Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2026 – 04:51 AM EDT

PDB ID	:	8FC1 / pdb_00008fc1
Title	:	Crystal structure of the Thermus thermophilus 70S ribosome in complex with protein Y, hygromycin A, and erythromycin at 2.50A resolution
Authors	:	Chen, C.-W.; Syroegin, E.A.; Svetlov, M.S.; Polikanov, Y.S.
Deposited on	:	2022-12-01
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:

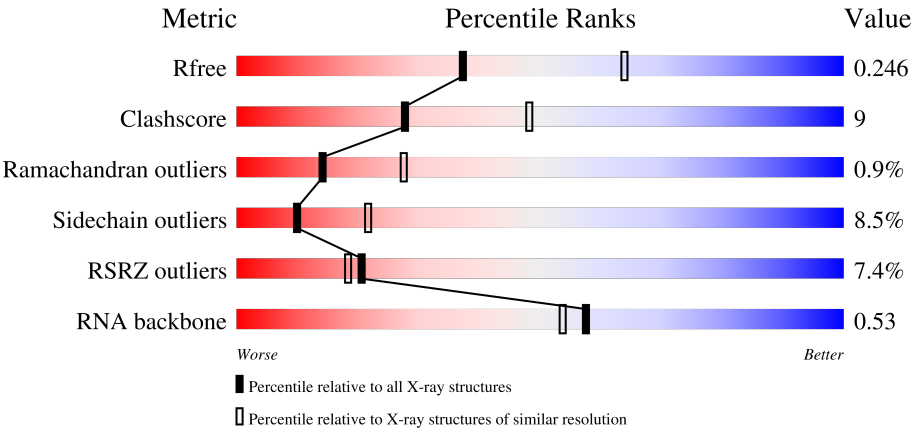
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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.



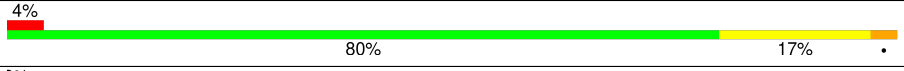
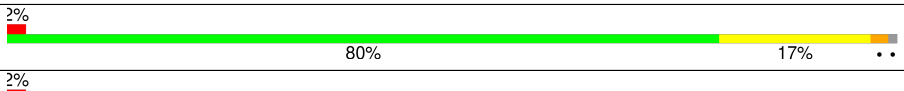
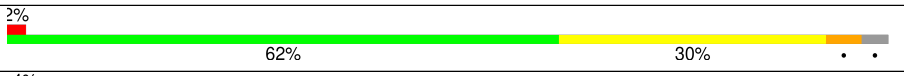
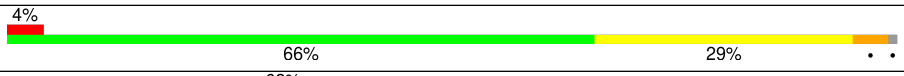
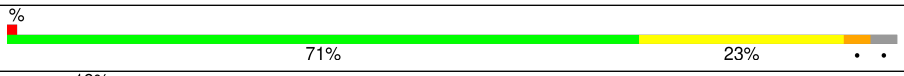
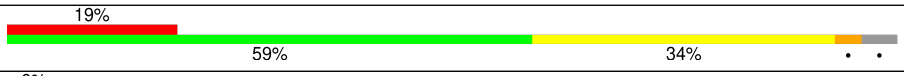
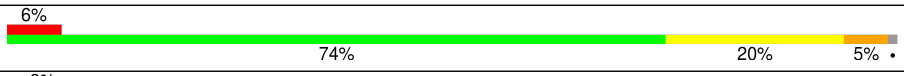
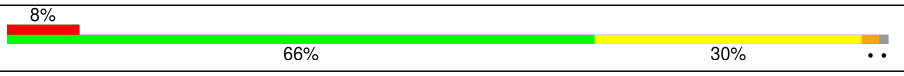
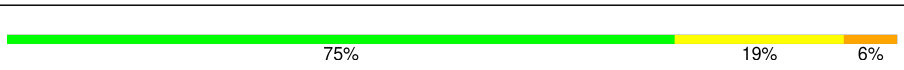
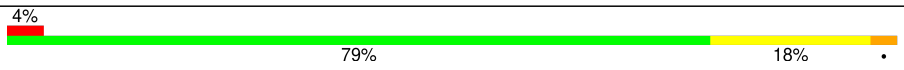
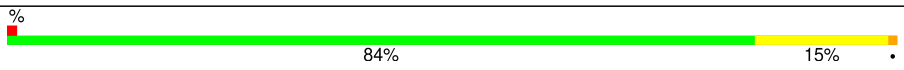
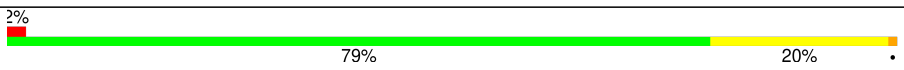
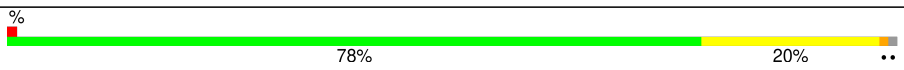
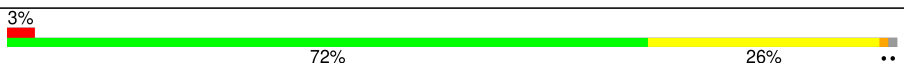
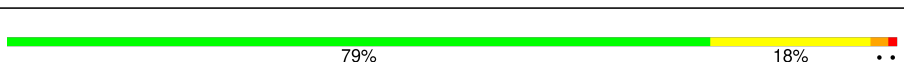
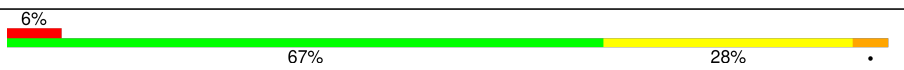
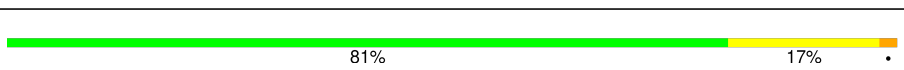
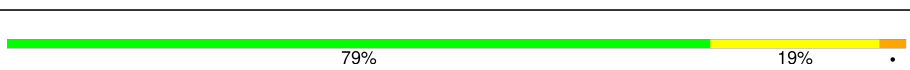
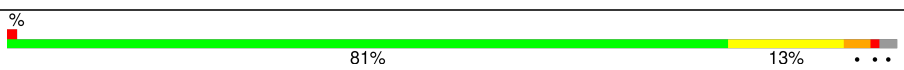
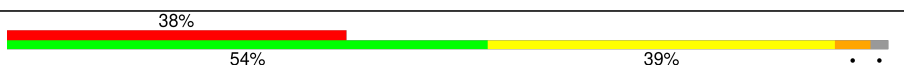
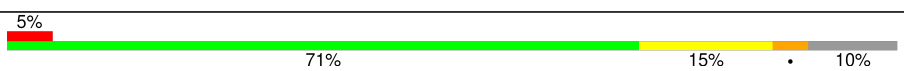
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)
RNA backbone	3983	1003 (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 <=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	3% 66% 27% 6%
1	2A	2915	4% 58% 33% 7%
2	1B	121	% 71% 24%
2	2B	121	5% 45% 45% 9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	1D	276	
3	2D	276	
4	1E	206	
4	2E	206	
5	1F	210	
5	2F	210	
6	1G	182	
6	2G	182	
7	1H	180	
7	2H	180	
8	1I	148	
8	2I	148	
9	1N	140	
9	2N	140	
10	1O	122	
10	2O	122	
11	1P	150	
11	2P	150	
12	1Q	141	
12	2Q	141	
13	1R	118	
13	2R	118	
14	1S	112	
14	2S	112	
15	1T	146	

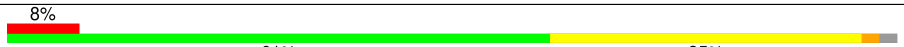
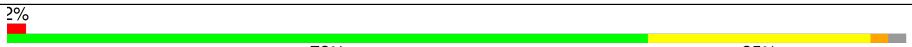
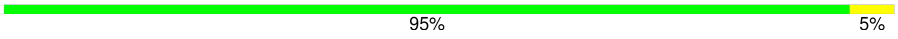
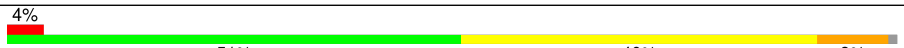
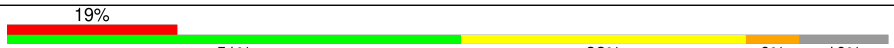
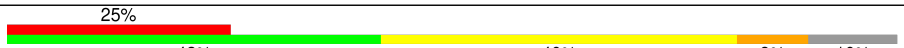
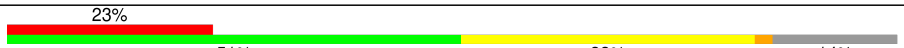
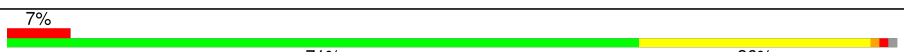
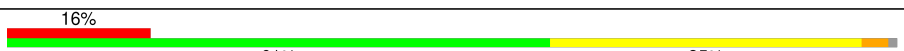
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	2T	146	2% 71% 19% 10%
16	1U	118	% 84% 14%
16	2U	118	69% 27%
17	1V	101	% 77% 21%
17	2V	101	3% 77% 19%
18	1W	113	2% 81% 15%
18	2W	113	4% 78% 19%
19	1X	96	3% 74% 20% 5%
19	2X	96	4% 77% 18%
20	1Y	110	3% 75% 22%
20	2Y	110	15% 68% 25%
21	1Z	206	4% 73% 23%
21	2Z	206	18% 62% 33%
22	10	85	2% 80% 9% 9%
22	20	85	8% 79% 11% 9%
23	11	98	% 76% 22%
23	21	98	2% 76% 20%
24	12	72	3% 78% 18%
24	22	72	% 67% 29%
25	13	60	2% 75% 22%
25	23	60	5% 62% 33%
26	14	71	20% 63% 23% 10%
26	24	71	65% 37% 51% 10%
27	15	60	72% 22% 5%
27	25	60	2% 77% 22%

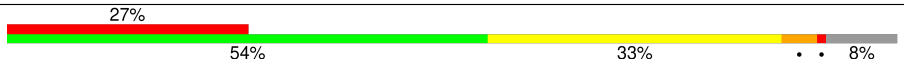
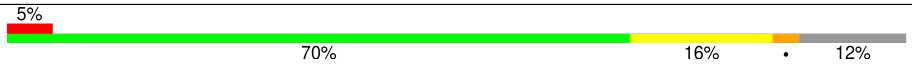
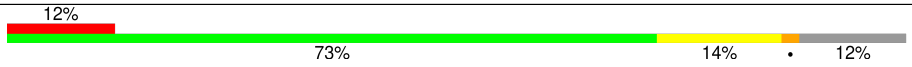
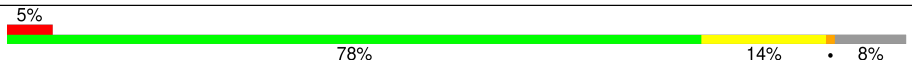
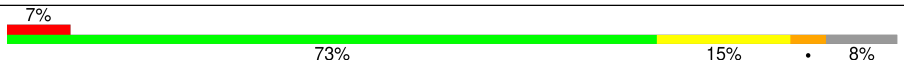
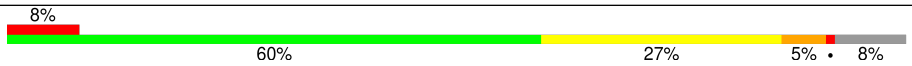
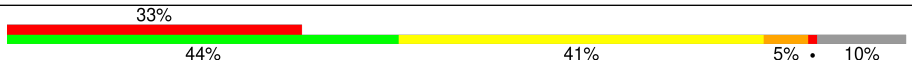
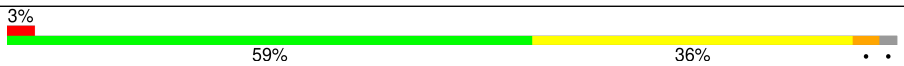
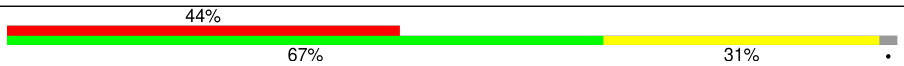
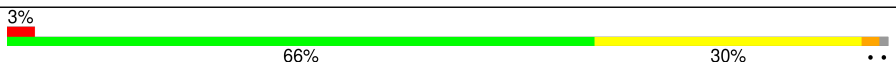
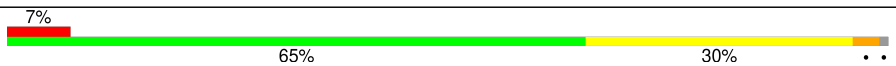
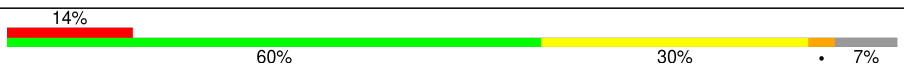
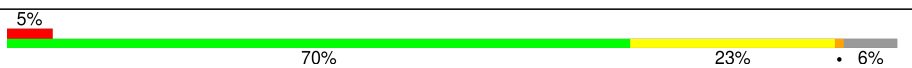
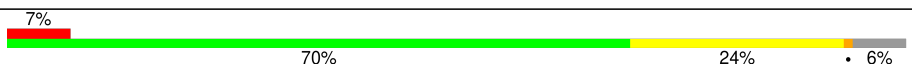
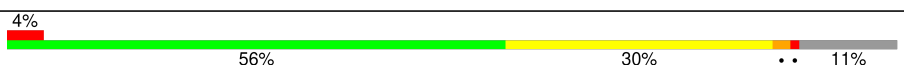
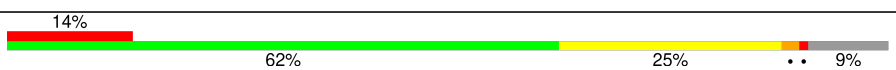
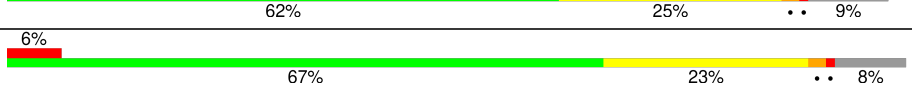
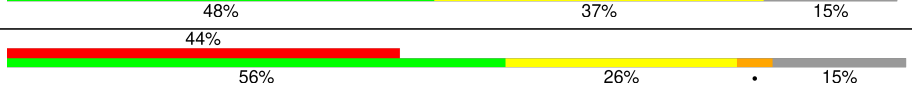
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	16	54	
28	26	54	
29	17	49	
29	27	49	
30	18	65	
30	28	65	
31	19	37	
31	29	37	
32	1a	1521	
32	2a	1521	
33	1b	256	
33	2b	256	
34	1c	239	
34	2c	239	
35	1d	209	
35	2d	209	
36	1e	162	
36	2e	162	
37	1f	101	
37	2f	101	
38	1g	156	
38	2g	156	
39	1h	138	
39	2h	138	
40	1i	128	

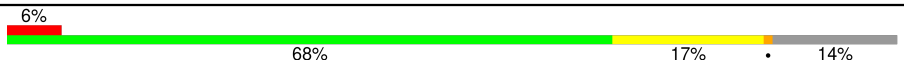
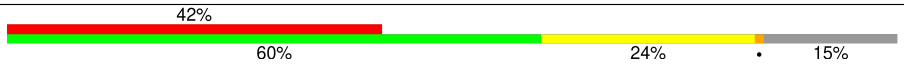
Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	1y	113	
53	2y	113	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	MG	1a	1877	-	-	-	X
54	MG	2a	3006	-	-	-	X
54	MG	2a	3010	-	-	-	X
57	MPD	1a	1880	-	-	X	-

2 Entry composition (i)

There are 61 unique types of molecules in this entry. The entry contains 296967 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	2872	Total	C	N	O	P	0	0	0
			61869	27540	11574	19884	2871			
1	2A	2867	Total	C	N	O	P	0	0	0
			61758	27491	11552	19850	2865			

- 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
			2572	1145	476	832	119			
2	2B	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

- 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
			2131	1346	422	360	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
			1426	916	253	253	4			
6	2G	181	Total	C	N	O	S	0	0	0
			1424	912	259	249	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	173	Total	C	N	O	S	0	0	0
			1324	842	247	234	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	1I	147	Total	C	N	O	S	0	0	0
			1094	699	191	203	1			
8	2I	146	Total	C	N	O	S	0	0	0
			1076	687	186	202	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
			1121	722	208	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 933	C 588	N 171	O 170	S 4	0	0	0

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	1S	110	Total 877	C 553	N 175	O 149	0	0	0
14	2S	110	Total 870	C 549	N 173	O 148	0	0	0

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

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

- 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
			775	498	141	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
			810	520	153	131	6			
20	2Y	107	Total	C	N	O	S	0	0	0
			810	519	153	132	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	1Z	203	Total	C	N	O	S	0	0	0
			1587	1011	282	292	2			
21	2Z	201	Total	C	N	O	S	0	0	0
			1557	995	274	286	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			
22	20	77	Total	C	N	O	S	0	0	0
			608	375	129	103	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
			754	475	148	130	1			
23	21	97	Total	C	N	O	S	0	0	0
			759	478	149	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
			592	368	119	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
			546	346	96	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
			536	342	98	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
			459	288	90	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	1504	Total	C	N	O	P	0	0	0
			32331	14396	5990	10441	1504			

- 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
			1842	1175	330	332	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
			1558	979	305	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
			1665	1043	329	286	7			
35	2d	208	Total	C	N	O	S	0	0	0
			1668	1047	330	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
			1133	716	214	199	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
			814	516	144	151	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
			1235	769	244	216	6			
38	2g	155	Total	C	N	O	S	0	0	0
			1229	766	241	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
			1098	694	210	192	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
			986	625	193	168			
40	2i	126	Total	C	N	O	0	0	0
			966	613	186	167			

- 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
			719	446	142	131			
41	2j	96	Total	C	N	O	0	0	0
			710	442	137	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
			834	520	156	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	116	Total	C	N	O	S	0	0	0
			914	564	189	159	2			
44	2m	114	Total	C	N	O	S	0	0	0
			895	550	186	157	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
			648	415	120	111	2			
50	2s	83	Total	C	N	O	S	0	0	0
			645	410	118	115	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
			732	449	157	124	2			
51	2t	98	Total	C	N	O	S	0	0	0
			733	451	154	126	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 protein called Ribosome-associated inhibitor A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1y	97	Total 764	C 478	N 144	O 139	S 3	0	0	0
53	2y	96	Total 749	C 468	N 141	O 137	S 3	0	0	0

- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	1A	1040	Total 1040	Mg 1040	0	0
54	1B	29	Total 29	Mg 29	0	0
54	1D	18	Total 18	Mg 18	0	0
54	1E	8	Total 8	Mg 8	0	0
54	1F	18	Total 18	Mg 18	0	0
54	1G	4	Total 4	Mg 4	0	0
54	1H	2	Total 2	Mg 2	0	0
54	1N	4	Total 4	Mg 4	0	0
54	1O	1	Total 1	Mg 1	0	0
54	1P	5	Total 5	Mg 5	0	0
54	1Q	5	Total 5	Mg 5	0	0
54	1R	5	Total 5	Mg 5	0	0
54	1T	5	Total 5	Mg 5	0	0
54	1U	7	Total 7	Mg 7	0	0
54	1V	6	Total 6	Mg 6	0	0
54	1W	3	Total 3	Mg 3	0	0
54	1Y	1	Total 1	Mg 1	0	0
54	1Z	1	Total 1	Mg 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	10	8	Total Mg 8 8	0	0
54	11	5	Total Mg 5 5	0	0
54	13	3	Total Mg 3 3	0	0
54	14	1	Total Mg 1 1	0	0
54	15	8	Total Mg 8 8	0	0
54	17	6	Total Mg 6 6	0	0
54	18	2	Total Mg 2 2	0	0
54	19	2	Total Mg 2 2	0	0
54	1a	279	Total Mg 279 279	0	0
54	1b	1	Total Mg 1 1	0	0
54	1d	5	Total Mg 5 5	0	0
54	1e	3	Total Mg 3 3	0	0
54	1f	2	Total Mg 2 2	0	0
54	1g	3	Total Mg 3 3	0	0
54	1h	2	Total Mg 2 2	0	0
54	1i	1	Total Mg 1 1	0	0
54	1k	1	Total Mg 1 1	0	0
54	1l	2	Total Mg 2 2	0	0
54	1m	2	Total Mg 2 2	0	0
54	1n	2	Total Mg 2 2	0	0
54	1o	1	Total Mg 1 1	0	0

Continued on next page...

Continued from previous page...

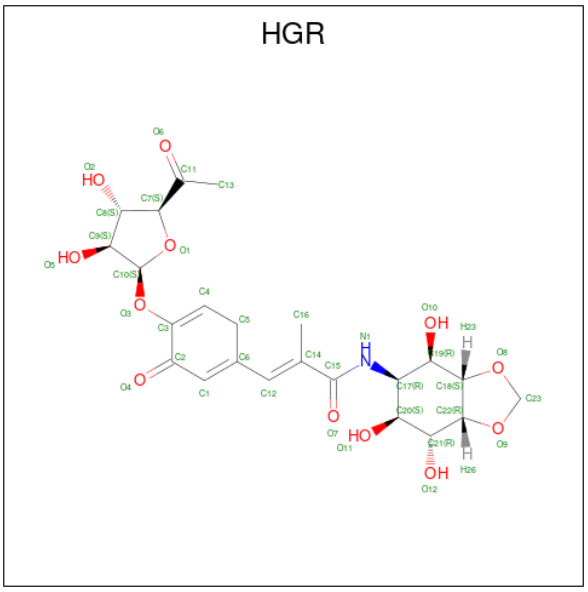
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	1t	1	Total Mg 1 1	0	0
54	1y	3	Total Mg 3 3	0	0
54	2A	730	Total Mg 730 730	0	0
54	2B	18	Total Mg 18 18	0	0
54	2D	13	Total Mg 13 13	0	0
54	2E	6	Total Mg 6 6	0	0
54	2F	4	Total Mg 4 4	0	0
54	2G	2	Total Mg 2 2	0	0
54	2I	1	Total Mg 1 1	0	0
54	2O	2	Total Mg 2 2	0	0
54	2P	1	Total Mg 1 1	0	0
54	2Q	1	Total Mg 1 1	0	0
54	2R	3	Total Mg 3 3	0	0
54	2T	3	Total Mg 3 3	0	0
54	2U	1	Total Mg 1 1	0	0
54	2V	2	Total Mg 2 2	0	0
54	2W	2	Total Mg 2 2	0	0
54	2X	1	Total Mg 1 1	0	0
54	2Y	1	Total Mg 1 1	0	0
54	20	1	Total Mg 1 1	0	0
54	21	2	Total Mg 2 2	0	0

Continued on next page...

Continued from previous page...

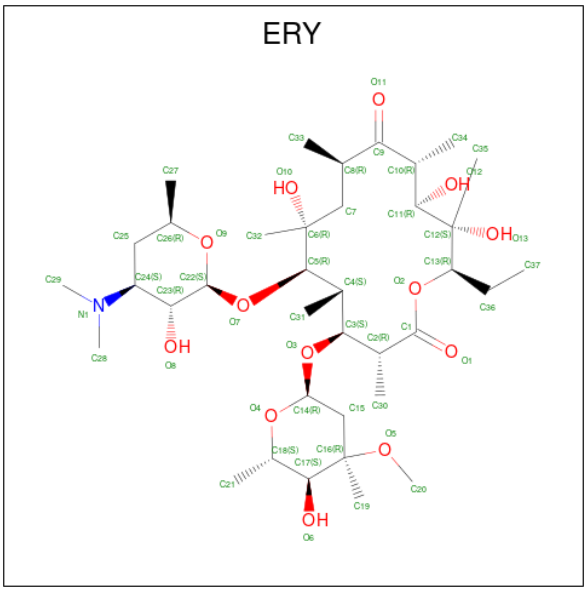
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	23	1	Total Mg 1 1	0	0
54	25	3	Total Mg 3 3	0	0
54	27	2	Total Mg 2 2	0	0
54	28	2	Total Mg 2 2	0	0
54	2a	190	Total Mg 190 190	0	0
54	2e	2	Total Mg 2 2	0	0
54	2f	1	Total Mg 1 1	0	0
54	2j	1	Total Mg 1 1	0	0
54	2k	1	Total Mg 1 1	0	0
54	2n	1	Total Mg 1 1	0	0
54	2r	2	Total Mg 2 2	0	0
54	2t	1	Total Mg 1 1	0	0
54	2y	1	Total Mg 1 1	0	0

- Molecule 55 is Hygromycin A (CCD ID: HGR) (formula: $C_{23}H_{29}NO_{12}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	1A	1	Total C N O 36 23 1 12	0	0
55	2A	1	Total C N O 36 23 1 12	0	0

- Molecule 56 is ERYTHROMYCIN A (CCD ID: ERY) (formula: $C_{37}H_{67}NO_{13}$) (labeled as "Ligand of Interest" by depositor).



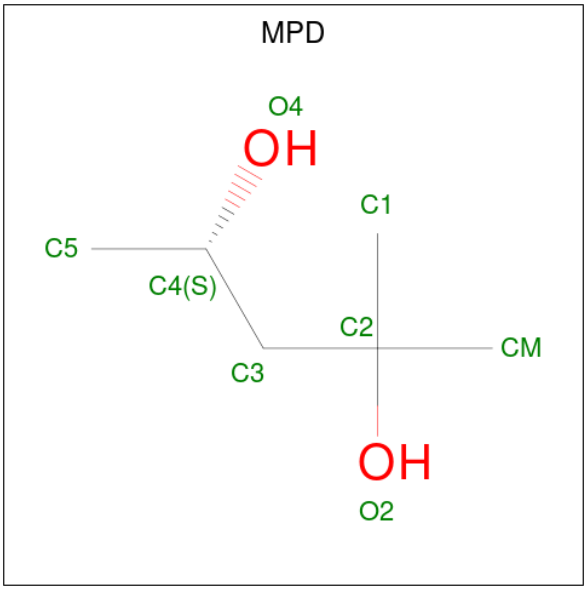
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	1A	1	Total C N O 51 37 1 13	0	0

Continued on next page...

Continued from previous page...

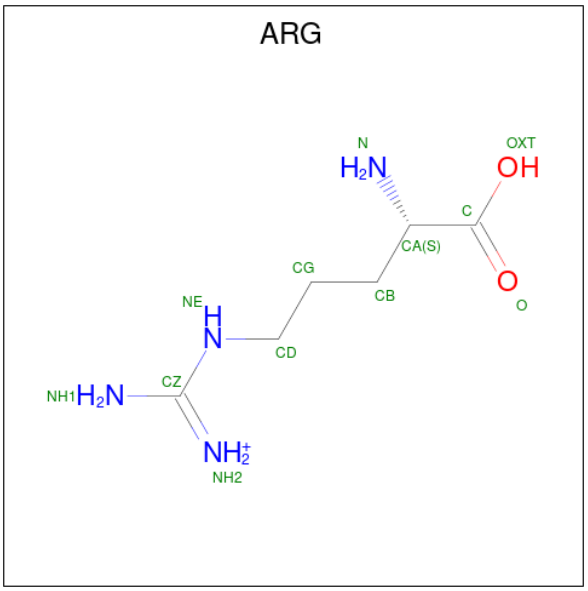
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	2A	1	Total C N O 51 37 1 13	0	0

- Molecule 57 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	1A	1	Total C O 8 6 2	0	0
57	1T	1	Total C O 8 6 2	0	0
57	18	1	Total C O 8 6 2	0	0
57	1a	1	Total C O 8 6 2	0	0
57	2A	1	Total C O 8 6 2	0	0
57	2A	1	Total C O 8 6 2	0	0
57	2B	1	Total C O 8 6 2	0	0

- Molecule 58 is ARGININE (CCD ID: ARG) (formula: $C_6H_{15}N_4O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	1B	1	Total C N O 12 6 4 2	0	0
58	1F	1	Total C N O 12 6 4 2	0	0

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

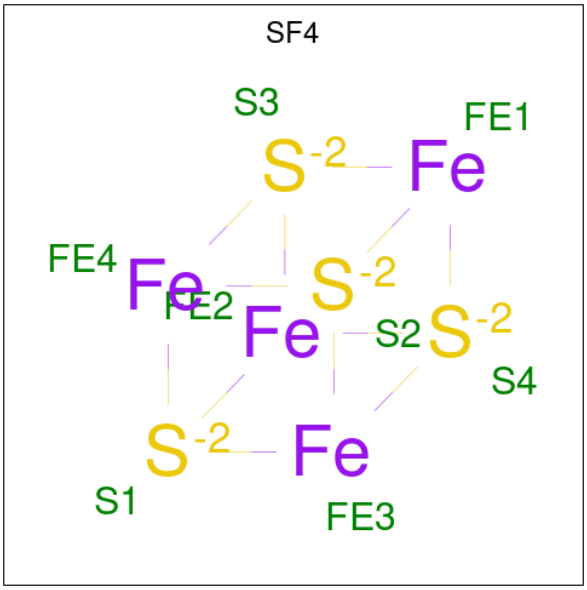
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	1Y	1	Total Zn 1 1	0	0
59	14	1	Total Zn 1 1	0	0
59	15	1	Total Zn 1 1	0	0
59	16	1	Total Zn 1 1	0	0
59	19	1	Total Zn 1 1	0	0
59	1n	1	Total Zn 1 1	0	0
59	2Y	1	Total Zn 1 1	0	0
59	24	1	Total Zn 1 1	0	0
59	25	1	Total Zn 1 1	0	0
59	26	1	Total Zn 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	29	1	Total Zn 1 1	0	0
59	2n	1	Total Zn 1 1	0	0

- Molecule 60 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 61 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	3898	Total O 3898 3898	0	0
61	1B	94	Total O 94 94	0	0
61	1D	103	Total O 103 103	0	0
61	1E	68	Total O 68 68	0	0
61	1F	64	Total O 64 64	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1G	16	Total O 16 16	0	0
61	1H	15	Total O 15 15	0	0
61	1I	5	Total O 5 5	0	0
61	1N	45	Total O 45 45	0	0
61	1O	22	Total O 22 22	0	0
61	1P	56	Total O 56 56	0	0
61	1Q	37	Total O 37 37	0	0
61	1R	29	Total O 29 29	0	0
61	1S	12	Total O 12 12	0	0
61	1T	37	Total O 37 37	0	0
61	1U	41	Total O 41 41	0	0
61	1V	34	Total O 34 34	0	0
61	1W	27	Total O 27 27	0	0
61	1X	27	Total O 27 27	0	0
61	1Y	16	Total O 16 16	0	0
61	1Z	5	Total O 5 5	0	0
61	10	21	Total O 21 21	0	0
61	11	28	Total O 28 28	0	0
61	12	14	Total O 14 14	0	0
61	13	22	Total O 22 22	0	0
61	14	4	Total O 4 4	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	15	25	Total O 25 25	0	0
61	16	21	Total O 21 21	0	0
61	17	13	Total O 13 13	0	0
61	18	23	Total O 23 23	0	0
61	19	2	Total O 2 2	0	0
61	1a	447	Total O 447 447	0	0
61	1b	1	Total O 1 1	0	0
61	1c	2	Total O 2 2	0	0
61	1d	9	Total O 9 9	0	0
61	1e	5	Total O 5 5	0	0
61	1f	1	Total O 1 1	0	0
61	1h	1	Total O 1 1	0	0
61	1j	1	Total O 1 1	0	0
61	1l	3	Total O 3 3	0	0
61	1o	2	Total O 2 2	0	0
61	1p	2	Total O 2 2	0	0
61	1y	1	Total O 1 1	0	0
61	2A	1941	Total O 1941 1941	0	0
61	2B	45	Total O 45 45	0	0
61	2D	45	Total O 45 45	0	0
61	2E	25	Total O 25 25	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2F	15	Total O 15 15	0	0
61	2G	2	Total O 2 2	0	0
61	2H	1	Total O 1 1	0	0
61	2I	1	Total O 1 1	0	0
61	2N	3	Total O 3 3	0	0
61	2O	10	Total O 10 10	0	0
61	2P	19	Total O 19 19	0	0
61	2Q	13	Total O 13 13	0	0
61	2R	17	Total O 17 17	0	0
61	2T	6	Total O 6 6	0	0
61	2U	7	Total O 7 7	0	0
61	2V	4	Total O 4 4	0	0
61	2W	20	Total O 20 20	0	0
61	2X	7	Total O 7 7	0	0
61	2Y	2	Total O 2 2	0	0
61	2Z	7	Total O 7 7	0	0
61	20	5	Total O 5 5	0	0
61	21	15	Total O 15 15	0	0
61	22	1	Total O 1 1	0	0
61	23	2	Total O 2 2	0	0
61	25	7	Total O 7 7	0	0

Continued on next page...

Continued from previous page...

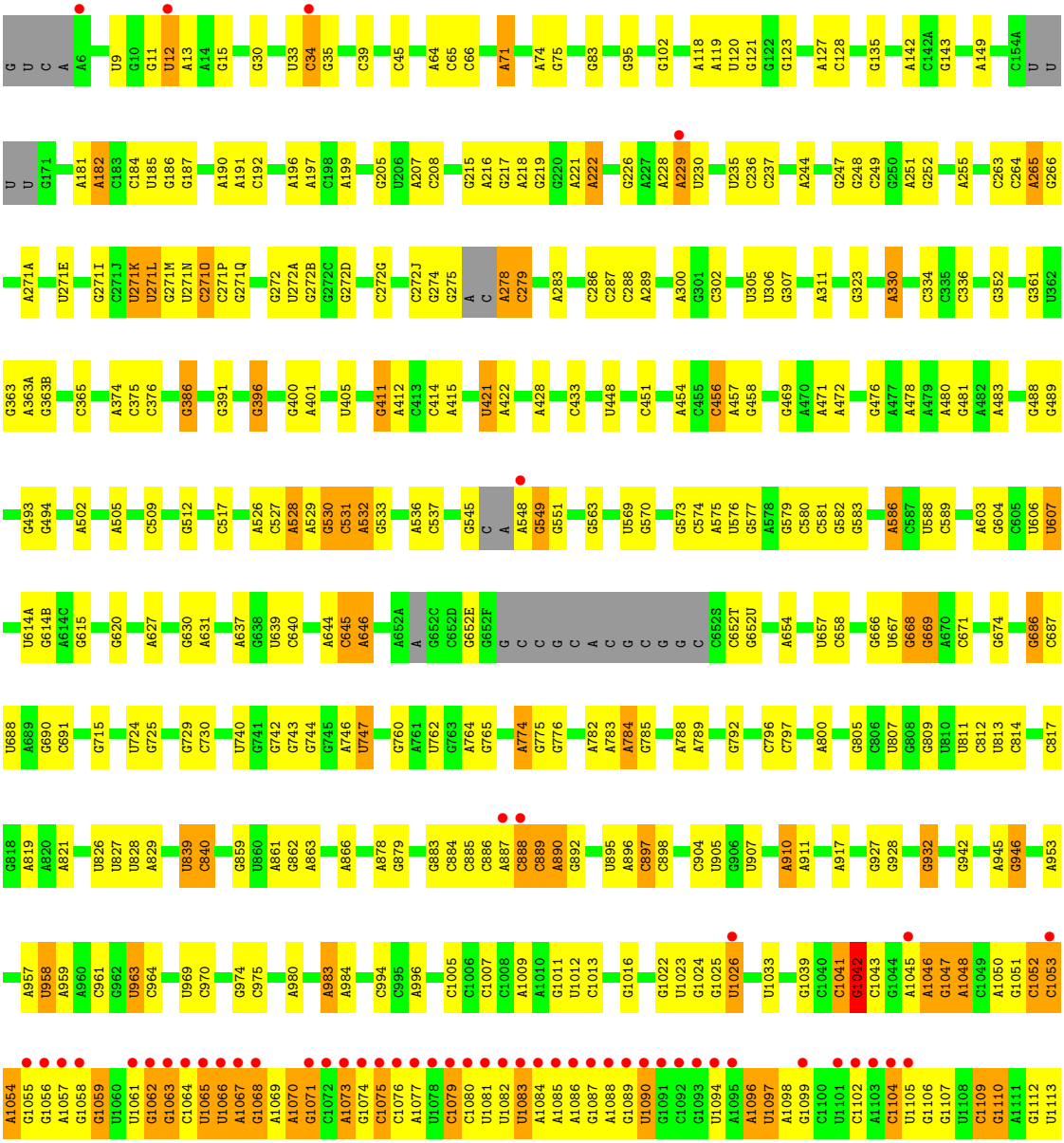
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	26	2	Total O 2 2	0	0
61	27	8	Total O 8 8	0	0
61	28	9	Total O 9 9	0	0
61	2a	266	Total O 266 266	0	0
61	2d	4	Total O 4 4	0	0
61	2e	1	Total O 1 1	0	0
61	2l	1	Total O 1 1	0	0
61	2o	2	Total O 2 2	0	0
61	2q	1	Total O 1 1	0	0
61	2r	3	Total O 3 3	0	0
61	2u	1	Total O 1 1	0	0

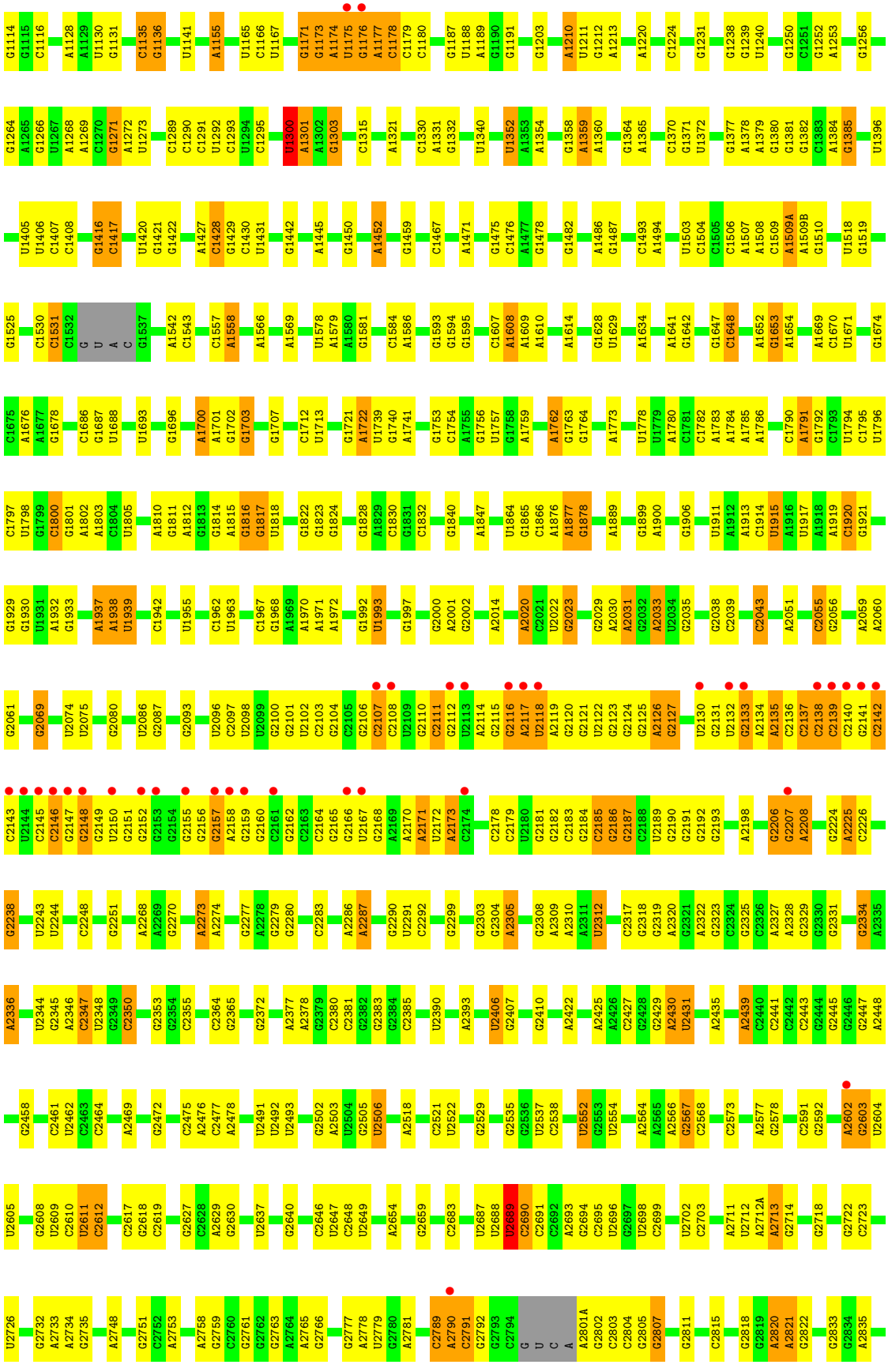
3 Residue-property plots (i)

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

- Molecule 1: 23S Ribosomal RNA

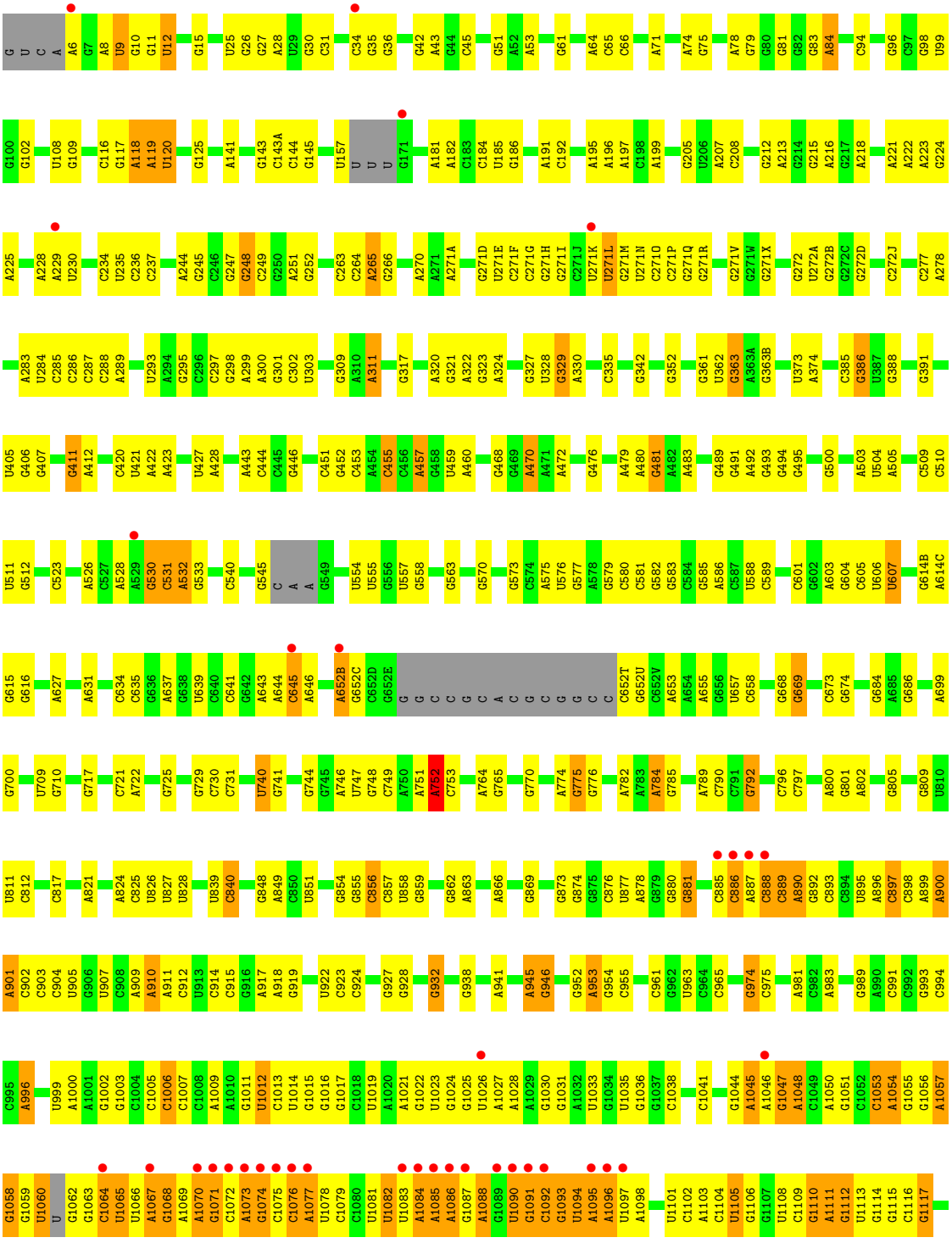
Chain 1A:

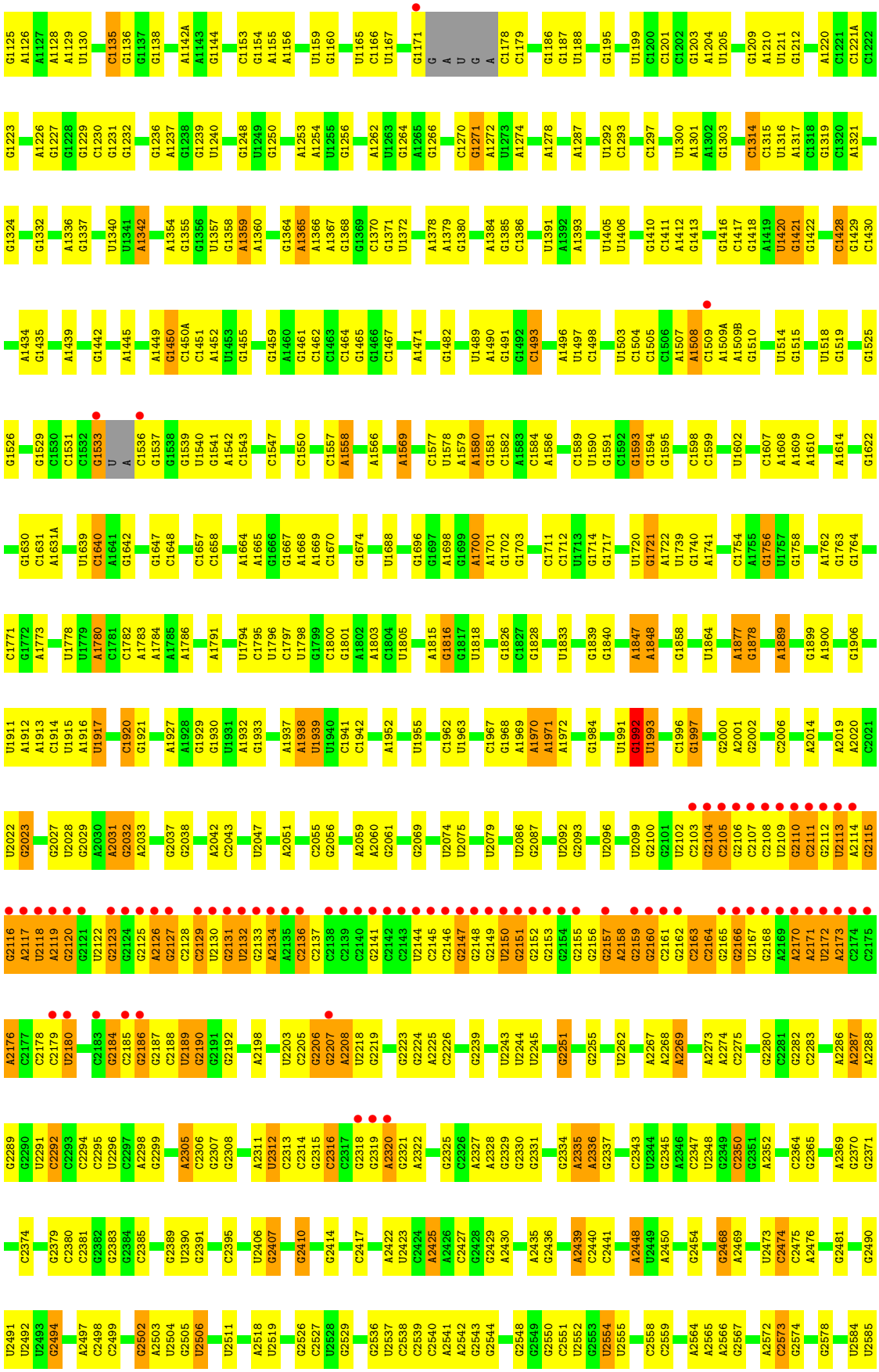


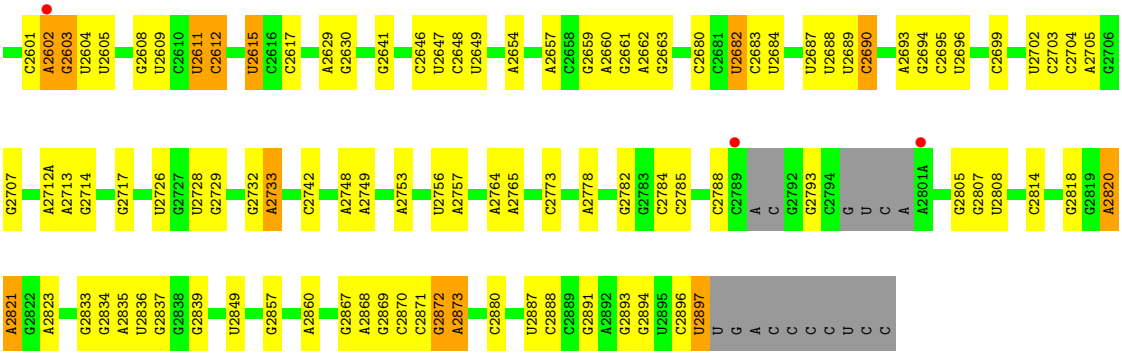


• Molecule 1: 23S Ribosomal RNA

Chain 2A:

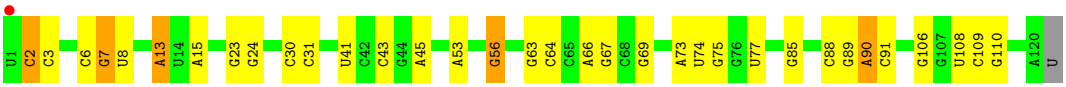






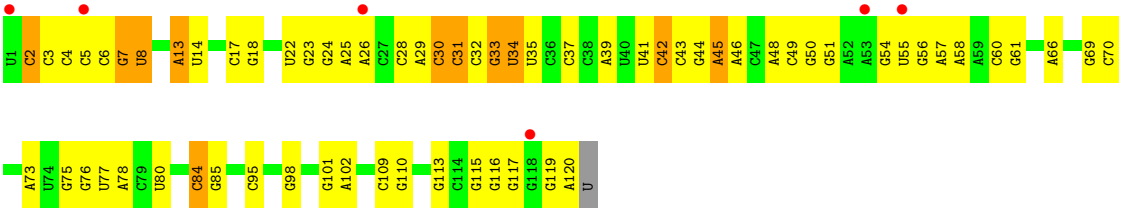
• Molecule 2: 5S Ribosomal RNA

Chain 1B:



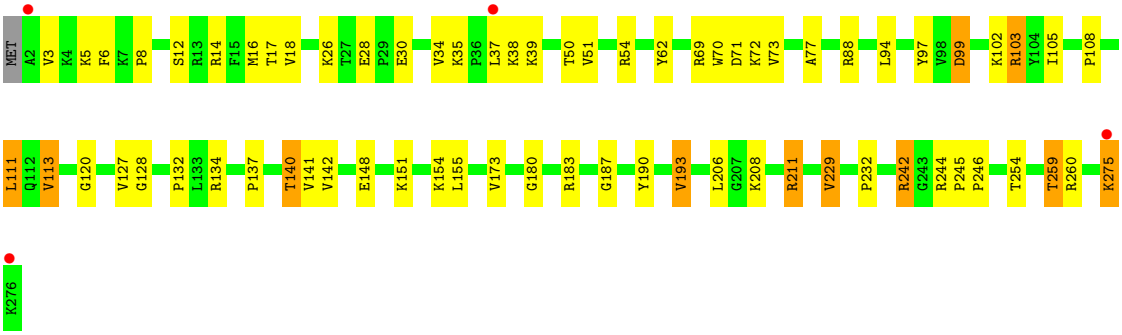
• Molecule 2: 5S Ribosomal RNA

Chain 2B:



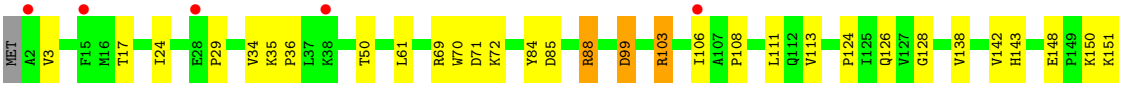
• Molecule 3: 50S ribosomal protein L2

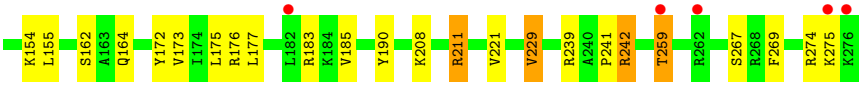
Chain 1D:



• Molecule 3: 50S ribosomal protein L2

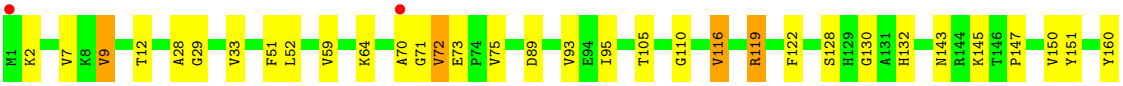
Chain 2D:

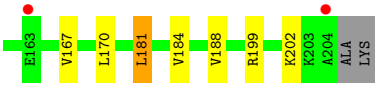




• Molecule 4: 50S ribosomal protein L3

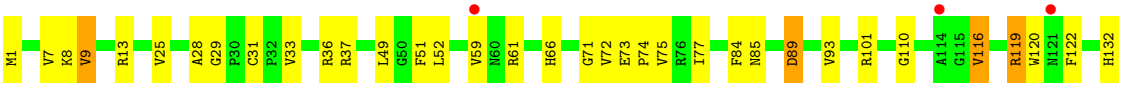
Chain 1E:

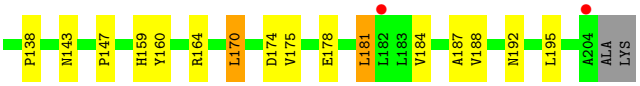




• Molecule 4: 50S ribosomal protein L3

Chain 2E:



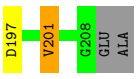


• Molecule 5: 50S ribosomal protein L4

Chain 1F:

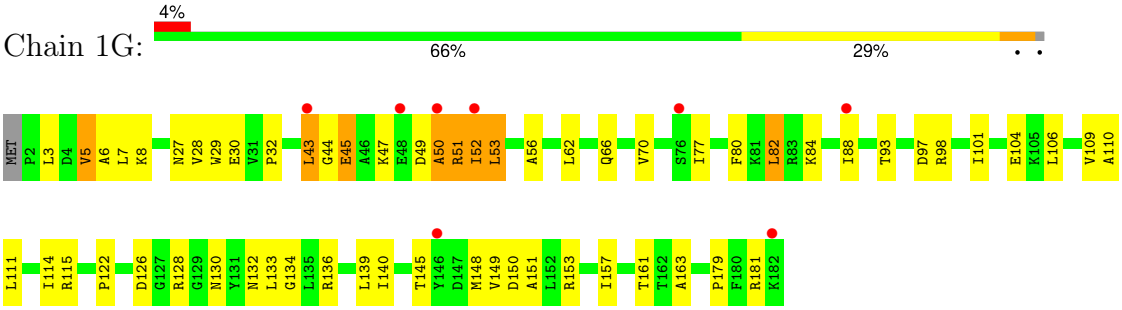
• Molecule 5: 50S ribosomal protein L4

Chain 2F:



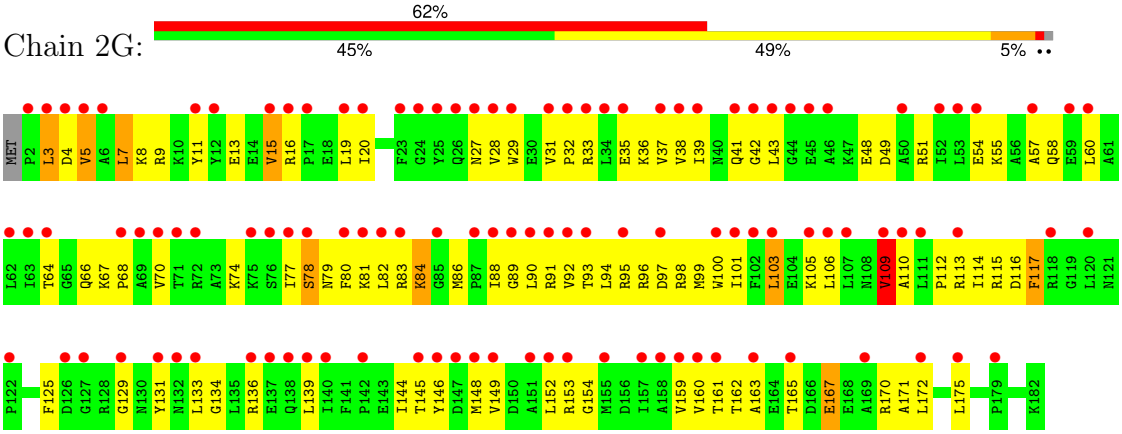
• Molecule 6: 50S ribosomal protein L5

Chain 1G:



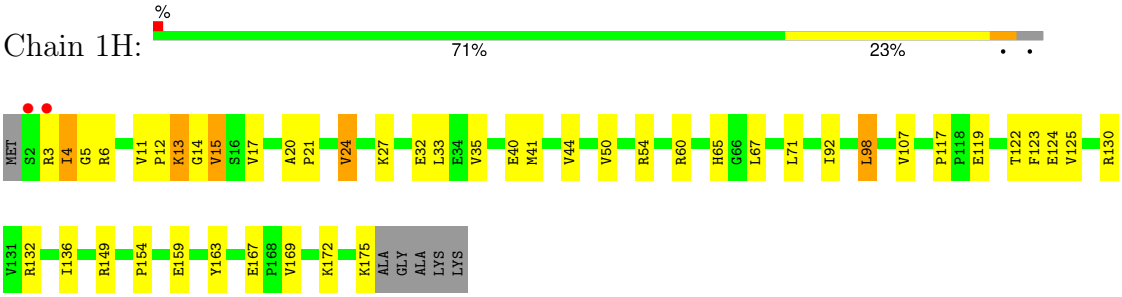
• Molecule 6: 50S ribosomal protein L5

Chain 2G:



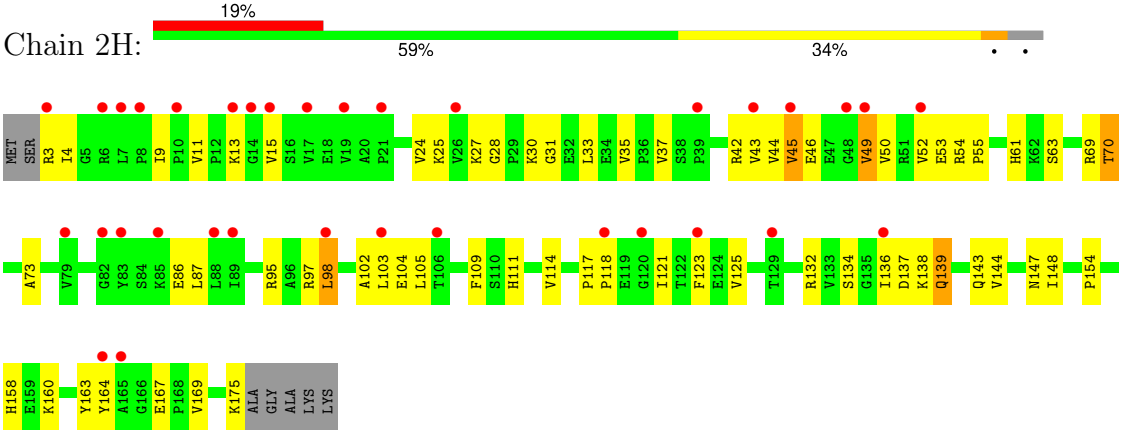
• Molecule 7: 50S ribosomal protein L6

Chain 1H:



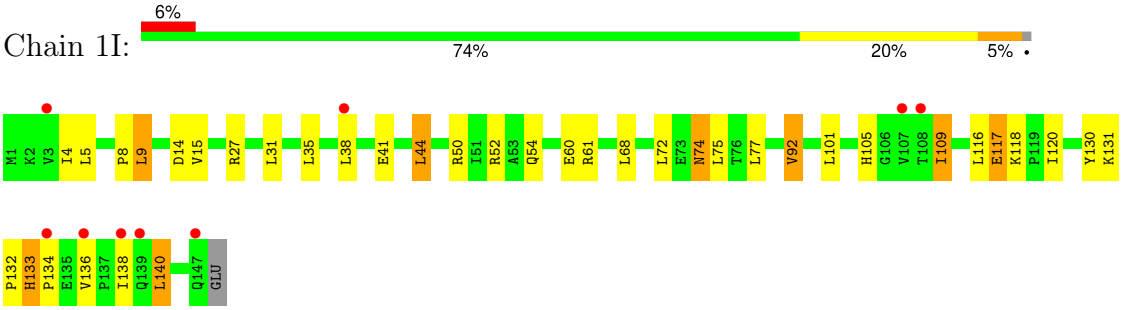
• Molecule 7: 50S ribosomal protein L6

Chain 2H:



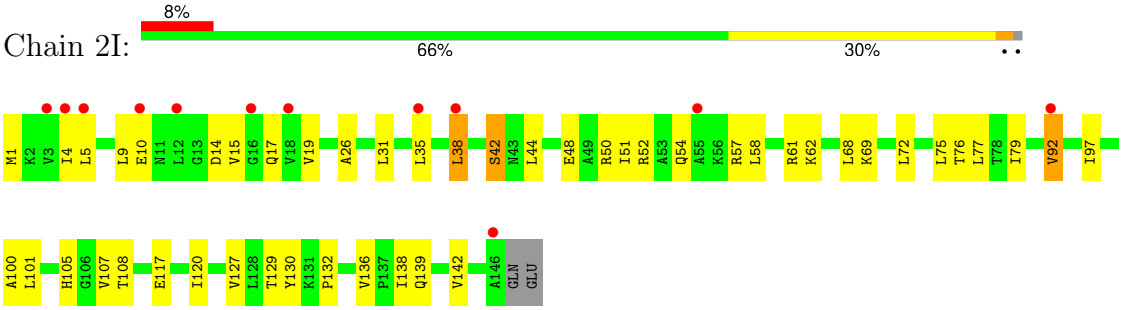
• Molecule 8: 50S ribosomal protein L9

Chain 1I:



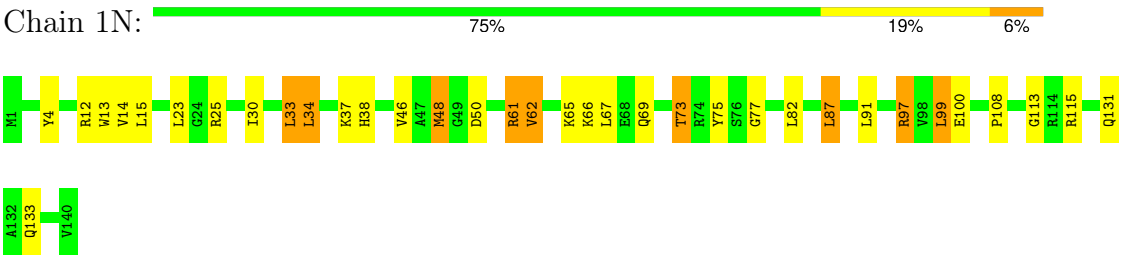
• Molecule 8: 50S ribosomal protein L9

Chain 2I:



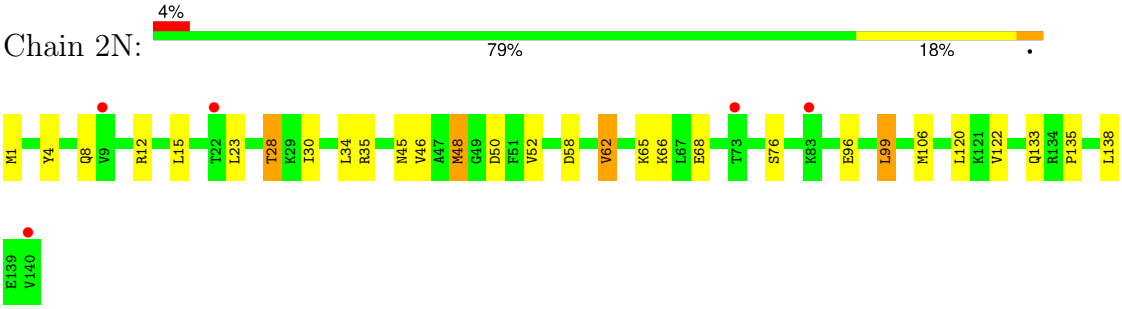
• Molecule 9: 50S ribosomal protein L13

Chain 1N:



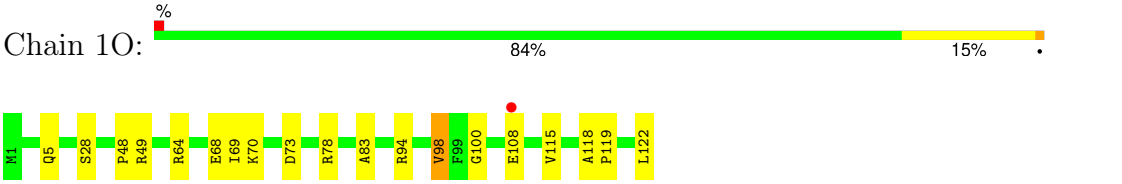
• Molecule 9: 50S ribosomal protein L13

Chain 2N:



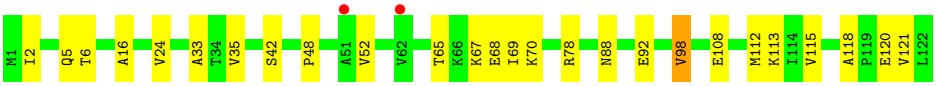
• Molecule 10: 50S ribosomal protein L14

Chain 1O:



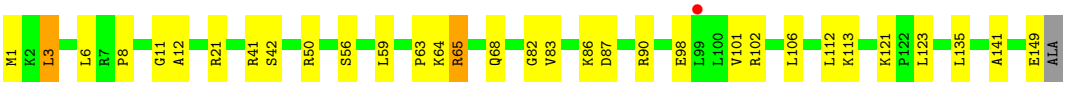
• Molecule 10: 50S ribosomal protein L14

Chain 2O:



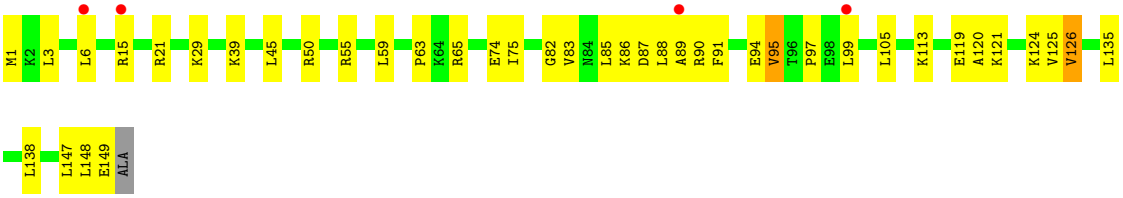
• Molecule 11: 50S ribosomal protein L15

Chain 1P:



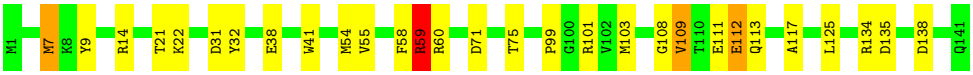
• Molecule 11: 50S ribosomal protein L15

Chain 2P:



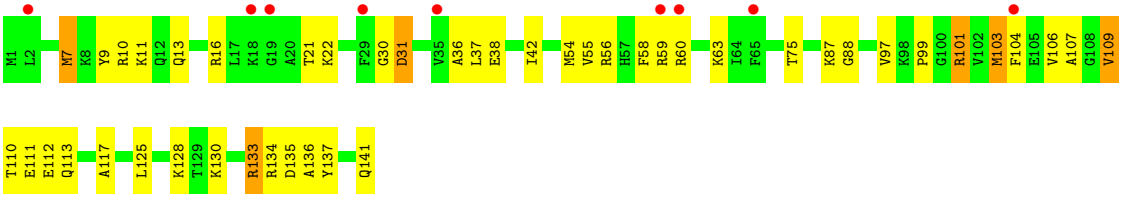
• Molecule 12: 50S ribosomal protein L16

Chain 1Q:



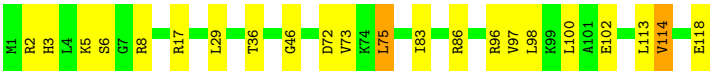
• Molecule 12: 50S ribosomal protein L16

Chain 2Q:



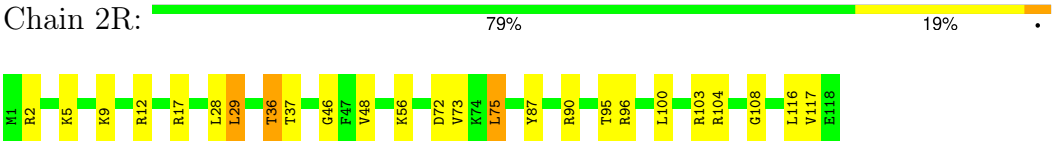
• Molecule 13: 50S ribosomal protein L17

