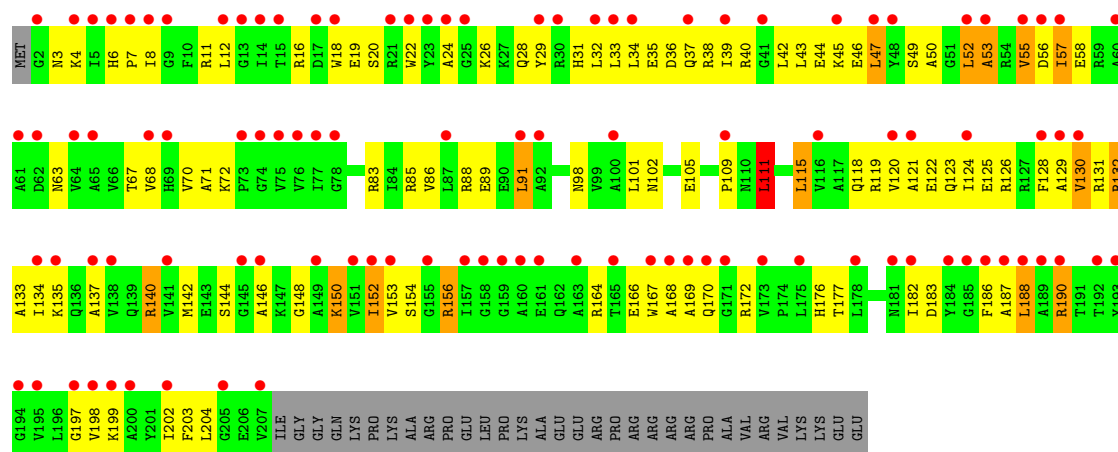




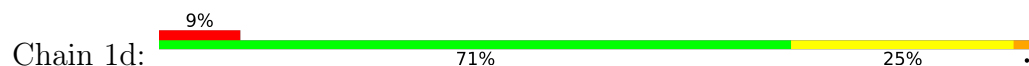
- Molecule 34: 30S ribosomal protein S3



- Molecule 34: 30S ribosomal protein S3

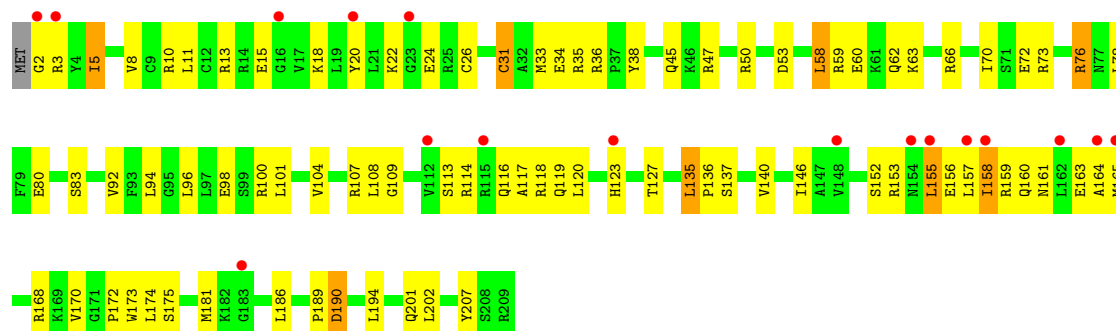


- Molecule 35: 30S ribosomal protein S4

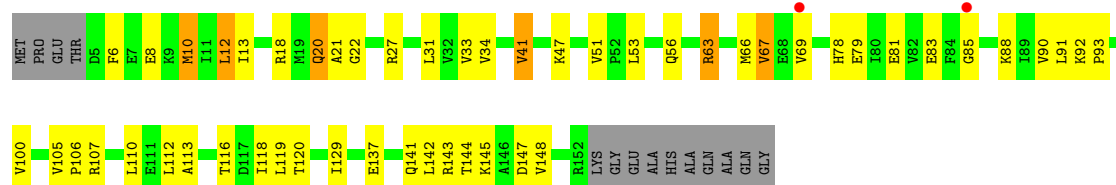




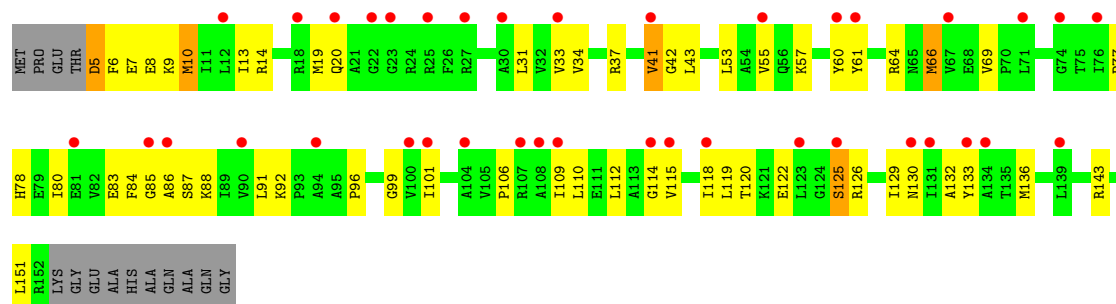
- Molecule 35: 30S ribosomal protein S4



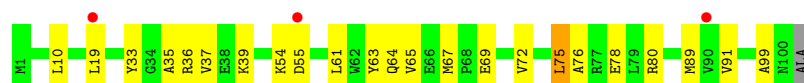
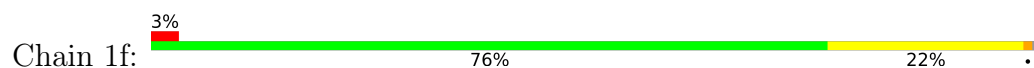
- Molecule 36: 30S ribosomal protein S5



- Molecule 36: 30S ribosomal protein S5



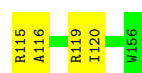
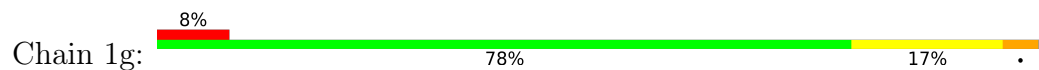
- Molecule 37: 30S ribosomal protein S6



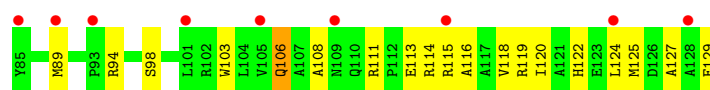
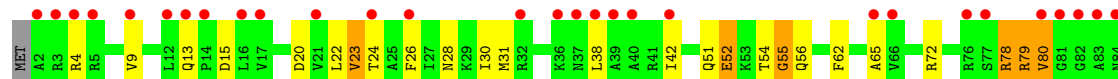
- Molecule 37: 30S ribosomal protein S6



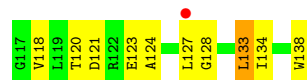
- Molecule 38: 30S ribosomal protein S7



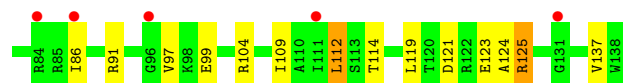
- Molecule 38: 30S ribosomal protein S7



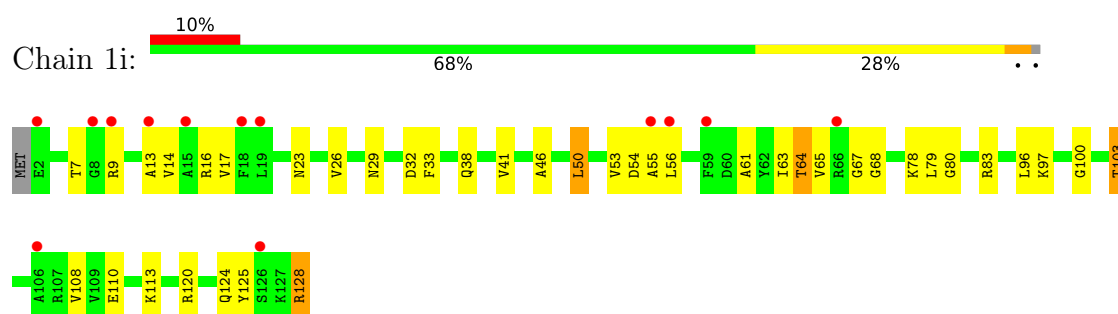
- Molecule 39: 30S ribosomal protein S8



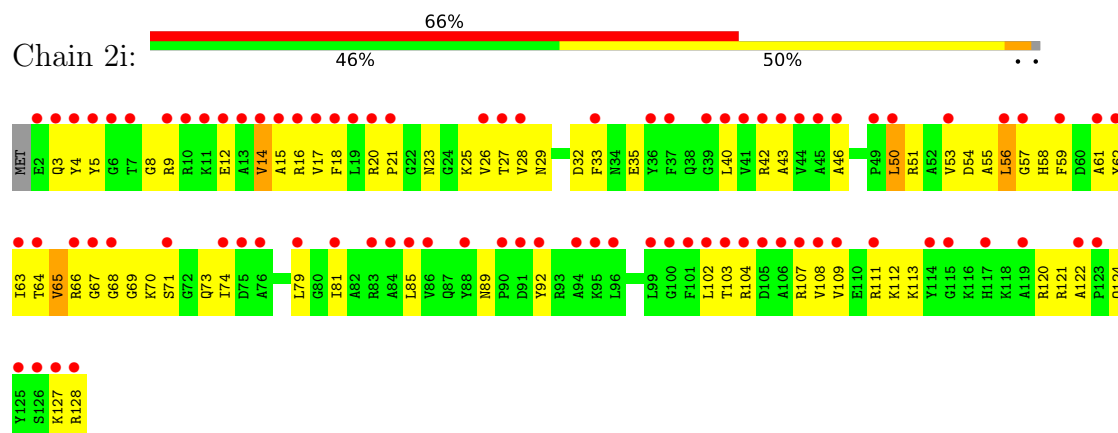
- Molecule 39: 30S ribosomal protein S8



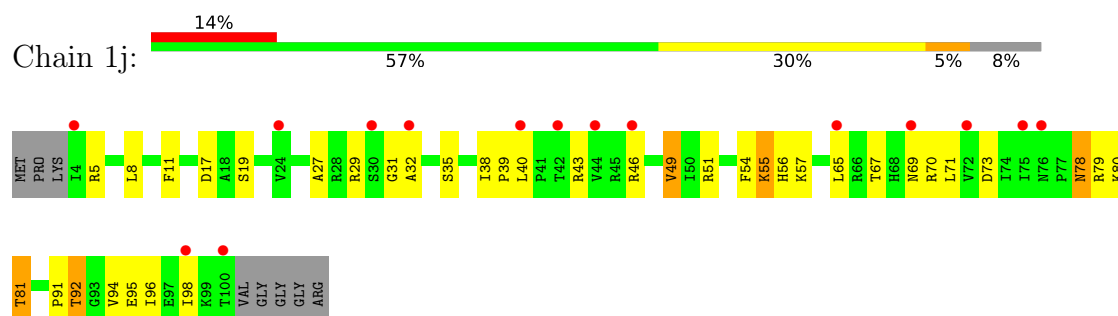
- Molecule 40: 30S ribosomal protein S9



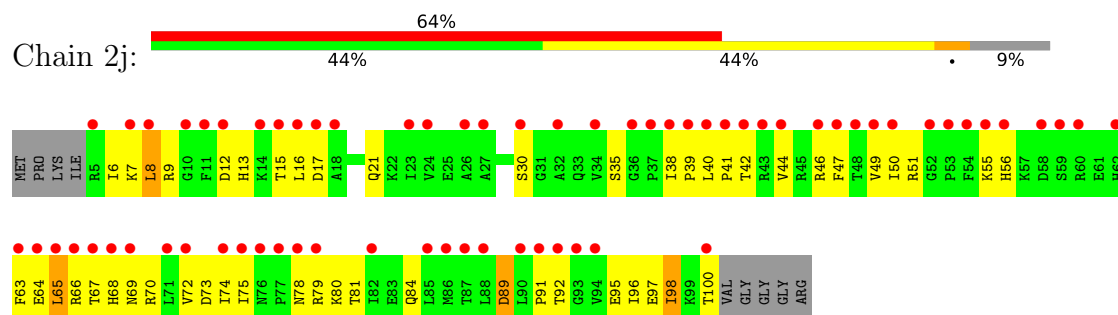
- Molecule 40: 30S ribosomal protein S9



- Molecule 41: 30S ribosomal protein S10

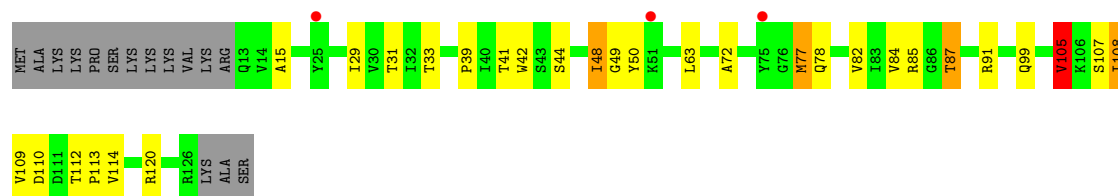


- Molecule 41: 30S ribosomal protein S10

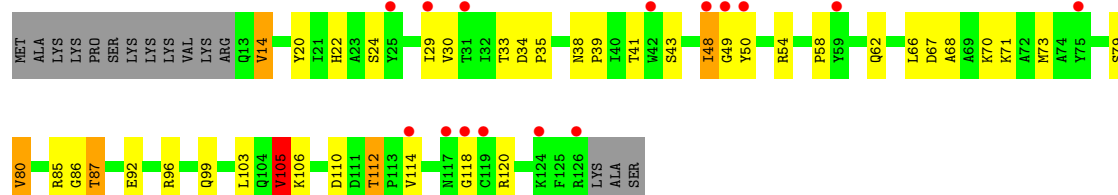


- Molecule 42: 30S ribosomal protein S11

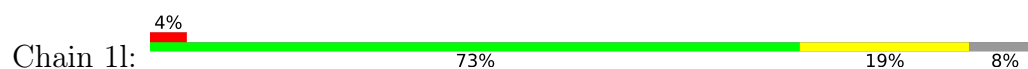




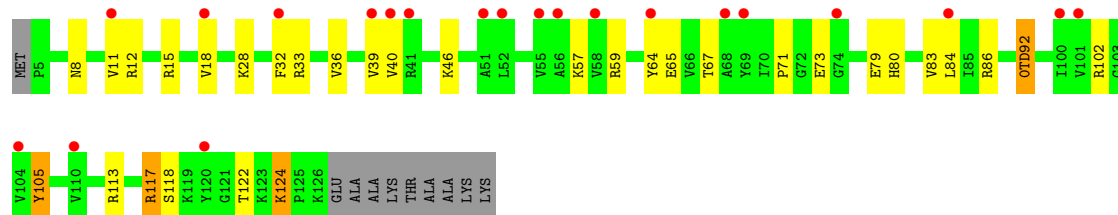
- Molecule 42: 30S ribosomal protein S11



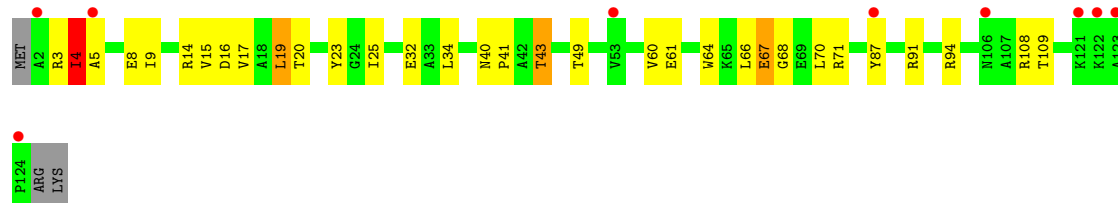
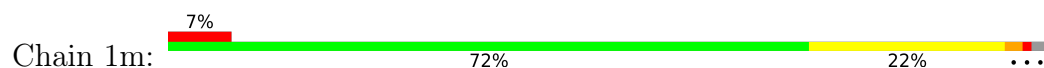
- Molecule 43: 30S ribosomal protein S12



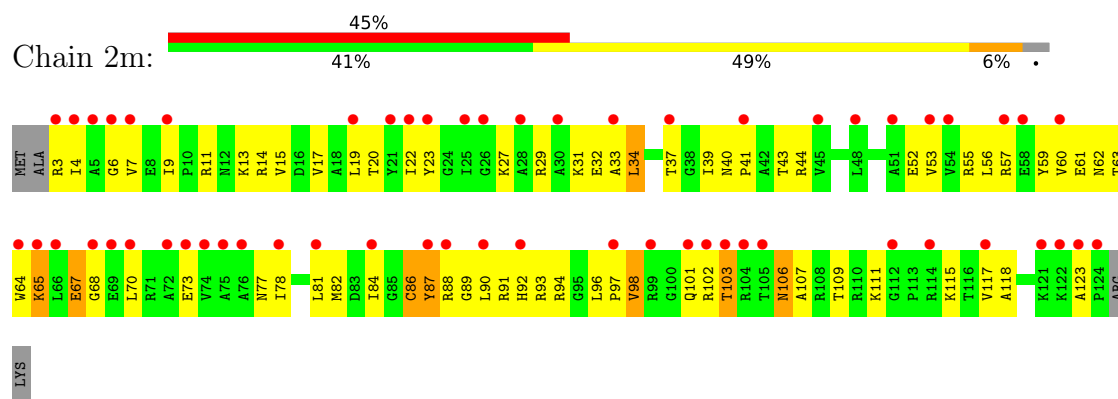
- Molecule 43: 30S ribosomal protein S12



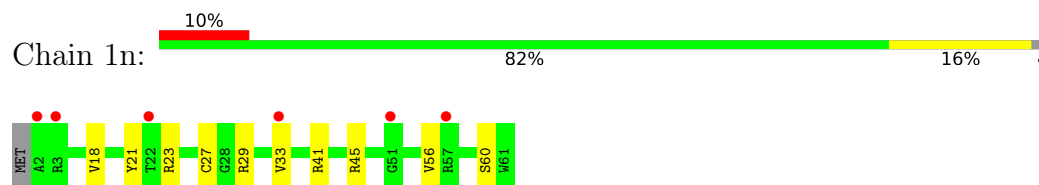
- Molecule 44: 30S ribosomal protein S13



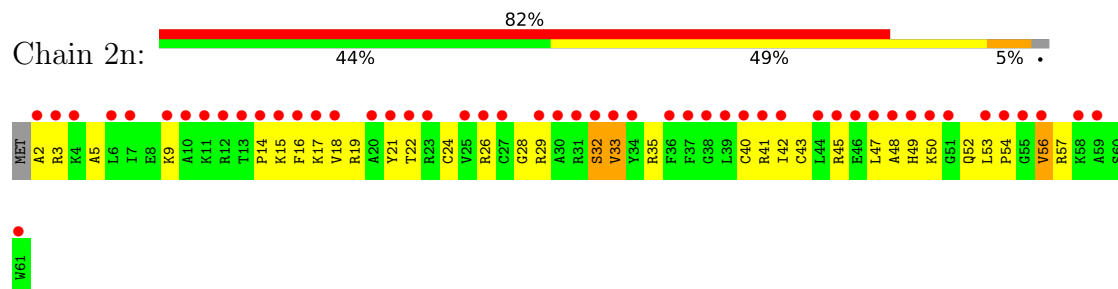
- Molecule 44: 30S ribosomal protein S13



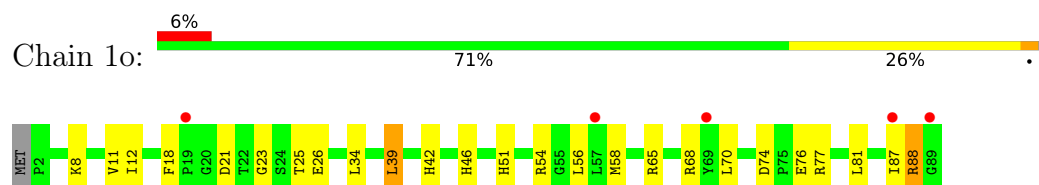
- Molecule 45: 30S ribosomal protein S14 type Z



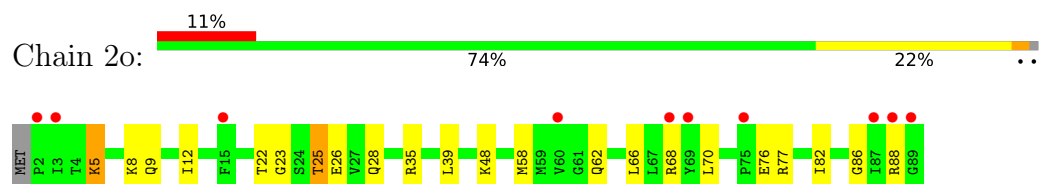
- Molecule 45: 30S ribosomal protein S14 type Z



- Molecule 46: 30S ribosomal protein S15

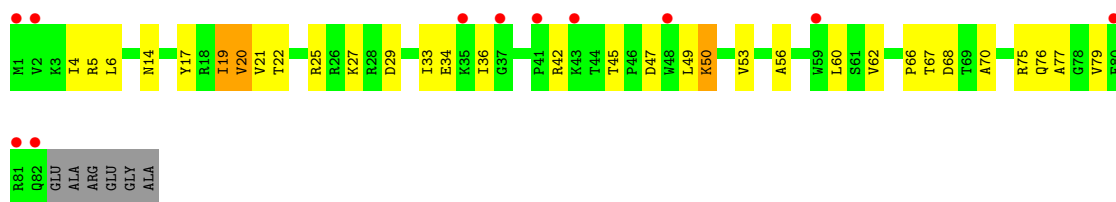


- Molecule 46: 30S ribosomal protein S15

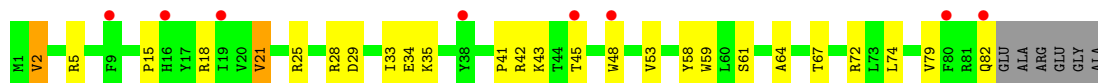


- Molecule 47: 30S ribosomal protein S16





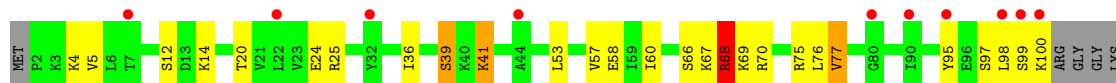
- Molecule 47: 30S ribosomal protein S16



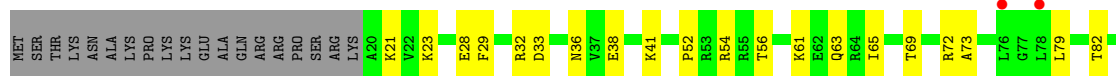
- Molecule 48: 30S ribosomal protein S17



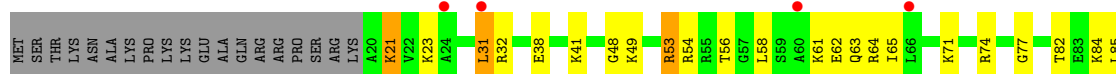
- Molecule 48: 30S ribosomal protein S17



- Molecule 49: 30S ribosomal protein S18

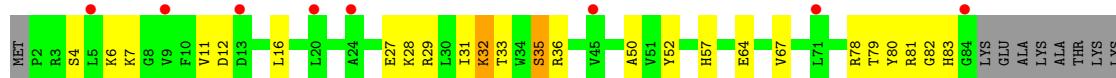


- Molecule 49: 30S ribosomal protein S18

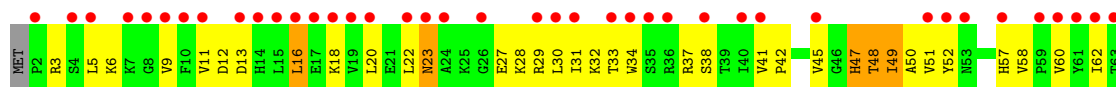




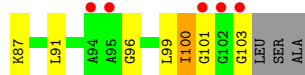
- Molecule 50: 30S ribosomal protein S19



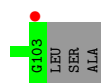
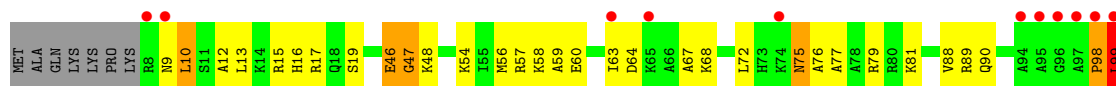
- Molecule 50: 30S ribosomal protein S19



- Molecule 51: 30S ribosomal protein S20



- Molecule 51: 30S ribosomal protein S20

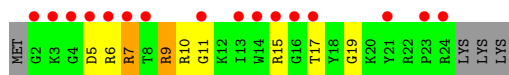


- Molecule 52: 30S ribosomal protein Thx





- Molecule 52: 30S ribosomal protein Thx



- Molecule 53: mRNA



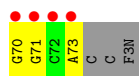
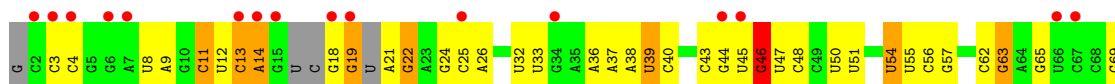
- Molecule 53: mRNA



- Molecule 54: A-site tRNA



- Molecule 54: A-site tRNA



- Molecule 55: P-site tRNA





• Molecule 55: P-site tRNA



• Molecule 56: E-site tRNA



• Molecule 56: E-site tRNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.86Å 449.80Å 621.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	198.84 – 2.50 198.84 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (198.84-2.50) 99.8 (198.84-2.50)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 2.52Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.224 , 0.268 0.226 , 0.270	Depositor DCC
R_{free} test set	100061 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	51.2	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 63.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	299504	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% 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: 7MG, 31H, OMC, 4OC, 6IF, K, MG, OMU, 4SU, M2G, 5MC, UR3, 0TD, ZN, SF4, 2MA, MIA, MA6, 2MG, 5MU, OMG, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1A	0.28	0/69011	0.48	1/107720 (0.0%)
1	2A	0.21	1/67295 (0.0%)	0.40	2/105042 (0.0%)
2	1B	0.22	0/2882	0.42	0/4494
2	2B	0.21	0/2879	0.39	0/4487
3	1D	0.27	0/2186	0.52	0/2944
3	2D	0.22	0/2186	0.45	0/2944
4	1E	0.27	0/1592	0.49	0/2149
4	2E	0.23	0/1592	0.45	0/2149
5	1F	0.26	0/1619	0.47	0/2193
5	2F	0.20	0/1615	0.45	2/2188 (0.1%)
6	1G	0.21	0/1448	0.44	0/1957
6	2G	0.20	0/1453	0.43	0/1963
7	1H	0.21	0/1356	0.41	0/1834
7	2H	0.19	0/1356	0.37	0/1834
8	1I	0.18	0/1112	0.40	0/1514
8	2I	0.20	0/1079	0.43	0/1475
9	1N	0.25	0/1144	0.46	0/1543
9	2N	0.19	0/1144	0.41	0/1543
10	1O	0.25	0/943	0.45	0/1269
10	2O	0.18	0/943	0.40	0/1269
11	1P	0.26	0/1152	0.52	0/1533
11	2P	0.21	0/1152	0.48	0/1533
12	1Q	0.27	0/1143	0.49	0/1527
12	2Q	0.21	0/1143	0.45	0/1527
13	1R	0.29	0/982	0.49	0/1312
13	2R	0.20	0/982	0.47	0/1312
14	1S	0.21	0/883	0.45	0/1176
14	2S	0.22	0/880	0.51	0/1172
15	1T	0.25	0/1105	0.49	0/1477
15	2T	0.21	0/1097	0.44	0/1468
16	1U	0.30	0/977	0.50	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.20	0/977	0.41	0/1301
17	1V	0.26	0/782	0.50	0/1049
17	2V	0.17	0/782	0.39	0/1049
18	1W	0.29	0/897	0.45	0/1205
18	2W	0.21	0/897	0.39	0/1205
19	1X	0.26	0/764	0.52	0/1025
19	2X	0.21	0/764	0.50	0/1025
20	1Y	0.23	0/819	0.50	0/1095
20	2Y	0.19	0/819	0.48	0/1095
21	1Z	0.23	0/1267	0.49	1/1717 (0.1%)
21	2Z	0.22	0/1299	0.44	0/1763
22	10	0.26	0/662	0.51	0/881
22	20	0.21	0/662	0.45	0/881
23	11	0.24	0/762	0.43	0/1014
23	21	0.21	0/762	0.44	0/1014
24	12	0.23	0/590	0.43	0/781
24	22	0.19	0/590	0.38	0/781
25	13	0.25	0/474	0.47	0/635
25	23	0.20	0/469	0.41	0/630
26	14	0.26	0/565	0.53	0/761
26	24	0.25	0/545	0.54	0/737
27	15	0.27	0/469	0.51	0/635
27	25	0.22	0/469	0.46	0/635
28	16	0.26	0/460	0.46	0/613
28	26	0.21	0/456	0.48	0/608
29	17	0.29	0/426	0.52	0/561
29	27	0.22	0/426	0.48	0/561
30	18	0.26	0/525	0.48	0/691
30	28	0.18	0/525	0.39	0/691
31	19	0.26	0/310	0.48	0/407
31	29	0.18	0/310	0.41	0/407
32	1a	0.20	0/35795	0.39	1/55864 (0.0%)
32	2a	0.20	0/35886	0.39	0/56005
33	1b	0.21	0/1881	0.49	0/2542
33	2b	0.24	0/1860	0.52	0/2518
34	1c	0.20	0/1572	0.40	0/2126
34	2c	0.23	0/1566	0.46	0/2119
35	1d	0.19	0/1685	0.44	0/2262
35	2d	0.20	0/1704	0.45	0/2284
36	1e	0.20	0/1145	0.45	0/1543
36	2e	0.21	0/1149	0.46	0/1548
37	1f	0.19	0/823	0.39	0/1115
37	2f	0.19	0/829	0.42	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.19	0/1250	0.41	0/1679
38	2g	0.20	0/1254	0.39	0/1683
39	1h	0.19	0/1108	0.40	0/1494
39	2h	0.18	0/1108	0.41	0/1494
40	1i	0.20	0/1002	0.49	0/1346
40	2i	0.22	0/997	0.47	0/1343
41	1j	0.19	0/722	0.42	0/982
41	2j	0.24	0/727	0.48	0/988
42	1k	0.20	0/844	0.40	0/1145
42	2k	0.16	0/848	0.36	0/1149
43	1l	0.21	0/937	0.42	0/1260
43	2l	0.19	0/937	0.43	0/1260
44	1m	0.22	0/969	0.47	0/1302
44	2m	0.22	0/961	0.48	0/1291
45	1n	0.20	0/501	0.42	0/664
45	2n	0.22	0/501	0.44	0/664
46	1o	0.19	0/739	0.37	0/985
46	2o	0.16	0/739	0.39	0/985
47	1p	0.19	0/697	0.45	0/939
47	2p	0.19	0/693	0.44	0/935
48	1q	0.20	0/836	0.42	0/1117
48	2q	0.19	0/836	0.44	0/1117
49	1r	0.21	0/560	0.43	0/746
49	2r	0.18	0/560	0.42	0/746
50	1s	0.19	0/667	0.51	0/900
50	2s	0.26	0/661	0.60	0/893
51	1t	0.19	0/730	0.47	0/965
51	2t	0.20	0/729	0.44	0/965
52	1u	0.17	0/203	0.40	0/266
52	2u	0.19	0/203	0.43	0/266
53	1v	0.22	0/310	0.35	0/480
53	2v	0.18	0/310	0.32	0/480
54	1w	0.27	1/1537 (0.1%)	0.40	0/2390
54	2w	0.29	1/1487 (0.1%)	0.43	0/2311
55	1x	0.27	0/1700	0.42	0/2650
55	2x	0.25	0/1700	0.38	0/2650
56	1y	0.25	1/1606 (0.1%)	0.42	0/2497
56	2y	0.25	0/1583	0.40	0/2459
All	All	0.23	4/316502 (0.0%)	0.43	7/473837 (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
51	1t	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	1y	8	4SU	O3'-P	5.15	1.61	1.56
1	2A	2552	OMU	O3'-P	5.14	1.61	1.56
54	1w	8	4SU	O3'-P	5.13	1.61	1.56
54	2w	8	4SU	O3'-P	5.04	1.61	1.56

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	1Z	53	ILE	N-CA-C	-8.15	104.65	111.91
1	1A	1992	G	C2'-C3'-O3'	6.74	119.61	109.50
1	2A	1992	G	C2'-C3'-O3'	5.43	117.65	109.50
32	1a	266	G	C2'-C3'-O3'	5.28	117.42	109.50
5	2F	21	ALA	CA-C-N	5.18	131.03	121.70
5	2F	21	ALA	C-N-CA	5.18	131.03	121.70
1	2A	752	A	C2'-C3'-O3'	5.16	117.24	109.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
51	1t	99	LEU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61852	0	31197	568	0
1	2A	60322	0	30426	677	0
2	1B	2577	0	1305	21	0
2	2B	2575	0	1303	52	0
3	1D	2136	0	2218	35	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	2D	2136	0	2218	35	0
4	1E	1559	0	1618	30	0
4	2E	1559	0	1618	25	0
5	1F	1584	0	1625	31	0
5	2F	1580	0	1619	43	0
6	1G	1423	0	1436	32	0
6	2G	1428	0	1438	74	0
7	1H	1330	0	1407	26	0
7	2H	1330	0	1407	35	0
8	1I	1097	0	1140	23	0
8	2I	1064	0	1082	44	0
9	1N	1117	0	1184	20	0
9	2N	1117	0	1184	21	0
10	1O	933	0	996	15	0
10	2O	933	0	996	21	0
11	1P	1135	0	1212	28	0
11	2P	1135	0	1212	28	0
12	1Q	1122	0	1179	20	0
12	2Q	1122	0	1179	38	0
13	1R	968	0	1033	14	0
13	2R	968	0	1033	16	0
14	1S	873	0	927	15	0
14	2S	870	0	923	46	0
15	1T	1091	0	1151	16	0
15	2T	1083	0	1136	33	0
16	1U	959	0	1019	12	0
16	2U	959	0	1019	14	0
17	1V	771	0	830	9	0
17	2V	771	0	830	19	0
18	1W	886	0	940	6	0
18	2W	886	0	940	13	0
19	1X	750	0	814	12	0
19	2X	750	0	814	24	0
20	1Y	806	0	881	15	0
20	2Y	806	0	881	21	0
21	1Z	1240	0	1240	32	0
21	2Z	1271	0	1273	58	0
22	10	653	0	674	14	0
22	20	653	0	674	20	0
23	11	755	0	826	14	0
23	21	755	0	826	15	0
24	12	588	0	643	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	22	588	0	643	15	0
25	13	469	0	518	7	0
25	23	464	0	514	8	0
26	14	552	0	533	21	0
26	24	532	0	503	31	0
27	15	455	0	465	5	0
27	25	455	0	465	11	0
28	16	453	0	473	12	0
28	26	449	0	469	12	0
29	17	418	0	467	5	0
29	27	418	0	467	11	0
30	18	517	0	582	14	0
30	28	517	0	582	17	0
31	19	307	0	335	7	0
31	29	307	0	335	12	0
32	1a	32246	0	16295	378	0
32	2a	32327	0	16339	575	0
33	1b	1846	0	1867	55	0
33	2b	1825	0	1828	93	0
34	1c	1548	0	1535	29	0
34	2c	1542	0	1517	83	0
35	1d	1655	0	1672	32	0
35	2d	1674	0	1714	67	0
36	1e	1129	0	1185	36	0
36	2e	1133	0	1191	37	0
37	1f	810	0	804	16	0
37	2f	816	0	808	22	0
38	1g	1231	0	1238	18	0
38	2g	1235	0	1249	41	0
39	1h	1088	0	1126	24	0
39	2h	1088	0	1126	27	0
40	1i	983	0	986	24	0
40	2i	978	0	966	52	0
41	1j	709	0	650	29	0
41	2j	714	0	672	33	0
42	1k	829	0	825	15	0
42	2k	833	0	836	25	0
43	1l	932	0	981	13	0
43	2l	932	0	981	19	0
44	1m	958	0	1002	19	0
44	2m	950	0	988	57	0
45	1n	492	0	529	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	2n	492	0	529	27	0
46	1o	728	0	760	15	0
46	2o	728	0	760	14	0
47	1p	681	0	697	23	0
47	2p	677	0	686	19	0
48	1q	823	0	891	19	0
48	2q	823	0	891	19	0
49	1r	555	0	618	14	0
49	2r	555	0	618	19	0
50	1s	652	0	662	16	0
50	2s	646	0	644	45	0
51	1t	728	0	798	26	0
51	2t	727	0	796	28	0
52	1u	199	0	208	7	0
52	2u	199	0	208	8	0
53	1v	277	0	140	1	0
53	2v	277	0	140	3	0
54	1w	1530	0	786	17	0
54	2w	1482	0	755	21	0
55	1x	1635	0	839	7	0
55	2x	1635	0	839	12	0
56	1y	1585	0	804	21	0
56	2y	1565	0	795	27	0
57	10	8	0	0	0	0
57	11	5	0	0	0	0
57	12	2	0	0	0	0
57	13	4	0	0	0	0
57	14	1	0	0	0	0
57	15	9	0	0	0	0
57	16	1	0	0	0	0
57	17	6	0	0	0	0
57	18	6	0	0	0	0
57	19	1	0	0	0	0
57	1A	1108	0	0	0	0
57	1B	36	0	0	0	0
57	1D	12	0	0	0	0
57	1E	16	0	0	0	0
57	1F	12	0	0	0	0
57	1G	5	0	0	0	0
57	1I	1	0	0	0	0
57	1N	6	0	0	0	0
57	1O	6	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	1P	6	0	0	0	0
57	1Q	6	0	0	0	0
57	1R	4	0	0	0	0
57	1S	3	0	0	0	0
57	1T	2	0	0	0	0
57	1U	9	0	0	0	0
57	1V	6	0	0	0	0
57	1W	6	0	0	0	0
57	1X	5	0	0	0	0
57	1Y	4	0	0	0	0
57	1Z	3	0	0	0	0
57	1a	229	0	0	0	0
57	1b	2	0	0	0	0
57	1d	1	0	0	0	0
57	1e	2	0	0	0	0
57	1f	1	0	0	0	0
57	1l	3	0	0	0	0
57	1m	1	0	0	0	0
57	1n	2	0	0	0	0
57	1r	1	0	0	0	0
57	1t	1	0	0	0	0
57	1v	1	0	0	0	0
57	1w	5	0	0	0	0
57	1x	15	0	0	0	0
57	1y	4	0	0	0	0
57	20	3	0	0	0	0
57	21	1	0	0	0	0
57	23	2	0	0	0	0
57	25	3	0	0	0	0
57	26	1	0	0	0	0
57	27	3	0	0	0	0
57	28	3	0	0	0	0
57	2A	729	0	0	0	0
57	2B	18	0	0	0	0
57	2D	6	0	0	0	0
57	2E	7	0	0	0	0
57	2F	6	0	0	0	0
57	2G	1	0	0	0	0
57	2N	1	0	0	0	0
57	2O	1	0	0	0	0
57	2Q	1	0	0	0	0
57	2R	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	2T	3	0	0	0	0
57	2W	1	0	0	0	0
57	2X	1	0	0	0	0
57	2Y	1	0	0	0	0
57	2Z	1	0	0	0	0
57	2a	186	0	0	0	0
57	2d	1	0	0	0	0
57	2e	1	0	0	0	0
57	2f	2	0	0	0	0
57	2l	3	0	0	0	0
57	2q	3	0	0	0	0
57	2r	1	0	0	0	0
57	2t	1	0	0	0	0
57	2v	1	0	0	0	0
57	2w	1	0	0	0	0
57	2x	5	0	0	0	0
57	2y	3	0	0	0	0
58	1A	32	0	0	2	0
58	2A	32	0	0	0	0
59	14	1	0	0	0	0
59	15	1	0	0	0	0
59	16	1	0	0	0	0
59	19	1	0	0	0	0
59	1Y	1	0	0	0	0
59	1n	1	0	0	0	0
59	24	1	0	0	0	0
59	25	1	0	0	0	0
59	26	1	0	0	0	0
59	29	1	0	0	0	0
59	2Y	1	0	0	0	0
59	2n	1	0	0	0	0
60	1d	8	0	0	0	0
60	2d	8	0	0	1	0
61	2A	1	0	0	0	0
62	10	10	0	0	0	0
62	11	12	0	0	1	0
62	12	4	0	0	0	0
62	13	5	0	0	1	0
62	15	7	0	0	0	0
62	16	1	0	0	0	0
62	17	8	0	0	1	0
62	18	10	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	1A	2122	0	0	77	0
62	1B	69	0	0	3	0
62	1D	24	0	0	0	0
62	1E	27	0	0	0	0
62	1F	18	0	0	1	0
62	1G	7	0	0	0	0
62	1H	2	0	0	0	0
62	1N	4	0	0	1	0
62	1O	7	0	0	1	0
62	1P	20	0	0	2	0
62	1Q	8	0	0	0	0
62	1R	10	0	0	2	0
62	1S	4	0	0	0	0
62	1T	8	0	0	0	0
62	1U	10	0	0	1	0
62	1V	9	0	0	0	0
62	1W	7	0	0	0	0
62	1X	7	0	0	1	0
62	1Y	3	0	0	0	0
62	1Z	1	0	0	0	0
62	1a	361	0	0	25	0
62	1b	1	0	0	0	0
62	1d	1	0	0	0	0
62	1e	1	0	0	0	0
62	1g	1	0	0	0	0
62	1l	4	0	0	0	0
62	1m	2	0	0	0	0
62	1q	4	0	0	0	0
62	1u	1	0	0	1	0
62	1v	5	0	0	0	0
62	1w	6	0	0	0	0
62	1x	16	0	0	1	0
62	1y	2	0	0	0	0
62	20	2	0	0	0	0
62	21	3	0	0	0	0
62	23	2	0	0	0	0
62	25	2	0	0	1	0
62	26	1	0	0	0	0
62	27	2	0	0	0	0
62	28	6	0	0	0	0
62	29	1	0	0	0	0
62	2A	968	0	0	65	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	2B	15	0	0	0	0
62	2D	16	0	0	4	0
62	2E	9	0	0	0	0
62	2F	9	0	0	0	0
62	2I	1	0	0	0	0
62	2N	1	0	0	0	0
62	2O	2	0	0	0	0
62	2P	10	0	0	1	0
62	2Q	1	0	0	0	0
62	2R	3	0	0	0	0
62	2T	2	0	0	0	0
62	2W	1	0	0	0	0
62	2X	3	0	0	1	0
62	2Y	1	0	0	0	0
62	2a	51	0	0	6	0
62	2d	1	0	0	0	0
62	2i	1	0	0	0	0
62	2j	1	0	0	0	0
62	2l	3	0	0	0	0
62	2p	1	0	0	0	0
62	2t	2	0	0	0	0
62	2x	3	0	0	0	0
62	2y	8	0	0	1	0
All	All	299504	0	196651	4204	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 (4204) 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	1.32	1.26
6:1G:21:ARG:HA	6:1G:21:ARG:HH11	1.20	1.02
1:1A:1082:U:O4	1:1A:1086:A:N1	1.93	1.01
1:2A:2138:C:N4	1:2A:2153:G:H1	1.61	0.98
32:1a:1002:G:H3'	32:1a:1003:G:H4'	1.45	0.97
1:1A:1057:A:H61	1:1A:1081:U:H3	1.12	0.97
32:2a:1133:G:H1	32:2a:1141:C:H42	1.10	0.97
1:1A:2499:C:OP1	62:1A:4203:HOH:O	1.82	0.96
1:2A:2099:U:H3	1:2A:2190:G:H1	0.97	0.95
1:2A:2589:A:OP1	62:2A:3803:HOH:O	1.83	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2B:7:G:H21	14:2S:38:GLN:HE22	1.14	0.94
1:2A:2138:C:H42	1:2A:2153:G:H1	0.95	0.93
1:1A:1054:A:N6	1:1A:1105:U:H3	1.67	0.93
1:1A:1058:G:H1	1:1A:1080:C:N4	1.67	0.92
29:27:24:THR:HG22	29:27:27:GLY:H	1.32	0.91
1:1A:2100:G:H1	1:1A:2189:U:H3	0.98	0.91
1:1A:2427:C:OP1	62:1A:4204:HOH:O	1.88	0.91
1:1A:1058:G:H1	1:1A:1080:C:H42	1.09	0.91
10:2O:48:PRO:HB3	32:2a:1422:G:H5''	1.51	0.90
33:2b:69:LEU:HB3	33:2b:162:ILE:HG22	1.52	0.90
1:2A:784:A:OP2	62:2A:3803:HOH:O	1.90	0.90
54:1w:26:A:H61	54:1w:44:G:H1	1.18	0.88
56:2y:18:G:N2	56:2y:55:PSU:N3	2.23	0.86
1:2A:783:A:OP2	62:2A:3803:HOH:O	1.92	0.86
1:1A:1057:A:N6	1:1A:1081:U:H3	1.74	0.86
29:17:24:THR:HG22	29:17:27:GLY:H	1.40	0.84
38:2g:113:GLU:HG2	38:2g:119:ARG:HG2	1.57	0.84
32:2a:1286:A:H8	32:2a:1287:A:H4'	1.41	0.84
33:2b:16:HIS:HB2	33:2b:204:ASN:HB3	1.58	0.84
1:2A:1689:A:H62	1:2A:1698:A:H2	1.26	0.84
1:1A:2136:C:N4	1:1A:2155:G:N1	2.26	0.84
32:2a:1295:G:O2'	44:2m:14:ARG:NH1	2.10	0.83
1:1A:11:G:H2'	1:1A:12:U:H5''	1.59	0.83
40:2i:46:ALA:HB2	40:2i:74:ILE:HG23	1.58	0.83
1:1A:2136:C:N3	1:1A:2155:G:C2	2.47	0.82
44:2m:23:TYR:HB3	44:2m:67:GLU:HA	1.59	0.82
1:1A:2136:C:N3	1:1A:2155:G:N2	2.27	0.82
26:24:61:ARG:HG2	50:2s:42:PRO:HG3	1.60	0.82
32:1a:1027:C:C2	32:1a:1034:G:N2	2.47	0.82
1:1A:1058:G:N2	1:1A:1080:C:N3	2.25	0.82
1:2A:1204:A:H2	1:2A:1241:A:H62	1.27	0.82
34:2c:70:VAL:HG12	34:2c:72:LYS:H	1.45	0.82
1:2A:2049:G:N7	62:2A:3824:HOH:O	2.13	0.81
38:2g:78:ARG:HD3	38:2g:79:ARG:H	1.46	0.81
10:2O:35:VAL:HG11	10:2O:103:ALA:HB3	1.61	0.81
56:2y:55:PSU:HN1	56:2y:57:G:H5''	1.45	0.81
1:1A:631:A:OP1	11:1P:65:ARG:NH1	2.14	0.81
34:2c:131:ARG:HH21	34:2c:135:LYS:HZ2	1.29	0.81
32:1a:1189:C:OP1	41:1j:51:ARG:NH2	2.13	0.80
32:1a:1025:U:O2	32:1a:1036:G:O6	1.98	0.80
32:2a:1286:A:C8	32:2a:1287:A:H4'	2.17	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:2j:49:VAL:HG23	45:2n:41:ARG:HB2	1.64	0.80
32:2a:922:G:H4'	36:2e:20:GLN:HA	1.62	0.80
32:2a:1348:U:H4'	40:2i:120:ARG:HG3	1.64	0.80
1:1A:1669:A:OP2	62:1A:4206:HOH:O	2.00	0.80
1:2A:10:G:O2'	1:2A:2801(A):A:N7	2.13	0.80
8:2I:62:LYS:HE3	8:2I:133:HIS:HE1	1.47	0.80
32:2a:975:A:H4'	32:2a:976:G:H5''	1.62	0.80
1:2A:805:G:OP1	62:2A:3804:HOH:O	2.00	0.80
41:1j:27:ALA:HA	41:1j:81:THR:HG21	1.63	0.79
1:2A:500:G:N1	1:2A:503:A:OP2	2.16	0.79
1:2A:2206:G:H3'	1:2A:2207:G:C8	2.17	0.79
1:1A:1798:U:H5'	3:1D:259:THR:HG22	1.64	0.79
56:2y:18:G:H22	56:2y:55:PSU:HN3	1.27	0.79
44:2m:3:ARG:N	44:2m:7:VAL:O	2.16	0.79
1:2A:2296:U:OP2	14:2S:9:ARG:NH2	2.16	0.79
50:2s:50:ALA:HB1	50:2s:57:HIS:HB3	1.65	0.79
1:1A:1541:G:OP2	62:1A:4205:HOH:O	1.99	0.79
1:2A:2345:G:H4'	1:2A:2346:A:H5''	1.65	0.79
35:2d:153:ARG:HH21	35:2d:181:MET:HG3	1.45	0.79
1:1A:2550:G:OP1	62:1A:4206:HOH:O	2.00	0.78
32:2a:1129:C:O2'	32:2a:1130:A:N7	2.15	0.78
32:2a:1105:A:H2'	32:2a:1106:G:H8	1.48	0.78
1:1A:2142:C:N3	1:1A:2149:G:O6	2.16	0.78
41:1j:38:ILE:HD11	41:1j:71:LEU:HD23	1.65	0.78
1:2A:500:G:H22	1:2A:503:A:H5'	1.48	0.78
1:1A:376:C:OP1	62:1A:4207:HOH:O	2.01	0.78
1:2A:2127:G:C6	1:2A:2161:C:N4	2.52	0.78
1:2A:2807:G:N1	1:2A:2893:G:O6	2.13	0.78
34:2c:88:ARG:HA	34:2c:91:LEU:HD13	1.65	0.78
1:1A:279:C:H42	1:1A:361:G:H1	1.32	0.78
56:1y:51:U:H3	56:1y:63:G:H1	1.28	0.78
40:2i:121:ARG:NH1	40:2i:122:ALA:O	2.16	0.78
32:1a:1505:G:OP2	62:1a:1903:HOH:O	2.02	0.78
1:2A:631:A:OP1	11:2P:65:ARG:NH1	2.15	0.77
32:2a:1376:U:H2'	32:2a:1377:A:H8	1.48	0.77
1:2A:852:G:H2'	1:2A:853:G:H8	1.50	0.77
32:2a:953:G:H5'	32:2a:965:A:H61	1.48	0.77
1:1A:1203:G:O6	62:1A:4208:HOH:O	2.01	0.77
4:1E:110:GLY:O	62:1R:301:HOH:O	2.02	0.77
32:1a:405:U:O4	35:1d:2:GLY:N	2.18	0.77
32:2a:950:U:H3	32:2a:1231:G:H1	1.32	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1054:A:N6	1:1A:1105:U:N3	2.31	0.77
32:1a:664:G:H22	32:1a:741:G:H1	1.33	0.77
50:1s:27:GLU:HB2	50:1s:28:LYS:HA	1.67	0.77
5:2F:137:LYS:HA	5:2F:140:LEU:HD12	1.66	0.76
1:1A:1670:C:OP2	62:1A:4206:HOH:O	2.03	0.76
1:2A:1147:C:H2'	1:2A:1148:A:H8	1.50	0.76
52:1u:5:ASP:OD2	62:1u:101:HOH:O	2.03	0.76
32:2a:1133:G:H1	32:2a:1141:C:N4	1.83	0.76
55:2x:50:U:H3	55:2x:64:G:H1	1.34	0.76
26:14:15:ILE:HG13	26:14:21:VAL:HG12	1.67	0.76
32:1a:975:A:H4'	32:1a:976:G:H5''	1.66	0.76
33:2b:189:ASP:N	33:2b:189:ASP:OD1	2.19	0.76
1:2A:2127:G:N1	1:2A:2161:C:N4	2.33	0.75
12:1Q:111:GLU:OE2	12:1Q:133:ARG:NH2	2.17	0.75
1:2A:1801:G:OP2	3:2D:154:LYS:NZ	2.19	0.75
1:2A:131:G:OP1	62:2A:3806:HOH:O	2.04	0.75
33:1b:77:ALA:HB2	33:1b:211:ILE:HD13	1.69	0.75
1:2A:1693:U:O2'	3:2D:14:ARG:NH2	2.20	0.75
8:1I:92:VAL:HG13	8:1I:120:ILE:HB	1.68	0.75
1:2A:2805:G:H2'	1:2A:2807:G:C8	2.21	0.75
35:2d:18:LYS:NZ	35:2d:31:CYS:SG	2.59	0.75
1:1A:1065:U:O2	1:1A:1073:A:N6	2.19	0.75
1:1A:1647:G:OP1	62:1A:4209:HOH:O	2.05	0.75
10:1O:35:VAL:HG11	10:1O:103:ALA:HB3	1.68	0.75
28:16:13:CYS:SG	28:16:47:THR:HG21	2.26	0.75
34:2c:63:ASN:HB3	34:2c:98:ASN:HD22	1.52	0.75
1:1A:1058:G:N2	1:1A:1081:U:O2	2.19	0.75
43:2l:32:PHE:HB3	43:2l:84:LEU:HD11	1.68	0.75
14:2S:67:ARG:HG2	14:2S:71:ARG:HD2	1.68	0.74
32:1a:972:C:O2'	41:1j:55:LYS:O	2.06	0.74
1:2A:962:G:OP1	62:2A:3805:HOH:O	2.05	0.74
21:2Z:30:ASN:HD22	21:2Z:90:VAL:HB	1.51	0.74
32:2a:1166:G:N2	32:2a:1170:A:OP2	2.19	0.74
10:1O:36:GLY:O	62:1O:301:HOH:O	2.05	0.74
21:2Z:19:ARG:NH1	21:2Z:84:GLU:O	2.21	0.74
42:2k:48:ILE:O	42:2k:50:TYR:N	2.20	0.74
1:2A:948:G:OP1	62:2A:3805:HOH:O	2.06	0.74
32:2a:64:G:H4'	32:2a:65:U:H3'	1.69	0.74
41:2j:42:THR:HG22	41:2j:68:HIS:HA	1.70	0.74
42:2k:54:ARG:HH22	56:2y:39:PSU:H4'	1.51	0.74
1:2A:80:G:H1	1:2A:106:C:H42	1.35	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:624:C:OP1	62:2A:3807:HOH:O	2.05	0.74
15:2T:105:LEU:HB2	15:2T:110:ILE:HG13	1.68	0.74
1:2A:1452:A:OP2	62:2A:3808:HOH:O	2.06	0.74
34:2c:20:SER:HB3	34:2c:22:TRP:HE1	1.53	0.74
1:1A:2350:C:OP2	62:1A:4210:HOH:O	2.05	0.74
1:1A:2690:C:OP1	13:1R:17:ARG:NH2	2.20	0.74
1:1A:1271:G:OP2	62:1A:4209:HOH:O	2.04	0.74
1:1A:2140:C:N3	1:1A:2151:G:O6	2.20	0.74
11:1P:42:SER:O	62:1P:301:HOH:O	2.05	0.74
32:2a:1029:C:N3	32:2a:1032:G:N2	2.36	0.74
54:2w:18:G:O2'	54:2w:57:G:N2	2.20	0.74
1:2A:963:U:OP2	62:2A:3805:HOH:O	2.04	0.73
32:1a:892:A:OP2	62:1a:1904:HOH:O	2.05	0.73
1:2A:1434:A:H61	1:2A:1558:A:H62	1.34	0.73
32:2a:673:G:H2'	32:2a:674:G:C8	2.22	0.73
42:2k:99:GLN:HG2	42:2k:105:VAL:HG21	1.69	0.73
1:2A:1812:A:OP2	62:2A:3809:HOH:O	2.06	0.73
26:24:24:THR:OG1	26:24:25:TYR:N	2.20	0.73
32:2a:984:C:H2'	32:2a:985:C:H6	1.52	0.73
17:2V:62:LEU:HD11	17:2V:95:LEU:HB2	1.71	0.73
50:2s:77:THR:HG23	50:2s:78:ARG:HG3	1.70	0.73
1:1A:2139:C:H42	1:1A:2152:G:H1	1.33	0.73
1:1A:826:U:OP1	62:1A:4204:HOH:O	2.06	0.73
1:1A:1315:C:OP2	62:1A:4211:HOH:O	2.06	0.73
44:1m:23:TYR:HB3	44:1m:67:GLU:HA	1.71	0.73
54:1w:26:A:N6	54:1w:44:G:H1	1.87	0.73
1:1A:1252:G:N7	16:1U:36:ARG:NH1	2.36	0.73
19:2X:8:ILE:O	24:22:36:ARG:NH2	2.21	0.73
5:2F:122:LYS:NZ	5:2F:152:GLU:OE2	2.21	0.73
6:1G:21:ARG:HA	6:1G:21:ARG:NH1	2.02	0.72
1:2A:1037:G:H1	1:2A:1118:C:H42	1.37	0.72
1:2A:2127:G:N1	1:2A:2161:C:C4	2.56	0.72
1:1A:1332:G:OP1	62:1A:4211:HOH:O	2.08	0.72
1:1A:1693:U:O2'	3:1D:14:ARG:NH2	2.23	0.72
44:2m:78:ILE:HA	44:2m:81:LEU:HD12	1.69	0.72
6:2G:64:THR:HB	6:2G:94:LEU:HD21	1.70	0.72
23:21:52:ARG:HH21	23:21:57:GLU:HB2	1.54	0.72
1:1A:1075:C:H2'	1:1A:1076:C:H2'	1.71	0.72
1:2A:2134:A:O2'	1:2A:2159:G:N2	2.22	0.72
34:2c:111:LEU:HD21	34:2c:146:ALA:HB2	1.70	0.72
40:2i:15:ALA:HB2	40:2i:65:VAL:HG23	1.71	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:1h:34:GLU:OE1	39:1h:37:ARG:NH1	2.23	0.72
1:2A:882:G:H1	1:2A:894:C:H42	1.38	0.72
18:1W:25:ARG:NH2	18:1W:74:ALA:O	2.23	0.72
3:2D:125:ILE:HB	37:2f:81:ILE:HD11	1.70	0.72
1:1A:582:G:OP2	62:1A:4212:HOH:O	2.08	0.72
35:1d:98:GLU:OE1	35:1d:103:ASN:ND2	2.22	0.72
56:1y:8:4SU:H4'	56:1y:48:C:H4'	1.72	0.72
2:2B:24:G:N3	2:2B:26:A:N6	2.37	0.72
1:1A:1359:A:H2'	1:1A:1360:A:H5'	1.72	0.71
3:2D:71:ASP:HB2	3:2D:103:ARG:HH12	1.53	0.71
32:2a:1216:G:H5''	45:2n:5:ALA:HB2	1.71	0.71
36:2e:33:VAL:HG13	36:2e:112:LEU:HD22	1.72	0.71
1:1A:2683:C:O2	10:1O:70:LYS:NZ	2.19	0.71
32:1a:1314:C:OP2	50:1s:4:SER:OG	2.07	0.71
32:1a:1255:G:N7	41:1j:43:ARG:NH2	2.38	0.71
36:1e:137:GLU:HG3	36:1e:141:GLN:HE21	1.55	0.71
1:2A:2319:G:H22	14:2S:3:ARG:HH11	1.37	0.71
14:2S:25:ARG:HB3	14:2S:40:ILE:HB	1.72	0.71
1:2A:2430:A:OP2	62:2A:3810:HOH:O	2.08	0.71
1:2A:586:A:N1	1:2A:809:G:O2'	2.23	0.71
32:2a:564:C:O2'	39:2h:91:ARG:NH2	2.19	0.71
44:2m:3:ARG:NH2	44:2m:9:ILE:O	2.24	0.71
6:2G:41:GLN:HG2	6:2G:43:LEU:HD22	1.73	0.71
32:2a:1029:C:C4	32:2a:1032:G:N1	2.56	0.71
1:1A:1013:C:OP2	62:1A:4215:HOH:O	2.09	0.71
1:2A:89:G:H3'	1:2A:90:U:H5''	1.71	0.71
2:2B:20:C:N4	2:2B:63:G:O6	2.16	0.71
33:2b:73:THR:OG1	33:2b:95:GLN:O	2.09	0.71
1:1A:2821:A:OP2	62:1R:301:HOH:O	2.08	0.71
26:14:16:CYS:SG	26:14:17:GLY:N	2.63	0.71
1:2A:1271:G:OP2	62:2A:3811:HOH:O	2.08	0.71
1:2A:2138:C:N3	1:2A:2153:G:N2	2.35	0.71
27:25:40:LYS:NZ	27:25:44:THR:O	2.23	0.71
33:2b:16:HIS:HB3	33:2b:210:SER:HB2	1.72	0.71
1:1A:1993:U:OP2	62:1A:4213:HOH:O	2.09	0.70
32:2a:1029:C:N4	32:2a:1032:G:N1	2.39	0.70
1:2A:106:C:H1'	20:2Y:1:MET:HE2	1.73	0.70
5:2F:21:ALA:HB3	5:2F:22:ALA:HA	1.73	0.70
21:2Z:31:ARG:HH11	21:2Z:94:GLU:HG2	1.56	0.70
1:1A:880:G:H2'	1:1A:881:G:H8	1.53	0.70
1:2A:2127:G:N2	1:2A:2161:C:N3	2.38	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:2I:3:VAL:HG12	8:2I:38:LEU:HA	1.73	0.70
1:1A:582:G:N7	62:1A:4262:HOH:O	2.23	0.70
1:2A:1779:U:OP2	62:2A:3813:HOH:O	2.10	0.70
32:2a:1274:G:N2	32:2a:1275:A:N7	2.35	0.70
38:2g:20:ASP:HB3	38:2g:23:VAL:HB	1.72	0.70
1:1A:880:G:H2'	1:1A:881:G:C8	2.26	0.70
1:1A:2277:G:OP2	22:10:10:THR:HG21	1.91	0.70
34:1c:20:SER:HB2	34:1c:40:ARG:HH22	1.55	0.70
42:1k:99:GLN:HG3	42:1k:105:VAL:HG11	1.73	0.70
1:2A:955:C:OP1	12:2Q:87:LYS:NZ	2.21	0.70
1:1A:1840:G:N7	62:1A:4267:HOH:O	2.25	0.70
49:2r:38:GLU:HA	49:2r:41:LYS:HE3	1.73	0.70
1:1A:1664:A:OP1	62:1A:4214:HOH:O	2.09	0.70
39:1h:120:THR:H	39:1h:123:GLU:HB2	1.56	0.70
1:2A:531:C:OP1	1:2A:561:G:N1	2.25	0.70
1:2A:2365:G:N7	30:28:39:LYS:NZ	2.39	0.70
1:2A:1648:C:OP1	62:2A:3811:HOH:O	2.09	0.70
32:2a:533:A:OP1	62:2a:1801:HOH:O	2.09	0.70
1:1A:1506:C:H2'	1:1A:1507:A:H8	1.56	0.69
6:2G:44:GLY:N	6:2G:88:ILE:O	2.24	0.69
32:2a:1219:U:OP1	45:2n:19:ARG:NH1	2.25	0.69
39:1h:43:GLY:O	39:1h:64:LYS:NZ	2.23	0.69
1:2A:2127:G:C2	1:2A:2161:C:N3	2.61	0.69
30:28:33:ASN:HA	30:28:36:LYS:HD2	1.73	0.69
1:1A:2049:G:N7	62:1A:4269:HOH:O	2.25	0.69
1:2A:1153:C:OP1	16:2U:92:ARG:NH2	2.26	0.69
21:2Z:130:PRO:HA	21:2Z:133:ILE:HG13	1.74	0.69
1:2A:947:G:OP2	62:2A:3815:HOH:O	2.10	0.69
1:2A:2448:A:OP1	62:2A:3814:HOH:O	2.10	0.69
1:2A:2379:G:O2'	14:2S:17:ARG:NH1	2.20	0.69
40:2i:28:VAL:HG22	40:2i:63:ILE:HB	1.74	0.69
1:1A:1094:U:N3	1:1A:1097:U:OP2	2.26	0.69
8:1I:130:TYR:HB3	8:1I:138:ILE:HB	1.75	0.69
32:1a:1391:U:OP2	62:1a:1906:HOH:O	2.10	0.69
1:2A:450:G:O6	62:2A:3812:HOH:O	2.08	0.69
1:2A:1798:U:H5'	3:2D:259:THR:HG22	1.74	0.69
32:2a:656:C:O2'	46:2o:28:GLN:OE1	2.09	0.69
32:2a:1329:A:OP2	52:2u:7:ARG:NH1	2.24	0.69
1:1A:1823:G:OP1	3:1D:54:ARG:NH1	2.26	0.69
1:1A:2222:G:OP2	62:1A:4219:HOH:O	2.11	0.69
1:2A:1254:A:OP2	62:2A:3816:HOH:O	2.10	0.69

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	1.75	0.69
1:2A:1762:A:N1	62:2A:3861:HOH:O	2.26	0.69
32:2a:1118:C:N3	32:2a:1156:G:N2	2.41	0.69
1:2A:775:G:O3'	62:2A:3817:HOH:O	2.11	0.68
1:2A:1389:G:N7	62:2A:3857:HOH:O	2.26	0.68
33:2b:118:LEU:HD11	33:2b:138:LEU:HD23	1.74	0.68
1:1A:773:U:OP1	62:1A:4218:HOH:O	2.11	0.68
1:1A:1082:U:N3	1:1A:1086:A:N6	2.09	0.68
32:1a:1086:U:H3	32:1a:1099:G:H22	1.41	0.68
1:2A:179:G:N7	62:2A:3854:HOH:O	2.25	0.68
1:2A:2759:G:OP2	62:2A:3820:HOH:O	2.11	0.68
32:2a:1012:U:H2'	32:2a:1013:G:C8	2.28	0.68
32:2a:1149:C:O2'	32:2a:1280:A:N1	2.22	0.68
1:1A:123:G:OP2	62:1A:4216:HOH:O	2.10	0.68
1:1A:2629:A:O2'	1:1A:2630:G:OP2	2.09	0.68
47:1p:19:ILE:HD12	47:1p:36:ILE:HG13	1.76	0.68
52:1u:6:ARG:HG2	52:1u:15:ARG:HD2	1.74	0.68
1:2A:449:A:OP2	62:2A:3818:HOH:O	2.11	0.68
1:2A:2577:A:H5''	1:2A:2578:G:H5'	1.75	0.68
1:2A:751:A:OP1	62:2A:3819:HOH:O	2.11	0.68
32:1a:36:C:OP1	43:1l:123:LYS:NZ	2.26	0.68
32:1a:1224:G:OP1	62:1a:1907:HOH:O	2.10	0.68
12:1Q:97:VAL:HG11	12:1Q:103:MET:HE3	1.75	0.68
32:1a:1435:G:H2'	32:1a:1436:U:C6	2.29	0.68
36:1e:144:THR:H	36:1e:147:ASP:HB2	1.57	0.68
8:2I:5:LEU:HD11	8:2I:19:VAL:HG22	1.76	0.68
34:2c:6:HIS:ND1	45:2n:49:HIS:HB3	2.07	0.68
1:1A:1469:A:OP2	62:1A:4220:HOH:O	2.12	0.68
19:1X:35:THR:HG22	19:1X:38:GLU:H	1.58	0.68
32:2a:942:G:N2	40:2i:124:GLN:OE1	2.23	0.68
32:2a:1402:4OC:HM22	32:2a:1403:C:H5'	1.74	0.68
1:2A:2114:A:H62	1:2A:2115:G:H21	1.42	0.68
26:24:58:ARG:HD2	50:2s:68:GLY:H	1.59	0.68
32:2a:1004:A:N6	32:2a:1037:C:O2	2.23	0.68
50:1s:12:ASP:OD2	50:1s:35:SER:OG	2.12	0.67
32:1a:1356:G:H2'	32:1a:1357:A:C8	2.29	0.67
1:2A:1634:A:OP1	62:2A:3821:HOH:O	2.12	0.67
1:2A:1816:G:O6	3:2D:35:LYS:NZ	2.22	0.67
1:2A:1352:U:OP2	62:2A:3823:HOH:O	2.13	0.67
32:2a:1279:A:O2'	32:2a:1281:U:OP2	2.12	0.67
7:1H:3:ARG:HE	7:1H:54:ARG:HH12	1.42	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1346:A:OP1	40:1i:120:ARG:NH1	2.24	0.67
1:2A:789:A:N1	62:2A:3862:HOH:O	2.26	0.67
1:2A:911:A:OP1	62:2A:3822:HOH:O	2.12	0.67
1:2A:2166:G:O6	1:2A:2171:A:N6	2.28	0.67
2:2B:22:U:H3	2:2B:61:G:H1	1.41	0.67
5:2F:103:LYS:HA	5:2F:106:ARG:HD3	1.76	0.67
1:1A:2448:A:OP1	62:1A:4203:HOH:O	2.13	0.67
5:1F:61:GLY:O	62:1F:401:HOH:O	2.13	0.67
2:2B:50:G:OP1	14:2S:63:THR:N	2.27	0.67
33:2b:21:ARG:HA	33:2b:39:ILE:HA	1.77	0.67
1:1A:878:A:N6	1:1A:899:A:O2'	2.28	0.67
1:1A:2121:G:H1	1:1A:2177:C:H42	1.42	0.67
2:2B:41:U:H5	6:2G:70:VAL:H	1.41	0.67
8:2I:122:GLU:O	8:2I:126:TYR:OH	2.13	0.67
32:2a:1273:G:H3'	32:2a:1274:G:H8	1.59	0.67
1:1A:570:G:O6	62:1A:4203:HOH:O	2.12	0.67
26:24:14:ILE:HD12	26:24:31:ILE:HB	1.76	0.67
36:1e:20:GLN:NE2	36:1e:21:ALA:O	2.27	0.67
1:2A:1378:A:O2'	1:2A:1380:G:N7	2.24	0.67
1:2A:2857:G:N2	1:2A:2860:A:OP2	2.27	0.67
6:2G:106:LEU:HA	6:2G:110:ALA:HB3	1.77	0.67
6:1G:21:ARG:C	6:1G:21:ARG:HD3	2.19	0.67
32:1a:536:C:OP2	62:1a:1909:HOH:O	2.12	0.67
1:2A:1021:A:H62	1:2A:1141:U:H3	1.41	0.67
1:2A:1449:A:O2'	1:2A:1529:G:N2	2.25	0.67
32:2a:266:G:H5''	32:2a:268:C:H41	1.60	0.67
47:2p:15:PRO:HD2	47:2p:42:ARG:HD2	1.77	0.67
1:1A:2447:G:OP2	62:1A:4221:HOH:O	2.12	0.66
32:1a:189(K):U:H2'	32:1a:189(L):G:C8	2.30	0.66
32:1a:1108:G:O6	62:1a:1905:HOH:O	2.10	0.66
1:2A:2110:G:OP1	1:2A:2118:U:N3	2.28	0.66
1:2A:2135:A:N1	1:2A:2156:G:O2'	2.28	0.66
1:1A:1069:A:H1'	1:1A:1096:A:H4'	1.76	0.66
1:1A:2849:U:OP2	15:1T:95:ARG:NH1	2.28	0.66
43:1l:70:ILE:HG12	43:1l:100:ILE:HD12	1.77	0.66
10:2O:24:VAL:HG13	10:2O:33:ALA:HB2	1.75	0.66
32:2a:1347:G:H5''	40:2i:107:ARG:HB3	1.76	0.66
50:2s:38:SER:HB2	50:2s:71:LEU:HD22	1.76	0.66
1:1A:1143:A:OP2	62:1A:4223:HOH:O	2.14	0.66
1:2A:2206:G:H5''	1:2A:2207:G:N7	2.10	0.66
1:2A:2306:C:N4	6:2G:42:GLY:O	2.28	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1013:G:N2	32:2a:1016:A:OP2	2.28	0.66
36:2e:8:GLU:HG2	36:2e:34:VAL:HG23	1.77	0.66
38:2g:22:LEU:HG	38:2g:62:PHE:HE2	1.61	0.66
1:1A:2206:G:H3'	1:1A:2207:G:C8	2.29	0.66
5:2F:185:ASP:HA	5:2F:188:ARG:HD3	1.78	0.66
11:2P:39:LYS:HB2	11:2P:45:LEU:HD13	1.76	0.66
1:1A:1342:A:OP2	62:1A:4217:HOH:O	2.13	0.66
33:1b:30:ARG:HH21	33:1b:194:PRO:HB2	1.61	0.66
33:1b:33:TYR:HB2	33:1b:43:ASP:HB2	1.77	0.66
32:2a:1128:C:O2'	32:2a:1147:C:N3	2.24	0.66
41:2j:30:SER:O	41:2j:81:THR:OG1	2.13	0.66
1:1A:1453:U:OP1	13:1R:77:ARG:NH1	2.27	0.66
32:2a:737:A:H1'	37:2f:73:ASN:HD21	1.61	0.66
32:2a:976:G:H5'	32:2a:1358:U:O2'	1.95	0.66
33:2b:119:GLU:OE2	33:2b:153:ARG:NH1	2.29	0.66
1:1A:2469:A:O3'	12:1Q:56:ARG:NH1	2.29	0.66
34:1c:82:GLU:OE2	34:1c:85:ARG:NH1	2.29	0.66
5:2F:116:ASP:OD2	11:2P:1:MET:N	2.28	0.66
32:2a:661:G:H1	32:2a:744:C:H42	1.44	0.66
44:2m:84:ILE:HG13	44:2m:86:CYS:HB3	1.76	0.66
6:2G:63:ILE:HD11	6:2G:144:ILE:HG13	1.77	0.66
32:1a:613:C:H2'	32:1a:614:A:H8	1.61	0.66
32:1a:982:U:OP2	45:1n:23:ARG:NH2	2.29	0.66
32:1a:1414:U:H3	32:1a:1486:G:H1	1.44	0.66
1:2A:994:C:OP1	16:2U:53:ARG:NH2	2.28	0.66
32:2a:1178:G:N2	32:2a:1181:G:OP2	2.28	0.66
32:2a:1309:G:O3'	44:2m:77:ASN:ND2	2.29	0.66
35:2d:72:GLU:OE2	35:2d:207:TYR:OH	2.13	0.66
1:1A:1113:U:H2'	1:1A:1114:G:H8	1.61	0.66
1:1A:2033:A:OP1	62:1A:4227:HOH:O	2.14	0.65
1:2A:1141:U:OP2	9:2N:63:THR:OG1	2.14	0.65
1:2A:1507:A:O2'	1:2A:1508:A:O4'	2.14	0.65
1:2A:2127:G:N2	1:2A:2161:C:C2	2.64	0.65
3:2D:2:ALA:N	3:2D:200:ASP:OD2	2.29	0.65
1:1A:2163:C:OP1	1:1A:2165:G:N2	2.29	0.65
1:2A:2343:C:HO2'	1:2A:2373:G:HO2'	1.43	0.65
45:2n:32:SER:O	45:2n:32:SER:OG	2.13	0.65
1:1A:882:G:H1	1:1A:894:C:H42	1.44	0.65
7:1H:86:GLU:HG3	7:1H:132:ARG:HH21	1.60	0.65
32:1a:542:G:OP1	35:1d:10:ARG:NH2	2.29	0.65
12:2Q:37:LEU:HD11	12:2Q:130:LYS:HB2	1.76	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:2e:122:GLU:O	36:2e:126:ARG:NH1	2.29	0.65
1:1A:2687:U:OP2	62:1A:4224:HOH:O	2.14	0.65
32:1a:1398:A:O2'	62:1a:1911:HOH:O	2.14	0.65
26:24:40:HIS:HB3	26:24:43:TYR:HB2	1.79	0.65
1:1A:2863:C:OP2	62:1A:4228:HOH:O	2.14	0.65
10:1O:2:ILE:HD12	10:1O:6:THR:HG21	1.78	0.65
32:1a:567:G:N3	62:1a:1938:HOH:O	2.30	0.65
34:1c:3:ASN:OD1	34:1c:3:ASN:N	2.29	0.65
40:2i:17:VAL:HA	40:2i:63:ILE:HG12	1.78	0.65
1:1A:2409:G:O2'	62:1A:4226:HOH:O	2.14	0.65
1:1A:2428:G:OP1	62:1A:4204:HOH:O	2.15	0.65
1:2A:1890:A:OP2	62:2A:3825:HOH:O	2.14	0.65
1:2A:2138:C:H2'	1:2A:2139:C:O4'	1.97	0.65
1:2A:2753:A:N3	31:29:15:LYS:NZ	2.44	0.65
32:2a:1330:U:H4'	44:2m:23:TYR:CZ	2.31	0.65
6:2G:69:ALA:HB3	6:2G:91:ARG:HH21	1.62	0.65
15:2T:60:THR:HG22	15:2T:77:PRO:HA	1.79	0.65
2:1B:105:A:OP1	21:1Z:72:ARG:NH1	2.29	0.65
21:2Z:23:LYS:HD2	21:2Z:40:ASP:HA	1.78	0.65
32:2a:236:G:O2'	48:2q:4:LYS:NZ	2.30	0.65
41:2j:44:VAL:HG23	41:2j:66:ARG:HB3	1.79	0.65
1:1A:2142:C:O2	1:1A:2149:G:N1	2.21	0.65
32:1a:1356:G:O6	62:1a:1908:HOH:O	2.12	0.65
1:2A:1313:U:OP1	62:2A:3826:HOH:O	2.14	0.65
1:2A:2042:A:OP1	62:2A:3827:HOH:O	2.14	0.65
1:1A:2102:U:H3	1:1A:2187:G:H1	1.45	0.64
23:11:2:SER:OG	62:11:201:HOH:O	2.14	0.64
24:12:17:SER:N	24:12:20:GLU:OE1	2.29	0.64
32:1a:118:U:O4	62:1a:1910:HOH:O	2.13	0.64
20:2Y:55:TYR:H	20:2Y:56:PRO:HD3	1.61	0.64
28:26:23:THR:OG1	28:26:24:GLU:N	2.28	0.64
32:2a:1387:G:H2'	32:2a:1388:C:C6	2.32	0.64
1:1A:1418:G:OP2	62:1A:4230:HOH:O	2.15	0.64
1:1A:2749:A:OP1	7:1H:3:ARG:NH1	2.31	0.64
26:14:46:GLN:O	26:14:48:ARG:N	2.29	0.64
32:1a:1118:C:OP1	40:1i:9:ARG:NH1	2.29	0.64
1:2A:1188:U:H4'	17:2V:79:VAL:HG22	1.80	0.64
33:2b:188:ALA:HB1	33:2b:192:SER:HB2	1.77	0.64
43:1l:52:LEU:O	43:1l:54:LYS:NZ	2.27	0.64
1:2A:2318:G:H21	14:2S:3:ARG:NE	1.96	0.64
1:2A:2801(A):A:H3'	1:2A:2802:G:H5'	1.79	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:2l:71:PRO:O	43:2l:102:ARG:NH1	2.28	0.64
2:1B:92:C:OP1	21:1Z:79:ARG:NH1	2.31	0.64
1:2A:2110:G:H3'	1:2A:2111:C:H5'	1.78	0.64
1:2A:2819:G:N7	62:2A:3873:HOH:O	2.29	0.64
17:2V:60:GLU:HB2	17:2V:97:LYS:HE2	1.77	0.64
32:2a:1412:C:H2'	32:2a:1413:A:C8	2.32	0.64
6:1G:126:ASP:HB3	6:1G:128:ARG:H	1.62	0.64
6:2G:15:VAL:HG21	6:2G:176:LEU:HD23	1.78	0.64
6:2G:146:TYR:HD2	44:2m:11:ARG:HH22	1.45	0.64
32:2a:582:U:OP1	46:2o:68:ARG:NH2	2.27	0.64
32:2a:1122:U:N3	32:2a:1123:A:N7	2.45	0.64
1:1A:2575:C:OP2	62:1A:4229:HOH:O	2.14	0.64
1:1A:2801(A):A:H1'	1:1A:2895:U:H1'	1.80	0.64
11:1P:39:LYS:HG3	11:1P:45:LEU:HD22	1.79	0.64
32:1a:1373:G:H5''	38:1g:36:LYS:HE2	1.79	0.64
41:1j:8:LEU:HD22	41:1j:96:ILE:HG22	1.79	0.64
10:2O:68:GLU:OE1	10:2O:78:ARG:NH1	2.31	0.64
32:2a:157:G:H1	32:2a:164:U:H3	1.44	0.64
42:2k:22:HIS:HB3	42:2k:29:ILE:HB	1.78	0.64
1:1A:1300:U:H4'	1:1A:1301:A:H5''	1.80	0.64
1:1A:2331:G:N7	62:1A:4292:HOH:O	2.29	0.64
32:1a:376:G:O3'	47:1p:5:ARG:NH1	2.29	0.64
33:2b:27:LYS:HB3	33:2b:194:PRO:HD2	1.79	0.64
34:2c:47:LEU:HD12	34:2c:68:VAL:HG11	1.80	0.64
3:1D:206:LEU:HD22	3:1D:211:ARG:HG2	1.80	0.64
37:1f:89:MET:HE1	49:1r:72:ARG:HB3	1.78	0.64
32:2a:1240:U:N3	38:2g:30:ILE:O	2.24	0.64
38:2g:108:ALA:HA	38:2g:111:ARG:HD2	1.79	0.64
1:1A:2156:G:H2'	1:1A:2157:G:C2	2.33	0.64
1:1A:2785:C:OP1	4:1E:41:LYS:NZ	2.31	0.64
10:1O:64:ARG:HG2	10:1O:79:PHE:CG	2.33	0.64
33:1b:166:ASP:HB3	33:1b:169:LYS:HB3	1.79	0.64
1:2A:925:C:H2'	1:2A:926:A:H8	1.61	0.64
1:2A:2788:C:OP1	4:2E:61:ARG:NH2	2.30	0.64
7:2H:159:GLU:HG3	7:2H:169:VAL:HG11	1.80	0.64
32:2a:442:C:H42	32:2a:492:G:H1	1.46	0.64
33:2b:98:LEU:HB2	33:2b:101:MET:HE3	1.78	0.64
34:2c:39:ILE:HG22	34:2c:43:LEU:HD11	1.80	0.64
48:2q:95:TYR:HA	48:2q:98:LEU:HD12	1.78	0.64
7:1H:121:ILE:HG13	7:1H:144:VAL:HG21	1.80	0.64
1:2A:1800:C:OP2	3:2D:183:ARG:NH2	2.30	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2705:A:OP2	62:2A:3830:HOH:O	2.15	0.64
7:2H:164:TYR:HB2	7:2H:167:GLU:HB2	1.79	0.64
19:2X:53:LYS:HB3	19:2X:82:GLN:HB3	1.80	0.64
32:2a:504:C:OP1	62:2a:1802:HOH:O	2.15	0.64
32:2a:1136:U:OP2	32:2a:1137:C:N4	2.30	0.64
39:1h:21:LYS:O	39:1h:65:TYR:OH	2.16	0.63
1:2A:2589:A:OP2	62:2A:3828:HOH:O	2.15	0.63
1:2A:2619:C:OP1	4:2E:152:LYS:NZ	2.31	0.63
35:1d:144:ASP:N	35:1d:144:ASP:OD1	2.29	0.63
4:2E:9:VAL:HB	15:2T:3:ARG:HG2	1.80	0.63
32:2a:1239:A:H62	32:2a:1299:A:N6	1.96	0.63
14:2S:35:ILE:H	14:2S:53:SER:HB3	1.63	0.63
25:13:44:ARG:O	25:13:48:GLU:HG3	1.97	0.63
33:1b:82:ARG:NH1	33:1b:92:TYR:OH	2.31	0.63
46:1o:74:ASP:HB3	46:1o:77:ARG:HB2	1.81	0.63
1:2A:1796:U:H2'	1:2A:1797:C:C6	2.33	0.63
2:2B:43:C:OP1	26:24:6:HIS:NE2	2.29	0.63
40:2i:8:GLY:HA2	40:2i:79:LEU:HD23	1.80	0.63
56:2y:14:A:H61	56:2y:21:A:H2	1.46	0.63
32:1a:642:A:N3	39:1h:113:SER:OG	2.23	0.63
28:26:12:GLU:OE2	28:26:19:ARG:NH1	2.31	0.63
32:2a:117:G:OP2	62:2a:1803:HOH:O	2.16	0.63
32:2a:1025:U:H3	32:2a:1036:G:H1	1.45	0.63
32:2a:1318:A:OP1	50:2s:3:ARG:NH2	2.24	0.63
25:13:7:LYS:HE3	25:13:32:GLN:HE21	1.62	0.63
32:1a:79:G:C6	32:1a:90:U:O2	2.52	0.63
32:2a:664:G:H22	32:2a:741:G:H1	1.45	0.63
41:2j:40:LEU:HB2	41:2j:69:ASN:HB3	1.79	0.63
44:2m:19:LEU:HD21	44:2m:56:LEU:HD21	1.78	0.63
34:1c:6:HIS:HD2	34:1c:8:ILE:H	1.46	0.63
5:2F:53:THR:HG23	5:2F:55:GLY:H	1.64	0.63
6:2G:15:VAL:HG22	6:2G:175:LEU:HB3	1.81	0.63
19:2X:50:LYS:HB3	19:2X:87:GLN:HE22	1.63	0.63
34:2c:50:ALA:HB1	34:2c:70:VAL:HG11	1.81	0.63
50:2s:13:ASP:HA	50:2s:16:LEU:HB3	1.81	0.63
6:1G:77:ILE:HG22	6:1G:80:PHE:H	1.62	0.63
32:1a:1270:C:OP2	52:1u:24:ARG:NH2	2.31	0.63
20:2Y:9:LYS:NZ	20:2Y:28:LYS:O	2.29	0.63
33:2b:19:HIS:ND1	33:2b:20:GLU:OE2	2.27	0.63
1:1A:2612:C:OP2	27:15:2:ALA:N	2.32	0.63
51:1t:22:ARG:O	51:1t:26:ASN:ND2	2.28	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:2E:116:VAL:HG13	4:2E:122:PHE:HB2	1.80	0.63
33:2b:219:VAL:HA	33:2b:222:ILE:HG12	1.80	0.63
1:1A:2136:C:C2	1:1A:2155:G:N2	2.67	0.62
12:1Q:20:ALA:HB2	21:1Z:79:ARG:HG3	1.81	0.62
41:1j:5:ARG:NH2	41:1j:73:ASP:OD2	2.28	0.62
33:2b:74:LYS:O	33:2b:78:GLN:NE2	2.32	0.62
1:1A:1588:C:H2'	1:1A:1589:C:H6	1.65	0.62
5:1F:53:THR:HG23	5:1F:55:GLY:H	1.63	0.62
13:1R:67:LEU:HD13	13:1R:76:VAL:HG21	1.81	0.62
50:1s:11:VAL:HG11	50:1s:16:LEU:HB2	1.82	0.62
1:2A:1420:U:O2'	1:2A:1421:G:OP1	2.11	0.62
35:2d:15:GLU:OE2	35:2d:66:ARG:NH1	2.33	0.62
40:2i:21:PRO:HA	40:2i:59:PHE:HA	1.81	0.62
1:1A:1991:U:H2'	1:1A:1992:G:H5''	1.81	0.62
2:1B:25:A:OP2	62:1B:301:HOH:O	2.15	0.62
10:1O:110:GLY:HA2	10:1O:112:MET:HE2	1.80	0.62
1:2A:322:A:OP2	5:2F:169:ASN:HB2	1.99	0.62
1:2A:2136:C:N4	1:2A:2155:G:H1	1.97	0.62
15:2T:30:VAL:HG22	15:2T:86:ILE:HG12	1.80	0.62
34:2c:44:GLU:HA	34:2c:52:LEU:HD23	1.82	0.62
36:2e:80:ILE:HG22	36:2e:91:LEU:HB2	1.81	0.62
49:1r:73:ALA:HB1	49:1r:79:LEU:HD13	1.81	0.62
1:2A:2327:A:H2'	1:2A:2328:A:C8	2.33	0.62
41:2j:78:ASN:O	41:2j:80:LYS:N	2.32	0.62
31:19:2:LYS:HE2	31:19:31:LYS:O	2.00	0.62
32:1a:1352:C:OP1	52:1u:3:LYS:NZ	2.28	0.62
35:1d:173:TRP:CD1	35:1d:173:TRP:H	2.18	0.62
21:2Z:4:ARG:NH2	21:2Z:66:SER:OG	2.32	0.62
32:2a:1212:U:H5'	32:2a:1213:A:C8	2.34	0.62
50:2s:27:GLU:OE1	50:2s:28:LYS:NZ	2.28	0.62
1:2A:1019:U:H3	1:2A:1142(A):A:H62	1.46	0.62
33:2b:52:GLU:O	33:2b:56:ARG:NH1	2.33	0.62
41:2j:8:LEU:HB3	41:2j:96:ILE:HG23	1.80	0.62
47:2p:5:ARG:HH21	47:2p:28:ARG:HA	1.62	0.62
21:2Z:98:MET:O	21:2Z:126:VAL:N	2.32	0.62
32:2a:289:G:OP2	62:2a:1803:HOH:O	2.16	0.62
37:2f:95:GLU:O	49:2r:32:ARG:NH1	2.33	0.62
1:1A:2839:G:H5'	13:1R:46:GLY:HA2	1.82	0.62
1:1A:1062:G:P	1:1A:1070:A:H1'	2.39	0.62
32:1a:410:G:OP1	35:1d:30:LYS:NZ	2.29	0.62
54:1w:60:U:H5''	54:1w:61:C:H5	1.63	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2291:U:OP1	1:2A:2380:C:O2'	2.15	0.62
1:1A:1076:C:O2'	1:1A:1077:A:N7	2.31	0.62
11:1P:124:LYS:HA	11:1P:144:GLU:HB3	1.82	0.62
1:1A:1174:A:H4'	1:1A:1175:U:OP1	1.98	0.61
42:2k:54:ARG:NH2	56:2y:39:PSU:H4'	2.15	0.61
32:1a:1292:U:OP2	38:1g:41:ARG:NH2	2.33	0.61
56:2y:14:A:O2'	56:2y:15:G:OP1	2.15	0.61
1:1A:952:G:OP1	12:1Q:16:ARG:NH2	2.33	0.61
1:1A:1039:G:H1	1:1A:1116:C:H42	1.48	0.61
1:1A:2503:2MA:H8	58:1A:4109:6IF:O	2.00	0.61
32:1a:598:U:H2'	32:1a:599:C:H6	1.65	0.61
1:2A:271(G):C:H2'	1:2A:271(H):G:C8	2.36	0.61
32:2a:794:A:OP1	62:2a:1804:HOH:O	2.16	0.61
21:1Z:11:GLU:O	21:1Z:36:LYS:NZ	2.30	0.61
1:2A:1652:A:OP1	13:2R:8:ARG:NH1	2.31	0.61
1:2A:1688:U:O2	1:2A:1700:A:H5'	2.00	0.61
1:2A:2135:A:C8	1:2A:2136:C:H5	2.17	0.61
1:2A:2206:G:H3'	1:2A:2207:G:H8	1.64	0.61
1:1A:2789:C:O2	1:1A:2894:G:N1	2.32	0.61
8:1I:38:LEU:HD23	8:1I:38:LEU:H	1.65	0.61
32:1a:1239:A:H62	32:1a:1299:A:N6	1.99	0.61
32:1a:69:G:H2'	32:1a:70:G:C8	2.36	0.61
32:1a:193:C:H2'	32:1a:194:C:H6	1.65	0.61
32:1a:582:U:OP1	46:1o:68:ARG:NH2	2.33	0.61
32:2a:972:C:O2'	41:2j:55:LYS:O	2.18	0.61
32:2a:1029:C:N4	32:2a:1032:G:H1	1.98	0.61
33:2b:92:TYR:CE2	33:2b:151:GLY:HA3	2.36	0.61
50:2s:11:VAL:O	50:2s:13:ASP:N	2.34	0.61
6:1G:3:LEU:O	6:1G:8:LYS:NZ	2.23	0.61
32:1a:1194:U:H4'	36:1e:22:GLY:HA2	1.83	0.61
32:2a:192:U:H4'	51:2t:57:ARG:HD2	1.80	0.61
32:2a:426:G:OP1	35:2d:38:TYR:OH	2.14	0.61
4:1E:36:ARG:NH1	4:1E:85:ASN:OD1	2.33	0.61
32:1a:1370:G:N7	62:1a:1939:HOH:O	2.31	0.61
22:20:15:ASP:OD1	22:20:16:SER:N	2.30	0.61
4:1E:105:THR:OG1	4:1E:199:ARG:NH2	2.34	0.61
40:1i:110:GLU:OE2	40:1i:113:LYS:NZ	2.31	0.61
42:1k:48:ILE:O	42:1k:50:TYR:N	2.34	0.61
1:2A:1345:C:OP2	62:2A:3832:HOH:O	2.16	0.61
35:2d:165:MET:SD	35:2d:168:ARG:HD2	2.40	0.61
35:2d:175:SER:HB3	35:2d:186:LEU:HD21	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:2h:7:ALA:O	39:2h:11:THR:OG1	2.18	0.61
32:2a:8:A:H5'	36:2e:101:ILE:HG22	1.83	0.61
32:2a:473:G:H2'	32:2a:474:G:H8	1.66	0.61
1:1A:602:G:O2'	1:1A:655:A:N6	2.34	0.60
33:1b:18:GLY:HA3	33:1b:42:ILE:HG13	1.83	0.60
39:1h:10:LEU:HD22	39:1h:83:ILE:HD11	1.82	0.60
48:1q:67:LYS:O	48:1q:68:ARG:HB2	1.99	0.60
1:2A:878:A:N6	1:2A:899:A:O2'	2.34	0.60
1:2A:2100:G:H2'	1:2A:2101:G:H8	1.64	0.60
1:2A:2431:U:OP1	62:2A:3831:HOH:O	2.16	0.60
8:2I:92:VAL:HG13	8:2I:120:ILE:HB	1.82	0.60
32:2a:35:G:O2'	43:2I:118:SER:O	2.17	0.60
32:2a:1005:A:H5''	32:2a:1006:C:C5	2.36	0.60
32:2a:1119:C:OP2	40:2i:9:ARG:NH2	2.32	0.60
32:2a:1387:G:H2'	32:2a:1388:C:H6	1.66	0.60
38:2g:133:GLY:HA2	38:2g:136:LYS:HB2	1.82	0.60
1:1A:1971:A:OP1	62:1A:4237:HOH:O	2.17	0.60
7:1H:3:ARG:HG2	7:1H:6:ARG:HE	1.67	0.60
33:2b:54:THR:HG23	33:2b:199:TYR:HB3	1.83	0.60
33:2b:155:LEU:HD11	33:2b:159:PRO:HG3	1.82	0.60
34:2c:120:VAL:HG22	34:2c:133:ALA:HB1	1.83	0.60
1:1A:1800:C:OP1	3:1D:260:ARG:NH2	2.34	0.60
4:1E:143:ASN:HD22	4:1E:147:PRO:HD2	1.66	0.60
54:1w:51:U:H2'	54:1w:52:G:C8	2.36	0.60
24:22:29:LYS:HG2	24:22:57:ILE:HD13	1.83	0.60
32:2a:562:C:H1'	43:2I:15:ARG:HB3	1.83	0.60
35:2d:108:LEU:HD21	35:2d:174:LEU:HB3	1.82	0.60
5:1F:165:ARG:HA	5:1F:168:ARG:HD2	1.82	0.60
11:1P:59:LEU:HD13	30:18:58:ILE:HD13	1.82	0.60
32:1a:674:G:H2'	32:1a:675:A:H8	1.67	0.60
49:1r:32:ARG:HA	49:1r:69:THR:HG21	1.83	0.60
56:1y:9:A:O3'	56:1y:45:U:O2'	2.19	0.60
37:2f:8:ILE:HD13	37:2f:26:ILE:HD13	1.82	0.60
48:1q:66:SER:O	48:1q:70:ARG:NH1	2.34	0.60
1:2A:958:U:OP2	12:2Q:14:ARG:NE	2.34	0.60
1:2A:1507:A:O2'	1:2A:1508:A:O5'	2.19	0.60
1:2A:1861:G:H1	1:2A:1881:C:H42	1.48	0.60
22:20:11:ARG:O	22:20:14:ARG:NH2	2.32	0.60
44:2m:60:VAL:HA	44:2m:63:THR:HB	1.83	0.60
1:1A:2128:C:N4	1:1A:2161:C:N3	2.49	0.60
43:1I:71:PRO:O	43:1I:102:ARG:NH1	2.34	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:1o:39:LEU:HD13	46:1o:56:LEU:HB2	1.83	0.60
2:2B:3:C:H2'	2:2B:4:C:C6	2.37	0.60
6:2G:38:VAL:HG22	6:2G:93:THR:HG23	1.84	0.60
12:2Q:32:TYR:OH	12:2Q:111:GLU:OE2	2.19	0.60
19:2X:60:ARG:HH22	29:27:47:ARG:HH22	1.47	0.60
26:24:46:GLN:C	26:24:48:ARG:H	2.10	0.60
32:2a:1055:A:N7	32:2a:1200:C:N4	2.47	0.60
51:2t:56:MET:HG3	51:2t:88:VAL:HG21	1.84	0.60
1:2A:974:G:OP1	1:2A:1187:G:O2'	2.16	0.60
32:2a:148:G:H2'	32:2a:149:A:H8	1.65	0.60
44:2m:37:THR:HG21	44:2m:56:LEU:HD13	1.82	0.60
1:1A:1827:C:C2'	1:1A:1828:G:H5'	2.32	0.60
1:1A:2646:C:H2'	1:1A:2647:U:O4'	2.01	0.60
21:1Z:7:ALA:HB2	21:1Z:59:LEU:HD22	1.84	0.60
40:1i:128:ARG:NH2	55:1x:33:U:OP2	2.35	0.60
1:2A:1670:C:OP1	62:2A:3833:HOH:O	2.16	0.60
32:2a:742:G:OP2	46:2o:35:ARG:NH2	2.27	0.60
32:2a:913:A:OP1	43:2l:46:LYS:NZ	2.34	0.60
32:2a:1261:A:O2'	32:2a:1283:G:OP1	2.14	0.60
1:1A:1027:A:N3	62:1A:4300:HOH:O	2.31	0.60
1:1A:1044:G:H5'	1:1A:1045:A:OP2	2.02	0.60
1:1A:2023:G:H5'	1:1A:2617:C:H4'	1.83	0.60
2:1B:66:A:H61	2:1B:108:U:H2'	1.67	0.60
19:1X:31:HIS:CD2	19:1X:33:LYS:H	2.20	0.60
28:26:32:ASN:N	28:26:32:ASN:OD1	2.34	0.60
32:2a:839:U:H3'	32:2a:840:C:H5'	1.84	0.60
32:2a:1305:G:N2	32:2a:1331:G:H1'	2.17	0.60
19:1X:31:HIS:HD2	19:1X:33:LYS:H	1.50	0.60
32:1a:673:G:H2'	32:1a:674:G:C8	2.37	0.60
32:1a:920:U:H2'	32:1a:921:U:C6	2.36	0.60
32:1a:1531:A:H8	32:1a:1531:A:O5'	1.85	0.60
1:2A:1778:U:OP1	62:2A:3834:HOH:O	2.17	0.60
10:2O:64:ARG:NH1	10:2O:81:ASP:OD2	2.35	0.60
32:2a:1368:G:OP1	40:2i:111:ARG:NH2	2.34	0.60
44:2m:34:LEU:HD13	44:2m:41:PRO:HB3	1.83	0.60
49:2r:31:LEU:HD23	49:2r:31:LEU:H	1.67	0.60
1:1A:1399:C:OP1	19:1X:25:LYS:NZ	2.35	0.59
1:1A:2328:A:H2'	1:1A:2329:G:C8	2.37	0.59
1:1A:2406:U:OP1	62:1A:4236:HOH:O	2.17	0.59
1:2A:1665:A:OP2	62:2A:3829:HOH:O	2.15	0.59
5:2F:184:TYR:CE2	5:2F:188:ARG:HD2	2.37	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:2I:69:LYS:HG3	8:2I:138:ILE:HG12	1.83	0.59
19:2X:35:THR:HG22	19:2X:38:GLU:H	1.66	0.59
1:1A:1796:U:H2'	1:1A:1797:C:C6	2.37	0.59
3:1D:72:LYS:NZ	3:1D:99:ASP:OD2	2.30	0.59
9:1N:73:THR:HG22	9:1N:84:LYS:HG2	1.84	0.59
46:1o:54:ARG:HG2	46:1o:58:MET:HE2	1.84	0.59
1:2A:1803:A:O2'	3:2D:259:THR:HG21	2.01	0.59
6:2G:32:PRO:HB2	6:2G:172:LEU:HD13	1.83	0.59
7:2H:25:LYS:HD2	7:2H:34:GLU:HG2	1.85	0.59
1:1A:530:G:OP2	62:1A:4235:HOH:O	2.17	0.59
26:14:55:ARG:N	26:14:56:VAL:HA	2.18	0.59
32:1a:1021:G:O2'	32:1a:1022:G:O5'	2.12	0.59
1:2A:2183:C:H2'	1:2A:2184:G:H8	1.67	0.59
7:2H:113:VAL:HG11	7:2H:151:ILE:HD13	1.84	0.59
2:2B:11:C:OP2	2:2B:12:C:N4	2.32	0.59
15:2T:127:ALA:C	15:2T:129:ARG:H	2.10	0.59
34:2c:7:PRO:HB2	34:2c:182:ILE:HD11	1.84	0.59
50:2s:28:LYS:HB3	50:2s:29:ARG:CB	2.33	0.59
1:1A:2384:G:N7	62:1A:4304:HOH:O	2.32	0.59
15:1T:16:ARG:NH1	15:1T:83:ILE:O	2.26	0.59
25:13:18:ASP:OD1	25:13:18:ASP:N	2.31	0.59
36:1e:18:ARG:HH11	36:1e:27:ARG:HH12	1.49	0.59
1:2A:1181:C:H2'	1:2A:1182:A:C8	2.37	0.59
12:2Q:16:ARG:HG2	12:2Q:18:LYS:HE2	1.84	0.59
12:2Q:60:ARG:NH1	54:2w:54:5MU:OP2	2.35	0.59
32:2a:1279:A:H4'	32:2a:1280:A:OP1	2.03	0.59
14:1S:20:ARG:NH2	22:10:51:VAL:O	2.35	0.59
32:1a:1391:U:H2'	32:1a:1392:G:C8	2.37	0.59
26:24:46:GLN:HG2	26:24:48:ARG:H	1.68	0.59
32:2a:653:A:OP1	39:2h:56:LYS:NZ	2.23	0.59
32:2a:1353:G:OP1	52:2u:10:ARG:NH1	2.35	0.59
34:2c:125:GLU:HB2	34:2c:190:ARG:HH21	1.67	0.59
1:1A:2344:U:OP1	28:16:37:ARG:NH1	2.35	0.59
32:1a:953:G:H5'	32:1a:965:A:H61	1.67	0.59
36:1e:110:LEU:HD13	36:1e:118:ILE:HG21	1.84	0.59
1:2A:2121:G:H1	1:2A:2177:C:H42	1.51	0.59
1:2A:2136:C:N3	1:2A:2155:G:N2	2.47	0.59
2:2B:15:A:OP2	2:2B:69:G:N2	2.35	0.59
6:2G:108:ASN:HA	26:24:37:SER:HB2	1.85	0.59
8:2I:81:VAL:O	8:2I:146:ALA:HA	2.02	0.59
32:2a:406:G:H21	35:2d:119:GLN:HE22	1.51	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:947:G:O3'	44:2m:109:THR:OG1	2.20	0.59
32:2a:1010:G:N2	32:2a:1020:U:O2'	2.35	0.59
33:2b:17:PHE:HA	33:2b:44:LEU:HD11	1.85	0.59
1:1A:1057:A:N6	1:1A:1087:G:OP1	2.35	0.59
46:1o:25:THR:HG21	46:1o:70:LEU:HB2	1.84	0.59
32:2a:921:U:O2	36:2e:19:MET:HB2	2.02	0.59
34:2c:164:ARG:NH2	34:2c:166:GLU:OE2	2.35	0.59
41:2j:47:PHE:N	41:2j:63:PHE:O	2.29	0.59
55:2x:40:C:H2'	55:2x:41:C:H6	1.68	0.59
1:1A:998:C:OP1	62:1A:4232:HOH:O	2.16	0.59
6:1G:122:PRO:HG3	6:1G:182:LYS:H	1.68	0.59
47:1p:60:LEU:HD11	47:1p:66:PRO:HD3	1.85	0.59
3:2D:8:PRO:HB3	3:2D:14:ARG:HG3	1.85	0.59
10:2O:115:VAL:HG13	10:2O:121:VAL:HG21	1.84	0.59
36:2e:110:LEU:HD13	36:2e:118:ILE:HD13	1.84	0.59
1:1A:8:A:H2'	1:1A:9:U:C6	2.37	0.59
1:1A:1779:U:OP2	62:1A:4231:HOH:O	2.16	0.59
8:1I:4:ILE:HG12	8:1I:18:VAL:HG22	1.83	0.59
1:2A:276:A:H5''	1:2A:277:C:H5'	1.84	0.59
1:2A:890:A:H2'	1:2A:892:G:H8	1.68	0.59
34:2c:58:GLU:HB3	41:2j:92:THR:HG21	1.85	0.59
1:1A:2121:G:O6	1:1A:2176:A:N6	2.36	0.58
6:1G:11:TYR:OH	6:1G:32:PRO:O	2.20	0.58
33:2b:216:SER:O	33:2b:220:ASP:N	2.28	0.58
42:2k:86:GLY:H	42:2k:112:THR:HG1	1.50	0.58
43:2l:39:VAL:HB	43:2l:57:LYS:HB2	1.85	0.58
1:1A:1405:U:H2'	1:1A:1406:U:C6	2.39	0.58
56:1y:19:G:N2	56:1y:56:C:N3	2.52	0.58
8:2I:93:THR:HG22	8:2I:119:PRO:HB3	1.85	0.58
32:2a:920:U:H2'	32:2a:921:U:C6	2.38	0.58
1:1A:668:G:H5'	1:1A:669:G:OP2	2.02	0.58
1:1A:1786:A:H1'	1:1A:1938:A:N6	2.17	0.58
23:11:18:ILE:HG12	23:11:37:ILE:HG12	1.86	0.58
1:2A:2683:C:O2	10:2O:70:LYS:NZ	2.30	0.58
26:24:10:VAL:HG13	26:24:12:ALA:HB2	1.85	0.58
32:2a:1132:C:H2'	32:2a:1133:G:C8	2.38	0.58
33:2b:178:ARG:HH22	39:2h:68:ARG:HH22	1.52	0.58
1:1A:1356:G:OP2	62:1A:4233:HOH:O	2.16	0.58
1:1A:1371:G:O6	62:1A:4225:HOH:O	2.14	0.58
1:1A:2139:C:N4	1:1A:2152:G:H1	2.00	0.58
1:1A:2185:C:H2'	1:1A:2186:G:C8	2.38	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1500:A:OP1	62:1a:1913:HOH:O	2.16	0.58
51:1t:57:ARG:HH12	51:1t:100:ILE:HD12	1.69	0.58
1:2A:1593:G:H2'	1:2A:1594:G:C8	2.38	0.58
15:2T:26:ASP:OD1	15:2T:120:ARG:NH2	2.35	0.58
32:2a:936:C:H2'	32:2a:937:A:O4'	2.04	0.58
44:2m:91:ARG:HB2	44:2m:98:VAL:HG13	1.86	0.58
15:1T:127:ALA:C	15:1T:129:ARG:H	2.11	0.58
34:1c:181:ASN:HD21	34:1c:204:LEU:HD12	1.68	0.58
36:1e:78:HIS:HD2	39:1h:104:ARG:HD2	1.67	0.58
1:2A:1264:G:OP1	27:25:19:ARG:NH2	2.32	0.58
2:2B:75:G:N2	21:2Z:87:ASP:OD1	2.36	0.58
3:2D:180:GLY:HA3	3:2D:275:LYS:HG2	1.86	0.58
8:2I:93:THR:OG1	8:2I:96:ASP:OD1	2.18	0.58
49:2r:53:ARG:HA	49:2r:56:THR:HG1	1.68	0.58
1:1A:2787:C:H1'	4:1E:62:PRO:HG3	1.84	0.58
1:1A:2790:A:H3'	1:1A:2790:A:N3	2.18	0.58
5:1F:125:LEU:HD23	5:1F:194:MET:HB2	1.86	0.58
36:1e:10:MET:HE2	36:1e:13:ILE:HD11	1.86	0.58
1:2A:2404:C:O3'	11:2P:77:ARG:NH2	2.36	0.58
41:2j:6:ILE:HG12	41:2j:98:ILE:HG13	1.86	0.58
41:2j:64:GLU:OE2	41:2j:66:ARG:NE	2.34	0.58
1:1A:2810:A:N6	1:1A:2891:G:O2'	2.35	0.58
32:1a:123:C:OP1	32:1a:311:C:O2'	2.19	0.58
1:2A:1156:A:OP2	62:2A:3837:HOH:O	2.17	0.58
17:2V:98:GLU:OE2	17:2V:100:ARG:NH1	2.36	0.58
34:2c:123:GLN:O	34:2c:128:PHE:HB2	2.03	0.58
40:2i:85:LEU:HB3	40:2i:92:TYR:HD2	1.68	0.58
48:2q:57:VAL:HG12	48:2q:76:LEU:HA	1.84	0.58
32:1a:1025:U:C2	32:1a:1036:G:O6	2.57	0.58
1:2A:852:G:H2'	1:2A:853:G:C8	2.34	0.58
32:2a:1366:C:H2'	32:2a:1367:C:C6	2.39	0.58
34:2c:123:GLN:HA	34:2c:126:ARG:HD2	1.85	0.58
1:1A:1113:U:H2'	1:1A:1114:G:C8	2.37	0.58
1:1A:1827:C:H2'	1:1A:1828:G:H5'	1.85	0.58
32:1a:755:G:OP2	46:1o:65:ARG:HD2	2.03	0.58
34:1c:131:ARG:HH11	34:1c:166:GLU:HG3	1.67	0.58
36:1e:79:GLU:HG3	36:1e:93:PRO:HD2	1.85	0.58
44:1m:34:LEU:HD13	44:1m:41:PRO:HA	1.86	0.58
47:1p:4:ILE:HB	47:1p:66:PRO:HA	1.85	0.58
10:2O:35:VAL:HG23	10:2O:65:THR:HG23	1.85	0.58
32:2a:397:A:N7	32:2a:547:A:O2'	2.36	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:707:C:H2'	32:2a:708:C:C6	2.38	0.58
39:2h:28:ALA:HB3	39:2h:57:PRO:HB2	1.86	0.58
32:1a:1328:C:OP2	52:1u:7:ARG:NH1	2.36	0.58
33:1b:84:GLU:OE1	33:1b:87:ARG:NH1	2.37	0.58
6:2G:43:LEU:HD21	6:2G:153:ARG:HD2	1.85	0.58
9:2N:58:ASP:N	9:2N:58:ASP:OD1	2.37	0.58
14:2S:67:ARG:O	14:2S:71:ARG:HG3	2.04	0.58
32:2a:909:A:N3	32:2a:1413:A:O2'	2.30	0.58
1:1A:1087:G:H2'	1:1A:1089:G:C8	2.38	0.57
1:1A:1688:U:O2	1:1A:1700:A:H5'	2.04	0.57
3:1D:71:ASP:HB2	3:1D:103:ARG:HH12	1.69	0.57
21:1Z:23:LYS:HD3	21:1Z:40:ASP:HA	1.86	0.57
32:1a:79:G:O6	32:1a:90:U:C2	2.56	0.57
38:1g:22:LEU:HG	38:1g:62:PHE:HE2	1.68	0.57
1:2A:2317:C:N4	1:2A:2318:G:O6	2.37	0.57
7:2H:51:ARG:HH12	7:2H:53:GLU:HG2	1.67	0.57
44:2m:13:LYS:HA	44:2m:44:ARG:HH11	1.69	0.57
1:1A:2141:G:O6	1:1A:2150:U:O2	2.22	0.57
5:1F:116:ASP:OD1	5:1F:119:ARG:NH2	2.36	0.57
1:2A:779:U:O4	62:2A:3836:HOH:O	2.17	0.57
1:2A:2328:A:H2'	1:2A:2329:G:C8	2.39	0.57
21:2Z:154:ASP:OD1	21:2Z:154:ASP:N	2.28	0.57
32:2a:890:G:O2'	32:2a:906:G:O6	2.18	0.57
36:2e:6:PHE:HB3	36:2e:34:VAL:HG22	1.86	0.57
36:2e:92:LYS:HB3	36:2e:119:LEU:HB2	1.84	0.57
38:2g:153:HIS:CE1	42:2k:58:PRO:HD2	2.39	0.57
44:2m:86:CYS:O	44:2m:89:GLY:N	2.33	0.57
1:2A:987:G:O2'	1:2A:1000:A:N3	2.36	0.57
17:2V:10:LYS:NZ	17:2V:23:GLU:OE2	2.37	0.57
32:2a:997:U:H3	32:2a:1044:A:H61	1.52	0.57
32:2a:1119:C:H2'	32:2a:1120:G:H8	1.68	0.57
32:2a:1257:U:O4	45:2n:17:LYS:NZ	2.37	0.57
34:2c:125:GLU:O	34:2c:190:ARG:NH2	2.38	0.57
5:1F:185:ASP:HA	5:1F:188:ARG:HD3	1.86	0.57
34:1c:56:ASP:HB2	34:1c:67:THR:HB	1.86	0.57
1:2A:674:G:H1'	5:2F:74:ARG:HD3	1.86	0.57
1:2A:2114:A:H2	1:2A:2171:A:N6	2.02	0.57
10:2O:76:ALA:HB3	15:2T:75:ILE:HB	1.87	0.57
32:2a:297:G:N2	32:2a:300:A:OP2	2.38	0.57
32:2a:1326:C:OP1	52:2u:17:THR:OG1	2.18	0.57
36:2e:87:SER:OG	36:2e:125:SER:O	2.17	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2106:G:H1	1:1A:2183:C:H42	1.51	0.57
1:1A:2134:A:O2'	1:1A:2135:A:OP1	2.20	0.57
32:1a:1300:G:N7	62:1a:1944:HOH:O	2.32	0.57
46:1o:11:VAL:HG21	46:1o:34:LEU:HD22	1.86	0.57
50:1s:31:ILE:O	50:1s:50:ALA:N	2.31	0.57
32:2a:280:C:N3	48:2q:39:SER:OG	2.37	0.57
32:1a:67:C:H2'	32:1a:68:G:C8	2.39	0.57
32:1a:955:U:O4	62:1a:1912:HOH:O	2.15	0.57
32:1a:1005:A:OP2	32:1a:1024:G:N2	2.37	0.57
1:2A:652(A):A:H3'	1:2A:652(B):A:H5''	1.86	0.57
1:2A:2184:G:H2'	1:2A:2185:C:C6	2.40	0.57
1:2A:2292:C:OP1	14:2S:17:ARG:NH2	2.35	0.57
15:2T:117:ASP:OD2	15:2T:120:ARG:NE	2.33	0.57
17:2V:43:GLU:OE1	17:2V:43:GLU:N	2.38	0.57
32:2a:19:C:H5''	36:2e:86:ALA:HB1	1.87	0.57
32:2a:1128:C:H1'	32:2a:1147:C:H42	1.68	0.57
32:2a:1275:A:H3'	32:2a:1276:G:H8	1.70	0.57
32:1a:324:G:N7	62:1a:1945:HOH:O	2.33	0.57
32:1a:869:G:OP2	62:1a:1914:HOH:O	2.18	0.57
1:2A:1033:U:OP1	31:29:9:ARG:NH2	2.35	0.57
1:2A:1889:A:H2'	1:2A:1890:A:C8	2.40	0.57
10:2O:20:MET:HE3	10:2O:44:LYS:HE3	1.87	0.57
15:2T:29:ARG:HB3	15:2T:87:ASP:HB2	1.86	0.57
32:2a:1182:G:H4'	32:2a:1183:A:H5''	1.85	0.57
38:2g:54:THR:O	38:2g:56:GLN:N	2.38	0.57
37:1f:10:LEU:HD23	37:1f:61:LEU:HD13	1.87	0.57
41:1j:49:VAL:HG23	45:1n:41:ARG:HB2	1.87	0.57
1:2A:2316:C:O2'	6:2G:128:ARG:NH2	2.34	0.57
35:2d:15:GLU:HB3	35:2d:63:LYS:HG2	1.85	0.57
1:1A:1358:G:OP2	62:1A:4241:HOH:O	2.18	0.57
1:1A:2567:G:H2'	1:1A:2568:C:C6	2.39	0.57
8:1I:38:LEU:HD11	23:11:75:GLU:HG3	1.85	0.57
32:1a:474:G:H5'	32:1a:475:G:OP2	2.05	0.57
32:1a:757:U:H2'	32:1a:758:G:O4'	2.04	0.57
1:2A:646:A:H2'	1:2A:647:G:O4'	2.04	0.57
1:2A:1919:A:O2'	32:2a:1517:G:N3	2.37	0.57
32:2a:417:C:H2'	32:2a:418:C:C6	2.39	0.57
34:2c:36:ASP:HA	34:2c:39:ILE:HD12	1.86	0.57
4:1E:97:LYS:N	4:1E:100:GLU:OE2	2.36	0.57
49:1r:38:GLU:HA	49:1r:41:LYS:HE2	1.87	0.57
1:2A:888:C:OP1	44:2m:93:ARG:NH1	2.37	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2376:A:N3	14:2S:106:ARG:NH2	2.53	0.57
1:2A:2537:U:H2'	1:2A:2538:C:C6	2.40	0.57
21:2Z:45:ASP:OD1	21:2Z:49:ARG:NE	2.38	0.57
32:2a:673:G:O3'	37:2f:87:ARG:NH2	2.38	0.57
32:2a:1360:A:OP2	45:2n:35:ARG:NH2	2.38	0.57
36:2e:43:LEU:HD11	36:2e:132:ALA:HB1	1.87	0.57
3:1D:183:ARG:HG3	3:1D:270:ILE:HD13	1.87	0.56
5:2F:155:LEU:HB2	5:2F:189:THR:HG21	1.86	0.56
6:2G:145:THR:HG22	6:2G:146:TYR:H	1.70	0.56
32:2a:674:G:H2'	32:2a:675:A:H8	1.70	0.56
1:2A:614(B):G:H2'	5:2F:44:ARG:HH11	1.70	0.56
1:2A:2125:G:H1'	1:2A:2173:A:N6	2.20	0.56
4:2E:9:VAL:HG22	4:2E:25:VAL:HB	1.86	0.56
14:2S:10:ARG:HH21	14:2S:91:PRO:HB2	1.70	0.56
32:2a:404:U:H2'	32:2a:405:U:C6	2.40	0.56
32:2a:1414:U:H3	32:2a:1486:G:H1	1.52	0.56
40:2i:50:LEU:HD12	40:2i:51:ARG:HG3	1.87	0.56
47:2p:53:VAL:HG23	47:2p:79:VAL:HG22	1.86	0.56
1:1A:579:G:H2'	1:1A:580:C:C6	2.41	0.56
5:1F:133:ASN:N	5:1F:138:GLU:OE1	2.32	0.56
7:1H:154:PRO:HB3	7:1H:163:TYR:CZ	2.41	0.56
11:1P:50:ARG:HD3	30:18:7:HIS:CD2	2.40	0.56
17:1V:43:GLU:OE1	17:1V:43:GLU:N	2.37	0.56
32:1a:848:C:H2'	32:1a:849:C:H6	1.70	0.56
33:1b:61:LEU:HD11	33:1b:160:ASP:HB2	1.87	0.56
38:1g:70:LYS:HG2	38:1g:96:GLN:HB3	1.87	0.56
42:1k:29:ILE:HG23	42:1k:44:SER:HB3	1.87	0.56
42:1k:82:VAL:HB	42:1k:108:ILE:HG13	1.88	0.56
47:1p:53:VAL:HG13	47:1p:79:VAL:HG22	1.86	0.56
54:1w:51:U:H2'	54:1w:52:G:H8	1.71	0.56
56:1y:18:G:O2'	56:1y:57:G:O6	2.19	0.56
1:2A:1579:A:H2'	1:2A:1580:A:C8	2.39	0.56
1:2A:2127:G:C2	1:2A:2161:C:C4	2.93	0.56
1:2A:2176:A:H2'	1:2A:2177:C:C6	2.39	0.56
32:2a:130:A:N3	32:2a:263:A:O2'	2.33	0.56
32:2a:352:C:O2'	32:2a:354:G:OP1	2.23	0.56
32:2a:1190:G:O2'	34:2c:3:ASN:HB2	2.05	0.56
32:2a:1263:C:C4	32:2a:1272:G:O6	2.57	0.56
33:2b:164:VAL:HG23	33:2b:186:ALA:HB2	1.86	0.56
38:2g:65:ALA:HB1	38:2g:127:ALA:HB3	1.87	0.56
46:2o:70:LEU:HD11	46:2o:77:ARG:HB3	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:956:G:O6	62:1A:4234:HOH:O	2.16	0.56
1:1A:1701:A:OP2	62:1A:4243:HOH:O	2.18	0.56
1:2A:307:G:N1	1:2A:310:A:OP2	2.37	0.56
1:2A:307:G:H21	1:2A:330:A:H62	1.52	0.56
1:2A:2637:U:OP1	4:2E:82:ARG:NH1	2.39	0.56
6:2G:17:PRO:HA	6:2G:20:ILE:HD12	1.86	0.56
21:2Z:48:PHE:CE1	21:2Z:52:SER:HA	2.41	0.56
32:2a:533:A:O2'	32:2a:535:A:OP2	2.19	0.56
32:2a:1272:G:N2	32:2a:1273:G:C8	2.72	0.56
1:1A:81:G:HO2'	1:1A:295:G:HO2'	1.52	0.56
1:1A:1173:G:N1	1:1A:1176:G:OP2	2.37	0.56
1:1A:2128:C:N3	1:1A:2160:G:N2	2.53	0.56
1:1A:2777:G:O6	62:1A:4239:HOH:O	2.17	0.56
32:1a:270:A:H2'	32:1a:271:C:C6	2.41	0.56
32:2a:1060:C:H5''	41:2j:51:ARG:HG2	1.88	0.56
33:2b:150:SER:OG	33:2b:151:GLY:N	2.38	0.56
34:2c:52:LEU:HD12	34:2c:53:ALA:H	1.70	0.56
1:1A:2126:A:N3	1:1A:2127:G:H1'	2.20	0.56
1:2A:2130:U:H3	1:2A:2159:G:H1	1.54	0.56
1:2A:2320:A:H1'	1:2A:2321:G:C2	2.40	0.56
32:2a:417:C:H2'	32:2a:418:C:H6	1.71	0.56
32:2a:564:C:HO2'	39:2h:91:ARG:HH22	1.50	0.56
32:2a:953:G:H5'	32:2a:965:A:N6	2.20	0.56
33:2b:88:ALA:HB2	33:2b:219:VAL:HG13	1.87	0.56
1:1A:286:C:H2'	1:1A:287:C:C6	2.41	0.56
1:1A:1047:G:H2'	1:1A:1110:G:H22	1.70	0.56
1:1A:2185:C:H2'	1:1A:2186:G:H8	1.70	0.56
1:1A:2336:A:H61	22:10:43:THR:CG2	2.18	0.56
10:1O:48:PRO:HB3	32:1a:1422:G:H5''	1.88	0.56
17:1V:74:LYS:HB2	17:1V:83:ARG:HB2	1.87	0.56
26:14:53:GLU:CD	26:14:54:GLY:H	2.14	0.56
33:1b:119:GLU:HG3	33:1b:153:ARG:HH12	1.70	0.56
36:1e:69:VAL:HG11	36:1e:113:ALA:HB1	1.88	0.56
38:1g:78:ARG:HE	38:1g:79:ARG:HE	1.53	0.56
49:1r:52:PRO:HB2	49:1r:54:ARG:HG2	1.88	0.56
1:2A:2133:G:O2'	1:2A:2157:G:N2	2.38	0.56
2:2B:13:A:N1	2:2B:69:G:O2'	2.34	0.56
32:2a:448:A:P	32:2a:485:G:H22	2.28	0.56
32:2a:1226:C:O2'	44:2m:111:LYS:NZ	2.36	0.56
1:1A:1045:A:OP1	1:1A:1045:A:H4'	2.06	0.56
1:2A:1450:G:H1	1:2A:1462:C:H42	1.53	0.56