Chain 1R:



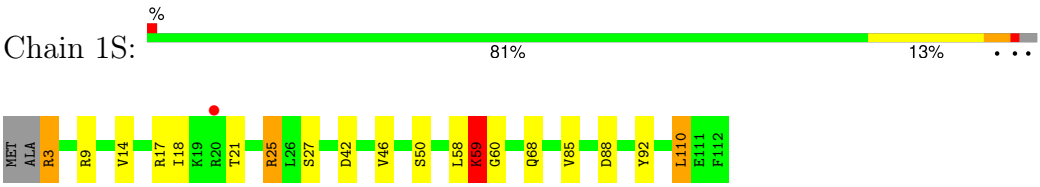
• Molecule 13: 50S ribosomal protein L17

Chain 2R:



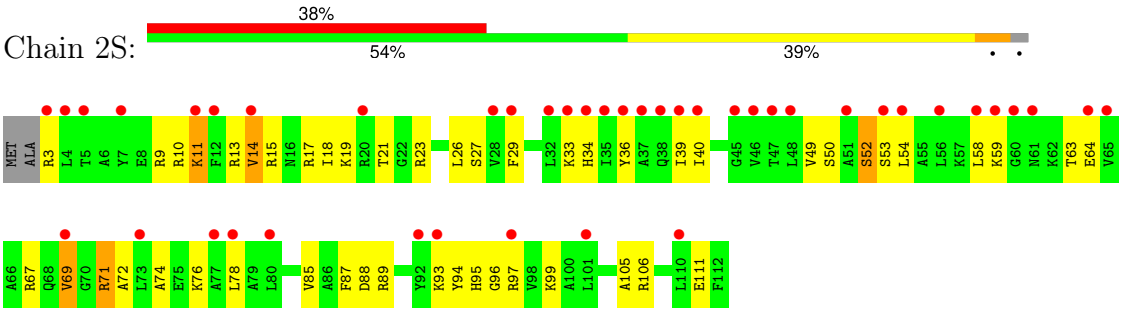
• Molecule 14: 50S ribosomal protein L18

Chain 1S:



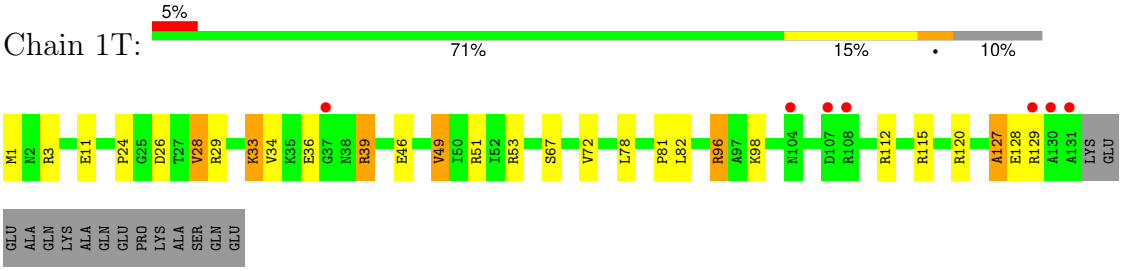
• Molecule 14: 50S ribosomal protein L18

Chain 2S:



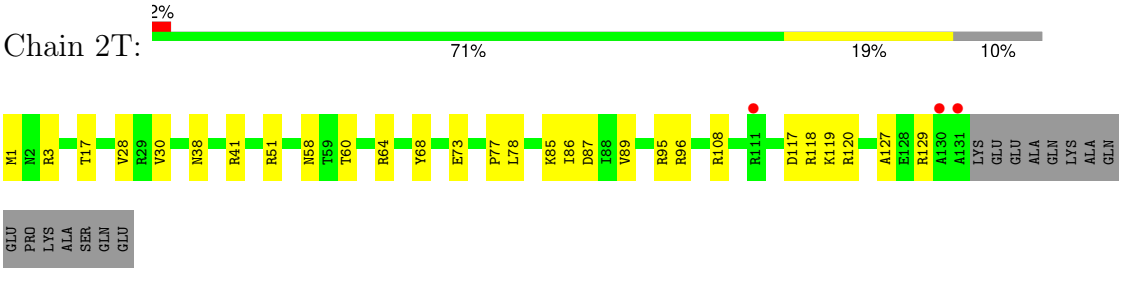
• Molecule 15: 50S ribosomal protein L19

Chain 1T:



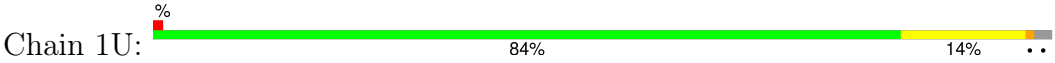
• Molecule 15: 50S ribosomal protein L19

Chain 2T:



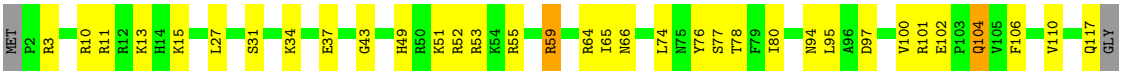
• Molecule 16: 50S ribosomal protein L20

Chain 1U:



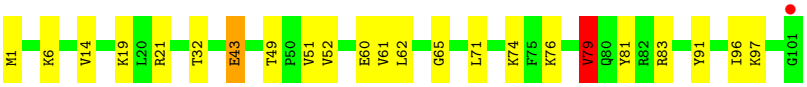
• Molecule 16: 50S ribosomal protein L20

Chain 2U:



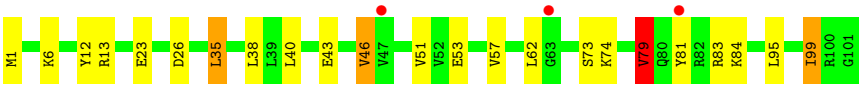
• Molecule 17: 50S ribosomal protein L21

Chain 1V:



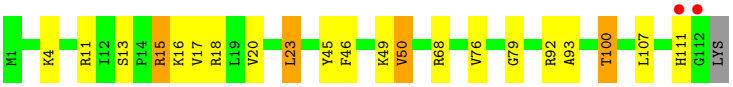
• Molecule 17: 50S ribosomal protein L21

Chain 2V:



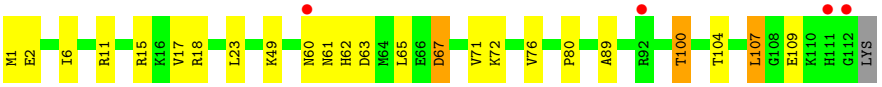
• Molecule 18: 50S ribosomal protein L22

Chain 1W:



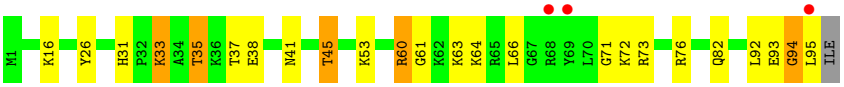
• Molecule 18: 50S ribosomal protein L22

Chain 2W:



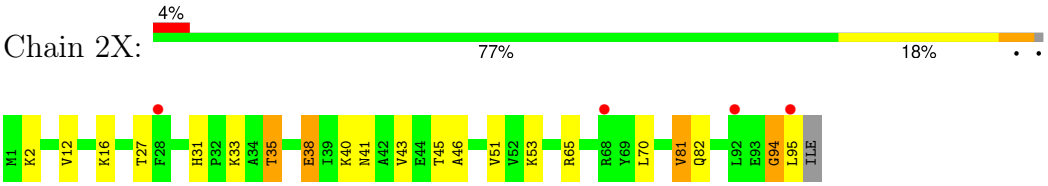
• Molecule 19: 50S ribosomal protein L23

Chain 1X:



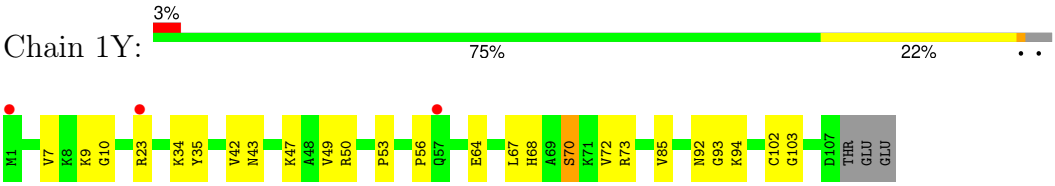
• Molecule 19: 50S ribosomal protein L23

Chain 2X:



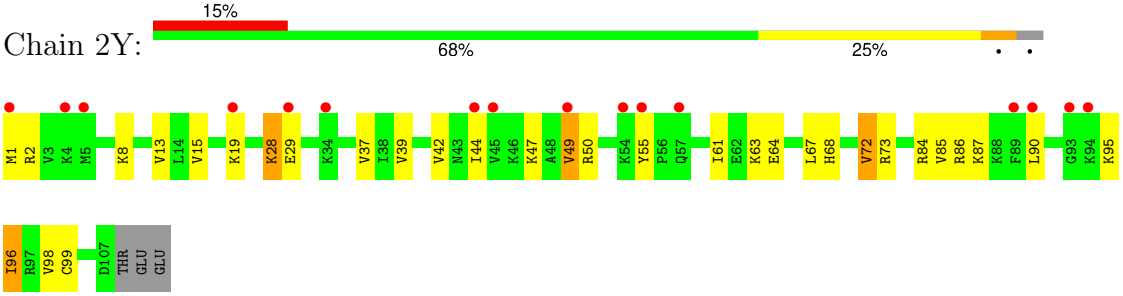
• Molecule 20: 50S ribosomal protein L24

Chain 1Y:



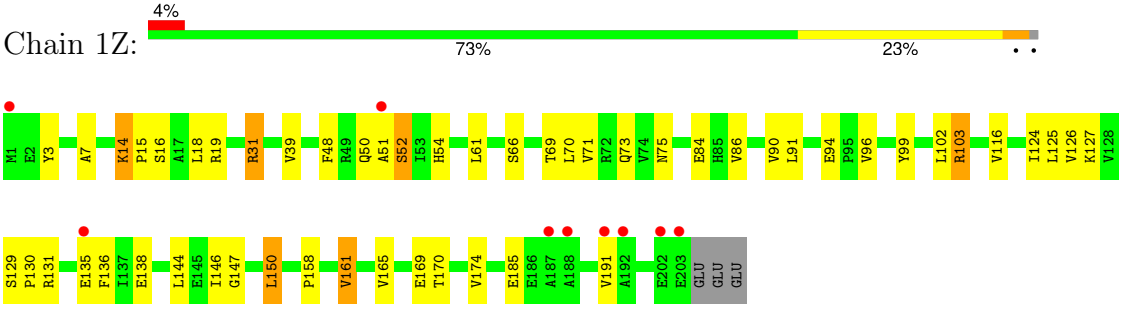
• Molecule 20: 50S ribosomal protein L24

Chain 2Y:



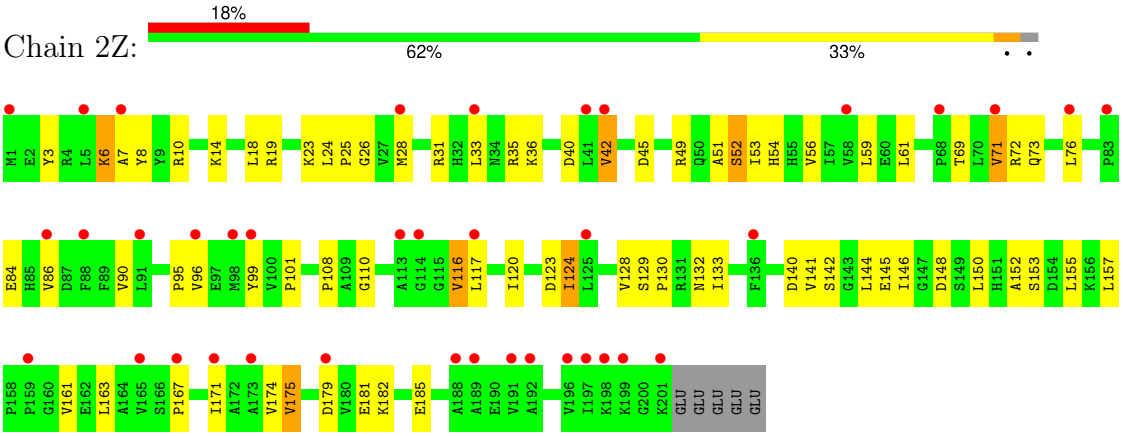
• Molecule 21: 50S ribosomal protein L25

Chain 1Z:



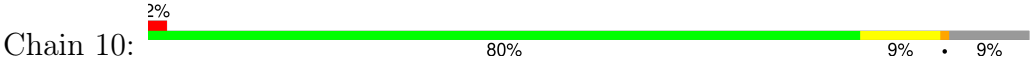
• Molecule 21: 50S ribosomal protein L25

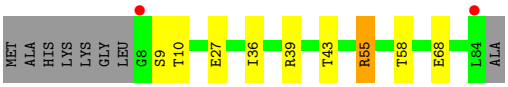
Chain 2Z:



• Molecule 22: 50S ribosomal protein L27

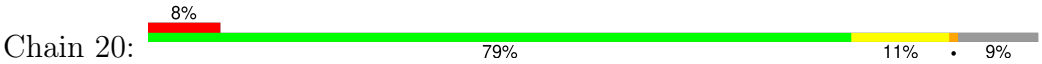
Chain 10:

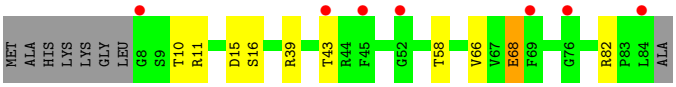




• Molecule 22: 50S ribosomal protein L27

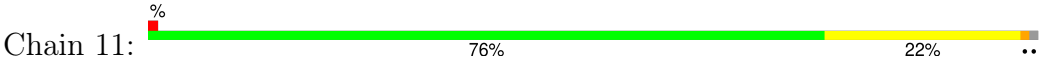
Chain 20:

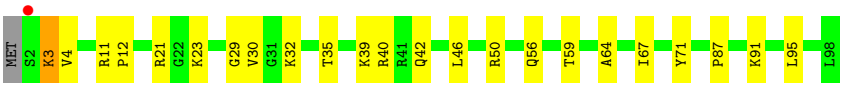




• Molecule 23: 50S ribosomal protein L28

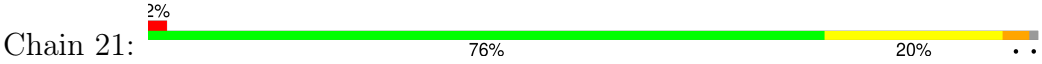
Chain 11:





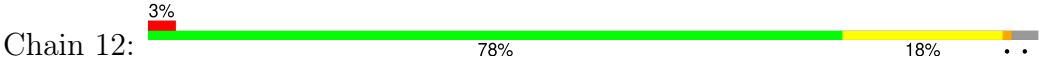
• Molecule 23: 50S ribosomal protein L28

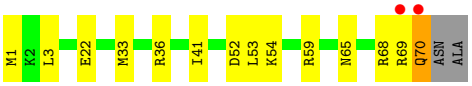
Chain 21:



• Molecule 24: 50S ribosomal protein L29

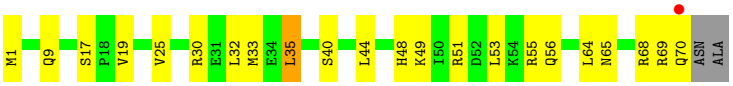
Chain 12:





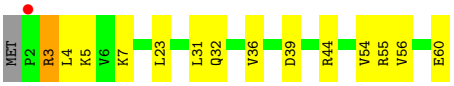
• Molecule 24: 50S ribosomal protein L29

Chain 22:



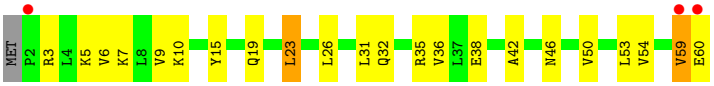
• Molecule 25: 50S ribosomal protein L30

Chain 13:



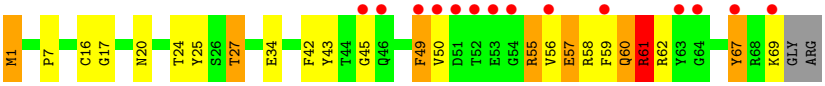
• Molecule 25: 50S ribosomal protein L30

Chain 23:



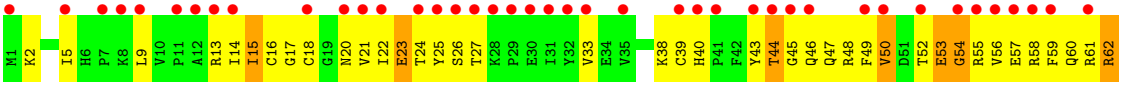
• Molecule 26: 50S ribosomal protein L31

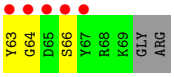
Chain 14:



• Molecule 26: 50S ribosomal protein L31

Chain 24:



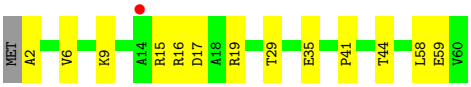


• Molecule 27: 50S ribosomal protein L32

Chain 15:

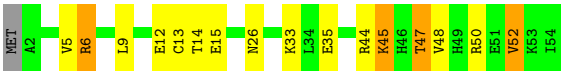
• Molecule 27: 50S ribosomal protein L32

Chain 25:



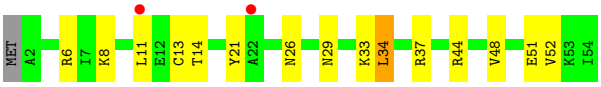
• Molecule 28: 50S ribosomal protein L33

Chain 16:



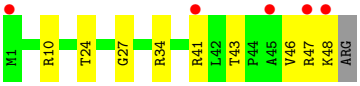
• Molecule 28: 50S ribosomal protein L33

Chain 26:



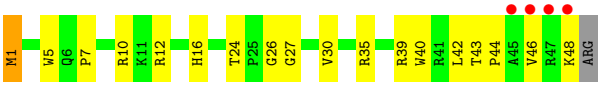
• Molecule 29: 50S ribosomal protein L34

Chain 17:



• Molecule 29: 50S ribosomal protein L34

Chain 27:

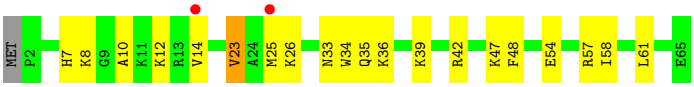


• Molecule 30: 50S ribosomal protein L35

Chain 18:

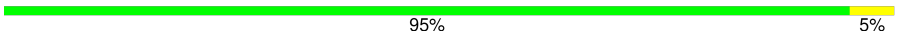
• Molecule 30: 50S ribosomal protein L35

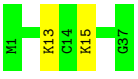
Chain 28:



• Molecule 31: 50S ribosomal protein L36

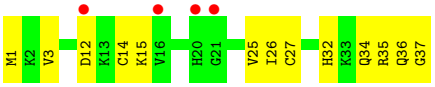
Chain 19:





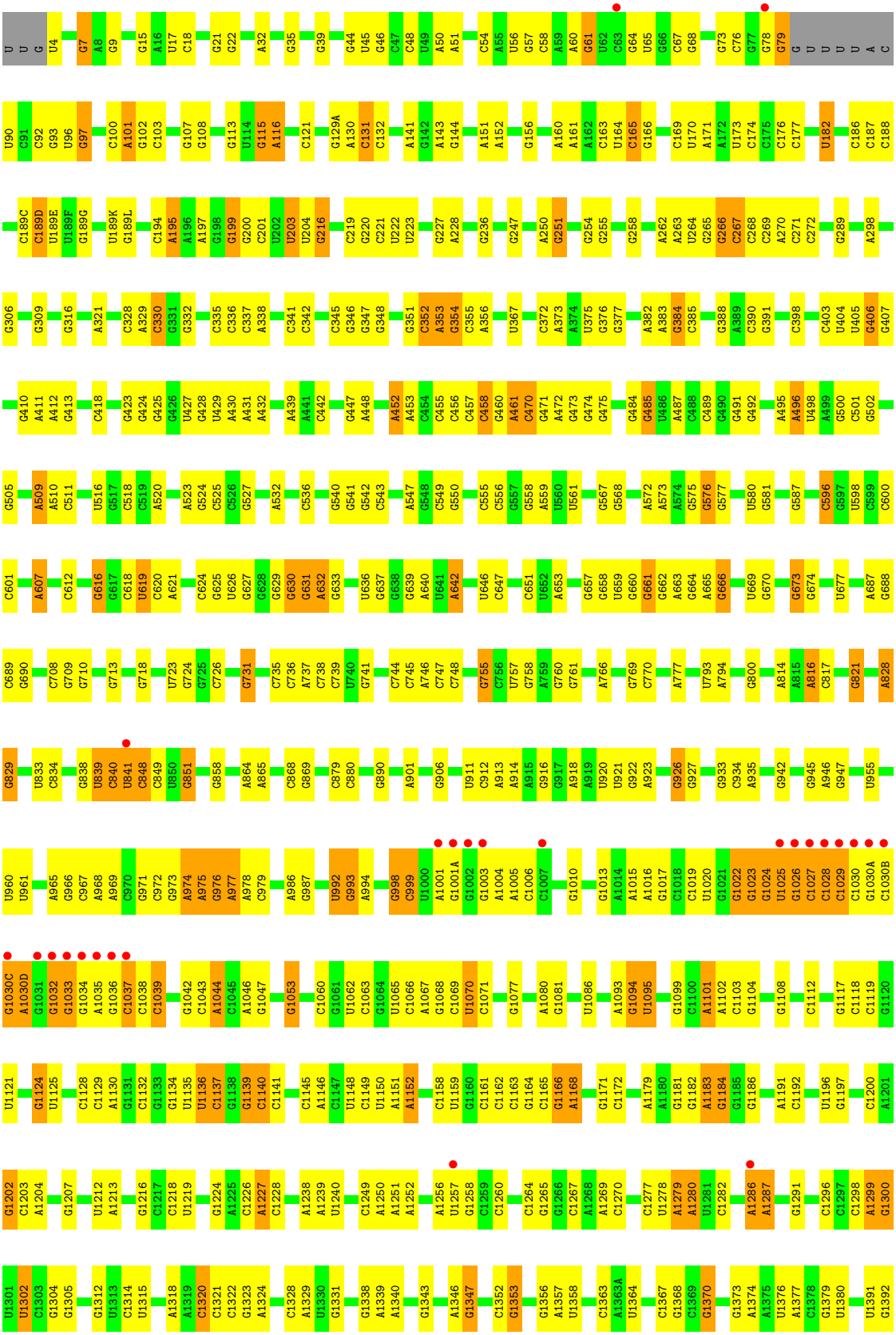
• Molecule 31: 50S ribosomal protein L36

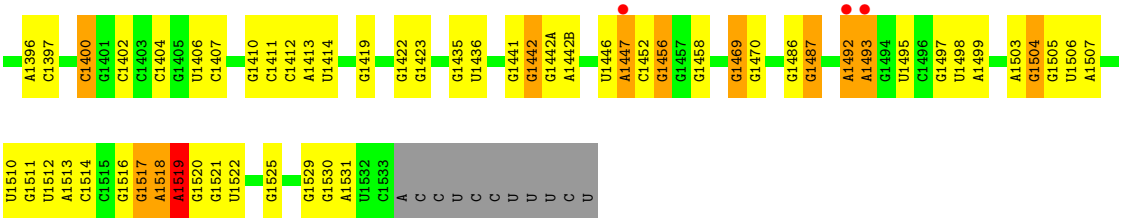
Chain 29:



• Molecule 32: 16S Ribosomal RNA

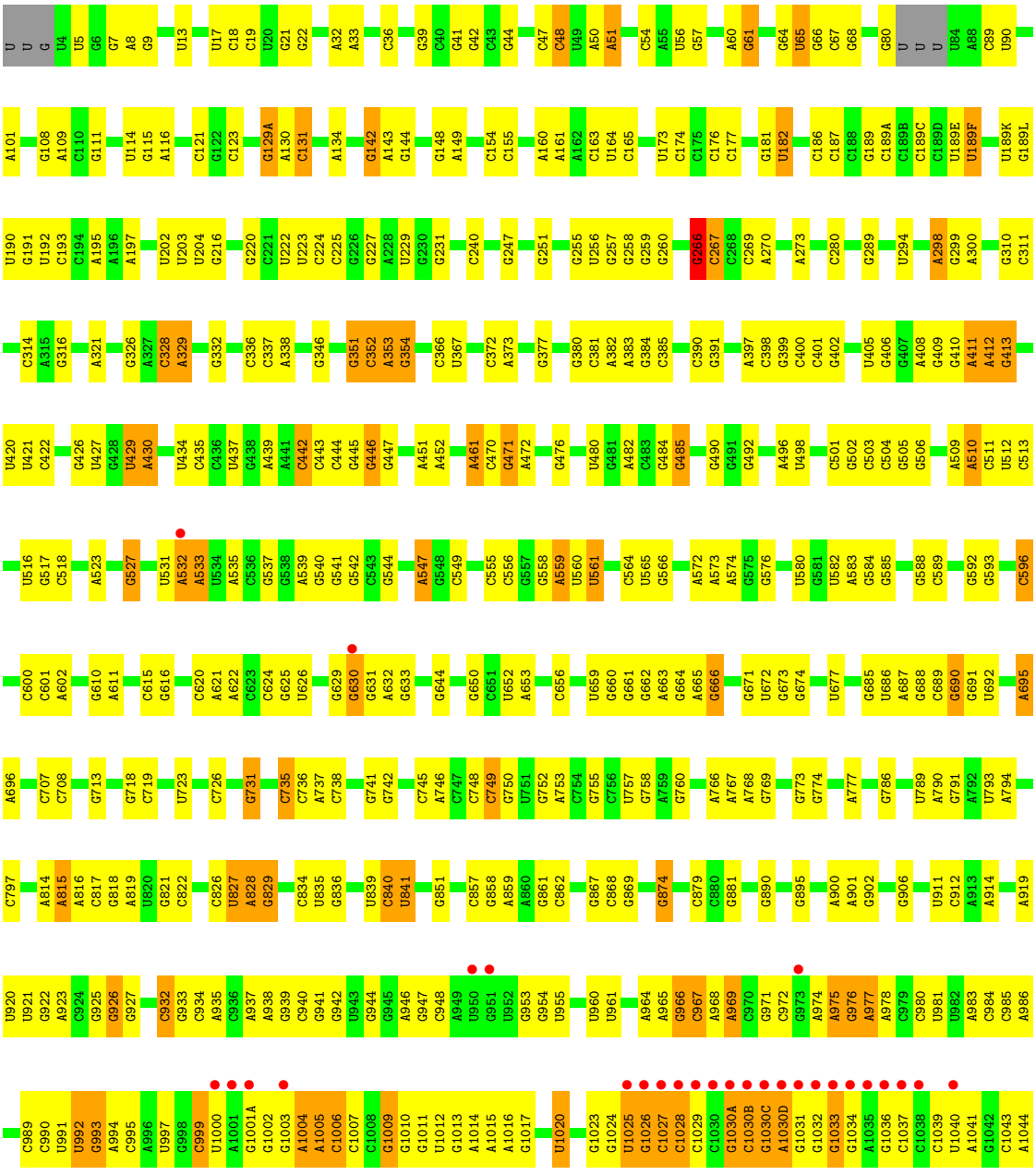
Chain 1a:

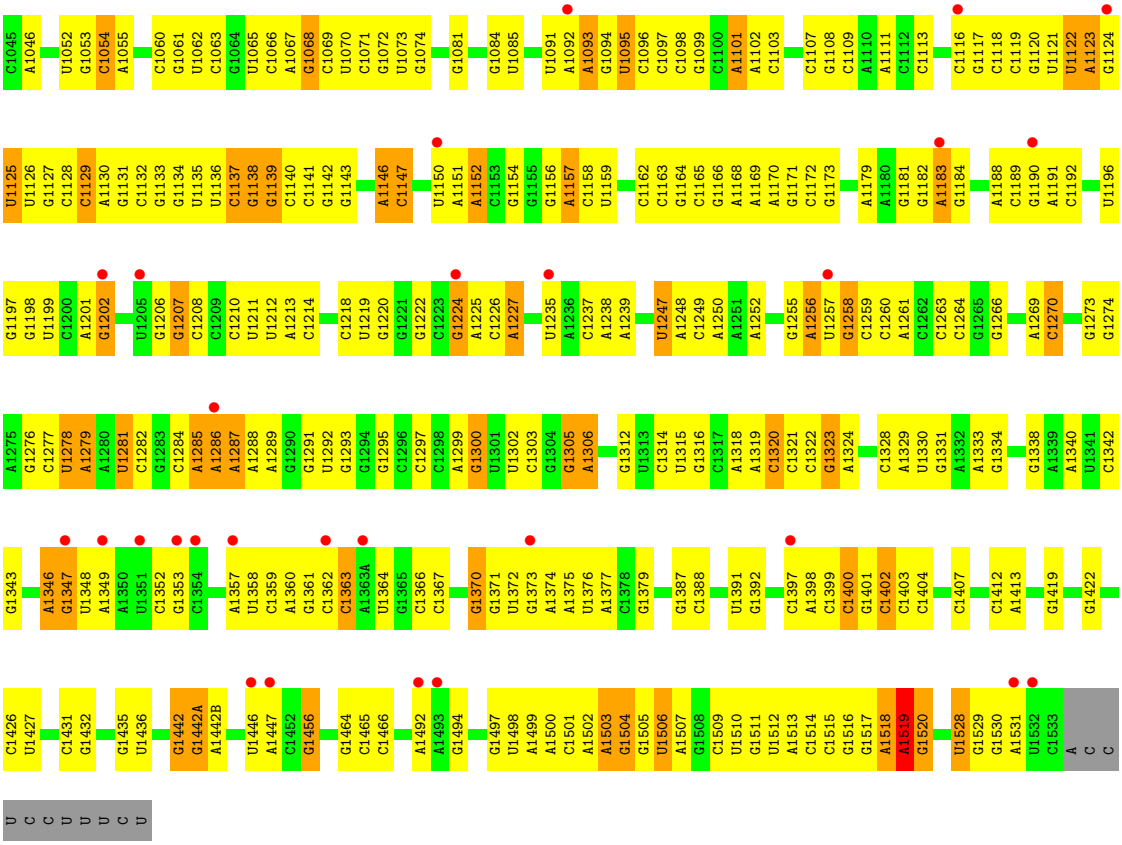




• Molecule 32: 16S Ribosomal RNA

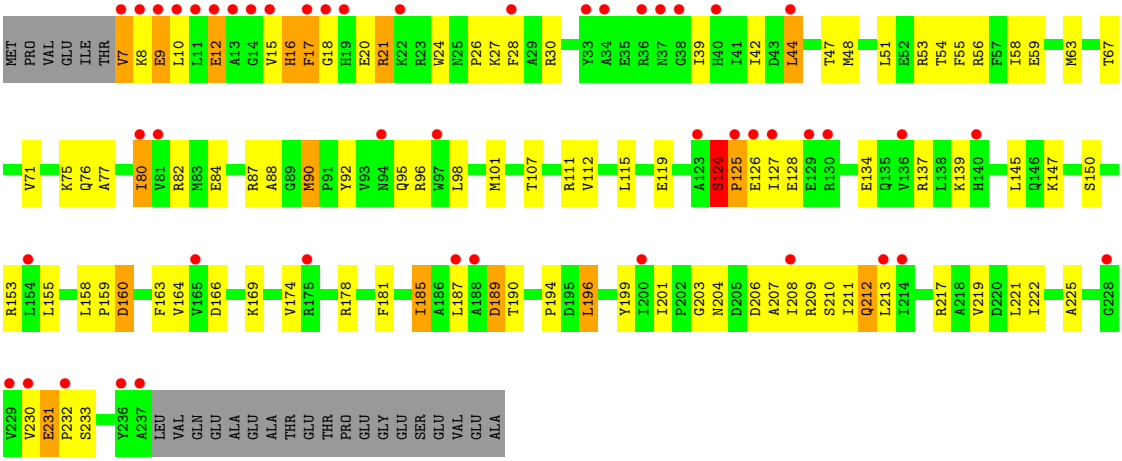
Chain 2a:





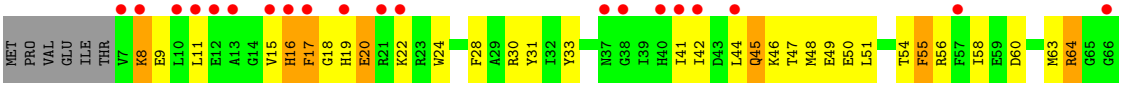
• Molecule 33: 30S ribosomal protein S2

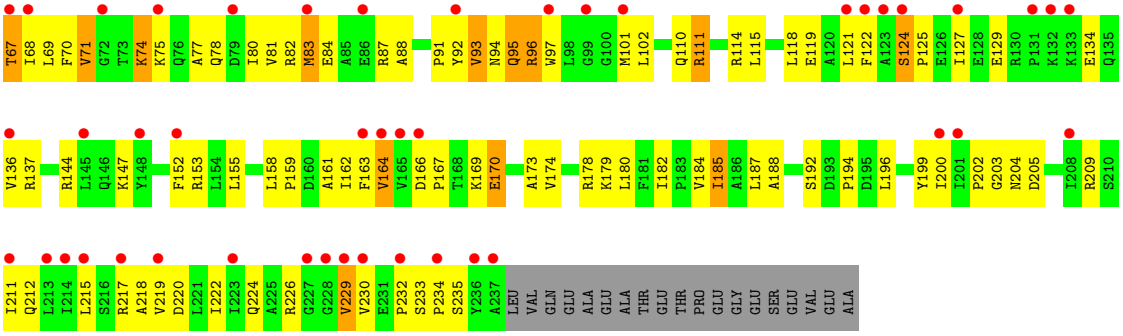
Chain 1b:



• Molecule 33: 30S ribosomal protein S2

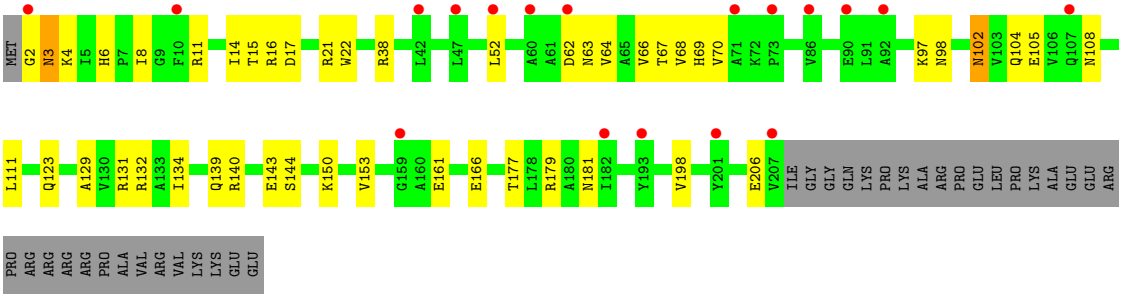
Chain 2b:





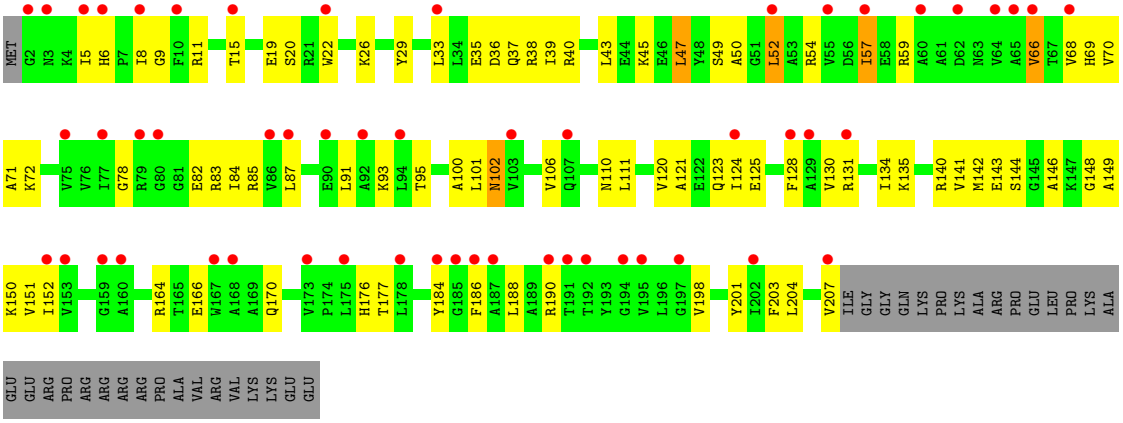
• Molecule 34: 30S ribosomal protein S3

Chain 1c:



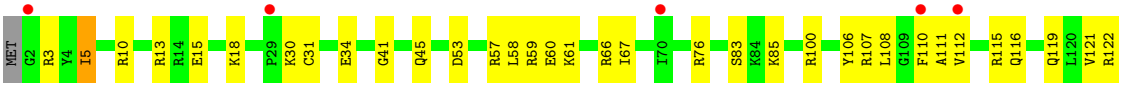
• Molecule 34: 30S ribosomal protein S3

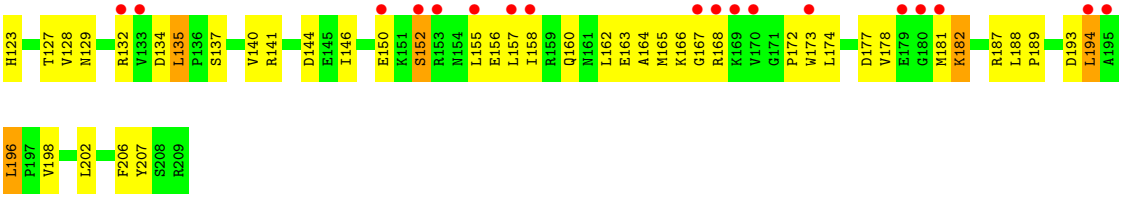
Chain 2c:



• Molecule 35: 30S ribosomal protein S4

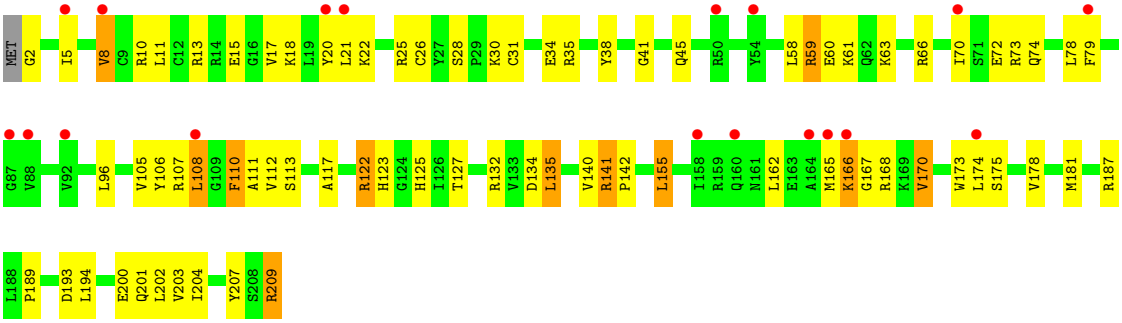
Chain 1d:





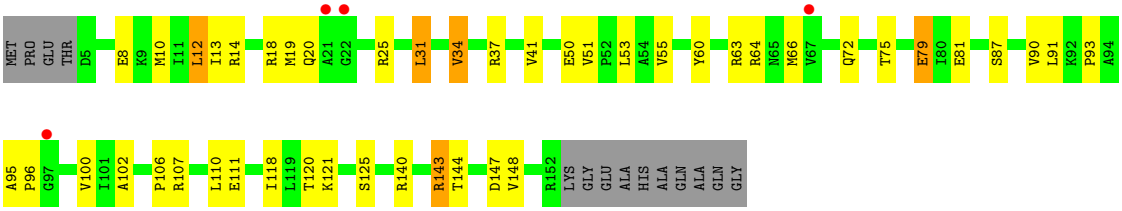
• Molecule 35: 30S ribosomal protein S4

Chain 2d:



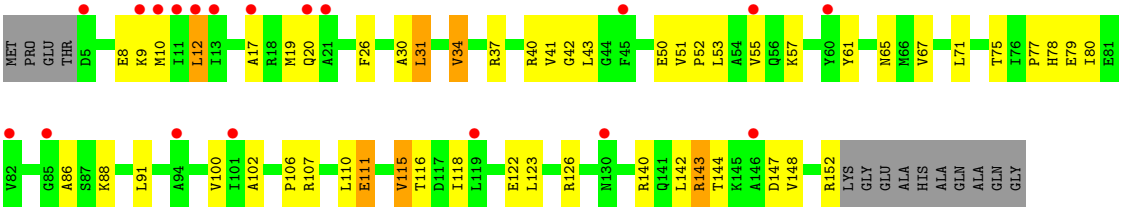
• Molecule 36: 30S ribosomal protein S5

Chain 1e:



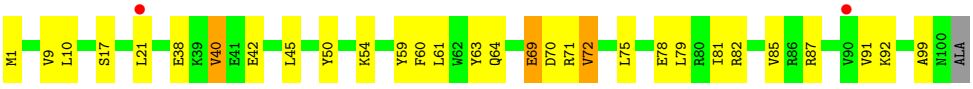
• Molecule 36: 30S ribosomal protein S5

Chain 2e:



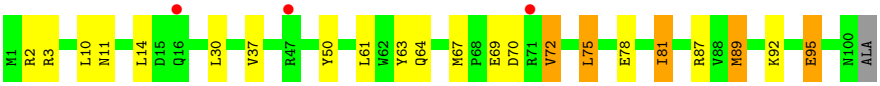
• Molecule 37: 30S ribosomal protein S6

Chain 1f:



• Molecule 37: 30S ribosomal protein S6

Chain 2f:

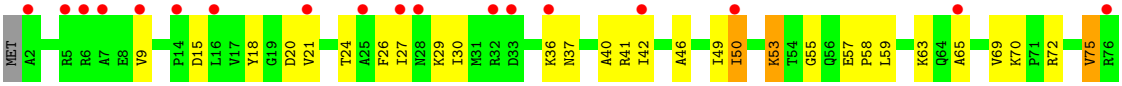


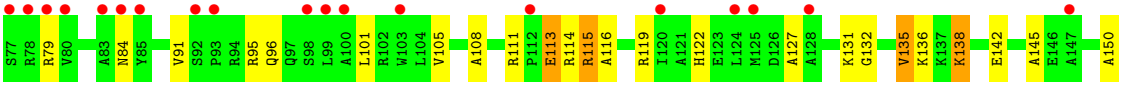
• Molecule 38: 30S ribosomal protein S7

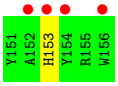
Chain 1g:

• Molecule 38: 30S ribosomal protein S7

Chain 2g:

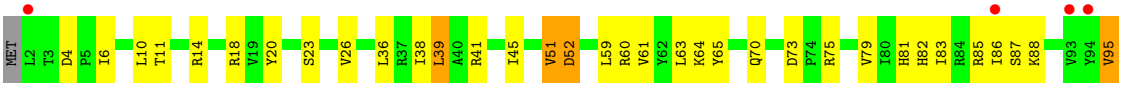


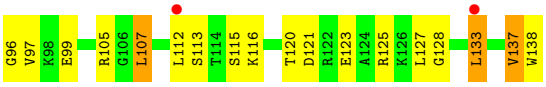




• Molecule 39: 30S ribosomal protein S8

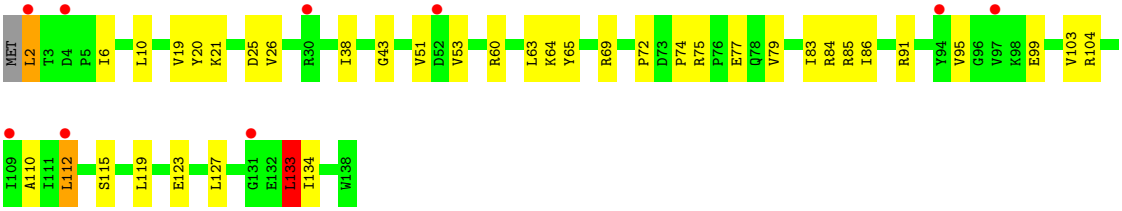
Chain 1h:



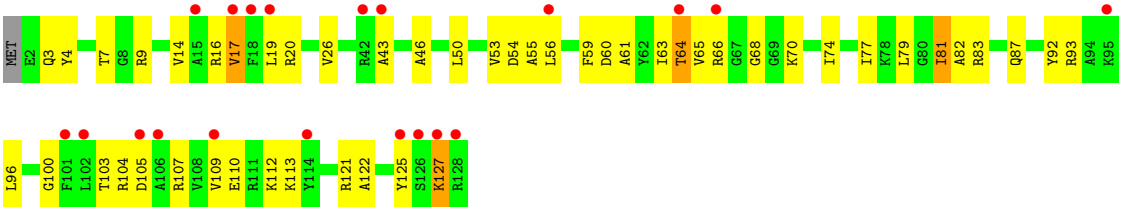


• Molecule 39: 30S ribosomal protein S8

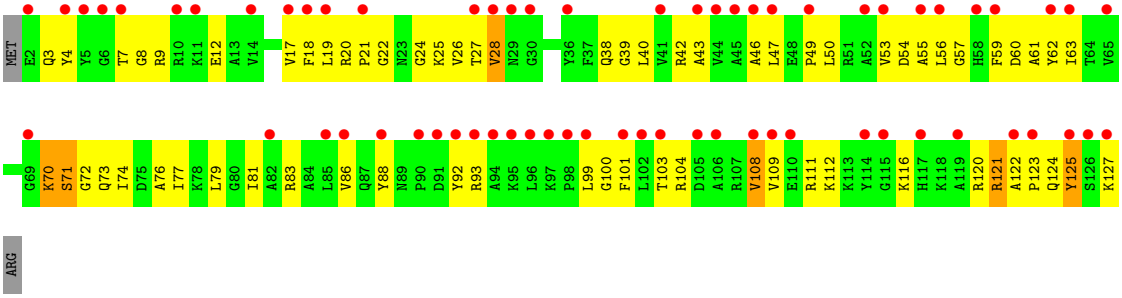
Chain 2h:



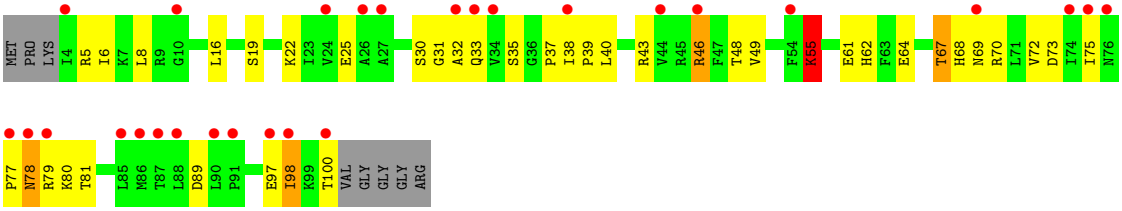
• Molecule 40: 30S ribosomal protein S9



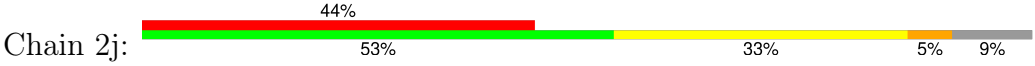
• Molecule 40: 30S ribosomal protein S9

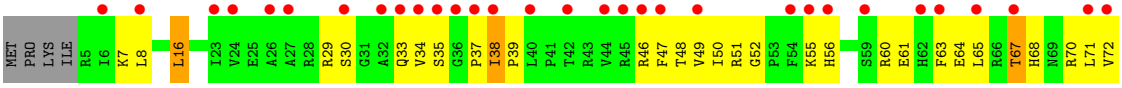


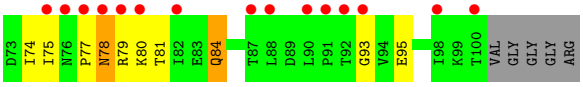
• Molecule 41: 30S ribosomal protein S10



• Molecule 41: 30S ribosomal protein S10

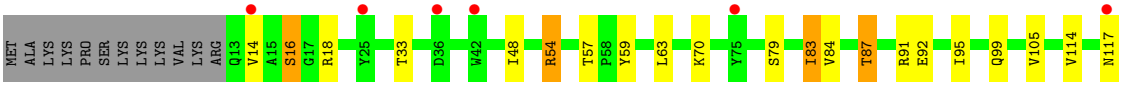


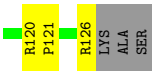




• Molecule 42: 30S ribosomal protein S11

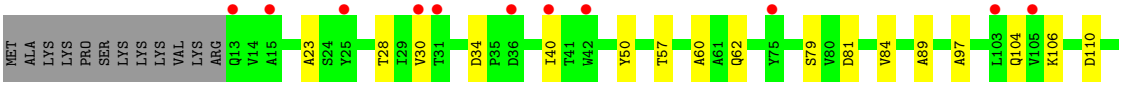
Chain 1k:

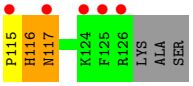




• Molecule 42: 30S ribosomal protein S11

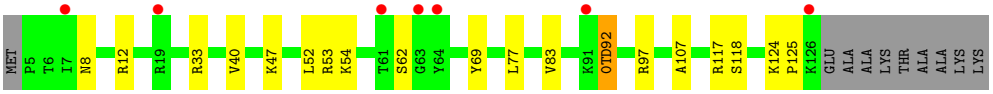
Chain 2k:





• Molecule 43: 30S ribosomal protein S12

Chain 1l:

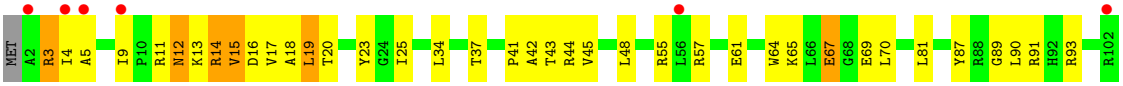


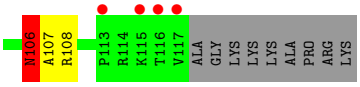
• Molecule 43: 30S ribosomal protein S12

Chain 2l:

• Molecule 44: 30S ribosomal protein S13

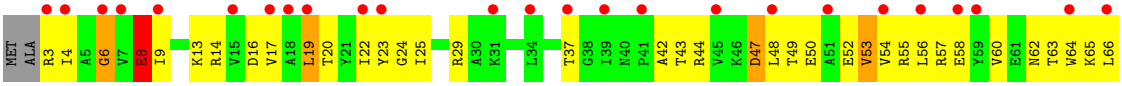
Chain 1m:

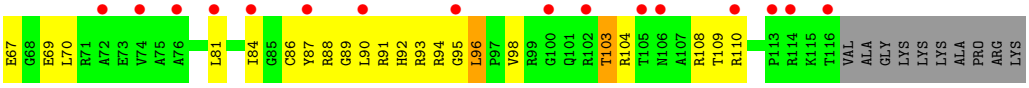




• Molecule 44: 30S ribosomal protein S13

Chain 2m:



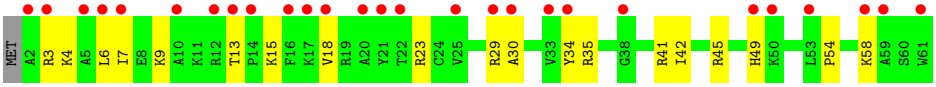


• Molecule 45: 30S ribosomal protein S14 type Z

Chain 1n:

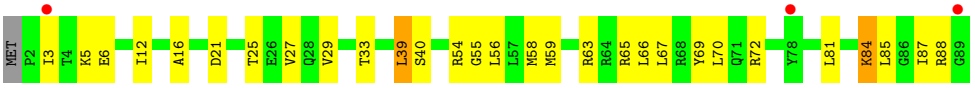
• Molecule 45: 30S ribosomal protein S14 type Z

Chain 2n:



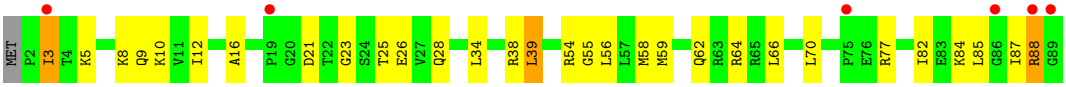
• Molecule 46: 30S ribosomal protein S15

Chain 1o:



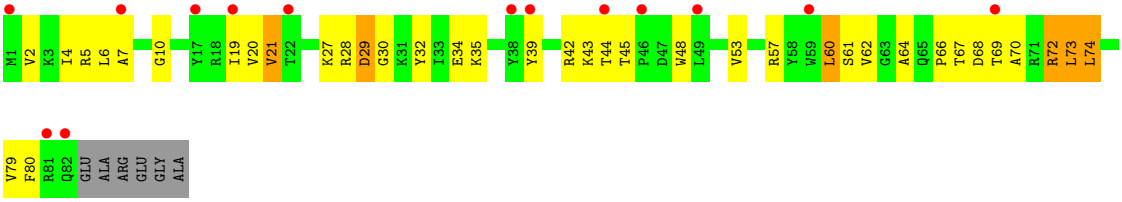
• Molecule 46: 30S ribosomal protein S15

Chain 2o:

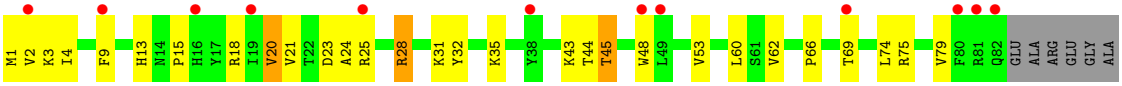


• Molecule 47: 30S ribosomal protein S16

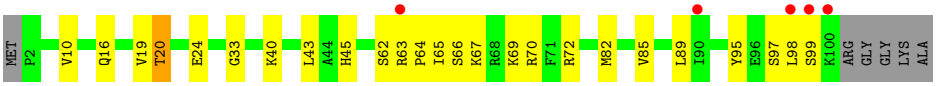
Chain 1p:



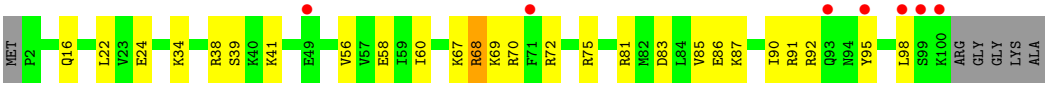
• Molecule 47: 30S ribosomal protein S16



• Molecule 48: 30S ribosomal protein S17

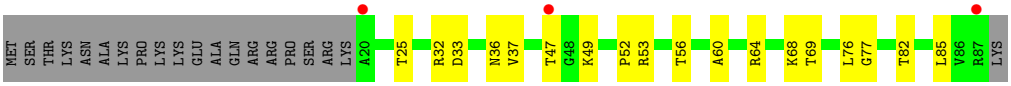


• Molecule 48: 30S ribosomal protein S17

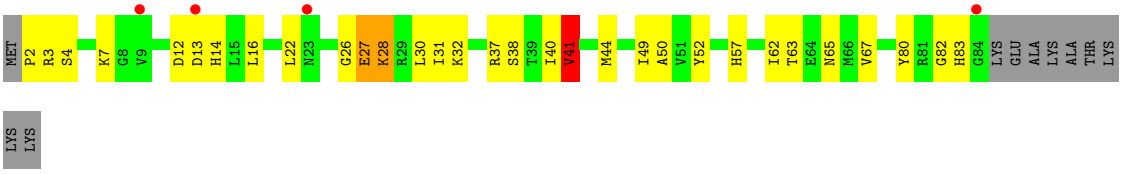


• Molecule 49: 30S ribosomal protein S18

• Molecule 49: 30S ribosomal protein S18

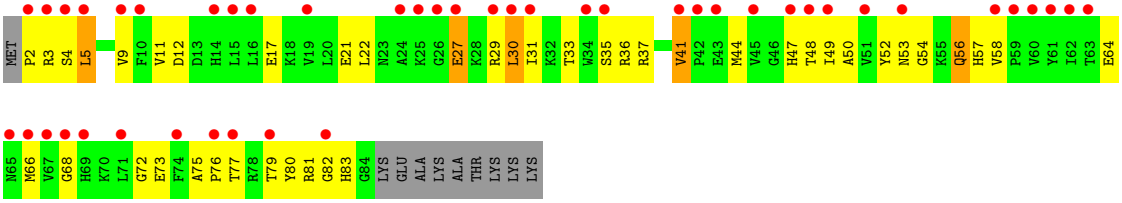


• Molecule 50: 30S ribosomal protein S19



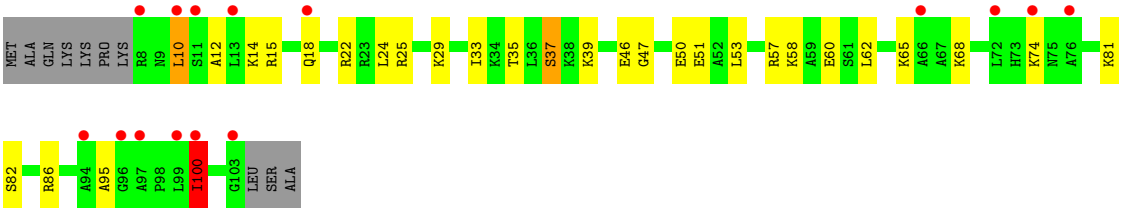
• Molecule 50: 30S ribosomal protein S19

Chain 2s:



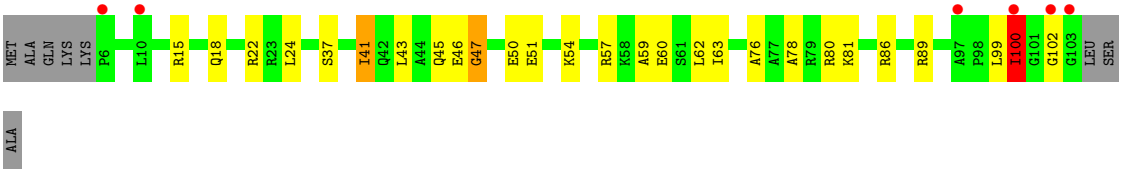
• Molecule 51: 30S ribosomal protein S20

Chain 1t:



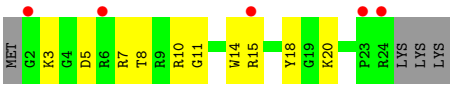
• Molecule 51: 30S ribosomal protein S20

Chain 2t:



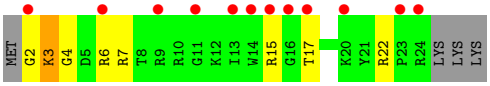
• Molecule 52: 30S ribosomal protein Thx

Chain 1u:



• Molecule 52: 30S ribosomal protein Thx

Chain 2u:

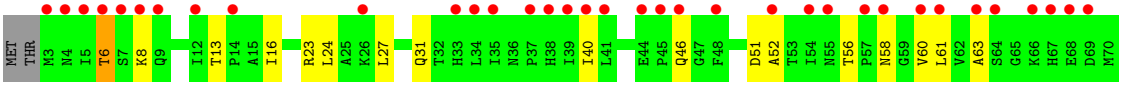


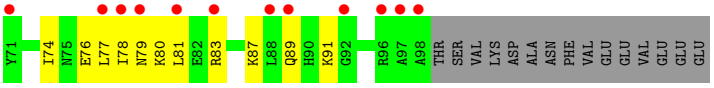
• Molecule 53: Ribosome-associated inhibitor A

Chain 1y:

• Molecule 53: Ribosome-associated inhibitor A

Chain 2y:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	208.57Å 448.58Å 617.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	151.65 – 2.50 151.65 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (151.65-2.50) 99.9 (151.65-2.50)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.22 (at 2.52Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.206 , 0.246 0.206 , 0.246	Depositor DCC
R_{free} test set	98630 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	57.6	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 64.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	296967	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.54% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MA6, PSU, HGR, G7M, 2MG, 5MC, OMC, ERY, OMG, UR3, 2MA, 4OC, 5MU, MPD, 0TD, ZN, 2MU, M2G, MG, SF4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	1A	0.31	0/69030	0.49	5/107750 (0.0%)
1	2A	0.24	0/68902	0.43	2/107548 (0.0%)
2	1B	0.25	0/2876	0.44	0/4486
2	2B	0.21	0/2878	0.40	0/4490
3	1D	0.30	0/2181	0.55	0/2940
3	2D	0.24	0/2186	0.48	0/2944
4	1E	0.27	0/1592	0.51	0/2149
4	2E	0.21	0/1592	0.45	0/2149
5	1F	0.26	0/1619	0.50	0/2193
5	2F	0.22	0/1615	0.48	0/2188
6	1G	0.21	0/1451	0.41	0/1961
6	2G	0.23	0/1449	0.44	0/1957
7	1H	0.23	0/1356	0.44	0/1834
7	2H	0.19	0/1350	0.40	0/1826
8	1I	0.20	0/1109	0.42	0/1512
8	2I	0.17	0/1091	0.40	0/1490
9	1N	0.27	0/1148	0.48	0/1547
9	2N	0.19	0/1144	0.38	0/1543
10	1O	0.28	0/943	0.47	0/1269
10	2O	0.23	0/943	0.47	0/1269
11	1P	0.28	0/1152	0.52	0/1533
11	2P	0.22	0/1152	0.45	0/1533
12	1Q	0.28	0/1143	0.49	0/1527
12	2Q	0.19	0/1143	0.43	0/1527
13	1R	0.29	0/982	0.53	0/1312
13	2R	0.25	0/982	0.46	0/1312
14	1S	0.23	0/887	0.46	0/1180
14	2S	0.20	0/880	0.45	0/1172
15	1T	0.26	0/1105	0.50	0/1477
15	2T	0.21	0/1097	0.45	0/1468
16	1U	0.30	0/977	0.53	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
16	2U	0.19	0/977	0.40	0/1301
17	1V	0.27	0/786	0.47	0/1053
17	2V	0.20	0/782	0.40	0/1049
18	1W	0.29	0/897	0.46	0/1205
18	2W	0.23	0/897	0.43	0/1205
19	1X	0.28	0/764	0.52	0/1025
19	2X	0.21	0/764	0.44	0/1025
20	1Y	0.26	0/823	0.52	0/1099
20	2Y	0.20	0/823	0.46	0/1100
21	1Z	0.23	0/1620	0.46	0/2200
21	2Z	0.20	0/1590	0.45	0/2162
22	10	0.29	0/616	0.54	0/821
22	20	0.20	0/616	0.45	0/821
23	11	0.27	0/761	0.46	0/1013
23	21	0.23	0/766	0.41	0/1018
24	12	0.23	0/590	0.45	0/781
24	22	0.21	0/594	0.43	0/785
25	13	0.28	0/474	0.52	0/635
25	23	0.19	0/469	0.40	0/630
26	14	0.26	0/559	0.59	0/754
26	24	0.30	0/549	0.70	0/741
27	15	0.32	0/473	0.60	0/639
27	25	0.26	0/469	0.45	0/635
28	16	0.26	0/460	0.50	0/613
28	26	0.21	0/456	0.45	0/608
29	17	0.33	0/426	0.50	0/561
29	27	0.25	0/426	0.50	0/561
30	18	0.27	0/525	0.51	0/691
30	28	0.21	0/525	0.41	0/691
31	19	0.31	0/310	0.50	0/407
31	29	0.20	0/310	0.42	0/407
32	1a	0.21	0/35795	0.40	0/55864
32	2a	0.20	1/35890 (0.0%)	0.39	2/56012 (0.0%)
33	1b	0.22	0/1876	0.48	0/2533
33	2b	0.25	0/1860	0.51	2/2518 (0.1%)
34	1c	0.19	0/1582	0.42	0/2137
34	2c	0.22	0/1566	0.41	0/2119
35	1d	0.20	0/1695	0.44	0/2274
35	2d	0.19	0/1698	0.42	0/2277
36	1e	0.21	0/1149	0.44	0/1548
36	2e	0.20	0/1149	0.41	0/1548
37	1f	0.21	0/827	0.40	0/1120
37	2f	0.20	0/829	0.41	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	1g	0.19	0/1254	0.40	0/1683
38	2g	0.20	0/1248	0.40	0/1676
39	1h	0.19	0/1118	0.42	0/1506
39	2h	0.17	0/1108	0.40	0/1494
40	1i	0.20	0/1005	0.46	0/1351
40	2i	0.23	0/985	0.47	0/1329
41	1j	0.24	0/732	0.40	0/993
41	2j	0.23	0/723	0.41	0/984
42	1k	0.20	0/849	0.45	0/1150
42	2k	0.20	0/848	0.44	0/1149
43	1l	0.20	0/937	0.43	0/1260
43	2l	0.18	0/937	0.40	0/1260
44	1m	0.19	0/924	0.46	0/1242
44	2m	0.23	0/905	0.46	0/1217
45	1n	0.20	0/501	0.48	0/664
45	2n	0.21	0/501	0.43	0/664
46	1o	0.20	0/739	0.40	0/985
46	2o	0.21	0/739	0.40	0/985
47	1p	0.20	0/697	0.49	0/939
47	2p	0.20	0/693	0.45	0/935
48	1q	0.21	0/836	0.42	0/1117
48	2q	0.21	0/836	0.41	0/1117
49	1r	0.21	0/560	0.52	0/746
49	2r	0.20	0/560	0.38	0/746
50	1s	0.19	0/663	0.51	1/895 (0.1%)
50	2s	0.22	0/660	0.44	0/893
51	1t	0.21	0/734	0.50	0/969
51	2t	0.19	0/736	0.42	0/976
52	1u	0.21	0/203	0.48	0/266
52	2u	0.23	0/203	0.48	0/266
53	1y	0.20	0/776	0.40	0/1048
53	2y	0.20	0/761	0.37	0/1030
All	All	0.25	1/309939 (0.0%)	0.44	12/463231 (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
26	14	0	1
26	24	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
33	1b	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2a	1498	UR3	O3'-P	5.25	1.61	1.56

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1042	G	OP1-P-O3'	-8.93	81.21	108.00
1	1A	1042	G	OP2-P-O3'	-6.96	87.13	108.00
50	1s	41	VAL	CB-CA-C	6.42	115.62	109.33
33	2b	232	PRO	CA-C-N	6.00	138.01	120.97
33	2b	232	PRO	C-N-CA	6.00	138.01	120.97
1	2A	1992	G	C2'-C3'-O3'	5.94	118.41	109.50
32	2a	266	G	C2'-C3'-O3'	5.70	118.05	109.50
1	1A	512	G	O4'-C1'-N9	5.43	116.34	108.20
32	2a	266	G	P-O3'-C3'	5.33	128.19	120.20
1	1A	1300	U	C4'-C3'-O3'	5.32	117.38	109.40
1	2A	752	A	C2'-C3'-O3'	5.28	117.43	109.50
1	1A	2689	U	C4'-C3'-O3'	5.14	117.11	109.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	14	67	TYR	Peptide
33	1b	231	GLU	Peptide
26	24	18	CYS	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.

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61869	0	31205	610	0
1	2A	61758	0	31152	750	0
2	1B	2572	0	1305	24	0
2	2B	2573	0	1306	60	0
3	1D	2131	0	2207	54	0
3	2D	2136	0	2218	36	0
4	1E	1559	0	1618	27	0
4	2E	1559	0	1618	36	0
5	1F	1584	0	1625	26	0
5	2F	1580	0	1619	52	0
6	1G	1426	0	1445	42	0
6	2G	1424	0	1441	89	0
7	1H	1330	0	1407	26	0
7	2H	1324	0	1402	41	0
8	1I	1094	0	1127	25	0
8	2I	1076	0	1094	29	0
9	1N	1121	0	1195	25	0
9	2N	1117	0	1184	20	0
10	1O	933	0	996	13	0
10	2O	933	0	996	18	0
11	1P	1135	0	1212	25	0
11	2P	1135	0	1212	28	0
12	1Q	1122	0	1179	19	0
12	2Q	1122	0	1179	28	0
13	1R	968	0	1033	16	0
13	2R	968	0	1033	16	0
14	1S	877	0	938	17	0
14	2S	870	0	923	30	0
15	1T	1091	0	1151	21	0
15	2T	1083	0	1136	25	0
16	1U	959	0	1019	15	0
16	2U	959	0	1019	26	0
17	1V	775	0	841	16	0
17	2V	771	0	830	16	0
18	1W	886	0	940	14	0
18	2W	886	0	940	11	0
19	1X	750	0	814	18	0
19	2X	750	0	814	15	0
20	1Y	810	0	892	16	0
20	2Y	810	0	887	21	0
21	1Z	1587	0	1598	31	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	2Z	1557	0	1564	49	0
22	10	608	0	622	9	0
22	20	608	0	622	4	0
23	11	754	0	823	13	0
23	21	759	0	837	18	0
24	12	588	0	643	11	0
24	22	592	0	654	10	0
25	13	469	0	518	8	0
25	23	464	0	514	14	0
26	14	546	0	522	21	0
26	24	536	0	514	36	0
27	15	459	0	476	11	0
27	25	455	0	465	7	0
28	16	453	0	473	7	0
28	26	449	0	469	8	0
29	17	418	0	467	5	0
29	27	418	0	467	10	0
30	18	517	0	582	15	0
30	28	517	0	582	16	0
31	19	307	0	335	1	0
31	29	307	0	335	10	0
32	1a	32246	0	16295	415	0
32	2a	32331	0	16338	532	0
33	1b	1842	0	1862	65	0
33	2b	1825	0	1828	86	0
34	1c	1558	0	1557	33	0
34	2c	1542	0	1517	62	0
35	1d	1665	0	1687	56	0
35	2d	1668	0	1703	58	0
36	1e	1133	0	1191	29	0
36	2e	1133	0	1191	36	0
37	1f	814	0	808	17	0
37	2f	816	0	808	16	0
38	1g	1235	0	1249	20	0
38	2g	1229	0	1238	30	0
39	1h	1098	0	1143	39	0
39	2h	1088	0	1126	22	0
40	1i	986	0	990	34	0
40	2i	966	0	953	51	0
41	1j	719	0	672	26	0
41	2j	710	0	661	30	0
42	1k	834	0	838	20	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	2k	833	0	836	11	0
43	1l	932	0	981	14	0
43	2l	932	0	981	18	0
44	1m	914	0	954	33	0
44	2m	895	0	920	45	0
45	1n	492	0	529	19	0
45	2n	492	0	529	17	0
46	1o	728	0	760	18	0
46	2o	728	0	760	20	0
47	1p	681	0	697	28	0
47	2p	677	0	686	21	0
48	1q	823	0	891	18	0
48	2q	823	0	891	18	0
49	1r	555	0	618	9	0
49	2r	555	0	618	12	0
50	1s	648	0	658	20	0
50	2s	645	0	635	39	0
51	1t	732	0	809	24	0
51	2t	733	0	795	17	0
52	1u	199	0	208	7	0
52	2u	199	0	208	7	0
53	1y	764	0	786	17	0
53	2y	749	0	757	18	0
54	10	8	0	0	0	0
54	11	5	0	0	0	0
54	13	3	0	0	0	0
54	14	1	0	0	0	0
54	15	8	0	0	0	0
54	17	6	0	0	0	0
54	18	2	0	0	0	0
54	19	2	0	0	0	0
54	1A	1040	0	0	0	0
54	1B	29	0	0	0	0
54	1D	18	0	0	0	0
54	1E	8	0	0	0	0
54	1F	18	0	0	0	0
54	1G	4	0	0	0	0
54	1H	2	0	0	0	0
54	1N	4	0	0	0	0
54	1O	1	0	0	0	0
54	1P	5	0	0	0	0
54	1Q	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	1R	5	0	0	0	0
54	1T	5	0	0	0	0
54	1U	7	0	0	0	0
54	1V	6	0	0	0	0
54	1W	3	0	0	0	0
54	1Y	1	0	0	0	0
54	1Z	1	0	0	0	0
54	1a	279	0	0	0	0
54	1b	1	0	0	0	0
54	1d	5	0	0	0	0
54	1e	3	0	0	0	0
54	1f	2	0	0	0	0
54	1g	3	0	0	0	0
54	1h	2	0	0	0	0
54	1i	1	0	0	0	0
54	1k	1	0	0	0	0
54	1l	2	0	0	0	0
54	1m	2	0	0	0	0
54	1n	2	0	0	0	0
54	1o	1	0	0	0	0
54	1t	1	0	0	0	0
54	1y	3	0	0	0	0
54	20	1	0	0	0	0
54	21	2	0	0	0	0
54	23	1	0	0	0	0
54	25	3	0	0	0	0
54	27	2	0	0	0	0
54	28	2	0	0	0	0
54	2A	730	0	0	0	0
54	2B	18	0	0	0	0
54	2D	13	0	0	0	0
54	2E	6	0	0	0	0
54	2F	4	0	0	0	0
54	2G	2	0	0	0	0
54	2I	1	0	0	0	0
54	2O	2	0	0	0	0
54	2P	1	0	0	0	0
54	2Q	1	0	0	0	0
54	2R	3	0	0	0	0
54	2T	3	0	0	0	0
54	2U	1	0	0	0	0
54	2V	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	2W	2	0	0	0	0
54	2X	1	0	0	0	0
54	2Y	1	0	0	0	0
54	2a	190	0	0	0	0
54	2e	2	0	0	0	0
54	2f	1	0	0	0	0
54	2j	1	0	0	0	0
54	2k	1	0	0	0	0
54	2n	1	0	0	0	0
54	2r	2	0	0	0	0
54	2t	1	0	0	0	0
54	2y	1	0	0	0	0
55	1A	36	0	29	1	0
55	2A	36	0	29	1	0
56	1A	51	0	67	0	0
56	2A	51	0	67	1	0
57	18	8	0	14	3	0
57	1A	8	0	14	1	0
57	1T	8	0	14	0	0
57	1a	8	0	13	6	0
57	2A	16	0	28	0	0
57	2B	8	0	14	0	0
58	1B	12	0	12	0	0
58	1F	12	0	12	1	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	10	21	0	0	1	0
61	11	28	0	0	1	0
61	12	14	0	0	2	0
61	13	22	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	14	4	0	0	0	0
61	15	25	0	0	0	0
61	16	21	0	0	0	0
61	17	13	0	0	0	0
61	18	23	0	0	1	0
61	19	2	0	0	0	0
61	1A	3898	0	0	87	0
61	1B	94	0	0	2	0
61	1D	103	0	0	2	0
61	1E	68	0	0	1	0
61	1F	64	0	0	0	0
61	1G	16	0	0	0	0
61	1H	15	0	0	0	0
61	1I	5	0	0	0	0
61	1N	45	0	0	1	0
61	1O	22	0	0	1	0
61	1P	56	0	0	3	0
61	1Q	37	0	0	1	0
61	1R	29	0	0	0	0
61	1S	12	0	0	2	0
61	1T	37	0	0	3	0
61	1U	41	0	0	4	0
61	1V	34	0	0	1	0
61	1W	27	0	0	1	0
61	1X	27	0	0	1	0
61	1Y	16	0	0	1	0
61	1Z	5	0	0	0	0
61	1a	447	0	0	18	0
61	1b	1	0	0	0	0
61	1c	2	0	0	0	0
61	1d	9	0	0	2	0
61	1e	5	0	0	1	0
61	1f	1	0	0	0	0
61	1h	1	0	0	0	0
61	1j	1	0	0	0	0
61	1l	3	0	0	1	0
61	1o	2	0	0	0	0
61	1p	2	0	0	0	0
61	1y	1	0	0	0	0
61	20	5	0	0	0	0
61	21	15	0	0	0	0
61	22	1	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	23	2	0	0	0	0
61	25	7	0	0	1	0
61	26	2	0	0	0	0
61	27	8	0	0	0	0
61	28	9	0	0	1	0
61	2A	1941	0	0	97	0
61	2B	45	0	0	13	0
61	2D	45	0	0	0	0
61	2E	25	0	0	1	0
61	2F	15	0	0	0	0
61	2G	2	0	0	0	0
61	2H	1	0	0	0	0
61	2I	1	0	0	0	0
61	2N	3	0	0	1	0
61	2O	10	0	0	0	0
61	2P	19	0	0	1	0
61	2Q	13	0	0	0	0
61	2R	17	0	0	2	0
61	2T	6	0	0	0	0
61	2U	7	0	0	0	0
61	2V	4	0	0	1	0
61	2W	20	0	0	0	0
61	2X	7	0	0	0	0
61	2Y	2	0	0	0	0
61	2Z	7	0	0	0	0
61	2a	266	0	0	18	0
61	2d	4	0	0	0	0
61	2e	1	0	0	0	0
61	2l	1	0	0	0	0
61	2o	2	0	0	0	0
61	2q	1	0	0	0	0
61	2r	3	0	0	0	0
61	2u	1	0	0	0	0
All	All	296967	0	194709	4218	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 (4218) 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	1.38	1.21
1:1A:1082:U:O4	1:1A:1086:A:N1	1.98	0.95
1:1A:1798:U:H5'	3:1D:259:THR:HG22	1.48	0.95
10:2O:48:PRO:HB3	32:2a:1422:G:H5"	1.49	0.94
1:2A:2100:G:H1	1:2A:2189:U:H3	1.11	0.94
1:2A:1798:U:H5'	3:2D:259:THR:HG22	1.50	0.94
1:1A:1054:A:H61	1:1A:1105:U:H3	1.16	0.93
1:2A:511:U:OP2	61:2A:3801:HOH:O	1.85	0.93
20:1Y:92:ASN:HB2	20:1Y:94:LYS:H	1.35	0.91
32:1a:201:C:H42	32:1a:216:G:H1	1.14	0.91
32:1a:73:G:H1	32:1a:96:U:H3	0.95	0.90
32:1a:1086:U:H3	32:1a:1099:G:H22	1.21	0.89
1:2A:2427:C:OP1	61:2A:3802:HOH:O	1.91	0.88
1:2A:510:C:OP1	61:2A:3801:HOH:O	1.91	0.87
1:2A:2131:G:H5"	1:2A:2132:U:H5'	1.55	0.87
1:2A:585:G:OP2	61:2A:3803:HOH:O	1.92	0.86
3:1D:242:ARG:HG3	3:1D:242:ARG:HH11	1.39	0.85
1:2A:2099:U:H3	1:2A:2190:G:H1	1.23	0.85
23:11:50:ARG:HG2	23:11:59:THR:HG22	1.58	0.85
32:2a:1295:G:O2'	44:2m:14:ARG:NH1	2.10	0.85
1:2A:1782:C:OP1	61:2A:3804:HOH:O	1.95	0.84
1:2A:2527:C:N4	61:2A:3805:HOH:O	2.09	0.84
8:1I:92:VAL:HG13	8:1I:120:ILE:HB	1.59	0.84
1:2A:1264:G:OP1	27:25:19:ARG:NH2	2.09	0.84
1:2A:2807:G:N1	1:2A:2893:G:O6	2.10	0.84
1:1A:1669:A:OP2	61:1A:4101:HOH:O	1.95	0.83
4:2E:110:GLY:O	61:2R:301:HOH:O	1.94	0.83
50:1s:50:ALA:HB1	50:1s:57:HIS:HB3	1.62	0.82
32:1a:1025:U:C2	32:1a:1036:G:O6	2.31	0.82
1:1A:2143:C:N3	1:1A:2148:G:O6	2.13	0.82
1:1A:2822:G:OP2	61:1A:4102:HOH:O	1.96	0.82
11:1P:141:ALA:HA	25:23:38:GLU:HG2	1.61	0.82
1:1A:330:A:H2	1:1A:1210:A:HO2'	1.23	0.82
32:2a:1286:A:H8	32:2a:1287:A:H4'	1.44	0.82
32:1a:1441:G:H5"	32:1a:1442:G:H5'	1.60	0.81
1:2A:2122:U:H3	1:2A:2176:A:H61	1.27	0.81
1:2A:2536:G:O6	61:2A:3805:HOH:O	1.99	0.81
1:1A:2102:U:O2	1:1A:2187:G:O6	1.97	0.81
1:2A:2296:U:OP2	14:2S:9:ARG:NH2	2.13	0.81
6:2G:161:THR:HG22	6:2G:163:ALA:H	1.45	0.81
32:2a:1505:G:OP1	61:2a:3202:HOH:O	1.97	0.81
21:2Z:99:TYR:HB3	21:2Z:123:ASP:HB2	1.63	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:2b:91:PRO:HG3	33:2b:155:LEU:HD13	1.61	0.81
6:1G:161:THR:HG22	6:1G:163:ALA:H	1.44	0.80
46:1o:54:ARG:HG2	46:1o:58:MET:HE2	1.61	0.80
41:1j:49:VAL:HG23	45:1n:41:ARG:HB2	1.63	0.80
32:2a:36:C:OP1	43:2l:123:LYS:NZ	2.13	0.80
1:2A:512:G:N7	61:2A:3801:HOH:O	2.14	0.80
26:24:59:PHE:HA	26:24:61:ARG:N	1.97	0.80
10:1O:48:PRO:HB3	32:1a:1422:G:H5"	1.64	0.79
38:2g:113:GLU:HG3	38:2g:119:ARG:HG2	1.64	0.79
1:1A:1175:U:OP1	1:1A:1177:A:N6	2.15	0.79
16:1U:33:ARG:NH1	61:1U:301:HOH:O	2.16	0.79
32:1a:664:G:H22	32:1a:741:G:H1	1.29	0.79
1:2A:2156:G:N7	1:2A:2157:G:N2	2.31	0.79
40:2i:4:TYR:HB2	40:2i:19:LEU:HB2	1.64	0.79
32:1a:975:A:H4'	32:1a:976:G:H5"	1.63	0.79
1:1A:1047:G:H2'	1:1A:1110:G:H22	1.47	0.79
39:2h:64:LYS:HG2	39:2h:79:VAL:HG21	1.63	0.79
32:1a:266:G:H5'	32:1a:268:C:H41	1.48	0.79
32:1a:1004:A:OP1	32:1a:1024:G:N2	2.16	0.79
32:2a:975:A:H4'	32:2a:976:G:H5"	1.64	0.79
1:2A:2839:G:H5'	13:2R:46:GLY:HA2	1.66	0.78
8:2I:92:VAL:HG23	8:2I:120:ILE:HB	1.65	0.78
33:2b:93:VAL:HG21	33:2b:97:TRP:HD1	1.48	0.78
1:1A:1671:U:O4	61:1A:4101:HOH:O	2.02	0.78
1:2A:1647:G:OP1	61:2A:3806:HOH:O	2.00	0.78
1:2A:2365:G:N7	30:28:39:LYS:NZ	2.32	0.78
26:24:59:PHE:HA	26:24:61:ARG:H	1.48	0.78
40:2i:3:GLN:HE21	40:2i:20:ARG:HE	1.29	0.78
2:1B:23:G:O6	61:1B:301:HOH:O	2.01	0.78
34:1c:179:ARG:NH1	34:1c:206:GLU:OE1	2.16	0.78
2:2B:49:C:OP1	61:2B:301:HOH:O	2.01	0.78
12:2Q:75:THR:HG21	12:2Q:87:LYS:HE3	1.65	0.78
32:2a:1500:A:OP1	61:2a:3202:HOH:O	2.02	0.78
36:2e:122:GLU:O	36:2e:126:ARG:NH1	2.17	0.78
1:2A:2141:G:O6	1:2A:2150:U:O2	2.02	0.78
1:1A:631:A:OP1	11:1P:65:ARG:NH1	2.15	0.78
44:2m:94:ARG:HB3	44:2m:96:LEU:HD12	1.64	0.78
19:1X:31:HIS:HD2	19:1X:33:LYS:H	1.29	0.77
32:2a:390:C:O3'	47:2p:28:ARG:NH2	2.17	0.77
1:2A:994:C:OP1	16:2U:53:ARG:NH2	2.16	0.77
1:2A:2494:G:OP2	61:2A:3807:HOH:O	2.01	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1D:108:PRO:HD2	3:1D:111:LEU:HG	1.66	0.77
1:2A:641:C:O2'	1:2A:2350:C:OP1	2.01	0.77
4:1E:70:ALA:O	4:1E:72:VAL:N	2.17	0.77
32:2a:1292:U:OP2	38:2g:41:ARG:NH2	2.16	0.77
1:1A:1865:G:OP1	61:1A:4103:HOH:O	2.01	0.77
32:2a:1286:A:C8	32:2a:1287:A:H4'	2.21	0.77
1:2A:1271:G:OP2	61:2A:3806:HOH:O	2.02	0.76
1:2A:775:G:O3'	61:2A:3808:HOH:O	2.03	0.76
37:2f:67:MET:HE1	37:2f:75:LEU:HD22	1.67	0.76
21:1Z:144:LEU:HD21	21:1Z:150:LEU:HD13	1.66	0.76
29:27:24:THR:HG23	29:27:27:GLY:H	1.50	0.76
41:2j:49:VAL:HG23	45:2n:41:ARG:HB2	1.68	0.76
1:1A:1082:U:N3	1:1A:1086:A:N6	2.09	0.76
1:2A:2748:A:H5'	7:2H:4:ILE:HD12	1.66	0.76
1:1A:1024:G:OP2	61:1A:4105:HOH:O	2.04	0.76
35:1d:15:GLU:OE2	35:1d:66:ARG:NH1	2.19	0.76
1:1A:826:U:OP1	61:1A:4104:HOH:O	2.02	0.75
32:2a:1118:C:OP1	40:2i:9:ARG:NH1	2.20	0.75
14:1S:59:LYS:HD2	14:1S:60:GLY:H	1.50	0.75
1:1A:1085:A:O2'	1:1A:1104:C:O2'	2.04	0.75
25:13:3:ARG:NH1	25:13:60:GLU:OE2	2.19	0.75
32:1a:1108:G:O6	61:1a:1901:HOH:O	2.04	0.75
41:1j:35:SER:HB3	41:1j:73:ASP:HB2	1.68	0.75
32:2a:1346:A:OP1	40:2i:120:ARG:NH1	2.20	0.75
32:1a:1003:G:H2'	32:1a:1004:A:H4'	1.67	0.75
32:2a:1352:C:H42	32:2a:1370:G:H1	1.34	0.75
1:1A:1648:C:OP1	61:1A:4106:HOH:O	2.05	0.74
1:2A:2206:G:H3'	1:2A:2207:G:H8	1.51	0.74
36:1e:107:ARG:NH1	61:1e:301:HOH:O	2.19	0.74
1:2A:1314:C:OP1	61:2A:3809:HOH:O	2.03	0.74
51:1t:33:ILE:O	51:1t:37:SER:OG	2.06	0.74
32:1a:1025:U:O2	32:1a:1036:G:O6	2.03	0.74
35:2d:18:LYS:NZ	35:2d:31:CYS:SG	2.61	0.74
51:2t:50:GLU:HG3	51:2t:100:ILE:HD11	1.70	0.74
1:2A:1023:U:OP2	61:2A:3810:HOH:O	2.05	0.74
1:2A:1602:U:O4	61:2A:3811:HOH:O	2.06	0.74
1:2A:2000:G:OP2	61:2A:3812:HOH:O	2.06	0.74
1:2A:2602:A:H1'	1:2A:2603:G:H5"	1.68	0.74
46:2o:54:ARG:HG2	46:2o:58:MET:HE2	1.68	0.74
1:2A:1315:C:OP2	61:2A:3809:HOH:O	2.04	0.74
21:2Z:33:LEU:HD11	21:2Z:90:VAL:HG21	1.70	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:2s:50:ALA:HB1	50:2s:57:HIS:HB3	1.69	0.73
33:2b:119:GLU:HG3	33:2b:153:ARG:HH22	1.51	0.73
32:1a:406:G:H21	35:1d:119:GLN:HE22	1.36	0.73
21:2Z:152:ALA:HA	21:2Z:155:LEU:HD13	1.70	0.73
33:2b:122:PHE:HA	33:2b:127:ILE:HG12	1.71	0.73
32:1a:596:C:OP2	61:1a:1902:HOH:O	2.05	0.73
33:1b:9:GLU:HG3	33:1b:217:ARG:HH22	1.53	0.73
35:2d:122:ARG:NH1	35:2d:134:ASP:O	2.22	0.73
32:1a:1414:U:H3	32:1a:1486:G:H1	1.37	0.73
32:2a:596:C:O2	32:2a:644:G:N2	2.19	0.73
24:12:22:GLU:OE2	24:12:68:ARG:NH2	2.22	0.73
1:1A:2143:C:O2	1:1A:2148:G:N1	2.22	0.73
32:2a:559:A:OP1	36:2e:126:ARG:NH2	2.21	0.73
32:2a:1003:G:H2'	32:2a:1004:A:H4'	1.70	0.73
32:1a:501:C:OP1	43:1l:117:ARG:NH2	2.21	0.73
1:2A:2548:G:N7	61:2A:3862:HOH:O	2.21	0.72
33:2b:166:ASP:HB3	33:2b:169:LYS:HB3	1.70	0.72
1:1A:2427:C:OP1	61:1A:4104:HOH:O	2.07	0.72
9:1N:46:VAL:HG23	9:1N:48:MET:HG2	1.71	0.72
6:2G:35:GLU:HG3	6:2G:36:LYS:HG3	1.70	0.72
1:1A:1832:C:OP2	61:1A:4107:HOH:O	2.06	0.72
32:2a:1507:A:N6	32:2a:1528:U:O4	2.15	0.72
1:1A:135:G:N7	61:1A:4153:HOH:O	2.22	0.72
1:1A:1321:A:N1	61:1A:4149:HOH:O	2.22	0.72
21:1Z:14:LYS:HE2	21:1Z:15:PRO:HD2	1.71	0.72
51:1t:57:ARG:HH22	51:1t:100:ILE:HD12	1.55	0.72
53:2y:40:ILE:HB	53:2y:51:ASP:HB2	1.70	0.72
1:1A:123:G:OP2	61:1A:4108:HOH:O	2.06	0.72
1:1A:1300:U:H4'	1:1A:1301:A:H5'	1.71	0.72
1:1A:1381:G:N7	61:1A:4156:HOH:O	2.22	0.72
5:2F:21:ALA:HB3	5:2F:22:ALA:HA	1.71	0.72
1:1A:2821:A:OP2	61:1A:4102:HOH:O	2.06	0.72
6:2G:41:GLN:HG3	6:2G:60:LEU:HD12	1.71	0.72
10:2O:115:VAL:HG13	10:2O:121:VAL:HG21	1.72	0.72
21:2Z:19:ARG:NH1	21:2Z:84:GLU:O	2.22	0.72
26:24:9:LEU:HD23	26:24:27:THR:HG23	1.71	0.72
32:2a:1518:MA6:H93	32:2a:1519:MA6:H102	1.71	0.72
1:1A:1823:G:OP1	3:1D:54:ARG:NH1	2.21	0.72
32:1a:1518:MA6:H93	32:1a:1519:MA6:H92	1.70	0.72
32:2a:427:U:OP1	35:2d:13:ARG:NH2	2.23	0.72
43:2l:57:LYS:HE2	43:2l:65:GLU:HG2	1.70	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1315:C:OP2	61:1A:4109:HOH:O	2.07	0.72
1:2A:143:G:H4'	19:2X:35:THR:HG21	1.72	0.72
48:1q:67:LYS:HA	48:1q:70:ARG:HH21	1.54	0.71
1:1A:2116:G:OP2	1:1A:2166:G:N2	2.23	0.71
36:1e:37:ARG:HH12	36:1e:111:GLU:HG2	1.55	0.71
18:2W:67:ASP:OD1	18:2W:67:ASP:N	2.23	0.71
32:2a:366:C:N3	61:2a:3214:HOH:O	2.21	0.71
1:1A:1054:A:N6	1:1A:1105:U:H3	1.85	0.71
1:1A:1176:G:H1'	1:1A:1177:A:H5'	1.72	0.71
1:2A:11:G:H2'	1:2A:12:U:H5'	1.72	0.71
1:2A:731:C:OP1	61:2A:3816:HOH:O	2.09	0.71
32:2a:673:G:H2'	32:2a:674:G:C8	2.24	0.71
1:2A:1026:U:OP1	61:2A:3810:HOH:O	2.09	0.71
1:2A:2102:U:O2	1:2A:2187:G:O6	2.08	0.71
23:21:51:VAL:HG11	23:21:74:VAL:HG21	1.73	0.71
26:24:16:CYS:SG	26:24:17:GLY:N	2.63	0.71
1:1A:994:C:OP1	16:1U:53:ARG:NH2	2.23	0.71
1:2A:2551:C:OP2	61:2A:3814:HOH:O	2.07	0.71
1:1A:1059:G:O6	1:1A:1079:C:N3	2.23	0.71
1:1A:1023:U:OP2	61:1A:4105:HOH:O	2.09	0.71
6:1G:115:ARG:HB3	6:1G:136:ARG:HH22	1.56	0.71
1:1A:400:G:N7	61:1A:4152:HOH:O	2.22	0.70
33:1b:15:VAL:HG11	33:1b:213:LEU:HD13	1.72	0.70
23:21:50:ARG:HG2	23:21:59:THR:HG22	1.72	0.70
36:2e:144:THR:H	36:2e:147:ASP:HB2	1.56	0.70
50:1s:49:ILE:HG12	50:1s:62:ILE:HD11	1.73	0.70
1:1A:1026:U:OP1	61:1A:4105:HOH:O	2.10	0.70
21:2Z:69:THR:HG22	21:2Z:90:VAL:HA	1.74	0.70
32:2a:1285:A:H4'	32:2a:1286:A:H5'	1.73	0.70
1:1A:365:C:OP2	61:1A:4113:HOH:O	2.09	0.70
1:1A:2447:G:OP2	61:1A:4111:HOH:O	2.09	0.70
1:2A:792:G:O6	61:2A:3813:HOH:O	2.07	0.70
1:2A:1050:A:H2'	1:2A:1051:G:H8	1.57	0.70
32:1a:992:U:H4'	32:1a:993:G:H5'	1.74	0.70
5:2F:30:PRO:HB3	11:2P:1:MET:HE1	1.74	0.70
35:2d:30:LYS:HG2	35:2d:35:ARG:HH21	1.56	0.70
1:2A:407:G:OP2	61:2A:3817:HOH:O	2.09	0.70
9:2N:50:ASP:OD1	61:2N:201:HOH:O	2.09	0.70
33:2b:8:LYS:HG2	33:2b:9:GLU:H	1.56	0.70
28:16:13:CYS:SG	28:16:47:THR:HG21	2.32	0.70
1:2A:1418:G:N7	61:2A:3885:HOH:O	2.25	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2104:G:O6	1:2A:2185:C:N3	2.25	0.70
32:2a:1198:G:OP1	61:2a:3203:HOH:O	2.10	0.70
1:1A:2763:G:OP2	61:1A:4110:HOH:O	2.09	0.70
7:1H:124:GLU:HG3	7:1H:132:ARG:HB3	1.74	0.70
32:2a:1052:U:O2'	32:2a:1055:A:OP2	2.07	0.70
32:2a:1376:U:H2'	32:2a:1377:A:H8	1.55	0.70
35:2d:166:LYS:C	35:2d:166:LYS:HZ2	2.00	0.70
1:2A:965:C:OP2	61:2A:3815:HOH:O	2.09	0.69
1:2A:2584:U:H2'	1:2A:2585:U:H2'	1.75	0.69
1:1A:2464:C:O2'	61:1A:4112:HOH:O	2.09	0.69
35:1d:155:LEU:HB3	35:1d:158:ILE:HG12	1.73	0.69
39:1h:120:THR:H	39:1h:123:GLU:HB2	1.56	0.69
1:2A:2115:G:H22	1:2A:2119:A:H5'	1.56	0.69
3:2D:108:PRO:HB3	3:2D:143:HIS:CE1	2.28	0.69
40:2i:7:THR:O	40:2i:83:ARG:NH1	2.25	0.69
1:1A:927:G:N7	61:1A:4174:HOH:O	2.25	0.69
32:1a:1094:G:OP1	61:1a:1903:HOH:O	2.10	0.69
1:2A:2782:G:OP2	61:2A:3821:HOH:O	2.11	0.69
8:1I:68:LEU:HD21	8:1I:109:ILE:HD11	1.73	0.69
5:2F:20:LEU:HD23	5:2F:21:ALA:H	1.57	0.69
32:2a:944:G:N1	32:2a:1338:G:OP2	2.23	0.69
1:1A:809:G:OP1	61:1A:4115:HOH:O	2.10	0.69
1:1A:1016:G:N7	61:1A:4179:HOH:O	2.26	0.69
1:2A:452:G:OP2	61:2A:3820:HOH:O	2.11	0.69
1:2A:881:G:H1	1:2A:895:U:H3	1.41	0.69
15:2T:95:ARG:HG2	15:2T:95:ARG:HH11	1.56	0.69
1:1A:307:G:H21	1:1A:330:A:H62	1.39	0.69
32:1a:407:G:H5"	35:1d:115:ARG:HB3	1.74	0.69
1:2A:955:C:OP1	12:2Q:87:LYS:NZ	2.23	0.69
1:2A:1912:A:OP1	61:2A:3822:HOH:O	2.11	0.69
1:2A:2206:G:H3'	1:2A:2207:G:C8	2.27	0.69
2:2B:58:A:OP2	61:2B:303:HOH:O	2.11	0.69
6:2G:60:LEU:HD13	6:2G:68:PRO:HG3	1.73	0.69
32:2a:1278:U:H5"	32:2a:1279:A:H5'	1.73	0.69
6:1G:139:LEU:HD21	6:1G:149:VAL:HG11	1.74	0.69
29:17:24:THR:HG23	29:17:27:GLY:H	1.55	0.69
32:1a:79:G:N1	32:1a:90:U:N3	2.40	0.69
32:1a:587:G:N7	61:1a:1916:HOH:O	2.24	0.69
36:1e:8:GLU:HG2	36:1e:34:VAL:HG23	1.75	0.69
39:1h:41:ARG:NH2	39:1h:123:GLU:OE2	2.25	0.69
1:1A:762:U:OP1	61:1A:4116:HOH:O	2.11	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:2H:143:GLN:NE2	7:2H:147:ASN:OD1	2.24	0.69
33:1b:185:ILE:HG22	33:1b:199:TYR:HB2	1.76	0.68
32:2a:559:A:H4'	32:2a:560:U:H3'	1.74	0.68
1:1A:279:C:H42	1:1A:361:G:H1	1.41	0.68
33:1b:67:THR:HA	33:1b:90:MET:HE2	1.75	0.68
27:25:16:ARG:NH1	27:25:17:ASP:OD1	2.27	0.68
1:1A:376:C:OP1	61:1A:4114:HOH:O	2.10	0.68
1:1A:1173:G:O2'	1:1A:1174:A:O5'	2.11	0.68
44:2m:24:GLY:HA3	44:2m:66:LEU:HD12	1.76	0.68
1:1A:1069:A:H5'	1:1A:1070:A:C2	2.28	0.68
1:2A:84:A:N1	1:2A:98:G:O2'	2.26	0.68
26:24:48:ARG:HD2	26:24:52:THR:HA	1.74	0.68
40:2i:42:ARG:NH1	40:2i:71:SER:O	2.27	0.68
61:1A:4102:HOH:O	4:1E:110:GLY:O	2.12	0.68
7:1H:159:GLU:HG2	7:1H:169:VAL:HG11	1.75	0.68
1:2A:826:U:OP1	61:2A:3802:HOH:O	2.12	0.68
2:2B:98:G:OP2	61:2B:302:HOH:O	2.10	0.68
3:1D:88:ARG:NH1	61:1D:401:HOH:O	2.24	0.68
32:1a:473:G:H2'	32:1a:474:G:H8	1.59	0.68
32:1a:1182:G:H4'	32:1a:1183:A:H5'	1.75	0.68
2:2B:75:G:N2	61:2B:310:HOH:O	2.26	0.68
13:2R:103:ARG:NH1	13:2R:108:GLY:O	2.26	0.68
1:2A:2150:U:H2'	1:2A:2151:G:C8	2.29	0.68
12:2Q:109:VAL:HG13	12:2Q:113:GLN:HB3	1.75	0.68
48:2q:67:LYS:HA	48:2q:70:ARG:HH21	1.58	0.68
1:1A:2390:U:OP2	61:1A:4119:HOH:O	2.12	0.68
1:2A:1771:C:OP1	61:2A:3824:HOH:O	2.12	0.68
1:1A:219:G:OP2	61:1A:4120:HOH:O	2.12	0.68
5:2F:192:LEU:HD13	5:2F:194:MET:HE2	1.75	0.68
32:2a:1129:C:H2'	32:2a:1139:G:N7	2.09	0.68
1:1A:2125:G:O2'	1:1A:2173:A:N6	2.26	0.67
32:1a:612:C:O2	32:1a:629:G:N2	2.28	0.67
1:2A:1007:C:OP1	9:2N:35:ARG:NH1	2.27	0.67
1:2A:1371:G:O6	61:2A:3823:HOH:O	2.11	0.67
10:2O:24:VAL:HG13	10:2O:33:ALA:HB2	1.74	0.67
32:2a:677:U:H3	32:2a:713:G:H22	1.39	0.67
1:1A:2350:C:OP2	61:1A:4118:HOH:O	2.12	0.67
1:2A:2646:C:OP2	1:2A:2732:G:O2'	2.10	0.67
2:2B:28:C:OP1	14:2S:36:TYR:OH	2.10	0.67
14:2S:39:ILE:HB	14:2S:49:VAL:HG22	1.76	0.67
32:2a:861:G:OP1	39:2h:75:ARG:NH2	2.27	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:2i:121:ARG:NH1	40:2i:122:ALA:O	2.27	0.67
9:1N:100:GLU:OE2	61:1N:301:HOH:O	2.13	0.67
21:1Z:144:LEU:HD11	21:1Z:150:LEU:HD22	1.74	0.67
32:1a:1015:A:H2'	32:1a:1016:A:C8	2.30	0.67
18:2W:18:ARG:NH1	18:2W:76:VAL:O	2.27	0.67
33:2b:77:ALA:HB2	33:2b:211:ILE:HD13	1.77	0.67
32:1a:1179:A:OP2	40:1i:93:ARG:NH2	2.20	0.67
1:2A:1094:U:H4'	1:2A:1096:A:H62	1.60	0.67
8:2I:77:LEU:HD13	8:2I:101:LEU:HG	1.75	0.67
50:2s:36:ARG:HH12	50:2s:75:ALA:HB3	1.59	0.67
7:1H:27:LYS:HG2	7:1H:32:GLU:HG2	1.75	0.67
32:1a:453:A:O2'	47:1p:68:ASP:O	2.12	0.67
1:2A:989:G:O2'	61:2A:3826:HOH:O	2.12	0.67
1:2A:1324:G:N7	61:2A:3889:HOH:O	2.26	0.67
26:24:48:ARG:O	26:24:50:VAL:N	2.26	0.67
32:1a:598:U:O4	61:1a:1902:HOH:O	2.09	0.67
1:2A:271(L):U:H5'	8:2I:50:ARG:HH22	1.60	0.67
32:2a:134:A:N6	47:2p:25:ARG:HH22	1.93	0.67
32:2a:954:G:H21	32:2a:1227:A:H62	1.41	0.67
32:2a:976:G:H5'	32:2a:1358:U:O2'	1.95	0.67
32:1a:946:A:H2'	32:1a:947:G:C8	2.29	0.67
6:2G:97:ASP:HA	6:2G:100:TRP:HD1	1.60	0.67
1:1A:2270:G:O6	61:1A:4117:HOH:O	2.11	0.67
1:2A:84:A:H5'	20:2Y:8:LYS:HB3	1.75	0.67
1:2A:1631(A):A:N6	61:2A:3891:HOH:O	2.26	0.67
32:1a:1374:A:OP1	38:1g:36:LYS:NZ	2.28	0.67
1:2A:1153:C:OP2	61:2A:3825:HOH:O	2.12	0.67
41:2j:38:ILE:HG12	41:2j:71:LEU:HB3	1.77	0.67
49:2r:32:ARG:HA	49:2r:69:THR:HG21	1.75	0.67
3:1D:71:ASP:HB3	3:1D:103:ARG:HH22	1.60	0.66
32:1a:922:G:H4'	36:1e:20:GLN:HA	1.77	0.66
1:2A:674:G:OP2	61:2A:3819:HOH:O	2.11	0.66
1:2A:2306:C:N4	6:2G:42:GLY:O	2.28	0.66
1:2A:2707:G:OP1	61:2A:3827:HOH:O	2.12	0.66
4:2E:77:ILE:HD13	4:2E:195:LEU:HD22	1.77	0.66
39:2h:86:ILE:HG21	39:2h:133:LEU:HD13	1.76	0.66
1:1A:1332:G:OP1	61:1A:4109:HOH:O	2.14	0.66
1:2A:1069:A:H2'	1:2A:1073:A:N7	2.10	0.66
3:2D:72:LYS:NZ	3:2D:99:ASP:OD2	2.26	0.66
5:2F:101:LEU:HD12	5:2F:102:PRO:HD2	1.77	0.66
32:2a:535:A:OP1	61:2a:3204:HOH:O	2.12	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2839:G:H5'	13:1R:46:GLY:HA2	1.77	0.66
44:1m:12:ASN:O	44:1m:44:ARG:NH1	2.29	0.66
48:1q:45:HIS:HD2	48:1q:65:ILE:HG12	1.60	0.66
32:2a:1376:U:H2'	32:2a:1377:A:C8	2.29	0.66
41:2j:61:GLU:OE2	45:2n:58:LYS:NZ	2.27	0.66
1:2A:2502:G:N7	61:2A:3903:HOH:O	2.28	0.66
1:1A:1757:U:OP1	61:1A:4122:HOH:O	2.14	0.66
1:1A:2637:U:OP2	61:1A:4121:HOH:O	2.13	0.66
47:1p:43:LYS:HG2	47:1p:48:TRP:CE2	2.31	0.66
1:2A:1968:G:N7	61:2A:3907:HOH:O	2.28	0.66
32:2a:656:C:O2'	46:2o:28:GLN:OE1	2.11	0.66
33:2b:15:VAL:HB	33:2b:209:ARG:HB3	1.75	0.66
48:2q:22:LEU:HD13	48:2q:41:LYS:HG2	1.76	0.66
1:2A:1101:U:H2'	1:2A:1102:C:H6	1.60	0.66
1:1A:529:A:N1	61:1A:4216:HOH:O	2.29	0.66
1:1A:1670:C:OP2	61:1A:4101:HOH:O	2.12	0.66
19:1X:53:LYS:HB3	19:1X:82:GLN:HB3	1.78	0.66
39:1h:86:ILE:HD12	39:1h:133:LEU:HD22	1.78	0.66
47:1p:53:VAL:HG13	47:1p:79:VAL:HG12	1.77	0.66
1:2A:2504:U:OP2	61:2A:3828:HOH:O	2.14	0.66
6:2G:11:TYR:HA	6:2G:15:VAL:HG22	1.77	0.66
1:1A:1064:C:C4	1:1A:1074:G:O6	2.48	0.66
32:1a:1129:C:O2'	32:1a:1139:G:N7	2.21	0.66
33:1b:166:ASP:HB3	33:1b:169:LYS:HB3	1.78	0.66
32:2a:895:G:N7	61:2a:3233:HOH:O	2.28	0.66
32:2a:1005:A:OP2	32:2a:1024:G:N2	2.28	0.66
32:2a:1456:G:N1	51:2t:51:GLU:OE2	2.27	0.66
6:1G:49:ASP:O	6:1G:51:ARG:N	2.28	0.66
1:2A:2499:C:N3	61:2A:3910:HOH:O	2.28	0.66
6:2G:33:ARG:HE	6:2G:162:THR:HG21	1.60	0.66
26:24:46:GLN:O	26:24:48:ARG:N	2.28	0.66
9:1N:73:THR:HG23	9:1N:82:LEU:HD11	1.77	0.66
35:1d:85:LYS:O	61:1d:401:HOH:O	2.14	0.66
33:2b:217:ARG:HA	33:2b:220:ASP:HB2	1.78	0.66
1:1A:278:A:O2'	1:1A:279:C:OP1	2.12	0.65
3:1D:69:ARG:NH2	3:1D:128:GLY:O	2.29	0.65
8:1I:130:TYR:HB3	8:1I:138:ILE:HB	1.77	0.65
1:2A:2168:G:O2'	1:2A:2170:A:N7	2.28	0.65
32:2a:1226:C:N4	44:2m:104:ARG:HD2	2.11	0.65
32:2a:1402:4OC:HM22	32:2a:1403:C:H5'	1.77	0.65
35:2d:60:GLU:HG3	35:2d:202:LEU:HD12	1.79	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:2k:117:ASN:N	42:2k:117:ASN:OD1	2.29	0.65
1:1A:1816:G:O6	3:1D:35:LYS:NZ	2.28	0.65
1:1A:1937:A:H1'	1:1A:1939:5MU:H72	1.77	0.65
15:1T:39:ARG:NH1	61:1T:302:HOH:O	2.29	0.65
53:1y:49:VAL:HG22	53:1y:66:LYS:HG2	1.78	0.65
14:2S:34:HIS:O	14:2S:97:ARG:NH2	2.29	0.65
38:2g:135:VAL:HA	38:2g:138:LYS:HB3	1.78	0.65
40:2i:26:VAL:HG22	40:2i:61:ALA:HB3	1.76	0.65
7:1H:3:ARG:HG2	7:1H:6:ARG:HG3	1.77	0.65
19:1X:31:HIS:CD2	19:1X:33:LYS:H	2.13	0.65
32:1a:376:G:H4'	47:1p:5:ARG:HH11	1.60	0.65
40:1i:7:THR:O	40:1i:83:ARG:NH1	2.29	0.65
1:2A:299:A:N1	1:2A:322:A:O2'	2.26	0.65
12:2Q:11:LYS:NZ	12:2Q:88:GLY:O	2.22	0.65
32:2a:769:G:H4'	32:2a:1513:A:H4'	1.78	0.65
1:2A:2821:A:OP2	61:2R:301:HOH:O	2.13	0.65
1:1A:2815:C:H5'	27:15:29:THR:HG21	1.79	0.65
1:2A:323:G:HO2'	1:2A:1205:U:H3	1.43	0.65
5:2F:17:ARG:HH12	5:2F:19:GLU:HG3	1.62	0.65
40:1i:17:VAL:HB	40:1i:63:ILE:HG12	1.78	0.65
1:2A:1507:A:O2'	1:2A:1508:A:O5'	2.14	0.65
1:2A:2126:A:H4'	1:2A:2127:G:O5'	1.95	0.65
1:1A:1382:G:N7	61:1A:4197:HOH:O	2.28	0.65
32:1a:176:C:H2'	32:1a:177:C:H6	1.62	0.65
32:1a:189(K):U:H2'	32:1a:189(L):G:H8	1.62	0.65
5:1F:53:THR:CG2	5:1F:55:GLY:H	2.10	0.65
1:2A:362:U:O2'	1:2A:363:G:H5'	1.97	0.65
8:2I:72:LEU:HD21	8:2I:107:VAL:HG11	1.77	0.65
1:2A:2683:C:O2	10:2O:70:LYS:NZ	2.22	0.65
32:2a:148:G:H2'	32:2a:149:A:H8	1.61	0.65
32:2a:942:G:N2	40:2i:124:GLN:OE1	2.29	0.65
33:2b:74:LYS:NZ	33:2b:205:ASP:O	2.30	0.65
26:14:16:CYS:SG	26:14:17:GLY:N	2.70	0.65
24:22:9:GLN:O	61:22:101:HOH:O	2.15	0.65
32:1a:186:C:H2'	32:1a:187:C:C6	2.33	0.64
1:2A:1365:A:O2'	23:21:11:ARG:NH1	2.30	0.64
1:2A:2105:C:N4	1:2A:2106:G:O6	2.30	0.64
1:2A:2255:G:OP2	61:2A:3831:HOH:O	2.14	0.64
1:2A:2407:G:OP1	61:2A:3833:HOH:O	2.15	0.64
32:2a:1189:C:OP1	41:2j:51:ARG:NH2	2.29	0.64
17:1V:74:LYS:HB2	17:1V:83:ARG:HB2	1.78	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1009:A:OP2	61:2A:3830:HOH:O	2.14	0.64
32:2a:1164:G:H1	32:2a:1172:C:N4	1.93	0.64
32:1a:800:G:N7	61:1a:1931:HOH:O	2.29	0.64
1:2A:1105:U:H2'	1:2A:1106:G:H8	1.62	0.64
6:2G:38:VAL:HG22	6:2G:93:THR:HB	1.79	0.64
32:2a:222:U:H2'	32:2a:223:U:C6	2.32	0.64
32:2a:1068:G:N2	32:2a:1191:A:N3	2.45	0.64
32:2a:1435:G:H2'	32:2a:1436:U:C6	2.31	0.64
33:2b:111:ARG:HH11	33:2b:111:ARG:HA	1.61	0.64
33:1b:82:ARG:NH1	33:1b:92:TYR:OH	2.30	0.64
8:2I:77:LEU:HD23	8:2I:142:VAL:HG13	1.79	0.64
19:1X:41:ASN:O	19:1X:45:THR:HG23	1.96	0.64
36:1e:8:GLU:OE2	36:1e:63:ARG:NH2	2.30	0.64
46:1o:33:THR:HG21	46:1o:85:LEU:HD22	1.79	0.64
33:2b:16:HIS:HB2	33:2b:204:ASN:HB3	1.78	0.64
2:1B:30:C:OP1	61:1B:302:HOH:O	2.15	0.64
5:1F:192:LEU:HD13	5:1F:194:MET:HE2	1.78	0.64
32:1a:316:G:OP2	32:1a:351:G:O2'	2.15	0.64
38:1g:148:ASN:HD22	42:1k:54:ARG:HH22	1.46	0.64
1:2A:526:A:OP1	61:2A:3829:HOH:O	2.14	0.64
18:2W:71:VAL:HA	18:2W:107:LEU:HD12	1.79	0.64
34:2c:110:ASN:OD1	34:2c:140:ARG:NH1	2.30	0.64
11:1P:59:LEU:HD21	30:18:10:ALA:HB2	1.79	0.64
1:2A:991:C:OP2	61:2A:3834:HOH:O	2.15	0.64
3:2D:69:ARG:NH2	3:2D:128:GLY:O	2.31	0.64
5:2F:122:LYS:NZ	5:2F:152:GLU:OE2	2.31	0.64
1:1A:2133:G:H3'	1:1A:2157:G:H21	1.63	0.64
1:1A:2183:C:H2'	1:1A:2184:G:C8	2.33	0.64
32:2a:1352:C:OP1	52:2u:3:LYS:NZ	2.31	0.64
32:1a:17:U:H2'	32:1a:18:C:C6	2.33	0.64
32:1a:271:C:H2'	32:1a:272:C:H6	1.62	0.64
32:2a:413:G:N7	35:2d:35:ARG:NH1	2.46	0.64
32:1a:186:C:H2'	32:1a:187:C:H6	1.62	0.63
32:1a:1033:G:H2'	32:1a:1034:G:H8	1.61	0.63
51:1t:14:LYS:HG2	51:1t:18:GLN:HE21	1.63	0.63
1:2A:1025:G:C4	1:2A:1135:C:H1'	2.33	0.63
1:2A:2112:G:H2'	1:2A:2113:U:C6	2.33	0.63
32:2a:977:A:O3'	32:2a:980:C:N4	2.31	0.63
34:2c:71:ALA:HA	34:2c:106:VAL:HB	1.79	0.63
41:2j:33:GLN:H	41:2j:75:ILE:H	1.45	0.63
32:1a:1304:G:OP2	61:1a:1904:HOH:O	2.15	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:1i:50:LEU:HD13	40:1i:56:LEU:HA	1.79	0.63
1:2A:1064:C:H3'	1:2A:1065:U:C5'	2.27	0.63
32:2a:1352:C:N4	32:2a:1370:G:H1	1.97	0.63
38:2g:91:VAL:HG13	38:2g:95:ARG:HG2	1.80	0.63
26:14:57:GLU:HB2	26:14:58:ARG:HA	1.79	0.63
1:2A:1941:C:OP2	61:2A:3832:HOH:O	2.14	0.63
38:2g:27:ILE:HD12	38:2g:40:ALA:HA	1.79	0.63
40:2i:21:PRO:HA	40:2i:59:PHE:HA	1.79	0.63
47:1p:20:VAL:HG23	47:1p:35:LYS:HA	1.80	0.63
50:1s:63:THR:OG1	50:1s:65:ASN:OD1	2.16	0.63
5:2F:11:VAL:HG22	5:2F:125:LEU:HB2	1.81	0.63
32:2a:410:G:OP1	35:2d:30:LYS:NZ	2.30	0.63
35:2d:166:LYS:HZ2	35:2d:167:GLY:N	1.95	0.63
7:1H:20:ALA:HB1	7:1H:21:PRO:HD2	1.79	0.63
14:1S:3:ARG:NH2	61:1S:203:HOH:O	2.30	0.63
32:1a:1135:U:H4'	32:1a:1136:U:H5	1.64	0.63
32:1a:1412:C:H2'	32:1a:1413:A:C8	2.33	0.63
1:2A:1199:U:OP1	61:2A:3835:HOH:O	2.15	0.63
44:2m:91:ARG:HB2	44:2m:98:VAL:HG12	1.78	0.63
32:1a:677:U:H3	32:1a:713:G:H22	1.46	0.63
1:2A:1014:U:H2'	1:2A:1015:G:H8	1.63	0.63
46:1o:39:LEU:HD13	46:1o:56:LEU:HB2	1.81	0.63
1:2A:2615:U:OP1	61:2A:3836:HOH:O	2.15	0.63
14:2S:15:ARG:HB3	14:2S:19:LYS:HE3	1.81	0.63
21:1Z:158:PRO:HG2	21:1Z:161:VAL:HG11	1.81	0.63
32:1a:100:C:H2'	32:1a:101:A:C8	2.33	0.63
1:2A:583:G:N7	61:2A:3929:HOH:O	2.31	0.63
1:2A:1378:A:OP1	29:27:10:ARG:NH2	2.32	0.63
32:2a:41:G:H2'	32:2a:42:G:C8	2.33	0.63
32:2a:111:G:OP2	61:2a:3205:HOH:O	2.15	0.63
33:2b:67:THR:HG23	33:2b:159:PRO:HA	1.81	0.63
40:2i:53:VAL:O	40:2i:55:ALA:N	2.32	0.63
1:1A:1509(A):A:H2'	1:1A:1509(B):A:O4'	1.99	0.62
2:1B:77:U:OP1	21:1Z:19:ARG:NH2	2.32	0.62
32:1a:347:G:C8	57:1a:1880:MPD:H53	2.34	0.62
6:2G:115:ARG:HB2	6:2G:136:ARG:HH21	1.64	0.62
32:2a:402:G:O2'	32:2a:620:C:N3	2.29	0.62
32:2a:862:C:H1'	32:2a:874:G:H5"	1.81	0.62
32:2a:1237:C:HO2'	32:2a:1300:G:H1	1.46	0.62
61:2a:3231:HOH:O	43:2l:54:LYS:NZ	2.31	0.62
36:2e:102:ALA:HB1	36:2e:106:PRO:HG2	1.79	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:53:A:OP2	61:2A:3837:HOH:O	2.15	0.62
1:2A:1607:C:N4	1:2A:1622:G:OP2	2.28	0.62
2:2B:116:G:N7	61:2B:314:HOH:O	2.31	0.62
32:2a:17:U:H2'	32:2a:18:C:C6	2.34	0.62
34:2c:35:GLU:OE2	34:2c:59:ARG:NH2	2.31	0.62
35:2d:79:PHE:HE1	35:2d:204:ILE:HD13	1.64	0.62
1:1A:588:U:H2'	1:1A:589:C:C6	2.34	0.62
1:2A:2379:G:O2'	14:2S:17:ARG:NH1	2.27	0.62
11:2P:91:PHE:O	11:2P:121:LYS:NZ	2.32	0.62
12:2Q:135:ASP:OD2	12:2Q:136:ALA:N	2.29	0.62
1:1A:715:G:C2	46:1o:56:LEU:HD21	2.33	0.62
1:1A:2820:A:OP2	13:1R:2:ARG:NH2	2.32	0.62
32:1a:1435:G:H2'	32:1a:1436:U:C6	2.34	0.62
33:1b:134:GLU:HG3	33:1b:137:ARG:HH21	1.64	0.62
1:2A:468:G:O2'	5:2F:62:ARG:NH2	2.32	0.62
6:2G:145:THR:HG22	6:2G:148:MET:HE3	1.80	0.62
1:1A:226:G:H21	1:1A:228:A:H62	1.47	0.62
1:2A:2805:G:H2'	1:2A:2807:G:C8	2.34	0.62
32:2a:142:G:H2'	32:2a:143:A:H8	1.65	0.62
44:2m:65:LYS:HE3	44:2m:69:GLU:HB3	1.80	0.62
1:1A:1069:A:H4'	1:1A:1070:A:H5"	1.81	0.62
32:1a:1003:G:C2'	32:1a:1004:A:H4'	2.29	0.62
35:1d:172:PRO:HB2	35:1d:187:ARG:HH21	1.64	0.62
49:1r:32:ARG:HA	49:1r:69:THR:HG21	1.81	0.62
4:2E:59:VAL:HG21	4:2E:74:PRO:HB3	1.82	0.62
32:2a:1062:U:H2'	32:2a:1063:C:C6	2.35	0.62
34:2c:124:ILE:HD12	34:2c:130:VAL:HG22	1.81	0.62
46:2o:39:LEU:HD13	46:2o:56:LEU:HB2	1.80	0.62
19:1X:35:THR:HG22	19:1X:38:GLU:H	1.65	0.62
1:2A:918:A:H5"	2:2B:98:G:O2'	1.99	0.62
32:2a:1239:A:H62	32:2a:1299:A:H62	1.48	0.62
1:1A:942:G:O6	61:1A:4126:HOH:O	2.16	0.62
1:1A:1053:C:N3	1:1A:1106:G:O6	2.32	0.62
1:1A:1187:G:H5"	17:1V:81:TYR:CE1	2.34	0.62
15:1T:127:ALA:C	15:1T:129:ARG:H	2.07	0.62
35:1d:18:LYS:NZ	35:1d:31:CYS:SG	2.73	0.62
1:2A:530:G:N1	1:2A:2023:G:OP1	2.29	0.62
14:2S:93:LYS:HG2	14:2S:95:HIS:HB2	1.82	0.62
32:2a:1360:A:OP2	45:2n:35:ARG:NH2	2.33	0.62
32:1a:1158:C:H5	32:1a:1181:G:H1	1.44	0.62
1:2A:309:G:N3	1:2A:329:G:O2'	2.32	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2125:G:O2'	1:2A:2173:A:N6	2.33	0.62
44:1m:11:ARG:HA	44:1m:45:VAL:HB	1.82	0.62
34:2c:19:GLU:HB3	34:2c:40:ARG:HH12	1.65	0.62
44:2m:58:GLU:O	44:2m:62:ASN:ND2	2.32	0.62
46:2o:25:THR:HG21	46:2o:70:LEU:HB2	1.80	0.62
1:2A:1011:G:OP2	16:2U:66:ASN:ND2	2.32	0.61
1:2A:1332:G:OP1	61:2A:3809:HOH:O	2.16	0.61
1:2A:2749:A:OP1	7:2H:3:ARG:NH1	2.33	0.61
32:2a:41:G:H2'	32:2a:42:G:H8	1.65	0.61
1:1A:1271:G:OP2	61:1A:4106:HOH:O	2.16	0.61
21:1Z:136:PHE:HE1	21:1Z:138:GLU:HG3	1.65	0.61
1:2A:1803:A:O2'	3:2D:259:THR:HG21	1.99	0.61
1:1A:1069:A:H5'	1:1A:1070:A:H2	1.65	0.61
1:1A:2139:C:H42	1:1A:2152:G:H1	1.47	0.61
1:2A:607:U:OP1	5:2F:102:PRO:HA	2.01	0.61
1:2A:1840:G:OP2	61:2A:3841:HOH:O	2.16	0.61
1:2A:2112:G:H2'	1:2A:2113:U:H6	1.64	0.61
34:2c:8:ILE:HG12	34:2c:184:TYR:HB3	1.81	0.61
1:1A:271(L):U:OP1	8:1I:50:ARG:NH2	2.26	0.61
24:12:65:ASN:OD1	24:12:69:ARG:NH1	2.34	0.61
27:15:16:ARG:HG3	27:15:17:ASP:N	2.14	0.61
34:2c:111:LEU:HD22	34:2c:146:ALA:HB2	1.83	0.61
1:1A:2023:G:H5'	1:1A:2617:C:H4'	1.80	0.61
20:1Y:92:ASN:N	20:1Y:93:GLY:HA2	2.14	0.61
33:1b:17:PHE:HB3	33:1b:44:LEU:HD21	1.80	0.61
1:2A:1053:C:H2'	1:2A:1054:A:H8	1.66	0.61
1:2A:2113:U:H3	1:2A:2168:G:H5'	1.65	0.61
1:2A:2753:A:N3	31:29:15:LYS:NZ	2.47	0.61
32:2a:601:C:H2'	32:2a:602:A:H8	1.64	0.61
33:2b:71:VAL:HG23	33:2b:164:VAL:HA	1.82	0.61
1:1A:1830:C:OP2	61:1A:4124:HOH:O	2.16	0.61
11:1P:42:SER:O	61:1P:301:HOH:O	2.16	0.61
32:1a:1112:C:H1'	34:1c:179:ARG:HE	1.66	0.61
34:1c:6:HIS:HD2	34:1c:8:ILE:H	1.47	0.61
2:2B:117:G:N7	61:2B:315:HOH:O	2.31	0.61
32:2a:255:G:OP1	48:2q:69:LYS:NZ	2.25	0.61
32:2a:662:G:H2'	32:2a:663:A:C8	2.36	0.61
32:1a:262:A:H2'	32:1a:263:A:C8	2.35	0.61
48:1q:20:THR:HG23	48:1q:43:LEU:HD12	1.83	0.61
6:2G:19:LEU:HD13	6:2G:32:PRO:HD2	1.83	0.61
12:2Q:10:ARG:HG2	12:2Q:11:LYS:HG2	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2S:74:ALA:HB2	14:2S:105:ALA:HA	1.83	0.61
32:2a:1510:U:H2'	32:2a:1511:G:C8	2.34	0.61
33:2b:83:MET:HE1	33:2b:235:SER:HA	1.82	0.61
1:1A:2207:G:O2'	1:1A:2208:A:OP1	2.18	0.61
33:1b:181:PHE:HB3	39:1h:70:GLN:HE21	1.66	0.61
1:2A:1239:G:OP1	61:2A:3840:HOH:O	2.16	0.61
1:2A:1754:C:P	15:2T:96:ARG:HH12	2.24	0.61
32:2a:565:U:OP2	32:2a:566:G:O2'	2.16	0.61
33:2b:58:ILE:HD11	33:2b:185:ILE:HG12	1.83	0.61
32:2a:461:A:O2'	32:2a:471:G:N7	2.29	0.61
33:2b:44:LEU:HA	33:2b:47:THR:HG22	1.82	0.61
1:1A:1378:A:OP1	29:17:10:ARG:NH2	2.34	0.60
1:1A:1840:G:N7	61:1A:4235:HOH:O	2.31	0.60
1:1A:1877:A:H5'	1:1A:1878:G:OP2	2.01	0.60
32:1a:965:A:OP2	53:1y:8:LYS:NZ	2.34	0.60
33:1b:98:LEU:HG	33:1b:101:MET:HE3	1.83	0.60
41:1j:35:SER:N	41:1j:73:ASP:O	2.27	0.60
1:2A:668:G:H5'	1:2A:669:G:OP2	2.01	0.60
1:2A:2469:A:H4'	12:2Q:56:ARG:HG2	1.83	0.60
32:2a:1003:G:H3'	32:2a:1003:G:N3	2.16	0.60
43:2l:28:LYS:HB2	43:2l:33:ARG:HH21	1.67	0.60
53:2y:23:ARG:HG3	53:2y:78:ILE:HG13	1.81	0.60
11:1P:87:ASP:O	11:1P:90:ARG:NH1	2.34	0.60
32:1a:976:G:H5'	32:1a:1358:U:O2'	2.01	0.60
32:1a:1218:C:H2'	32:1a:1219:U:C6	2.35	0.60
36:1e:81:GLU:HG2	36:1e:90:VAL:HG22	1.82	0.60
1:2A:483:A:H5"	20:2Y:50:ARG:HD3	1.81	0.60
1:2A:489:G:N7	18:2W:49:LYS:NZ	2.49	0.60
1:2A:1006:C:OP2	61:2A:3839:HOH:O	2.16	0.60
3:2D:108:PRO:HD2	3:2D:111:LEU:HD22	1.82	0.60
33:2b:54:THR:HG23	33:2b:199:TYR:HB3	1.82	0.60
1:1A:483:A:H5"	20:1Y:50:ARG:HH11	1.66	0.60
46:1o:55:GLY:HA2	46:1o:58:MET:HE3	1.83	0.60
1:2A:2122:U:H3	1:2A:2176:A:N6	1.97	0.60
2:2B:54:G:H21	6:2G:29:TRP:HZ2	1.49	0.60
12:2Q:31:ASP:OD1	12:2Q:134:ARG:NH1	2.34	0.60
1:1A:2126:A:H4'	1:1A:2127:G:O5'	2.00	0.60
1:2A:271(H):G:H2'	1:2A:271(I):G:H8	1.66	0.60
1:2A:2134:A:N6	1:2A:2156:G:O2'	2.35	0.60
30:28:34:TRP:O	61:28:201:HOH:O	2.16	0.60
32:2a:316:G:OP2	32:2a:351:G:O2'	2.19	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1174:A:H1'	1:1A:1175:U:H5'	1.82	0.60
1:1A:1508:A:H4'	1:1A:1509(A):A:C5	2.37	0.60
32:1a:945:G:OP1	61:1a:1908:HOH:O	2.17	0.60
34:1c:62:ASP:O	34:1c:98:ASN:ND2	2.33	0.60
1:2A:81:G:N7	61:2A:3925:HOH:O	2.30	0.60
32:2a:992:U:H4'	32:2a:993:G:O5'	2.01	0.60
1:1A:607:U:OP1	5:1F:102:PRO:HA	2.02	0.60
15:1T:29:ARG:HG3	15:1T:46:GLU:HB2	1.83	0.60
26:14:7:PRO:HB2	26:14:27:THR:HG21	1.83	0.60
1:2A:271(R):G:H5"	23:21:97:LEU:HD21	1.82	0.60
1:2A:2206:G:H5"	1:2A:2207:G:C8	2.37	0.60
32:2a:224:C:H2'	32:2a:225:C:H6	1.67	0.60
41:2j:8:LEU:HB2	41:2j:70:ARG:HB2	1.83	0.60
1:1A:2243:U:H2'	1:1A:2244:U:C6	2.37	0.60
32:1a:189(K):U:H2'	32:1a:189(L):G:C8	2.37	0.60
32:1a:1456:G:N1	51:1t:51:GLU:OE2	2.32	0.60
42:1k:92:GLU:OE1	49:1r:87:ARG:NH2	2.34	0.60
26:24:24:THR:OG1	26:24:25:TYR:N	2.35	0.60
48:2q:67:LYS:O	48:2q:69:LYS:N	2.34	0.60
44:1m:17:VAL:O	44:1m:20:THR:OG1	2.16	0.60
1:2A:1105:U:H2'	1:2A:1106:G:C8	2.36	0.60
1:2A:2130:U:H2'	1:2A:2158:A:N1	2.16	0.60
6:2G:7:LEU:HD23	6:2G:100:TRP:HE3	1.67	0.60
32:2a:601:C:H2'	32:2a:602:A:C8	2.37	0.60
33:2b:80:ILE:HD11	33:2b:212:GLN:HE21	1.67	0.60
2:1B:8:U:O3'	14:1S:25:ARG:NH2	2.35	0.60
53:1y:52:ALA:HB2	53:1y:77:LEU:HD21	1.84	0.60
4:2E:116:VAL:HG13	4:2E:122:PHE:HB2	1.84	0.60
32:2a:1025:U:O2'	32:2a:1026:G:N7	2.35	0.60
43:2l:60:LEU:HD11	43:2l:66:VAL:HG22	1.82	0.60
4:1E:116:VAL:HG13	4:1E:122:PHE:HB2	1.83	0.60
7:1H:3:ARG:NH1	7:1H:5:GLY:H	2.00	0.60
10:1O:73:ASP:HB2	15:1T:82:LEU:HD13	1.83	0.60
18:1W:4:LYS:NZ	61:1W:303:HOH:O	2.33	0.60
32:1a:651:C:OP1	61:1a:1906:HOH:O	2.16	0.60
1:2A:2023:G:H5'	1:2A:2617:C:H4'	1.84	0.60
1:2A:2602:A:H1'	1:2A:2603:G:C5'	2.32	0.60
9:2N:96:GLU:HB2	9:2N:122:VAL:HG12	1.83	0.60
40:2i:28:VAL:HG13	40:2i:63:ILE:HB	1.82	0.60
48:1q:95:TYR:HA	48:1q:98:LEU:HD12	1.84	0.59
1:2A:1405:U:H2'	1:2A:1406:U:C6	2.36	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1634:A:OP2	61:1A:4123:HOH:O	2.16	0.59
30:18:15:LYS:HB3	57:18:103:MPD:H53	1.84	0.59
32:1a:973:G:H3'	32:1a:974:A:H5"	1.84	0.59
33:1b:12:GLU:O	33:1b:15:VAL:HG12	2.02	0.59
7:1H:40:GLU:OE1	7:1H:60:ARG:NH1	2.32	0.59
26:14:16:CYS:HB3	26:14:20:ASN:HB3	1.83	0.59
32:1a:1352:C:OP1	52:1u:3:LYS:NZ	2.28	0.59
1:2A:1639:U:H2'	1:2A:1640:C:H5"	1.83	0.59
6:2G:38:VAL:HG13	6:2G:93:THR:HG22	1.85	0.59
32:2a:148:G:H2'	32:2a:149:A:C8	2.37	0.59
32:2a:1305:G:OP1	52:2u:2:GLY:N	2.36	0.59
32:2a:1513:A:H2'	32:2a:1514:C:C6	2.37	0.59
1:1A:1178:C:H2'	1:1A:1179:C:C6	2.38	0.59
8:1I:77:LEU:HD22	8:1I:101:LEU:HG	1.84	0.59
26:14:55:ARG:H	26:14:56:VAL:HA	1.68	0.59
32:2a:1291:G:H4'	40:2i:39:GLY:HA3	1.85	0.59
33:2b:93:VAL:HG21	33:2b:97:TRP:CD1	2.34	0.59
32:1a:626:U:H2'	32:1a:627:G:C8	2.37	0.59
32:1a:1286:A:H2'	32:1a:1287:A:H4'	1.84	0.59
40:1i:26:VAL:HA	40:1i:61:ALA:HB3	1.85	0.59
1:2A:271(H):G:H2'	1:2A:271(I):G:C8	2.37	0.59
1:2A:1084:A:H8	1:2A:1085:A:H4'	1.66	0.59
6:2G:57:ALA:HB2	6:2G:90:LEU:HD23	1.84	0.59
41:2j:63:PHE:HE1	45:2n:58:LYS:HG2	1.67	0.59
48:2q:81:ARG:NH1	48:2q:83:ASP:OD1	2.35	0.59
53:2y:52:ALA:HB2	53:2y:77:LEU:HD21	1.84	0.59
1:1A:2406:U:OP1	61:1A:4125:HOH:O	2.16	0.59
15:1T:33:LYS:HG2	15:1T:82:LEU:HD23	1.84	0.59
19:1X:60:ARG:NH1	29:17:47:ARG:HH22	2.00	0.59
33:1b:16:HIS:HB3	33:1b:210:SER:HB2	1.84	0.59
43:1l:33:ARG:HE	43:1l:62:SER:HB3	1.67	0.59
36:2e:110:LEU:HD13	36:2e:118:ILE:HG21	1.84	0.59
38:2g:15:ASP:OD1	38:2g:20:ASP:N	2.35	0.59
40:2i:40:LEU:HD23	40:2i:74:ILE:HD11	1.83	0.59
1:1A:796:C:H2'	1:1A:797:C:C6	2.38	0.59
46:1o:25:THR:HG21	46:1o:70:LEU:HB2	1.85	0.59
35:2d:15:GLU:OE2	35:2d:66:ARG:NH1	2.35	0.59
36:2e:100:VAL:O	36:2e:107:ARG:NH2	2.28	0.59
1:1A:1300:U:H4'	1:1A:1301:A:C5'	2.32	0.59
2:2B:33:G:H1'	2:2B:50:G:H22	1.68	0.59
32:2a:953:G:N7	44:2m:104:ARG:NH2	2.51	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:14:56:VAL:HB	26:14:60:GLN:HG2	1.83	0.59
40:1i:4:TYR:HB2	40:1i:19:LEU:HB2	1.83	0.59
1:2A:669:G:O6	61:2A:3842:HOH:O	2.16	0.59
61:2B:305:HOH:O	6:2G:67:LYS:N	2.36	0.59
14:2S:50:SER:O	14:2S:76:LYS:NZ	2.27	0.59
1:1A:958:U:H5"	12:1Q:14:ARG:HD3	1.84	0.59
8:2I:130:TYR:HB3	8:2I:138:ILE:HB	1.83	0.59
9:2N:4:TYR:O	16:2U:64:ARG:NH2	2.24	0.59
12:1Q:103:MET:HE1	12:1Q:125:LEU:HD13	1.85	0.58
17:1V:1:MET:HE1	17:1V:43:GLU:HB2	1.83	0.58
41:1j:8:LEU:HB2	41:1j:70:ARG:HB2	1.85	0.58
1:2A:1278:A:OP1	13:2R:36:THR:HG23	2.03	0.58
12:2Q:103:MET:HE3	12:2Q:125:LEU:HD13	1.84	0.58
32:2a:1305:G:N2	32:2a:1331:G:H1'	2.18	0.58
53:2y:58:ASN:ND2	53:2y:89:GLN:OE1	2.36	0.58
4:1E:29:GLY:HA3	61:1E:410:HOH:O	2.01	0.58
1:2A:2693:A:H2'	1:2A:2694:G:H8	1.68	0.58
32:2a:922:G:H4'	36:2e:20:GLN:HA	1.83	0.58
1:1A:1011:G:OP1	16:1U:77:SER:HB2	2.04	0.58
32:1a:330:C:OP2	61:1a:1905:HOH:O	2.16	0.58
32:1a:473:G:H2'	32:1a:474:G:C8	2.38	0.58
1:2A:1076:C:H4'	1:2A:1077:A:OP1	2.02	0.58
61:2A:3842:HOH:O	5:2F:53:THR:HG21	2.03	0.58
6:2G:3:LEU:HD23	6:2G:3:LEU:H	1.68	0.58
38:2g:69:VAL:HG22	38:2g:135:VAL:HG12	1.84	0.58
7:1H:11:VAL:HG21	7:1H:50:VAL:HG23	1.84	0.58
1:2A:922:U:H2'	1:2A:923:C:C6	2.38	0.58
1:2A:2152:G:H2'	1:2A:2153:G:C8	2.39	0.58
21:2Z:153:SER:HB3	21:2Z:167:PRO:HB3	1.84	0.58
32:2a:986:A:N3	50:2s:52:TYR:OH	2.31	0.58
32:2a:1366:C:O2'	41:2j:60:ARG:NH2	2.37	0.58
34:2c:6:HIS:HB3	45:2n:49:HIS:HD2	1.67	0.58
34:2c:142:MET:HG3	34:2c:170:GLN:HB3	1.86	0.58
38:2g:75:VAL:HG13	38:2g:145:ALA:HA	1.86	0.58
1:1A:1364:G:N7	23:11:3:LYS:HE2	2.17	0.58
1:1A:1647:G:OP1	61:1A:4106:HOH:O	2.17	0.58
47:1p:57:ARG:HH21	47:1p:79:VAL:HA	1.69	0.58
1:2A:2111:C:H42	1:2A:2147:G:H22	1.50	0.58
2:2B:102:A:OP2	61:2B:304:HOH:O	2.17	0.58
14:2S:58:LEU:HG	14:2S:59:LYS:H	1.67	0.58
40:2i:22:GLY:H	40:2i:59:PHE:HA	1.69	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1486:A:H2'	1:1A:1487:G:H8	1.69	0.58
13:1R:97:VAL:HG22	13:1R:114:VAL:HG13	1.85	0.58
32:1a:1510:U:H2'	32:1a:1511:G:C8	2.38	0.58
38:1g:75:VAL:HG21	38:1g:144:MET:HG2	1.85	0.58
1:2A:2602:A:H4'	1:2A:2603:G:OP1	2.04	0.58
5:2F:143:ALA:HB1	5:2F:148:LEU:HB2	1.84	0.58
32:2a:181:G:N2	32:2a:182:U:O4	2.27	0.58
39:2h:10:LEU:HD22	39:2h:83:ILE:HD11	1.86	0.58
1:1A:1053:C:O2	1:1A:1106:G:N1	2.36	0.58
1:1A:2291:U:H2'	1:1A:2292:C:C6	2.39	0.58
6:2G:101:ILE:HG22	6:2G:105:LYS:HE2	1.85	0.58
32:2a:1084:G:H5'	32:2a:1102:A:OP2	2.04	0.58
33:2b:178:ARG:HH22	39:2h:74:PRO:HB3	1.69	0.58
50:2s:31:ILE:HB	50:2s:49:ILE:HG13	1.85	0.58
1:1A:2882:A:OP1	13:1R:96:ARG:HD3	2.04	0.58
2:1B:66:A:H61	2:1B:108:U:H2'	1.69	0.58
3:1D:137:PRO:O	3:1D:140:THR:HG23	2.04	0.58
25:13:7:LYS:HE3	25:13:32:GLN:HE21	1.69	0.58
33:1b:67:THR:N	33:1b:160:ASP:OD1	2.36	0.58
1:2A:885:C:H2'	1:2A:886:C:O4'	2.04	0.58
5:2F:164:ARG:O	5:2F:168:ARG:HG3	2.04	0.58
19:2X:53:LYS:HB3	19:2X:82:GLN:HB3	1.85	0.58
32:2a:1004:A:H5"	32:2a:1025:U:C5	2.39	0.58
41:2j:77:PRO:O	41:2j:81:THR:OG1	2.20	0.58
1:1A:1025:G:C4	1:1A:1135:C:H1'	2.38	0.58
1:1A:2096:U:H2'	1:1A:2097:C:C6	2.39	0.58
1:1A:2119:A:N6	1:1A:2171:A:N7	2.51	0.58
33:1b:231:GLU:HB3	33:1b:232:PRO:CD	2.32	0.58
1:2A:770:G:OP2	61:2A:3845:HOH:O	2.17	0.58
1:2A:1062:G:H2'	1:2A:1063:G:H8	1.68	0.58
1:2A:1371:G:HO2'	1:2A:1372:U:H5	1.52	0.58
1:2A:1514:U:H2'	1:2A:1515:G:H8	1.69	0.58
1:2A:2327:A:H2'	1:2A:2328:A:C8	2.38	0.58
1:2A:2565:A:OP1	61:2A:3843:HOH:O	2.17	0.58
1:2A:2657:A:O3'	7:2H:160:LYS:NZ	2.37	0.58
34:2c:78:GLY:HA3	34:2c:83:ARG:H	1.68	0.58
1:1A:1056:G:N1	1:1A:1102:C:OP2	2.34	0.58
1:1A:2125:G:H22	1:1A:2172:U:H5"	1.67	0.58
24:22:1:MET:SD	24:22:56:GLN:NE2	2.77	0.58
34:2c:66:VAL:HB	34:2c:101:LEU:HD12	1.86	0.58
1:1A:2319:G:N2	14:1S:3:ARG:HA	2.19	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1059:G:OP2	1:2A:1060:U:H2'	2.04	0.57
1:2A:1507:A:O2'	1:2A:1508:A:O4'	2.22	0.57
32:2a:426:G:OP1	35:2d:38:TYR:OH	2.12	0.57
32:1a:1305:G:N2	32:1a:1331:G:H1'	2.19	0.57
44:1m:23:TYR:HB3	44:1m:67:GLU:HA	1.86	0.57
6:2G:36:LYS:HE3	6:2G:95:ARG:HH12	1.69	0.57
35:2d:165:MET:SD	35:2d:168:ARG:NH1	2.77	0.57
11:1P:90:ARG:HG2	11:1P:90:ARG:HH11	1.69	0.57
40:1i:125:TYR:HE1	40:1i:127:LYS:HG3	1.69	0.57
6:2G:80:PHE:O	6:2G:82:LEU:N	2.37	0.57
32:2a:1010:G:H2'	32:2a:1011:G:H8	1.68	0.57
32:2a:1263:C:H2'	32:2a:1264:C:H6	1.69	0.57
49:2r:47:THR:HG23	49:2r:49:LYS:HG3	1.86	0.57
1:1A:184:C:H2'	1:1A:185:U:C6	2.39	0.57
1:1A:517:C:OP1	27:15:16:ARG:NH2	2.29	0.57
1:1A:897:C:H2'	1:1A:898:C:C6	2.40	0.57
1:1A:2110:G:H5"	1:1A:2111:C:H5	1.70	0.57
5:1F:64:ILE:HG21	5:1F:78:ILE:HG23	1.86	0.57
35:1d:177:ASP:HB3	35:1d:182:LYS:HG3	1.87	0.57
44:1m:15:VAL:HG11	44:1m:48:LEU:HD21	1.86	0.57
1:2A:11:G:C2'	1:2A:12:U:H5'	2.34	0.57
1:2A:588:U:H2'	1:2A:589:C:C6	2.39	0.57
1:2A:1226:A:OP1	17:2V:84:LYS:NZ	2.32	0.57
17:2V:40:LEU:HB2	17:2V:46:VAL:HG13	1.87	0.57
1:1A:1048:A:OP2	1:1A:1109:C:N4	2.38	0.57
1:1A:2107:C:N3	1:1A:2182:G:O6	2.37	0.57
1:1A:2327:A:H2'	1:1A:2328:A:C8	2.38	0.57
25:13:39:ASP:OD2	25:13:44:ARG:NH2	2.37	0.57
32:1a:1016:A:OP1	45:1n:15:LYS:NZ	2.37	0.57
32:1a:1356:G:H2'	32:1a:1357:A:C8	2.40	0.57
1:2A:1087:G:H22	1:2A:1102:C:H42	1.52	0.57
1:2A:1796:U:H2'	1:2A:1797:C:C6	2.39	0.57
7:2H:42:ARG:HB3	7:2H:53:GLU:HB2	1.84	0.57
21:2Z:179:ASP:O	21:2Z:182:LYS:HG2	2.03	0.57
36:2e:57:LYS:HG2	36:2e:61:TYR:CE2	2.39	0.57
52:2u:6:ARG:HD3	52:2u:15:ARG:NH1	2.20	0.57
1:1A:1295:C:OP2	61:1A:4131:HOH:O	2.17	0.57
19:1X:76:ARG:NH1	61:1X:102:HOH:O	2.37	0.57
32:1a:410:G:OP1	35:1d:30:LYS:NZ	2.30	0.57
32:1a:1400:5MC:C2	53:1y:63:ALA:HA	2.39	0.57
39:1h:10:LEU:HD22	39:1h:83:ILE:HD11	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:301:G:OP2	20:2Y:84:ARG:NH2	2.37	0.57
1:2A:1188:U:H4'	17:2V:79:VAL:HG22	1.85	0.57
11:2P:87:ASP:O	11:2P:90:ARG:NH1	2.37	0.57
32:2a:977:A:N6	32:2a:1224:G:OP1	2.34	0.57
43:2l:49:ASN:ND2	43:2l:92:0TD:SB	2.77	0.57
1:1A:1056:G:H5"	1:1A:1057:A:O4'	2.03	0.57
1:1A:1430:C:H2'	1:1A:1431:U:C6	2.38	0.57
1:1A:1817:G:OP1	3:1D:88:ARG:NH2	2.37	0.57
1:1A:2377:A:H2'	1:1A:2378:A:C8	2.39	0.57
1:1A:2610:C:O2'	61:1A:4130:HOH:O	2.17	0.57
2:2B:75:G:O3'	21:2Z:10:ARG:NH2	2.38	0.57
34:2c:6:HIS:CE1	34:2c:8:ILE:HB	2.40	0.57
34:2c:54:ARG:HB2	34:2c:69:HIS:HB2	1.86	0.57
1:1A:336:C:O2'	20:1Y:35:TYR:OH	2.22	0.57
1:1A:1803:A:O2'	3:1D:259:THR:HG21	2.04	0.57
1:1A:2683:C:O2	10:1O:70:LYS:NZ	2.29	0.57
3:1D:17:THR:O	3:1D:211:ARG:NH2	2.35	0.57
1:2A:1991:U:H2'	1:2A:1992:G:H5"	1.85	0.57
1:2A:2690:C:OP1	13:2R:17:ARG:NH2	2.38	0.57
1:2A:2805:G:H2'	1:2A:2807:G:H8	1.70	0.57
21:2Z:10:ARG:HB3	21:2Z:36:LYS:HB3	1.86	0.57
1:1A:1518:U:H2'	1:1A:1519:G:O4'	2.05	0.57
4:1E:143:ASN:HD22	4:1E:147:PRO:HD3	1.69	0.57
6:1G:27:ASN:HB3	6:1G:30:GLU:HG3	1.87	0.57
8:1I:109:ILE:HG13	8:1I:130:TYR:CZ	2.40	0.57
32:1a:1240:U:OP2	38:1g:116:ALA:N	2.38	0.57
1:2A:2857:G:N2	1:2A:2860:A:OP2	2.33	0.57
2:2B:75:G:H22	21:2Z:73:GLN:NE2	2.03	0.57
6:2G:16:ARG:O	6:2G:20:ILE:HG13	2.04	0.57
32:2a:632:A:H5'	32:2a:633:G:OP2	2.04	0.57
33:2b:162:ILE:HD11	33:2b:184:VAL:HG22	1.87	0.57
34:2c:6:HIS:CD2	45:2n:49:HIS:HB3	2.39	0.57
34:2c:102:ASN:OD1	34:2c:102:ASN:N	2.38	0.57
38:2g:79:ARG:HA	38:2g:84:ASN:HA	1.86	0.57
50:2s:11:VAL:HG12	50:2s:12:ASP:H	1.70	0.57
1:1A:911:A:H2'	12:1Q:9:TYR:OH	2.05	0.57
34:1c:108:ASN:ND2	34:1c:144:SER:OG	2.27	0.57
25:23:7:LYS:HE3	25:23:32:GLN:HE21	1.70	0.57
32:2a:56:U:H2'	32:2a:57:G:C8	2.40	0.57
32:2a:67:C:H2'	32:2a:68:G:C8	2.40	0.57
33:2b:8:LYS:HG3	33:2b:48:MET:HG2	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:2b:42:ILE:HD13	33:2b:203:GLY:HA2	1.86	0.57
1:1A:456:C:H4'	61:1A:4654:HOH:O	2.04	0.56
1:1A:1165:U:H2'	1:1A:1166:C:C6	2.39	0.56
32:1a:600:C:H2'	32:1a:601:C:H6	1.70	0.56
32:1a:769:G:H4'	32:1a:1513:A:H4'	1.87	0.56
32:1a:840:C:H4'	32:1a:841:U:OP2	2.03	0.56
33:1b:76:GLN:NE2	33:1b:206:ASP:OD1	2.38	0.56
39:1h:112:LEU:HD22	39:1h:133:LEU:HA	1.86	0.56
1:2A:1050:A:H2'	1:2A:1051:G:C8	2.40	0.56
61:2A:3878:HOH:O	11:2P:55:ARG:NH2	2.38	0.56
3:2D:164:GLN:OE1	3:2D:176:ARG:NH2	2.38	0.56
14:2S:94:TYR:OH	14:2S:106:ARG:NH1	2.38	0.56
32:2a:1069:C:O2'	32:2a:1192:C:O2	2.19	0.56
32:2a:1329:A:OP2	52:2u:7:ARG:NH1	2.28	0.56
33:2b:174:VAL:O	33:2b:178:ARG:HG2	2.05	0.56
32:1a:222:U:H2'	32:1a:223:U:C6	2.40	0.56
39:1h:95:VAL:HB	39:1h:99:GLU:HG3	1.87	0.56
51:1t:57:ARG:HH12	51:1t:100:ILE:HD12	1.71	0.56
1:2A:749:C:OP2	61:2A:3844:HOH:O	2.17	0.56
1:2A:1081:U:H2'	1:2A:1082:U:O2	2.05	0.56
1:2A:2537:U:H2'	1:2A:2538:C:C6	2.40	0.56
7:2H:13:LYS:HA	7:2H:15:VAL:H	1.70	0.56
32:2a:405:U:O4	35:2d:2:GLY:N	2.38	0.56
1:1A:330:A:H2	1:1A:1210:A:O2'	1.85	0.56
1:1A:1406:U:H2'	1:1A:1407:C:C6	2.40	0.56
1:1A:2114:A:H1'	1:1A:2168:G:H5'	1.87	0.56
1:1A:2789:C:H1'	1:1A:2892:A:H2	1.71	0.56
1:1A:2791:C:H2'	1:1A:2792:G:C8	2.40	0.56
3:1D:71:ASP:HB3	3:1D:103:ARG:NH2	2.20	0.56
5:1F:184:TYR:CE2	5:1F:188:ARG:HD2	2.39	0.56
12:1Q:22:LYS:NZ	61:1Q:301:HOH:O	2.39	0.56
32:1a:972:C:OP1	61:1a:1909:HOH:O	2.18	0.56
37:1f:50:TYR:OH	49:1r:74:ARG:O	2.21	0.56
1:2A:911:A:H2'	12:2Q:9:TYR:OH	2.04	0.56
1:2A:1019:U:OP1	1:2A:1035:U:O2'	2.20	0.56
1:2A:2110:G:OP1	1:2A:2118:U:N3	2.37	0.56
5:2F:155:LEU:HD11	5:2F:176:LEU:HD12	1.87	0.56
15:2T:85:LYS:NZ	15:2T:87:ASP:OD2	2.38	0.56
18:2W:1:MET:HE2	18:2W:62:HIS:HB3	1.86	0.56
21:2Z:157:LEU:HD11	21:2Z:163:LEU:HB2	1.88	0.56
26:24:59:PHE:CA	26:24:61:ARG:H	2.15	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:28:34:TRP:CE2	30:28:35:GLN:HB3	2.41	0.56
32:2a:1070:U:H2'	32:2a:1071:C:H6	1.71	0.56
32:2a:1201:A:H4'	32:2a:1202:G:H5"	1.87	0.56
44:2m:48:LEU:HD23	44:2m:53:VAL:HG12	1.87	0.56
15:1T:24:PRO:HA	15:1T:49:VAL:HG22	1.88	0.56
36:1e:91:LEU:HB3	36:1e:118:ILE:HD11	1.87	0.56
38:1g:113:GLU:HG2	38:1g:119:ARG:HG2	1.88	0.56
1:2A:1798:U:OP2	3:2D:274:ARG:NH2	2.39	0.56
2:2B:8:U:H3	2:2B:113:G:H1	1.52	0.56
32:2a:164:U:H2'	32:2a:165:C:C6	2.41	0.56
38:2g:46:ALA:HA	38:2g:49:ILE:HD12	1.87	0.56
1:1A:414:C:H2'	1:1A:415:A:C8	2.40	0.56
1:1A:2577:A:H5'	27:15:3:LYS:HE3	1.86	0.56
30:18:30:ARG:HD3	61:18:219:HOH:O	2.05	0.56
32:1a:489:C:OP1	35:1d:132:ARG:NH2	2.39	0.56
32:1a:673:G:H2'	32:1a:674:G:C8	2.40	0.56
32:1a:737:A:H2'	32:1a:738:C:C6	2.40	0.56
33:1b:189:ASP:OD1	33:1b:189:ASP:N	2.37	0.56
1:2A:1073:A:H2'	1:2A:1074:G:C8	2.40	0.56
1:2A:2134:A:H8	1:2A:2156:G:H21	1.52	0.56
1:1A:288:C:H2'	1:1A:289:A:H8	1.69	0.56
1:1A:1067:A:H3'	1:1A:1067:A:N3	2.21	0.56
32:1a:45:U:H2'	32:1a:46:G:C8	2.40	0.56
32:1a:56:U:H2'	32:1a:57:G:C8	2.39	0.56
32:1a:266:G:H5"	32:1a:267:C:C5	2.41	0.56
32:1a:355:C:O2'	32:1a:388:G:N3	2.31	0.56
32:1a:1003:G:N2	32:1a:1004:A:H1'	2.21	0.56
33:1b:119:GLU:OE2	33:1b:153:ARG:NH1	2.34	0.56
1:2A:1324:G:O2'	61:2A:3847:HOH:O	2.18	0.56
1:2A:1533:G:N2	1:2A:1536:C:N3	2.53	0.56
32:2a:890:G:O2'	32:2a:906:G:O6	2.20	0.56
34:2c:29:TYR:OH	45:2n:54:PRO:O	2.20	0.56
1:1A:2336:A:H61	22:10:43:THR:CG2	2.19	0.56
11:1P:63:PRO:HD3	30:18:27:THR:HG22	1.87	0.56
32:1a:839:U:H1'	32:1a:840:C:OP1	2.06	0.56
2:2B:13:A:N1	2:2B:69:G:O2'	2.38	0.56
6:2G:106:LEU:HA	6:2G:110:ALA:HB3	1.87	0.56
32:2a:1030(A):G:H1'	32:2a:1030(C):G:N7	2.20	0.56
39:2h:123:GLU:O	39:2h:127:LEU:HG	2.06	0.56
1:1A:323:G:C8	5:1F:171:PRO:HG3	2.41	0.56
1:1A:489:G:N7	18:1W:49:LYS:NZ	2.54	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1141:U:OP1	9:1N:25:ARG:NH1	2.39	0.56
11:1P:63:PRO:HG2	30:18:25:MET:HB2	1.88	0.56
39:1h:14:ARG:NH1	39:1h:83:ILE:O	2.37	0.56
1:2A:2184:G:N1	1:2A:2185:C:O2	2.39	0.56
7:2H:154:PRO:HB3	7:2H:163:TYR:CE1	2.41	0.56
32:2a:1266:G:N2	32:2a:1269:A:OP2	2.36	0.56
34:2c:47:LEU:HD13	34:2c:68:VAL:HG11	1.87	0.56
61:1A:4102:HOH:O	13:1R:3:HIS:NE2	2.33	0.56
11:1P:50:ARG:HD3	30:18:7:HIS:CD2	2.41	0.56
1:2A:459:U:H5"	29:27:40:TRP:CD2	2.41	0.56
1:2A:2006:C:OP2	61:2A:3850:HOH:O	2.18	0.56
3:2D:71:ASP:OD2	3:2D:103:ARG:NH2	2.31	0.56
36:2e:77:PRO:HD2	36:2e:142:LEU:HD22	1.88	0.56
1:1A:1340:U:OP1	19:1X:16:LYS:NZ	2.36	0.56
1:1A:1530:C:HO2'	1:1A:1531:C:H6	1.52	0.56
1:1A:2646:C:H2'	1:1A:2647:U:O4'	2.06	0.56
5:1F:185:ASP:HA	5:1F:188:ARG:HD3	1.87	0.56
1:2A:1439:A:OP1	61:2A:3846:HOH:O	2.18	0.56
1:2A:2836:U:H2'	1:2A:2837:G:C8	2.41	0.56
32:2a:1142:G:H3'	32:2a:1143:G:H8	1.71	0.56
1:2A:2849:U:OP2	15:2T:95:ARG:NH1	2.39	0.55
43:2l:89:ARG:HH21	43:2l:91:LYS:HA	1.71	0.55
7:1H:3:ARG:NH2	7:1H:65:HIS:HB3	2.20	0.55
32:1a:828:A:H2'	32:1a:829:G:O4'	2.06	0.55
1:2A:271(V):G:O6	61:2A:3848:HOH:O	2.18	0.55
1:2A:2079:U:O3'	23:21:35:THR:OG1	2.23	0.55
32:2a:108:G:C6	51:2t:15:ARG:HG2	2.40	0.55
36:2e:71:LEU:HD21	36:2e:115:VAL:HG22	1.87	0.55
1:1A:2130:U:O2'	1:1A:2133:G:O2'	2.21	0.55
1:1A:2372:G:O6	61:1A:4127:HOH:O	2.16	0.55
36:1e:140:ARG:O	36:1e:143:ARG:NH2	2.40	0.55
1:2A:528:A:O2'	61:2A:3851:HOH:O	2.18	0.55
1:2A:2299:G:N1	1:2A:2318:G:N7	2.55	0.55
2:2B:14:U:OP2	2:2B:70:C:O2'	2.21	0.55
21:2Z:23:LYS:HD3	21:2Z:40:ASP:HA	1.88	0.55
39:2h:103:VAL:HG21	39:2h:110:ALA:HB2	1.89	0.55
1:1A:2506:U:O2	55:1A:4041:HGR:H23	2.06	0.55
2:1B:7:G:H5"	2:1B:7:G:H8	1.72	0.55
35:1d:128:VAL:HG12	35:1d:129:ASN:HD22	1.71	0.55
3:2D:175:LEU:HD12	3:2D:185:VAL:HG21	1.88	0.55
25:23:59:VAL:HG12	25:23:60:GLU:H	1.72	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:2m:14:ARG:HE	44:2m:42:ALA:HA	1.71	0.55
1:1A:1047:G:H2'	1:1A:1110:G:N2	2.19	0.55
3:1D:148:GLU:HB2	3:1D:151:LYS:HD2	1.88	0.55
32:1a:1442:G:H2'	32:1a:1442:G:N3	2.22	0.55
1:2A:674:G:H1'	5:2F:74:ARG:HD3	1.87	0.55
1:2A:1816:G:O6	3:2D:35:LYS:NZ	2.30	0.55
1:2A:2305:A:H5"	6:2G:134:GLY:HA3	1.89	0.55
30:28:23:VAL:HG11	30:28:47:LYS:HD3	1.88	0.55
32:2a:1222:G:OP2	32:2a:1322:C:N4	2.39	0.55
1:1A:2304:G:H22	1:1A:2312:U:H3	1.55	0.55
6:1G:43:LEU:O	6:1G:45:GLU:HG2	2.06	0.55
7:1H:41:MET:HE2	7:1H:65:HIS:HA	1.88	0.55
32:1a:1504:G:OP1	32:1a:1507:A:H4'	2.07	0.55
37:1f:69:GLU:O	37:1f:72:VAL:HG12	2.07	0.55
48:1q:45:HIS:CD2	48:1q:65:ILE:HG12	2.40	0.55
5:2F:64:ILE:HG21	5:2F:78:ILE:HG23	1.87	0.55
6:2G:15:VAL:HB	6:2G:175:LEU:HB3	1.88	0.55
8:2I:9:LEU:HD21	8:2I:35:LEU:HD13	1.89	0.55
27:25:15:ARG:NH1	61:25:201:HOH:O	2.28	0.55
32:2a:382:A:H2'	32:2a:383:A:C8	2.42	0.55
32:2a:544:G:OP1	35:2d:59:ARG:NH2	2.40	0.55
21:1Z:125:LEU:HB3	21:1Z:165:VAL:HG13	1.88	0.55
32:1a:640:A:O2'	39:1h:115:SER:O	2.25	0.55
33:1b:125:PRO:HB2	33:1b:128:GLU:H	1.70	0.55
1:2A:271(E):U:H2'	1:2A:271(F):C:C6	2.42	0.55
1:2A:1073:A:H2'	1:2A:1074:G:H8	1.72	0.55
8:2I:5:LEU:HD11	8:2I:19:VAL:HG22	1.89	0.55
17:2V:6:LYS:HB2	17:2V:38:LEU:HD11	1.87	0.55
32:2a:664:G:H22	32:2a:741:G:H1	1.53	0.55
1:1A:1063:G:H5"	1:1A:1065:U:H5	1.72	0.55
4:1E:170:LEU:HB3	4:1E:184:VAL:HG22	1.89	0.55
34:1c:131:ARG:HH11	34:1c:166:GLU:HG3	1.71	0.55
49:1r:47:THR:HA	49:1r:83:GLU:HB2	1.89	0.55
32:2a:1005:A:H1'	32:2a:1025:U:C2	2.42	0.55
32:2a:1093:A:N3	32:2a:1109:C:O2'	2.38	0.55
32:2a:1142:G:H2'	32:2a:1143:G:O4'	2.07	0.55
42:2k:23:ALA:HB2	42:2k:28:THR:HG23	1.88	0.55
1:1A:1068:G:O2'	1:1A:1096:A:H4'	2.05	0.55
20:1Y:92:ASN:H	20:1Y:92:ASN:HD22	1.55	0.55
44:1m:87:TYR:HA	44:1m:90:LEU:HD12	1.87	0.55
26:24:61:ARG:HH12	50:2s:9:VAL:HG21	1.71	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:2c:134:ILE:HG23	34:2c:151:VAL:HB	1.89	0.55
39:2h:51:VAL:HG11	39:2h:60:ARG:HH11	1.71	0.55
1:1A:121:G:H4'	1:1A:149:A:H5'	1.89	0.55
9:1N:30:ILE:HG22	9:1N:34:LEU:HD22	1.88	0.55
20:1Y:102:CYS:SG	20:1Y:103:GLY:N	2.79	0.55
25:13:3:ARG:HD3	25:13:60:GLU:CD	2.31	0.55
32:1a:44:G:OP2	61:1a:1911:HOH:O	2.18	0.55
32:1a:406:G:H21	35:1d:119:GLN:NE2	2.02	0.55
32:1a:757:U:H2'	32:1a:758:G:O4'	2.06	0.55
1:2A:657:U:H2'	1:2A:658:C:C6	2.42	0.55
1:2A:1292:U:H2'	1:2A:1293:C:C6	2.42	0.55
1:2A:1642:G:N7	61:2A:3952:HOH:O	2.34	0.55
1:2A:1815:A:OP2	61:2A:3849:HOH:O	2.18	0.55
32:2a:48:C:OP2	61:2a:3206:HOH:O	2.18	0.55
32:2a:1004:A:H5"	32:2a:1025:U:C4	2.41	0.55
1:1A:1231:G:N7	61:1A:4258:HOH:O	2.33	0.54
32:1a:1251:A:H2'	32:1a:1252:A:C8	2.42	0.54
36:1e:148:VAL:HG21	39:1h:107:LEU:HB3	1.87	0.54
1:2A:212:G:H2'	1:2A:213:A:O4'	2.07	0.54
1:2A:1156:A:O4'	16:2U:51:LYS:NZ	2.40	0.54
8:2I:4:ILE:HD11	8:2I:44:LEU:HD23	1.88	0.54
32:2a:1218:C:H2'	32:2a:1219:U:C6	2.41	0.54
32:2a:1269:A:N1	32:2a:1312:G:O2'	2.35	0.54
35:2d:173:TRP:CD1	35:2d:189:PRO:HG3	2.41	0.54
1:1A:1702:G:N7	61:1A:4255:HOH:O	2.33	0.54
1:1A:1800:C:OP1	3:1D:260:ARG:NH2	2.40	0.54
32:1a:1140:C:H2'	32:1a:1141:C:H6	1.73	0.54
32:1a:1312:G:N7	50:1s:2:PRO:HD2	2.22	0.54
33:1b:163:PHE:HA	33:1b:185:ILE:HG12	1.88	0.54
40:1i:110:GLU:OE2	40:1i:113:LYS:NZ	2.40	0.54
1:2A:1035:U:H2'	1:2A:1036:G:C8	2.42	0.54
5:2F:53:THR:HG23	5:2F:55:GLY:H	1.72	0.54
35:2d:72:GLU:OE2	35:2d:207:TYR:OH	2.22	0.54
32:1a:79:G:N2	32:1a:90:U:O2	2.39	0.54
42:1k:54:ARG:O	42:1k:57:THR:OG1	2.20	0.54
1:2A:361:G:O2'	1:2A:362:U:H5'	2.08	0.54
3:2D:106:ILE:HD11	3:2D:143:HIS:HD2	1.71	0.54
7:2H:9:ILE:HD11	7:2H:50:VAL:HB	1.88	0.54
11:2P:94:GLU:HG3	11:2P:124:LYS:HD3	1.88	0.54
32:2a:584:G:H5'	48:2q:91:ARG:HH22	1.71	0.54
34:2c:39:ILE:HG23	34:2c:91:LEU:HD11	1.88	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:2t:57:ARG:HH22	51:2t:100:ILE:HD12	1.72	0.54
1:1A:1778:U:H2'	1:1A:1784:A:N6	2.23	0.54
1:1A:2328:A:H2'	1:1A:2329:G:C8	2.42	0.54
32:1a:642:A:N3	39:1h:113:SER:OG	2.32	0.54
2:2B:57:A:H1'	6:2G:29:TRP:HB2	1.89	0.54
21:2Z:116:VAL:HG13	21:2Z:175:VAL:HG23	1.90	0.54
32:2a:696:A:N1	32:2a:797:C:O2'	2.36	0.54
34:2c:50:ALA:HB1	34:2c:70:VAL:HG11	1.90	0.54
44:2m:37:THR:HB	44:2m:55:ARG:HD2	1.89	0.54
1:1A:1405:U:H2'	1:1A:1406:U:C6	2.43	0.54
1:1A:2690:C:OP1	13:1R:17:ARG:NH2	2.39	0.54
8:1I:14:ASP:OD1	8:1I:15:VAL:N	2.40	0.54
32:1a:1069:C:OP2	61:1a:1910:HOH:O	2.18	0.54
1:2A:2115:G:H21	1:2A:2171:A:H61	1.54	0.54
1:1A:286:C:H2'	1:1A:287:C:C6	2.43	0.54
1:1A:760:G:OP1	61:1A:4132:HOH:O	2.18	0.54
1:1A:2331:G:O2'	1:1A:2336:A:N1	2.36	0.54
5:1F:53:THR:HG22	5:1F:55:GLY:H	1.72	0.54
23:11:56:GLN:HE21	23:11:87:PRO:HG3	1.73	0.54
32:1a:347:G:H8	57:1a:1880:MPD:H53	1.69	0.54
1:2A:1250:G:H5"	61:2A:5379:HOH:O	2.07	0.54
1:2A:2104:G:H21	1:2A:2105:C:N4	2.06	0.54
2:2B:6:C:H4'	2:2B:28:C:H5'	1.90	0.54
6:2G:55:LYS:HA	6:2G:58:GLN:HB3	1.90	0.54
32:2a:629:G:H2'	32:2a:630:G:O4'	2.08	0.54
32:2a:1006:C:H2'	32:2a:1007:C:C6	2.43	0.54
33:2b:69:LEU:HB3	33:2b:162:ILE:HG22	1.89	0.54
12:1Q:21:THR:HG21	12:1Q:101:ARG:HB2	1.89	0.54
17:1V:21:ARG:HD3	17:1V:91:TYR:CD1	2.43	0.54
17:1V:43:GLU:OE1	17:1V:43:GLU:N	2.40	0.54
32:1a:57:G:H2'	32:1a:58:C:C6	2.42	0.54
32:1a:169:C:H2'	32:1a:170:U:H6	1.71	0.54
32:1a:1030(C):G:H2'	32:1a:1030(D):A:H8	1.72	0.54
32:1a:1300:G:N7	61:1a:1939:HOH:O	2.34	0.54
33:1b:30:ARG:HH22	33:1b:194:PRO:HB2	1.72	0.54
37:1f:91:VAL:HG11	49:1r:72:ARG:HH12	1.73	0.54
40:1i:92:TYR:O	40:1i:96:LEU:HB2	2.07	0.54
32:2a:1135:U:H2'	32:2a:1137:C:N3	2.23	0.54
33:2b:102:LEU:HD23	33:2b:182:ILE:HD12	1.90	0.54
44:2m:3:ARG:N	44:2m:8:GLU:HA	2.22	0.54
44:2m:19:LEU:HD21	44:2m:56:LEU:HD21	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:890:G:O2'	32:1a:906:G:O6	2.17	0.54
32:1a:1456:G:O3'	51:1t:39:LYS:NZ	2.41	0.54
1:2A:577:G:O2'	1:2A:1254:A:OP1	2.25	0.54
6:2G:77:ILE:HG21	6:2G:80:PHE:CD2	2.43	0.54
9:2N:46:VAL:HG23	9:2N:48:MET:HG2	1.90	0.54
26:24:59:PHE:HB2	26:24:62:ARG:HH21	1.72	0.54
32:2a:539:A:H2'	32:2a:540:G:C8	2.43	0.54
32:2a:1374:A:OP1	38:2g:36:LYS:NZ	2.33	0.54
34:2c:11:ARG:NH2	34:2c:177:THR:O	2.41	0.54
1:1A:1064:C:C2	1:1A:1074:G:N1	2.74	0.54
32:1a:177:C:OP1	51:1t:65:LYS:NZ	2.37	0.54
35:1d:173:TRP:CD1	35:1d:173:TRP:H	2.25	0.54
1:2A:1316:U:H2'	1:2A:1317:A:C8	2.43	0.54
1:2A:2717:G:O2'	15:2T:96:ARG:HD3	2.08	0.54
2:2B:42:C:C4	2:2B:43:C:C4	2.96	0.54
5:2F:184:TYR:CE2	5:2F:188:ARG:HD2	2.43	0.54
11:2P:63:PRO:HG2	30:28:25:MET:HB2	1.90	0.54
16:2U:34:LYS:NZ	16:2U:37:GLU:OE1	2.35	0.54
41:2j:50:ILE:HG22	41:2j:52:GLY:H	1.73	0.54
1:1A:579:G:H2'	1:1A:580:C:C6	2.43	0.54
1:1A:1786:A:H1'	1:1A:1938:A:N6	2.23	0.54
1:1A:2691:C:OP2	61:1A:4136:HOH:O	2.19	0.54
36:1e:50:GLU:HB2	36:1e:53:LEU:HD13	1.89	0.54
47:1p:42:ARG:HB3	47:1p:44:THR:HG23	1.90	0.54
1:2A:752:A:H3'	29:27:1:MET:HE1	1.90	0.54
1:2A:2687:U:H2'	1:2A:2688:U:O4'	2.08	0.54
15:2T:127:ALA:C	15:2T:129:ARG:H	2.14	0.54
21:2Z:3:TYR:CD2	21:2Z:51:ALA:HB2	2.43	0.54
21:2Z:10:ARG:NH1	21:2Z:26:GLY:O	2.41	0.54
32:2a:1030(C):G:H2'	32:2a:1030(D):A:C8	2.43	0.54
32:2a:1128:C:H1'	32:2a:1147:C:H42	1.73	0.54
1:1A:2102:U:C2	1:1A:2187:G:O6	2.60	0.53
2:1B:106:G:H5'	21:1Z:31:ARG:HG2	1.89	0.53
4:1E:73:GLU:H	4:1E:73:GLU:CD	2.16	0.53
32:1a:636:U:H2'	32:1a:637:G:H8	1.72	0.53
32:1a:920:U:H2'	32:1a:921:U:C6	2.43	0.53
32:1a:1003:G:C2	32:1a:1004:A:H1'	2.42	0.53
33:1b:87:ARG:HD2	33:1b:233:SER:HB2	1.89	0.53
1:2A:1090:U:H2'	1:2A:1091:G:H8	1.72	0.53
2:2B:42:C:O2'	61:2B:305:HOH:O	2.18	0.53
6:2G:109:VAL:HG21	26:24:14:ILE:HG21	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:29:1:MET:HE3	31:29:35:ARG:HB2	1.89	0.53
32:2a:1367:C:H4'	41:2j:48:THR:HG21	1.90	0.53
40:2i:99:LEU:HB3	40:2i:101:PHE:CE1	2.43	0.53
1:1A:1509(B):A:H2'	1:1A:1510:G:O4'	2.08	0.53
1:1A:1721:G:H8	1:1A:1741:A:H62	1.57	0.53
32:1a:1277:C:O2'	32:1a:1279:A:H1'	2.08	0.53
37:1f:61:LEU:HD23	37:1f:63:TYR:OH	2.08	0.53
41:1j:22:LYS:NZ	41:1j:89:ASP:O	2.30	0.53
1:2A:1525:G:H2'	1:2A:1526:G:C8	2.43	0.53
1:2A:2319:G:H22	14:2S:3:ARG:HD3	1.73	0.53
6:2G:15:VAL:HB	6:2G:175:LEU:HD23	1.90	0.53
15:2T:108:ARG:NH1	32:2a:1464:G:OP1	2.41	0.53
29:27:35:ARG:HG3	29:27:42:LEU:HD11	1.90	0.53
32:2a:1023:G:H3'	32:2a:1024:G:H8	1.74	0.53
41:2j:16:LEU:HD12	41:2j:68:HIS:HB2	1.90	0.53
44:2m:50:GLU:HA	44:2m:53:VAL:HG22	1.89	0.53
1:1A:1796:U:H2'	1:1A:1797:C:C6	2.42	0.53
1:1A:2646:C:OP2	1:1A:2732:G:O2'	2.24	0.53
6:1G:98:ARG:CZ	26:14:1:MET:HE3	2.39	0.53
32:1a:501:C:H2'	32:1a:502:G:C8	2.43	0.53
32:1a:1391:U:H2'	32:1a:1392:G:C8	2.42	0.53
35:1d:163:GLU:O	35:1d:166:LYS:HB2	2.08	0.53
1:2A:586:A:N1	1:2A:809:G:O2'	2.38	0.53
1:2A:2294:C:P	14:2S:89:ARG:HH22	2.30	0.53
1:2A:2564:A:C2	1:2A:2647:U:H4'	2.43	0.53
7:2H:164:TYR:HB2	7:2H:167:GLU:HB2	1.91	0.53
12:2Q:54:MET:HG2	12:2Q:117:ALA:HB1	1.89	0.53
32:2a:748:C:H4'	32:2a:749:C:O5'	2.09	0.53
32:2a:965:A:O2'	53:2y:40:ILE:HG21	2.07	0.53
32:2a:1158:C:N4	32:2a:1181:G:O6	2.41	0.53
32:2a:1305:G:O2'	32:2a:1331:G:N2	2.42	0.53
32:2a:1371:G:OP1	40:2i:12:GLU:HB2	2.09	0.53
32:2a:1375:A:H4'	38:2g:29:LYS:HE3	1.89	0.53
1:1A:910:A:N1	1:1A:2277:G:H1'	2.24	0.53
1:1A:1052:C:H42	1:1A:1107:G:H1	1.57	0.53
1:1A:2759:G:N7	61:1A:4256:HOH:O	2.33	0.53
26:14:34:GLU:HB2	44:1m:57:ARG:CZ	2.38	0.53
32:1a:626:U:H2'	32:1a:627:G:H8	1.72	0.53
32:1a:1003:G:N2	32:1a:1004:A:N3	2.56	0.53
33:1b:84:GLU:HB3	33:1b:219:VAL:HG21	1.90	0.53
53:1y:33:HIS:CE1	53:1y:35:ILE:HG12	2.42	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1493:C:N4	1:2A:2206:G:O2'	2.41	0.53
1:2A:2788:C:OP1	4:2E:61:ARG:NH2	2.41	0.53
3:2D:108:PRO:HG2	3:2D:111:LEU:HB2	1.90	0.53
21:2Z:129:SER:HB3	21:2Z:132:ASN:HB2	1.89	0.53
32:2a:266:G:O2'	32:2a:267:C:OP2	2.17	0.53
32:2a:745:C:H2'	32:2a:746:A:H8	1.74	0.53
1:1A:1614:A:OP2	61:1A:4133:HOH:O	2.18	0.53
9:1N:62:VAL:HG22	9:1N:66:LYS:HD2	1.90	0.53
37:1f:75:LEU:O	37:1f:79:LEU:HG	2.09	0.53
52:1u:14:TRP:HE3	52:1u:15:ARG:HG3	1.73	0.53
1:2A:862:G:O2'	2:2B:78:A:N3	2.42	0.53
1:2A:1056:G:H5"	1:2A:1057:A:H5'	1.90	0.53
1:2A:1187:G:H5'	17:2V:81:TYR:CE1	2.44	0.53
1:2A:2104:G:O6	1:2A:2185:C:C4	2.61	0.53
1:2A:2749:A:H1'	7:2H:63:SER:HB3	1.91	0.53
2:2B:45:A:H2'	2:2B:46:A:H8	1.71	0.53
6:2G:171:ALA:O	6:2G:175:LEU:N	2.36	0.53
26:24:40:HIS:HB3	26:24:43:TYR:CD2	2.43	0.53
32:2a:390:C:H2'	32:2a:391:G:C8	2.43	0.53
32:2a:984:C:H2'	32:2a:985:C:H6	1.73	0.53
32:2a:1503:A:H5'	32:2a:1531:A:H1'	1.90	0.53
41:2j:37:PRO:HA	41:2j:72:VAL:HG22	1.91	0.53
1:1A:184:C:H2'	1:1A:185:U:H6	1.73	0.53
1:1A:1330:C:OP1	61:1A:4135:HOH:O	2.19	0.53
15:1T:51:ARG:HG3	15:1T:98:LYS:HE3	1.91	0.53
15:1T:81:PRO:O	61:1T:301:HOH:O	2.19	0.53
21:1Z:3:TYR:CD2	21:1Z:51:ALA:HB2	2.44	0.53
33:1b:155:LEU:HD11	33:1b:159:PRO:HG3	1.90	0.53
35:1d:140:VAL:HG11	35:1d:146:ILE:HD11	1.91	0.53
41:1j:16:LEU:HD22	41:1j:68:HIS:HB2	1.91	0.53
50:1s:12:ASP:HB3	50:1s:14:HIS:CD2	2.43	0.53
5:2F:108:LYS:O	5:2F:112:MET:HG3	2.08	0.53
32:2a:54:C:N4	32:2a:353:A:OP2	2.38	0.53
32:2a:273:A:H1'	48:2q:16:GLN:NE2	2.24	0.53
32:2a:1031:G:H2'	32:2a:1032:G:C8	2.43	0.53
33:2b:84:GLU:HB3	33:2b:219:VAL:HG21	1.90	0.53
34:2c:20:SER:HB2	34:2c:40:ARG:HH21	1.73	0.53
35:2d:25:ARG:NH1	35:2d:30:LYS:O	2.42	0.53
1:1A:1754:C:OP1	15:1T:96:ARG:NH1	2.42	0.53
1:1A:2114:A:O2'	1:1A:2167:U:O3'	2.22	0.53
6:2G:167:GLU:HA	6:2G:170:ARG:HB3	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:2H:154:PRO:HB3	7:2H:163:TYR:CZ	2.44	0.53
32:2a:1030(A):G:H2'	32:2a:1030(B):C:H5"	1.91	0.53
1:1A:2115:G:H2'	1:1A:2117:A:N6	2.24	0.53
32:1a:164:U:H2'	32:1a:165:C:C6	2.44	0.53
33:1b:16:HIS:HB2	33:1b:204:ASN:HB3	1.90	0.53
41:1j:37:PRO:HA	41:1j:72:VAL:HG12	1.90	0.53
43:1l:53:ARG:HB3	43:1l:69:TYR:HE1	1.72	0.53
46:1o:84:LYS:O	46:1o:84:LYS:HD3	2.09	0.53
1:2A:800:A:H8	1:2A:800:A:OP1	1.92	0.53
1:2A:1110:G:H1'	1:2A:1111:A:C8	2.43	0.53
1:2A:1113:U:H2'	1:2A:1114:G:C8	2.43	0.53
1:2A:1266:G:O5'	18:2W:15:ARG:NH2	2.41	0.53
1:2A:1780:A:OP1	61:2A:3804:HOH:O	2.19	0.53
1:2A:2152:G:H2'	1:2A:2153:G:H8	1.73	0.53
2:2B:85:G:OP1	61:2B:306:HOH:O	2.19	0.53
25:23:5:LYS:HG3	25:23:36:VAL:HG22	1.91	0.53
32:2a:1314:C:OP2	50:2s:4:SER:OG	2.19	0.53
44:2m:95:GLY:O	44:2m:110:ARG:HG3	2.09	0.53
1:1A:272(J):C:H2'	1:1A:274:G:H8	1.73	0.53
3:1D:8:PRO:HB3	3:1D:14:ARG:HG3	1.90	0.53
32:1a:194:C:H2'	32:1a:195:A:H5"	1.90	0.53
32:1a:1124:G:N2	32:1a:1125:U:O4	2.36	0.53
35:2d:162:LEU:HD13	35:2d:181:MET:HG2	1.90	0.53
44:2m:13:LYS:HA	44:2m:44:ARG:HH11	1.74	0.53
50:2s:52:TYR:HA	50:2s:56:GLN:O	2.09	0.53
5:1F:53:THR:HG23	5:1F:55:GLY:H	1.74	0.53
32:1a:1166:G:H5'	32:1a:1168:A:OP2	2.09	0.53
35:1d:83:SER:O	61:1d:402:HOH:O	2.18	0.53
36:1e:10:MET:SD	36:1e:13:ILE:HD11	2.49	0.53
40:1i:46:ALA:HB2	40:1i:74:ILE:HG23	1.91	0.53
1:2A:1514:U:H2'	1:2A:1515:G:C8	2.44	0.53
1:2A:1593:G:H2'	1:2A:1594:G:C8	2.44	0.53
1:1A:1266:G:O5'	18:1W:15:ARG:NH2	2.42	0.52
1:1A:1416:G:O2'	1:1A:1417:C:OP2	2.20	0.52
21:1Z:70:LEU:HG	21:1Z:91:LEU:HD11	1.92	0.52
36:1e:102:ALA:HB1	36:1e:106:PRO:HG2	1.89	0.52
41:1j:30:SER:HB3	41:1j:81:THR:HG22	1.90	0.52
43:1l:54:LYS:HD2	43:1l:54:LYS:N	2.24	0.52
44:1m:11:ARG:O	44:1m:13:LYS:N	2.41	0.52
51:1t:10:LEU:HB3	51:1t:12:ALA:H	1.74	0.52
1:2A:1359:A:H61	1:2A:1372:U:H3	1.56	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:185:U:H4'	1:1A:218:A:H4'	1.91	0.52
1:1A:2334:G:H5'	14:1S:9:ARG:HG2	1.91	0.52
3:1D:127:VAL:HA	3:1D:193:VAL:HG22	1.90	0.52
32:1a:461:A:O2'	32:1a:470:C:H5'	2.10	0.52
32:1a:1202:G:O4'	45:1n:29:ARG:NH1	2.39	0.52
1:2A:874:G:O2'	21:2Z:120:ILE:HD11	2.09	0.52
1:2A:2474:C:OP2	1:2A:2475:C:N4	2.40	0.52
3:2D:71:ASP:CG	3:2D:103:ARG:HH22	2.16	0.52
32:2a:662:G:O2'	32:2a:836:G:OP1	2.27	0.52
32:2a:1013:G:N2	32:2a:1016:A:OP2	2.39	0.52
32:2a:1068:G:H8	32:2a:1068:G:OP2	1.91	0.52
40:2i:77:ILE:O	40:2i:81:ILE:HG22	2.09	0.52
40:2i:100:GLY:O	40:2i:103:THR:HG22	2.09	0.52
1:1A:2149:G:H2'	1:1A:2150:U:C6	2.44	0.52
4:1E:7:VAL:HG23	4:1E:51:PHE:HE2	1.74	0.52
32:1a:376:G:H5"	47:1p:5:ARG:HD2	1.91	0.52
32:1a:1318:A:OP1	50:1s:7:LYS:NZ	2.41	0.52
44:1m:65:LYS:HG2	44:1m:69:GLU:HG2	1.92	0.52
1:2A:1047:G:H2'	1:2A:1110:G:H22	1.74	0.52
12:2Q:111:GLU:OE2	12:2Q:133:ARG:NH2	2.42	0.52
15:2T:60:THR:HG22	15:2T:77:PRO:HA	1.91	0.52
32:2a:933:G:N2	32:2a:935:A:O4'	2.43	0.52
1:1A:2138:C:N3	1:1A:2139:C:N4	2.57	0.52
9:1N:4:TYR:CD2	16:1U:100:VAL:HG11	2.44	0.52
24:12:65:ASN:O	24:12:69:ARG:HG3	2.10	0.52
1:2A:1028:A:N6	1:2A:1125:G:H2'	2.24	0.52
1:2A:2206:G:H5"	1:2A:2207:G:N7	2.24	0.52
19:2X:46:ALA:HB1	24:22:33:MET:HE1	1.91	0.52
32:2a:1003:G:C5	32:2a:1004:A:H1'	2.44	0.52
36:2e:80:ILE:HG22	36:2e:91:LEU:HB2	1.92	0.52
1:1A:2055:C:O2	61:1A:4128:HOH:O	2.17	0.52
1:1A:2683:C:OP1	15:1T:53:ARG:NH2	2.42	0.52
1:1A:2791:C:H2'	1:1A:2792:G:H8	1.74	0.52
32:1a:96:U:H2'	32:1a:97:G:C8	2.44	0.52
42:1k:48:ILE:HD13	42:1k:63:LEU:HD12	1.92	0.52
44:1m:11:ARG:C	44:1m:13:LYS:H	2.17	0.52
1:2A:1916:A:H2'	1:2A:1917:PSU:O4'	2.10	0.52
1:2A:1920:OMC:HM22	1:2A:1921:G:H5'	1.92	0.52
1:2A:2115:G:N2	1:2A:2171:A:H61	2.07	0.52
4:2E:143:ASN:HD22	4:2E:147:PRO:HD3	1.74	0.52
6:2G:36:LYS:HD2	6:2G:160:VAL:HG21	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:741:G:H5"	46:2o:59:MET:HE1	1.91	0.52
34:2c:36:ASP:OD1	34:2c:57:ILE:HD12	2.08	0.52
53:2y:87:LYS:O	53:2y:91:LYS:HB2	2.09	0.52
1:1A:226:G:N2	1:1A:228:A:H62	2.08	0.52
1:1A:614(A):U:H5'	58:1F:319:ARG:HG2	1.91	0.52
1:1A:1062:G:H2'	1:1A:1063:G:H8	1.75	0.52
11:1P:82:GLY:HA2	11:1P:113:LYS:O	2.09	0.52
26:14:59:PHE:O	26:14:62:ARG:HG2	2.09	0.52
32:1a:1013:G:N2	32:1a:1016:A:OP2	2.42	0.52
32:1a:1158:C:H5	32:1a:1181:G:N1	2.05	0.52
32:1a:1298:C:P	38:1g:114:ARG:HH22	2.33	0.52
34:1c:11:ARG:HB3	34:1c:15:THR:HB	1.92	0.52
48:1q:67:LYS:HA	48:1q:70:ARG:NH2	2.24	0.52
1:2A:1364:G:OP2	23:21:3:LYS:HG3	2.10	0.52
2:2B:77:U:OP1	21:2Z:19:ARG:NH2	2.42	0.52
23:21:53:VAL:HG22	23:21:74:VAL:HG13	1.90	0.52
24:22:65:ASN:OD1	24:22:69:ARG:NH1	2.43	0.52
34:2c:9:GLY:HA3	45:2n:49:HIS:HA	1.91	0.52
43:2l:32:PHE:HB3	43:2l:84:LEU:HD11	1.92	0.52
45:2n:23:ARG:NH1	45:2n:30:ALA:HB2	2.23	0.52
46:2o:70:LEU:HD11	46:2o:77:ARG:HB2	1.92	0.52
1:1A:1653:G:H3'	13:1R:2:ARG:HD3	1.91	0.52
1:1A:2319:G:H22	14:1S:3:ARG:HA	1.74	0.52
6:1G:101:ILE:HD13	26:14:25:TYR:HB2	1.92	0.52
23:11:32:LYS:NZ	61:11:205:HOH:O	2.42	0.52
32:1a:1022:G:H5'	32:1a:1023:G:OP2	2.09	0.52
32:1a:1103:C:OP1	33:1b:96:ARG:NH2	2.43	0.52
1:2A:1525:G:H2'	1:2A:1526:G:H8	1.75	0.52
1:2A:2189:U:H2'	1:2A:2190:G:H8	1.74	0.52
1:2A:2319:G:N2	14:2S:3:ARG:HD3	2.24	0.52
32:2a:932:C:H2'	32:2a:933:G:H8	1.74	0.52
32:2a:1061:G:O4'	41:2j:56:HIS:ND1	2.43	0.52
34:2c:6:HIS:HB3	45:2n:49:HIS:CD2	2.45	0.52
34:2c:20:SER:OG	34:2c:22:TRP:NE1	2.43	0.52
1:1A:639:U:H2'	1:1A:640:C:C6	2.45	0.52
1:1A:1721:G:H2'	1:1A:1740:G:O6	2.09	0.52
32:1a:102:G:O2'	32:1a:151:A:N3	2.35	0.52
32:1a:558:G:O6	61:1a:1907:HOH:O	2.16	0.52
32:1a:1239:A:H62	32:1a:1299:A:N6	2.07	0.52
33:1b:88:ALA:HB2	33:1b:219:VAL:HG13	1.90	0.52
40:1i:121:ARG:NH1	40:1i:122:ALA:O	2.42	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2312:U:H5'	6:2G:88:ILE:HD11	1.91	0.52
1:2A:2313:C:H4'	6:2G:91:ARG:HD3	1.92	0.52
1:2A:2684:U:OP2	61:2A:3853:HOH:O	2.19	0.52
32:2a:269:C:H2'	32:2a:270:A:C8	2.45	0.52
32:2a:737:A:H2'	32:2a:738:C:C6	2.44	0.52
32:2a:1015:A:O3'	45:2n:15:LYS:NZ	2.43	0.52
32:2a:1028:C:C2	32:2a:1033:G:N1	2.78	0.52
1:1A:1641:A:H2'	1:1A:1642:G:O4'	2.10	0.52
18:1W:79:GLY:HA3	18:1W:100:THR:HG22	1.91	0.52
32:1a:269:C:H2'	32:1a:270:A:C8	2.45	0.52
36:1e:144:THR:H	36:1e:147:ASP:HB2	1.75	0.52
1:2A:218:A:C2	1:2A:235:U:H4'	2.44	0.52
1:2A:1067:A:H4'	1:2A:1068:G:OP2	2.09	0.52
32:2a:828:A:N6	32:2a:858:G:O2'	2.42	0.52
32:2a:1263:C:H2'	32:2a:1264:C:C6	2.44	0.52
6:1G:66:GLN:NE2	6:1G:93:THR:O	2.42	0.52
12:1Q:54:MET:HG2	12:1Q:117:ALA:HB1	1.91	0.52
32:1a:1125:U:H4'	41:1j:5:ARG:NH2	2.25	0.52
33:1b:15:VAL:HG13	33:1b:16:HIS:HD2	1.75	0.52
1:2A:119:A:H4'	1:2A:120:U:OP1	2.09	0.52
1:2A:1518:U:H2'	1:2A:1519:G:O4'	2.10	0.52
7:2H:55:PRO:HG2	7:2H:61:HIS:CE1	2.45	0.52
1:1A:666:G:H1'	30:18:4:MET:HE3	1.91	0.51
1:1A:1379:A:H4'	1:1A:1380:G:OP2	2.10	0.51
1:2A:297:C:OP1	20:2Y:87:LYS:HG3	2.09	0.51
1:2A:1359:A:N3	1:2A:1359:A:H5'	2.25	0.51
6:2G:16:ARG:NH1	6:2G:31:VAL:HG21	2.25	0.51
20:2Y:55:TYR:CZ	20:2Y:61:ILE:HG21	2.46	0.51
21:2Z:6:LYS:HD3	21:2Z:8:TYR:HE2	1.75	0.51
32:2a:224:C:H2'	32:2a:225:C:C6	2.46	0.51
32:2a:719:C:O2'	49:2r:49:LYS:HB3	2.09	0.51
32:2a:1010:G:H2'	32:2a:1011:G:C8	2.45	0.51
1:1A:217:G:OP2	61:1A:4134:HOH:O	2.18	0.51
1:1A:531:C:H4'	1:1A:532:A:H5"	1.92	0.51
1:1A:1486:A:H2'	1:1A:1487:G:C8	2.45	0.51
1:1A:2319:G:H22	14:1S:3:ARG:NH1	2.07	0.51
32:1a:270:A:H2'	32:1a:271:C:C6	2.46	0.51
32:1a:1513:A:H2'	32:1a:1514:C:C6	2.46	0.51
1:2A:265:A:N1	1:2A:427:U:O2'	2.42	0.51
1:2A:300:A:OP1	20:2Y:86:ARG:NH2	2.43	0.51
2:2B:24:G:H4'	2:2B:25:A:C8	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:2i:4:TYR:O	40:2i:19:LEU:N	2.23	0.51
1:1A:644:A:H4'	1:1A:645:C:H5	1.76	0.51
1:1A:1268:A:H2'	1:1A:1269:A:O4'	2.11	0.51
1:1A:1721:G:H5'	1:1A:1722:A:OP2	2.09	0.51
6:1G:50:ALA:C	6:1G:52:ILE:H	2.16	0.51
21:1Z:14:LYS:HZ3	21:1Z:16:SER:H	1.58	0.51
32:1a:1077:G:N2	32:1a:1080:A:OP2	2.42	0.51
1:2A:1074:G:C2	1:2A:1075:C:H1'	2.46	0.51
32:2a:632:A:H5"	32:2a:632:A:H8	1.75	0.51
33:2b:158:LEU:HD21	33:2b:180:LEU:HD13	1.92	0.51
38:2g:53:LYS:HE3	38:2g:122:HIS:NE2	2.26	0.51
1:1A:1063:G:H2'	1:1A:1063:G:N3	2.26	0.51
1:1A:2147:G:H2'	1:1A:2148:G:H4'	1.93	0.51
32:1a:1239:A:H62	32:1a:1299:A:H61	1.59	0.51
38:1g:27:ILE:HD12	38:1g:40:ALA:HA	1.93	0.51
1:2A:251:A:C5	1:2A:252:G:H1'	2.46	0.51
1:2A:1057:A:N7	1:2A:1086:A:H2'	2.25	0.51
1:2A:2059:A:OP2	61:2A:3855:HOH:O	2.19	0.51
1:2A:2206:G:H8	1:2A:2207:G:N7	2.08	0.51
1:2A:2267:A:H5"	1:2A:2268:A:H5'	1.91	0.51
2:2B:23:G:O6	61:2B:307:HOH:O	2.19	0.51
6:2G:68:PRO:HA	6:2G:92:VAL:HB	1.91	0.51
21:2Z:40:ASP:OD2	21:2Z:42:VAL:HG13	2.10	0.51
42:2k:116:HIS:N	42:2k:117:ASN:HA	2.26	0.51
1:1A:272(J):C:H2'	1:1A:274:G:C8	2.45	0.51
32:1a:7:G:H21	36:1e:121:LYS:HG2	1.76	0.51
32:1a:731:G:H5'	32:1a:766:A:H4'	1.92	0.51
1:2A:247:G:H4'	1:2A:386:G:C5	2.46	0.51
1:2A:1754:C:OP1	15:2T:96:ARG:NH1	2.39	0.51
1:2A:2286:A:H4'	1:2A:2287:A:O4'	2.11	0.51
1:2A:2867:G:OP2	15:2T:119:LYS:NZ	2.38	0.51
5:2F:178:PRO:HB2	5:2F:201:VAL:HG21	1.91	0.51
26:24:20:ASN:ND2	26:24:38:LYS:HD2	2.25	0.51
32:2a:273:A:H1'	48:2q:16:GLN:HE21	1.75	0.51
34:2c:37:GLN:HA	34:2c:40:ARG:HG3	1.92	0.51
35:2d:187:ARG:NH2	35:2d:193:ASP:OD2	2.43	0.51
1:1A:271(Q):G:O6	61:1A:4129:HOH:O	2.17	0.51
32:1a:176:C:H2'	32:1a:177:C:C6	2.43	0.51
35:1d:162:LEU:HD13	35:1d:181:MET:HG2	1.93	0.51
1:2A:747:U:O2	1:2A:2014:A:H1'	2.11	0.51
1:2A:1489:U:HO2'	1:2A:1490:A:H8	1.58	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2G:112:PRO:HG3	26:24:43:TYR:HE2	1.74	0.51
7:2H:24:VAL:HG13	7:2H:37:VAL:HG21	1.93	0.51
8:2I:26:ALA:HB1	8:2I:31:LEU:HD13	1.92	0.51
9:2N:4:TYR:CD2	16:2U:100:VAL:HG11	2.45	0.51
13:2R:95:THR:HG22	13:2R:116:LEU:HD23	1.91	0.51
25:23:9:VAL:HG12	25:23:32:GLN:HE22	1.75	0.51
38:2g:132:GLY:O	38:2g:136:LYS:HG2	2.10	0.51
47:2p:13:HIS:C	47:2p:15:PRO:HD3	2.36	0.51
1:1A:904:C:O2'	21:1Z:169:GLU:OE2	2.25	0.51
32:1a:710:G:H5"	37:1f:54:LYS:HE3	1.93	0.51
32:1a:1277:C:H1'	32:1a:1282:C:O2	2.11	0.51
1:2A:248:G:OP1	61:2A:3854:HOH:O	2.19	0.51
1:2A:903:C:H2'	1:2A:904:C:C6	2.45	0.51
1:2A:1786:A:H1'	1:2A:1938:A:N6	2.26	0.51
1:2A:2171:A:H4'	1:2A:2172:U:OP1	2.10	0.51
2:2B:55:U:HO2'	6:2G:29:TRP:CD1	2.29	0.51
6:2G:19:LEU:HG	6:2G:175:LEU:HD22	1.93	0.51
21:2Z:128:VAL:HG12	21:2Z:161:VAL:HA	1.92	0.51
32:2a:377:G:OP1	47:2p:3:LYS:HD3	2.11	0.51
32:2a:1151:A:O2'	32:2a:1152:A:H8	1.93	0.51
38:2g:65:ALA:HB1	38:2g:127:ALA:HB3	1.91	0.51
1:1A:1084:A:H2	1:1A:1105:U:H1'	1.75	0.51
1:1A:1899:G:N3	1:1A:1899:G:H2'	2.25	0.51
1:1A:2186:G:H5'	1:1A:2187:G:OP2	2.10	0.51
26:14:55:ARG:N	26:14:56:VAL:HA	2.26	0.51
32:1a:131:C:H2'	32:1a:132:C:C6	2.46	0.51
37:1f:78:GLU:O	37:1f:81:ILE:HG22	2.11	0.51
1:2A:78:A:H2'	1:2A:79:G:C8	2.46	0.51
1:2A:288:C:H2'	1:2A:289:A:H8	1.76	0.51
1:2A:1165:U:H2'	1:2A:1166:C:C6	2.46	0.51
1:2A:2661:G:H2'	1:2A:2662:A:C8	2.46	0.51
26:24:58:ARG:HH21	50:2s:68:GLY:H	1.56	0.51
28:26:6:ARG:NH1	28:26:26:ASN:HB2	2.26	0.51
32:2a:560:U:H4'	32:2a:561:U:O5'	2.11	0.51
32:2a:923:A:O2'	32:2a:1399:C:OP2	2.24	0.51
32:2a:1103:C:OP1	33:2b:96:ARG:NH2	2.41	0.51
32:2a:1182:G:H4'	32:2a:1183:A:H3'	1.93	0.51
32:2a:1247:U:H1'	32:2a:1291:G:N2	2.26	0.51
32:2a:1512:U:H2'	32:2a:1513:A:C8	2.46	0.51
36:2e:17:ALA:HA	36:2e:26:PHE:HA	1.92	0.51
51:2t:60:GLU:HG3	51:2t:81:LYS:HD2	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1D:72:LYS:NZ	3:1D:99:ASP:OD2	2.37	0.51
28:16:15:GLU:OE1	28:16:45:LYS:NZ	2.44	0.51
32:1a:7:G:H5'	32:1a:298:A:O4'	2.10	0.51
32:1a:636:U:H2'	32:1a:637:G:C8	2.45	0.51
33:1b:115:LEU:HD13	33:1b:145:LEU:HB3	1.93	0.51
47:1p:27:LYS:HG3	47:1p:30:GLY:HA3	1.92	0.51
1:2A:1087:G:H22	1:2A:1102:C:N4	2.08	0.51
21:2Z:52:SER:OG	21:2Z:54:HIS:ND1	2.43	0.51
26:24:50:VAL:HG11	44:2m:64:TRP:C	2.36	0.51
37:2f:61:LEU:HD13	37:2f:63:TYR:OH	2.11	0.51
44:2m:87:TYR:N	50:2s:73:GLU:O	2.44	0.51
1:1A:686:G:N2	1:1A:788:A:H61	2.10	0.51
1:1A:2116:G:H1	1:1A:2165:G:H22	1.58	0.51
4:1E:9:VAL:HB	15:1T:3:ARG:HG2	1.92	0.51
6:1G:179:PRO:HG3	26:14:43:TYR:OH	2.11	0.51
32:1a:67:C:H2'	32:1a:68:G:C8	2.46	0.51
32:1a:1027:C:H2'	32:1a:1028:C:C5	2.46	0.51
36:1e:110:LEU:HD13	36:1e:118:ILE:HG21	1.93	0.51
38:1g:50:ILE:HD11	38:1g:58:PRO:HA	1.93	0.51
39:1h:14:ARG:O	39:1h:18:ARG:HG2	2.11	0.51
1:2A:2646:C:H2'	1:2A:2647:U:O4'	2.10	0.51
16:2U:49:HIS:HA	16:2U:52:ARG:HG2	1.93	0.51
32:2a:1249:C:O2'	40:2i:73:GLN:NE2	2.44	0.51
35:2d:166:LYS:HA	35:2d:178:VAL:HG21	1.92	0.51
1:1A:1094:U:O2'	1:1A:1096:A:N7	2.40	0.50
32:1a:575:G:O2'	32:1a:821:G:H5'	2.10	0.50
39:1h:64:LYS:HG2	39:1h:79:VAL:HG21	1.93	0.50
1:2A:500:G:N1	1:2A:503:A:OP2	2.44	0.50
19:2X:2:LYS:NZ	19:2X:38:GLU:OE2	2.38	0.50
21:2Z:53:ILE:HG22	21:2Z:71:VAL:HB	1.93	0.50
32:2a:51:A:N1	32:2a:314:C:O2'	2.43	0.50
1:1A:272:G:O2'	1:1A:421:U:OP2	2.18	0.50
6:1G:32:PRO:HB3	6:1G:163:ALA:HB2	1.91	0.50
13:1R:118:GLU:H	13:1R:118:GLU:CD	2.19	0.50
30:18:47:LYS:NZ	57:18:103:MPD:H51	2.27	0.50
32:1a:735:C:H2'	32:1a:736:C:H6	1.76	0.50
1:2A:1274:A:N3	1:2A:1297:C:H1'	2.26	0.50
1:2A:1803:A:H4'	3:2D:259:THR:HG23	1.94	0.50
6:2G:66:GLN:HG2	6:2G:92:VAL:HG21	1.93	0.50
7:2H:11:VAL:HG21	7:2H:50:VAL:HG23	1.92	0.50
21:2Z:124:ILE:HD13	21:2Z:155:LEU:HD22	1.91	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:2h:6:ILE:O	39:2h:10:LEU:HG	2.11	0.50
1:1A:1939:5MU:OP1	1:1A:2604:U:O2'	2.27	0.50
1:1A:2102:U:O2	1:1A:2187:G:C6	2.64	0.50
1:1A:2207:G:H2'	1:1A:2208:A:C2	2.47	0.50
17:1V:6:LYS:HG2	61:1V:313:HOH:O	2.12	0.50
32:1a:744:C:O2'	32:1a:851:G:N2	2.43	0.50
32:1a:1004:A:C5	32:1a:1037:C:C2	3.00	0.50
32:1a:1010:G:N2	32:1a:1020:U:H1'	2.26	0.50
34:1c:66:VAL:HG12	34:1c:68:VAL:HG23	1.94	0.50
35:1d:3:ARG:NH1	35:1d:5:ILE:HG22	2.26	0.50
53:1y:23:ARG:NH1	53:1y:26:LYS:HD2	2.27	0.50
1:2A:1014:U:H2'	1:2A:1015:G:C8	2.46	0.50
1:2A:2273:A:H2'	1:2A:2274:A:C8	2.47	0.50
1:2A:2602:A:N6	61:2A:3995:HOH:O	2.37	0.50
11:2P:95:VAL:HG23	11:2P:125:VAL:HA	1.92	0.50
15:2T:1:MET:HE2	15:2T:3:ARG:HG3	1.93	0.50
23:21:59:THR:O	23:21:91:LYS:NZ	2.44	0.50
23:21:83:GLU:OE1	23:21:83:GLU:N	2.44	0.50
32:2a:384:G:H2'	32:2a:385:C:C6	2.47	0.50
32:2a:1137:C:O2	32:2a:1138:G:N2	2.44	0.50
33:2b:55:PHE:CE1	33:2b:218:ALA:HA	2.47	0.50
40:2i:86:VAL:HG11	40:2i:93:ARG:HH21	1.75	0.50
1:1A:2133:G:H3'	1:1A:2157:G:N2	2.26	0.50
1:1A:2336:A:H61	22:10:43:THR:HG22	1.76	0.50
28:16:44:ARG:HG2	28:16:44:ARG:HH11	1.75	0.50
37:1f:69:GLU:H	37:1f:69:GLU:CD	2.18	0.50
1:2A:1688:U:O2	1:2A:1700:A:H5'	2.11	0.50
6:2G:11:TYR:CZ	6:2G:16:ARG:HD3	2.46	0.50
26:24:64:GLY:C	26:24:66:SER:H	2.18	0.50
1:1A:251:A:C5	1:1A:252:G:H1'	2.46	0.50
4:1E:167:VAL:HG12	4:1E:170:LEU:HD11	1.93	0.50
7:1H:154:PRO:HB3	7:1H:163:TYR:CZ	2.46	0.50
11:1P:106:LEU:HD22	11:1P:112:LEU:HD13	1.94	0.50
32:1a:390:C:H2'	32:1a:391:G:C8	2.47	0.50
32:1a:1353:G:OP1	52:1u:10:ARG:NH1	2.44	0.50
33:1b:96:ARG:HG2	33:1b:98:LEU:HD23	1.93	0.50
39:1h:6:ILE:HB	39:1h:85:ARG:NH1	2.26	0.50
1:2A:1110:G:H1'	1:2A:1111:A:H8	1.75	0.50
2:2B:29:A:H2'	2:2B:30:C:O4'	2.12	0.50
2:2B:57:A:OP2	61:2B:303:HOH:O	2.19	0.50
15:2T:95:ARG:HG2	15:2T:95:ARG:NH1	2.26	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:13:U:OP1	61:2a:3208:HOH:O	2.20	0.50
32:2a:624:C:H2'	32:2a:625:G:H8	1.77	0.50
32:2a:946:A:H2'	32:2a:947:G:C8	2.46	0.50
32:2a:1028:C:C2'	32:2a:1033:G:H22	2.24	0.50
32:2a:1316:G:N2	32:2a:1318:A:H3'	2.27	0.50
35:2d:201:GLN:NE2	36:2e:116:THR:O	2.35	0.50
1:1A:1803:A:H4'	3:1D:259:THR:HG23	1.94	0.50
26:14:61:ARG:HG3	26:14:62:ARG:H	1.76	0.50
32:1a:169:C:H2'	32:1a:170:U:C6	2.46	0.50
33:1b:15:VAL:HG23	33:1b:209:ARG:HD2	1.92	0.50
34:1c:102:ASN:HD22	34:1c:102:ASN:N	2.10	0.50
46:1o:6:GLU:H	46:1o:6:GLU:CD	2.19	0.50
1:2A:1589:C:H2'	1:2A:1590:U:C6	2.46	0.50
7:2H:98:LEU:HD22	7:2H:125:VAL:HG23	1.92	0.50
19:2X:65:ARG:HE	19:2X:70:LEU:HD21	1.77	0.50
32:2a:574:A:OP2	61:2a:3207:HOH:O	2.19	0.50
32:2a:1030(A):G:H1'	32:2a:1030(C):G:C5	2.46	0.50
32:2a:1323:G:H4'	32:2a:1363:C:N3	2.25	0.50
33:2b:127:ILE:C	33:2b:129:GLU:H	2.19	0.50
36:2e:52:PRO:HG2	36:2e:53:LEU:HD12	1.93	0.50
40:2i:71:SER:HA	40:2i:74:ILE:HD12	1.94	0.50
1:1A:620:G:N3	1:1A:620:G:H5'	2.27	0.50
8:1I:72:LEU:C	8:1I:74:ASN:H	2.19	0.50
8:1I:133:HIS:ND1	8:1I:134:PRO:O	2.41	0.50
32:1a:108:G:C6	51:1t:15:ARG:HG2	2.45	0.50
4:2E:178:GLU:CD	4:2E:178:GLU:H	2.20	0.50
5:2F:154:VAL:HA	5:2F:191:ARG:HB2	1.94	0.50
6:2G:41:GLN:NE2	6:2G:154:GLY:O	2.37	0.50
8:2I:1:MET:HE2	8:2I:38:LEU:HD21	1.94	0.50
26:24:46:GLN:HB3	26:24:48:ARG:CZ	2.42	0.50
30:28:26:LYS:HD2	30:28:48:PHE:CD2	2.46	0.50
32:2a:164:U:H2'	32:2a:165:C:H6	1.77	0.50
32:2a:946:A:O2'	32:2a:1333:A:N3	2.42	0.50
32:2a:1002:G:H2'	32:2a:1003:G:C8	2.47	0.50
32:2a:1121:U:C2'	32:2a:1122:U:H5'	2.42	0.50
1:1A:586:A:N1	1:1A:809:G:O2'	2.38	0.50
1:1A:1359:A:N6	1:1A:1372:U:H3	2.10	0.50
7:1H:24:VAL:HG22	7:1H:35:VAL:HB	1.94	0.50
14:1S:27:SER:HA	14:1S:88:ASP:HB3	1.94	0.50
40:1i:16:ARG:HH11	40:1i:64:THR:HG21	1.77	0.50
40:1i:50:LEU:HA	40:1i:53:VAL:HG22	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:774:A:H2'	1:2A:774:A:N3	2.27	0.50
1:2A:1096:A:H2'	1:2A:1097:U:H6	1.77	0.50
1:2A:2693:A:H2'	1:2A:2694:G:C8	2.45	0.50
32:2a:420:U:H2'	32:2a:422:C:C5	2.47	0.50
32:2a:547:A:OP1	61:2a:3209:HOH:O	2.20	0.50
32:2a:707:C:H2'	32:2a:708:C:C6	2.46	0.50
34:2c:110:ASN:O	34:2c:141:VAL:HG22	2.12	0.50
36:2e:53:LEU:HD12	36:2e:53:LEU:H	1.77	0.50
49:2r:33:ASP:OD2	49:2r:36:ASN:HB2	2.11	0.50
1:1A:1175:U:O2'	1:1A:1176:G:O5'	2.29	0.50
1:1A:1968:G:OP1	61:1A:4139:HOH:O	2.19	0.50
1:1A:2290:G:OP2	61:1A:4137:HOH:O	2.19	0.50
1:1A:2355:C:H1'	22:10:39:ARG:HH21	1.75	0.50
1:1A:2811:G:N2	1:1A:2891:G:H1'	2.27	0.50
18:1W:23:LEU:HD22	27:15:25:LEU:HD12	1.94	0.50
32:1a:452:A:H4'	47:1p:72:ARG:NH1	2.27	0.50
36:1e:100:VAL:O	36:1e:107:ARG:NH2	2.44	0.50
41:1j:78:ASN:O	41:1j:80:LYS:N	2.45	0.50
43:1l:117:ARG:NH1	61:1l:301:HOH:O	2.43	0.50
1:2A:271(D):G:H2'	1:2A:271(E):U:C6	2.47	0.50
1:2A:1063:G:HO2'	1:2A:1064:C:H6	1.58	0.50
1:2A:1316:U:H2'	1:2A:1317:A:H8	1.75	0.50
1:2A:1366:A:OP1	23:21:3:LYS:NZ	2.45	0.50
1:2A:2134:A:H8	1:2A:2156:G:N2	2.10	0.50
1:2A:2166:G:H2'	1:2A:2167:U:O4'	2.12	0.50
32:2a:56:U:H2'	32:2a:57:G:H8	1.75	0.50
32:2a:580:U:H5"	46:2o:58:MET:HG2	1.94	0.50
32:2a:815:A:N7	32:2a:1509:C:O2'	2.41	0.50
32:2a:1255:G:O3'	32:2a:1258:G:H1'	2.12	0.50
34:2c:131:ARG:NH2	36:2e:50:GLU:HG3	2.27	0.50
36:2e:140:ARG:O	36:2e:143:ARG:NH2	2.45	0.50
40:2i:25:LYS:H	40:2i:60:ASP:CB	2.24	0.50
48:2q:95:TYR:HA	48:2q:98:LEU:HD12	1.93	0.50
1:1A:207:A:H2'	1:1A:208:C:O4'	2.12	0.49
1:1A:878:A:H2'	1:1A:879:G:H5'	1.94	0.49
1:1A:2171:A:H1'	1:1A:2172:U:C6	2.47	0.49
12:1Q:108:GLY:HA3	21:1Z:116:VAL:HG13	1.94	0.49
32:1a:129(A):G:C6	32:1a:189(E):U:H4'	2.47	0.49
32:1a:1412:C:H2'	32:1a:1413:A:H8	1.77	0.49
34:1c:108:ASN:HD21	34:1c:144:SER:HG	1.55	0.49
39:1h:73:ASP:OD1	39:1h:75:ARG:NH1	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:1j:62:HIS:HB3	45:1n:59:ALA:HB3	1.93	0.49
1:2A:897:C:H2'	1:2A:898:C:C6	2.47	0.49
2:2B:31:C:H4'	6:2G:29:TRP:CH2	2.46	0.49
5:2F:11:VAL:HB	5:2F:18:ARG:HG2	1.94	0.49
32:2a:940:C:H2'	32:2a:941:G:C8	2.47	0.49
32:2a:1108:G:H5'	34:2c:176:HIS:HD2	1.75	0.49
35:2d:170:VAL:HG13	35:2d:174:LEU:HB2	1.94	0.49
36:2e:50:GLU:HB2	36:2e:53:LEU:HD13	1.93	0.49
41:2j:63:PHE:HZ	45:2n:49:HIS:CE1	2.30	0.49
44:2m:14:ARG:HH21	44:2m:42:ALA:HA	1.77	0.49
1:1A:2353:G:N7	61:1A:4280:HOH:O	2.35	0.49
32:1a:1118:C:H1'	32:1a:1179:A:C4	2.47	0.49
1:2A:385:C:O2'	1:2A:388:G:N2	2.45	0.49
2:2B:25:A:H2'	2:2B:26:A:C8	2.46	0.49
12:2Q:36:ALA:HB2	12:2Q:103:MET:SD	2.53	0.49
32:2a:1273:G:H3'	32:2a:1274:G:H8	1.77	0.49
32:2a:1347:G:N2	32:2a:1373:G:H2'	2.26	0.49
33:2b:18:GLY:HA2	33:2b:42:ILE:HD12	1.94	0.49
33:2b:82:ARG:HB3	33:2b:92:TYR:CZ	2.45	0.49
36:2e:88:LYS:HE2	36:2e:123:LEU:HD12	1.93	0.49
1:1A:247:G:H4'	1:1A:386:G:C5	2.46	0.49
1:1A:2069:G:N7	61:1A:4283:HOH:O	2.35	0.49
1:1A:2870:C:H2'	1:1A:2871:C:O4'	2.12	0.49
6:1G:150:ASP:CG	6:1G:151:ALA:H	2.20	0.49
10:1O:118:ALA:O	57:1a:1880:MPD:H12	2.12	0.49
32:1a:662:G:H2'	32:1a:663:A:C8	2.47	0.49
32:1a:745:C:H2'	32:1a:746:A:C8	2.46	0.49
32:1a:955:U:O2'	50:1s:83:HIS:HD2	1.96	0.49
1:2A:108:U:OP1	1:2A:293:U:O2'	2.30	0.49
16:2U:43:GLY:HA3	17:2V:73:SER:HB3	1.94	0.49
27:25:41:PRO:O	27:25:44:THR:OG1	2.25	0.49
32:2a:1002:G:C2	32:2a:1003:G:N7	2.79	0.49
32:2a:1320:C:H2'	32:2a:1321:C:O4'	2.12	0.49
34:2c:148:GLY:HA3	34:2c:203:PHE:HB3	1.93	0.49
1:1A:644:A:H4'	1:1A:645:C:C5	2.48	0.49
1:1A:1053:C:H2'	1:1A:1054:A:C8	2.47	0.49
12:1Q:14:ARG:HG2	12:1Q:41:TRP:HH2	1.76	0.49
32:1a:738:C:H2'	32:1a:739:C:C6	2.47	0.49
32:1a:1016:A:H2'	32:1a:1017:G:O4'	2.11	0.49
32:1a:1267:C:O2	52:1u:20:LYS:HE2	2.12	0.49
32:1a:1525:G:OP1	42:1k:120:ARG:NH2	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1c:134:ILE:HD11	34:1c:153:VAL:HB	1.94	0.49
40:1i:79:LEU:HD22	40:1i:104:ARG:HB2	1.94	0.49
4:2E:174:ASP:OD1	4:2E:175:VAL:N	2.46	0.49
13:2R:2:ARG:NH1	13:2R:5:LYS:O	2.44	0.49
32:2a:921:U:O2	36:2e:19:MET:HB2	2.12	0.49
32:2a:1202:G:O4'	45:2n:29:ARG:NH1	2.45	0.49
47:2p:1:MET:N	47:2p:1:MET:SD	2.82	0.49
1:1A:1814:G:H4'	3:1D:51:VAL:HG21	1.95	0.49
1:1A:2461:C:H2'	1:1A:2462:U:C6	2.48	0.49
12:1Q:32:TYR:OH	12:1Q:111:GLU:OE2	2.24	0.49
17:1V:60:GLU:OE1	17:1V:97:LYS:NZ	2.33	0.49
19:1X:63:LYS:O	19:1X:64:LYS:HD3	2.13	0.49
32:1a:1323:G:H2'	32:1a:1324:A:C8	2.47	0.49
40:1i:105:ASP:HB2	40:1i:107:ARG:HG3	1.94	0.49
45:1n:7:ILE:HD11	45:1n:28:GLY:HA3	1.93	0.49
46:1o:87:ILE:HG22	46:1o:88:ARG:N	2.27	0.49
1:2A:96:G:H4'	24:22:48:HIS:CD2	2.47	0.49
1:2A:643:A:N1	1:2A:2369:A:O2'	2.41	0.49
1:2A:1086:A:OP1	1:2A:1104:C:O2'	2.30	0.49
1:2A:1581:G:H2'	1:2A:1582:C:O4'	2.12	0.49
2:2B:60:C:H2'	2:2B:61:G:H8	1.78	0.49
5:2F:178:PRO:HB2	5:2F:201:VAL:CG2	2.42	0.49
7:2H:3:ARG:HE	7:2H:54:ARG:NH1	2.09	0.49
32:2a:437:U:H5'	35:2d:155:LEU:HD21	1.94	0.49
32:2a:750:G:N3	46:2o:23:GLY:HA3	2.27	0.49
32:2a:1016:A:O5'	32:2a:1016:A:H8	1.95	0.49
1:1A:1210:A:H5"	1:1A:1212:G:O4'	2.13	0.49
2:1B:75:G:H22	21:1Z:73:GLN:NE2	2.11	0.49
6:1G:115:ARG:HB3	6:1G:136:ARG:NH2	2.27	0.49
32:1a:1101:A:H4'	32:1a:1102:A:O5'	2.13	0.49
32:1a:1183:A:H3'	32:1a:1184:G:C5'	2.43	0.49
34:1c:139:GLN:HE21	34:1c:143:GLU:HG3	1.78	0.49
1:2A:1178:C:H2'	1:2A:1179:C:C6	2.47	0.49
1:2A:2526:G:H5'	1:2A:2742:C:O2'	2.12	0.49
1:2A:2784:C:H1'	4:2E:37:ARG:HH12	1.77	0.49
5:2F:120:GLU:HB2	5:2F:122:LYS:HG2	1.93	0.49
20:2Y:39:VAL:HB	20:2Y:42:VAL:HB	1.94	0.49
32:2a:123:C:OP1	32:2a:311:C:O2'	2.28	0.49
32:2a:280:C:N3	48:2q:39:SER:OG	2.44	0.49
32:2a:1119:C:H2'	32:2a:1120:G:C8	2.48	0.49
46:2o:82:ILE:HB	46:2o:87:ILE:HB	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:2r:53:ARG:NH1	49:2r:60:ALA:HB2	2.28	0.49
51:2t:18:GLN:O	51:2t:22:ARG:HG3	2.13	0.49
1:1A:288:C:H2'	1:1A:289:A:C8	2.47	0.49
16:1U:86:ALA:O	17:1V:49:THR:HG23	2.13	0.49
32:1a:755:G:OP2	46:1o:65:ARG:HD2	2.12	0.49
1:2A:652(B):A:H61	1:2A:655:A:H1'	1.78	0.49
1:2A:2022:U:O2'	1:2A:2617:C:H5'	2.12	0.49
21:2Z:150:LEU:HB2	21:2Z:171:ILE:HD11	1.94	0.49
32:2a:1287:A:C6	32:2a:1288:A:C6	3.01	0.49
33:2b:222:ILE:O	33:2b:226:ARG:HB2	2.13	0.49
1:1A:1224:C:OP1	61:1A:4140:HOH:O	2.20	0.49
1:1A:2698:U:H2'	1:1A:2699:C:C6	2.48	0.49
29:17:24:THR:HG23	29:17:27:GLY:N	2.26	0.49
32:1a:1128:C:H4'	32:1a:1148:U:O2	2.13	0.49
1:2A:1996:C:H4'	1:2A:1997:G:OP1	2.11	0.49
6:2G:4:ASP:HA	6:2G:8:LYS:HE2	1.93	0.49
20:2Y:28:LYS:NZ	20:2Y:64:GLU:OE1	2.39	0.49
32:2a:353:A:H5'	32:2a:353:A:H8	1.77	0.49
32:2a:437:U:O2'	35:2d:125:HIS:HE1	1.95	0.49
32:2a:938:A:N6	32:2a:939:G:C6	2.80	0.49
32:2a:986:A:H1'	50:2s:54:GLY:O	2.12	0.49
50:2s:81:ARG:HB2	50:2s:81:ARG:NH1	2.27	0.49
1:1A:1009:A:OP2	9:1N:37:LYS:NZ	2.39	0.49
3:1D:26:LYS:HE2	3:1D:28:GLU:O	2.12	0.49
6:1G:126:ASP:HB3	6:1G:128:ARG:H	1.78	0.49
32:1a:501:C:H1'	32:1a:549:C:H1'	1.95	0.49
1:2A:272:G:N7	1:2A:421:U:H2'	2.28	0.49
5:2F:185:ASP:HA	5:2F:188:ARG:HD3	1.95	0.49
32:2a:731:G:H5'	32:2a:766:A:H4'	1.94	0.49
32:2a:741:G:H2'	32:2a:742:G:O4'	2.13	0.49
32:2a:1118:C:N3	32:2a:1156:G:N2	2.61	0.49
32:2a:1391:U:H2'	32:2a:1392:G:C8	2.48	0.49
33:2b:87:ARG:CZ	33:2b:233:SER:HB2	2.43	0.49
42:2k:115:PRO:C	42:2k:117:ASN:HA	2.38	0.49
50:2s:22:LEU:HD22	50:2s:27:GLU:HA	1.95	0.49
1:1A:1264:G:OP1	27:15:19:ARG:NH2	2.22	0.49
1:1A:1452:A:H5"	61:1A:5982:HOH:O	2.13	0.49
14:1S:25:ARG:NH1	14:1S:42:ASP:OD1	2.46	0.49
15:1T:127:ALA:O	15:1T:129:ARG:N	2.46	0.49
30:18:62:LEU:HB3	30:18:65:GLU:HG2	1.95	0.49
32:1a:352:C:OP2	61:1a:1912:HOH:O	2.20	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:1j:40:LEU:HB2	41:1j:69:ASN:HB2	1.93	0.49
1:2A:236:C:H2'	1:2A:237:C:C6	2.48	0.49
1:2A:245:G:O6	30:28:8:LYS:NZ	2.42	0.49
1:2A:2059:A:O2'	5:2F:69:HIS:HD2	1.95	0.49
1:2A:2104:G:N1	1:2A:2185:C:O2	2.45	0.49
1:2A:2179:C:C4	1:2A:2180:U:C4	3.01	0.49
5:2F:116:ASP:OD2	11:2P:1:MET:N	2.34	0.49
31:29:14:CYS:HA	31:29:27:CYS:HB2	1.94	0.49
32:2a:42:G:H5"	61:2a:3307:HOH:O	2.11	0.49
32:2a:1164:G:H1	32:2a:1172:C:H42	1.61	0.49
33:2b:179:LYS:HA	39:2h:72:PRO:HG3	1.95	0.49
39:2h:20:TYR:HA	39:2h:65:TYR:CZ	2.47	0.49
48:2q:58:GLU:OE1	48:2q:75:ARG:NE	2.46	0.49
1:1A:1688:U:O2	1:1A:1700:A:H5'	2.12	0.48
1:1A:2098:U:H3	1:1A:2191:G:H1	1.60	0.48
36:1e:60:TYR:CZ	36:1e:64:ARG:HD3	2.48	0.48
39:1h:10:LEU:HD12	39:1h:85:ARG:HD2	1.94	0.48
1:2A:2611:U:H6	1:2A:2611:U:H5'	1.78	0.48
5:2F:187:VAL:HG12	11:2P:3:LEU:HD12	1.94	0.48
17:2V:1:MET:HB3	17:2V:99:ILE:HD12	1.94	0.48
33:2b:119:GLU:CD	33:2b:153:ARG:HH12	2.20	0.48
33:2b:211:ILE:O	33:2b:215:LEU:HB2	2.13	0.48
38:2g:72:ARG:NH1	38:2g:142:GLU:OE2	2.46	0.48
40:2i:125:TYR:HE1	40:2i:127:LYS:HB3	1.78	0.48
44:2m:108:ARG:HD3	44:2m:108:ARG:HA	1.60	0.48
1:1A:1045:A:H5'	1:1A:1046:A:H5'	1.94	0.48
1:1A:2611:U:C4	27:15:3:LYS:HG2	2.47	0.48
15:1T:127:ALA:C	15:1T:129:ARG:N	2.71	0.48
20:1Y:68:HIS:ND1	20:1Y:70:SER:HB3	2.28	0.48
22:10:27:GLU:HG3	22:10:68:GLU:HA	1.95	0.48
32:1a:1093:A:O2'	32:1a:1095:U:OP1	2.28	0.48
38:1g:91:VAL:HG12	38:1g:95:ARG:HB3	1.94	0.48
41:1j:49:VAL:HG21	45:1n:41:ARG:O	2.13	0.48
1:2A:30:G:H2'	1:2A:31:C:C6	2.48	0.48
1:2A:144:C:H2'	1:2A:145:G:H8	1.77	0.48
1:2A:1048:A:N1	1:2A:1112:G:O2'	2.41	0.48
3:2D:124:PRO:HB2	3:2D:126:GLN:HG2	1.96	0.48
6:2G:9:ARG:O	6:2G:13:GLU:HB2	2.13	0.48
7:2H:46:GLU:HB2	7:2H:49:VAL:HG12	1.94	0.48
7:2H:109:PHE:C	7:2H:111:HIS:H	2.20	0.48
14:2S:26:LEU:HD22	14:2S:87:PHE:CD1	2.47	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:975:A:N1	41:2j:48:THR:HB	2.28	0.48
32:2a:1070:U:OP1	36:2e:20:GLN:NE2	2.47	0.48
32:2a:1442:G:H2'	32:2a:1442:G:N3	2.28	0.48
1:1A:244:A:C2	1:1A:255:A:C4	3.01	0.48
1:1A:1815:A:OP2	3:1D:54:ARG:NH2	2.46	0.48
1:1A:2100:G:H1	1:1A:2189:U:H3	1.61	0.48
1:1A:2162:G:H1'	1:1A:2173:A:H1'	1.95	0.48
13:1R:83:ILE:O	13:1R:86:ARG:HG2	2.12	0.48
32:1a:620:C:C2	35:1d:135:LEU:HG	2.47	0.48
32:1a:1161:C:H2'	32:1a:1162:C:C6	2.49	0.48
32:1a:1264:C:H2'	32:1a:1265:G:C8	2.47	0.48
33:1b:42:ILE:HD12	33:1b:203:GLY:HA2	1.95	0.48
35:1d:156:GLU:O	35:1d:160:GLN:HG2	2.13	0.48
35:1d:173:TRP:CE3	35:1d:174:LEU:HG	2.48	0.48
40:1i:9:ARG:HG2	40:1i:14:VAL:HG13	1.96	0.48
53:1y:3:MET:HE2	53:1y:3:MET:HB3	1.73	0.48
12:2Q:58:PHE:O	12:2Q:60:ARG:N	2.43	0.48
32:2a:1151:A:N3	41:2j:39:PRO:HG3	2.28	0.48
33:2b:48:MET:HA	33:2b:51:LEU:HD12	1.95	0.48
34:2c:57:ILE:HG12	34:2c:66:VAL:HG13	1.94	0.48
52:2u:15:ARG:HB3	52:2u:17:THR:HG23	1.93	0.48
1:1A:1693:U:H1'	3:1D:14:ARG:NH1	2.28	0.48
1:1A:2110:G:OP1	1:1A:2118:U:N3	2.47	0.48
7:1H:41:MET:HE1	7:1H:54:ARG:HB3	1.95	0.48
32:1a:1004:A:N7	32:1a:1036:G:N1	2.61	0.48
33:1b:115:LEU:O	33:1b:119:GLU:HG2	2.13	0.48
37:1f:91:VAL:HG11	49:1r:72:ARG:NH1	2.27	0.48
1:2A:236:C:H2'	1:2A:237:C:H6	1.79	0.48
1:2A:322:A:OP2	5:2F:169:ASN:HB2	2.13	0.48
11:2P:85:LEU:HD13	11:2P:120:ALA:HB2	1.95	0.48
20:2Y:15:VAL:HG21	20:2Y:42:VAL:HG11	1.95	0.48
26:24:59:PHE:HB2	26:24:62:ARG:NH2	2.27	0.48
32:2a:1002:G:N3	32:2a:1003:G:N7	2.62	0.48
32:2a:1235:U:O2'	32:2a:1305:G:O5'	2.31	0.48
1:1A:2096:U:H3	1:1A:2193:G:H1	1.62	0.48
1:1A:2124:G:H2'	1:1A:2125:G:H5'	1.96	0.48
32:1a:448:A:P	32:1a:485:G:H22	2.37	0.48
34:1c:15:THR:HG22	34:1c:16:ARG:HG3	1.95	0.48
48:1q:10:VAL:HG13	48:1q:19:VAL:HB	1.95	0.48
51:1t:18:GLN:O	51:1t:22:ARG:HG3	2.14	0.48
1:2A:263:C:H2'	1:2A:264:C:O4'	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:523:C:H4'	1:2A:540:C:O2	2.14	0.48
1:2A:855:G:H2'	1:2A:856:C:C6	2.48	0.48
1:2A:2136:C:C6	1:2A:2137:C:H5	2.32	0.48
1:2A:2262:U:H4'	1:2A:2328:A:C2	2.48	0.48
3:2D:85:ASP:OD2	3:2D:88:ARG:HD2	2.13	0.48
15:2T:64:ARG:HB2	15:2T:73:GLU:HG2	1.96	0.48
32:2a:444:C:H2'	32:2a:445:G:H8	1.77	0.48
32:2a:1005:A:O2'	32:2a:1036:G:N2	2.45	0.48
32:2a:1188:A:H2'	32:2a:1189:C:O4'	2.13	0.48
32:2a:1359:C:O2'	32:2a:1361:G:N7	2.46	0.48
34:2c:120:VAL:O	34:2c:124:ILE:HG12	2.14	0.48
38:2g:70:LYS:HB3	38:2g:96:GLN:OE1	2.13	0.48
42:2k:110:ASP:HB3	49:2r:85:LEU:HB3	1.94	0.48
1:1A:729:G:C6	3:1D:208:LYS:HB2	2.48	0.48
1:1A:1050:A:H2'	1:1A:1051:G:O4'	2.14	0.48
1:1A:2345:G:N3	1:1A:2381:C:H2'	2.28	0.48
21:1Z:103:ARG:HD3	21:1Z:136:PHE:CD1	2.48	0.48
32:1a:1117:G:H4'	40:1i:104:ARG:NH1	2.29	0.48
32:1a:1486:G:H2'	32:1a:1487:G:O4'	2.13	0.48
38:1g:54:THR:O	38:1g:56:GLN:N	2.46	0.48
40:1i:50:LEU:O	40:1i:54:ASP:N	2.46	0.48
44:1m:19:LEU:HB3	44:1m:25:ILE:HG21	1.95	0.48
1:2A:1420:U:O2'	1:2A:1421:G:OP1	2.30	0.48
7:2H:9:ILE:HG13	7:2H:50:VAL:O	2.14	0.48
32:2a:187:C:O2'	51:2t:89:ARG:HD3	2.13	0.48
32:2a:620:C:C2	35:2d:135:LEU:HG	2.48	0.48
1:1A:375:C:H2'	1:1A:376:C:C6	2.49	0.48
1:1A:1083:U:H1'	1:1A:1086:A:N6	2.28	0.48
1:1A:2849:U:H4'	1:1A:2868:A:C2	2.48	0.48
2:1B:2:C:H2'	2:1B:3:C:C6	2.49	0.48
32:1a:491:G:H2'	32:1a:492:G:O4'	2.14	0.48
32:1a:542:G:H5'	35:1d:41:GLY:HA3	1.96	0.48
32:1a:624:C:H2'	32:1a:625:G:H8	1.78	0.48
34:1c:17:ASP:OD2	34:1c:21:ARG:HD3	2.13	0.48
37:1f:82:ARG:HB2	37:1f:85:VAL:HG23	1.96	0.48
1:2A:2648:C:H2'	1:2A:2649:U:C6	2.49	0.48
14:2S:15:ARG:O	14:2S:19:LYS:HG2	2.14	0.48
26:24:57:GLU:HA	26:24:58:ARG:HA	1.59	0.48
44:2m:16:ASP:OD1	44:2m:16:ASP:N	2.42	0.48
44:2m:84:ILE:HG13	44:2m:86:CYS:H	1.79	0.48
1:1A:1113:U:H2'	1:1A:1114:G:C8	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1131:G:H21	9:1N:73:THR:CG2	2.26	0.48
1:1A:2080:G:OP1	23:11:35:THR:HG21	2.14	0.48
9:1N:65:LYS:HE2	9:1N:69:GLN:NE2	2.29	0.48
30:18:26:LYS:HD2	30:18:48:PHE:CD2	2.49	0.48
32:1a:199:G:H2'	32:1a:200:G:C8	2.49	0.48
32:1a:664:G:N2	32:1a:741:G:H1	2.07	0.48
34:1c:3:ASN:OD1	34:1c:3:ASN:N	2.46	0.48
44:1m:5:ALA:HB1	44:1m:61:GLU:HG2	1.96	0.48
30:28:54:GLU:OE1	30:28:57:ARG:NH1	2.46	0.48
32:2a:1108:G:H5'	34:2c:176:HIS:CD2	2.49	0.48
33:2b:166:ASP:O	33:2b:170:GLU:HG2	2.13	0.48
36:2e:152:ARG:HB3	39:2h:43:GLY:HA3	1.95	0.48
40:2i:40:LEU:HD21	40:2i:70:LYS:HB3	1.95	0.48
41:2j:46:ARG:HA	41:2j:64:GLU:HA	1.96	0.48
1:1A:1805:U:O2	3:1D:50:THR:HB	2.14	0.48
1:1A:1932:A:H2'	1:1A:1933:G:O4'	2.14	0.48
1:1A:2805:G:H2'	1:1A:2807:G:H8	1.77	0.48
61:1A:6449:HOH:O	3:1D:38:LYS:HE3	2.13	0.48
3:1D:113:VAL:HG12	61:1D:482:HOH:O	2.14	0.48
18:1W:68:ARG:HH11	18:1W:111:HIS:HA	1.77	0.48
25:13:7:LYS:HE3	25:13:32:GLN:NE2	2.29	0.48
32:1a:474:G:H2'	32:1a:475:G:C8	2.48	0.48
51:1t:57:ARG:NH2	51:1t:100:ILE:HD12	2.26	0.48
1:2A:954:G:H5"	12:2Q:13:GLN:HB3	1.96	0.48
1:2A:1096:A:H2'	1:2A:1097:U:C6	2.48	0.48
1:2A:2119:A:H61	1:2A:2168:G:H21	1.61	0.48
1:2A:2291:U:O2'	1:2A:2374:C:O2	2.29	0.48
1:2A:2660:A:H2'	1:2A:2661:G:O4'	2.13	0.48
1:2A:2870:C:H2'	1:2A:2871:C:O4'	2.14	0.48
9:2N:1:MET:HE1	16:2U:94:ASN:ND2	2.29	0.48
32:2a:1119:C:H2'	32:2a:1120:G:H8	1.79	0.48
1:1A:1354:A:OP2	61:1A:4141:HOH:O	2.20	0.48
1:1A:2206:G:H5'	1:1A:2207:G:C5	2.48	0.48
1:1A:2430:A:N3	1:1A:2430:A:H2'	2.27	0.48
1:1A:2439:A:H5'	1:1A:2439:A:C8	2.49	0.48
32:1a:1228:C:P	44:1m:108:ARG:HH22	2.37	0.48
34:1c:63:ASN:HB3	34:1c:98:ASN:HB2	1.96	0.48
37:1f:42:GLU:OE2	37:1f:59:TYR:OH	2.24	0.48
42:1k:18:ARG:HD3	42:1k:83:ILE:HD11	1.96	0.48
1:2A:729:G:C6	3:2D:208:LYS:HB2	2.49	0.48
6:2G:48:GLU:HA	6:2G:51:ARG:HH21	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:2P:126:VAL:HG12	11:2P:148:LEU:HG	1.95	0.48
13:2R:87:TYR:OH	13:2R:117:VAL:O	2.28	0.48
21:2Z:140:ASP:OD1	21:2Z:142:SER:OG	2.24	0.48
26:24:59:PHE:CE2	50:2s:64:GLU:HB2	2.49	0.48
32:2a:558:G:OP1	61:2a:3210:HOH:O	2.20	0.48
32:2a:920:U:H2'	32:2a:921:U:C6	2.48	0.48
32:2a:922:G:N3	32:2a:1398:A:H2	2.12	0.48
33:2b:45:GLN:O	33:2b:49:GLU:HG2	2.14	0.48
34:2c:186:PHE:CZ	34:2c:188:LEU:HD13	2.49	0.48
35:2d:15:GLU:HB3	35:2d:63:LYS:HG2	1.96	0.48
1:1A:1055:G:N1	1:1A:1104:C:O2	2.47	0.47
1:1A:1239:G:H2'	1:1A:1240:U:O4'	2.14	0.47
1:1A:1593:G:H2'	1:1A:1594:G:C8	2.49	0.47
1:1A:1707:G:N7	61:1A:4289:HOH:O	2.36	0.47
1:1A:2151:G:C2	1:1A:2152:G:H1'	2.49	0.47
16:1U:30:LYS:N	16:1U:30:LYS:HD2	2.29	0.47
22:10:36:ILE:HD12	22:10:58:THR:HG21	1.96	0.47
32:1a:271:C:H2'	32:1a:272:C:C6	2.47	0.47
46:1o:55:GLY:O	46:1o:59:MET:HG3	2.14	0.47
1:2A:223:A:O2'	1:2A:420:C:O2	2.31	0.47
1:2A:854:G:H2'	1:2A:855:G:H8	1.79	0.47
8:2I:57:ARG:O	8:2I:61:ARG:HG2	2.14	0.47
8:2I:129:THR:HG22	8:2I:139:GLN:OE1	2.14	0.47
21:2Z:7:ALA:HB2	21:2Z:59:LEU:HD22	1.95	0.47
32:2a:451:A:N6	32:2a:480:U:H2'	2.28	0.47
32:2a:1141:C:H2'	32:2a:1142:G:H8	1.79	0.47
32:2a:1239:A:O2'	38:2g:114:ARG:O	2.24	0.47
32:2a:1277:C:O2'	32:2a:1279:A:C8	2.65	0.47
32:2a:1312:G:H5'	50:2s:5:LEU:HD21	1.94	0.47
32:2a:1324:A:O4'	32:2a:1362:C:H4'	2.13	0.47
35:2d:22:LYS:HD2	60:2d:501:SF4:S3	2.54	0.47
1:1A:279:C:N4	1:1A:361:G:H1	2.12	0.47
1:1A:774:A:N3	1:1A:774:A:H2'	2.28	0.47
1:1A:1155:A:OP1	16:1U:55:ARG:HD3	2.13	0.47
20:1Y:92:ASN:HB2	20:1Y:94:LYS:N	2.16	0.47
25:13:4:LEU:O	25:13:36:VAL:HA	2.14	0.47
32:1a:580:U:H2'	32:1a:581:G:O4'	2.14	0.47
32:1a:1250:A:H4'	40:1i:68:GLY:N	2.30	0.47
33:1b:71:VAL:HB	33:1b:164:VAL:HG22	1.96	0.47
39:1h:116:LYS:HD3	39:1h:127:LEU:HD22	1.97	0.47
40:1i:16:ARG:HD3	40:1i:64:THR:HG21	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:1k:99:GLN:HG2	42:1k:105:VAL:HG21	1.96	0.47
44:1m:3:ARG:HD2	44:1m:9:ILE:HG12	1.95	0.47
47:1p:39:TYR:CZ	47:1p:73:LEU:HD21	2.48	0.47
53:1y:55:ASN:OD1	53:1y:60:VAL:HG12	2.14	0.47
1:2A:994:C:O2'	1:2A:996:A:OP1	2.28	0.47
1:2A:1939:5MU:OP1	1:2A:2604:U:O2'	2.32	0.47
1:2A:2162:G:H4'	1:2A:2172:U:O2'	2.13	0.47
1:2A:2189:U:H2'	1:2A:2190:G:C8	2.49	0.47
2:2B:55:U:H1'	6:2G:29:TRP:HE1	1.80	0.47
11:2P:85:LEU:HA	11:2P:88:LEU:HD12	1.97	0.47
21:2Z:108:PRO:HG3	21:2Z:141:VAL:HB	1.96	0.47
32:2a:995:C:N3	32:2a:1046:A:O2'	2.44	0.47
32:2a:1226:C:H3'	44:2m:96:LEU:HD21	1.96	0.47
35:2d:61:LYS:HD2	35:2d:207:TYR:OH	2.14	0.47
53:2y:76:GLU:HA	53:2y:79:ASN:ND2	2.30	0.47
1:1A:249:C:O2'	11:1P:64:LYS:NZ	2.27	0.47
1:1A:2322:A:H2'	1:1A:2323:G:O4'	2.15	0.47
3:1D:242:ARG:HD2	3:1D:246:PRO:HG3	1.96	0.47
6:1G:43:LEU:C	6:1G:45:GLU:H	2.23	0.47
1:2A:2031:A:C6	1:2A:2498:C:H1'	2.49	0.47
5:2F:33:LEU:HD22	5:2F:112:MET:HE3	1.95	0.47
6:2G:145:THR:HG22	6:2G:148:MET:HG2	1.95	0.47
19:2X:94:GLY:HA3	19:2X:95:LEU:C	2.39	0.47
32:2a:401:C:OP2	35:2d:73:ARG:NH2	2.47	0.47
32:2a:409:G:H2'	32:2a:410:G:O4'	2.14	0.47
32:2a:947:G:H2'	32:2a:948:C:O4'	2.14	0.47
32:2a:1014:A:C2	32:2a:1219:U:H1'	2.48	0.47
1:1A:620:G:N3	1:1A:620:G:H2'	2.29	0.47
1:1A:690:G:H2'	1:1A:691:C:C6	2.50	0.47
1:1A:2000:G:OP1	13:1R:5:LYS:NZ	2.47	0.47
1:1A:2564:A:C2	1:1A:2647:U:H4'	2.49	0.47
4:1E:28:ALA:HB3	4:1E:93:VAL:HG12	1.96	0.47
28:16:35:GLU:OE2	28:16:50:ARG:NH1	2.44	0.47
35:1d:129:ASN:HD21	35:1d:144:ASP:HB3	1.79	0.47
1:2A:271(Q):G:H2'	1:2A:271(R):G:H8	1.79	0.47
1:2A:1055:G:H2'	1:2A:1056:G:O4'	2.15	0.47
1:2A:1069:A:C2	1:2A:1073:A:H5'	2.49	0.47
1:2A:1336:A:H2'	1:2A:1337:G:C8	2.49	0.47
1:2A:1410:G:H2'	1:2A:1411:C:C6	2.48	0.47
1:2A:1669:A:H5"	1:2A:2550:G:OP1	2.14	0.47
1:2A:1794:U:H2'	1:2A:1795:C:C6	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:2H:52:VAL:HG11	7:2H:69:ARG:HB2	1.96	0.47
32:2a:7:G:H5'	32:2a:298:A:O4'	2.13	0.47
37:2f:50:TYR:CE2	49:2r:77:GLY:HA2	2.49	0.47
43:2l:7:ILE:HG21	48:2q:34:LYS:HB2	1.96	0.47
1:1A:1686:C:H2'	1:1A:1687:G:O4'	2.14	0.47
12:1Q:31:ASP:OD1	12:1Q:134:ARG:NH1	2.47	0.47
13:1R:96:ARG:NH2	13:1R:118:GLU:OE2	2.48	0.47
32:1a:933:G:OP2	38:1g:3:ARG:HB2	2.15	0.47
32:1a:1047:G:H5"	45:1n:4:LYS:HD2	1.97	0.47
35:1d:196:LEU:O	35:1d:198:VAL:N	2.42	0.47
1:2A:2104:G:N7	1:2A:2186:G:C2	2.83	0.47
1:2A:2572:A:OP1	1:2A:2574:G:O2'	2.30	0.47
10:2O:120:GLU:HB2	15:2T:68:TYR:HE2	1.80	0.47
12:2Q:37:LEU:HD21	12:2Q:130:LYS:HE2	1.97	0.47
26:24:61:ARG:NH1	50:2s:9:VAL:HG21	2.29	0.47
32:2a:1165:C:H2'	32:2a:1166:G:O4'	2.14	0.47
1:1A:264:C:O2'	1:1A:265:A:H2'	2.15	0.47
1:1A:2074:U:H2'	1:1A:2075:U:C6	2.49	0.47
3:1D:77:ALA:HB2	3:1D:97:TYR:CD1	2.50	0.47
32:1a:524:G:H2'	32:1a:525:C:C6	2.49	0.47
32:1a:864:A:H2'	32:1a:865:A:C8	2.49	0.47
32:1a:977:A:H2'	32:1a:978:A:H5"	1.97	0.47
33:1b:9:GLU:OE2	33:1b:217:ARG:NH1	2.43	0.47
37:1f:99:ALA:O	49:1r:28:GLU:HA	2.15	0.47
41:1j:5:ARG:NE	41:1j:73:ASP:OD1	2.31	0.47
1:2A:601:C:O2'	1:2A:605:C:OP1	2.27	0.47
1:2A:2682:U:O2'	15:2T:58:ASN:ND2	2.47	0.47
3:2D:267:SER:C	3:2D:269:PHE:H	2.22	0.47
4:2E:73:GLU:H	4:2E:73:GLU:CD	2.19	0.47
6:2G:42:GLY:HA2	6:2G:89:GLY:HA2	1.95	0.47
6:2G:64:THR:HB	6:2G:94:LEU:HD21	1.96	0.47
7:2H:102:ALA:HA	7:2H:117:PRO:HD3	1.96	0.47
32:2a:222:U:H2'	32:2a:223:U:H6	1.76	0.47
32:2a:1292:U:H5'	40:2i:38:GLN:OE1	2.14	0.47
32:2a:1431:C:H2'	32:2a:1432:G:O4'	2.14	0.47
1:1A:127:A:H5"	1:1A:128:C:C6	2.50	0.47
1:1A:1475:G:H2'	1:1A:1476:C:C6	2.48	0.47
1:1A:1790:C:H5"	1:1A:1791:A:OP1	2.15	0.47
1:1A:1864:U:OP1	1:1A:2410:G:O2'	2.29	0.47
1:1A:2155:G:H3'	1:1A:2156:G:H8	1.80	0.47