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	2.41	0.56
1:2A:2191:G:H2'	1:2A:2192:G:O4'	2.06	0.56
32:2a:539:A:H2'	32:2a:540:G:C8	2.40	0.56
44:2m:73:GLU:O	44:2m:77:ASN:HB2	2.06	0.56
1:1A:588:U:H2'	1:1A:589:C:C6	2.40	0.56
1:1A:2136:C:N4	1:1A:2155:G:H1	2.04	0.56
9:1N:73:THR:HB	9:1N:82:LEU:HD11	1.87	0.56
41:1j:65:LEU:HD13	45:1n:56:VAL:HG13	1.87	0.56
1:2A:2136:C:N4	1:2A:2155:G:N1	2.54	0.56
1:2A:2880:C:O3'	13:2R:90:ARG:NH1	2.39	0.56
30:28:14:VAL:HG13	30:28:22:VAL:HG13	1.88	0.56
32:2a:1411:C:H2'	32:2a:1412:C:C6	2.41	0.56
35:2d:15:GLU:OE2	35:2d:59:ARG:NH1	2.38	0.56
46:2o:25:THR:HG21	46:2o:70:LEU:HB2	1.88	0.56
20:1Y:102:CYS:SG	20:1Y:103:GLY:N	2.79	0.56
34:1c:125:GLU:HG3	34:1c:189:ALA:HB1	1.87	0.56
1:2A:301:G:OP2	20:2Y:84:ARG:NH2	2.36	0.56
1:2A:1769:G:O2'	1:2A:1958:C:OP1	2.24	0.56
6:2G:39:ILE:HG13	6:2G:157:ILE:HG23	1.88	0.56
26:24:60:GLN:O	26:24:62:ARG:NH1	2.38	0.56
32:2a:1245:A:H2'	32:2a:1246:C:O4'	2.06	0.56
42:2k:14:VAL:HG11	42:2k:35:PRO:HD3	1.88	0.56
50:2s:32:LYS:HB3	50:2s:57:HIS:CE1	2.41	0.56
1:1A:887:A:H2	1:1A:889:C:H3'	1.71	0.55
1:1A:1406:U:H2'	1:1A:1407:C:C6	2.41	0.55
1:1A:2305:A:H5''	6:1G:134:GLY:HA3	1.87	0.55
21:1Z:1:MET:H2	21:1Z:3:TYR:HE2	1.54	0.55
32:1a:1346:A:N1	32:1a:1374:A:H5''	2.20	0.55
21:2Z:54:HIS:NE2	21:2Z:123:ASP:OD2	2.34	0.55
44:2m:107:ALA:HB3	44:2m:111:LYS:HE3	1.87	0.55
56:2y:30:G:H2'	56:2y:31:A:H8	1.71	0.55
1:1A:1178:C:H2'	1:1A:1179:C:C6	2.42	0.55
1:2A:285:C:H42	1:2A:356:G:H1	1.54	0.55
1:2A:524:U:H2'	1:2A:525:U:C6	2.42	0.55
1:2A:900:A:O2'	1:2A:901:A:OP1	2.23	0.55
2:2B:1:U:H2'	2:2B:2:C:H6	1.71	0.55
6:2G:33:ARG:O	6:2G:161:THR:HG23	2.05	0.55
11:2P:92:GLU:OE2	11:2P:121:LYS:NZ	2.25	0.55
32:2a:56:U:H2'	32:2a:57:G:C8	2.41	0.55
32:2a:148:G:H2'	32:2a:149:A:C8	2.42	0.55
32:2a:1268:A:N3	32:2a:1326:C:O2'	2.37	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:2b:223:ILE:HA	33:2b:226:ARG:HD3	1.88	0.55
37:2f:69:GLU:O	37:2f:72:VAL:HG12	2.06	0.55
7:1H:17:VAL:HG11	7:1H:50:VAL:HG11	1.88	0.55
1:2A:903:C:H2'	1:2A:904:C:C6	2.41	0.55
1:2A:2035:G:OP1	62:2A:3840:HOH:O	2.18	0.55
12:2Q:110:THR:HB	12:2Q:113:GLN:H	1.70	0.55
28:26:25:LYS:HE3	28:26:27:LYS:HA	1.88	0.55
33:2b:74:LYS:NZ	33:2b:206:ASP:OD1	2.39	0.55
1:1A:1587:A:H2'	1:1A:1588:C:C6	2.42	0.55
5:1F:101:LEU:HD23	5:1F:106:ARG:HG3	1.88	0.55
7:1H:33:LEU:HD21	7:1H:136:ILE:HG13	1.88	0.55
32:1a:37:U:O2'	32:1a:547:A:N1	2.40	0.55
48:1q:57:VAL:HG12	48:1q:76:LEU:HA	1.88	0.55
7:2H:56:SER:HB3	7:2H:61:HIS:HD1	1.70	0.55
28:26:6:ARG:NH1	28:26:26:ASN:HB2	2.21	0.55
33:2b:81:VAL:HB	33:2b:94:ASN:HD21	1.71	0.55
39:2h:21:LYS:O	39:2h:65:TYR:OH	2.23	0.55
1:1A:2306:C:O2	62:1A:4222:HOH:O	2.14	0.55
32:1a:1456:G:O3'	51:1t:39:LYS:NZ	2.40	0.55
32:2a:501:C:H2'	32:2a:502:G:H8	1.71	0.55
32:2a:1137:C:O2	32:2a:1138:G:N2	2.40	0.55
32:2a:1347:G:HO2'	32:2a:1373:G:H1	1.54	0.55
40:2i:14:VAL:HG23	40:2i:66:ARG:HG3	1.89	0.55
14:1S:11:LYS:O	14:1S:15:ARG:HB2	2.07	0.55
1:2A:2805:G:H2'	1:2A:2807:G:H8	1.72	0.55
6:2G:15:VAL:HA	6:2G:175:LEU:HD22	1.87	0.55
8:2I:4:ILE:HG12	8:2I:18:VAL:HG22	1.88	0.55
11:2P:50:ARG:HD3	30:28:7:HIS:CD2	2.42	0.55
32:2a:921:U:O2'	36:2e:19:MET:O	2.22	0.55
32:2a:946:A:H2'	32:2a:947:G:C8	2.42	0.55
1:1A:1588:C:H2'	1:1A:1589:C:C6	2.42	0.55
32:1a:56:U:H2'	32:1a:57:G:C8	2.42	0.55
33:1b:84:GLU:HA	33:1b:87:ARG:HD3	1.89	0.55
34:1c:177:THR:HG22	34:1c:180:ALA:H	1.72	0.55
1:2A:18:C:O2'	1:2A:554:U:OP1	2.25	0.55
1:2A:300:A:OP1	20:2Y:86:ARG:NH2	2.32	0.55
6:2G:44:GLY:HA2	6:2G:88:ILE:HG22	1.88	0.55
32:2a:17:U:H2'	32:2a:18:C:C6	2.41	0.55
32:2a:1298:C:OP2	38:2g:114:ARG:NH2	2.29	0.55
33:2b:16:HIS:CG	33:2b:17:PHE:N	2.75	0.55
1:1A:1482:G:H2'	1:1A:1484:G:H8	1.72	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2218:U:O4'	23:11:52:ARG:NH2	2.39	0.55
32:1a:159:G:O2'	32:1a:161:A:N7	2.28	0.55
32:1a:1037:C:H2'	32:1a:1038:C:C6	2.41	0.55
32:1a:1145:C:H4'	32:1a:1146:A:H5'	1.89	0.55
33:1b:52:GLU:OE2	33:1b:56:ARG:NH2	2.40	0.55
1:2A:894:C:O2'	1:2A:895:U:H5''	2.07	0.55
18:2W:2:GLU:OE2	18:2W:72:LYS:NZ	2.34	0.55
32:2a:1030(A):G:N1	32:2a:1030(D):A:OP2	2.37	0.55
32:2a:1376:U:OP1	38:2g:98:SER:OG	2.24	0.55
34:2c:19:GLU:O	34:2c:57:ILE:N	2.36	0.55
40:2i:3:GLN:HE21	40:2i:20:ARG:CZ	2.20	0.55
25:13:29:ARG:HD2	62:13:204:HOH:O	2.07	0.55
32:1a:186:C:H2'	32:1a:187:C:C6	2.42	0.55
32:1a:236:G:OP1	48:1q:40:LYS:NZ	2.40	0.55
32:1a:1037:C:H2'	32:1a:1038:C:H6	1.71	0.55
1:2A:1794:U:H2'	1:2A:1795:C:H6	1.72	0.55
32:2a:708:C:H2'	32:2a:709:G:H8	1.72	0.55
1:1A:1058:G:N1	1:1A:1080:C:N4	2.31	0.55
1:1A:2243:U:H2'	1:1A:2244:U:C6	2.42	0.55
32:1a:130:A:N3	32:1a:263:A:O2'	2.36	0.55
32:1a:1004:A:H5''	32:1a:1025:U:H5	1.71	0.55
32:1a:1412:C:H2'	32:1a:1413:A:C8	2.41	0.55
36:1e:78:HIS:HE1	36:1e:143:ARG:H	1.53	0.55
39:1h:51:VAL:HG12	39:1h:52:ASP:H	1.72	0.55
2:2B:19:G:H2'	2:2B:20:C:O4'	2.07	0.55
5:2F:20:LEU:HD12	5:2F:125:LEU:HD13	1.89	0.55
6:2G:7:LEU:HD13	6:2G:104:GLU:HA	1.89	0.55
21:2Z:145:GLU:H	21:2Z:148:ASP:HB2	1.71	0.55
32:2a:278:G:OP2	48:2q:41:LYS:NZ	2.25	0.55
32:2a:437:U:H5'	35:2d:155:LEU:HD21	1.89	0.55
33:2b:178:ARG:NH2	39:2h:68:ARG:HH22	2.04	0.55
1:1A:1028:A:N6	1:1A:1125:G:H2'	2.22	0.54
1:1A:2430:A:N3	1:1A:2430:A:H2'	2.23	0.54
51:1t:10:LEU:HB3	51:1t:12:ALA:H	1.72	0.54
1:2A:947:G:H2'	1:2A:948:G:C8	2.43	0.54
2:2B:42:C:O2'	6:2G:67:LYS:O	2.18	0.54
2:2B:113:G:N2	14:2S:45:GLY:O	2.34	0.54
6:2G:113:ARG:NH2	6:2G:139:LEU:O	2.40	0.54
14:2S:15:ARG:O	14:2S:19:LYS:HG2	2.08	0.54
19:2X:94:GLY:H	19:2X:95:LEU:C	2.15	0.54
32:2a:573:A:N3	32:2a:883:C:O2'	2.36	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:2t:9:ASN:O	51:2t:10:LEU:HB2	2.07	0.54
56:2y:7:A:O2'	56:2y:49:C:O4'	2.24	0.54
11:1P:95:VAL:HB	11:1P:100:LEU:HD11	1.89	0.54
1:2A:878:A:H61	1:2A:899:A:H1'	1.71	0.54
1:2A:2060:A:N3	62:2A:3891:HOH:O	2.33	0.54
1:2A:2595:G:N7	62:2A:3896:HOH:O	2.34	0.54
1:2A:2839:G:H5'	13:2R:46:GLY:HA2	1.89	0.54
14:2S:38:GLN:NE2	14:2S:47:THR:OG1	2.40	0.54
21:2Z:52:SER:OG	21:2Z:53:ILE:N	2.39	0.54
32:2a:473:G:H2'	32:2a:474:G:C8	2.42	0.54
32:2a:1062:U:H2'	32:2a:1063:C:C6	2.42	0.54
32:2a:1314:C:OP1	50:2s:6:LYS:NZ	2.33	0.54
34:2c:152:ILE:HG22	34:2c:167:TRP:HB3	1.89	0.54
56:2y:55:PSU:N1	56:2y:57:G:H5''	2.20	0.54
1:1A:84:A:H5''	20:1Y:8:LYS:HE3	1.88	0.54
1:1A:961:C:OP2	62:1A:4244:HOH:O	2.18	0.54
1:1A:2140:C:O2	1:1A:2151:G:N1	2.28	0.54
1:1A:2319:G:H22	14:1S:3:ARG:NE	2.04	0.54
32:1a:448:A:OP2	32:1a:485:G:N1	2.23	0.54
32:1a:1039:C:H2'	32:1a:1040:U:C6	2.43	0.54
35:1d:162:LEU:HD13	35:1d:181:MET:HG2	1.89	0.54
37:1f:37:VAL:HA	37:1f:65:VAL:HG12	1.89	0.54
39:1h:112:LEU:HA	39:1h:134:ILE:HG12	1.88	0.54
1:2A:2161:C:H2'	1:2A:2162:G:O4'	2.07	0.54
1:2A:2683:C:OP1	15:2T:53:ARG:NH2	2.37	0.54
3:2D:183:ARG:HG3	3:2D:270:ILE:HD13	1.89	0.54
32:2a:532:A:N1	34:2c:156:ARG:NH1	2.45	0.54
32:2a:1109:C:H2'	32:2a:1110:A:O4'	2.07	0.54
1:1A:1494:A:OP1	62:1A:4242:HOH:O	2.18	0.54
47:1p:67:THR:H	47:1p:70:ALA:HB3	1.73	0.54
54:1w:70:G:C2	54:1w:71:G:H1'	2.43	0.54
1:2A:2104:G:H1	1:2A:2185:C:H42	1.56	0.54
26:24:40:HIS:CD2	26:24:41:PRO:HD2	2.42	0.54
32:2a:757:U:H2'	32:2a:758:G:O4'	2.07	0.54
32:2a:1040:U:H2'	32:2a:1041:A:H8	1.72	0.54
51:2t:10:LEU:HD23	51:2t:12:ALA:HB2	1.88	0.54
3:1D:12:SER:HB3	3:1D:208:LYS:HB3	1.89	0.54
5:1F:64:ILE:HD11	5:1F:75:HIS:HB2	1.88	0.54
5:1F:184:TYR:CE2	5:1F:188:ARG:HD2	2.42	0.54
6:1G:126:ASP:HB2	6:1G:130:ASN:H	1.72	0.54
32:1a:942:G:H21	40:1i:124:GLN:NE2	2.06	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:1h:73:ASP:OD1	39:1h:75:ARG:NE	2.41	0.54
6:2G:114:ILE:HA	6:2G:140:ILE:HD11	1.90	0.54
8:2I:14:ASP:N	8:2I:17:GLN:OE1	2.30	0.54
32:2a:1218:C:H2'	32:2a:1219:U:C6	2.43	0.54
50:2s:64:GLU:OE2	50:2s:65:ASN:ND2	2.41	0.54
1:1A:1165:U:H2'	1:1A:1166:C:C6	2.42	0.54
1:1A:1803:A:O2'	3:1D:259:THR:HG21	2.08	0.54
8:1I:76:THR:HG22	8:1I:141:LYS:HB2	1.89	0.54
1:2A:1581:G:H2'	1:2A:1582:C:O4'	2.07	0.54
5:2F:143:ALA:HB1	5:2F:148:LEU:HB2	1.89	0.54
7:2H:24:VAL:HG13	7:2H:37:VAL:HG21	1.89	0.54
35:2d:107:ARG:HH12	35:2d:194:LEU:HD23	1.73	0.54
38:2g:133:GLY:O	38:2g:137:LYS:N	2.33	0.54
21:1Z:7:ALA:O	21:1Z:62:PRO:HD3	2.08	0.54
33:1b:82:ARG:NH1	33:1b:86:GLU:OE2	2.40	0.54
1:2A:84:A:H5'	20:2Y:8:LYS:HG2	1.88	0.54
1:2A:271(G):C:H2'	1:2A:271(H):G:H8	1.71	0.54
1:2A:2502:G:N7	62:2A:3895:HOH:O	2.33	0.54
6:2G:16:ARG:O	6:2G:20:ILE:HG13	2.07	0.54
19:2X:31:HIS:CD2	19:2X:33:LYS:H	2.25	0.54
32:2a:390:C:O3'	47:2p:28:ARG:NH2	2.41	0.54
33:2b:114:ARG:HD2	33:2b:117:GLU:HB3	1.89	0.54
33:2b:200:ILE:HG22	33:2b:202:PRO:HD3	1.90	0.54
40:2i:40:LEU:HD23	40:2i:42:ARG:H	1.71	0.54
54:2w:11:C:H2'	54:2w:12:U:H6	1.73	0.54
18:1W:4:LYS:HD3	18:1W:6:ILE:HD11	1.90	0.54
32:1a:1277:C:O2'	32:1a:1279:A:H1'	2.07	0.54
37:1f:67:MET:HE1	37:1f:75:LEU:HD12	1.88	0.54
49:1r:21:LYS:NZ	49:1r:54:ARG:O	2.40	0.54
1:2A:1509(B):A:H2'	1:2A:1510:G:H8	1.73	0.54
2:2B:114:C:H2'	2:2B:115:G:C8	2.43	0.54
23:21:56:GLN:HE21	23:21:87:PRO:HG3	1.71	0.54
44:2m:40:ASN:HD22	44:2m:43:THR:HG23	1.73	0.54
1:1A:882:G:H4'	54:1w:19:G:O6	2.07	0.54
1:1A:1047:G:H2'	1:1A:1110:G:N2	2.22	0.54
1:1A:2125:G:N1	1:1A:2172:U:OP1	2.35	0.54
1:1A:2368:C:OP2	62:1A:4240:HOH:O	2.18	0.54
3:1D:108:PRO:HB3	3:1D:143:HIS:CE1	2.42	0.54
23:11:50:ARG:HG2	23:11:59:THR:HG22	1.88	0.54
1:2A:1449:A:HO2'	1:2A:1529:G:H21	1.53	0.54
8:2I:133:HIS:HD2	8:2I:134:PRO:HD2	1.72	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2S:33:LYS:HB3	14:2S:34:HIS:CD2	2.43	0.54
32:2a:1411:C:H2'	32:2a:1412:C:H6	1.73	0.54
34:2c:71:ALA:CB	34:2c:109:PRO:HB3	2.38	0.54
1:1A:884:C:H42	1:1A:892:G:H1	1.56	0.54
8:1I:75:LEU:HD22	8:1I:105:HIS:CD2	2.43	0.54
17:1V:76:LYS:HB2	17:1V:81:TYR:HB3	1.90	0.54
32:1a:22:G:H4'	32:1a:885:G:C8	2.43	0.54
32:1a:971:G:N2	32:1a:1363(A):A:OP2	2.37	0.54
40:1i:53:VAL:O	40:1i:55:ALA:N	2.33	0.54
51:1t:50:GLU:HA	51:1t:100:ILE:HG12	1.89	0.54
1:2A:2120:G:H2'	1:2A:2121:G:H8	1.73	0.54
1:2A:2377:A:H2'	1:2A:2378:A:C8	2.43	0.54
7:2H:56:SER:HB3	7:2H:61:HIS:ND1	2.23	0.54
35:2d:157:LEU:O	35:2d:161:ASN:ND2	2.38	0.54
38:2g:79:ARG:HH21	38:2g:80:VAL:HA	1.74	0.54
44:2m:67:GLU:HG3	44:2m:68:GLY:N	2.23	0.54
54:2w:43:C:H2'	54:2w:44:G:C8	2.43	0.54
1:1A:2727:G:O2'	10:1O:70:LYS:NZ	2.40	0.53
32:1a:1510:U:H2'	32:1a:1511:G:C8	2.43	0.53
1:2A:71:A:N7	19:2X:31:HIS:HE1	2.06	0.53
1:2A:764:A:H5'	3:2D:210:GLY:HA2	1.90	0.53
6:2G:61:ALA:HB1	26:24:7:PRO:HG3	1.89	0.53
8:2I:50:ARG:O	8:2I:54:GLN:N	2.40	0.53
9:2N:30:ILE:HG23	9:2N:52:VAL:HG11	1.90	0.53
34:2c:142:MET:HG3	34:2c:170:GLN:HB3	1.88	0.53
35:2d:50:ARG:HH12	36:2e:10:MET:HG3	1.73	0.53
32:1a:316:G:OP2	32:1a:351:G:O2'	2.25	0.53
1:2A:892:G:H3'	1:2A:893:C:H5''	1.91	0.53
1:2A:2314:C:H2'	1:2A:2315:G:C8	2.43	0.53
12:2Q:37:LEU:HD21	12:2Q:130:LYS:HE2	1.90	0.53
19:2X:47:PHE:HZ	24:22:37:PHE:HE2	1.57	0.53
44:2m:23:TYR:O	44:2m:67:GLU:N	2.41	0.53
1:1A:534:U:H2'	1:1A:535:C:C6	2.44	0.53
1:1A:1498:C:OP1	62:1A:4245:HOH:O	2.19	0.53
1:1A:2128:C:N4	1:1A:2160:G:N1	2.56	0.53
1:1A:2153:G:H2'	1:1A:2154:G:C8	2.43	0.53
10:1O:97:ARG:NH1	32:1a:339:C:OP2	2.40	0.53
24:12:9:GLN:HE22	24:12:56:GLN:HB3	1.73	0.53
32:1a:299:G:H2'	32:1a:300:A:C8	2.43	0.53
1:2A:1149:G:H2'	1:2A:1150:C:C6	2.43	0.53
1:2A:2074:U:H2'	1:2A:2075:U:C6	2.43	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1352:C:H2'	32:2a:1353:G:C8	2.44	0.53
33:2b:185:ILE:HG22	33:2b:199:TYR:HB2	1.90	0.53
39:2h:19:VAL:HG23	39:2h:21:LYS:HG3	1.90	0.53
41:2j:89:ASP:O	41:2j:91:PRO:HD3	2.09	0.53
1:1A:899:A:H2'	1:1A:899:A:N3	2.23	0.53
7:1H:149:ARG:HH12	7:1H:167:GLU:CD	2.16	0.53
32:1a:69:G:H2'	32:1a:70:G:H8	1.71	0.53
32:1a:134:A:H61	47:1p:25:ARG:HH12	1.56	0.53
32:1a:373:A:H2'	32:1a:374:A:H8	1.72	0.53
1:2A:247:G:H4'	1:2A:386:G:C5	2.43	0.53
1:2A:860:U:H1'	1:2A:2268:A:H5'	1.89	0.53
1:2A:918:A:C5	1:2A:919:G:H1'	2.43	0.53
1:2A:2131:G:C8	1:2A:2133:G:C2	2.96	0.53
21:2Z:156:LYS:HE3	21:2Z:158:PRO:HD3	1.89	0.53
32:2a:437:U:H5''	35:2d:155:LEU:HD11	1.89	0.53
32:2a:748:C:H4'	32:2a:749:C:O5'	2.08	0.53
44:2m:90:LEU:HD11	44:2m:94:ARG:HH11	1.74	0.53
54:2w:51:U:H3	54:2w:63:G:H1	1.55	0.53
1:1A:1278:A:OP1	13:1R:36:THR:HG23	2.08	0.53
1:1A:2870:C:H2'	1:1A:2871:C:O4'	2.09	0.53
32:1a:946:A:H2'	32:1a:947:G:C8	2.44	0.53
33:1b:76:GLN:H	33:1b:76:GLN:CD	2.16	0.53
1:2A:93:G:H2'	1:2A:94:C:C6	2.44	0.53
1:2A:2162:G:H4'	1:2A:2172:U:H2'	1.89	0.53
3:2D:108:PRO:HB3	3:2D:143:HIS:CE1	2.44	0.53
32:2a:129(A):G:C6	32:2a:189(E):U:H4'	2.43	0.53
32:2a:1066:C:H2'	32:2a:1067:A:C8	2.43	0.53
32:2a:1273:G:H3'	32:2a:1274:G:C8	2.43	0.53
33:2b:105:PHE:O	33:2b:107:THR:N	2.38	0.53
42:2k:110:ASP:HB3	49:2r:85:LEU:HB3	1.90	0.53
3:1D:148:GLU:HB2	3:1D:151:LYS:HD2	1.91	0.53
40:1i:56:LEU:H	40:1i:56:LEU:HD12	1.74	0.53
1:2A:2111:C:N4	1:2A:2144:U:O2'	2.35	0.53
1:2A:2129:C:C4	1:2A:2159:G:N1	2.77	0.53
8:2I:55:ALA:HA	8:2I:58:LEU:HB3	1.90	0.53
8:2I:72:LEU:HD21	8:2I:107:VAL:HG11	1.89	0.53
9:2N:15:LEU:HD23	9:2N:137:LYS:HD2	1.90	0.53
32:2a:115:G:H4'	32:2a:116:A:O5'	2.07	0.53
32:2a:420:U:H2'	32:2a:422:C:C5	2.44	0.53
32:2a:1072:G:H2'	32:2a:1073:U:C6	2.43	0.53
1:1A:1187:G:H5''	17:1V:81:TYR:CE1	2.44	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1G:38:VAL:HG22	6:1G:93:THR:HG23	1.90	0.53
32:1a:103:C:O2'	32:1a:172:A:N1	2.42	0.53
32:1a:1033:G:H2'	32:1a:1034:G:H8	1.74	0.53
42:1k:87:THR:O	42:1k:87:THR:OG1	2.15	0.53
1:2A:1147:C:H2'	1:2A:1148:A:C8	2.38	0.53
1:2A:2114:A:H1'	1:2A:2168:G:O2'	2.09	0.53
6:2G:33:ARG:HE	6:2G:162:THR:HG21	1.73	0.53
22:20:70:GLN:HE21	22:20:72:ARG:HD2	1.74	0.53
1:1A:184:C:H2'	1:1A:185:U:C6	2.44	0.53
1:1A:839:U:H2'	1:1A:840:C:C6	2.44	0.53
1:1A:1176:G:N2	1:1A:1178:C:OP2	2.42	0.53
1:1A:1778:U:OP1	62:1A:4246:HOH:O	2.19	0.53
1:1A:1918:A:N6	62:1A:4388:HOH:O	2.42	0.53
1:1A:2145:C:H3'	1:1A:2146:C:H5'	1.90	0.53
7:1H:101:ARG:HH12	7:1H:122:THR:HA	1.74	0.53
18:1W:1:MET:HE2	18:1W:62:HIS:HB3	1.91	0.53
32:1a:890:G:O2'	32:1a:906:G:O6	2.26	0.53
32:1a:1106:G:O3'	34:1c:172:ARG:HB2	2.09	0.53
32:1a:1402:4OC:HM22	32:1a:1403:C:H5'	1.91	0.53
32:1a:1456:G:N2	51:1t:51:GLU:OE2	2.34	0.53
1:2A:2117:A:N6	1:2A:2171:A:N1	2.55	0.53
1:2A:2137:C:H42	1:2A:2154:G:H1	1.57	0.53
1:2A:2646:C:H2'	1:2A:2647:U:O4'	2.09	0.53
8:2I:37:VAL:HG12	8:2I:38:LEU:HD12	1.90	0.53
21:2Z:151:HIS:HD2	21:2Z:168:GLU:C	2.17	0.53
32:2a:130:A:O2'	32:2a:131:C:O5'	2.27	0.53
32:2a:1348:U:H2'	32:2a:1349:A:H8	1.74	0.53
40:2i:26:VAL:HG13	40:2i:61:ALA:HB3	1.90	0.53
40:2i:29:ASN:ND2	40:2i:65:VAL:O	2.40	0.53
43:2l:28:LYS:HE2	43:2l:64:TYR:HE2	1.74	0.53
47:2p:28:ARG:NH1	47:2p:29:ASP:OD2	2.42	0.53
56:2y:14:A:H3'	56:2y:15:G:C8	2.44	0.53
1:1A:2478:A:H5'	31:19:31:LYS:HD3	1.91	0.53
12:1Q:139:GLU:OE2	21:1Z:122:ARG:HD2	2.08	0.53
32:1a:271:C:H2'	32:1a:272:C:C6	2.44	0.53
32:1a:1136:U:H5''	32:1a:1137:C:C2	2.44	0.53
56:1y:55:PSU:N3	56:1y:57:G:H5'	2.24	0.53
32:2a:1321:C:H4'	44:2m:87:TYR:CZ	2.44	0.53
50:2s:49:ILE:HG22	50:2s:62:ILE:HD11	1.91	0.53
1:1A:882:G:H4'	54:1w:19:G:C6	2.44	0.53
1:1A:2319:G:N1	14:1S:3:ARG:HA	2.24	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:828:A:H2'	32:1a:829:G:O4'	2.08	0.53
50:1s:27:GLU:OE1	50:1s:27:GLU:N	2.38	0.53
1:2A:568:U:H5'	1:2A:945:A:N1	2.23	0.53
1:2A:2099:U:O2	1:2A:2190:G:N2	2.38	0.53
6:2G:63:ILE:HD13	6:2G:143:GLU:HB2	1.91	0.53
9:2N:96:GLU:CD	9:2N:96:GLU:H	2.17	0.53
11:2P:39:LYS:HG3	11:2P:45:LEU:HD22	1.91	0.53
32:2a:457:C:H2'	32:2a:458:C:C6	2.44	0.53
32:2a:984:C:H2'	32:2a:985:C:C6	2.40	0.53
32:2a:1002:G:N3	32:2a:1003:G:H1'	2.24	0.53
32:2a:1118:C:H1'	32:2a:1179:A:C5	2.44	0.53
33:2b:16:HIS:HB2	33:2b:204:ASN:HD22	1.74	0.53
35:2d:47:ARG:HB3	35:2d:47:ARG:HH11	1.72	0.53
48:2q:58:GLU:OE2	48:2q:75:ARG:NH2	2.42	0.53
1:1A:271(K):U:H1'	8:1I:50:ARG:CZ	2.39	0.52
1:1A:2108:C:H2'	1:1A:2109:U:H6	1.73	0.52
1:1A:2869:G:H2'	1:1A:2870:C:O4'	2.09	0.52
32:1a:1442:G:H2'	32:1a:1442:G:N3	2.24	0.52
1:2A:1952:A:OP1	10:2O:42:SER:OG	2.24	0.52
7:2H:137:ASP:HB3	7:2H:140:LYS:HB3	1.92	0.52
8:2I:62:LYS:HE3	8:2I:133:HIS:CE1	2.37	0.52
32:2a:447:G:O6	32:2a:485:G:O2'	2.23	0.52
32:2a:833:U:H2'	32:2a:834:C:C6	2.44	0.52
33:2b:124:SER:HB3	33:2b:125:PRO:HD3	1.91	0.52
35:2d:22:LYS:O	35:2d:113:SER:HB3	2.09	0.52
36:2e:7:GLU:OE1	36:2e:37:ARG:NH2	2.28	0.52
48:2q:67:LYS:O	48:2q:68:ARG:HB2	2.09	0.52
1:1A:7:G:H2'	1:1A:8:A:O4'	2.10	0.52
1:1A:2355:C:H1'	22:10:39:ARG:HH21	1.74	0.52
32:1a:167:G:H2'	32:1a:168:G:C8	2.43	0.52
32:1a:584:G:H5'	48:1q:91:ARG:HH21	1.74	0.52
32:1a:1025:U:O2	32:1a:1036:G:C6	2.62	0.52
32:1a:1343:G:H2'	32:1a:1344:C:C6	2.44	0.52
32:1a:1499:A:OP2	62:1a:1903:HOH:O	2.19	0.52
15:2T:84:GLN:HG2	15:2T:85:LYS:HG2	1.91	0.52
32:2a:222:U:H2'	32:2a:223:U:C6	2.45	0.52
32:2a:646:U:H2'	32:2a:647:C:C6	2.44	0.52
32:2a:663:A:O3'	49:2r:64:ARG:NH2	2.39	0.52
32:2a:1118:C:OP1	40:2i:104:ARG:NH1	2.41	0.52
32:2a:1376:U:H2'	32:2a:1377:A:C8	2.38	0.52
34:2c:71:ALA:HB1	34:2c:109:PRO:HB3	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:2p:18:ARG:HD3	47:2p:35:LYS:HD2	1.90	0.52
1:1A:84:A:H5'	20:1Y:8:LYS:HG2	1.90	0.52
1:1A:247:G:H4'	1:1A:386:G:C5	2.44	0.52
1:1A:1062:G:H2'	1:1A:1063:G:C8	2.44	0.52
1:1A:1518:U:H2'	1:1A:1519:G:O4'	2.08	0.52
1:1A:2155:G:H2'	1:1A:2155:G:N3	2.24	0.52
6:1G:15:VAL:HG22	6:1G:175:LEU:HB3	1.92	0.52
16:1U:83:LEU:HD12	16:1U:113:ALA:HB2	1.92	0.52
32:1a:976:G:H5'	32:1a:1358:U:O2'	2.09	0.52
36:1e:41:VAL:HG23	36:1e:67:VAL:HG12	1.91	0.52
1:2A:8:A:H2'	1:2A:9:U:C6	2.44	0.52
1:2A:118:A:N3	1:2A:178:G:H1'	2.24	0.52
1:2A:2794:C:N4	1:2A:2802:G:O6	2.42	0.52
32:2a:56:U:H2'	32:2a:57:G:H8	1.74	0.52
32:2a:237:C:H5''	48:2q:25:ARG:CZ	2.39	0.52
32:2a:1513:A:H2'	32:2a:1514:C:C6	2.44	0.52
40:2i:33:PHE:HE2	40:2i:43:ALA:HB1	1.74	0.52
1:1A:441:U:O2	5:1F:46:ARG:NH2	2.38	0.52
1:1A:1069:A:O4'	1:1A:1096:A:O2'	2.28	0.52
1:1A:2788:C:OP1	4:1E:61:ARG:NH2	2.43	0.52
26:14:58:ARG:O	26:14:61:ARG:N	2.43	0.52
32:1a:963:G:H5'	62:1a:2024:HOH:O	2.08	0.52
33:1b:59:GLU:HB2	33:1b:221:LEU:HD21	1.92	0.52
1:2A:910:A:C5	12:2Q:13:GLN:HG3	2.44	0.52
1:2A:1159:U:H2'	1:2A:1160:G:H8	1.75	0.52
2:2B:1:U:H2'	2:2B:2:C:C6	2.44	0.52
32:2a:865:A:H5'	32:2a:1078:U:H5	1.73	0.52
41:2j:69:ASN:O	41:2j:70:ARG:NH1	2.37	0.52
42:2k:73:MET:HG2	42:2k:103:LEU:HD21	1.91	0.52
56:2y:65:G:H2'	56:2y:66:U:C6	2.44	0.52
1:1A:414:C:H2'	1:1A:415:A:C8	2.45	0.52
4:1E:7:VAL:HG23	4:1E:51:PHE:HE2	1.73	0.52
33:1b:118:LEU:HB3	33:1b:142:LEU:HD12	1.91	0.52
33:1b:155:LEU:HD11	33:1b:159:PRO:HG3	1.92	0.52
37:1f:39:LYS:HB2	37:1f:64:GLN:HB3	1.92	0.52
1:2A:252:G:OP1	11:2P:50:ARG:NH1	2.40	0.52
1:2A:2286:A:OP1	28:26:29:ASN:ND2	2.42	0.52
26:24:53:GLU:HG2	26:24:55:ARG:H	1.74	0.52
32:2a:544:G:OP1	35:2d:59:ARG:NH2	2.32	0.52
35:2d:47:ARG:HB3	35:2d:47:ARG:NH1	2.24	0.52
38:2g:26:PHE:CZ	38:2g:30:ILE:HD11	2.44	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:2m:33:ALA:HB1	44:2m:59:TYR:HE2	1.74	0.52
49:2r:48:GLY:O	49:2r:74:ARG:NH2	2.42	0.52
51:1t:87:LYS:O	51:1t:91:LEU:HG	2.09	0.52
1:2A:84:A:H5'	20:2Y:8:LYS:HE3	1.92	0.52
1:2A:300:A:P	20:2Y:86:ARG:HH22	2.31	0.52
17:2V:40:LEU:HD11	17:2V:101:GLY:HA3	1.91	0.52
28:26:8:LYS:HD3	30:28:34:TRP:CD2	2.43	0.52
32:2a:1097:C:O2'	32:2a:1169:A:N3	2.42	0.52
32:2a:1203:C:H2'	32:2a:1204:A:H8	1.75	0.52
33:2b:217:ARG:HA	33:2b:220:ASP:HB2	1.91	0.52
40:2i:85:LEU:HB3	40:2i:92:TYR:CD2	2.44	0.52
43:2l:8:ASN:O	43:2l:12:ARG:HG3	2.10	0.52
11:1P:39:LYS:HB2	11:1P:45:LEU:HD13	1.90	0.52
11:1P:59:LEU:HD11	30:18:10:ALA:HA	1.91	0.52
36:1e:6:PHE:HB3	36:1e:34:VAL:HG22	1.90	0.52
43:1l:117:ARG:HB3	43:1l:122:THR:HB	1.92	0.52
48:1q:26:GLN:HE21	48:1q:37:LYS:HE3	1.74	0.52
1:2A:36:G:OP1	62:2A:3839:HOH:O	2.18	0.52
1:2A:1030:G:OP2	12:2Q:128:LYS:NZ	2.42	0.52
32:2a:1002:G:C2	32:2a:1003:G:H1'	2.45	0.52
34:2c:34:LEU:HD11	34:2c:38:ARG:HH21	1.74	0.52
10:1O:89:ASN:H	10:1O:89:ASN:ND2	2.08	0.52
28:16:18:ARG:HD2	28:16:42:TRP:CD1	2.45	0.52
32:1a:259:G:OP2	51:1t:83:ARG:NH1	2.43	0.52
33:1b:48:MET:HA	33:1b:51:LEU:HB2	1.92	0.52
40:1i:32:ASP:OD1	40:1i:33:PHE:N	2.42	0.52
6:2G:53:LEU:HB3	6:2G:56:ALA:HB3	1.92	0.52
12:2Q:137:TYR:CE1	21:2Z:83:PRO:HG3	2.44	0.52
32:2a:545:C:O2'	32:2a:549:C:OP1	2.21	0.52
1:1A:528:A:O2'	1:1A:529:A:H5'	2.10	0.52
1:1A:911:A:H2'	12:1Q:9:TYR:OH	2.10	0.52
1:1A:2831:G:P	4:1E:58:ARG:HH21	2.33	0.52
32:1a:1381:U:H1'	38:1g:79:ARG:HG2	1.91	0.52
43:1l:77:LEU:HD21	43:1l:107:ALA:HB2	1.92	0.52
1:2A:668:G:H5'	1:2A:669:G:OP2	2.10	0.52
1:2A:2314:C:H2'	1:2A:2315:G:H8	1.74	0.52
7:2H:15:VAL:HG11	7:2H:76:VAL:HG23	1.91	0.52
8:2I:130:TYR:HD2	8:2I:138:ILE:HD12	1.74	0.52
32:2a:501:C:H2'	32:2a:502:G:C8	2.45	0.52
32:2a:1060:C:O2'	41:2j:56:HIS:ND1	2.43	0.52
1:1A:1025:G:C4	1:1A:1135:C:H1'	2.45	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2347:C:H2'	1:1A:2348:U:C6	2.45	0.52
32:1a:341:C:H2'	32:1a:342:C:C6	2.45	0.52
32:1a:438:G:H4'	35:1d:123:HIS:CE1	2.45	0.52
32:1a:456:C:H2'	32:1a:457:C:C6	2.44	0.52
32:1a:715:A:H2'	32:1a:716:A:C8	2.45	0.52
1:2A:271(E):U:H2'	1:2A:271(F):C:C6	2.45	0.52
1:2A:2114:A:H62	1:2A:2115:G:N2	2.07	0.52
1:2A:2238:G:H5''	62:2A:4395:HOH:O	2.10	0.52
32:2a:1310:G:H5'	44:2m:77:ASN:HD21	1.75	0.52
33:2b:47:THR:O	33:2b:51:LEU:N	2.42	0.52
35:2d:146:ILE:HD12	35:2d:146:ILE:H	1.74	0.52
1:1A:2564:A:C2	1:1A:2647:U:H4'	2.45	0.51
17:1V:98:GLU:OE2	17:1V:100:ARG:NH1	2.43	0.51
29:17:33:ARG:NH2	62:17:201:HOH:O	2.43	0.51
32:1a:377:G:OP1	47:1p:5:ARG:HD2	2.10	0.51
40:1i:26:VAL:HG13	40:1i:61:ALA:HB3	1.92	0.51
1:2A:527:C:N4	1:2A:2779:U:OP2	2.42	0.51
1:2A:2291:U:H2'	1:2A:2292:C:C6	2.45	0.51
2:2B:119:G:H5'	2:2B:120:A:OP2	2.09	0.51
4:2E:77:ILE:HG21	4:2E:195:LEU:HD11	1.92	0.51
5:2F:18:ARG:NH1	5:2F:127:GLU:OE2	2.43	0.51
32:2a:662:G:H2'	32:2a:663:A:H8	1.76	0.51
32:2a:714:G:H2'	32:2a:715:A:C8	2.45	0.51
32:2a:957:U:H2'	32:2a:959:A:OP2	2.09	0.51
32:2a:1129:C:P	40:2i:66:ARG:HH12	2.33	0.51
32:2a:1239:A:H62	32:2a:1299:A:H62	1.58	0.51
33:2b:101:MET:HG2	33:2b:108:ILE:HG21	1.91	0.51
35:2d:114:ARG:O	35:2d:118:ARG:N	2.39	0.51
39:2h:17:THR:HA	39:2h:65:TYR:HE1	1.74	0.51
1:1A:1095:A:N6	1:1A:1097:U:O2	2.44	0.51
11:1P:138:LEU:HD23	11:1P:145:PRO:HB3	1.92	0.51
21:1Z:136:PHE:O	21:1Z:137:ILE:HG13	2.10	0.51
32:1a:1263:C:H2'	32:1a:1264:C:C6	2.46	0.51
34:1c:71:ALA:O	34:1c:73:PRO:HD3	2.10	0.51
1:2A:1278:A:OP1	13:2R:36:THR:HG23	2.11	0.51
8:2I:14:ASP:O	8:2I:17:GLN:HB2	2.09	0.51
28:26:10:LEU:HG	28:26:54:ILE:HG13	1.92	0.51
32:2a:157:G:H2'	32:2a:158:G:H8	1.75	0.51
32:2a:983:A:H3'	32:2a:983:A:N3	2.25	0.51
33:2b:50:GLU:HB3	33:2b:200:ILE:O	2.10	0.51
42:2k:43:SER:HB3	42:2k:68:ALA:HB2	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:2w:13:C:H4'	54:2w:14:A:OP1	2.09	0.51
1:1A:1641:A:H2'	1:1A:1642:G:O4'	2.10	0.51
1:2A:1837:C:OP1	32:2a:784:C:H4'	2.10	0.51
1:2A:2875:C:O2'	15:2T:2:ASN:OD1	2.27	0.51
7:2H:25:LYS:HE2	7:2H:27:LYS:HE3	1.92	0.51
9:2N:21:LYS:NZ	9:2N:140:VAL:OXT	2.44	0.51
11:2P:95:VAL:HG23	11:2P:100:LEU:HD11	1.92	0.51
12:2Q:111:GLU:O	12:2Q:115:MET:HG2	2.10	0.51
14:2S:35:ILE:HG22	14:2S:101:LEU:HD12	1.93	0.51
25:23:12:PRO:HB2	25:23:20:LYS:HG2	1.90	0.51
32:2a:427:U:OP1	35:2d:13:ARG:NH1	2.43	0.51
32:2a:438:G:H4'	35:2d:123:HIS:CE1	2.45	0.51
32:2a:1272:G:N2	32:2a:1273:G:N7	2.57	0.51
32:2a:1401:G:OP1	53:2v:18:G:O2'	2.25	0.51
47:2p:43:LYS:HG2	47:2p:48:TRP:CG	2.45	0.51
1:1A:1243:G:O2'	11:1P:7:ARG:NH2	2.44	0.51
1:1A:1364:G:P	23:11:3:LYS:HG3	2.51	0.51
5:1F:53:THR:CG2	5:1F:55:GLY:H	2.22	0.51
15:1T:108:ARG:HH21	15:1T:112:ARG:HD3	1.75	0.51
32:1a:191:G:N3	51:1t:103:GLY:HA2	2.25	0.51
32:1a:598:U:H2'	32:1a:599:C:C6	2.45	0.51
34:1c:11:ARG:NH2	34:1c:177:THR:O	2.44	0.51
44:1m:3:ARG:HD2	44:1m:9:ILE:HG12	1.92	0.51
1:2A:709:U:H2'	1:2A:710:G:C8	2.46	0.51
26:24:58:ARG:HG3	50:2s:65:ASN:HA	1.92	0.51
31:29:25:VAL:HB	31:29:34:GLN:HB2	1.92	0.51
35:2d:152:SER:O	35:2d:158:ILE:HD11	2.11	0.51
42:2k:41:THR:HG21	42:2k:71:LYS:HB2	1.91	0.51
49:2r:58:LEU:HB2	49:2r:63:GLN:HE21	1.74	0.51
1:1A:2156:G:OP2	1:1A:2156:G:H8	1.94	0.51
4:1E:116:VAL:HG13	4:1E:122:PHE:HB2	1.92	0.51
14:1S:48:LEU:HD23	14:1S:82:ILE:HD11	1.93	0.51
32:1a:848:C:H2'	32:1a:849:C:C6	2.45	0.51
51:1t:47:GLY:HA2	51:1t:48:LYS:C	2.36	0.51
1:2A:774:A:H2'	1:2A:774:A:N3	2.26	0.51
1:2A:1824:G:N3	3:2D:254:THR:OG1	2.43	0.51
1:2A:2136:C:O2'	1:2A:2137:C:O5'	2.29	0.51
2:2B:2:C:H2'	2:2B:3:C:H6	1.75	0.51
23:21:86:SER:OG	23:21:89:GLU:OE2	2.25	0.51
32:2a:865:A:H5'	32:2a:1078:U:C5	2.45	0.51
37:2f:100:ASN:ND2	49:2r:23:LYS:HE3	2.26	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:2g:89:MET:SD	38:2g:155:ARG:HB2	2.50	0.51
32:1a:271:C:H2'	32:1a:272:C:H6	1.76	0.51
32:1a:1250:A:O3'	40:1i:67:GLY:HA2	2.11	0.51
32:1a:1303:C:OP2	62:1a:1917:HOH:O	2.20	0.51
37:1f:35:ALA:HB2	37:1f:67:MET:HE2	1.92	0.51
1:2A:1410:G:H2'	1:2A:1411:C:C6	2.45	0.51
1:2A:1899:G:H2'	1:2A:1899:G:N3	2.25	0.51
7:2H:3:ARG:NH1	7:2H:4:ILE:H	2.08	0.51
8:2I:1:MET:N	8:2I:20:ASP:OD1	2.29	0.51
12:2Q:65:PHE:HB2	12:2Q:105:GLU:HB2	1.92	0.51
32:2a:1442:G:H2'	32:2a:1442:G:N3	2.25	0.51
33:2b:149:LEU:HD22	33:2b:152:PHE:CD2	2.46	0.51
40:2i:23:ASN:OD1	40:2i:25:LYS:HG2	2.09	0.51
1:1A:946:G:OP1	62:1A:4248:HOH:O	2.19	0.51
19:1X:94:GLY:H	19:1X:95:LEU:HB2	1.76	0.51
21:1Z:72:ARG:NH2	21:1Z:97:GLU:O	2.44	0.51
1:2A:1754:C:H5	15:2T:96:ARG:NH2	2.08	0.51
34:2c:6:HIS:HD2	34:2c:7:PRO:HD2	1.76	0.51
51:2t:64:ASP:OD2	51:2t:81:LYS:NZ	2.28	0.51
1:1A:1273:U:OP1	62:1A:4247:HOH:O	2.19	0.51
1:1A:2245:U:O2'	1:1A:2436:G:OP2	2.25	0.51
2:1B:23:G:O6	62:1B:302:HOH:O	2.19	0.51
3:1D:146:GLU:HB2	3:1D:189:CYS:HB3	1.93	0.51
26:14:61:ARG:HD3	50:1s:67:VAL:HG12	1.93	0.51
36:1e:79:GLU:HG2	36:1e:92:LYS:HG2	1.92	0.51
46:1o:18:PHE:CE2	46:1o:21:ASP:HB2	2.45	0.51
1:2A:2135:A:OP1	1:2A:2160:G:H1'	2.10	0.51
1:2A:2391:G:O6	1:2A:2425:A:H8	1.94	0.51
5:2F:154:VAL:HG22	5:2F:191:ARG:HB2	1.93	0.51
21:2Z:27:VAL:HG12	21:2Z:85:HIS:HE1	1.76	0.51
31:29:10:ILE:HD12	31:29:32:HIS:HA	1.91	0.51
33:2b:60:ASP:O	33:2b:64:ARG:HG2	2.11	0.51
1:1A:34:C:H5''	1:1A:35:G:OP2	2.10	0.51
1:1A:242:G:C8	30:18:5:LYS:HG2	2.45	0.51
1:1A:922:U:H2'	1:1A:923:C:C6	2.46	0.51
1:1A:1055:G:H2'	1:1A:1056:G:O4'	2.11	0.51
19:1X:53:LYS:HB3	19:1X:82:GLN:HB3	1.93	0.51
32:1a:202:U:H3'	32:1a:203:U:C5	2.46	0.51
32:1a:1038:C:O2'	32:1a:1039:C:H5'	2.11	0.51
33:1b:185:ILE:HG22	33:1b:199:TYR:HB2	1.93	0.51
39:1h:2:LEU:HD22	39:1h:3:THR:H	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1364:G:OP2	23:21:61:ARG:NH1	2.43	0.51
1:2A:1651:G:H2'	1:2A:1652:A:O4'	2.09	0.51
21:2Z:106:GLY:HA3	21:2Z:141:VAL:HB	1.92	0.51
32:2a:1518:MA6:H93	32:2a:1519:MA6:H92	1.93	0.51
50:2s:80:TYR:O	50:2s:82:GLY:N	2.42	0.51
1:1A:2110:G:O2'	1:1A:2120:G:OP2	2.28	0.51
1:1A:2331:G:O2'	22:10:43:THR:HG22	2.11	0.51
1:1A:2331:G:O2'	1:1A:2336:A:N1	2.39	0.51
28:16:9:LEU:HD13	28:16:51:GLU:HG3	1.93	0.51
32:1a:222:U:H2'	32:1a:223:U:C6	2.46	0.51
35:1d:178:VAL:C	35:1d:180:GLY:H	2.18	0.51
37:1f:69:GLU:H	37:1f:69:GLU:CD	2.19	0.51
1:2A:2022:U:O2'	1:2A:2617:C:H5'	2.11	0.51
1:2A:2128:C:H2'	1:2A:2129:C:O4'	2.11	0.51
1:2A:2133:G:HO2'	1:2A:2157:G:N2	2.09	0.51
7:2H:149:ARG:HD2	7:2H:164:TYR:CE2	2.46	0.51
32:2a:109:A:C6	32:2a:326:G:C6	2.99	0.51
32:2a:737:A:H2'	32:2a:738:C:C6	2.46	0.51
32:2a:1148:U:H5'	40:2i:16:ARG:HD2	1.92	0.51
55:2x:31:G:H3'	55:2x:32:5MC:HM53	1.92	0.51
1:1A:1062:G:H22	1:1A:1077:A:N6	2.09	0.50
32:1a:92:C:H2'	32:1a:93:G:C8	2.46	0.50
32:1a:748:C:H4'	32:1a:749:C:O5'	2.11	0.50
34:1c:153:VAL:HG22	34:1c:198:VAL:HG13	1.93	0.50
35:1d:79:PHE:HE1	35:1d:204:ILE:HG12	1.76	0.50
51:1t:56:MET:HE3	51:1t:85:MET:HG2	1.93	0.50
56:1y:56:C:H2'	56:1y:57:G:O4'	2.10	0.50
1:2A:1316:U:H2'	1:2A:1317:A:H8	1.75	0.50
2:2B:28:C:H2'	2:2B:29:A:O4'	2.11	0.50
3:2D:148:GLU:HB2	3:2D:151:LYS:HD2	1.94	0.50
26:24:45:GLY:C	26:24:47:GLN:H	2.19	0.50
32:2a:559:A:OP1	36:2e:126:ARG:NH2	2.44	0.50
32:2a:719:C:O2'	49:2r:49:LYS:HB3	2.10	0.50
32:2a:1065:U:H3	32:2a:1109:C:C5'	2.23	0.50
32:2a:1183:A:O2'	32:2a:1185:G:OP2	2.28	0.50
41:2j:13:HIS:HB3	41:2j:68:HIS:CE1	2.45	0.50
1:1A:71:A:N7	19:1X:31:HIS:HE1	2.09	0.50
1:1A:639:U:H2'	1:1A:640:C:C6	2.46	0.50
1:1A:969:U:H2'	1:1A:970:C:C6	2.46	0.50
1:1A:2175:C:H2'	1:1A:2176:A:O4'	2.12	0.50
6:1G:64:THR:HB	6:1G:94:LEU:HD11	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:96:U:H2'	32:1a:97:G:C8	2.46	0.50
32:1a:429:U:O2'	35:1d:22:LYS:NZ	2.44	0.50
32:1a:1003:G:H2'	32:1a:1004:A:N3	2.27	0.50
32:1a:1239:A:H62	32:1a:1299:A:H62	1.59	0.50
1:2A:892:G:H3'	1:2A:893:C:C5'	2.41	0.50
1:2A:1886:C:H2'	1:2A:1887:C:H6	1.75	0.50
1:2A:2119:A:N1	1:2A:2170:A:H2'	2.26	0.50
1:2A:2345:G:N3	1:2A:2381:C:H2'	2.25	0.50
1:2A:2408:U:H2'	1:2A:2409:G:C8	2.46	0.50
7:2H:150:ALA:HA	7:2H:153:LYS:HG3	1.93	0.50
32:2a:1261:A:H5'	32:2a:1284:C:OP1	2.11	0.50
33:2b:18:GLY:HA2	33:2b:42:ILE:HG13	1.94	0.50
56:2y:55:PSU:HN1	56:2y:57:G:C5'	2.19	0.50
1:1A:8:A:H2'	1:1A:9:U:H6	1.76	0.50
21:1Z:126:VAL:HG12	21:1Z:128:VAL:HB	1.94	0.50
28:16:26:ASN:HD21	28:16:28:ARG:NH2	2.08	0.50
32:1a:445:G:H2'	32:1a:446:G:C8	2.47	0.50
1:2A:855:G:O2'	22:20:27:GLU:OE2	2.24	0.50
1:2A:1116:C:H2'	1:2A:1117:G:C8	2.46	0.50
10:2O:53:LYS:N	10:2O:56:ASP:OD2	2.28	0.50
32:2a:1427:U:H2'	32:2a:1428:A:C8	2.46	0.50
50:2s:58:VAL:O	50:2s:60:VAL:HG23	2.12	0.50
1:1A:323:G:C8	5:1F:171:PRO:HG3	2.46	0.50
1:1A:818:G:H5'	1:1A:839:U:OP1	2.11	0.50
1:1A:1066:U:H2'	1:1A:1068:G:OP2	2.11	0.50
32:1a:104:G:H2'	32:1a:105:G:H5''	1.93	0.50
32:1a:925:G:H1'	32:1a:1502:A:C4	2.46	0.50
32:1a:1125:U:H4'	41:1j:5:ARG:NH2	2.26	0.50
32:1a:1144:G:N2	32:1a:1146:A:H62	2.09	0.50
32:1a:1286:A:C8	32:1a:1287:A:H4'	2.46	0.50
36:1e:78:HIS:CD2	39:1h:104:ARG:HD2	2.46	0.50
44:1m:15:VAL:O	44:1m:19:LEU:HD22	2.10	0.50
50:1s:50:ALA:HB1	50:1s:57:HIS:HB3	1.92	0.50
54:1w:9:A:O2'	54:1w:10:G:N7	2.44	0.50
1:2A:800:A:H8	1:2A:800:A:OP1	1.95	0.50
1:2A:1028:A:N6	1:2A:1125:G:H2'	2.25	0.50
1:2A:2364:C:OP1	22:20:55:ARG:NH1	2.39	0.50
7:2H:86:GLU:HG3	7:2H:132:ARG:HH21	1.77	0.50
10:2O:63:VAL:HG12	10:2O:106:LEU:HD11	1.92	0.50
21:2Z:102:LEU:HD22	21:2Z:137:ILE:HB	1.93	0.50
32:2a:967:5MC:H2'	32:2a:968:A:C8	2.47	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:979:C:O2	45:2n:19:ARG:HG2	2.12	0.50
32:2a:1135:U:H2'	32:2a:1137:C:N3	2.26	0.50
45:2n:32:SER:O	45:2n:40:CYS:HA	2.11	0.50
1:1A:1364:G:OP2	23:11:3:LYS:HG3	2.12	0.50
1:1A:1580:A:OP2	1:1A:1580:A:H8	1.95	0.50
5:1F:164:ARG:HD2	5:1F:175:THR:HG23	1.94	0.50
7:1H:96:ALA:HB2	7:1H:105:LEU:HD23	1.93	0.50
9:1N:77:GLY:O	62:1N:301:HOH:O	2.19	0.50
32:1a:877:C:H5''	39:1h:88:LYS:HD3	1.91	0.50
32:1a:1036:G:H3'	32:1a:1037:C:C6	2.46	0.50
32:1a:1456:G:H22	51:1t:51:GLU:CD	2.18	0.50
32:1a:1518:MA6:H93	32:1a:1519:MA6:H92	1.92	0.50
33:1b:155:LEU:HD21	33:1b:159:PRO:HD3	1.93	0.50
38:1g:74:GLU:HG2	38:1g:91:VAL:HG22	1.94	0.50
1:2A:194:G:N7	62:2A:3902:HOH:O	2.35	0.50
1:2A:2836:U:H2'	1:2A:2837:G:C8	2.46	0.50
6:2G:97:ASP:HA	6:2G:100:TRP:HD1	1.76	0.50
6:2G:111:LEU:HA	6:2G:114:ILE:HD12	1.94	0.50
27:25:2:ALA:N	62:25:201:HOH:O	2.44	0.50
32:2a:743:U:H2'	32:2a:744:C:C6	2.47	0.50
35:2d:173:TRP:CD2	35:2d:189:PRO:HB3	2.47	0.50
45:2n:48:ALA:HB2	45:2n:53:LEU:HD12	1.94	0.50
51:2t:47:GLY:HA2	51:2t:48:LYS:C	2.37	0.50
1:1A:1405:U:H2'	1:1A:1406:U:H6	1.75	0.50
1:1A:1828:G:H8	1:1A:1828:G:OP2	1.95	0.50
1:1A:2312:U:OP1	6:1G:73:ALA:HA	2.12	0.50
21:1Z:103:ARG:O	21:1Z:138:GLU:HA	2.11	0.50
26:14:53:GLU:HB2	26:14:55:ARG:C	2.37	0.50
36:1e:81:GLU:HG2	36:1e:90:VAL:HG22	1.93	0.50
39:1h:56:LYS:HB2	39:1h:58:TYR:HE2	1.77	0.50
41:1j:40:LEU:HB2	41:1j:69:ASN:HB2	1.94	0.50
54:1w:13:C:H2'	54:1w:14:A:H5''	1.93	0.50
1:2A:2059:A:H2'	1:2A:2503:2MA:HM23	1.94	0.50
6:2G:135:LEU:HB2	6:2G:155:MET:HE3	1.92	0.50
32:2a:1189:C:O2'	34:2c:176:HIS:ND1	2.31	0.50
34:2c:150:LYS:HG3	34:2c:169:ALA:HB2	1.94	0.50
35:2d:33:MET:HB2	60:2d:302:SF4:S2	2.51	0.50
35:2d:98:GLU:HG3	35:2d:194:LEU:HD21	1.94	0.50
50:2s:30:LEU:HA	50:2s:48:THR:O	2.12	0.50
56:2y:18:G:N1	56:2y:55:PSU:C4	2.78	0.50
32:1a:585:G:O6	62:1a:1915:HOH:O	2.19	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:973:G:H3'	32:1a:974:A:H5''	1.94	0.50
32:1a:1273:G:H3'	32:1a:1274:G:H8	1.76	0.50
48:1q:50:LYS:HE2	48:1q:51:TYR:CZ	2.46	0.50
56:1y:8:4SU:H4'	56:1y:48:C:C4'	2.42	0.50
1:2A:242:G:C8	30:28:5:LYS:HG2	2.47	0.50
1:2A:1183:G:H5''	25:23:30:ARG:NH2	2.26	0.50
1:2A:1225:G:H4'	17:2V:84:LYS:HG2	1.93	0.50
1:2A:1899:G:O2'	1:2A:1900:A:OP2	2.30	0.50
1:2A:2320:A:N3	1:2A:2320:A:H2'	2.27	0.50
1:2A:2611:U:C4	27:25:3:LYS:HG2	2.47	0.50
1:2A:2823:A:OP1	4:2E:159:HIS:NE2	2.44	0.50
6:2G:41:GLN:O	6:2G:43:LEU:N	2.45	0.50
32:2a:1104:G:H4'	33:2b:111:ARG:HH21	1.76	0.50
32:2a:1423:G:H2'	32:2a:1424:C:H6	1.77	0.50
39:2h:73:ASP:OD1	39:2h:75:ARG:NE	2.43	0.50
42:2k:87:THR:O	42:2k:87:THR:OG1	2.25	0.50
1:1A:1156:A:OP1	16:1U:55:ARG:NH1	2.43	0.50
1:1A:1762:A:H2'	62:1A:5722:HOH:O	2.12	0.50
1:1A:2120:G:O2'	1:1A:2121:G:H5'	2.11	0.50
1:1A:2404:C:O3'	11:1P:77:ARG:NH2	2.45	0.50
4:1E:5:LEU:HD12	4:1E:51:PHE:HB2	1.94	0.50
4:1E:72:VAL:HG12	4:1E:73:GLU:O	2.12	0.50
32:1a:396:G:O2'	32:1a:398:C:OP1	2.15	0.50
32:1a:453:A:O2'	47:1p:68:ASP:O	2.30	0.50
32:1a:1032:G:H2'	32:1a:1033:G:O4'	2.12	0.50
32:1a:1039:C:H2'	32:1a:1040:U:H6	1.76	0.50
32:1a:1136:U:H5''	32:1a:1137:C:N3	2.27	0.50
1:2A:275:G:H2'	1:2A:276:A:O4'	2.11	0.50
1:2A:896:A:H1'	54:2w:56:C:H5'	1.92	0.50
1:2A:2185:C:H2'	1:2A:2186:G:O4'	2.12	0.50
8:2I:130:TYR:HB3	8:2I:138:ILE:HB	1.94	0.50
21:2Z:30:ASN:HA	21:2Z:89:PHE:HE1	1.77	0.50
32:2a:288:A:H2'	32:2a:289:G:H4'	1.94	0.50
32:2a:1100:C:H2'	32:2a:1102:A:O5'	2.12	0.50
41:2j:80:LYS:O	41:2j:84:GLN:HG3	2.11	0.50
1:1A:2136:C:N4	1:1A:2155:G:C6	2.72	0.50
1:1A:2464:C:H1'	62:1A:5742:HOH:O	2.11	0.50
2:1B:96:U:O4	62:1B:303:HOH:O	2.19	0.50
11:1P:111:ARG:HB3	11:1P:128:HIS:CG	2.46	0.50
21:1Z:3:TYR:CD2	21:1Z:51:ALA:HB2	2.46	0.50
24:12:3:LEU:O	24:12:7:ARG:HG3	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1027:C:N1	32:1a:1034:G:N2	2.59	0.50
32:1a:1080:A:OP1	36:1e:47:LYS:HD3	2.12	0.50
32:1a:1240:U:OP2	38:1g:116:ALA:N	2.45	0.50
32:1a:1458:G:H5''	51:1t:31:SER:HB2	1.93	0.50
50:1s:36:ARG:NH1	50:1s:52:TYR:O	2.40	0.50
1:2A:30:G:H2'	1:2A:31:C:C6	2.47	0.50
1:2A:2319:G:H22	14:2S:3:ARG:NH1	2.09	0.50
19:2X:26:TYR:HB3	19:2X:92:LEU:HD22	1.93	0.50
21:2Z:54:HIS:HE2	21:2Z:123:ASP:CG	2.20	0.50
32:2a:1376:U:P	38:2g:94:ARG:HH22	2.34	0.50
50:2s:37:ARG:O	50:2s:70:LYS:NZ	2.37	0.50
1:1A:1379:A:H4'	1:1A:1380:G:OP2	2.11	0.49
1:1A:2687:U:H2'	1:1A:2688:U:O4'	2.11	0.49
9:1N:75:TYR:CE2	9:1N:77:GLY:HA2	2.47	0.49
12:1Q:68:ILE:HD13	12:1Q:103:MET:HG2	1.94	0.49
20:1Y:43:ASN:HB3	20:1Y:65:ALA:HB3	1.92	0.49
32:1a:202:U:H3'	32:1a:203:U:C6	2.47	0.49
32:1a:1030(B):C:H2'	32:1a:1030(C):G:H5'	1.94	0.49
32:1a:1503:A:N3	53:1v:13:A:N6	2.60	0.49
35:1d:140:VAL:HG21	35:1d:146:ILE:HD11	1.93	0.49
1:2A:2454:G:O6	62:2A:3841:HOH:O	2.18	0.49
23:21:83:GLU:N	23:21:83:GLU:OE2	2.45	0.49
32:2a:397:A:H3'	32:2a:397:A:N3	2.27	0.49
32:2a:736:C:H2'	32:2a:737:A:C8	2.47	0.49
38:2g:79:ARG:NH2	38:2g:80:VAL:HA	2.26	0.49
42:2k:33:THR:HA	42:2k:39:PRO:HA	1.93	0.49
47:2p:43:LYS:HG2	47:2p:48:TRP:CD2	2.47	0.49
54:2w:19:G:N2	54:2w:57:G:H1'	2.27	0.49
1:1A:800:A:H8	1:1A:800:A:OP1	1.94	0.49
1:1A:938:G:OP2	30:18:52:LYS:NZ	2.44	0.49
1:1A:1796:U:H2'	1:1A:1797:C:H6	1.76	0.49
9:1N:58:ASP:OD1	9:1N:58:ASP:N	2.43	0.49
16:1U:74:LEU:HD12	16:1U:74:LEU:H	1.77	0.49
16:1U:108:GLU:O	16:1U:112:ARG:HG2	2.11	0.49
21:1Z:152:ALA:HB1	21:1Z:163:LEU:HD11	1.94	0.49
32:1a:1004:A:H5''	32:1a:1025:U:C5	2.47	0.49
36:1e:145:LYS:HA	36:1e:148:VAL:HG22	1.93	0.49
56:1y:38:A:H2'	56:1y:39:PSU:O4'	2.12	0.49
1:2A:218:A:C2	1:2A:235:U:H4'	2.46	0.49
1:2A:236:C:H2'	1:2A:237:C:C6	2.47	0.49
1:2A:597:U:H2'	1:2A:598:G:H8	1.75	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:625:G:N7	11:2P:107:LYS:NZ	2.56	0.49
1:2A:2401:U:OP1	28:26:18:ARG:NH2	2.44	0.49
8:2I:77:LEU:HB3	8:2I:142:VAL:HG13	1.94	0.49
26:24:41:PRO:HG3	26:24:49:PHE:CE1	2.47	0.49
32:2a:1026:G:O6	32:2a:1036:G:N2	2.45	0.49
1:1A:1063:G:H2'	1:1A:1064:C:C5	2.47	0.49
32:1a:17:U:H2'	32:1a:18:C:C6	2.48	0.49
32:1a:456:C:H2'	32:1a:457:C:H6	1.78	0.49
32:1a:977:A:O2'	32:1a:981:U:N3	2.44	0.49
33:1b:54:THR:HG23	33:1b:199:TYR:HB3	1.93	0.49
41:1j:55:LYS:O	41:1j:57:LYS:N	2.45	0.49
1:2A:1025:G:C4	1:2A:1135:C:H1'	2.48	0.49
5:2F:120:GLU:OE2	5:2F:122:LYS:HG3	2.12	0.49
7:2H:144:VAL:O	7:2H:148:ILE:HG13	2.12	0.49
12:2Q:78:PRO:HG2	12:2Q:81:VAL:HG11	1.93	0.49
17:2V:40:LEU:HD12	17:2V:46:VAL:HG21	1.94	0.49
32:2a:662:G:H2'	32:2a:663:A:C8	2.46	0.49
32:2a:1023:G:H3'	32:2a:1024:G:H8	1.77	0.49
32:2a:1105:A:H2'	32:2a:1106:G:C8	2.38	0.49
32:2a:1119:C:H2'	32:2a:1120:G:C8	2.47	0.49
34:2c:83:ARG:C	34:2c:85:ARG:H	2.20	0.49
35:2d:22:LYS:HB2	35:2d:26:CYS:SG	2.52	0.49
37:2f:61:LEU:HD22	37:2f:63:TYR:CZ	2.47	0.49
56:2y:18:G:N2	56:2y:55:PSU:HN3	1.95	0.49
21:1Z:41:LEU:HD11	21:1Z:83:PRO:HG2	1.95	0.49
32:1a:184:G:H2'	32:1a:185:A:H8	1.77	0.49
32:1a:406:G:N3	35:1d:119:GLN:NE2	2.60	0.49
32:1a:627:G:O2'	32:1a:628:G:H5'	2.12	0.49
32:1a:1027:C:C4	32:1a:1034:G:N1	2.80	0.49
40:1i:9:ARG:HG2	40:1i:14:VAL:HG12	1.94	0.49
55:1x:8:4SU:O2	55:1x:21:A:H2	1.94	0.49
1:2A:1231:G:H2'	1:2A:1232:G:H8	1.77	0.49
1:2A:2164:C:C4	1:2A:2165:G:H1'	2.48	0.49
11:2P:95:VAL:HG22	11:2P:125:VAL:HG23	1.95	0.49
14:2S:39:ILE:HG21	14:2S:82:ILE:HD13	1.94	0.49
18:2W:17:VAL:HG11	18:2W:103:ILE:HD11	1.94	0.49
32:2a:1510:U:H2'	32:2a:1511:G:C8	2.47	0.49
34:2c:11:ARG:NH2	34:2c:177:THR:O	2.44	0.49
55:2x:23:C:H2'	55:2x:24:U:C6	2.48	0.49
56:2y:18:G:N2	56:2y:55:PSU:C4	2.75	0.49
1:1A:360:G:OP1	62:1A:4250:HOH:O	2.20	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1297:C:OP1	1:1A:2710:C:H4'	2.13	0.49
1:1A:1372:U:H2'	1:1A:1373:A:O4'	2.13	0.49
10:1O:20:MET:HE3	10:1O:44:LYS:HE3	1.94	0.49
32:1a:1095:U:P	32:1a:1108:G:H1	2.35	0.49
2:2B:2:C:H2'	2:2B:3:C:C6	2.47	0.49
2:2B:24:G:O2'	2:2B:56:G:N7	2.43	0.49
12:2Q:35:VAL:HG22	12:2Q:102:VAL:HG22	1.95	0.49
13:2R:97:VAL:HG22	13:2R:114:VAL:HG13	1.95	0.49
26:24:59:PHE:HE2	50:2s:64:GLU:HB2	1.77	0.49
32:2a:993:G:N3	32:2a:993:G:H2'	2.27	0.49
33:2b:187:LEU:HD23	33:2b:188:ALA:N	2.28	0.49
34:2c:31:HIS:O	34:2c:35:GLU:HB3	2.12	0.49
1:1A:898:C:N4	1:1A:899:A:N7	2.60	0.49
1:1A:1253:A:OP1	62:1A:4249:HOH:O	2.19	0.49
32:1a:161:A:N1	32:1a:347:G:O2'	2.42	0.49
38:1g:27:ILE:HD13	38:1g:40:ALA:HA	1.95	0.49
1:2A:2319:G:N2	14:2S:3:ARG:HD2	2.27	0.49
8:2I:45:LYS:O	8:2I:49:ALA:N	2.41	0.49
32:2a:1097:C:H1'	32:2a:1170:A:H1'	1.94	0.49
32:2a:1521:G:H2'	32:2a:1522:U:C6	2.47	0.49
1:1A:568:U:H5'	1:1A:945:A:N6	2.28	0.49
1:1A:729:G:C6	3:1D:208:LYS:HB2	2.48	0.49
1:1A:1077:A:H2'	1:1A:1078:U:H4'	1.95	0.49
9:1N:62:VAL:CG2	9:1N:66:LYS:HD2	2.42	0.49
23:11:26:ARG:HG3	23:11:27:GLU:HG3	1.94	0.49
32:1a:667:G:H4'	46:1o:51:HIS:ND1	2.27	0.49
32:1a:1504:G:OP1	32:1a:1507:A:H4'	2.13	0.49
34:1c:15:THR:HG21	34:1c:181:ASN:HA	1.94	0.49
1:2A:854:G:H2'	1:2A:855:G:H8	1.78	0.49
1:2A:928:G:H8	1:2A:928:G:O5'	1.95	0.49
1:2A:1502:C:H2'	1:2A:1503:U:H6	1.78	0.49
5:2F:53:THR:HG23	5:2F:55:GLY:N	2.26	0.49
6:2G:15:VAL:HG13	6:2G:175:LEU:HD13	1.94	0.49
16:2U:113:ALA:O	16:2U:117:GLN:HG2	2.11	0.49
21:2Z:40:ASP:OD2	21:2Z:43:GLU:N	2.42	0.49
32:2a:189(K):U:H2'	32:2a:189(L):G:C8	2.48	0.49
32:2a:821:G:H2'	32:2a:822:C:C6	2.47	0.49
32:2a:1346:A:H61	32:2a:1374:A:H3'	1.78	0.49
1:1A:1798:U:H5'	3:1D:259:THR:CG2	2.41	0.49
1:1A:2121:G:H1	1:1A:2177:C:N4	2.08	0.49
6:1G:106:LEU:HA	6:1G:110:ALA:HB3	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1291:G:O2'	40:1i:38:GLN:OE1	2.29	0.49
39:1h:35:ILE:HD13	39:1h:118:VAL:HG11	1.95	0.49
1:2A:27:G:N2	1:2A:512:G:H1'	2.27	0.49
1:2A:212:G:H2'	1:2A:213:A:O4'	2.13	0.49
1:2A:492:A:H2'	1:2A:493:G:O4'	2.13	0.49
1:2A:1358:G:O2'	1:2A:1373:A:N6	2.45	0.49
1:2A:1359:A:H2'	1:2A:1360:A:H5'	1.94	0.49
1:2A:2680:C:H1'	4:2E:187:ALA:HB1	1.94	0.49
1:2A:2787:C:H1'	4:2E:62:PRO:HG3	1.94	0.49
9:2N:138:LEU:HB3	9:2N:140:VAL:HG13	1.93	0.49
12:2Q:85:LYS:HD3	22:20:7:LEU:HD22	1.94	0.49
32:2a:559:A:H4'	32:2a:560:U:H3'	1.94	0.49
32:2a:1015:A:H2'	32:2a:1016:A:C8	2.48	0.49
34:2c:29:TYR:OH	45:2n:54:PRO:O	2.30	0.49
1:1A:657:U:H2'	1:1A:658:C:C6	2.48	0.49
5:1F:31:HIS:NE2	5:1F:35:GLU:OE2	2.45	0.49
13:1R:97:VAL:HG22	13:1R:114:VAL:HG13	1.94	0.49
33:1b:20:GLU:HG2	33:1b:23:ARG:NH1	2.28	0.49
36:1e:12:LEU:HB3	36:1e:31:LEU:HB2	1.94	0.49
36:1e:78:HIS:CE1	36:1e:143:ARG:H	2.30	0.49
40:1i:79:LEU:HG	40:1i:83:ARG:HD2	1.93	0.49
47:1p:47:ASP:OD1	47:1p:47:ASP:N	2.46	0.49
1:2A:1633:G:OP2	62:2A:3844:HOH:O	2.20	0.49
1:2A:1924:C:H4'	55:2x:13:C:O2'	2.13	0.49
6:2G:161:THR:HG22	6:2G:163:ALA:H	1.77	0.49
14:2S:56:LEU:HB3	14:2S:58:LEU:HD12	1.94	0.49
21:2Z:98:MET:HE3	21:2Z:100:VAL:HB	1.94	0.49
22:20:52:GLY:O	22:20:59:LEU:HA	2.13	0.49
24:22:37:PHE:O	24:22:40:SER:OG	2.31	0.49
32:2a:134:A:H61	47:2p:25:ARG:NH1	2.11	0.49
32:2a:828:A:H2'	32:2a:829:G:O4'	2.12	0.49
32:2a:1346:A:N1	32:2a:1374:A:H5''	2.27	0.49
32:2a:1435:G:H2'	32:2a:1436:U:C6	2.48	0.49
32:2a:1490:C:H2'	32:2a:1491:G:O4'	2.12	0.49
1:1A:1188:U:H4'	17:1V:79:VAL:HG22	1.94	0.49
32:1a:399:G:H2'	32:1a:400:C:C6	2.48	0.49
33:1b:12:GLU:O	33:1b:15:VAL:HG22	2.12	0.49
44:1m:40:ASN:O	44:1m:43:THR:OG1	2.30	0.49
45:1n:27:CYS:SG	45:1n:29:ARG:HB2	2.53	0.49
1:2A:184:C:H2'	1:2A:185:U:C6	2.48	0.49
1:2A:481:G:O5'	20:2Y:47:LYS:NZ	2.40	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2F:31:HIS:HB2	11:2P:9:ASN:OD1	2.12	0.49
19:2X:84:ALA:HB3	19:2X:87:GLN:NE2	2.28	0.49
32:2a:382:A:H2'	32:2a:383:A:C8	2.48	0.49
32:2a:660:G:H1	32:2a:745:C:H42	1.61	0.49
32:2a:1033:G:H2'	32:2a:1034:G:H8	1.76	0.49
33:2b:15:VAL:HG23	33:2b:16:HIS:HD2	1.78	0.49
39:2h:12:ARG:NH1	39:2h:27:PRO:HD3	2.28	0.49
50:2s:27:GLU:HB2	50:2s:28:LYS:HA	1.95	0.49
1:1A:271(M):G:O2'	1:1A:271(N):U:H5''	2.13	0.48
2:1B:11:C:OP2	22:10:72:ARG:NH2	2.35	0.48
52:1u:5:ASP:O	52:1u:11:GLY:HA3	2.13	0.48
55:1x:8:4SU:O5'	55:1x:8:4SU:H6	2.13	0.48
4:2E:28:ALA:HB3	4:2E:93:VAL:HG12	1.95	0.48
9:2N:20:GLY:HA2	9:2N:61:ARG:NH2	2.28	0.48
12:2Q:36:ALA:HB2	12:2Q:103:MET:SD	2.52	0.48
32:2a:1005:A:H3'	32:2a:1006:C:C6	2.48	0.48
32:2a:1190:G:H5'	34:2c:176:HIS:HE1	1.78	0.48
35:2d:20:TYR:HD1	35:2d:26:CYS:HB3	1.78	0.48
42:2k:80:VAL:HG22	42:2k:105:VAL:HA	1.95	0.48
24:12:7:ARG:O	24:12:11:GLU:HG3	2.14	0.48
1:2A:1042:G:H3'	1:2A:1043:C:H6	1.78	0.48
3:2D:232:PRO:O	62:2D:402:HOH:O	2.19	0.48
7:2H:3:ARG:HE	7:2H:54:ARG:HH12	1.60	0.48
21:2Z:47:VAL:O	21:2Z:50:GLN:NE2	2.46	0.48
21:2Z:61:LEU:HB2	21:2Z:65:GLN:O	2.14	0.48
32:2a:137:C:H2'	32:2a:138:G:H8	1.78	0.48
32:2a:821:G:H2'	32:2a:822:C:H6	1.77	0.48
32:2a:1218:C:OP2	45:2n:9:LYS:NZ	2.46	0.48
32:2a:1371:G:O3'	40:2i:69:GLY:HA3	2.13	0.48
36:2e:60:TYR:CZ	36:2e:64:ARG:HD3	2.48	0.48
40:2i:17:VAL:HG11	40:2i:81:ILE:HA	1.95	0.48
43:2l:79:GLU:HG2	43:2l:80:HIS:CE1	2.48	0.48
47:2p:21:VAL:HG22	47:2p:33:ILE:HB	1.94	0.48
50:2s:51:VAL:HB	50:2s:75:ALA:HB2	1.95	0.48
50:2s:66:MET:HB2	50:2s:74:PHE:CZ	2.48	0.48
1:1A:229:A:H5''	1:1A:230:U:H5'	1.95	0.48
1:1A:1803:A:H4'	3:1D:259:THR:HG23	1.94	0.48
8:1I:12:LEU:HD22	8:1I:19:VAL:HG21	1.94	0.48
21:1Z:150:LEU:HG	21:1Z:151:HIS:H	1.77	0.48
31:19:2:LYS:HD3	31:19:4:ARG:NH2	2.29	0.48
32:1a:57:G:H2'	32:1a:58:C:C6	2.47	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:677:U:H3	32:1a:713:G:H22	1.59	0.48
32:1a:1305:G:N2	32:1a:1331:G:H1'	2.29	0.48
1:2A:570:G:H2'	1:2A:2030:A:C5	2.48	0.48
1:2A:848:G:H2'	1:2A:849:A:C8	2.48	0.48
1:2A:1239:G:H2'	1:2A:1240:U:O4'	2.13	0.48
1:2A:2010:G:H5''	18:2W:42:ARG:HB2	1.95	0.48
6:2G:5:VAL:HG23	6:2G:8:LYS:H	1.78	0.48
12:2Q:26:TYR:O	12:2Q:67:ARG:NH1	2.43	0.48
15:2T:102:ILE:HB	15:2T:110:ILE:HG12	1.96	0.48
21:2Z:30:ASN:ND2	21:2Z:90:VAL:HB	2.25	0.48
23:21:50:ARG:HD2	23:21:57:GLU:OE2	2.13	0.48
34:2c:120:VAL:HG23	34:2c:137:ALA:HB2	1.95	0.48
54:2w:39:PSU:H2'	54:2w:40:C:C6	2.49	0.48
2:1B:75:G:H22	21:1Z:73:GLN:NE2	2.11	0.48
3:1D:166:GLN:HB2	3:1D:174:ILE:HG22	1.94	0.48
9:1N:42:TRP:CH2	9:1N:44:PRO:HB3	2.48	0.48
25:13:7:LYS:HB2	25:13:34:GLU:HG3	1.94	0.48
26:14:40:HIS:CD2	26:14:41:PRO:HD2	2.48	0.48
32:1a:1179:A:O3'	40:1i:103:THR:HB	2.13	0.48
1:2A:271(Q):G:H2'	1:2A:271(R):G:C8	2.47	0.48
1:2A:296:C:O3'	20:2Y:95:LYS:NZ	2.47	0.48
2:2B:24:G:H4'	2:2B:25:A:C8	2.48	0.48
12:2Q:16:ARG:HG3	12:2Q:17:LEU:H	1.79	0.48
12:2Q:45:GLN:N	12:2Q:45:GLN:OE1	2.45	0.48
12:2Q:82:ARG:HH21	22:20:4:LYS:HG3	1.77	0.48
13:2R:38:VAL:HG22	13:2R:112:ALA:HB2	1.95	0.48
32:2a:537:G:H5''	43:2l:113:ARG:NH1	2.29	0.48
32:2a:859:A:H2'	32:2a:860:A:O4'	2.12	0.48
32:2a:1366:C:H2'	32:2a:1367:C:H6	1.75	0.48
33:2b:51:LEU:O	33:2b:55:PHE:HB2	2.13	0.48
40:2i:112:LYS:NZ	40:2i:113:LYS:O	2.46	0.48
1:1A:1256:G:H1'	5:1F:82:ILE:HD11	1.96	0.48
32:1a:877:C:OP1	39:1h:88:LYS:NZ	2.27	0.48
32:1a:881:G:P	43:1l:12:ARG:HH22	2.36	0.48
32:1a:1278:U:H5'	32:1a:1279:A:O4'	2.13	0.48
32:1a:1410:G:H2'	32:1a:1411:C:C6	2.48	0.48
55:1x:12:G:OP2	62:1x:201:HOH:O	2.19	0.48
1:2A:1509(B):A:H2'	1:2A:1510:G:C8	2.48	0.48
1:2A:2478:A:OP2	31:29:2:LYS:NZ	2.33	0.48
2:2B:42:C:C4	2:2B:43:C:C4	3.01	0.48
2:2B:105:A:H5'	2:2B:106:G:OP2	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2Z:6:LYS:HE3	21:2Z:8:TYR:HE2	1.79	0.48
32:2a:412:A:O4'	35:2d:35:ARG:NH2	2.47	0.48
32:2a:448:A:OP2	32:2a:485:G:N2	2.45	0.48
32:2a:1030(A):G:N2	32:2a:1030(C):G:H3'	2.27	0.48
32:2a:1031:G:H2'	32:2a:1032:G:C8	2.49	0.48
33:2b:83:MET:HE2	33:2b:234:PRO:HG3	1.96	0.48
40:2i:127:LYS:O	40:2i:128:ARG:HB3	2.14	0.48
1:1A:272(A):U:HO2'	1:1A:272(B):G:P	2.34	0.48
7:1H:9:ILE:HB	7:1H:50:VAL:HG23	1.96	0.48
32:1a:964:A:OP1	62:1a:1919:HOH:O	2.20	0.48
44:1m:87:TYR:O	44:1m:91:ARG:HG2	2.13	0.48
51:1t:39:LYS:HG2	51:1t:55:ILE:HG21	1.96	0.48
1:2A:1608:A:H1'	1:2A:1610:A:OP2	2.14	0.48
1:2A:2847:U:OP1	15:2T:98:LYS:NZ	2.47	0.48
2:2B:17:C:H2'	2:2B:18:G:O4'	2.14	0.48
15:2T:73:GLU:OE2	15:2T:103:ARG:NE	2.37	0.48
21:2Z:51:ALA:O	21:2Z:52:SER:HB3	2.13	0.48
23:21:65:SER:HB2	23:21:66:HIS:ND1	2.28	0.48
29:27:24:THR:HG22	29:27:27:GLY:N	2.14	0.48
30:28:26:LYS:HD2	30:28:48:PHE:CD2	2.49	0.48
32:2a:954:G:H2'	32:2a:955:U:O4'	2.13	0.48
32:2a:1201:A:H4'	32:2a:1202:G:O5'	2.14	0.48
32:2a:1203:C:OP1	45:2n:3:ARG:NE	2.45	0.48
32:2a:1370:G:N7	40:2i:109:VAL:HG11	2.28	0.48
32:2a:1381:U:O2'	38:2g:79:ARG:HD3	2.13	0.48
35:2d:114:ARG:HA	35:2d:117:ALA:HB3	1.96	0.48
40:2i:9:ARG:HG2	40:2i:14:VAL:HG12	1.94	0.48
40:2i:71:SER:HA	40:2i:74:ILE:HD12	1.95	0.48
43:2l:59:ARG:HA	43:2l:65:GLU:HA	1.95	0.48
1:1A:226:G:N2	1:1A:228:A:H62	2.11	0.48
1:1A:1094:U:H1'	1:1A:1097:U:C4	2.49	0.48
1:1A:2336:A:H61	22:10:43:THR:HG22	1.79	0.48
1:1A:2611:U:C4	27:15:3:LYS:HG2	2.48	0.48
2:1B:88:C:H2'	2:1B:89:G:O4'	2.13	0.48
36:1e:33:VAL:HG13	36:1e:112:LEU:HD12	1.96	0.48
1:2A:250:G:C6	1:2A:251:A:C6	3.01	0.48
1:2A:1932:A:H2'	1:2A:1933:G:O4'	2.14	0.48
1:2A:2394:C:N3	56:2y:76:A:O2'	2.35	0.48
5:2F:165:ARG:HG2	5:2F:168:ARG:NH2	2.28	0.48
8:2I:38:LEU:O	8:2I:40:THR:N	2.47	0.48
26:24:41:PRO:HG3	26:24:49:PHE:CZ	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1051:C:H2'	32:2a:1052:U:C6	2.49	0.48
34:2c:121:ALA:HB1	34:2c:188:LEU:O	2.13	0.48
39:2h:7:ALA:HA	39:2h:10:LEU:HD12	1.95	0.48
41:2j:8:LEU:HD12	41:2j:16:LEU:HD22	1.95	0.48
45:2n:24:CYS:O	45:2n:28:GLY:N	2.40	0.48
56:2y:9:A:H4'	56:2y:46:7MG:H5'	1.94	0.48
1:1A:196:A:H2'	1:1A:196:A:N3	2.29	0.48
1:1A:278:A:OP2	1:1A:278:A:H8	1.97	0.48
1:1A:2001:A:H2'	1:1A:2002:G:C8	2.48	0.48
1:1A:2747:G:O6	1:1A:2755:C:H5''	2.14	0.48
30:18:62:LEU:HB3	30:18:65:GLU:CG	2.44	0.48
32:1a:1021:G:HO2'	32:1a:1022:G:P	2.34	0.48
32:1a:1030(C):G:H2'	32:1a:1030(D):A:C8	2.49	0.48
44:1m:5:ALA:HA	44:1m:61:GLU:OE2	2.14	0.48
1:2A:863:A:H2'	1:2A:864:G:C8	2.48	0.48
1:2A:1805:U:O2	3:2D:50:THR:HB	2.14	0.48
1:2A:1847:A:H3'	1:2A:1848:A:H5'	1.96	0.48
1:2A:2126:A:N6	1:2A:2162:G:O2'	2.44	0.48
1:2A:2238:G:H2'	1:2A:2238:G:N3	2.29	0.48
1:2A:2258:C:O2'	1:2A:2427:C:OP2	2.28	0.48
5:2F:129:PHE:CD2	5:2F:163:VAL:HG21	2.49	0.48
6:2G:112:PRO:HG3	26:24:43:TYR:CE1	2.48	0.48
6:2G:114:ILE:HB	6:2G:117:PHE:HD1	1.78	0.48
7:2H:20:ALA:HB3	7:2H:23:ARG:HG3	1.96	0.48
8:2I:71:ILE:O	8:2I:75:LEU:HG	2.13	0.48
11:2P:63:PRO:HG2	30:28:25:MET:HB2	1.95	0.48
32:2a:9:G:H2'	32:2a:10:A:H8	1.78	0.48
32:2a:1052:U:O2'	32:2a:1055:A:OP2	2.20	0.48
32:2a:1128:C:O2'	32:2a:1129:C:OP1	2.32	0.48
34:2c:182:ILE:HG22	34:2c:203:PHE:HA	1.96	0.48
34:2c:183:ASP:HB2	34:2c:204:LEU:HD11	1.94	0.48
50:2s:28:LYS:HZ2	50:2s:47:HIS:HA	1.79	0.48
1:1A:620:G:N3	1:1A:620:G:H5'	2.29	0.48
1:1A:894:C:H2'	1:1A:895:U:O4'	2.14	0.48
1:1A:1062:G:H8	1:1A:1070:A:H4'	1.79	0.48
1:1A:1105:U:H2'	1:1A:1106:G:H8	1.78	0.48
7:1H:20:ALA:HB1	7:1H:21:PRO:HD2	1.96	0.48
26:14:62:ARG:C	26:14:63:TYR:CG	2.92	0.48
44:1m:108:ARG:HD3	44:1m:108:ARG:HA	1.65	0.48
56:1y:4:C:H2'	56:1y:5:G:O4'	2.14	0.48
1:2A:1607:C:H5''	1:2A:1608:A:H5'	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2S:11:LYS:HG3	14:2S:91:PRO:HB3	1.95	0.48
20:2Y:76:CYS:HA	20:2Y:106:LEU:HD23	1.96	0.48
32:2a:716:A:N3	42:2k:118:GLY:HA2	2.29	0.48
32:2a:1095:U:C4	32:2a:1096:C:C4	3.02	0.48
32:2a:1111:A:N1	34:2c:177:THR:OG1	2.32	0.48
1:1A:1508:A:O2'	1:1A:1509:C:H5''	2.14	0.48
9:1N:15:LEU:HB2	9:1N:135:PRO:HB2	1.96	0.48
32:1a:1129:C:O2'	32:1a:1139:G:N7	2.41	0.48
36:1e:106:PRO:O	36:1e:110:LEU:HG	2.14	0.48
40:1i:16:ARG:HH11	40:1i:64:THR:HG21	1.79	0.48
1:2A:95:G:O2'	24:22:48:HIS:ND1	2.41	0.48
1:2A:1371:G:O6	62:2A:3843:HOH:O	2.19	0.48
1:2A:1406:U:H2'	1:2A:1407:C:C6	2.48	0.48
1:2A:2646:C:OP2	1:2A:2732:G:O2'	2.30	0.48
30:28:26:LYS:HB2	30:28:44:LYS:O	2.14	0.48
32:2a:524:G:H2'	32:2a:525:C:C6	2.49	0.48
32:2a:1142:G:H2'	32:2a:1143:G:O4'	2.14	0.48
32:2a:1456:G:O6	51:2t:54:LYS:NZ	2.42	0.48
37:2f:36:ARG:NH2	37:2f:38:GLU:OE2	2.47	0.48
40:2i:81:ILE:O	40:2i:85:LEU:HG	2.14	0.48
47:2p:58:TYR:O	47:2p:61:SER:OG	2.17	0.48
56:2y:55:PSU:H6	56:2y:57:G:OP2	1.97	0.48
1:1A:2136:C:C4	1:1A:2155:G:N1	2.82	0.47
11:1P:2:LYS:HG2	11:1P:3:LEU:N	2.29	0.47
32:1a:162:A:N7	32:1a:163:C:H1'	2.29	0.47
32:1a:542:G:P	35:1d:10:ARG:HH22	2.37	0.47
32:1a:1356:G:H2'	32:1a:1357:A:H8	1.76	0.47
37:1f:76:ALA:O	37:1f:80:ARG:HG3	2.14	0.47
47:1p:6:LEU:HB3	47:1p:17:TYR:CD1	2.49	0.47
1:2A:918:A:N3	2:2B:80:U:O2'	2.41	0.47
3:2D:253:GLN:HG3	62:2D:412:HOH:O	2.13	0.47
12:2Q:43:THR:HA	12:2Q:94:VAL:HG12	1.94	0.47
15:2T:28:VAL:HG13	15:2T:86:ILE:HG23	1.96	0.47
32:2a:457:C:H2'	32:2a:458:C:H6	1.78	0.47
32:2a:1003:G:N2	32:2a:1025:U:O4	2.47	0.47
46:2o:26:GLU:N	46:2o:26:GLU:OE1	2.47	0.47
11:1P:97:PRO:HD3	11:1P:126:VAL:O	2.14	0.47
21:1Z:8:TYR:HB2	21:1Z:38:TYR:CE2	2.49	0.47
32:1a:182:U:C4	32:1a:183:G:H1'	2.49	0.47
32:1a:505:G:N7	62:1a:1950:HOH:O	2.35	0.47
32:1a:1302:U:C5	44:1m:17:VAL:HG21	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:1i:17:VAL:HA	40:1i:63:ILE:HG23	1.96	0.47
46:1o:8:LYS:O	46:1o:12:ILE:HG13	2.15	0.47
1:2A:2518:A:OP2	62:2A:3842:HOH:O	2.19	0.47
1:2A:2690:C:OP1	13:2R:17:ARG:NH2	2.47	0.47
1:2A:2871:C:N4	62:2A:3983:HOH:O	2.46	0.47
15:2T:109:GLU:HG2	15:2T:112:ARG:NH2	2.29	0.47
18:2W:83:LYS:HE3	18:2W:97:LYS:HE3	1.96	0.47
21:2Z:53:ILE:CD1	21:2Z:99:TYR:HB2	2.44	0.47
32:2a:1004:A:N3	32:2a:1038:C:C2	2.82	0.47
32:2a:1118:C:H1'	32:2a:1179:A:C4	2.49	0.47
32:2a:1203:C:H2'	32:2a:1204:A:C8	2.49	0.47
32:2a:1271:G:C2	32:2a:1272:G:N7	2.82	0.47
32:2a:1301:U:O2'	32:2a:1302:U:H5'	2.13	0.47
33:2b:27:LYS:O	33:2b:194:PRO:HG2	2.14	0.47
34:2c:12:LEU:HG	34:2c:18:TRP:CH2	2.49	0.47
35:2d:135:LEU:C	35:2d:137:SER:H	2.22	0.47
1:1A:207:A:H2'	1:1A:208:C:O4'	2.14	0.47
1:1A:1095:A:H62	1:1A:1097:U:H3	1.60	0.47
1:1A:1996:C:H4'	1:1A:1997:G:OP1	2.13	0.47
1:1A:2145:C:C3'	1:1A:2146:C:H5'	2.43	0.47
1:1A:2791:C:H2'	1:1A:2792:G:C8	2.49	0.47
2:1B:29:A:O2'	2:1B:58:A:N1	2.46	0.47
14:1S:14:VAL:O	14:1S:18:ILE:HG12	2.14	0.47
32:1a:1062:U:H2'	32:1a:1063:C:C6	2.48	0.47
32:1a:1118:C:H1'	32:1a:1179:A:C4	2.48	0.47
32:1a:1179:A:H2'	32:1a:1180:A:O4'	2.15	0.47
37:1f:61:LEU:HD23	37:1f:63:TYR:OH	2.14	0.47
40:1i:46:ALA:HA	40:1i:78:LYS:HB2	1.95	0.47
1:2A:370:G:N7	62:2A:3908:HOH:O	2.36	0.47
1:2A:1336:A:H2'	1:2A:1337:G:C8	2.50	0.47
1:2A:2590:A:O3'	3:2D:239:ARG:NH2	2.47	0.47
2:2B:7:G:H5'	14:2S:29:PHE:CE2	2.50	0.47
8:2I:1:MET:N	8:2I:21:VAL:O	2.38	0.47
18:2W:68:ARG:NH1	18:2W:111:HIS:HA	2.30	0.47
23:21:26:ARG:HG3	23:21:27:GLU:HG3	1.97	0.47
32:2a:328:C:H4'	32:2a:329:A:H5'	1.95	0.47
32:2a:815:A:N7	32:2a:1509:C:O2'	2.37	0.47
32:2a:1263:C:N3	32:2a:1272:G:O6	2.47	0.47
33:2b:12:GLU:O	33:2b:15:VAL:HG22	2.13	0.47
34:2c:22:TRP:HZ3	34:2c:24:ALA:HB2	1.79	0.47
35:2d:76:ARG:O	35:2d:80:GLU:HG2	2.13	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:2l:84:LEU:HB2	43:2l:105:TYR:CE2	2.49	0.47
1:1A:443:A:H1'	1:1A:1201:C:O4'	2.14	0.47
1:1A:1054:A:N1	1:1A:1105:U:O2	2.48	0.47
1:1A:2483:C:N3	12:1Q:124:LYS:NZ	2.61	0.47
24:12:16:LEU:HD12	24:12:21:LEU:HD23	1.96	0.47
42:1k:72:ALA:HB1	42:1k:77:MET:HG2	1.96	0.47
1:2A:297:C:H2'	1:2A:298:G:O4'	2.13	0.47
1:2A:1300:U:H4'	1:2A:1301:A:H5'	1.96	0.47
1:2A:1796:U:H2'	1:2A:1797:C:H6	1.78	0.47
1:2A:2114:A:H2	1:2A:2171:A:H61	1.61	0.47
7:2H:25:LYS:HE3	7:2H:32:GLU:HB2	1.97	0.47
11:2P:138:LEU:HG	11:2P:143:GLY:HA3	1.95	0.47
28:26:38:LYS:HB3	28:26:38:LYS:HE3	1.73	0.47
32:2a:858:G:O6	32:2a:869:G:H3'	2.14	0.47
32:2a:1084:G:H5'	32:2a:1102:A:OP2	2.14	0.47
32:2a:1305:G:O2'	32:2a:1331:G:N2	2.47	0.47
32:2a:1423:G:H2'	32:2a:1424:C:C6	2.48	0.47
33:2b:28:PHE:CD1	33:2b:194:PRO:HG3	2.49	0.47
1:1A:272:G:N7	1:1A:421:U:H2'	2.29	0.47
1:1A:288:C:H2'	1:1A:289:A:H8	1.80	0.47
1:1A:1003:G:O2'	1:1A:1010:A:N1	2.40	0.47
4:1E:128:SER:OG	4:1E:129:HIS:N	2.48	0.47
8:1I:92:VAL:HG11	8:1I:144:VAL:HG11	1.96	0.47
12:1Q:85:LYS:HG2	22:10:7:LEU:HB3	1.96	0.47
23:11:56:GLN:HE21	23:11:87:PRO:HG3	1.80	0.47
32:1a:165:C:H2'	32:1a:166:G:C8	2.49	0.47
32:1a:636:U:H2'	32:1a:637:G:H8	1.78	0.47
1:2A:1412:A:H2'	1:2A:1413:G:C8	2.48	0.47
1:2A:2294:C:P	14:2S:89:ARG:HH22	2.38	0.47
1:2A:2870:C:H2'	1:2A:2871:C:O4'	2.14	0.47
9:2N:73:THR:HG22	9:2N:84:LYS:HG2	1.95	0.47
10:2O:120:GLU:HB2	15:2T:68:TYR:HE2	1.79	0.47
21:2Z:99:TYR:HB3	21:2Z:123:ASP:HB3	1.96	0.47
32:2a:1085:U:H3'	32:2a:1086:U:C5	2.49	0.47
40:2i:20:ARG:HH22	40:2i:62:TYR:HB3	1.80	0.47
44:2m:3:ARG:HH22	44:2m:11:ARG:HG3	1.79	0.47
54:2w:9:A:H8	54:2w:11:C:H41	1.60	0.47
1:1A:570:G:H2'	1:1A:2030:A:N7	2.30	0.47
1:1A:576:U:H2'	1:1A:577:G:C8	2.49	0.47
1:1A:1712:C:H2'	1:1A:1713:U:O4'	2.14	0.47
1:1A:2417:C:OP1	11:1P:65:ARG:NH2	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1E:9:VAL:HB	15:1T:3:ARG:HG2	1.96	0.47
4:1E:111:ARG:HG3	13:1R:1:MET:SD	2.55	0.47
19:1X:26:TYR:HB3	19:1X:92:LEU:HD22	1.96	0.47
21:1Z:48:PHE:HE1	21:1Z:71:VAL:HG11	1.78	0.47
32:1a:7:G:H5''	32:1a:298:A:O4'	2.14	0.47
32:1a:96:U:H2'	32:1a:97:G:H8	1.80	0.47
32:1a:258:G:H2'	32:1a:259:G:H8	1.79	0.47
32:1a:382:A:H2'	32:1a:383:A:C8	2.50	0.47
41:1j:78:ASN:O	41:1j:80:LYS:N	2.47	0.47
42:1k:91:ARG:NH1	42:1k:110:ASP:OD1	2.47	0.47
1:2A:597:U:H2'	1:2A:598:G:C8	2.49	0.47
1:2A:643:A:N1	1:2A:2369:A:O2'	2.46	0.47
1:2A:2155:G:N7	1:2A:2156:G:H1'	2.30	0.47
2:2B:75:G:H22	21:2Z:73:GLN:NE2	2.13	0.47
12:2Q:7:MET:HE1	12:2Q:73:PRO:HG3	1.96	0.47
13:2R:33:ARG:NH2	13:2R:115:GLU:OE1	2.38	0.47
21:2Z:17:ALA:HA	21:2Z:20:ARG:HB3	1.95	0.47
21:2Z:53:ILE:HG22	21:2Z:71:VAL:HG23	1.97	0.47
21:2Z:94:GLU:H	21:2Z:94:GLU:CD	2.22	0.47
32:2a:438:G:N1	32:2a:495:A:OP2	2.35	0.47
34:2c:67:THR:HA	34:2c:102:ASN:HB2	1.97	0.47
55:2x:8:4SU:O2	55:2x:21:A:H2	1.97	0.47
1:1A:1045:A:OP1	1:1A:1046:A:H3'	2.14	0.47
1:1A:1810:A:H2'	1:1A:1811:G:O4'	2.14	0.47
1:1A:2153:G:H2'	1:1A:2154:G:H8	1.78	0.47
3:1D:83:GLU:OE1	3:1D:104:TYR:OH	2.26	0.47
5:1F:184:TYR:O	5:1F:188:ARG:HG3	2.15	0.47
15:1T:16:ARG:NH2	15:1T:18:ASP:OD2	2.48	0.47
30:18:62:LEU:HB3	30:18:65:GLU:HG3	1.96	0.47
32:1a:11:G:O2'	32:1a:506:G:N2	2.45	0.47
32:1a:933:G:OP2	38:1g:3:ARG:HB2	2.14	0.47
32:1a:1002:G:H3'	32:1a:1003:G:C4'	2.30	0.47
32:1a:1370:G:C2	32:1a:1371:G:C8	3.02	0.47
36:1e:100:VAL:O	36:1e:107:ARG:NH1	2.48	0.47
37:1f:99:ALA:HB1	49:1r:23:LYS:HZ2	1.79	0.47
40:1i:17:VAL:HG11	40:1i:80:GLY:C	2.40	0.47
47:1p:14:ASN:HA	47:1p:42:ARG:NH2	2.30	0.47
1:2A:361:G:O2'	1:2A:362:U:H5'	2.15	0.47
1:2A:861:A:N3	2:2B:79:C:O2'	2.44	0.47
1:2A:1012:U:C5	9:2N:28:THR:HG21	2.49	0.47
1:2A:1020:A:N1	1:2A:1141:U:O2'	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1487:G:H2'	1:2A:1488:G:O4'	2.13	0.47
1:2A:2166:G:H3'	1:2A:2167:U:H5''	1.96	0.47
1:2A:2802:G:C5	1:2A:2803:C:H1'	2.50	0.47
2:2B:14:U:OP2	2:2B:70:C:O2'	2.24	0.47
6:2G:7:LEU:HD23	6:2G:100:TRP:HE3	1.80	0.47
6:2G:36:LYS:HD3	6:2G:95:ARG:NH2	2.30	0.47
11:2P:54:GLY:O	62:2P:201:HOH:O	2.20	0.47
15:2T:18:ASP:OD1	15:2T:18:ASP:N	2.32	0.47
16:2U:104:GLN:NE2	16:2U:105:VAL:HG23	2.29	0.47
21:2Z:73:GLN:O	21:2Z:87:ASP:N	2.44	0.47
32:2a:79:G:H1	32:2a:90:U:H3	1.62	0.47
32:2a:542:G:OP1	35:2d:10:ARG:NH1	2.45	0.47
32:2a:1003:G:H2'	32:2a:1004:A:O4'	2.14	0.47
32:2a:1120:G:C6	32:2a:1121:U:C4	3.02	0.47
32:2a:1272:G:N2	32:2a:1273:G:C5	2.82	0.47
35:2d:58:LEU:O	35:2d:62:GLN:HG2	2.15	0.47
38:2g:22:LEU:HG	38:2g:62:PHE:CE2	2.45	0.47
38:2g:51:GLN:O	38:2g:55:GLY:HA2	2.15	0.47
48:2q:99:SER:OG	48:2q:100:LYS:N	2.47	0.47
49:2r:21:LYS:HD3	49:2r:21:LYS:HA	1.55	0.47
51:2t:77:ALA:O	51:2t:81:LYS:HG3	2.14	0.47
56:2y:19:G:O3'	62:2y:201:HOH:O	2.20	0.47
1:1A:2537:U:H2'	1:1A:2538:C:C6	2.50	0.47
1:1A:2791:C:H5'	1:1A:2893:G:N2	2.30	0.47
12:1Q:103:MET:HE1	12:1Q:127:ILE:HD11	1.97	0.47
15:1T:60:THR:HG22	15:1T:77:PRO:HA	1.97	0.47
32:1a:7:G:H2'	36:1e:119:LEU:HD22	1.95	0.47
32:1a:473:G:H2'	32:1a:474:G:C8	2.49	0.47
32:1a:674:G:H2'	32:1a:675:A:C8	2.46	0.47
32:1a:1030(B):C:H2'	32:1a:1030(B):C:O2	2.15	0.47
32:1a:1529:G:H4'	32:1a:1530:G:OP2	2.15	0.47
33:1b:16:HIS:HD2	33:1b:204:ASN:H	1.63	0.47
51:1t:47:GLY:N	51:1t:48:LYS:HB2	2.29	0.47
1:2A:489:G:N7	18:2W:49:LYS:NZ	2.63	0.47
1:2A:511:U:H4'	1:2A:1235:G:H4'	1.95	0.47
1:2A:641:C:H42	1:2A:647:G:H1	1.63	0.47
1:2A:900:A:H2'	1:2A:901:A:C8	2.50	0.47
1:2A:902:C:H2'	1:2A:903:C:C6	2.50	0.47
1:2A:1359:A:H2	1:2A:1372:U:O4	1.97	0.47
6:2G:64:THR:HG22	6:2G:94:LEU:HD11	1.95	0.47
8:2I:77:LEU:HD12	8:2I:140:LEU:HD21	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:2V:76:LYS:HB2	17:2V:81:TYR:HD2	1.80	0.47
21:2Z:99:TYR:HB3	21:2Z:123:ASP:CB	2.44	0.47
32:2a:1250:A:H4'	40:2i:68:GLY:H	1.80	0.47
50:2s:20:LEU:HA	50:2s:23:ASN:ND2	2.29	0.47
1:1A:1686:C:H2'	1:1A:1687:G:O4'	2.15	0.47
5:1F:74:ARG:H	5:1F:74:ARG:HG3	1.41	0.47
8:1I:76:THR:CG2	8:1I:141:LYS:HE2	2.45	0.47
19:1X:92:LEU:O	19:1X:94:GLY:N	2.47	0.47
20:1Y:8:LYS:HD3	20:1Y:97:ARG:NH1	2.30	0.47
32:1a:1026:G:N7	32:1a:1035:A:H2	2.13	0.47
32:1a:1304:G:C6	32:1a:1305:G:N1	2.83	0.47
41:1j:11:PHE:HE1	41:1j:67:THR:HG22	1.79	0.47
1:2A:144:C:H2'	1:2A:145:G:H8	1.80	0.47
1:2A:245:G:O6	30:28:8:LYS:NZ	2.44	0.47
1:2A:332:A:O2'	1:2A:334:C:OP2	2.30	0.47
1:2A:1035:U:H2'	1:2A:1036:G:C8	2.50	0.47
1:2A:2483:C:H2'	1:2A:2484:G:O4'	2.15	0.47
4:2E:47:VAL:HG21	4:2E:86:PRO:HD3	1.97	0.47
13:2R:118:GLU:CD	13:2R:118:GLU:H	2.22	0.47
14:2S:18:ILE:O	14:2S:21:THR:OG1	2.28	0.47
32:2a:653:A:H5''	32:2a:653:A:N3	2.30	0.47
32:2a:1033:G:H2'	32:2a:1034:G:C8	2.50	0.47
32:2a:1294:G:H2'	32:2a:1295:G:C8	2.50	0.47
32:2a:1299:A:H2'	32:2a:1299:A:N3	2.29	0.47
32:2a:1503:A:H2	53:2v:13:A:N7	2.13	0.47
33:2b:97:TRP:HH2	33:2b:102:LEU:HG	1.79	0.47
44:2m:81:LEU:HD22	44:2m:88:ARG:HE	1.79	0.47
51:2t:60:GLU:HG3	51:2t:81:LYS:HD2	1.97	0.47
1:1A:1038:C:H42	1:1A:1117:G:H1	1.62	0.47
3:1D:85:ASP:OD2	3:1D:88:ARG:HD2	2.15	0.47
7:1H:13:LYS:HA	7:1H:14:GLY:HA2	1.60	0.47
32:1a:1347:G:O2'	32:1a:1373:G:O6	2.31	0.47
33:1b:146:GLN:O	33:1b:150:SER:HB3	2.15	0.47
41:1j:38:ILE:CG1	41:1j:71:LEU:HB3	2.45	0.47
56:1y:18:G:C2	56:1y:58:A:C5	3.03	0.47
1:2A:340:A:H2'	1:2A:341:G:O4'	2.15	0.47
1:2A:1112:G:H2'	1:2A:1113:U:O4'	2.15	0.47
5:2F:157:VAL:HB	5:2F:194:MET:HG2	1.97	0.47
6:2G:151:ALA:HB3	6:2G:153:ARG:NH1	2.30	0.47
26:24:58:ARG:O	26:24:61:ARG:HB2	2.15	0.47
32:2a:382:A:H2'	32:2a:383:A:H8	1.80	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:565:U:OP2	32:2a:566:G:O2'	2.21	0.47
32:2a:937:A:H1'	32:2a:1379:G:N2	2.30	0.47
32:2a:980:C:H1'	45:2n:19:ARG:HA	1.97	0.47
32:2a:1124:G:H4'	41:2j:38:ILE:HD11	1.96	0.47
32:2a:1228:C:OP1	44:2m:115:LYS:N	2.46	0.47
1:1A:581:C:H5''	62:1U:303:HOH:O	2.14	0.46
1:1A:1104:C:H2'	1:1A:1105:U:C6	2.50	0.46
1:1A:1176:G:H21	1:1A:1178:C:P	2.38	0.46
1:1A:1268:A:C2	1:1A:2013:A:C4	3.03	0.46
1:1A:1594:G:H2'	1:1A:1595:G:O4'	2.16	0.46
1:1A:2693:A:H2'	1:1A:2694:G:H8	1.79	0.46
1:1A:2889:C:H2'	1:1A:2891:G:O4'	2.15	0.46
32:1a:134:A:H61	47:1p:25:ARG:NH1	2.13	0.46
32:1a:148:G:H2'	32:1a:149:A:C8	2.50	0.46
33:1b:114:ARG:NE	33:1b:141:GLU:OE2	2.46	0.46
49:1r:61:LYS:O	49:1r:65:ILE:HG12	2.15	0.46
1:2A:1019:U:HO2'	1:2A:1021:A:H2	1.61	0.46
1:2A:1263:U:C4	1:2A:1264:G:C6	3.03	0.46
1:2A:1266:G:O5'	18:2W:15:ARG:NH2	2.48	0.46
1:2A:1379:A:H4'	1:2A:1380:G:OP2	2.16	0.46
7:2H:13:LYS:HA	7:2H:14:GLY:HA2	1.64	0.46
32:2a:450:G:H4'	47:2p:41:PRO:HB2	1.95	0.46
32:2a:958:A:H5''	32:2a:959:A:OP2	2.14	0.46
33:2b:8:LYS:HE3	33:2b:51:LEU:HD13	1.97	0.46
33:2b:16:HIS:CB	33:2b:204:ASN:HB3	2.39	0.46
1:1A:224:G:H2'	1:1A:225:A:O4'	2.14	0.46
1:1A:2136:C:C4	1:1A:2155:G:C2	3.03	0.46
4:1E:52:LEU:O	4:1E:76:ARG:N	2.44	0.46
12:1Q:59:ARG:C	12:1Q:61:GLY:H	2.23	0.46
32:1a:1258:G:H2'	32:1a:1259:C:H6	1.81	0.46
32:1a:1289:A:OP1	52:1u:9:ARG:NH2	2.48	0.46
1:2A:921:G:C6	1:2A:922:U:C4	3.04	0.46
1:2A:1996:C:H4'	1:2A:1997:G:OP1	2.15	0.46
9:2N:38:HIS:CD2	9:2N:39:ARG:HG3	2.51	0.46
16:2U:76:TYR:CZ	16:2U:80:ILE:HG13	2.50	0.46
16:2U:83:LEU:HD12	16:2U:113:ALA:HB2	1.98	0.46
32:2a:429:U:H1'	32:2a:430:A:H5''	1.98	0.46
32:2a:593:G:N2	62:2a:1808:HOH:O	2.33	0.46
32:2a:1271:G:N2	32:2a:1272:G:N7	2.63	0.46
44:2m:13:LYS:HA	44:2m:44:ARG:NH1	2.29	0.46
46:2o:5:LYS:O	46:2o:9:GLN:HG2	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:2q:66:SER:HB3	48:2q:69:LYS:HB2	1.97	0.46
1:1A:298:G:H5''	1:1A:299:A:OP1	2.16	0.46
1:1A:1503:U:H2'	1:1A:1504:C:C6	2.50	0.46
1:1A:1750:G:O2'	1:1A:2860:A:N1	2.46	0.46
1:1A:2629:A:HO2'	1:1A:2630:G:P	2.37	0.46
2:1B:73:A:N1	21:1Z:34:ASN:ND2	2.62	0.46
32:1a:1001(A):G:H2'	32:1a:1002:G:O4'	2.15	0.46
1:2A:154(A):C:H42	1:2A:171:G:H1	1.62	0.46
1:2A:658:C:H2'	1:2A:659:C:C6	2.50	0.46
1:2A:900:A:H2'	1:2A:901:A:H8	1.80	0.46
1:2A:984:A:H5''	1:2A:985:C:H5	1.81	0.46
1:2A:1798:U:C5'	3:2D:259:THR:HG22	2.42	0.46
1:2A:2129:C:N3	1:2A:2159:G:N2	2.63	0.46
1:2A:2387:U:H1'	22:20:41:ARG:HE	1.80	0.46
5:2F:118:ALA:C	5:2F:120:GLU:H	2.23	0.46
15:2T:6:LEU:O	15:2T:10:VAL:HG23	2.15	0.46
32:2a:472:A:HO2'	47:2p:82:GLN:H	1.61	0.46
32:2a:743:U:H2'	32:2a:744:C:H6	1.81	0.46
32:2a:986:A:N3	50:2s:52:TYR:OH	2.42	0.46
32:2a:1219:U:O2'	50:2s:34:TRP:HB3	2.14	0.46
33:2b:15:VAL:O	33:2b:17:PHE:N	2.43	0.46
34:2c:42:LEU:HA	34:2c:45:LYS:NZ	2.31	0.46
34:2c:131:ARG:NH2	34:2c:135:LYS:HZ2	2.05	0.46
52:2u:6:ARG:HB3	52:2u:15:ARG:HD2	1.97	0.46
1:1A:64:A:O3'	19:1X:71:GLY:HA3	2.15	0.46
1:1A:764:A:H5'	3:1D:210:GLY:HA2	1.98	0.46
1:1A:1794:U:H2'	1:1A:1795:C:C6	2.50	0.46
12:1Q:16:ARG:HG3	12:1Q:17:LEU:H	1.79	0.46
22:10:70:GLN:HE21	22:10:72:ARG:HD2	1.79	0.46
27:15:48:GLU:O	27:15:60:VAL:HG11	2.15	0.46
32:1a:26:A:O2'	35:1d:209:ARG:NH2	2.48	0.46
34:1c:66:VAL:HG23	34:1c:101:LEU:HA	1.96	0.46
34:1c:98:ASN:N	34:1c:98:ASN:OD1	2.48	0.46
56:1y:65:G:C6	56:1y:66:U:C4	3.02	0.46
1:2A:1125:G:H5'	31:29:37:GLY:HA2	1.96	0.46
1:2A:1231:G:H2'	1:2A:1232:G:C8	2.50	0.46
1:2A:1412:A:H2'	1:2A:1413:G:H8	1.81	0.46
1:2A:1913:A:H4'	1:2A:1914:C:O5'	2.15	0.46
1:2A:2758:A:C2	1:2A:2759:G:H1'	2.51	0.46
3:2D:108:PRO:HG2	3:2D:111:LEU:HB2	1.98	0.46
6:2G:42:GLY:HA2	6:2G:89:GLY:HA3	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2G:152:LEU:H	6:2G:152:LEU:HD12	1.80	0.46
16:2U:108:GLU:O	16:2U:112:ARG:HG2	2.16	0.46
19:2X:31:HIS:HD2	19:2X:33:LYS:H	1.63	0.46
21:2Z:99:TYR:HA	21:2Z:124:ILE:O	2.14	0.46
32:2a:187:C:O2'	51:2t:89:ARG:NH2	2.48	0.46
32:2a:423:G:H3'	32:2a:423:G:N3	2.30	0.46
32:2a:1268:A:H4'	52:2u:19:GLY:HA2	1.97	0.46
34:2c:39:ILE:O	34:2c:43:LEU:HG	2.15	0.46
34:2c:137:ALA:HA	34:2c:140:ARG:NH1	2.31	0.46
49:2r:58:LEU:HB2	49:2r:63:GLN:NE2	2.29	0.46
50:2s:49:ILE:CG2	50:2s:62:ILE:HD11	2.45	0.46
1:1A:796:C:H2'	1:1A:797:C:C6	2.50	0.46
1:1A:1092:C:C2'	1:1A:1093:G:H5'	2.45	0.46
21:1Z:150:LEU:HD21	21:1Z:154:ASP:HB2	1.97	0.46
32:1a:262:A:H2'	32:1a:263:A:C8	2.51	0.46
39:1h:86:ILE:HD12	39:1h:133:LEU:HG	1.98	0.46
1:2A:1187:G:H5'	17:2V:81:TYR:CE1	2.50	0.46
1:2A:1591:G:H2'	1:2A:1592:C:C6	2.51	0.46
1:2A:2145:C:O2'	1:2A:2147:G:N7	2.48	0.46
1:2A:2704:C:H2'	1:2A:2705:A:O4'	2.15	0.46
1:2A:2849:U:H4'	1:2A:2868:A:C2	2.51	0.46
15:2T:118:ARG:HG2	32:2a:1442(A):G:C8	2.50	0.46
32:2a:938:A:N3	32:2a:1376:U:O2'	2.45	0.46
34:2c:88:ARG:O	34:2c:91:LEU:HB2	2.15	0.46
37:2f:33:TYR:HE2	37:2f:78:GLU:HG2	1.81	0.46
38:2g:103:TRP:CH2	38:2g:141:VAL:HG21	2.50	0.46
1:1A:907:U:HO2'	12:1Q:101:ARG:HH22	1.60	0.46
1:1A:1173:G:OP2	1:1A:1173:G:H2'	2.15	0.46
1:1A:2124:G:H1	1:1A:2174:C:H42	1.63	0.46
5:1F:150:GLY:HA2	5:1F:172:TRP:CD2	2.51	0.46
19:1X:57:LEU:HA	62:1X:201:HOH:O	2.14	0.46
32:1a:648:A:H2'	32:1a:649:G:H8	1.81	0.46
33:1b:163:PHE:HA	33:1b:185:ILE:HG12	1.98	0.46
38:1g:26:PHE:O	38:1g:30:ILE:HG13	2.16	0.46
56:1y:13:C:H2'	56:1y:14:A:H5''	1.96	0.46
1:2A:249:C:O2	30:28:12:LYS:NZ	2.36	0.46
1:2A:993:G:N2	17:2V:23:GLU:OE2	2.48	0.46
1:2A:2655:G:O2'	1:2A:2664:G:O6	2.28	0.46
21:2Z:121:HIS:N	21:2Z:171:ILE:O	2.48	0.46
26:24:44:THR:O	26:24:46:GLN:N	2.45	0.46
32:2a:1027:C:N4	32:2a:1036:G:O6	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:2b:27:LYS:HD3	33:2b:193:ASP:OD1	2.15	0.46
41:2j:12:ASP:O	41:2j:15:THR:OG1	2.33	0.46
48:2q:67:LYS:HA	48:2q:70:ARG:HH12	1.81	0.46
50:2s:22:LEU:O	50:2s:27:GLU:N	2.49	0.46
56:2y:2:C:H2'	56:2y:3:C:H6	1.80	0.46
1:1A:458:G:O2'	1:1A:469:G:O6	2.31	0.46
1:1A:1649:G:O2'	13:1R:107:ASP:OD2	2.26	0.46
1:1A:2345:G:N3	1:1A:2381:C:H2'	2.31	0.46
2:1B:31:C:H4'	6:1G:29:TRP:CH2	2.51	0.46
9:1N:60:ILE:O	9:1N:61:ARG:NH1	2.49	0.46
32:1a:1031:G:H2'	32:1a:1032:G:C8	2.51	0.46
32:1a:1112:C:H1'	34:1c:179:ARG:NH1	2.31	0.46
32:1a:1124:G:H5''	41:1j:35:SER:OG	2.16	0.46
32:1a:1148:U:O4'	40:1i:16:ARG:HD2	2.15	0.46
33:1b:132:LYS:O	33:1b:136:VAL:HG13	2.16	0.46
1:2A:186:G:H2'	1:2A:187:G:H8	1.81	0.46
1:2A:2100:G:H2'	1:2A:2101:G:C8	2.48	0.46
2:2B:34:U:O4	2:2B:44:G:O2'	2.32	0.46
8:2I:8:PRO:HB3	8:2I:15:VAL:H	1.81	0.46
19:2X:60:ARG:HH22	29:27:47:ARG:NH2	2.13	0.46
22:20:48:GLY:HA3	22:20:80:HIS:ND1	2.31	0.46
32:2a:359:U:H2'	32:2a:360:A:C8	2.50	0.46
32:2a:600:C:H2'	32:2a:601:C:C6	2.51	0.46
32:2a:1155:G:H2'	32:2a:1156:G:C8	2.50	0.46
33:2b:102:LEU:HD12	33:2b:176:GLU:HB2	1.97	0.46
34:2c:24:ALA:HB3	34:2c:29:TYR:CD1	2.50	0.46
35:2d:163:GLU:C	35:2d:165:MET:H	2.23	0.46
44:2m:82:MET:HE2	44:2m:92:HIS:HB3	1.97	0.46
1:1A:721:C:H2'	1:1A:722:A:C8	2.51	0.46
1:1A:1057:A:C8	1:1A:1086:A:C8	3.04	0.46
1:1A:1266:G:O6	18:1W:13:SER:OG	2.19	0.46
1:1A:1783:A:H5'	1:1A:2608:G:H4'	1.98	0.46
7:1H:157:TYR:CE1	7:1H:172:LYS:HG3	2.50	0.46
32:1a:434:U:H2'	32:1a:435:C:C6	2.51	0.46
32:1a:1183:A:O2'	32:1a:1184:G:OP1	2.32	0.46
42:1k:33:THR:HA	42:1k:39:PRO:HA	1.97	0.46
56:1y:55:PSU:O5'	56:1y:55:PSU:H6	1.99	0.46
1:2A:887:A:O2'	1:2A:889:C:OP2	2.26	0.46
1:2A:1915:5MU:H2'	1:2A:1916:A:O4'	2.15	0.46
1:2A:2065:C:H2'	1:2A:2066:C:C6	2.51	0.46
6:2G:56:ALA:HA	6:2G:59:GLU:CD	2.40	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:2W:18:ARG:HG2	18:2W:76:VAL:HB	1.98	0.46
32:2a:546:G:OP1	35:2d:73:ARG:HG3	2.16	0.46
32:2a:939:G:O2'	32:2a:1375:A:N3	2.48	0.46
32:2a:1132:C:H2'	32:2a:1133:G:H8	1.81	0.46
32:2a:1250:A:OP1	40:2i:67:GLY:N	2.40	0.46
33:2b:103:THR:HG23	33:2b:176:GLU:HB3	1.98	0.46
34:2c:63:ASN:HB2	34:2c:98:ASN:HB2	1.98	0.46
35:2d:20:TYR:CD1	35:2d:26:CYS:HB3	2.51	0.46
38:2g:115:ARG:O	38:2g:119:ARG:HG3	2.15	0.46
41:2j:35:SER:HB3	41:2j:73:ASP:H	1.81	0.46
41:2j:74:ILE:HD12	41:2j:74:ILE:HA	1.84	0.46
44:2m:81:LEU:HD11	44:2m:88:ARG:HH21	1.80	0.46
1:1A:284:U:H2'	1:1A:285:C:C6	2.51	0.46
1:1A:1051:G:H2'	1:1A:1052:C:O4'	2.15	0.46
1:1A:2097:C:H2'	1:1A:2098:U:C6	2.51	0.46
1:1A:2820:A:C5	13:1R:4:LEU:HD11	2.51	0.46
3:1D:35:LYS:HD3	3:1D:64:ILE:HD11	1.97	0.46
4:1E:47:VAL:HG22	4:1E:84:PHE:O	2.16	0.46
22:10:5:LYS:O	22:10:7:LEU:HD12	2.16	0.46
31:19:25:VAL:HB	31:19:34:GLN:HB2	1.98	0.46
32:1a:7:G:O2'	36:1e:120:THR:O	2.34	0.46
32:1a:79:G:O6	32:1a:90:U:O2	2.32	0.46
32:1a:382:A:H2'	32:1a:383:A:H8	1.79	0.46
32:1a:1525:G:P	42:1k:120:ARG:HH22	2.39	0.46
35:1d:61:LYS:HD2	35:1d:207:TYR:OH	2.15	0.46
39:1h:124:ALA:O	39:1h:128:GLY:N	2.48	0.46
41:1j:19:SER:OG	41:1j:91:PRO:HD2	2.16	0.46
1:2A:827:U:O2'	1:2A:2068:U:C2	2.68	0.46
1:2A:956:G:H2'	1:2A:957:A:H2'	1.98	0.46
1:2A:1697:G:OP2	1:2A:1698:A:O2'	2.30	0.46
2:2B:55:U:O3'	6:2G:27:ASN:ND2	2.48	0.46
11:2P:28:GLY:O	11:2P:30:THR:N	2.47	0.46
15:2T:27:THR:HG22	15:2T:89:VAL:HB	1.98	0.46
26:24:17:GLY:N	26:24:33:VAL:O	2.48	0.46
32:2a:620:C:C2	35:2d:135:LEU:HG	2.51	0.46
32:2a:937:A:H1'	32:2a:1379:G:H22	1.81	0.46
32:2a:951:G:N7	44:2m:102:ARG:NH2	2.64	0.46
32:2a:994:A:O2'	32:2a:995:C:H5'	2.16	0.46
32:2a:1040:U:C2	32:2a:1041:A:C8	3.04	0.46
32:2a:1371:G:OP1	40:2i:12:GLU:HB3	2.16	0.46
38:2g:115:ARG:HH11	38:2g:118:VAL:HG21	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:2g:116:ALA:O	38:2g:120:ILE:HG13	2.15	0.46
39:2h:121:ASP:HB2	39:2h:125:ARG:NH2	2.31	0.46
44:2m:92:HIS:CE1	44:2m:98:VAL:HG11	2.51	0.46
1:1A:1069:A:H4'	1:1A:1070:A:H5''	1.98	0.46
1:1A:2139:C:N3	1:1A:2152:G:N2	2.63	0.46
2:1B:8:U:O3'	14:1S:25:ARG:NH2	2.38	0.46
18:1W:86:LEU:HB2	18:1W:96:ILE:HD12	1.98	0.46
21:1Z:138:GLU:H	21:1Z:156:LYS:HZ1	1.64	0.46
32:1a:390:C:H2'	32:1a:391:G:C8	2.51	0.46
32:1a:909:A:H2'	32:1a:910:C:O4'	2.16	0.46
33:1b:119:GLU:O	33:1b:123:ALA:HB2	2.16	0.46
39:1h:41:ARG:NH2	39:1h:123:GLU:OE2	2.49	0.46
40:1i:13:ALA:HB2	40:1i:68:GLY:HA3	1.98	0.46
41:1j:39:PRO:HA	41:1j:70:ARG:HD3	1.96	0.46
42:1k:15:ALA:O	42:1k:78:GLN:N	2.44	0.46
51:1t:34:LYS:HE3	51:1t:80:ARG:HH22	1.80	0.46
1:2A:263:C:H2'	1:2A:264:C:O4'	2.16	0.46
1:2A:2630:G:H2'	1:2A:2631:G:H8	1.81	0.46
2:2B:98:G:H3'	2:2B:99:G:H8	1.81	0.46
20:2Y:55:TYR:N	20:2Y:56:PRO:HD3	2.28	0.46
32:2a:114:U:H2'	32:2a:115:G:C8	2.51	0.46
37:2f:70:ASP:OD1	37:2f:71:ARG:HG3	2.15	0.46
40:2i:58:HIS:H	40:2i:58:HIS:CD2	2.35	0.46
45:2n:26:ARG:HD3	45:2n:43:CYS:HB3	1.98	0.46
48:2q:12:SER:HB3	48:2q:20:THR:HB	1.98	0.46
51:2t:9:ASN:OD1	51:2t:9:ASN:N	2.49	0.46
54:2w:25:C:H2'	54:2w:26:A:C8	2.51	0.46
1:1A:55:G:O2'	1:1A:127:A:N1	2.42	0.45
1:1A:185:U:H4'	1:1A:218:A:H4'	1.98	0.45
1:1A:1952:A:C6	1:1A:1953:A:N1	2.84	0.45
1:1A:2693:A:H2'	1:1A:2694:G:C8	2.51	0.45
5:1F:196:LEU:HD23	5:1F:196:LEU:HA	1.80	0.45
8:1I:77:LEU:HD21	8:1I:100:ALA:HB3	1.97	0.45
20:1Y:55:TYR:N	20:1Y:56:PRO:HD3	2.31	0.45
32:1a:339:C:H2'	32:1a:340:U:C6	2.51	0.45
34:1c:181:ASN:ND2	34:1c:204:LEU:HD12	2.29	0.45
1:2A:94(A):G:H2'	1:2A:95:G:O4'	2.16	0.45
1:2A:479:A:N3	1:2A:481:G:H5''	2.31	0.45
1:2A:692:C:O2'	3:2D:38:LYS:NZ	2.49	0.45
1:2A:2192:G:H5'	1:2A:2193:G:OP2	2.16	0.45
1:2A:2693:A:H2'	1:2A:2694:G:H8	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:2E:9:VAL:HG13	4:2E:25:VAL:O	2.17	0.45
7:2H:20:ALA:HB1	7:2H:23:ARG:HH11	1.81	0.45
7:2H:30:LYS:HE3	7:2H:30:LYS:HB3	1.83	0.45
32:2a:20:U:H2'	32:2a:21:G:O4'	2.16	0.45
32:2a:977:A:H2'	32:2a:978:A:H5''	1.99	0.45
32:2a:1122:U:C2	32:2a:1123:A:C8	3.04	0.45
32:2a:1343:G:H2'	32:2a:1344:C:C6	2.52	0.45
54:2w:21:A:O2'	54:2w:22:G:OP1	2.33	0.45
1:1A:75:G:H4'	24:12:55:ARG:NH1	2.31	0.45
1:1A:2096:U:H3	1:1A:2193:G:H1	1.64	0.45
1:1A:2140:C:N3	1:1A:2151:G:C6	2.84	0.45
1:1A:2312:U:H5'	6:1G:88:ILE:HD11	1.97	0.45
3:1D:218:ARG:HB3	3:1D:219:PRO:HD2	1.97	0.45
9:1N:30:ILE:HG23	9:1N:52:VAL:HG11	1.98	0.45
20:1Y:106:LEU:O	20:1Y:107:ASP:HB2	2.16	0.45
26:14:56:VAL:HG22	26:14:60:GLN:HG3	1.98	0.45
48:1q:53:LEU:HD23	48:1q:82:MET:HE1	1.98	0.45
1:2A:8:A:H2'	1:2A:9:U:H6	1.81	0.45
1:2A:582:G:H2'	1:2A:583:G:C8	2.50	0.45
1:2A:645:C:H5''	1:2A:646:A:OP2	2.15	0.45
1:2A:918:A:C6	1:2A:919:G:H1'	2.51	0.45
22:20:70:GLN:HE21	22:20:72:ARG:CD	2.29	0.45
32:2a:659:U:H2'	32:2a:660:G:O4'	2.16	0.45
32:2a:814:A:H2'	32:2a:816:A:H5''	1.97	0.45
32:2a:1221:G:O3'	50:2s:77:THR:OG1	2.34	0.45
32:2a:1525:G:OP1	42:2k:120:ARG:NH2	2.48	0.45
33:2b:192:SER:O	33:2b:194:PRO:HD3	2.16	0.45
35:2d:3:ARG:NH1	35:2d:5:ILE:HG13	2.32	0.45
35:2d:36:ARG:HD2	35:2d:38:TYR:OH	2.16	0.45
51:2t:54:LYS:HB3	51:2t:54:LYS:HE2	1.73	0.45
1:1A:223:A:N1	1:1A:407:G:O2'	2.45	0.45
1:1A:687:C:H5''	29:17:2:LYS:HE2	1.98	0.45
1:1A:1237:A:OP1	62:1A:4251:HOH:O	2.21	0.45
1:1A:1816:G:O6	3:1D:35:LYS:NZ	2.48	0.45
1:1A:2849:U:P	15:1T:95:ARG:HH12	2.39	0.45
17:1V:14:VAL:HB	17:1V:96:ILE:HG13	1.99	0.45
32:1a:986:A:H2'	32:1a:987:G:O4'	2.16	0.45
33:1b:67:THR:N	33:1b:160:ASP:OD1	2.49	0.45
1:2A:832:G:H5'	11:2P:45:LEU:HD11	1.99	0.45
1:2A:1364:G:P	23:21:3:LYS:HG3	2.55	0.45
1:2A:2070:G:H2'	1:2A:2071:A: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:2142:C:H2'	1:2A:2143:C:C6	2.51	0.45
1:2A:2821:A:H2'	1:2A:2822:G:C8	2.51	0.45
11:2P:121:LYS:HB3	11:2P:123:LEU:HD13	1.98	0.45
19:2X:60:ARG:HH22	29:27:47:ARG:HH12	1.62	0.45
32:2a:532:A:H2'	32:2a:532:A:N3	2.31	0.45
32:2a:942:G:C2	32:2a:1342:C:C2	3.03	0.45
32:2a:1004:A:H5''	32:2a:1024:G:H22	1.81	0.45
32:2a:1241:G:H2'	32:2a:1242:C:C6	2.51	0.45
39:2h:121:ASP:N	39:2h:121:ASP:OD1	2.49	0.45
23:11:8:SER:HB3	23:11:66:HIS:CD2	2.52	0.45
28:16:6:ARG:HD3	28:16:24:GLU:OE2	2.16	0.45
32:1a:300:A:O2'	32:1a:564:C:N3	2.43	0.45
32:1a:769:G:H4'	32:1a:1513:A:H4'	1.98	0.45
35:1d:122:ARG:HD2	35:1d:122:ARG:HA	1.69	0.45
36:1e:142:LEU:O	36:1e:143:ARG:NH1	2.43	0.45
39:1h:23:SER:OG	39:1h:24:THR:N	2.49	0.45
44:1m:16:ASP:OD1	44:1m:16:ASP:N	2.49	0.45
44:1m:67:GLU:HG3	44:1m:71:ARG:NH2	2.31	0.45
51:1t:39:LYS:HE3	51:1t:39:LYS:HB2	1.87	0.45
54:1w:9:A:H8	54:1w:11:C:H41	1.63	0.45
1:2A:375:C:H2'	1:2A:376:C:C6	2.52	0.45
1:2A:479:A:H4'	1:2A:480:A:OP1	2.17	0.45
1:2A:639:U:H2'	1:2A:640:C:C6	2.50	0.45
1:2A:884:C:H3'	1:2A:885:C:C6	2.52	0.45
1:2A:1405:U:H2'	1:2A:1406:U:C6	2.51	0.45
1:2A:1991:U:H2'	1:2A:1992:G:H5''	1.97	0.45
1:2A:2115:G:H4'	1:2A:2167:U:N3	2.31	0.45
1:2A:2129:C:N4	1:2A:2159:G:C6	2.84	0.45
1:2A:2630:G:H2'	1:2A:2631:G:C8	2.51	0.45
4:2E:50:GLY:HA2	4:2E:77:ILE:O	2.16	0.45
6:2G:112:PRO:HG3	26:24:43:TYR:CZ	2.52	0.45