4:1E:105:THR:OG1	4:1E:199:ARG:NH2	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:11:23:LYS:HB3	23:11:29:GLY:HA3	1.97	0.47
32:1a:382:A:H2'	32:1a:383:A:H8	1.79	0.47
32:1a:738:C:H2'	32:1a:739:C:H6	1.79	0.47
32:1a:1062:U:H2'	32:1a:1063:C:C6	2.49	0.47
33:1b:21:ARG:HA	33:1b:39:ILE:HA	1.97	0.47
39:1h:39:LEU:HD12	39:1h:39:LEU:HA	1.78	0.47
41:1j:61:GLU:OE2	45:1n:58:LYS:NZ	2.31	0.47
1:2A:373:U:H2'	1:2A:374:A:H8	1.80	0.47
1:2A:557:U:O2	9:2N:45:ASN:HB2	2.15	0.47
1:2A:1364:G:P	23:21:3:LYS:HG3	2.55	0.47
1:2A:1647:G:H3'	1:2A:1647:G:OP2	2.14	0.47
2:2B:33:G:C6	2:2B:34:U:C4	3.02	0.47
4:2E:8:LYS:HG2	4:2E:192:ASN:HA	1.97	0.47
5:2F:32:LEU:HB3	5:2F:112:MET:HE1	1.96	0.47
14:2S:14:VAL:O	14:2S:18:ILE:HG12	2.15	0.47
19:2X:12:VAL:HG21	19:2X:27:THR:HG22	1.96	0.47
24:22:35:LEU:HD11	24:22:49:LYS:HB3	1.96	0.47
32:2a:437:U:O2'	35:2d:123:HIS:HD2	1.98	0.47
32:2a:984:C:H2'	32:2a:985:C:C6	2.49	0.47
32:2a:1001(A):G:H2'	32:2a:1002:G:O4'	2.15	0.47
32:2a:1252:A:H61	32:2a:1285:A:H61	1.61	0.47
32:2a:1412:C:H2'	32:2a:1413:A:C8	2.49	0.47
38:2g:26:PHE:O	38:2g:30:ILE:HG13	2.15	0.47
41:2j:51:ARG:O	45:2n:45:ARG:NH1	2.48	0.47
46:2o:55:GLY:HA2	46:2o:58:MET:HE3	1.97	0.47
2:1B:66:A:N6	2:1B:108:U:H2'	2.29	0.47
12:1Q:21:THR:HG21	12:1Q:101:ARG:N	2.29	0.47
32:1a:60:A:N1	32:1a:107:G:O2'	2.42	0.47
32:1a:472:A:H5"	47:1p:80:PHE:HB3	1.97	0.47
32:1a:858:G:O6	32:1a:869:G:H3'	2.14	0.47
1:2A:286:C:H2'	1:2A:287:C:C6	2.50	0.47
1:2A:811:U:H2'	11:2P:21:ARG:HA	1.97	0.47
1:2A:1342:A:OP2	61:2A:3811:HOH:O	2.20	0.47
1:2A:1889:A:O2'	1:2A:2087:G:H5'	2.14	0.47
1:2A:1952:A:OP1	10:2O:42:SER:OG	2.30	0.47
1:2A:2391:G:O6	1:2A:2425:A:H8	1.98	0.47
1:2A:2849:U:H4'	1:2A:2868:A:C2	2.49	0.47
56:2A:3732:ERY:H321	56:2A:3732:ERY:H8	1.69	0.47
14:2S:36:TYR:HA	14:2S:52:SER:HA	1.97	0.47
21:2Z:95:PRO:HA	21:2Z:129:SER:HA	1.96	0.47
32:2a:501:C:H1'	32:2a:549:C:H1'	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1123:A:C2	41:2j:39:PRO:HD2	2.49	0.47
32:2a:1362:C:H2'	32:2a:1363:C:H5"	1.97	0.47
34:2c:150:LYS:HB3	34:2c:201:TYR:HB2	1.96	0.47
35:2d:20:TYR:HD1	35:2d:26:CYS:HB3	1.79	0.47
40:2i:72:GLY:O	40:2i:76:ALA:N	2.45	0.47
1:1A:191:A:H2'	1:1A:192:C:C6	2.50	0.47
1:1A:2687:U:H2'	1:1A:2688:U:O4'	2.13	0.47
8:1I:31:LEU:HD21	8:1I:38:LEU:HG	1.97	0.47
32:1a:431:A:H2'	32:1a:432:A:O4'	2.14	0.47
44:1m:57:ARG:O	44:1m:61:GLU:HG3	2.15	0.47
47:1p:2:VAL:HG13	47:1p:64:ALA:HA	1.97	0.47
1:2A:323:G:C8	5:2F:171:PRO:HG3	2.50	0.47
1:2A:1711:C:H2'	1:2A:1712:C:C6	2.49	0.47
1:2A:2155:G:C2	1:2A:2156:G:H1'	2.50	0.47
5:2F:172:TRP:H	5:2F:172:TRP:CD1	2.32	0.47
12:2Q:137:TYR:O	12:2Q:141:GLN:NE2	2.43	0.47
32:2a:537:G:H5"	43:2l:113:ARG:NH1	2.29	0.47
32:2a:542:G:OP1	35:2d:10:ARG:NH1	2.37	0.47
32:2a:911:U:H2'	32:2a:912:C:C6	2.50	0.47
34:2c:83:ARG:O	34:2c:87:LEU:N	2.43	0.47
40:2i:18:PHE:CD2	40:2i:62:TYR:HD2	2.33	0.47
44:2m:92:HIS:CE1	44:2m:98:VAL:HG11	2.49	0.47
1:1A:1055:G:O6	1:1A:1104:C:N3	2.48	0.47
1:1A:1176:G:H4'	1:1A:1177:A:OP1	2.14	0.47
6:1G:62:LEU:HD12	6:1G:148:MET:HE1	1.96	0.47
32:1a:337:C:H2'	32:1a:338:A:C8	2.50	0.47
40:1i:100:GLY:O	40:1i:103:THR:HG22	2.14	0.47
1:2A:271(K):U:O2	8:2I:50:ARG:HD2	2.15	0.47
1:2A:839:U:H2'	1:2A:840:C:C6	2.50	0.47
1:2A:919:G:N2	1:2A:2269:A:OP2	2.48	0.47
1:2A:1064:C:H3'	1:2A:1065:U:H5'	1.95	0.47
1:2A:1391:U:O2	1:2A:1393:A:H8	1.97	0.47
3:2D:17:THR:O	3:2D:211:ARG:NH2	2.48	0.47
32:2a:1348:U:H4'	40:2i:120:ARG:HD2	1.97	0.47
32:2a:1519:MA6:H92	32:2a:1520:G:O2'	2.15	0.47
34:2c:131:ARG:O	34:2c:135:LYS:HG2	2.15	0.47
34:2c:149:ALA:HA	34:2c:201:TYR:O	2.15	0.47
38:2g:113:GLU:H	38:2g:113:GLU:HG2	1.43	0.47
47:2p:53:VAL:HG13	47:2p:79:VAL:HA	1.95	0.47
52:2u:2:GLY:C	52:2u:4:GLY:H	2.23	0.47
1:1A:222:A:H3'	1:1A:421:U:H5'	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:458:G:O2'	1:1A:469:G:O6	2.32	0.46
1:1A:1096:A:H3'	1:1A:1097:U:H5"	1.97	0.46
1:1A:1171:G:H5'	61:1A:4742:HOH:O	2.14	0.46
1:1A:1753:G:N1	1:1A:1756:G:OP2	2.47	0.46
9:1N:61:ARG:HA	9:1N:61:ARG:HD3	1.64	0.46
32:1a:353:A:H5'	32:1a:353:A:H8	1.80	0.46
32:1a:998:G:H2'	32:1a:999:C:C6	2.50	0.46
32:1a:1376:U:H2'	32:1a:1377:A:C8	2.50	0.46
35:1d:107:ARG:HG3	35:1d:173:TRP:HH2	1.79	0.46
38:1g:111:ARG:NH1	38:1g:113:GLU:OE2	2.37	0.46
48:1q:85:VAL:O	48:1q:89:LEU:HG	2.14	0.46
50:1s:32:LYS:HA	50:1s:50:ALA:HB3	1.97	0.46
1:2A:1125:G:H5'	31:29:37:GLY:HA2	1.97	0.46
1:2A:2506:U:O2	55:2A:3731:HGR:H23	2.16	0.46
6:2G:36:LYS:HE3	6:2G:95:ARG:NH1	2.30	0.46
7:2H:3:ARG:HE	7:2H:54:ARG:HH12	1.63	0.46
7:2H:117:PRO:HG3	7:2H:123:PHE:CE2	2.50	0.46
10:2O:88:ASN:HD21	10:2O:92:GLU:HB2	1.79	0.46
30:28:8:LYS:HB3	30:28:12:LYS:HE3	1.96	0.46
32:2a:130:A:O2'	32:2a:131:C:O5'	2.29	0.46
32:2a:560:U:H5'	32:2a:566:G:N2	2.30	0.46
32:2a:592:G:H2'	32:2a:593:G:H8	1.80	0.46
32:2a:659:U:H2'	32:2a:660:G:O4'	2.15	0.46
32:2a:1400:5MC:C2	53:2y:63:ALA:HA	2.50	0.46
32:2a:1465:C:H2'	32:2a:1466:C:O4'	2.16	0.46
41:2j:78:ASN:O	41:2j:80:LYS:N	2.48	0.46
44:2m:92:HIS:HA	44:2m:110:ARG:HH21	1.79	0.46
53:2y:74:ILE:O	53:2y:78:ILE:HG12	2.15	0.46
1:1A:530:G:N1	1:1A:2023:G:OP1	2.37	0.46
1:1A:1177:A:H2'	1:1A:1177:A:N3	2.29	0.46
8:1I:116:LEU:HD11	8:1I:120:ILE:HG13	1.98	0.46
12:1Q:7:MET:HE2	12:1Q:7:MET:HB2	1.72	0.46
32:1a:309:G:O2'	32:1a:607:A:N1	2.46	0.46
32:1a:335:C:H2'	32:1a:336:C:C6	2.50	0.46
32:1a:1033:G:H2'	32:1a:1034:G:C8	2.45	0.46
33:1b:124:SER:HA	33:1b:125:PRO:HA	1.56	0.46
40:1i:77:ILE:O	40:1i:81:ILE:HG23	2.15	0.46
1:2A:328:U:H4'	20:2Y:68:HIS:CD2	2.50	0.46
1:2A:2410:G:N7	61:2A:3969:HOH:O	2.35	0.46
1:2A:2833:G:H4'	1:2A:2834:G:OP2	2.15	0.46
2:2B:84:C:OP1	25:23:15:TYR:OH	2.26	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2F:195:ASP:OD1	5:2F:196:LEU:N	2.47	0.46
15:2T:119:LYS:HB2	32:2a:1442(A):G:N2	2.30	0.46
19:2X:40:LYS:HG3	19:2X:51:VAL:HB	1.97	0.46
32:2a:1092:A:C5	32:2a:1183:A:N7	2.83	0.46
33:2b:178:ARG:HB3	39:2h:72:PRO:HA	1.97	0.46
34:2c:22:TRP:HA	41:2j:93:GLY:HA2	1.97	0.46
34:2c:70:VAL:HG12	34:2c:72:LYS:N	2.30	0.46
35:2d:70:ILE:HD11	35:2d:74:GLN:HB3	1.97	0.46
36:2e:43:LEU:O	36:2e:65:ASN:ND2	2.42	0.46
40:2i:50:LEU:HB3	40:2i:56:LEU:HA	1.97	0.46
44:2m:47:ASP:OD2	44:2m:47:ASP:N	2.46	0.46
1:1A:2299:G:N7	61:1A:4296:HOH:O	2.36	0.46
32:1a:73:G:N2	32:1a:96:U:O2	2.40	0.46
32:1a:375:U:OP1	47:1p:69:THR:HG21	2.16	0.46
32:1a:1148:U:O3'	40:1i:14:VAL:HG11	2.16	0.46
32:1a:1492:A:P	43:1l:47:LYS:HE3	2.56	0.46
1:2A:300:A:P	20:2Y:86:ARG:HH21	2.38	0.46
1:2A:910:A:C5	12:2Q:13:GLN:HG3	2.49	0.46
1:2A:1166:C:H2'	1:2A:1167:U:C6	2.50	0.46
1:2A:1428:C:O2'	1:2A:1569:A:OP2	2.21	0.46
5:2F:32:LEU:HD22	5:2F:112:MET:HE2	1.96	0.46
10:2O:2:ILE:HD12	10:2O:6:THR:HG21	1.97	0.46
15:2T:127:ALA:C	15:2T:129:ARG:N	2.73	0.46
21:2Z:179:ASP:HB3	21:2Z:182:LYS:HE3	1.98	0.46
32:2a:926:G:C6	53:2y:87:LYS:HG3	2.50	0.46
32:2a:1226:C:OP2	44:2m:91:ARG:NH1	2.38	0.46
37:2f:30:LEU:HD23	37:2f:75:LEU:HD11	1.97	0.46
41:2j:8:LEU:HB3	41:2j:16:LEU:HD22	1.97	0.46
51:2t:43:LEU:O	51:2t:47:GLY:N	2.48	0.46
1:1A:582:G:H2'	1:1A:583:G:C8	2.51	0.46
3:1D:102:LYS:C	3:1D:103:ARG:HG2	2.40	0.46
7:1H:98:LEU:HD13	7:1H:125:VAL:HG23	1.96	0.46
9:1N:13:TRP:CE2	9:1N:133:GLN:HG2	2.51	0.46
16:1U:33:ARG:NH2	61:1U:302:HOH:O	2.26	0.46
18:1W:46:PHE:O	18:1W:50:VAL:HG23	2.16	0.46
28:16:6:ARG:NH1	28:16:26:ASN:HB2	2.30	0.46
30:18:23:VAL:CG1	30:18:47:LYS:HD3	2.46	0.46
32:1a:266:G:H2'	32:1a:266:G:N3	2.29	0.46
39:1h:51:VAL:HG12	39:1h:52:ASP:H	1.79	0.46
41:1j:48:THR:OG1	41:1j:62:HIS:ND1	2.48	0.46
1:2A:99:U:O4	20:2Y:8:LYS:NZ	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:271(Q):G:H2'	1:2A:271(R):G:C8	2.51	0.46
1:2A:321:G:OP1	5:2F:135:LYS:NZ	2.48	0.46
1:2A:873:G:N2	1:2A:905:U:C2	2.83	0.46
1:2A:1115:G:H2'	1:2A:1116:C:C6	2.51	0.46
21:2Z:96:VAL:N	21:2Z:128:VAL:O	2.35	0.46
32:2a:176:C:H2'	32:2a:177:C:C6	2.51	0.46
32:2a:857:C:H2'	32:2a:858:G:O4'	2.15	0.46
32:2a:964:A:N3	32:2a:969:A:O2'	2.44	0.46
32:2a:1333:A:H2'	32:2a:1334:G:O4'	2.15	0.46
32:2a:1360:A:H2'	32:2a:1361:G:O4'	2.15	0.46
32:2a:1503:A:OP1	32:2a:1531:A:O2'	2.33	0.46
34:2c:123:GLN:O	34:2c:128:PHE:HB2	2.14	0.46
34:2c:188:LEU:HD12	34:2c:188:LEU:HA	1.73	0.46
36:2e:57:LYS:HG2	36:2e:61:TYR:HE2	1.80	0.46
36:2e:78:HIS:CE1	36:2e:142:LEU:HD23	2.51	0.46
41:2j:56:HIS:N	41:2j:56:HIS:CD2	2.82	0.46
1:1A:1054:A:N1	1:1A:1105:U:O2	2.48	0.46
2:1B:15:A:OP1	2:1B:108:U:O2'	2.30	0.46
6:1G:110:ALA:HB1	6:1G:140:ILE:HG22	1.98	0.46
15:1T:112:ARG:HG3	15:1T:115:ARG:HH21	1.81	0.46
32:1a:425:G:O3'	35:1d:45:GLN:NE2	2.48	0.46
35:1d:116:GLN:CD	35:1d:157:LEU:HD21	2.41	0.46
42:1k:87:THR:O	42:1k:87:THR:OG1	2.31	0.46
1:2A:81:G:HO2'	1:2A:295:G:HO2'	1.63	0.46
1:2A:1031:G:H21	31:29:36:GLN:HE22	1.62	0.46
1:2A:1063:G:H1	1:2A:1075:C:H42	1.63	0.46
1:2A:1227:G:OP1	16:2U:13:LYS:HG2	2.16	0.46
1:2A:2074:U:H2'	1:2A:2075:U:C6	2.50	0.46
1:2A:2136:C:H2'	1:2A:2137:C:C6	2.51	0.46
1:2A:2704:C:H2'	1:2A:2705:A:O4'	2.16	0.46
1:2A:2887:U:H2'	1:2A:2888:C:H6	1.81	0.46
23:21:4:VAL:HG11	23:21:11:ARG:HH21	1.80	0.46
24:22:51:ARG:O	24:22:55:ARG:HG3	2.16	0.46
31:29:25:VAL:HB	31:29:34:GLN:HB2	1.97	0.46
32:2a:142:G:H2'	32:2a:143:A:C8	2.46	0.46
32:2a:154:C:H2'	32:2a:155:C:H6	1.81	0.46
32:2a:600:C:H2'	32:2a:601:C:C6	2.51	0.46
32:2a:940:C:H2'	32:2a:941:G:H8	1.79	0.46
53:2y:6:THR:HG22	53:2y:40:ILE:HG23	1.97	0.46
1:1A:1289:C:H2'	1:1A:1290:C:C6	2.51	0.46
26:14:59:PHE:CE2	50:1s:67:VAL:HG21	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:382:A:H2'	32:1a:383:A:C8	2.51	0.46
32:1a:1380:U:C4	38:1g:3:ARG:HG2	2.51	0.46
37:1f:91:VAL:HG12	37:1f:92:LYS:O	2.15	0.46
39:1h:95:VAL:HG23	39:1h:96:GLY:O	2.15	0.46
43:1l:52:LEU:O	43:1l:54:LYS:NZ	2.42	0.46
1:2A:65:C:H2'	1:2A:66:C:C6	2.51	0.46
1:2A:1025:G:H3'	1:2A:1026:U:H5'	1.97	0.46
1:2A:1464:C:H2'	1:2A:1465:G:C8	2.51	0.46
1:2A:1590:U:H2'	1:2A:1591:G:C8	2.51	0.46
1:2A:1993:U:OP2	61:2A:3857:HOH:O	2.19	0.46
1:2A:2116:G:OP1	1:2A:2117:A:N6	2.49	0.46
1:2A:2370:G:C6	1:2A:2371:G:C6	3.04	0.46
1:2A:2395:C:O2'	23:21:30:VAL:HG13	2.16	0.46
26:24:13:ARG:NH1	26:24:23:GLU:HB3	2.31	0.46
26:24:15:ILE:HG23	26:24:21:VAL:HG12	1.97	0.46
32:2a:1039:C:H2'	32:2a:1040:U:O4'	2.15	0.46
32:2a:1111:A:N1	34:2c:177:THR:OG1	2.38	0.46
32:2a:1172:C:H2'	32:2a:1173:G:H8	1.81	0.46
32:2a:1357:A:O2'	45:2n:34:TYR:HE1	1.99	0.46
44:2m:20:THR:HA	44:2m:25:ILE:O	2.15	0.46
1:1A:784:A:C6	3:1D:229:VAL:HG11	2.50	0.46
1:1A:969:U:H2'	1:1A:970:C:C6	2.51	0.46
1:1A:2114:A:H3'	1:1A:2115:G:C8	2.50	0.46
1:1A:2140:C:H2'	1:1A:2141:G:H8	1.81	0.46
1:1A:2303:G:O2'	6:1G:132:ASN:ND2	2.41	0.46
32:1a:73:G:H2'	32:1a:76:C:C6	2.50	0.46
32:1a:639:G:H2'	32:1a:640:A:H8	1.81	0.46
32:1a:1151:A:O2'	32:1a:1152:A:H8	1.99	0.46
32:1a:1318:A:H5"	50:1s:3:ARG:NH1	2.30	0.46
39:1h:51:VAL:HG21	39:1h:60:ARG:HD2	1.98	0.46
1:2A:234:C:H2'	1:2A:235:U:C6	2.51	0.46
1:2A:889:C:O2'	1:2A:890:A:H8	1.99	0.46
1:2A:2162:G:H1'	1:2A:2173:A:H1'	1.97	0.46
12:2Q:42:ILE:HG13	12:2Q:97:VAL:HG21	1.98	0.46
14:2S:33:LYS:HB2	14:2S:34:HIS:CD2	2.51	0.46
17:2V:62:LEU:HD11	17:2V:95:LEU:HB2	1.98	0.46
22:20:39:ARG:HD3	22:20:58:THR:HG23	1.97	0.46
32:2a:1107:C:C4	32:2a:1108:G:C8	3.04	0.46
32:2a:1504:G:OP1	32:2a:1507:A:H4'	2.16	0.46
33:2b:63:MET:HE2	33:2b:63:MET:HB3	1.82	0.46
39:2h:19:VAL:HG23	39:2h:21:LYS:HD3	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:2k:34:ASP:HB3	42:2k:40:ILE:HD11	1.97	0.46
48:2q:67:LYS:C	48:2q:69:LYS:H	2.23	0.46
1:1A:2820:A:P	13:1R:2:ARG:HH22	2.39	0.46
2:1B:88:C:H2'	2:1B:89:G:O4'	2.16	0.46
3:1D:69:ARG:HD2	3:1D:105:ILE:HG21	1.98	0.46
5:1F:155:LEU:HD11	5:1F:176:LEU:HD12	1.97	0.46
6:1G:114:ILE:HG12	6:1G:140:ILE:HD13	1.97	0.46
33:1b:7:VAL:HG12	33:1b:217:ARG:HD2	1.96	0.46
34:1c:15:THR:HG21	34:1c:181:ASN:HA	1.98	0.46
34:1c:108:ASN:HD22	34:1c:111:LEU:HG	1.81	0.46
1:2A:284:U:H2'	1:2A:285:C:C6	2.50	0.46
1:2A:2163:C:H5"	1:2A:2164:C:OP2	2.16	0.46
1:2A:2328:A:H2'	1:2A:2329:G:C8	2.50	0.46
1:2A:2820:A:OP1	13:2R:2:ARG:NH2	2.48	0.46
9:2N:4:TYR:HB2	16:2U:101:ARG:NH1	2.30	0.46
10:2O:112:MET:HE2	10:2O:112:MET:H	1.81	0.46
10:2O:113:LYS:HB2	10:2O:113:LYS:HE3	1.72	0.46
12:2Q:30:GLY:HA2	12:2Q:107:ALA:HB2	1.98	0.46
26:24:64:GLY:C	26:24:66:SER:N	2.72	0.46
32:2a:786:G:C2	32:2a:797:C:C2	3.04	0.46
32:2a:1036:G:H3'	32:2a:1037:C:H6	1.81	0.46
40:2i:26:VAL:HA	40:2i:61:ALA:O	2.16	0.46
51:2t:57:ARG:HH12	51:2t:100:ILE:HB	1.79	0.46
1:1A:1071:G:O2'	1:1A:1089:G:H2'	2.16	0.46
1:1A:1919:A:N1	32:1a:1495:U:O2'	2.39	0.46
1:1A:1993:U:H4'	4:1E:128:SER:OG	2.16	0.46
1:1A:2145:C:H5"	1:1A:2146:C:C5	2.51	0.46
6:1G:5:VAL:HG22	6:1G:8:LYS:H	1.81	0.46
9:1N:108:PRO:O	9:1N:113:GLY:HA3	2.16	0.46
11:1P:8:PRO:HB2	11:1P:12:ALA:HB3	1.98	0.46
32:1a:624:C:O3'	47:1p:10:GLY:HA2	2.16	0.46
1:2A:1058:G:H2'	1:2A:1059:G:C8	2.51	0.46
1:2A:2092:U:OP1	61:2A:3863:HOH:O	2.21	0.46
1:2A:2291:U:H2'	1:2A:2292:C:C6	2.51	0.46
1:2A:2352:A:N6	1:2A:2365:G:O2'	2.49	0.46
1:2A:2417:C:OP1	11:2P:65:ARG:NH2	2.49	0.46
1:2A:2641:G:H5"	9:2N:76:SER:HB3	1.98	0.46
2:2B:3:C:H2'	2:2B:4:C:C6	2.50	0.46
8:2I:69:LYS:HB2	8:2I:138:ILE:HG12	1.97	0.46
12:2Q:7:MET:HB2	12:2Q:7:MET:HE3	1.76	0.46
14:2S:27:SER:HA	14:2S:88:ASP:HB3	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:23:10:LYS:HB3	25:23:53:LEU:HA	1.97	0.46
32:2a:735:C:H2'	32:2a:736:C:H6	1.80	0.46
32:2a:1515:C:H2'	32:2a:1516:G:H8	1.80	0.46
33:2b:47:THR:HB	33:2b:202:PRO:HG2	1.96	0.46
34:2c:5:ILE:HG12	34:2c:6:HIS:H	1.81	0.46
35:2d:38:TYR:CE1	35:2d:45:GLN:HG3	2.51	0.46
37:2f:11:ASN:HB3	37:2f:14:LEU:HG	1.98	0.46
1:1A:9:U:H3	1:1A:2629:A:H2	1.56	0.46
1:1A:143:G:H1'	19:1X:37:THR:HG21	1.98	0.46
1:1A:1179:C:H2'	1:1A:1180:C:H6	1.80	0.46
1:1A:1919:A:O2'	32:1a:1517:G:N3	2.47	0.46
1:1A:2753:A:N3	31:19:15:LYS:NZ	2.64	0.46
19:1X:31:HIS:HD2	19:1X:33:LYS:N	2.07	0.46
32:1a:35:G:O2'	43:1l:118:SER:O	2.24	0.46
32:1a:620:C:H2'	32:1a:621:A:O4'	2.16	0.46
32:1a:1347:G:N2	32:1a:1373:G:H2'	2.30	0.46
35:1d:164:ALA:O	35:1d:168:ARG:NH1	2.45	0.46
1:2A:1069:A:C5	1:2A:1095:A:H4'	2.51	0.46
1:2A:2295:C:H5	14:2S:13:ARG:HH22	1.64	0.46
1:2A:2814:C:HO2'	27:25:29:THR:HG1	1.63	0.46
2:2B:17:C:H2'	2:2B:18:G:O4'	2.16	0.46
21:2Z:117:LEU:HD21	21:2Z:141:VAL:HG11	1.98	0.46
26:24:58:ARG:NH2	50:2s:68:GLY:H	2.14	0.46
32:2a:294:U:OP1	32:2a:610:G:O2'	2.27	0.46
32:2a:625:G:H2'	32:2a:626:U:H6	1.80	0.46
32:2a:662:G:H2'	32:2a:663:A:H8	1.78	0.46
32:2a:1347:G:N1	32:2a:1374:A:OP2	2.31	0.46
33:2b:19:HIS:O	33:2b:20:GLU:HB2	2.15	0.46
33:2b:33:TYR:N	33:2b:41:ILE:O	2.38	0.46
33:2b:75:LYS:HA	33:2b:78:GLN:HB2	1.97	0.46
34:2c:82:GLU:HA	34:2c:85:ARG:HH12	1.81	0.46
1:1A:11:G:H2'	1:1A:12:U:H5"	1.97	0.45
1:1A:305:U:H2'	1:1A:306:U:C6	2.52	0.45
1:1A:1022:G:N7	9:1N:66:LYS:HE2	2.31	0.45
1:1A:1097:U:H2'	1:1A:1098:A:O4'	2.17	0.45
1:1A:1810:A:H2'	1:1A:1811:G:O4'	2.16	0.45
1:1A:2139:C:N4	1:1A:2152:G:H1	2.11	0.45
1:1A:2805:G:H2'	1:1A:2807:G:C8	2.50	0.45
6:1G:122:PRO:HD3	6:1G:181:ARG:HG2	1.98	0.45
21:1Z:19:ARG:NH1	21:1Z:84:GLU:O	2.49	0.45
32:1a:418:C:H1'	32:1a:540:G:O2'	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:632:A:H5'	32:1a:633:G:OP2	2.16	0.45
32:1a:1469:G:N7	61:1a:1940:HOH:O	2.36	0.45
34:1c:11:ARG:NH2	34:1c:177:THR:O	2.49	0.45
38:1g:149:ARG:HD2	42:1k:59:TYR:CZ	2.52	0.45
47:1p:7:ALA:HB1	47:1p:29:ASP:HA	1.98	0.45
1:2A:2047:U:O2'	1:2A:2823:A:N1	2.46	0.45
1:2A:2540:C:H2'	1:2A:2541:A:O4'	2.16	0.45
2:2B:32:C:C4	2:2B:33:G:C8	3.04	0.45
32:2a:839:U:H5"	32:2a:840:C:H5	1.81	0.45
32:2a:1349:A:H5"	40:2i:121:ARG:HB2	1.97	0.45
33:2b:24:TRP:CD1	33:2b:24:TRP:H	2.34	0.45
33:2b:111:ARG:HA	33:2b:111:ARG:HD3	1.72	0.45
33:2b:114:ARG:O	33:2b:118:LEU:N	2.47	0.45
1:1A:228:A:H8	1:1A:229:A:H5'	1.82	0.45
1:1A:271(E):U:O4	61:1A:4138:HOH:O	2.19	0.45
1:1A:839:U:H1'	1:1A:1191:G:H1'	1.98	0.45
1:1A:1385:G:O2'	1:1A:1396:U:O2	2.27	0.45
4:1E:2:LYS:HB2	4:1E:95:ILE:HD12	1.98	0.45
4:1E:28:ALA:HB3	4:1E:93:VAL:CG1	2.46	0.45
4:1E:59:VAL:HG12	4:1E:64:LYS:HG3	1.97	0.45
14:1S:14:VAL:O	14:1S:18:ILE:HG12	2.17	0.45
17:1V:21:ARG:HD3	17:1V:91:TYR:CE1	2.52	0.45
20:1Y:9:LYS:HA	20:1Y:10:GLY:HA2	1.63	0.45
21:1Z:3:TYR:CE2	21:1Z:51:ALA:HB2	2.50	0.45
22:10:43:THR:O	22:10:43:THR:HG23	2.16	0.45
32:1a:352:C:O2'	32:1a:354:G:OP1	2.30	0.45
32:1a:646:U:H2'	32:1a:647:C:C6	2.51	0.45
33:1b:77:ALA:HB2	33:1b:211:ILE:HG21	1.97	0.45
35:1d:61:LYS:HD3	35:1d:206:PHE:CD2	2.51	0.45
44:1m:81:LEU:O	44:1m:89:GLY:HA3	2.15	0.45
1:2A:898:C:H2'	1:2A:899:A:O4'	2.16	0.45
1:2A:1030:G:OP2	12:2Q:128:LYS:NZ	2.44	0.45
1:2A:2336:A:H61	22:20:43:THR:CG2	2.29	0.45
1:2A:2364:C:H2'	1:2A:2365:G:O4'	2.16	0.45
1:2A:2648:C:H2'	1:2A:2649:U:H6	1.81	0.45
11:2P:59:LEU:HD11	30:28:10:ALA:HA	1.97	0.45
18:2W:2:GLU:OE2	18:2W:72:LYS:NZ	2.35	0.45
21:2Z:59:LEU:HD12	21:2Z:69:THR:HG21	1.97	0.45
26:24:58:ARG:HA	26:24:58:ARG:HD2	1.85	0.45
32:2a:540:G:C6	32:2a:541:G:C5	3.04	0.45
46:2o:3:ILE:HG21	46:2o:34:LEU:HD21	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:2t:41:ILE:H	51:2t:41:ILE:HG12	1.28	0.45
1:1A:888:C:H6	1:1A:888:C:H2'	1.49	0.45
1:1A:1359:A:H61	1:1A:1372:U:H3	1.64	0.45
1:1A:2286:A:H4'	1:1A:2287:A:O4'	2.16	0.45
1:1A:2839:G:H5'	13:1R:46:GLY:CA	2.46	0.45
6:1G:5:VAL:HG13	6:1G:8:LYS:HE2	1.98	0.45
9:1N:67:LEU:HD23	9:1N:87:LEU:HD13	1.98	0.45
9:1N:75:TYR:CE2	9:1N:77:GLY:HA2	2.52	0.45
10:1O:64:ARG:HB2	10:1O:83:ALA:HB3	1.99	0.45
32:1a:108:G:N1	51:1t:15:ARG:HG2	2.31	0.45
32:1a:346:G:N3	57:1a:1880:MPD:O4	2.50	0.45
33:1b:27:LYS:O	33:1b:30:ARG:NH1	2.50	0.45
36:1e:90:VAL:O	36:1e:120:THR:HA	2.16	0.45
1:2A:974:G:N2	61:2A:3826:HOH:O	2.22	0.45
1:2A:999:U:OP2	61:2A:3825:HOH:O	2.21	0.45
1:2A:1031:G:N2	31:29:36:GLN:HE22	2.15	0.45
1:2A:2490:G:O6	61:2A:3864:HOH:O	2.21	0.45
1:2A:2647:U:H2'	1:2A:2648:C:C6	2.51	0.45
1:2A:2823:A:OP1	4:2E:159:HIS:NE2	2.45	0.45
4:2E:181:LEU:HD12	4:2E:181:LEU:HA	1.66	0.45
7:2H:137:ASP:OD1	7:2H:138:LYS:N	2.49	0.45
28:26:11:LEU:HB2	28:26:21:TYR:HB2	1.97	0.45
28:26:33:LYS:HA	28:26:33:LYS:HD3	1.82	0.45
31:29:32:HIS:O	31:29:34:GLN:HG3	2.16	0.45
32:2a:352:C:H4'	32:2a:354:G:OP1	2.16	0.45
32:2a:767:A:H2'	32:2a:768:A:O4'	2.17	0.45
32:2a:834:C:H2'	32:2a:835:U:H6	1.81	0.45
32:2a:881:G:P	43:2l:12:ARG:HH22	2.39	0.45
32:2a:939:G:H2'	32:2a:940:C:C6	2.51	0.45
32:2a:1348:U:H2'	32:2a:1349:A:H8	1.81	0.45
36:2e:8:GLU:HG2	36:2e:34:VAL:HG23	1.99	0.45
44:2m:53:VAL:O	44:2m:57:ARG:N	2.42	0.45
46:2o:10:LYS:HE3	46:2o:10:LYS:HB2	1.77	0.45
47:2p:74:LEU:HD23	47:2p:79:VAL:HG11	1.98	0.45
1:1A:570:G:H2'	1:1A:2030:A:N7	2.32	0.45
1:1A:2023:G:H4'	1:1A:2617:C:O3'	2.16	0.45
4:1E:181:LEU:HD12	4:1E:181:LEU:HA	1.69	0.45
19:1X:26:TYR:HB3	19:1X:92:LEU:HD22	1.98	0.45
21:1Z:52:SER:C	21:1Z:54:HIS:H	2.24	0.45
29:17:34:ARG:NH1	29:17:41:ARG:O	2.49	0.45
32:1a:403:C:OP1	35:1d:137:SER:OG	2.35	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1148:U:H2'	32:1a:1149:C:O4'	2.15	0.45
32:1a:1249:C:O4'	40:1i:70:LYS:HE3	2.17	0.45
32:1a:1304:G:C6	32:1a:1305:G:N1	2.84	0.45
32:1a:1368:G:OP2	40:1i:112:LYS:HG3	2.15	0.45
46:1o:16:ALA:HB1	46:1o:21:ASP:HB3	1.98	0.45
48:1q:62:SER:HB3	48:1q:72:ARG:HH11	1.82	0.45
48:1q:82:MET:HA	48:1q:85:VAL:HG22	1.99	0.45
1:2A:234:C:H2'	1:2A:235:U:H6	1.82	0.45
1:2A:635:C:O2'	1:2A:639:U:OP1	2.26	0.45
1:2A:1087:G:H2'	1:2A:1088:A:H5'	1.97	0.45
6:2G:16:ARG:CZ	6:2G:31:VAL:HG21	2.47	0.45
7:2H:45:VAL:HA	7:2H:50:VAL:HG22	1.97	0.45
16:2U:97:ASP:O	16:2U:101:ARG:HG3	2.17	0.45
16:2U:104:GLN:CD	16:2U:104:GLN:H	2.24	0.45
18:2W:80:PRO:O	18:2W:100:THR:HB	2.16	0.45
26:24:53:GLU:OE1	26:24:54:GLY:N	2.49	0.45
32:2a:143:A:H4'	32:2a:144:G:C8	2.52	0.45
32:2a:560:U:H6	32:2a:560:U:H2'	1.47	0.45
32:2a:1073:U:H2'	32:2a:1074:G:C8	2.52	0.45
32:2a:1157:A:H4'	32:2a:1158:C:O5'	2.16	0.45
32:2a:1198:G:H2'	32:2a:1199:U:C6	2.52	0.45
32:2a:1237:C:O3'	32:2a:1300:G:N2	2.44	0.45
32:2a:1318:A:O2'	50:2s:37:ARG:HB2	2.17	0.45
34:2c:43:LEU:HD22	34:2c:47:LEU:HD12	1.98	0.45
1:1A:1084:A:C2	1:1A:1105:U:H1'	2.51	0.45
1:1A:1429:G:H2'	1:1A:1430:C:C6	2.52	0.45
1:1A:2022:U:O2'	1:1A:2617:C:H5'	2.17	0.45
12:1Q:38:GLU:HA	12:1Q:99:PRO:HG3	1.97	0.45
33:1b:18:GLY:HA3	33:1b:42:ILE:HG13	1.97	0.45
41:1j:39:PRO:HA	41:1j:70:ARG:HD3	1.98	0.45
1:2A:1022:G:N7	9:2N:66:LYS:HE2	2.31	0.45
1:2A:2028:U:H2'	1:2A:2029:G:O4'	2.17	0.45
1:2A:2037:G:H2'	1:2A:2038:G:C8	2.52	0.45
1:2A:2119:A:O2'	1:2A:2120:G:H5'	2.17	0.45
2:2B:50:G:OP1	14:2S:63:THR:N	2.47	0.45
4:2E:29:GLY:HA3	61:2E:408:HOH:O	2.16	0.45
32:2a:434:U:H2'	32:2a:435:C:C6	2.51	0.45
32:2a:826:C:H2'	32:2a:827:U:C6	2.52	0.45
38:2g:59:LEU:HD11	38:2g:63:LYS:HE2	1.98	0.45
50:2s:17:GLU:O	50:2s:21:GLU:N	2.36	0.45
1:1A:1359:A:N1	1:1A:1372:U:C4	2.84	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1784:A:H4'	1:1A:1785:A:O5'	2.17	0.45
1:1A:2748:A:H5'	7:1H:4:ILE:HD13	1.97	0.45
4:1E:143:ASN:HD22	4:1E:147:PRO:CD	2.28	0.45
11:1P:98:GLU:HG3	11:1P:102:ARG:CZ	2.47	0.45
14:1S:58:LEU:HA	14:1S:58:LEU:HD23	1.69	0.45
20:1Y:23:ARG:HD3	61:1Y:315:HOH:O	2.15	0.45
32:1a:865:A:H2	32:1a:918:A:H4'	1.82	0.45
32:1a:901:A:O2'	32:1a:1513:A:OP1	2.31	0.45
35:1d:60:GLU:HG3	35:1d:202:LEU:HD12	1.98	0.45
41:1j:6:ILE:HA	41:1j:97:GLU:O	2.16	0.45
47:1p:74:LEU:O	47:1p:79:VAL:HG22	2.17	0.45
1:2A:443:A:H1'	1:2A:1201:C:O4'	2.15	0.45
1:2A:479:A:N3	1:2A:481:G:H5"	2.32	0.45
1:2A:848:G:H2'	1:2A:849:A:C8	2.52	0.45
1:2A:888:C:OP1	44:2m:93:ARG:HD2	2.16	0.45
1:2A:2111:C:N4	1:2A:2147:G:H22	2.13	0.45
6:2G:39:ILE:HD11	6:2G:60:LEU:HD21	1.98	0.45
6:2G:77:ILE:HG22	6:2G:80:PHE:H	1.81	0.45
8:2I:50:ARG:O	8:2I:54:GLN:HG2	2.15	0.45
25:23:7:LYS:HE3	25:23:32:GLN:NE2	2.32	0.45
46:2o:84:LYS:HA	46:2o:84:LYS:HD2	1.73	0.45
51:2t:59:ALA:O	51:2t:63:ILE:HG13	2.16	0.45
1:1A:263:C:H2'	1:1A:264:C:O4'	2.17	0.45
1:1A:271(K):U:H4'	1:1A:271(L):U:OP2	2.14	0.45
1:1A:1301:A:C8	1:1A:1303:G:C8	3.04	0.45
1:1A:1712:C:H2'	1:1A:1713:U:O4'	2.16	0.45
1:1A:1802:A:N1	1:1A:1822:G:H1'	2.31	0.45
1:1A:2443:C:OP1	5:1F:68:LYS:HD3	2.16	0.45
1:1A:2602:A:H4'	1:1A:2603:G:OP1	2.15	0.45
2:1B:30:C:H2'	2:1B:31:C:H5'	1.98	0.45
21:1Z:102:LEU:HD11	21:1Z:124:ILE:HB	1.99	0.45
25:13:55:ARG:HD3	61:13:220:HOH:O	2.16	0.45
32:1a:407:G:OP1	35:1d:115:ARG:HD3	2.17	0.45
32:1a:616:G:OP2	35:1d:141:ARG:NH2	2.48	0.45
32:1a:1302:U:OP1	44:1m:13:LYS:HE3	2.16	0.45
33:1b:84:GLU:OE1	33:1b:87:ARG:NH1	2.45	0.45
34:1c:153:VAL:HG22	34:1c:198:VAL:HG22	1.98	0.45
37:1f:38:GLU:HB2	37:1f:64:GLN:HG2	1.99	0.45
41:1j:67:THR:O	41:1j:67:THR:OG1	2.33	0.45
44:1m:4:ILE:HA	44:1m:5:ALA:HA	1.72	0.45
47:1p:60:LEU:HD11	47:1p:66:PRO:HD3	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:1s:41:VAL:HG12	50:1s:44:MET:HG3	1.99	0.45
1:2A:1450:G:H2'	1:2A:1450(A):C:C6	2.52	0.45
1:2A:1657:C:H2'	1:2A:1658:C:C6	2.51	0.45
2:2B:4:C:H2'	2:2B:5:C:C6	2.52	0.45
4:2E:9:VAL:HB	15:2T:3:ARG:HG2	1.97	0.45
32:2a:691:G:H1'	32:2a:696:A:N6	2.31	0.45
32:2a:983:A:H3'	32:2a:983:A:N3	2.32	0.45
32:2a:1226:C:O4'	50:2s:83:HIS:HE1	1.99	0.45
32:2a:1401:G:N7	53:2y:83:ARG:NH1	2.65	0.45
43:2l:8:ASN:O	43:2l:12:ARG:HG3	2.17	0.45
1:1A:526:A:O2'	1:1A:2043:C:O2	2.31	0.45
1:1A:1098:A:H3'	1:1A:1099:G:H8	1.81	0.45
1:1A:1174:A:C1'	1:1A:1175:U:H5'	2.46	0.45
1:1A:1358:G:O2'	1:1A:1359:A:H5"	2.16	0.45
1:1A:1641:A:OP2	61:1A:4144:HOH:O	2.21	0.45
1:1A:1783:A:H5'	1:1A:2608:G:H4'	1.98	0.45
4:1E:12:THR:OG1	15:1T:11:GLU:OE2	2.32	0.45
32:1a:708:C:H2'	32:1a:709:G:H8	1.82	0.45
53:1y:70:MET:HE2	53:1y:70:MET:HB3	1.84	0.45
1:2A:1503:U:H2'	1:2A:1504:C:C6	2.52	0.45
1:2A:1598:C:H2'	1:2A:1599:C:H6	1.81	0.45
1:2A:1668:A:H4'	1:2A:1669:A:O5'	2.16	0.45
1:2A:1899:G:H2'	1:2A:1899:G:N3	2.32	0.45
1:2A:2104:G:O6	1:2A:2186:G:C5	2.69	0.45
5:2F:29:ASN:HB3	5:2F:112:MET:HE1	1.98	0.45
6:2G:146:TYR:O	6:2G:149:VAL:HG22	2.17	0.45
7:2H:28:GLY:N	7:2H:31:GLY:O	2.50	0.45
7:2H:70:THR:HA	7:2H:73:ALA:HB3	1.99	0.45
8:2I:5:LEU:HD23	8:2I:9:LEU:HD13	1.98	0.45
19:2X:41:ASN:O	19:2X:45:THR:HG23	2.16	0.45
19:2X:65:ARG:HB3	19:2X:70:LEU:HD23	1.99	0.45
21:2Z:146:ILE:HA	21:2Z:174:VAL:HG12	1.97	0.45
32:2a:501:C:H2'	32:2a:502:G:C8	2.52	0.45
32:2a:965:A:C8	53:2y:8:LYS:HD2	2.52	0.45
32:2a:1012:U:H2'	32:2a:1013:G:O4'	2.17	0.45
1:1A:862:G:H2'	1:1A:863:A:O4'	2.17	0.45
1:1A:963:U:H2'	1:1A:964:C:C6	2.52	0.45
1:1A:2165:G:H2'	1:1A:2166:G:C8	2.52	0.45
1:1A:2779:U:H5'	1:1A:2781:A:O4'	2.17	0.45
6:1G:43:LEU:O	6:1G:45:GLU:N	2.50	0.45
6:1G:82:LEU:HD21	6:1G:88:ILE:HG21	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:1V:65:GLY:HA3	17:1V:91:TYR:CZ	2.52	0.45
32:1a:911:U:OP2	43:1l:97:ARG:NH2	2.49	0.45
32:1a:1036:G:H5"	32:1a:1037:C:C5	2.51	0.45
33:1b:150:SER:O	33:1b:153:ARG:HG2	2.17	0.45
36:1e:79:GLU:HG3	36:1e:93:PRO:HD2	1.99	0.45
39:1h:23:SER:HA	39:1h:61:VAL:O	2.17	0.45
41:1j:31:GLY:HA2	41:1j:32:ALA:HA	1.47	0.45
1:2A:271(P):C:O3'	8:2I:42:SER:HB2	2.17	0.45
1:2A:796:C:H2'	1:2A:797:C:C6	2.51	0.45
1:2A:888:C:H2'	1:2A:889:C:N3	2.32	0.45
1:2A:1016:G:H2'	1:2A:1017:G:O4'	2.17	0.45
1:2A:1826:G:H4'	3:2D:242:ARG:CZ	2.47	0.45
1:2A:2742:C:OP1	31:29:35:ARG:HD3	2.17	0.45
1:2A:2849:U:OP2	15:2T:95:ARG:HG2	2.16	0.45
6:2G:115:ARG:HB2	6:2G:136:ARG:NH2	2.29	0.45
16:2U:49:HIS:O	16:2U:53:ARG:N	2.47	0.45
32:2a:757:U:H2'	32:2a:758:G:O4'	2.17	0.45
33:2b:92:TYR:HE1	33:2b:94:ASN:HB2	1.82	0.45
35:2d:10:ARG:HA	35:2d:13:ARG:HB2	1.98	0.45
35:2d:105:VAL:HG13	35:2d:110:PHE:HB2	1.98	0.45
40:2i:125:TYR:CE1	40:2i:127:LYS:HB3	2.52	0.45
44:2m:81:LEU:HD13	44:2m:88:ARG:HD2	1.98	0.45
1:1A:813:U:H2'	1:1A:814:C:C6	2.52	0.45
1:1A:2119:A:H2	1:1A:2171:A:H5'	1.82	0.45
1:1A:2155:G:H3'	1:1A:2156:G:C8	2.52	0.45
5:1F:24:LEU:HD21	5:1F:199:TRP:HH2	1.82	0.45
7:1H:11:VAL:HG13	7:1H:15:VAL:HG22	1.98	0.45
8:1I:109:ILE:HA	8:1I:109:ILE:HD12	1.73	0.45
18:1W:13:SER:HB3	18:1W:16:LYS:HD2	1.99	0.45
32:1a:264:U:H4'	48:1q:63:ARG:HD2	1.97	0.45
32:1a:455:C:O5'	32:1a:455:C:H6	1.99	0.45
39:1h:123:GLU:O	39:1h:127:LEU:HD12	2.15	0.45
43:1l:8:ASN:O	43:1l:12:ARG:HG3	2.17	0.45
51:1t:25:ARG:O	51:1t:29:LYS:HG3	2.17	0.45
1:2A:468:G:N7	29:27:39:ARG:NH2	2.60	0.45
1:2A:1422:G:H1'	1:2A:1496:A:N1	2.32	0.45
1:2A:1796:U:H2'	1:2A:1797:C:H6	1.82	0.45
1:2A:2320:A:N3	1:2A:2320:A:H2'	2.31	0.45
1:2A:2887:U:H2'	1:2A:2888:C:C6	2.52	0.45
32:2a:411:A:O2'	32:2a:413:G:H5'	2.16	0.45
32:2a:625:G:OP1	47:2p:9:PHE:HB3	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1226:C:H4'	50:2s:80:TYR:CZ	2.52	0.45
32:2a:1318:A:H5"	50:2s:3:ARG:NH2	2.32	0.45
32:2a:1401:G:OP1	53:2y:80:LYS:HE2	2.17	0.45
33:2b:101:MET:C	33:2b:102:LEU:HD12	2.42	0.45
51:2t:37:SER:O	51:2t:41:ILE:HG12	2.16	0.45
1:1A:478:A:C6	1:1A:480:A:C6	3.05	0.44
1:1A:527:C:H4'	1:1A:528:A:O5'	2.17	0.44
1:1A:1557:C:H5"	1:1A:1558:A:OP2	2.17	0.44
1:1A:2121:G:H2'	1:1A:2122:U:C6	2.52	0.44
1:1A:2136:C:C2	1:1A:2137:C:H5	2.35	0.44
3:1D:70:TRP:HB3	3:1D:190:TYR:CE2	2.52	0.44
6:1G:6:ALA:HB3	6:1G:104:GLU:OE2	2.18	0.44
15:1T:28:VAL:O	15:1T:46:GLU:HA	2.17	0.44
32:1a:236:G:OP1	48:1q:40:LYS:NZ	2.41	0.44
32:1a:346:G:N2	57:1a:1880:MPD:O4	2.50	0.44
32:1a:555:C:H2'	32:1a:556:C:C6	2.52	0.44
36:1e:95:ALA:HB1	36:1e:96:PRO:HD2	1.98	0.44
41:1j:55:LYS:H	41:1j:55:LYS:HG3	1.44	0.44
46:1o:29:VAL:HB	46:1o:81:LEU:HD21	1.99	0.44
1:2A:576:U:H2'	1:2A:577:G:C8	2.52	0.44
1:2A:1116:C:H2'	1:2A:1117:G:O4'	2.16	0.44
1:2A:1639:U:C2'	1:2A:1640:C:H5"	2.47	0.44
1:2A:1739:U:O2'	1:2A:1740:G:H8	2.00	0.44
1:2A:2134:A:C5	1:2A:2157:G:H5'	2.52	0.44
5:2F:132:VAL:CG2	5:2F:163:VAL:HG22	2.47	0.44
6:2G:41:GLN:HE22	6:2G:153:ARG:HB3	1.81	0.44
8:2I:48:GLU:HG3	8:2I:52:ARG:NH1	2.31	0.44
22:20:68:GLU:OE1	22:20:82:ARG:HD3	2.18	0.44
32:2a:1004:A:N7	32:2a:1037:C:H2'	2.32	0.44
32:2a:1009:G:C2	32:2a:1010:G:C8	3.05	0.44
32:2a:1328:C:H2'	32:2a:1329:A:O4'	2.17	0.44
33:2b:55:PHE:HE1	33:2b:218:ALA:HA	1.82	0.44
34:2c:35:GLU:HA	34:2c:38:ARG:HG3	1.98	0.44
38:2g:26:PHE:HE1	38:2g:105:VAL:HG22	1.81	0.44
41:2j:46:ARG:HG2	41:2j:64:GLU:HB3	1.98	0.44
1:1A:811:U:H2'	11:1P:21:ARG:HA	2.00	0.44
1:1A:888:C:H5'	44:1m:93:ARG:HD2	1.99	0.44
1:1A:1007:C:OP1	9:1N:37:LYS:NZ	2.49	0.44
1:1A:2038:G:H2'	1:1A:2039:C:O4'	2.16	0.44
1:1A:2167:U:H2'	1:1A:2168:G:C8	2.52	0.44
5:1F:167:ALA:HB1	5:1F:173:VAL:HG11	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1H:17:VAL:HG21	7:1H:50:VAL:HG21	1.99	0.44
12:1Q:109:VAL:HG22	12:1Q:113:GLN:CD	2.42	0.44
16:1U:16:LYS:HB3	16:1U:16:LYS:HE2	1.84	0.44
32:1a:67:C:O2'	32:1a:171:A:H1'	2.18	0.44
32:1a:255:G:H1'	48:1q:16:GLN:OE1	2.18	0.44
32:1a:458:C:H2'	32:1a:460:G:C8	2.52	0.44
33:1b:7:VAL:O	33:1b:9:GLU:N	2.51	0.44
35:1d:122:ARG:HD2	35:1d:122:ARG:HA	1.68	0.44
40:1i:56:LEU:HD23	40:1i:56:LEU:H	1.82	0.44
51:1t:100:ILE:H	51:1t:100:ILE:HG12	1.49	0.44
1:2A:191:A:H2'	1:2A:192:C:C6	2.52	0.44
1:2A:848:G:OP1	61:2A:3860:HOH:O	2.20	0.44
1:2A:1590:U:H2'	1:2A:1591:G:H8	1.82	0.44
1:2A:2184:G:H2'	1:2A:2185:C:O4'	2.17	0.44
1:2A:2223:G:OP1	3:2D:172:TYR:OH	2.28	0.44
5:2F:129:PHE:CD2	5:2F:163:VAL:HG21	2.52	0.44
6:2G:74:LYS:O	6:2G:84:LYS:NZ	2.51	0.44
9:2N:30:ILE:HG23	9:2N:52:VAL:HG11	1.99	0.44
10:2O:98:VAL:HG22	10:2O:118:ALA:HA	1.99	0.44
26:24:26:SER:OG	26:24:27:THR:N	2.49	0.44
32:2a:21:G:OP1	61:2a:3212:HOH:O	2.21	0.44
32:2a:839:U:H5"	32:2a:840:C:C5	2.52	0.44
32:2a:999:C:H2'	32:2a:1000:U:H6	1.82	0.44
32:2a:1224:G:C6	32:2a:1322:C:O4'	2.69	0.44
32:2a:1305:G:H22	32:2a:1331:G:H1'	1.80	0.44
35:2d:78:LEU:HD22	35:2d:96:LEU:HB3	1.98	0.44
38:2g:108:ALA:HA	38:2g:111:ARG:HD2	1.99	0.44
1:1A:1174:A:H4'	1:1A:1175:U:OP1	2.16	0.44
1:1A:1352:U:OP2	61:1A:4142:HOH:O	2.21	0.44
1:1A:2029:G:H2'	1:1A:2031:A:OP1	2.17	0.44
1:1A:2611:U:H5'	1:1A:2611:U:H6	1.82	0.44
5:1F:129:PHE:CD2	5:1F:163:VAL:HG21	2.53	0.44
15:1T:96:ARG:NH2	61:1T:306:HOH:O	2.50	0.44
18:1W:20:VAL:O	18:1W:23:LEU:HB2	2.17	0.44
32:1a:520:A:N1	32:1a:536:C:H1'	2.32	0.44
32:1a:1320:C:H2'	32:1a:1321:C:O4'	2.16	0.44
32:1a:1516:G:N1	32:1a:1519:MA6:OP2	2.48	0.44
33:1b:24:TRP:CZ3	33:1b:26:PRO:HA	2.52	0.44
35:1d:61:LYS:HD2	35:1d:207:TYR:OH	2.17	0.44
37:1f:60:PHE:O	37:1f:61:LEU:HD12	2.18	0.44
39:1h:4:ASP:OD1	39:1h:85:ARG:NH1	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2001:A:H2'	1:2A:2002:G:C8	2.52	0.44
1:2A:2159:G:H2'	1:2A:2160:G:O4'	2.17	0.44
1:2A:2167:U:H2'	1:2A:2168:G:C4	2.52	0.44
1:2A:2519:U:OP2	61:2A:3866:HOH:O	2.21	0.44
2:2B:22:U:H3	2:2B:61:G:H1	1.64	0.44
6:2G:37:VAL:HG21	6:2G:103:LEU:HD21	1.98	0.44
6:2G:54:GLU:O	6:2G:58:GLN:N	2.42	0.44
7:2H:25:LYS:HE3	7:2H:27:LYS:HE2	1.99	0.44
10:2O:68:GLU:HB3	10:2O:78:ARG:HB2	1.98	0.44
11:2P:50:ARG:HD3	30:28:7:HIS:CD2	2.52	0.44
11:2P:82:GLY:HA2	11:2P:113:LYS:O	2.17	0.44
16:2U:78:THR:HG22	16:2U:117:GLN:HE22	1.82	0.44
19:2X:31:HIS:CD2	19:2X:33:LYS:H	2.34	0.44
32:2a:8:A:C5	35:2d:209:ARG:HA	2.52	0.44
32:2a:472:A:OP1	47:2p:75:ARG:NH1	2.50	0.44
32:2a:615:C:H2'	32:2a:616:G:O4'	2.17	0.44
32:2a:673:G:O3'	37:2f:87:ARG:NH2	2.51	0.44
32:2a:691:G:H2'	32:2a:692:U:C6	2.52	0.44
32:2a:937:A:H1'	32:2a:1379:G:N2	2.33	0.44
32:2a:1071:C:H2'	32:2a:1072:G:C8	2.53	0.44
33:2b:212:GLN:CD	33:2b:235:SER:HB3	2.42	0.44
35:2d:189:PRO:HB2	35:2d:194:LEU:HD11	1.99	0.44
36:2e:31:LEU:HD23	36:2e:31:LEU:HA	1.78	0.44
40:2i:116:LYS:HA	40:2i:123:PRO:HD3	1.99	0.44
1:1A:236:C:H2'	1:1A:237:C:C6	2.52	0.44
1:1A:300:A:H2'	1:1A:334:C:H1'	1.98	0.44
1:1A:480:A:OP2	20:1Y:47:LYS:NZ	2.50	0.44
1:1A:606:U:H4'	1:1A:658:C:H4'	1.98	0.44
1:1A:645:C:H5'	1:1A:646:A:OP2	2.17	0.44
1:1A:1058:G:H8	1:1A:1058:G:O5'	2.01	0.44
1:1A:2143:C:N3	1:1A:2148:G:C6	2.84	0.44
30:18:15:LYS:HB3	57:18:103:MPD:C5	2.47	0.44
32:1a:428:G:OP2	35:1d:10:ARG:NH1	2.50	0.44
32:1a:501:C:H2'	32:1a:502:G:H8	1.81	0.44
32:1a:926:G:O6	53:1y:87:LYS:HE2	2.17	0.44
32:1a:1095:U:OP2	32:1a:1108:G:N1	2.46	0.44
32:1a:1458:G:OP1	51:1t:35:THR:OG1	2.29	0.44
34:1c:52:LEU:HD12	34:1c:52:LEU:HA	1.83	0.44
36:1e:12:LEU:HB3	36:1e:31:LEU:HB2	1.99	0.44
51:1t:14:LYS:O	51:1t:18:GLN:HG3	2.17	0.44
1:2A:302:C:H2'	1:2A:303:U:C6	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:652(T):C:H2'	1:2A:652(U):G:H8	1.83	0.44
1:2A:1045:A:H5'	1:2A:1047:G:O5'	2.16	0.44
1:2A:1102:C:H2'	1:2A:1103:A:C8	2.52	0.44
1:2A:1847:A:H3'	1:2A:1848:A:H5'	2.00	0.44
1:2A:2128:C:H5'	1:2A:2129:C:OP2	2.18	0.44
1:2A:2773:C:OP1	4:2E:164:ARG:NE	2.51	0.44
2:2B:66:A:H61	2:2B:109:C:H5"	1.82	0.44
4:2E:119:ARG:HD2	4:2E:120:TRP:CE2	2.52	0.44
6:2G:139:LEU:HA	6:2G:144:ILE:HB	1.99	0.44
7:2H:139:GLN:O	7:2H:143:GLN:N	2.41	0.44
20:2Y:67:LEU:HA	20:2Y:67:LEU:HD23	1.77	0.44
32:2a:745:C:H2'	32:2a:746:A:C8	2.52	0.44
32:2a:1060:C:H2'	32:2a:1061:G:H8	1.81	0.44
32:2a:1255:G:N1	32:2a:1279:A:N7	2.65	0.44
35:2d:173:TRP:NE1	35:2d:189:PRO:HG3	2.33	0.44
37:2f:89:MET:HB3	49:2r:76:LEU:HD21	1.99	0.44
37:2f:89:MET:HE3	49:2r:76:LEU:HG	1.99	0.44
38:2g:42:ILE:HD13	38:2g:116:ALA:HB3	1.99	0.44
40:2i:8:GLY:HA2	40:2i:79:LEU:HB3	1.99	0.44
44:2m:17:VAL:O	44:2m:20:THR:OG1	2.31	0.44
1:1A:1866:C:H2'	1:1A:1876:A:O4'	2.18	0.44
8:1I:27:ARG:HD2	23:11:71:TYR:CE2	2.52	0.44
12:1Q:58:PHE:O	12:1Q:60:ARG:N	2.50	0.44
12:1Q:112:GLU:HG3	12:1Q:113:GLN:N	2.32	0.44
24:12:70:GLN:H	24:12:70:GLN:HG3	1.55	0.44
32:1a:1028:C:H2'	32:1a:1029:C:H4'	1.99	0.44
32:1a:1446:U:O2'	32:1a:1447:A:H3'	2.17	0.44
39:1h:18:ARG:NH2	39:1h:81:HIS:O	2.50	0.44
1:2A:1092:C:H2'	1:2A:1092:C:O2	2.17	0.44
1:2A:1450:G:H2'	1:2A:1450(A):C:H6	1.81	0.44
1:2A:2118:U:O2'	1:2A:2119:A:H5"	2.17	0.44
1:2A:2243:U:H2'	1:2A:2244:U:C6	2.53	0.44
1:2A:2298:A:N6	1:2A:2318:G:C8	2.86	0.44
2:2B:95:C:N4	61:2B:323:HOH:O	2.50	0.44
5:2F:132:VAL:HA	5:2F:138:GLU:HB3	2.00	0.44
25:23:19:GLN:O	25:23:23:LEU:HD22	2.18	0.44
32:2a:176:C:H2'	32:2a:177:C:H6	1.82	0.44
32:2a:531:U:O3'	32:2a:532:A:H4'	2.17	0.44
32:2a:978:A:OP1	32:2a:1361:G:N2	2.45	0.44
32:2a:1054:C:H4'	32:2a:1055:A:O5'	2.17	0.44
32:2a:1169:A:H2'	32:2a:1170:A:C8	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:2b:70:PHE:CD1	33:2b:163:PHE:HB3	2.53	0.44
34:2c:111:LEU:HD21	34:2c:144:SER:HB2	1.99	0.44
36:2e:37:ARG:HH12	36:2e:111:GLU:HG2	1.82	0.44
1:1A:34:C:O2'	1:1A:35:G:O4'	2.35	0.44
1:1A:819:A:C4	1:1A:1189:A:C2	3.05	0.44
1:1A:2309:A:H2'	1:1A:2310:A:H8	1.82	0.44
1:1A:2693:A:H2'	1:1A:2694:G:H8	1.83	0.44
2:1B:13:A:N1	2:1B:69:G:O2'	2.49	0.44
6:1G:97:ASP:O	6:1G:101:ILE:HG13	2.18	0.44
8:1I:9:LEU:HD21	8:1I:35:LEU:HD13	2.00	0.44
23:11:3:LYS:HG3	23:11:4:VAL:HG23	1.99	0.44
32:1a:60:A:H4'	32:1a:61:G:H5'	2.00	0.44
32:1a:79:G:O6	32:1a:90:U:O4	2.36	0.44
32:1a:254:G:H21	48:1q:16:GLN:NE2	2.16	0.44
32:1a:624:C:H2'	32:1a:625:G:C8	2.52	0.44
33:1b:174:VAL:O	33:1b:178:ARG:HG3	2.17	0.44
35:1d:173:TRP:CD2	35:1d:189:PRO:HG3	2.52	0.44
38:1g:48:LYS:O	38:1g:52:GLU:HG2	2.18	0.44
1:2A:143:G:H2'	1:2A:143(A):C:C6	2.52	0.44
1:2A:729:G:C5	3:2D:208:LYS:HB2	2.52	0.44
1:2A:817:C:H4'	1:2A:932:G:C5	2.53	0.44
1:2A:1091:G:H2'	1:2A:1091:G:N3	2.33	0.44
1:2A:1111:A:O2'	1:2A:1112:G:H4'	2.18	0.44
1:2A:1187:G:N2	1:2A:1188:U:O4	2.51	0.44
1:2A:2497:A:H5"	61:2A:3935:HOH:O	2.17	0.44
3:2D:148:GLU:HB2	3:2D:151:LYS:HD2	2.00	0.44
4:2E:28:ALA:HB3	4:2E:93:VAL:CG1	2.48	0.44
7:2H:86:GLU:OE2	7:2H:132:ARG:NH2	2.50	0.44
20:2Y:90:LEU:HD21	20:2Y:96:ILE:HG12	1.99	0.44
22:20:15:ASP:OD1	22:20:16:SER:N	2.50	0.44
28:26:8:LYS:HD3	30:28:34:TRP:CD2	2.53	0.44
29:27:26:GLY:O	29:27:30:VAL:HG23	2.17	0.44
30:28:33:ASN:HA	30:28:36:LYS:HD2	2.00	0.44
32:2a:1291:G:OP1	38:2g:37:ASN:ND2	2.51	0.44
50:2s:80:TYR:CZ	50:2s:82:GLY:HA2	2.52	0.44
53:2y:61:LEU:HB3	53:2y:81:LEU:HD22	2.00	0.44
1:1A:483:A:O2'	20:1Y:49:VAL:O	2.32	0.44
1:1A:668:G:H5'	1:1A:669:G:OP2	2.17	0.44
1:1A:2893:G:H4'	1:1A:2894:G:O5'	2.17	0.44
6:1G:179:PRO:HB2	26:14:42:PHE:HE2	1.82	0.44
10:1O:100:GLY:O	10:1O:119:PRO:HD2	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:227:G:H2'	32:1a:228:A:O4'	2.18	0.44
32:1a:427:U:OP1	35:1d:13:ARG:NH1	2.44	0.44
32:1a:1492:A:H4'	32:1a:1493:A:C2	2.52	0.44
42:1k:16:SER:HG	42:1k:79:SER:HG	1.58	0.44
1:2A:116:C:H2'	1:2A:117:G:O4'	2.18	0.44
1:2A:144:C:H2'	1:2A:145:G:C8	2.53	0.44
1:2A:480:A:OP2	20:2Y:47:LYS:HD3	2.18	0.44
1:2A:1359:A:N6	1:2A:1372:U:H3	2.14	0.44
1:2A:1756:G:H4'	1:2A:1758:G:O4'	2.18	0.44
1:2A:2439:A:H5'	1:2A:2439:A:C8	2.53	0.44
6:2G:129:GLY:O	6:2G:161:THR:HB	2.18	0.44
8:2I:4:ILE:HA	8:2I:17:GLN:O	2.18	0.44
12:2Q:137:TYR:HB3	21:2Z:76:LEU:HD21	2.00	0.44
13:2R:12:ARG:O	13:2R:17:ARG:NH1	2.51	0.44
15:2T:30:VAL:HG22	15:2T:86:ILE:HG12	1.99	0.44
23:21:8:SER:HB3	23:21:66:HIS:CD2	2.52	0.44
24:22:64:LEU:O	24:22:68:ARG:HG2	2.18	0.44
26:24:2:LYS:HD2	26:24:5:ILE:HD13	2.00	0.44
32:2a:384:G:H2'	32:2a:385:C:H6	1.81	0.44
32:2a:555:C:H2'	32:2a:556:C:C6	2.52	0.44
32:2a:901:A:O2'	32:2a:1513:A:OP1	2.32	0.44
32:2a:1005:A:H5"	32:2a:1006:C:C5	2.52	0.44
32:2a:1032:G:C2'	32:2a:1033:G:H5'	2.47	0.44
32:2a:1101:A:H4'	32:2a:1102:A:O5'	2.17	0.44
32:2a:1151:A:O4'	41:2j:39:PRO:HB2	2.17	0.44
34:2c:164:ARG:NH1	34:2c:166:GLU:OE1	2.51	0.44
39:2h:104:ARG:HD3	39:2h:104:ARG:HA	1.83	0.44
50:2s:44:MET:HA	50:2s:47:HIS:ND1	2.33	0.44
1:1A:667:U:O2	30:18:2:PRO:HD2	2.17	0.44
1:1A:2115:G:N3	1:1A:2117:A:N6	2.61	0.44
1:1A:2445:G:OP1	5:1F:74:ARG:NH2	2.50	0.44
61:1A:5156:HOH:O	5:1F:74:ARG:HG3	2.17	0.44
5:1F:12:LEU:HD13	5:1F:124:LEU:HD11	2.00	0.44
6:1G:50:ALA:C	6:1G:52:ILE:N	2.76	0.44
23:11:3:LYS:O	23:11:12:PRO:HD3	2.16	0.44
32:1a:1162:C:H2'	32:1a:1163:C:H6	1.83	0.44
35:1d:111:ALA:HB1	35:1d:116:GLN:HB3	1.99	0.44
39:1h:6:ILE:O	39:1h:10:LEU:HG	2.18	0.44
39:1h:20:TYR:HA	39:1h:65:TYR:CZ	2.52	0.44
44:1m:37:THR:O	44:1m:55:ARG:NH1	2.22	0.44
1:2A:271(A):A:N1	1:2A:272(D):G:O2'	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1064:C:H5	1:2A:1065:U:C6	2.35	0.44
1:2A:1155:A:H5"	16:2U:55:ARG:HD3	2.00	0.44
1:2A:1270:C:H5"	1:2A:1271:G:O5'	2.18	0.44
1:2A:1580:A:H8	1:2A:1580:A:OP2	2.01	0.44
1:2A:1833:U:O2'	1:2A:1969:A:N1	2.31	0.44
1:2A:2315:G:H2'	1:2A:2316:C:C6	2.53	0.44
1:2A:2335:A:C8	1:2A:2337:G:C5	3.05	0.44
6:2G:41:GLN:HG3	6:2G:60:LEU:CD1	2.45	0.44
13:2R:36:THR:HG22	13:2R:37:THR:H	1.83	0.44
15:2T:117:ASP:OD2	15:2T:120:ARG:NE	2.31	0.44
32:2a:338:A:H2	32:2a:351:G:H22	1.66	0.44
32:2a:1096:C:H2'	32:2a:1097:C:H6	1.83	0.44
32:2a:1170:A:N6	32:2a:1171:G:N3	2.66	0.44
33:2b:54:THR:O	33:2b:58:ILE:HG12	2.17	0.44
36:2e:10:MET:HE2	36:2e:55:VAL:HG11	2.00	0.44
1:1A:65:C:H2'	1:1A:66:C:H6	1.81	0.44
1:1A:2140:C:H2'	1:1A:2141:G:C8	2.52	0.44
1:1A:2618:G:H21	4:1E:150:VAL:HG21	1.83	0.44
1:1A:2803:C:H2'	1:1A:2804:C:C6	2.53	0.44
3:1D:12:SER:HB3	3:1D:208:LYS:HB3	1.99	0.44
5:1F:104:LYS:O	5:1F:108:LYS:HB2	2.18	0.44
12:1Q:135:ASP:N	12:1Q:138:ASP:OD2	2.47	0.44
21:1Z:14:LYS:NZ	21:1Z:16:SER:H	2.16	0.44
32:1a:495:A:H4'	32:1a:496:A:OP1	2.17	0.44
32:1a:500:G:H2'	32:1a:501:C:C6	2.53	0.44
32:1a:669:U:H2'	32:1a:670:G:C8	2.53	0.44
32:1a:838:G:H5'	32:1a:839:U:OP2	2.17	0.44
32:1a:1338:G:H2'	32:1a:1339:A:C8	2.53	0.44
32:1a:1470:G:N7	61:1a:1944:HOH:O	2.36	0.44
34:1c:108:ASN:ND2	34:1c:111:LEU:HG	2.32	0.44
1:2A:923:C:H2'	1:2A:924:C:C6	2.52	0.44
1:2A:1053:C:H2'	1:2A:1054:A:C8	2.50	0.44
1:2A:1063:G:O2'	1:2A:1064:C:H6	2.01	0.44
1:2A:1093:G:O6	1:2A:1094:U:N3	2.51	0.44
1:2A:2554:U:H2'	1:2A:2555:U:C6	2.53	0.44
2:2B:45:A:C4	2:2B:46:A:C8	3.06	0.44
6:2G:19:LEU:HD23	6:2G:19:LEU:HA	1.80	0.44
7:2H:97:ARG:NH2	7:2H:104:GLU:OE1	2.51	0.44
16:2U:11:ARG:O	16:2U:15:LYS:HG3	2.17	0.44
17:2V:74:LYS:HB2	17:2V:83:ARG:HB2	1.99	0.44
21:2Z:45:ASP:OD1	21:2Z:49:ARG:NE	2.49	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1372:U:OP1	40:2i:72:GLY:N	2.50	0.44
33:2b:110:GLN:O	33:2b:111:ARG:NH1	2.51	0.44
35:2d:108:LEU:HD12	35:2d:108:LEU:HA	1.81	0.44
35:2d:111:ALA:HB3	35:2d:117:ALA:HB2	1.98	0.44
40:2i:49:PRO:HG2	40:2i:81:ILE:HG23	2.00	0.44
44:2m:43:THR:HG22	44:2m:44:ARG:O	2.17	0.44
48:2q:67:LYS:HG2	48:2q:68:ARG:HG3	2.00	0.44
1:1A:1105:U:H2'	1:1A:1106:G:C8	2.52	0.43
1:1A:1203:G:H5'	11:1P:3:LEU:HD23	1.99	0.43
6:1G:77:ILE:HG21	6:1G:80:PHE:CD2	2.53	0.43
10:1O:28:SER:OG	61:1O:301:HOH:O	2.20	0.43
14:1S:110:LEU:HA	14:1S:110:LEU:HD12	1.74	0.43
32:1a:619:U:N3	35:1d:134:ASP:OD1	2.43	0.43
32:1a:747:C:H3'	32:1a:748:C:C6	2.53	0.43
32:1a:1400:5MC:N3	53:1y:63:ALA:HA	2.32	0.43
33:1b:55:PHE:CD1	33:1b:58:ILE:HD12	2.53	0.43
33:1b:230:VAL:HG22	33:1b:231:GLU:H	1.82	0.43
39:1h:97:VAL:HG21	39:1h:128:GLY:HA2	1.99	0.43
51:1t:53:LEU:HB2	51:1t:100:ILE:HG13	2.00	0.43
1:2A:888:C:H2'	1:2A:889:C:C4	2.53	0.43
1:2A:1449:A:N3	1:2A:1529:G:H1'	2.33	0.43
1:2A:1504:C:H2'	1:2A:1505:C:C6	2.52	0.43
1:2A:2032:G:OP2	1:2A:2454:G:O2'	2.30	0.43
1:2A:2051:A:H5'	1:2A:2578:G:O4'	2.18	0.43
1:2A:2311:A:H5"	6:2G:77:ILE:HD11	1.99	0.43
3:2D:70:TRP:CE2	3:2D:150:LYS:HD3	2.52	0.43
6:2G:5:VAL:HG23	6:2G:8:LYS:H	1.83	0.43
11:2P:55:ARG:HA	61:2P:301:HOH:O	2.18	0.43
21:2Z:51:ALA:O	21:2Z:52:SER:C	2.61	0.43
32:2a:189:G:C5	32:2a:189(A):C:C4	3.06	0.43
32:2a:192:U:O2'	51:2t:60:GLU:OE1	2.27	0.43
32:2a:881:G:OP2	43:2l:12:ARG:NH2	2.51	0.43
32:2a:1250:A:N3	32:2a:1370:G:O2'	2.45	0.43
33:2b:24:TRP:H	33:2b:24:TRP:HD1	1.66	0.43
33:2b:50:GLU:O	33:2b:54:THR:N	2.28	0.43
33:2b:95:GLN:HG3	33:2b:147:LYS:O	2.18	0.43
33:2b:229:VAL:HG12	33:2b:230:VAL:H	1.83	0.43
1:1A:286:C:H2'	1:1A:287:C:H6	1.82	0.43
1:1A:654:A:OP2	61:1A:4146:HOH:O	2.21	0.43
1:1A:2086:U:H2'	1:1A:2087:G:C8	2.54	0.43
19:1X:61:GLY:HA3	19:1X:73:ARG:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:10:55:ARG:H	22:10:55:ARG:HG3	1.45	0.43
32:1a:54:C:N4	32:1a:353:A:OP2	2.47	0.43
32:1a:103:C:OP2	51:1t:14:LYS:NZ	2.51	0.43
32:1a:1025:U:O2'	32:1a:1026:G:O4'	2.28	0.43
32:1a:1328:C:H2'	32:1a:1329:A:O4'	2.18	0.43
33:1b:47:THR:HG22	33:1b:51:LEU:HD12	2.00	0.43
39:1h:11:THR:OG1	39:1h:14:ARG:NH2	2.51	0.43
42:1k:92:GLU:HA	42:1k:95:ILE:HD12	1.99	0.43
48:1q:43:LEU:HB3	48:1q:69:LYS:HG2	1.99	0.43
51:1t:50:GLU:O	51:1t:100:ILE:HD11	2.17	0.43
1:2A:8:A:H2'	1:2A:9:U:H6	1.83	0.43
1:2A:297:C:H2'	1:2A:298:G:O4'	2.17	0.43
1:2A:904:C:H2'	1:2A:905:U:C6	2.54	0.43
1:2A:993:G:N2	17:2V:23:GLU:OE2	2.51	0.43
1:2A:1864:U:OP1	1:2A:2410:G:O2'	2.25	0.43
1:2A:1932:A:H2'	1:2A:1933:G:O4'	2.18	0.43
1:2A:2313:C:H2'	1:2A:2314:C:C6	2.53	0.43
1:2A:2468:G:C2	1:2A:2481:G:N3	2.86	0.43
3:2D:24:ILE:HD13	3:2D:84:TYR:HB2	2.01	0.43
11:2P:135:LEU:HA	11:2P:135:LEU:HD23	1.76	0.43
17:2V:43:GLU:OE1	17:2V:43:GLU:N	2.51	0.43
28:26:6:ARG:HH11	28:26:26:ASN:HB2	1.83	0.43
32:2a:192:U:H2'	32:2a:193:C:C6	2.52	0.43
32:2a:828:A:H2'	32:2a:829:G:O4'	2.18	0.43
32:2a:1210:C:H2'	32:2a:1211:U:H5"	2.00	0.43
1:1A:30:G:OP1	61:1A:4143:HOH:O	2.21	0.43
1:1A:39:C:O2	5:1F:46:ARG:NH2	2.44	0.43
1:1A:186:G:H2'	1:1A:187:G:H8	1.83	0.43
1:1A:1045:A:OP1	1:1A:1045:A:H4'	2.18	0.43
1:1A:2119:A:C6	1:1A:2171:A:C5	3.06	0.43
61:1A:4416:HOH:O	24:12:54:LYS:NZ	2.49	0.43
2:1B:24:G:N7	2:1B:56:G:H2'	2.34	0.43
11:1P:68:GLN:HG3	61:1P:308:HOH:O	2.19	0.43
19:1X:66:LEU:HD12	19:1X:66:LEU:HA	1.81	0.43
23:11:11:ARG:HG3	23:11:12:PRO:HD2	2.01	0.43
24:12:1:MET:N	24:12:52:ASP:OD2	2.45	0.43
32:1a:540:G:H2'	32:1a:541:G:O4'	2.19	0.43
32:1a:1034:G:H2'	32:1a:1035:A:O4'	2.19	0.43
34:1c:129:ALA:HB3	34:1c:132:ARG:HD2	2.00	0.43
39:1h:121:ASP:HB2	39:1h:125:ARG:NH2	2.33	0.43
40:1i:20:ARG:O	40:1i:60:ASP:N	2.41	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:583:G:OP2	16:2U:10:ARG:HD2	2.18	0.43
1:2A:900:A:H2'	1:2A:901:A:O4'	2.18	0.43
1:2A:1063:G:N2	1:2A:1076:C:O2'	2.51	0.43
1:2A:1104:C:H2'	1:2A:1105:U:C6	2.52	0.43
1:2A:1231:G:H2'	1:2A:1232:G:C8	2.53	0.43
1:2A:1540:U:H2'	1:2A:1541:G:O4'	2.18	0.43
1:2A:1579:A:H2'	1:2A:1580:A:C8	2.53	0.43
6:2G:16:ARG:HD2	6:2G:16:ARG:HA	1.65	0.43
9:2N:62:VAL:HG11	9:2N:66:LYS:HB2	1.98	0.43
26:24:59:PHE:HE2	50:2s:64:GLU:HB2	1.82	0.43
29:27:12:ARG:NH2	29:27:44:PRO:HB3	2.33	0.43
32:2a:442:C:H42	32:2a:492:G:H1	1.66	0.43
34:2c:84:ILE:HA	34:2c:87:LEU:HD12	2.00	0.43
35:2d:200:GLU:HA	35:2d:203:VAL:HG23	2.01	0.43
44:2m:29:ARG:HD3	44:2m:64:TRP:CE2	2.53	0.43
46:2o:5:LYS:O	46:2o:9:GLN:HG2	2.17	0.43
1:1A:142:A:N1	1:1A:1595:G:O2'	2.46	0.43
1:1A:574:C:N3	4:1E:145:LYS:NZ	2.62	0.43
1:1A:630:G:OP1	30:18:47:LYS:NZ	2.48	0.43
10:1O:70:LYS:HB3	10:1O:70:LYS:HE2	1.81	0.43
21:1Z:69:THR:HG22	21:1Z:90:VAL:HA	1.99	0.43
32:1a:265:G:H5'	48:1q:64:PRO:O	2.18	0.43
32:1a:868:C:H2'	32:1a:869:G:O4'	2.19	0.43
32:1a:986:A:N3	50:1s:52:TYR:OH	2.49	0.43
39:1h:86:ILE:HG21	39:1h:133:LEU:HD13	2.00	0.43
39:1h:116:LYS:HZ3	39:1h:127:LEU:HD23	1.83	0.43
51:1t:82:SER:O	51:1t:86:ARG:HG3	2.17	0.43
52:1u:5:ASP:O	52:1u:11:GLY:HA3	2.18	0.43
1:2A:270:A:OP2	1:2A:271(X):G:N1	2.34	0.43
1:2A:470:A:OP1	5:2F:59:TYR:HE1	2.02	0.43
1:2A:606:U:H4'	1:2A:658:C:H4'	2.00	0.43
1:2A:784:A:C8	1:2A:792:G:C5	3.06	0.43
1:2A:1783:A:H5'	1:2A:2608:G:H4'	2.01	0.43
5:2F:32:LEU:O	5:2F:36:VAL:HG23	2.18	0.43
12:2Q:103:MET:HB3	12:2Q:104:PHE:CD2	2.53	0.43
21:2Z:14:LYS:HB3	21:2Z:14:LYS:HE2	1.75	0.43
21:2Z:152:ALA:O	21:2Z:155:LEU:HB2	2.18	0.43
32:2a:19:C:H5"	36:2e:86:ALA:HB3	1.99	0.43
32:2a:537:G:N7	61:2a:3253:HOH:O	2.37	0.43
32:2a:938:A:C6	32:2a:939:G:C5	3.06	0.43
32:2a:1070:U:H2'	32:2a:1071:C:C6	2.50	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1126:U:C4'	32:2a:1281:U:H1'	2.49	0.43
34:2c:20:SER:HB2	34:2c:40:ARG:NH2	2.34	0.43
37:2f:69:GLU:H	37:2f:69:GLU:CD	2.22	0.43
40:2i:28:VAL:HA	40:2i:63:ILE:O	2.19	0.43
43:2l:103:GLY:N	43:2l:107:ALA:O	2.49	0.43
48:2q:67:LYS:HA	48:2q:70:ARG:NH2	2.30	0.43
1:1A:807:U:OP2	11:1P:41:ARG:NH2	2.50	0.43
1:1A:887:A:H1'	1:1A:888:C:H3'	2.01	0.43
1:1A:2273:A:H2'	1:1A:2274:A:C8	2.53	0.43
1:1A:2648:C:H2'	1:1A:2649:U:C6	2.53	0.43
8:1I:61:ARG:HB3	8:1I:133:HIS:HD2	1.82	0.43
32:1a:660:G:C2	32:1a:746:A:C2	3.07	0.43
32:1a:1192:C:OP2	34:1c:4:LYS:NZ	2.51	0.43
32:1a:1291:G:OP1	38:1g:37:ASN:ND2	2.50	0.43
32:1a:1343:G:H4'	40:1i:122:ALA:HB3	2.01	0.43
33:1b:54:THR:O	33:1b:58:ILE:HG13	2.18	0.43
47:1p:20:VAL:HG21	47:1p:32:TYR:CG	2.54	0.43
1:2A:65:C:H2'	1:2A:66:C:H6	1.82	0.43
1:2A:78:A:H2'	1:2A:79:G:H8	1.84	0.43
1:2A:784:A:N6	3:2D:229:VAL:HG11	2.33	0.43
1:2A:1002:G:H2'	1:2A:1003:G:O4'	2.19	0.43
1:2A:1111:A:C2	1:2A:1112:G:H1'	2.54	0.43
1:2A:1262:A:O2'	61:2A:3859:HOH:O	2.20	0.43
1:2A:1550:C:OP1	1:2A:1720:U:O2'	2.21	0.43
1:2A:1639:U:H4'	1:2A:2699:C:H4'	2.01	0.43
1:2A:2086:U:H2'	1:2A:2087:G:C8	2.54	0.43
1:2A:2291:U:OP1	1:2A:2380:C:O2'	2.33	0.43
1:2A:2612:C:OP2	27:25:2:ALA:N	2.52	0.43
1:2A:2785:C:O2'	4:2E:66:HIS:ND1	2.48	0.43
4:2E:89:ASP:OD1	4:2E:89:ASP:N	2.52	0.43
6:2G:36:LYS:H	6:2G:160:VAL:HB	1.83	0.43
8:2I:79:ILE:HG21	8:2I:92:VAL:HG11	2.00	0.43
21:2Z:157:LEU:HD13	21:2Z:161:VAL:HG12	2.00	0.43
32:2a:114:U:H2'	32:2a:115:G:C8	2.53	0.43
32:2a:620:C:H2'	32:2a:621:A:O4'	2.18	0.43
32:2a:1387:G:H2'	32:2a:1388:C:C6	2.54	0.43
44:2m:91:ARG:HH22	44:2m:103:THR:HG21	1.83	0.43
47:2p:1:MET:O	47:2p:24:ALA:HB2	2.19	0.43
52:2u:17:THR:O	52:2u:22:ARG:NH1	2.45	0.43
1:1A:71:A:N7	19:1X:31:HIS:HE1	2.16	0.43
1:1A:271(P):C:H2'	1:1A:271(Q):G:O4'	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1252:G:N3	16:1U:33:ARG:HG2	2.33	0.43
3:1D:71:ASP:CB	3:1D:103:ARG:HH22	2.29	0.43
10:1O:49:ARG:HH12	32:1a:1423:G:P	2.41	0.43
15:1T:26:ASP:OD1	15:1T:120:ARG:NH2	2.39	0.43
21:1Z:75:ASN:O	21:1Z:84:GLU:HG2	2.18	0.43
32:1a:141:A:H1'	32:1a:182:U:O2	2.18	0.43
32:1a:1003:G:H2'	32:1a:1004:A:C4'	2.43	0.43
33:1b:196:LEU:HA	33:1b:196:LEU:HD12	1.75	0.43
35:1d:187:ARG:NH2	35:1d:193:ASP:OD2	2.49	0.43
45:1n:33:VAL:HA	45:1n:40:CYS:HA	1.99	0.43
50:1s:13:ASP:HA	50:1s:16:LEU:HB3	1.99	0.43
1:2A:1055:G:H3'	1:2A:1056:G:H8	1.83	0.43
1:2A:1354:A:H2'	1:2A:1355:G:O4'	2.18	0.43
1:2A:1434:A:H2'	1:2A:1435:G:C8	2.53	0.43
1:2A:1498:C:O4'	1:2A:1577:C:H4'	2.19	0.43
2:2B:76:G:N2	2:2B:101:G:O6	2.48	0.43
3:2D:155:LEU:HD13	3:2D:177:LEU:HD22	2.01	0.43
6:2G:82:LEU:HA	6:2G:86:MET:SD	2.58	0.43
7:2H:98:LEU:HD12	7:2H:98:LEU:HA	1.81	0.43
11:2P:147:LEU:HD23	11:2P:148:LEU:O	2.18	0.43
13:2R:9:LYS:O	13:2R:17:ARG:HD3	2.18	0.43
19:2X:65:ARG:HE	19:2X:70:LEU:CD2	2.32	0.43
32:2a:512:U:H2'	32:2a:513:C:C6	2.53	0.43
32:2a:1218:C:OP2	45:2n:9:LYS:NZ	2.28	0.43
32:2a:1258:G:H2'	32:2a:1259:C:C6	2.53	0.43
32:2a:1505:G:H4'	32:2a:1506:U:H5"	2.01	0.43
34:2c:52:LEU:HA	34:2c:70:VAL:HG22	2.00	0.43
46:2o:8:LYS:O	46:2o:12:ILE:HG13	2.19	0.43
1:1A:1055:G:N1	1:1A:1104:C:C2	2.86	0.43
1:1A:1292:U:H2'	1:1A:1293:C:C6	2.54	0.43
7:1H:154:PRO:HB3	7:1H:163:TYR:CE1	2.53	0.43
24:12:3:LEU:HD23	24:12:3:LEU:HA	1.72	0.43
32:1a:113:G:O4'	32:1a:354:G:H4'	2.18	0.43
32:1a:689:C:H2'	32:1a:690:G:O4'	2.18	0.43
47:1p:29:ASP:OD1	47:1p:29:ASP:N	2.52	0.43
47:1p:57:ARG:HE	47:1p:79:VAL:HA	1.84	0.43
1:2A:491:G:H2'	1:2A:492:A:C8	2.54	0.43
1:2A:854:G:H2'	1:2A:855:G:C8	2.53	0.43
1:2A:1340:U:OP1	19:2X:16:LYS:NZ	2.51	0.43
1:2A:1805:U:O2	3:2D:50:THR:HB	2.18	0.43
1:2A:1877:A:H5'	1:2A:1878:G:OP2	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2695:C:H2'	1:2A:2696:U:C6	2.54	0.43
2:2B:7:G:H4'	14:2S:29:PHE:CD2	2.54	0.43
8:2I:77:LEU:HD11	8:2I:100:ALA:HB3	2.01	0.43
11:2P:87:ASP:HB3	11:2P:105:LEU:HD13	2.00	0.43
11:2P:97:PRO:HD3	11:2P:126:VAL:O	2.17	0.43
13:2R:72:ASP:HB3	13:2R:75:LEU:HB3	2.00	0.43
17:2V:53:GLU:H	17:2V:53:GLU:HG2	1.67	0.43
21:2Z:130:PRO:C	21:2Z:132:ASN:H	2.25	0.43
23:21:83:GLU:HA	23:21:84:GLY:HA2	1.66	0.43
32:2a:692:U:H1'	32:2a:695:A:N7	2.33	0.43
32:2a:1093:A:N3	32:2a:1095:U:H5'	2.34	0.43
32:2a:1146:A:H2'	32:2a:1147:C:O4'	2.19	0.43
32:2a:1342:C:H2'	32:2a:1343:G:C8	2.54	0.43
35:2d:38:TYR:OH	35:2d:45:GLN:NE2	2.51	0.43
36:2e:51:VAL:O	36:2e:55:VAL:HG23	2.18	0.43
51:2t:76:ALA:O	51:2t:80:ARG:HG3	2.18	0.43
1:1A:536:A:H2'	1:1A:537:C:C6	2.54	0.43
1:1A:724:U:H2'	1:1A:725:G:O4'	2.19	0.43
1:1A:1071:G:H1'	1:1A:1089:G:H2'	2.01	0.43
1:1A:1422:G:H4'	1:1A:1493:C:OP1	2.19	0.43
1:1A:1614:A:C2	18:1W:93:ALA:HB2	2.54	0.43
1:1A:2627:G:N2	1:1A:2777:G:OP2	2.50	0.43
1:1A:2640:G:OP1	9:1N:97:ARG:NH2	2.42	0.43
14:1S:59:LYS:H	14:1S:59:LYS:HG3	1.52	0.43
17:1V:14:VAL:HB	17:1V:96:ILE:HG13	2.00	0.43
21:1Z:14:LYS:HD3	21:1Z:16:SER:OG	2.19	0.43
27:15:35:GLU:HG2	27:15:51:TYR:CD1	2.54	0.43
32:1a:567:G:H2'	32:1a:568:G:O4'	2.18	0.43
32:1a:1043:C:H2'	32:1a:1044:A:O4'	2.19	0.43
42:1k:99:GLN:HG2	42:1k:105:VAL:HG11	1.99	0.43
1:2A:422:A:H2'	1:2A:423:A:C8	2.54	0.43
1:2A:1056:G:H21	1:2A:1103:A:H62	1.67	0.43
1:2A:1090:U:H2'	1:2A:1091:G:C8	2.53	0.43
1:2A:1096:A:C8	1:2A:1097:U:H5	2.36	0.43
1:2A:1509(B):A:H2'	1:2A:1510:G:O4'	2.18	0.43
1:2A:2019:A:N7	27:25:9:LYS:HE2	2.34	0.43
4:2E:28:ALA:HB3	4:2E:93:VAL:HG12	2.01	0.43
11:2P:89:ALA:HA	11:2P:121:LYS:HD3	2.00	0.43
12:2Q:21:THR:HG23	12:2Q:99:PRO:O	2.19	0.43
13:2R:28:LEU:HD23	13:2R:48:VAL:HG21	2.01	0.43
19:2X:43:VAL:HG11	19:2X:81:VAL:HG21	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:23:46:ASN:O	25:23:50:VAL:HG22	2.19	0.43
32:2a:953:G:C2	32:2a:954:G:H1'	2.54	0.43
32:2a:1126:U:H4'	32:2a:1281:U:H1'	2.01	0.43
38:2g:150:ALA:HB1	42:2k:57:THR:HG21	2.00	0.43
1:1A:569:U:C4	1:1A:570:G:C6	3.07	0.43
1:1A:645:C:O2	1:1A:645:C:H2'	2.19	0.43
1:1A:747:U:O2	1:1A:2014:A:H1'	2.18	0.43
1:1A:1289:C:H2'	1:1A:1290:C:H6	1.84	0.43
1:1A:1358:G:N2	1:1A:1372:U:C5	2.87	0.43
1:1A:1427:A:H4'	1:1A:1428:C:O4'	2.19	0.43
1:1A:2033:A:O2'	1:1A:2035:G:OP2	2.34	0.43
1:1A:2718:G:O2'	1:1A:2847:U:OP1	2.32	0.43
57:1A:4043:MPD:H4	57:1A:4043:MPD:HM2	1.73	0.43
8:1I:4:ILE:HD11	8:1I:44:LEU:HD13	2.00	0.43
8:1I:133:HIS:HD1	8:1I:133:HIS:C	2.27	0.43
9:1N:23:LEU:HD12	9:1N:99:LEU:HD23	2.00	0.43
18:1W:45:TYR:CZ	18:1W:49:LYS:HE3	2.54	0.43
32:1a:1070:U:H2'	32:1a:1071:C:H6	1.83	0.43
33:1b:63:MET:HB3	33:1b:225:ALA:HB1	2.00	0.43
34:1c:62:ASP:O	34:1c:97:LYS:HB2	2.18	0.43
39:1h:82:HIS:O	39:1h:137:VAL:HA	2.19	0.43
47:1p:20:VAL:HG21	47:1p:32:TYR:CD2	2.54	0.43
1:2A:42:G:H2'	1:2A:43:A:O4'	2.18	0.43
1:2A:271(F):C:H2'	1:2A:271(G):C:C6	2.53	0.43
1:2A:391:G:H1'	1:2A:411:G:O4'	2.19	0.43
1:2A:1012:U:C5	9:2N:28:THR:HG21	2.53	0.43
1:2A:1539:G:H2'	1:2A:1540:U:C6	2.54	0.43
1:2A:1721:G:H8	1:2A:1741:A:H62	1.65	0.43
1:2A:2659:G:P	7:2H:158:HIS:HE2	2.42	0.43
61:2A:3940:HOH:O	3:2D:239:ARG:NH2	2.52	0.43
61:2A:4049:HOH:O	5:2F:74:ARG:HD2	2.17	0.43
2:2B:28:C:H2'	2:2B:29:A:O4'	2.19	0.43
4:2E:9:VAL:HG13	4:2E:25:VAL:O	2.19	0.43
4:2E:119:ARG:HG2	4:2E:160:TYR:HB2	2.01	0.43
8:2I:75:LEU:HD11	8:2I:105:HIS:ND1	2.34	0.43
21:2Z:52:SER:OG	21:2Z:53:ILE:N	2.50	0.43
32:2a:160:A:H2'	32:2a:161:A:O4'	2.19	0.43
32:2a:1067:A:H8	32:2a:1067:A:O5'	2.01	0.43
32:2a:1091:U:H2'	32:2a:1093:A:OP2	2.18	0.43
32:2a:1314:C:N4	50:2s:2:PRO:O	2.51	0.43
32:2a:1516:G:N1	32:2a:1519:MA6:OP2	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:2j:80:LYS:O	41:2j:84:GLN:HB3	2.18	0.43
1:1A:228:A:H2'	1:1A:230:U:O4'	2.19	0.43
1:1A:488:G:O2'	18:1W:49:LYS:NZ	2.50	0.43
1:1A:671:C:N4	61:1A:4668:HOH:O	2.52	0.43
1:1A:957:A:N1	1:1A:2458:G:H4'	2.34	0.43
1:1A:2116:G:H1	1:1A:2165:G:N2	2.16	0.43
1:1A:2142:C:H2'	1:1A:2143:C:C6	2.54	0.43
1:1A:2185:C:H2'	1:1A:2186:G:O4'	2.19	0.43
2:1B:43:C:H5"	26:14:1:MET:HG2	2.01	0.43
6:1G:126:ASP:N	6:1G:130:ASN:O	2.43	0.43
8:1I:8:PRO:HD3	8:1I:15:VAL:HB	2.01	0.43
20:1Y:53:PRO:O	20:1Y:56:PRO:HD3	2.19	0.43
32:1a:152:A:N6	32:1a:170:U:C2	2.87	0.43
32:1a:219:C:H2'	32:1a:220:G:O4'	2.18	0.43
32:1a:576:G:O6	32:1a:880:C:O2'	2.31	0.43
32:1a:757:U:O2'	32:1a:879:C:O2	2.32	0.43
32:1a:1005:A:C2	32:1a:1025:U:H1'	2.53	0.43
32:1a:1269:A:H5'	52:1u:18:TYR:O	2.19	0.43
34:1c:150:LYS:HB2	34:1c:150:LYS:HE3	1.88	0.43
41:1j:5:ARG:NH2	41:1j:73:ASP:OD2	2.32	0.43
1:2A:476:G:N1	1:2A:479:A:OP2	2.50	0.43
1:2A:1221(A):C:C2	1:2A:1229:G:C2	3.07	0.43
1:2A:1366:A:H2'	1:2A:1367:A:O4'	2.19	0.43
1:2A:1614:A:P	1:2A:1614:A:H8	2.42	0.43
4:2E:7:VAL:HG23	4:2E:51:PHE:HE2	1.83	0.43
8:2I:130:TYR:HD2	8:2I:138:ILE:HD12	1.84	0.43
10:2O:16:ALA:HB2	10:2O:52:VAL:HG21	2.01	0.43
16:2U:106:PHE:O	16:2U:110:VAL:HG23	2.19	0.43
32:2a:33:A:N3	43:2l:32:PHE:HE2	2.16	0.43
32:2a:399:G:H2'	32:2a:400:C:C6	2.53	0.43
32:2a:718:G:C8	42:2k:116:HIS:HB3	2.53	0.43
32:2a:1093:A:OP2	32:2a:1093:A:H8	2.01	0.43
32:2a:1289:A:N1	32:2a:1371:G:O2'	2.38	0.43
34:2c:8:ILE:HD11	34:2c:184:TYR:H	1.82	0.43
37:2f:70:ASP:OD1	37:2f:70:ASP:N	2.46	0.43
38:2g:114:ARG:HB2	38:2g:115:ARG:NH2	2.34	0.43
40:2i:3:GLN:NE2	40:2i:20:ARG:HH21	2.17	0.43
47:2p:53:VAL:HG13	47:2p:79:VAL:HG22	2.01	0.43
50:2s:33:THR:HG22	50:2s:50:ALA:O	2.19	0.43
51:2t:57:ARG:NH2	51:2t:100:ILE:HG21	2.34	0.43
1:1A:2591:C:H2'	1:1A:2592:G:C8	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1D:70:TRP:HB3	3:1D:190:TYR:CZ	2.54	0.42
3:1D:232:PRO:HB3	3:1D:244:ARG:CZ	2.48	0.42
4:1E:119:ARG:HG2	4:1E:160:TYR:CG	2.53	0.42
7:1H:117:PRO:HG3	7:1H:123:PHE:CD2	2.54	0.42
32:1a:21:G:H2'	32:1a:22:G:C8	2.54	0.42
32:1a:266:G:H5"	32:1a:267:C:H5	1.83	0.42
32:1a:911:U:H2'	32:1a:912:C:C6	2.54	0.42
32:1a:922:G:C6	32:1a:923:A:C6	3.07	0.42
32:1a:1005:A:H8	32:1a:1005:A:O5'	2.02	0.42
32:1a:1226:C:H4'	50:1s:80:TYR:OH	2.18	0.42
33:1b:77:ALA:HA	33:1b:80:ILE:HG23	2.00	0.42
35:1d:121:VAL:O	35:1d:134:ASP:HA	2.19	0.42
35:1d:150:GLU:C	35:1d:152:SER:H	2.27	0.42
46:1o:87:ILE:HG22	46:1o:88:ARG:H	1.84	0.42
1:2A:446:G:OP1	16:2U:3:ARG:NH1	2.52	0.42
1:2A:483:A:O2'	20:2Y:49:VAL:O	2.30	0.42
1:2A:1721:G:H2'	1:2A:1740:G:O6	2.17	0.42
1:2A:2042:A:OP1	61:2A:3865:HOH:O	2.21	0.42
1:2A:2186:G:N1	1:2A:2187:G:C5	2.87	0.42
1:2A:2390:U:O2'	1:2A:2391:G:H5'	2.19	0.42
1:2A:2808:U:N3	1:2A:2893:G:O6	2.51	0.42
3:2D:106:ILE:HD11	3:2D:143:HIS:CD2	2.53	0.42
6:2G:58:GLN:C	6:2G:60:LEU:H	2.27	0.42
6:2G:114:ILE:HB	6:2G:117:PHE:HB2	2.01	0.42
7:2H:103:LEU:HB2	7:2H:123:PHE:CD2	2.54	0.42
9:2N:62:VAL:HG13	9:2N:66:LYS:HD2	2.01	0.42
15:2T:41:ARG:NH2	32:2a:346:G:OP1	2.47	0.42
21:2Z:72:ARG:HD3	21:2Z:72:ARG:HA	1.76	0.42
32:2a:583:A:H2'	32:2a:584:G:O4'	2.19	0.42
32:2a:1097:C:H2'	32:2a:1098:C:C6	2.53	0.42
32:2a:1122:U:C4	32:2a:1123:A:N7	2.87	0.42
32:2a:1426:C:H2'	32:2a:1427:U:H6	1.84	0.42
33:2b:115:LEU:O	33:2b:119:GLU:HG2	2.19	0.42
34:2c:186:PHE:HZ	34:2c:188:LEU:HD13	1.82	0.42
1:1A:471:A:H2'	1:1A:472:A:O4'	2.19	0.42
1:1A:729:G:C5	3:1D:208:LYS:HB2	2.55	0.42
1:1A:2790:A:H2'	1:1A:2790:A:N3	2.34	0.42
3:1D:134:ARG:HG3	3:1D:187:GLY:O	2.18	0.42
10:1O:68:GLU:HB3	10:1O:78:ARG:HB2	2.00	0.42
32:1a:203:U:H5'	32:1a:216:G:N2	2.35	0.42
32:1a:629:G:H2'	32:1a:630:G:O4'	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:1e:51:VAL:O	36:1e:55:VAL:HG23	2.19	0.42
45:1n:24:CYS:HB2	45:1n:40:CYS:HB3	2.01	0.42
53:1y:24:LEU:HD23	53:1y:24:LEU:HA	1.88	0.42
1:2A:35:G:H2'	1:2A:36:G:O4'	2.19	0.42
1:2A:244:A:H4'	11:2P:74:GLU:HB2	2.01	0.42
1:2A:851:U:O2'	25:23:42:ALA:O	2.37	0.42
1:2A:1070:A:H2'	1:2A:1071:G:C8	2.54	0.42
1:2A:1412:A:H2'	1:2A:1413:G:C8	2.54	0.42
1:2A:1670:C:OP1	61:2A:3867:HOH:O	2.21	0.42
4:2E:7:VAL:HG23	4:2E:51:PHE:CE2	2.54	0.42
5:2F:150:GLY:HA2	5:2F:172:TRP:CD2	2.54	0.42
6:2G:3:LEU:O	6:2G:8:LYS:NZ	2.40	0.42
11:2P:39:LYS:HD2	11:2P:45:LEU:HD11	2.00	0.42
32:2a:154:C:H2'	32:2a:155:C:C6	2.54	0.42
32:2a:664:G:P	49:2r:64:ARG:HH21	2.41	0.42
32:2a:980:C:H3'	32:2a:981:U:C6	2.54	0.42
32:2a:1099:G:OP2	33:2b:144:ARG:NH2	2.52	0.42
33:2b:28:PHE:HE1	33:2b:192:SER:HB2	1.84	0.42
35:2d:110:PHE:N	35:2d:110:PHE:CD1	2.85	0.42
1:1A:64:A:O3'	19:1X:71:GLY:HA3	2.19	0.42
1:1A:302:C:P	20:1Y:73:ARG:HH22	2.42	0.42
1:1A:363(A):A:H2'	1:1A:363(B):G:C8	2.54	0.42
1:1A:674:G:O2'	5:1F:74:ARG:HD3	2.19	0.42
1:1A:743:G:OP1	4:1E:130:GLY:HA2	2.19	0.42
1:1A:1371:G:H2'	1:1A:1372:U:H5	1.85	0.42
1:1A:1503:U:H2'	1:1A:1504:C:H6	1.84	0.42
61:1A:7088:HOH:O	18:1W:92:ARG:HD2	2.18	0.42
5:1F:64:ILE:HD11	5:1F:75:HIS:HB2	2.00	0.42
7:1H:13:LYS:HA	7:1H:14:GLY:HA2	1.53	0.42
10:1O:115:VAL:O	57:1a:1880:MPD:H13	2.20	0.42
11:1P:98:GLU:HG3	11:1P:102:ARG:NH2	2.33	0.42
32:1a:92:C:H2'	32:1a:93:G:C8	2.55	0.42
32:1a:250:A:H4'	32:1a:251:G:O5'	2.18	0.42
32:1a:376:G:H2'	32:1a:377:G:H8	1.84	0.42
1:2A:184:C:H2'	1:2A:185:U:C6	2.54	0.42
1:2A:897:C:H2'	1:2A:898:C:H6	1.82	0.42
1:2A:981:A:N1	1:2A:2027:G:O2'	2.48	0.42
1:2A:2144:U:O2'	1:2A:2147:G:N1	2.50	0.42
1:2A:2149:G:C2	1:2A:2150:U:H1'	2.55	0.42
3:2D:29:PRO:HB2	3:2D:34:VAL:HG11	2.01	0.42
10:2O:35:VAL:HG13	10:2O:65:THR:HG23	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:22:65:ASN:O	24:22:69:ARG:HG3	2.18	0.42
26:24:20:ASN:HD21	26:24:38:LYS:HD2	1.83	0.42
32:2a:189(K):U:H2'	32:2a:189(L):G:C8	2.55	0.42
32:2a:942:G:C2	32:2a:1342:C:C2	3.07	0.42
32:2a:1330:U:H2'	32:2a:1331:G:H5'	2.02	0.42
33:2b:15:VAL:HG23	33:2b:16:HIS:HD2	1.84	0.42
48:2q:38:ARG:HD3	48:2q:38:ARG:HA	1.87	0.42
3:1D:16:MET:HE3	3:1D:16:MET:HB2	1.81	0.42
3:1D:38:LYS:HD2	3:1D:38:LYS:HA	1.63	0.42
4:1E:119:ARG:HG2	4:1E:160:TYR:HB2	2.01	0.42
6:1G:50:ALA:O	6:1G:52:ILE:N	2.52	0.42
17:1V:76:LYS:HB2	17:1V:81:TYR:HB3	2.01	0.42
26:14:50:VAL:HG21	44:1m:64:TRP:C	2.45	0.42
32:1a:189(D):C:H2'	32:1a:189(E):U:O4'	2.20	0.42
32:1a:376:G:OP1	47:1p:5:ARG:HB2	2.20	0.42
32:1a:1029:C:N3	32:1a:1032:G:O6	2.53	0.42
32:1a:1128:C:H5"	40:1i:66:ARG:HH22	1.84	0.42
32:1a:1171:G:H2'	32:1a:1172:C:C6	2.55	0.42
32:1a:1186:G:O3'	40:1i:113:LYS:HE2	2.18	0.42
34:1c:22:TRP:CH2	45:1n:54:PRO:HG2	2.54	0.42
50:1s:80:TYR:CZ	50:1s:82:GLY:HA2	2.55	0.42
1:2A:673:C:H5"	5:2F:81:PRO:HD2	2.00	0.42
1:2A:1062:G:N7	1:2A:1070:A:H1'	2.34	0.42
1:2A:1248:G:C5	16:2U:3:ARG:HB2	2.55	0.42
3:2D:35:LYS:HB2	3:2D:36:PRO:HD2	2.02	0.42
12:2Q:38:GLU:HA	12:2Q:99:PRO:HG3	2.00	0.42
18:2W:6:ILE:HG12	18:2W:104:THR:HG23	2.02	0.42
32:2a:80:G:N2	32:2a:90:U:H1'	2.34	0.42
32:2a:129(A):G:C6	32:2a:189(E):U:H4'	2.54	0.42
32:2a:443:C:H2'	32:2a:444:C:C6	2.55	0.42
32:2a:1030(D):A:N7	32:2a:1031:G:C4	2.87	0.42
32:2a:1124:G:H4'	32:2a:1125:U:OP1	2.19	0.42
32:2a:1515:C:H2'	32:2a:1516:G:C8	2.53	0.42
33:2b:161:ALA:HB1	33:2b:185:ILE:HD11	2.01	0.42
33:2b:162:ILE:O	33:2b:185:ILE:HD12	2.19	0.42
41:2j:16:LEU:HD23	41:2j:16:LEU:HA	1.83	0.42
44:2m:4:ILE:O	44:2m:6:GLY:N	2.44	0.42
44:2m:25:ILE:HG23	44:2m:29:ARG:HB2	2.01	0.42
1:1A:548:A:N6	17:1V:19:LYS:H	2.17	0.42
1:1A:839:U:H2'	1:1A:840:C:C6	2.54	0.42
1:1A:1075:C:OP1	12:1Q:59:ARG:NH2	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1759:A:H1'	1:1A:2711:A:C2	2.54	0.42
1:1A:1818:U:O4	3:1D:154:LYS:HD3	2.19	0.42
1:1A:2689:U:H4'	1:1A:2690:C:H5'	2.01	0.42
6:1G:3:LEU:HD22	26:14:25:TYR:CE1	2.54	0.42
7:1H:12:PRO:O	7:1H:15:VAL:HG13	2.19	0.42
26:14:24:THR:OG1	26:14:25:TYR:N	2.52	0.42
32:1a:460:G:N2	32:1a:471:G:N7	2.67	0.42
32:1a:986:A:H2'	32:1a:987:G:O4'	2.19	0.42
32:1a:1070:U:H2'	32:1a:1071:C:C6	2.54	0.42
32:1a:1410:G:H2'	32:1a:1411:C:C6	2.54	0.42
34:1c:69:HIS:HA	34:1c:104:GLN:HB3	2.00	0.42
44:1m:108:ARG:HD3	44:1m:108:ARG:HA	1.81	0.42
50:1s:22:LEU:HD12	50:1s:31:ILE:HD11	2.02	0.42
1:2A:2330:G:H2'	1:2A:2331:G:O4'	2.19	0.42
1:2A:2573:C:H3'	61:2A:4221:HOH:O	2.19	0.42
2:2B:55:U:O3'	6:2G:27:ASN:ND2	2.52	0.42
5:2F:179:GLU:CD	5:2F:179:GLU:H	2.28	0.42
7:2H:103:LEU:O	7:2H:114:VAL:HA	2.20	0.42
8:2I:62:LYS:HG3	8:2I:136:VAL:HG21	2.01	0.42
10:2O:120:GLU:HB2	15:2T:68:TYR:CE2	2.55	0.42
14:2S:11:LYS:HE3	14:2S:15:ARG:HH22	1.84	0.42
32:2a:328:C:H4'	32:2a:329:A:H5'	2.01	0.42
32:2a:671:G:H2'	32:2a:672:U:O4'	2.19	0.42
32:2a:814:A:N7	32:2a:816:A:C4	2.87	0.42
32:2a:818:G:O2'	32:2a:819:A:H5'	2.19	0.42
33:2b:51:LEU:O	33:2b:55:PHE:HB2	2.19	0.42
34:2c:121:ALA:HB2	34:2c:198:VAL:HG21	2.02	0.42
36:2e:40:ARG:HA	36:2e:67:VAL:O	2.19	0.42
47:2p:43:LYS:C	47:2p:45:THR:H	2.27	0.42
1:1A:1607:C:H4'	1:1A:1608:A:O5'	2.19	0.42
1:1A:1762:A:H2'	61:1A:7353:HOH:O	2.20	0.42
1:1A:2142:C:O2	1:1A:2149:G:N1	2.51	0.42
1:1A:2292:C:OP1	14:1S:17:ARG:NH2	2.52	0.42
8:1I:131:LYS:HB2	8:1I:131:LYS:HE3	1.84	0.42
20:1Y:42:VAL:HG11	20:1Y:67:LEU:HD11	2.00	0.42
32:1a:631:G:H2'	32:1a:632:A:C8	2.55	0.42
33:1b:16:HIS:CG	33:1b:17:PHE:N	2.87	0.42
37:1f:9:VAL:HB	37:1f:87:ARG:HB2	2.02	0.42
39:1h:81:HIS:N	39:1h:138:TRP:O	2.53	0.42
1:2A:12:U:O2	1:2A:12:U:H2'	2.20	0.42
1:2A:721:C:H2'	1:2A:722:A:C8	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:740:U:H2'	1:2A:741:G:C8	2.54	0.42
1:2A:839:U:H2'	1:2A:840:C:H6	1.84	0.42
1:2A:910:A:C6	1:2A:911:A:C6	3.08	0.42
1:2A:927:G:H2'	1:2A:928:G:O4'	2.18	0.42
1:2A:1027:A:C6	1:2A:1126:A:C4	3.08	0.42
1:2A:1035:U:H2'	1:2A:1036:G:H8	1.85	0.42
1:2A:1138:G:N3	9:2N:106:MET:HE2	2.35	0.42
1:2A:1159:U:H2'	1:2A:1160:G:H8	1.84	0.42
1:2A:1702:G:H2'	1:2A:1703:G:O4'	2.20	0.42
1:2A:2134:A:O2'	1:2A:2159:G:H1'	2.20	0.42
6:2G:32:PRO:HB3	6:2G:163:ALA:HB2	2.00	0.42
7:2H:163:TYR:CE1	7:2H:169:VAL:HG22	2.54	0.42
10:2O:112:MET:HE2	10:2O:112:MET:HB2	1.80	0.42
32:2a:542:G:H5'	35:2d:41:GLY:HA3	2.01	0.42
32:2a:757:U:OP1	32:2a:822:C:O2'	2.31	0.42
32:2a:1009:G:H2'	32:2a:1009:G:N3	2.35	0.42
32:2a:1010:G:C2	32:2a:1020:U:H1'	2.55	0.42
32:2a:1220:G:O3'	50:2s:36:ARG:HD3	2.19	0.42
32:2a:1276:G:H2'	32:2a:1277:C:C6	2.55	0.42
35:2d:20:TYR:CD1	35:2d:26:CYS:HB3	2.54	0.42
36:2e:12:LEU:O	36:2e:30:ALA:HA	2.19	0.42
36:2e:143:ARG:HD2	39:2h:77:GLU:OE2	2.19	0.42
37:2f:95:GLU:O	49:2r:32:ARG:HD2	2.19	0.42
40:2i:25:LYS:H	40:2i:60:ASP:HB3	1.84	0.42
42:2k:79:SER:HB2	42:2k:104:GLN:HB3	2.02	0.42
47:2p:4:ILE:HA	47:2p:20:VAL:O	2.20	0.42
47:2p:43:LYS:HA	47:2p:48:TRP:CB	2.50	0.42
48:2q:41:LYS:NZ	48:2q:92:ARG:HH21	2.16	0.42
1:1A:1628:G:H2'	1:1A:1629:U:C6	2.54	0.42
1:1A:1790:C:H2'	1:1A:1791:A:C5	2.54	0.42
1:1A:2695:C:H2'	1:1A:2696:U:C6	2.55	0.42
1:1A:2722:G:H2'	1:1A:2723:C:C6	2.55	0.42
14:1S:92:TYR:OH	61:1S:201:HOH:O	2.21	0.42
24:12:59:ARG:NH2	61:12:102:HOH:O	2.52	0.42
32:1a:130:A:H1'	32:1a:263:A:O2'	2.19	0.42
32:1a:1216:G:H5"	45:1n:5:ALA:HB2	2.00	0.42
39:1h:39:LEU:HB3	39:1h:45:ILE:HG12	2.01	0.42
47:1p:4:ILE:HG22	47:1p:19:ILE:HD11	2.00	0.42
1:2A:61:G:OP1	24:22:51:ARG:NH2	2.52	0.42
1:2A:1064:C:H42	1:2A:1074:G:H1	1.66	0.42
1:2A:2122:U:H2'	1:2A:2123:G:H8	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2282:G:H4'	1:2A:2389:G:O2'	2.19	0.42
4:2E:1:MET:O	4:2E:84:PHE:HB2	2.19	0.42
6:2G:112:PRO:HG3	26:24:43:TYR:CE2	2.54	0.42
9:2N:120:LEU:HG	9:2N:122:VAL:HG23	2.02	0.42
20:2Y:13:VAL:HB	20:2Y:72:VAL:HG13	2.01	0.42
25:23:26:LEU:O	25:23:35:ARG:NE	2.49	0.42
26:24:44:THR:O	26:24:46:GLN:N	2.53	0.42
32:2a:588:G:H4'	39:2h:2:LEU:HD23	2.02	0.42
32:2a:768:A:OP2	61:2a:3213:HOH:O	2.21	0.42
32:2a:1002:G:N2	32:2a:1039:C:C2	2.88	0.42
32:2a:1118:C:H1'	32:2a:1179:A:C4	2.55	0.42
35:2d:110:PHE:N	35:2d:110:PHE:HD1	2.18	0.42
51:2t:51:GLU:HA	51:2t:54:LYS:HE2	2.01	0.42
1:1A:744:G:OP1	4:1E:132:HIS:ND1	2.44	0.42
1:1A:817:C:H4'	1:1A:932:G:C5	2.55	0.42
1:1A:1052:C:N4	1:1A:1107:G:H1	2.16	0.42
1:1A:1113:U:H2'	1:1A:1114:G:H8	1.84	0.42
1:1A:2114:A:H3'	1:1A:2115:G:H8	1.85	0.42
1:1A:2431:U:OP1	61:1A:4147:HOH:O	2.22	0.42
1:1A:2693:A:H2'	1:1A:2694:G:C8	2.55	0.42
1:1A:2751:G:H4'	7:1H:4:ILE:HD11	2.01	0.42
3:1D:26:LYS:NZ	3:1D:30:GLU:OE1	2.53	0.42
9:1N:12:ARG:NH1	9:1N:50:ASP:OD2	2.53	0.42
32:1a:79:G:C2	32:1a:90:U:O2	2.72	0.42
32:1a:384:G:H2'	32:1a:385:C:C6	2.54	0.42
32:1a:447:G:O6	32:1a:485:G:O2'	2.32	0.42
32:1a:1406:U:O2	32:1a:1517:G:N2	2.49	0.42
32:1a:1516:G:H2'	32:1a:1518:MA6:OP2	2.20	0.42
33:1b:18:GLY:HA2	33:1b:204:ASN:HB2	2.02	0.42
33:1b:53:ARG:HA	33:1b:56:ARG:NH1	2.35	0.42
1:2A:652(T):C:H2'	1:2A:652(U):G:C8	2.55	0.42
1:2A:684:G:OP1	29:27:16:HIS:ND1	2.46	0.42
1:2A:748:G:C8	18:2W:89:ALA:HB1	2.55	0.42
1:2A:824:A:H2'	1:2A:825:C:O4'	2.19	0.42
1:2A:862:G:H2'	1:2A:863:A:O4'	2.20	0.42
1:2A:1005:C:H2'	1:2A:1006:C:C6	2.55	0.42
1:2A:1068:G:H3'	1:2A:1096:A:OP2	2.18	0.42
1:2A:1203:G:C6	1:2A:1204:A:N6	2.88	0.42
1:2A:1287:A:O4'	13:2R:104:ARG:HD3	2.20	0.42
1:2A:1593:G:H2'	1:2A:1594:G:H8	1.83	0.42
1:2A:1630:G:H2'	1:2A:1631:C:C6	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1667:G:O2'	1:2A:1991:U:O4	2.31	0.42
1:2A:2519:U:C2	1:2A:2542:A:C6	3.08	0.42
1:2A:2728:U:H2'	1:2A:2729:G:C8	2.55	0.42
6:2G:83:ARG:H	6:2G:86:MET:CE	2.31	0.42
11:2P:6:LEU:HD23	11:2P:6:LEU:HA	1.80	0.42
32:2a:259:G:H2'	32:2a:260:G:O4'	2.20	0.42
32:2a:584:G:O6	61:2a:3211:HOH:O	2.20	0.42
32:2a:666:G:H5'	32:2a:726:C:H1'	2.01	0.42
32:2a:1027:C:C4	32:2a:1034:G:O6	2.72	0.42
32:2a:1132:C:H2'	32:2a:1133:G:O4'	2.20	0.42
32:2a:1269:A:H2	32:2a:1312:G:N3	2.18	0.42
33:2b:30:ARG:HG3	33:2b:31:TYR:CD1	2.55	0.42
33:2b:167:PRO:HD3	33:2b:187:LEU:O	2.19	0.42
37:2f:3:ARG:HD3	37:2f:64:GLN:HE21	1.85	0.42
1:1A:1041:C:H5'	1:1A:1042:G:OP2	2.20	0.42
1:1A:1503:U:H2'	1:1A:1504:C:C6	2.54	0.42
1:1A:2156:G:H2'	1:1A:2157:G:O4'	2.20	0.42
1:1A:2522:U:O2'	1:1A:2647:U:OP1	2.32	0.42
3:1D:206:LEU:HD22	3:1D:211:ARG:HG2	2.00	0.42
11:1P:121:LYS:O	11:1P:123:LEU:N	2.53	0.42
19:1X:93:GLU:O	19:1X:95:LEU:HD13	2.19	0.42
21:1Z:48:PHE:CE1	21:1Z:71:VAL:HG11	2.54	0.42
21:1Z:146:ILE:HA	21:1Z:147:GLY:HA2	1.73	0.42
22:10:10:THR:HA	61:10:213:HOH:O	2.18	0.42
32:1a:456:C:H2'	32:1a:457:C:C6	2.54	0.42
32:1a:974:A:P	45:1n:29:ARG:HH21	2.42	0.42
36:1e:87:SER:OG	36:1e:125:SER:O	2.35	0.42
53:1y:26:LYS:HD3	53:1y:78:ILE:HG21	2.01	0.42
1:2A:27:G:N2	1:2A:512:G:H1'	2.34	0.42
1:2A:801:G:OP2	5:2F:55:GLY:HA2	2.20	0.42
1:2A:918:A:N3	2:2B:80:U:O2'	2.49	0.42
1:2A:1186:G:OP1	61:2A:3869:HOH:O	2.22	0.42
1:2A:1509(B):A:H8	1:2A:1509(B):A:O5'	2.03	0.42
1:2A:1714:G:H2'	1:2A:1717:G:H8	1.85	0.42
1:2A:2115:G:H3'	1:2A:2116:G:C5'	2.50	0.42
1:2A:2203:U:H2'	1:2A:2205:C:C6	2.54	0.42
1:2A:2539:C:H4'	31:29:3:VAL:HG21	2.01	0.42
1:2A:2680:C:H1'	4:2E:187:ALA:HB1	2.02	0.42
1:2A:2869:G:H2'	1:2A:2870:C:O4'	2.18	0.42
5:2F:183:VAL:O	5:2F:187:VAL:HG23	2.19	0.42
6:2G:144:ILE:HA	6:2G:148:MET:SD	2.60	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:2H:118:PRO:HD2	7:2H:121:ILE:HB	2.02	0.42
14:2S:53:SER:OG	14:2S:54:LEU:N	2.53	0.42
23:21:67:ILE:N	23:21:68:PRO:HD2	2.35	0.42
32:2a:471:G:H2'	32:2a:472:A:H8	1.84	0.42
32:2a:611:A:H2	32:2a:630:G:N2	2.18	0.42
32:2a:1119:C:P	40:2i:9:ARG:HH22	2.43	0.42
32:2a:1207:2MG:H2'	32:2a:1208:C:H6	1.85	0.42
33:2b:15:VAL:O	33:2b:17:PHE:N	2.52	0.42
39:2h:103:VAL:CG2	39:2h:110:ALA:HB2	2.50	0.42
49:2r:52:PRO:O	49:2r:56:THR:HG23	2.20	0.42
53:2y:27:LEU:HD11	53:2y:81:LEU:HD13	2.01	0.42
1:1A:493:G:H2'	1:1A:494:G:O4'	2.20	0.42
1:1A:1171:G:H3'	1:1A:1173:G:H5'	2.01	0.42
1:1A:1377:G:H2'	61:1A:6635:HOH:O	2.20	0.42
1:1A:2171:A:H1'	1:1A:2172:U:C5	2.55	0.42
1:1A:2305:A:H5"	6:1G:134:GLY:HA3	2.02	0.42
1:1A:2887:U:H2'	1:1A:2888:C:C6	2.54	0.42
2:1B:2:C:H2'	2:1B:3:C:H6	1.84	0.42
3:1D:245:PRO:HA	3:1D:246:PRO:HD3	1.93	0.42
9:1N:48:MET:HE3	9:1N:48:MET:C	2.45	0.42
10:1O:122:LEU:HD13	15:1T:72:VAL:HG11	2.02	0.42
15:1T:1:MET:HE2	15:1T:3:ARG:HG3	2.01	0.42
17:1V:49:THR:HG22	17:1V:49:THR:O	2.19	0.42
20:1Y:34:LYS:O	20:1Y:34:LYS:HD3	2.20	0.42
21:1Z:91:LEU:HD22	21:1Z:130:PRO:HG3	2.01	0.42
27:15:20:ARG:HG2	27:15:23:HIS:CE1	2.55	0.42
32:1a:410:G:P	35:1d:30:LYS:HZ1	2.41	0.42
32:1a:1164:G:H2'	32:1a:1165:C:C6	2.54	0.42
32:1a:1296:C:H4'	32:1a:1302:U:C4	2.55	0.42
32:1a:1492:A:H4'	32:1a:1493:A:C6	2.54	0.42
35:1d:172:PRO:HB2	35:1d:187:ARG:NH2	2.34	0.42
36:1e:20:GLN:NE2	36:1e:25:ARG:HD2	2.35	0.42
43:1l:40:VAL:HG11	43:1l:77:LEU:O	2.20	0.42
53:1y:3:MET:HG3	53:1y:37:PRO:HG2	2.02	0.42
1:2A:1461:G:H2'	1:2A:1462:C:C6	2.54	0.42
1:2A:2019:A:O4'	16:2U:34:LYS:HE2	2.20	0.42
1:2A:2092:U:H4'	1:2A:2093:G:O5'	2.19	0.42
1:2A:2660:A:N7	7:2H:175:LYS:NZ	2.57	0.42
1:2A:2732:G:H3'	1:2A:2733:A:O4'	2.19	0.42
21:2Z:24:LEU:HA	21:2Z:25:PRO:HD3	1.92	0.42
32:2a:109:A:C6	32:2a:326:G:C6	3.08	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:539:A:C6	32:2a:540:G:C6	3.08	0.42
36:2e:17:ALA:HB2	36:2e:26:PHE:CD1	2.55	0.42
44:2m:20:THR:C	44:2m:22:ILE:H	2.28	0.42
50:2s:50:ALA:CB	50:2s:57:HIS:HB3	2.45	0.42
1:1A:2723:C:OP1	13:1R:3:HIS:ND1	2.44	0.41
3:1D:34:VAL:HA	3:1D:62:TYR:O	2.20	0.41
5:1F:64:ILE:HD12	5:1F:65:TRP:CZ3	2.55	0.41
7:1H:33:LEU:HD21	7:1H:136:ILE:HG13	2.01	0.41
9:1N:33:LEU:HD12	9:1N:38:HIS:CE1	2.55	0.41
11:1P:6:LEU:HA	11:1P:6:LEU:HD23	1.75	0.41
24:12:53:LEU:HD23	24:12:53:LEU:HA	1.87	0.41
32:1a:404:U:H2'	32:1a:405:U:C6	2.55	0.41
32:1a:1118:C:H2'	32:1a:1119:C:C6	2.55	0.41
32:1a:1492:A:H4'	32:1a:1493:A:N1	2.35	0.41
32:1a:1521:G:H2'	32:1a:1522:U:C6	2.55	0.41
35:1d:188:LEU:HD23	35:1d:188:LEU:HA	1.92	0.41
45:1n:53:LEU:HB2	45:1n:56:VAL:HB	2.02	0.41
1:2A:335:C:H4'	20:2Y:73:ARG:NH1	2.34	0.41
1:2A:1665:A:H4'	10:2O:67:LYS:HB2	2.02	0.41
1:2A:1970:A:N1	61:2A:3977:HOH:O	2.36	0.41
1:2A:2695:C:H2'	1:2A:2696:U:H6	1.84	0.41
2:2B:37:C:N3	2:2B:48:A:O2'	2.49	0.41
2:2B:45:A:H2'	2:2B:46:A:C8	2.54	0.41
4:2E:13:ARG:HG2	15:2T:58:ASN:HD21	1.84	0.41
5:2F:149:ASP:N	5:2F:149:ASP:OD1	2.52	0.41
6:2G:42:GLY:HA2	6:2G:89:GLY:CA	2.50	0.41
14:2S:23:ARG:NH1	14:2S:85:VAL:H	2.17	0.41
32:2a:1501:C:OP2	32:2a:1504:G:O2'	2.25	0.41
32:2a:1512:U:H2'	32:2a:1513:A:H8	1.83	0.41
33:2b:167:PRO:HG3	33:2b:188:ALA:HB2	2.02	0.41
33:2b:180:LEU:C	33:2b:182:ILE:H	2.28	0.41
41:2j:38:ILE:HD13	41:2j:71:LEU:HD22	2.02	0.41
42:2k:50:TYR:HD2	42:2k:60:ALA:HB2	1.85	0.41
42:2k:62:GLN:HG3	42:2k:97:ALA:HB2	2.02	0.41
47:2p:18:ARG:HG2	47:2p:35:LYS:HE3	2.02	0.41
1:1A:218:A:C2	1:1A:235:U:H4'	2.55	0.41
1:1A:374:A:C2	1:1A:401:A:C4	3.09	0.41
1:1A:2120:G:C2	1:1A:2179:C:C2	3.09	0.41
1:1A:2552:2MU:O5'	1:1A:2552:2MU:H6	2.21	0.41
1:1A:2612:C:OP2	27:15:2:ALA:N	2.53	0.41
2:1B:66:A:H61	2:1B:109:C:H5"	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1D:132:PRO:HG3	3:1D:190:TYR:CE2	2.56	0.41
11:1P:86:LYS:HG3	11:1P:87:ASP:N	2.35	0.41
17:1V:71:LEU:HA	17:1V:71:LEU:HD23	1.84	0.41
32:1a:165:C:H2'	32:1a:166:G:C8	2.55	0.41
32:1a:189(C):C:H2'	32:1a:189(D):C:O4'	2.20	0.41
32:1a:448:A:C4	32:1a:487:A:C2	3.07	0.41
32:1a:458:C:H2'	32:1a:460:G:H8	1.85	0.41
32:1a:1068:G:N2	32:1a:1191:A:N3	2.63	0.41
32:1a:1469:G:H2'	32:1a:1470:G:C8	2.55	0.41
35:1d:119:GLN:HG3	35:1d:123:HIS:CE1	2.55	0.41
38:1g:12:LEU:O	38:1g:21:VAL:HG12	2.20	0.41
42:1k:99:GLN:HE21	42:1k:105:VAL:HG21	1.85	0.41
44:1m:4:ILE:HG22	44:1m:57:ARG:HE	1.86	0.41
44:1m:34:LEU:HD13	44:1m:41:PRO:HA	2.01	0.41
49:1r:47:THR:HG23	49:1r:49:LYS:HG3	2.02	0.41
50:1s:27:GLU:CB	50:1s:28:LYS:HB3	2.50	0.41
1:2A:952:G:C6	1:2A:953:A:N7	2.88	0.41
1:2A:1970:A:H4'	1:2A:1971:A:OP1	2.19	0.41
1:2A:2543:G:H2'	1:2A:2544:G:C8	2.54	0.41
2:2B:34:U:O4	2:2B:44:G:O2'	2.28	0.41
2:2B:60:C:H2'	2:2B:61:G:C8	2.55	0.41
3:2D:70:TRP:HB3	3:2D:190:TYR:CE2	2.54	0.41
4:2E:101:ARG:HA	4:2E:170:LEU:O	2.21	0.41
6:2G:125:PHE:CE1	6:2G:131:TYR:HB2	2.55	0.41
21:2Z:110:GLY:HA3	21:2Z:174:VAL:HG11	2.02	0.41
29:27:5:TRP:CD1	29:27:7:PRO:HD3	2.55	0.41
32:2a:42:G:O2'	32:2a:622:A:N1	2.47	0.41
32:2a:299:G:H2'	32:2a:300:A:C8	2.56	0.41
32:2a:391:G:P	47:2p:28:ARG:HH22	2.42	0.41
32:2a:408:A:H4'	35:2d:112:VAL:HG21	2.02	0.41
32:2a:1004:A:N6	32:2a:1037:C:C6	2.88	0.41
32:2a:1122:U:C2	32:2a:1123:A:C8	3.09	0.41
32:2a:1270:C:O2'	32:2a:1314:C:H5'	2.21	0.41
35:2d:11:LEU:O	35:2d:15:GLU:HG2	2.20	0.41
40:2i:8:GLY:CA	40:2i:79:LEU:HB3	2.51	0.41
45:2n:6:LEU:HA	45:2n:9:LYS:HB2	2.02	0.41
46:2o:87:ILE:HG22	46:2o:88:ARG:N	2.35	0.41
1:1A:861:A:H2'	1:1A:862:G:O4'	2.21	0.41
1:1A:2147:G:H2'	1:1A:2148:G:C4'	2.50	0.41
1:1A:2151:G:H2'	1:1A:2152:G:O4'	2.20	0.41
2:1B:90:A:N7	2:1B:91:C:H1'	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1I:9:LEU:HA	8:1I:9:LEU:HD13	1.70	0.41
8:1I:117:GLU:HG3	8:1I:118:LYS:H	1.86	0.41
8:1I:132:PRO:HD2	8:1I:136:VAL:O	2.21	0.41
32:1a:457:C:H2'	32:1a:458:C:H6	1.84	0.41
33:1b:219:VAL:HA	33:1b:222:ILE:HD12	2.01	0.41
35:1d:108:LEU:HD23	35:1d:110:PHE:CZ	2.55	0.41
36:1e:66:MET:HE3	36:1e:66:MET:HB3	1.82	0.41
40:1i:55:ALA:HB1	40:1i:59:PHE:CD2	2.55	0.41
1:2A:185:U:H2'	1:2A:186:G:C8	2.55	0.41
1:2A:858:U:O2	1:2A:2268:A:H2'	2.21	0.41
1:2A:2784:C:H1'	4:2E:37:ARG:NH1	2.35	0.41
1:2A:2872:G:O2'	1:2A:2873:A:H5'	2.19	0.41
26:24:13:ARG:HA	26:24:22:ILE:O	2.21	0.41
32:2a:736:C:H2'	32:2a:737:A:C8	2.55	0.41
32:2a:978:A:O2'	32:2a:1322:C:N3	2.45	0.41
32:2a:1320:C:C2	50:2s:72:GLY:HA3	2.55	0.41
33:2b:11:LEU:HD12	33:2b:217:ARG:HH12	1.85	0.41
34:2c:70:VAL:HG12	34:2c:72:LYS:H	1.86	0.41
39:2h:95:VAL:HB	39:2h:99:GLU:HG3	2.01	0.41
44:2m:66:LEU:O	44:2m:70:LEU:HB3	2.19	0.41
50:2s:12:ASP:OD2	50:2s:35:SER:OG	2.36	0.41
1:1A:271(L):U:H4'	8:1I:50:ARG:NH1	2.36	0.41
1:1A:889:C:O2'	1:1A:890:A:O5'	2.34	0.41
1:1A:927:G:H2'	1:1A:928:G:O4'	2.19	0.41
1:1A:980:A:C4	1:1A:1136:G:O4'	2.73	0.41
1:1A:1069:A:O2'	1:1A:1073:A:C6	2.71	0.41
1:1A:1652:A:C2'	1:1A:1653:G:H5'	2.50	0.41
1:1A:2347:C:H2'	1:1A:2348:U:C6	2.55	0.41
1:1A:2734:A:H2'	1:1A:2735:G:O4'	2.20	0.41
2:1B:41:U:H5	6:1G:70:VAL:O	2.04	0.41
3:1D:97:TYR:C	3:1D:99:ASP:N	2.78	0.41
4:1E:119:ARG:CG	4:1E:160:TYR:HB2	2.50	0.41
11:1P:11:GLY:O	61:1P:302:HOH:O	2.22	0.41
32:1a:848:C:H2'	32:1a:849:C:O4'	2.21	0.41
33:1b:187:LEU:HD12	33:1b:201:ILE:O	2.20	0.41
51:1t:60:GLU:HG3	51:1t:81:LYS:HE3	2.01	0.41
1:2A:118:A:C8	1:2A:119:A:C8	3.09	0.41
1:2A:311:A:C6	1:2A:328:U:C4	3.07	0.41
1:2A:581:C:H2'	1:2A:582:G:C8	2.55	0.41
1:2A:699:A:H2'	1:2A:700:G:O4'	2.20	0.41
1:2A:874:G:OP1	12:2Q:63:LYS:NZ	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2168:G:H22	1:2A:2171:A:H2'	1.85	0.41
1:2A:2251:OMG:C8	1:2A:2450:A:H4'	2.55	0.41
6:2G:70:VAL:HG23	6:2G:90:LEU:HD12	2.03	0.41
6:2G:78:SER:OG	6:2G:79:ASN:N	2.54	0.41
16:2U:102:GLU:OE2	17:2V:13:ARG:NH1	2.32	0.41
20:2Y:87:LYS:HB3	20:2Y:95:LYS:HD2	2.02	0.41
21:2Z:144:LEU:HD11	21:2Z:150:LEU:HG	2.02	0.41
25:23:3:ARG:HG2	25:23:38:GLU:HA	2.02	0.41
32:2a:64:G:H4'	32:2a:65:U:H3'	2.01	0.41
32:2a:229:U:O2'	47:2p:23:ASP:OD2	2.35	0.41
32:2a:381:C:H2'	32:2a:382:A:O4'	2.20	0.41
32:2a:445:G:H2'	32:2a:446:G:O4'	2.19	0.41
32:2a:504:C:H1'	32:2a:510:A:C4	2.55	0.41
32:2a:685:G:O2'	32:2a:686:U:H5'	2.21	0.41
32:2a:790:A:H4'	53:2y:31:GLN:OE1	2.20	0.41
32:2a:841:U:H6	32:2a:841:U:P	2.43	0.41
32:2a:1189:C:H5"	34:2c:5:ILE:HD12	2.02	0.41
32:2a:1206:G:C6	32:2a:1207:2MG:C6	3.08	0.41
32:2a:1297:C:OP2	44:2m:44:ARG:NH2	2.52	0.41
37:2f:2:ARG:CZ	37:2f:69:GLU:HG2	2.50	0.41
44:2m:3:ARG:HB2	44:2m:9:ILE:H	1.85	0.41
47:2p:43:LYS:HA	47:2p:48:TRP:HB2	2.02	0.41
1:1A:2378:A:H2'	14:1S:21:THR:HG21	2.02	0.41
1:1A:2472:G:H2'	1:1A:2475:C:H42	1.86	0.41
1:1A:2521:C:C4	1:1A:2522:U:C4	3.09	0.41
2:1B:31:C:H4'	6:1G:29:TRP:CH2	2.56	0.41
7:1H:98:LEU:HD12	7:1H:98:LEU:HA	1.86	0.41
16:1U:76:TYR:CZ	16:1U:80:ILE:HG13	2.55	0.41
32:1a:115:G:H4'	32:1a:116:A:O5'	2.19	0.41
32:1a:160:A:H2'	32:1a:161:A:O4'	2.19	0.41
32:1a:411:A:OP1	35:1d:30:LYS:NZ	2.38	0.41
32:1a:523:A:N1	43:1l:92:0TD:H6	2.34	0.41
42:1k:70:LYS:HE2	42:1k:70:LYS:HB2	1.86	0.41
1:2A:25:U:C4	1:2A:26:G:C6	3.09	0.41
1:2A:821:A:H2'	1:2A:946:G:H5"	2.02	0.41
1:2A:1762:A:N6	61:2A:4205:HOH:O	2.54	0.41
1:2A:2104:G:O6	1:2A:2185:C:C2	2.73	0.41
4:2E:31:CYS:HB3	4:2E:49:LEU:HB3	2.01	0.41
9:2N:15:LEU:HB2	9:2N:135:PRO:HB2	2.03	0.41
14:2S:95:HIS:C	14:2S:99:LYS:HB2	2.45	0.41
32:2a:189(F):U:C4	48:2q:72:ARG:NH1	2.88	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:380:G:C2	32:2a:384:G:C6	3.08	0.41
32:2a:503:C:OP2	43:2l:116:SER:OG	2.29	0.41
32:2a:517:G:N1	32:2a:533:A:OP2	2.41	0.41
32:2a:1122:U:N3	32:2a:1123:A:N7	2.69	0.41
32:2a:1225:A:H2'	32:2a:1226:C:C5	2.55	0.41
33:2b:83:MET:SD	33:2b:234:PRO:HB2	2.60	0.41
40:2i:127:LYS:HE3	53:2y:60:VAL:HG21	2.01	0.41
50:2s:2:PRO:HB2	50:2s:3:ARG:H	1.56	0.41
50:2s:41:VAL:N	50:2s:44:MET:HE3	2.36	0.41
1:1A:576:U:H2'	1:1A:577:G:C8	2.55	0.41
1:1A:1098:A:H2'	1:1A:1099:G:O4'	2.19	0.41
1:1A:1740:G:H2'	1:1A:1741:A:C8	2.55	0.41
1:1A:1794:U:H2'	1:1A:1795:C:C6	2.55	0.41
1:1A:2106:G:C4	1:1A:2107:C:H1'	2.56	0.41
1:1A:2224:G:H4'	1:1A:2226:C:C2	2.56	0.41
1:1A:2537:U:H2'	1:1A:2538:C:C6	2.56	0.41
1:1A:2567:G:H2'	1:1A:2568:C:C6	2.55	0.41
1:1A:2619:C:H4'	4:1E:151:TYR:O	2.20	0.41
2:1B:6:C:H2'	2:1B:7:G:H5"	2.01	0.41
11:1P:3:LEU:HD12	11:1P:3:LEU:HA	1.92	0.41
16:1U:29:SER:C	16:1U:30:LYS:HD2	2.45	0.41
16:1U:117:GLN:H	16:1U:117:GLN:HG2	1.60	0.41
19:1X:94:GLY:HA3	19:1X:95:LEU:C	2.46	0.41
32:1a:130:A:C8	48:1q:63:ARG:HG3	2.56	0.41
32:1a:542:G:P	35:1d:10:ARG:HH22	2.43	0.41
32:1a:1038:C:H2'	32:1a:1039:C:C6	2.55	0.41
33:1b:87:ARG:NH1	33:1b:233:SER:OG	2.53	0.41
33:1b:189:ASP:HB2	33:1b:190:THR:H	1.72	0.41
34:1c:123:GLN:HE22	34:1c:140:ARG:HH12	1.67	0.41
35:1d:194:LEU:HA	35:1d:194:LEU:HD13	1.63	0.41
38:1g:106:GLN:O	38:1g:110:GLN:HG2	2.20	0.41
46:1o:63:ARG:HG2	46:1o:67:LEU:HD12	2.02	0.41
1:2A:192:C:O2'	1:2A:802:A:N3	2.49	0.41
1:2A:554:U:C4	1:2A:555:U:C4	3.08	0.41
1:2A:570:G:H5"	61:2A:5156:HOH:O	2.19	0.41
1:2A:907:U:H4'	12:2Q:101:ARG:HH22	1.86	0.41
1:2A:1024:G:C6	1:2A:1025:G:C6	3.09	0.41
1:2A:1101:U:H2'	1:2A:1102:C:C6	2.47	0.41
1:2A:2307:G:H8	1:2A:2307:G:OP1	2.03	0.41
1:2A:2511:U:O2'	4:2E:138:PRO:O	2.34	0.41
2:2B:39:A:O2'	2:2B:46:A:N1	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2F:53:THR:HG23	5:2F:55:GLY:N	2.35	0.41
32:2a:181:G:H4'	32:2a:182:U:H5'	2.02	0.41
32:2a:310:G:H4'	47:2p:31:LYS:HD3	2.02	0.41
32:2a:336:C:H2'	32:2a:337:C:C6	2.55	0.41
32:2a:685:G:C2	32:2a:686:U:C4	3.08	0.41
33:2b:134:GLU:HA	33:2b:137:ARG:NH2	2.34	0.41
38:2g:50:ILE:HD11	38:2g:58:PRO:HA	2.03	0.41
39:2h:112:LEU:HA	39:2h:134:ILE:HG12	2.01	0.41
40:2i:24:GLY:HA3	40:2i:57:GLY:HA2	2.01	0.41
40:2i:46:ALA:HB2	40:2i:74:ILE:HG23	2.03	0.41
44:2m:89:GLY:O	44:2m:93:ARG:HG3	2.20	0.41
1:1A:476:G:H4'	1:1A:502:A:N1	2.36	0.41
1:1A:527:C:N3	1:1A:2779:U:H2'	2.36	0.41
1:1A:581:C:H2'	1:1A:582:G:C8	2.56	0.41
1:1A:657:U:H2'	1:1A:658:C:C6	2.56	0.41
1:1A:1131:G:H21	9:1N:73:THR:HG21	1.86	0.41
1:1A:1188:U:H4'	17:1V:79:VAL:HG22	2.01	0.41
1:1A:1678:G:H5"	1:1A:1678:G:N3	2.35	0.41
1:1A:2162:G:H4'	1:1A:2172:U:O2'	2.21	0.41
1:1A:2183:C:H2'	1:1A:2184:G:H8	1.83	0.41
5:1F:12:LEU:HD12	5:1F:12:LEU:HA	1.83	0.41
6:1G:53:LEU:O	6:1G:56:ALA:N	2.49	0.41
24:12:33:MET:HG3	24:12:36:ARG:NH2	2.36	0.41
25:13:5:LYS:HG3	25:13:36:VAL:HG22	2.03	0.41
32:1a:509:A:N3	32:1a:543:C:O2'	2.45	0.41
32:1a:814:A:H2'	32:1a:816:A:H5"	2.01	0.41
32:1a:1003:G:O2'	32:1a:1004:A:H4'	2.21	0.41
32:1a:1069:C:O2'	32:1a:1192:C:H1'	2.21	0.41
33:1b:75:LYS:HA	33:1b:75:LYS:HD2	1.92	0.41
33:1b:207:ALA:O	33:1b:211:ILE:HG13	2.20	0.41
37:1f:70:ASP:OD1	37:1f:71:ARG:HG3	2.21	0.41
48:1q:66:SER:O	48:1q:70:ARG:NH2	2.53	0.41
51:1t:65:LYS:O	51:1t:68:LYS:HB2	2.21	0.41
53:1y:6:THR:OG1	53:1y:38:HIS:HE1	2.03	0.41
1:2A:579:G:H2'	1:2A:580:C:C6	2.56	0.41
1:2A:614(C):A:C4	5:2F:180:GLY:HA2	2.54	0.41
1:2A:901:A:H2'	1:2A:902:C:O4'	2.20	0.41
1:2A:945:A:C4	1:2A:2448:A:C2	3.08	0.41
1:2A:1112:G:H2'	1:2A:1113:U:O4'	2.21	0.41
1:2A:1178:C:H2'	1:2A:1179:C:H6	1.86	0.41
1:2A:1410:G:H2'	1:2A:1411:C:H6	1.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1557:C:H5”	1:2A:1558:A:OP2	2.21	0.41
1:2A:2168:G:H2’	1:2A:2170:A:OP2	2.21	0.41
1:2A:2286:A:OP1	28:26:29:ASN:ND2	2.54	0.41
1:2A:2345:G:N3	1:2A:2381:C:H2’	2.36	0.41
1:2A:2544:G:H1’	1:2A:2646:C:H4’	2.02	0.41
2:2B:2:C:H2’	2:2B:3:C:C6	2.55	0.41
2:2B:42:C:N3	6:2G:91:ARG:NH1	2.68	0.41
5:2F:129:PHE:HD2	5:2F:163:VAL:HG21	1.86	0.41
6:2G:93:THR:O	6:2G:93:THR:OG1	2.37	0.41
8:2I:14:ASP:OD1	8:2I:15:VAL:N	2.50	0.41
8:2I:48:GLU:HG3	8:2I:52:ARG:HH11	1.85	0.41
8:2I:132:PRO:HD2	8:2I:136:VAL:O	2.21	0.41
11:2P:138:LEU:HD12	11:2P:138:LEU:HA	1.93	0.41
16:2U:76:TYR:CZ	16:2U:80:ILE:HG13	2.55	0.41
32:2a:192:U:H2’	32:2a:193:C:H6	1.86	0.41
32:2a:429:U:H4’	32:2a:430:A:O5’	2.21	0.41
32:2a:512:U:H2’	32:2a:513:C:H6	1.86	0.41
44:2m:49:THR:O	44:2m:52:GLU:N	2.53	0.41
50:2s:41:VAL:O	50:2s:44:MET:HB2	2.21	0.41
1:1A:396:G:H1’	23:11:42:GLN:HB3	2.02	0.41
1:1A:1066:U:O4	1:1A:1069:A:H2’	2.20	0.41
1:1A:1089:G:N2	1:1A:1090:U:O4	2.51	0.41
1:1A:1379:A:H1’	61:1A:5148:HOH:O	2.20	0.41
1:1A:1920:OMC:HM22	1:1A:1921:G:O4’	2.21	0.41
1:1A:2119:A:C6	1:1A:2170:A:C6	3.09	0.41
1:1A:2119:A:O2’	1:1A:2120:G:H5’	2.20	0.41
1:1A:2801(A):A:H1’	1:1A:2895:U:H1’	2.02	0.41
1:1A:2889:C:H2’	1:1A:2891:G:O4’	2.20	0.41
2:1B:74:U:H2’	2:1B:75:G:O4’	2.20	0.41
6:1G:106:LEU:O	6:1G:111:LEU:HG	2.21	0.41
18:1W:18:ARG:NH1	18:1W:76:VAL:O	2.54	0.41
32:1a:15:G:H21	36:1e:18:ARG:HA	1.85	0.41
32:1a:660:G:OP1	46:1o:5:LYS:HE2	2.21	0.41
32:1a:661:G:H1	32:1a:744:C:H42	1.69	0.41
32:1a:1080:A:H5’	36:1e:14:ARG:NH2	2.36	0.41
32:1a:1124:G:N7	32:1a:1145:C:O2’	2.49	0.41
32:1a:1302:U:C5	44:1m:17:VAL:HG21	2.56	0.41
32:1a:1314:C:H2’	32:1a:1315:U:C6	2.56	0.41
33:1b:95:GLN:HG3	33:1b:147:LYS:O	2.20	0.41
40:1i:43:ALA:HA	40:1i:74:ILE:HD13	2.03	0.41
43:1l:77:LEU:HD21	43:1l:107:ALA:HA	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:1m:14:ARG:CZ	44:1m:42:ALA:HA	2.51	0.41
47:1p:70:ALA:O	47:1p:74:LEU:HD12	2.21	0.41
53:1y:55:ASN:HA	53:1y:60:VAL:HA	2.03	0.41
1:2A:1239:G:H2'	1:2A:1240:U:O4'	2.21	0.41
1:2A:1778:U:H2'	1:2A:1784:A:N6	2.35	0.41
1:2A:2335:A:C8	1:2A:2337:G:N7	2.88	0.41
2:2B:43:C:C4	2:2B:45:A:N6	2.89	0.41
6:2G:103:LEU:HA	6:2G:106:LEU:HB3	2.03	0.41
13:2R:29:LEU:HD12	13:2R:29:LEU:HA	1.83	0.41
13:2R:56:LYS:NZ	13:2R:90:ARG:O	2.53	0.41
14:2S:10:ARG:O	14:2S:14:VAL:HG13	2.21	0.41
32:2a:954:G:C5	32:2a:955:U:C4	3.08	0.41
32:2a:1004:A:H5"	32:2a:1025:U:O4	2.20	0.41
33:2b:30:ARG:NH2	33:2b:194:PRO:HB2	2.36	0.41
35:2d:22:LYS:O	35:2d:113:SER:HB3	2.21	0.41
38:2g:101:LEU:O	38:2g:105:VAL:HG23	2.20	0.41
46:2o:26:GLU:OE1	46:2o:26:GLU:N	2.50	0.41
46:2o:62:GLN:O	46:2o:66:LEU:HD13	2.21	0.41
50:2s:50:ALA:HA	50:2s:58:VAL:O	2.21	0.41
1:1A:391:G:H1'	1:1A:411:G:O4'	2.21	0.41
1:1A:548:A:O2'	1:1A:549:G:OP1	2.32	0.41
1:1A:829:A:N7	1:1A:2248:C:H5'	2.36	0.41
1:1A:2059:A:O2'	5:1F:69:HIS:HD2	2.03	0.41
1:1A:2238:G:N3	1:1A:2238:G:H2'	2.35	0.41
1:1A:2319:G:H22	14:1S:3:ARG:CZ	2.34	0.41
1:1A:2627:G:O2'	1:1A:2781:A:N1	2.45	0.41
1:1A:2881:C:H2'	1:1A:2882:A:O4'	2.21	0.41
3:1D:242:ARG:HG3	3:1D:242:ARG:NH1	2.14	0.41
5:1F:150:GLY:HA2	5:1F:172:TRP:CD2	2.56	0.41
6:1G:110:ALA:O	6:1G:140:ILE:HG23	2.21	0.41
7:1H:149:ARG:NH1	7:1H:167:GLU:OE2	2.54	0.41
15:1T:127:ALA:O	15:1T:128:GLU:HB3	2.20	0.41
21:1Z:96:VAL:O	21:1Z:127:LYS:HA	2.21	0.41
27:15:56:LYS:HE3	27:15:58:LEU:O	2.21	0.41
32:1a:4:U:O4	39:1h:105:ARG:HD3	2.21	0.41
32:1a:405:U:H5"	32:1a:495:A:H2	1.86	0.41
32:1a:658:G:H2'	32:1a:659:U:C6	2.56	0.41
32:1a:735:C:H2'	32:1a:736:C:C6	2.54	0.41
32:1a:760:G:H2'	32:1a:761:G:H5'	2.02	0.41
32:1a:975:A:N6	32:1a:1367:C:O4'	2.53	0.41
32:1a:1019:C:H2'	32:1a:1020:U:O4'	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1162:C:H2'	32:1a:1163:C:C6	2.56	0.41
32:1a:1226:C:H4'	32:1a:1227:A:OP1	2.21	0.41
32:1a:1353:G:C2	32:1a:1370:G:C2	3.08	0.41
32:1a:1396:A:C2	36:1e:19:MET:HG3	2.56	0.41
33:1b:208:ILE:O	33:1b:212:GLN:HB3	2.21	0.41
33:1b:231:GLU:HB3	33:1b:232:PRO:HD3	2.02	0.41
35:1d:53:ASP:O	35:1d:57:ARG:HG3	2.21	0.41
35:1d:106:TYR:HE2	35:1d:107:ARG:NH1	2.19	0.41
35:1d:165:MET:SD	35:1d:168:ARG:HG3	2.61	0.41
41:1j:33:GLN:O	41:1j:75:ILE:N	2.54	0.41
41:1j:46:ARG:NH2	41:1j:64:GLU:OE1	2.54	0.41
43:1l:124:LYS:HA	43:1l:125:PRO:HD3	1.94	0.41
44:1m:9:ILE:HB	44:1m:18:ALA:HB1	2.03	0.41
44:1m:16:ASP:OD1	44:1m:17:VAL:N	2.54	0.41
44:1m:87:TYR:O	44:1m:91:ARG:HG2	2.20	0.41
46:1o:12:ILE:HG23	46:1o:27:VAL:HG11	2.03	0.41
47:1p:4:ILE:HG12	47:1p:21:VAL:HB	2.02	0.41
51:1t:58:LYS:HD2	51:1t:58:LYS:HA	1.77	0.41
51:1t:74:LYS:HB3	51:1t:74:LYS:HE3	1.95	0.41
1:2A:323:G:H1'	1:2A:1205:U:O2	2.19	0.41
1:2A:455:C:N3	1:2A:472:A:H2'	2.36	0.41
1:2A:493:G:H2'	1:2A:494:G:O4'	2.21	0.41
1:2A:531:C:H4'	1:2A:532:A:H5"	2.03	0.41
1:2A:631:A:OP1	11:2P:65:ARG:NH1	2.54	0.41
1:2A:725:G:O6	61:2A:3852:HOH:O	2.19	0.41
1:2A:890:A:H2'	1:2A:892:G:O4'	2.21	0.41
1:2A:1153:C:H2'	1:2A:1154:G:O4'	2.21	0.41
1:2A:1209:G:O2'	1:2A:1237:A:N1	2.39	0.41
1:2A:1429:G:H2'	1:2A:1430:C:C6	2.56	0.41
1:2A:2348:U:OP2	30:28:42:ARG:NH2	2.52	0.41
4:2E:119:ARG:HB3	4:2E:120:TRP:CD1	2.56	0.41
6:2G:96:ARG:N	6:2G:99:MET:HE2	2.35	0.41
8:2I:77:LEU:HD22	8:2I:97:ILE:HG23	2.03	0.41
10:2O:88:ASN:ND2	10:2O:92:GLU:HB2	2.36	0.41
16:2U:65:ILE:HD11	16:2U:95:LEU:HB2	2.02	0.41
19:2X:35:THR:HG22	19:2X:38:GLU:H	1.85	0.41
20:2Y:44:ILE:HA	20:2Y:63:LYS:O	2.20	0.41
23:21:51:VAL:HG12	23:21:53:VAL:HG23	2.03	0.41
28:26:34:LEU:HB2	28:26:51:GLU:HB2	2.02	0.41
32:2a:412:A:N7	35:2d:35:ARG:HD3	2.35	0.41
32:2a:490:G:P	35:2d:132:ARG:HH22	2.44	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:582:U:C2	32:2a:760:G:C6	3.09	0.41
32:2a:789:U:H2'	32:2a:791:G:OP2	2.21	0.41
32:2a:867:G:H2'	32:2a:868:C:H6	1.86	0.41
32:2a:991:U:H2'	32:2a:1212:U:C4	2.56	0.41
32:2a:1113:C:O5'	32:2a:1113:C:H6	2.04	0.41
32:2a:1150:U:O4	32:2a:1151:A:N6	2.54	0.41
32:2a:1260:C:O5'	32:2a:1284:C:H4'	2.21	0.41
33:2b:88:ALA:HB2	33:2b:219:VAL:HG13	2.02	0.41
33:2b:164:VAL:HG23	33:2b:170:GLU:HG3	2.01	0.41
34:2c:125:GLU:HG2	34:2c:190:ARG:O	2.21	0.41
35:2d:11:LEU:HD23	35:2d:66:ARG:HB3	2.03	0.41
35:2d:166:LYS:NZ	35:2d:167:GLY:N	2.64	0.41
37:2f:2:ARG:NE	37:2f:69:GLU:HG2	2.35	0.41
37:2f:78:GLU:O	37:2f:81:ILE:HB	2.21	0.41
38:2g:18:TYR:CD1	38:2g:59:LEU:HB2	2.55	0.41
40:2i:9:ARG:HB2	40:2i:104:ARG:HE	1.85	0.41
40:2i:53:VAL:HG11	40:2i:92:TYR:OH	2.21	0.41
41:2j:67:THR:O	41:2j:67:THR:OG1	2.33	0.41
43:2l:46:LYS:HG2	43:2l:92:0TD:O	2.21	0.41
50:2s:44:MET:HA	50:2s:47:HIS:CE1	2.56	0.41
1:1A:83:G:OP1	61:1A:4148:HOH:O	2.22	0.41
1:1A:271(A):A:N1	1:1A:272(D):G:O2'	2.46	0.41
1:1A:583:G:OP2	16:1U:10:ARG:HD2	2.20	0.41
1:1A:884:C:H3'	1:1A:885:C:H6	1.86	0.41
1:1A:983:A:C6	1:1A:984:A:N1	2.89	0.41
1:1A:1065:U:O2'	1:1A:1066:U:O4'	2.36	0.41
1:1A:1166:C:H2'	1:1A:1167:U:C6	2.56	0.41
1:1A:1213:A:H1'	1:1A:1238:G:N3	2.36	0.41
1:1A:1824:G:N3	3:1D:254:THR:OG1	2.54	0.41
1:1A:2020:A:OP2	61:1A:4150:HOH:O	2.22	0.41
1:1A:2051:A:H5'	1:1A:2578:G:O4'	2.21	0.41
1:1A:2344:U:H4'	61:1A:6800:HOH:O	2.21	0.41
1:1A:2492:U:H2'	1:1A:2493:U:C6	2.56	0.41
1:1A:2659:G:O2'	7:1H:175:LYS:NZ	2.53	0.41
1:1A:2712:U:O2'	1:1A:2713:A:H5'	2.21	0.41
6:1G:133:LEU:HD11	6:1G:157:ILE:HD12	2.02	0.41
26:14:69:LYS:HE2	26:14:69:LYS:HB3	1.89	0.41
32:1a:221:C:H2'	32:1a:222:U:H6	1.86	0.41
32:1a:657:G:C2	32:1a:658:G:C8	3.09	0.41
32:1a:979:C:O2	45:1n:19:ARG:HG2	2.21	0.41
32:1a:1186:G:H21	45:1n:61:TRP:C	2.29	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1525:G:P	42:1k:120:ARG:HH22	2.43	0.41
34:1c:15:THR:CG2	34:1c:181:ASN:HA	2.51	0.41
35:1d:108:LEU:HB3	35:1d:110:PHE:CE1	2.56	0.41
36:1e:72:GLN:O	36:1e:75:THR:HG22	2.20	0.41
40:1i:81:ILE:HG13	40:1i:82:ALA:N	2.31	0.41
42:1k:95:ILE:O	42:1k:99:GLN:HG3	2.21	0.41
44:1m:14:ARG:NH2	44:1m:16:ASP:OD2	2.48	0.41
46:1o:69:TYR:HA	46:1o:72:ARG:NH2	2.36	0.41
49:1r:52:PRO:O	49:1r:56:THR:HG23	2.21	0.41
1:2A:108:U:H2'	1:2A:109:G:C8	2.56	0.41
1:2A:185:U:H4'	1:2A:218:A:H4'	2.02	0.41
1:2A:643:A:C8	28:26:44:ARG:NH1	2.89	0.41
1:2A:744:G:OP1	4:2E:132:HIS:ND1	2.45	0.41
1:2A:909:A:H2'	1:2A:912:C:C5	2.56	0.41
1:2A:1292:U:H2'	1:2A:1293:C:H6	1.85	0.41
1:2A:1357:U:H2'	1:2A:1358:G:O4'	2.21	0.41
1:2A:1379:A:H4'	1:2A:1380:G:OP2	2.21	0.41
1:2A:1818:U:O2'	3:2D:154:LYS:O	2.22	0.41
1:2A:2558:C:H2'	1:2A:2559:C:O4'	2.21	0.41
2:2B:115:G:H2'	2:2B:116:G:O4'	2.21	0.41
6:2G:110:ALA:O	6:2G:113:ARG:N	2.54	0.41
14:2S:69:VAL:HA	14:2S:72:ALA:HB3	2.03	0.41
30:28:58:ILE:HA	30:28:61:LEU:HD12	2.02	0.41
32:2a:60:A:H4'	32:2a:61:G:O5'	2.21	0.41
32:2a:190:U:H2'	32:2a:191:G:H8	1.86	0.41
32:2a:585:G:N3	32:2a:879:C:H4'	2.36	0.41
32:2a:652:U:O4	32:2a:752:G:O2'	2.36	0.41
34:2c:19:GLU:C	34:2c:40:ARG:HH22	2.29	0.41
35:2d:8:VAL:HG22	35:2d:21:LEU:HD13	2.02	0.41
40:2i:111:ARG:HG2	40:2i:112:LYS:O	2.21	0.41
1:1A:271(O):C:H2'	1:1A:271(P):C:C6	2.57	0.40
1:1A:307:G:N2	1:1A:330:A:H62	2.13	0.40
1:1A:821:A:H2'	1:1A:946:G:H5"	2.03	0.40
1:1A:1702:G:H2'	1:1A:1703:G:O4'	2.21	0.40
1:1A:1794:U:H2'	1:1A:1795:C:H6	1.86	0.40
1:1A:2116:G:P	1:1A:2166:G:H21	2.44	0.40
1:1A:2820:A:O2'	1:1A:2821:A:OP1	2.38	0.40
3:1D:6:PHE:HE2	3:1D:18:VAL:HG13	1.86	0.40
3:1D:180:GLY:HA3	3:1D:275:LYS:HG2	2.03	0.40
10:1O:98:VAL:HG22	10:1O:118:ALA:HA	2.03	0.40
12:1Q:71:ASP:OD1	12:1Q:71:ASP:N	2.49	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1R:72:ASP:HB3	13:1R:75:LEU:HB2	2.02	0.40
16:1U:36:ARG:NH2	61:1U:307:HOH:O	2.54	0.40
26:14:43:TYR:O	26:14:45:GLY:N	2.54	0.40
32:1a:64:G:H4'	32:1a:65:U:H3'	2.03	0.40
32:1a:474:G:H2'	32:1a:475:G:H8	1.86	0.40
32:1a:666:G:H5'	32:1a:726:C:H1'	2.03	0.40
32:1a:1060:C:C5	34:1c:2:GLY:HA3	2.56	0.40
32:1a:1203:C:H2'	32:1a:1204:A:O4'	2.21	0.40
32:1a:1329:A:N7	52:1u:7:ARG:NH2	2.69	0.40
32:1a:1347:G:H22	32:1a:1374:A:P	2.44	0.40
34:1c:97:LYS:HB3	34:1c:97:LYS:HE2	1.92	0.40
38:1g:153:HIS:C	38:1g:155:ARG:H	2.30	0.40
41:1j:61:GLU:OE2	45:1n:49:HIS:HE1	2.04	0.40
44:1m:13:LYS:C	44:1m:44:ARG:HD2	2.45	0.40
50:1s:3:ARG:HE	50:1s:7:LYS:HB2	1.86	0.40
53:1y:23:ARG:HA	53:1y:23:ARG:HD2	1.71	0.40
1:2A:27:G:O2'	1:2A:28:A:OP2	2.33	0.40
1:2A:207:A:H2'	1:2A:208:C:O4'	2.21	0.40
1:2A:459:U:H2'	1:2A:460:A:H8	1.86	0.40
1:2A:1223:G:N2	1:2A:1226:A:OP2	2.47	0.40
1:2A:2245:U:O2'	1:2A:2436:G:OP2	2.32	0.40
2:2B:44:G:OP1	6:2G:98:ARG:NH2	2.54	0.40
4:2E:36:ARG:NH1	4:2E:85:ASN:OD1	2.49	0.40
7:2H:144:VAL:O	7:2H:148:ILE:HG13	2.21	0.40
14:2S:67:ARG:HD2	14:2S:71:ARG:HH22	1.86	0.40
15:2T:127:ALA:O	15:2T:129:ARG:HG3	2.21	0.40
21:2Z:28:MET:HE1	21:2Z:61:LEU:HD11	2.03	0.40
32:2a:523:A:N1	43:2l:92:0TD:H6	2.36	0.40
32:2a:689:C:H2'	32:2a:690:G:O4'	2.20	0.40
32:2a:900:A:H2'	32:2a:901:A:C8	2.56	0.40
32:2a:947:G:O2'	32:2a:1306:A:H4'	2.21	0.40
32:2a:953:G:H2'	32:2a:954:G:O4'	2.20	0.40
33:2b:60:ASP:OD2	33:2b:64:ARG:NH2	2.54	0.40
44:2m:49:THR:O	44:2m:53:VAL:HG13	2.21	0.40
1:1A:83:G:N2	1:1A:102:G:H1'	2.36	0.40
1:1A:686:G:H21	1:1A:788:A:H61	1.67	0.40
1:1A:861:A:C2	1:1A:917:A:C4	3.10	0.40
1:1A:1080:C:H2'	1:1A:1081:U:C6	2.56	0.40
1:1A:2093:G:C6	1:1A:2225:A:C8	3.09	0.40
1:1A:2869:G:H2'	1:1A:2870:C:O4'	2.21	0.40
5:1F:157:VAL:O	5:1F:194:MET:HA	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:1P:135:LEU:HD23	11:1P:135:LEU:HA	1.88	0.40
21:1Z:116:VAL:O	21:1Z:174:VAL:HA	2.22	0.40
28:16:12:GLU:OE1	28:16:52:VAL:HG21	2.20	0.40
28:16:33:LYS:HD3	28:16:33:LYS:HA	1.82	0.40
32:1a:376:G:H4'	47:1p:5:ARG:NH1	2.34	0.40
32:1a:718:G:H5'	42:1k:117:ASN:HB2	2.03	0.40
32:1a:833:U:H2'	32:1a:834:C:C6	2.56	0.40
33:1b:28:PHE:CD1	33:1b:190:THR:HA	2.56	0.40
39:1h:36:LEU:HD12	39:1h:59:LEU:HD13	2.03	0.40
44:1m:106:ASN:HB2	44:1m:107:ALA:H	1.44	0.40
1:2A:11:G:N7	61:2A:3993:HOH:O	2.37	0.40
1:2A:1021:A:H61	1:2A:1142(A):A:N6	2.19	0.40
1:2A:1451:C:H4'	1:2A:1452:A:C8	2.57	0.40
1:2A:2224:G:H4'	1:2A:2226:C:C2	2.56	0.40
1:2A:2820:A:O2'	1:2A:2821:A:OP1	2.38	0.40
2:2B:119:G:C6	2:2B:120:A:C6	3.09	0.40
7:2H:117:PRO:HA	7:2H:118:PRO:HD3	1.87	0.40
17:2V:35:LEU:HB2	17:2V:57:VAL:HG22	2.04	0.40
21:2Z:130:PRO:O	21:2Z:133:ILE:HG13	2.21	0.40
21:2Z:145:GLU:HB2	21:2Z:148:ASP:OD2	2.21	0.40
32:2a:109:A:H2'	32:2a:326:G:N2	2.36	0.40
32:2a:256:U:H2'	32:2a:257:G:C8	2.57	0.40
32:2a:625:G:H2'	32:2a:626:U:C6	2.56	0.40
32:2a:966:M2G:H2'	32:2a:967:5MC:O4'	2.21	0.40
32:2a:1276:G:H2'	32:2a:1277:C:H6	1.86	0.40
32:2a:1292:U:H2'	32:2a:1293:G:O4'	2.22	0.40
35:2d:141:ARG:HB3	35:2d:142:PRO:HD2	2.03	0.40
37:2f:69:GLU:O	37:2f:72:VAL:HG13	2.22	0.40
50:2s:22:LEU:HD23	50:2s:22:LEU:HA	1.93	0.40
1:1A:414:C:H2'	1:1A:415:A:H8	1.85	0.40
1:1A:687:C:H2'	1:1A:688:U:O4'	2.21	0.40
1:1A:742:G:H4'	1:1A:1676:A:H5'	2.04	0.40
1:1A:1059:G:N1	1:1A:1079:C:O2	2.34	0.40
1:1A:1068:G:H2'	1:1A:1069:A:C8	2.56	0.40
1:1A:1250:G:H5"	61:1U:324:HOH:O	2.20	0.40
1:1A:2001:A:H2'	1:1A:2002:G:C8	2.57	0.40
1:1A:2135:A:H4'	1:1A:2160:G:H4'	2.03	0.40
1:1A:2317:C:H2'	1:1A:2318:G:O4'	2.22	0.40
1:1A:2331:G:O2'	22:10:43:THR:HG22	2.22	0.40
1:1A:2345:G:H4'	1:1A:2346:A:H5"	2.03	0.40
1:1A:2364:C:H2'	1:1A:2365:G:O4'	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1I:140:LEU:HD23	8:1I:140:LEU:HA	1.91	0.40
9:1N:87:LEU:HD22	9:1N:91:LEU:HG	2.03	0.40
21:1Z:7:ALA:HA	21:1Z:39:VAL:HG12	2.02	0.40
21:1Z:54:HIS:HD2	21:1Z:99:TYR:O	2.04	0.40
23:11:64:ALA:HA	23:11:67:ILE:HG13	2.03	0.40
24:12:36:ARG:HD3	61:12:108:HOH:O	2.20	0.40
30:18:28:GLY:O	30:18:36:LYS:NZ	2.53	0.40
32:1a:1004:A:O4'	32:1a:1025:U:N3	2.55	0.40
32:1a:1149:C:O2'	32:1a:1280:A:N1	2.52	0.40
35:1d:59:ARG:HH21	35:1d:66:ARG:HH12	1.69	0.40
40:1i:3:GLN:HE21	40:1i:20:ARG:HE	1.69	0.40
42:1k:18:ARG:HB2	42:1k:33:THR:OG1	2.22	0.40
45:1n:26:ARG:HD3	45:1n:43:CYS:HB3	2.03	0.40
1:2A:83:G:O2'	1:2A:102:G:N2	2.55	0.40
1:2A:249:C:O2	30:28:12:LYS:NZ	2.40	0.40
1:2A:320:A:H4'	1:2A:322:A:C8	2.56	0.40
1:2A:557:U:H2'	1:2A:558:G:H8	1.87	0.40
1:2A:644:A:H4'	1:2A:645:C:C5	2.56	0.40
1:2A:751:A:C6	1:2A:789:A:C5	3.09	0.40
1:2A:1024:G:O2'	1:2A:1144:G:O2'	2.37	0.40
1:2A:1698:A:C8	1:2A:1700:A:O4'	2.75	0.40
1:2A:2187:G:N7	1:2A:2188:C:C4	2.90	0.40
32:2a:559:A:H5"	32:2a:560:U:H3'	2.03	0.40
32:2a:955:U:O2'	50:2s:83:HIS:HD2	2.04	0.40
32:2a:1162:C:H2'	32:2a:1163:C:H6	1.86	0.40
32:2a:1261:A:H5'	32:2a:1284:C:OP1	2.21	0.40
33:2b:97:TRP:CH2	33:2b:173:ALA:HA	2.56	0.40
34:2c:91:LEU:C	34:2c:93:LYS:H	2.29	0.40
39:2h:69:ARG:HD3	39:2h:75:ARG:O	2.21	0.40
44:2m:50:GLU:O	44:2m:54:VAL:HG22	2.21	0.40
46:2o:16:ALA:HB1	46:2o:21:ASP:HB3	2.03	0.40
46:2o:85:LEU:HB2	46:2o:87:ILE:HG13	2.03	0.40
1:1A:190:A:OP2	23:11:39:LYS:HE3	2.21	0.40
1:1A:1175:U:O3'	1:1A:1176:G:H4'	2.21	0.40
1:1A:1330:C:O2'	1:1A:1331:A:H5'	2.21	0.40
1:1A:1792:G:O2'	1:1A:1830:C:OP1	2.33	0.40
3:1D:5:LYS:HE3	3:1D:5:LYS:HB3	1.85	0.40
3:1D:73:VAL:HG13	3:1D:120:GLY:HA3	2.04	0.40
8:1I:105:HIS:CD2	8:1I:105:HIS:N	2.90	0.40
9:1N:131:GLN:H	9:1N:131:GLN:HG2	1.55	0.40
32:1a:188:C:O5'	32:1a:188:C:H6	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:341:C:H2'	32:1a:342:C:C6	2.57	0.40
32:1a:345:C:H5'	32:1a:346:G:C5	2.57	0.40
32:1a:1004:A:N7	32:1a:1036:G:C2	2.89	0.40
34:1c:14:ILE:HD11	45:1n:57:ARG:HH21	1.86	0.40
39:1h:36:LEU:HA	39:1h:39:LEU:HB2	2.04	0.40
41:1j:98:ILE:H	41:1j:98:ILE:HG13	1.71	0.40
50:1s:4:SER:HB2	50:1s:7:LYS:HG3	2.03	0.40
50:1s:40:ILE:HA	50:1s:44:MET:SD	2.61	0.40
1:2A:453:C:O2	1:2A:457:A:O2'	2.39	0.40
1:2A:709:U:H2'	1:2A:710:G:C8	2.55	0.40
1:2A:1009:A:O4'	16:2U:59:ARG:HG2	2.21	0.40
1:2A:1075:C:H2'	1:2A:1076:C:H5'	2.02	0.40
1:2A:1188:U:C4'	17:2V:79:VAL:HG22	2.49	0.40
1:2A:1971:A:C4	3:2D:241:PRO:HD3	2.56	0.40
6:2G:19:LEU:HD11	6:2G:172:LEU:HB2	2.03	0.40
9:2N:58:ASP:OD1	9:2N:58:ASP:N	2.54	0.40
32:2a:186:C:H5'	51:2t:78:ALA:HB1	2.04	0.40
32:2a:858:G:O6	32:2a:869:G:H3'	2.22	0.40
32:2a:925:G:H1'	32:2a:1502:A:C4	2.56	0.40
32:2a:939:G:C6	32:2a:940:C:N4	2.90	0.40
32:2a:1084:G:C5	32:2a:1085:U:C4	3.09	0.40
32:2a:1116:C:O2'	40:2i:108:VAL:HG21	2.21	0.40
32:2a:1131:G:H2'	32:2a:1132:C:C6	2.55	0.40
32:2a:1190:G:H5'	34:2c:176:HIS:CE1	2.56	0.40
32:2a:1278:U:H5'	32:2a:1279:A:C4	2.56	0.40
32:2a:1346:A:H5"	40:2i:120:ARG:NH1	2.36	0.40
33:2b:46:LYS:HA	33:2b:49:GLU:HG3	2.02	0.40
33:2b:153:ARG:HE	33:2b:153:ARG:HB2	1.73	0.40
36:2e:34:VAL:O	36:2e:42:GLY:N	2.53	0.40
39:2h:25:ASP:OD1	39:2h:25:ASP:N	2.55	0.40
47:2p:4:ILE:O	47:2p:66:PRO:HA	2.20	0.40
47:2p:18:ARG:NH1	47:2p:32:TYR:OH	2.54	0.40
1:1A:182:A:H2	1:1A:433:C:O2	2.04	0.40
1:1A:800:A:H8	1:1A:800:A:OP1	2.04	0.40
1:1A:904:C:H2'	1:1A:905:U:C6	2.56	0.40
1:1A:1291:C:H2'	1:1A:1292:U:H6	1.87	0.40
1:1A:1408:C:C2	1:1A:1595:G:N2	2.89	0.40
1:1A:2101:G:H2'	1:1A:2102:U:O4'	2.21	0.40
1:1A:2291:U:OP1	1:1A:2380:C:O2'	2.38	0.40
2:1B:77:U:P	21:1Z:19:ARG:HH22	2.44	0.40
6:1G:3:LEU:O	6:1G:8:LYS:NZ	2.27	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1G:106:LEU:HA	6:1G:110:ALA:HB3	2.04	0.40
13:1R:98:LEU:HB2	13:1R:113:LEU:HD11	2.04	0.40
32:1a:1053:G:N7	32:1a:1200:C:H5"	2.37	0.40
32:1a:1136:U:H5"	32:1a:1137:C:O2	2.22	0.40
32:1a:1511:G:H2'	32:1a:1512:U:O4'	2.20	0.40
38:1g:6:ARG:H	38:1g:6:ARG:HG3	1.73	0.40
39:1h:87:SER:C	39:1h:88:LYS:HG2	2.47	0.40
42:1k:84:VAL:HG11	42:1k:91:ARG:HD2	2.02	0.40
42:1k:121:PRO:HG2	42:1k:126:ARG:HG2	2.04	0.40
44:1m:4:ILE:HG22	44:1m:57:ARG:NE	2.36	0.40
47:1p:60:LEU:HA	47:1p:60:LEU:HD12	1.88	0.40
1:2A:6:A:H61	1:2A:2897:U:H3	1.70	0.40
1:2A:224:G:H2'	1:2A:225:A:O4'	2.22	0.40
1:2A:495:G:N3	18:2W:61:ASN:ND2	2.69	0.40
1:2A:876:C:H2'	1:2A:877:U:C6	2.56	0.40
1:2A:1000:A:H62	1:2A:1154:G:H2'	1.86	0.40
1:2A:1359:A:N1	1:2A:1372:U:O4	2.54	0.40
1:2A:2207:G:H3'	1:2A:2208:A:H5"	2.04	0.40
4:2E:9:VAL:HG22	4:2E:25:VAL:HB	2.03	0.40
7:2H:24:VAL:HG22	7:2H:35:VAL:HB	2.04	0.40
9:2N:23:LEU:HD12	9:2N:99:LEU:HD23	2.03	0.40
17:2V:23:GLU:HB2	61:2V:301:HOH:O	2.21	0.40
20:2Y:37:VAL:HG21	20:2Y:72:VAL:HG21	2.03	0.40
23:21:51:VAL:N	23:21:58:ILE:O	2.51	0.40
25:23:5:LYS:HB3	25:23:5:LYS:HE2	1.92	0.40
32:2a:447:G:O6	32:2a:485:G:O2'	2.38	0.40
32:2a:1122:U:O2'	32:2a:1123:A:H5'	2.22	0.40
32:2a:1168:A:H8	32:2a:1168:A:O5'	2.05	0.40
32:2a:1172:C:H2'	32:2a:1173:G:C8	2.56	0.40
32:2a:1256:A:H61	32:2a:1278:U:C1'	2.34	0.40
32:2a:1279:A:H2'	32:2a:1279:A:N3	2.36	0.40
32:2a:1323:G:H4'	32:2a:1363:C:C2	2.57	0.40
33:2b:152:PHE:CE1	33:2b:155:LEU:HD23	2.57	0.40
33:2b:211:ILE:H	33:2b:211:ILE:HG13	1.57	0.40
50:2s:53:ASN:ND2	50:2s:76:PRO:O	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	1D	273/276 (99%)	258 (94%)	14 (5%)	1 (0%)	30 49
3	2D	273/276 (99%)	257 (94%)	15 (6%)	1 (0%)	30 49
4	1E	202/206 (98%)	191 (95%)	9 (4%)	2 (1%)	12 24
4	2E	202/206 (98%)	192 (95%)	8 (4%)	2 (1%)	12 24
5	1F	201/210 (96%)	197 (98%)	3 (2%)	1 (0%)	24 43
5	2F	201/210 (96%)	190 (94%)	10 (5%)	1 (0%)	24 43
6	1G	179/182 (98%)	163 (91%)	12 (7%)	4 (2%)	5 9
6	2G	179/182 (98%)	149 (83%)	26 (14%)	4 (2%)	5 9
7	1H	172/180 (96%)	161 (94%)	10 (6%)	1 (1%)	21 38
7	2H	171/180 (95%)	148 (86%)	23 (14%)	0	100 100
8	1I	145/148 (98%)	128 (88%)	16 (11%)	1 (1%)	18 34
8	2I	144/148 (97%)	130 (90%)	13 (9%)	1 (1%)	18 34
9	1N	138/140 (99%)	133 (96%)	5 (4%)	0	100 100
9	2N	138/140 (99%)	134 (97%)	4 (3%)	0	100 100
10	1O	120/122 (98%)	113 (94%)	6 (5%)	1 (1%)	16 31
10	2O	120/122 (98%)	112 (93%)	7 (6%)	1 (1%)	16 31
11	1P	147/150 (98%)	141 (96%)	6 (4%)	0	100 100
11	2P	147/150 (98%)	140 (95%)	6 (4%)	1 (1%)	18 34
12	1Q	139/141 (99%)	134 (96%)	4 (3%)	1 (1%)	18 34
12	2Q	139/141 (99%)	130 (94%)	9 (6%)	0	100 100
13	1R	116/118 (98%)	114 (98%)	2 (2%)	0	100 100
13	2R	116/118 (98%)	113 (97%)	3 (3%)	0	100 100
14	1S	108/112 (96%)	102 (94%)	5 (5%)	1 (1%)	14 27
14	2S	108/112 (96%)	96 (89%)	11 (10%)	1 (1%)	14 27
15	1T	129/146 (88%)	120 (93%)	8 (6%)	1 (1%)	16 31

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
15	2T	129/146 (88%)	122 (95%)	7 (5%)	0	100 100
16	1U	114/118 (97%)	114 (100%)	0	0	100 100
16	2U	114/118 (97%)	114 (100%)	0	0	100 100
17	1V	99/101 (98%)	95 (96%)	2 (2%)	2 (2%)	6 10
17	2V	99/101 (98%)	95 (96%)	3 (3%)	1 (1%)	12 24
18	1W	110/113 (97%)	110 (100%)	0	0	100 100
18	2W	110/113 (97%)	108 (98%)	2 (2%)	0	100 100
19	1X	93/96 (97%)	90 (97%)	2 (2%)	1 (1%)	11 22
19	2X	93/96 (97%)	87 (94%)	5 (5%)	1 (1%)	11 22
20	1Y	105/110 (96%)	95 (90%)	10 (10%)	0	100 100
20	2Y	105/110 (96%)	99 (94%)	6 (6%)	0	100 100
21	1Z	201/206 (98%)	186 (92%)	14 (7%)	1 (0%)	24 43
21	2Z	199/206 (97%)	177 (89%)	20 (10%)	2 (1%)	12 24
22	10	75/85 (88%)	71 (95%)	4 (5%)	0	100 100
22	20	75/85 (88%)	71 (95%)	4 (5%)	0	100 100
23	11	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	11 22
23	21	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	11 22
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100 100
24	22	68/72 (94%)	64 (94%)	4 (6%)	0	100 100
25	13	57/60 (95%)	56 (98%)	1 (2%)	0	100 100
25	23	57/60 (95%)	54 (95%)	3 (5%)	0	100 100
26	14	67/71 (94%)	53 (79%)	10 (15%)	4 (6%)	1 1
26	24	67/71 (94%)	45 (67%)	15 (22%)	7 (10%)	0 0
27	15	57/60 (95%)	57 (100%)	0	0	100 100
27	25	57/60 (95%)	54 (95%)	2 (4%)	1 (2%)	6 12
28	16	51/54 (94%)	49 (96%)	2 (4%)	0	100 100
28	26	51/54 (94%)	46 (90%)	5 (10%)	0	100 100
29	17	46/49 (94%)	46 (100%)	0	0	100 100
29	27	46/49 (94%)	46 (100%)	0	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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
31	19	35/37 (95%)	35 (100%)	0	0	100 100
31	29	35/37 (95%)	33 (94%)	2 (6%)	0	100 100
33	1b	229/256 (90%)	193 (84%)	28 (12%)	8 (4%)	3 4
33	2b	229/256 (90%)	191 (83%)	32 (14%)	6 (3%)	4 7
34	1c	204/239 (85%)	188 (92%)	15 (7%)	1 (0%)	24 43
34	2c	204/239 (85%)	176 (86%)	26 (13%)	2 (1%)	12 24
35	1d	206/209 (99%)	188 (91%)	17 (8%)	1 (0%)	24 43
35	2d	206/209 (99%)	197 (96%)	9 (4%)	0	100 100
36	1e	146/162 (90%)	137 (94%)	9 (6%)	0	100 100
36	2e	146/162 (90%)	138 (94%)	8 (6%)	0	100 100
37	1f	98/101 (97%)	93 (95%)	4 (4%)	1 (1%)	12 24
37	2f	98/101 (97%)	93 (95%)	5 (5%)	0	100 100
38	1g	153/156 (98%)	148 (97%)	4 (3%)	1 (1%)	18 34
38	2g	153/156 (98%)	142 (93%)	9 (6%)	2 (1%)	9 18
39	1h	135/138 (98%)	129 (96%)	6 (4%)	0	100 100
39	2h	135/138 (98%)	124 (92%)	10 (7%)	1 (1%)	18 34
40	1i	125/128 (98%)	113 (90%)	11 (9%)	1 (1%)	16 31
40	2i	124/128 (97%)	107 (86%)	14 (11%)	3 (2%)	4 8
41	1j	95/105 (90%)	78 (82%)	13 (14%)	4 (4%)	2 2
41	2j	94/105 (90%)	80 (85%)	10 (11%)	4 (4%)	2 2
42	1k	112/129 (87%)	104 (93%)	8 (7%)	0	100 100
42	2k	112/129 (87%)	100 (89%)	11 (10%)	1 (1%)	14 27
43	1l	119/132 (90%)	115 (97%)	4 (3%)	0	100 100
43	2l	119/132 (90%)	112 (94%)	7 (6%)	0	100 100
44	1m	114/126 (90%)	103 (90%)	7 (6%)	4 (4%)	3 4
44	2m	112/126 (89%)	100 (89%)	8 (7%)	4 (4%)	2 3
45	1n	58/61 (95%)	56 (97%)	2 (3%)	0	100 100
45	2n	58/61 (95%)	56 (97%)	2 (3%)	0	100 100
46	1o	86/89 (97%)	83 (96%)	3 (4%)	0	100 100
46	2o	86/89 (97%)	79 (92%)	6 (7%)	1 (1%)	10 20
47	1p	80/88 (91%)	70 (88%)	9 (11%)	1 (1%)	9 18