32:2a:404:U:OP2	35:2d:118:ARG:NH2	2.49	0.45
32:2a:580:U:H5''	46:2o:58:MET:HG2	1.99	0.45
32:2a:818:G:N2	32:2a:873:A:OP1	2.47	0.45
32:2a:1247:U:H1'	32:2a:1291:G:N2	2.32	0.45
32:2a:1256:A:OP1	34:2c:26:LYS:NZ	2.49	0.45
33:2b:26:PRO:C	33:2b:28:PHE:H	2.23	0.45
35:2d:155:LEU:HD23	35:2d:156:GLU:N	2.31	0.45
35:2d:159:ARG:O	35:2d:163:GLU:HB2	2.16	0.45
36:2e:33:VAL:HG21	36:2e:109:ILE:HA	1.98	0.45
37:2f:82:ARG:HE	37:2f:82:ARG:HB3	1.59	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:2g:106:GLN:H	38:2g:106:GLN:HG2	1.40	0.45
39:2h:9:MET:HG3	39:2h:26:VAL:HG21	1.98	0.45
41:2j:7:LYS:HG2	41:2j:9:ARG:NH1	2.31	0.45
52:2u:5:ASP:O	52:2u:11:GLY:HA3	2.16	0.45
1:1A:484:C:OP1	20:1Y:51:VAL:HG22	2.17	0.45
1:1A:2591:C:H2'	1:1A:2592:G:C8	2.52	0.45
3:1D:79:VAL:HG12	3:1D:113:VAL:HA	1.99	0.45
26:14:15:ILE:HB	26:14:32:TYR:CD1	2.52	0.45
32:1a:433:C:H2'	32:1a:434:U:C6	2.52	0.45
33:1b:28:PHE:CD2	33:1b:190:THR:HA	2.51	0.45
1:2A:68:G:H2'	1:2A:69:C:O4'	2.17	0.45
1:2A:196:A:N3	1:2A:196:A:H2'	2.32	0.45
1:2A:232:G:H8	1:2A:232:G:OP2	2.00	0.45
1:2A:589:C:H2'	1:2A:590:A:C8	2.52	0.45
1:2A:1751:C:O2'	1:2A:2861:G:O2'	2.28	0.45
1:2A:2134:A:H2'	1:2A:2134:A:N3	2.30	0.45
7:2H:10:PRO:O	7:2H:12:PRO:HD3	2.17	0.45
7:2H:35:VAL:HG13	7:2H:71:LEU:HD22	1.98	0.45
8:2I:130:TYR:CE2	8:2I:132:PRO:HB3	2.52	0.45
23:21:23:LYS:HB3	23:21:29:GLY:HA3	1.98	0.45
32:2a:406:G:H21	35:2d:119:GLN:NE2	2.15	0.45
32:2a:661:G:N2	32:2a:744:C:N3	2.55	0.45
36:2e:9:LYS:HD3	36:2e:9:LYS:HA	1.65	0.45
1:1A:1041:C:H42	1:1A:1114:G:H1	1.63	0.45
1:1A:1178:C:H2'	1:1A:1179:C:H6	1.81	0.45
1:1A:1721:G:H2'	1:1A:1722:A:H2'	1.98	0.45
1:1A:2106:G:H1	1:1A:2183:C:N4	2.14	0.45
1:1A:2849:U:H4'	1:1A:2868:A:C2	2.51	0.45
6:1G:108:ASN:HB3	26:14:22:ILE:HD13	1.97	0.45
12:1Q:77:LYS:NZ	12:1Q:86:GLY:O	2.50	0.45
47:1p:49:LEU:HD12	47:1p:50:LYS:H	1.82	0.45
51:1t:13:LEU:HD12	51:1t:14:LYS:N	2.31	0.45
1:2A:307:G:N7	62:2A:3912:HOH:O	2.36	0.45
1:2A:2118:U:C4	1:2A:2149:G:H1'	2.52	0.45
5:2F:178:PRO:HB3	5:2F:198:ALA:HA	1.99	0.45
7:2H:123:PHE:O	7:2H:124:GLU:HG3	2.17	0.45
7:2H:154:PRO:HB3	7:2H:163:TYR:CZ	2.52	0.45
14:2S:52:SER:HB2	14:2S:55:ALA:HB3	1.99	0.45
15:2T:41:ARG:NH1	32:2a:346:G:OP1	2.50	0.45
21:2Z:53:ILE:HD11	21:2Z:99:TYR:HB2	1.98	0.45
25:23:6:VAL:HG22	25:23:56:VAL:HG12	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:27:24:THR:O	29:27:28:ARG:HG3	2.17	0.45
32:2a:107:G:H2'	32:2a:108:G:O4'	2.17	0.45
32:2a:157:G:N2	32:2a:164:U:O2	2.35	0.45
32:2a:1029:C:N4	32:2a:1031:G:C6	2.85	0.45
33:2b:185:ILE:HG22	33:2b:199:TYR:HD2	1.82	0.45
35:2d:92:VAL:O	35:2d:96:LEU:HG	2.17	0.45
46:2o:8:LYS:O	46:2o:12:ILE:HG13	2.16	0.45
54:2w:45:U:H5''	54:2w:46:7MG:OP2	2.15	0.45
1:1A:226:G:H21	1:1A:228:A:H62	1.64	0.45
1:1A:1876:A:H2'	1:1A:1877:A:C8	2.51	0.45
1:1A:2871:C:N3	62:1A:4331:HOH:O	2.36	0.45
10:1O:73:ASP:HB2	15:1T:82:LEU:HD13	1.99	0.45
13:1R:36:THR:HG22	13:1R:37:THR:H	1.80	0.45
32:1a:165:C:H2'	32:1a:166:G:H8	1.82	0.45
32:1a:430:A:OP2	35:1d:8:VAL:HG12	2.16	0.45
1:2A:644:A:H4'	1:2A:645:C:N4	2.32	0.45
1:2A:1364:G:OP2	23:21:3:LYS:HG3	2.16	0.45
6:2G:117:PHE:CE2	6:2G:119:GLY:HA2	2.52	0.45
9:2N:13:TRP:CE2	9:2N:133:GLN:HG2	2.50	0.45
12:2Q:53:ALA:HB1	12:2Q:120:ILE:HG22	1.99	0.45
17:2V:71:LEU:HD23	17:2V:71:LEU:HA	1.77	0.45
18:2W:4:LYS:HD3	18:2W:6:ILE:HD11	1.98	0.45
32:2a:9:G:H2'	32:2a:10:A:C8	2.51	0.45
32:2a:399:G:H2'	32:2a:400:C:C6	2.51	0.45
32:2a:427:U:OP2	35:2d:36:ARG:NH2	2.50	0.45
32:2a:1294:G:H2'	32:2a:1295:G:H8	1.82	0.45
36:2e:129:ILE:HG22	36:2e:133:TYR:HE2	1.81	0.45
44:2m:39:ILE:HG12	44:2m:52:GLU:HG2	1.97	0.45
50:2s:31:ILE:HD12	50:2s:31:ILE:HA	1.82	0.45
1:1A:580:C:H2'	1:1A:581:C:C6	2.51	0.45
7:1H:98:LEU:HG	7:1H:125:VAL:HG23	1.99	0.45
11:1P:1:MET:HE2	11:1P:1:MET:HB2	1.66	0.45
15:1T:127:ALA:C	15:1T:129:ARG:N	2.73	0.45
20:1Y:6:HIS:H	20:1Y:6:HIS:CD2	2.34	0.45
24:12:64:LEU:HD11	24:12:68:ARG:HE	1.82	0.45
26:14:59:PHE:CD2	50:1s:64:GLU:HB3	2.52	0.45
32:1a:629:G:H2'	32:1a:630:G:O4'	2.17	0.45
32:1a:1125:U:H4'	41:1j:5:ARG:HH22	1.82	0.45
33:1b:133:LYS:HE3	33:1b:133:LYS:C	2.42	0.45
47:1p:4:ILE:HD12	47:1p:60:LEU:HD13	1.99	0.45
54:1w:5:G:H2'	54:1w:6:G:C8	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1434:A:N6	1:2A:1558:A:H62	2.07	0.45
1:2A:2126:A:H4'	1:2A:2127:G:OP2	2.16	0.45
1:2A:2164:C:C5	1:2A:2165:G:H1'	2.51	0.45
5:2F:24:LEU:HB3	5:2F:115:ALA:HB2	1.99	0.45
5:2F:108:LYS:O	5:2F:112:MET:HG3	2.17	0.45
21:2Z:104:PHE:HD2	21:2Z:139:VAL:HB	1.81	0.45
30:28:34:TRP:CE2	30:28:35:GLN:HB3	2.51	0.45
33:2b:120:ALA:O	33:2b:125:PRO:HD2	2.16	0.45
34:2c:53:ALA:HB2	34:2c:115:LEU:CD1	2.46	0.45
39:2h:45:ILE:HG21	39:2h:61:VAL:HG12	1.98	0.45
40:2i:16:ARG:HB2	40:2i:64:THR:CG2	2.47	0.45
1:1A:2291:U:H2'	1:1A:2292:C:C6	2.52	0.45
6:1G:21:ARG:HH11	6:1G:21:ARG:CA	2.09	0.45
7:1H:3:ARG:HE	7:1H:54:ARG:NH1	2.12	0.45
10:1O:34:THR:OG1	10:1O:35:VAL:N	2.49	0.45
25:13:55:ARG:C	25:13:55:ARG:HE	2.25	0.45
28:16:12:GLU:OE1	28:16:52:VAL:HG11	2.16	0.45
32:1a:162:A:C8	32:1a:163:C:H1'	2.52	0.45
32:1a:1328:C:H2'	32:1a:1329:A:O4'	2.17	0.45
33:1b:16:HIS:HB2	33:1b:204:ASN:CB	2.47	0.45
34:1c:18:TRP:H	34:1c:18:TRP:HE3	1.63	0.45
55:1x:58:A:H4'	55:1x:59:A:OP1	2.17	0.45
1:2A:143:G:H2'	1:2A:143(A):C:C6	2.52	0.45
1:2A:362:U:O2'	1:2A:363:G:H5'	2.17	0.45
1:2A:1131:G:O6	1:2A:2040:C:H1'	2.17	0.45
1:2A:1812:A:H5''	62:2A:3809:HOH:O	2.16	0.45
1:2A:1851:U:H2'	1:2A:1852:C:O4'	2.17	0.45
1:2A:2120:G:H2'	1:2A:2121:G:C8	2.51	0.45
1:2A:2343:C:O3'	1:2A:2373:G:H4'	2.16	0.45
1:2A:2461:C:H2'	1:2A:2462:U:C6	2.52	0.45
1:2A:2572:A:OP1	1:2A:2574:G:O2'	2.33	0.45
6:2G:111:LEU:HD23	6:2G:117:PHE:CZ	2.52	0.45
6:2G:173:LEU:HB3	6:2G:178:PHE:CD1	2.52	0.45
6:2G:173:LEU:O	6:2G:178:PHE:HD1	2.00	0.45
7:2H:9:ILE:HB	7:2H:50:VAL:HG23	1.97	0.45
21:2Z:77:ASP:CG	21:2Z:80:ARG:HH11	2.24	0.45
26:24:46:GLN:O	26:24:48:ARG:N	2.49	0.45
32:2a:45:U:H2'	32:2a:46:G:C8	2.52	0.45
32:2a:662:G:O2'	32:2a:836:G:OP1	2.35	0.45
32:2a:1133:G:N2	32:2a:1141:C:N3	2.55	0.45
34:2c:152:ILE:HG13	34:2c:199:LYS:HB2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:2n:47:LEU:O	45:2n:50:LYS:HG2	2.17	0.45
47:2p:41:PRO:O	47:2p:43:LYS:HE2	2.17	0.45
50:2s:80:TYR:O	50:2s:81:ARG:HG2	2.16	0.45
11:1P:95:VAL:HG22	11:1P:125:VAL:HB	1.98	0.45
26:14:54:GLY:N	26:14:55:ARG:HA	2.30	0.45
32:1a:1077:G:N2	32:1a:1080:A:OP2	2.42	0.45
38:1g:51:GLN:O	38:1g:55:GLY:HA2	2.16	0.45
40:1i:29:ASN:OD1	40:1i:65:VAL:N	2.46	0.45
48:1q:87:LYS:HD3	48:1q:87:LYS:HA	1.78	0.45
1:2A:1022:G:H22	1:2A:1142(A):A:H2	1.54	0.45
1:2A:1512:U:H2'	1:2A:1513:C:C6	2.52	0.45
1:2A:1786:A:H1'	1:2A:1938:A:N6	2.31	0.45
6:2G:142:PRO:HG2	6:2G:143:GLU:OE2	2.16	0.45
7:2H:154:PRO:HB3	7:2H:163:TYR:CE1	2.52	0.45
32:2a:141:A:H1'	32:2a:182:U:O2	2.17	0.45
32:2a:551:U:H2'	32:2a:552:U:C6	2.52	0.45
32:2a:1502:A:H5'	32:2a:1504:G:N7	2.32	0.45
33:2b:186:ALA:O	33:2b:201:ILE:HG13	2.16	0.45
36:2e:5:ASP:N	36:2e:5:ASP:OD1	2.50	0.45
38:2g:42:ILE:HG22	38:2g:120:ILE:HD12	1.99	0.45
40:2i:50:LEU:HD13	40:2i:56:LEU:HA	1.99	0.45
44:2m:37:THR:O	44:2m:55:ARG:NH1	2.38	0.45
44:2m:57:ARG:O	44:2m:61:GLU:HB2	2.17	0.45
50:2s:80:TYR:CZ	50:2s:82:GLY:HA2	2.52	0.45
1:1A:795:C:H2'	1:1A:796:C:C6	2.53	0.44
1:1A:1721:G:H8	1:1A:1721:G:O5'	2.00	0.44
1:1A:2251:OMG:HM23	1:1A:2251:OMG:H1'	1.82	0.44
32:1a:250:A:H4'	32:1a:251:G:O5'	2.16	0.44
32:1a:713:G:H2'	32:1a:714:G:C8	2.52	0.44
32:1a:736:C:H2'	32:1a:737:A:C8	2.53	0.44
1:2A:859:G:O2'	1:2A:916:G:O6	2.31	0.44
1:2A:887:A:H4'	1:2A:888:C:C5	2.52	0.44
1:2A:971:C:H2'	1:2A:972:G:O4'	2.17	0.44
1:2A:1721:G:H2'	1:2A:1740:G:O6	2.17	0.44
1:2A:2406:U:C2	11:2P:72:PRO:HG2	2.52	0.44
2:2B:110:G:C2'	2:2B:111:G:H5'	2.46	0.44
4:2E:23:VAL:HG21	4:2E:183:LEU:HD23	1.99	0.44
6:2G:61:ALA:HA	6:2G:66:GLN:O	2.17	0.44
32:2a:1097:C:O4'	32:2a:1170:A:O2'	2.33	0.44
32:2a:1289:A:OP1	52:2u:9:ARG:NH2	2.50	0.44
32:2a:1502:A:C8	32:2a:1505:G:N2	2.85	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1518:MA6:H93	32:2a:1519:MA6:C9	2.46	0.44
34:2c:183:ASP:N	34:2c:202:ILE:O	2.26	0.44
35:2d:104:VAL:HG21	35:2d:140:VAL:HG21	1.98	0.44
50:2s:80:TYR:C	50:2s:82:GLY:H	2.23	0.44
55:2x:50:U:H2'	55:2x:51:C:C6	2.52	0.44
1:1A:2117:A:O2'	1:1A:2118:U:H5''	2.16	0.44
20:1Y:90:LEU:HD21	20:1Y:96:ILE:HD13	1.99	0.44
32:1a:1223:C:OP2	50:1s:78:ARG:NH2	2.37	0.44
41:1j:54:PHE:CD2	41:1j:55:LYS:HB3	2.52	0.44
48:1q:53:LEU:HB3	48:1q:82:MET:HE1	1.99	0.44
49:1r:52:PRO:O	49:1r:56:THR:HG23	2.17	0.44
1:2A:136:G:H1	1:2A:143(A):C:H42	1.66	0.44
1:2A:862:G:H2'	1:2A:863:A:O4'	2.17	0.44
1:2A:919:G:N2	1:2A:2269:A:OP2	2.50	0.44
1:2A:938:G:OP2	30:28:52:LYS:NZ	2.41	0.44
5:2F:158:THR:HB	5:2F:195:ASP:HB2	1.98	0.44
12:2Q:31:ASP:HA	12:2Q:134:ARG:HH11	1.82	0.44
19:2X:35:THR:O	19:2X:39:ILE:HG13	2.17	0.44
21:2Z:71:VAL:HA	21:2Z:87:ASP:O	2.18	0.44
26:24:53:GLU:C	26:24:55:ARG:H	2.26	0.44
30:28:34:TRP:CG	30:28:35:GLN:N	2.86	0.44
32:2a:863:U:H2'	32:2a:865:A:OP2	2.17	0.44
32:2a:1014:A:OP2	50:2s:18:LYS:NZ	2.50	0.44
32:2a:1189:C:OP1	41:2j:51:ARG:NH2	2.47	0.44
34:2c:134:ILE:HG22	34:2c:168:ALA:HB3	1.98	0.44
40:2i:29:ASN:OD1	40:2i:64:THR:HA	2.17	0.44
46:2o:48:LYS:HD3	46:2o:48:LYS:HA	1.62	0.44
56:2y:33:U:H2'	56:2y:35:A:OP2	2.18	0.44
56:2y:58:A:H4'	56:2y:59:U:OP1	2.17	0.44
1:1A:887:A:C2	1:1A:889:C:H3'	2.51	0.44
1:1A:994:C:OP1	16:1U:53:ARG:NH2	2.50	0.44
1:1A:2181:G:O2'	1:1A:2182:G:OP1	2.33	0.44
1:1A:2467:C:H4'	12:1Q:123:HIS:CD2	2.51	0.44
1:1A:2723:C:OP1	13:1R:3:HIS:ND1	2.51	0.44
5:1F:129:PHE:CD2	5:1F:163:VAL:HG21	2.52	0.44
16:1U:104:GLN:NE2	16:1U:105:VAL:HG23	2.33	0.44
28:16:35:GLU:OE2	28:16:50:ARG:NH1	2.48	0.44
32:1a:189:G:C6	32:1a:189(L):G:N1	2.85	0.44
32:1a:539:A:H2'	32:1a:540:G:C8	2.51	0.44
32:1a:1456:G:C4	51:1t:55:ILE:HD11	2.53	0.44
33:1b:109:SER:O	33:1b:112:VAL:HG22	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:1j:35:SER:HB3	41:1j:73:ASP:HB2	2.00	0.44
47:1p:22:THR:HA	47:1p:33:ILE:HD12	1.98	0.44
1:2A:455:C:N3	1:2A:472:A:H2'	2.32	0.44
1:2A:493:G:H2'	1:2A:494:G:O4'	2.17	0.44
1:2A:1005:C:H2'	1:2A:1006:C:C6	2.53	0.44
1:2A:1235:G:C6	1:2A:1236:G:N1	2.85	0.44
1:2A:1847:A:H4'	1:2A:1848:A:OP2	2.18	0.44
1:2A:2320:A:H1'	1:2A:2321:G:N2	2.32	0.44
8:2I:59:ALA:HA	8:2I:62:LYS:HD2	1.98	0.44
8:2I:88:ILE:HD11	8:2I:144:VAL:HG11	1.99	0.44
11:2P:85:LEU:HA	11:2P:88:LEU:HD12	1.98	0.44
14:2S:10:ARG:NH2	14:2S:91:PRO:O	2.49	0.44
16:2U:66:ASN:O	16:2U:70:ARG:HG3	2.16	0.44
22:20:31:VAL:HG22	22:20:65:GLY:O	2.17	0.44
32:2a:258:G:H2'	32:2a:259:G:H8	1.81	0.44
32:2a:390:C:H4'	47:2p:28:ARG:HH21	1.83	0.44
32:2a:671:G:H2'	32:2a:672:U:O4'	2.17	0.44
32:2a:707:C:H2'	32:2a:708:C:H6	1.83	0.44
32:2a:1142:G:H3'	32:2a:1143:G:H8	1.82	0.44
32:2a:1151:A:O2'	32:2a:1152:A:H8	1.99	0.44
32:2a:1226:C:H6	44:2m:103:THR:HB	1.82	0.44
32:2a:1323:G:H2'	32:2a:1324:A:C8	2.53	0.44
39:2h:12:ARG:HD3	39:2h:26:VAL:HG22	2.00	0.44
45:2n:15:LYS:HE2	45:2n:16:PHE:CE2	2.52	0.44
51:2t:98:PRO:O	51:2t:99:LEU:HB2	2.17	0.44
1:1A:862:G:H2'	1:1A:863:A:O4'	2.18	0.44
1:1A:956:G:H2'	1:1A:957:A:H2'	1.98	0.44
1:1A:2142:C:N3	1:1A:2149:G:C6	2.85	0.44
1:1A:2404:C:C2'	1:1A:2405:G:H5'	2.47	0.44
6:1G:106:LEU:HD12	6:1G:110:ALA:HB3	2.00	0.44
8:1I:48:GLU:OE1	8:1I:52:ARG:NH1	2.51	0.44
9:1N:62:VAL:HG22	9:1N:66:LYS:HD2	1.98	0.44
32:1a:45:U:H2'	32:1a:46:G:C8	2.52	0.44
32:1a:194:C:H2'	32:1a:195:A:H5''	1.99	0.44
32:1a:662:G:H2'	32:1a:663:A:C8	2.53	0.44
32:1a:1033:G:C4	32:1a:1034:G:C8	3.06	0.44
32:1a:1427:U:H2'	32:1a:1428:A:C8	2.52	0.44
33:1b:150:SER:OG	33:1b:151:GLY:N	2.51	0.44
43:1l:113:ARG:HB3	43:1l:122:THR:HG21	1.98	0.44
46:1o:88:ARG:HA	46:1o:88:ARG:HD2	1.79	0.44
47:1p:75:ARG:C	47:1p:77:ALA:H	2.26	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:656:G:H2'	1:2A:657:U:O4'	2.18	0.44
1:2A:667:U:O2	30:28:2:PRO:HD2	2.17	0.44
1:2A:797:C:H2'	1:2A:798:G:O4'	2.18	0.44
1:2A:1193:G:OP1	11:2P:14:LYS:NZ	2.41	0.44
1:2A:2123:G:H2'	1:2A:2124:G:C8	2.52	0.44
1:2A:2273:A:H2'	1:2A:2274:A:C8	2.53	0.44
1:2A:2712:U:OP1	1:2A:2714:G:H4'	2.18	0.44
5:2F:20:LEU:HD23	5:2F:20:LEU:HA	1.86	0.44
17:2V:55:ALA:HA	17:2V:101:GLY:HA2	1.99	0.44
21:2Z:126:VAL:HG13	21:2Z:161:VAL:HG23	1.99	0.44
21:2Z:144:LEU:HD13	21:2Z:150:LEU:HD23	1.99	0.44
32:2a:981:U:H5'	45:2n:21:TYR:CE2	2.53	0.44
32:2a:1002:G:H1	32:2a:1038:C:H42	1.65	0.44
32:2a:1187:G:OP1	40:2i:113:LYS:NZ	2.50	0.44
34:2c:131:ARG:NH1	34:2c:166:GLU:OE1	2.46	0.44
35:2d:201:GLN:HE21	36:2e:99:GLY:HA2	1.83	0.44
36:2e:41:VAL:O	36:2e:66:MET:HA	2.17	0.44
44:2m:65:LYS:O	44:2m:70:LEU:HD12	2.17	0.44
1:1A:90:U:H1'	1:1A:92:A:C8	2.53	0.44
1:1A:185:U:H2'	1:1A:186:G:C8	2.53	0.44
1:1A:1385:G:O2'	1:1A:1396:U:O2	2.31	0.44
1:1A:1427:A:H4'	1:1A:1428:C:O4'	2.18	0.44
1:1A:1429:G:H2'	1:1A:1430:C:C6	2.52	0.44
1:1A:1508:A:O2'	1:1A:1509:C:OP1	2.26	0.44
1:1A:2698:U:H2'	1:1A:2699:C:C6	2.53	0.44
5:1F:34:TRP:CZ3	11:1P:8:PRO:HB3	2.52	0.44
8:1I:93:THR:H	8:1I:96:ASP:HB2	1.82	0.44
14:1S:34:HIS:O	14:1S:97:ARG:NH2	2.51	0.44
19:1X:12:VAL:HG21	19:1X:27:THR:HG22	1.98	0.44
22:10:29:GLN:O	22:10:67:VAL:HG23	2.17	0.44
32:1a:1074:G:O2'	32:1a:1101:A:N1	2.34	0.44
1:2A:96:G:H4'	24:22:48:HIS:CD2	2.52	0.44
1:2A:911:A:H2'	12:2Q:9:TYR:OH	2.18	0.44
1:2A:1007:C:OP1	9:2N:35:ARG:NH1	2.43	0.44
1:2A:1496:A:OP2	1:2A:1496:A:H8	2.00	0.44
1:2A:2693:A:H2'	1:2A:2694:G:C8	2.53	0.44
3:2D:237:GLU:OE2	62:2D:403:HOH:O	2.21	0.44
4:2E:174:ASP:OD1	4:2E:175:VAL:N	2.48	0.44
8:2I:48:GLU:HA	8:2I:51:ILE:HG22	2.00	0.44
12:2Q:2:LEU:HB3	12:2Q:69:PHE:CE1	2.53	0.44
14:2S:3:ARG:NH1	14:2S:4:LEU:H	2.16	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:266:G:H2'	32:2a:266:G:N3	2.33	0.44
42:2k:58:PRO:O	42:2k:62:GLN:N	2.44	0.44
43:2l:28:LYS:HB2	43:2l:33:ARG:HH21	1.82	0.44
46:2o:62:GLN:O	46:2o:66:LEU:HG	2.17	0.44
1:1A:686:G:N2	1:1A:788:A:H61	2.15	0.44
1:1A:736:C:OP1	62:1A:4255:HOH:O	2.21	0.44
1:1A:897:C:H4'	54:1w:55:PSU:O3'	2.17	0.44
1:1A:2788:C:P	4:1E:61:ARG:HH21	2.41	0.44
1:1A:2820:A:P	13:1R:2:ARG:HH22	2.40	0.44
6:1G:43:LEU:C	6:1G:45:GLU:H	2.26	0.44
7:1H:149:ARG:NH2	7:1H:167:GLU:OE2	2.44	0.44
9:1N:108:PRO:O	9:1N:113:GLY:HA3	2.17	0.44
32:1a:1258:G:H2'	32:1a:1259:C:C6	2.53	0.44
1:2A:1394:U:C4	1:2A:1395:A:C5	3.06	0.44
1:2A:2141:G:C2	1:2A:2142:C:H1'	2.53	0.44
1:2A:2307:G:H8	1:2A:2307:G:OP1	2.00	0.44
1:2A:2579:C:H2'	1:2A:2580:U:O4'	2.18	0.44
1:2A:2865:U:OP2	1:2A:2866:U:O2'	2.28	0.44
4:2E:60:ASN:CG	4:2E:62:PRO:HD2	2.43	0.44
21:2Z:29:TYR:HB3	21:2Z:34:ASN:HD22	1.82	0.44
32:2a:728:A:H2'	32:2a:729:A:C8	2.53	0.44
32:2a:1074:G:O2'	32:2a:1101:A:N1	2.48	0.44
32:2a:1079:G:O3'	36:2e:14:ARG:NH2	2.50	0.44
34:2c:37:GLN:HE22	45:2n:52:GLN:HB3	1.83	0.44
39:2h:112:LEU:HD11	39:2h:124:ALA:HB2	2.00	0.44
1:1A:271(K):U:H1'	8:1I:50:ARG:NH1	2.33	0.44
1:1A:753:C:H2'	1:1A:754:C:H6	1.82	0.44
1:1A:875:G:H2'	1:1A:876:C:O4'	2.17	0.44
1:1A:875:G:O2'	21:1Z:151:HIS:HE1	2.00	0.44
1:1A:1778:U:H2'	1:1A:1784:A:N6	2.32	0.44
1:1A:2188:C:H2'	1:1A:2189:U:O4'	2.18	0.44
2:1B:57:A:H1'	6:1G:29:TRP:HB2	2.00	0.44
2:1B:103:G:H21	21:1Z:73:GLN:HE22	1.65	0.44
5:1F:132:VAL:HA	5:1F:138:GLU:HB3	2.00	0.44
11:1P:63:PRO:HD3	30:18:27:THR:HG22	2.00	0.44
14:1S:110:LEU:HA	14:1S:110:LEU:HD12	1.83	0.44
15:1T:113:LYS:HA	15:1T:113:LYS:HD3	1.83	0.44
23:11:44:PRO:HB2	23:11:46:LEU:HD12	1.99	0.44
26:14:29:PRO:O	26:14:30:GLU:HG3	2.17	0.44
32:1a:110:C:H2'	32:1a:111:G:O4'	2.17	0.44
32:1a:432:A:H3'	32:1a:433:C:H6	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1456:G:O6	51:1t:54:LYS:NZ	2.35	0.44
34:1c:33:LEU:O	34:1c:37:GLN:HG2	2.18	0.44
43:1l:53:ARG:HD2	43:1l:93:LEU:HD11	1.99	0.44
51:1t:64:ASP:OD2	51:1t:81:LYS:HD3	2.18	0.44
1:2A:647:G:H8	1:2A:647:G:O5'	2.01	0.44
1:2A:945:A:C4	1:2A:2448:A:C2	3.05	0.44
1:2A:956:G:H5''	12:2Q:77:LYS:HD2	1.99	0.44
1:2A:1116:C:H2'	1:2A:1117:G:H8	1.81	0.44
1:2A:1291:C:H2'	1:2A:1292:U:C6	2.53	0.44
1:2A:2116:G:N1	1:2A:2162:G:OP1	2.51	0.44
1:2A:2129:C:N4	1:2A:2159:G:N1	2.66	0.44
9:2N:123:TYR:CE2	9:2N:129:PRO:HD2	2.52	0.44
15:2T:65:LYS:HE3	15:2T:67:SER:HB2	1.98	0.44
21:2Z:70:LEU:O	21:2Z:89:PHE:N	2.40	0.44
29:27:5:TRP:CD1	29:27:7:PRO:HD3	2.52	0.44
32:2a:892:A:O2'	32:2a:1415:G:H4'	2.18	0.44
32:2a:1157:A:H4'	32:2a:1158:C:O5'	2.18	0.44
33:2b:16:HIS:CB	33:2b:210:SER:HB2	2.45	0.44
34:2c:40:ARG:NH2	34:2c:55:VAL:O	2.49	0.44
34:2c:124:ILE:HG21	34:2c:130:VAL:HG13	2.00	0.44
38:2g:26:PHE:O	38:2g:30:ILE:HD12	2.18	0.44
46:2o:82:ILE:O	46:2o:86:GLY:N	2.51	0.44
55:2x:58:A:H4'	55:2x:59:A:OP1	2.17	0.44
1:1A:428:A:H8	1:1A:428:A:OP2	2.01	0.44
1:1A:763:G:OP1	62:1A:4254:HOH:O	2.21	0.44
1:1A:1957:C:H2'	1:1A:1958:C:C6	2.53	0.44
4:1E:108:SER:O	4:1E:162:ALA:HA	2.18	0.44
32:1a:185:A:H2'	32:1a:186:C:C6	2.53	0.44
32:1a:432:A:H3'	32:1a:433:C:C6	2.53	0.44
32:1a:473:G:H2'	32:1a:474:G:H8	1.83	0.44
41:1j:55:LYS:HD3	41:1j:56:HIS:CE1	2.52	0.44
44:1m:17:VAL:O	44:1m:20:THR:OG1	2.26	0.44
44:1m:25:ILE:HD11	44:1m:60:VAL:HG13	1.98	0.44
1:2A:740:U:H2'	1:2A:741:G:C8	2.53	0.44
1:2A:2032:G:OP2	1:2A:2454:G:O2'	2.28	0.44
12:2Q:3:MET:HE3	12:2Q:3:MET:HB2	1.87	0.44
13:2R:62:ALA:O	13:2R:66:VAL:HG23	2.18	0.44
14:2S:11:LYS:O	14:2S:15:ARG:HB2	2.18	0.44
15:2T:127:ALA:C	15:2T:129:ARG:N	2.76	0.44
19:2X:4:ALA:HB1	19:2X:42:ALA:HA	1.99	0.44
26:24:13:ARG:HA	26:24:22:ILE:O	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1002:G:C6	32:2a:1003:G:H8	2.36	0.44
32:2a:1009:G:H22	32:2a:1021:G:H1'	1.83	0.44
32:2a:1298:C:P	38:2g:114:ARG:HH22	2.39	0.44
40:2i:32:ASP:O	40:2i:35:GLU:HG2	2.18	0.44
41:2j:46:ARG:HG2	41:2j:64:GLU:HB3	2.00	0.44
1:1A:185:U:H2'	1:1A:186:G:H8	1.83	0.44
1:1A:1059:G:OP2	1:1A:1060:U:H3'	2.18	0.44
1:1A:2121:G:H2'	1:1A:2122:U:C6	2.53	0.44
1:1A:2377:A:H2'	1:1A:2378:A:C8	2.53	0.44
4:1E:79:ARG:HD3	4:1E:79:ARG:HA	1.80	0.44
32:1a:1168:A:H2'	32:1a:1169:A:C8	2.53	0.44
32:1a:1286:A:H2'	32:1a:1287:A:H4'	1.98	0.44
38:1g:113:GLU:CG	38:1g:119:ARG:HG2	2.47	0.44
1:2A:40:C:H2'	1:2A:41:C:C6	2.52	0.44
1:2A:106:C:O2	1:2A:294:A:O2'	2.34	0.44
1:2A:518:G:H2'	1:2A:519:U:C6	2.53	0.44
1:2A:1188:U:C4'	17:2V:79:VAL:HG22	2.47	0.44
1:2A:2096:U:H2'	1:2A:2097:C:C6	2.52	0.44
5:2F:176:LEU:HD23	5:2F:176:LEU:HA	1.80	0.44
12:2Q:11:LYS:NZ	12:2Q:88:GLY:O	2.40	0.44
20:2Y:35:TYR:CE2	20:2Y:69:ALA:HB3	2.53	0.44
25:23:4:LEU:O	25:23:36:VAL:HA	2.17	0.44
32:2a:54:C:N4	32:2a:353:A:OP2	2.46	0.44
32:2a:441:A:H3'	32:2a:442:C:C6	2.52	0.44
32:2a:1226:C:H4'	50:2s:80:TYR:CZ	2.53	0.44
32:2a:1264:C:O5'	32:2a:1264:C:H6	2.01	0.44
50:2s:20:LEU:HA	50:2s:20:LEU:HD23	1.86	0.44
54:2w:9:A:H8	54:2w:11:C:N4	2.16	0.44
1:1A:2126:A:H4'	1:1A:2127:G:OP1	2.18	0.43
2:1B:24:G:N7	2:1B:56:G:H2'	2.33	0.43
20:1Y:9:LYS:HA	20:1Y:10:GLY:HA2	1.65	0.43
32:1a:294:U:OP1	32:1a:610:G:O2'	2.35	0.43
32:1a:1053:G:N7	32:1a:1200:C:H5''	2.33	0.43
35:1d:150:GLU:C	35:1d:152:SER:H	2.25	0.43
40:1i:100:GLY:O	40:1i:103:THR:HG23	2.17	0.43
50:1s:4:SER:HB3	50:1s:7:LYS:HG3	2.00	0.43
1:2A:191:A:H2'	1:2A:192:C:C6	2.52	0.43
1:2A:1547:C:H2'	1:2A:1548:C:C6	2.53	0.43
1:2A:1790:C:H5''	1:2A:1791:A:OP1	2.17	0.43
8:2I:3:VAL:O	8:2I:18:VAL:HA	2.18	0.43
12:2Q:66:ILE:HG12	12:2Q:104:PHE:CD1	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:2X:44:GLU:OE2	62:2X:201:HOH:O	2.20	0.43
23:21:77:ALA:O	23:21:80:LEU:HB2	2.18	0.43
24:22:25:VAL:HG13	24:22:57:ILE:HG23	1.98	0.43
32:2a:404:U:O4	35:2d:2:GLY:N	2.51	0.43
32:2a:437:U:C5'	35:2d:155:LEU:HD21	2.48	0.43
32:2a:658:G:O4'	46:2o:22:THR:HB	2.18	0.43
32:2a:1216:G:OP1	45:2n:2:ALA:HA	2.17	0.43
35:2d:100:ARG:O	35:2d:104:VAL:HG13	2.18	0.43
37:2f:50:TYR:CE2	49:2r:77:GLY:HA2	2.53	0.43
38:2g:114:ARG:HB2	38:2g:115:ARG:NH2	2.33	0.43
42:2k:92:GLU:O	42:2k:96:ARG:HD2	2.18	0.43
1:1A:744:G:OP1	62:1A:4252:HOH:O	2.21	0.43
1:1A:2336:A:H61	22:10:43:THR:HG21	1.83	0.43
11:1P:125:VAL:HG13	11:1P:138:LEU:HD21	2.00	0.43
15:1T:74:ARG:HG2	15:1T:76:PHE:CZ	2.53	0.43
27:15:8:LYS:O	27:15:9:LYS:HD2	2.19	0.43
29:17:12:ARG:NH2	29:17:44:PRO:HB3	2.32	0.43
32:1a:993:G:H2'	32:1a:995:C:H41	1.82	0.43
33:1b:19:HIS:HA	33:1b:39:ILE:HG23	2.00	0.43
33:1b:80:ILE:O	33:1b:84:GLU:HG2	2.18	0.43
37:1f:33:TYR:OH	37:1f:78:GLU:HG3	2.18	0.43
41:1j:5:ARG:HG3	41:1j:71:LEU:HD11	2.00	0.43
1:2A:1042:G:H3'	1:2A:1043:C:C6	2.53	0.43
1:2A:2001:A:OP1	13:2R:9:LYS:NZ	2.49	0.43
1:2A:2274:A:C5	1:2A:2276:G:C8	3.06	0.43
4:2E:50:GLY:HA3	4:2E:75:VAL:HG21	1.99	0.43
9:2N:73:THR:HA	9:2N:83:LYS:O	2.18	0.43
11:2P:82:GLY:HA2	11:2P:113:LYS:O	2.17	0.43
14:2S:19:LYS:O	14:2S:21:THR:N	2.41	0.43
32:2a:335:C:O2'	32:2a:1433:A:N3	2.44	0.43
32:2a:408:A:H2'	32:2a:409:G:O4'	2.18	0.43
32:2a:1133:G:H2'	32:2a:1134:G:H8	1.82	0.43
32:2a:1187:G:C6	32:2a:1188:A:C6	3.06	0.43
32:2a:1446:U:H2'	32:2a:1452:C:C5	2.53	0.43
35:2d:163:GLU:O	35:2d:165:MET:N	2.51	0.43
43:2l:11:VAL:HG11	48:2q:36:ILE:HG21	2.00	0.43
1:1A:1055:G:OP2	1:1A:1055:G:H8	2.01	0.43
1:1A:1105:U:H2'	1:1A:1106:G:C8	2.52	0.43
1:1A:1899:G:N3	1:1A:1899:G:H2'	2.32	0.43
1:1A:2151:G:C6	1:1A:2152:G:C6	3.06	0.43
2:1B:78:A:C2	2:1B:100:A:C4	3.06	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1Q:16:ARG:HG2	12:1Q:18:LYS:HE2	2.00	0.43
32:1a:67:C:H4'	32:1a:172:A:O4'	2.18	0.43
32:1a:116:A:OP1	62:1a:1918:HOH:O	2.20	0.43
32:1a:445:G:H2'	32:1a:446:G:H8	1.81	0.43
35:1d:158:ILE:H	35:1d:158:ILE:HG13	1.40	0.43
42:1k:48:ILE:HD12	42:1k:63:LEU:HB2	2.00	0.43
44:1m:3:ARG:HG2	44:1m:8:GLU:HA	1.98	0.43
1:2A:731:C:OP1	62:2A:3846:HOH:O	2.21	0.43
1:2A:1009:A:O4'	16:2U:59:ARG:HD2	2.18	0.43
1:2A:1357:U:H2'	1:2A:1358:G:O4'	2.18	0.43
1:2A:1479:G:H1'	1:2A:1558:A:OP1	2.18	0.43
1:2A:2105:C:H2'	1:2A:2106:G:C8	2.54	0.43
1:2A:2630:G:H1	1:2A:2788:C:H42	1.67	0.43
2:2B:66:A:N6	2:2B:108:U:H3'	2.33	0.43
3:2D:218:ARG:HB3	3:2D:219:PRO:HD2	2.01	0.43
5:2F:192:LEU:HD12	5:2F:193:VAL:H	1.83	0.43
6:2G:29:TRP:HA	6:2G:33:ARG:HH12	1.82	0.43
6:2G:107:LEU:HD21	6:2G:178:PHE:CZ	2.53	0.43
6:2G:125:PHE:HB3	6:2G:166:ASP:CG	2.44	0.43
20:2Y:44:ILE:HA	20:2Y:63:LYS:O	2.18	0.43
32:2a:90:U:H2'	32:2a:91:C:C6	2.53	0.43
32:2a:646:U:H2'	32:2a:647:C:H6	1.83	0.43
32:2a:1328:C:O2'	44:2m:29:ARG:NE	2.50	0.43
39:2h:13:ILE:O	39:2h:17:THR:HG23	2.19	0.43
49:2r:61:LYS:O	49:2r:65:ILE:HG12	2.18	0.43
1:1A:518:G:H2'	1:1A:519:U:C6	2.53	0.43
1:1A:545:G:H4'	1:1A:545:G:OP1	2.18	0.43
1:1A:593:G:H4'	30:18:4:MET:HE2	2.01	0.43
1:1A:1514:U:H2'	1:1A:1515:G:C8	2.53	0.43
1:1A:2661:G:H2'	1:1A:2662:A:C8	2.53	0.43
4:1E:47:VAL:O	4:1E:80:GLU:HA	2.18	0.43
7:1H:3:ARG:NH2	7:1H:65:HIS:HB3	2.34	0.43
30:18:25:MET:HE3	30:18:25:MET:HB3	1.90	0.43
32:1a:341:C:H2'	32:1a:342:C:H6	1.83	0.43
32:1a:1346:A:H61	32:1a:1374:A:H3'	1.84	0.43
35:1d:53:ASP:HB3	35:1d:57:ARG:NH1	2.33	0.43
35:1d:111:ALA:HA	35:1d:161:ASN:ND2	2.33	0.43
54:1w:60:U:H3'	54:1w:61:C:H6	1.83	0.43
55:1x:61:C:H2'	55:1x:62:C:H6	1.83	0.43
1:2A:141:A:C8	1:2A:1408:C:O2'	2.71	0.43
1:2A:1262:A:H2	27:25:10:LYS:HD2	1.82	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2114:A:H1'	1:2A:2168:G:HO2'	1.83	0.43
1:2A:2126:A:O2'	1:2A:2162:G:N2	2.51	0.43
1:2A:2814:C:HO2'	27:25:29:THR:HG1	1.62	0.43
1:2A:2888:C:H2'	1:2A:2889:C:C6	2.53	0.43
3:2D:275:LYS:HD2	3:2D:276:LYS:HB2	2.00	0.43
9:2N:28:THR:HG22	9:2N:29:LYS:N	2.33	0.43
12:2Q:130:LYS:HE2	12:2Q:130:LYS:HB3	1.74	0.43
15:2T:16:ARG:NH2	15:2T:18:ASP:OD2	2.51	0.43
15:2T:51:ARG:HG3	15:2T:98:LYS:HD2	1.99	0.43
19:2X:43:VAL:HG21	19:2X:81:VAL:HG11	2.00	0.43
20:2Y:9:LYS:HA	20:2Y:10:GLY:HA2	1.59	0.43
21:2Z:24:LEU:HD12	21:2Z:25:PRO:HD2	1.99	0.43
31:29:13:LYS:HA	31:29:13:LYS:HD3	1.76	0.43
32:2a:523:A:H61	43:2l:92:0TD:CG	2.31	0.43
32:2a:664:G:N2	32:2a:741:G:H1	2.12	0.43
32:2a:673:G:H2'	32:2a:674:G:H8	1.81	0.43
37:2f:12:PRO:HG3	37:2f:57:GLN:C	2.43	0.43
38:2g:152:ALA:O	38:2g:155:ARG:HD3	2.19	0.43
42:2k:20:TYR:O	42:2k:30:VAL:HA	2.18	0.43
50:2s:41:VAL:HG23	50:2s:42:PRO:HD2	2.01	0.43
1:1A:2143:C:H2'	1:1A:2144:U:O4'	2.18	0.43
1:1A:2784:C:H1'	4:1E:37:ARG:NH1	2.34	0.43
15:1T:108:ARG:NH2	15:1T:112:ARG:HD3	2.33	0.43
32:1a:728:A:H2'	32:1a:729:A:C8	2.53	0.43
32:1a:735:C:H2'	32:1a:736:C:H6	1.82	0.43
39:1h:116:LYS:HD3	39:1h:127:LEU:HD13	2.01	0.43
42:1k:41:THR:OG1	42:1k:42:TRP:N	2.50	0.43
1:2A:144:C:H2'	1:2A:145:G:C8	2.54	0.43
1:2A:1186:G:C2	1:2A:1187:G:H1'	2.53	0.43
1:2A:2184:G:H2'	1:2A:2185:C:H6	1.83	0.43
2:2B:7:G:H2'	2:2B:8:U:O4'	2.18	0.43
3:2D:141:VAL:HG12	3:2D:162:SER:HB2	2.00	0.43
14:2S:11:LYS:HE3	14:2S:15:ARG:NH1	2.33	0.43
19:2X:47:PHE:HZ	24:22:37:PHE:CE2	2.36	0.43
22:20:36:ILE:HD13	22:20:58:THR:HG21	2.00	0.43
25:23:10:LYS:HB3	25:23:53:LEU:HA	2.00	0.43
32:2a:176:C:H2'	32:2a:177:C:H6	1.82	0.43
32:2a:452:A:H4'	47:2p:72:ARG:HH21	1.83	0.43
32:2a:607:A:H2'	32:2a:608:A:O4'	2.18	0.43
32:2a:994:A:C2'	32:2a:995:C:H5'	2.48	0.43
32:2a:1051:C:H2'	32:2a:1052:U:H6	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1095:U:H2'	32:2a:1096:C:C6	2.54	0.43
32:2a:1163:C:C2	32:2a:1174:G:C2	3.06	0.43
32:2a:1190:G:C5'	34:2c:176:HIS:HE1	2.32	0.43
32:2a:1404:5MC:O2	32:2a:1519:MA6:O2'	2.29	0.43
34:2c:85:ARG:O	34:2c:89:GLU:N	2.51	0.43
36:2e:53:LEU:HD12	36:2e:53:LEU:H	1.83	0.43
47:2p:21:VAL:HG13	47:2p:34:GLU:HB3	2.00	0.43
1:1A:272(A):U:O2'	1:1A:272(B):G:O5'	2.18	0.43
1:1A:1268:A:H2'	1:1A:1269:A:O4'	2.18	0.43
1:1A:1794:U:H2'	1:1A:1795:C:H6	1.82	0.43
1:1A:2206:G:H5''	1:1A:2207:G:C5	2.53	0.43
62:1A:4929:HOH:O	5:1F:74:ARG:HG3	2.19	0.43
3:1D:9:TYR:CE1	3:1D:13:ARG:HG3	2.53	0.43
3:1D:145:VAL:HG11	3:1D:175:LEU:HD11	2.00	0.43
6:1G:97:ASP:O	6:1G:101:ILE:HG13	2.19	0.43
7:1H:3:ARG:HH21	7:1H:65:HIS:HB3	1.84	0.43
33:1b:155:LEU:HD12	33:1b:155:LEU:HA	1.76	0.43
44:1m:3:ARG:HG3	44:1m:4:ILE:N	2.33	0.43
1:2A:236:C:H2'	1:2A:237:C:H6	1.83	0.43
1:2A:253:C:O2'	62:2A:3847:HOH:O	2.21	0.43
1:2A:480:A:O2'	20:2Y:46:LYS:O	2.35	0.43
1:2A:927:G:H2'	1:2A:928:G:O4'	2.18	0.43
1:2A:1260:G:C6	1:2A:1261:C:C4	3.06	0.43
1:2A:1462:C:H4'	1:2A:2703:C:H5'	2.01	0.43
1:2A:1833:U:O2'	1:2A:1969:A:N1	2.35	0.43
1:2A:2121:G:H1	1:2A:2177:C:N4	2.17	0.43
2:2B:74:U:H3'	2:2B:75:G:H5''	2.00	0.43
2:2B:114:C:H2'	2:2B:115:G:H8	1.81	0.43
8:2I:48:GLU:HG3	8:2I:52:ARG:NH1	2.34	0.43
10:2O:64:ARG:NH2	10:2O:99:PHE:O	2.51	0.43
13:2R:67:LEU:HD13	13:2R:76:VAL:HG21	2.00	0.43
16:2U:8:VAL:HG23	16:2U:11:ARG:NH2	2.34	0.43
18:2W:86:LEU:HD22	18:2W:96:ILE:HD11	2.00	0.43
21:2Z:95:PRO:HA	21:2Z:129:SER:HA	2.00	0.43
21:2Z:159:PRO:HA	21:2Z:160:GLY:HA2	1.71	0.43
21:2Z:171:ILE:H	21:2Z:171:ILE:HG13	1.61	0.43
22:20:53:MET:HG2	22:20:57:PHE:HA	2.00	0.43
32:2a:46:G:O2'	32:2a:365:U:H1'	2.18	0.43
32:2a:108:G:C6	51:2t:15:ARG:HG2	2.54	0.43
32:2a:137:C:H2'	32:2a:138:G:C8	2.54	0.43
32:2a:707:C:OP1	42:2k:85:ARG:NH1	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1068:G:H8	32:2a:1068:G:OP2	2.02	0.43
32:2a:1427:U:H2'	32:2a:1428:A:H8	1.83	0.43
34:2c:22:TRP:CH2	34:2c:32:LEU:HB3	2.53	0.43
44:2m:14:ARG:H	44:2m:14:ARG:HG3	1.57	0.43
48:2q:57:VAL:HA	48:2q:77:VAL:HG23	2.00	0.43
1:1A:1190:G:OP1	11:1P:30:THR:OG1	2.33	0.43
1:1A:1432:C:H2'	1:1A:1433:U:O4'	2.19	0.43
1:1A:1889:A:H2'	1:1A:1890:A:C8	2.54	0.43
32:1a:42:G:H2'	32:1a:43:C:O4'	2.19	0.43
32:1a:57:G:H2'	32:1a:58:C:H6	1.83	0.43
32:1a:73:G:C6	32:1a:76:C:C4	3.06	0.43
32:1a:167:G:H2'	32:1a:168:G:H8	1.81	0.43
32:1a:737:A:H2'	32:1a:738:C:C6	2.53	0.43
32:1a:750:G:N3	46:1o:23:GLY:HA3	2.33	0.43
32:1a:1530:G:OP1	62:1a:1920:HOH:O	2.21	0.43
42:1k:85:ARG:HD3	42:1k:113:PRO:HD3	2.01	0.43
48:1q:7:THR:OG1	48:1q:58:GLU:HG2	2.19	0.43
1:2A:443:A:H1'	1:2A:1201:C:O4'	2.18	0.43
1:2A:587:C:P	11:2P:21:ARG:HH22	2.41	0.43
1:2A:879:G:H2'	1:2A:879:G:N3	2.34	0.43
1:2A:1371:G:H2'	1:2A:1372:U:H5	1.84	0.43
1:2A:2019:A:N7	27:25:9:LYS:HE2	2.34	0.43
1:2A:2356:C:OP1	22:20:24:LYS:NZ	2.36	0.43
1:2A:2552:OMU:H6	1:2A:2552:OMU:O5'	2.19	0.43
1:2A:2647:U:H2'	1:2A:2648:C:C6	2.53	0.43
5:2F:32:LEU:HB3	5:2F:112:MET:HE1	2.01	0.43
14:2S:63:THR:O	14:2S:66:ALA:HB3	2.19	0.43
14:2S:67:ARG:HH12	14:2S:103:GLU:HB3	1.83	0.43
26:24:34:GLU:OE1	44:2m:3:ARG:HA	2.18	0.43
32:2a:7:G:H5'	32:2a:298:A:O4'	2.19	0.43
32:2a:416:G:C5	32:2a:417:C:C4	3.06	0.43
32:2a:719:C:H42	49:2r:71:LYS:HE2	1.83	0.43
32:2a:1085:U:H3'	32:2a:1086:U:C6	2.53	0.43
32:2a:1168:A:H2'	32:2a:1169:A:C8	2.54	0.43
33:2b:114:ARG:HD2	33:2b:114:ARG:HA	1.64	0.43
34:2c:186:PHE:CZ	34:2c:188:LEU:HD13	2.54	0.43
39:2h:51:VAL:HG11	39:2h:60:ARG:NH1	2.33	0.43
40:2i:57:GLY:C	40:2i:59:PHE:H	2.26	0.43
48:2q:53:LEU:HD12	48:2q:53:LEU:HA	1.90	0.43
50:2s:28:LYS:HA	50:2s:28:LYS:HD3	1.80	0.43
54:2w:25:C:H2'	54:2w:26:A:H8	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:2w:56:C:H2'	54:2w:57:G:O4'	2.18	0.43
56:2y:58:A:O2'	56:2y:60:U:OP2	2.27	0.43
1:1A:1069:A:H2'	1:1A:1073:A:C8	2.53	0.43
1:1A:1567:A:OP2	3:1D:84:TYR:OH	2.31	0.43
2:1B:74:U:H2'	2:1B:75:G:O4'	2.19	0.43
3:1D:13:ARG:HA	3:1D:16:MET:HE3	2.00	0.43
11:1P:63:PRO:HG2	30:18:25:MET:HB2	2.00	0.43
11:1P:126:VAL:HG22	11:1P:146:VAL:HB	2.01	0.43
15:1T:118:ARG:HG2	32:1a:1442(A):G:C8	2.53	0.43
24:12:16:LEU:HB3	24:12:20:GLU:HB2	2.00	0.43
32:1a:219:C:H2'	32:1a:220:G:O4'	2.19	0.43
32:1a:404:U:H2'	32:1a:405:U:C6	2.54	0.43
34:1c:89:GLU:O	34:1c:93:LYS:N	2.41	0.43
36:1e:8:GLU:OE2	36:1e:63:ARG:NH2	2.52	0.43
36:1e:18:ARG:NH1	36:1e:27:ARG:HH12	2.14	0.43
56:1y:6:G:O6	56:1y:7:A:N6	2.52	0.43
56:1y:59:U:OP1	56:1y:60:U:H5	2.01	0.43
1:2A:271(H):G:H2'	1:2A:271(I):G:H8	1.83	0.43
1:2A:1291:C:H2'	1:2A:1292:U:H6	1.83	0.43
1:2A:1410:G:H2'	1:2A:1411:C:H6	1.82	0.43
1:2A:2529:G:O6	31:29:31:LYS:NZ	2.52	0.43
2:2B:24:G:N7	2:2B:56:G:H2'	2.33	0.43
2:2B:115:G:H2'	2:2B:116:G:O4'	2.19	0.43
6:2G:123:ASN:C	6:2G:125:PHE:H	2.25	0.43
13:2R:88:ARG:HG2	13:2R:89:ASP:OD1	2.18	0.43
16:2U:76:TYR:HH	16:2U:92:ARG:HE	1.61	0.43
32:2a:250:A:H4'	32:2a:251:G:O5'	2.19	0.43
32:2a:359:U:H2'	32:2a:360:A:H8	1.83	0.43
32:2a:458:C:H2'	32:2a:460:G:O4'	2.18	0.43
32:2a:701:C:OP1	32:2a:702:A:O2'	2.28	0.43
32:2a:814:A:N7	32:2a:816:A:C4	2.87	0.43
32:2a:967:5MC:H2'	32:2a:968:A:N7	2.34	0.43
32:2a:977:A:H2'	32:2a:977:A:N3	2.33	0.43
32:2a:1263:C:H3'	32:2a:1263:C:H6	1.84	0.43
32:2a:1324:A:O4'	32:2a:1362:C:H4'	2.19	0.43
35:2d:101:LEU:HA	35:2d:104:VAL:HG22	2.01	0.43
35:2d:116:GLN:O	35:2d:120:LEU:HG	2.18	0.43
1:1A:286:C:H2'	1:1A:287:C:H6	1.83	0.43
1:1A:883:G:H21	1:1A:893:C:H42	1.65	0.43
1:1A:1709:U:H2'	1:1A:1710:C:C6	2.53	0.43
3:1D:206:LEU:HD23	3:1D:206:LEU:HA	1.81	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1I:81:VAL:HG21	8:1I:88:ILE:HD13	2.01	0.43
8:1I:127:VAL:HA	8:1I:140:LEU:O	2.19	0.43
9:1N:67:LEU:O	9:1N:88:GLU:HG3	2.19	0.43
32:1a:66:G:O4'	32:1a:173:U:C4	2.72	0.43
32:1a:688:G:H2'	32:1a:689:C:H6	1.83	0.43
33:1b:15:VAL:HB	33:1b:209:ARG:HG3	2.01	0.43
33:1b:16:HIS:CG	33:1b:17:PHE:N	2.87	0.43
34:1c:119:ARG:NH1	34:1c:123:GLN:HE21	2.16	0.43
35:1d:101:LEU:HB2	35:1d:138:TYR:HB3	2.01	0.43
50:1s:32:LYS:HB3	50:1s:32:LYS:HE2	1.80	0.43
54:1w:5:G:H2'	54:1w:6:G:H8	1.83	0.43
1:2A:271(P):C:H4'	8:2I:42:SER:O	2.18	0.43
1:2A:912:C:OP1	12:2Q:8:LYS:NZ	2.36	0.43
1:2A:1264:G:H2'	1:2A:2014:A:N6	2.34	0.43
1:2A:2393:A:H2'	1:2A:2394:C:O4'	2.19	0.43
1:2A:2401:U:P	28:26:18:ARG:HH21	2.42	0.43
6:2G:62:LEU:HB3	6:2G:143:GLU:HB3	2.01	0.43
6:2G:135:LEU:HG	6:2G:157:ILE:HD11	2.01	0.43
16:2U:29:SER:OG	16:2U:30:LYS:NZ	2.24	0.43
24:22:51:ARG:HE	24:22:51:ARG:HB2	1.51	0.43
32:2a:409:G:OP1	35:2d:24:GLU:N	2.51	0.43
32:2a:560:U:H5'	32:2a:566:G:N2	2.33	0.43
32:2a:737:A:H5'	37:2f:90:VAL:O	2.19	0.43
32:2a:1134:G:N1	32:2a:1135:U:H1'	2.34	0.43
32:2a:1333:A:H2'	32:2a:1334:G:O4'	2.19	0.43
33:2b:111:ARG:HH11	33:2b:111:ARG:HA	1.84	0.43
35:2d:160:GLN:HE21	35:2d:160:GLN:HB3	1.62	0.43
36:2e:83:GLU:HA	36:2e:88:LYS:HA	2.01	0.43
39:2h:64:LYS:HG2	39:2h:79:VAL:HG21	2.00	0.43
41:2j:63:PHE:HE2	45:2n:45:ARG:HA	1.83	0.43
1:1A:492:A:H2'	1:1A:493:G:O4'	2.18	0.43
1:1A:880:G:C2'	1:1A:881:G:H8	2.28	0.43
1:1A:1062:G:N2	1:1A:1077:A:H61	2.17	0.43
1:1A:1762:A:N1	62:1A:4340:HOH:O	2.37	0.43
1:1A:2038:G:O6	62:1A:4256:HOH:O	2.22	0.43
10:1O:63:VAL:HG12	10:1O:106:LEU:HD11	1.99	0.43
13:1R:28:LEU:HD23	13:1R:48:VAL:HG21	2.01	0.43
16:1U:81:HIS:CE1	16:1U:85:LYS:HD2	2.54	0.43
21:1Z:151:HIS:HA	21:1Z:170:THR:HA	2.00	0.43
23:11:44:PRO:HB2	23:11:46:LEU:CD1	2.49	0.43
32:1a:1261:A:H3'	32:1a:1262:C:C6	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:1f:35:ALA:HA	37:1f:67:MET:HB3	2.01	0.43
39:1h:110:ALA:HB3	39:1h:121:ASP:HB3	2.01	0.43
1:2A:686:G:N2	1:2A:788:A:H61	2.17	0.43
1:2A:884:C:H3'	1:2A:885:C:H6	1.84	0.43
1:2A:1266:G:O4'	18:2W:15:ARG:NH2	2.50	0.43
6:2G:77:ILE:HG21	6:2G:80:PHE:CD2	2.54	0.43
6:2G:122:PRO:O	6:2G:125:PHE:HD2	2.02	0.43
8:2I:45:LYS:O	8:2I:48:GLU:N	2.51	0.43
8:2I:102:SER:O	8:2I:106:GLY:N	2.46	0.43
8:2I:124:GLY:H	8:2I:144:VAL:HB	1.84	0.43
12:2Q:12:GLN:NE2	12:2Q:72:LYS:HG3	2.34	0.43
21:2Z:69:THR:HG22	21:2Z:90:VAL:HG22	2.01	0.43
24:22:31:GLU:HB3	24:22:53:LEU:HD21	2.00	0.43
32:2a:395:C:H2'	32:2a:396:G:C8	2.53	0.43
32:2a:1060:C:H2'	32:2a:1061:G:H8	1.82	0.43
32:2a:1095:U:H2'	32:2a:1096:C:O4'	2.18	0.43
32:2a:1310:G:H5'	44:2m:77:ASN:ND2	2.34	0.43
32:2a:1328:C:H2'	32:2a:1329:A:O4'	2.19	0.43
34:2c:120:VAL:CG2	34:2c:137:ALA:HB2	2.49	0.43
35:2d:38:TYR:CE1	35:2d:45:GLN:HG3	2.53	0.43
35:2d:172:PRO:HD2	35:2d:173:TRP:CZ3	2.54	0.43
37:2f:97:PHE:HE2	49:2r:62:GLU:HG2	1.84	0.43
38:2g:113:GLU:HG3	38:2g:118:VAL:HG12	1.99	0.43
39:2h:3:THR:O	39:2h:5:PRO:HD3	2.19	0.43
39:2h:119:LEU:HB3	39:2h:123:GLU:HB2	2.00	0.43
41:2j:9:ARG:HH22	41:2j:69:ASN:HD21	1.67	0.43
41:2j:47:PHE:HB2	41:2j:63:PHE:HB2	2.00	0.43
45:2n:29:ARG:CZ	45:2n:42:ILE:HD11	2.49	0.43
1:1A:479:A:N3	1:1A:481:G:H5''	2.34	0.42
1:1A:570:G:H2'	1:1A:2030:A:C5	2.54	0.42
1:1A:2445:G:OP1	5:1F:74:ARG:NH2	2.48	0.42
1:1A:2779:U:H5'	1:1A:2781:A:O4'	2.19	0.42
1:1A:2811:G:N2	1:1A:2891:G:H1'	2.34	0.42
32:1a:116:A:H8	32:1a:116:A:O5'	2.02	0.42
32:1a:193:C:H2'	32:1a:194:C:C6	2.49	0.42
46:1o:42:HIS:CE1	46:1o:46:HIS:CD2	3.07	0.42
1:2A:82:G:H5''	1:2A:296:C:H5'	2.00	0.42
1:2A:816:C:H2'	1:2A:817:C:H6	1.83	0.42
1:2A:1399:C:H2'	1:2A:1400:G:H8	1.84	0.42
1:2A:2070:G:H2'	1:2A:2071:A:H8	1.84	0.42
6:2G:114:ILE:HG13	6:2G:140:ILE:HG12	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:23:7:LYS:HE3	25:23:32:GLN:HE21	1.84	0.42
31:29:27:CYS:SG	31:29:28:GLU:N	2.92	0.42
32:2a:683:G:H2'	32:2a:684:A:O4'	2.20	0.42
32:2a:840:C:H4'	32:2a:841:U:OP1	2.19	0.42
32:2a:976:G:C8	32:2a:1358:U:C2	3.06	0.42
32:2a:1084:G:C5	32:2a:1085:U:C4	3.07	0.42
32:2a:1176:A:H2'	32:2a:1177:G:C8	2.54	0.42
34:2c:8:ILE:HG23	34:2c:16:ARG:HG2	2.01	0.42
36:2e:37:ARG:HB3	36:2e:114:GLY:HA2	2.01	0.42
47:2p:2:VAL:HG13	47:2p:64:ALA:HA	2.01	0.42
48:2q:24:GLU:HA	48:2q:39:SER:HA	2.01	0.42
52:2u:15:ARG:HB2	52:2u:17:THR:HG23	2.00	0.42
1:1A:1071:G:H1'	1:1A:1089:G:H2'	1.99	0.42
1:1A:1639:U:O2'	1:1A:2699:C:H4'	2.19	0.42
1:1A:2286:A:H4'	1:1A:2287:A:O4'	2.20	0.42
1:1A:2328:A:H2'	1:1A:2329:G:H8	1.84	0.42
1:1A:2667:C:H2'	1:1A:2668:G:O4'	2.18	0.42
1:1A:2802:G:H2'	1:1A:2803:C:C6	2.54	0.42
7:1H:3:ARG:NH1	7:1H:5:GLY:H	2.16	0.42
32:1a:109:A:H2'	32:1a:326:G:N2	2.33	0.42
32:1a:958:A:C6	32:1a:959:A:N1	2.87	0.42
32:1a:1017:G:H2'	32:1a:1018:C:C6	2.54	0.42
32:1a:1327:C:H2'	32:1a:1328:C:C6	2.54	0.42
33:1b:208:ILE:HD13	33:1b:208:ILE:H	1.83	0.42
1:2A:1423:G:H2'	1:2A:1424:G:H8	1.83	0.42
1:2A:2507:C:H5''	1:2A:2573:C:N4	2.34	0.42
1:2A:2552:OMU:H2'	1:2A:2554:U:OP2	2.18	0.42
2:2B:30:C:OP2	14:2S:32:LEU:HD11	2.20	0.42
3:2D:16:MET:HG3	3:2D:206:LEU:O	2.19	0.42
6:2G:93:THR:HG22	6:2G:95:ARG:HG3	2.00	0.42
7:2H:118:PRO:HD2	7:2H:121:ILE:HB	2.01	0.42
14:2S:15:ARG:HB3	14:2S:19:LYS:NZ	2.34	0.42
21:2Z:55:HIS:CE1	21:2Z:135:GLU:HB2	2.54	0.42
32:2a:176:C:H2'	32:2a:177:C:C6	2.53	0.42
32:2a:762:C:H2'	32:2a:763:G:H8	1.84	0.42
32:2a:1030(A):G:N2	32:2a:1030(D):A:OP2	2.52	0.42
32:2a:1092:A:H5''	38:2g:4:ARG:NH1	2.33	0.42
38:2g:52:GLU:H	38:2g:52:GLU:HG2	1.68	0.42
38:2g:120:ILE:O	38:2g:124:LEU:HB2	2.19	0.42
44:2m:6:GLY:HA3	44:2m:67:GLU:CD	2.44	0.42
50:2s:50:ALA:HA	50:2s:58:VAL:O	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:249:C:O2	30:18:12:LYS:NZ	2.38	0.42
1:1A:512:G:N1	62:1A:4307:HOH:O	2.32	0.42
1:1A:1039:G:H1	1:1A:1116:C:N4	2.14	0.42
1:1A:1359:A:H2	1:1A:1372:U:O4	2.01	0.42
1:1A:2791:C:H2'	1:1A:2792:G:H8	1.84	0.42
8:1I:10:GLU:H	8:1I:10:GLU:HG3	1.36	0.42
17:1V:71:LEU:HD23	17:1V:71:LEU:HA	1.96	0.42
21:1Z:138:GLU:H	21:1Z:156:LYS:NZ	2.18	0.42
32:1a:461:A:O2'	32:1a:470:C:H5'	2.19	0.42
32:1a:982:U:H4'	32:1a:983:A:O5'	2.18	0.42
32:1a:1284:C:H3'	32:1a:1285:A:H8	1.84	0.42
33:1b:87:ARG:HD2	33:1b:233:SER:HB3	2.01	0.42
33:1b:193:ASP:HB3	33:1b:196:LEU:HD22	2.00	0.42
44:1m:4:ILE:HA	44:1m:5:ALA:HA	1.81	0.42
46:1o:18:PHE:CZ	46:1o:21:ASP:HB2	2.53	0.42
50:1s:33:THR:OG1	50:1s:35:SER:HB2	2.18	0.42
55:1x:19:G:H4'	55:1x:20:U:OP2	2.19	0.42
1:2A:880:G:H2'	1:2A:881:G:H8	1.84	0.42
1:2A:1753:G:N1	1:2A:1756:G:OP2	2.46	0.42
1:2A:1864:U:OP1	1:2A:2410:G:O2'	2.30	0.42
1:2A:1946:U:H2'	1:2A:1947:C:C6	2.54	0.42
2:2B:33:G:C6	2:2B:34:U:C4	3.07	0.42
6:2G:127:GLY:H	6:2G:166:ASP:CG	2.27	0.42
9:2N:15:LEU:HB2	9:2N:135:PRO:HB2	2.01	0.42
10:2O:80:ASP:OD2	15:2T:64:ARG:NH2	2.52	0.42
11:2P:118:GLY:O	11:2P:137:LYS:NZ	2.47	0.42
12:2Q:81:VAL:HG12	22:20:5:LYS:HD3	2.01	0.42
14:2S:35:ILE:HD11	14:2S:97:ARG:HE	1.84	0.42
19:2X:12:VAL:HG22	19:2X:29:TRP:CE2	2.54	0.42
24:22:8:LYS:O	24:22:12:GLU:HB2	2.19	0.42
32:2a:920:U:H2'	32:2a:921:U:H6	1.81	0.42
32:2a:1125:U:O2'	32:2a:1126:U:H2'	2.19	0.42
32:2a:1386:G:C2	32:2a:1387:G:N7	2.87	0.42
32:2a:1507:A:OP2	53:2v:13:A:N6	2.52	0.42
33:2b:133:LYS:O	33:2b:137:ARG:HB2	2.20	0.42
55:2x:40:C:H2'	55:2x:41:C:C6	2.51	0.42
1:1A:795:C:H2'	1:1A:796:C:H6	1.84	0.42
1:1A:1358:G:N2	1:1A:1372:U:C5	2.86	0.42
1:1A:1359:A:C2	1:1A:1372:U:O4	2.73	0.42
1:1A:2528:U:H5''	31:19:31:LYS:HE2	2.02	0.42
1:1A:2590:A:H2'	1:1A:2591:C:C6	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1S:10:ARG:O	14:1S:14:VAL:HG13	2.19	0.42
33:1b:16:HIS:HB2	33:1b:204:ASN:HB3	2.02	0.42
37:1f:99:ALA:O	49:1r:28:GLU:HA	2.18	0.42
40:1i:50:LEU:HD13	40:1i:56:LEU:HA	2.01	0.42
41:1j:17:ASP:OD1	41:1j:70:ARG:NE	2.52	0.42
1:2A:271(K):U:H4'	1:2A:271(L):U:OP1	2.20	0.42
1:2A:1667:G:O2'	1:2A:1991:U:O4	2.30	0.42
1:2A:1779:U:H2'	62:2A:4198:HOH:O	2.18	0.42
1:2A:2647:U:H2'	1:2A:2648:C:H6	1.84	0.42
4:2E:54:GLN:OE1	4:2E:55:ASN:N	2.51	0.42
5:2F:32:LEU:O	5:2F:36:VAL:HG23	2.20	0.42
5:2F:33:LEU:HG	5:2F:112:MET:HE3	2.01	0.42
21:2Z:53:ILE:HA	21:2Z:71:VAL:HG23	2.02	0.42
26:24:67:TYR:HD2	50:2s:9:VAL:HB	1.84	0.42
32:2a:986:A:H2'	32:2a:987:G:O4'	2.19	0.42
34:2c:86:VAL:HA	34:2c:89:GLU:HG2	2.01	0.42
35:2d:60:GLU:HG3	35:2d:202:LEU:HD12	2.01	0.42
36:2e:84:PHE:N	36:2e:87:SER:O	2.50	0.42
36:2e:143:ARG:NE	39:2h:77:GLU:OE2	2.49	0.42
38:2g:122:HIS:HA	38:2g:125:MET:HE3	2.00	0.42
38:2g:152:ALA:O	38:2g:155:ARG:NH1	2.51	0.42
44:2m:31:LYS:HA	44:2m:34:LEU:HD12	2.01	0.42
1:1A:44:G:H5''	1:1A:45:C:OP1	2.18	0.42
1:1A:687:C:H1'	29:17:4:THR:HG22	2.01	0.42
1:1A:784:A:C6	3:1D:229:VAL:HG11	2.54	0.42
1:1A:1082:U:C4	1:1A:1086:A:N1	2.79	0.42
1:1A:2319:G:H1	14:1S:3:ARG:HA	1.83	0.42
20:1Y:49:VAL:HG11	20:1Y:61:ILE:HG12	2.00	0.42
21:1Z:93:ASP:HB3	21:1Z:131:ARG:HH22	1.84	0.42
32:1a:236:G:H5''	48:1q:42:TYR:OH	2.19	0.42
32:1a:685:G:C2	32:1a:686:U:C4	3.07	0.42
32:1a:1033:G:C2'	32:1a:1034:G:H8	2.32	0.42
36:1e:105:VAL:HB	36:1e:106:PRO:HD3	2.02	0.42
1:2A:615:G:OP1	5:2F:40:GLN:HG2	2.20	0.42
1:2A:660:G:H5'	5:2F:99:TYR:CE1	2.55	0.42
1:2A:1012:U:H5	9:2N:28:THR:HG21	1.84	0.42
1:2A:1857:G:C6	1:2A:1858:G:N1	2.86	0.42
1:2A:2206:G:H3'	1:2A:2207:G:N7	2.35	0.42
3:2D:227:ASN:C	3:2D:234:GLY:HA3	2.45	0.42
4:2E:33:VAL:HG11	4:2E:36:ARG:CZ	2.49	0.42
17:2V:1:MET:CE	17:2V:44:LYS:H	2.31	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:20:23:VAL:HG22	22:20:38:VAL:HG22	2.01	0.42
24:22:51:ARG:O	24:22:55:ARG:HG3	2.20	0.42
32:2a:631:G:H2'	32:2a:632:A:H8	1.83	0.42
32:2a:719:C:N4	49:2r:71:LYS:HE2	2.35	0.42
32:2a:1372:U:H2'	32:2a:1373:G:O4'	2.18	0.42
32:2a:1412:C:H2'	32:2a:1413:A:H8	1.82	0.42
33:2b:58:ILE:H	33:2b:58:ILE:HG12	1.72	0.42
33:2b:63:MET:HG3	33:2b:225:ALA:HB1	2.02	0.42
40:2i:53:VAL:HG23	40:2i:55:ALA:H	1.83	0.42
41:2j:65:LEU:HD13	45:2n:56:VAL:HG22	2.01	0.42
48:2q:14:LYS:H	48:2q:14:LYS:HG2	1.60	0.42
1:1A:191:A:H2'	1:1A:192:C:C6	2.54	0.42
1:1A:1489:U:HO2'	1:1A:1490:A:H8	1.67	0.42
1:1A:1932:A:H2'	1:1A:1933:G:O4'	2.19	0.42
1:1A:2093:G:C6	1:1A:2225:A:C8	3.08	0.42
3:1D:145:VAL:HG12	3:1D:146:GLU:O	2.20	0.42
4:1E:181:LEU:HD12	4:1E:181:LEU:HA	1.77	0.42
6:1G:105:LYS:NZ	26:14:25:TYR:O	2.44	0.42
11:1P:79:ARG:HE	11:1P:79:ARG:HB2	1.75	0.42
26:14:63:TYR:N	26:14:64:GLY:HA2	2.33	0.42
30:18:33:ASN:HA	30:18:36:LYS:HD2	2.02	0.42
32:1a:690:G:C6	32:1a:691:G:C6	3.08	0.42
35:1d:109:GLY:HA3	35:1d:165:MET:SD	2.59	0.42
36:1e:83:GLU:HG2	36:1e:88:LYS:HG3	2.00	0.42
46:1o:26:GLU:HG3	46:1o:81:LEU:HD22	2.02	0.42
51:1t:50:GLU:HG3	51:1t:100:ILE:HG23	2.01	0.42
56:1y:48:C:OP1	56:1y:48:C:H2'	2.20	0.42
1:2A:1359:A:C2	1:2A:1372:U:O4	2.73	0.42
1:2A:1429:G:H2'	1:2A:1430:C:C6	2.54	0.42
1:2A:2001:A:H2'	1:2A:2002:G:C8	2.55	0.42
1:2A:2125:G:H1'	1:2A:2173:A:H61	1.85	0.42
1:2A:2497:A:H5''	62:2A:4041:HOH:O	2.19	0.42
6:2G:43:LEU:HD13	6:2G:43:LEU:HA	1.90	0.42
21:2Z:31:ARG:NH1	21:2Z:94:GLU:HG2	2.30	0.42
32:2a:1004:A:C6	32:2a:1037:C:H1'	2.55	0.42
32:2a:1452:C:H5'	32:2a:1457:G:H1'	2.02	0.42
33:2b:92:TYR:CZ	33:2b:151:GLY:HA3	2.54	0.42
34:2c:32:LEU:HD23	34:2c:32:LEU:HA	1.79	0.42
42:2k:67:ASP:O	42:2k:71:LYS:HG3	2.19	0.42
44:2m:20:THR:C	44:2m:22:ILE:H	2.27	0.42
1:1A:897:C:N3	1:1A:898:C:N4	2.67	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1230:C:H2'	1:1A:1231:G:C8	2.54	0.42
1:1A:2287:A:O2'	1:1A:2289:G:N7	2.51	0.42
1:1A:2590:A:H2'	1:1A:2591:C:H6	1.84	0.42
1:1A:2626:C:H2'	1:1A:2627:G:O4'	2.19	0.42
5:1F:28:ILE:O	5:1F:30:PRO:HD3	2.20	0.42
26:14:57:GLU:HA	26:14:58:ARG:HA	1.85	0.42
28:16:38:LYS:HE3	28:16:38:LYS:HB3	1.81	0.42
32:1a:258:G:H2'	32:1a:259:G:C8	2.54	0.42
32:1a:684:A:H2'	32:1a:685:G:O4'	2.20	0.42
32:1a:711:G:OP1	37:1f:54:LYS:NZ	2.30	0.42
32:1a:721:G:H4'	32:1a:722:A:O4'	2.20	0.42
32:1a:743:U:H2'	32:1a:744:C:C6	2.54	0.42
32:1a:1266:G:N2	32:1a:1270:C:N3	2.68	0.42
34:1c:6:HIS:CD2	34:1c:8:ILE:HB	2.55	0.42
35:1d:119:GLN:HG2	35:1d:123:HIS:CD2	2.54	0.42
43:1l:53:ARG:HB3	43:1l:69:TYR:HE1	1.85	0.42
1:2A:125:G:H21	29:27:48:LYS:HG2	1.85	0.42
1:2A:312:G:H4'	1:2A:331:A:N3	2.35	0.42
1:2A:565:C:H2'	1:2A:566:U:O4'	2.19	0.42
1:2A:700:G:O2'	1:2A:1632:A:N3	2.48	0.42
1:2A:1913:A:N6	54:2w:38:A:H5'	2.35	0.42
1:2A:2127:G:H22	1:2A:2160:G:H22	1.65	0.42
1:2A:2270:G:H2'	1:2A:2271:G:O4'	2.19	0.42
1:2A:2313:C:H4'	6:2G:91:ARG:HG3	2.02	0.42
1:2A:2468:G:C4	1:2A:2481:G:C2	3.07	0.42
5:2F:184:TYR:O	5:2F:188:ARG:HG3	2.20	0.42
6:2G:172:LEU:O	6:2G:176:LEU:HG	2.19	0.42
15:2T:8:LYS:HA	15:2T:8:LYS:HD3	1.85	0.42
17:2V:85:LYS:HE2	17:2V:85:LYS:HB2	1.92	0.42
20:2Y:60:PHE:O	20:2Y:61:ILE:HD13	2.20	0.42
32:2a:194:C:H2'	32:2a:195:A:H5''	2.01	0.42
32:2a:1263:C:H1'	32:2a:1273:G:N2	2.34	0.42
32:2a:1304:G:C6	32:2a:1305:G:N1	2.88	0.42
32:2a:1403:C:H1'	32:2a:1500:A:N1	2.34	0.42
33:2b:7:VAL:HB	33:2b:9:GLU:HG2	2.01	0.42
33:2b:87:ARG:NH2	33:2b:220:ASP:OD1	2.49	0.42
33:2b:144:ARG:NH2	33:2b:148:TYR:OH	2.52	0.42
34:2c:187:ALA:O	34:2c:198:VAL:HB	2.20	0.42
35:2d:31:CYS:SG	35:2d:33:MET:N	2.92	0.42
38:2g:28:ASN:HA	38:2g:31:MET:HE2	2.01	0.42
55:2x:23:C:H2'	55:2x:24:U:H6	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:27:G:N2	1:1A:512:G:H1'	2.35	0.42
1:1A:143:G:H2'	1:1A:143(A):C:C6	2.54	0.42
1:1A:1851:U:H2'	1:1A:1852:C:O4'	2.20	0.42
1:1A:2320:A:H2'	1:1A:2320:A:N3	2.35	0.42
7:1H:86:GLU:HG3	7:1H:132:ARG:NH2	2.31	0.42
21:1Z:104:PHE:CD2	21:1Z:104:PHE:N	2.86	0.42
28:16:28:ARG:NH1	28:16:29:ASN:OD1	2.53	0.42
31:19:17:ILE:HG12	31:19:24:TYR:HB2	2.02	0.42
32:1a:175:C:H5'	51:1t:25:ARG:NH1	2.34	0.42
32:1a:938:A:C6	32:1a:939:G:C5	3.08	0.42
32:1a:1002:G:N7	32:1a:1003:G:H1'	2.34	0.42
32:1a:1073:U:O2'	33:1b:104:ASN:OD1	2.30	0.42
33:1b:27:LYS:HB2	33:1b:194:PRO:HD2	2.01	0.42
35:1d:13:ARG:HB3	35:1d:38:TYR:O	2.20	0.42
43:1l:42:THR:HA	43:1l:53:ARG:O	2.20	0.42
1:2A:35:G:H2'	1:2A:36:G:O4'	2.20	0.42
1:2A:262:A:H2'	1:2A:263:C:O4'	2.19	0.42
1:2A:1027:A:C6	1:2A:1126:A:C4	3.08	0.42
1:2A:1641:A:H2'	1:2A:1642:G:O4'	2.20	0.42
1:2A:2115:G:O2'	1:2A:2117:A:N7	2.29	0.42
3:2D:121:PRO:HB3	3:2D:135:PHE:CE2	2.55	0.42
32:2a:491:G:H2'	32:2a:492:G:O4'	2.20	0.42
32:2a:1004:A:N1	32:2a:1037:C:C2	2.88	0.42
33:2b:57:PHE:CD2	33:2b:185:ILE:HG21	2.54	0.42
33:2b:118:LEU:HD21	33:2b:138:LEU:HB3	2.02	0.42
34:2c:144:SER:C	34:2c:146:ALA:H	2.28	0.42
51:2t:59:ALA:O	51:2t:63:ILE:HG13	2.19	0.42
1:1A:1085:A:C6	1:1A:1086:A:C8	3.08	0.42
1:1A:1092:C:H2'	1:1A:1093:G:H5'	2.01	0.42
1:1A:1937:A:H1'	1:1A:1939:5MU:H72	2.02	0.42
1:1A:2189:U:H5'	1:1A:2190:G:OP2	2.20	0.42
1:1A:2366:A:H2'	1:1A:2367:G:O4'	2.20	0.42
1:1A:2648:C:H2'	1:1A:2649:U:C6	2.55	0.42
6:1G:116:ASP:OD2	44:1m:68:GLY:HA3	2.19	0.42
11:1P:18:ARG:NE	62:1P:304:HOH:O	2.53	0.42
32:1a:44:G:H2'	32:1a:45:U:O4'	2.20	0.42
32:1a:109:A:C6	32:1a:326:G:C6	3.07	0.42
32:1a:295:C:H2'	32:1a:296:U:O4'	2.20	0.42
32:1a:532:A:N6	32:1a:1206:G:O2'	2.53	0.42
32:1a:1101:A:H4'	32:1a:1102:A:O5'	2.20	0.42
32:1a:1261:A:H3'	32:1a:1262:C:H6	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1c:12:LEU:HA	34:1c:12:LEU:HD23	1.77	0.42
41:1j:31:GLY:HA3	41:1j:32:ALA:HA	1.87	0.42
1:2A:65:C:O2'	1:2A:456:C:N3	2.51	0.42
1:2A:731:C:H5''	62:2A:3846:HOH:O	2.18	0.42
1:2A:1514:U:H2'	1:2A:1515:G:H8	1.85	0.42
1:2A:1912:A:O2'	32:2a:1494:G:O2'	2.33	0.42
1:2A:1957:C:H2'	1:2A:1958:C:C6	2.54	0.42
1:2A:2741:A:H2'	1:2A:2742:C:O4'	2.19	0.42
2:2B:83:G:N1	2:2B:94:C:N3	2.43	0.42
6:2G:125:PHE:CE1	6:2G:131:TYR:HB2	2.55	0.42
11:2P:135:LEU:HD23	11:2P:135:LEU:HA	1.80	0.42
18:2W:12:ILE:O	18:2W:101:SER:OG	2.33	0.42
21:2Z:138:GLU:H	21:2Z:156:LYS:HZ3	1.67	0.42
32:2a:157:G:H2'	32:2a:158:G:C8	2.54	0.42
32:2a:630:G:H2'	32:2a:631:G:H8	1.85	0.42
32:2a:750:G:N3	46:2o:23:GLY:HA3	2.35	0.42
32:2a:772:U:H2'	32:2a:773:G:O4'	2.20	0.42
32:2a:957:U:O2'	32:2a:959:A:N7	2.49	0.42
34:2c:118:GLN:HA	34:2c:121:ALA:HB3	2.02	0.42
34:2c:119:ARG:HE	34:2c:140:ARG:NH2	2.18	0.42
34:2c:154:SER:HB3	34:2c:197:GLY:HA3	2.02	0.42
39:2h:60:ARG:HG2	39:2h:62:TYR:CZ	2.55	0.42
51:2t:67:ALA:HA	51:2t:72:LEU:O	2.19	0.42
2:1B:66:A:N6	2:1B:108:U:H2'	2.34	0.42
8:1I:12:LEU:HA	8:1I:12:LEU:HD23	1.80	0.42
10:1O:4:PRO:O	10:1O:5:GLN:HB2	2.20	0.42
20:1Y:92:ASN:CG	20:1Y:94:LYS:HG2	2.45	0.42
24:12:44:LEU:HD12	24:12:44:LEU:HA	1.94	0.42
27:15:20:ARG:C	27:15:22:HIS:H	2.28	0.42
32:1a:343:U:O2'	32:1a:344:A:H2'	2.19	0.42
32:1a:616:G:O2'	32:1a:617:G:H5'	2.20	0.42
32:1a:950:U:H2'	32:1a:951:G:C8	2.55	0.42
32:1a:1112:C:H1'	34:1c:179:ARG:HH11	1.84	0.42
36:1e:27:ARG:NH1	36:1e:27:ARG:HB2	2.35	0.42
37:1f:99:ALA:HB3	49:1r:29:PHE:CE1	2.55	0.42
41:1j:65:LEU:HB2	45:1n:56:VAL:HG12	2.02	0.42
1:2A:71:A:H5''	1:2A:73:A:C8	2.55	0.42
1:2A:97:C:OP1	24:22:2:LYS:NZ	2.51	0.42
1:2A:171:G:H2'	1:2A:172:C:C6	2.54	0.42
1:2A:880:G:N1	1:2A:898:C:O2	2.53	0.42
1:2A:1420:U:HO2'	1:2A:1421:G:P	2.39	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1628:G:H2'	1:2A:1629:U:C6	2.55	0.42
1:2A:1647:G:P	1:2A:1647:G:H3'	2.60	0.42
1:2A:1710:C:H5'	1:2A:2859:G:H1'	2.02	0.42
1:2A:2298:A:N6	1:2A:2299:G:N3	2.68	0.42
1:2A:2758:A:C4	7:2H:67:LEU:HD21	2.55	0.42
5:2F:139:PHE:CG	5:2F:167:ALA:HB2	2.55	0.42
8:2I:129:THR:HG22	8:2I:139:GLN:HG3	2.02	0.42
11:2P:97:PRO:HD3	11:2P:126:VAL:O	2.20	0.42
20:2Y:5:MET:HG2	20:2Y:30:VAL:HG11	2.01	0.42
23:21:40:ARG:NH2	23:21:42:GLN:HG2	2.35	0.42
32:2a:196:A:OP1	51:2t:68:LYS:NZ	2.41	0.42
32:2a:949:A:C6	32:2a:950:U:C4	3.08	0.42
32:2a:1004:A:N6	32:2a:1037:C:H1'	2.35	0.42
32:2a:1026:G:H5'	32:2a:1027:C:O5'	2.19	0.42
32:2a:1330:U:H4'	44:2m:23:TYR:CE2	2.54	0.42
32:2a:1509:C:H2'	32:2a:1510:U:O4'	2.19	0.42
32:2a:1528:U:O3'	32:2a:1529:G:H3'	2.19	0.42
33:2b:8:LYS:HB3	33:2b:217:ARG:HG3	2.02	0.42
35:2d:109:GLY:HA3	35:2d:165:MET:HG3	2.01	0.42
40:2i:9:ARG:HG2	40:2i:14:VAL:HA	2.01	0.42
42:2k:79:SER:OG	42:2k:106:LYS:NZ	2.53	0.42
45:2n:50:LYS:HG3	45:2n:52:GLN:HG3	2.01	0.42
51:2t:13:LEU:O	51:2t:17:ARG:HG2	2.20	0.42
54:2w:24:G:H2'	54:2w:25:C:O4'	2.20	0.42
54:2w:33:U:N3	54:2w:36:A:OP2	2.52	0.42
1:1A:214:G:O2'	1:1A:216:A:O3'	2.38	0.41
1:1A:1062:G:H22	1:1A:1077:A:H61	1.66	0.41
1:1A:1913:A:H4'	1:1A:1914:C:H5''	2.01	0.41
1:1A:2235:G:N7	62:1A:4342:HOH:O	2.37	0.41
1:1A:2285:C:OP2	28:16:6:ARG:NH2	2.42	0.41
1:1A:2820:A:OP2	13:1R:2:ARG:NH2	2.53	0.41
4:1E:101:ARG:CZ	4:1E:171:GLU:HB2	2.50	0.41
5:1F:14:PRO:HD2	5:1F:127:GLU:OE1	2.20	0.41
7:1H:154:PRO:HB3	7:1H:163:TYR:CE1	2.54	0.41
8:1I:27:ARG:HD3	23:11:71:TYR:CE2	2.55	0.41
32:1a:265:G:H5'	48:1q:64:PRO:O	2.20	0.41
32:1a:865:A:H2	32:1a:918:A:H4'	1.85	0.41
32:1a:955:U:O2'	50:1s:83:HIS:HD2	2.03	0.41
32:1a:1134:G:H5'	32:1a:1135:U:OP2	2.19	0.41
32:1a:1144:G:H21	32:1a:1146:A:H62	1.68	0.41
36:1e:31:LEU:HD23	36:1e:31:LEU:HA	1.89	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:1r:33:ASP:OD2	49:1r:36:ASN:HB2	2.19	0.41
51:1t:59:ALA:O	51:1t:63:ILE:HG13	2.20	0.41
51:1t:100:ILE:HB	51:1t:101:GLY:H	1.70	0.41
11:2P:90:ARG:NH1	11:2P:105:LEU:HD11	2.35	0.41
15:2T:94:ALA:HB1	15:2T:99:LEU:HD21	2.01	0.41
15:2T:107:ASP:O	15:2T:111:ARG:HG3	2.20	0.41
19:2X:60:ARG:NH2	29:27:47:ARG:HH22	2.17	0.41
32:2a:389:A:H2'	32:2a:389:A:N3	2.34	0.41
32:2a:741:G:H2'	32:2a:742:G:O4'	2.20	0.41
32:2a:940:C:H2'	32:2a:941:G:C8	2.54	0.41
33:2b:57:PHE:HD2	33:2b:58:ILE:HD13	1.85	0.41
33:2b:98:LEU:HD13	33:2b:101:MET:HE3	2.02	0.41
34:2c:20:SER:HB3	34:2c:22:TRP:NE1	2.30	0.41
34:2c:122:GLU:HA	34:2c:125:GLU:HG2	2.02	0.41
36:2e:86:ALA:HB3	36:2e:130:ASN:ND2	2.35	0.41
43:2l:57:LYS:HG2	43:2l:67:THR:HG22	2.02	0.41
43:2l:117:ARG:HB3	43:2l:122:THR:HB	2.02	0.41
51:2t:46:GLU:H	51:2t:46:GLU:HG3	1.73	0.41
56:2y:68:C:H2'	56:2y:69:G:O4'	2.18	0.41
1:1A:484:C:H2'	1:1A:485:C:C6	2.55	0.41
1:1A:747:U:O2	1:1A:2014:A:H1'	2.19	0.41
1:1A:1072:C:H5''	1:1A:1073:A:OP1	2.20	0.41
1:1A:1093:G:H3'	1:1A:1094:U:H5''	2.01	0.41
1:1A:2052:G:H4'	4:1E:143:ASN:O	2.21	0.41
1:1A:2422:A:O4'	56:1y:76:A:N6	2.53	0.41
6:1G:179:PRO:HG3	26:14:43:TYR:OH	2.20	0.41
7:1H:24:VAL:HG11	7:1H:43:VAL:HG21	2.02	0.41
8:1I:9:LEU:HA	8:1I:9:LEU:HD12	1.77	0.41
11:1P:38:GLN:O	11:1P:40:SER:N	2.46	0.41
21:1Z:101:PRO:HA	21:1Z:123:ASP:HB3	2.02	0.41
32:1a:19:C:H2'	32:1a:20:U:C6	2.55	0.41
32:1a:92:C:H2'	32:1a:93:G:H8	1.85	0.41
32:1a:737:A:H2'	32:1a:738:C:H6	1.85	0.41
32:1a:924:C:H2'	32:1a:925:G:C8	2.55	0.41
32:1a:1158:C:C2	32:1a:1160:G:C8	3.08	0.41
32:1a:1511:G:H2'	32:1a:1512:U:O4'	2.20	0.41
33:1b:189:ASP:HB3	33:1b:203:GLY:O	2.21	0.41
48:1q:45:HIS:CD2	48:1q:65:ILE:HG21	2.55	0.41
56:1y:54:5MU:OP2	56:1y:54:5MU:H71	2.20	0.41
1:2A:744:G:OP1	4:2E:132:HIS:ND1	2.53	0.41
1:2A:864:G:OP2	12:2Q:22:LYS:HE3	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:867:C:H2'	1:2A:868:U:H6	1.85	0.41
1:2A:988:A:N7	62:2A:3923:HOH:O	2.37	0.41
1:2A:1469:A:H2'	1:2A:1470:G:O4'	2.20	0.41
1:2A:2439:A:N6	55:2x:76:31H:OP1	2.53	0.41
8:2I:117:GLU:CD	8:2I:118:LYS:H	2.28	0.41
10:2O:66:LYS:N	10:2O:82:ASN:OD1	2.47	0.41
21:2Z:98:MET:N	21:2Z:126:VAL:O	2.51	0.41
27:25:51:TYR:CE2	27:25:56:LYS:HD2	2.55	0.41
32:2a:433:C:H2'	32:2a:434:U:H6	1.85	0.41
32:2a:952:U:H2'	32:2a:953:G:C8	2.56	0.41
32:2a:1029:C:N4	32:2a:1032:G:C6	2.88	0.41
32:2a:1296:C:H5''	44:2m:44:ARG:HH22	1.84	0.41
33:2b:126:GLU:H	33:2b:126:GLU:CD	2.26	0.41
35:2d:18:LYS:HE3	35:2d:26:CYS:O	2.20	0.41
37:2f:69:GLU:CD	37:2f:69:GLU:H	2.24	0.41
41:2j:17:ASP:OD2	41:2j:70:ARG:NE	2.52	0.41
1:1A:278:A:H2'	1:1A:279:C:C6	2.55	0.41
1:1A:530:G:N1	1:1A:2023:G:OP1	2.36	0.41
1:1A:1477:A:C2	1:1A:1515:G:C2	3.09	0.41
1:1A:2119:A:O2'	1:1A:2120:G:H5''	2.20	0.41
5:1F:164:ARG:O	5:1F:168:ARG:HB3	2.21	0.41
32:1a:1489:G:H2'	32:1a:1490:C:O4'	2.20	0.41
33:1b:78:GLN:HE21	33:1b:95:GLN:HA	1.86	0.41
56:1y:24:G:H2'	56:1y:25:C:C6	2.55	0.41
1:2A:211:A:H2'	1:2A:212:G:O4'	2.20	0.41
1:2A:856:C:HO2'	1:2A:857:C:P	2.43	0.41
1:2A:1783:A:H5'	1:2A:2608:G:H4'	2.03	0.41
7:2H:20:ALA:HB1	7:2H:21:PRO:HD2	2.01	0.41
8:2I:84:GLY:C	8:2I:86:THR:H	2.28	0.41
16:2U:16:LYS:HB3	16:2U:16:LYS:HE2	1.79	0.41
19:2X:60:ARG:NH2	29:27:47:ARG:HH12	2.19	0.41
32:2a:429:U:O3'	35:2d:22:LYS:NZ	2.53	0.41
32:2a:495:A:H1'	32:2a:496:A:H5''	2.00	0.41
32:2a:971:G:OP1	32:2a:971:G:H3'	2.21	0.41
32:2a:1123:A:N3	41:2j:39:PRO:HD2	2.35	0.41
32:2a:1254:C:O4'	32:2a:1356:G:H5''	2.20	0.41
32:2a:1267:C:N3	32:2a:1327:C:H4'	2.35	0.41
34:2c:186:PHE:HZ	34:2c:188:LEU:HD13	1.85	0.41
37:2f:61:LEU:HD13	37:2f:63:TYR:OH	2.20	0.41
38:2g:111:ARG:HB3	38:2g:113:GLU:OE1	2.20	0.41
54:2w:50:U:C2	54:2w:65:G:C2	3.07	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:370:G:H8	1:1A:370:G:OP2	2.03	0.41
1:1A:582:G:H2'	1:1A:583:G:C8	2.56	0.41
1:1A:1359:A:N3	1:1A:1359:A:H5'	2.36	0.41
1:1A:2629:A:H1'	1:1A:2630:G:O5'	2.21	0.41
3:1D:35:LYS:HB2	3:1D:36:PRO:HD2	2.01	0.41
9:1N:4:TYR:CG	16:1U:100:VAL:HG11	2.56	0.41
32:1a:377:G:P	47:1p:5:ARG:HH11	2.43	0.41
32:1a:502:G:H2'	32:1a:503:C:O4'	2.20	0.41
32:1a:646:U:H2'	32:1a:647:C:C6	2.56	0.41
33:1b:48:MET:HE2	33:1b:48:MET:HB3	1.87	0.41
36:1e:78:HIS:HE1	36:1e:142:LEU:HA	1.85	0.41
54:1w:48:C:C2	54:1w:59:U:H1'	2.56	0.41
1:2A:848:G:C2	1:2A:933:A:H1'	2.56	0.41
1:2A:1266:G:O2'	1:2A:2012:G:O6	2.35	0.41
1:2A:1778:U:H2'	1:2A:1784:A:N6	2.36	0.41
1:2A:2334:G:H4'	1:2A:2335:A:OP2	2.21	0.41
4:2E:72:VAL:HG12	4:2E:73:GLU:O	2.20	0.41
5:2F:11:VAL:HG22	5:2F:125:LEU:HD12	2.01	0.41
6:2G:103:LEU:O	6:2G:107:LEU:HG	2.20	0.41
8:2I:110:ASP:H	8:2I:130:TYR:HE1	1.69	0.41
12:2Q:1:MET:HG2	12:2Q:44:ALA:HB1	2.02	0.41
33:2b:118:LEU:O	33:2b:122:PHE:HB3	2.20	0.41
36:2e:57:LYS:O	36:2e:61:TYR:HD2	2.04	0.41
37:2f:12:PRO:HG3	37:2f:57:GLN:O	2.20	0.41
51:2t:58:LYS:HA	51:2t:58:LYS:HD2	1.75	0.41
1:1A:1292:U:H2'	1:1A:1293:C:C6	2.55	0.41
1:1A:2022:U:O2'	1:1A:2617:C:H5'	2.20	0.41
1:1A:2051:A:H5'	1:1A:2578:G:O4'	2.20	0.41
1:1A:2134:A:OP1	1:1A:2156:G:N2	2.54	0.41
1:1A:2272:U:H5''	1:1A:2273:A:OP1	2.21	0.41
1:1A:2573:C:OP1	62:1A:4229:HOH:O	2.22	0.41
4:1E:40:GLU:CD	4:1E:40:GLU:H	2.27	0.41
14:1S:11:LYS:HG3	14:1S:91:PRO:HD3	2.03	0.41
18:1W:62:HIS:O	18:1W:64:MET:HG3	2.20	0.41
24:12:31:GLU:O	24:12:35:LEU:HG	2.21	0.41
32:1a:119:A:H4'	32:1a:120:A:C8	2.55	0.41
32:1a:266:G:N3	32:1a:266:G:H5''	2.35	0.41
32:1a:473:G:OP2	47:1p:75:ARG:NH1	2.53	0.41
32:1a:1029:C:H41	32:1a:1030(A):G:N2	2.18	0.41
33:1b:93:VAL:HG11	33:1b:97:TRP:CD1	2.55	0.41
34:1c:6:HIS:HA	34:1c:7:PRO:HD3	1.96	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:1s:80:TYR:CZ	50:1s:82:GLY:HA2	2.55	0.41
1:2A:577:G:O2'	1:2A:1254:A:OP1	2.34	0.41
1:2A:606:U:H4'	1:2A:658:C:H4'	2.03	0.41
1:2A:925:C:H2'	1:2A:926:A:C8	2.49	0.41
1:2A:2232:U:P	23:21:40:ARG:HH12	2.42	0.41
3:2D:159:ALA:HB1	3:2D:198:ASN:O	2.19	0.41
9:2N:9:VAL:HG11	9:2N:39:ARG:NH2	2.35	0.41
10:2O:2:ILE:HB	10:2O:33:ALA:HB3	2.02	0.41
12:2Q:81:VAL:HB	22:20:7:LEU:HD21	2.03	0.41
17:2V:60:GLU:CB	17:2V:97:LYS:HE2	2.49	0.41
32:2a:582:U:C2	32:2a:760:G:C6	3.09	0.41
32:2a:997:U:H3	32:2a:1044:A:N6	2.16	0.41
32:2a:1094:G:O2'	32:2a:1108:G:N2	2.54	0.41
32:2a:1249:C:O4'	40:2i:70:LYS:HE3	2.20	0.41
32:2a:1250:A:H4'	40:2i:68:GLY:N	2.36	0.41
33:2b:67:THR:HB	33:2b:159:PRO:HA	2.02	0.41
33:2b:71:VAL:O	33:2b:164:VAL:HG12	2.20	0.41
40:2i:65:VAL:HG21	40:2i:73:GLN:HB3	2.03	0.41
44:2m:123:ALA:HB2	54:2w:39:PSU:O4'	2.19	0.41
1:1A:764:A:H5'	3:1D:210:GLY:CA	2.50	0.41
1:1A:1028:A:H61	1:1A:1125:G:H2'	1.83	0.41
1:1A:1056:G:H1'	1:1A:1103:A:H61	1.85	0.41
1:1A:1173:G:O2'	1:1A:1174:A:O4'	2.33	0.41
1:1A:1240:U:H3'	62:1A:5761:HOH:O	2.21	0.41
1:1A:1482:G:H2'	1:1A:1484:G:C8	2.53	0.41
1:1A:1547:C:H2'	1:1A:1548:C:H6	1.86	0.41
1:1A:2134:A:N3	1:1A:2159:G:O2'	2.34	0.41
7:1H:144:VAL:O	7:1H:148:ILE:HG13	2.21	0.41
30:18:52:LYS:N	30:18:53:PRO:HD2	2.36	0.41
32:1a:9:G:C6	32:1a:26:A:N6	2.89	0.41
32:1a:431:A:H2'	32:1a:432:A:O4'	2.21	0.41
32:1a:967:5MC:H4'	40:1i:125:TYR:HE1	1.85	0.41
33:1b:133:LYS:O	33:1b:136:VAL:HG22	2.20	0.41
35:1d:182:LYS:HB2	35:1d:182:LYS:HE3	1.84	0.41
37:1f:91:VAL:HG11	49:1r:72:ARG:NH1	2.36	0.41
47:1p:60:LEU:HD12	47:1p:60:LEU:HA	1.81	0.41
48:1q:14:LYS:H	48:1q:14:LYS:HG2	1.56	0.41
1:2A:322:A:OP1	5:2F:168:ARG:HD2	2.20	0.41
1:2A:2286:A:H4'	1:2A:2287:A:O4'	2.21	0.41
1:2A:2503:2MA:H4'	1:2A:2504:U:OP1	2.20	0.41
4:2E:4:ILE:HD11	4:2E:29:GLY:HA2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2F:39:TRP:NE1	5:2F:99:TYR:O	2.51	0.41
5:2F:40:GLN:HE22	5:2F:184:TYR:H	1.69	0.41
17:2V:1:MET:HE2	17:2V:43:GLU:H	1.85	0.41
25:23:5:LYS:NZ	25:23:34:GLU:OE2	2.52	0.41
26:24:9:LEU:HD23	26:24:9:LEU:HA	1.87	0.41
32:2a:158:G:C2'	32:2a:159:G:H5'	2.50	0.41
32:2a:629:G:H2'	32:2a:630:G:O4'	2.21	0.41
32:2a:664:G:P	49:2r:64:ARG:HH21	2.42	0.41
32:2a:1517:G:N7	32:2a:1518:MA6:H103	2.35	0.41
33:2b:84:GLU:O	33:2b:219:VAL:HG21	2.21	0.41
33:2b:118:LEU:HD23	33:2b:142:LEU:HB2	2.02	0.41
33:2b:144:ARG:HA	33:2b:144:ARG:HD2	1.80	0.41
37:2f:24:GLU:O	37:2f:28:ARG:N	2.40	0.41
42:2k:66:LEU:O	42:2k:70:LYS:HG3	2.21	0.41
51:2t:75:ASN:HD22	51:2t:75:ASN:N	2.18	0.41
56:2y:14:A:N6	56:2y:21:A:H2	2.17	0.41
1:1A:607:U:OP1	5:1F:102:PRO:HA	2.21	0.41
1:1A:1083:U:N3	1:1A:1085:A:H5''	2.35	0.41
1:1A:1647:G:P	1:1A:1647:G:H3'	2.59	0.41
1:1A:2334:G:H4'	1:1A:2335:A:OP2	2.21	0.41
1:1A:2359:C:H2'	1:1A:2360:A:O4'	2.21	0.41
7:1H:45:VAL:HA	7:1H:50:VAL:HG12	2.01	0.41
15:1T:24:PRO:HD3	15:1T:52:ILE:HD12	2.03	0.41
20:1Y:5:MET:HG2	20:1Y:30:VAL:HG11	2.03	0.41
31:19:32:HIS:O	31:19:34:GLN:HG3	2.21	0.41
32:1a:279:A:N6	48:1q:98:LEU:HB2	2.35	0.41
32:1a:280:C:N3	48:1q:38:ARG:HA	2.35	0.41
32:1a:582:U:H2'	32:1a:583:A:C8	2.56	0.41
32:1a:1160:G:H22	32:1a:1176:A:H2	1.68	0.41
34:1c:87:LEU:O	34:1c:91:LEU:HB2	2.20	0.41
1:2A:748:G:C8	18:2W:89:ALA:HB1	2.55	0.41
1:2A:796:C:H2'	1:2A:797:C:C6	2.56	0.41
1:2A:1178:C:H2'	1:2A:1179:C:C6	2.55	0.41
1:2A:1843:C:H5'	3:2D:253:GLN:OE1	2.21	0.41
2:2B:3:C:H2'	2:2B:4:C:H6	1.83	0.41
3:2D:239:ARG:NH1	62:2D:406:HOH:O	2.48	0.41
7:2H:102:ALA:HB2	7:2H:116:GLU:HG3	2.03	0.41
10:2O:98:VAL:O	10:2O:119:PRO:HD3	2.21	0.41
22:20:72:ARG:HB2	22:20:75:LEU:HB2	2.03	0.41
31:29:29:ASN:HB3	31:29:32:HIS:ND1	2.35	0.41
32:2a:15:G:H2'	32:2a:16:A:O4'	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:64:G:C4'	32:2a:65:U:H3'	2.45	0.41
32:2a:390:C:H2'	32:2a:391:G:C8	2.56	0.41
32:2a:431:A:H2'	32:2a:432:A:C8	2.55	0.41
32:2a:762:C:H2'	32:2a:763:G:C8	2.56	0.41
32:2a:857:C:H2'	32:2a:858:G:O4'	2.19	0.41
32:2a:971:G:H1'	32:2a:1365:G:O2'	2.20	0.41
32:2a:1009:G:N2	32:2a:1021:G:H1'	2.36	0.41
33:2b:19:HIS:HB2	33:2b:204:ASN:HB2	2.02	0.41
33:2b:139:LYS:O	33:2b:143:GLU:HB2	2.21	0.41
33:2b:167:PRO:HG2	33:2b:192:SER:HB3	2.01	0.41
44:2m:94:ARG:HG2	44:2m:96:LEU:HD21	2.03	0.41
51:2t:68:LYS:HE2	51:2t:68:LYS:HB3	1.77	0.41
1:1A:910:A:N3	1:1A:2264:C:O2'	2.44	0.41
1:1A:1266:G:O2'	1:1A:2012:G:O6	2.36	0.41
1:1A:1570:A:H2'	1:1A:1571:A:C8	2.56	0.41
1:1A:2065:C:H2'	1:1A:2066:C:C6	2.55	0.41
1:1A:2846:G:H2'	1:1A:2847:U:O4'	2.21	0.41
8:1I:92:VAL:HG22	8:1I:120:ILE:HD12	2.02	0.41
11:1P:89:ALA:HA	11:1P:121:LYS:HE2	2.03	0.41
14:1S:71:ARG:NH1	14:1S:107:GLU:OE2	2.51	0.41
16:1U:46:ALA:O	16:1U:50:ARG:HG2	2.21	0.41
28:16:18:ARG:HD2	28:16:42:TRP:CG	2.55	0.41
32:1a:736:C:H2'	32:1a:737:A:H8	1.86	0.41
32:1a:1075:C:OP1	33:1b:179:LYS:NZ	2.53	0.41
32:1a:1079:G:C6	32:1a:1080:A:N6	2.88	0.41
32:1a:1346:A:C2'	38:1g:10:ARG:HH22	2.34	0.41
32:1a:1525:G:OP1	42:1k:120:ARG:NH2	2.54	0.41
33:1b:16:HIS:HB3	33:1b:210:SER:HB2	2.03	0.41
33:1b:122:PHE:HD1	33:1b:122:PHE:HA	1.75	0.41
48:1q:83:ASP:OD1	48:1q:83:ASP:N	2.52	0.41
48:1q:86:GLU:O	48:1q:90:ILE:HG13	2.20	0.41
56:1y:19:G:N1	56:1y:56:C:N4	2.65	0.41
1:2A:489:G:H2'	1:2A:491:G:O4'	2.20	0.41
1:2A:819:A:C4	1:2A:1189:A:C2	3.09	0.41
1:2A:1003:G:N2	1:2A:1153:C:C2	2.88	0.41
1:2A:1011:G:OP2	16:2U:66:ASN:ND2	2.50	0.41
1:2A:2543:G:H2'	1:2A:2544:G:C8	2.56	0.41
1:2A:2567:G:H2'	1:2A:2568:C:C6	2.55	0.41
1:2A:2722:G:H2'	1:2A:2723:C:C6	2.55	0.41
2:2B:60:C:H2'	2:2B:61:G:C8	2.56	0.41
5:2F:116:ASP:O	5:2F:120:GLU:HG2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:2I:2:LYS:HA	8:2I:20:ASP:HA	2.03	0.41
32:2a:521:G:H4'	43:2I:73:GLU:HG2	2.03	0.41
32:2a:1058:G:H1	32:2a:1199:U:H3	1.69	0.41
32:2a:1235:U:O2'	32:2a:1305:G:O5'	2.39	0.41
32:2a:1512:U:H2'	32:2a:1513:A:C8	2.56	0.41
33:2b:165:VAL:HA	33:2b:187:LEU:HB3	2.02	0.41
36:2e:43:LEU:HD22	36:2e:136:MET:HG3	2.03	0.41
40:2i:15:ALA:CB	40:2i:65:VAL:HG23	2.47	0.41
44:2m:29:ARG:HD3	44:2m:64:TRP:CE2	2.56	0.41
51:2t:90:GLN:HE21	51:2t:90:GLN:HB3	1.75	0.41
1:1A:718:A:H3'	1:1A:719:C:H6	1.85	0.41
1:1A:1060:U:H3	1:1A:1088:A:H8	1.60	0.41
1:1A:1064:C:H2'	1:1A:1065:U:H5'	2.03	0.41
1:1A:2803:C:H2'	1:1A:2804:C:C6	2.56	0.41
4:1E:9:VAL:HG22	4:1E:25:VAL:HB	2.02	0.41
6:1G:4:ASP:OD2	6:1G:9:ARG:NH1	2.52	0.41
6:1G:25:TYR:CZ	6:1G:32:PRO:HD3	2.56	0.41
6:1G:155:MET:HE2	6:1G:155:MET:HB3	2.00	0.41
8:1I:124:GLY:H	8:1I:144:VAL:HG23	1.84	0.41
12:1Q:10:ARG:HH11	12:1Q:11:LYS:HE3	1.86	0.41
12:1Q:82:ARG:NH2	22:10:4:LYS:HG3	2.35	0.41
14:1S:37:ALA:HB3	14:1S:73:LEU:HD13	2.02	0.41
32:1a:19:C:H2'	32:1a:20:U:H6	1.85	0.41
32:1a:189(D):C:H2'	32:1a:189(E):U:O4'	2.20	0.41
32:1a:977:A:H1'	32:1a:982:U:O4	2.21	0.41
32:1a:1027:C:H5	32:1a:1028:C:C4	2.39	0.41
32:1a:1060:C:OP1	45:1n:45:ARG:NH2	2.51	0.41
32:1a:1273:G:H3'	32:1a:1274:G:C8	2.54	0.41
33:1b:21:ARG:O	33:1b:23:ARG:HG2	2.21	0.41
33:1b:162:ILE:O	33:1b:185:ILE:HG12	2.21	0.41
34:1c:22:TRP:NE1	34:1c:59:ARG:HD2	2.36	0.41
34:1c:110:ASN:OD1	34:1c:110:ASN:N	2.54	0.41
35:1d:125:HIS:HD2	35:1d:152:SER:OG	2.03	0.41
38:1g:31:MET:HG3	38:1g:36:LYS:HA	2.02	0.41
38:1g:113:GLU:H	38:1g:113:GLU:HG2	1.59	0.41
41:1j:5:ARG:HE	41:1j:5:ARG:HB2	1.72	0.41
51:1t:18:GLN:O	51:1t:22:ARG:HG3	2.20	0.41
1:2A:21:A:H2'	1:2A:22:C:O4'	2.21	0.41
1:2A:443:A:H5''	1:2A:444:C:OP1	2.21	0.41
1:2A:448:U:O4	1:2A:583:G:H1'	2.21	0.41
1:2A:721:C:H2'	1:2A:722:A:C8	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:999:U:O2'	1:2A:1000:A:H5'	2.21	0.41
1:2A:1450:G:H1	1:2A:1462:C:N4	2.17	0.41
1:2A:1450:G:H2'	1:2A:1450(A):C:H6	1.86	0.41
1:2A:1502:C:H2'	1:2A:1503:U:C6	2.54	0.41
1:2A:1546:C:H5'	1:2A:1547:C:O5'	2.21	0.41
1:2A:2116:G:H8	1:2A:2166:G:H22	1.68	0.41
1:2A:2180:U:H2'	1:2A:2181:G:O4'	2.21	0.41
1:2A:2218:U:N3	23:21:55:GLY:O	2.54	0.41
1:2A:2526:G:H5'	1:2A:2742:C:O2'	2.20	0.41
1:2A:2732:G:OP1	4:2E:203:LYS:NZ	2.40	0.41
1:2A:2831:G:OP1	1:2A:2834:G:H4'	2.21	0.41
2:2B:29:A:P	14:2S:32:LEU:HG	2.60	0.41
8:2I:62:LYS:HB2	8:2I:133:HIS:CE1	2.56	0.41
10:2O:26:LYS:O	10:2O:30:ALA:HB2	2.21	0.41
11:2P:2:LYS:HG2	11:2P:3:LEU:N	2.36	0.41
14:2S:77:ALA:O	14:2S:81:GLY:N	2.32	0.41
27:25:20:ARG:C	27:25:22:HIS:H	2.29	0.41
30:28:11:LYS:HA	30:28:11:LYS:HD2	1.92	0.41
32:2a:64:G:H4'	32:2a:65:U:C3'	2.46	0.41
32:2a:434:U:H2'	32:2a:435:C:C6	2.56	0.41
32:2a:448:A:OP2	32:2a:485:G:N1	2.49	0.41
32:2a:631:G:H2'	32:2a:632:A:C8	2.56	0.41
32:2a:791:G:C6	32:2a:792:A:N7	2.89	0.41
32:2a:826:C:H2'	32:2a:827:U:C6	2.56	0.41
32:2a:918:A:H2'	32:2a:919:A:C8	2.55	0.41
32:2a:1064:G:O6	32:2a:1191:A:N6	2.53	0.41
32:2a:1349:A:C4	32:2a:1350:A:C8	3.09	0.41
32:2a:1401:G:H2'	32:2a:1402:4OC:O4'	2.21	0.41
33:2b:92:TYR:N	33:2b:151:GLY:O	2.39	0.41
34:2c:40:ARG:HE	34:2c:55:VAL:HG22	1.86	0.41
34:2c:85:ARG:CZ	34:2c:85:ARG:HB3	2.51	0.41
34:2c:148:GLY:HA3	34:2c:203:PHE:HB3	2.02	0.41
37:2f:14:LEU:HD22	37:2f:18:GLN:HB3	2.03	0.41
40:2i:4:TYR:O	40:2i:18:PHE:HA	2.20	0.41
45:2n:22:THR:HG23	45:2n:33:VAL:HG21	2.03	0.41
47:2p:59:TRP:HB3	47:2p:64:ALA:CB	2.51	0.41
48:2q:66:SER:O	48:2q:70:ARG:NH1	2.52	0.41
49:2r:53:ARG:HA	49:2r:56:THR:OG1	2.20	0.41
50:2s:18:LYS:HD3	50:2s:31:ILE:HG12	2.03	0.41
50:2s:20:LEU:HD23	50:2s:23:ASN:ND2	2.36	0.41
50:2s:32:LYS:HG2	50:2s:50:ALA:HB3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:396:G:H1'	23:11:42:GLN:HB3	2.03	0.41
1:1A:2646:C:OP2	1:1A:2732:G:O2'	2.30	0.41
9:1N:12:ARG:HB3	9:1N:50:ASP:OD1	2.21	0.41
9:1N:67:LEU:HD12	9:1N:67:LEU:HA	1.80	0.41
12:1Q:12:GLN:NE2	12:1Q:72:LYS:HG3	2.36	0.41
21:1Z:3:TYR:CE2	21:1Z:51:ALA:HB2	2.56	0.41
22:10:82:ARG:HA	22:10:83:PRO:HD3	1.94	0.41
26:14:49:PHE:HD1	26:14:49:PHE:HA	1.75	0.41
32:1a:1134:G:N3	32:1a:1134:G:H2'	2.36	0.41
35:1d:63:LYS:HB2	35:1d:63:LYS:HE3	1.87	0.41
36:1e:31:LEU:HD11	36:1e:129:ILE:HA	2.03	0.41
36:1e:91:LEU:HB3	36:1e:118:ILE:HD11	2.02	0.41
39:1h:81:HIS:HB2	39:1h:138:TRP:CD1	2.55	0.41
41:1j:46:ARG:HH11	41:1j:46:ARG:HB2	1.86	0.41
42:1k:84:VAL:HG11	42:1k:91:ARG:HD2	2.02	0.41
1:2A:230:U:H2'	1:2A:231:C:C6	2.56	0.41
1:2A:1518:U:H2'	1:2A:1519:G:O4'	2.21	0.41
1:2A:1529:G:O6	1:2A:1530:C:N4	2.53	0.41
1:2A:1639:U:H4'	1:2A:2699:C:H4'	2.03	0.41
1:2A:2584:U:H2'	1:2A:2585:U:C6	2.56	0.41
1:2A:2695:C:H2'	1:2A:2696:U:C6	2.56	0.41
14:2S:10:ARG:NH2	14:2S:91:PRO:HB2	2.34	0.41
31:29:20:HIS:O	31:29:22:ARG:N	2.52	0.41
32:2a:120:A:C6	32:2a:122:G:C2	3.09	0.41
32:2a:452:A:O2'	32:2a:453:A:OP2	2.25	0.41
32:2a:838:G:N2	32:2a:840:C:H5''	2.36	0.41
32:2a:1060:C:HO2'	41:2j:56:HIS:CG	2.36	0.41
32:2a:1103:C:C2	32:2a:1104:G:C8	3.09	0.41
32:2a:1287:A:H2'	32:2a:1288:A:C8	2.56	0.41
34:2c:129:ALA:HB3	34:2c:132:ARG:HD2	2.02	0.41
34:2c:150:LYS:HE3	34:2c:169:ALA:HB2	2.02	0.41
36:2e:34:VAL:HG12	36:2e:42:GLY:HA3	2.03	0.41
44:2m:17:VAL:HG12	44:2m:27:LYS:NZ	2.36	0.41
48:2q:66:SER:HB3	48:2q:69:LYS:HD3	2.03	0.41
55:2x:20:U:H4'	55:2x:21:A:OP1	2.21	0.41
1:1A:412:A:O5'	1:1A:412:A:H8	2.04	0.40
1:1A:764:A:O4'	3:1D:213:ARG:HG3	2.21	0.40
1:1A:2233:U:H2'	1:1A:2234:G:C8	2.56	0.40
2:1B:13:A:N1	2:1B:69:G:O2'	2.41	0.40
2:1B:33:G:C2	2:1B:50:G:C2	3.10	0.40
5:1F:135:LYS:HB3	5:1F:135:LYS:HE3	1.90	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1U:76:TYR:CE2	16:1U:80:ILE:HG13	2.56	0.40
20:1Y:11:ASP:HA	20:1Y:26:LYS:HZ2	1.86	0.40
21:1Z:146:ILE:HA	21:1Z:147:GLY:HA2	1.70	0.40
32:1a:418:C:H2'	32:1a:419:C:C6	2.57	0.40
32:1a:789:U:O2'	62:1a:1923:HOH:O	2.22	0.40
32:1a:1360:A:H8	32:1a:1360:A:OP1	2.04	0.40
39:1h:64:LYS:HD2	39:1h:79:VAL:HG21	2.03	0.40
43:1l:33:ARG:HE	43:1l:62:SER:HB3	1.86	0.40
47:1p:20:VAL:HG22	47:1p:34:GLU:O	2.20	0.40
1:2A:557:U:O2	9:2N:45:ASN:HB2	2.21	0.40
1:2A:900:A:HO2'	1:2A:901:A:P	2.44	0.40
1:2A:1754:C:OP1	15:2T:96:ARG:NH1	2.54	0.40
1:2A:2318:G:H21	14:2S:3:ARG:CZ	2.35	0.40
1:2A:2882:A:OP1	13:2R:96:ARG:NE	2.51	0.40
2:2B:41:U:O4	6:2G:70:VAL:HB	2.20	0.40
6:2G:125:PHE:HB3	6:2G:166:ASP:OD2	2.21	0.40
9:2N:67:LEU:O	9:2N:88:GLU:HG3	2.21	0.40
14:2S:16:ASN:HA	14:2S:19:LYS:HG3	2.03	0.40
14:2S:69:VAL:HG13	14:2S:101:LEU:HG	2.03	0.40
22:20:10:THR:HG22	22:20:12:ASN:H	1.85	0.40
24:22:22:GLU:OE2	24:22:68:ARG:NH2	2.55	0.40
25:23:46:ASN:O	25:23:50:VAL:HG22	2.21	0.40
27:25:57:VAL:HG12	27:25:58:LEU:HD13	2.03	0.40
32:2a:501:C:OP2	43:2l:124:LYS:NZ	2.34	0.40
32:2a:1157:A:H5'	32:2a:1158:C:C6	2.56	0.40
32:2a:1161:C:H2'	32:2a:1162:C:C6	2.56	0.40
32:2a:1179:A:H2'	32:2a:1180:A:O4'	2.21	0.40
33:2b:83:MET:HE2	33:2b:83:MET:HB3	1.80	0.40
33:2b:177:ALA:HB1	33:2b:182:ILE:O	2.21	0.40
36:2e:78:HIS:ND1	39:2h:104:ARG:HD2	2.36	0.40
38:2g:42:ILE:HD13	38:2g:116:ALA:HB3	2.03	0.40
1:1A:1914:C:H2'	1:1A:1915:5MU:O4'	2.22	0.40
1:1A:2029:G:OP2	62:1A:4257:HOH:O	2.22	0.40
1:1A:2110:G:C5	1:1A:2120:G:C8	3.09	0.40
1:1A:2139:C:H2'	1:1A:2140:C:O4'	2.21	0.40
1:1A:2327:A:H2'	1:1A:2328:A:C8	2.56	0.40
1:1A:2689:U:H4'	1:1A:2690:C:H5'	2.02	0.40
15:1T:127:ALA:O	15:1T:128:GLU:HB3	2.20	0.40
17:1V:34:GLU:HB3	17:1V:56:SER:OG	2.21	0.40
32:1a:186:C:H2'	32:1a:187:C:H6	1.84	0.40
32:1a:911:U:H2'	32:1a:912:C:C6	2.57	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1068:G:H8	32:1a:1068:G:OP2	2.03	0.40
35:1d:52:SER:O	35:1d:56:VAL:HG13	2.21	0.40
36:1e:41:VAL:O	36:1e:66:MET:HA	2.21	0.40
38:1g:50:ILE:HG13	38:1g:61:VAL:HG11	2.03	0.40
43:1l:7:ILE:O	43:1l:11:VAL:HG23	2.21	0.40
44:1m:66:LEU:O	44:1m:67:GLU:C	2.64	0.40
54:1w:18:G:HO2'	54:1w:57:G:H22	1.61	0.40
1:2A:105:C:H2'	1:2A:106:C:C6	2.56	0.40
1:2A:784:A:N6	3:2D:229:VAL:HG11	2.36	0.40
1:2A:918:A:O2'	2:2B:97:G:N2	2.48	0.40
1:2A:1512:U:H2'	1:2A:1513:C:H6	1.86	0.40
1:2A:2405:G:O2'	1:2A:2411:A:N6	2.50	0.40
6:2G:68:PRO:HB2	6:2G:90:LEU:HB3	2.03	0.40
7:2H:76:VAL:HA	7:2H:79:VAL:HG22	2.04	0.40
10:2O:25:LEU:HD12	10:2O:38:VAL:HG12	2.02	0.40
13:2R:72:ASP:HB3	13:2R:75:LEU:HB3	2.02	0.40
21:2Z:171:ILE:HD12	21:2Z:172:ALA:H	1.84	0.40
26:24:46:GLN:C	26:24:48:ARG:N	2.77	0.40
27:25:35:GLU:HG3	27:25:51:TYR:CD1	2.57	0.40
28:26:9:LEU:HA	28:26:54:ILE:HB	2.04	0.40
30:28:26:LYS:HG2	30:28:46:ARG:O	2.21	0.40
32:2a:37:U:H2'	32:2a:38:G:O4'	2.21	0.40
32:2a:266:G:H5''	32:2a:268:C:N4	2.32	0.40
32:2a:504:C:H1'	32:2a:510:A:C4	2.56	0.40
32:2a:612:C:O2	32:2a:629:G:N2	2.54	0.40
32:2a:780:A:H1'	32:2a:803:G:N2	2.36	0.40
34:2c:22:TRP:CZ2	45:2n:54:PRO:HG2	2.56	0.40
36:2e:43:LEU:HD13	36:2e:136:MET:HG2	2.02	0.40
44:2m:23:TYR:CE2	44:2m:70:LEU:HD22	2.57	0.40
44:2m:97:PRO:HB3	44:2m:101:GLN:HB2	2.02	0.40
51:2t:10:LEU:HD12	51:2t:10:LEU:HA	1.91	0.40
1:1A:142(A):C:H2'	1:1A:143:G:O4'	2.21	0.40
1:1A:1006:C:C2	1:1A:1138:G:N2	2.89	0.40
1:1A:1252:G:N3	16:1U:33:ARG:HG2	2.36	0.40
1:1A:2086:U:H2'	1:1A:2087:G:C8	2.56	0.40
1:1A:2101:G:H1	1:1A:2188:C:H42	1.69	0.40
1:1A:2630:G:H2'	1:1A:2631:G:O4'	2.21	0.40
1:1A:2679:A:H4'	4:1E:165:VAL:HG11	2.02	0.40
1:1A:2838:G:C2	1:1A:2881:C:C2	3.10	0.40
4:1E:2:LYS:HB2	4:1E:95:ILE:HD12	2.04	0.40
5:1F:154:VAL:HG22	5:1F:191:ARG:HB2	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1G:18:GLU:HG3	6:1G:22:ARG:HD3	2.02	0.40
9:1N:15:LEU:HB3	9:1N:137:LYS:HA	2.02	0.40
9:1N:137:LYS:HE2	9:1N:139:GLU:OE2	2.21	0.40
32:1a:262:A:C6	32:1a:263:A:C6	3.09	0.40
35:1d:189:PRO:HB3	35:1d:193:ASP:CB	2.51	0.40
1:2A:125:G:O6	29:27:10:ARG:NH1	2.54	0.40
1:2A:1316:U:H2'	1:2A:1317:A:C8	2.56	0.40
1:2A:2184:G:O2'	1:2A:2185:C:H5'	2.21	0.40
2:2B:118:G:C5	2:2B:119:G:C8	3.10	0.40
3:2D:26:LYS:HE2	3:2D:28:GLU:O	2.21	0.40
7:2H:148:ILE:HG13	7:2H:148:ILE:H	1.64	0.40
14:2S:24:LEU:HD23	14:2S:24:LEU:HA	1.85	0.40
19:2X:11:PRO:HD3	24:22:37:PHE:CD1	2.56	0.40
32:2a:22:G:H5'	32:2a:885:G:OP2	2.21	0.40
32:2a:395:C:H2'	32:2a:396:G:H8	1.87	0.40
32:2a:652:U:O4	32:2a:752:G:O2'	2.27	0.40
32:2a:685:G:N2	32:2a:704:A:OP2	2.43	0.40
32:2a:994:A:N7	32:2a:1216:G:H4'	2.35	0.40
32:2a:1010:G:N1	32:2a:1020:U:H1'	2.36	0.40
32:2a:1413:A:H2'	32:2a:1414:U:O4'	2.21	0.40
32:2a:1424:C:H2'	32:2a:1425:U:O4'	2.22	0.40
33:2b:214:ILE:HD13	33:2b:214:ILE:HA	1.71	0.40
50:2s:30:LEU:HD11	50:2s:50:ALA:HB2	2.02	0.40
1:1A:27:G:C2	1:1A:512:G:N3	2.89	0.40
1:1A:1086:A:O3'	1:1A:1087:G:C8	2.74	0.40
1:1A:1164:G:H2'	1:1A:1165:U:C6	2.56	0.40
1:1A:2190:G:C2	1:1A:2191:G:C8	3.09	0.40
1:1A:2505:G:OP1	58:1A:4109:6IF:OAM	2.39	0.40
9:1N:73:THR:HA	9:1N:83:LYS:O	2.21	0.40
32:1a:130:A:O2'	32:1a:131:C:O5'	2.40	0.40
32:1a:233:C:H2'	32:1a:234:C:H6	1.86	0.40
32:1a:1291:G:OP1	38:1g:37:ASN:ND2	2.54	0.40
35:1d:166:LYS:NZ	35:1d:179:GLU:OE2	2.53	0.40
45:1n:21:TYR:OH	45:1n:23:ARG:NH1	2.54	0.40
47:1p:56:ALA:O	47:1p:60:LEU:HB2	2.21	0.40
49:1r:63:GLN:HE21	49:1r:63:GLN:HA	1.87	0.40
1:2A:298:G:H5''	1:2A:299:A:OP1	2.21	0.40
1:2A:1268:A:H2'	1:2A:1269:A:O4'	2.20	0.40
1:2A:2364:C:H2'	1:2A:2365:G:O4'	2.22	0.40
2:2B:40:U:O2'	2:2B:41:U:H5'	2.22	0.40
4:2E:1:MET:HE3	4:2E:199:ARG:HD2	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:2R:54:LEU:HD23	13:2R:54:LEU:HA	1.92	0.40
20:2Y:8:LYS:HD3	20:2Y:97:ARG:NH1	2.37	0.40
31:29:7:VAL:HG12	31:29:34:GLN:HB3	2.03	0.40
32:2a:159:G:OP2	32:2a:159:G:H8	2.04	0.40
32:2a:263:A:OP1	51:2t:79:ARG:NH1	2.54	0.40
32:2a:300:A:O5'	32:2a:300:A:H8	2.05	0.40
32:2a:949:A:H1'	32:2a:1364:U:H3	1.85	0.40
32:2a:1252:A:H2'	32:2a:1253:G:O4'	2.20	0.40
32:2a:1266:G:N2	32:2a:1269:A:OP2	2.40	0.40
33:2b:159:PRO:HB2	33:2b:161:ALA:O	2.22	0.40
35:2d:190:ASP:O	35:2d:194:LEU:HD12	2.21	0.40
36:2e:106:PRO:O	36:2e:110:LEU:HG	2.21	0.40
40:2i:5:TYR:CD1	40:2i:18:PHE:HE1	2.40	0.40
44:2m:117:VAL:HG22	44:2m:118:ALA:H	1.86	0.40
56:2y:26:A:N1	56:2y:44:G:O6	2.54	0.40
1:1A:53:A:H2'	1:1A:54:G:O4'	2.21	0.40
1:1A:558:G:OP1	9:1N:111:PRO:HD2	2.21	0.40
1:1A:699:A:H2'	1:1A:700:G:O4'	2.22	0.40
1:1A:1668:A:H4'	1:1A:1669:A:O5'	2.20	0.40
1:1A:1773:A:H2'	1:1A:1774:C:O4'	2.21	0.40
1:1A:1814:G:H4'	3:1D:51:VAL:HG21	2.04	0.40
1:1A:1866:C:H2'	1:1A:1876:A:O4'	2.21	0.40
6:1G:21:ARG:HD3	6:1G:21:ARG:O	2.21	0.40
6:1G:165:THR:OG1	6:1G:168:GLU:HG3	2.20	0.40
14:1S:25:ARG:O	14:1S:39:ILE:HA	2.21	0.40
25:13:7:LYS:HE3	25:13:32:GLN:NE2	2.33	0.40
32:1a:100:C:H2'	32:1a:101:A:C8	2.56	0.40
32:1a:1015:A:H2'	32:1a:1016:A:C8	2.57	0.40
32:1a:1016:A:H2'	32:1a:1017:G:O4'	2.21	0.40
32:1a:1194:U:H2'	32:1a:1195:C:C6	2.56	0.40
41:1j:92:THR:O	41:1j:94:VAL:N	2.49	0.40
44:1m:15:VAL:HG13	44:1m:43:THR:O	2.21	0.40
1:2A:116:C:H2'	1:2A:117:G:O4'	2.22	0.40
1:2A:328:U:H4'	20:2Y:68:HIS:CD2	2.57	0.40
1:2A:1593:G:H2'	1:2A:1594:G:H8	1.82	0.40
1:2A:1599:C:OP1	19:2X:36:LYS:HG3	2.21	0.40
1:2A:1848:A:C6	32:2a:702:A:C6	3.10	0.40
1:2A:2751:G:H8	7:2H:2:SER:N	2.19	0.40
5:2F:21:ALA:CB	5:2F:22:ALA:HA	2.48	0.40
14:2S:19:LYS:HG2	14:2S:19:LYS:H	1.61	0.40
14:2S:62:LYS:HA	14:2S:65:VAL:HG22	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:2Y:5:MET:HB2	20:2Y:5:MET:HE2	1.82	0.40
32:2a:259:G:H2'	32:2a:260:G:O4'	2.21	0.40
32:2a:528:C:H5'	32:2a:529:G:OP2	2.20	0.40
32:2a:985:C:H2'	32:2a:986:A:C8	2.57	0.40
32:2a:1374:A:O2'	38:2g:28:ASN:HB3	2.21	0.40
32:2a:1467:G:H8	32:2a:1467:G:O5'	2.04	0.40
35:2d:11:LEU:HD23	35:2d:66:ARG:HB3	2.04	0.40
37:2f:62:TRP:CH2	37:2f:64:GLN:HB2	2.56	0.40
42:2k:34:ASP:OD2	42:2k:38:ASN:HB2	2.22	0.40
51:2t:16:HIS:O	51:2t:19:SER:OG	2.24	0.40
51:2t:72:LEU:HG	51:2t:76:ALA:HB3	2.04	0.40
51:2t:72:LEU:HD12	51:2t:72:LEU:HA	1.83	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	258 (94%)	14 (5%)	1 (0%)	30	49
3	2D	273/276 (99%)	253 (93%)	20 (7%)	0	100	100
4	1E	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	24	43
4	2E	202/206 (98%)	186 (92%)	15 (7%)	1 (0%)	24	43
5	1F	201/210 (96%)	195 (97%)	5 (2%)	1 (0%)	24	43
5	2F	201/210 (96%)	187 (93%)	12 (6%)	2 (1%)	12	24
6	1G	179/182 (98%)	166 (93%)	12 (7%)	1 (1%)	21	38
6	2G	179/182 (98%)	154 (86%)	22 (12%)	3 (2%)	7	13
7	1H	172/180 (96%)	162 (94%)	10 (6%)	0	100	100
7	2H	172/180 (96%)	156 (91%)	15 (9%)	1 (1%)	21	38

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	1I	144/148 (97%)	132 (92%)	12 (8%)	0	100	100
8	2I	144/148 (97%)	123 (85%)	19 (13%)	2 (1%)	9	17
9	1N	138/140 (99%)	131 (95%)	7 (5%)	0	100	100
9	2N	138/140 (99%)	129 (94%)	8 (6%)	1 (1%)	18	34
10	1O	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
10	2O	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
11	1P	147/150 (98%)	135 (92%)	9 (6%)	3 (2%)	6	10
11	2P	147/150 (98%)	127 (86%)	15 (10%)	5 (3%)	3	4
12	1Q	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
12	2Q	139/141 (99%)	126 (91%)	13 (9%)	0	100	100
13	1R	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
13	2R	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
14	1S	108/112 (96%)	103 (95%)	5 (5%)	0	100	100
14	2S	108/112 (96%)	96 (89%)	8 (7%)	4 (4%)	2	3
15	1T	129/146 (88%)	121 (94%)	7 (5%)	1 (1%)	16	31
15	2T	129/146 (88%)	123 (95%)	6 (5%)	0	100	100
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	110 (96%)	4 (4%)	0	100	100
17	1V	99/101 (98%)	93 (94%)	5 (5%)	1 (1%)	12	24
17	2V	99/101 (98%)	92 (93%)	6 (6%)	1 (1%)	12	24
18	1W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
18	2W	110/113 (97%)	107 (97%)	3 (3%)	0	100	100
19	1X	93/96 (97%)	88 (95%)	3 (3%)	2 (2%)	5	9
19	2X	93/96 (97%)	88 (95%)	4 (4%)	1 (1%)	11	22
20	1Y	105/110 (96%)	97 (92%)	7 (7%)	1 (1%)	12	24
20	2Y	105/110 (96%)	99 (94%)	3 (3%)	3 (3%)	3	5
21	1Z	148/206 (72%)	125 (84%)	21 (14%)	2 (1%)	9	17
21	2Z	156/206 (76%)	122 (78%)	33 (21%)	1 (1%)	21	38
22	10	81/85 (95%)	78 (96%)	3 (4%)	0	100	100
22	20	81/85 (95%)	73 (90%)	7 (9%)	1 (1%)	10	20
23	11	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	11	22