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
47	2p	80/88 (91%)	69 (86%)	10 (12%)	1 (1%)	9 18
48	1q	97/105 (92%)	87 (90%)	9 (9%)	1 (1%)	12 24
48	2q	97/105 (92%)	89 (92%)	7 (7%)	1 (1%)	12 24
49	1r	66/88 (75%)	63 (96%)	3 (4%)	0	100 100
49	2r	66/88 (75%)	64 (97%)	2 (3%)	0	100 100
50	1s	81/93 (87%)	69 (85%)	10 (12%)	2 (2%)	4 7
50	2s	81/93 (87%)	68 (84%)	11 (14%)	2 (2%)	4 7
51	1t	94/106 (89%)	87 (93%)	4 (4%)	3 (3%)	3 4
51	2t	96/106 (91%)	88 (92%)	5 (5%)	3 (3%)	3 5
52	1u	21/27 (78%)	21 (100%)	0	0	100 100
52	2u	21/27 (78%)	16 (76%)	4 (19%)	1 (5%)	2 2
53	1y	95/113 (84%)	95 (100%)	0	0	100 100
53	2y	94/113 (83%)	90 (96%)	4 (4%)	0	100 100
All	All	11629/12354 (94%)	10793 (93%)	728 (6%)	108 (1%)	14 27