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	21	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	11	22
24	12	68/72 (94%)	68 (100%)	0	0	100	100
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%)	52 (91%)	4 (7%)	1 (2%)	6	12
26	14	67/71 (94%)	54 (81%)	8 (12%)	5 (8%)	1	0
26	24	67/71 (94%)	47 (70%)	17 (25%)	3 (4%)	2	2
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
27	25	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
28	16	51/54 (94%)	51 (100%)	0	0	100	100
28	26	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
29	17	46/49 (94%)	45 (98%)	1 (2%)	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%)	61 (98%)	1 (2%)	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	33 (94%)	1 (3%)	1 (3%)	3	5
33	1b	229/256 (90%)	190 (83%)	31 (14%)	8 (4%)	3	4
33	2b	229/256 (90%)	180 (79%)	40 (18%)	9 (4%)	2	3
34	1c	204/239 (85%)	180 (88%)	23 (11%)	1 (0%)	24	43
34	2c	204/239 (85%)	169 (83%)	31 (15%)	4 (2%)	6	10
35	1d	206/209 (99%)	187 (91%)	18 (9%)	1 (0%)	24	43
35	2d	206/209 (99%)	187 (91%)	17 (8%)	2 (1%)	12	24
36	1e	146/162 (90%)	133 (91%)	12 (8%)	1 (1%)	18	34
36	2e	146/162 (90%)	125 (86%)	17 (12%)	4 (3%)	4	6
37	1f	98/101 (97%)	91 (93%)	7 (7%)	0	100	100
37	2f	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
38	1g	153/156 (98%)	139 (91%)	12 (8%)	2 (1%)	9	18
38	2g	153/156 (98%)	135 (88%)	16 (10%)	2 (1%)	9	18
39	1h	135/138 (98%)	126 (93%)	9 (7%)	0	100	100
39	2h	135/138 (98%)	122 (90%)	12 (9%)	1 (1%)	18	34

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	1i	125/128 (98%)	112 (90%)	12 (10%)	1 (1%)	16	31
40	2i	125/128 (98%)	101 (81%)	23 (18%)	1 (1%)	16	31
41	1j	95/105 (90%)	81 (85%)	11 (12%)	3 (3%)	3	4
41	2j	94/105 (90%)	76 (81%)	14 (15%)	4 (4%)	2	2
42	1k	112/129 (87%)	99 (88%)	10 (9%)	3 (3%)	4	6
42	2k	112/129 (87%)	100 (89%)	10 (9%)	2 (2%)	6	12
43	1l	119/132 (90%)	111 (93%)	8 (7%)	0	100	100
43	2l	119/132 (90%)	110 (92%)	8 (7%)	1 (1%)	16	31
44	1m	121/126 (96%)	109 (90%)	10 (8%)	2 (2%)	7	13
44	2m	120/126 (95%)	97 (81%)	21 (18%)	2 (2%)	7	13
45	1n	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
45	2n	58/61 (95%)	51 (88%)	6 (10%)	1 (2%)	7	13
46	1o	86/89 (97%)	81 (94%)	3 (4%)	2 (2%)	5	8
46	2o	86/89 (97%)	79 (92%)	6 (7%)	1 (1%)	10	20
47	1p	80/88 (91%)	73 (91%)	6 (8%)	1 (1%)	9	18
47	2p	80/88 (91%)	71 (89%)	9 (11%)	0	100	100
48	1q	97/105 (92%)	92 (95%)	5 (5%)	0	100	100
48	2q	97/105 (92%)	86 (89%)	10 (10%)	1 (1%)	12	24
49	1r	66/88 (75%)	62 (94%)	4 (6%)	0	100	100
49	2r	66/88 (75%)	61 (92%)	5 (8%)	0	100	100
50	1s	81/93 (87%)	71 (88%)	8 (10%)	2 (2%)	4	7
50	2s	81/93 (87%)	64 (79%)	15 (18%)	2 (2%)	4	7
51	1t	94/106 (89%)	85 (90%)	6 (6%)	3 (3%)	3	4
51	2t	94/106 (89%)	87 (93%)	3 (3%)	4 (4%)	2	2
52	1u	21/27 (78%)	21 (100%)	0	0	100	100
52	2u	21/27 (78%)	13 (62%)	8 (38%)	0	100	100
All	All	11370/12128 (94%)	10356 (91%)	891 (8%)	123 (1%)	11	22

All (123) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
11	1P	38	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	1Z	52	SER
21	1Z	163	LEU
23	11	3	LYS
26	14	47	GLN
33	1b	22	LYS
33	1b	126	GLU
38	1g	80	VAL
44	1m	67	GLU
50	1s	81	ARG
6	2G	51	ARG
8	2I	10	GLU
11	2P	36	LYS
20	2Y	55	TYR
33	2b	17	PHE
33	2b	123	ALA
38	2g	80	VAL
50	2s	81	ARG
11	1P	36	LYS
17	1V	79	VAL
19	1X	93	GLU
26	14	57	GLU
26	14	62	ARG
33	1b	17	PHE
36	1e	85	GLY
41	1j	79	ARG
42	1k	49	GLY
42	1k	77	MET
46	1o	88	ARG
5	2F	130	ALA
6	2G	42	GLY
11	2P	29	LYS
11	2P	44	GLY
14	2S	96	GLY
17	2V	79	VAL
19	2X	94	GLY
21	2Z	146	ILE
23	21	3	LYS
33	2b	74	LYS
36	2e	77	PRO
38	2g	55	GLY
41	2j	79	ARG
42	2k	49	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
46	2o	88	ARG
48	2q	68	ARG
50	2s	12	ASP
4	1E	52	LEU
20	1Y	54	LYS
26	14	49	PHE
33	1b	8	LYS
41	1j	29	ARG
50	1s	29	ARG
51	1t	47	GLY
4	2E	52	LEU
6	2G	47	LYS
7	2H	47	GLU
8	2I	39	ALA
11	2P	45	LEU
14	2S	20	ARG
14	2S	84	GLN
20	2Y	54	LYS
22	20	73	GLY
26	24	49	PHE
33	2b	9	GLU
33	2b	16	HIS
33	2b	20	GLU
34	2c	111	LEU
35	2d	164	ALA
39	2h	68	ARG
42	2k	105	VAL
43	2l	105	TYR
3	1D	262	ARG
15	1T	37	GLY
33	1b	155	LEU
38	1g	52	GLU
40	1i	54	ASP
41	1j	78	ASN
46	1o	87	ILE
47	1p	76	GLN
51	1t	96	GLY
5	2F	146	ALA
11	2P	38	GLN
26	24	11	PRO
26	24	39	CYS
33	2b	106	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	2b	126	GLU
34	2c	53	ALA
34	2c	91	LEU
44	2m	87	TYR
45	2n	14	PRO
51	2t	10	LEU
51	2t	98	PRO
6	1G	43	LEU
11	1P	29	LYS
19	1X	2	LYS
26	14	53	GLU
33	1b	124	SER
33	1b	129	GLU
33	1b	231	GLU
34	1c	107	GLN
35	1d	88	VAL
51	1t	100	ILE
9	2N	8	GLN
14	2S	32	LEU
34	2c	156	ARG
36	2e	85	GLY
40	2i	56	LEU
41	2j	75	ILE
44	2m	106	ASN
51	2t	99	LEU
25	23	59	VAL
33	2b	231	GLU
36	2e	96	PRO
41	2j	41	PRO
44	1m	4	ILE
42	1k	105	VAL
35	2d	136	PRO
41	2j	50	ILE
31	29	21	GLY
36	2e	69	VAL
51	2t	47	GLY
20	2Y	27	VAL

5.3.2 Protein sidechains ⓘ

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	215/218 (99%)	199 (93%)	16 (7%)	13	27
3	2D	215/218 (99%)	204 (95%)	11 (5%)	21	43
4	1E	164/166 (99%)	151 (92%)	13 (8%)	11	24
4	2E	164/166 (99%)	151 (92%)	13 (8%)	11	24
5	1F	160/166 (96%)	143 (89%)	17 (11%)	6	14
5	2F	159/166 (96%)	152 (96%)	7 (4%)	25	50
6	1G	143/156 (92%)	129 (90%)	14 (10%)	7	16
6	2G	143/156 (92%)	125 (87%)	18 (13%)	4	9
7	1H	144/148 (97%)	133 (92%)	11 (8%)	12	26
7	2H	144/148 (97%)	125 (87%)	19 (13%)	4	8
8	1I	113/124 (91%)	91 (80%)	22 (20%)	1	2
8	2I	105/124 (85%)	92 (88%)	13 (12%)	4	9
9	1N	118/119 (99%)	110 (93%)	8 (7%)	14	31
9	2N	118/119 (99%)	109 (92%)	9 (8%)	12	26
10	1O	100/100 (100%)	96 (96%)	4 (4%)	28	54
10	2O	100/100 (100%)	96 (96%)	4 (4%)	28	54
11	1P	115/116 (99%)	107 (93%)	8 (7%)	14	29
11	2P	115/116 (99%)	104 (90%)	11 (10%)	8	17
12	1Q	111/111 (100%)	105 (95%)	6 (5%)	20	41
12	2Q	111/111 (100%)	102 (92%)	9 (8%)	11	23
13	1R	101/101 (100%)	98 (97%)	3 (3%)	36	64
13	2R	101/101 (100%)	96 (95%)	5 (5%)	22	44
14	1S	86/88 (98%)	77 (90%)	9 (10%)	6	14
14	2S	85/88 (97%)	70 (82%)	15 (18%)	2	3
15	1T	115/127 (91%)	112 (97%)	3 (3%)	40	68
15	2T	113/127 (89%)	107 (95%)	6 (5%)	20	42
16	1U	93/94 (99%)	85 (91%)	8 (9%)	10	21
16	2U	93/94 (99%)	85 (91%)	8 (9%)	10	21
17	1V	80/82 (98%)	76 (95%)	4 (5%)	22	44

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	2V	80/82 (98%)	71 (89%)	9 (11%)	5	12
18	1W	90/92 (98%)	86 (96%)	4 (4%)	25	50
18	2W	90/92 (98%)	86 (96%)	4 (4%)	25	50
19	1X	77/78 (99%)	74 (96%)	3 (4%)	28	55
19	2X	77/78 (99%)	74 (96%)	3 (4%)	28	55
20	1Y	85/91 (93%)	79 (93%)	6 (7%)	13	29
20	2Y	85/91 (93%)	76 (89%)	9 (11%)	6	14
21	1Z	135/179 (75%)	122 (90%)	13 (10%)	8	17
21	2Z	137/179 (76%)	116 (85%)	21 (15%)	3	5
22	10	65/67 (97%)	63 (97%)	2 (3%)	35	62
22	20	65/67 (97%)	61 (94%)	4 (6%)	16	34
23	11	80/83 (96%)	79 (99%)	1 (1%)	61	82
23	21	80/83 (96%)	75 (94%)	5 (6%)	16	34
24	12	65/67 (97%)	61 (94%)	4 (6%)	16	34
24	22	65/67 (97%)	59 (91%)	6 (9%)	8	19
25	13	51/52 (98%)	44 (86%)	7 (14%)	3	7
25	23	50/52 (96%)	47 (94%)	3 (6%)	17	36
26	14	59/63 (94%)	51 (86%)	8 (14%)	3	8
26	24	53/63 (84%)	43 (81%)	10 (19%)	1	3
27	15	50/52 (96%)	47 (94%)	3 (6%)	17	36
27	25	50/52 (96%)	48 (96%)	2 (4%)	28	54
28	16	51/52 (98%)	46 (90%)	5 (10%)	7	16
28	26	50/52 (96%)	48 (96%)	2 (4%)	28	54
29	17	41/42 (98%)	37 (90%)	4 (10%)	7	16
29	27	41/42 (98%)	36 (88%)	5 (12%)	5	10
30	18	54/55 (98%)	52 (96%)	2 (4%)	30	57
30	28	54/55 (98%)	51 (94%)	3 (6%)	19	39
31	19	34/34 (100%)	32 (94%)	2 (6%)	18	37
31	29	34/34 (100%)	33 (97%)	1 (3%)	37	65
33	1b	192/220 (87%)	166 (86%)	26 (14%)	4	8
33	2b	187/220 (85%)	158 (84%)	29 (16%)	2	5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	1c	142/188 (76%)	129 (91%)	13 (9%)	8	19
34	2c	140/188 (74%)	117 (84%)	23 (16%)	2	4
35	1d	169/181 (93%)	150 (89%)	19 (11%)	6	12
35	2d	173/181 (96%)	156 (90%)	17 (10%)	7	16
36	1e	113/123 (92%)	103 (91%)	10 (9%)	9	20
36	2e	114/123 (93%)	103 (90%)	11 (10%)	8	17
37	1f	84/90 (93%)	79 (94%)	5 (6%)	17	36
37	2f	85/90 (94%)	79 (93%)	6 (7%)	13	29
38	1g	119/127 (94%)	107 (90%)	12 (10%)	7	15
38	2g	120/127 (94%)	105 (88%)	15 (12%)	4	9
39	1h	114/119 (96%)	104 (91%)	10 (9%)	9	20
39	2h	114/119 (96%)	99 (87%)	15 (13%)	4	8
40	1i	90/99 (91%)	80 (89%)	10 (11%)	6	12
40	2i	89/99 (90%)	80 (90%)	9 (10%)	7	15
41	1j	66/92 (72%)	60 (91%)	6 (9%)	9	19
41	2j	69/92 (75%)	59 (86%)	10 (14%)	3	6
42	1k	82/99 (83%)	73 (89%)	9 (11%)	6	13
42	2k	83/99 (84%)	75 (90%)	8 (10%)	8	17
43	1l	96/108 (89%)	93 (97%)	3 (3%)	35	62
43	2l	96/108 (89%)	89 (93%)	7 (7%)	13	27
44	1m	93/101 (92%)	83 (89%)	10 (11%)	6	13
44	2m	92/101 (91%)	80 (87%)	12 (13%)	4	8
45	1n	49/50 (98%)	46 (94%)	3 (6%)	17	35
45	2n	49/50 (98%)	44 (90%)	5 (10%)	7	15
46	1o	78/80 (98%)	76 (97%)	2 (3%)	40	68
46	2o	78/80 (98%)	74 (95%)	4 (5%)	21	43
47	1p	69/74 (93%)	61 (88%)	8 (12%)	5	11
47	2p	68/74 (92%)	63 (93%)	5 (7%)	13	27
48	1q	94/97 (97%)	87 (93%)	7 (7%)	13	27
48	2q	94/97 (97%)	87 (93%)	7 (7%)	13	27
49	1r	59/77 (77%)	58 (98%)	1 (2%)	53	78

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	2r	59/77 (77%)	53 (90%)	6 (10%)	7	15
50	1s	69/80 (86%)	65 (94%)	4 (6%)	18	38
50	2s	67/80 (84%)	56 (84%)	11 (16%)	2	4
51	1t	70/82 (85%)	65 (93%)	5 (7%)	13	29
51	2t	70/82 (85%)	67 (96%)	3 (4%)	26	51
52	1u	18/22 (82%)	17 (94%)	1 (6%)	19	39
52	2u	18/22 (82%)	16 (89%)	2 (11%)	6	12
All	All	9303/10064 (92%)	8489 (91%)	814 (9%)	9	21