All (108) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	1E	71	GLY
5	1F	130	ALA
6	1G	47	LYS
6	1G	50	ALA
26	14	49	PHE
41	1j	55	LYS
44	1m	3	ARG
51	1t	95	ALA
5	2F	130	ALA
6	2G	81	LYS
21	2Z	52	SER
33	2b	20	GLU
44	2m	67	GLU
3	1D	275	LYS
6	1G	51	ARG
21	1Z	52	SER
33	1b	8	LYS
33	1b	124	SER
38	1g	55	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	1j	79	ARG
51	1t	47	GLY
4	2E	71	GLY
8	2I	10	GLU
14	2S	96	GLY
17	2V	79	VAL
19	2X	94	GLY
26	24	45	GLY
26	24	47	GLN
26	24	54	GLY
26	24	62	ARG
38	2g	55	GLY
40	2i	54	ASP
41	2j	35	SER
41	2j	55	LYS
41	2j	78	ASN
44	2m	8	GLU
4	1E	52	LEU
12	1Q	59	ARG
15	1T	127	ALA
26	14	57	GLU
33	1b	17	PHE
33	1b	20	GLU
33	1b	21	ARG
34	1c	3	ASN
41	1j	77	PRO
50	1s	27	GLU
51	1t	100	ILE
6	2G	78	SER
23	21	3	LYS
26	24	49	PHE
33	2b	17	PHE
33	2b	95	GLN
33	2b	125	PRO
34	2c	95	THR
38	2g	53	LYS
39	2h	133	LEU
40	2i	121	ARG
41	2j	79	ARG
42	2k	89	ALA
44	2m	6	GLY
47	2p	44	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	2s	29	ARG
51	2t	100	ILE
52	2u	3	LYS
10	1O	5	GLN
17	1V	43	GLU
19	1X	94	GLY
33	1b	125	PRO
41	1j	78	ASN
44	1m	12	ASN
44	1m	67	GLU
44	1m	106	ASN
47	1p	28	ARG
4	2E	52	LEU
6	2G	117	PHE
27	25	35	GLU
34	2c	100	ALA
40	2i	43	ALA
44	2m	23	TYR
48	2q	68	ARG
50	2s	30	LEU
51	2t	47	GLY
51	2t	102	GLY
14	1S	59	LYS
23	11	3	LYS
26	14	55	ARG
26	14	61	ARG
33	1b	16	HIS
3	2D	275	LYS
10	2O	5	GLN
11	2P	29	LYS
26	24	39	CYS
26	24	55	ARG
33	2b	16	HIS
8	1I	117	GLU
35	1d	167	GLY
46	2o	88	ARG
7	1H	92	ILE
17	1V	79	VAL
6	1G	44	GLY
33	1b	127	ILE
40	1i	109	VAL
50	1s	26	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	2G	109	VAL
33	2b	124	SER
48	1q	33	GLY
21	2Z	101	PRO
37	1f	40	VAL