All (814) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	16	MET
3	1D	32	SER
3	1D	34	VAL
3	1D	37	LEU
3	1D	88	ARG
3	1D	106	ILE
3	1D	113	VAL
3	1D	122	ASP
3	1D	155	LEU
3	1D	162	SER
3	1D	173	VAL
3	1D	221	VAL
3	1D	229	VAL
3	1D	242	ARG
3	1D	259	THR
3	1D	273	ARG
4	1E	9	VAL
4	1E	12	THR
4	1E	41	LYS
4	1E	45	THR
4	1E	47	VAL
4	1E	73	GLU
4	1E	77	ILE
4	1E	90	THR
4	1E	93	VAL
4	1E	116	VAL
4	1E	181	LEU
4	1E	184	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	1E	188	VAL
5	1F	12	LEU
5	1F	24	LEU
5	1F	27	GLU
5	1F	53	THR
5	1F	57	VAL
5	1F	70	THR
5	1F	74	ARG
5	1F	88	VAL
5	1F	132	VAL
5	1F	140	LEU
5	1F	144	LYS
5	1F	162	LEU
5	1F	168	ARG
5	1F	175	THR
5	1F	183	VAL
5	1F	192	LEU
5	1F	201	VAL
6	1G	3	LEU
6	1G	5	VAL
6	1G	7	LEU
6	1G	21	ARG
6	1G	31	VAL
6	1G	43	LEU
6	1G	82	LEU
6	1G	109	VAL
6	1G	126	ASP
6	1G	133	LEU
6	1G	139	LEU
6	1G	140	ILE
6	1G	149	VAL
6	1G	159	VAL
7	1H	24	VAL
7	1H	33	LEU
7	1H	45	VAL
7	1H	49	VAL
7	1H	76	VAL
7	1H	95	ARG
7	1H	113	VAL
7	1H	119	GLU
7	1H	122	THR
7	1H	124	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	1H	127	GLU
8	1I	1	MET
8	1I	5	LEU
8	1I	9	LEU
8	1I	10	GLU
8	1I	38	LEU
8	1I	40	THR
8	1I	41	GLU
8	1I	44	LEU
8	1I	47	LEU
8	1I	68	LEU
8	1I	85	GLU
8	1I	92	VAL
8	1I	95	LYS
8	1I	101	LEU
8	1I	108	THR
8	1I	109	ILE
8	1I	116	LEU
8	1I	117	GLU
8	1I	122	GLU
8	1I	133	HIS
8	1I	140	LEU
8	1I	142	VAL
9	1N	1	MET
9	1N	5	VAL
9	1N	14	VAL
9	1N	28	THR
9	1N	48	MET
9	1N	58	ASP
9	1N	67	LEU
9	1N	134	ARG
10	1O	28	SER
10	1O	52	VAL
10	1O	69	ILE
10	1O	89	ASN
11	1P	1	MET
11	1P	7	ARG
11	1P	15	ARG
11	1P	45	LEU
11	1P	76	LYS
11	1P	95	VAL
11	1P	119	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	1P	125	VAL
12	1Q	7	MET
12	1Q	56	ARG
12	1Q	75	THR
12	1Q	109	VAL
12	1Q	127	ILE
12	1Q	133	ARG
13	1R	36	THR
13	1R	67	LEU
13	1R	114	VAL
14	1S	14	VAL
14	1S	15	ARG
14	1S	36	TYR
14	1S	49	VAL
14	1S	50	SER
14	1S	68	GLN
14	1S	73	LEU
14	1S	85	VAL
14	1S	110	LEU
15	1T	28	VAL
15	1T	36	GLU
15	1T	49	VAL
16	1U	8	VAL
16	1U	31	SER
16	1U	74	LEU
16	1U	84	LYS
16	1U	85	LYS
16	1U	95	LEU
16	1U	100	VAL
16	1U	111	GLU
17	1V	6	LYS
17	1V	61	VAL
17	1V	79	VAL
17	1V	100	ARG
18	1W	11	ARG
18	1W	15	ARG
18	1W	17	VAL
18	1W	96	ILE
19	1X	35	THR
19	1X	70	LEU
19	1X	72	LYS
20	1Y	37	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	1Y	61	ILE
20	1Y	72	VAL
20	1Y	91	GLU
20	1Y	99	CYS
20	1Y	106	LEU
21	1Z	18	LEU
21	1Z	49	ARG
21	1Z	56	VAL
21	1Z	104	PHE
21	1Z	128	VAL
21	1Z	129	SER
21	1Z	136	PHE
21	1Z	139	VAL
21	1Z	154	ASP
21	1Z	155	LEU
21	1Z	161	VAL
21	1Z	169	GLU
21	1Z	170	THR
22	10	7	LEU
22	10	10	THR
23	11	35	THR
24	12	3	LEU
24	12	4	SER
24	12	19	VAL
24	12	40	SER
25	13	18	ASP
25	13	23	LEU
25	13	35	ARG
25	13	54	VAL
25	13	55	ARG
25	13	58	VAL
25	13	60	GLU
26	14	47	GLN
26	14	49	PHE
26	14	52	THR
26	14	53	GLU
26	14	59	PHE
26	14	60	GLN
26	14	63	TYR
26	14	67	TYR
27	15	6	VAL
27	15	35	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	15	40	LYS
28	16	9	LEU
28	16	19	ARG
28	16	24	GLU
28	16	44	ARG
28	16	47	THR
29	17	24	THR
29	17	32	LYS
29	17	43	THR
29	17	46	VAL
30	18	14	VAL
30	18	52	LYS
31	19	17	ILE
31	19	18	ARG
33	1b	7	VAL
33	1b	8	LYS
33	1b	12	GLU
33	1b	17	PHE
33	1b	35	GLU
33	1b	39	ILE
33	1b	54	THR
33	1b	64	ARG
33	1b	76	GLN
33	1b	80	ILE
33	1b	95	GLN
33	1b	108	ILE
33	1b	112	VAL
33	1b	127	ILE
33	1b	133	LYS
33	1b	160	ASP
33	1b	185	ILE
33	1b	192	SER
33	1b	196	LEU
33	1b	200	ILE
33	1b	208	ILE
33	1b	215	LEU
33	1b	219	VAL
33	1b	221	LEU
33	1b	223	ILE
33	1b	233	SER
34	1c	3	ASN
34	1c	8	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	1c	28	GLN
34	1c	68	VAL
34	1c	70	VAL
34	1c	82	GLU
34	1c	91	LEU
34	1c	98	ASN
34	1c	178	LEU
34	1c	192	THR
34	1c	195	VAL
34	1c	198	VAL
34	1c	201	TYR
35	1d	3	ARG
35	1d	5	ILE
35	1d	17	VAL
35	1d	19	LEU
35	1d	49	ARG
35	1d	77	ASN
35	1d	83	SER
35	1d	88	VAL
35	1d	115	ARG
35	1d	135	LEU
35	1d	140	VAL
35	1d	144	ASP
35	1d	158	ILE
35	1d	177	ASP
35	1d	178	VAL
35	1d	188	LEU
35	1d	193	ASP
35	1d	194	LEU
35	1d	200	GLU
36	1e	10	MET
36	1e	12	LEU
36	1e	20	GLN
36	1e	41	VAL
36	1e	51	VAL
36	1e	53	LEU
36	1e	56	GLN
36	1e	63	ARG
36	1e	67	VAL
36	1e	116	THR
37	1f	19	LEU
37	1f	36	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	1f	55	ASP
37	1f	72	VAL
37	1f	75	LEU
38	1g	12	LEU
38	1g	31	MET
38	1g	50	ILE
38	1g	57	GLU
38	1g	61	VAL
38	1g	78	ARG
38	1g	79	ARG
38	1g	104	LEU
38	1g	110	GLN
38	1g	113	GLU
38	1g	115	ARG
38	1g	120	ILE
39	1h	2	LEU
39	1h	23	SER
39	1h	29	SER
39	1h	51	VAL
39	1h	52	ASP
39	1h	54	ASP
39	1h	83	ILE
39	1h	86	ILE
39	1h	112	LEU
39	1h	133	LEU
40	1i	7	THR
40	1i	23	ASN
40	1i	41	VAL
40	1i	50	LEU
40	1i	64	THR
40	1i	96	LEU
40	1i	97	LYS
40	1i	103	THR
40	1i	108	VAL
40	1i	128	ARG
41	1j	49	VAL
41	1j	55	LYS
41	1j	81	THR
41	1j	92	THR
41	1j	95	GLU
41	1j	98	ILE
42	1k	31	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
42	1k	48	ILE
42	1k	87	THR
42	1k	105	VAL
42	1k	107	SER
42	1k	108	ILE
42	1k	109	VAL
42	1k	112	THR
42	1k	114	VAL
43	1l	18	VAL
43	1l	40	VAL
43	1l	83	VAL
44	1m	4	ILE
44	1m	14	ARG
44	1m	19	LEU
44	1m	32	GLU
44	1m	43	THR
44	1m	49	THR
44	1m	64	TRP
44	1m	70	LEU
44	1m	94	ARG
44	1m	109	THR
45	1n	18	VAL
45	1n	33	VAL
45	1n	60	SER
46	1o	39	LEU
46	1o	76	GLU
47	1p	19	ILE
47	1p	20	VAL
47	1p	21	VAL
47	1p	27	LYS
47	1p	29	ASP
47	1p	45	THR
47	1p	50	LYS
47	1p	62	VAL
48	1q	9	VAL
48	1q	35	VAL
48	1q	36	ILE
48	1q	53	LEU
48	1q	57	VAL
48	1q	97	SER
48	1q	98	LEU
49	1r	82	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	1s	6	LYS
50	1s	32	LYS
50	1s	35	SER
50	1s	79	THR
51	1t	10	LEU
51	1t	24	LEU
51	1t	29	LYS
51	1t	71	THR
51	1t	84	LEU
52	1u	20	LYS
3	2D	3	VAL
3	2D	106	ILE
3	2D	113	VAL
3	2D	141	VAL
3	2D	173	VAL
3	2D	204	ILE
3	2D	221	VAL
3	2D	229	VAL
3	2D	242	ARG
3	2D	259	THR
3	2D	275	LYS
4	2E	1	MET
4	2E	7	VAL
4	2E	9	VAL
4	2E	12	THR
4	2E	38	THR
4	2E	47	VAL
4	2E	87	GLU
4	2E	90	THR
4	2E	104	VAL
4	2E	116	VAL
4	2E	134	ILE
4	2E	181	LEU
4	2E	184	VAL
5	2F	28	ILE
5	2F	96	ASP
5	2F	106	ARG
5	2F	145	GLU
5	2F	157	VAL
5	2F	165	ARG
5	2F	179	GLU
6	2G	3	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	2G	7	LEU
6	2G	18	GLU
6	2G	28	VAL
6	2G	39	ILE
6	2G	43	LEU
6	2G	51	ARG
6	2G	53	LEU
6	2G	60	LEU
6	2G	91	ARG
6	2G	111	LEU
6	2G	123	ASN
6	2G	140	ILE
6	2G	148	MET
6	2G	152	LEU
6	2G	155	MET
6	2G	168	GLU
6	2G	175	LEU
7	2H	23	ARG
7	2H	24	VAL
7	2H	45	VAL
7	2H	49	VAL
7	2H	50	VAL
7	2H	70	THR
7	2H	71	LEU
7	2H	81	GLU
7	2H	85	LYS
7	2H	103	LEU
7	2H	115	VAL
7	2H	122	THR
7	2H	124	GLU
7	2H	125	VAL
7	2H	129	THR
7	2H	133	VAL
7	2H	134	SER
7	2H	136	ILE
7	2H	141	VAL
8	2I	15	VAL
8	2I	37	VAL
8	2I	38	LEU
8	2I	58	LEU
8	2I	61	ARG
8	2I	77	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	2I	82	ARG
8	2I	85	GLU
8	2I	92	VAL
8	2I	117	GLU
8	2I	125	GLU
8	2I	127	VAL
8	2I	142	VAL
9	2N	1	MET
9	2N	14	VAL
9	2N	22	THR
9	2N	28	THR
9	2N	48	MET
9	2N	62	VAL
9	2N	63	THR
9	2N	67	LEU
9	2N	134	ARG
10	2O	21	CYS
10	2O	28	SER
10	2O	52	VAL
10	2O	96	THR
11	2P	7	ARG
11	2P	45	LEU
11	2P	65	ARG
11	2P	70	GLN
11	2P	75	ILE
11	2P	95	VAL
11	2P	96	THR
11	2P	98	GLU
11	2P	117	GLU
11	2P	125	VAL
11	2P	135	LEU
12	2Q	6	ARG
12	2Q	7	MET
12	2Q	31	ASP
12	2Q	56	ARG
12	2Q	60	ARG
12	2Q	68	ILE
12	2Q	106	VAL
12	2Q	109	VAL
12	2Q	110	THR
13	2R	6	SER
13	2R	24	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	2R	67	LEU
13	2R	113	LEU
13	2R	114	VAL
14	2S	4	LEU
14	2S	5	THR
14	2S	15	ARG
14	2S	27	SER
14	2S	44	LYS
14	2S	47	THR
14	2S	49	VAL
14	2S	53	SER
14	2S	58	LEU
14	2S	63	THR
14	2S	64	GLU
14	2S	73	LEU
14	2S	85	VAL
14	2S	98	VAL
14	2S	103	GLU
15	2T	9	LEU
15	2T	15	VAL
15	2T	49	VAL
15	2T	50	ILE
15	2T	104	ASN
15	2T	107	ASP
16	2U	5	LYS
16	2U	31	SER
16	2U	65	ILE
16	2U	74	LEU
16	2U	85	LYS
16	2U	95	LEU
16	2U	111	GLU
16	2U	114	LYS
17	2V	1	MET
17	2V	7	THR
17	2V	14	VAL
17	2V	28	GLU
17	2V	56	SER
17	2V	61	VAL
17	2V	79	VAL
17	2V	95	LEU
17	2V	98	GLU
18	2W	11	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	2W	17	VAL
18	2W	67	ASP
18	2W	109	GLU
19	2X	1	MET
19	2X	35	THR
19	2X	81	VAL
20	2Y	7	VAL
20	2Y	11	ASP
20	2Y	49	VAL
20	2Y	72	VAL
20	2Y	85	VAL
20	2Y	91	GLU
20	2Y	97	ARG
20	2Y	98	VAL
20	2Y	106	LEU
21	2Z	5	LEU
21	2Z	18	LEU
21	2Z	42	VAL
21	2Z	46	LYS
21	2Z	47	VAL
21	2Z	56	VAL
21	2Z	70	LEU
21	2Z	71	VAL
21	2Z	74	VAL
21	2Z	96	VAL
21	2Z	98	MET
21	2Z	121	HIS
21	2Z	123	ASP
21	2Z	126	VAL
21	2Z	141	VAL
21	2Z	145	GLU
21	2Z	154	ASP
21	2Z	155	LEU
21	2Z	161	VAL
21	2Z	170	THR
21	2Z	171	ILE
22	20	7	LEU
22	20	11	ARG
22	20	36	ILE
22	20	68	GLU
23	21	46	LEU
23	21	65	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
23	21	75	GLU
23	21	89	GLU
23	21	98	LEU
24	22	3	LEU
24	22	11	GLU
24	22	12	GLU
24	22	21	LEU
24	22	66	GLU
24	22	70	GLN
25	23	31	LEU
25	23	56	VAL
25	23	59	VAL
26	24	8	LYS
26	24	23	GLU
26	24	24	THR
26	24	34	GLU
26	24	49	PHE
26	24	56	VAL
26	24	59	PHE
26	24	63	TYR
26	24	67	TYR
26	24	68	ARG
27	25	6	VAL
27	25	58	LEU
28	26	23	THR
28	26	32	ASN
29	27	1	MET
29	27	24	THR
29	27	41	ARG
29	27	43	THR
29	27	46	VAL
30	28	14	VAL
30	28	34	TRP
30	28	37	SER
31	29	33	LYS
33	2b	10	LEU
33	2b	16	HIS
33	2b	44	LEU
33	2b	47	THR
33	2b	55	PHE
33	2b	58	ILE
33	2b	67	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	2b	68	ILE
33	2b	71	VAL
33	2b	76	GLN
33	2b	90	MET
33	2b	94	ASN
33	2b	95	GLN
33	2b	98	LEU
33	2b	107	THR
33	2b	112	VAL
33	2b	115	LEU
33	2b	127	ILE
33	2b	164	VAL
33	2b	184	VAL
33	2b	185	ILE
33	2b	189	ASP
33	2b	196	LEU
33	2b	201	ILE
33	2b	204	ASN
33	2b	214	ILE
33	2b	223	ILE
33	2b	229	VAL
33	2b	236	TYR
34	2c	4	LYS
34	2c	28	GLN
34	2c	33	LEU
34	2c	46	GLU
34	2c	47	LEU
34	2c	49	SER
34	2c	52	LEU
34	2c	55	VAL
34	2c	56	ASP
34	2c	57	ILE
34	2c	101	LEU
34	2c	105	GLU
34	2c	111	LEU
34	2c	115	LEU
34	2c	130	VAL
34	2c	132	ARG
34	2c	140	ARG
34	2c	150	LYS
34	2c	152	ILE
34	2c	153	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	2c	172	ARG
34	2c	188	LEU
34	2c	190	ARG
35	2d	5	ILE
35	2d	8	VAL
35	2d	31	CYS
35	2d	34	GLU
35	2d	53	ASP
35	2d	58	LEU
35	2d	70	ILE
35	2d	76	ARG
35	2d	78	LEU
35	2d	83	SER
35	2d	94	LEU
35	2d	127	THR
35	2d	135	LEU
35	2d	155	LEU
35	2d	158	ILE
35	2d	170	VAL
35	2d	190	ASP
36	2e	5	ASP
36	2e	10	MET
36	2e	13	ILE
36	2e	31	LEU
36	2e	41	VAL
36	2e	55	VAL
36	2e	66	MET
36	2e	115	VAL
36	2e	120	THR
36	2e	125	SER
36	2e	151	LEU
37	2f	19	LEU
37	2f	31	GLU
37	2f	45	LEU
37	2f	63	TYR
37	2f	64	GLN
37	2f	69	GLU
38	2g	9	VAL
38	2g	13	GLN
38	2g	15	ASP
38	2g	23	VAL
38	2g	24	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	2g	38	LEU
38	2g	52	GLU
38	2g	72	ARG
38	2g	78	ARG
38	2g	79	ARG
38	2g	106	GLN
38	2g	129	GLU
38	2g	142	GLU
38	2g	146	GLU
38	2g	155	ARG
39	2h	2	LEU
39	2h	11	THR
39	2h	37	ARG
39	2h	51	VAL
39	2h	52	ASP
39	2h	60	ARG
39	2h	61	VAL
39	2h	86	ILE
39	2h	97	VAL
39	2h	99	GLU
39	2h	109	ILE
39	2h	112	LEU
39	2h	114	THR
39	2h	125	ARG
39	2h	137	VAL
40	2i	14	VAL
40	2i	27	THR
40	2i	50	LEU
40	2i	54	ASP
40	2i	65	VAL
40	2i	89	ASN
40	2i	102	LEU
40	2i	103	THR
40	2i	108	VAL
41	2j	8	LEU
41	2j	21	GLN
41	2j	65	LEU
41	2j	67	THR
41	2j	72	VAL
41	2j	89	ASP
41	2j	95	GLU
41	2j	97	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	2j	98	ILE
41	2j	100	THR
42	2k	14	VAL
42	2k	24	SER
42	2k	48	ILE
42	2k	80	VAL
42	2k	87	THR
42	2k	105	VAL
42	2k	112	THR
42	2k	114	VAL
43	2l	18	VAL
43	2l	36	VAL
43	2l	40	VAL
43	2l	83	VAL
43	2l	86	ARG
43	2l	117	ARG
43	2l	124	LYS
44	2m	4	ILE
44	2m	15	VAL
44	2m	32	GLU
44	2m	34	LEU
44	2m	53	VAL
44	2m	62	ASN
44	2m	65	LYS
44	2m	67	GLU
44	2m	86	CYS
44	2m	98	VAL
44	2m	103	THR
44	2m	106	ASN
45	2n	18	VAL
45	2n	32	SER
45	2n	33	VAL
45	2n	56	VAL
45	2n	57	ARG
46	2o	5	LYS
46	2o	25	THR
46	2o	39	LEU
46	2o	76	GLU
47	2p	2	VAL
47	2p	21	VAL
47	2p	45	THR
47	2p	67	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
47	2p	74	LEU
48	2q	5	VAL
48	2q	39	SER
48	2q	41	LYS
48	2q	60	ILE
48	2q	68	ARG
48	2q	77	VAL
48	2q	97	SER
49	2r	21	LYS
49	2r	31	LEU
49	2r	53	ARG
49	2r	54	ARG
49	2r	82	THR
49	2r	84	LYS
50	2s	5	LEU
50	2s	16	LEU
50	2s	23	ASN
50	2s	33	THR
50	2s	45	VAL
50	2s	47	HIS
50	2s	48	THR
50	2s	49	ILE
50	2s	71	LEU
50	2s	81	ARG
50	2s	83	HIS
51	2t	46	GLU
51	2t	75	ASN
51	2t	99	LEU
52	2u	7	ARG
52	2u	9	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (156) such sidechains are listed below:

Mol	Chain	Res	Type
5	1F	69	HIS
6	1G	26	GLN
6	1G	108	ASN
9	1N	94	HIS
9	1N	131	GLN
10	1O	89	ASN
12	1Q	12	GLN
12	1Q	113	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	1Q	123	HIS
13	1R	71	GLN
15	1T	58	ASN
15	1T	90	GLN
16	1U	81	HIS
16	1U	94	ASN
19	1X	31	HIS
19	1X	82	GLN
20	1Y	6	HIS
21	1Z	34	ASN
21	1Z	73	GLN
21	1Z	75	ASN
21	1Z	151	HIS
22	10	70	GLN
23	11	56	GLN
24	12	9	GLN
24	12	43	GLN
25	13	32	GLN
26	14	40	HIS
26	14	47	GLN
28	16	20	ASN
33	1b	40	HIS
33	1b	78	GLN
33	1b	224	GLN
34	1c	6	HIS
34	1c	118	GLN
34	1c	123	GLN
34	1c	162	GLN
34	1c	170	GLN
34	1c	181	ASN
35	1d	74	GLN
35	1d	77	ASN
35	1d	116	GLN
35	1d	123	HIS
35	1d	125	HIS
35	1d	201	GLN
36	1e	20	GLN
36	1e	38	GLN
36	1e	78	HIS
36	1e	141	GLN
37	1f	57	GLN
37	1f	73	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	1f	100	ASN
38	1g	13	GLN
38	1g	28	ASN
38	1g	106	GLN
40	1i	31	GLN
40	1i	34	ASN
40	1i	58	HIS
40	1i	124	GLN
41	1j	21	GLN
41	1j	56	HIS
42	1k	116	HIS
43	1l	99	HIS
44	1m	77	ASN
44	1m	92	HIS
46	1o	46	HIS
46	1o	50	HIS
47	1p	16	HIS
48	1q	26	GLN
48	1q	45	HIS
48	1q	93	GLN
49	1r	63	GLN
50	1s	57	HIS
50	1s	83	HIS
51	1t	45	GLN
51	1t	73	HIS
5	2F	40	GLN
5	2F	69	HIS
6	2G	26	GLN
6	2G	108	ASN
6	2G	132	ASN
8	2I	133	HIS
9	2N	101	HIS
11	2P	70	GLN
12	2Q	12	GLN
13	2R	31	HIS
13	2R	50	HIS
13	2R	71	GLN
14	2S	38	GLN
15	2T	43	GLN
15	2T	58	ASN
15	2T	90	GLN
16	2U	72	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	2U	94	ASN
18	2W	60	ASN
18	2W	62	HIS
19	2X	31	HIS
19	2X	82	GLN
20	2Y	6	HIS
21	2Z	34	ASN
21	2Z	55	HIS
22	20	50	ASN
22	20	70	GLN
23	21	56	GLN
25	23	32	GLN
33	2b	76	GLN
33	2b	94	ASN
33	2b	135	GLN
34	2c	37	GLN
34	2c	98	ASN
34	2c	104	GLN
34	2c	136	GLN
35	2d	77	ASN
35	2d	116	GLN
35	2d	119	GLN
35	2d	123	HIS
35	2d	125	HIS
35	2d	160	GLN
35	2d	199	ASN
36	2e	38	GLN
36	2e	73	ASN
36	2e	78	HIS
36	2e	130	ASN
36	2e	141	GLN
37	2f	7	ASN
37	2f	73	ASN
37	2f	84	ASN
37	2f	100	ASN
38	2g	28	ASN
38	2g	86	GLN
38	2g	106	GLN
38	2g	148	ASN
40	2i	3	GLN
40	2i	58	HIS
41	2j	21	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	2j	33	GLN
41	2j	69	ASN
42	2k	26	ASN
42	2k	78	GLN
42	2k	104	GLN
42	2k	116	HIS
42	2k	117	ASN
43	2l	99	HIS
44	2m	12	ASN
44	2m	62	ASN
44	2m	77	ASN
46	2o	9	GLN
48	2q	93	GLN
49	2r	63	GLN
50	2s	23	ASN
50	2s	47	HIS
50	2s	56	GLN
50	2s	69	HIS
51	2t	18	GLN
51	2t	45	GLN
51	2t	75	ASN
51	2t	90	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	436 (15%)	25 (0%)
1	2A	2791/2915 (95%)	463 (16%)	25 (0%)
2	1B	119/121 (98%)	8 (6%)	0
2	2B	118/121 (97%)	27 (22%)	0
32	1a	1497/1521 (98%)	235 (15%)	0
32	2a	1501/1521 (98%)	302 (20%)	0
53	1v	12/24 (50%)	1 (8%)	0
53	2v	12/24 (50%)	1 (8%)	0
54	1w	69/76 (90%)	20 (28%)	0
54	2w	66/76 (86%)	16 (24%)	0
55	1x	74/77 (96%)	8 (10%)	0
55	2x	74/77 (96%)	9 (12%)	0
56	1y	72/76 (94%)	24 (33%)	0
56	2y	70/76 (92%)	17 (24%)	0
All	All	9339/9620 (97%)	1567 (16%)	50 (0%)

All (1567) 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	71	A
1	1A	74	A
1	1A	75	G
1	1A	84	A
1	1A	118	A
1	1A	119	A
1	1A	120	U
1	1A	154(A)	C
1	1A	196	A
1	1A	199	A
1	1A	205	G
1	1A	214	G
1	1A	215	G
1	1A	216	A
1	1A	222	A
1	1A	228	A
1	1A	229	A
1	1A	233	A
1	1A	248	G
1	1A	269	U
1	1A	271(K)	U
1	1A	271(L)	U
1	1A	271(M)	G
1	1A	271(O)	C
1	1A	271(S)	G
1	1A	272(A)	U
1	1A	272(B)	G
1	1A	272(H)	C
1	1A	274	G
1	1A	275	G
1	1A	279	C
1	1A	311	A
1	1A	329	G
1	1A	330	A
1	1A	352	G
1	1A	363	G
1	1A	363(A)	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	363(B)	G
1	1A	380	U
1	1A	386	G
1	1A	396	G
1	1A	405	U
1	1A	411	G
1	1A	428	A
1	1A	444	C
1	1A	448	U
1	1A	451	C
1	1A	454	A
1	1A	455	C
1	1A	456	C
1	1A	457	A
1	1A	479	A
1	1A	481	G
1	1A	494	G
1	1A	504	U
1	1A	505	A
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	563	G
1	1A	573	G
1	1A	575	A
1	1A	586	A
1	1A	592	G
1	1A	603	A
1	1A	604	G
1	1A	607	U
1	1A	614(A)	U
1	1A	614(B)	G
1	1A	615	G
1	1A	616	G
1	1A	627	A
1	1A	637	A
1	1A	645	C
1	1A	646	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	652(A)	A
1	1A	652(D)	C
1	1A	652(E)	G
1	1A	652(F)	G
1	1A	652(T)	C
1	1A	669	G
1	1A	686	G
1	1A	730	C
1	1A	740	U
1	1A	746	A
1	1A	747	U
1	1A	764	A
1	1A	774	A
1	1A	775	G
1	1A	776	G
1	1A	782	A
1	1A	783	A
1	1A	784	A
1	1A	785	G
1	1A	789	A
1	1A	790	C
1	1A	792	G
1	1A	805	G
1	1A	812	C
1	1A	819	A
1	1A	824	A
1	1A	827	U
1	1A	828	U
1	1A	855	G
1	1A	859	G
1	1A	866	A
1	1A	879	G
1	1A	880	G
1	1A	882	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	889	C
1	1A	890	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	894	C
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	915	C
1	1A	932	G
1	1A	945	A
1	1A	946	G
1	1A	953	A
1	1A	959	A
1	1A	961	C
1	1A	974	G
1	1A	975	C
1	1A	983	A
1	1A	996	A
1	1A	1005	C
1	1A	1012	U
1	1A	1013	C
1	1A	1025	G
1	1A	1026	U
1	1A	1033	U
1	1A	1038	C
1	1A	1041	C
1	1A	1043	C
1	1A	1045	A
1	1A	1046	A
1	1A	1047	G
1	1A	1054	A
1	1A	1055	G
1	1A	1057	A
1	1A	1058	G
1	1A	1059	G
1	1A	1063	G
1	1A	1066	U
1	1A	1069	A
1	1A	1070	A
1	1A	1071	G
1	1A	1073	A
1	1A	1075	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1076	C
1	1A	1078	U
1	1A	1079	C
1	1A	1081	U
1	1A	1083	U
1	1A	1087	G
1	1A	1088	A
1	1A	1089	G
1	1A	1090	U
1	1A	1091	G
1	1A	1093	G
1	1A	1094	U
1	1A	1099	G
1	1A	1100	C
1	1A	1101	U
1	1A	1110	G
1	1A	1111	A
1	1A	1112	G
1	1A	1115	G
1	1A	1116	C
1	1A	1117	G
1	1A	1128	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	1220	A
1	1A	1253	A
1	1A	1256	G
1	1A	1271	G
1	1A	1272	A
1	1A	1273	U
1	1A	1300	U
1	1A	1301	A
1	1A	1303	G
1	1A	1345	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	1445	A
1	1A	1450	G
1	1A	1455	G
1	1A	1461	G
1	1A	1467	C
1	1A	1473	G
1	1A	1482	G
1	1A	1493	C
1	1A	1494	A
1	1A	1508	A
1	1A	1509	C
1	1A	1509(A)	A
1	1A	1532	C
1	1A	1540	U
1	1A	1541	G
1	1A	1543	C
1	1A	1554	A
1	1A	1558	A
1	1A	1566	A
1	1A	1569	A
1	1A	1578	U
1	1A	1581	G
1	1A	1584	C
1	1A	1586	A
1	1A	1608	A
1	1A	1609	A
1	1A	1610	A
1	1A	1647	G
1	1A	1648	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1674	G
1	1A	1700	A
1	1A	1701	A
1	1A	1703	G
1	1A	1722	A
1	1A	1739	U
1	1A	1746	G
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	1847	A
1	1A	1861	G
1	1A	1877	A
1	1A	1878	G
1	1A	1889	A
1	1A	1900	A
1	1A	1906	G
1	1A	1929	G
1	1A	1930	G
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	1993	U
1	1A	1997	G
1	1A	2020	A
1	1A	2023	G
1	1A	2031	A
1	1A	2032	G
1	1A	2033	A
1	1A	2043	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	2098	U
1	1A	2101	G
1	1A	2108	C
1	1A	2110	G
1	1A	2112	G
1	1A	2113	U
1	1A	2116	G
1	1A	2119	A
1	1A	2121	G
1	1A	2122	U
1	1A	2126	A
1	1A	2127	G
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	2146	C
1	1A	2147	G
1	1A	2150	U
1	1A	2151	G
1	1A	2156	G
1	1A	2157	G
1	1A	2158	A
1	1A	2159	G
1	1A	2165	G
1	1A	2166	G
1	1A	2168	G
1	1A	2171	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	2207	G
1	1A	2208	A
1	1A	2218	U
1	1A	2219	G
1	1A	2225	A
1	1A	2235	G
1	1A	2238	G
1	1A	2239	G
1	1A	2268	A
1	1A	2269	A
1	1A	2273	A
1	1A	2283	C
1	1A	2287	A
1	1A	2305	A
1	1A	2307	G
1	1A	2308	G
1	1A	2312	U
1	1A	2313	C
1	1A	2320	A
1	1A	2325	G
1	1A	2334	G
1	1A	2336	A
1	1A	2347	C
1	1A	2354	G
1	1A	2361	A
1	1A	2379	G
1	1A	2383	G
1	1A	2385	C
1	1A	2405	G
1	1A	2406	U
1	1A	2407	G
1	1A	2422	A
1	1A	2423	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2425	A
1	1A	2429	G
1	1A	2430	A
1	1A	2431	U
1	1A	2435	A
1	1A	2439	A
1	1A	2441	C
1	1A	2448	A
1	1A	2474	C
1	1A	2476	A
1	1A	2478	A
1	1A	2502	G
1	1A	2505	G
1	1A	2518	A
1	1A	2529	G
1	1A	2535	G
1	1A	2554	U
1	1A	2566	A
1	1A	2567	G
1	1A	2573	C
1	1A	2578	G
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	2654	A
1	1A	2689	U
1	1A	2690	C
1	1A	2691	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	2758	A
1	1A	2764	A
1	1A	2765	A
1	1A	2778	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2790	A
1	1A	2791	C
1	1A	2792	G
1	1A	2793	G
1	1A	2794	C
1	1A	2802	G
1	1A	2804	C
1	1A	2810	A
1	1A	2820	A
1	1A	2821	A
1	1A	2835	A
1	1A	2872	G
1	1A	2880	C
1	1A	2892	A
1	1A	2894	G
1	1A	2895	U
2	1B	12	C
2	1B	32	C
2	1B	35	U
2	1B	56	G
2	1B	57	A
2	1B	73	A
2	1B	85	G
2	1B	110	G
32	1a	7	G
32	1a	9	G
32	1a	32	A
32	1a	39	G
32	1a	47	C
32	1a	48	C
32	1a	51	A
32	1a	52	G
32	1a	61	G
32	1a	70	G
32	1a	79	G
32	1a	91	C
32	1a	98	G
32	1a	101	A
32	1a	105	G
32	1a	115	G
32	1a	116	A
32	1a	120	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	121	C
32	1a	131	C
32	1a	145	G
32	1a	147	G
32	1a	162	A
32	1a	163	C
32	1a	174	C
32	1a	182	U
32	1a	189(J)	G
32	1a	195	A
32	1a	197	A
32	1a	199	G
32	1a	201	C
32	1a	202	U
32	1a	203	U
32	1a	204	U
32	1a	222	U
32	1a	247	G
32	1a	251	G
32	1a	266	G
32	1a	267	C
32	1a	289	G
32	1a	318	G
32	1a	328	C
32	1a	329	A
32	1a	332	G
32	1a	342	C
32	1a	348	G
32	1a	351	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	414	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	461	A
32	1a	470	C
32	1a	471	G
32	1a	474	G
32	1a	485	G
32	1a	496	A
32	1a	498	U
32	1a	505	G
32	1a	509	A
32	1a	510	A
32	1a	511	C
32	1a	518	C
32	1a	524	G
32	1a	527	7MG
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	628	G
32	1a	630	G
32	1a	653	A
32	1a	665	A
32	1a	687	A
32	1a	688	G
32	1a	695	A
32	1a	723	U
32	1a	724	G
32	1a	731	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	749	C
32	1a	752	G
32	1a	753	A
32	1a	755	G
32	1a	766	A
32	1a	777	A
32	1a	792	A
32	1a	793	U
32	1a	794	A
32	1a	815	A
32	1a	817	C
32	1a	821	G
32	1a	827	U
32	1a	828	A
32	1a	840	C
32	1a	841	U
32	1a	851	G
32	1a	870	U
32	1a	874	G
32	1a	876	G
32	1a	877	C
32	1a	914	A
32	1a	916	G
32	1a	926	G
32	1a	927	G
32	1a	934	C
32	1a	942	G
32	1a	958	A
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	1000	U
32	1a	1003	G
32	1a	1005	A
32	1a	1006	C
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	1039	C
32	1a	1044	A
32	1a	1045	C
32	1a	1053	G
32	1a	1068	G
32	1a	1081	G
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1121	U
32	1a	1123	A
32	1a	1125	U
32	1a	1134	G
32	1a	1137	C
32	1a	1138	G
32	1a	1139	G
32	1a	1146	A
32	1a	1152	A
32	1a	1159	U
32	1a	1183	A
32	1a	1184	G
32	1a	1196	U
32	1a	1197	G
32	1a	1202	G
32	1a	1214	C
32	1a	1227	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	1236	A
32	1a	1238	A
32	1a	1250	A
32	1a	1256	A
32	1a	1257	U
32	1a	1260	C
32	1a	1270	C
32	1a	1275	A
32	1a	1276	G
32	1a	1278	U
32	1a	1279	A
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	1305	G
32	1a	1312	G
32	1a	1320	C
32	1a	1322	C
32	1a	1338	G
32	1a	1340	A
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	1381	U
32	1a	1397	C
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
32	1a	1492	A
32	1a	1494	G
32	1a	1497	G
32	1a	1503	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	1504	G
32	1a	1506	U
32	1a	1517	G
32	1a	1519	MA6
32	1a	1529	G
32	1a	1530	G
32	1a	1532	U
53	1v	13	A
54	1w	2	C
54	1w	7	A
54	1w	8	4SU
54	1w	14	A
54	1w	19	G
54	1w	20	U
54	1w	21	A
54	1w	23	A
54	1w	24	G
54	1w	45	U
54	1w	46	7MG
54	1w	47	U
54	1w	48	C
54	1w	50	U
54	1w	62	C
54	1w	63	G
54	1w	64	A
54	1w	68	C
54	1w	70	G
54	1w	73	A
55	1x	9	G
55	1x	14	A
55	1x	18	G
55	1x	19	G
55	1x	21	A
55	1x	38	A
55	1x	47	U
55	1x	61	C
56	1y	6	G
56	1y	8	4SU
56	1y	9	A
56	1y	13	C
56	1y	14	A
56	1y	15	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
56	1y	19	G
56	1y	20	U
56	1y	21	A
56	1y	35	A
56	1y	36	A
56	1y	44	G
56	1y	45	U
56	1y	46	7MG
56	1y	48	C
56	1y	53	G
56	1y	54	5MU
56	1y	56	C
56	1y	57	G
56	1y	59	U
56	1y	64	A
56	1y	65	G
56	1y	69	G
56	1y	70	G
1	2A	8	A
1	2A	15	G
1	2A	16	G
1	2A	34	C
1	2A	35	G
1	2A	45	C
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	79	G
1	2A	84	A
1	2A	90	U
1	2A	94	C
1	2A	95	G
1	2A	100	G
1	2A	102	G
1	2A	118	A
1	2A	119	A
1	2A	120	U
1	2A	125	G
1	2A	154(A)	C
1	2A	157	U
1	2A	173	G
1	2A	181	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	221	A
1	2A	222	A
1	2A	225	A
1	2A	228	A
1	2A	229	A
1	2A	230	U
1	2A	232	G
1	2A	233	A
1	2A	248	G
1	2A	250	G
1	2A	264	C
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	277	C
1	2A	278	A
1	2A	304	G
1	2A	311	A
1	2A	317	G
1	2A	324	A
1	2A	327	G
1	2A	329	G
1	2A	330	A
1	2A	333	G
1	2A	352	G
1	2A	354	G
1	2A	363	G
1	2A	363(B)	G
1	2A	363(E)	U
1	2A	372	G
1	2A	380	U
1	2A	386	G
1	2A	399	G
1	2A	403	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	411	G
1	2A	421	U
1	2A	422	A
1	2A	444	C
1	2A	454	A
1	2A	455	C
1	2A	457	A
1	2A	481	G
1	2A	503	A
1	2A	504	U
1	2A	505	A
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	562	U
1	2A	563	G
1	2A	568	U
1	2A	573	G
1	2A	575	A
1	2A	588	U
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	626	U
1	2A	627	A
1	2A	634	C
1	2A	637	A
1	2A	645	C
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	669	G
1	2A	686	G
1	2A	715	G
1	2A	717	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	726	G
1	2A	730	C
1	2A	752	A
1	2A	753	C
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	805	G
1	2A	812	C
1	2A	819	A
1	2A	827	U
1	2A	828	U
1	2A	832	G
1	2A	857	C
1	2A	859	G
1	2A	874	G
1	2A	877	U
1	2A	878	A
1	2A	879	G
1	2A	880	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	896	A
1	2A	900	A
1	2A	901	A
1	2A	910	A
1	2A	914	C
1	2A	917	A
1	2A	919	G
1	2A	932	G
1	2A	941	A
1	2A	945	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	946	G
1	2A	953	A
1	2A	959	A
1	2A	961	C
1	2A	974	G
1	2A	975	C
1	2A	983	A
1	2A	996	A
1	2A	997	G
1	2A	999	U
1	2A	1012	U
1	2A	1013	C
1	2A	1017	G
1	2A	1021	A
1	2A	1022	G
1	2A	1023	U
1	2A	1025	G
1	2A	1026	U
1	2A	1027	A
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	1133	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	1210	A
1	2A	1211	U
1	2A	1212	G
1	2A	1220	A
1	2A	1221	C
1	2A	1229	G
1	2A	1241	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1242	A
1	2A	1244	G
1	2A	1248	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	1380	G
1	2A	1384	A
1	2A	1385	G
1	2A	1386	C
1	2A	1416	G
1	2A	1417	C
1	2A	1421	G
1	2A	1427	A
1	2A	1428	C
1	2A	1437	C
1	2A	1445	A
1	2A	1449	A
1	2A	1450	G
1	2A	1460	A
1	2A	1466	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1531	C
1	2A	1532	C
1	2A	1533	G
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	1586	A
1	2A	1608	A
1	2A	1609	A
1	2A	1610	A
1	2A	1616	A
1	2A	1647	G
1	2A	1648	C
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	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A
1	2A	1780	A
1	2A	1782	C
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1816	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	1889	A
1	2A	1900	A
1	2A	1906	G
1	2A	1914	C
1	2A	1929	G
1	2A	1930	G
1	2A	1936	A
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	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	2043	C
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2062	A
1	2A	2069	G
1	2A	2106	G
1	2A	2110	G
1	2A	2111	C
1	2A	2113	U
1	2A	2116	G
1	2A	2117	A
1	2A	2120	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	2131	G
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2135	A
1	2A	2137	C
1	2A	2138	C
1	2A	2139	C
1	2A	2140	C
1	2A	2141	G
1	2A	2142	C
1	2A	2146	C
1	2A	2150	U
1	2A	2156	G
1	2A	2157	G
1	2A	2158	A
1	2A	2159	G
1	2A	2161	C
1	2A	2165	G
1	2A	2166	G
1	2A	2167	U
1	2A	2168	G
1	2A	2170	A
1	2A	2172	U
1	2A	2174	C
1	2A	2176	A
1	2A	2178	C
1	2A	2182	G
1	2A	2185	C
1	2A	2189	U
1	2A	2192	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2218	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2225	A
1	2A	2239	G
1	2A	2269	A
1	2A	2275	C
1	2A	2278	A
1	2A	2280	G
1	2A	2283	C
1	2A	2287	A
1	2A	2288	A
1	2A	2298	A
1	2A	2305	A
1	2A	2308	G
1	2A	2312	U
1	2A	2315	G
1	2A	2319	G
1	2A	2320	A
1	2A	2325	G
1	2A	2327	A
1	2A	2334	G
1	2A	2336	A
1	2A	2341	G
1	2A	2346	A
1	2A	2347	C
1	2A	2350	C
1	2A	2354	G
1	2A	2376	A
1	2A	2379	G
1	2A	2383	G
1	2A	2385	C
1	2A	2388	A
1	2A	2403	C
1	2A	2406	U
1	2A	2425	A
1	2A	2429	G
1	2A	2430	A
1	2A	2434	A
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2445	G
1	2A	2448	A
1	2A	2460	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2465	C
1	2A	2469	A
1	2A	2476	A
1	2A	2490	G
1	2A	2491	U
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	2534	A
1	2A	2554	U
1	2A	2555	U
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2577	A
1	2A	2578	G
1	2A	2602	A
1	2A	2609	U
1	2A	2611	U
1	2A	2612	C
1	2A	2630	G
1	2A	2634	G
1	2A	2652	C
1	2A	2654	A
1	2A	2673	G
1	2A	2689	U
1	2A	2690	C
1	2A	2702	U
1	2A	2703	C
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	2751	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2757	A
1	2A	2758	A
1	2A	2761	G
1	2A	2764	A
1	2A	2765	A
1	2A	2766	G
1	2A	2778	A
1	2A	2789	C
1	2A	2793	G
1	2A	2803	C
1	2A	2820	A
1	2A	2821	A
1	2A	2835	A
1	2A	2850	A
1	2A	2872	G
1	2A	2880	C
1	2A	2892	A
1	2A	2894	G
1	2A	2897	U
2	2B	2	C
2	2B	8	U
2	2B	12	C
2	2B	17	C
2	2B	19	G
2	2B	33	G
2	2B	34	U
2	2B	35	U
2	2B	38	C
2	2B	41	U
2	2B	42	C
2	2B	56	G
2	2B	58	A
2	2B	67	G
2	2B	69	G
2	2B	73	A
2	2B	74	U
2	2B	75	G
2	2B	84	C
2	2B	85	G
2	2B	89	G
2	2B	106	G
2	2B	108	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2B	110	G
2	2B	111	G
2	2B	116	G
2	2B	120	A
32	2a	9	G
32	2a	16	A
32	2a	22	G
32	2a	26	A
32	2a	32	A
32	2a	39	G
32	2a	47	C
32	2a	48	C
32	2a	50	A
32	2a	51	A
32	2a	54	C
32	2a	65	U
32	2a	66	G
32	2a	73	G
32	2a	88	A
32	2a	89	C
32	2a	101	A
32	2a	116	A
32	2a	121	C
32	2a	131	C
32	2a	142	G
32	2a	143	A
32	2a	159	G
32	2a	163	C
32	2a	182	U
32	2a	189(F)	U
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	267	C
32	2a	289	G
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	349	A
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	384	G
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	412	A
32	2a	413	G
32	2a	414	A
32	2a	421	U
32	2a	423	G
32	2a	424	G
32	2a	429	U
32	2a	430	A
32	2a	441	A
32	2a	442	C
32	2a	452	A
32	2a	461	A
32	2a	470	C
32	2a	471	G
32	2a	484	G
32	2a	485	G
32	2a	496	A
32	2a	498	U
32	2a	499	A
32	2a	505	G
32	2a	509	A
32	2a	510	A
32	2a	511	C
32	2a	517	G
32	2a	518	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	521	G
32	2a	527	7MG
32	2a	531	U
32	2a	532	A
32	2a	533	A
32	2a	547	A
32	2a	559	A
32	2a	562	C
32	2a	564	C
32	2a	572	A
32	2a	573	A
32	2a	574	A
32	2a	575	G
32	2a	576	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	687	A
32	2a	688	G
32	2a	695	A
32	2a	702	A
32	2a	703	G
32	2a	720	C
32	2a	721	G
32	2a	723	U
32	2a	731	G
32	2a	742	G
32	2a	748	C
32	2a	749	C
32	2a	755	G
32	2a	760	G
32	2a	774	G
32	2a	777	A
32	2a	787	A
32	2a	792	A
32	2a	793	U
32	2a	794	A
32	2a	805	C
32	2a	816	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	817	C
32	2a	821	G
32	2a	828	A
32	2a	840	C
32	2a	841	U
32	2a	853	G
32	2a	855	G
32	2a	859	A
32	2a	871	U
32	2a	872	A
32	2a	887	G
32	2a	902	G
32	2a	914	A
32	2a	926	G
32	2a	927	G
32	2a	932	C
32	2a	934	C
32	2a	935	A
32	2a	942	G
32	2a	958	A
32	2a	960	U
32	2a	961	U
32	2a	963	G
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	984	C
32	2a	992	U
32	2a	993	G
32	2a	994	A
32	2a	995	C
32	2a	997	U
32	2a	999	C
32	2a	1001	A
32	2a	1002	G
32	2a	1003	G
32	2a	1004	A
32	2a	1005	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1006	C
32	2a	1009	G
32	2a	1011	G
32	2a	1012	U
32	2a	1016	A
32	2a	1017	G
32	2a	1020	U
32	2a	1021	G
32	2a	1022	G
32	2a	1023	G
32	2a	1025	U
32	2a	1026	G
32	2a	1027	C
32	2a	1028	C
32	2a	1029	C
32	2a	1030	C
32	2a	1030(A)	G
32	2a	1031	G
32	2a	1033	G
32	2a	1035	A
32	2a	1039	C
32	2a	1040	U
32	2a	1046	A
32	2a	1050	G
32	2a	1051	C
32	2a	1052	U
32	2a	1053	G
32	2a	1054	C
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1077	G
32	2a	1078	U
32	2a	1079	G
32	2a	1081	G
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	1105	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1108	G
32	2a	1109	C
32	2a	1113	C
32	2a	1122	U
32	2a	1124	G
32	2a	1125	U
32	2a	1129	C
32	2a	1130	A
32	2a	1132	C
32	2a	1133	G
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1146	A
32	2a	1147	C
32	2a	1149	C
32	2a	1152	A
32	2a	1157	A
32	2a	1158	C
32	2a	1159	U
32	2a	1172	C
32	2a	1182	G
32	2a	1184	G
32	2a	1191	A
32	2a	1196	U
32	2a	1197	G
32	2a	1202	G
32	2a	1207	2MG
32	2a	1211	U
32	2a	1212	U
32	2a	1213	A
32	2a	1219	U
32	2a	1227	A
32	2a	1236	A
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1261	A
32	2a	1262	C
32	2a	1264	C
32	2a	1270	C
32	2a	1272	G
32	2a	1273	G
32	2a	1277	C
32	2a	1279	A
32	2a	1280	A
32	2a	1283	G
32	2a	1287	A
32	2a	1293	G
32	2a	1294	G
32	2a	1299	A
32	2a	1300	G
32	2a	1302	U
32	2a	1303	C
32	2a	1305	G
32	2a	1306	A
32	2a	1313	U
32	2a	1320	C
32	2a	1323	G
32	2a	1336	C
32	2a	1346	A
32	2a	1347	G
32	2a	1350	A
32	2a	1354	C
32	2a	1363	C
32	2a	1364	U
32	2a	1368	G
32	2a	1370	G
32	2a	1397	C
32	2a	1406	U
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1442(B)	A
32	2a	1447	A
32	2a	1452	C
32	2a	1456	G
32	2a	1492	A
32	2a	1494	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1497	G
32	2a	1504	G
32	2a	1506	U
32	2a	1507	A
32	2a	1517	G
32	2a	1518	MA6
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
54	2w	3	C
54	2w	4	C
54	2w	11	C
54	2w	13	C
54	2w	14	A
54	2w	19	G
54	2w	22	G
54	2w	46	7MG
54	2w	47	U
54	2w	48	C
54	2w	62	C
54	2w	63	G
54	2w	69	G
54	2w	70	G
54	2w	71	G
54	2w	73	A
55	2x	9	G
55	2x	13	C
55	2x	18	G
55	2x	19	G
55	2x	21	A
55	2x	42	G
55	2x	47	U
55	2x	59	A
55	2x	61	C
56	2y	2	C
56	2y	15	G
56	2y	19	G
56	2y	25	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
56	2y	26	A
56	2y	27	G
56	2y	45	U
56	2y	48	C
56	2y	49	C
56	2y	52	G
56	2y	53	G
56	2y	54	5MU
56	2y	56	C
56	2y	58	A
56	2y	60	U
56	2y	69	G
56	2y	70	G

All (50) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	195	A
1	1A	196	A
1	1A	266	G
1	1A	278	A
1	1A	548	A
1	1A	746	A
1	1A	774	A
1	1A	974	G
1	1A	1067	A
1	1A	1142(A)	A
1	1A	1174	A
1	1A	1176	G
1	1A	1379	A
1	1A	1442	G
1	1A	1508	A
1	1A	1608	A
1	1A	1992	G
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	2629	A
1	1A	2689	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	827	U
1	2A	856	C
1	2A	900	A
1	2A	1026	U
1	2A	1210	A
1	2A	1240	U
1	2A	1379	A
1	2A	1420	U
1	2A	1442	G
1	2A	1530	C
1	2A	1653	G
1	2A	1913	A
1	2A	1992	G
1	2A	2119	A
1	2A	2126	A
1	2A	2689	U
1	2A	2756	U

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

86 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	$\# Z > 2$
1	PSU	1A	1911	1	18,21,22	1.43	2 (11%)	21,30,33	2.16	4 (19%)
54	4SU	2w	8	54	18,21,22	1.66	3 (16%)	25,30,33	2.15	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	M2G	1a	966	32	24,27,28	1.30	3 (12%)	33,40,43	1.89	5 (15%)
56	7MG	1y	46	56	23,26,27	1.33	4 (17%)	27,39,42	2.64	7 (25%)
1	PSU	1A	1917	1	18,21,22	1.37	3 (16%)	21,30,33	2.04	3 (14%)
32	PSU	2a	516	32	18,21,22	1.37	2 (11%)	21,30,33	1.98	4 (19%)
55	PSU	1x	55	55	18,21,22	1.33	2 (11%)	21,30,33	2.20	3 (14%)
1	OMG	1A	2251	57,1,55	23,26,27	1.26	3 (13%)	32,38,41	1.95	7 (21%)
56	5MU	2y	54	56	19,22,23	1.51	4 (21%)	27,32,35	1.98	8 (29%)
54	PSU	2w	39	54	18,21,22	1.37	2 (11%)	21,30,33	1.90	3 (14%)
55	5MU	1x	54	55	19,22,23	1.42	6 (31%)	27,32,35	1.82	6 (22%)
54	MIA	1w	37	54	28,31,32	2.28	6 (21%)	38,44,47	2.71	12 (31%)
1	PSU	1A	2605	57,1	18,21,22	1.43	4 (22%)	21,30,33	2.02	4 (19%)
56	4SU	2y	8	56	18,21,22	1.70	4 (22%)	25,30,33	2.17	5 (20%)
55	5MC	2x	32	55	19,22,23	1.63	3 (15%)	26,32,35	1.26	4 (15%)
1	PSU	2A	2605	1	18,21,22	1.31	3 (16%)	21,30,33	2.02	4 (19%)
54	4SU	1w	8	54	18,21,22	1.82	5 (27%)	25,30,33	2.02	4 (16%)
1	5MC	1A	1962	57,1	19,22,23	1.65	3 (15%)	26,32,35	1.14	3 (11%)
32	4OC	1a	1402	32	20,23,24	0.75	0	25,32,35	1.04	2 (8%)
54	PSU	2w	32	54	18,21,22	1.34	2 (11%)	21,30,33	1.95	3 (14%)
1	5MU	1A	1915	1	19,22,23	1.39	6 (31%)	27,32,35	2.20	6 (22%)
32	PSU	1a	516	32	18,21,22	1.44	2 (11%)	21,30,33	1.98	4 (19%)
55	5MU	2x	54	55	19,22,23	1.45	5 (26%)	27,32,35	2.15	6 (22%)
32	MA6	2a	1518	32	23,26,27	0.42	0	33,38,41	2.05	9 (27%)
32	5MC	2a	1407	32	19,22,23	1.69	3 (15%)	26,32,35	1.22	3 (11%)
1	5MU	2A	1939	57,1	19,22,23	1.42	5 (26%)	27,32,35	2.27	6 (22%)
54	7MG	1w	46	54	23,26,27	1.39	2 (8%)	27,39,42	2.55	7 (25%)
32	5MC	2a	967	32	19,22,23	1.71	3 (15%)	26,32,35	1.10	2 (7%)
1	PSU	2A	1917	1	18,21,22	1.39	2 (11%)	21,30,33	2.09	5 (23%)
56	PSU	1y	32	56	18,21,22	1.37	2 (11%)	21,30,33	1.99	3 (14%)
32	2MG	2a	1207	32	23,26,27	1.28	4 (17%)	33,38,41	2.11	6 (18%)
55	PSU	2x	55	55	18,21,22	1.39	2 (11%)	21,30,33	2.07	4 (19%)
56	PSU	1y	39	56	18,21,22	1.42	2 (11%)	21,30,33	1.89	3 (14%)
54	7MG	2w	46	54	23,26,27	1.36	2 (8%)	27,39,42	2.51	8 (29%)
1	5MC	2A	1962	1	19,22,23	1.65	3 (15%)	26,32,35	1.14	2 (7%)
54	PSU	2w	55	54	18,21,22	1.39	2 (11%)	21,30,33	2.01	3 (14%)
32	4OC	2a	1402	32,57	20,23,24	0.79	0	25,32,35	1.14	3 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMC	1A	1920	1	19,22,23	0.81	0	25,31,34	1.07	2 (8%)
1	OMC	2A	1920	1	19,22,23	0.77	0	25,31,34	0.84	0
32	5MC	2a	1400	32	19,22,23	1.67	3 (15%)	26,32,35	1.20	3 (11%)
32	5MC	2a	1404	32	19,22,23	1.67	3 (15%)	26,32,35	1.18	3 (11%)
55	4SU	2x	8	55	18,21,22	1.99	5 (27%)	25,30,33	1.49	5 (20%)
32	5MC	1a	1407	32	19,22,23	1.56	3 (15%)	26,32,35	1.16	3 (11%)
32	MA6	2a	1519	32	23,26,27	0.42	0	33,38,41	2.08	9 (27%)
54	5MU	2w	54	54	19,22,23	1.44	5 (26%)	27,32,35	1.76	6 (22%)
1	OMU	1A	2552	57,1	19,22,23	1.23	3 (15%)	25,31,34	1.81	5 (20%)
1	OMU	2A	2552	57,1	19,22,23	1.29	3 (15%)	25,31,34	1.99	6 (24%)
32	UR3	2a	1498	32	19,22,23	0.99	1 (5%)	26,32,35	1.79	3 (11%)
1	5MU	2A	1915	1	19,22,23	1.46	5 (26%)	27,32,35	2.05	6 (22%)
55	4SU	1x	8	55	18,21,22	2.05	6 (33%)	25,30,33	1.33	3 (12%)
54	MIA	2w	37	54	24,27,32	1.99	5 (20%)	32,39,47	2.50	10 (31%)
1	5MU	1A	1939	1	19,22,23	1.45	5 (26%)	27,32,35	2.12	7 (25%)
32	MA6	1a	1518	32	23,26,27	0.40	0	33,38,41	2.06	9 (27%)
56	MIA	2y	37	56	21,24,32	1.61	3 (14%)	30,35,47	2.09	10 (33%)
56	PSU	1y	55	56	18,21,22	1.34	2 (11%)	21,30,33	2.02	3 (14%)
56	PSU	2y	32	56	18,21,22	1.36	2 (11%)	21,30,33	2.01	3 (14%)
54	PSU	1w	55	54	18,21,22	1.45	2 (11%)	21,30,33	2.03	4 (19%)
1	2MA	1A	2503	57,1	22,25,26	1.54	4 (18%)	32,37,40	2.29	8 (25%)
54	PSU	1w	32	57,54	18,21,22	1.37	2 (11%)	21,30,33	1.94	3 (14%)
1	2MA	2A	2503	57,1	22,25,26	1.49	4 (18%)	32,37,40	2.34	8 (25%)
43	0TD	2l	92	43	8,9,10	4.57	1 (12%)	6,11,13	5.09	3 (50%)
32	7MG	1a	527	32,57	23,26,27	1.46	4 (17%)	27,39,42	2.54	7 (25%)
1	5MC	2A	1942	1	19,22,23	1.69	3 (15%)	26,32,35	1.18	2 (7%)
32	5MC	1a	1404	32	19,22,23	1.73	3 (15%)	26,32,35	1.13	3 (11%)
1	5MC	1A	1942	57,1	19,22,23	1.43	3 (15%)	26,32,35	1.20	2 (7%)
54	5MU	1w	54	54	19,22,23	1.39	5 (26%)	27,32,35	1.97	6 (22%)
1	OMG	2A	2251	1,55	23,26,27	1.20	3 (13%)	32,38,41	1.93	6 (18%)
32	7MG	2a	527	32,57	23,26,27	1.33	4 (17%)	27,39,42	2.62	7 (25%)
1	PSU	2A	1911	1	18,21,22	1.37	2 (11%)	21,30,33	1.95	3 (14%)
54	PSU	1w	39	54	18,21,22	1.29	2 (11%)	21,30,33	2.16	4 (19%)
55	31H	2x	76	57,55	31,34,35	1.18	3 (9%)	35,47,50	2.06	12 (34%)
43	0TD	1l	92	43	8,9,10	4.51	1 (12%)	6,11,13	5.91	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	M2G	2a	966	32	24,27,28	1.32	4 (16%)	33,40,43	1.97	6 (18%)
32	UR3	1a	1498	32	19,22,23	1.03	1 (5%)	26,32,35	1.80	3 (11%)
56	5MU	1y	54	56	19,22,23	1.46	4 (21%)	27,32,35	1.58	5 (18%)
32	5MC	1a	967	32	19,22,23	1.60	3 (15%)	26,32,35	1.14	2 (7%)
56	PSU	2y	39	56	18,21,22	1.35	2 (11%)	21,30,33	1.89	4 (19%)
56	4SU	1y	8	56	18,21,22	1.81	5 (27%)	25,30,33	2.11	4 (16%)
32	2MG	1a	1207	32	23,26,27	1.22	2 (8%)	33,38,41	2.31	9 (27%)
56	MIA	1y	37	56	21,24,32	1.61	3 (14%)	30,35,47	2.02	9 (30%)
55	31H	1x	76	57,55	31,34,35	1.15	3 (9%)	35,47,50	2.05	12 (34%)
32	MA6	1a	1519	32	23,26,27	0.43	0	33,38,41	2.14	9 (27%)
56	PSU	2y	55	56	18,21,22	1.34	3 (16%)	21,30,33	2.00	4 (19%)
56	7MG	2y	46	56	23,26,27	1.34	2 (8%)	27,39,42	2.71	7 (25%)
55	5MC	1x	32	55	19,22,23	1.84	3 (15%)	26,32,35	1.24	3 (11%)
32	5MC	1a	1400	32	19,22,23	1.67	3 (15%)	26,32,35	1.13	3 (11%)

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
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
56	7MG	1y	46	56	-	4/7/37/38	0/3/3/3
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	57,1,55	-	0/9/27/28	0/3/3/3
56	5MU	2y	54	56	-	3/7/25/26	0/2/2/2
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
55	5MU	1x	54	55	-	0/7/25/26	0/2/2/2
54	MIA	1w	37	54	-	4/15/33/34	0/3/3/3
1	PSU	1A	2605	57,1	-	0/7/25/26	0/2/2/2
56	4SU	2y	8	56	-	0/7/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	57,1	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	4OC	1a	1402	32	-	0/9/29/30	0/2/2/2
54	PSU	2w	32	54	-	2/7/25/26	0/2/2/2
1	5MU	1A	1915	1	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	1/11/29/30	0/3/3/3
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	57,1	-	0/7/25/26	0/2/2/2
54	7MG	1w	46	54	-	3/7/37/38	0/3/3/3
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	1/7/25/26	0/2/2/2
56	PSU	1y	32	56	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	4/9/27/28	0/3/3/3
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
56	PSU	1y	39	56	-	0/7/25/26	0/2/2/2
54	7MG	2w	46	54	-	1/7/37/38	0/3/3/3
1	5MC	2A	1962	1	-	2/7/25/26	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32,57	-	2/9/29/30	0/2/2/2
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
55	4SU	2x	8	55	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	3/11/29/30	0/3/3/3
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
1	OMU	1A	2552	57,1	-	0/9/27/28	0/2/2/2
1	OMU	2A	2552	57,1	-	0/9/27/28	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
54	MIA	2w	37	54	-	0/11/29/34	0/3/3/3
1	5MU	1A	1939	1	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3
56	MIA	2y	37	56	-	0/7/25/34	0/3/3/3
56	PSU	1y	55	56	-	1/7/25/26	0/2/2/2
56	PSU	2y	32	56	-	0/7/25/26	0/2/2/2
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
1	2MA	1A	2503	57,1	-	2/7/25/26	0/3/3/3
54	PSU	1w	32	57,54	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MA	2A	2503	57,1	-	1/7/25/26	0/3/3/3
43	0TD	2l	92	43	-	4/7/12/14	-
32	7MG	1a	527	32,57	-	3/7/37/38	0/3/3/3
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
1	5MC	1A	1942	57,1	-	0/7/25/26	0/2/2/2
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	1,55	-	0/9/27/28	0/3/3/3
32	7MG	2a	527	32,57	-	3/7/37/38	0/3/3/3
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
55	31H	2x	76	57,55	-	3/22/40/41	0/3/3/3
43	0TD	1l	92	43	-	2/7/12/14	-
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
56	5MU	1y	54	56	-	2/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
56	PSU	2y	39	56	-	0/7/25/26	0/2/2/2
56	4SU	1y	8	56	-	3/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	1/9/27/28	0/3/3/3
56	MIA	1y	37	56	-	0/7/25/34	0/3/3/3
55	31H	1x	76	57,55	-	4/22/40/41	0/3/3/3
32	MA6	1a	1519	32	-	3/11/29/30	0/3/3/3
56	PSU	2y	55	56	-	4/7/25/26	0/2/2/2
56	7MG	2y	46	56	-	3/7/37/38	0/3/3/3
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	2/7/25/26	0/2/2/2

All (247) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.52	1.69	1.82
43	1l	92	0TD	CB-SB	-12.30	1.69	1.82
54	1w	37	MIA	C13-C14	6.88	1.53	1.32
55	1x	32	5MC	C5-C4	6.83	1.49	1.44
54	1w	37	MIA	C2-S10	-6.39	1.70	1.75
32	1a	1404	5MC	C5-C4	6.37	1.48	1.44
32	2a	967	5MC	C5-C4	6.27	1.48	1.44
1	2A	1942	5MC	C5-C4	6.14	1.48	1.44
32	2a	1407	5MC	C5-C4	6.09	1.48	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1a	1400	5MC	C5-C4	6.07	1.48	1.44
32	2a	1400	5MC	C5-C4	6.06	1.48	1.44
32	2a	1404	5MC	C5-C4	6.04	1.48	1.44
1	2A	1962	5MC	C5-C4	5.97	1.48	1.44
1	1A	1962	5MC	C5-C4	5.95	1.48	1.44
54	2w	37	MIA	C2-S10	-5.81	1.70	1.75
32	1a	967	5MC	C5-C4	5.80	1.48	1.44
55	2x	32	5MC	C5-C4	5.69	1.48	1.44
32	1a	1407	5MC	C5-C4	5.67	1.48	1.44
56	1y	37	MIA	C5-C4	5.07	1.48	1.39
54	2w	37	MIA	C5-C4	5.01	1.48	1.39
56	2y	37	MIA	C5-C4	4.96	1.47	1.39
56	1y	8	4SU	C4-S4	-4.87	1.60	1.68
54	1w	37	MIA	C5-C4	4.83	1.47	1.39
54	1w	8	4SU	C4-S4	-4.80	1.60	1.68
1	1A	1942	5MC	C5-C4	4.74	1.47	1.44
56	2y	8	4SU	C4-S4	-4.65	1.60	1.68
55	1x	8	4SU	C4-N3	-4.62	1.32	1.37
1	1A	2503	2MA	C5-C4	4.51	1.47	1.39
55	2x	8	4SU	C4-N3	-4.51	1.33	1.37
54	2w	8	4SU	C4-S4	-4.50	1.60	1.68
55	2x	8	4SU	C4-S4	-4.36	1.61	1.68
55	1x	8	4SU	C4-S4	-4.30	1.61	1.68
1	2A	2503	2MA	C5-C4	4.29	1.46	1.39
54	1w	55	PSU	C6-C5	4.16	1.39	1.35
56	1y	39	PSU	C6-C5	4.05	1.39	1.35
54	2w	55	PSU	C6-C5	3.97	1.39	1.35
54	2w	46	7MG	C4-N9	-3.96	1.33	1.37
32	1a	527	7MG	C4-N9	-3.92	1.33	1.37
56	1y	32	PSU	C6-C5	3.90	1.39	1.35
32	1a	516	PSU	C6-C5	3.89	1.39	1.35
56	2y	32	PSU	C6-C5	3.86	1.39	1.35
55	2x	55	PSU	C6-C5	3.82	1.39	1.35
55	1x	76	31H	C5-N7	-3.81	1.32	1.39
55	2x	76	31H	C5-N7	-3.81	1.32	1.39
32	2a	516	PSU	C6-C5	3.74	1.39	1.35
54	2w	32	PSU	C6-C5	3.74	1.39	1.35
54	2w	39	PSU	C6-C5	3.68	1.39	1.35
54	1w	46	7MG	C4-N9	-3.65	1.33	1.37
1	1A	1911	PSU	C6-C5	3.61	1.39	1.35
56	2y	39	PSU	C6-C5	3.60	1.39	1.35
55	1x	8	4SU	C2-N3	-3.59	1.31	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	2605	PSU	C6-C5	3.58	1.39	1.35
1	2A	1917	PSU	C6-C5	3.56	1.39	1.35
56	2y	46	7MG	C5-C4	3.55	1.48	1.37
54	1w	32	PSU	C6-C5	3.52	1.39	1.35
1	1A	1917	PSU	C6-C5	3.52	1.39	1.35
54	1w	46	7MG	C5-C4	3.47	1.48	1.37
56	1y	46	7MG	C5-C4	3.45	1.48	1.37
56	1y	8	4SU	C4-N3	-3.43	1.34	1.37
54	1w	39	PSU	C6-C5	3.39	1.39	1.35
32	2a	966	M2G	C5-C4	3.36	1.48	1.38
32	1a	527	7MG	C5-C4	3.36	1.48	1.37
56	1y	55	PSU	C6-C5	3.33	1.39	1.35
55	2x	76	31H	C5-C4	-3.31	1.33	1.39
32	2a	1207	2MG	C5-C4	3.30	1.47	1.38
54	2w	46	7MG	C5-C4	3.28	1.47	1.37
32	2a	527	7MG	C5-C4	3.28	1.47	1.37
56	2y	54	5MU	C2-N1	3.27	1.43	1.38
55	1x	55	PSU	C6-C5	3.26	1.38	1.35
1	1A	2251	OMG	C5-C4	3.25	1.47	1.38
56	2y	55	PSU	C6-C5	3.23	1.38	1.35
1	2A	1911	PSU	C6-C5	3.22	1.38	1.35
55	1x	8	4SU	C5-C4	-3.22	1.38	1.42
1	1A	2605	PSU	C6-C5	3.22	1.38	1.35
55	1x	76	31H	C5-C4	-3.15	1.33	1.39
32	1a	966	M2G	C5-C4	3.14	1.47	1.38
54	1w	8	4SU	C4-N3	-3.13	1.34	1.37
1	2A	2251	OMG	C5-C4	3.09	1.47	1.38
55	2x	8	4SU	C2-N3	-3.08	1.32	1.38
1	2A	1915	5MU	C6-C5	3.08	1.39	1.34
56	2y	54	5MU	C6-C5	3.03	1.39	1.34
1	2A	1942	5MC	C6-C5	3.01	1.39	1.34
55	2x	54	5MU	C6-C5	3.01	1.39	1.34
32	2a	527	7MG	C4-N9	-3.01	1.34	1.37
56	1y	54	5MU	C6-C5	3.00	1.39	1.34
54	2w	37	MIA	C5-C6	2.99	1.49	1.41
32	1a	1207	2MG	C5-C4	2.98	1.46	1.38
54	2w	8	4SU	C4-N3	-2.96	1.34	1.37
56	1y	37	MIA	C5-C6	2.96	1.49	1.41
32	2a	1404	5MC	C6-C5	2.96	1.39	1.34
1	1A	1942	5MC	C6-C5	2.95	1.39	1.34
1	1A	1939	5MU	C2-N3	-2.93	1.32	1.38
54	2w	54	5MU	C6-C5	2.90	1.39	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	2y	37	MIA	C5-C6	2.90	1.49	1.41
32	1a	1400	5MC	C6-C5	2.89	1.39	1.34
55	2x	8	4SU	C5-C4	-2.89	1.39	1.42
56	1y	54	5MU	C4-N3	-2.86	1.33	1.38
32	2a	966	M2G	C2-N2	2.86	1.40	1.35
55	2x	32	5MC	C6-C5	2.85	1.39	1.34
1	1A	1911	PSU	C4-N3	-2.85	1.33	1.38
54	1w	54	5MU	C6-C5	2.83	1.39	1.34
1	1A	2605	PSU	C4-N3	-2.81	1.33	1.38
32	2a	967	5MC	C6-C5	2.81	1.39	1.34
1	1A	1939	5MU	C4-N3	-2.80	1.33	1.38
1	2A	1939	5MU	C4-N3	-2.80	1.33	1.38
55	1x	54	5MU	C6-C5	2.80	1.39	1.34
54	1w	37	MIA	C5-C6	2.78	1.48	1.41
55	1x	54	5MU	C4-N3	-2.78	1.33	1.38
32	1a	1404	5MC	C6-C5	2.77	1.39	1.34
1	2A	2552	OMU	C4-N3	-2.77	1.33	1.38
55	1x	32	5MC	C6-C5	2.75	1.39	1.34
1	1A	1962	5MC	C6-C5	2.72	1.39	1.34
1	1A	2552	OMU	C4-N3	-2.72	1.34	1.38
1	2A	1962	5MC	C6-C5	2.72	1.39	1.34
1	2A	1939	5MU	C6-C5	2.72	1.39	1.34
1	1A	1939	5MU	C6-N1	-2.69	1.33	1.38
32	2a	1407	5MC	C6-C5	2.68	1.39	1.34
1	1A	2503	2MA	C5-C6	2.67	1.48	1.41
1	2A	1911	PSU	C4-N3	-2.67	1.33	1.38
32	1a	966	M2G	C6-N1	-2.66	1.33	1.38
1	2A	1917	PSU	C4-N3	-2.65	1.33	1.38
1	2A	1939	5MU	C2-N3	-2.65	1.33	1.38
1	1A	1915	5MU	C4-N3	-2.64	1.33	1.38
32	1a	516	PSU	C4-N3	-2.64	1.33	1.38
32	2a	1400	5MC	C6-C5	2.63	1.38	1.34
32	1a	967	5MC	C6-C5	2.63	1.38	1.34
1	2A	1915	5MU	C4-N3	-2.63	1.33	1.38
56	2y	8	4SU	C4-N3	-2.62	1.34	1.37
56	2y	8	4SU	C5-C4	-2.62	1.39	1.42
55	2x	54	5MU	C4-C5	2.61	1.49	1.44
32	1a	966	M2G	C2-N2	2.60	1.39	1.35
1	1A	1939	5MU	C6-C5	2.60	1.38	1.34
55	2x	54	5MU	C4-N3	-2.60	1.34	1.38
1	2A	2552	OMU	C5-C4	2.60	1.49	1.43
1	1A	1915	5MU	C2-N1	2.59	1.42	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1x	76	31H	C5-C6	-2.59	1.33	1.41
54	1w	54	5MU	C4-N3	-2.57	1.34	1.38
32	1a	1407	5MC	C6-C5	2.57	1.38	1.34
1	2A	1915	5MU	C4-C5	2.57	1.49	1.44
1	1A	1917	PSU	C4-N3	-2.54	1.34	1.38
56	2y	37	MIA	C8-N7	2.54	1.36	1.31
56	2y	39	PSU	C4-N3	-2.53	1.34	1.38
32	1a	527	7MG	C8-N9	2.53	1.47	1.45
1	1A	2251	OMG	C5-N7	-2.53	1.34	1.39
55	1x	32	5MC	C6-N1	-2.51	1.33	1.38
54	2w	54	5MU	C4-N3	-2.50	1.34	1.38
54	2w	39	PSU	C4-N3	-2.50	1.34	1.38
54	1w	8	4SU	C2-N1	2.50	1.42	1.38
54	1w	32	PSU	C4-N3	-2.49	1.34	1.38
56	1y	37	MIA	C8-N7	2.49	1.36	1.31
1	2A	2503	2MA	C5-N7	-2.48	1.34	1.39
54	1w	55	PSU	C4-N3	-2.48	1.34	1.38
1	2A	1939	5MU	C6-N1	-2.48	1.33	1.38
56	1y	39	PSU	C4-N3	-2.47	1.34	1.38
56	1y	32	PSU	C4-N3	-2.47	1.34	1.38
32	1a	1498	UR3	C2-N1	2.47	1.41	1.38
56	2y	54	5MU	C4-N3	-2.46	1.34	1.38
32	1a	1207	2MG	C6-N1	-2.45	1.34	1.38
1	1A	1915	5MU	C6-C5	2.45	1.38	1.34
32	2a	1207	2MG	C6-N1	-2.45	1.34	1.38
1	1A	1962	5MC	C6-N1	-2.44	1.33	1.38
56	2y	32	PSU	C4-N3	-2.44	1.34	1.38
54	2w	55	PSU	C4-N3	-2.44	1.34	1.38
54	1w	37	MIA	C8-N7	2.43	1.36	1.31
54	2w	54	5MU	C4-C5	2.43	1.48	1.44
55	2x	55	PSU	C4-N3	-2.43	1.34	1.38
54	1w	8	4SU	C5-C4	-2.43	1.39	1.42
1	2A	2251	OMG	C6-N1	-2.42	1.34	1.38
32	2a	1407	5MC	C6-N1	-2.42	1.33	1.38
55	2x	76	31H	C5-C6	-2.42	1.34	1.41
1	1A	2251	OMG	C6-N1	-2.40	1.34	1.38
56	1y	55	PSU	C4-N3	-2.39	1.34	1.38
56	2y	54	5MU	C4-C5	2.38	1.48	1.44
54	2w	54	5MU	C2-N1	2.38	1.42	1.38
1	2A	2503	2MA	C5-C6	2.37	1.47	1.41
32	2a	966	M2G	C6-N1	-2.37	1.34	1.38
54	1w	54	5MU	C4-C5	2.36	1.48	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	2x	54	5MU	C2-N1	2.36	1.42	1.38
32	2a	1207	2MG	C2-N3	2.35	1.36	1.32
56	2y	55	PSU	C4-N3	-2.35	1.34	1.38
1	2A	1915	5MU	C2-N1	2.32	1.42	1.38
1	1A	2605	PSU	C2-N3	-2.32	1.33	1.37
32	2a	1400	5MC	C6-N1	-2.32	1.34	1.38
56	1y	54	5MU	C4-C5	2.30	1.48	1.44
56	1y	46	7MG	C4-N9	-2.30	1.35	1.37
1	2A	2251	OMG	C5-N7	-2.29	1.34	1.39
54	2w	37	MIA	C8-N7	2.29	1.36	1.31
32	2a	516	PSU	C4-N3	-2.29	1.34	1.38
56	1y	8	4SU	C2-N3	-2.29	1.34	1.38
1	2A	1962	5MC	C6-N1	-2.28	1.34	1.38
54	2w	32	PSU	C4-N3	-2.28	1.34	1.38
56	1y	46	7MG	C6-N1	-2.28	1.34	1.38
1	1A	1915	5MU	C4-C5	2.26	1.48	1.44
1	1A	2503	2MA	C5-N7	-2.26	1.35	1.39
1	1A	1939	5MU	C4-C5	2.26	1.48	1.44
54	1w	39	PSU	C4-N3	-2.24	1.34	1.38
56	1y	8	4SU	C5-C4	-2.24	1.39	1.42
56	2y	8	4SU	C2-N1	2.24	1.42	1.38
56	1y	54	5MU	C2-N1	2.23	1.42	1.38
32	1a	1404	5MC	C6-N1	-2.22	1.34	1.38
54	2w	8	4SU	C5-C4	-2.22	1.39	1.42
55	2x	32	5MC	C6-N1	-2.22	1.34	1.38
54	1w	37	MIA	C5-N7	-2.22	1.35	1.39
32	1a	527	7MG	C6-N1	-2.22	1.34	1.38
55	1x	54	5MU	C4-C5	2.21	1.48	1.44
56	2y	46	7MG	C6-N1	-2.21	1.34	1.38
32	1a	1400	5MC	C6-N1	-2.20	1.34	1.38
1	1A	2503	2MA	C8-N7	2.20	1.35	1.31
1	2A	1942	5MC	C6-N1	-2.18	1.34	1.38
1	1A	1915	5MU	C6-N1	-2.18	1.34	1.38
32	1a	967	5MC	C6-N1	-2.17	1.34	1.38
1	2A	2503	2MA	C8-N7	2.17	1.35	1.31
54	2w	37	MIA	C5-N7	-2.16	1.35	1.39
1	1A	2552	OMU	C5-C4	2.16	1.48	1.43
32	2a	527	7MG	C6-N1	-2.16	1.34	1.38
56	1y	46	7MG	C8-N9	2.16	1.47	1.45
55	1x	54	5MU	C2-N3	-2.16	1.34	1.38
32	2a	527	7MG	C5-C6	2.15	1.48	1.43
1	2A	2605	PSU	C4-N3	-2.15	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2w	54	5MU	C2-N3	-2.14	1.34	1.38
55	1x	8	4SU	O2-C2	2.13	1.26	1.23
32	2a	1498	UR3	C6-C5	2.13	1.40	1.35
55	1x	54	5MU	C2-N1	2.11	1.41	1.38
55	2x	8	4SU	C2-N1	2.11	1.41	1.38
32	2a	967	5MC	C6-N1	-2.11	1.34	1.38
1	1A	2605	PSU	C2-N1	-2.10	1.33	1.36
54	1w	8	4SU	C2-N3	-2.10	1.34	1.38
1	1A	1942	5MC	C6-N1	-2.10	1.34	1.38
1	2A	1915	5MU	C6-N1	-2.09	1.34	1.38
1	1A	1915	5MU	C2-N3	-2.08	1.34	1.38
32	2a	966	M2G	C5-N7	-2.08	1.34	1.39
1	1A	1917	PSU	C2-N3	-2.08	1.34	1.37
1	1A	2552	OMU	C6-C5	2.08	1.39	1.35
55	1x	54	5MU	C6-N1	-2.08	1.34	1.38
32	1a	1407	5MC	C6-N1	-2.08	1.34	1.38
1	2A	1939	5MU	C4-C5	2.07	1.48	1.44
1	2A	2605	PSU	C2-N3	-2.07	1.34	1.37
54	1w	54	5MU	C2-N3	-2.06	1.34	1.38
55	2x	54	5MU	C6-N1	-2.06	1.34	1.38
32	2a	1207	2MG	C5-N7	-2.06	1.34	1.39
54	1w	54	5MU	C2-N1	2.06	1.41	1.38
1	2A	2552	OMU	C6-C5	2.05	1.39	1.35
55	1x	8	4SU	C6-C5	2.05	1.39	1.35
32	2a	1404	5MC	C6-N1	-2.05	1.34	1.38
55	1x	55	PSU	C4-N3	-2.04	1.35	1.38
56	2y	55	PSU	C2-N1	-2.01	1.34	1.36
56	1y	8	4SU	C6-C5	2.00	1.39	1.35

All (432) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	-13.89	77.39	102.36
43	2l	92	0TD	CSB-SB-CB	-11.47	81.74	102.36
56	2y	46	7MG	N9-C4-N3	9.49	139.37	125.46
56	1y	46	7MG	N9-C4-N3	9.26	139.03	125.46
54	1w	37	MIA	C12-C13-C14	-8.77	111.27	127.01
54	2w	37	MIA	C5-C4-N3	-8.76	117.95	127.18
32	2a	527	7MG	N9-C4-N3	8.68	138.18	125.46
32	1a	527	7MG	N9-C4-N3	8.61	138.08	125.46
54	1w	46	7MG	N9-C4-N3	8.60	138.06	125.46
1	2A	2503	2MA	C5-C4-N3	-7.99	118.76	127.18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1w	37	MIA	C5-C4-N3	-7.83	118.93	127.18
54	2w	46	7MG	N9-C4-N3	7.82	136.92	125.46
1	1A	2503	2MA	C5-C4-N3	-7.71	119.06	127.18
32	2a	1498	UR3	C4-N3-C2	-7.28	118.72	124.58
32	1a	1207	2MG	C2-N3-C4	7.27	121.09	112.00
54	2w	37	MIA	N3-C4-N9	6.98	135.85	126.99
1	1A	1911	PSU	N1-C2-N3	6.86	122.40	115.17
32	2a	1207	2MG	C2-N3-C4	6.84	120.56	112.00
32	1a	1498	UR3	C4-N3-C2	-6.82	119.09	124.58
1	2A	1917	PSU	N1-C2-N3	6.81	122.35	115.17
1	2A	2503	2MA	N3-C4-N9	6.74	135.55	126.99
55	1x	55	PSU	N1-C2-N3	6.74	122.28	115.17
32	2a	966	M2G	C5-C4-N3	-6.68	117.76	128.39
55	2x	55	PSU	N1-C2-N3	6.62	122.16	115.17
54	2w	8	4SU	C4-N3-C2	-6.55	121.03	127.31
1	1A	2503	2MA	N3-C4-N9	6.54	135.29	126.99
56	1y	8	4SU	C4-N3-C2	-6.45	121.13	127.31
1	1A	2605	PSU	N1-C2-N3	6.41	121.93	115.17
54	1w	39	PSU	N1-C2-N3	6.41	121.92	115.17
56	2y	32	PSU	N1-C2-N3	6.28	121.79	115.17
32	2a	1207	2MG	C5-C4-N3	-6.24	118.45	128.39
56	1y	55	PSU	N1-C2-N3	6.24	121.75	115.17
32	1a	516	PSU	N1-C2-N3	6.23	121.74	115.17
56	2y	55	PSU	N1-C2-N3	6.18	121.69	115.17
1	1A	1917	PSU	N1-C2-N3	6.16	121.67	115.17
56	1y	32	PSU	N1-C2-N3	6.15	121.66	115.17
32	2a	516	PSU	N1-C2-N3	6.11	121.62	115.17
54	2w	55	PSU	N1-C2-N3	6.07	121.58	115.17
32	1a	966	M2G	C5-C4-N3	-6.07	118.73	128.39
54	2w	32	PSU	N1-C2-N3	6.06	121.56	115.17
54	1w	55	PSU	N1-C2-N3	6.04	121.54	115.17
1	2A	1911	PSU	N1-C2-N3	6.03	121.53	115.17
54	1w	32	PSU	N1-C2-N3	6.02	121.52	115.17
54	1w	37	MIA	N3-C4-N9	6.01	134.62	126.99
55	2x	76	31H	N1-C2-N3	-6.01	119.49	128.58
1	1A	2251	OMG	C5-C4-N3	-6.00	118.84	128.39
56	2y	8	4SU	C4-N3-C2	-5.98	121.58	127.31
1	2A	2605	PSU	N1-C2-N3	5.95	121.45	115.17
56	1y	39	PSU	N1-C2-N3	5.95	121.45	115.17
32	1a	1207	2MG	C5-C4-N3	-5.94	118.94	128.39
54	2w	39	PSU	N1-C2-N3	5.93	121.42	115.17
1	2A	2251	OMG	C5-C4-N3	-5.89	119.02	128.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1w	8	4SU	C4-N3-C2	-5.86	121.70	127.31
56	2y	39	PSU	N1-C2-N3	5.79	121.27	115.17
54	2w	46	7MG	N9-C8-N7	-5.77	95.21	103.37
55	1x	76	31H	N1-C2-N3	-5.75	119.88	128.58
56	1y	37	MIA	C5-C4-N3	-5.71	118.85	126.72
1	2A	1939	5MU	C4-N3-C2	-5.63	119.95	127.34
1	2A	2552	OMU	N3-C2-N1	5.60	122.18	114.89
56	1y	8	4SU	C5-C4-N3	5.59	119.95	114.75
56	2y	37	MIA	C5-C4-N3	-5.59	119.03	126.72
32	2a	527	7MG	N9-C8-N7	-5.57	95.48	103.37
54	1w	8	4SU	C5-C4-N3	5.55	119.91	114.75
56	1y	46	7MG	C5-C4-N3	-5.53	117.75	128.13
56	2y	46	7MG	C5-C4-N3	-5.52	117.76	128.13
54	1w	46	7MG	N9-C8-N7	-5.45	95.66	103.37
55	2x	54	5MU	N3-C2-N1	5.42	121.94	114.89
1	1A	2552	OMU	N3-C2-N1	5.40	121.92	114.89
1	1A	1915	5MU	C4-N3-C2	-5.36	120.31	127.34
56	2y	8	4SU	C5-C4-N3	5.30	119.68	114.75
55	2x	54	5MU	C4-N3-C2	-5.28	120.41	127.34
32	2a	966	M2G	N9-C4-N3	5.28	136.51	125.95
54	2w	8	4SU	C5-C4-N3	5.28	119.66	114.75
32	2a	527	7MG	C5-C4-N3	-5.25	118.27	128.13
1	2A	1915	5MU	N3-C2-N1	5.19	121.65	114.89
1	2A	1939	5MU	C5-C4-N3	5.18	119.83	115.32
32	2a	1518	MA6	N1-C2-N3	-5.17	120.76	128.58
32	1a	527	7MG	C5-C4-N3	-5.15	118.46	128.13
56	2y	46	7MG	N9-C8-N7	-5.13	96.10	103.37
1	2A	1939	5MU	N3-C2-N1	5.13	121.57	114.89
55	2x	76	31H	C5-C4-N3	-5.04	119.77	126.72
1	1A	1915	5MU	N3-C2-N1	5.03	121.43	114.89
55	1x	76	31H	C5-C4-N3	-5.01	119.82	126.72
32	1a	1519	MA6	N1-C2-N3	-5.01	121.00	128.58
1	2A	1915	5MU	C4-N3-C2	-5.00	120.78	127.34
1	1A	2251	OMG	C2-N3-C4	4.95	120.82	112.30
1	1A	1915	5MU	C5-C4-N3	4.95	119.62	115.32
1	1A	1939	5MU	C4-N3-C2	-4.93	120.87	127.34
32	1a	527	7MG	N9-C8-N7	-4.93	96.39	103.37
56	1y	46	7MG	N9-C8-N7	-4.93	96.39	103.37
54	1w	46	7MG	C5-C4-N3	-4.87	119.00	128.13
32	2a	1519	MA6	N1-C2-N3	-4.86	121.23	128.58
32	1a	1518	MA6	N1-C2-N3	-4.80	121.32	128.58
1	1A	1939	5MU	C5-C4-N3	4.77	119.47	115.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2251	OMG	N9-C4-N3	4.76	135.47	125.95
54	1w	54	5MU	N3-C2-N1	4.73	121.05	114.89
1	2A	2251	OMG	N9-C4-N3	4.73	135.41	125.95
54	1w	54	5MU	C4-N3-C2	-4.72	121.16	127.34
32	2a	1519	MA6	C5-C4-N3	-4.69	120.26	126.72
1	2A	2251	OMG	C2-N3-C4	4.69	120.38	112.30
32	1a	966	M2G	N9-C4-N3	4.67	135.30	125.95
54	1w	39	PSU	C4-N3-C2	-4.66	119.95	126.37
1	2A	2552	OMU	C4-N3-C2	-4.64	120.85	126.61
32	2a	966	M2G	C2-N3-C4	4.64	121.09	112.51
55	1x	55	PSU	O2-C2-N1	-4.60	118.05	122.79
55	1x	54	5MU	N3-C2-N1	4.59	120.87	114.89
56	2y	8	4SU	C5-C4-S4	-4.59	119.06	124.31
56	2y	46	7MG	C2-N3-C4	4.58	120.19	112.30
32	2a	1207	2MG	N9-C4-N3	4.56	135.07	125.95
54	2w	46	7MG	C5-C4-N3	-4.53	119.63	128.13
32	1a	1519	MA6	C5-C4-N3	-4.52	120.49	126.72
32	2a	527	7MG	C2-N3-C4	4.49	120.03	112.30
56	1y	46	7MG	C2-N3-C4	4.48	120.02	112.30
32	2a	1518	MA6	C5-C4-N3	-4.47	120.56	126.72
56	2y	54	5MU	C4-N3-C2	-4.47	121.48	127.34
56	2y	37	MIA	N3-C4-N9	4.46	134.75	127.17
56	1y	37	MIA	N3-C4-N9	4.46	134.75	127.17
56	2y	54	5MU	C5-C4-N3	4.44	119.18	115.32
32	1a	1518	MA6	C5-C4-N3	-4.43	120.61	126.72
1	2A	1939	5MU	C5-C6-N1	-4.41	118.53	123.31
56	2y	54	5MU	N3-C2-N1	4.39	120.60	114.89
1	1A	1939	5MU	N3-C2-N1	4.38	120.60	114.89
1	2A	1939	5MU	O4-C4-C5	-4.38	119.91	124.92
54	1w	54	5MU	C5-C4-N3	4.37	119.12	115.32
32	1a	966	M2G	C2-N3-C4	4.33	120.52	112.51
1	2A	2605	PSU	C4-N3-C2	-4.31	120.44	126.37
54	2w	8	4SU	N3-C2-N1	4.30	120.48	114.89
32	1a	527	7MG	C2-N3-C4	4.29	119.69	112.30
1	1A	1939	5MU	C5-C6-N1	-4.29	118.65	123.31
1	1A	1911	PSU	C4-N3-C2	-4.27	120.49	126.37
55	2x	54	5MU	C5-C4-N3	4.23	119.00	115.32
1	2A	1915	5MU	C5-C4-N3	4.21	118.98	115.32
54	1w	37	MIA	C15-C14-C13	-4.20	110.05	122.66
54	2w	46	7MG	C2-N3-C4	4.20	119.53	112.30
1	1A	1915	5MU	O4-C4-C5	-4.20	120.12	124.92
56	1y	8	4SU	N3-C2-N1	4.18	120.34	114.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1w	39	PSU	O2-C2-N1	-4.18	118.48	122.79
1	1A	2552	OMU	C4-N3-C2	-4.17	121.44	126.61
55	2x	55	PSU	C4-N3-C2	-4.15	120.65	126.37
1	1A	1917	PSU	C4-N3-C2	-4.12	120.69	126.37
55	1x	54	5MU	C4-N3-C2	-4.11	121.94	127.34
32	1a	1519	MA6	C5-N7-C8	4.10	109.90	103.45
55	1x	55	PSU	C4-N3-C2	-4.10	120.72	126.37
32	1a	1207	2MG	C6-C5-N7	4.08	137.72	130.29
32	2a	1518	MA6	C2-N1-C6	4.07	121.78	111.83
1	2A	1917	PSU	C4-N3-C2	-4.06	120.77	126.37
54	1w	46	7MG	C2-N3-C4	4.05	119.27	112.30
32	1a	1519	MA6	C4-C5-N7	-4.04	105.97	110.58
54	2w	54	5MU	N3-C2-N1	4.04	120.15	114.89
56	1y	32	PSU	C4-N3-C2	-4.03	120.81	126.37
32	1a	1518	MA6	C2-N1-C6	4.03	121.67	111.83
32	2a	1519	MA6	C4-C5-N7	-4.02	105.99	110.58
56	2y	54	5MU	O4-C4-C5	-4.01	120.33	124.92
56	2y	55	PSU	O2-C2-N1	-4.01	118.65	122.79
56	1y	55	PSU	O2-C2-N1	-3.97	118.69	122.79
54	2w	55	PSU	C4-N3-C2	-3.96	120.91	126.37
32	1a	1518	MA6	C5-N7-C8	3.95	109.65	103.45
32	2a	1519	MA6	C2-N1-C6	3.94	121.46	111.83
32	1a	1519	MA6	C2-N1-C6	3.94	121.46	111.83
56	2y	32	PSU	C4-N3-C2	-3.94	120.94	126.37
1	1A	1911	PSU	O2-C2-N1	-3.91	118.76	122.79
1	1A	1939	5MU	O4-C4-C5	-3.90	120.45	124.92
56	1y	55	PSU	C4-N3-C2	-3.89	121.01	126.37
32	2a	1519	MA6	C5-N7-C8	3.89	109.56	103.45
54	2w	32	PSU	C4-N3-C2	-3.89	121.02	126.37
55	1x	32	5MC	C5-C6-N1	-3.87	119.11	123.31
54	1w	55	PSU	O2-C2-N1	-3.86	118.81	122.79
56	1y	54	5MU	N3-C2-N1	3.85	119.90	114.89
1	1A	2605	PSU	C4-N3-C2	-3.85	121.07	126.37
54	2w	54	5MU	C4-N3-C2	-3.84	122.30	127.34
54	2w	54	5MU	C5-C4-N3	3.84	118.66	115.32
54	1w	54	5MU	O4-C4-C5	-3.83	120.53	124.92
32	2a	516	PSU	C4-N3-C2	-3.83	121.09	126.37
56	2y	55	PSU	C4-N3-C2	-3.82	121.11	126.37
32	1a	1518	MA6	C4-C5-N7	-3.80	106.23	110.58
56	2y	39	PSU	C4-N3-C2	-3.80	121.14	126.37
32	1a	516	PSU	C4-N3-C2	-3.80	121.14	126.37
56	2y	37	MIA	N3-C2-N1	-3.78	122.86	128.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1915	5MU	O4-C4-C5	-3.78	120.60	124.92
1	2A	1911	PSU	O2-C2-N1	-3.77	118.90	122.79
43	2l	92	0TD	OD2-CG-CB	3.77	121.29	113.15
56	1y	37	MIA	C2-N3-C4	3.76	121.00	111.83
55	2x	54	5MU	C5-C6-N1	-3.74	119.25	123.31
56	2y	37	MIA	C4-C5-N7	-3.73	106.32	110.58
56	2y	37	MIA	C2-N3-C4	3.72	120.92	111.83
32	1a	1207	2MG	N9-C4-N3	3.70	133.35	125.95
54	2w	39	PSU	C4-N3-C2	-3.70	121.28	126.37
56	2y	8	4SU	N3-C2-N1	3.69	119.70	114.89
55	2x	54	5MU	O4-C4-C5	-3.69	120.69	124.92
54	1w	32	PSU	O2-C2-N1	-3.69	118.98	122.79
56	1y	37	MIA	N3-C2-N1	-3.68	123.01	128.58
32	2a	1518	MA6	C5-N7-C8	3.67	109.22	103.45
1	1A	1942	5MC	C5-C6-N1	-3.66	119.33	123.31
55	2x	8	4SU	C1'-N1-C2	3.66	124.17	117.59
54	1w	32	PSU	C4-N3-C2	-3.65	121.34	126.37
1	2A	1942	5MC	C5-C6-N1	-3.65	119.35	123.31
54	2w	37	MIA	C2-N3-C4	3.65	121.84	112.29
1	2A	1911	PSU	C4-N3-C2	-3.64	121.35	126.37
32	2a	1400	5MC	C5-C6-N1	-3.64	119.36	123.31
1	1A	2552	OMU	O2-C2-N1	-3.64	118.06	122.80
32	1a	1519	MA6	N9-C8-N7	-3.63	108.79	113.94
1	2A	2552	OMU	O2-C2-N1	-3.62	118.08	122.80
54	1w	37	MIA	C6-C5-N7	3.61	136.37	132.43
56	1y	37	MIA	C4-C5-N7	-3.61	106.45	110.58
54	1w	37	MIA	C16-C14-C13	-3.61	111.82	122.66
55	1x	54	5MU	O4-C4-C5	-3.58	120.82	124.92
55	1x	8	4SU	C6-C5-C4	-3.57	116.86	119.95
32	1a	1519	MA6	C2-N3-C4	3.56	120.53	111.83
32	2a	1518	MA6	C2-N3-C4	3.56	120.53	111.83
54	2w	54	5MU	O4-C4-C5	-3.56	120.85	124.92
32	2a	1518	MA6	C4-C5-N7	-3.54	106.53	110.58
55	1x	54	5MU	C5-C4-N3	3.54	118.40	115.32
54	1w	8	4SU	N3-C2-N1	3.54	119.50	114.89
32	1a	1518	MA6	N9-C8-N7	-3.54	108.92	113.94
32	2a	1407	5MC	C5-C6-N1	-3.53	119.48	123.31
32	2a	1519	MA6	C2-N3-C4	3.53	120.44	111.83
54	1w	37	MIA	C2-N3-C4	3.52	121.52	112.29
56	1y	39	PSU	C4-N3-C2	-3.51	121.53	126.37
1	1A	1917	PSU	O2-C2-N1	-3.51	119.17	122.79
55	2x	55	PSU	O2-C2-N1	-3.50	119.18	122.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1w	55	PSU	C4-N3-C2	-3.48	121.58	126.37
54	2w	8	4SU	C5-C4-S4	-3.43	120.39	124.31
54	2w	37	MIA	C4-C5-N7	-3.42	106.67	110.58
32	2a	1404	5MC	C5-C6-N1	-3.42	119.60	123.31
54	2w	55	PSU	O2-C2-N1	-3.42	119.27	122.79
32	1a	1404	5MC	C5-C6-N1	-3.42	119.60	123.31
1	2A	2503	2MA	N6-C6-N1	3.41	121.63	117.03
55	1x	76	31H	N9-C8-N7	-3.41	109.10	113.94
32	1a	1400	5MC	C5-C6-N1	-3.41	119.61	123.31
32	2a	516	PSU	O2-C2-N1	-3.40	119.28	122.79
55	2x	76	31H	C2-N3-C4	3.40	120.14	111.83
1	2A	1915	5MU	C5-C6-N1	-3.40	119.62	123.31
54	1w	37	MIA	C4-C5-N7	-3.38	106.71	110.58
56	2y	32	PSU	O2-C2-N1	-3.38	119.30	122.79
55	2x	8	4SU	C5-C4-N3	3.37	117.89	114.75
55	1x	76	31H	C2-N3-C4	3.36	120.04	111.83
54	2w	32	PSU	O2-C2-N1	-3.35	119.33	122.79
32	1a	1518	MA6	C2-N3-C4	3.35	120.01	111.83
55	2x	76	31H	N9-C8-N7	-3.34	109.20	113.94
56	1y	54	5MU	C4-N3-C2	-3.33	122.98	127.34
32	1a	1207	2MG	C4-C5-N7	-3.33	105.40	110.67
32	1a	1498	UR3	C5-C4-N3	3.32	119.41	115.04
56	1y	54	5MU	C5-C4-N3	3.31	118.20	115.32
54	1w	8	4SU	C5-C4-S4	-3.30	120.54	124.31
32	2a	1518	MA6	N9-C8-N7	-3.30	109.26	113.94
1	2A	2503	2MA	C4-N9-C8	3.28	109.18	105.74
32	2a	1407	5MC	C5-C4-N3	-3.28	118.40	121.75
32	2a	1519	MA6	N9-C8-N7	-3.26	109.31	113.94
32	1a	966	M2G	C6-C5-N7	3.26	136.22	130.29
1	1A	1915	5MU	C5-C6-N1	-3.24	119.79	123.31
1	2A	1917	PSU	O2-C2-N1	-3.22	119.47	122.79
32	1a	516	PSU	O2-C2-N1	-3.21	119.47	122.79
1	1A	1962	5MC	C5-C4-N3	-3.21	118.46	121.75
1	2A	1962	5MC	C5-C6-N1	-3.21	119.83	123.31
32	1a	1207	2MG	N1-C2-N2	3.20	119.82	116.56
1	1A	2605	PSU	O2-C2-N1	-3.19	119.50	122.79
1	1A	2503	2MA	C4-C5-N7	-3.18	106.94	110.58
32	2a	967	5MC	C5-C6-N1	-3.17	119.87	123.31
32	1a	1407	5MC	C5-C6-N1	-3.13	119.92	123.31
32	2a	1207	2MG	C6-C5-N7	3.12	135.98	130.29
1	1A	1939	5MU	O2-C2-N1	-3.12	118.73	122.80
55	1x	76	31H	CA-N-CN	-3.12	118.02	122.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2503	2MA	C4-C5-N7	-3.12	107.02	110.58
32	2a	1498	UR3	C5-C4-N3	3.11	119.14	115.04
54	1w	54	5MU	C5-C6-N1	-3.09	119.95	123.31
1	1A	2503	2MA	C4-N9-C8	3.09	108.98	105.74
56	1y	32	PSU	O2-C2-N1	-3.09	119.60	122.79
1	1A	2503	2MA	C2-N1-C6	3.08	122.83	118.10
43	1l	92	0TD	OD2-CG-CB	3.06	119.75	113.15
1	1A	1942	5MC	C5-C4-N3	-3.06	118.62	121.75
54	2w	39	PSU	O2-C2-N1	-3.04	119.65	122.79
32	1a	1407	5MC	C5-C4-N3	-3.04	118.64	121.75
55	2x	76	31H	C4'-O4'-C1'	-3.03	102.78	109.47
55	2x	32	5MC	C5-C4-N3	-3.02	118.65	121.75
1	2A	1942	5MC	C5-C4-N3	-3.02	118.66	121.75
56	1y	39	PSU	O2-C2-N1	-3.01	119.68	122.79
55	1x	76	31H	C5-N7-C8	2.99	108.15	103.45
56	2y	37	MIA	C4-N9-C8	2.99	108.88	105.74
56	2y	39	PSU	O2-C2-N1	-2.98	119.71	122.79
32	1a	1402	4OC	C6-C5-C4	2.98	120.59	117.00
55	2x	32	5MC	C5-C6-N1	-2.96	120.10	123.31
55	1x	32	5MC	C5-C4-N3	-2.96	118.72	121.75
1	1A	2251	OMG	C6-C5-N7	2.95	135.65	130.29
1	1A	2503	2MA	N6-C6-N1	2.94	120.99	117.03
32	1a	967	5MC	C5-C6-N1	-2.93	120.13	123.31
32	2a	527	7MG	C5-C6-N1	2.93	116.09	110.94
56	1y	54	5MU	O4-C4-C5	-2.93	121.57	124.92
56	2y	54	5MU	C5-C6-N1	-2.93	120.14	123.31
1	2A	2552	OMU	C2'-C1'-N1	-2.92	108.70	114.24
32	2a	1404	5MC	C5-C4-N3	-2.92	118.76	121.75
54	2w	37	MIA	C12-N6-C6	-2.92	120.14	122.85
55	2x	54	5MU	O2-C2-N1	-2.91	119.01	122.80
55	1x	54	5MU	C5-C6-N1	-2.88	120.19	123.31
1	2A	2251	OMG	C6-C5-N7	2.87	135.51	130.29
55	2x	76	31H	C5-N7-C8	2.85	107.94	103.45
54	2w	37	MIA	C6-C5-N7	2.84	135.52	132.43
32	2a	1518	MA6	N3-C4-N9	2.83	131.98	127.17
55	1x	8	4SU	C5-C4-N3	2.82	117.38	114.75
55	2x	76	31H	C5-C4-N9	2.81	108.88	105.81
32	1a	967	5MC	C5-C4-N3	-2.79	118.89	121.75
32	1a	1207	2MG	N2-C2-N3	-2.79	116.96	120.51
55	1x	76	31H	C4'-O4'-C1'	-2.79	103.31	109.47
54	1w	37	MIA	N3-C2-N1	-2.78	121.92	127.00
32	1a	1518	MA6	N3-C4-N9	2.78	131.89	127.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	2y	37	MIA	C5-N7-C8	2.75	107.78	103.45
32	1a	527	7MG	C5-C6-N1	2.75	115.78	110.94
32	1a	1404	5MC	C5-C4-N3	-2.74	118.95	121.75
43	2l	92	0TD	OD1-CG-CB	-2.73	116.71	122.44
56	2y	46	7MG	C5-C4-N9	-2.73	102.83	106.33
1	1A	1920	OMC	O2-C2-N3	-2.73	118.03	122.33
1	1A	1962	5MC	C5-C6-N1	-2.72	120.36	123.31
1	2A	2605	PSU	O2-C2-N1	-2.72	119.98	122.79
32	1a	1519	MA6	N3-C4-N9	2.72	131.79	127.17
55	1x	76	31H	C5-C4-N9	2.71	108.77	105.81
32	2a	1519	MA6	N3-C4-N9	2.70	131.76	127.17
32	2a	1498	UR3	C3U-N3-C4	2.69	121.60	117.87
54	2w	54	5MU	C5-C6-N1	-2.69	120.39	123.31
32	2a	1207	2MG	C4-C5-N7	-2.67	106.44	110.67
54	1w	37	MIA	C2-N1-C6	2.65	122.58	117.54
56	1y	37	MIA	C5-N7-C8	2.65	107.62	103.45
54	2w	46	7MG	C5-C6-N1	2.65	115.60	110.94
54	1w	46	7MG	C5-C4-N9	-2.65	102.94	106.33
56	1y	8	4SU	C5-C4-S4	-2.63	121.30	124.31
32	1a	1400	5MC	C5-C4-N3	-2.63	119.06	121.75
32	2a	967	5MC	C5-C4-N3	-2.62	119.06	121.75
1	2A	2552	OMU	C5-C4-N3	2.62	118.47	114.80
32	1a	1498	UR3	C1'-N1-C2	2.61	121.31	117.04
32	2a	966	M2G	C6-C5-N7	2.61	135.04	130.29
1	2A	2503	2MA	C2-N1-C6	2.60	122.10	118.10
56	1y	46	7MG	C5-C6-N1	2.58	115.48	110.94
54	1w	55	PSU	C6-C5-C4	-2.57	116.44	118.17
54	2w	37	MIA	C5-N7-C8	2.55	107.46	103.45
55	2x	32	5MC	O2-C2-N3	-2.55	118.31	122.33
1	1A	2251	OMG	O6-C6-C5	-2.54	119.81	126.53
1	2A	2503	2MA	C5-N7-C8	2.54	107.44	103.45
56	2y	8	4SU	C1'-N1-C2	2.54	122.15	117.59
1	2A	2251	OMG	O6-C6-C5	-2.54	119.83	126.53
55	2x	76	31H	C6-C5-C4	2.53	120.63	117.18
32	1a	1518	MA6	C4-C5-C6	2.53	118.52	115.91
56	2y	46	7MG	C5-C6-N1	2.52	115.37	110.94
32	2a	1400	5MC	C5-C4-N3	-2.51	119.18	121.75
1	1A	2552	OMU	C5-C4-N3	2.51	118.31	114.80
55	1x	8	4SU	O2-C2-N1	2.50	126.05	122.80
55	1x	76	31H	N3-C4-N9	2.50	131.41	127.17
1	1A	2503	2MA	C5-N7-C8	2.49	107.36	103.45
32	1a	966	M2G	C4-C5-N7	-2.48	106.73	110.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1519	MA6	C4-C5-C6	2.48	118.47	115.91
54	2w	37	MIA	N3-C2-N1	-2.48	122.48	127.00
56	1y	54	5MU	C5-C6-N1	-2.47	120.63	123.31
55	2x	8	4SU	O2-C2-N1	2.46	126.00	122.80
55	2x	76	31H	N3-C4-N9	2.46	131.34	127.17
1	2A	1939	5MU	O2-C2-N1	-2.45	119.61	122.80
56	1y	46	7MG	C5-C4-N9	-2.44	103.21	106.33
54	1w	37	MIA	C5-N7-C8	2.42	107.26	103.45
56	2y	54	5MU	C1'-N1-C2	2.42	121.94	117.59
55	2x	76	31H	CA-N-CN	-2.42	119.10	122.82
55	1x	32	5MC	CM5-C5-C6	-2.41	119.59	122.85
54	1w	46	7MG	C5-C6-N1	2.40	115.16	110.94
1	2A	1962	5MC	C5-C4-N3	-2.39	119.30	121.75
56	1y	37	MIA	C4-N9-C8	2.39	108.25	105.74
1	1A	2552	OMU	O4-C4-C5	-2.38	121.06	125.16
32	2a	516	PSU	O4'-C1'-C2'	2.37	108.42	105.15
54	1w	54	5MU	O2-C2-N1	-2.36	119.72	122.80
55	2x	8	4SU	O2-C2-N3	-2.34	117.18	121.49
1	2A	1915	5MU	O2-C2-N1	-2.33	119.76	122.80
55	2x	8	4SU	C6-C5-C4	-2.33	117.93	119.95
56	2y	54	5MU	O2-C2-N3	-2.32	117.21	121.49
32	1a	527	7MG	O6-C6-C5	-2.31	121.94	127.62
1	2A	2503	2MA	N9-C8-N7	-2.30	110.67	113.94
32	2a	1402	4OC	O2-C2-N3	-2.30	118.70	122.33
32	2a	966	M2G	C4-C5-N7	-2.30	107.03	110.67
1	1A	1962	5MC	CM5-C5-C6	-2.30	119.74	122.85
1	1A	1915	5MU	C5M-C5-C4	2.28	121.22	118.78
54	2w	46	7MG	O6-C6-C5	-2.27	122.04	127.62
32	1a	527	7MG	C5-C4-N9	-2.26	103.44	106.33
54	2w	46	7MG	C5-C4-N9	-2.25	103.45	106.33
54	1w	37	MIA	C4-N9-C8	2.24	108.09	105.74
55	1x	76	31H	C6-C5-C4	2.24	120.23	117.18
54	2w	37	MIA	C2-N1-C6	2.23	121.78	117.54
56	2y	55	PSU	O4'-C1'-C2'	2.23	108.23	105.15
1	2A	2251	OMG	C4-C5-N7	-2.22	107.14	110.67
55	1x	76	31H	OCN-CN-N	-2.22	119.58	125.32
32	2a	1404	5MC	O2-C2-N3	-2.22	118.83	122.33
32	2a	1402	4OC	C6-C5-C4	2.22	119.67	117.00
54	2w	37	MIA	C4-N9-C8	2.22	108.07	105.74
1	2A	1917	PSU	C5-C6-N1	-2.22	119.06	122.14
32	2a	966	M2G	O6-C6-C5	-2.21	120.69	126.53
56	2y	37	MIA	N9-C8-N7	-2.21	110.80	113.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1920	OMC	C1'-N1-C2	2.21	123.32	118.44
56	2y	37	MIA	C6-C5-N7	2.20	136.34	132.09
32	2a	1518	MA6	C4-C5-C6	2.20	118.18	115.91
32	1a	1207	2MG	C8-N7-C5	2.19	108.16	104.26
1	1A	1911	PSU	C5-C6-N1	-2.19	119.10	122.14
32	2a	527	7MG	C5-C4-N9	-2.19	103.53	106.33
32	2a	1400	5MC	O2-C2-N3	-2.18	118.89	122.33
54	2w	54	5MU	C5M-C5-C4	2.18	121.11	118.78
55	1x	76	31H	C4-C5-N7	-2.18	108.09	110.58
54	2w	46	7MG	C6-C5-C4	-2.17	118.58	122.40
54	2w	8	4SU	O2-C2-N1	-2.17	119.97	122.80
32	1a	1519	MA6	C4-C5-C6	2.16	118.14	115.91
55	2x	55	PSU	C5-C6-N1	-2.16	119.15	122.14
56	1y	37	MIA	C6-C5-N7	2.14	136.22	132.09
54	1w	46	7MG	O6-C6-C5	-2.14	122.37	127.62
1	2A	2552	OMU	O4-C4-C5	-2.13	121.50	125.16
56	2y	37	MIA	C2-N1-C6	2.11	122.19	118.73
56	1y	46	7MG	O6-C6-C5	-2.10	122.46	127.62
55	2x	76	31H	C4-C5-N7	-2.10	108.18	110.58
1	1A	2605	PSU	C5-C6-N1	-2.09	119.24	122.14
32	1a	516	PSU	O4'-C1'-C2'	2.09	108.04	105.15
56	2y	46	7MG	O4'-C1'-N9	-2.09	106.45	109.30
56	2y	39	PSU	C5-C6-N1	-2.08	119.25	122.14
1	1A	2251	OMG	C4-C5-N7	-2.08	107.37	110.67
54	1w	39	PSU	C5-C6-N1	-2.08	119.26	122.14
56	2y	54	5MU	C1'-N1-C6	-2.07	117.73	121.15
32	1a	1207	2MG	C2-N1-C6	-2.07	122.04	124.55
1	2A	1917	PSU	O2-C2-N3	-2.07	118.18	121.86
32	1a	1402	4OC	C5-C6-N1	-2.07	118.47	121.84
55	1x	54	5MU	O2-C2-N1	-2.07	120.11	122.80
32	2a	1407	5MC	O2-C2-N3	-2.07	119.07	122.33
32	1a	1400	5MC	O2-C2-N3	-2.06	119.08	122.33
55	2x	76	31H	OCN-CN-N	-2.06	119.99	125.32
32	2a	1207	2MG	C2-N1-C6	-2.05	122.07	124.55
32	1a	1404	5MC	CM5-C5-C6	-2.05	120.08	122.85
55	2x	32	5MC	C1'-N1-C6	-2.04	117.78	121.15
32	2a	527	7MG	O6-C6-C5	-2.04	122.61	127.62
1	1A	2503	2MA	N9-C8-N7	-2.03	111.05	113.94
1	1A	2251	OMG	C5-C6-N1	2.03	118.42	113.25
1	1A	1939	5MU	C5M-C5-C4	2.03	120.94	118.78
1	2A	2605	PSU	C5-C6-N1	-2.02	119.33	122.14
56	1y	37	MIA	C2-N1-C6	2.01	122.03	118.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1407	5MC	CM5-C5-C6	-2.01	120.13	122.85
32	2a	1402	4OC	CM4-N4-C4	-2.00	118.54	122.45

There are no chirality outliers.

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	1l	92	0TD	CA-CB-SB-CSB
43	1l	92	0TD	CG-CB-SB-CSB
56	1y	46	7MG	C4'-C5'-O5'-P
43	2l	92	0TD	O-C-CA-CB
43	2l	92	0TD	CG-CB-SB-CSB
56	2y	54	5MU	C3'-C4'-C5'-O5'
56	2y	54	5MU	O4'-C4'-C5'-O5'
56	2y	55	PSU	C2'-C1'-C5-C4
56	2y	55	PSU	C2'-C1'-C5-C6
32	1a	1207	2MG	N3-C2-N2-CM2
32	2a	1207	2MG	O4'-C4'-C5'-O5'
32	2a	1207	2MG	N1-C2-N2-CM2
32	2a	1207	2MG	N3-C2-N2-CM2
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1519	MA6	O4'-C4'-C5'-O5'
54	1w	37	MIA	C12-C13-C14-C16
32	2a	1207	2MG	C3'-C4'-C5'-O5'
32	2a	1402	4OC	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
55	1x	76	31H	C3'-C4'-C5'-O5'
55	2x	76	31H	C3'-C4'-C5'-O5'
56	1y	8	4SU	C3'-C4'-C5'-O5'
56	1y	8	4SU	O4'-C4'-C5'-O5'
32	1a	527	7MG	C3'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
55	1x	76	31H	C4'-C5'-O5'-P
56	2y	46	7MG	O4'-C1'-N9-C4
32	2a	527	7MG	C3'-C4'-C5'-O5'
56	1y	54	5MU	O4'-C4'-C5'-O5'
32	1a	527	7MG	O4'-C4'-C5'-O5'
32	1a	1400	5MC	O4'-C4'-C5'-O5'
55	1x	76	31H	O4'-C4'-C5'-O5'
55	2x	76	31H	O4'-C4'-C5'-O5'
32	2a	1402	4OC	C3'-C4'-C5'-O5'
54	2w	32	PSU	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
54	2w	46	7MG	C4'-C5'-O5'-P
32	2a	527	7MG	O4'-C4'-C5'-O5'
54	1w	46	7MG	C3'-C4'-C5'-O5'
56	1y	46	7MG	C2'-C1'-N9-C8
56	2y	46	7MG	C2'-C1'-N9-C8
55	1x	76	31H	CA-CB-CG-SD
54	1w	37	MIA	N1-C2-S10-C11
56	1y	46	7MG	C3'-C4'-C5'-O5'
54	1w	46	7MG	O4'-C4'-C5'-O5'
1	2A	1917	PSU	O4'-C4'-C5'-O5'
56	2y	46	7MG	O4'-C1'-N9-C8
32	2a	1519	MA6	C4'-C5'-O5'-P
54	1w	46	7MG	C4'-C5'-O5'-P
55	2x	76	31H	C4'-C5'-O5'-P
56	1y	55	PSU	O4'-C1'-C5-C4
56	2y	55	PSU	O4'-C1'-C5-C4
32	1a	1400	5MC	C3'-C4'-C5'-O5'
54	1w	37	MIA	N3-C2-S10-C11
32	1a	1519	MA6	C4'-C5'-O5'-P
54	1w	37	MIA	N6-C12-C13-C14
32	1a	527	7MG	C4'-C5'-O5'-P
56	1y	46	7MG	O4'-C1'-N9-C8
32	2a	527	7MG	C4'-C5'-O5'-P
1	1A	2503	2MA	O4'-C4'-C5'-O5'
43	2l	92	0TD	CA-CB-SB-CSB
43	2l	92	0TD	SB-CB-CG-OD2
56	1y	8	4SU	C4'-C5'-O5'-P
1	1A	2503	2MA	C4'-C5'-O5'-P
56	2y	55	PSU	O4'-C1'-C5-C6
56	1y	54	5MU	C3'-C4'-C5'-O5'
1	2A	1962	5MC	C2'-C1'-N1-C6
1	2A	2503	2MA	O4'-C4'-C5'-O5'
1	2A	1962	5MC	O4'-C1'-N1-C6
1	1A	1920	OMC	C2'-C1'-N1-C2
54	2w	32	PSU	C3'-C4'-C5'-O5'
56	2y	54	5MU	C2'-C1'-N1-C2
32	2a	1518	MA6	O4'-C4'-C5'-O5'

There are no ring outliers.

32 monomers are involved in 49 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1A	2251	OMG	1	0
54	2w	39	PSU	2	0
55	2x	32	5MC	1	0
32	1a	1402	4OC	1	0
1	1A	1915	5MU	1	0
32	2a	1518	MA6	3	0
32	2a	967	5MC	2	0
56	1y	39	PSU	1	0
54	2w	46	7MG	1	0
32	2a	1402	4OC	2	0
32	2a	1404	5MC	1	0
55	2x	8	4SU	1	0
32	2a	1519	MA6	3	0
54	2w	54	5MU	1	0
1	2A	2552	OMU	2	0
1	2A	1915	5MU	1	0
55	1x	8	4SU	2	0
1	1A	1939	5MU	1	0
32	1a	1518	MA6	1	0
56	1y	55	PSU	2	0
54	1w	55	PSU	1	0
1	1A	2503	2MA	1	0
1	2A	2503	2MA	2	0
43	2l	92	0TD	1	0
55	2x	76	31H	1	0
56	1y	54	5MU	1	0
32	1a	967	5MC	1	0
56	2y	39	PSU	2	0
56	1y	8	4SU	2	0
32	1a	1519	MA6	1	0
56	2y	55	PSU	9	0
56	2y	46	7MG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2586 ligands modelled in this entry, 2582 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
60	SF4	1d	302	35	0,12,12	-	-	-	-	-
58	6IF	1A	4109	-	30,34,34	1.02	1 (3%)	30,49,49	1.18	3 (10%)
58	6IF	2A	3731	-	30,34,34	0.77	0	30,49,49	1.08	3 (10%)
60	SF4	2d	302	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
60	SF4	1d	302	35	-	-	0/6/5/5
58	6IF	1A	4109	-	-	4/22/65/65	0/3/3/3
58	6IF	2A	3731	-	-	2/22/65/65	0/3/3/3
60	SF4	2d	302	35	-	-	0/6/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	1A	4109	6IF	CG-CB	-2.40	1.49	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	1A	4109	6IF	CBB-CBA-CAY	-3.07	110.73	116.68
58	1A	4109	6IF	CAK-CAI-CAG	-2.96	110.28	114.17
58	2A	3731	6IF	CBB-CBA-CAY	-2.74	111.37	116.68
58	2A	3731	6IF	CD2-CAY-CAX	-2.51	110.03	113.78
58	2A	3731	6IF	CAK-CAI-CAG	-2.38	111.04	114.17
58	1A	4109	6IF	CD2-CAY-CAX	-2.04	110.74	113.78

There are no chirality outliers.

All (6) torsion outliers are listed below:

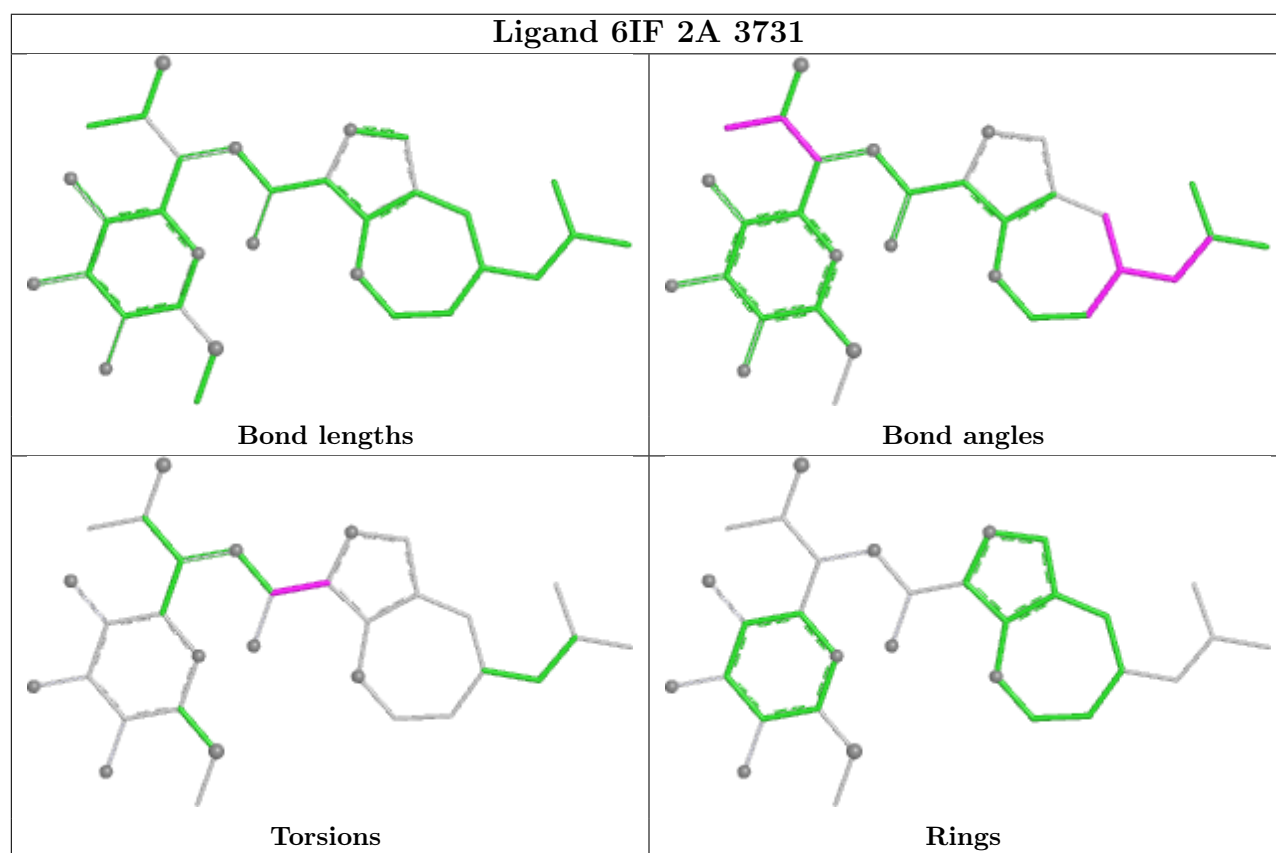
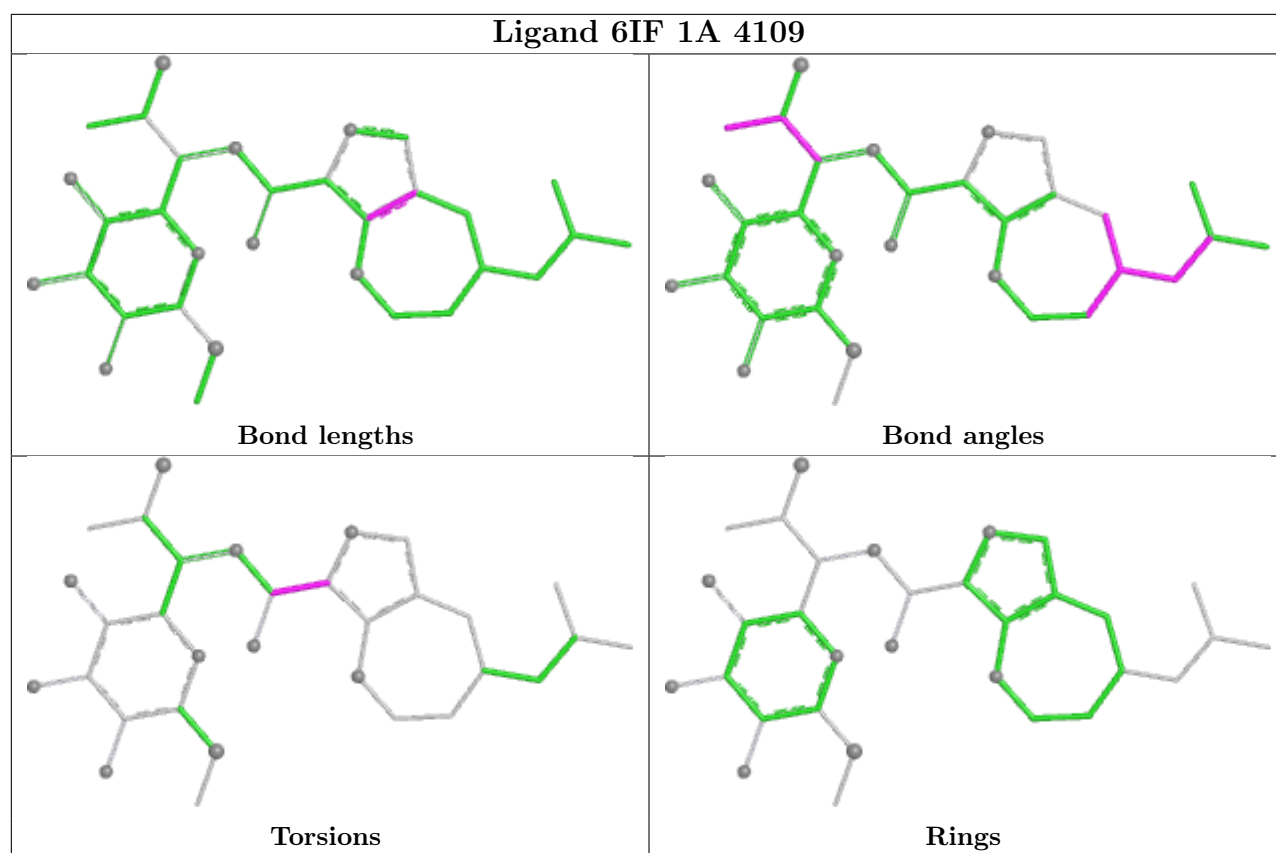
Mol	Chain	Res	Type	Atoms
58	1A	4109	6IF	O-C-CA-CB
58	1A	4109	6IF	NAH-C-CA-CB
58	2A	3731	6IF	NAH-C-CA-CB
58	1A	4109	6IF	NAH-C-CA-N
58	1A	4109	6IF	O-C-CA-N
58	2A	3731	6IF	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	1A	4109	6IF	2	0
60	2d	302	SF4	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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%)	-0.57	129 (4%)	38	33	19, 36, 89, 102	0
1	2A	2789/2915 (95%)	0.01	109 (3%)	43	38	34, 57, 89, 99	0
2	1B	120/121 (99%)	-0.47	0	100	100	29, 47, 62, 82	0
2	2B	120/121 (99%)	1.29	18 (15%)	5	4	62, 80, 88, 92	0
3	1D	275/276 (99%)	-0.16	2 (0%)	84	81	21, 37, 51, 74	0
3	2D	275/276 (99%)	0.38	6 (2%)	62	58	33, 52, 64, 81	0
4	1E	204/206 (99%)	-0.13	0	100	100	18, 40, 58, 71	0
4	2E	204/206 (99%)	0.41	2 (0%)	79	76	33, 56, 68, 74	0
5	1F	203/210 (96%)	-0.03	1 (0%)	87	85	20, 41, 65, 79	0
5	2F	203/210 (96%)	0.69	6 (2%)	52	48	35, 66, 77, 83	0
6	1G	181/182 (99%)	0.57	6 (3%)	49	45	38, 56, 69, 83	0
6	2G	181/182 (99%)	1.86	79 (43%)	0	0	72, 79, 83, 88	0
7	1H	174/180 (96%)	0.26	2 (1%)	78	75	36, 52, 63, 67	0
7	2H	174/180 (96%)	1.55	43 (24%)	2	1	66, 78, 85, 88	0
8	1I	146/148 (98%)	0.90	4 (2%)	56	51	45, 70, 79, 83	0
8	2I	146/148 (98%)	1.16	11 (7%)	20	18	53, 71, 79, 83	0
9	1N	140/140 (100%)	-0.05	1 (0%)	84	81	24, 39, 56, 71	0
9	2N	140/140 (100%)	0.82	8 (5%)	29	26	45, 63, 75, 79	0
10	1O	122/122 (100%)	-0.10	0	100	100	25, 40, 57, 62	0
10	2O	122/122 (100%)	0.53	1 (0%)	82	80	47, 57, 69, 73	0
11	1P	149/150 (99%)	0.11	2 (1%)	75	71	20, 44, 65, 71	0
11	2P	149/150 (99%)	0.85	9 (6%)	27	24	38, 65, 79, 83	0
12	1Q	141/141 (100%)	0.06	3 (2%)	63	59	28, 41, 56, 70	0
12	2Q	141/141 (100%)	1.30	28 (19%)	3	2	49, 66, 76, 83	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%)	-0.25	0 100 100	25, 33, 46, 54	0
13	2R	118/118 (100%)	0.27	0 100 100	39, 50, 60, 64	0
14	1S	110/112 (98%)	0.16	0 100 100	37, 48, 58, 64	0
14	2S	110/112 (98%)	1.76	39 (35%) 1 1	65, 74, 79, 81	0
15	1T	131/146 (89%)	0.14	3 (2%) 61 57	33, 44, 65, 70	0
15	2T	131/146 (89%)	0.56	3 (2%) 61 57	50, 59, 71, 78	0
16	1U	116/118 (98%)	-0.36	1 (0%) 81 78	21, 29, 47, 62	0
16	2U	116/118 (98%)	0.72	2 (1%) 69 65	46, 61, 74, 83	0
17	1V	101/101 (100%)	-0.25	1 (0%) 79 76	22, 39, 56, 64	0
17	2V	101/101 (100%)	0.84	5 (4%) 34 30	42, 70, 75, 81	0
18	1W	112/113 (99%)	-0.30	0 100 100	22, 31, 50, 73	0
18	2W	112/113 (99%)	0.30	3 (2%) 56 51	40, 50, 67, 85	0
19	1X	95/96 (98%)	-0.09	2 (2%) 63 59	25, 37, 56, 76	0
19	2X	95/96 (98%)	0.97	9 (9%) 14 12	45, 59, 73, 83	0
20	1Y	107/110 (97%)	0.24	1 (0%) 81 78	34, 47, 64, 71	0
20	2Y	107/110 (97%)	1.12	12 (11%) 10 8	56, 69, 79, 84	0
21	1Z	154/206 (74%)	0.82	15 (9%) 13 11	38, 61, 78, 84	0
21	2Z	160/206 (77%)	1.95	67 (41%) 0 0	65, 78, 87, 89	0
22	10	83/85 (97%)	0.33	7 (8%) 17 15	27, 37, 66, 79	0
22	20	83/85 (97%)	1.48	19 (22%) 2 1	46, 65, 76, 82	0
23	11	97/98 (98%)	0.20	1 (1%) 79 76	27, 43, 66, 71	0
23	21	97/98 (98%)	0.51	4 (4%) 41 37	40, 53, 71, 75	0
24	12	70/72 (97%)	0.27	1 (1%) 73 70	35, 47, 57, 70	0
24	22	70/72 (97%)	1.10	9 (12%) 7 6	59, 69, 76, 78	0
25	13	59/60 (98%)	-0.17	0 100 100	24, 34, 57, 74	0
25	23	59/60 (98%)	0.81	1 (1%) 69 65	54, 64, 74, 82	0
26	14	69/71 (97%)	1.06	13 (18%) 3 2	48, 69, 83, 87	0
26	24	69/71 (97%)	2.18	35 (50%) 0 0	75, 82, 88, 95	0
27	15	59/60 (98%)	-0.39	1 (1%) 69 65	20, 30, 52, 62	0
27	25	59/60 (98%)	0.17	0 100 100	35, 49, 61, 74	0
28	16	53/54 (98%)	-0.12	0 100 100	29, 42, 54, 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%)	0.85	3 (5%) 29 26	54, 62, 68, 73	0
29	17	48/49 (97%)	-0.26	1 (2%) 63 59	21, 27, 55, 61	0
29	27	48/49 (97%)	0.21	3 (6%) 26 23	32, 42, 64, 67	0
30	18	64/65 (98%)	-0.17	0 100 100	28, 34, 41, 55	0
30	28	64/65 (98%)	0.61	2 (3%) 51 47	46, 56, 62, 68	0
31	19	37/37 (100%)	-0.11	0 100 100	29, 38, 54, 56	0
31	29	37/37 (100%)	1.09	4 (10%) 11 9	59, 67, 75, 76	0
32	1a	1488/1521 (97%)	0.19	37 (2%) 58 54	35, 64, 87, 99	0
32	2a	1491/1521 (98%)	0.82	152 (10%) 12 10	52, 76, 92, 101	0
33	1b	231/256 (90%)	1.22	39 (16%) 4 3	62, 74, 82, 86	0
33	2b	231/256 (90%)	2.09	119 (51%) 0 0	71, 82, 87, 89	0
34	1c	206/239 (86%)	0.88	8 (3%) 43 38	56, 68, 76, 82	0
34	2c	206/239 (86%)	2.11	106 (51%) 0 0	72, 82, 88, 93	0
35	1d	208/209 (99%)	0.94	18 (8%) 16 14	52, 68, 75, 79	0
35	2d	208/209 (99%)	1.06	17 (8%) 17 15	61, 70, 77, 80	0
36	1e	148/162 (91%)	0.49	2 (1%) 73 70	49, 62, 70, 76	0
36	2e	148/162 (91%)	1.57	38 (25%) 1 1	68, 76, 81, 87	0
37	1f	100/101 (99%)	0.69	3 (3%) 52 48	52, 64, 71, 74	0
37	2f	100/101 (99%)	0.87	2 (2%) 65 61	63, 70, 75, 79	0
38	1g	155/156 (99%)	0.92	12 (7%) 19 17	56, 67, 75, 81	0
38	2g	155/156 (99%)	1.60	42 (27%) 1 1	69, 77, 83, 86	0
39	1h	137/138 (99%)	0.69	4 (2%) 53 49	53, 64, 71, 79	0
39	2h	137/138 (99%)	1.37	22 (16%) 4 4	70, 77, 81, 82	0
40	1i	127/128 (99%)	1.20	13 (10%) 12 10	49, 72, 78, 83	0
40	2i	127/128 (99%)	2.40	85 (66%) 0 0	72, 81, 86, 87	0
41	1j	97/105 (92%)	1.24	15 (15%) 5 4	58, 74, 80, 83	0
41	2j	96/105 (91%)	2.58	67 (69%) 0 0	76, 83, 87, 90	0
42	1k	114/129 (88%)	0.66	3 (2%) 57 52	45, 63, 74, 77	0
42	2k	114/129 (88%)	1.24	15 (13%) 7 6	61, 73, 79, 82	0
43	1l	121/132 (91%)	0.49	5 (4%) 41 37	45, 54, 64, 75	0
43	2l	121/132 (91%)	1.28	21 (17%) 4 3	55, 70, 77, 80	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%)	0.97	9 (7%) 21 19	54, 66, 74, 84	0
44	2m	122/126 (96%)	2.08	57 (46%) 0 0	72, 80, 85, 88	0
45	1n	60/61 (98%)	1.14	6 (10%) 12 10	55, 65, 70, 74	0
45	2n	60/61 (98%)	3.27	50 (83%) 0 0	76, 83, 87, 89	0
46	1o	88/89 (98%)	0.80	5 (5%) 29 26	50, 61, 71, 74	0
46	2o	88/89 (98%)	1.13	10 (11%) 10 8	63, 72, 80, 83	0
47	1p	82/88 (93%)	1.31	11 (13%) 7 5	56, 68, 74, 82	0
47	2p	82/88 (93%)	1.08	8 (9%) 13 11	57, 67, 74, 78	0
48	1q	99/105 (94%)	0.92	1 (1%) 79 76	52, 64, 72, 76	0
48	2q	99/105 (94%)	0.97	10 (10%) 12 10	61, 71, 78, 81	0
49	1r	68/88 (77%)	0.65	3 (4%) 39 34	54, 64, 75, 77	0
49	2r	68/88 (77%)	0.96	4 (5%) 28 24	65, 72, 78, 83	0
50	1s	83/93 (89%)	1.10	8 (9%) 13 11	61, 69, 78, 81	0
50	2s	83/93 (89%)	2.65	57 (68%) 0 0	76, 84, 88, 91	0
51	1t	96/106 (90%)	1.18	15 (15%) 5 4	58, 67, 74, 79	0
51	2t	96/106 (90%)	0.92	12 (12%) 8 6	58, 69, 76, 78	0
52	1u	23/27 (85%)	1.24	2 (8%) 16 14	57, 63, 67, 71	0
52	2u	23/27 (85%)	2.69	16 (69%) 0 0	76, 79, 83, 84	0
53	1v	13/24 (54%)	0.84	3 (23%) 2 1	49, 65, 82, 92	0
53	2v	13/24 (54%)	1.70	4 (30%) 1 1	75, 83, 93, 97	0
54	1w	64/76 (84%)	1.03	8 (12%) 8 6	64, 85, 97, 101	0
54	2w	62/76 (81%)	1.66	20 (32%) 1 1	84, 92, 98, 103	0
55	1x	71/77 (92%)	0.19	0 100 100	28, 60, 80, 86	0
55	2x	71/77 (92%)	0.75	2 (2%) 55 50	46, 79, 89, 90	0
56	1y	67/76 (88%)	0.86	6 (8%) 15 13	38, 85, 93, 95	0
56	2y	66/76 (86%)	1.09	4 (6%) 27 23	54, 91, 94, 98	0
All	All	20867/21748 (95%)	0.48	1913 (9%) 14 13	18, 63, 86, 103	0

All (1913) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
45	1n	2	ALA	8.2
41	2j	47	PHE	7.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
21	1Z	141	VAL	7.7
44	1m	2	ALA	6.9
44	2m	124	PRO	6.7
22	10	6	GLY	6.6
34	2c	2	GLY	6.3
22	10	7	LEU	6.3
44	1m	124	PRO	6.3
40	2i	45	ALA	6.2
45	2n	25	VAL	6.2
45	2n	2	ALA	6.1
21	2Z	174	VAL	6.0
22	10	3	HIS	6.0
50	2s	2	PRO	5.8
45	2n	34	TYR	5.8
40	2i	14	VAL	5.8
38	2g	16	LEU	5.8
26	24	51	ASP	5.7
33	2b	185	ILE	5.6
40	2i	102	LEU	5.6
1	1A	1094	U	5.4
51	1t	103	GLY	5.3
45	2n	21	TYR	5.2
45	2n	7	ILE	5.2
52	2u	6	ARG	5.2
41	2j	65	LEU	5.1
33	2b	163	PHE	5.1
38	2g	80	VAL	5.1
26	24	49	PHE	5.0
21	2Z	146	ILE	5.0
50	2s	82	GLY	5.0
45	2n	38	GLY	5.0
40	2i	9	ARG	4.9
22	10	4	LYS	4.9
21	2Z	173	ALA	4.9
45	2n	37	PHE	4.9
52	2u	14	TRP	4.8
21	1Z	146	ILE	4.8
33	2b	237	ALA	4.8
1	2A	2803	C	4.8
41	2j	67	THR	4.8
32	2a	1033	G	4.8
44	2m	102	ARG	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
21	2Z	144	LEU	4.8
6	2G	20	ILE	4.7
1	2A	2155	G	4.7
32	2a	1220	G	4.7
36	2e	22	GLY	4.7
1	1A	2803	C	4.7
32	1a	1035	A	4.7
50	2s	9	VAL	4.6
45	2n	14	PRO	4.6
34	2c	194	GLY	4.6
41	2j	59	SER	4.6
33	2b	201	ILE	4.6
41	2j	32	ALA	4.6
6	2G	19	LEU	4.6
45	2n	3	ARG	4.5
1	1A	1096	A	4.5
50	2s	13	ASP	4.5
32	1a	1034	G	4.5
52	2u	2	GLY	4.5
38	1g	80	VAL	4.5
32	2a	1219	U	4.5
44	2m	90	LEU	4.5
34	2c	124	ILE	4.4
54	1w	71	G	4.4
1	1A	1057	A	4.4
32	1a	1027	C	4.4
54	2w	73	A	4.4
40	2i	5	TYR	4.4
33	2b	71	VAL	4.3
33	2b	187	LEU	4.3
1	2A	2147	G	4.3
50	2s	80	TYR	4.3
38	1g	82	GLY	4.3
41	2j	74	ILE	4.3
22	20	2	ALA	4.3
26	24	32	TYR	4.3
41	2j	40	LEU	4.3
45	2n	53	LEU	4.3
40	2i	126	SER	4.3
41	2j	36	GLY	4.2
21	2Z	171	ILE	4.2
39	2h	2	LEU	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
45	2n	39	LEU	4.2
7	1H	2	SER	4.2
1	2A	2802	G	4.2
34	2c	167	TRP	4.2
50	2s	22	LEU	4.2
38	2g	83	ALA	4.2
44	2m	123	ALA	4.2
41	2j	41	PRO	4.2
43	2l	55	VAL	4.2
22	20	3	HIS	4.2
33	1b	228	GLY	4.2
33	2b	184	VAL	4.2
33	2b	188	ALA	4.2
34	2c	189	ALA	4.1
26	24	56	VAL	4.1
33	2b	57	PHE	4.1
6	1G	146	TYR	4.1
45	2n	42	ILE	4.1
21	2Z	150	LEU	4.1
50	2s	4	SER	4.1
50	2s	31	ILE	4.1
50	2s	71	LEU	4.1
32	2a	1149	C	4.0
33	2b	161	ALA	4.0
45	2n	59	ALA	4.0
41	2j	76	ASN	4.0
34	2c	33	LEU	4.0
40	2i	99	LEU	4.0
50	2s	15	LEU	4.0
41	2j	63	PHE	4.0
44	1m	123	ALA	4.0
34	2c	5	ILE	4.0
26	24	35	VAL	4.0
1	2A	2112	G	4.0
22	20	69	PHE	4.0
50	2s	16	LEU	4.0
34	2c	195	VAL	4.0
38	1g	83	ALA	4.0
45	2n	30	ALA	4.0
1	2A	2154	G	4.0
45	2n	55	GLY	4.0
34	2c	188	LEU	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	2c	73	PRO	4.0
40	2i	11	LYS	3.9
21	2Z	172	ALA	3.9
32	1a	1036	G	3.9
34	2c	157	ILE	3.9
32	2a	1150	U	3.9
45	2n	6	LEU	3.9
45	2n	33	VAL	3.9
52	2u	15	ARG	3.9
14	2S	7	TYR	3.9
44	2m	4	ILE	3.9
1	2A	2133	G	3.9
19	1X	95	LEU	3.9
21	1Z	149	SER	3.9
1	1A	1078	U	3.9
1	1A	1081	U	3.9
45	2n	16	PHE	3.9
43	2l	56	ALA	3.9
41	2j	93	GLY	3.9
1	2A	2793	G	3.9
7	2H	52	VAL	3.9
32	2a	1034	G	3.9
40	2i	108	VAL	3.9
1	1A	888	C	3.9
12	2Q	121	ALA	3.9
34	2c	87	LEU	3.9
6	2G	28	VAL	3.9
50	2s	11	VAL	3.9
1	2A	2804	C	3.8
33	2b	70	PHE	3.8
32	1a	1025	U	3.8
1	1A	885	C	3.8
1	1A	1087	G	3.8
32	2a	1224	G	3.8
44	1m	122	LYS	3.8
45	2n	29	ARG	3.8
38	2g	12	LEU	3.8
50	2s	38	SER	3.8
50	1s	9	VAL	3.8
53	2v	24	A	3.8
22	10	5	LYS	3.8
52	2u	3	LYS	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
50	2s	52	TYR	3.8
32	2a	1223	C	3.8
34	2c	52	LEU	3.8
40	2i	41	VAL	3.8
41	2j	68	HIS	3.8
43	2l	32	PHE	3.8
14	2S	35	ILE	3.8
1	1A	2792	G	3.8
39	2h	9	MET	3.8
33	2b	165	VAL	3.7
45	2n	31	ARG	3.7
34	2c	8	ILE	3.7
1	1A	1064	C	3.7
41	2j	42	THR	3.7
32	1a	630	G	3.7
45	2n	40	CYS	3.7
12	2Q	104	PHE	3.7
14	2S	29	PHE	3.7
33	1b	227	GLY	3.7
6	2G	3	LEU	3.7
19	2X	92	LEU	3.7
45	2n	44	LEU	3.7
1	1A	896	A	3.7
44	2m	23	TYR	3.7
50	2s	34	TRP	3.7
1	2A	2111	C	3.7
34	2c	15	THR	3.7
50	2s	35	SER	3.7
44	2m	78	ILE	3.7
33	2b	97	TRP	3.7
33	2b	236	TYR	3.7
33	2b	152	PHE	3.7
1	1A	2793	G	3.7
40	2i	49	PRO	3.7
32	1a	1531	A	3.6
7	2H	45	VAL	3.6
44	2m	60	VAL	3.6
40	1i	15	ALA	3.6
50	2s	24	ALA	3.6
21	1Z	104	PHE	3.6
21	1Z	150	LEU	3.6
38	2g	84	ASN	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	2159	G	3.6
1	2A	652(B)	A	3.6
3	1D	276	LYS	3.6
41	2j	55	LYS	3.6
1	1A	2174	C	3.6
32	2a	1116	C	3.6
39	1h	2	LEU	3.6
51	1t	13	LEU	3.6
40	2i	105	ASP	3.6
42	2k	119	CYS	3.6
1	1A	1068	G	3.6
36	2e	115	VAL	3.6
50	2s	79	THR	3.6
1	2A	2169	A	3.6
23	1l	2	SER	3.6
45	2n	47	LEU	3.6
33	2b	193	ASP	3.6
50	2s	14	HIS	3.6
1	2A	2805	G	3.6
1	2A	2894	G	3.6
54	2w	71	G	3.6
23	2l	2	SER	3.6
38	2g	82	GLY	3.6
40	2i	19	LEU	3.6
33	2b	234	PRO	3.6
1	1A	2111	C	3.5
54	2w	3	C	3.5
40	2i	125	TYR	3.5
1	1A	1059	G	3.5
6	2G	163	ALA	3.5
32	1a	1023	G	3.5
11	2P	109	GLY	3.5
34	2c	158	GLY	3.5
34	2c	185	GLY	3.5
40	2i	39	GLY	3.5
1	2A	2173	A	3.5
33	2b	21	ARG	3.5
41	2j	34	VAL	3.5
41	2j	88	LEU	3.5
44	2m	81	LEU	3.5
54	1w	73	A	3.5
45	2n	50	LYS	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	2a	1218	C	3.5
54	2w	72	C	3.5
33	1b	229	VAL	3.5
14	2S	52	SER	3.5
1	1A	1095	A	3.5
32	2a	1001(A)	G	3.5
52	2u	5	ASP	3.5
6	2G	159	VAL	3.5
1	1A	2794	C	3.5
1	2A	2128	C	3.5
1	2A	2109	U	3.5
33	1b	10	LEU	3.5
19	2X	69	TYR	3.5
38	1g	85	TYR	3.5
38	2g	154	TYR	3.5
42	2k	50	TYR	3.5
1	1A	1058	G	3.4
1	2A	2156	G	3.4
32	1a	1030(A)	G	3.4
44	2m	53	VAL	3.4
45	2n	13	THR	3.4
44	2m	70	LEU	3.4
7	2H	39	PRO	3.4
34	2c	155	GLY	3.4
38	2g	14	PRO	3.4
7	2H	2	SER	3.4
14	2S	92	TYR	3.4
32	1a	1532	U	3.4
33	2b	208	ILE	3.4
38	2g	85	TYR	3.4
14	2S	12	PHE	3.4
40	2i	101	PHE	3.4
40	2i	10	ARG	3.4
40	2i	42	ARG	3.4
1	1A	2112	G	3.4
33	1b	230	VAL	3.4
34	2c	153	VAL	3.4
41	2j	49	VAL	3.4
22	20	7	LEU	3.4
22	20	5	LYS	3.4
40	2i	90	PRO	3.4
50	2s	68	GLY	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
15	1T	130	ALA	3.4
1	2A	2143	C	3.4
1	2A	2145	C	3.4
34	2c	48	TYR	3.4
45	2n	36	PHE	3.4
32	2a	1503	A	3.4
26	14	56	VAL	3.4
50	2s	77	THR	3.4
1	2A	2115	G	3.4
12	2Q	10	ARG	3.4
26	14	58	ARG	3.4
1	2A	2138	C	3.4
6	2G	29	TRP	3.4
34	2c	170	GLN	3.4
6	2G	15	VAL	3.4
41	2j	48	THR	3.4
43	2l	104	VAL	3.4
44	2m	103	THR	3.4
34	2c	145	GLY	3.4
34	2c	137	ALA	3.4
36	2e	109	ILE	3.4
40	1i	66	ARG	3.4
45	2n	26	ARG	3.4
50	2s	75	ALA	3.4
26	24	66	SER	3.4
1	1A	2190	G	3.3
1	2A	2127	G	3.3
32	1a	1026	G	3.3
32	2a	1036	G	3.3
32	2a	1190	G	3.3
32	2a	1202	G	3.3
1	1A	1066	U	3.3
33	2b	122	PHE	3.3
45	2n	61	TRP	3.3
42	2k	114	VAL	3.3
31	29	37	GLY	3.3
21	2Z	164	ALA	3.3
34	2c	39	ILE	3.3
41	2j	26	ALA	3.3
51	1t	11	SER	3.3
47	1p	80	PHE	3.3
1	1A	2152	G	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	1a	1024	G	3.3
1	2A	1536	C	3.3
32	2a	1030(B)	C	3.3
40	2i	96	LEU	3.3
7	2H	17	VAL	3.3
33	2b	112	VAL	3.3
45	2n	18	VAL	3.3
6	1G	48	GLU	3.3
34	2c	152	ILE	3.3
40	2i	81	ILE	3.3
51	2t	97	ALA	3.3
1	1A	1093	G	3.3
1	1A	2115	G	3.3
1	2A	2125	G	3.3
2	2B	23	G	3.3
32	2a	1030(A)	G	3.3
1	2A	2174	C	3.3
38	2g	76	ARG	3.3
45	2n	54	PRO	3.3
40	2i	103	THR	3.3
36	2e	74	GLY	3.3
8	1I	146	ALA	3.3
19	2X	91	ALA	3.3
44	2m	72	ALA	3.3
1	2A	2126	A	3.3
40	2i	18	PHE	3.3
26	14	63	TYR	3.3
8	2I	75	LEU	3.3
34	2c	175	LEU	3.3
11	1P	149	GLU	3.3
21	2Z	121	HIS	3.3
21	2Z	165	VAL	3.3
33	1b	136	VAL	3.3
1	2A	2136	C	3.3
33	2b	223	ILE	3.3
21	2Z	21	ALA	3.3
34	2c	129	ALA	3.3
34	2c	160	ALA	3.3
34	2c	168	ALA	3.3
40	2i	76	ALA	3.3
32	2a	983	A	3.2
44	2m	66	LEU	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
50	2s	59	PRO	3.2
33	2b	93	VAL	3.2
44	2m	7	VAL	3.2
22	20	43	THR	3.2
1	1A	1176	G	3.2
1	2A	2146	C	3.2
1	2A	2896	C	3.2
33	1b	237	ALA	3.2
44	2m	5	ALA	3.2
12	2Q	65	PHE	3.2
1	1A	1098	A	3.2
1	1A	2119	A	3.2
8	2I	82	ARG	3.2
21	2Z	155	LEU	3.2
34	2c	6	HIS	3.2
34	1c	2	GLY	3.2
34	2c	77	ILE	3.2
40	2i	13	ALA	3.2
32	1a	1028	C	3.2
32	1a	1001(A)	G	3.2
32	2a	1032	G	3.2
56	1y	18	G	3.2
12	2Q	60	ARG	3.2
26	24	55	ARG	3.2
41	2j	37	PRO	3.2
26	24	40	HIS	3.2
22	20	4	LYS	3.2
29	27	48	LYS	3.2
40	2i	62	TYR	3.2
45	2n	17	LYS	3.2
1	1A	1060	U	3.2
33	2b	172	ILE	3.2
34	2c	187	ALA	3.2
52	1u	24	ARG	3.2
52	2u	24	ARG	3.2
1	1A	2804	C	3.2
1	2A	2139	C	3.2
54	2w	4	C	3.2
21	2Z	143	GLY	3.2
34	2c	9	GLY	3.2
34	2c	55	VAL	3.2
34	2c	198	VAL	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
41	2j	44	VAL	3.2
46	2o	60	VAL	3.2
52	2u	11	GLY	3.2
21	2Z	170	THR	3.2
32	2a	950	U	3.2
41	2j	38	ILE	3.2
50	2s	62	ILE	3.2
35	1d	195	ALA	3.1
44	2m	121	LYS	3.1
32	2a	1038	C	3.1
40	2i	123	PRO	3.1
33	2b	10	LEU	3.1
33	2b	221	LEU	3.1
6	2G	146	TYR	3.1
33	2b	89	GLY	3.1
43	2l	39	VAL	3.1
33	1b	127	ILE	3.1
1	1A	1065	U	3.1
8	2I	146	ALA	3.1
22	10	2	ALA	3.1
51	1t	74	LYS	3.1
26	14	59	PHE	3.1
52	2u	23	PRO	3.1
40	2i	79	LEU	3.1
19	2X	94	GLY	3.1
34	2c	171	GLY	3.1
40	2i	17	VAL	3.1
40	2i	100	GLY	3.1
40	2i	109	VAL	3.1
42	2k	49	GLY	3.1
44	2m	6	GLY	3.1
45	2n	51	GLY	3.1
32	2a	1117	G	3.1
34	2c	192	THR	3.1
38	2g	42	ILE	3.1
41	2j	75	ILE	3.1
50	2s	63	THR	3.1
6	2G	50	ALA	3.1
6	2G	57	ALA	3.1
45	2n	11	LYS	3.1
34	2c	161	GLU	3.1
6	2G	4	ASP	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
6	2G	102	PHE	3.1
41	2j	77	PRO	3.1
45	2n	49	HIS	3.1
33	2b	149	LEU	3.1
47	2p	48	TRP	3.1
41	2j	78	ASN	3.1
40	2i	67	GLY	3.1
21	2Z	141	VAL	3.1
33	2b	200	ILE	3.1
41	2j	87	THR	3.1
42	2k	48	ILE	3.1
1	1A	1089	G	3.1
1	1A	2117	A	3.1
1	1A	2151	G	3.1
1	1A	2805	G	3.1
32	2a	1363(A)	A	3.1
32	2a	1358	U	3.1
33	2b	55	PHE	3.1
36	2e	125	SER	3.1
50	1s	84	GLY	3.1
50	2s	84	GLY	3.1
27	15	60	VAL	3.1
1	1A	1075	C	3.1
3	2D	276	LYS	3.0
32	2a	1030	C	3.1
40	2i	63	ILE	3.1
33	2b	123	ALA	3.0
33	2b	199	TYR	3.0
32	1a	1003	G	3.0
32	2a	973	G	3.0
33	2b	91	PRO	3.0
52	1u	23	PRO	3.0
6	2G	62	LEU	3.0
33	2b	118	LEU	3.0
12	2Q	30	GLY	3.0
6	2G	38	VAL	3.0
33	2b	230	VAL	3.0
29	17	45	ALA	3.0
35	2d	164	ALA	3.0
40	2i	92	TYR	3.0
44	2m	87	TYR	3.0
1	1A	2158	A	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	1a	1503	A	3.0
32	2a	1092	A	3.0
6	2G	172	LEU	3.0
33	2b	213	LEU	3.0
32	1a	1033	G	3.0
43	2l	110	VAL	3.0
3	2D	2	ALA	3.0
36	2e	104	ALA	3.0
47	1p	1	MET	3.0
1	1A	1100	C	3.0
33	2b	31	TYR	3.0
54	1w	72	C	3.0
8	1I	38	LEU	3.0
1	1A	1086	A	3.0
1	1A	1097	U	3.0
1	2A	2113	U	3.0
32	2a	1016	A	3.0
34	2c	190	ARG	3.0
40	2i	91	ASP	3.0
41	2j	11	PHE	3.0
50	2s	10	PHE	3.0
1	1A	1062	G	3.0
19	1X	94	GLY	3.0
6	2G	160	VAL	3.0
21	1Z	1	MET	3.0
34	2c	149	ALA	3.0
38	2g	40	ALA	3.0
44	2m	76	ALA	3.0
40	2i	21	PRO	3.0
26	24	25	TYR	3.0
7	2H	60	ARG	3.0
1	1A	34	C	3.0
21	2Z	5	LEU	3.0
26	24	9	LEU	3.0
41	2j	43	ARG	3.0
32	2a	980	C	3.0
21	2Z	154	ASP	3.0
1	1A	1070	A	3.0
1	1A	1077	A	3.0
1	1A	2114	A	3.0
1	2A	2170	A	3.0
36	2e	114	GLY	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	2H	9	ILE	2.9
34	2c	14	ILE	2.9
41	2j	82	ILE	2.9
44	2m	22	ILE	2.9
20	2Y	1	MET	2.9
32	2a	1216	G	2.9
48	2q	7	THR	2.9
33	1b	97	TRP	2.9
40	1i	106	ALA	2.9
41	2j	62	HIS	2.9
44	2m	104	ARG	2.9
21	2Z	99	TYR	2.9
26	14	69	LYS	2.9
40	2i	36	TYR	2.9
32	2a	1359	C	2.9
48	2q	99	SER	2.9
36	2e	130	ASN	2.9
12	2Q	47	ILE	2.9
34	2c	182	ILE	2.9
50	2s	41	VAL	2.9
33	2b	67	THR	2.9
33	2b	73	THR	2.9
6	2G	73	ALA	2.9
33	2b	13	ALA	2.9
34	2c	24	ALA	2.9
34	2c	53	ALA	2.9
34	2c	65	ALA	2.9
1	1A	2160	G	2.9
1	2A	883	G	2.9
2	2B	119	G	2.9
21	2Z	167	PRO	2.9
26	24	7	PRO	2.9
32	2a	1356	G	2.9
45	2n	23	ARG	2.9
46	1o	19	PRO	2.9
54	2w	15	G	2.9
41	2j	90	LEU	2.9
50	1s	5	LEU	2.9
50	2s	20	LEU	2.9
21	2Z	136	PHE	2.9
14	2S	31	SER	2.9
56	1y	20	U	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
43	1l	29	GLY	2.9
52	2u	16	GLY	2.9
1	1A	2135	A	2.9
1	2A	896	A	2.9
21	2Z	168	GLU	2.9
40	2i	28	VAL	2.9
41	1j	44	VAL	2.9
40	2i	83	ARG	2.9
45	2n	22	THR	2.9
34	2c	200	ALA	2.9
50	2s	18	LYS	2.9
50	2s	76	PRO	2.9
14	2S	54	LEU	2.9
33	2b	11	LEU	2.9
34	2c	12	LEU	2.9
41	2j	85	LEU	2.9
35	1d	173	TRP	2.9
32	2a	976	G	2.9
32	2a	1026	G	2.9
26	24	63	TYR	2.9
43	1l	64	TYR	2.9
47	2p	38	TYR	2.9
21	1Z	166	SER	2.9
1	1A	2167	U	2.9
1	1A	2145	C	2.9
1	1A	2896	C	2.9
1	2A	885	C	2.9
26	24	31	ILE	2.9
46	2o	3	ILE	2.9
1	1A	1073	A	2.9
7	2H	37	VAL	2.9
14	2S	46	VAL	2.9
32	2a	1251	A	2.9
33	1b	130	ARG	2.9
45	2n	45	ARG	2.9
50	2s	19	VAL	2.9
6	2G	74	LYS	2.9
34	2c	146	ALA	2.9
6	2G	152	LEU	2.9
21	2Z	33	LEU	2.9
34	2c	18	TRP	2.9
1	1A	1056	G	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	1099	G	2.9
7	2H	41	MET	2.9
1	1A	2897	U	2.8
1	2A	1026	U	2.8
1	2A	2118	U	2.8
1	2A	2167	U	2.8
3	2D	38	LYS	2.8
6	2G	101	ILE	2.8
35	1d	122	ARG	2.8
44	1m	121	LYS	2.8
50	2s	40	ILE	2.8
35	2d	112	VAL	2.8
36	2e	33	VAL	2.8
38	2g	21	VAL	2.8
41	2j	72	VAL	2.8
33	1b	131	PRO	2.8
33	2b	168	THR	2.8
34	2c	163	ALA	2.8
7	2H	64	LEU	2.8
33	2b	44	LEU	2.8
38	2g	38	LEU	2.8
41	2j	86	MET	2.8
21	1Z	136	PHE	2.8
26	14	32	TYR	2.8
34	2c	184	TYR	2.8
34	2c	13	GLY	2.8
38	2g	4	ARG	2.8
38	2g	5	ARG	2.8
44	2m	122	LYS	2.8
51	1t	102	GLY	2.8
51	2t	8	ARG	2.8
32	2a	953	G	2.8
32	2a	1002	G	2.8
50	2s	23	ASN	2.8
6	2G	92	VAL	2.8
34	2c	68	VAL	2.8
6	2G	17	PRO	2.8
41	2j	100	THR	2.8
44	2m	105	THR	2.8
6	1G	50	ALA	2.8
6	2G	158	ALA	2.8
20	2Y	105	ALA	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	2a	1217	C	2.8
43	2l	51	ALA	2.8
32	2a	965	A	2.8
33	2b	215	LEU	2.8
39	2h	63	LEU	2.8
6	2G	48	GLU	2.8
34	2c	62	ASP	2.8
14	2S	57	LYS	2.8
21	2Z	72	ARG	2.8
40	1i	59	PHE	2.8
6	2G	12	TYR	2.8
26	24	17	GLY	2.8
36	1e	85	GLY	2.8
38	2g	81	GLY	2.8
40	2i	4	TYR	2.8
40	2i	115	GLY	2.8
21	1Z	120	ILE	2.8
33	2b	80	ILE	2.8
14	2S	14	VAL	2.8
26	14	50	VAL	2.8
33	2b	131	PRO	2.8
33	2b	197	VAL	2.8
54	1w	1	G	2.8
56	2y	57	G	2.8
1	2A	2144	U	2.8
41	1j	100	THR	2.8
52	2u	17	THR	2.8
54	1w	20	U	2.8
15	1T	131	ALA	2.8
33	1b	120	ALA	2.8
43	2l	84	LEU	2.8
49	1r	78	LEU	2.8
1	1A	2138	C	2.8
32	2a	979	C	2.8
20	1Y	1	MET	2.8
32	1a	1447	A	2.8
32	2a	969	A	2.8
32	2a	994	A	2.8
50	2s	66	MET	2.8
40	2i	20	ARG	2.8
45	1n	3	ARG	2.8
14	2S	34	HIS	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
38	2g	26	PHE	2.8
14	2S	96	GLY	2.8
7	2H	89	ILE	2.8
26	24	15	ILE	2.8
42	2k	25	TYR	2.8
42	2k	75	TYR	2.8
50	2s	61	TYR	2.8
21	2Z	105	VAL	2.8
25	23	2	PRO	2.8
33	1b	7	VAL	2.8
41	2j	53	PRO	2.8
44	2m	117	VAL	2.8
1	1A	2132	U	2.8
11	2P	6	LEU	2.8
33	2b	98	LEU	2.8
40	2i	106	ALA	2.8
41	2j	71	LEU	2.8
50	2s	5	LEU	2.8
32	2a	1222	G	2.8
3	2D	275	LYS	2.8
16	1U	117	GLN	2.8
21	1Z	119	GLU	2.8
33	2b	175	ARG	2.8
44	2m	3	ARG	2.8
50	2s	78	ARG	2.8
1	1A	2173	A	2.8
32	2a	1035	A	2.8
53	1v	12	A	2.8
53	1v	13	A	2.8
12	1Q	61	GLY	2.7
7	2H	72	ILE	2.7
33	2b	148	TYR	2.7
44	2m	97	PRO	2.7
21	2Z	74	VAL	2.7
50	2s	60	VAL	2.7
33	2b	121	LEU	2.7
39	2h	3	THR	2.7
49	2r	66	LEU	2.7
14	2S	37	ALA	2.7
44	2m	33	ALA	2.7
1	1A	2113	U	2.7
1	1A	2150	U	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	614(A)	U	2.7
33	2b	22	LYS	2.7
42	2k	124	LYS	2.7
45	2n	9	LYS	2.7
19	2X	68	ARG	2.7
33	2b	86	GLU	2.7
1	2A	2893	G	2.7
32	1a	1032	G	2.7
32	2a	1310	G	2.7
45	2n	27	CYS	2.7
1	1A	2129	C	2.7
2	2B	53	A	2.7
32	1a	1030(D)	A	2.7
32	2a	1183	A	2.7
21	2Z	88	PHE	2.7
26	24	64	GLY	2.7
34	2c	128	PHE	2.7
41	2j	54	PHE	2.7
52	2u	4	GLY	2.7
21	2Z	53	ILE	2.7
33	2b	222	ILE	2.7
33	1b	232	PRO	2.7
34	2c	7	PRO	2.7
39	2h	67	PRO	2.7
7	2H	79	VAL	2.7
33	2b	15	VAL	2.7
33	2b	92	TYR	2.7
36	2e	123	LEU	2.7
49	2r	60	ALA	2.7
14	2S	20	ARG	2.7
45	2n	41	ARG	2.7
26	24	30	GLU	2.7
21	2Z	87	ASP	2.7
39	2h	4	ASP	2.7
1	2A	2318	G	2.7
33	1b	18	GLY	2.7
33	2b	72	GLY	2.7
41	2j	52	GLY	2.7
54	1w	70	G	2.7
1	1A	1076	C	2.7
1	1A	2136	C	2.7
21	1Z	171	ILE	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	1a	1008	C	2.7
32	2a	1027	C	2.7
32	2a	1285	A	2.7
33	2b	162	ILE	2.7
21	2Z	68	PRO	2.7
47	1p	41	PRO	2.7
6	2G	111	LEU	2.7
21	2Z	125	LEU	2.7
29	27	45	ALA	2.7
36	2e	108	ALA	2.7
38	2g	65	ALA	2.7
40	2i	27	THR	2.7
40	2i	46	ALA	2.7
40	2i	104	ARG	2.7
44	2m	58	GLU	2.7
1	1A	2130	U	2.7
1	2A	2132	U	2.7
32	2a	982	U	2.7
46	1o	89	GLY	2.7
6	2G	114	ILE	2.7
33	2b	17	PHE	2.7
34	2c	134	ILE	2.7
34	2c	202	ILE	2.7
36	2e	118	ILE	2.7
40	2i	59	PHE	2.7
26	24	29	PRO	2.7
1	2A	652(U)	G	2.7
1	2A	2134	A	2.7
32	2a	975	A	2.7
32	2a	1021	G	2.7
1	2A	2137	C	2.7
32	2a	1115	C	2.7
32	2a	1260	C	2.7
50	2s	7	LYS	2.7
33	2b	174	VAL	2.7
33	2b	229	VAL	2.7
36	2e	12	LEU	2.7
39	2h	10	LEU	2.7
40	1i	19	LEU	2.7
50	2s	45	VAL	2.7
21	2Z	152	ALA	2.7
40	2i	61	ALA	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
44	2m	75	ALA	2.7
51	2t	103	GLY	2.6
26	24	42	PHE	2.6
33	2b	39	ILE	2.6
33	2b	214	ILE	2.6
41	2j	91	PRO	2.6
1	1A	1088	A	2.6
1	2A	1445	A	2.6
19	2X	95	LEU	2.6
1	1A	2128	C	2.6
33	1b	15	VAL	2.6
33	2b	142	LEU	2.6
35	2d	148	VAL	2.6
35	2d	155	LEU	2.6
50	1s	20	LEU	2.6
1	1A	2802	G	2.6
1	2A	2110	G	2.6
1	2A	2166	G	2.6
26	14	57	GLU	2.6
32	1a	1031	G	2.6
38	2g	77	SER	2.6
56	2y	56	C	2.6
8	2I	53	ALA	2.6
14	2S	72	ALA	2.6
33	2b	88	ALA	2.6
39	2h	58	TYR	2.6
44	1m	87	TYR	2.6
47	1p	82	GLN	2.6
22	10	8	GLY	2.6
26	24	65	ASP	2.6
32	2a	1196	U	2.6
7	2H	136	ILE	2.6
26	14	49	PHE	2.6
41	1j	75	ILE	2.6
41	2j	50	ILE	2.6
29	27	47	ARG	2.6
33	2b	48	MET	2.6
38	2g	32	ARG	2.6
7	2H	107	VAL	2.6
32	2a	974	A	2.6
26	24	27	THR	2.6
32	2a	1114	C	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	2b	77	ALA	2.6
1	1A	2141	G	2.6
38	2g	151	TYR	2.6
40	2i	117	HIS	2.6
42	2k	42	TRP	2.6
33	2b	75	LYS	2.6
38	2g	36	LYS	2.6
6	1G	21	ARG	2.6
23	2l	68	PRO	2.6
32	2a	1532	U	2.6
12	2Q	64	ILE	2.6
44	2m	9	ILE	2.6
50	2s	36	ARG	2.6
6	2G	23	PHE	2.6
34	2c	186	PHE	2.6
47	2p	80	PHE	2.6
22	20	84	LEU	2.6
33	1b	9	GLU	2.6
33	1b	134	GLU	2.6
43	2l	52	LEU	2.6
21	2Z	42	VAL	2.6
34	2c	64	VAL	2.6
40	2i	44	VAL	2.6
50	2s	53	ASN	2.6
40	1i	126	SER	2.6
1	1A	1069	A	2.6
6	2G	64	THR	2.6
38	2g	2	ALA	2.6
32	2a	1286	A	2.6
34	2c	69	HIS	2.6
1	1A	897	C	2.6
1	2A	2175	C	2.6
2	2B	62	C	2.6
14	2S	36	TYR	2.6
32	2a	999	C	2.6
32	2a	1019	C	2.6
34	2c	23	TYR	2.6
44	2m	21	TYR	2.6
1	1A	2162	G	2.6
1	2A	2157	G	2.6
32	2a	1221	G	2.6
44	2m	64	TRP	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
54	2w	18	G	2.6
6	2G	147	ASP	2.6
35	1d	2	GLY	2.6
35	2d	2	GLY	2.6
36	2e	107	ARG	2.6
46	2o	89	GLY	2.6
14	2S	40	ILE	2.6
35	2d	158	ILE	2.6
7	2H	88	LEU	2.6
14	2S	32	LEU	2.6
21	2Z	76	LEU	2.6
24	22	66	GLU	2.6
40	1i	2	GLU	2.6
49	2r	31	LEU	2.6
50	1s	71	LEU	2.6
34	2c	173	VAL	2.6
38	2g	17	VAL	2.6
38	2g	66	VAL	2.6
6	2G	145	THR	2.6
26	24	24	THR	2.6
38	2g	39	ALA	2.6
49	2r	24	ALA	2.6
50	2s	33	THR	2.6
7	2H	94	TYR	2.6
17	2V	91	TYR	2.6
22	20	26	TYR	2.6
33	1b	236	TYR	2.6
40	2i	114	TYR	2.6
1	1A	889	C	2.5
6	2G	21	ARG	2.5
22	20	77	ARG	2.5
40	2i	128	ARG	2.5
56	1y	56	C	2.5
12	2Q	1	MET	2.5
33	2b	232	PRO	2.5
50	2s	8	GLY	2.5
1	1A	1063	G	2.5
1	2A	2124	G	2.5
26	24	14	ILE	2.5
32	2a	1024	G	2.5
33	2b	108	ILE	2.5
56	2y	18	G	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	2F	24	LEU	2.5
7	2H	71	LEU	2.5
32	1a	1000	U	2.5
32	2a	961	U	2.5
32	2a	1205	U	2.5
35	2d	162	LEU	2.5
38	2g	124	LEU	2.5
40	2i	56	LEU	2.5
22	20	79	VAL	2.5
34	2c	138	VAL	2.5
44	2m	101	GLN	2.5
33	2b	16	HIS	2.5
4	2E	204	ALA	2.5
41	2j	27	ALA	2.5
44	2m	30	ALA	2.5
51	1t	95	ALA	2.5
24	22	7	ARG	2.5
35	2d	115	ARG	2.5
38	2g	115	ARG	2.5
47	1p	81	ARG	2.5
1	2A	2158	A	2.5
7	2H	83	TYR	2.5
26	24	43	TYR	2.5
32	2a	986	A	2.5
32	2a	1250	A	2.5
32	2a	1357	A	2.5
53	1v	24	A	2.5
1	1A	2142	C	2.5
32	2a	1277	C	2.5
38	1g	81	GLY	2.5
51	1t	101	GLY	2.5
35	1d	5	ILE	2.5
35	1d	150	GLU	2.5
1	1A	1071	G	2.5
1	2A	1533	G	2.5
2	2B	118	G	2.5
32	2a	951	G	2.5
32	2a	1031	G	2.5
32	2a	1048	G	2.5
36	2e	71	LEU	2.5
44	2m	19	LEU	2.5
1	1A	1175	U	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	2H	115	VAL	2.5
8	2I	81	VAL	2.5
21	2Z	27	VAL	2.5
44	1m	53	VAL	2.5
45	2n	10	ALA	2.5
6	2G	161	THR	2.5
21	2Z	16	SER	2.5
44	2m	37	THR	2.5
35	1d	191	ARG	2.5
41	2j	79	ARG	2.5
7	2H	128	PRO	2.5
34	2c	109	PRO	2.5
51	2t	98	PRO	2.5
1	1A	2790	A	2.5
1	2A	899	A	2.5
15	2T	69	GLY	2.5
21	2Z	106	GLY	2.5
31	29	21	GLY	2.5
10	2O	81	ASP	2.5
32	2a	1044	A	2.5
34	2c	78	GLY	2.5
35	2d	183	GLY	2.5
50	2s	26	GLY	2.5
33	2b	166	ASP	2.5
6	2G	77	ILE	2.5
40	2i	12	GLU	2.5
32	2a	972	C	2.5
54	2w	2	C	2.5
54	2w	67	C	2.5
6	2G	7	LEU	2.5
6	2G	178	PHE	2.5
14	2S	101	LEU	2.5
38	2g	101	LEU	2.5
40	2i	40	LEU	2.5
41	2j	8	LEU	2.5
14	2S	33	LYS	2.5
44	2m	65	LYS	2.5
1	1A	1082	U	2.5
1	1A	2109	U	2.5
32	2a	1065	U	2.5
36	2e	67	VAL	2.5
38	2g	37	ASN	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
41	1j	72	VAL	2.5
42	2k	117	ASN	2.5
44	1m	106	ASN	2.5
1	1A	2125	G	2.5
32	2a	1124	G	2.5
32	2a	1276	G	2.5
6	2G	136	ARG	2.5
41	2j	46	ARG	2.5
45	2n	32	SER	2.5
33	2b	202	PRO	2.5
6	2G	44	GLY	2.5
12	2Q	61	GLY	2.5
34	2c	29	TYR	2.5
39	2h	48	TYR	2.5
44	2m	69	GLU	2.5
36	2e	76	ILE	2.5
1	1A	2801(A)	A	2.5
1	1A	2892	A	2.5
1	2A	6	A	2.5
1	2A	229	A	2.5
1	2A	1847	A	2.5
32	2a	959	A	2.5
54	2w	7	A	2.5
21	2Z	41	LEU	2.5
33	2b	154	LEU	2.5
41	1j	65	LEU	2.5
45	2n	15	LYS	2.5
8	2I	54	GLN	2.5
1	1A	1080	C	2.5
1	2A	2140	C	2.5
32	2a	1018	C	2.5
32	2a	1054	C	2.5
6	2G	31	VAL	2.5
16	2U	90	VAL	2.5
34	2c	130	VAL	2.5
36	2e	100	VAL	2.5
44	2m	54	VAL	2.5
6	2G	51	ARG	2.5
38	1g	4	ARG	2.5
38	2g	3	ARG	2.5
33	2b	173	ALA	2.5
45	2n	48	ALA	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
14	2S	5	THR	2.5
34	2c	165	THR	2.5
1	2A	2141	G	2.5
1	2A	2807	G	2.5
32	2a	1053	G	2.5
51	1t	70	SER	2.5
21	1Z	169	GLU	2.4
36	2e	23	GLY	2.4
6	2G	63	ILE	2.4
6	2G	97	ASP	2.4
14	2S	94	TYR	2.4
26	24	28	LYS	2.4
41	1j	4	ILE	2.4
45	2n	58	LYS	2.4
6	2G	139	LEU	2.4
33	2b	51	LEU	2.4
33	2b	138	LEU	2.4
34	2c	32	LEU	2.4
37	2f	21	LEU	2.4
40	1i	56	LEU	2.4
50	2s	30	LEU	2.4
51	2t	99	LEU	2.4
21	2Z	32	HIS	2.4
32	1a	344	A	2.4
36	2e	27	ARG	2.4
44	2m	88	ARG	2.4
2	2B	27	C	2.4
21	2Z	139	VAL	2.4
31	29	16	VAL	2.4
32	2a	1037	C	2.4
34	2c	116	VAL	2.4
36	2e	41	VAL	2.4
45	2n	56	VAL	2.4
1	2A	1113	U	2.4
1	2A	2897	U	2.4
14	2S	66	ALA	2.4
32	2a	1126	U	2.4
33	1b	34	ALA	2.4
35	2d	165	MET	2.4
41	2j	18	ALA	2.4
40	2i	2	GLU	2.4
1	1A	2120	G	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	2121	G	2.4
1	1A	2207	G	2.4
1	2A	2168	G	2.4
32	2a	1127	G	2.4
47	1p	37	GLY	2.4
36	2e	101	ILE	2.4
40	2i	74	ILE	2.4
41	2j	23	ILE	2.4
6	2G	131	TYR	2.4
20	2Y	55	TYR	2.4
22	20	59	LEU	2.4
34	2c	178	LEU	2.4
12	2Q	59	ARG	2.4
40	2i	111	ARG	2.4
46	2o	88	ARG	2.4
1	2A	2310	A	2.4
2	2B	120	A	2.4
32	2a	1236	A	2.4
6	2G	130	ASN	2.4
7	2H	44	VAL	2.4
12	2Q	106	VAL	2.4
26	24	33	VAL	2.4
30	28	34	TRP	2.4
33	2b	136	VAL	2.4
34	2c	207	VAL	2.4
36	2e	55	VAL	2.4
39	1h	93	VAL	2.4
43	1l	18	VAL	2.4
43	2l	101	VAL	2.4
51	1t	75	ASN	2.4
1	1A	884	C	2.4
1	1A	1079	C	2.4
1	2A	867	C	2.4
7	2H	165	ALA	2.4
32	1a	1029	C	2.4
32	2a	1043	C	2.4
32	2a	1118	C	2.4
33	2b	186	ALA	2.4
34	2c	60	ALA	2.4
51	1t	12	ALA	2.4
1	2A	271(K)	U	2.4
1	2A	2130	U	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	2B	55	U	2.4
33	2b	210	SER	2.4
34	2c	135	LYS	2.4
36	2e	81	GLU	2.4
46	2o	75	PRO	2.4
18	2W	112	GLY	2.4
1	1A	2110	G	2.4
1	1A	2131	G	2.4
1	2A	1170	G	2.4
6	2G	41	GLN	2.4
8	1I	72	LEU	2.4
34	2c	91	LEU	2.4
43	2l	41	ARG	2.4
42	2k	59	TYR	2.4
48	2q	95	TYR	2.4
33	1b	17	PHE	2.4
14	2S	49	VAL	2.4
22	20	31	VAL	2.4
40	2i	53	VAL	2.4
1	2A	2119	A	2.4
32	2a	1093	A	2.4
32	2a	1151	A	2.4
35	2d	154	ASN	2.4
40	2i	122	ALA	2.4
2	2B	6	C	2.4
6	2G	32	PRO	2.4
22	20	68	GLU	2.4
45	2n	4	LYS	2.4
52	2u	8	THR	2.4
32	2a	1119	C	2.4
33	2b	99	GLY	2.4
40	2i	68	GLY	2.4
6	2G	140	ILE	2.4
21	2Z	124	ILE	2.4
26	24	5	ILE	2.4
6	2G	133	LEU	2.4
14	2S	58	LEU	2.4
21	1Z	121	HIS	2.4
21	2Z	102	LEU	2.4
33	2b	69	LEU	2.4
37	1f	55	ASP	2.4
44	2m	57	ARG	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	2149	G	2.4
6	2G	80	PHE	2.4
6	2G	148	MET	2.4
7	2H	123	PHE	2.4
21	2Z	3	TYR	2.4
32	1a	1021	G	2.4
32	2a	1061	G	2.4
36	2e	61	TYR	2.4
54	2w	44	G	2.4
6	2G	149	VAL	2.4
21	2Z	71	VAL	2.4
34	2c	75	VAL	2.4
39	2h	61	VAL	2.4
50	2s	67	VAL	2.4
12	2Q	22	LYS	2.4
1	2A	2117	A	2.4
32	2a	996	A	2.4
32	2a	1049	U	2.3
1	1A	1092	C	2.3
17	2V	9	GLY	2.3
32	2a	985	C	2.3
6	2G	157	ILE	2.3
9	2N	85	ILE	2.3
34	2c	21	ARG	2.3
41	2j	5	ARG	2.3
42	2k	29	ILE	2.3
45	2n	12	ARG	2.3
50	2s	81	ARG	2.3
11	1P	100	LEU	2.3
33	1b	187	LEU	2.3
33	1b	213	LEU	2.3
35	2d	157	LEU	2.3
40	2i	85	LEU	2.3
41	2j	56	HIS	2.3
41	2j	58	ASP	2.3
44	2m	48	LEU	2.3
46	1o	57	LEU	2.3
50	2s	69	HIS	2.3
12	2Q	7	MET	2.3
26	24	67	TYR	2.3
33	1b	33	TYR	2.3
6	2G	182	LYS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	2H	133	VAL	2.3
14	2S	69	VAL	2.3
14	2S	98	VAL	2.3
21	2Z	96	VAL	2.3
33	2b	139	LYS	2.3
34	2c	141	VAL	2.3
39	2h	19	VAL	2.3
50	2s	51	VAL	2.3
1	1A	2894	G	2.3
18	2W	60	ASN	2.3
32	1a	1002	G	2.3
32	2a	963	G	2.3
32	2a	1323	G	2.3
6	2G	110	ALA	2.3
35	1d	179	GLU	2.3
48	2q	44	ALA	2.3
17	2V	50	PRO	2.3
42	2k	31	THR	2.3
32	1a	1001	A	2.3
32	1a	1286	A	2.3
53	2v	12	A	2.3
53	2v	13	A	2.3
12	2Q	15	GLY	2.3
21	2Z	147	GLY	2.3
40	2i	57	GLY	2.3
41	2j	60	ARG	2.3
32	2a	1070	U	2.3
34	2c	37	GLN	2.3
40	2i	3	GLN	2.3
5	2F	181	LEU	2.3
8	2I	68	LEU	2.3
33	2b	145	LEU	2.3
40	2i	50	LEU	2.3
50	2s	83	HIS	2.3
52	2u	13	ILE	2.3
1	2A	888	C	2.3
6	2G	126	ASP	2.3
32	2a	1249	C	2.3
12	2Q	103	MET	2.3
6	2G	141	PHE	2.3
40	2i	33	PHE	2.3
47	1p	35	LYS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
35	1d	138	TYR	2.3
36	2e	90	VAL	2.3
4	2E	73	GLU	2.3
17	2V	93	GLU	2.3
21	2Z	17	ALA	2.3
33	2b	171	ALA	2.3
41	2j	39	PRO	2.3
44	2m	41	PRO	2.3
1	1A	1074	G	2.3
1	1A	2133	G	2.3
1	2A	1171	G	2.3
26	24	52	THR	2.3
38	1g	5	ARG	2.3
41	2j	66	ARG	2.3
54	2w	70	G	2.3
1	2A	866	A	2.3
1	2A	2171	A	2.3
2	2B	25	A	2.3
6	2G	100	TRP	2.3
14	2S	53	SER	2.3
21	2Z	166	SER	2.3
32	2a	977	A	2.3
32	2a	1001	A	2.3
32	2a	1004	A	2.3
32	2a	1280	A	2.3
32	2a	1306	A	2.3
34	2c	22	TRP	2.3
35	1d	23	GLY	2.3
35	2d	23	GLY	2.3
44	2m	112	GLY	2.3
7	2H	103	LEU	2.3
14	2S	80	LEU	2.3
16	2U	88	ILE	2.3
21	2Z	157	LEU	2.3
28	26	7	ILE	2.3
33	1b	118	LEU	2.3
33	2b	41	ILE	2.3
34	2c	57	ILE	2.3
35	1d	21	LEU	2.3
35	1d	194	LEU	2.3
51	1t	55	ILE	2.3
51	2t	63	ILE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	2118	U	2.3
32	2a	1307	U	2.3
33	2b	101	MET	2.3
1	2A	2129	C	2.3
1	2A	2164	C	2.3
1	2A	2794	C	2.3
32	2a	948	C	2.3
32	2a	1045	C	2.3
34	2c	4	LYS	2.3
50	2s	74	PHE	2.3
7	2H	19	VAL	2.3
33	2b	170	GLU	2.3
34	1c	90	GLU	2.3
34	1c	207	VAL	2.3
43	2l	18	VAL	2.3
46	1o	69	TYR	2.3
47	1p	2	VAL	2.3
6	2G	2	PRO	2.3
6	2G	87	PRO	2.3
7	2H	12	PRO	2.3
34	2c	181	ASN	2.3
36	2e	94	ALA	2.3
46	2o	2	PRO	2.3
36	2e	25	ARG	2.3
52	2u	7	ARG	2.3
26	24	44	THR	2.3
34	1c	15	THR	2.3
21	1Z	147	GLY	2.3
33	2b	228	GLY	2.3
34	2c	41	GLY	2.3
40	2i	6	GLY	2.3
41	2j	10	GLY	2.3
1	1A	883	G	2.3
1	1A	2100	G	2.3
2	2B	103	G	2.3
32	2a	987	G	2.3
41	1j	30	SER	2.3
33	2b	196	LEU	2.3
35	1d	188	LEU	2.3
43	2l	100	ILE	2.3
44	2m	84	ILE	2.3
47	1p	48	TRP	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
47	2p	19	ILE	2.3
51	1t	10	LEU	2.3
1	2A	2801(A)	A	2.3
23	21	78	LYS	2.3
33	1b	133	LYS	2.3
54	2w	66	U	2.3
1	1A	2140	C	2.3
7	2H	124	GLU	2.3
11	2P	149	GLU	2.3
33	2b	7	VAL	2.3
38	2g	9	VAL	2.3
49	1r	86	VAL	2.3
22	20	72	ARG	2.3
26	14	67	TYR	2.3
35	2d	3	ARG	2.3
38	1g	79	ARG	2.3
40	2i	66	ARG	2.3
33	2b	85	ALA	2.2
40	2i	94	ALA	2.2
19	2X	35	THR	2.2
11	2P	26	GLY	2.2
26	14	54	GLY	2.2
26	14	64	GLY	2.2
34	2c	74	GLY	2.2
43	1l	63	GLY	2.2
47	2p	82	GLN	2.2
7	2H	84	SER	2.2
7	2H	171	LEU	2.2
12	2Q	66	ILE	2.2
12	2Q	127	ILE	2.2
14	2S	59	LYS	2.2
20	2Y	5	MET	2.2
21	2Z	1	MET	2.2
24	22	3	LEU	2.2
33	2b	127	ILE	2.2
34	1c	202	ILE	2.2
40	2i	95	LYS	2.2
40	2i	127	LYS	2.2
51	2t	74	LYS	2.2
1	1A	548	A	2.2
1	1A	2171	A	2.2
33	2b	220	ASP	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	2c	17	ASP	2.2
54	2w	14	A	2.2
1	2A	882	G	2.2
32	2a	587	G	2.2
32	2a	993	G	2.2
32	2a	1233	G	2.2
56	2y	15	G	2.2
1	2A	2895	U	2.2
32	2a	1040	U	2.2
7	2H	53	GLU	2.2
40	2i	37	PHE	2.2
2	2B	4	C	2.2
5	2F	6	VAL	2.2
6	2G	109	VAL	2.2
7	2H	15	VAL	2.2
9	2N	9	VAL	2.2
20	2Y	85	VAL	2.2
33	2b	53	ARG	2.2
33	2b	81	VAL	2.2
34	2c	76	VAL	2.2
42	2k	126	ARG	2.2
43	2l	40	VAL	2.2
54	1w	4	C	2.2
8	2I	49	ALA	2.2
12	2Q	49	ALA	2.2
33	2b	34	ALA	2.2
33	2b	207	ALA	2.2
36	2e	30	ALA	2.2
38	1g	2	ALA	2.2
38	2g	109	ASN	2.2
40	2i	15	ALA	2.2
12	2Q	26	TYR	2.2
36	2e	133	TYR	2.2
43	2l	64	TYR	2.2
43	2l	69	TYR	2.2
48	2q	32	TYR	2.2
52	2u	21	TYR	2.2
21	2Z	151	HIS	2.2
35	2d	123	HIS	2.2
45	1n	22	THR	2.2
3	1D	275	LYS	2.2
11	2P	118	GLY	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
9	2N	112	LEU	2.2
34	2c	47	LEU	2.2
41	2j	16	LEU	2.2
33	1b	223	ILE	2.2
33	2b	211	ILE	2.2
34	1c	124	ILE	2.2
47	1p	59	TRP	2.2
1	1A	1046	A	2.2
32	2a	1005	A	2.2
32	2a	1225	A	2.2
1	1A	895	U	2.2
1	2A	2150	U	2.2
32	2a	1020	U	2.2
1	1A	1055	G	2.2
1	1A	1091	G	2.2
1	2A	11	G	2.2
1	2A	2116	G	2.2
1	2A	2165	G	2.2
11	2P	79	ARG	2.2
14	2S	13	ARG	2.2
14	2S	97	ARG	2.2
14	2S	28	VAL	2.2
20	2Y	45	VAL	2.2
33	1b	125	PRO	2.2
33	2b	159	PRO	2.2
38	2g	93	PRO	2.2
43	2l	11	VAL	2.2
1	1A	1072	C	2.2
1	2A	884	C	2.2
11	2P	127	ALA	2.2
32	1a	999	C	2.2
32	2a	970	C	2.2
33	2b	37	ASN	2.2
34	2c	169	ALA	2.2
39	2h	28	ALA	2.2
41	2j	69	ASN	2.2
51	1t	9	ASN	2.2
51	2t	94	ALA	2.2
51	2t	95	ALA	2.2
34	2c	193	TYR	2.2
34	2c	199	LYS	2.2
41	2j	7	LYS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
41	2j	14	LYS	2.2
6	2G	165	THR	2.2
9	2N	22	THR	2.2
42	1k	25	TYR	2.2
42	1k	75	TYR	2.2
47	2p	45	THR	2.2
14	2S	90	GLY	2.2
35	1d	157	LEU	2.2
44	2m	68	GLY	2.2
39	2h	45	ILE	2.2
48	2q	90	ILE	2.2
6	2G	76	SER	2.2
40	2i	71	SER	2.2
6	2G	35	GLU	2.2
7	2H	159	GLU	2.2
45	2n	46	GLU	2.2
6	2G	128	ARG	2.2
33	2b	96	ARG	2.2
1	1A	1067	A	2.2
1	1A	2170	A	2.2
1	1A	2189	U	2.2
32	2a	964	A	2.2
32	2a	978	A	2.2
32	2a	997	U	2.2
32	2a	1315	U	2.2
55	2x	47	U	2.2
12	2Q	29	PHE	2.2
7	2H	43	VAL	2.2
8	2I	19	VAL	2.2
20	2Y	7	VAL	2.2
21	2Z	161	VAL	2.2
24	22	19	VAL	2.2
33	2b	164	VAL	2.2
40	2i	26	VAL	2.2
1	1A	880	G	2.2
1	2A	1115	G	2.2
1	2A	2151	G	2.2
32	2a	1064	G	2.2
47	1p	43	LYS	2.2
54	2w	34	G	2.2
12	2Q	136	ALA	2.2
14	2S	100	ALA	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
38	2g	128	ALA	2.2
36	2e	20	GLN	2.2
1	2A	886	C	2.2
7	2H	67	LEU	2.2
32	1a	1030	C	2.2
32	1a	1037	C	2.2
32	2a	1066	C	2.2
32	2a	1321	C	2.2
32	2a	1354	C	2.2
35	2d	16	GLY	2.2
35	2d	20	TYR	2.2
40	2i	64	THR	2.2
41	2j	15	THR	2.2
41	2j	92	THR	2.2
33	1b	221	LEU	2.2
36	2e	85	GLY	2.2
37	2f	61	LEU	2.2
51	2t	96	GLY	2.2
21	2Z	137	ILE	2.2
39	2h	35	ILE	2.2
33	2b	192	SER	2.2
9	2N	68	GLU	2.2
44	2m	73	GLU	2.2
6	2G	95	ARG	2.2
7	2H	3	ARG	2.2
12	1Q	60	ARG	2.2
21	2Z	81	ARG	2.2
34	2c	30	ARG	2.2
51	1t	8	ARG	2.2
7	2H	21	PRO	2.2
1	1A	1083	U	2.2
1	2A	2135	A	2.1
26	24	2	LYS	2.2
6	2G	70	VAL	2.1
32	2a	1000	U	2.2
32	2a	1232	U	2.2
32	2a	1235	U	2.2
32	2a	1257	U	2.2
41	2j	24	VAL	2.1
44	2m	45	VAL	2.1
48	1q	23	VAL	2.1
8	2I	1	MET	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
15	2T	130	ALA	2.1
40	2i	84	ALA	2.1
44	2m	92	HIS	2.1
45	2n	20	ALA	2.1
47	2p	16	HIS	2.1
51	1t	94	ALA	2.1
1	1A	2116	G	2.1
1	2A	2792	G	2.1
5	1F	208	GLY	2.1
21	1Z	102	LEU	2.1
21	2Z	18	LEU	2.1
54	2w	19	G	2.1
55	2x	70	G	2.1
56	1y	19	G	2.1
33	1b	41	ILE	2.1
36	2e	131	ILE	2.1
40	2i	88	TYR	2.1
43	2l	120	TYR	2.1
46	2o	87	ILE	2.1
1	1A	2791	C	2.1
1	2A	652(V)	C	2.1
32	2a	1263	C	2.1
12	1Q	6	ARG	2.1
12	2Q	5	ARG	2.1
20	2Y	91	GLU	2.1
21	2Z	4	ARG	2.1
33	1b	129	GLU	2.1
40	2i	107	ARG	2.1
41	1j	46	ARG	2.1
45	1n	57	ARG	2.1
50	2s	17	GLU	2.1
33	2b	233	SER	2.1
50	2s	29	ARG	2.1
11	2P	76	LYS	2.1
48	2q	100	LYS	2.1
24	22	37	PHE	2.1
9	1N	140	VAL	2.1
21	2Z	90	VAL	2.1
26	24	10	VAL	2.1
26	24	50	VAL	2.1
38	2g	156	TRP	2.1
40	2i	86	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
41	2j	94	VAL	2.1
44	2m	74	VAL	2.1
50	1s	45	VAL	2.1
1	1A	1103	A	2.1
1	1A	1177	A	2.1
1	2A	2320	A	2.1
2	2B	26	A	2.1
12	2Q	113	GLN	2.1
56	1y	45	U	2.1
32	2a	1110	A	2.1
32	2a	1447	A	2.1
34	2c	100	ALA	2.1
36	2e	86	ALA	2.1
40	2i	43	ALA	2.1
53	2v	14	A	2.1
41	1j	69	ASN	2.1
6	2G	175	LEU	2.1
17	2V	94	LEU	2.1
28	26	9	LEU	2.1
33	2b	103	THR	2.1
34	2c	197	GLY	2.1
36	2e	139	LEU	2.1
39	1h	71	GLY	2.1
40	2i	7	THR	2.1
41	1j	40	LEU	2.1
44	2m	26	GLY	2.1
41	1j	98	ILE	2.1
44	2m	25	ILE	2.1
12	2Q	32	TYR	2.1
1	1A	275	G	2.1
1	1A	2165	G	2.1
1	2A	2153	G	2.1
1	2A	2162	G	2.1
20	2Y	29	GLU	2.1
21	2Z	138	GLU	2.1
33	2b	141	GLU	2.1
36	2e	60	TYR	2.1
39	2h	30	ARG	2.1
39	2h	84	ARG	2.1
44	2m	114	ARG	2.1
32	2a	1017	G	2.1
32	2a	1182	G	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	2D	71	ASP	2.1
32	2a	1234	C	2.1
34	2c	56	ASP	2.1
41	2j	12	ASP	2.1
54	1w	3	C	2.1
34	2c	45	LYS	2.1
5	2F	14	PRO	2.1
21	2Z	159	PRO	2.1
26	24	11	PRO	2.1
33	2b	167	PRO	2.1
33	2b	83	MET	2.1
47	2p	9	PHE	2.1
8	1l	107	VAL	2.1
24	22	70	GLN	2.1
33	1b	71	VAL	2.1
38	1g	86	GLN	2.1
38	2g	105	VAL	2.1
1	1A	1026	U	2.1
6	2G	171	ALA	2.1
19	2X	46	ALA	2.1
21	2Z	51	ALA	2.1
32	1a	204	U	2.1
41	1j	32	ALA	2.1
44	2m	51	ALA	2.1
41	1j	76	ASN	2.1
1	2A	2114	A	2.1
14	2S	48	LEU	2.1
21	2Z	91	LEU	2.1
22	20	22	GLY	2.1
28	26	11	LEU	2.1
32	1a	172	A	2.1
32	2a	1015	A	2.1
33	2b	180	LEU	2.1
34	2c	205	GLY	2.1
38	1g	12	LEU	2.1
39	1h	127	LEU	2.1
43	2l	74	GLY	2.1
48	2q	80	GLY	2.1
48	2q	98	LEU	2.1
44	2m	99	ARG	2.1
9	2N	60	ILE	2.1
26	24	22	ILE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
38	1g	90	GLU	2.1
46	1o	87	ILE	2.1
6	2G	11	TYR	2.1
33	2b	33	TYR	2.1
7	1H	175	LYS	2.1
39	2h	54	ASP	2.1
42	1k	51	LYS	2.1
7	2H	16	SER	2.1
33	1b	124	SER	2.1
50	1s	13	ASP	2.1
1	2A	614(B)	G	2.1
1	2A	2159	G	2.1
2	2B	18	G	2.1
2	2B	117	G	2.1
32	2a	1185	G	2.1
56	1y	15	G	2.1
1	1A	2161	C	2.1
2	2B	32	C	2.1
32	1a	1030(B)	C	2.1
32	2a	1189	C	2.1
32	2a	1322	C	2.1
33	2b	194	PRO	2.1
9	2N	1	MET	2.1
6	1G	80	PHE	2.1
7	2H	76	VAL	2.1
12	2Q	52	VAL	2.1
22	20	45	PHE	2.1
22	20	66	VAL	2.1
34	2c	120	VAL	2.1
36	1e	69	VAL	2.1
40	1i	18	PHE	2.1
20	2Y	78	ALA	2.1
33	2b	225	ALA	2.1
40	1i	55	ALA	2.1
1	1A	271(K)	U	2.1
1	1A	1963	U	2.1
12	2Q	6	ARG	2.1
17	1V	101	GLY	2.1
22	20	6	GLY	2.1
23	21	79	GLY	2.1
24	12	69	ARG	2.1
35	1d	135	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	2b	227	GLY	2.1
40	1i	8	GLY	2.1
40	1i	9	ARG	2.1
46	2o	68	ARG	2.1
48	2q	22	LEU	2.1
49	1r	76	LEU	2.1
54	2w	45	U	2.1
38	2g	24	THR	2.1
1	1A	229	A	2.1
32	2a	532	A	2.1
32	2a	1014	A	2.1
32	2a	1180	A	2.1
33	1b	32	ILE	2.1
33	1b	214	ILE	2.1
30	28	29	LYS	2.1
33	2b	27	LYS	2.1
35	1d	22	LYS	2.1
51	2t	65	LYS	2.1
33	2b	160	ASP	2.1
34	1c	193	TYR	2.1
41	2j	17	ASP	2.1
46	2o	69	TYR	2.1
21	2Z	153	SER	2.1
6	2G	68	PRO	2.1
6	2G	122	PRO	2.1
21	2Z	28	MET	2.1
1	1A	881	G	2.0
1	1A	886	C	2.1
1	1A	898	C	2.1
1	1A	2143	C	2.1
1	2A	271(M)	G	2.0
1	2A	652(T)	C	2.1
31	29	20	HIS	2.1
1	2A	2319	G	2.0
2	2B	19	G	2.0
32	2a	927	G	2.0
32	2a	1069	C	2.1
32	2a	1384	C	2.1
38	2g	13	GLN	2.0
54	2w	6	G	2.0
19	2X	81	VAL	2.0
21	2Z	86	VAL	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	2c	151	VAL	2.0
7	2H	170	ARG	2.0
14	2S	102	ALA	2.0
15	1T	115	ARG	2.0
35	1d	3	ARG	2.0
38	2g	152	ALA	2.0
40	2i	16	ARG	2.0
40	2i	119	ALA	2.0
43	2l	68	ALA	2.0
50	1s	24	ALA	2.0
6	1G	139	LEU	2.0
24	22	35	LEU	2.0
5	2F	208	GLY	2.0
15	2T	128	GLU	2.0
33	2b	134	GLU	2.0
33	2b	231	GLU	2.0
41	2j	64	GLU	2.0
50	2s	72	GLY	2.0
1	1A	12	U	2.0
6	2G	162	THR	2.0
7	2H	175	LYS	2.0
32	1a	1257	U	2.0
32	2a	1083	U	2.0
33	1b	22	LYS	2.0
39	2h	86	ILE	2.0
41	1j	42	THR	2.0
2	2B	52	A	2.0
20	2Y	53	PRO	2.0
6	2G	86	MET	2.0
20	2Y	57	GLN	2.0
26	14	60	GLN	2.0
33	1b	224	GLN	2.0
1	1A	2108	C	2.0
1	1A	2146	C	2.0
1	2A	897	C	2.0
3	2D	268	ARG	2.0
6	2G	98	ARG	2.0
9	2N	61	ARG	2.0
32	2a	1262	C	2.0
32	2a	1366	C	2.0
32	2a	1383	C	2.0
34	1c	106	VAL	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
36	2e	18	ARG	2.0
37	1f	90	VAL	2.0
41	1j	24	VAL	2.0
43	2l	58	VAL	2.0
45	1n	33	VAL	2.0
46	2o	15	PHE	2.0
54	2w	13	C	2.0
54	2w	25	C	2.0
1	2A	652(C)	G	2.0
1	2A	2131	G	2.0
1	2A	2206	G	2.0
1	2A	2315	G	2.0
6	2G	43	LEU	2.0
6	2G	53	LEU	2.0
6	2G	151	ALA	2.0
32	2a	971	G	2.0
32	2a	1094	G	2.0
7	2H	7	LEU	2.0
11	2P	105	LEU	2.0
12	2Q	2	LEU	2.0
14	2S	4	LEU	2.0
21	2Z	11	GLU	2.0
24	22	5	GLU	2.0
24	22	60	LEU	2.0
33	1b	11	LEU	2.0
33	1b	188	ALA	2.0
34	2c	34	LEU	2.0
34	2c	61	ALA	2.0
34	2c	92	ALA	2.0
34	2c	121	ALA	2.0
36	2e	134	ALA	2.0
37	1f	19	LEU	2.0
39	2h	36	LEU	2.0
40	1i	13	ALA	2.0
44	1m	5	ALA	2.0
44	2m	28	ALA	2.0
8	2I	87	LYS	2.0
33	2b	14	GLY	2.0
34	2c	25	GLY	2.0
34	2c	159	GLY	2.0
35	1d	169	LYS	2.0
39	2h	96	GLY	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
39	2h	131	GLY	2.0
42	2k	118	GLY	2.0
43	1l	126	LYS	2.0
45	1n	51	GLY	2.0
51	2t	9	ASN	2.0
21	2Z	57	ILE	2.0
39	2h	111	ILE	2.0
32	2a	991	U	2.0
32	2a	1148	U	2.0
1	2A	528	A	2.0
32	1a	160	A	2.0
32	2a	1157	A	2.0
32	2a	1289	A	2.0
38	2g	89	MET	2.0
40	2i	75	ASP	2.0
5	2F	15	SER	2.0
18	2W	111	HIS	2.0
21	2Z	29	TYR	2.0
21	2Z	149	SER	2.0
41	2j	30	SER	2.0
50	2s	57	HIS	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	7MG	2w	46	24/25	0.55	0.16	80,91,98,112	0
56	7MG	2y	46	24/25	0.61	0.18	86,94,100,112	0
54	7MG	1w	46	24/25	0.63	0.16	77,86,96,115	0
56	PSU	2y	55	20/21	0.64	0.17	87,95,102,109	0
56	7MG	1y	46	24/25	0.65	0.17	80,89,98,108	0
54	4SU	2w	8	20/21	0.65	0.15	87,95,103,113	0
56	4SU	2y	8	20/21	0.70	0.15	88,92,98,104	0
56	5MU	2y	54	21/22	0.72	0.17	88,92,99,117	0
56	PSU	1y	55	20/21	0.76	0.15	83,88,100,106	0
56	5MU	1y	54	21/22	0.76	0.15	78,83,92,101	0
32	2MG	2a	1207	24/25	0.77	0.16	79,87,95,98	0
56	MIA	2y	37	22/30	0.77	0.13	76,84,93,104	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	4SU	1y	8	20/21	0.79	0.13	83,87,95,95	0
54	PSU	2w	55	20/21	0.79	0.13	81,87,92,98	0
54	5MU	2w	54	21/22	0.80	0.14	78,82,90,92	0
56	PSU	2y	32	20/21	0.80	0.14	71,82,95,95	0
56	MIA	1y	37	22/30	0.82	0.13	65,74,81,86	0
32	PSU	2a	516	20/21	0.83	0.14	79,81,87,89	0
54	PSU	2w	32	20/21	0.83	0.14	82,88,94,98	0
1	5MU	2A	1915	21/22	0.83	0.14	71,75,81,92	0
56	PSU	2y	39	20/21	0.84	0.11	78,81,93,96	0
55	5MU	2x	54	21/22	0.85	0.13	77,81,89,99	0
54	PSU	1w	55	20/21	0.86	0.11	63,81,85,87	0
54	PSU	2w	39	20/21	0.86	0.11	79,84,88,89	0
54	4SU	1w	8	20/21	0.86	0.12	78,82,90,94	0
54	MIA	2w	37	25/30	0.87	0.14	78,85,89,102	0
55	4SU	2x	8	20/21	0.87	0.14	74,79,83,91	0
32	M2G	2a	966	25/26	0.87	0.18	60,70,84,89	0
55	PSU	2x	55	20/21	0.87	0.11	75,81,83,89	0
56	PSU	1y	39	20/21	0.88	0.12	70,76,82,83	0
43	0TD	2l	92	10/11	0.88	0.13	67,69,75,87	0
54	PSU	1w	32	20/21	0.89	0.12	68,73,86,90	0
32	5MC	2a	967	21/22	0.89	0.15	68,73,80,84	0
1	PSU	2A	1917	20/21	0.89	0.10	62,70,76,83	0
32	4OC	2a	1402	22/23	0.90	0.12	58,66,73,76	0
32	5MC	2a	1404	21/22	0.90	0.12	59,64,67,71	0
56	PSU	1y	32	20/21	0.90	0.10	73,76,81,82	0
43	0TD	1l	92	10/11	0.90	0.11	44,53,57,69	0
55	PSU	1x	55	20/21	0.91	0.11	46,61,70,71	0
55	5MC	2x	32	21/22	0.91	0.14	68,74,78,81	0
54	MIA	1w	37	29/30	0.92	0.12	55,64,74,79	0
1	PSU	2A	1911	20/21	0.92	0.11	54,63,72,74	0
55	5MU	1x	54	21/22	0.92	0.10	59,65,71,77	0
54	5MU	1w	54	21/22	0.93	0.10	61,72,78,81	0
54	PSU	1w	39	20/21	0.93	0.09	63,74,77,81	0
32	7MG	2a	527	24/25	0.93	0.11	60,67,73,83	0
32	5MC	2a	1400	21/22	0.93	0.13	71,74,78,82	0
32	UR3	2a	1498	21/22	0.93	0.12	60,63,70,74	0
32	5MC	2a	1407	21/22	0.94	0.11	55,59,64,65	0
1	5MU	1A	1915	21/22	0.94	0.09	40,55,60,62	0
32	MA6	2a	1518	24/25	0.94	0.12	52,67,72,73	0
32	MA6	2a	1519	24/25	0.94	0.13	51,66,71,73	0
1	OMC	2A	1920	21/22	0.95	0.09	59,64,68,69	0
1	5MC	2A	1962	21/22	0.95	0.10	42,50,58,66	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	M2G	1a	966	25/26	0.95	0.10	47,54,60,64	0
55	4SU	1x	8	20/21	0.95	0.09	55,61,65,65	0
32	PSU	1a	516	20/21	0.95	0.09	58,62,67,69	0
1	5MC	2A	1942	21/22	0.96	0.09	50,56,64,64	0
32	5MC	1a	967	21/22	0.96	0.10	50,56,63,64	0
55	5MC	1x	32	21/22	0.96	0.10	48,53,59,68	0
32	7MG	1a	527	24/25	0.96	0.09	40,48,52,57	0
32	2MG	1a	1207	24/25	0.96	0.09	56,65,68,72	0
1	5MU	2A	1939	21/22	0.96	0.08	35,39,47,48	0
32	MA6	1a	1519	24/25	0.96	0.09	35,41,45,52	0
1	5MC	1A	1942	21/22	0.96	0.08	33,40,46,48	0
1	PSU	1A	1917	20/21	0.97	0.07	39,48,54,59	0
1	PSU	1A	1911	20/21	0.97	0.08	36,45,52,52	0
1	OMG	2A	2251	24/25	0.97	0.09	39,42,46,48	0
32	5MC	1a	1400	21/22	0.97	0.09	43,51,56,63	0
1	2MA	2A	2503	23/24	0.97	0.09	29,37,42,45	0
32	4OC	1a	1402	22/23	0.97	0.08	39,48,54,54	0
1	PSU	2A	2605	20/21	0.97	0.07	33,40,43,47	0
32	5MC	1a	1404	21/22	0.97	0.08	38,42,46,50	0
1	OMC	1A	1920	21/22	0.97	0.09	38,45,50,52	0
55	31H	2x	76	32/33	0.97	0.09	40,48,54,68	0
32	MA6	1a	1518	24/25	0.98	0.08	31,42,46,48	0
1	2MA	1A	2503	23/24	0.98	0.06	14,20,24,26	0
1	5MU	1A	1939	21/22	0.98	0.07	22,28,33,34	0
1	OMU	1A	2552	21/22	0.98	0.07	23,30,35,38	0
1	OMU	2A	2552	21/22	0.98	0.07	39,44,49,59	0
32	5MC	1a	1407	21/22	0.98	0.08	33,40,45,49	0
1	PSU	1A	2605	20/21	0.98	0.06	21,26,30,32	0
32	UR3	1a	1498	21/22	0.98	0.06	38,41,43,47	0
55	31H	1x	76	32/33	0.98	0.07	22,29,37,42	10
1	5MC	1A	1962	21/22	0.98	0.06	27,34,40,50	0
1	OMG	1A	2251	24/25	0.99	0.05	22,26,30,32	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(Å ²)	Q<0.9
57	MG	2A	3525	1/1	0.50	0.23	84,84,84,84	0
57	MG	2A	3556	1/1	0.50	0.32	80,80,80,80	0
57	MG	2A	3552	1/1	0.52	0.27	79,79,79,79	0
57	MG	2A	3560	1/1	0.60	0.23	64,64,64,64	0
57	MG	2a	1616	1/1	0.60	0.32	80,80,80,80	0
57	MG	2A	3555	1/1	0.62	0.23	73,73,73,73	0
57	MG	2A	3601	1/1	0.63	0.27	72,72,72,72	0
57	MG	2A	3617	1/1	0.64	0.22	43,43,43,43	0
57	MG	2A	3550	1/1	0.64	0.23	63,63,63,63	0
57	MG	2A	3533	1/1	0.66	0.21	72,72,72,72	0
57	MG	2a	1658	1/1	0.66	0.23	78,78,78,78	0
57	MG	2a	1739	1/1	0.66	0.44	75,75,75,75	0
57	MG	2A	3582	1/1	0.67	0.20	75,75,75,75	0
57	MG	2A	3543	1/1	0.68	0.26	62,62,62,62	0
57	MG	1A	3436	1/1	0.68	0.46	77,77,77,77	0
57	MG	1A	4063	1/1	0.68	0.15	70,70,70,70	0
57	MG	2a	1636	1/1	0.69	0.23	81,81,81,81	0
57	MG	1A	3728	1/1	0.69	0.18	63,63,63,63	0
57	MG	1x	114	1/1	0.69	0.18	70,70,70,70	0
57	MG	1a	1824	1/1	0.70	0.23	79,79,79,79	0
57	MG	1Y	203	1/1	0.71	0.15	84,84,84,84	0
57	MG	1a	1741	1/1	0.71	0.33	79,79,79,79	0
57	MG	2A	3341	1/1	0.71	0.33	63,63,63,63	0
57	MG	2A	3166	1/1	0.72	0.20	59,59,59,59	0
57	MG	2A	3656	1/1	0.72	0.15	64,64,64,64	0
57	MG	2A	3588	1/1	0.73	0.26	71,71,71,71	0
57	MG	1A	3692	1/1	0.73	0.20	63,63,63,63	0
57	MG	2A	3378	1/1	0.73	0.20	63,63,63,63	0
57	MG	2A	3512	1/1	0.73	0.18	42,42,42,42	0
57	MG	1B	234	1/1	0.74	0.17	67,67,67,67	0
57	MG	2A	3544	1/1	0.74	0.23	68,68,68,68	0
57	MG	1A	3716	1/1	0.74	0.17	37,37,37,37	0
57	MG	2A	3356	1/1	0.74	0.23	76,76,76,76	0
57	MG	2A	3681	1/1	0.74	0.19	47,47,47,47	0
57	MG	2G	201	1/1	0.74	0.23	76,76,76,76	0
57	MG	1A	3542	1/1	0.74	0.26	66,66,66,66	0
57	MG	1a	1758	1/1	0.74	0.16	69,69,69,69	0
57	MG	2a	1646	1/1	0.74	0.41	76,76,76,76	0
57	MG	1A	3811	1/1	0.74	0.17	58,58,58,58	0
57	MG	1A	3415	1/1	0.74	0.20	63,63,63,63	0
57	MG	2a	1753	1/1	0.74	0.33	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
57	MG	1a	1642	1/1	0.75	0.29	78,78,78,78	0
57	MG	1a	1721	1/1	0.75	0.32	81,81,81,81	0
57	MG	2A	3404	1/1	0.75	0.25	67,67,67,67	0
57	MG	1A	3876	1/1	0.75	0.21	57,57,57,57	0
57	MG	2A	3722	1/1	0.75	0.14	78,78,78,78	0
57	MG	1A	3819	1/1	0.75	0.25	58,58,58,58	0
57	MG	1A	4074	1/1	0.76	0.16	64,64,64,64	0
57	MG	2A	3551	1/1	0.76	0.17	79,79,79,79	0
57	MG	1a	1781	1/1	0.76	0.26	71,71,71,71	0
57	MG	2A	3615	1/1	0.76	0.15	74,74,74,74	0
57	MG	2A	3540	1/1	0.76	0.17	66,66,66,66	0
57	MG	2A	3624	1/1	0.76	0.15	76,76,76,76	0
57	MG	2A	3486	1/1	0.76	0.17	54,54,54,54	0
57	MG	1y	102	1/1	0.76	0.16	88,88,88,88	0
57	MG	2v	101	1/1	0.76	0.30	77,77,77,77	0
57	MG	1A	3290	1/1	0.77	0.18	54,54,54,54	0
57	MG	20	102	1/1	0.77	0.22	63,63,63,63	0
57	MG	2A	3452	1/1	0.77	0.24	73,73,73,73	0
57	MG	1A	3719	1/1	0.77	0.17	46,46,46,46	0
57	MG	2a	1637	1/1	0.77	0.24	73,73,73,73	0
57	MG	2A	3496	1/1	0.77	0.24	66,66,66,66	0
57	MG	2A	3575	1/1	0.77	0.21	74,74,74,74	0
57	MG	1Z	3702	1/1	0.77	0.10	70,70,70,70	0
57	MG	1a	1637	1/1	0.77	0.32	76,76,76,76	0
57	MG	2B	214	1/1	0.77	0.19	70,70,70,70	0
57	MG	2A	3149	1/1	0.78	0.19	53,53,53,53	0
57	MG	2A	3409	1/1	0.78	0.19	51,51,51,51	0
57	MG	2A	3589	1/1	0.78	0.14	58,58,58,58	0
57	MG	1a	1683	1/1	0.78	0.21	72,72,72,72	0
57	MG	1A	4046	1/1	0.78	0.15	53,53,53,53	0
57	MG	1A	3514	1/1	0.78	0.21	65,65,65,65	0
57	MG	1a	1659	1/1	0.78	0.28	74,74,74,74	0
57	MG	2A	3446	1/1	0.79	0.19	53,53,53,53	0
57	MG	1A	3338	1/1	0.79	0.24	51,51,51,51	0
57	MG	1F	308	1/1	0.79	0.13	49,49,49,49	0
57	MG	2A	3263	1/1	0.79	0.27	72,72,72,72	0
57	MG	1A	3548	1/1	0.79	0.22	52,52,52,52	0
57	MG	1w	104	1/1	0.79	0.13	69,69,69,69	0
57	MG	2a	1640	1/1	0.79	0.17	76,76,76,76	0
57	MG	2A	3638	1/1	0.79	0.14	67,67,67,67	0
57	MG	1A	3756	1/1	0.79	0.26	63,63,63,63	0
57	MG	1A	4095	1/1	0.79	0.17	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
57	MG	2A	3687	1/1	0.79	0.11	69,69,69,69	0
57	MG	2A	3028	1/1	0.79	0.13	59,59,59,59	0
57	MG	1A	4058	1/1	0.80	0.14	44,44,44,44	0
57	MG	1y	104	1/1	0.80	0.11	87,87,87,87	0
57	MG	2A	3415	1/1	0.80	0.11	37,37,37,37	0
57	MG	2A	3707	1/1	0.80	0.19	72,72,72,72	0
57	MG	1a	1739	1/1	0.80	0.43	73,73,73,73	0
57	MG	2A	3111	1/1	0.80	0.29	64,64,64,64	0
57	MG	2B	217	1/1	0.80	0.24	76,76,76,76	0
57	MG	1A	3401	1/1	0.80	0.11	77,77,77,77	0
57	MG	2A	3493	1/1	0.80	0.20	70,70,70,70	0
57	MG	1A	3437	1/1	0.80	0.15	47,47,47,47	0
57	MG	2a	1619	1/1	0.80	0.14	64,64,64,64	0
57	MG	2a	1626	1/1	0.80	0.31	71,71,71,71	0
57	MG	2A	3175	1/1	0.80	0.32	71,71,71,71	0
57	MG	1A	3562	1/1	0.80	0.21	62,62,62,62	0
57	MG	2A	3532	1/1	0.80	0.13	78,78,78,78	0
57	MG	2a	1644	1/1	0.80	0.12	61,61,61,61	0
57	MG	2A	3606	1/1	0.80	0.26	74,74,74,74	0
57	MG	2A	3299	1/1	0.80	0.33	64,64,64,64	0
57	MG	2a	1663	1/1	0.80	0.18	74,74,74,74	0
57	MG	1A	3892	1/1	0.80	0.15	31,31,31,31	0
57	MG	2a	1742	1/1	0.80	0.30	65,65,65,65	0
57	MG	1A	3365	1/1	0.80	0.14	60,60,60,60	0
57	MG	1a	1720	1/1	0.80	0.21	67,67,67,67	0
57	MG	2x	102	1/1	0.80	0.31	77,77,77,77	0
57	MG	2A	3397	1/1	0.81	0.20	74,74,74,74	0
57	MG	2A	3047	1/1	0.81	0.26	69,69,69,69	0
57	MG	2A	3407	1/1	0.81	0.29	69,69,69,69	0
57	MG	1A	4101	1/1	0.81	0.14	43,43,43,43	0
57	MG	2a	1629	1/1	0.81	0.23	74,74,74,74	0
57	MG	1A	3635	1/1	0.81	0.21	58,58,58,58	0
57	MG	1a	1678	1/1	0.81	0.25	64,64,64,64	0
57	MG	1b	302	1/1	0.81	0.21	80,80,80,80	0
57	MG	2A	3256	1/1	0.81	0.35	75,75,75,75	0
57	MG	1E	314	1/1	0.81	0.12	62,62,62,62	0
57	MG	1A	3553	1/1	0.81	0.17	62,62,62,62	0
57	MG	2A	3719	1/1	0.81	0.23	62,62,62,62	0
57	MG	1A	3531	1/1	0.81	0.14	69,69,69,69	0
57	MG	2A	3723	1/1	0.81	0.17	69,69,69,69	0
57	MG	2A	3514	1/1	0.81	0.23	68,68,68,68	0
57	MG	1A	3761	1/1	0.81	0.12	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
57	MG	1A	4044	1/1	0.81	0.13	53,53,53,53	0
57	MG	1y	103	1/1	0.82	0.31	77,77,77,77	0
57	MG	2A	3579	1/1	0.82	0.12	70,70,70,70	0
57	MG	2A	3302	1/1	0.82	0.22	64,64,64,64	0
57	MG	1A	3476	1/1	0.82	0.26	70,70,70,70	0
57	MG	2A	3354	1/1	0.82	0.13	71,71,71,71	0
57	MG	2A	3001	1/1	0.82	0.37	57,57,57,57	0
57	MG	1A	4088	1/1	0.82	0.11	64,64,64,64	0
57	MG	1A	3903	1/1	0.82	0.12	23,23,23,23	0
57	MG	2a	1633	1/1	0.82	0.41	67,67,67,67	0
57	MG	2a	1635	1/1	0.82	0.33	67,67,67,67	0
57	MG	2A	3052	1/1	0.82	0.29	66,66,66,66	0
57	MG	1A	3777	1/1	0.82	0.13	31,31,31,31	0
57	MG	2A	3635	1/1	0.82	0.18	55,55,55,55	0
57	MG	1a	1670	1/1	0.82	0.30	66,66,66,66	0
57	MG	2A	3547	1/1	0.82	0.12	55,55,55,55	0
57	MG	2a	1649	1/1	0.82	0.20	66,66,66,66	0
57	MG	1A	4045	1/1	0.82	0.22	56,56,56,56	0
57	MG	2A	3445	1/1	0.82	0.14	48,48,48,48	0
57	MG	2a	1670	1/1	0.82	0.20	63,63,63,63	0
57	MG	2a	1696	1/1	0.82	0.18	66,66,66,66	0
57	MG	1A	3533	1/1	0.82	0.12	81,81,81,81	0
57	MG	1A	3164	1/1	0.82	0.23	55,55,55,55	0
57	MG	2A	3481	1/1	0.82	0.13	63,63,63,63	0
57	MG	2a	1784	1/1	0.82	0.16	71,71,71,71	0
57	MG	1A	3758	1/1	0.82	0.13	62,62,62,62	0
57	MG	2B	206	1/1	0.82	0.20	68,68,68,68	0
57	MG	1A	3490	1/1	0.83	0.21	63,63,63,63	0
57	MG	1A	3689	1/1	0.83	0.17	50,50,50,50	0
57	MG	2A	3303	1/1	0.83	0.34	59,59,59,59	0
57	MG	1x	108	1/1	0.83	0.24	68,68,68,68	0
57	MG	1A	3232	1/1	0.83	0.15	62,62,62,62	0
57	MG	1A	4048	1/1	0.83	0.18	53,53,53,53	0
57	MG	1A	3696	1/1	0.83	0.14	53,53,53,53	0
57	MG	1A	3026	1/1	0.83	0.17	63,63,63,63	0
57	MG	2a	1621	1/1	0.83	0.22	78,78,78,78	0
57	MG	1A	3016	1/1	0.83	0.25	56,56,56,56	0
57	MG	1A	3572	1/1	0.83	0.14	51,51,51,51	0
57	MG	1A	3900	1/1	0.83	0.12	37,37,37,37	0
57	MG	1A	4100	1/1	0.83	0.15	62,62,62,62	0
57	MG	2A	3057	1/1	0.83	0.14	61,61,61,61	0
57	MG	2A	3110	1/1	0.83	0.19	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3605	1/1	0.83	0.16	70,70,70,70	0
57	MG	1a	1722	1/1	0.83	0.33	64,64,64,64	0
57	MG	2A	3607	1/1	0.83	0.14	60,60,60,60	0
57	MG	1A	3597	1/1	0.83	0.09	35,35,35,35	0
57	MG	1B	202	1/1	0.83	0.24	61,61,61,61	0
57	MG	2A	3170	1/1	0.83	0.09	57,57,57,57	0
57	MG	2a	1665	1/1	0.83	0.29	67,67,67,67	0
57	MG	1A	3931	1/1	0.83	0.13	72,72,72,72	0
57	MG	2a	1692	1/1	0.83	0.21	74,74,74,74	0
57	MG	2A	3224	1/1	0.83	0.15	58,58,58,58	0
57	MG	2a	1709	1/1	0.83	0.26	78,78,78,78	0
57	MG	2A	3226	1/1	0.83	0.21	74,74,74,74	0
57	MG	2A	3230	1/1	0.83	0.29	63,63,63,63	0
57	MG	1A	4019	1/1	0.83	0.12	35,35,35,35	0
57	MG	2a	1775	1/1	0.83	0.33	76,76,76,76	0
57	MG	2a	1778	1/1	0.83	0.22	72,72,72,72	0
57	MG	2A	3259	1/1	0.83	0.28	71,71,71,71	0
57	MG	1A	4037	1/1	0.83	0.18	72,72,72,72	0
57	MG	2A	3268	1/1	0.83	0.21	54,54,54,54	0
57	MG	1A	3268	1/1	0.84	0.10	57,57,57,57	0
57	MG	1A	3538	1/1	0.84	0.33	65,65,65,65	0
57	MG	2A	3300	1/1	0.84	0.33	64,64,64,64	0
57	MG	15	108	1/1	0.84	0.14	40,40,40,40	0
57	MG	1a	1628	1/1	0.84	0.23	61,61,61,61	0
57	MG	2A	3059	1/1	0.84	0.30	61,61,61,61	0
57	MG	2A	3343	1/1	0.84	0.28	58,58,58,58	0
57	MG	2A	3539	1/1	0.84	0.14	66,66,66,66	0
57	MG	2A	3632	1/1	0.84	0.16	64,64,64,64	0
57	MG	1A	4028	1/1	0.84	0.10	66,66,66,66	0
57	MG	1A	3205	1/1	0.84	0.16	59,59,59,59	0
57	MG	2a	1653	1/1	0.84	0.44	69,69,69,69	0
57	MG	1B	212	1/1	0.84	0.11	59,59,59,59	0
57	MG	1a	1669	1/1	0.84	0.17	57,57,57,57	0
57	MG	1A	3529	1/1	0.84	0.23	66,66,66,66	0
57	MG	1a	1676	1/1	0.84	0.17	64,64,64,64	0
57	MG	2A	3716	1/1	0.84	0.17	60,60,60,60	0
57	MG	2A	3216	1/1	0.84	0.28	60,60,60,60	0
57	MG	1A	3255	1/1	0.84	0.10	61,61,61,61	0
57	MG	2a	1711	1/1	0.84	0.41	71,71,71,71	0
57	MG	2a	1724	1/1	0.84	0.30	65,65,65,65	0
57	MG	2a	1728	1/1	0.84	0.36	64,64,64,64	0
57	MG	1A	4093	1/1	0.84	0.13	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1a	1696	1/1	0.84	0.31	72,72,72,72	0
57	MG	2A	3563	1/1	0.84	0.15	61,61,61,61	0
57	MG	2a	1756	1/1	0.84	0.41	73,73,73,73	0
57	MG	1a	1717	1/1	0.84	0.20	66,66,66,66	0
57	MG	1S	203	1/1	0.84	0.10	63,63,63,63	0
57	MG	2a	1779	1/1	0.84	0.31	62,62,62,62	0
57	MG	2A	3581	1/1	0.84	0.16	63,63,63,63	0
57	MG	2A	3003	1/1	0.84	0.28	61,61,61,61	0
57	MG	2A	3491	1/1	0.84	0.14	70,70,70,70	0
57	MG	1a	1791	1/1	0.85	0.15	56,56,56,56	0
57	MG	1A	3363	1/1	0.85	0.15	63,63,63,63	0
57	MG	1A	4086	1/1	0.85	0.18	49,49,49,49	0
57	MG	1a	1640	1/1	0.85	0.18	61,61,61,61	0
57	MG	1A	3942	1/1	0.85	0.10	49,49,49,49	0
57	MG	2A	3260	1/1	0.85	0.17	61,61,61,61	0
57	MG	1A	3988	1/1	0.85	0.12	60,60,60,60	0
57	MG	1A	3813	1/1	0.85	0.14	53,53,53,53	0
57	MG	1A	4027	1/1	0.85	0.23	65,65,65,65	0
57	MG	1A	3358	1/1	0.85	0.16	82,82,82,82	0
57	MG	1A	3822	1/1	0.85	0.12	42,42,42,42	0
57	MG	2a	1618	1/1	0.85	0.13	73,73,73,73	0
57	MG	1a	1682	1/1	0.85	0.30	63,63,63,63	0
57	MG	2a	1620	1/1	0.85	0.19	79,79,79,79	0
57	MG	2A	3021	1/1	0.85	0.26	70,70,70,70	0
57	MG	1A	3837	1/1	0.85	0.14	52,52,52,52	0
57	MG	1a	1692	1/1	0.85	0.40	74,74,74,74	0
57	MG	1B	228	1/1	0.85	0.23	73,73,73,73	0
57	MG	2A	3562	1/1	0.85	0.11	46,46,46,46	0
57	MG	1A	3589	1/1	0.85	0.22	58,58,58,58	0
57	MG	2A	3383	1/1	0.85	0.11	55,55,55,55	0
57	MG	2A	3386	1/1	0.85	0.26	72,72,72,72	0
57	MG	1A	3429	1/1	0.85	0.19	58,58,58,58	0
57	MG	2A	3398	1/1	0.85	0.10	44,44,44,44	0
57	MG	2a	1647	1/1	0.85	0.18	76,76,76,76	0
57	MG	2A	3583	1/1	0.85	0.17	55,55,55,55	0
57	MG	2A	3062	1/1	0.85	0.15	58,58,58,58	0
57	MG	1A	3708	1/1	0.85	0.12	34,34,34,34	0
57	MG	2A	3594	1/1	0.85	0.12	66,66,66,66	0
57	MG	1O	201	1/1	0.85	0.12	72,72,72,72	0
57	MG	1A	4049	1/1	0.85	0.12	59,59,59,59	0
57	MG	2a	1678	1/1	0.85	0.28	76,76,76,76	0
57	MG	2A	3428	1/1	0.85	0.23	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
57	MG	2a	1694	1/1	0.85	0.12	60,60,60,60	0
57	MG	1A	3610	1/1	0.85	0.16	57,57,57,57	0
57	MG	2A	3168	1/1	0.85	0.27	67,67,67,67	0
57	MG	1A	3914	1/1	0.85	0.17	62,62,62,62	0
57	MG	2a	1716	1/1	0.85	0.10	56,56,56,56	0
57	MG	2A	3478	1/1	0.85	0.23	64,64,64,64	0
57	MG	2A	3628	1/1	0.85	0.17	66,66,66,66	0
57	MG	1A	4065	1/1	0.85	0.19	50,50,50,50	0
57	MG	2A	3187	1/1	0.85	0.16	56,56,56,56	0
57	MG	2A	3490	1/1	0.85	0.13	48,48,48,48	0
57	MG	2A	3640	1/1	0.85	0.17	66,66,66,66	0
57	MG	2a	1766	1/1	0.85	0.33	62,62,62,62	0
57	MG	2a	1767	1/1	0.85	0.24	57,57,57,57	0
57	MG	2A	3648	1/1	0.85	0.14	76,76,76,76	0
57	MG	2A	3654	1/1	0.85	0.19	52,52,52,52	0
57	MG	2A	3193	1/1	0.85	0.32	66,66,66,66	0
57	MG	2a	1780	1/1	0.85	0.16	67,67,67,67	0
57	MG	2A	3212	1/1	0.85	0.22	66,66,66,66	0
57	MG	1a	1784	1/1	0.85	0.15	69,69,69,69	0
57	MG	2A	3703	1/1	0.85	0.17	67,67,67,67	0
57	MG	1A	3092	1/1	0.86	0.13	59,59,59,59	0
57	MG	1a	1708	1/1	0.86	0.19	58,58,58,58	0
57	MG	1a	1715	1/1	0.86	0.16	59,59,59,59	0
57	MG	1A	3724	1/1	0.86	0.22	64,64,64,64	0
57	MG	2A	3050	1/1	0.86	0.17	56,56,56,56	0
57	MG	2a	1609	1/1	0.86	0.23	68,68,68,68	0
57	MG	1A	3457	1/1	0.86	0.12	59,59,59,59	0
57	MG	1A	3915	1/1	0.86	0.12	46,46,46,46	0
57	MG	2A	3058	1/1	0.86	0.20	55,55,55,55	0
57	MG	2A	3359	1/1	0.86	0.22	63,63,63,63	0
57	MG	2A	3373	1/1	0.86	0.29	62,62,62,62	0
57	MG	1A	3312	1/1	0.86	0.14	56,56,56,56	0
57	MG	1a	1734	1/1	0.86	0.25	54,54,54,54	0
57	MG	2A	3569	1/1	0.86	0.18	61,61,61,61	0
57	MG	2A	3091	1/1	0.86	0.14	56,56,56,56	0
57	MG	2A	3101	1/1	0.86	0.26	69,69,69,69	0
57	MG	1A	3932	1/1	0.86	0.13	70,70,70,70	0
57	MG	1A	3938	1/1	0.86	0.10	32,32,32,32	0
57	MG	1a	1623	1/1	0.86	0.24	68,68,68,68	0
57	MG	1a	1759	1/1	0.86	0.13	58,58,58,58	0
57	MG	1a	1760	1/1	0.86	0.13	80,80,80,80	0
57	MG	2A	3591	1/1	0.86	0.17	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
57	MG	2A	3419	1/1	0.86	0.11	51,51,51,51	0
57	MG	2A	3598	1/1	0.86	0.12	57,57,57,57	0
57	MG	2a	1659	1/1	0.86	0.22	62,62,62,62	0
57	MG	1A	3202	1/1	0.86	0.11	48,48,48,48	0
57	MG	2A	3442	1/1	0.86	0.21	69,69,69,69	0
57	MG	1A	3848	1/1	0.86	0.13	50,50,50,50	0
57	MG	2a	1677	1/1	0.86	0.43	71,71,71,71	0
57	MG	1A	4094	1/1	0.86	0.12	41,41,41,41	0
57	MG	2a	1686	1/1	0.86	0.21	69,69,69,69	0
57	MG	2A	3449	1/1	0.86	0.17	48,48,48,48	0
57	MG	2A	3188	1/1	0.86	0.15	52,52,52,52	0
57	MG	2A	3461	1/1	0.86	0.10	65,65,65,65	0
57	MG	2A	3466	1/1	0.86	0.11	54,54,54,54	0
57	MG	2A	3476	1/1	0.86	0.18	52,52,52,52	0
57	MG	1A	3855	1/1	0.86	0.13	56,56,56,56	0
57	MG	2a	1722	1/1	0.86	0.25	56,56,56,56	0
57	MG	2A	3210	1/1	0.86	0.26	69,69,69,69	0
57	MG	2a	1727	1/1	0.86	0.28	71,71,71,71	0
57	MG	1a	1829	1/1	0.86	0.27	60,60,60,60	0
57	MG	1A	4097	1/1	0.86	0.17	64,64,64,64	0
57	MG	1r	101	1/1	0.86	0.21	68,68,68,68	0
57	MG	1A	3869	1/1	0.86	0.11	48,48,48,48	0
57	MG	1A	3874	1/1	0.86	0.16	58,58,58,58	0
57	MG	2A	3506	1/1	0.86	0.17	46,46,46,46	0
57	MG	2A	3692	1/1	0.86	0.10	71,71,71,71	0
57	MG	1A	3509	1/1	0.86	0.09	44,44,44,44	0
57	MG	2A	3706	1/1	0.86	0.27	56,56,56,56	0
57	MG	1A	3878	1/1	0.86	0.16	41,41,41,41	0
57	MG	1A	3886	1/1	0.86	0.13	50,50,50,50	0
57	MG	1B	230	1/1	0.86	0.16	75,75,75,75	0
57	MG	2l	201	1/1	0.86	0.26	70,70,70,70	0
57	MG	1A	3398	1/1	0.86	0.14	67,67,67,67	0
57	MG	2A	3275	1/1	0.86	0.25	65,65,65,65	0
57	MG	1A	3659	1/1	0.87	0.12	69,69,69,69	0
57	MG	2A	3094	1/1	0.87	0.23	66,66,66,66	0
57	MG	1A	4096	1/1	0.87	0.29	54,54,54,54	0
57	MG	1a	1702	1/1	0.87	0.33	67,67,67,67	0
57	MG	2A	3460	1/1	0.87	0.16	73,73,73,73	0
57	MG	1A	3489	1/1	0.87	0.12	61,61,61,61	0
57	MG	2A	3114	1/1	0.87	0.19	64,64,64,64	0
57	MG	1A	4098	1/1	0.87	0.13	54,54,54,54	0
57	MG	2A	3477	1/1	0.87	0.23	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
57	MG	2A	3160	1/1	0.87	0.20	59,59,59,59	0
57	MG	2B	204	1/1	0.87	0.24	67,67,67,67	0
57	MG	1A	3348	1/1	0.87	0.19	58,58,58,58	0
57	MG	2B	211	1/1	0.87	0.26	62,62,62,62	0
57	MG	2A	3167	1/1	0.87	0.13	57,57,57,57	0
57	MG	1A	3827	1/1	0.87	0.21	61,61,61,61	0
57	MG	2B	218	1/1	0.87	0.21	64,64,64,64	0
57	MG	1A	3956	1/1	0.87	0.12	26,26,26,26	0
57	MG	2Z	301	1/1	0.87	0.24	76,76,76,76	0
57	MG	20	101	1/1	0.87	0.31	62,62,62,62	0
57	MG	1A	3508	1/1	0.87	0.11	53,53,53,53	0
57	MG	26	101	1/1	0.87	0.22	61,61,61,61	0
57	MG	28	102	1/1	0.87	0.24	59,59,59,59	0
57	MG	2a	1603	1/1	0.87	0.15	65,65,65,65	0
57	MG	1A	4008	1/1	0.87	0.12	28,28,28,28	0
57	MG	2a	1611	1/1	0.87	0.22	66,66,66,66	0
57	MG	1A	3845	1/1	0.87	0.14	50,50,50,50	0
57	MG	1B	233	1/1	0.87	0.16	73,73,73,73	0
57	MG	2A	3199	1/1	0.87	0.35	64,64,64,64	0
57	MG	1A	3847	1/1	0.87	0.15	58,58,58,58	0
57	MG	1A	3158	1/1	0.87	0.10	49,49,49,49	0
57	MG	1A	4031	1/1	0.87	0.11	58,58,58,58	0
57	MG	1a	1763	1/1	0.87	0.18	70,70,70,70	0
57	MG	1a	1778	1/1	0.87	0.17	64,64,64,64	0
57	MG	1A	3335	1/1	0.87	0.21	54,54,54,54	0
57	MG	2A	3231	1/1	0.87	0.24	65,65,65,65	0
57	MG	2A	3243	1/1	0.87	0.14	52,52,52,52	0
57	MG	2A	3251	1/1	0.87	0.22	71,71,71,71	0
57	MG	1O	206	1/1	0.87	0.10	64,64,64,64	0
57	MG	1R	201	1/1	0.87	0.14	56,56,56,56	0
57	MG	1A	4038	1/1	0.87	0.23	57,57,57,57	0
57	MG	1a	1828	1/1	0.87	0.25	59,59,59,59	0
57	MG	1A	3469	1/1	0.87	0.16	56,56,56,56	0
57	MG	2a	1656	1/1	0.87	0.18	84,84,84,84	0
57	MG	2A	3274	1/1	0.87	0.26	48,48,48,48	0
57	MG	1A	3530	1/1	0.87	0.15	55,55,55,55	0
57	MG	2A	3288	1/1	0.87	0.26	60,60,60,60	0
57	MG	2A	3570	1/1	0.87	0.15	57,57,57,57	0
57	MG	2a	1668	1/1	0.87	0.32	71,71,71,71	0
57	MG	1f	201	1/1	0.87	0.17	55,55,55,55	0
57	MG	15	105	1/1	0.87	0.19	54,54,54,54	0
57	MG	1A	3310	1/1	0.87	0.33	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
57	MG	1A	3604	1/1	0.87	0.12	47,47,47,47	0
57	MG	2A	3304	1/1	0.87	0.40	70,70,70,70	0
57	MG	2A	3313	1/1	0.87	0.21	55,55,55,55	0
57	MG	1A	3609	1/1	0.87	0.13	56,56,56,56	0
57	MG	2a	1698	1/1	0.87	0.17	62,62,62,62	0
57	MG	2a	1705	1/1	0.87	0.18	66,66,66,66	0
57	MG	1a	1629	1/1	0.87	0.10	51,51,51,51	0
57	MG	1a	1630	1/1	0.87	0.27	59,59,59,59	0
57	MG	1a	1636	1/1	0.87	0.24	76,76,76,76	0
57	MG	1A	4050	1/1	0.87	0.11	57,57,57,57	0
57	MG	1A	3478	1/1	0.87	0.18	60,60,60,60	0
57	MG	2A	3375	1/1	0.87	0.30	45,45,45,45	0
57	MG	1A	3895	1/1	0.87	0.14	35,35,35,35	0
57	MG	2A	3613	1/1	0.87	0.12	56,56,56,56	0
57	MG	2a	1740	1/1	0.87	0.35	69,69,69,69	0
57	MG	1A	3534	1/1	0.87	0.12	58,58,58,58	0
57	MG	1A	3901	1/1	0.87	0.08	29,29,29,29	0
57	MG	1A	4081	1/1	0.87	0.11	58,58,58,58	0
57	MG	1a	1675	1/1	0.87	0.12	58,58,58,58	0
57	MG	2A	3055	1/1	0.87	0.20	65,65,65,65	0
57	MG	1A	3778	1/1	0.87	0.11	34,34,34,34	0
57	MG	1A	3906	1/1	0.87	0.27	46,46,46,46	0
57	MG	1A	3781	1/1	0.87	0.08	16,16,16,16	0
57	MG	1A	3652	1/1	0.87	0.18	60,60,60,60	0
57	MG	2A	3651	1/1	0.87	0.15	57,57,57,57	0
57	MG	2A	3082	1/1	0.87	0.21	60,60,60,60	0
57	MG	2A	3087	1/1	0.87	0.23	70,70,70,70	0
57	MG	2A	3668	1/1	0.87	0.11	53,53,53,53	0
57	MG	2x	103	1/1	0.87	0.17	66,66,66,66	0
57	MG	2A	3051	1/1	0.88	0.18	68,68,68,68	0
57	MG	2E	302	1/1	0.88	0.25	66,66,66,66	0
57	MG	1A	3535	1/1	0.88	0.11	69,69,69,69	0
57	MG	1A	3208	1/1	0.88	0.11	64,64,64,64	0
57	MG	2A	3293	1/1	0.88	0.25	53,53,53,53	0
57	MG	1a	1709	1/1	0.88	0.46	67,67,67,67	0
57	MG	1a	1712	1/1	0.88	0.12	79,79,79,79	0
57	MG	1A	3541	1/1	0.88	0.21	45,45,45,45	0
57	MG	2A	3060	1/1	0.88	0.22	58,58,58,58	0
57	MG	2a	1606	1/1	0.88	0.16	71,71,71,71	0
57	MG	1O	204	1/1	0.88	0.10	64,64,64,64	0
57	MG	2A	3071	1/1	0.88	0.23	58,58,58,58	0
57	MG	1A	3520	1/1	0.88	0.20	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
57	MG	1A	3844	1/1	0.88	0.09	33,33,33,33	0
57	MG	1S	201	1/1	0.88	0.39	46,46,46,46	0
57	MG	2A	3355	1/1	0.88	0.24	68,68,68,68	0
57	MG	1A	3917	1/1	0.88	0.17	56,56,56,56	0
57	MG	2a	1622	1/1	0.88	0.23	68,68,68,68	0
57	MG	2A	3100	1/1	0.88	0.17	60,60,60,60	0
57	MG	1A	3611	1/1	0.88	0.17	48,48,48,48	0
57	MG	2a	1631	1/1	0.88	0.21	64,64,64,64	0
57	MG	1A	3622	1/1	0.88	0.16	53,53,53,53	0
57	MG	1A	3480	1/1	0.88	0.21	74,74,74,74	0
57	MG	2A	3382	1/1	0.88	0.10	52,52,52,52	0
57	MG	1A	3941	1/1	0.88	0.08	60,60,60,60	0
57	MG	2A	3122	1/1	0.88	0.24	48,48,48,48	0
57	MG	2A	3127	1/1	0.88	0.18	66,66,66,66	0
57	MG	17	103	1/1	0.88	0.10	48,48,48,48	0
57	MG	1a	1603	1/1	0.88	0.15	64,64,64,64	0
57	MG	1a	1607	1/1	0.88	0.31	62,62,62,62	0
57	MG	2a	1650	1/1	0.88	0.22	74,74,74,74	0
57	MG	1A	4082	1/1	0.88	0.12	44,44,44,44	0
57	MG	2a	1655	1/1	0.88	0.21	73,73,73,73	0
57	MG	1A	3650	1/1	0.88	0.08	26,26,26,26	0
57	MG	1A	3950	1/1	0.88	0.12	58,58,58,58	0
57	MG	1A	3867	1/1	0.88	0.13	49,49,49,49	0
57	MG	2A	3178	1/1	0.88	0.12	57,57,57,57	0
57	MG	2A	3180	1/1	0.88	0.12	56,56,56,56	0
57	MG	2A	3619	1/1	0.88	0.09	44,44,44,44	0
57	MG	2A	3622	1/1	0.88	0.11	51,51,51,51	0
57	MG	1a	1827	1/1	0.88	0.36	70,70,70,70	0
57	MG	2A	3627	1/1	0.88	0.11	72,72,72,72	0
57	MG	1A	3977	1/1	0.88	0.14	53,53,53,53	0
57	MG	1A	3438	1/1	0.88	0.12	43,43,43,43	0
57	MG	1A	3997	1/1	0.88	0.11	38,38,38,38	0
57	MG	2A	3207	1/1	0.88	0.12	56,56,56,56	0
57	MG	1A	4002	1/1	0.88	0.09	86,86,86,86	0
57	MG	2a	1703	1/1	0.88	0.20	65,65,65,65	0
57	MG	2A	3470	1/1	0.88	0.11	62,62,62,62	0
57	MG	2A	3475	1/1	0.88	0.20	58,58,58,58	0
57	MG	1a	1643	1/1	0.88	0.28	69,69,69,69	0
57	MG	1A	3767	1/1	0.88	0.21	50,50,50,50	0
57	MG	2a	1718	1/1	0.88	0.17	65,65,65,65	0
57	MG	1A	3163	1/1	0.88	0.15	50,50,50,50	0
57	MG	2A	3225	1/1	0.88	0.28	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
57	MG	1A	3676	1/1	0.88	0.14	31,31,31,31	0
57	MG	1A	4107	1/1	0.88	0.19	65,65,65,65	0
57	MG	2a	1729	1/1	0.88	0.28	63,63,63,63	0
57	MG	2a	1730	1/1	0.88	0.40	72,72,72,72	0
57	MG	1A	3679	1/1	0.88	0.12	31,31,31,31	0
57	MG	1A	3889	1/1	0.88	0.11	40,40,40,40	0
57	MG	2A	3244	1/1	0.88	0.13	65,65,65,65	0
57	MG	2A	3714	1/1	0.88	0.17	73,73,73,73	0
57	MG	2A	3499	1/1	0.88	0.20	55,55,55,55	0
57	MG	2A	3717	1/1	0.88	0.15	57,57,57,57	0
57	MG	1a	1681	1/1	0.88	0.23	71,71,71,71	0
57	MG	1A	4035	1/1	0.88	0.10	80,80,80,80	0
57	MG	1A	3799	1/1	0.88	0.08	38,38,38,38	0
57	MG	2B	203	1/1	0.88	0.16	62,62,62,62	0
57	MG	2A	3517	1/1	0.88	0.13	49,49,49,49	0
57	MG	2a	1781	1/1	0.88	0.16	67,67,67,67	0
57	MG	1a	1684	1/1	0.88	0.10	58,58,58,58	0
57	MG	2B	207	1/1	0.88	0.18	71,71,71,71	0
57	MG	2q	203	1/1	0.88	0.14	74,74,74,74	0
57	MG	1A	3342	1/1	0.88	0.23	62,62,62,62	0
57	MG	1A	3274	1/1	0.88	0.12	52,52,52,52	0
57	MG	2A	3537	1/1	0.88	0.11	60,60,60,60	0
57	MG	2B	209	1/1	0.89	0.21	65,65,65,65	0
57	MG	1A	3863	1/1	0.89	0.08	50,50,50,50	0
57	MG	1A	3959	1/1	0.89	0.09	48,48,48,48	0
57	MG	2A	3214	1/1	0.89	0.26	69,69,69,69	0
57	MG	1A	3967	1/1	0.89	0.11	49,49,49,49	0
57	MG	2A	3218	1/1	0.89	0.10	53,53,53,53	0
57	MG	1A	3554	1/1	0.89	0.26	58,58,58,58	0
57	MG	1A	3555	1/1	0.89	0.23	59,59,59,59	0
57	MG	1A	3776	1/1	0.89	0.10	28,28,28,28	0
57	MG	1w	105	1/1	0.89	0.23	70,70,70,70	0
57	MG	1x	103	1/1	0.89	0.11	61,61,61,61	0
57	MG	2A	3235	1/1	0.89	0.14	60,60,60,60	0
57	MG	2A	3239	1/1	0.89	0.12	55,55,55,55	0
57	MG	1A	3532	1/1	0.89	0.15	71,71,71,71	0
57	MG	1x	110	1/1	0.89	0.15	69,69,69,69	0
57	MG	1a	1665	1/1	0.89	0.09	55,55,55,55	0
57	MG	1A	3245	1/1	0.89	0.16	59,59,59,59	0
57	MG	1A	3574	1/1	0.89	0.25	48,48,48,48	0
57	MG	1a	1673	1/1	0.89	0.19	65,65,65,65	0
57	MG	1A	3251	1/1	0.89	0.12	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
57	MG	2A	3265	1/1	0.89	0.18	56,56,56,56	0
57	MG	1A	3891	1/1	0.89	0.13	46,46,46,46	0
57	MG	2a	1625	1/1	0.89	0.11	57,57,57,57	0
57	MG	2A	3016	1/1	0.89	0.21	73,73,73,73	0
57	MG	1B	224	1/1	0.89	0.14	70,70,70,70	0
57	MG	1a	1680	1/1	0.89	0.24	70,70,70,70	0
57	MG	2A	3290	1/1	0.89	0.20	45,45,45,45	0
57	MG	1A	4029	1/1	0.89	0.11	77,77,77,77	0
57	MG	1A	3808	1/1	0.89	0.09	20,20,20,20	0
57	MG	1A	3511	1/1	0.89	0.10	64,64,64,64	0
57	MG	1A	3405	1/1	0.89	0.18	46,46,46,46	0
57	MG	1a	1691	1/1	0.89	0.25	72,72,72,72	0
57	MG	1A	3027	1/1	0.89	0.18	69,69,69,69	0
57	MG	2A	3306	1/1	0.89	0.33	62,62,62,62	0
57	MG	2a	1648	1/1	0.89	0.15	69,69,69,69	0
57	MG	1A	4042	1/1	0.89	0.16	60,60,60,60	0
57	MG	2A	3340	1/1	0.89	0.14	52,52,52,52	0
57	MG	1A	3428	1/1	0.89	0.14	56,56,56,56	0
57	MG	1A	3459	1/1	0.89	0.17	70,70,70,70	0
57	MG	2A	3352	1/1	0.89	0.17	56,56,56,56	0
57	MG	1A	3828	1/1	0.89	0.31	34,34,34,34	0
57	MG	2A	3603	1/1	0.89	0.16	60,60,60,60	0
57	MG	1A	3619	1/1	0.89	0.09	27,27,27,27	0
57	MG	1A	3549	1/1	0.89	0.34	65,65,65,65	0
57	MG	2a	1666	1/1	0.89	0.11	59,59,59,59	0
57	MG	1A	3731	1/1	0.89	0.10	40,40,40,40	0
57	MG	2A	3368	1/1	0.89	0.27	63,63,63,63	0
57	MG	2a	1672	1/1	0.89	0.22	70,70,70,70	0
57	MG	1A	4053	1/1	0.89	0.09	28,28,28,28	0
57	MG	1A	3733	1/1	0.89	0.09	53,53,53,53	0
57	MG	2a	1679	1/1	0.89	0.20	66,66,66,66	0
57	MG	2a	1681	1/1	0.89	0.13	68,68,68,68	0
57	MG	13	103	1/1	0.89	0.15	57,57,57,57	0
57	MG	1a	1724	1/1	0.89	0.41	72,72,72,72	0
57	MG	2a	1693	1/1	0.89	0.19	78,78,78,78	0
57	MG	2A	3103	1/1	0.89	0.10	64,64,64,64	0
57	MG	2a	1695	1/1	0.89	0.23	64,64,64,64	0
57	MG	2A	3625	1/1	0.89	0.21	65,65,65,65	0
57	MG	1A	4059	1/1	0.89	0.14	70,70,70,70	0
57	MG	2a	1699	1/1	0.89	0.38	73,73,73,73	0
57	MG	1A	3937	1/1	0.89	0.12	52,52,52,52	0
57	MG	1A	3626	1/1	0.89	0.10	10,10,10,10	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	1706	1/1	0.89	0.19	71,71,71,71	0
57	MG	1a	1742	1/1	0.89	0.22	56,56,56,56	0
57	MG	2a	1710	1/1	0.89	0.14	59,59,59,59	0
57	MG	2A	3637	1/1	0.89	0.15	67,67,67,67	0
57	MG	2a	1714	1/1	0.89	0.25	74,74,74,74	0
57	MG	2A	3126	1/1	0.89	0.27	67,67,67,67	0
57	MG	1a	1744	1/1	0.89	0.23	67,67,67,67	0
57	MG	2a	1719	1/1	0.89	0.23	67,67,67,67	0
57	MG	2a	1720	1/1	0.89	0.14	65,65,65,65	0
57	MG	18	3406	1/1	0.89	0.21	53,53,53,53	0
57	MG	2A	3152	1/1	0.89	0.22	55,55,55,55	0
57	MG	2A	3422	1/1	0.89	0.14	62,62,62,62	0
57	MG	1A	3854	1/1	0.89	0.13	51,51,51,51	0
57	MG	1A	3493	1/1	0.89	0.10	46,46,46,46	0
57	MG	1a	1616	1/1	0.89	0.11	63,63,63,63	0
57	MG	2A	3685	1/1	0.89	0.15	46,46,46,46	0
57	MG	1a	1771	1/1	0.89	0.11	56,56,56,56	0
57	MG	2a	1741	1/1	0.89	0.21	45,45,45,45	0
57	MG	1a	1622	1/1	0.89	0.26	63,63,63,63	0
57	MG	1a	1779	1/1	0.89	0.09	55,55,55,55	0
57	MG	2a	1754	1/1	0.89	0.33	57,57,57,57	0
57	MG	1A	3945	1/1	0.89	0.13	60,60,60,60	0
57	MG	2A	3179	1/1	0.89	0.23	68,68,68,68	0
57	MG	2A	3710	1/1	0.89	0.29	60,60,60,60	0
57	MG	2a	1770	1/1	0.89	0.30	65,65,65,65	0
57	MG	2a	1773	1/1	0.89	0.20	64,64,64,64	0
57	MG	2A	3712	1/1	0.89	0.17	58,58,58,58	0
57	MG	2a	1777	1/1	0.89	0.23	73,73,73,73	0
57	MG	2A	3462	1/1	0.89	0.10	67,67,67,67	0
57	MG	1a	1625	1/1	0.89	0.27	54,54,54,54	0
57	MG	1a	1788	1/1	0.89	0.09	85,85,85,85	0
57	MG	1a	1627	1/1	0.89	0.18	59,59,59,59	0
57	MG	2A	3190	1/1	0.89	0.24	40,40,40,40	0
57	MG	1a	1796	1/1	0.89	0.12	45,45,45,45	0
57	MG	1A	3857	1/1	0.89	0.17	51,51,51,51	0
57	MG	2A	3201	1/1	0.89	0.14	77,77,77,77	0
57	MG	2A	3203	1/1	0.89	0.13	63,63,63,63	0
57	MG	1A	3955	1/1	0.89	0.09	25,25,25,25	0
57	MG	2y	102	1/1	0.89	0.08	81,81,81,81	0
57	MG	2y	103	1/1	0.89	0.28	58,58,58,58	0
57	MG	2A	3128	1/1	0.90	0.16	61,61,61,61	0
57	MG	2A	3426	1/1	0.90	0.11	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
57	MG	1A	3165	1/1	0.90	0.12	45,45,45,45	0
57	MG	2A	3438	1/1	0.90	0.12	31,31,31,31	0
57	MG	1A	3169	1/1	0.90	0.25	62,62,62,62	0
57	MG	1A	3182	1/1	0.90	0.10	51,51,51,51	0
57	MG	1a	1745	1/1	0.90	0.15	68,68,68,68	0
57	MG	1a	1748	1/1	0.90	0.16	60,60,60,60	0
57	MG	2B	213	1/1	0.90	0.21	64,64,64,64	0
57	MG	2A	3451	1/1	0.90	0.12	60,60,60,60	0
57	MG	2B	215	1/1	0.90	0.18	65,65,65,65	0
57	MG	2B	216	1/1	0.90	0.27	75,75,75,75	0
57	MG	1A	3359	1/1	0.90	0.17	62,62,62,62	0
57	MG	18	3405	1/1	0.90	0.16	48,48,48,48	0
57	MG	2A	3171	1/1	0.90	0.10	47,47,47,47	0
57	MG	2E	306	1/1	0.90	0.11	57,57,57,57	0
57	MG	2A	3174	1/1	0.90	0.13	60,60,60,60	0
57	MG	1A	3361	1/1	0.90	0.14	60,60,60,60	0
57	MG	2A	3468	1/1	0.90	0.14	67,67,67,67	0
57	MG	2A	3177	1/1	0.90	0.30	60,60,60,60	0
57	MG	1a	1601	1/1	0.90	0.29	66,66,66,66	0
57	MG	27	101	1/1	0.90	0.25	63,63,63,63	0
57	MG	1A	3460	1/1	0.90	0.18	55,55,55,55	0
57	MG	2a	1602	1/1	0.90	0.31	71,71,71,71	0
57	MG	1a	1605	1/1	0.90	0.11	59,59,59,59	0
57	MG	1A	3809	1/1	0.90	0.07	34,34,34,34	0
57	MG	2a	1607	1/1	0.90	0.23	69,69,69,69	0
57	MG	1A	3930	1/1	0.90	0.08	72,72,72,72	0
57	MG	2A	3485	1/1	0.90	0.09	32,32,32,32	0
57	MG	1A	3467	1/1	0.90	0.17	64,64,64,64	0
57	MG	1A	4064	1/1	0.90	0.12	68,68,68,68	0
57	MG	1A	3294	1/1	0.90	0.07	30,30,30,30	0
57	MG	1A	3933	1/1	0.90	0.15	33,33,33,33	0
57	MG	1a	1800	1/1	0.90	0.12	47,47,47,47	0
57	MG	1A	4080	1/1	0.90	0.15	52,52,52,52	0
57	MG	1A	3540	1/1	0.90	0.19	34,34,34,34	0
57	MG	1A	3820	1/1	0.90	0.13	46,46,46,46	0
57	MG	1a	1632	1/1	0.90	0.30	59,59,59,59	0
57	MG	2a	1630	1/1	0.90	0.40	74,74,74,74	0
57	MG	1b	301	1/1	0.90	0.09	80,80,80,80	0
57	MG	2A	3518	1/1	0.90	0.09	54,54,54,54	0
57	MG	2A	3519	1/1	0.90	0.19	59,59,59,59	0
57	MG	2A	3523	1/1	0.90	0.22	60,60,60,60	0
57	MG	1A	3666	1/1	0.90	0.09	44,44,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3530	1/1	0.90	0.14	67,67,67,67	0
57	MG	2a	1642	1/1	0.90	0.23	59,59,59,59	0
57	MG	1A	3673	1/1	0.90	0.09	49,49,49,49	0
57	MG	1a	1638	1/1	0.90	0.15	50,50,50,50	0
57	MG	1v	101	1/1	0.90	0.20	71,71,71,71	0
57	MG	1w	101	1/1	0.90	0.18	76,76,76,76	0
57	MG	1w	103	1/1	0.90	0.15	63,63,63,63	0
57	MG	1A	4090	1/1	0.90	0.11	50,50,50,50	0
57	MG	2a	1651	1/1	0.90	0.15	58,58,58,58	0
57	MG	1A	3308	1/1	0.90	0.17	49,49,49,49	0
57	MG	2A	3240	1/1	0.90	0.17	57,57,57,57	0
57	MG	2A	3549	1/1	0.90	0.12	66,66,66,66	0
57	MG	1A	3376	1/1	0.90	0.23	58,58,58,58	0
57	MG	1a	1646	1/1	0.90	0.14	63,63,63,63	0
57	MG	2a	1661	1/1	0.90	0.21	71,71,71,71	0
57	MG	2A	3250	1/1	0.90	0.18	59,59,59,59	0
57	MG	1A	3547	1/1	0.90	0.20	52,52,52,52	0
57	MG	1x	113	1/1	0.90	0.19	72,72,72,72	0
57	MG	1a	1664	1/1	0.90	0.29	68,68,68,68	0
57	MG	1A	3378	1/1	0.90	0.14	53,53,53,53	0
57	MG	2a	1671	1/1	0.90	0.17	55,55,55,55	0
57	MG	2A	3261	1/1	0.90	0.12	54,54,54,54	0
57	MG	2a	1676	1/1	0.90	0.19	64,64,64,64	0
57	MG	1A	3957	1/1	0.90	0.10	62,62,62,62	0
57	MG	2A	3264	1/1	0.90	0.14	64,64,64,64	0
57	MG	1A	3483	1/1	0.90	0.15	41,41,41,41	0
57	MG	1A	3700	1/1	0.90	0.11	26,26,26,26	0
57	MG	2a	1684	1/1	0.90	0.17	76,76,76,76	0
57	MG	2a	1685	1/1	0.90	0.17	67,67,67,67	0
57	MG	2A	3273	1/1	0.90	0.11	58,58,58,58	0
57	MG	1A	3972	1/1	0.90	0.10	40,40,40,40	0
57	MG	1A	3974	1/1	0.90	0.07	24,24,24,24	0
57	MG	2A	3280	1/1	0.90	0.08	58,58,58,58	0
57	MG	2A	3286	1/1	0.90	0.20	48,48,48,48	0
57	MG	1A	3852	1/1	0.90	0.11	71,71,71,71	0
57	MG	1A	3383	1/1	0.90	0.12	53,53,53,53	0
57	MG	2A	3033	1/1	0.90	0.28	56,56,56,56	0
57	MG	1A	3996	1/1	0.90	0.12	26,26,26,26	0
57	MG	1A	3250	1/1	0.90	0.09	56,56,56,56	0
57	MG	2A	3301	1/1	0.90	0.17	57,57,57,57	0
57	MG	1A	3100	1/1	0.90	0.09	61,61,61,61	0
57	MG	1A	3723	1/1	0.90	0.09	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
57	MG	1a	1687	1/1	0.90	0.22	48,48,48,48	0
57	MG	2a	1712	1/1	0.90	0.19	68,68,68,68	0
57	MG	1a	1690	1/1	0.90	0.16	74,74,74,74	0
57	MG	2A	3616	1/1	0.90	0.16	42,42,42,42	0
57	MG	2A	3307	1/1	0.90	0.25	69,69,69,69	0
57	MG	2A	3309	1/1	0.90	0.27	56,56,56,56	0
57	MG	2A	3311	1/1	0.90	0.22	56,56,56,56	0
57	MG	2A	3623	1/1	0.90	0.20	58,58,58,58	0
57	MG	1A	3495	1/1	0.90	0.07	41,41,41,41	0
57	MG	2a	1726	1/1	0.90	0.42	68,68,68,68	0
57	MG	2A	3335	1/1	0.90	0.19	62,62,62,62	0
57	MG	1E	301	1/1	0.90	0.13	32,32,32,32	0
57	MG	1a	1693	1/1	0.90	0.11	69,69,69,69	0
57	MG	1a	1694	1/1	0.90	0.11	59,59,59,59	0
57	MG	2a	1733	1/1	0.90	0.38	57,57,57,57	0
57	MG	2a	1734	1/1	0.90	0.32	55,55,55,55	0
57	MG	2a	1737	1/1	0.90	0.40	64,64,64,64	0
57	MG	2A	3065	1/1	0.90	0.20	65,65,65,65	0
57	MG	1A	4023	1/1	0.90	0.08	41,41,41,41	0
57	MG	2A	3075	1/1	0.90	0.23	65,65,65,65	0
57	MG	1A	3318	1/1	0.90	0.08	50,50,50,50	0
57	MG	2a	1747	1/1	0.90	0.28	61,61,61,61	0
57	MG	2a	1748	1/1	0.90	0.35	62,62,62,62	0
57	MG	2A	3643	1/1	0.90	0.14	66,66,66,66	0
57	MG	1G	203	1/1	0.90	0.11	68,68,68,68	0
57	MG	1A	3006	1/1	0.90	0.14	54,54,54,54	0
57	MG	2a	1758	1/1	0.90	0.29	57,57,57,57	0
57	MG	2a	1761	1/1	0.90	0.29	59,59,59,59	0
57	MG	2a	1762	1/1	0.90	0.34	69,69,69,69	0
57	MG	2A	3369	1/1	0.90	0.31	61,61,61,61	0
57	MG	2A	3371	1/1	0.90	0.30	59,59,59,59	0
57	MG	2a	1768	1/1	0.90	0.26	61,61,61,61	0
57	MG	1a	1710	1/1	0.90	0.18	63,63,63,63	0
57	MG	1A	3421	1/1	0.90	0.10	57,57,57,57	0
57	MG	1A	3736	1/1	0.90	0.14	60,60,60,60	0
57	MG	1A	3747	1/1	0.90	0.20	49,49,49,49	0
57	MG	1A	3596	1/1	0.90	0.11	43,43,43,43	0
57	MG	2A	3694	1/1	0.90	0.12	41,41,41,41	0
57	MG	1S	202	1/1	0.90	0.12	46,46,46,46	0
57	MG	2A	3705	1/1	0.90	0.22	59,59,59,59	0
57	MG	2A	3388	1/1	0.90	0.16	53,53,53,53	0
57	MG	2a	1786	1/1	0.90	0.11	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3264	1/1	0.90	0.10	44,44,44,44	0
57	MG	2A	3116	1/1	0.90	0.21	64,64,64,64	0
57	MG	2A	3121	1/1	0.90	0.32	67,67,67,67	0
57	MG	1A	3519	1/1	0.90	0.12	52,52,52,52	0
57	MG	2A	3125	1/1	0.90	0.14	50,50,50,50	0
57	MG	2y	101	1/1	0.90	0.10	56,56,56,56	0
57	MG	1A	3339	1/1	0.90	0.13	54,54,54,54	0
57	MG	1Z	3703	1/1	0.90	0.17	52,52,52,52	0
59	ZN	24	501	1/1	0.90	0.14	135,135,135,135	0
57	MG	1A	3510	1/1	0.91	0.14	69,69,69,69	0
57	MG	1x	105	1/1	0.91	0.08	59,59,59,59	0
57	MG	1A	3060	1/1	0.91	0.17	49,49,49,49	0
57	MG	2A	3463	1/1	0.91	0.27	63,63,63,63	0
57	MG	1A	3408	1/1	0.91	0.13	48,48,48,48	0
57	MG	2A	3222	1/1	0.91	0.07	60,60,60,60	0
57	MG	2A	3469	1/1	0.91	0.14	65,65,65,65	0
57	MG	1x	111	1/1	0.91	0.13	62,62,62,62	0
57	MG	2F	306	1/1	0.91	0.07	62,62,62,62	0
57	MG	2A	3473	1/1	0.91	0.20	68,68,68,68	0
57	MG	1A	3647	1/1	0.91	0.08	35,35,35,35	0
57	MG	1A	3414	1/1	0.91	0.15	59,59,59,59	0
57	MG	1A	3061	1/1	0.91	0.15	50,50,50,50	0
57	MG	25	101	1/1	0.91	0.20	59,59,59,59	0
57	MG	1B	227	1/1	0.91	0.08	53,53,53,53	0
57	MG	2A	3232	1/1	0.91	0.17	62,62,62,62	0
57	MG	2A	3484	1/1	0.91	0.10	35,35,35,35	0
57	MG	1A	3655	1/1	0.91	0.09	33,33,33,33	0
57	MG	1B	229	1/1	0.91	0.11	61,61,61,61	0
57	MG	2a	1604	1/1	0.91	0.13	59,59,59,59	0
57	MG	1A	3657	1/1	0.91	0.08	27,27,27,27	0
57	MG	2A	3242	1/1	0.91	0.29	67,67,67,67	0
57	MG	2A	3005	1/1	0.91	0.25	62,62,62,62	0
57	MG	2A	3007	1/1	0.91	0.13	53,53,53,53	0
57	MG	2a	1613	1/1	0.91	0.19	63,63,63,63	0
57	MG	2A	3245	1/1	0.91	0.09	49,49,49,49	0
57	MG	2A	3247	1/1	0.91	0.10	53,53,53,53	0
57	MG	1A	3419	1/1	0.91	0.14	63,63,63,63	0
57	MG	2A	3513	1/1	0.91	0.14	45,45,45,45	0
57	MG	1A	3663	1/1	0.91	0.09	42,42,42,42	0
57	MG	2A	3255	1/1	0.91	0.13	55,55,55,55	0
57	MG	1A	3336	1/1	0.91	0.12	43,43,43,43	0
57	MG	1A	3018	1/1	0.91	0.12	36,36,36,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3522	1/1	0.91	0.28	66,66,66,66	0
57	MG	2A	3038	1/1	0.91	0.19	52,52,52,52	0
57	MG	2A	3524	1/1	0.91	0.10	72,72,72,72	0
57	MG	2A	3039	1/1	0.91	0.17	66,66,66,66	0
57	MG	2a	1634	1/1	0.91	0.18	72,72,72,72	0
57	MG	1E	315	1/1	0.91	0.12	59,59,59,59	0
57	MG	1A	3850	1/1	0.91	0.24	56,56,56,56	0
57	MG	1A	3093	1/1	0.91	0.13	58,58,58,58	0
57	MG	2A	3534	1/1	0.91	0.20	60,60,60,60	0
57	MG	1A	4010	1/1	0.91	0.17	27,27,27,27	0
57	MG	2a	1643	1/1	0.91	0.11	73,73,73,73	0
57	MG	2A	3053	1/1	0.91	0.32	74,74,74,74	0
57	MG	1A	4014	1/1	0.91	0.08	69,69,69,69	0
57	MG	2A	3542	1/1	0.91	0.12	69,69,69,69	0
57	MG	1A	3435	1/1	0.91	0.25	64,64,64,64	0
57	MG	1A	3180	1/1	0.91	0.22	56,56,56,56	0
57	MG	1A	3856	1/1	0.91	0.13	55,55,55,55	0
57	MG	1A	3256	1/1	0.91	0.11	66,66,66,66	0
57	MG	2A	3289	1/1	0.91	0.22	43,43,43,43	0
57	MG	2a	1654	1/1	0.91	0.13	65,65,65,65	0
57	MG	1A	3355	1/1	0.91	0.12	58,58,58,58	0
57	MG	1V	205	1/1	0.91	0.12	41,41,41,41	0
57	MG	2A	3297	1/1	0.91	0.15	56,56,56,56	0
57	MG	1A	3864	1/1	0.91	0.07	21,21,21,21	0
57	MG	1A	4033	1/1	0.91	0.08	80,80,80,80	0
57	MG	2A	3561	1/1	0.91	0.12	73,73,73,73	0
57	MG	1A	3444	1/1	0.91	0.13	65,65,65,65	0
57	MG	1A	3868	1/1	0.91	0.22	35,35,35,35	0
57	MG	2A	3565	1/1	0.91	0.09	75,75,75,75	0
57	MG	1a	1726	1/1	0.91	0.12	53,53,53,53	0
57	MG	1A	3707	1/1	0.91	0.11	33,33,33,33	0
57	MG	1A	3445	1/1	0.91	0.11	57,57,57,57	0
57	MG	1A	3449	1/1	0.91	0.17	41,41,41,41	0
57	MG	1A	3545	1/1	0.91	0.27	59,59,59,59	0
57	MG	2A	3107	1/1	0.91	0.16	62,62,62,62	0
57	MG	2A	3312	1/1	0.91	0.12	69,69,69,69	0
57	MG	2a	1680	1/1	0.91	0.10	62,62,62,62	0
57	MG	1A	3722	1/1	0.91	0.12	50,50,50,50	0
57	MG	2A	3316	1/1	0.91	0.25	53,53,53,53	0
57	MG	2A	3590	1/1	0.91	0.14	62,62,62,62	0
57	MG	2A	3318	1/1	0.91	0.21	48,48,48,48	0
57	MG	1A	3262	1/1	0.91	0.14	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
57	MG	2A	3339	1/1	0.91	0.18	56,56,56,56	0
57	MG	1a	1602	1/1	0.91	0.17	62,62,62,62	0
57	MG	1A	3098	1/1	0.91	0.23	58,58,58,58	0
57	MG	2A	3342	1/1	0.91	0.49	60,60,60,60	0
57	MG	2A	3119	1/1	0.91	0.14	49,49,49,49	0
57	MG	2A	3344	1/1	0.91	0.11	53,53,53,53	0
57	MG	2a	1702	1/1	0.91	0.27	57,57,57,57	0
57	MG	2A	3351	1/1	0.91	0.17	54,54,54,54	0
57	MG	2a	1704	1/1	0.91	0.13	56,56,56,56	0
57	MG	1A	3265	1/1	0.91	0.17	62,62,62,62	0
57	MG	1A	3191	1/1	0.91	0.16	51,51,51,51	0
57	MG	2a	1707	1/1	0.91	0.12	70,70,70,70	0
57	MG	1A	3194	1/1	0.91	0.35	36,36,36,36	0
57	MG	1A	3370	1/1	0.91	0.11	51,51,51,51	0
57	MG	1A	3559	1/1	0.91	0.12	55,55,55,55	0
57	MG	1A	3905	1/1	0.91	0.08	43,43,43,43	0
57	MG	1A	3754	1/1	0.91	0.09	59,59,59,59	0
57	MG	2a	1715	1/1	0.91	0.16	69,69,69,69	0
57	MG	2A	3370	1/1	0.91	0.16	60,60,60,60	0
57	MG	1A	3034	1/1	0.91	0.08	47,47,47,47	0
57	MG	2A	3372	1/1	0.91	0.12	54,54,54,54	0
57	MG	1a	1787	1/1	0.91	0.10	57,57,57,57	0
57	MG	2A	3374	1/1	0.91	0.24	40,40,40,40	0
57	MG	2A	3162	1/1	0.91	0.09	64,64,64,64	0
57	MG	2A	3164	1/1	0.91	0.24	61,61,61,61	0
57	MG	1A	3479	1/1	0.91	0.12	40,40,40,40	0
57	MG	1A	3148	1/1	0.91	0.22	38,38,38,38	0
57	MG	1A	3929	1/1	0.91	0.08	31,31,31,31	0
57	MG	1a	1797	1/1	0.91	0.09	56,56,56,56	0
57	MG	2a	1731	1/1	0.91	0.39	61,61,61,61	0
57	MG	2A	3653	1/1	0.91	0.09	54,54,54,54	0
57	MG	2A	3390	1/1	0.91	0.12	45,45,45,45	0
57	MG	2A	3394	1/1	0.91	0.13	50,50,50,50	0
57	MG	2A	3667	1/1	0.91	0.10	41,41,41,41	0
57	MG	2A	3395	1/1	0.91	0.12	63,63,63,63	0
57	MG	1a	1633	1/1	0.91	0.21	56,56,56,56	0
57	MG	1a	1823	1/1	0.91	0.14	61,61,61,61	0
57	MG	2a	1745	1/1	0.91	0.18	49,49,49,49	0
57	MG	1A	3379	1/1	0.91	0.21	52,52,52,52	0
57	MG	2A	3690	1/1	0.91	0.08	51,51,51,51	0
57	MG	2a	1749	1/1	0.91	0.53	68,68,68,68	0
57	MG	2a	1750	1/1	0.91	0.34	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	1752	1/1	0.91	0.34	52,52,52,52	0
57	MG	1A	3770	1/1	0.91	0.16	46,46,46,46	0
57	MG	1A	3484	1/1	0.91	0.13	43,43,43,43	0
57	MG	2A	3696	1/1	0.91	0.10	45,45,45,45	0
57	MG	1A	4092	1/1	0.91	0.13	63,63,63,63	0
57	MG	2a	1760	1/1	0.91	0.25	54,54,54,54	0
57	MG	1a	1641	1/1	0.91	0.21	52,52,52,52	0
57	MG	1A	3048	1/1	0.91	0.06	16,16,16,16	0
57	MG	2a	1763	1/1	0.91	0.24	64,64,64,64	0
57	MG	1A	3388	1/1	0.91	0.12	64,64,64,64	0
57	MG	2A	3708	1/1	0.91	0.11	56,56,56,56	0
57	MG	1A	3395	1/1	0.91	0.09	48,48,48,48	0
57	MG	2a	1769	1/1	0.91	0.27	60,60,60,60	0
57	MG	2A	3711	1/1	0.91	0.15	61,61,61,61	0
57	MG	2a	1771	1/1	0.91	0.24	61,61,61,61	0
57	MG	2A	3431	1/1	0.91	0.16	48,48,48,48	0
57	MG	2A	3434	1/1	0.91	0.08	36,36,36,36	0
57	MG	2a	1776	1/1	0.91	0.26	63,63,63,63	0
57	MG	2A	3715	1/1	0.91	0.17	68,68,68,68	0
57	MG	1t	201	1/1	0.91	0.12	53,53,53,53	0
57	MG	2A	3198	1/1	0.91	0.34	68,68,68,68	0
57	MG	2A	3444	1/1	0.91	0.14	64,64,64,64	0
57	MG	2A	3720	1/1	0.91	0.12	41,41,41,41	0
57	MG	1A	3397	1/1	0.91	0.26	42,42,42,42	0
57	MG	1a	1663	1/1	0.91	0.11	48,48,48,48	0
57	MG	2A	3724	1/1	0.91	0.20	44,44,44,44	0
57	MG	2A	3725	1/1	0.91	0.27	62,62,62,62	0
57	MG	2B	202	1/1	0.91	0.29	60,60,60,60	0
57	MG	1A	3212	1/1	0.91	0.12	42,42,42,42	0
57	MG	1A	3223	1/1	0.91	0.10	47,47,47,47	0
57	MG	1a	1667	1/1	0.91	0.21	56,56,56,56	0
57	MG	2A	3455	1/1	0.91	0.24	62,62,62,62	0
57	MG	2A	3457	1/1	0.91	0.14	53,53,53,53	0
57	MG	2A	3458	1/1	0.91	0.14	55,55,55,55	0
61	K	2A	3330	1/1	0.91	0.18	75,75,75,75	0
57	MG	2A	3358	1/1	0.92	0.13	59,59,59,59	0
57	MG	1A	3591	1/1	0.92	0.20	57,57,57,57	0
57	MG	2A	3361	1/1	0.92	0.16	55,55,55,55	0
57	MG	2A	3366	1/1	0.92	0.28	68,68,68,68	0
57	MG	1A	3357	1/1	0.92	0.16	48,48,48,48	0
57	MG	2A	3069	1/1	0.92	0.25	67,67,67,67	0
57	MG	1A	3498	1/1	0.92	0.17	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3073	1/1	0.92	0.08	47,47,47,47	0
57	MG	1A	3417	1/1	0.92	0.14	48,48,48,48	0
57	MG	2A	3076	1/1	0.92	0.11	53,53,53,53	0
57	MG	2A	3077	1/1	0.92	0.12	66,66,66,66	0
57	MG	2A	3080	1/1	0.92	0.12	45,45,45,45	0
57	MG	1A	3607	1/1	0.92	0.26	64,64,64,64	0
57	MG	2A	3083	1/1	0.92	0.15	55,55,55,55	0
57	MG	2A	3085	1/1	0.92	0.18	62,62,62,62	0
57	MG	2A	3384	1/1	0.92	0.13	40,40,40,40	0
57	MG	2A	3385	1/1	0.92	0.28	60,60,60,60	0
57	MG	2B	205	1/1	0.92	0.09	56,56,56,56	0
57	MG	1A	3921	1/1	0.92	0.24	36,36,36,36	0
57	MG	2A	3387	1/1	0.92	0.08	36,36,36,36	0
57	MG	2A	3089	1/1	0.92	0.18	46,46,46,46	0
57	MG	2B	210	1/1	0.92	0.19	61,61,61,61	0
57	MG	1A	3924	1/1	0.92	0.11	30,30,30,30	0
57	MG	2B	212	1/1	0.92	0.12	65,65,65,65	0
57	MG	1A	3926	1/1	0.92	0.12	41,41,41,41	0
57	MG	1A	3298	1/1	0.92	0.10	51,51,51,51	0
57	MG	1A	3766	1/1	0.92	0.17	59,59,59,59	0
57	MG	1A	3301	1/1	0.92	0.46	68,68,68,68	0
57	MG	2A	3104	1/1	0.92	0.20	50,50,50,50	0
57	MG	1A	4099	1/1	0.92	0.21	53,53,53,53	0
57	MG	1A	3769	1/1	0.92	0.06	16,16,16,16	0
57	MG	1A	3422	1/1	0.92	0.08	49,49,49,49	0
57	MG	2F	302	1/1	0.92	0.10	50,50,50,50	0
57	MG	1A	3772	1/1	0.92	0.09	20,20,20,20	0
57	MG	1A	3049	1/1	0.92	0.17	32,32,32,32	0
57	MG	1B	203	1/1	0.92	0.06	31,31,31,31	0
57	MG	2A	3120	1/1	0.92	0.25	70,70,70,70	0
57	MG	1B	204	1/1	0.92	0.28	63,63,63,63	0
57	MG	1B	206	1/1	0.92	0.20	47,47,47,47	0
57	MG	1B	208	1/1	0.92	0.28	59,59,59,59	0
57	MG	2A	3440	1/1	0.92	0.09	40,40,40,40	0
57	MG	1a	1703	1/1	0.92	0.19	51,51,51,51	0
57	MG	1a	1704	1/1	0.92	0.25	52,52,52,52	0
57	MG	1B	210	1/1	0.92	0.16	55,55,55,55	0
57	MG	2A	3141	1/1	0.92	0.28	54,54,54,54	0
57	MG	1B	211	1/1	0.92	0.09	50,50,50,50	0
57	MG	2A	3151	1/1	0.92	0.07	45,45,45,45	0
57	MG	1A	3086	1/1	0.92	0.11	35,35,35,35	0
57	MG	2a	1610	1/1	0.92	0.28	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
57	MG	2A	3454	1/1	0.92	0.09	59,59,59,59	0
57	MG	2A	3156	1/1	0.92	0.29	61,61,61,61	0
57	MG	2A	3158	1/1	0.92	0.26	67,67,67,67	0
57	MG	2a	1617	1/1	0.92	0.10	67,67,67,67	0
57	MG	1B	221	1/1	0.92	0.15	57,57,57,57	0
57	MG	1a	1714	1/1	0.92	0.15	46,46,46,46	0
57	MG	1B	222	1/1	0.92	0.07	51,51,51,51	0
57	MG	2A	3165	1/1	0.92	0.18	53,53,53,53	0
57	MG	1B	223	1/1	0.92	0.09	55,55,55,55	0
57	MG	2a	1623	1/1	0.92	0.24	68,68,68,68	0
57	MG	1a	1719	1/1	0.92	0.15	60,60,60,60	0
57	MG	1A	3104	1/1	0.92	0.10	36,36,36,36	0
57	MG	1A	3632	1/1	0.92	0.07	24,24,24,24	0
57	MG	1A	3634	1/1	0.92	0.11	52,52,52,52	0
57	MG	1A	3803	1/1	0.92	0.11	57,57,57,57	0
57	MG	1A	3807	1/1	0.92	0.12	26,26,26,26	0
57	MG	1a	1728	1/1	0.92	0.26	58,58,58,58	0
57	MG	1a	1729	1/1	0.92	0.11	65,65,65,65	0
57	MG	1B	232	1/1	0.92	0.11	43,43,43,43	0
57	MG	1a	1735	1/1	0.92	0.20	48,48,48,48	0
57	MG	2A	3482	1/1	0.92	0.15	63,63,63,63	0
57	MG	2A	3181	1/1	0.92	0.35	61,61,61,61	0
57	MG	2A	3185	1/1	0.92	0.13	72,72,72,72	0
57	MG	1A	3114	1/1	0.92	0.21	46,46,46,46	0
57	MG	1A	3374	1/1	0.92	0.24	43,43,43,43	0
57	MG	1A	3966	1/1	0.92	0.09	52,52,52,52	0
57	MG	2A	3192	1/1	0.92	0.12	54,54,54,54	0
57	MG	1E	303	1/1	0.92	0.21	44,44,44,44	0
57	MG	2A	3498	1/1	0.92	0.09	45,45,45,45	0
57	MG	2A	3195	1/1	0.92	0.13	38,38,38,38	0
57	MG	1E	307	1/1	0.92	0.20	49,49,49,49	0
57	MG	2A	3507	1/1	0.92	0.21	65,65,65,65	0
57	MG	1A	3649	1/1	0.92	0.11	50,50,50,50	0
57	MG	1A	3968	1/1	0.92	0.11	44,44,44,44	0
57	MG	2A	3202	1/1	0.92	0.15	48,48,48,48	0
57	MG	2A	3516	1/1	0.92	0.09	50,50,50,50	0
57	MG	2a	1660	1/1	0.92	0.19	56,56,56,56	0
57	MG	1A	3375	1/1	0.92	0.14	53,53,53,53	0
57	MG	1A	3442	1/1	0.92	0.21	46,46,46,46	0
57	MG	2A	3209	1/1	0.92	0.36	59,59,59,59	0
57	MG	1G	204	1/1	0.92	0.09	68,68,68,68	0
57	MG	1a	1767	1/1	0.92	0.19	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
57	MG	1N	205	1/1	0.92	0.13	54,54,54,54	0
57	MG	1a	1777	1/1	0.92	0.14	71,71,71,71	0
57	MG	2A	3529	1/1	0.92	0.12	73,73,73,73	0
57	MG	2A	3217	1/1	0.92	0.11	58,58,58,58	0
57	MG	2A	3531	1/1	0.92	0.12	53,53,53,53	0
57	MG	1A	3975	1/1	0.92	0.27	50,50,50,50	0
57	MG	1A	3653	1/1	0.92	0.13	72,72,72,72	0
57	MG	2A	3223	1/1	0.92	0.26	72,72,72,72	0
57	MG	2A	3535	1/1	0.92	0.11	59,59,59,59	0
57	MG	1A	3986	1/1	0.92	0.11	60,60,60,60	0
57	MG	2A	3538	1/1	0.92	0.09	58,58,58,58	0
57	MG	1P	205	1/1	0.92	0.24	49,49,49,49	0
57	MG	2a	1687	1/1	0.92	0.13	67,67,67,67	0
57	MG	2a	1691	1/1	0.92	0.14	58,58,58,58	0
57	MG	1a	1785	1/1	0.92	0.12	50,50,50,50	0
57	MG	1A	3327	1/1	0.92	0.17	45,45,45,45	0
57	MG	1A	3994	1/1	0.92	0.12	73,73,73,73	0
57	MG	1A	3330	1/1	0.92	0.22	52,52,52,52	0
57	MG	1a	1792	1/1	0.92	0.09	64,64,64,64	0
57	MG	2A	3236	1/1	0.92	0.14	63,63,63,63	0
57	MG	2A	3237	1/1	0.92	0.17	63,63,63,63	0
57	MG	1A	3331	1/1	0.92	0.21	54,54,54,54	0
57	MG	1T	202	1/1	0.92	0.10	51,51,51,51	0
57	MG	2A	3554	1/1	0.92	0.17	60,60,60,60	0
57	MG	1U	209	1/1	0.92	0.12	53,53,53,53	0
57	MG	1A	4001	1/1	0.92	0.07	28,28,28,28	0
57	MG	1W	201	1/1	0.92	0.17	44,44,44,44	0
57	MG	1A	3829	1/1	0.92	0.08	41,41,41,41	0
57	MG	2A	3246	1/1	0.92	0.27	66,66,66,66	0
57	MG	1Z	3701	1/1	0.92	0.10	60,60,60,60	0
57	MG	1A	3453	1/1	0.92	0.16	38,38,38,38	0
57	MG	1A	4009	1/1	0.92	0.09	16,16,16,16	0
57	MG	2A	3252	1/1	0.92	0.11	71,71,71,71	0
57	MG	10	103	1/1	0.92	0.06	47,47,47,47	0
57	MG	2a	1717	1/1	0.92	0.10	75,75,75,75	0
57	MG	10	107	1/1	0.92	0.11	59,59,59,59	0
57	MG	2A	3257	1/1	0.92	0.13	57,57,57,57	0
57	MG	1l	203	1/1	0.92	0.15	62,62,62,62	0
57	MG	2a	1721	1/1	0.92	0.29	47,47,47,47	0
57	MG	1A	3132	1/1	0.92	0.11	40,40,40,40	0
57	MG	2A	3586	1/1	0.92	0.11	39,39,39,39	0
57	MG	1A	4012	1/1	0.92	0.06	36,36,36,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3262	1/1	0.92	0.15	47,47,47,47	0
57	MG	1A	3670	1/1	0.92	0.07	24,24,24,24	0
57	MG	1A	3385	1/1	0.92	0.12	34,34,34,34	0
57	MG	1A	3248	1/1	0.92	0.13	57,57,57,57	0
57	MG	1A	4025	1/1	0.92	0.10	48,48,48,48	0
57	MG	1A	3391	1/1	0.92	0.14	51,51,51,51	0
57	MG	1A	3680	1/1	0.92	0.07	34,34,34,34	0
57	MG	2a	1735	1/1	0.92	0.33	61,61,61,61	0
57	MG	2a	1736	1/1	0.92	0.44	72,72,72,72	0
57	MG	1A	3269	1/1	0.92	0.32	53,53,53,53	0
57	MG	2a	1738	1/1	0.92	0.20	57,57,57,57	0
57	MG	1A	3691	1/1	0.92	0.09	32,32,32,32	0
57	MG	1A	3474	1/1	0.92	0.10	52,52,52,52	0
57	MG	1a	1610	1/1	0.92	0.08	57,57,57,57	0
57	MG	1a	1612	1/1	0.92	0.11	66,66,66,66	0
57	MG	1A	3137	1/1	0.92	0.16	40,40,40,40	0
57	MG	1y	101	1/1	0.92	0.06	68,68,68,68	0
57	MG	2A	3296	1/1	0.92	0.18	54,54,54,54	0
57	MG	2A	3621	1/1	0.92	0.20	48,48,48,48	0
57	MG	1A	3552	1/1	0.92	0.28	51,51,51,51	0
57	MG	2a	1751	1/1	0.92	0.41	59,59,59,59	0
57	MG	1A	3701	1/1	0.92	0.11	23,23,23,23	0
57	MG	1A	3703	1/1	0.92	0.15	68,68,68,68	0
57	MG	1A	3706	1/1	0.92	0.09	36,36,36,36	0
57	MG	1A	3277	1/1	0.92	0.18	35,35,35,35	0
57	MG	1A	3400	1/1	0.92	0.20	64,64,64,64	0
57	MG	2A	3630	1/1	0.92	0.24	61,61,61,61	0
57	MG	1A	3710	1/1	0.92	0.12	57,57,57,57	0
57	MG	2A	3008	1/1	0.92	0.13	56,56,56,56	0
57	MG	1A	3344	1/1	0.92	0.24	37,37,37,37	0
57	MG	2a	1764	1/1	0.92	0.42	67,67,67,67	0
57	MG	1A	3884	1/1	0.92	0.16	32,32,32,32	0
57	MG	2A	3026	1/1	0.92	0.10	54,54,54,54	0
57	MG	1A	3402	1/1	0.92	0.22	40,40,40,40	0
57	MG	2A	3645	1/1	0.92	0.08	47,47,47,47	0
57	MG	1A	4054	1/1	0.92	0.07	32,32,32,32	0
57	MG	2A	3314	1/1	0.92	0.12	52,52,52,52	0
57	MG	2A	3036	1/1	0.92	0.11	52,52,52,52	0
57	MG	1A	3560	1/1	0.92	0.15	63,63,63,63	0
57	MG	2A	3655	1/1	0.92	0.15	57,57,57,57	0
57	MG	2A	3323	1/1	0.92	0.30	52,52,52,52	0
57	MG	2A	3662	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
57	MG	1A	3561	1/1	0.92	0.08	55,55,55,55	0
57	MG	2A	3040	1/1	0.92	0.13	51,51,51,51	0
57	MG	2A	3671	1/1	0.92	0.09	53,53,53,53	0
57	MG	2a	1782	1/1	0.92	0.24	62,62,62,62	0
57	MG	2a	1783	1/1	0.92	0.14	73,73,73,73	0
57	MG	1A	4061	1/1	0.92	0.11	55,55,55,55	0
57	MG	2a	1785	1/1	0.92	0.27	69,69,69,69	0
57	MG	1A	3347	1/1	0.92	0.20	60,60,60,60	0
57	MG	2f	201	1/1	0.92	0.09	52,52,52,52	0
57	MG	1A	3893	1/1	0.92	0.09	32,32,32,32	0
57	MG	1a	1645	1/1	0.92	0.15	65,65,65,65	0
57	MG	1A	3207	1/1	0.92	0.15	61,61,61,61	0
57	MG	2w	101	1/1	0.92	0.16	55,55,55,55	0
57	MG	2A	3350	1/1	0.92	0.12	50,50,50,50	0
57	MG	1a	1651	1/1	0.92	0.22	66,66,66,66	0
57	MG	2A	3701	1/1	0.92	0.13	61,61,61,61	0
57	MG	1A	4068	1/1	0.92	0.06	25,25,25,25	0
57	MG	1A	3411	1/1	0.92	0.18	51,51,51,51	0
57	MG	1A	3253	1/1	0.92	0.20	49,49,49,49	0
57	MG	1A	3735	1/1	0.92	0.14	55,55,55,55	0
57	MG	1Q	203	1/1	0.93	0.11	55,55,55,55	0
57	MG	1Q	205	1/1	0.93	0.10	40,40,40,40	0
57	MG	2A	3400	1/1	0.93	0.08	42,42,42,42	0
57	MG	1a	1743	1/1	0.93	0.31	59,59,59,59	0
57	MG	2A	3153	1/1	0.93	0.18	57,57,57,57	0
57	MG	2A	3728	1/1	0.93	0.22	51,51,51,51	0
57	MG	2A	3730	1/1	0.93	0.14	66,66,66,66	0
57	MG	2B	201	1/1	0.93	0.16	64,64,64,64	0
57	MG	2A	3408	1/1	0.93	0.16	48,48,48,48	0
57	MG	1A	3671	1/1	0.93	0.09	24,24,24,24	0
57	MG	2A	3410	1/1	0.93	0.20	63,63,63,63	0
57	MG	1A	4011	1/1	0.93	0.10	19,19,19,19	0
57	MG	2A	3417	1/1	0.93	0.07	35,35,35,35	0
57	MG	1A	3846	1/1	0.93	0.18	60,60,60,60	0
57	MG	1a	1749	1/1	0.93	0.17	59,59,59,59	0
57	MG	1a	1752	1/1	0.93	0.08	56,56,56,56	0
57	MG	1a	1754	1/1	0.93	0.12	43,43,43,43	0
57	MG	1A	3433	1/1	0.93	0.12	41,41,41,41	0
57	MG	1A	3296	1/1	0.93	0.08	53,53,53,53	0
57	MG	2A	3435	1/1	0.93	0.16	56,56,56,56	0
57	MG	1U	202	1/1	0.93	0.19	40,40,40,40	0
57	MG	1A	4020	1/1	0.93	0.07	21,21,21,21	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3441	1/1	0.93	0.10	59,59,59,59	0
57	MG	1A	3677	1/1	0.93	0.07	25,25,25,25	0
57	MG	2E	301	1/1	0.93	0.15	59,59,59,59	0
57	MG	1A	3297	1/1	0.93	0.12	59,59,59,59	0
57	MG	2E	305	1/1	0.93	0.12	39,39,39,39	0
57	MG	1a	1776	1/1	0.93	0.35	70,70,70,70	0
57	MG	1Y	202	1/1	0.93	0.23	56,56,56,56	0
57	MG	1A	3053	1/1	0.93	0.09	37,37,37,37	0
57	MG	1A	3368	1/1	0.93	0.11	57,57,57,57	0
57	MG	2Q	201	1/1	0.93	0.08	53,53,53,53	0
57	MG	1A	3439	1/1	0.93	0.13	54,54,54,54	0
57	MG	1A	3246	1/1	0.93	0.13	57,57,57,57	0
57	MG	2A	3182	1/1	0.93	0.12	55,55,55,55	0
57	MG	10	102	1/1	0.93	0.18	47,47,47,47	0
57	MG	1a	1786	1/1	0.93	0.09	56,56,56,56	0
57	MG	1A	3543	1/1	0.93	0.26	50,50,50,50	0
57	MG	1A	4034	1/1	0.93	0.07	52,52,52,52	0
57	MG	1A	3373	1/1	0.93	0.12	60,60,60,60	0
57	MG	1A	3307	1/1	0.93	0.41	63,63,63,63	0
57	MG	1A	3247	1/1	0.93	0.32	62,62,62,62	0
57	MG	2A	3197	1/1	0.93	0.27	64,64,64,64	0
57	MG	1A	3183	1/1	0.93	0.13	70,70,70,70	0
57	MG	2a	1608	1/1	0.93	0.32	68,68,68,68	0
57	MG	1A	3870	1/1	0.93	0.10	41,41,41,41	0
57	MG	2A	3200	1/1	0.93	0.09	52,52,52,52	0
57	MG	1a	1813	1/1	0.93	0.07	68,68,68,68	0
57	MG	1a	1817	1/1	0.93	0.09	58,58,58,58	0
57	MG	1A	3873	1/1	0.93	0.07	40,40,40,40	0
57	MG	2A	3205	1/1	0.93	0.12	57,57,57,57	0
57	MG	1A	3550	1/1	0.93	0.26	47,47,47,47	0
57	MG	1a	1826	1/1	0.93	0.18	56,56,56,56	0
57	MG	1A	3454	1/1	0.93	0.12	62,62,62,62	0
57	MG	1A	3877	1/1	0.93	0.07	30,30,30,30	0
57	MG	1A	3311	1/1	0.93	0.25	50,50,50,50	0
57	MG	2A	3488	1/1	0.93	0.09	34,34,34,34	0
57	MG	1a	1606	1/1	0.93	0.14	53,53,53,53	0
57	MG	1A	3712	1/1	0.93	0.08	27,27,27,27	0
57	MG	1A	3187	1/1	0.93	0.08	44,44,44,44	0
57	MG	1A	3888	1/1	0.93	0.09	50,50,50,50	0
57	MG	1a	1613	1/1	0.93	0.11	65,65,65,65	0
57	MG	1A	3316	1/1	0.93	0.20	59,59,59,59	0
57	MG	2A	3501	1/1	0.93	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
57	MG	1A	3720	1/1	0.93	0.10	54,54,54,54	0
57	MG	1A	3188	1/1	0.93	0.24	32,32,32,32	0
57	MG	1A	3468	1/1	0.93	0.09	50,50,50,50	0
57	MG	2a	1638	1/1	0.93	0.22	57,57,57,57	0
57	MG	2a	1639	1/1	0.93	0.21	53,53,53,53	0
57	MG	1A	3320	1/1	0.93	0.17	57,57,57,57	0
57	MG	1A	3899	1/1	0.93	0.11	25,25,25,25	0
57	MG	2A	3233	1/1	0.93	0.16	57,57,57,57	0
57	MG	1x	102	1/1	0.93	0.09	33,33,33,33	0
57	MG	2a	1645	1/1	0.93	0.10	54,54,54,54	0
57	MG	1A	4071	1/1	0.93	0.09	46,46,46,46	0
57	MG	1A	3726	1/1	0.93	0.14	56,56,56,56	0
57	MG	2A	3238	1/1	0.93	0.13	63,63,63,63	0
57	MG	1x	106	1/1	0.93	0.25	69,69,69,69	0
57	MG	1A	3471	1/1	0.93	0.17	66,66,66,66	0
57	MG	1A	3325	1/1	0.93	0.15	52,52,52,52	0
57	MG	1A	3393	1/1	0.93	0.22	44,44,44,44	0
57	MG	1x	112	1/1	0.93	0.22	62,62,62,62	0
57	MG	1A	3587	1/1	0.93	0.07	37,37,37,37	0
57	MG	1A	3909	1/1	0.93	0.08	54,54,54,54	0
57	MG	2a	1657	1/1	0.93	0.14	65,65,65,65	0
57	MG	1A	3135	1/1	0.93	0.15	49,49,49,49	0
57	MG	1A	3746	1/1	0.93	0.08	51,51,51,51	0
57	MG	1A	3045	1/1	0.93	0.07	35,35,35,35	0
57	MG	1A	3919	1/1	0.93	0.12	64,64,64,64	0
57	MG	2A	3253	1/1	0.93	0.09	63,63,63,63	0
57	MG	2A	3254	1/1	0.93	0.11	48,48,48,48	0
57	MG	1A	3748	1/1	0.93	0.08	53,53,53,53	0
57	MG	1A	3752	1/1	0.93	0.08	21,21,21,21	0
57	MG	2A	3004	1/1	0.93	0.36	68,68,68,68	0
57	MG	1A	3594	1/1	0.93	0.14	43,43,43,43	0
57	MG	2A	3545	1/1	0.93	0.11	46,46,46,46	0
57	MG	2a	1674	1/1	0.93	0.15	65,65,65,65	0
57	MG	2a	1675	1/1	0.93	0.10	63,63,63,63	0
57	MG	1a	1657	1/1	0.93	0.20	52,52,52,52	0
57	MG	1a	1658	1/1	0.93	0.23	60,60,60,60	0
57	MG	2A	3009	1/1	0.93	0.11	45,45,45,45	0
57	MG	1A	3196	1/1	0.93	0.08	41,41,41,41	0
57	MG	1A	3481	1/1	0.93	0.17	50,50,50,50	0
57	MG	2A	3553	1/1	0.93	0.09	42,42,42,42	0
57	MG	1A	3261	1/1	0.93	0.16	62,62,62,62	0
57	MG	2A	3266	1/1	0.93	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
57	MG	1A	3039	1/1	0.93	0.21	56,56,56,56	0
57	MG	2A	3558	1/1	0.93	0.15	62,62,62,62	0
57	MG	2a	1689	1/1	0.93	0.17	48,48,48,48	0
57	MG	2A	3559	1/1	0.93	0.15	61,61,61,61	0
57	MG	2A	3269	1/1	0.93	0.16	65,65,65,65	0
57	MG	2A	3271	1/1	0.93	0.31	62,62,62,62	0
57	MG	2A	3029	1/1	0.93	0.11	54,54,54,54	0
57	MG	2A	3030	1/1	0.93	0.12	50,50,50,50	0
57	MG	2A	3564	1/1	0.93	0.15	56,56,56,56	0
57	MG	2a	1697	1/1	0.93	0.20	51,51,51,51	0
57	MG	1A	4105	1/1	0.93	0.09	47,47,47,47	0
57	MG	2A	3278	1/1	0.93	0.11	60,60,60,60	0
57	MG	2A	3035	1/1	0.93	0.12	31,31,31,31	0
57	MG	2A	3571	1/1	0.93	0.15	66,66,66,66	0
57	MG	2A	3572	1/1	0.93	0.08	69,69,69,69	0
57	MG	2A	3574	1/1	0.93	0.08	77,77,77,77	0
57	MG	2A	3285	1/1	0.93	0.26	44,44,44,44	0
57	MG	1A	3263	1/1	0.93	0.09	58,58,58,58	0
57	MG	1A	3040	1/1	0.93	0.11	39,39,39,39	0
57	MG	1a	1672	1/1	0.93	0.12	67,67,67,67	0
57	MG	1A	3111	1/1	0.93	0.11	33,33,33,33	0
57	MG	2A	3291	1/1	0.93	0.23	48,48,48,48	0
57	MG	2A	3041	1/1	0.93	0.21	63,63,63,63	0
57	MG	2A	3043	1/1	0.93	0.13	51,51,51,51	0
57	MG	1A	3494	1/1	0.93	0.09	41,41,41,41	0
57	MG	2A	3048	1/1	0.93	0.14	63,63,63,63	0
57	MG	2A	3049	1/1	0.93	0.18	63,63,63,63	0
57	MG	1A	3410	1/1	0.93	0.12	49,49,49,49	0
57	MG	1A	3496	1/1	0.93	0.13	43,43,43,43	0
57	MG	2A	3602	1/1	0.93	0.09	58,58,58,58	0
57	MG	1a	1679	1/1	0.93	0.21	60,60,60,60	0
57	MG	1A	3629	1/1	0.93	0.11	50,50,50,50	0
57	MG	1A	3630	1/1	0.93	0.07	23,23,23,23	0
57	MG	1A	3794	1/1	0.93	0.06	64,64,64,64	0
57	MG	2A	3609	1/1	0.93	0.15	53,53,53,53	0
57	MG	1B	216	1/1	0.93	0.09	38,38,38,38	0
57	MG	1A	3052	1/1	0.93	0.11	46,46,46,46	0
57	MG	1a	1686	1/1	0.93	0.15	51,51,51,51	0
57	MG	2a	1732	1/1	0.93	0.31	56,56,56,56	0
57	MG	1A	3800	1/1	0.93	0.09	20,20,20,20	0
57	MG	2A	3618	1/1	0.93	0.07	54,54,54,54	0
57	MG	2A	3063	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
57	MG	2A	3315	1/1	0.93	0.30	59,59,59,59	0
57	MG	2A	3064	1/1	0.93	0.14	59,59,59,59	0
57	MG	1A	3801	1/1	0.93	0.25	74,74,74,74	0
57	MG	1A	3501	1/1	0.93	0.07	46,46,46,46	0
57	MG	2A	3324	1/1	0.93	0.29	61,61,61,61	0
57	MG	2A	3626	1/1	0.93	0.16	66,66,66,66	0
57	MG	2A	3332	1/1	0.93	0.07	49,49,49,49	0
57	MG	1A	3412	1/1	0.93	0.12	51,51,51,51	0
57	MG	2A	3337	1/1	0.93	0.12	61,61,61,61	0
57	MG	1A	3970	1/1	0.93	0.09	52,52,52,52	0
57	MG	1A	3644	1/1	0.93	0.12	38,38,38,38	0
57	MG	1a	1695	1/1	0.93	0.14	64,64,64,64	0
57	MG	1A	3973	1/1	0.93	0.08	56,56,56,56	0
57	MG	1a	1697	1/1	0.93	0.17	59,59,59,59	0
57	MG	1a	1698	1/1	0.93	0.06	65,65,65,65	0
57	MG	2A	3346	1/1	0.93	0.20	43,43,43,43	0
57	MG	1A	3115	1/1	0.93	0.16	42,42,42,42	0
57	MG	1A	3217	1/1	0.93	0.08	46,46,46,46	0
57	MG	2a	1759	1/1	0.93	0.21	56,56,56,56	0
57	MG	1A	3349	1/1	0.93	0.23	49,49,49,49	0
57	MG	1D	312	1/1	0.93	0.14	37,37,37,37	0
57	MG	1A	3981	1/1	0.93	0.10	44,44,44,44	0
57	MG	1A	3352	1/1	0.93	0.15	49,49,49,49	0
57	MG	2A	3095	1/1	0.93	0.39	61,61,61,61	0
57	MG	2a	1765	1/1	0.93	0.46	68,68,68,68	0
57	MG	1A	3515	1/1	0.93	0.10	46,46,46,46	0
57	MG	2A	3360	1/1	0.93	0.41	63,63,63,63	0
57	MG	1E	312	1/1	0.93	0.10	25,25,25,25	0
57	MG	2A	3672	1/1	0.93	0.08	40,40,40,40	0
57	MG	2A	3365	1/1	0.93	0.33	61,61,61,61	0
57	MG	2A	3684	1/1	0.93	0.08	55,55,55,55	0
57	MG	1A	3420	1/1	0.93	0.12	41,41,41,41	0
57	MG	1a	1716	1/1	0.93	0.11	57,57,57,57	0
57	MG	1A	3823	1/1	0.93	0.08	61,61,61,61	0
57	MG	1A	3122	1/1	0.93	0.14	45,45,45,45	0
57	MG	1F	312	1/1	0.93	0.15	56,56,56,56	0
57	MG	2A	3695	1/1	0.93	0.10	62,62,62,62	0
57	MG	1G	202	1/1	0.93	0.17	56,56,56,56	0
57	MG	2A	3697	1/1	0.93	0.06	47,47,47,47	0
57	MG	1A	3999	1/1	0.93	0.07	24,24,24,24	0
57	MG	1A	3224	1/1	0.93	0.10	39,39,39,39	0
57	MG	2A	3704	1/1	0.93	0.08	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1a	1725	1/1	0.93	0.09	52,52,52,52	0
57	MG	1A	3426	1/1	0.93	0.09	60,60,60,60	0
57	MG	2e	201	1/1	0.93	0.08	72,72,72,72	0
57	MG	1A	4003	1/1	0.93	0.11	74,74,74,74	0
57	MG	2f	202	1/1	0.93	0.18	73,73,73,73	0
57	MG	2A	3124	1/1	0.93	0.18	62,62,62,62	0
57	MG	2l	203	1/1	0.93	0.14	56,56,56,56	0
57	MG	2A	3709	1/1	0.93	0.20	64,64,64,64	0
57	MG	1O	202	1/1	0.93	0.19	53,53,53,53	0
57	MG	1A	4004	1/1	0.93	0.07	54,54,54,54	0
57	MG	1A	3131	1/1	0.93	0.09	43,43,43,43	0
57	MG	1a	1736	1/1	0.93	0.30	54,54,54,54	0
57	MG	2A	3129	1/1	0.93	0.11	58,58,58,58	0
57	MG	2A	3138	1/1	0.93	0.11	53,53,53,53	0
57	MG	1A	3295	1/1	0.93	0.15	45,45,45,45	0
57	MG	2A	3718	1/1	0.93	0.10	57,57,57,57	0
57	MG	2A	3144	1/1	0.93	0.12	55,55,55,55	0
57	MG	2A	3393	1/1	0.94	0.12	48,48,48,48	0
57	MG	1A	3369	1/1	0.94	0.21	48,48,48,48	0
57	MG	2A	3140	1/1	0.94	0.37	63,63,63,63	0
57	MG	1R	204	1/1	0.94	0.10	36,36,36,36	0
57	MG	2A	3142	1/1	0.94	0.10	51,51,51,51	0
57	MG	1A	3097	1/1	0.94	0.06	37,37,37,37	0
57	MG	1a	1746	1/1	0.94	0.19	57,57,57,57	0
57	MG	2A	3406	1/1	0.94	0.10	66,66,66,66	0
57	MG	1A	3674	1/1	0.94	0.07	40,40,40,40	0
57	MG	1A	3539	1/1	0.94	0.09	38,38,38,38	0
57	MG	1a	1751	1/1	0.94	0.08	54,54,54,54	0
57	MG	1T	201	1/1	0.94	0.16	56,56,56,56	0
57	MG	2A	3413	1/1	0.94	0.12	58,58,58,58	0
57	MG	2A	3727	1/1	0.94	0.15	58,58,58,58	0
57	MG	1A	3443	1/1	0.94	0.23	52,52,52,52	0
57	MG	2A	3159	1/1	0.94	0.09	54,54,54,54	0
57	MG	2A	3418	1/1	0.94	0.08	43,43,43,43	0
57	MG	1A	4017	1/1	0.94	0.05	23,23,23,23	0
57	MG	2A	3161	1/1	0.94	0.12	55,55,55,55	0
57	MG	1A	4018	1/1	0.94	0.06	33,33,33,33	0
57	MG	1A	3371	1/1	0.94	0.12	50,50,50,50	0
57	MG	2A	3429	1/1	0.94	0.06	48,48,48,48	0
57	MG	1A	3144	1/1	0.94	0.16	46,46,46,46	0
57	MG	2A	3433	1/1	0.94	0.11	56,56,56,56	0
57	MG	1W	202	1/1	0.94	0.10	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
57	MG	1a	1769	1/1	0.94	0.08	57,57,57,57	0
57	MG	1Y	201	1/1	0.94	0.10	47,47,47,47	0
57	MG	2A	3439	1/1	0.94	0.09	51,51,51,51	0
57	MG	1A	3447	1/1	0.94	0.12	38,38,38,38	0
57	MG	1A	3448	1/1	0.94	0.17	62,62,62,62	0
57	MG	2A	3173	1/1	0.94	0.26	68,68,68,68	0
57	MG	2A	3443	1/1	0.94	0.08	41,41,41,41	0
57	MG	1A	3057	1/1	0.94	0.08	45,45,45,45	0
57	MG	1A	3693	1/1	0.94	0.09	22,22,22,22	0
57	MG	2A	3176	1/1	0.94	0.18	42,42,42,42	0
57	MG	1A	3859	1/1	0.94	0.15	43,43,43,43	0
57	MG	1A	4030	1/1	0.94	0.07	61,61,61,61	0
57	MG	2F	301	1/1	0.94	0.11	54,54,54,54	0
57	MG	1A	3861	1/1	0.94	0.14	35,35,35,35	0
57	MG	10	105	1/1	0.94	0.21	63,63,63,63	0
57	MG	1A	3195	1/1	0.94	0.25	52,52,52,52	0
57	MG	2O	201	1/1	0.94	0.13	70,70,70,70	0
57	MG	11	105	1/1	0.94	0.10	68,68,68,68	0
57	MG	2T	202	1/1	0.94	0.17	60,60,60,60	0
57	MG	2W	201	1/1	0.94	0.15	40,40,40,40	0
57	MG	2X	101	1/1	0.94	0.10	51,51,51,51	0
57	MG	12	101	1/1	0.94	0.07	39,39,39,39	0
57	MG	1A	3699	1/1	0.94	0.08	31,31,31,31	0
57	MG	14	101	1/1	0.94	0.13	64,64,64,64	0
57	MG	20	103	1/1	0.94	0.14	64,64,64,64	0
57	MG	1A	3062	1/1	0.94	0.21	48,48,48,48	0
57	MG	1A	3377	1/1	0.94	0.36	58,58,58,58	0
57	MG	1a	1812	1/1	0.94	0.11	62,62,62,62	0
57	MG	15	109	1/1	0.94	0.07	57,57,57,57	0
57	MG	2A	3196	1/1	0.94	0.18	52,52,52,52	0
57	MG	1a	1816	1/1	0.94	0.07	47,47,47,47	0
57	MG	2A	3472	1/1	0.94	0.10	34,34,34,34	0
57	MG	2a	1605	1/1	0.94	0.16	58,58,58,58	0
57	MG	1A	3702	1/1	0.94	0.07	26,26,26,26	0
57	MG	1a	1820	1/1	0.94	0.22	51,51,51,51	0
57	MG	1A	3314	1/1	0.94	0.26	59,59,59,59	0
57	MG	1A	3315	1/1	0.94	0.26	54,54,54,54	0
57	MG	1A	3462	1/1	0.94	0.09	61,61,61,61	0
57	MG	1A	3064	1/1	0.94	0.08	47,47,47,47	0
57	MG	2a	1612	1/1	0.94	0.18	59,59,59,59	0
57	MG	1A	3557	1/1	0.94	0.21	55,55,55,55	0
57	MG	2a	1615	1/1	0.94	0.20	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
57	MG	2A	3483	1/1	0.94	0.12	60,60,60,60	0
57	MG	1A	3711	1/1	0.94	0.10	30,30,30,30	0
57	MG	1A	3880	1/1	0.94	0.18	35,35,35,35	0
57	MG	1A	4052	1/1	0.94	0.12	31,31,31,31	0
57	MG	2A	3487	1/1	0.94	0.07	44,44,44,44	0
57	MG	1d	301	1/1	0.94	0.25	58,58,58,58	0
57	MG	2A	3489	1/1	0.94	0.10	43,43,43,43	0
57	MG	1e	201	1/1	0.94	0.12	67,67,67,67	0
57	MG	1A	3384	1/1	0.94	0.15	37,37,37,37	0
57	MG	1l	201	1/1	0.94	0.08	65,65,65,65	0
57	MG	2A	3495	1/1	0.94	0.09	38,38,38,38	0
57	MG	1l	202	1/1	0.94	0.09	64,64,64,64	0
57	MG	2A	3497	1/1	0.94	0.18	58,58,58,58	0
57	MG	2a	1632	1/1	0.94	0.28	60,60,60,60	0
57	MG	2A	3219	1/1	0.94	0.16	50,50,50,50	0
57	MG	1A	3317	1/1	0.94	0.13	42,42,42,42	0
57	MG	1A	3257	1/1	0.94	0.10	27,27,27,27	0
57	MG	1a	1615	1/1	0.94	0.15	58,58,58,58	0
57	MG	1A	3258	1/1	0.94	0.07	38,38,38,38	0
57	MG	2A	3509	1/1	0.94	0.17	41,41,41,41	0
57	MG	1A	4060	1/1	0.94	0.06	17,17,17,17	0
57	MG	2A	3227	1/1	0.94	0.20	59,59,59,59	0
57	MG	2A	3228	1/1	0.94	0.29	59,59,59,59	0
57	MG	1w	102	1/1	0.94	0.08	53,53,53,53	0
57	MG	1A	3568	1/1	0.94	0.11	34,34,34,34	0
57	MG	1A	4062	1/1	0.94	0.09	40,40,40,40	0
57	MG	1A	3321	1/1	0.94	0.09	35,35,35,35	0
57	MG	2A	3521	1/1	0.94	0.09	45,45,45,45	0
57	MG	1A	3259	1/1	0.94	0.09	48,48,48,48	0
57	MG	1A	3584	1/1	0.94	0.16	44,44,44,44	0
57	MG	1x	104	1/1	0.94	0.24	68,68,68,68	0
57	MG	1A	4066	1/1	0.94	0.14	46,46,46,46	0
57	MG	2A	3528	1/1	0.94	0.16	63,63,63,63	0
57	MG	1a	1631	1/1	0.94	0.24	62,62,62,62	0
57	MG	1x	107	1/1	0.94	0.11	51,51,51,51	0
57	MG	1A	4067	1/1	0.94	0.05	34,34,34,34	0
57	MG	1A	3326	1/1	0.94	0.12	51,51,51,51	0
57	MG	1A	3588	1/1	0.94	0.30	40,40,40,40	0
57	MG	1A	3067	1/1	0.94	0.09	48,48,48,48	0
57	MG	1A	3734	1/1	0.94	0.10	51,51,51,51	0
57	MG	1A	3328	1/1	0.94	0.14	41,41,41,41	0
57	MG	2A	3248	1/1	0.94	0.19	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
57	MG	1A	3206	1/1	0.94	0.07	34,34,34,34	0
57	MG	1A	3744	1/1	0.94	0.10	49,49,49,49	0
57	MG	2a	1667	1/1	0.94	0.17	52,52,52,52	0
57	MG	1A	3745	1/1	0.94	0.07	48,48,48,48	0
57	MG	1a	1644	1/1	0.94	0.09	58,58,58,58	0
57	MG	1A	3078	1/1	0.94	0.16	48,48,48,48	0
57	MG	2A	3002	1/1	0.94	0.26	58,58,58,58	0
57	MG	1A	3333	1/1	0.94	0.10	55,55,55,55	0
57	MG	1a	1648	1/1	0.94	0.13	49,49,49,49	0
57	MG	1a	1649	1/1	0.94	0.13	45,45,45,45	0
57	MG	2A	3006	1/1	0.94	0.22	46,46,46,46	0
57	MG	1A	3601	1/1	0.94	0.15	36,36,36,36	0
57	MG	1a	1652	1/1	0.94	0.09	45,45,45,45	0
57	MG	1a	1655	1/1	0.94	0.16	54,54,54,54	0
57	MG	2A	3010	1/1	0.94	0.18	62,62,62,62	0
57	MG	2a	1682	1/1	0.94	0.17	66,66,66,66	0
57	MG	1A	3749	1/1	0.94	0.07	50,50,50,50	0
57	MG	1A	3166	1/1	0.94	0.20	32,32,32,32	0
57	MG	2A	3023	1/1	0.94	0.27	41,41,41,41	0
57	MG	1A	3058	1/1	0.94	0.19	54,54,54,54	0
57	MG	2A	3027	1/1	0.94	0.08	46,46,46,46	0
57	MG	2a	1690	1/1	0.94	0.24	61,61,61,61	0
57	MG	1a	1660	1/1	0.94	0.14	65,65,65,65	0
57	MG	1A	3928	1/1	0.94	0.16	54,54,54,54	0
57	MG	1A	3170	1/1	0.94	0.10	45,45,45,45	0
57	MG	2A	3276	1/1	0.94	0.13	59,59,59,59	0
57	MG	2A	3567	1/1	0.94	0.07	68,68,68,68	0
57	MG	1A	3218	1/1	0.94	0.20	39,39,39,39	0
57	MG	1A	3413	1/1	0.94	0.13	33,33,33,33	0
57	MG	2A	3281	1/1	0.94	0.11	58,58,58,58	0
57	MG	1A	3765	1/1	0.94	0.07	42,42,42,42	0
57	MG	2a	1700	1/1	0.94	0.21	68,68,68,68	0
57	MG	2a	1701	1/1	0.94	0.06	75,75,75,75	0
57	MG	2A	3037	1/1	0.94	0.21	57,57,57,57	0
57	MG	2A	3287	1/1	0.94	0.23	48,48,48,48	0
57	MG	2A	3578	1/1	0.94	0.07	28,28,28,28	0
57	MG	1A	3613	1/1	0.94	0.08	36,36,36,36	0
57	MG	1a	1671	1/1	0.94	0.26	58,58,58,58	0
57	MG	1A	3934	1/1	0.94	0.08	32,32,32,32	0
57	MG	1B	201	1/1	0.94	0.17	51,51,51,51	0
57	MG	1A	3614	1/1	0.94	0.10	54,54,54,54	0
57	MG	2A	3044	1/1	0.94	0.12	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
57	MG	1A	3768	1/1	0.94	0.08	49,49,49,49	0
57	MG	1a	1677	1/1	0.94	0.13	64,64,64,64	0
57	MG	1A	3618	1/1	0.94	0.08	53,53,53,53	0
57	MG	2A	3593	1/1	0.94	0.05	47,47,47,47	0
57	MG	1A	3340	1/1	0.94	0.08	51,51,51,51	0
57	MG	2A	3595	1/1	0.94	0.10	40,40,40,40	0
57	MG	2A	3596	1/1	0.94	0.17	68,68,68,68	0
57	MG	1A	3620	1/1	0.94	0.09	39,39,39,39	0
57	MG	1A	3273	1/1	0.94	0.19	36,36,36,36	0
57	MG	1A	3087	1/1	0.94	0.14	48,48,48,48	0
57	MG	2A	3054	1/1	0.94	0.16	51,51,51,51	0
57	MG	2a	1725	1/1	0.94	0.28	66,66,66,66	0
57	MG	2A	3604	1/1	0.94	0.11	53,53,53,53	0
57	MG	1A	3181	1/1	0.94	0.15	47,47,47,47	0
57	MG	1A	3289	1/1	0.94	0.10	48,48,48,48	0
57	MG	1B	219	1/1	0.94	0.13	45,45,45,45	0
57	MG	1A	3958	1/1	0.94	0.09	52,52,52,52	0
57	MG	2A	3612	1/1	0.94	0.08	41,41,41,41	0
57	MG	1a	1689	1/1	0.94	0.20	60,60,60,60	0
57	MG	1A	3785	1/1	0.94	0.06	36,36,36,36	0
57	MG	1A	3964	1/1	0.94	0.12	43,43,43,43	0
57	MG	1A	3965	1/1	0.94	0.09	50,50,50,50	0
57	MG	1A	3225	1/1	0.94	0.13	49,49,49,49	0
57	MG	2A	3321	1/1	0.94	0.20	55,55,55,55	0
57	MG	1A	3291	1/1	0.94	0.12	53,53,53,53	0
57	MG	1A	3423	1/1	0.94	0.11	56,56,56,56	0
57	MG	1A	3643	1/1	0.94	0.16	59,59,59,59	0
57	MG	1A	3517	1/1	0.94	0.07	50,50,50,50	0
57	MG	2A	3336	1/1	0.94	0.28	49,49,49,49	0
57	MG	2a	1743	1/1	0.94	0.20	68,68,68,68	0
57	MG	2a	1744	1/1	0.94	0.29	55,55,55,55	0
57	MG	1A	3518	1/1	0.94	0.14	45,45,45,45	0
57	MG	2a	1746	1/1	0.94	0.21	58,58,58,58	0
57	MG	1a	1701	1/1	0.94	0.28	47,47,47,47	0
57	MG	2A	3078	1/1	0.94	0.10	41,41,41,41	0
57	MG	1A	3648	1/1	0.94	0.07	40,40,40,40	0
57	MG	1D	301	1/1	0.94	0.18	28,28,28,28	0
57	MG	2A	3634	1/1	0.94	0.10	39,39,39,39	0
57	MG	1A	3292	1/1	0.94	0.11	60,60,60,60	0
57	MG	2A	3636	1/1	0.94	0.08	51,51,51,51	0
57	MG	1a	1706	1/1	0.94	0.23	58,58,58,58	0
57	MG	2a	1755	1/1	0.94	0.32	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
57	MG	1a	1707	1/1	0.94	0.20	57,57,57,57	0
57	MG	2A	3348	1/1	0.94	0.18	58,58,58,58	0
57	MG	2A	3088	1/1	0.94	0.11	47,47,47,47	0
57	MG	1A	3089	1/1	0.94	0.18	50,50,50,50	0
57	MG	1A	3980	1/1	0.94	0.12	37,37,37,37	0
57	MG	2A	3650	1/1	0.94	0.08	52,52,52,52	0
57	MG	2A	3092	1/1	0.94	0.15	47,47,47,47	0
57	MG	2A	3652	1/1	0.94	0.10	80,80,80,80	0
57	MG	1A	3522	1/1	0.94	0.15	34,34,34,34	0
57	MG	1A	3527	1/1	0.94	0.11	47,47,47,47	0
57	MG	2A	3357	1/1	0.94	0.25	64,64,64,64	0
57	MG	2A	3096	1/1	0.94	0.24	51,51,51,51	0
57	MG	2A	3657	1/1	0.94	0.07	65,65,65,65	0
57	MG	2A	3660	1/1	0.94	0.10	54,54,54,54	0
57	MG	2A	3099	1/1	0.94	0.10	50,50,50,50	0
57	MG	2A	3666	1/1	0.94	0.10	54,54,54,54	0
57	MG	2a	1774	1/1	0.94	0.12	61,61,61,61	0
57	MG	1A	3987	1/1	0.94	0.10	40,40,40,40	0
57	MG	1A	3235	1/1	0.94	0.08	63,63,63,63	0
57	MG	2A	3362	1/1	0.94	0.15	38,38,38,38	0
57	MG	1A	3992	1/1	0.94	0.06	68,68,68,68	0
57	MG	2A	3674	1/1	0.94	0.06	50,50,50,50	0
57	MG	2A	3680	1/1	0.94	0.07	69,69,69,69	0
57	MG	1A	3993	1/1	0.94	0.12	64,64,64,64	0
57	MG	1G	201	1/1	0.94	0.13	39,39,39,39	0
57	MG	1A	3238	1/1	0.94	0.07	42,42,42,42	0
57	MG	1A	3059	1/1	0.94	0.07	31,31,31,31	0
57	MG	1A	3661	1/1	0.94	0.08	41,41,41,41	0
57	MG	1I	201	1/1	0.94	0.12	64,64,64,64	0
57	MG	2d	301	1/1	0.94	0.29	56,56,56,56	0
57	MG	1N	201	1/1	0.94	0.20	51,51,51,51	0
57	MG	1A	3998	1/1	0.94	0.12	36,36,36,36	0
57	MG	1A	3185	1/1	0.94	0.13	39,39,39,39	0
57	MG	2A	3377	1/1	0.94	0.27	56,56,56,56	0
57	MG	2A	3698	1/1	0.94	0.08	41,41,41,41	0
57	MG	2q	201	1/1	0.94	0.21	67,67,67,67	0
57	MG	1A	3004	1/1	0.94	0.08	26,26,26,26	0
57	MG	2r	101	1/1	0.94	0.11	61,61,61,61	0
57	MG	2t	201	1/1	0.94	0.17	45,45,45,45	0
57	MG	2A	3702	1/1	0.94	0.07	44,44,44,44	0
57	MG	1A	3305	1/1	0.94	0.06	29,29,29,29	0
57	MG	1O	205	1/1	0.94	0.11	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
57	MG	1A	3838	1/1	0.94	0.13	43,43,43,43	0
57	MG	2x	105	1/1	0.94	0.15	54,54,54,54	0
57	MG	1A	3841	1/1	0.94	0.12	40,40,40,40	0
57	MG	1A	4007	1/1	0.94	0.08	39,39,39,39	0
57	MG	1A	3842	1/1	0.94	0.11	55,55,55,55	0
57	MG	2A	3133	1/1	0.94	0.10	59,59,59,59	0
57	MG	2A	3135	1/1	0.94	0.10	54,54,54,54	0
57	MG	2A	3403	1/1	0.95	0.13	60,60,60,60	0
57	MG	2A	3143	1/1	0.95	0.09	53,53,53,53	0
57	MG	1A	3017	1/1	0.95	0.14	60,60,60,60	0
57	MG	2A	3145	1/1	0.95	0.10	56,56,56,56	0
57	MG	2A	3146	1/1	0.95	0.18	56,56,56,56	0
57	MG	2A	3147	1/1	0.95	0.09	54,54,54,54	0
57	MG	1A	3332	1/1	0.95	0.14	42,42,42,42	0
57	MG	2A	3150	1/1	0.95	0.16	57,57,57,57	0
57	MG	1A	3879	1/1	0.95	0.07	36,36,36,36	0
57	MG	1A	3198	1/1	0.95	0.12	40,40,40,40	0
57	MG	1a	1770	1/1	0.95	0.14	60,60,60,60	0
57	MG	2A	3155	1/1	0.95	0.08	47,47,47,47	0
57	MG	2A	3420	1/1	0.95	0.10	47,47,47,47	0
57	MG	1A	3881	1/1	0.95	0.06	29,29,29,29	0
57	MG	2A	3425	1/1	0.95	0.11	43,43,43,43	0
57	MG	1a	1772	1/1	0.95	0.18	68,68,68,68	0
57	MG	1A	3882	1/1	0.95	0.14	34,34,34,34	0
57	MG	1A	3381	1/1	0.95	0.09	49,49,49,49	0
57	MG	2B	208	1/1	0.95	0.18	62,62,62,62	0
57	MG	1A	3334	1/1	0.95	0.15	51,51,51,51	0
57	MG	1A	4047	1/1	0.95	0.06	27,27,27,27	0
57	MG	2A	3163	1/1	0.95	0.18	56,56,56,56	0
57	MG	1a	1780	1/1	0.95	0.08	60,60,60,60	0
57	MG	1l	102	1/1	0.95	0.08	49,49,49,49	0
57	MG	1a	1783	1/1	0.95	0.07	71,71,71,71	0
57	MG	1A	3101	1/1	0.95	0.07	33,33,33,33	0
57	MG	1A	3103	1/1	0.95	0.12	46,46,46,46	0
57	MG	1A	3740	1/1	0.95	0.09	44,44,44,44	0
57	MG	1A	4051	1/1	0.95	0.12	28,28,28,28	0
57	MG	2D	302	1/1	0.95	0.15	44,44,44,44	0
57	MG	2D	304	1/1	0.95	0.22	62,62,62,62	0
57	MG	1A	3743	1/1	0.95	0.09	62,62,62,62	0
57	MG	1A	3337	1/1	0.95	0.18	43,43,43,43	0
57	MG	2E	303	1/1	0.95	0.10	43,43,43,43	0
57	MG	2E	304	1/1	0.95	0.23	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
57	MG	1A	3621	1/1	0.95	0.11	38,38,38,38	0
57	MG	1a	1795	1/1	0.95	0.09	74,74,74,74	0
57	MG	1A	3525	1/1	0.95	0.12	49,49,49,49	0
57	MG	17	105	1/1	0.95	0.12	54,54,54,54	0
57	MG	1a	1799	1/1	0.95	0.08	55,55,55,55	0
57	MG	18	3401	1/1	0.95	0.16	54,54,54,54	0
57	MG	1a	1804	1/1	0.95	0.07	67,67,67,67	0
57	MG	18	3402	1/1	0.95	0.12	37,37,37,37	0
57	MG	2R	201	1/1	0.95	0.09	54,54,54,54	0
57	MG	1A	3623	1/1	0.95	0.07	42,42,42,42	0
57	MG	2A	3186	1/1	0.95	0.12	40,40,40,40	0
57	MG	1A	3171	1/1	0.95	0.27	41,41,41,41	0
57	MG	19	101	1/1	0.95	0.13	44,44,44,44	0
57	MG	2A	3189	1/1	0.95	0.16	43,43,43,43	0
57	MG	2A	3467	1/1	0.95	0.08	40,40,40,40	0
57	MG	1A	3252	1/1	0.95	0.07	53,53,53,53	0
57	MG	21	101	1/1	0.95	0.19	52,52,52,52	0
57	MG	1a	1821	1/1	0.95	0.08	58,58,58,58	0
57	MG	1A	3904	1/1	0.95	0.10	48,48,48,48	0
57	MG	2A	3194	1/1	0.95	0.09	52,52,52,52	0
57	MG	27	102	1/1	0.95	0.07	46,46,46,46	0
57	MG	27	103	1/1	0.95	0.07	40,40,40,40	0
57	MG	1A	3750	1/1	0.95	0.06	52,52,52,52	0
57	MG	2a	1601	1/1	0.95	0.15	53,53,53,53	0
57	MG	2A	3474	1/1	0.95	0.12	56,56,56,56	0
57	MG	1A	3176	1/1	0.95	0.10	35,35,35,35	0
57	MG	1A	3451	1/1	0.95	0.14	44,44,44,44	0
57	MG	1A	3633	1/1	0.95	0.13	42,42,42,42	0
57	MG	1A	3396	1/1	0.95	0.38	46,46,46,46	0
57	MG	1A	3760	1/1	0.95	0.10	36,36,36,36	0
57	MG	1A	4070	1/1	0.95	0.07	48,48,48,48	0
57	MG	1a	1614	1/1	0.95	0.29	54,54,54,54	0
57	MG	1A	3055	1/1	0.95	0.20	50,50,50,50	0
57	MG	1e	202	1/1	0.95	0.15	55,55,55,55	0
57	MG	2A	3206	1/1	0.95	0.06	44,44,44,44	0
57	MG	1A	4072	1/1	0.95	0.10	15,15,15,15	0
57	MG	1a	1618	1/1	0.95	0.07	48,48,48,48	0
57	MG	1a	1620	1/1	0.95	0.10	54,54,54,54	0
57	MG	1A	3920	1/1	0.95	0.12	32,32,32,32	0
57	MG	2A	3213	1/1	0.95	0.12	57,57,57,57	0
57	MG	2A	3492	1/1	0.95	0.12	56,56,56,56	0
57	MG	1n	101	1/1	0.95	0.30	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3494	1/1	0.95	0.07	39,39,39,39	0
57	MG	1n	102	1/1	0.95	0.15	55,55,55,55	0
57	MG	1A	4075	1/1	0.95	0.10	23,23,23,23	0
57	MG	2a	1624	1/1	0.95	0.13	59,59,59,59	0
57	MG	1a	1624	1/1	0.95	0.16	64,64,64,64	0
57	MG	1A	3456	1/1	0.95	0.18	54,54,54,54	0
57	MG	2a	1627	1/1	0.95	0.11	59,59,59,59	0
57	MG	2a	1628	1/1	0.95	0.08	83,83,83,83	0
57	MG	2A	3221	1/1	0.95	0.18	47,47,47,47	0
57	MG	1a	1626	1/1	0.95	0.17	52,52,52,52	0
57	MG	2A	3502	1/1	0.95	0.10	37,37,37,37	0
57	MG	2A	3503	1/1	0.95	0.08	50,50,50,50	0
57	MG	2A	3504	1/1	0.95	0.21	59,59,59,59	0
57	MG	1A	3343	1/1	0.95	0.09	59,59,59,59	0
57	MG	1A	3925	1/1	0.95	0.07	35,35,35,35	0
57	MG	1A	4083	1/1	0.95	0.12	43,43,43,43	0
57	MG	2A	3510	1/1	0.95	0.11	39,39,39,39	0
57	MG	1A	3537	1/1	0.95	0.09	48,48,48,48	0
57	MG	1x	101	1/1	0.95	0.08	47,47,47,47	0
57	MG	1A	3143	1/1	0.95	0.10	55,55,55,55	0
57	MG	2a	1641	1/1	0.95	0.19	63,63,63,63	0
57	MG	2A	3229	1/1	0.95	0.10	60,60,60,60	0
57	MG	1A	4089	1/1	0.95	0.10	53,53,53,53	0
57	MG	1A	3345	1/1	0.95	0.18	51,51,51,51	0
57	MG	1A	3306	1/1	0.95	0.15	44,44,44,44	0
57	MG	2A	3520	1/1	0.95	0.15	44,44,44,44	0
57	MG	1A	3463	1/1	0.95	0.06	45,45,45,45	0
57	MG	1A	3774	1/1	0.95	0.07	28,28,28,28	0
57	MG	1a	1639	1/1	0.95	0.18	43,43,43,43	0
57	MG	1A	3216	1/1	0.95	0.21	40,40,40,40	0
57	MG	1A	3406	1/1	0.95	0.11	51,51,51,51	0
57	MG	1A	3656	1/1	0.95	0.07	30,30,30,30	0
57	MG	1A	3779	1/1	0.95	0.11	26,26,26,26	0
57	MG	2A	3241	1/1	0.95	0.07	49,49,49,49	0
57	MG	1A	3939	1/1	0.95	0.08	36,36,36,36	0
57	MG	1x	115	1/1	0.95	0.09	68,68,68,68	0
57	MG	1A	3407	1/1	0.95	0.09	45,45,45,45	0
57	MG	1A	3470	1/1	0.95	0.10	37,37,37,37	0
57	MG	1A	4103	1/1	0.95	0.11	48,48,48,48	0
57	MG	1A	3786	1/1	0.95	0.08	61,61,61,61	0
57	MG	1a	1650	1/1	0.95	0.07	64,64,64,64	0
57	MG	2a	1664	1/1	0.95	0.14	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3790	1/1	0.95	0.06	29,29,29,29	0
57	MG	1A	3792	1/1	0.95	0.14	53,53,53,53	0
57	MG	1A	3024	1/1	0.95	0.13	45,45,45,45	0
57	MG	1A	3028	1/1	0.95	0.11	39,39,39,39	0
57	MG	2a	1669	1/1	0.95	0.16	52,52,52,52	0
57	MG	1A	3665	1/1	0.95	0.09	36,36,36,36	0
57	MG	1A	3220	1/1	0.95	0.07	40,40,40,40	0
57	MG	1B	207	1/1	0.95	0.17	62,62,62,62	0
57	MG	2a	1673	1/1	0.95	0.23	57,57,57,57	0
57	MG	1a	1661	1/1	0.95	0.07	50,50,50,50	0
57	MG	2A	3258	1/1	0.95	0.15	53,53,53,53	0
57	MG	1a	1662	1/1	0.95	0.12	63,63,63,63	0
57	MG	1A	3962	1/1	0.95	0.08	80,80,80,80	0
57	MG	1A	3802	1/1	0.95	0.11	58,58,58,58	0
57	MG	1A	3667	1/1	0.95	0.11	48,48,48,48	0
57	MG	1a	1666	1/1	0.95	0.23	65,65,65,65	0
57	MG	1A	3669	1/1	0.95	0.06	31,31,31,31	0
57	MG	1a	1668	1/1	0.95	0.07	57,57,57,57	0
57	MG	2a	1683	1/1	0.95	0.30	64,64,64,64	0
57	MG	1A	3221	1/1	0.95	0.09	45,45,45,45	0
57	MG	1A	3152	1/1	0.95	0.14	40,40,40,40	0
57	MG	2A	3032	1/1	0.95	0.04	33,33,33,33	0
57	MG	1A	3969	1/1	0.95	0.07	41,41,41,41	0
57	MG	2A	3272	1/1	0.95	0.13	61,61,61,61	0
57	MG	1A	3051	1/1	0.95	0.10	42,42,42,42	0
57	MG	1A	3162	1/1	0.95	0.27	33,33,33,33	0
57	MG	1A	3482	1/1	0.95	0.10	53,53,53,53	0
57	MG	1A	3416	1/1	0.95	0.06	43,43,43,43	0
57	MG	1A	3226	1/1	0.95	0.07	37,37,37,37	0
57	MG	1A	3488	1/1	0.95	0.17	38,38,38,38	0
57	MG	1A	3978	1/1	0.95	0.06	40,40,40,40	0
57	MG	2A	3573	1/1	0.95	0.10	57,57,57,57	0
57	MG	2A	3282	1/1	0.95	0.12	51,51,51,51	0
57	MG	2A	3283	1/1	0.95	0.19	43,43,43,43	0
57	MG	2A	3042	1/1	0.95	0.08	54,54,54,54	0
57	MG	1B	231	1/1	0.95	0.12	54,54,54,54	0
57	MG	1A	3824	1/1	0.95	0.15	55,55,55,55	0
57	MG	1A	3825	1/1	0.95	0.12	56,56,56,56	0
57	MG	1A	3982	1/1	0.95	0.12	57,57,57,57	0
57	MG	2A	3585	1/1	0.95	0.10	30,30,30,30	0
57	MG	1A	3984	1/1	0.95	0.08	56,56,56,56	0
57	MG	2A	3587	1/1	0.95	0.07	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1D	302	1/1	0.95	0.17	43,43,43,43	0
57	MG	2A	3292	1/1	0.95	0.25	49,49,49,49	0
57	MG	1D	311	1/1	0.95	0.10	52,52,52,52	0
57	MG	2A	3295	1/1	0.95	0.13	36,36,36,36	0
57	MG	1a	1688	1/1	0.95	0.12	64,64,64,64	0
57	MG	1A	3985	1/1	0.95	0.06	62,62,62,62	0
57	MG	2A	3298	1/1	0.95	0.38	58,58,58,58	0
57	MG	1A	3687	1/1	0.95	0.09	27,27,27,27	0
57	MG	1A	3230	1/1	0.95	0.08	40,40,40,40	0
57	MG	1E	306	1/1	0.95	0.12	29,29,29,29	0
57	MG	1A	3366	1/1	0.95	0.13	49,49,49,49	0
57	MG	1E	309	1/1	0.95	0.16	53,53,53,53	0
57	MG	1E	310	1/1	0.95	0.24	69,69,69,69	0
57	MG	2A	3305	1/1	0.95	0.35	67,67,67,67	0
57	MG	1E	311	1/1	0.95	0.09	38,38,38,38	0
57	MG	1A	3835	1/1	0.95	0.08	38,38,38,38	0
57	MG	1A	3492	1/1	0.95	0.12	36,36,36,36	0
57	MG	1A	3319	1/1	0.95	0.11	51,51,51,51	0
57	MG	2A	3066	1/1	0.95	0.09	51,51,51,51	0
57	MG	2A	3068	1/1	0.95	0.10	29,29,29,29	0
57	MG	1F	304	1/1	0.95	0.07	31,31,31,31	0
57	MG	1A	3694	1/1	0.95	0.06	36,36,36,36	0
57	MG	1F	309	1/1	0.95	0.12	40,40,40,40	0
57	MG	1A	3575	1/1	0.95	0.11	46,46,46,46	0
57	MG	2A	3620	1/1	0.95	0.08	43,43,43,43	0
57	MG	2A	3319	1/1	0.95	0.23	56,56,56,56	0
57	MG	1A	3579	1/1	0.95	0.13	59,59,59,59	0
57	MG	1A	3580	1/1	0.95	0.29	40,40,40,40	0
57	MG	1A	4000	1/1	0.95	0.08	28,28,28,28	0
57	MG	1A	3582	1/1	0.95	0.29	39,39,39,39	0
57	MG	2A	3334	1/1	0.95	0.23	55,55,55,55	0
57	MG	2A	3081	1/1	0.95	0.05	34,34,34,34	0
57	MG	1a	1711	1/1	0.95	0.21	57,57,57,57	0
57	MG	1G	205	1/1	0.95	0.07	53,53,53,53	0
57	MG	2A	3338	1/1	0.95	0.10	54,54,54,54	0
57	MG	2A	3633	1/1	0.95	0.05	34,34,34,34	0
57	MG	1a	1713	1/1	0.95	0.30	57,57,57,57	0
57	MG	1A	3189	1/1	0.95	0.07	30,30,30,30	0
57	MG	1A	3119	1/1	0.95	0.10	40,40,40,40	0
57	MG	1N	202	1/1	0.95	0.06	46,46,46,46	0
57	MG	1A	3849	1/1	0.95	0.07	37,37,37,37	0
57	MG	2A	3639	1/1	0.95	0.11	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
57	MG	1A	3704	1/1	0.95	0.09	21,21,21,21	0
57	MG	2A	3642	1/1	0.95	0.08	50,50,50,50	0
57	MG	2A	3345	1/1	0.95	0.25	54,54,54,54	0
57	MG	1A	3276	1/1	0.95	0.06	40,40,40,40	0
57	MG	2a	1757	1/1	0.95	0.11	59,59,59,59	0
57	MG	2A	3647	1/1	0.95	0.09	53,53,53,53	0
57	MG	1O	203	1/1	0.95	0.15	55,55,55,55	0
57	MG	2A	3649	1/1	0.95	0.06	53,53,53,53	0
57	MG	2A	3349	1/1	0.95	0.13	53,53,53,53	0
57	MG	1A	3236	1/1	0.95	0.15	27,27,27,27	0
57	MG	2A	3098	1/1	0.95	0.10	46,46,46,46	0
57	MG	1A	3288	1/1	0.95	0.20	46,46,46,46	0
57	MG	2A	3353	1/1	0.95	0.33	61,61,61,61	0
57	MG	1A	3502	1/1	0.95	0.08	60,60,60,60	0
57	MG	1A	3595	1/1	0.95	0.14	39,39,39,39	0
57	MG	2A	3102	1/1	0.95	0.06	55,55,55,55	0
57	MG	1A	4013	1/1	0.95	0.11	53,53,53,53	0
57	MG	1Q	204	1/1	0.95	0.11	54,54,54,54	0
57	MG	2A	3665	1/1	0.95	0.10	45,45,45,45	0
57	MG	2a	1772	1/1	0.95	0.15	57,57,57,57	0
57	MG	2A	3105	1/1	0.95	0.07	48,48,48,48	0
57	MG	2A	3106	1/1	0.95	0.10	50,50,50,50	0
57	MG	1a	1731	1/1	0.95	0.17	47,47,47,47	0
57	MG	2A	3108	1/1	0.95	0.07	43,43,43,43	0
57	MG	1A	3504	1/1	0.95	0.11	32,32,32,32	0
57	MG	1A	3713	1/1	0.95	0.05	14,14,14,14	0
57	MG	1A	3715	1/1	0.95	0.05	25,25,25,25	0
57	MG	1A	3506	1/1	0.95	0.09	41,41,41,41	0
57	MG	2A	3683	1/1	0.95	0.09	47,47,47,47	0
57	MG	2A	3118	1/1	0.95	0.14	39,39,39,39	0
57	MG	1A	3865	1/1	0.95	0.08	17,17,17,17	0
57	MG	1A	3718	1/1	0.95	0.10	36,36,36,36	0
57	MG	1A	3042	1/1	0.95	0.21	30,30,30,30	0
57	MG	1A	4026	1/1	0.95	0.07	42,42,42,42	0
57	MG	1A	3602	1/1	0.95	0.14	37,37,37,37	0
57	MG	1U	203	1/1	0.95	0.14	28,28,28,28	0
57	MG	1a	1747	1/1	0.95	0.17	57,57,57,57	0
57	MG	2A	3379	1/1	0.95	0.15	38,38,38,38	0
57	MG	1A	3721	1/1	0.95	0.06	45,45,45,45	0
57	MG	1V	202	1/1	0.95	0.29	38,38,38,38	0
57	MG	1A	3871	1/1	0.95	0.05	35,35,35,35	0
57	MG	2A	3130	1/1	0.95	0.15	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
57	MG	2A	3132	1/1	0.95	0.11	53,53,53,53	0
57	MG	1A	3434	1/1	0.95	0.28	52,52,52,52	0
57	MG	2A	3134	1/1	0.95	0.10	59,59,59,59	0
57	MG	2A	3389	1/1	0.95	0.06	24,24,24,24	0
57	MG	2x	101	1/1	0.95	0.15	48,48,48,48	0
57	MG	1A	3606	1/1	0.95	0.20	51,51,51,51	0
57	MG	2A	3137	1/1	0.95	0.15	58,58,58,58	0
57	MG	1a	1756	1/1	0.95	0.11	56,56,56,56	0
57	MG	2A	3139	1/1	0.95	0.09	37,37,37,37	0
57	MG	1a	1757	1/1	0.95	0.09	73,73,73,73	0
57	MG	1X	101	1/1	0.95	0.31	38,38,38,38	0
57	MG	1A	3130	1/1	0.95	0.13	74,74,74,74	0
57	MG	2A	3401	1/1	0.95	0.08	44,44,44,44	0
57	MG	1B	218	1/1	0.96	0.11	60,60,60,60	0
57	MG	1A	3102	1/1	0.96	0.25	42,42,42,42	0
57	MG	1B	220	1/1	0.96	0.09	50,50,50,50	0
57	MG	1A	3081	1/1	0.96	0.15	41,41,41,41	0
57	MG	1A	3658	1/1	0.96	0.05	31,31,31,31	0
57	MG	1A	3082	1/1	0.96	0.20	42,42,42,42	0
57	MG	1A	3322	1/1	0.96	0.13	29,29,29,29	0
57	MG	2A	3471	1/1	0.96	0.11	57,57,57,57	0
57	MG	1A	3805	1/1	0.96	0.05	19,19,19,19	0
57	MG	1A	3083	1/1	0.96	0.19	38,38,38,38	0
57	MG	2D	301	1/1	0.96	0.14	55,55,55,55	0
57	MG	1A	3112	1/1	0.96	0.09	33,33,33,33	0
57	MG	1A	3047	1/1	0.96	0.11	28,28,28,28	0
57	MG	2D	306	1/1	0.96	0.31	42,42,42,42	0
57	MG	1A	3544	1/1	0.96	0.24	45,45,45,45	0
57	MG	1A	3668	1/1	0.96	0.10	36,36,36,36	0
57	MG	1A	3002	1/1	0.96	0.07	50,50,50,50	0
57	MG	1A	3546	1/1	0.96	0.20	41,41,41,41	0
57	MG	2A	3011	1/1	0.96	0.05	44,44,44,44	0
57	MG	2A	3234	1/1	0.96	0.08	61,61,61,61	0
57	MG	2A	3015	1/1	0.96	0.11	46,46,46,46	0
57	MG	1B	236	1/1	0.96	0.07	40,40,40,40	0
57	MG	2F	304	1/1	0.96	0.24	47,47,47,47	0
57	MG	2F	305	1/1	0.96	0.28	47,47,47,47	0
57	MG	2A	3017	1/1	0.96	0.15	56,56,56,56	0
57	MG	2A	3018	1/1	0.96	0.07	41,41,41,41	0
57	MG	2N	201	1/1	0.96	0.09	57,57,57,57	0
57	MG	1A	3329	1/1	0.96	0.17	53,53,53,53	0
57	MG	2A	3022	1/1	0.96	0.07	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
57	MG	1A	3461	1/1	0.96	0.06	38,38,38,38	0
57	MG	2T	201	1/1	0.96	0.07	53,53,53,53	0
57	MG	2A	3024	1/1	0.96	0.07	40,40,40,40	0
57	MG	2T	203	1/1	0.96	0.10	48,48,48,48	0
57	MG	1D	305	1/1	0.96	0.08	35,35,35,35	0
57	MG	1D	308	1/1	0.96	0.07	48,48,48,48	0
57	MG	2Y	201	1/1	0.96	0.15	44,44,44,44	0
57	MG	1A	3167	1/1	0.96	0.07	39,39,39,39	0
57	MG	1A	3270	1/1	0.96	0.09	35,35,35,35	0
57	MG	1A	3826	1/1	0.96	0.06	31,31,31,31	0
57	MG	1A	3551	1/1	0.96	0.07	17,17,17,17	0
57	MG	1A	3464	1/1	0.96	0.21	48,48,48,48	0
57	MG	23	102	1/1	0.96	0.07	59,59,59,59	0
57	MG	1A	3466	1/1	0.96	0.21	49,49,49,49	0
57	MG	25	102	1/1	0.96	0.20	45,45,45,45	0
57	MG	2A	3500	1/1	0.96	0.09	38,38,38,38	0
57	MG	1A	3990	1/1	0.96	0.06	59,59,59,59	0
57	MG	1A	3831	1/1	0.96	0.04	24,24,24,24	0
57	MG	1A	3832	1/1	0.96	0.07	27,27,27,27	0
57	MG	28	101	1/1	0.96	0.07	46,46,46,46	0
57	MG	1A	3833	1/1	0.96	0.08	31,31,31,31	0
57	MG	28	103	1/1	0.96	0.09	75,75,75,75	0
57	MG	2A	3505	1/1	0.96	0.09	35,35,35,35	0
57	MG	1A	3995	1/1	0.96	0.09	44,44,44,44	0
57	MG	1A	3834	1/1	0.96	0.07	40,40,40,40	0
57	MG	2A	3508	1/1	0.96	0.06	41,41,41,41	0
57	MG	1A	3684	1/1	0.96	0.05	20,20,20,20	0
57	MG	1A	3685	1/1	0.96	0.08	21,21,21,21	0
57	MG	2A	3511	1/1	0.96	0.09	55,55,55,55	0
57	MG	1A	3394	1/1	0.96	0.19	24,24,24,24	0
57	MG	1F	310	1/1	0.96	0.12	30,30,30,30	0
57	MG	1A	3840	1/1	0.96	0.09	55,55,55,55	0
57	MG	2A	3515	1/1	0.96	0.07	47,47,47,47	0
57	MG	1A	3271	1/1	0.96	0.21	42,42,42,42	0
57	MG	1A	3690	1/1	0.96	0.08	56,56,56,56	0
57	MG	2a	1614	1/1	0.96	0.10	56,56,56,56	0
57	MG	1A	3556	1/1	0.96	0.07	52,52,52,52	0
57	MG	1A	3117	1/1	0.96	0.07	28,28,28,28	0
57	MG	1A	3088	1/1	0.96	0.11	34,34,34,34	0
57	MG	1a	1700	1/1	0.96	0.18	45,45,45,45	0
57	MG	2A	3270	1/1	0.96	0.19	49,49,49,49	0
57	MG	1A	3120	1/1	0.96	0.17	42,42,42,42	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3056	1/1	0.96	0.06	47,47,47,47	0
57	MG	1A	3399	1/1	0.96	0.08	51,51,51,51	0
57	MG	2A	3526	1/1	0.96	0.12	49,49,49,49	0
57	MG	2A	3527	1/1	0.96	0.14	51,51,51,51	0
57	MG	1A	3698	1/1	0.96	0.06	22,22,22,22	0
57	MG	1N	204	1/1	0.96	0.12	51,51,51,51	0
57	MG	1a	1705	1/1	0.96	0.24	49,49,49,49	0
57	MG	2A	3277	1/1	0.96	0.16	61,61,61,61	0
57	MG	1A	3475	1/1	0.96	0.06	47,47,47,47	0
57	MG	2A	3279	1/1	0.96	0.21	68,68,68,68	0
57	MG	1N	206	1/1	0.96	0.06	30,30,30,30	0
57	MG	1A	3563	1/1	0.96	0.16	34,34,34,34	0
57	MG	2A	3536	1/1	0.96	0.07	33,33,33,33	0
57	MG	1A	3853	1/1	0.96	0.05	55,55,55,55	0
57	MG	1A	3172	1/1	0.96	0.09	38,38,38,38	0
57	MG	2A	3284	1/1	0.96	0.17	52,52,52,52	0
57	MG	1A	4015	1/1	0.96	0.06	59,59,59,59	0
57	MG	1A	3571	1/1	0.96	0.05	28,28,28,28	0
57	MG	1A	3477	1/1	0.96	0.12	51,51,51,51	0
57	MG	1P	203	1/1	0.96	0.14	33,33,33,33	0
57	MG	1A	3281	1/1	0.96	0.15	28,28,28,28	0
57	MG	1A	3858	1/1	0.96	0.09	52,52,52,52	0
57	MG	1A	4022	1/1	0.96	0.04	30,30,30,30	0
57	MG	1A	3010	1/1	0.96	0.06	39,39,39,39	0
57	MG	1Q	206	1/1	0.96	0.10	34,34,34,34	0
57	MG	2A	3294	1/1	0.96	0.23	51,51,51,51	0
57	MG	1A	3179	1/1	0.96	0.12	34,34,34,34	0
57	MG	1R	203	1/1	0.96	0.13	42,42,42,42	0
57	MG	1A	3862	1/1	0.96	0.16	56,56,56,56	0
57	MG	1A	3227	1/1	0.96	0.21	36,36,36,36	0
57	MG	2A	3557	1/1	0.96	0.06	51,51,51,51	0
57	MG	1A	3709	1/1	0.96	0.07	23,23,23,23	0
57	MG	1A	3341	1/1	0.96	0.11	52,52,52,52	0
57	MG	1A	3866	1/1	0.96	0.10	34,34,34,34	0
57	MG	2A	3090	1/1	0.96	0.10	51,51,51,51	0
57	MG	1A	3228	1/1	0.96	0.23	24,24,24,24	0
57	MG	1A	3129	1/1	0.96	0.10	31,31,31,31	0
57	MG	2A	3093	1/1	0.96	0.23	57,57,57,57	0
57	MG	1A	3487	1/1	0.96	0.12	39,39,39,39	0
57	MG	1U	205	1/1	0.96	0.11	30,30,30,30	0
57	MG	1a	1737	1/1	0.96	0.20	44,44,44,44	0
57	MG	2A	3310	1/1	0.96	0.25	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3097	1/1	0.96	0.17	62,62,62,62	0
57	MG	1a	1738	1/1	0.96	0.26	62,62,62,62	0
57	MG	1A	3714	1/1	0.96	0.10	42,42,42,42	0
57	MG	1a	1740	1/1	0.96	0.21	57,57,57,57	0
57	MG	1A	3231	1/1	0.96	0.08	48,48,48,48	0
57	MG	2A	3576	1/1	0.96	0.07	70,70,70,70	0
57	MG	2A	3577	1/1	0.96	0.12	55,55,55,55	0
57	MG	1A	3091	1/1	0.96	0.15	25,25,25,25	0
57	MG	2A	3317	1/1	0.96	0.07	53,53,53,53	0
57	MG	1V	206	1/1	0.96	0.07	48,48,48,48	0
57	MG	1A	3346	1/1	0.96	0.15	41,41,41,41	0
57	MG	2A	3320	1/1	0.96	0.26	55,55,55,55	0
57	MG	1A	4043	1/1	0.96	0.06	42,42,42,42	0
57	MG	1W	204	1/1	0.96	0.08	35,35,35,35	0
57	MG	1W	206	1/1	0.96	0.07	34,34,34,34	0
57	MG	2A	3325	1/1	0.96	0.10	54,54,54,54	0
57	MG	2A	3326	1/1	0.96	0.09	65,65,65,65	0
57	MG	2A	3329	1/1	0.96	0.17	58,58,58,58	0
57	MG	1A	3875	1/1	0.96	0.06	24,24,24,24	0
57	MG	2A	3333	1/1	0.96	0.08	62,62,62,62	0
57	MG	1A	3491	1/1	0.96	0.22	57,57,57,57	0
57	MG	1A	3234	1/1	0.96	0.21	42,42,42,42	0
57	MG	2A	3113	1/1	0.96	0.07	42,42,42,42	0
57	MG	2a	1688	1/1	0.96	0.20	62,62,62,62	0
57	MG	1A	3013	1/1	0.96	0.17	30,30,30,30	0
57	MG	2A	3600	1/1	0.96	0.10	57,57,57,57	0
57	MG	1A	3019	1/1	0.96	0.19	43,43,43,43	0
57	MG	2A	3117	1/1	0.96	0.26	52,52,52,52	0
57	MG	1A	3351	1/1	0.96	0.09	40,40,40,40	0
57	MG	1A	3418	1/1	0.96	0.08	33,33,33,33	0
57	MG	1A	3725	1/1	0.96	0.04	16,16,16,16	0
57	MG	1A	3184	1/1	0.96	0.08	36,36,36,36	0
57	MG	1A	3500	1/1	0.96	0.15	49,49,49,49	0
57	MG	2A	3608	1/1	0.96	0.09	53,53,53,53	0
57	MG	1A	3302	1/1	0.96	0.31	54,54,54,54	0
57	MG	2A	3610	1/1	0.96	0.09	62,62,62,62	0
57	MG	2A	3611	1/1	0.96	0.14	55,55,55,55	0
57	MG	1a	1764	1/1	0.96	0.11	54,54,54,54	0
57	MG	2A	3347	1/1	0.96	0.17	39,39,39,39	0
57	MG	1a	1766	1/1	0.96	0.10	50,50,50,50	0
57	MG	1A	4056	1/1	0.96	0.07	44,44,44,44	0
57	MG	1l	103	1/1	0.96	0.09	39,39,39,39	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3356	1/1	0.96	0.07	46,46,46,46	0
57	MG	2a	1708	1/1	0.96	0.24	60,60,60,60	0
57	MG	1A	3303	1/1	0.96	0.16	38,38,38,38	0
57	MG	12	102	1/1	0.96	0.19	43,43,43,43	0
57	MG	13	102	1/1	0.96	0.06	47,47,47,47	0
57	MG	1A	3612	1/1	0.96	0.08	24,24,24,24	0
57	MG	13	104	1/1	0.96	0.07	51,51,51,51	0
57	MG	2A	3136	1/1	0.96	0.12	49,49,49,49	0
57	MG	1A	3095	1/1	0.96	0.04	32,32,32,32	0
57	MG	15	102	1/1	0.96	0.10	35,35,35,35	0
57	MG	15	104	1/1	0.96	0.24	28,28,28,28	0
57	MG	1A	3425	1/1	0.96	0.07	40,40,40,40	0
57	MG	15	107	1/1	0.96	0.09	31,31,31,31	0
57	MG	2A	3363	1/1	0.96	0.19	57,57,57,57	0
57	MG	1A	3896	1/1	0.96	0.09	44,44,44,44	0
57	MG	2a	1723	1/1	0.96	0.25	61,61,61,61	0
57	MG	1A	3615	1/1	0.96	0.08	25,25,25,25	0
57	MG	1A	3617	1/1	0.96	0.10	22,22,22,22	0
57	MG	1A	3136	1/1	0.96	0.11	28,28,28,28	0
57	MG	1a	1789	1/1	0.96	0.05	55,55,55,55	0
57	MG	1A	3360	1/1	0.96	0.09	33,33,33,33	0
57	MG	1A	3043	1/1	0.96	0.12	34,34,34,34	0
57	MG	1a	1794	1/1	0.96	0.06	56,56,56,56	0
57	MG	18	3404	1/1	0.96	0.12	42,42,42,42	0
57	MG	1A	4069	1/1	0.96	0.05	39,39,39,39	0
57	MG	2A	3644	1/1	0.96	0.04	54,54,54,54	0
57	MG	1A	3513	1/1	0.96	0.15	46,46,46,46	0
57	MG	1A	3432	1/1	0.96	0.07	39,39,39,39	0
57	MG	1A	3362	1/1	0.96	0.09	51,51,51,51	0
57	MG	2A	3380	1/1	0.96	0.07	54,54,54,54	0
57	MG	2A	3381	1/1	0.96	0.08	60,60,60,60	0
57	MG	1a	1801	1/1	0.96	0.07	51,51,51,51	0
57	MG	1A	3911	1/1	0.96	0.09	46,46,46,46	0
57	MG	1a	1809	1/1	0.96	0.06	63,63,63,63	0
57	MG	1A	3913	1/1	0.96	0.12	36,36,36,36	0
57	MG	1a	1604	1/1	0.96	0.16	54,54,54,54	0
57	MG	1A	4076	1/1	0.96	0.10	41,41,41,41	0
57	MG	1A	4078	1/1	0.96	0.05	28,28,28,28	0
57	MG	1a	1819	1/1	0.96	0.06	56,56,56,56	0
57	MG	1A	4079	1/1	0.96	0.15	55,55,55,55	0
57	MG	2A	3663	1/1	0.96	0.07	58,58,58,58	0
57	MG	2A	3392	1/1	0.96	0.07	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
57	MG	1A	3625	1/1	0.96	0.05	37,37,37,37	0
57	MG	1a	1611	1/1	0.96	0.11	28,28,28,28	0
57	MG	2A	3169	1/1	0.96	0.13	62,62,62,62	0
57	MG	2A	3670	1/1	0.96	0.06	38,38,38,38	0
57	MG	1A	3516	1/1	0.96	0.15	35,35,35,35	0
57	MG	1a	1825	1/1	0.96	0.09	49,49,49,49	0
57	MG	2A	3673	1/1	0.96	0.05	55,55,55,55	0
57	MG	2A	3172	1/1	0.96	0.07	51,51,51,51	0
57	MG	2A	3675	1/1	0.96	0.06	37,37,37,37	0
57	MG	1A	3755	1/1	0.96	0.06	17,17,17,17	0
57	MG	1A	3628	1/1	0.96	0.14	32,32,32,32	0
57	MG	2A	3682	1/1	0.96	0.07	44,44,44,44	0
57	MG	1A	3757	1/1	0.96	0.06	51,51,51,51	0
57	MG	1A	4087	1/1	0.96	0.19	55,55,55,55	0
57	MG	1a	1617	1/1	0.96	0.07	46,46,46,46	0
57	MG	1A	3139	1/1	0.96	0.09	39,39,39,39	0
57	MG	1a	1619	1/1	0.96	0.07	54,54,54,54	0
57	MG	1A	3759	1/1	0.96	0.04	33,33,33,33	0
57	MG	1A	3141	1/1	0.96	0.07	20,20,20,20	0
57	MG	1A	3033	1/1	0.96	0.11	27,27,27,27	0
57	MG	2A	3183	1/1	0.96	0.21	58,58,58,58	0
57	MG	2A	3184	1/1	0.96	0.21	37,37,37,37	0
57	MG	1A	3367	1/1	0.96	0.07	45,45,45,45	0
57	MG	1A	3072	1/1	0.96	0.24	52,52,52,52	0
57	MG	2A	3421	1/1	0.96	0.10	40,40,40,40	0
57	MG	1A	3313	1/1	0.96	0.09	52,52,52,52	0
57	MG	2A	3424	1/1	0.96	0.07	33,33,33,33	0
57	MG	1m	3001	1/1	0.96	0.09	57,57,57,57	0
57	MG	1A	3636	1/1	0.96	0.09	24,24,24,24	0
57	MG	2A	3427	1/1	0.96	0.07	37,37,37,37	0
57	MG	1A	3638	1/1	0.96	0.06	34,34,34,34	0
57	MG	1A	3639	1/1	0.96	0.05	27,27,27,27	0
57	MG	1A	3640	1/1	0.96	0.04	19,19,19,19	0
57	MG	1A	3936	1/1	0.96	0.12	55,55,55,55	0
57	MG	1A	3440	1/1	0.96	0.12	37,37,37,37	0
57	MG	1A	3528	1/1	0.96	0.15	47,47,47,47	0
57	MG	2A	3437	1/1	0.96	0.10	45,45,45,45	0
57	MG	1a	1635	1/1	0.96	0.12	59,59,59,59	0
57	MG	1A	3646	1/1	0.96	0.08	54,54,54,54	0
57	MG	1A	4106	1/1	0.96	0.12	43,43,43,43	0
57	MG	1A	3441	1/1	0.96	0.11	48,48,48,48	0
57	MG	1A	3146	1/1	0.96	0.17	29,29,29,29	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3046	1/1	0.96	0.12	30,30,30,30	0
57	MG	1A	3201	1/1	0.96	0.07	32,32,32,32	0
57	MG	2q	202	1/1	0.96	0.05	75,75,75,75	0
57	MG	2A	3204	1/1	0.96	0.10	48,48,48,48	0
57	MG	1A	3952	1/1	0.96	0.06	51,51,51,51	0
57	MG	2A	3447	1/1	0.96	0.04	39,39,39,39	0
57	MG	1B	205	1/1	0.96	0.05	44,44,44,44	0
57	MG	2A	3729	1/1	0.96	0.10	59,59,59,59	0
57	MG	2A	3450	1/1	0.96	0.06	44,44,44,44	0
57	MG	1A	3953	1/1	0.96	0.09	50,50,50,50	0
57	MG	1A	3150	1/1	0.96	0.15	32,32,32,32	0
57	MG	2x	104	1/1	0.96	0.17	52,52,52,52	0
57	MG	1A	3446	1/1	0.96	0.07	44,44,44,44	0
57	MG	1A	3791	1/1	0.96	0.08	48,48,48,48	0
57	MG	1A	3654	1/1	0.96	0.14	24,24,24,24	0
57	MG	1A	3203	1/1	0.96	0.09	22,22,22,22	0
58	6IF	2A	3731	32/32	0.96	0.08	28,36,41,45	0
59	ZN	14	102	1/1	0.96	0.08	97,97,97,97	0
57	MG	2A	3215	1/1	0.96	0.06	54,54,54,54	0
59	ZN	2n	501	1/1	0.96	0.07	95,95,95,95	0
57	MG	1A	3797	1/1	0.96	0.09	48,48,48,48	0
57	MG	1A	3324	1/1	0.97	0.11	38,38,38,38	0
57	MG	1A	3219	1/1	0.97	0.09	33,33,33,33	0
57	MG	1A	3991	1/1	0.97	0.10	50,50,50,50	0
57	MG	1A	3105	1/1	0.97	0.06	30,30,30,30	0
57	MG	1A	3107	1/1	0.97	0.29	34,34,34,34	0
57	MG	1A	3380	1/1	0.97	0.24	40,40,40,40	0
57	MG	1A	3108	1/1	0.97	0.14	26,26,26,26	0
57	MG	2A	3154	1/1	0.97	0.07	41,41,41,41	0
57	MG	1B	235	1/1	0.97	0.05	35,35,35,35	0
57	MG	1A	3109	1/1	0.97	0.06	38,38,38,38	0
57	MG	2A	3568	1/1	0.97	0.05	58,58,58,58	0
57	MG	1A	3523	1/1	0.97	0.19	34,34,34,34	0
57	MG	1A	3140	1/1	0.97	0.09	27,27,27,27	0
57	MG	1D	304	1/1	0.97	0.05	21,21,21,21	0
57	MG	1A	3624	1/1	0.97	0.07	21,21,21,21	0
57	MG	1D	307	1/1	0.97	0.06	36,36,36,36	0
57	MG	1A	3054	1/1	0.97	0.12	35,35,35,35	0
57	MG	1D	309	1/1	0.97	0.06	42,42,42,42	0
57	MG	1D	310	1/1	0.97	0.14	30,30,30,30	0
57	MG	1A	3386	1/1	0.97	0.11	24,24,24,24	0
57	MG	1A	3387	1/1	0.97	0.14	35,35,35,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3729	1/1	0.97	0.13	44,44,44,44	0
57	MG	2A	3580	1/1	0.97	0.05	49,49,49,49	0
57	MG	1A	3730	1/1	0.97	0.06	53,53,53,53	0
57	MG	2A	3364	1/1	0.97	0.07	47,47,47,47	0
57	MG	1A	4005	1/1	0.97	0.06	38,38,38,38	0
57	MG	1a	1656	1/1	0.97	0.06	43,43,43,43	0
57	MG	1A	4006	1/1	0.97	0.06	46,46,46,46	0
57	MG	1A	3066	1/1	0.97	0.05	25,25,25,25	0
57	MG	1A	3452	1/1	0.97	0.20	36,36,36,36	0
57	MG	1A	3631	1/1	0.97	0.08	27,27,27,27	0
57	MG	1A	3389	1/1	0.97	0.08	43,43,43,43	0
57	MG	1E	313	1/1	0.97	0.12	31,31,31,31	0
57	MG	1A	3390	1/1	0.97	0.07	45,45,45,45	0
57	MG	1A	3738	1/1	0.97	0.09	52,52,52,52	0
57	MG	1E	316	1/1	0.97	0.06	44,44,44,44	0
57	MG	1F	301	1/1	0.97	0.20	39,39,39,39	0
57	MG	1x	109	1/1	0.97	0.10	59,59,59,59	0
57	MG	1A	3739	1/1	0.97	0.08	50,50,50,50	0
57	MG	1A	3455	1/1	0.97	0.11	30,30,30,30	0
57	MG	1A	3279	1/1	0.97	0.16	30,30,30,30	0
57	MG	1A	3392	1/1	0.97	0.17	37,37,37,37	0
57	MG	1F	311	1/1	0.97	0.10	51,51,51,51	0
57	MG	1A	3458	1/1	0.97	0.05	35,35,35,35	0
57	MG	1A	3094	1/1	0.97	0.14	34,34,34,34	0
57	MG	1a	1674	1/1	0.97	0.23	66,66,66,66	0
57	MG	1A	3284	1/1	0.97	0.05	42,42,42,42	0
57	MG	1A	3642	1/1	0.97	0.05	23,23,23,23	0
57	MG	1A	3285	1/1	0.97	0.14	44,44,44,44	0
57	MG	1A	3286	1/1	0.97	0.12	35,35,35,35	0
57	MG	1A	3645	1/1	0.97	0.09	24,24,24,24	0
57	MG	1A	3287	1/1	0.97	0.06	39,39,39,39	0
57	MG	1A	3044	1/1	0.97	0.06	38,38,38,38	0
57	MG	2a	1652	1/1	0.97	0.09	55,55,55,55	0
57	MG	2A	3396	1/1	0.97	0.08	38,38,38,38	0
57	MG	1A	3465	1/1	0.97	0.16	54,54,54,54	0
57	MG	1A	3116	1/1	0.97	0.19	30,30,30,30	0
57	MG	2A	3399	1/1	0.97	0.07	35,35,35,35	0
57	MG	1A	3883	1/1	0.97	0.19	34,34,34,34	0
57	MG	1A	3084	1/1	0.97	0.15	27,27,27,27	0
57	MG	2A	3402	1/1	0.97	0.05	36,36,36,36	0
57	MG	1A	3885	1/1	0.97	0.22	39,39,39,39	0
57	MG	1A	3651	1/1	0.97	0.04	15,15,15,15	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2a	1662	1/1	0.97	0.06	55,55,55,55	0
57	MG	2A	3012	1/1	0.97	0.06	42,42,42,42	0
57	MG	2A	3013	1/1	0.97	0.05	53,53,53,53	0
57	MG	2A	3014	1/1	0.97	0.10	45,45,45,45	0
57	MG	2A	3208	1/1	0.97	0.11	58,58,58,58	0
57	MG	2A	3629	1/1	0.97	0.06	49,49,49,49	0
57	MG	1A	3887	1/1	0.97	0.14	30,30,30,30	0
57	MG	2A	3631	1/1	0.97	0.11	56,56,56,56	0
57	MG	2A	3411	1/1	0.97	0.10	44,44,44,44	0
57	MG	2A	3412	1/1	0.97	0.06	43,43,43,43	0
57	MG	1A	3233	1/1	0.97	0.06	36,36,36,36	0
57	MG	2A	3211	1/1	0.97	0.12	51,51,51,51	0
57	MG	2A	3416	1/1	0.97	0.09	50,50,50,50	0
57	MG	1A	3190	1/1	0.97	0.12	33,33,33,33	0
57	MG	1P	201	1/1	0.97	0.13	30,30,30,30	0
57	MG	2A	3019	1/1	0.97	0.10	30,30,30,30	0
57	MG	2A	3020	1/1	0.97	0.17	51,51,51,51	0
57	MG	1A	3403	1/1	0.97	0.05	27,27,27,27	0
57	MG	1A	3404	1/1	0.97	0.21	29,29,29,29	0
57	MG	1A	3008	1/1	0.97	0.07	24,24,24,24	0
57	MG	1A	3193	1/1	0.97	0.22	37,37,37,37	0
57	MG	2A	3025	1/1	0.97	0.20	56,56,56,56	0
57	MG	1A	3237	1/1	0.97	0.18	30,30,30,30	0
57	MG	1A	3898	1/1	0.97	0.05	43,43,43,43	0
57	MG	1A	3153	1/1	0.97	0.07	37,37,37,37	0
57	MG	1R	202	1/1	0.97	0.21	46,46,46,46	0
57	MG	2A	3432	1/1	0.97	0.08	68,68,68,68	0
57	MG	1A	3409	1/1	0.97	0.11	42,42,42,42	0
57	MG	1A	3773	1/1	0.97	0.05	31,31,31,31	0
57	MG	1A	3902	1/1	0.97	0.06	27,27,27,27	0
57	MG	2A	3034	1/1	0.97	0.06	40,40,40,40	0
57	MG	1A	3240	1/1	0.97	0.08	31,31,31,31	0
57	MG	2A	3659	1/1	0.97	0.06	77,77,77,77	0
57	MG	1A	3775	1/1	0.97	0.07	34,34,34,34	0
57	MG	1A	4055	1/1	0.97	0.04	46,46,46,46	0
57	MG	1A	3664	1/1	0.97	0.06	50,50,50,50	0
57	MG	2A	3664	1/1	0.97	0.05	48,48,48,48	0
57	MG	1A	4057	1/1	0.97	0.07	31,31,31,31	0
57	MG	1A	3558	1/1	0.97	0.06	47,47,47,47	0
57	MG	1A	3300	1/1	0.97	0.21	45,45,45,45	0
57	MG	1U	206	1/1	0.97	0.25	33,33,33,33	0
57	MG	1A	3910	1/1	0.97	0.10	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
57	MG	1A	3350	1/1	0.97	0.26	37,37,37,37	0
57	MG	2A	3046	1/1	0.97	0.10	46,46,46,46	0
57	MG	1A	3780	1/1	0.97	0.04	28,28,28,28	0
57	MG	1A	3243	1/1	0.97	0.10	42,42,42,42	0
57	MG	1A	3783	1/1	0.97	0.07	17,17,17,17	0
57	MG	2A	3678	1/1	0.97	0.05	50,50,50,50	0
57	MG	1a	1718	1/1	0.97	0.20	70,70,70,70	0
57	MG	1A	3784	1/1	0.97	0.05	22,22,22,22	0
57	MG	2A	3456	1/1	0.97	0.09	55,55,55,55	0
57	MG	2a	1713	1/1	0.97	0.17	62,62,62,62	0
57	MG	1W	203	1/1	0.97	0.14	35,35,35,35	0
57	MG	1A	3154	1/1	0.97	0.09	35,35,35,35	0
57	MG	2A	3459	1/1	0.97	0.07	41,41,41,41	0
57	MG	1W	205	1/1	0.97	0.08	34,34,34,34	0
57	MG	2A	3688	1/1	0.97	0.06	59,59,59,59	0
57	MG	1A	3157	1/1	0.97	0.06	34,34,34,34	0
57	MG	1A	3787	1/1	0.97	0.06	45,45,45,45	0
57	MG	1X	105	1/1	0.97	0.08	42,42,42,42	0
57	MG	1A	3788	1/1	0.97	0.04	21,21,21,21	0
57	MG	1A	3197	1/1	0.97	0.15	32,32,32,32	0
57	MG	1A	3672	1/1	0.97	0.07	23,23,23,23	0
57	MG	1A	3927	1/1	0.97	0.14	33,33,33,33	0
57	MG	1A	3569	1/1	0.97	0.17	44,44,44,44	0
57	MG	1A	3793	1/1	0.97	0.08	25,25,25,25	0
57	MG	10	101	1/1	0.97	0.13	38,38,38,38	0
57	MG	1A	3099	1/1	0.97	0.06	33,33,33,33	0
57	MG	2A	3067	1/1	0.97	0.05	38,38,38,38	0
57	MG	1A	3795	1/1	0.97	0.08	43,43,43,43	0
57	MG	10	104	1/1	0.97	0.14	34,34,34,34	0
57	MG	1A	3796	1/1	0.97	0.05	29,29,29,29	0
57	MG	2A	3072	1/1	0.97	0.08	48,48,48,48	0
57	MG	2A	3480	1/1	0.97	0.07	50,50,50,50	0
57	MG	1A	3675	1/1	0.97	0.08	33,33,33,33	0
57	MG	2A	3074	1/1	0.97	0.14	55,55,55,55	0
57	MG	2A	3713	1/1	0.97	0.05	44,44,44,44	0
57	MG	1A	3159	1/1	0.97	0.17	29,29,29,29	0
57	MG	1A	3935	1/1	0.97	0.06	68,68,68,68	0
57	MG	1A	3573	1/1	0.97	0.08	43,43,43,43	0
57	MG	1A	4085	1/1	0.97	0.08	32,32,32,32	0
57	MG	1A	3678	1/1	0.97	0.04	22,22,22,22	0
57	MG	13	101	1/1	0.97	0.07	36,36,36,36	0
57	MG	1A	3121	1/1	0.97	0.16	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2A	3721	1/1	0.97	0.17	45,45,45,45	0
57	MG	1A	3075	1/1	0.97	0.13	42,42,42,42	0
57	MG	2A	3084	1/1	0.97	0.11	50,50,50,50	0
57	MG	1A	3804	1/1	0.97	0.05	36,36,36,36	0
57	MG	2A	3086	1/1	0.97	0.12	34,34,34,34	0
57	MG	1a	1753	1/1	0.97	0.05	34,34,34,34	0
57	MG	1A	3204	1/1	0.97	0.07	34,34,34,34	0
57	MG	15	101	1/1	0.97	0.18	26,26,26,26	0
57	MG	1A	3126	1/1	0.97	0.22	36,36,36,36	0
57	MG	15	103	1/1	0.97	0.17	29,29,29,29	0
57	MG	1A	3946	1/1	0.97	0.04	53,53,53,53	0
57	MG	1A	3127	1/1	0.97	0.26	40,40,40,40	0
57	MG	1a	1761	1/1	0.97	0.08	42,42,42,42	0
57	MG	1A	3951	1/1	0.97	0.06	38,38,38,38	0
57	MG	1A	3424	1/1	0.97	0.25	53,53,53,53	0
57	MG	1A	3810	1/1	0.97	0.04	36,36,36,36	0
57	MG	17	101	1/1	0.97	0.04	29,29,29,29	0
57	MG	1a	1768	1/1	0.97	0.13	38,38,38,38	0
57	MG	1A	3364	1/1	0.97	0.10	43,43,43,43	0
57	MG	1A	3128	1/1	0.97	0.12	45,45,45,45	0
57	MG	1A	3815	1/1	0.97	0.04	24,24,24,24	0
57	MG	1A	3818	1/1	0.97	0.27	26,26,26,26	0
57	MG	18	3403	1/1	0.97	0.12	46,46,46,46	0
57	MG	1A	4102	1/1	0.97	0.12	46,46,46,46	0
57	MG	1A	3499	1/1	0.97	0.08	38,38,38,38	0
57	MG	1A	4104	1/1	0.97	0.14	49,49,49,49	0
57	MG	1A	3427	1/1	0.97	0.05	47,47,47,47	0
57	MG	2A	3109	1/1	0.97	0.12	42,42,42,42	0
57	MG	1A	3963	1/1	0.97	0.06	54,54,54,54	0
57	MG	2D	303	1/1	0.97	0.10	51,51,51,51	0
57	MG	1a	1782	1/1	0.97	0.07	52,52,52,52	0
57	MG	1A	3821	1/1	0.97	0.06	28,28,28,28	0
57	MG	1A	3077	1/1	0.97	0.09	24,24,24,24	0
57	MG	1A	3209	1/1	0.97	0.05	34,34,34,34	0
57	MG	2A	3308	1/1	0.97	0.17	52,52,52,52	0
57	MG	1A	3697	1/1	0.97	0.06	25,25,25,25	0
57	MG	1A	3503	1/1	0.97	0.18	45,45,45,45	0
57	MG	1A	3431	1/1	0.97	0.07	42,42,42,42	0
57	MG	1a	1608	1/1	0.97	0.07	50,50,50,50	0
57	MG	1a	1790	1/1	0.97	0.07	73,73,73,73	0
57	MG	1a	1609	1/1	0.97	0.20	48,48,48,48	0
57	MG	1A	3599	1/1	0.97	0.06	39,39,39,39	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3505	1/1	0.97	0.14	34,34,34,34	0
57	MG	1A	3210	1/1	0.97	0.08	38,38,38,38	0
57	MG	1A	3830	1/1	0.97	0.07	32,32,32,32	0
57	MG	1A	3603	1/1	0.97	0.06	47,47,47,47	0
57	MG	1A	3507	1/1	0.97	0.13	38,38,38,38	0
57	MG	1B	213	1/1	0.97	0.09	42,42,42,42	0
57	MG	2A	3322	1/1	0.97	0.22	48,48,48,48	0
57	MG	2A	3131	1/1	0.97	0.14	38,38,38,38	0
57	MG	1B	214	1/1	0.97	0.10	44,44,44,44	0
57	MG	1a	1803	1/1	0.97	0.12	68,68,68,68	0
57	MG	1B	215	1/1	0.97	0.06	35,35,35,35	0
57	MG	2A	3327	1/1	0.97	0.07	41,41,41,41	0
57	MG	2A	3328	1/1	0.97	0.10	38,38,38,38	0
57	MG	1A	3015	1/1	0.97	0.07	41,41,41,41	0
57	MG	1A	3979	1/1	0.97	0.09	27,27,27,27	0
57	MG	2A	3546	1/1	0.97	0.22	41,41,41,41	0
57	MG	1A	3090	1/1	0.97	0.08	53,53,53,53	0
57	MG	1A	3608	1/1	0.97	0.11	36,36,36,36	0
57	MG	1A	3080	1/1	0.97	0.12	38,38,38,38	0
57	MG	1a	1818	1/1	0.97	0.06	62,62,62,62	0
57	MG	1A	3133	1/1	0.97	0.13	39,39,39,39	0
57	MG	1A	3512	1/1	0.97	0.06	46,46,46,46	0
57	MG	1A	3267	1/1	0.97	0.10	31,31,31,31	0
57	MG	1B	226	1/1	0.97	0.06	37,37,37,37	0
57	MG	1A	3323	1/1	0.97	0.07	61,61,61,61	0
57	MG	1A	3200	1/1	0.98	0.03	31,31,31,31	0
57	MG	1A	3598	1/1	0.98	0.05	28,28,28,28	0
57	MG	1A	3037	1/1	0.98	0.18	31,31,31,31	0
57	MG	1A	3600	1/1	0.98	0.13	35,35,35,35	0
57	MG	2A	3367	1/1	0.98	0.18	39,39,39,39	0
57	MG	1A	3254	1/1	0.98	0.05	32,32,32,32	0
57	MG	1P	206	1/1	0.98	0.14	50,50,50,50	0
57	MG	1Q	201	1/1	0.98	0.09	29,29,29,29	0
57	MG	1Q	202	1/1	0.98	0.06	36,36,36,36	0
57	MG	1A	3123	1/1	0.98	0.14	31,31,31,31	0
57	MG	1A	3382	1/1	0.98	0.11	34,34,34,34	0
57	MG	1A	3124	1/1	0.98	0.14	32,32,32,32	0
57	MG	1A	3605	1/1	0.98	0.07	29,29,29,29	0
57	MG	2A	3376	1/1	0.98	0.24	47,47,47,47	0
57	MG	1A	3160	1/1	0.98	0.17	27,27,27,27	0
57	MG	1A	3161	1/1	0.98	0.10	27,27,27,27	0
57	MG	1A	3814	1/1	0.98	0.03	22,22,22,22	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3125	1/1	0.98	0.20	28,28,28,28	0
57	MG	1A	3705	1/1	0.98	0.07	38,38,38,38	0
57	MG	1A	3450	1/1	0.98	0.12	32,32,32,32	0
57	MG	2A	3191	1/1	0.98	0.19	36,36,36,36	0
57	MG	1A	3260	1/1	0.98	0.08	53,53,53,53	0
57	MG	1A	3940	1/1	0.98	0.05	35,35,35,35	0
57	MG	1A	3521	1/1	0.98	0.08	31,31,31,31	0
57	MG	1A	4077	1/1	0.98	0.04	31,31,31,31	0
57	MG	1A	3076	1/1	0.98	0.08	33,33,33,33	0
57	MG	1U	204	1/1	0.98	0.19	32,32,32,32	0
57	MG	1A	3020	1/1	0.98	0.10	44,44,44,44	0
57	MG	1A	3022	1/1	0.98	0.04	36,36,36,36	0
57	MG	2A	3599	1/1	0.98	0.04	36,36,36,36	0
57	MG	1U	207	1/1	0.98	0.13	32,32,32,32	0
57	MG	1A	3948	1/1	0.98	0.04	33,33,33,33	0
57	MG	1a	1699	1/1	0.98	0.15	44,44,44,44	0
57	MG	1A	3949	1/1	0.98	0.04	30,30,30,30	0
57	MG	1V	203	1/1	0.98	0.14	30,30,30,30	0
57	MG	1V	204	1/1	0.98	0.11	30,30,30,30	0
57	MG	1A	3041	1/1	0.98	0.12	27,27,27,27	0
57	MG	1A	4084	1/1	0.98	0.03	32,32,32,32	0
57	MG	1A	3616	1/1	0.98	0.07	40,40,40,40	0
57	MG	1A	3211	1/1	0.98	0.17	32,32,32,32	0
57	MG	1A	3266	1/1	0.98	0.14	41,41,41,41	0
57	MG	1A	3954	1/1	0.98	0.04	40,40,40,40	0
57	MG	2A	3405	1/1	0.98	0.04	24,24,24,24	0
57	MG	1A	3056	1/1	0.98	0.05	28,28,28,28	0
57	MG	2A	3614	1/1	0.98	0.16	45,45,45,45	0
57	MG	1A	3213	1/1	0.98	0.06	38,38,38,38	0
57	MG	1A	4091	1/1	0.98	0.06	57,57,57,57	0
57	MG	1X	102	1/1	0.98	0.05	27,27,27,27	0
57	MG	1X	104	1/1	0.98	0.12	33,33,33,33	0
57	MG	1A	3214	1/1	0.98	0.08	47,47,47,47	0
57	MG	1A	3168	1/1	0.98	0.14	38,38,38,38	0
57	MG	1A	3003	1/1	0.98	0.04	28,28,28,28	0
57	MG	2A	3414	1/1	0.98	0.04	55,55,55,55	0
57	MG	2A	3220	1/1	0.98	0.07	45,45,45,45	0
57	MG	1A	3961	1/1	0.98	0.04	52,52,52,52	0
57	MG	1Y	204	1/1	0.98	0.17	36,36,36,36	0
57	MG	1A	3025	1/1	0.98	0.05	34,34,34,34	0
57	MG	1A	3001	1/1	0.98	0.10	34,34,34,34	0
57	MG	1A	3836	1/1	0.98	0.06	34,34,34,34	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3275	1/1	0.98	0.15	39,39,39,39	0
57	MG	1A	3134	1/1	0.98	0.06	25,25,25,25	0
57	MG	2A	3423	1/1	0.98	0.10	26,26,26,26	0
57	MG	1A	3839	1/1	0.98	0.08	36,36,36,36	0
57	MG	1A	3174	1/1	0.98	0.16	25,25,25,25	0
57	MG	1a	1727	1/1	0.98	0.23	40,40,40,40	0
57	MG	1A	3727	1/1	0.98	0.07	27,27,27,27	0
57	MG	10	106	1/1	0.98	0.05	46,46,46,46	0
57	MG	2A	3045	1/1	0.98	0.12	26,26,26,26	0
57	MG	2A	3430	1/1	0.98	0.08	34,34,34,34	0
57	MG	1a	1730	1/1	0.98	0.14	43,43,43,43	0
57	MG	1A	3222	1/1	0.98	0.14	28,28,28,28	0
57	MG	2A	3641	1/1	0.98	0.05	52,52,52,52	0
57	MG	1a	1732	1/1	0.98	0.13	42,42,42,42	0
57	MG	1a	1733	1/1	0.98	0.25	50,50,50,50	0
57	MG	11	101	1/1	0.98	0.28	39,39,39,39	0
57	MG	2A	3436	1/1	0.98	0.09	36,36,36,36	0
57	MG	1A	3843	1/1	0.98	0.04	58,58,58,58	0
57	MG	1A	3280	1/1	0.98	0.21	38,38,38,38	0
57	MG	11	104	1/1	0.98	0.04	34,34,34,34	0
57	MG	1A	3009	1/1	0.98	0.03	22,22,22,22	0
57	MG	1A	4108	1/1	0.98	0.05	54,54,54,54	0
57	MG	1A	3283	1/1	0.98	0.44	35,35,35,35	0
57	MG	1A	3976	1/1	0.98	0.05	54,54,54,54	0
57	MG	1A	3732	1/1	0.98	0.07	25,25,25,25	0
57	MG	1A	3472	1/1	0.98	0.21	31,31,31,31	0
57	MG	1A	3473	1/1	0.98	0.06	35,35,35,35	0
57	MG	2A	3249	1/1	0.98	0.05	49,49,49,49	0
57	MG	2A	3448	1/1	0.98	0.09	42,42,42,42	0
57	MG	2A	3061	1/1	0.98	0.07	39,39,39,39	0
57	MG	2A	3661	1/1	0.98	0.04	62,62,62,62	0
57	MG	1A	3177	1/1	0.98	0.06	19,19,19,19	0
57	MG	1A	3851	1/1	0.98	0.06	34,34,34,34	0
57	MG	1A	3637	1/1	0.98	0.04	42,42,42,42	0
57	MG	2A	3453	1/1	0.98	0.04	24,24,24,24	0
57	MG	1B	209	1/1	0.98	0.08	36,36,36,36	0
57	MG	1A	3737	1/1	0.98	0.04	52,52,52,52	0
57	MG	1a	1750	1/1	0.98	0.10	44,44,44,44	0
57	MG	2A	3669	1/1	0.98	0.08	41,41,41,41	0
57	MG	1A	3178	1/1	0.98	0.04	31,31,31,31	0
57	MG	15	106	1/1	0.98	0.06	29,29,29,29	0
57	MG	2A	3070	1/1	0.98	0.04	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3005	1/1	0.98	0.06	37,37,37,37	0
57	MG	1A	3110	1/1	0.98	0.19	34,34,34,34	0
57	MG	1a	1755	1/1	0.98	0.10	43,43,43,43	0
57	MG	2A	3677	1/1	0.98	0.04	56,56,56,56	0
57	MG	1A	3741	1/1	0.98	0.06	26,26,26,26	0
57	MG	16	101	1/1	0.98	0.04	47,47,47,47	0
57	MG	1A	3989	1/1	0.98	0.10	57,57,57,57	0
57	MG	17	102	1/1	0.98	0.14	24,24,24,24	0
57	MG	2A	3267	1/1	0.98	0.10	38,38,38,38	0
57	MG	1A	3641	1/1	0.98	0.05	29,29,29,29	0
57	MG	2A	3079	1/1	0.98	0.12	54,54,54,54	0
57	MG	17	104	1/1	0.98	0.07	31,31,31,31	0
57	MG	1B	217	1/1	0.98	0.05	34,34,34,34	0
57	MG	2A	3689	1/1	0.98	0.06	64,64,64,64	0
57	MG	1A	3138	1/1	0.98	0.07	33,33,33,33	0
57	MG	2A	3691	1/1	0.98	0.05	30,30,30,30	0
57	MG	1a	1765	1/1	0.98	0.04	61,61,61,61	0
57	MG	2A	3693	1/1	0.98	0.03	63,63,63,63	0
57	MG	1A	3860	1/1	0.98	0.07	15,15,15,15	0
57	MG	1A	3229	1/1	0.98	0.20	31,31,31,31	0
57	MG	1A	3031	1/1	0.98	0.12	30,30,30,30	0
57	MG	1A	3032	1/1	0.98	0.26	26,26,26,26	0
57	MG	1A	3354	1/1	0.98	0.07	35,35,35,35	0
57	MG	2A	3699	1/1	0.98	0.12	48,48,48,48	0
57	MG	1A	3113	1/1	0.98	0.06	33,33,33,33	0
57	MG	1B	225	1/1	0.98	0.07	36,36,36,36	0
57	MG	1a	1774	1/1	0.98	0.03	50,50,50,50	0
57	MG	1a	1775	1/1	0.98	0.07	51,51,51,51	0
57	MG	1A	3142	1/1	0.98	0.08	38,38,38,38	0
57	MG	1A	3486	1/1	0.98	0.09	41,41,41,41	0
57	MG	1A	3753	1/1	0.98	0.08	29,29,29,29	0
57	MG	1A	3186	1/1	0.98	0.09	38,38,38,38	0
57	MG	1A	3065	1/1	0.98	0.12	36,36,36,36	0
57	MG	1A	3011	1/1	0.98	0.10	38,38,38,38	0
57	MG	1A	3872	1/1	0.98	0.05	42,42,42,42	0
57	MG	1A	3145	1/1	0.98	0.12	29,29,29,29	0
57	MG	1A	3299	1/1	0.98	0.04	30,30,30,30	0
57	MG	1A	3564	1/1	0.98	0.07	23,23,23,23	0
57	MG	1A	3565	1/1	0.98	0.06	49,49,49,49	0
57	MG	1A	3566	1/1	0.98	0.12	32,32,32,32	0
57	MG	1A	3762	1/1	0.98	0.03	40,40,40,40	0
57	MG	1D	303	1/1	0.98	0.07	40,40,40,40	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3050	1/1	0.98	0.12	35,35,35,35	0
57	MG	1A	3239	1/1	0.98	0.20	30,30,30,30	0
57	MG	1A	3660	1/1	0.98	0.09	46,46,46,46	0
57	MG	1A	3570	1/1	0.98	0.14	41,41,41,41	0
57	MG	1A	3662	1/1	0.98	0.04	36,36,36,36	0
57	MG	2A	3112	1/1	0.98	0.16	42,42,42,42	0
57	MG	1a	1621	1/1	0.98	0.05	45,45,45,45	0
57	MG	2A	3726	1/1	0.98	0.11	53,53,53,53	0
57	MG	1A	4016	1/1	0.98	0.03	21,21,21,21	0
57	MG	1A	3147	1/1	0.98	0.04	34,34,34,34	0
57	MG	1A	3771	1/1	0.98	0.09	44,44,44,44	0
57	MG	1A	3241	1/1	0.98	0.16	29,29,29,29	0
57	MG	1a	1802	1/1	0.98	0.05	52,52,52,52	0
57	MG	1A	3242	1/1	0.98	0.20	33,33,33,33	0
57	MG	1E	304	1/1	0.98	0.08	34,34,34,34	0
57	MG	1a	1806	1/1	0.98	0.10	68,68,68,68	0
57	MG	1a	1807	1/1	0.98	0.05	60,60,60,60	0
57	MG	1a	1808	1/1	0.98	0.04	49,49,49,49	0
57	MG	1E	305	1/1	0.98	0.09	28,28,28,28	0
57	MG	1a	1810	1/1	0.98	0.04	50,50,50,50	0
57	MG	1a	1811	1/1	0.98	0.09	67,67,67,67	0
57	MG	1A	3497	1/1	0.98	0.07	35,35,35,35	0
57	MG	1A	3192	1/1	0.98	0.17	30,30,30,30	0
57	MG	1a	1814	1/1	0.98	0.05	64,64,64,64	0
57	MG	1a	1815	1/1	0.98	0.04	64,64,64,64	0
57	MG	1A	3890	1/1	0.98	0.05	45,45,45,45	0
57	MG	1A	3577	1/1	0.98	0.07	21,21,21,21	0
57	MG	1A	3430	1/1	0.98	0.17	36,36,36,36	0
57	MG	1A	3244	1/1	0.98	0.04	37,37,37,37	0
57	MG	1A	3581	1/1	0.98	0.21	30,30,30,30	0
57	MG	1A	3071	1/1	0.98	0.05	16,16,16,16	0
57	MG	1a	1822	1/1	0.98	0.07	50,50,50,50	0
57	MG	1A	3583	1/1	0.98	0.12	44,44,44,44	0
57	MG	1A	4032	1/1	0.98	0.04	50,50,50,50	0
57	MG	2D	305	1/1	0.98	0.06	31,31,31,31	0
57	MG	1A	3782	1/1	0.98	0.04	47,47,47,47	0
57	MG	1F	302	1/1	0.98	0.08	31,31,31,31	0
57	MG	1F	303	1/1	0.98	0.11	31,31,31,31	0
57	MG	1A	3309	1/1	0.98	0.04	37,37,37,37	0
57	MG	1F	305	1/1	0.98	0.10	34,34,34,34	0
57	MG	1F	307	1/1	0.98	0.14	34,34,34,34	0
57	MG	2A	3148	1/1	0.98	0.11	37,37,37,37	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	2E	307	1/1	0.98	0.09	35,35,35,35	0
57	MG	1A	3585	1/1	0.98	0.23	33,33,33,33	0
57	MG	2A	3541	1/1	0.98	0.05	43,43,43,43	0
57	MG	2F	303	1/1	0.98	0.11	53,53,53,53	0
57	MG	1a	1647	1/1	0.98	0.09	52,52,52,52	0
57	MG	1A	4036	1/1	0.98	0.06	44,44,44,44	0
57	MG	1A	3586	1/1	0.98	0.07	32,32,32,32	0
57	MG	1A	3149	1/1	0.98	0.29	30,30,30,30	0
57	MG	1A	3372	1/1	0.98	0.12	32,32,32,32	0
57	MG	1A	3118	1/1	0.98	0.05	49,49,49,49	0
57	MG	2I	202	1/1	0.98	0.06	65,65,65,65	0
57	MG	2A	3548	1/1	0.98	0.05	57,57,57,57	0
57	MG	1a	1653	1/1	0.98	0.14	43,43,43,43	0
57	MG	2A	3157	1/1	0.98	0.06	53,53,53,53	0
57	MG	1A	3789	1/1	0.98	0.07	25,25,25,25	0
57	MG	1A	3907	1/1	0.98	0.07	43,43,43,43	0
57	MG	1A	3590	1/1	0.98	0.07	29,29,29,29	0
57	MG	1A	3682	1/1	0.98	0.05	19,19,19,19	0
57	MG	1A	3683	1/1	0.98	0.08	24,24,24,24	0
57	MG	1A	3012	1/1	0.98	0.04	27,27,27,27	0
57	MG	1A	3592	1/1	0.98	0.06	37,37,37,37	0
57	MG	1N	203	1/1	0.98	0.04	41,41,41,41	0
57	MG	1A	3593	1/1	0.98	0.06	34,34,34,34	0
57	MG	1A	3688	1/1	0.98	0.05	27,27,27,27	0
57	MG	23	101	1/1	0.98	0.06	52,52,52,52	0
57	MG	1A	3918	1/1	0.98	0.11	36,36,36,36	0
57	MG	1A	3249	1/1	0.98	0.15	34,34,34,34	0
58	6IF	1A	4109	32/32	0.98	0.07	18,25,31,31	0
57	MG	1A	3073	1/1	0.98	0.08	21,21,21,21	0
57	MG	25	103	1/1	0.98	0.08	56,56,56,56	0
59	ZN	2Y	202	1/1	0.98	0.04	95,95,95,95	0
57	MG	1A	3074	1/1	0.98	0.05	28,28,28,28	0
57	MG	1A	3923	1/1	0.98	0.04	33,33,33,33	0
60	SF4	1d	302	8/8	0.98	0.05	57,60,69,76	0
60	SF4	2d	302	8/8	0.98	0.04	62,75,82,85	0
57	MG	2A	3566	1/1	0.98	0.10	35,35,35,35	0
57	MG	1A	3272	1/1	0.99	0.12	38,38,38,38	0
57	MG	1A	3155	1/1	0.99	0.09	40,40,40,40	0
57	MG	17	106	1/1	0.99	0.03	43,43,43,43	0
57	MG	1A	3156	1/1	0.99	0.16	31,31,31,31	0
57	MG	2A	3331	1/1	0.99	0.11	25,25,25,25	0
57	MG	1A	3742	1/1	0.99	0.06	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
57	MG	1A	3007	1/1	0.99	0.04	39,39,39,39	0
57	MG	1A	3304	1/1	0.99	0.07	23,23,23,23	0
57	MG	1A	3023	1/1	0.99	0.07	18,18,18,18	0
57	MG	1A	3894	1/1	0.99	0.03	27,27,27,27	0
57	MG	1a	1762	1/1	0.99	0.04	41,41,41,41	0
57	MG	1A	3485	1/1	0.99	0.05	41,41,41,41	0
57	MG	1D	306	1/1	0.99	0.14	26,26,26,26	0
57	MG	1A	3014	1/1	0.99	0.10	23,23,23,23	0
57	MG	1U	201	1/1	0.99	0.11	30,30,30,30	0
57	MG	1A	3897	1/1	0.99	0.05	41,41,41,41	0
57	MG	1a	1685	1/1	0.99	0.04	43,43,43,43	0
57	MG	1A	3278	1/1	0.99	0.09	25,25,25,25	0
57	MG	1A	3627	1/1	0.99	0.09	37,37,37,37	0
57	MG	1A	4021	1/1	0.99	0.02	36,36,36,36	0
57	MG	1A	3960	1/1	0.99	0.04	42,42,42,42	0
57	MG	1A	3106	1/1	0.99	0.11	31,31,31,31	0
57	MG	1U	208	1/1	0.99	0.15	30,30,30,30	0
57	MG	1E	302	1/1	0.99	0.21	32,32,32,32	0
57	MG	1V	201	1/1	0.99	0.16	24,24,24,24	0
57	MG	1A	4024	1/1	0.99	0.08	33,33,33,33	0
57	MG	1A	3751	1/1	0.99	0.06	45,45,45,45	0
57	MG	1A	3798	1/1	0.99	0.02	36,36,36,36	0
57	MG	1A	3035	1/1	0.99	0.05	32,32,32,32	0
57	MG	1A	3063	1/1	0.99	0.05	26,26,26,26	0
57	MG	1E	308	1/1	0.99	0.03	30,30,30,30	0
57	MG	1A	3282	1/1	0.99	0.28	35,35,35,35	0
57	MG	1A	3036	1/1	0.99	0.10	23,23,23,23	0
57	MG	1A	3524	1/1	0.99	0.15	33,33,33,33	0
57	MG	1A	3908	1/1	0.99	0.05	28,28,28,28	0
57	MG	1A	3029	1/1	0.99	0.06	31,31,31,31	0
57	MG	1A	3971	1/1	0.99	0.03	43,43,43,43	0
57	MG	1A	3526	1/1	0.99	0.12	25,25,25,25	0
57	MG	1X	103	1/1	0.99	0.08	51,51,51,51	0
57	MG	1A	3806	1/1	0.99	0.07	21,21,21,21	0
57	MG	1a	1793	1/1	0.99	0.03	56,56,56,56	0
57	MG	1A	3912	1/1	0.99	0.03	30,30,30,30	0
57	MG	1A	3079	1/1	0.99	0.08	36,36,36,36	0
57	MG	1A	4039	1/1	0.99	0.04	45,45,45,45	0
57	MG	1A	4041	1/1	0.99	0.02	45,45,45,45	0
57	MG	1a	1798	1/1	0.99	0.05	64,64,64,64	0
57	MG	2A	3465	1/1	0.99	0.04	43,43,43,43	0
57	MG	1A	3038	1/1	0.99	0.20	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
57	MG	1F	306	1/1	0.99	0.13	28,28,28,28	0
57	MG	2A	3658	1/1	0.99	0.03	75,75,75,75	0
57	MG	1a	1634	1/1	0.99	0.10	31,31,31,31	0
57	MG	1A	3717	1/1	0.99	0.04	27,27,27,27	0
57	MG	1A	3096	1/1	0.99	0.12	22,22,22,22	0
57	MG	1A	3763	1/1	0.99	0.06	41,41,41,41	0
57	MG	1a	1805	1/1	0.99	0.03	40,40,40,40	0
57	MG	1A	3812	1/1	0.99	0.03	40,40,40,40	0
57	MG	1A	3764	1/1	0.99	0.02	25,25,25,25	0
57	MG	1A	3030	1/1	0.99	0.09	28,28,28,28	0
57	MG	1A	3983	1/1	0.99	0.05	50,50,50,50	0
57	MG	2A	3115	1/1	0.99	0.12	35,35,35,35	0
57	MG	1a	1723	1/1	0.99	0.14	38,38,38,38	0
57	MG	2A	3479	1/1	0.99	0.03	56,56,56,56	0
57	MG	1A	3922	1/1	0.99	0.02	20,20,20,20	0
57	MG	1A	3068	1/1	0.99	0.09	26,26,26,26	0
57	MG	2A	3031	1/1	0.99	0.06	53,53,53,53	0
57	MG	10	108	1/1	0.99	0.03	46,46,46,46	0
57	MG	1A	3816	1/1	0.99	0.03	36,36,36,36	0
57	MG	2A	3676	1/1	0.99	0.06	36,36,36,36	0
57	MG	2A	3391	1/1	0.99	0.07	43,43,43,43	0
57	MG	1A	3817	1/1	0.99	0.05	25,25,25,25	0
57	MG	2A	3679	1/1	0.99	0.04	45,45,45,45	0
57	MG	2A	3123	1/1	0.99	0.06	37,37,37,37	0
57	MG	1A	3215	1/1	0.99	0.16	38,38,38,38	0
57	MG	1A	3567	1/1	0.99	0.13	31,31,31,31	0
57	MG	1A	3681	1/1	0.99	0.05	41,41,41,41	0
57	MG	2A	3584	1/1	0.99	0.03	32,32,32,32	0
57	MG	1A	3069	1/1	0.99	0.11	21,21,21,21	0
57	MG	2A	3686	1/1	0.99	0.09	30,30,30,30	0
57	MG	1A	3151	1/1	0.99	0.12	31,31,31,31	0
57	MG	1A	3293	1/1	0.99	0.17	31,31,31,31	0
57	MG	1A	3536	1/1	0.99	0.05	48,48,48,48	0
57	MG	1a	1654	1/1	0.99	0.09	42,42,42,42	0
57	MG	1A	3686	1/1	0.99	0.04	26,26,26,26	0
57	MG	1A	3070	1/1	0.99	0.21	34,34,34,34	0
57	MG	2A	3592	1/1	0.99	0.03	52,52,52,52	0
57	MG	1A	3353	1/1	0.99	0.11	28,28,28,28	0
57	MG	1A	3173	1/1	0.99	0.12	29,29,29,29	0
57	MG	1A	3085	1/1	0.99	0.13	32,32,32,32	0
57	MG	1A	3576	1/1	0.99	0.15	24,24,24,24	0
57	MG	2A	3597	1/1	0.99	0.03	35,35,35,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	1A	3175	1/1	0.99	0.07	26,26,26,26	0
57	MG	2A	3700	1/1	0.99	0.03	58,58,58,58	0
57	MG	1P	202	1/1	0.99	0.10	25,25,25,25	0
57	MG	1A	3578	1/1	0.99	0.10	24,24,24,24	0
57	MG	1P	204	1/1	0.99	0.16	31,31,31,31	0
59	ZN	15	110	1/1	0.99	0.07	47,47,47,47	0
59	ZN	19	102	1/1	0.99	0.15	67,67,67,67	0
57	MG	1A	3021	1/1	0.99	0.04	22,22,22,22	0
57	MG	1A	3695	1/1	0.99	0.03	23,23,23,23	0
59	ZN	25	104	1/1	0.99	0.05	57,57,57,57	0
59	ZN	26	102	1/1	0.99	0.06	68,68,68,68	0
59	ZN	29	501	1/1	0.99	0.03	66,66,66,66	0
57	MG	1A	3943	1/1	0.99	0.05	51,51,51,51	0
57	MG	1A	3944	1/1	0.99	0.05	12,12,12,12	0
57	MG	1A	4073	1/1	0.99	0.07	28,28,28,28	0
57	MG	1A	3199	1/1	0.99	0.12	24,24,24,24	0
57	MG	1A	4040	1/1	1.00	0.05	24,24,24,24	0
57	MG	2A	3464	1/1	1.00	0.05	38,38,38,38	0
57	MG	1A	3916	1/1	1.00	0.03	35,35,35,35	0
59	ZN	1Y	205	1/1	1.00	0.02	57,57,57,57	0
57	MG	2A	3646	1/1	1.00	0.03	48,48,48,48	0
57	MG	1A	3947	1/1	1.00	0.09	29,29,29,29	0
59	ZN	16	102	1/1	1.00	0.03	41,41,41,41	0
57	MG	1a	1773	1/1	1.00	0.07	57,57,57,57	0
59	ZN	1n	103	1/1	1.00	0.04	63,63,63,63	0

6.5 Other polymers

There are no such residues in this entry.