5.3.2 Protein sidechains (i)

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	214/218 (98%)	195 (91%)	19 (9%)	9 20
3	2D	215/218 (99%)	199 (93%)	16 (7%)	13 27
4	1E	164/166 (99%)	154 (94%)	10 (6%)	17 35
4	2E	164/166 (99%)	153 (93%)	11 (7%)	15 31
5	1F	160/166 (96%)	144 (90%)	16 (10%)	7 15
5	2F	159/166 (96%)	140 (88%)	19 (12%)	5 11
6	1G	144/156 (92%)	132 (92%)	12 (8%)	10 22
6	2G	142/156 (91%)	126 (89%)	16 (11%)	5 12
7	1H	144/148 (97%)	131 (91%)	13 (9%)	9 19
7	2H	143/148 (97%)	129 (90%)	14 (10%)	7 16
8	1I	111/124 (90%)	98 (88%)	13 (12%)	5 11
8	2I	108/124 (87%)	98 (91%)	10 (9%)	8 18
9	1N	119/119 (100%)	107 (90%)	12 (10%)	7 15
9	2N	118/119 (99%)	107 (91%)	11 (9%)	8 18
10	1O	100/100 (100%)	96 (96%)	4 (4%)	28 54
10	2O	100/100 (100%)	97 (97%)	3 (3%)	36 64
11	1P	115/116 (99%)	108 (94%)	7 (6%)	17 35
11	2P	115/116 (99%)	106 (92%)	9 (8%)	11 24
12	1Q	111/111 (100%)	105 (95%)	6 (5%)	20 41
12	2Q	111/111 (100%)	98 (88%)	13 (12%)	5 11

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
13	1R	101/101 (100%)	92 (91%)	9 (9%)	9 20
13	2R	101/101 (100%)	95 (94%)	6 (6%)	18 37
14	1S	87/88 (99%)	79 (91%)	8 (9%)	8 19
14	2S	85/88 (97%)	75 (88%)	10 (12%)	5 11
15	1T	115/127 (91%)	106 (92%)	9 (8%)	11 24
15	2T	113/127 (89%)	106 (94%)	7 (6%)	16 34
16	1U	93/94 (99%)	89 (96%)	4 (4%)	26 51
16	2U	93/94 (99%)	87 (94%)	6 (6%)	15 32
17	1V	81/82 (99%)	75 (93%)	6 (7%)	13 27
17	2V	80/82 (98%)	73 (91%)	7 (9%)	9 20
18	1W	90/92 (98%)	83 (92%)	7 (8%)	11 24
18	2W	90/92 (98%)	80 (89%)	10 (11%)	6 12
19	1X	77/78 (99%)	72 (94%)	5 (6%)	15 32
19	2X	77/78 (99%)	74 (96%)	3 (4%)	28 55
20	1Y	86/91 (94%)	80 (93%)	6 (7%)	14 29
20	2Y	86/91 (94%)	75 (87%)	11 (13%)	4 9
21	1Z	169/179 (94%)	151 (89%)	18 (11%)	6 13
21	2Z	165/179 (92%)	152 (92%)	13 (8%)	11 24
22	10	61/67 (91%)	59 (97%)	2 (3%)	33 61
22	20	61/67 (91%)	57 (93%)	4 (7%)	15 32
23	11	79/83 (95%)	73 (92%)	6 (8%)	12 26
23	21	81/83 (98%)	75 (93%)	6 (7%)	13 27
24	12	65/67 (97%)	63 (97%)	2 (3%)	35 62
24	22	66/67 (98%)	56 (85%)	10 (15%)	3 5
25	13	51/52 (98%)	46 (90%)	5 (10%)	7 16
25	23	50/52 (96%)	45 (90%)	5 (10%)	7 15
26	14	58/63 (92%)	52 (90%)	6 (10%)	7 14
26	24	54/63 (86%)	45 (83%)	9 (17%)	2 4
27	15	51/52 (98%)	45 (88%)	6 (12%)	5 11
27	25	50/52 (96%)	47 (94%)	3 (6%)	17 36
28	16	51/52 (98%)	43 (84%)	8 (16%)	2 5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
28	26	50/52 (96%)	44 (88%)	6 (12%)	5 10
29	17	41/42 (98%)	38 (93%)	3 (7%)	13 27
29	27	41/42 (98%)	37 (90%)	4 (10%)	7 16
30	18	54/55 (98%)	52 (96%)	2 (4%)	30 57
30	28	54/55 (98%)	52 (96%)	2 (4%)	30 57
31	19	34/34 (100%)	33 (97%)	1 (3%)	37 65
31	29	34/34 (100%)	32 (94%)	2 (6%)	18 37
33	1b	191/220 (87%)	169 (88%)	22 (12%)	5 11
33	2b	187/220 (85%)	162 (87%)	25 (13%)	4 8
34	1c	144/188 (77%)	137 (95%)	7 (5%)	22 45
34	2c	140/188 (74%)	126 (90%)	14 (10%)	7 15
35	1d	171/181 (94%)	157 (92%)	14 (8%)	10 23
35	2d	172/181 (95%)	151 (88%)	21 (12%)	5 10
36	1e	114/123 (93%)	108 (95%)	6 (5%)	20 42
36	2e	114/123 (93%)	103 (90%)	11 (10%)	8 17
37	1f	85/90 (94%)	77 (91%)	8 (9%)	8 18
37	2f	85/90 (94%)	77 (91%)	8 (9%)	8 18
38	1g	120/127 (94%)	115 (96%)	5 (4%)	26 52
38	2g	119/127 (94%)	107 (90%)	12 (10%)	7 15
39	1h	116/119 (98%)	106 (91%)	10 (9%)	10 21
39	2h	114/119 (96%)	102 (90%)	12 (10%)	6 14
40	1i	91/99 (92%)	85 (93%)	6 (7%)	15 32
40	2i	88/99 (89%)	78 (89%)	10 (11%)	5 12
41	1j	68/92 (74%)	59 (87%)	9 (13%)	4 8
41	2j	68/92 (74%)	56 (82%)	12 (18%)	2 3
42	1k	83/99 (84%)	77 (93%)	6 (7%)	13 28
42	2k	83/99 (84%)	77 (93%)	6 (7%)	13 28
43	1l	96/108 (89%)	95 (99%)	1 (1%)	68 86
43	2l	96/108 (89%)	89 (93%)	7 (7%)	13 27
44	1m	90/101 (89%)	84 (93%)	6 (7%)	15 31
44	2m	87/101 (86%)	77 (88%)	10 (12%)	5 11

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
45	1n	49/50 (98%)	44 (90%)	5 (10%)	7 15
45	2n	49/50 (98%)	43 (88%)	6 (12%)	5 10
46	1o	78/80 (98%)	73 (94%)	5 (6%)	16 33
46	2o	78/80 (98%)	74 (95%)	4 (5%)	21 43
47	1p	69/74 (93%)	57 (83%)	12 (17%)	2 3
47	2p	68/74 (92%)	60 (88%)	8 (12%)	5 11
48	1q	94/97 (97%)	90 (96%)	4 (4%)	26 51
48	2q	94/97 (97%)	87 (93%)	7 (7%)	13 27
49	1r	59/77 (77%)	57 (97%)	2 (3%)	32 60
49	2r	59/77 (77%)	55 (93%)	4 (7%)	14 31
50	1s	68/80 (85%)	63 (93%)	5 (7%)	13 27
50	2s	67/80 (84%)	58 (87%)	9 (13%)	4 8
51	1t	71/82 (87%)	65 (92%)	6 (8%)	10 22
51	2t	70/82 (85%)	62 (89%)	8 (11%)	5 12
52	1u	18/22 (82%)	17 (94%)	1 (6%)	19 39
52	2u	18/22 (82%)	18 (100%)	0	100 100
53	1y	82/98 (84%)	81 (99%)	1 (1%)	63 83
53	2y	79/98 (81%)	73 (92%)	6 (8%)	12 26
All	All	9524/10260 (93%)	8712 (92%)	812 (8%)	10 22

All (812) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	3	VAL
3	1D	37	LEU
3	1D	39	LYS
3	1D	94	LEU
3	1D	99	ASP
3	1D	103	ARG
3	1D	111	LEU
3	1D	113	VAL
3	1D	140	THR
3	1D	141	VAL
3	1D	142	VAL
3	1D	155	LEU
3	1D	173	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	1D	183	ARG
3	1D	193	VAL
3	1D	211	ARG
3	1D	229	VAL
3	1D	242	ARG
3	1D	259	THR
4	1E	9	VAL
4	1E	33	VAL
4	1E	72	VAL
4	1E	75	VAL
4	1E	89	ASP
4	1E	116	VAL
4	1E	119	ARG
4	1E	181	LEU
4	1E	188	VAL
4	1E	202	LYS
5	1F	12	LEU
5	1F	24	LEU
5	1F	53	THR
5	1F	57	VAL
5	1F	74	ARG
5	1F	110	LEU
5	1F	125	LEU
5	1F	132	VAL
5	1F	140	LEU
5	1F	158	THR
5	1F	162	LEU
5	1F	170	LEU
5	1F	183	VAL
5	1F	192	LEU
5	1F	194	MET
5	1F	195	ASP
6	1G	5	VAL
6	1G	7	LEU
6	1G	28	VAL
6	1G	43	LEU
6	1G	45	GLU
6	1G	52	ILE
6	1G	53	LEU
6	1G	82	LEU
6	1G	84	LYS
6	1G	109	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	1G	145	THR
6	1G	153	ARG
7	1H	4	ILE
7	1H	13	LYS
7	1H	15	VAL
7	1H	24	VAL
7	1H	44	VAL
7	1H	67	LEU
7	1H	71	LEU
7	1H	98	LEU
7	1H	107	VAL
7	1H	119	GLU
7	1H	122	THR
7	1H	130	ARG
7	1H	172	LYS
8	1I	5	LEU
8	1I	9	LEU
8	1I	41	GLU
8	1I	44	LEU
8	1I	52	ARG
8	1I	54	GLN
8	1I	60	GLU
8	1I	74	ASN
8	1I	75	LEU
8	1I	92	VAL
8	1I	109	ILE
8	1I	133	HIS
8	1I	140	LEU
9	1N	14	VAL
9	1N	15	LEU
9	1N	33	LEU
9	1N	34	LEU
9	1N	48	MET
9	1N	61	ARG
9	1N	62	VAL
9	1N	73	THR
9	1N	87	LEU
9	1N	97	ARG
9	1N	99	LEU
9	1N	115	ARG
10	1O	69	ILE
10	1O	94	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	1O	98	VAL
10	1O	108	GLU
11	1P	1	MET
11	1P	3	LEU
11	1P	56	SER
11	1P	65	ARG
11	1P	83	VAL
11	1P	101	VAL
11	1P	149	GLU
12	1Q	7	MET
12	1Q	55	VAL
12	1Q	59	ARG
12	1Q	75	THR
12	1Q	109	VAL
12	1Q	112	GLU
13	1R	6	SER
13	1R	8	ARG
13	1R	29	LEU
13	1R	36	THR
13	1R	73	VAL
13	1R	75	LEU
13	1R	100	LEU
13	1R	102	GLU
13	1R	114	VAL
14	1S	3	ARG
14	1S	25	ARG
14	1S	46	VAL
14	1S	50	SER
14	1S	59	LYS
14	1S	68	GLN
14	1S	85	VAL
14	1S	110	LEU
15	1T	28	VAL
15	1T	33	LYS
15	1T	34	VAL
15	1T	36	GLU
15	1T	39	ARG
15	1T	49	VAL
15	1T	67	SER
15	1T	78	LEU
15	1T	96	ARG
16	1U	59	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	1U	74	LEU
16	1U	77	SER
16	1U	104	GLN
17	1V	32	THR
17	1V	51	VAL
17	1V	52	VAL
17	1V	61	VAL
17	1V	62	LEU
17	1V	79	VAL
18	1W	11	ARG
18	1W	15	ARG
18	1W	17	VAL
18	1W	23	LEU
18	1W	50	VAL
18	1W	100	THR
18	1W	107	LEU
19	1X	33	LYS
19	1X	35	THR
19	1X	45	THR
19	1X	60	ARG
19	1X	72	LYS
20	1Y	7	VAL
20	1Y	43	ASN
20	1Y	64	GLU
20	1Y	70	SER
20	1Y	72	VAL
20	1Y	85	VAL
21	1Z	14	LYS
21	1Z	18	LEU
21	1Z	31	ARG
21	1Z	50	GLN
21	1Z	61	LEU
21	1Z	66	SER
21	1Z	86	VAL
21	1Z	94	GLU
21	1Z	103	ARG
21	1Z	126	VAL
21	1Z	129	SER
21	1Z	131	ARG
21	1Z	135	GLU
21	1Z	150	LEU
21	1Z	161	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	1Z	170	THR
21	1Z	185	GLU
21	1Z	191	VAL
22	10	9	SER
22	10	55	ARG
23	11	21	ARG
23	11	30	VAL
23	11	40	ARG
23	11	46	LEU
23	11	91	LYS
23	11	95	LEU
24	12	41	ILE
24	12	70	GLN
25	13	3	ARG
25	13	23	LEU
25	13	31	LEU
25	13	54	VAL
25	13	56	VAL
26	14	1	MET
26	14	27	THR
26	14	49	PHE
26	14	60	GLN
26	14	61	ARG
26	14	67	TYR
27	15	6	VAL
27	15	16	ARG
27	15	26	THR
27	15	29	THR
27	15	58	LEU
27	15	60	VAL
28	16	5	VAL
28	16	6	ARG
28	16	9	LEU
28	16	14	THR
28	16	45	LYS
28	16	47	THR
28	16	48	VAL
28	16	52	VAL
29	17	43	THR
29	17	46	VAL
29	17	48	LYS
30	18	14	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	18	23	VAL
31	19	13	LYS
33	1b	7	VAL
33	1b	9	GLU
33	1b	10	LEU
33	1b	12	GLU
33	1b	44	LEU
33	1b	48	MET
33	1b	59	GLU
33	1b	80	ILE
33	1b	90	MET
33	1b	107	THR
33	1b	111	ARG
33	1b	112	VAL
33	1b	124	SER
33	1b	126	GLU
33	1b	139	LYS
33	1b	158	LEU
33	1b	160	ASP
33	1b	185	ILE
33	1b	189	ASP
33	1b	196	LEU
33	1b	212	GLN
33	1b	221	LEU
34	1c	38	ARG
34	1c	64	VAL
34	1c	67	THR
34	1c	70	VAL
34	1c	102	ASN
34	1c	105	GLU
34	1c	161	GLU
35	1d	5	ILE
35	1d	34	GLU
35	1d	58	LEU
35	1d	67	ILE
35	1d	76	ARG
35	1d	100	ARG
35	1d	112	VAL
35	1d	127	THR
35	1d	135	LEU
35	1d	152	SER
35	1d	178	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	1d	182	LYS
35	1d	194	LEU
35	1d	196	LEU
36	1e	12	LEU
36	1e	31	LEU
36	1e	34	VAL
36	1e	41	VAL
36	1e	79	GLU
36	1e	143	ARG
37	1f	1	MET
37	1f	10	LEU
37	1f	17	SER
37	1f	21	LEU
37	1f	40	VAL
37	1f	45	LEU
37	1f	69	GLU
37	1f	72	VAL
38	1g	6	ARG
38	1g	91	VAL
38	1g	104	LEU
38	1g	113	GLU
38	1g	138	LYS
39	1h	26	VAL
39	1h	38	ILE
39	1h	39	LEU
39	1h	51	VAL
39	1h	52	ASP
39	1h	63	LEU
39	1h	95	VAL
39	1h	107	LEU
39	1h	133	LEU
39	1h	137	VAL
40	1i	17	VAL
40	1i	64	THR
40	1i	65	VAL
40	1i	81	ILE
40	1i	87	GLN
40	1i	127	LYS
41	1j	19	SER
41	1j	25	GLU
41	1j	38	ILE
41	1j	43	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	1j	46	ARG
41	1j	55	LYS
41	1j	67	THR
41	1j	98	ILE
41	1j	100	THR
42	1k	14	VAL
42	1k	16	SER
42	1k	54	ARG
42	1k	83	ILE
42	1k	87	THR
42	1k	114	VAL
43	1l	83	VAL
44	1m	14	ARG
44	1m	15	VAL
44	1m	19	LEU
44	1m	43	THR
44	1m	70	LEU
44	1m	106	ASN
45	1n	3	ARG
45	1n	4	LYS
45	1n	7	ILE
45	1n	13	THR
45	1n	18	VAL
46	1o	3	ILE
46	1o	39	LEU
46	1o	40	SER
46	1o	66	LEU
46	1o	84	LYS
47	1p	6	LEU
47	1p	21	VAL
47	1p	29	ASP
47	1p	34	GLU
47	1p	45	THR
47	1p	60	LEU
47	1p	61	SER
47	1p	62	VAL
47	1p	67	THR
47	1p	72	ARG
47	1p	73	LEU
47	1p	74	LEU
48	1q	20	THR
48	1q	24	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
48	1q	97	SER
48	1q	99	SER
49	1r	25	THR
49	1r	37	VAL
50	1s	28	LYS
50	1s	30	LEU
50	1s	37	ARG
50	1s	38	SER
50	1s	41	VAL
51	1t	10	LEU
51	1t	24	LEU
51	1t	37	SER
51	1t	46	GLU
51	1t	62	LEU
51	1t	100	ILE
52	1u	8	THR
53	1y	60	VAL
3	2D	3	VAL
3	2D	61	LEU
3	2D	88	ARG
3	2D	99	ASP
3	2D	103	ARG
3	2D	113	VAL
3	2D	138	VAL
3	2D	142	VAL
3	2D	162	SER
3	2D	173	VAL
3	2D	183	ARG
3	2D	211	ARG
3	2D	221	VAL
3	2D	229	VAL
3	2D	242	ARG
3	2D	259	THR
4	2E	9	VAL
4	2E	33	VAL
4	2E	72	VAL
4	2E	75	VAL
4	2E	89	ASP
4	2E	116	VAL
4	2E	119	ARG
4	2E	170	LEU
4	2E	181	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	2E	184	VAL
4	2E	188	VAL
5	2F	20	LEU
5	2F	24	LEU
5	2F	33	LEU
5	2F	57	VAL
5	2F	74	ARG
5	2F	88	VAL
5	2F	126	VAL
5	2F	132	VAL
5	2F	136	THR
5	2F	157	VAL
5	2F	158	THR
5	2F	168	ARG
5	2F	170	LEU
5	2F	175	THR
5	2F	179	GLU
5	2F	183	VAL
5	2F	192	LEU
5	2F	197	ASP
5	2F	201	VAL
6	2G	3	LEU
6	2G	5	VAL
6	2G	7	LEU
6	2G	15	VAL
6	2G	28	VAL
6	2G	43	LEU
6	2G	49	ASP
6	2G	84	LYS
6	2G	103	LEU
6	2G	109	VAL
6	2G	116	ASP
6	2G	133	LEU
6	2G	152	LEU
6	2G	159	VAL
6	2G	165	THR
6	2G	167	GLU
7	2H	30	LYS
7	2H	33	LEU
7	2H	43	VAL
7	2H	44	VAL
7	2H	45	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	2H	49	VAL
7	2H	70	THR
7	2H	87	LEU
7	2H	95	ARG
7	2H	98	LEU
7	2H	105	LEU
7	2H	134	SER
7	2H	136	ILE
7	2H	139	GLN
8	2I	38	LEU
8	2I	42	SER
8	2I	51	ILE
8	2I	58	LEU
8	2I	68	LEU
8	2I	76	THR
8	2I	92	VAL
8	2I	108	THR
8	2I	117	GLU
8	2I	127	VAL
9	2N	8	GLN
9	2N	12	ARG
9	2N	28	THR
9	2N	34	LEU
9	2N	48	MET
9	2N	62	VAL
9	2N	65	LYS
9	2N	68	GLU
9	2N	99	LEU
9	2N	133	GLN
9	2N	138	LEU
10	2O	69	ILE
10	2O	98	VAL
10	2O	108	GLU
11	2P	15	ARG
11	2P	75	ILE
11	2P	83	VAL
11	2P	86	LYS
11	2P	95	VAL
11	2P	99	LEU
11	2P	119	GLU
11	2P	126	VAL
11	2P	149	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	2Q	7	MET
12	2Q	16	ARG
12	2Q	22	LYS
12	2Q	31	ASP
12	2Q	55	VAL
12	2Q	59	ARG
12	2Q	101	ARG
12	2Q	103	MET
12	2Q	106	VAL
12	2Q	109	VAL
12	2Q	110	THR
12	2Q	112	GLU
12	2Q	133	ARG
13	2R	29	LEU
13	2R	36	THR
13	2R	73	VAL
13	2R	75	LEU
13	2R	96	ARG
13	2R	100	LEU
14	2S	11	LYS
14	2S	14	VAL
14	2S	21	THR
14	2S	40	ILE
14	2S	52	SER
14	2S	64	GLU
14	2S	69	VAL
14	2S	71	ARG
14	2S	78	LEU
14	2S	111	GLU
15	2T	17	THR
15	2T	28	VAL
15	2T	38	ASN
15	2T	51	ARG
15	2T	78	LEU
15	2T	89	VAL
15	2T	118	ARG
16	2U	27	LEU
16	2U	31	SER
16	2U	59	ARG
16	2U	74	LEU
16	2U	77	SER
16	2U	104	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	2V	12	TYR
17	2V	26	ASP
17	2V	35	LEU
17	2V	46	VAL
17	2V	51	VAL
17	2V	79	VAL
17	2V	99	ILE
18	2W	11	ARG
18	2W	17	VAL
18	2W	23	LEU
18	2W	60	ASN
18	2W	63	ASP
18	2W	65	LEU
18	2W	67	ASP
18	2W	100	THR
18	2W	107	LEU
18	2W	109	GLU
19	2X	35	THR
19	2X	38	GLU
19	2X	81	VAL
20	2Y	1	MET
20	2Y	2	ARG
20	2Y	19	LYS
20	2Y	28	LYS
20	2Y	29	GLU
20	2Y	49	VAL
20	2Y	72	VAL
20	2Y	85	VAL
20	2Y	96	ILE
20	2Y	98	VAL
20	2Y	99	CYS
21	2Z	6	LYS
21	2Z	18	LEU
21	2Z	31	ARG
21	2Z	35	ARG
21	2Z	42	VAL
21	2Z	56	VAL
21	2Z	71	VAL
21	2Z	86	VAL
21	2Z	116	VAL
21	2Z	124	ILE
21	2Z	175	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	2Z	181	GLU
21	2Z	185	GLU
22	20	10	THR
22	20	11	ARG
22	20	66	VAL
22	20	68	GLU
23	21	4	VAL
23	21	11	ARG
23	21	21	ARG
23	21	40	ARG
23	21	62	VAL
23	21	95	LEU
24	22	17	SER
24	22	19	VAL
24	22	25	VAL
24	22	30	ARG
24	22	32	LEU
24	22	35	LEU
24	22	40	SER
24	22	44	LEU
24	22	53	LEU
24	22	70	GLN
25	23	6	VAL
25	23	23	LEU
25	23	31	LEU
25	23	54	VAL
25	23	59	VAL
26	24	15	ILE
26	24	23	GLU
26	24	33	VAL
26	24	44	THR
26	24	50	VAL
26	24	53	GLU
26	24	56	VAL
26	24	60	GLN
26	24	63	TYR
27	25	6	VAL
27	25	58	LEU
27	25	59	GLU
28	26	13	CYS
28	26	14	THR
28	26	34	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	26	37	ARG
28	26	48	VAL
28	26	52	VAL
29	27	1	MET
29	27	43	THR
29	27	46	VAL
29	27	48	LYS
30	28	14	VAL
30	28	23	VAL
31	29	12	ASP
31	29	26	ILE
33	2b	8	LYS
33	2b	22	LYS
33	2b	45	GLN
33	2b	55	PHE
33	2b	56	ARG
33	2b	64	ARG
33	2b	67	THR
33	2b	68	ILE
33	2b	71	VAL
33	2b	74	LYS
33	2b	81	VAL
33	2b	83	MET
33	2b	93	VAL
33	2b	96	ARG
33	2b	111	ARG
33	2b	121	LEU
33	2b	124	SER
33	2b	136	VAL
33	2b	164	VAL
33	2b	170	GLU
33	2b	185	ILE
33	2b	196	LEU
33	2b	200	ILE
33	2b	224	GLN
33	2b	229	VAL
34	2c	15	THR
34	2c	26	LYS
34	2c	33	LEU
34	2c	45	LYS
34	2c	47	LEU
34	2c	49	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	2c	52	LEU
34	2c	57	ILE
34	2c	66	VAL
34	2c	102	ASN
34	2c	143	GLU
34	2c	152	ILE
34	2c	204	LEU
34	2c	207	VAL
35	2d	5	ILE
35	2d	8	VAL
35	2d	17	VAL
35	2d	28	SER
35	2d	34	GLU
35	2d	58	LEU
35	2d	59	ARG
35	2d	106	TYR
35	2d	107	ARG
35	2d	108	LEU
35	2d	110	PHE
35	2d	122	ARG
35	2d	127	THR
35	2d	135	LEU
35	2d	140	VAL
35	2d	141	ARG
35	2d	155	LEU
35	2d	166	LYS
35	2d	170	VAL
35	2d	175	SER
35	2d	209	ARG
36	2e	9	LYS
36	2e	12	LEU
36	2e	31	LEU
36	2e	34	VAL
36	2e	41	VAL
36	2e	75	THR
36	2e	79	GLU
36	2e	111	GLU
36	2e	115	VAL
36	2e	143	ARG
36	2e	148	VAL
37	2f	10	LEU
37	2f	37	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	2f	72	VAL
37	2f	75	LEU
37	2f	81	ILE
37	2f	89	MET
37	2f	92	LYS
37	2f	95	GLU
38	2g	9	VAL
38	2g	21	VAL
38	2g	24	THR
38	2g	50	ILE
38	2g	57	GLU
38	2g	75	VAL
38	2g	113	GLU
38	2g	115	ARG
38	2g	131	LYS
38	2g	135	VAL
38	2g	138	LYS
38	2g	153	HIS
39	2h	2	LEU
39	2h	26	VAL
39	2h	38	ILE
39	2h	53	VAL
39	2h	63	LEU
39	2h	84	ARG
39	2h	85	ARG
39	2h	91	ARG
39	2h	112	LEU
39	2h	115	SER
39	2h	119	LEU
39	2h	133	LEU
40	2i	17	VAL
40	2i	27	THR
40	2i	28	VAL
40	2i	47	LEU
40	2i	70	LYS
40	2i	71	SER
40	2i	88	TYR
40	2i	108	VAL
40	2i	109	VAL
40	2i	125	TYR
41	2j	7	LYS
41	2j	16	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	2j	29	ARG
41	2j	30	SER
41	2j	34	VAL
41	2j	38	ILE
41	2j	47	PHE
41	2j	65	LEU
41	2j	67	THR
41	2j	74	ILE
41	2j	84	GLN
41	2j	95	GLU
42	2k	30	VAL
42	2k	81	ASP
42	2k	84	VAL
42	2k	106	LYS
42	2k	116	HIS
42	2k	117	ASN
43	2l	28	LYS
43	2l	33	ARG
43	2l	47	LYS
43	2l	81	SER
43	2l	83	VAL
43	2l	91	LYS
43	2l	123	LYS
44	2m	8	GLU
44	2m	19	LEU
44	2m	47	ASP
44	2m	53	VAL
44	2m	60	VAL
44	2m	63	THR
44	2m	90	LEU
44	2m	96	LEU
44	2m	103	THR
44	2m	109	THR
45	2n	3	ARG
45	2n	4	LYS
45	2n	7	ILE
45	2n	13	THR
45	2n	18	VAL
45	2n	42	ILE
46	2o	3	ILE
46	2o	38	ARG
46	2o	39	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
46	2o	64	ARG
47	2p	2	VAL
47	2p	20	VAL
47	2p	21	VAL
47	2p	28	ARG
47	2p	45	THR
47	2p	60	LEU
47	2p	62	VAL
47	2p	69	THR
48	2q	24	GLU
48	2q	56	VAL
48	2q	60	ILE
48	2q	85	VAL
48	2q	86	GLU
48	2q	87	LYS
48	2q	90	ILE
49	2r	25	THR
49	2r	37	VAL
49	2r	68	LYS
49	2r	82	THR
50	2s	5	LEU
50	2s	27	GLU
50	2s	30	LEU
50	2s	41	VAL
50	2s	48	THR
50	2s	56	GLN
50	2s	66	MET
50	2s	77	THR
50	2s	79	THR
51	2t	24	LEU
51	2t	41	ILE
51	2t	45	GLN
51	2t	46	GLU
51	2t	62	LEU
51	2t	86	ARG
51	2t	99	LEU
51	2t	100	ILE
53	2y	6	THR
53	2y	13	THR
53	2y	16	ILE
53	2y	24	LEU
53	2y	46	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	2y	56	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (139) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	126	GLN
3	1D	253	GLN
4	1E	143	ASN
5	1F	69	HIS
5	1F	203	GLN
5	1F	204	ASN
6	1G	26	GLN
6	1G	132	ASN
7	1H	139	GLN
8	1I	104	GLN
9	1N	38	HIS
9	1N	56	ASN
9	1N	69	GLN
13	1R	31	HIS
13	1R	61	HIS
15	1T	58	ASN
15	1T	123	GLN
16	1U	94	ASN
19	1X	31	HIS
19	1X	82	GLN
20	1Y	6	HIS
20	1Y	43	ASN
20	1Y	92	ASN
21	1Z	50	GLN
21	1Z	73	GLN
21	1Z	121	HIS
21	1Z	151	HIS
23	11	56	GLN
25	13	32	GLN
28	16	20	ASN
33	1b	40	HIS
33	1b	212	GLN
34	1c	6	HIS
34	1c	69	HIS
34	1c	102	ASN
34	1c	104	GLN
34	1c	108	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	1c	139	GLN
35	1d	45	GLN
35	1d	77	ASN
35	1d	119	GLN
35	1d	123	HIS
35	1d	129	ASN
36	1e	20	GLN
37	1f	100	ASN
38	1g	13	GLN
38	1g	28	ASN
38	1g	64	GLN
38	1g	148	ASN
39	1h	70	GLN
40	1i	3	GLN
40	1i	87	GLN
41	1j	13	HIS
41	1j	56	HIS
41	1j	69	ASN
42	1k	93	GLN
42	1k	99	GLN
42	1k	116	HIS
43	1l	99	HIS
45	1n	49	HIS
45	1n	52	GLN
46	1o	71	GLN
47	1p	13	HIS
47	1p	16	HIS
47	1p	76	GLN
48	1q	16	GLN
48	1q	45	HIS
48	1q	93	GLN
50	1s	14	HIS
50	1s	69	HIS
50	1s	83	HIS
51	1t	18	GLN
51	1t	75	ASN
53	1y	36	ASN
53	1y	38	HIS
3	2D	126	GLN
3	2D	253	GLN
4	2E	48	GLN
5	2F	69	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	2F	75	HIS
5	2F	133	ASN
6	2G	41	GLN
6	2G	132	ASN
8	2I	43	ASN
8	2I	133	HIS
9	2N	133	GLN
10	2O	89	ASN
12	2Q	12	GLN
14	2S	34	HIS
14	2S	68	GLN
15	2T	58	ASN
15	2T	84	GLN
16	2U	94	ASN
19	2X	82	GLN
20	2Y	57	GLN
21	2Z	73	GLN
21	2Z	75	ASN
21	2Z	121	HIS
25	23	32	GLN
33	2b	19	HIS
33	2b	37	ASN
33	2b	76	GLN
33	2b	95	GLN
33	2b	146	GLN
33	2b	212	GLN
33	2b	224	GLN
34	2c	98	ASN
34	2c	176	HIS
35	2d	77	ASN
35	2d	116	GLN
35	2d	125	HIS
35	2d	161	ASN
36	2e	20	GLN
36	2e	130	ASN
37	2f	73	ASN
37	2f	94	GLN
37	2f	100	ASN
38	2g	28	ASN
38	2g	64	GLN
38	2g	86	GLN
39	2h	82	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	2i	3	GLN
40	2i	58	HIS
41	2j	13	HIS
41	2j	68	HIS
41	2j	69	ASN
42	2k	104	GLN
43	2l	99	HIS
44	2m	62	ASN
45	2n	49	HIS
47	2p	13	HIS
48	2q	16	GLN
48	2q	26	GLN
48	2q	93	GLN
50	2s	83	HIS
53	2y	9	GLN
53	2y	33	HIS
53	2y	58	ASN
53	2y	79	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2865/2915 (98%)	403 (14%)	35 (1%)
1	2A	2858/2915 (98%)	463 (16%)	37 (1%)
2	1B	119/121 (98%)	13 (10%)	0
2	2B	119/121 (98%)	17 (14%)	0
32	1a	1497/1521 (98%)	246 (16%)	0
32	2a	1501/1521 (98%)	259 (17%)	0
All	All	8959/9114 (98%)	1401 (15%)	72 (0%)

All (1401) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	13	A
1	1A	15	G
1	1A	33	U
1	1A	34	C
1	1A	45	C
1	1A	71	A
1	1A	74	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	75	G
1	1A	95	G
1	1A	118	A
1	1A	119	A
1	1A	120	U
1	1A	181	A
1	1A	182	A
1	1A	196	A
1	1A	197	A
1	1A	199	A
1	1A	205	G
1	1A	215	G
1	1A	216	A
1	1A	221	A
1	1A	222	A
1	1A	229	A
1	1A	248	G
1	1A	265	A
1	1A	271(I)	G
1	1A	271(K)	U
1	1A	271(L)	U
1	1A	271(M)	G
1	1A	271(N)	U
1	1A	271(O)	C
1	1A	272(A)	U
1	1A	272(B)	G
1	1A	272(G)	C
1	1A	275	G
1	1A	279	C
1	1A	283	A
1	1A	311	A
1	1A	330	A
1	1A	352	G
1	1A	363	G
1	1A	386	G
1	1A	396	G
1	1A	405	U
1	1A	411	G
1	1A	412	A
1	1A	421	U
1	1A	422	A
1	1A	428	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	448	U
1	1A	451	C
1	1A	454	A
1	1A	456	C
1	1A	457	A
1	1A	481	G
1	1A	505	A
1	1A	509	C
1	1A	528	A
1	1A	530	G
1	1A	531	C
1	1A	532	A
1	1A	533	G
1	1A	545	G
1	1A	549	G
1	1A	551	G
1	1A	563	G
1	1A	573	G
1	1A	575	A
1	1A	586	A
1	1A	603	A
1	1A	604	G
1	1A	607	U
1	1A	614(B)	G
1	1A	615	G
1	1A	627	A
1	1A	637	A
1	1A	645	C
1	1A	646	A
1	1A	652(E)	G
1	1A	652(T)	C
1	1A	652(U)	G
1	1A	668	G
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	765	G
1	1A	775	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	776	G
1	1A	782	A
1	1A	783	A
1	1A	784	A
1	1A	785	G
1	1A	789	A
1	1A	792	G
1	1A	805	G
1	1A	812	C
1	1A	827	U
1	1A	828	U
1	1A	859	G
1	1A	866	A
1	1A	883	G
1	1A	886	C
1	1A	888	C
1	1A	889	C
1	1A	890	A
1	1A	892	G
1	1A	896	A
1	1A	897	C
1	1A	907	U
1	1A	910	A
1	1A	932	G
1	1A	945	A
1	1A	946	G
1	1A	953	A
1	1A	958	U
1	1A	959	A
1	1A	961	C
1	1A	963	U
1	1A	974	G
1	1A	975	C
1	1A	983	A
1	1A	996	A
1	1A	1005	C
1	1A	1012	U
1	1A	1013	C
1	1A	1026	U
1	1A	1033	U
1	1A	1039	G
1	1A	1041	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1042	G
1	1A	1043	C
1	1A	1046	A
1	1A	1047	G
1	1A	1048	A
1	1A	1052	C
1	1A	1053	C
1	1A	1054	A
1	1A	1059	G
1	1A	1061	U
1	1A	1062	G
1	1A	1063	G
1	1A	1065	U
1	1A	1066	U
1	1A	1067	A
1	1A	1068	G
1	1A	1070	A
1	1A	1071	G
1	1A	1073	A
1	1A	1075	C
1	1A	1076	C
1	1A	1077	A
1	1A	1079	C
1	1A	1083	U
1	1A	1087	G
1	1A	1088	A
1	1A	1090	U
1	1A	1096	A
1	1A	1097	U
1	1A	1104	C
1	1A	1109	C
1	1A	1110	G
1	1A	1112	G
1	1A	1116	C
1	1A	1128	A
1	1A	1130	U
1	1A	1135	C
1	1A	1136	G
1	1A	1155	A
1	1A	1171	G
1	1A	1173	G
1	1A	1174	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1175	U
1	1A	1176	G
1	1A	1177	A
1	1A	1178	C
1	1A	1210	A
1	1A	1211	U
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	1352	U
1	1A	1359	A
1	1A	1360	A
1	1A	1365	A
1	1A	1370	C
1	1A	1384	A
1	1A	1385	G
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	1452	A
1	1A	1459	G
1	1A	1467	C
1	1A	1471	A
1	1A	1478	G
1	1A	1482	G
1	1A	1494	A
1	1A	1506	C
1	1A	1507	A
1	1A	1509	C
1	1A	1509(A)	A
1	1A	1525	G
1	1A	1531	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1542	A
1	1A	1543	C
1	1A	1558	A
1	1A	1566	A
1	1A	1569	A
1	1A	1578	U
1	1A	1579	A
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	1648	C
1	1A	1654	A
1	1A	1674	G
1	1A	1696	G
1	1A	1700	A
1	1A	1701	A
1	1A	1703	G
1	1A	1722	A
1	1A	1739	U
1	1A	1762	A
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	1812	A
1	1A	1816	G
1	1A	1817	G
1	1A	1828	G
1	1A	1847	A
1	1A	1877	A
1	1A	1878	G
1	1A	1889	A
1	1A	1900	A
1	1A	1906	G
1	1A	1913	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1914	C
1	1A	1915	5MU
1	1A	1929	G
1	1A	1930	G
1	1A	1937	A
1	1A	1938	A
1	1A	1955	U
1	1A	1963	U
1	1A	1967	C
1	1A	1970	A
1	1A	1971	A
1	1A	1972	A
1	1A	1992	G
1	1A	1993	U
1	1A	1997	G
1	1A	2020	A
1	1A	2023	G
1	1A	2031	A
1	1A	2033	A
1	1A	2043	C
1	1A	2055	C
1	1A	2056	G
1	1A	2060	A
1	1A	2061	G
1	1A	2069	G
1	1A	2103	C
1	1A	2104	G
1	1A	2107	C
1	1A	2108	C
1	1A	2112	G
1	1A	2116	G
1	1A	2117	A
1	1A	2118	U
1	1A	2123	G
1	1A	2126	A
1	1A	2127	G
1	1A	2131	G
1	1A	2132	U
1	1A	2133	G
1	1A	2134	A
1	1A	2135	A
1	1A	2137	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2138	C
1	1A	2139	C
1	1A	2142	C
1	1A	2146	C
1	1A	2148	G
1	1A	2157	G
1	1A	2158	A
1	1A	2159	G
1	1A	2164	C
1	1A	2171	A
1	1A	2173	A
1	1A	2178	C
1	1A	2181	G
1	1A	2185	C
1	1A	2186	G
1	1A	2187	G
1	1A	2190	G
1	1A	2192	G
1	1A	2198	A
1	1A	2206	G
1	1A	2207	G
1	1A	2208	A
1	1A	2225	A
1	1A	2238	G
1	1A	2268	A
1	1A	2273	A
1	1A	2279	G
1	1A	2280	G
1	1A	2283	C
1	1A	2287	A
1	1A	2305	A
1	1A	2308	G
1	1A	2312	U
1	1A	2320	A
1	1A	2325	G
1	1A	2334	G
1	1A	2336	A
1	1A	2347	C
1	1A	2350	C
1	1A	2383	G
1	1A	2385	C
1	1A	2393	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2406	U
1	1A	2407	G
1	1A	2422	A
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	2469	A
1	1A	2476	A
1	1A	2477	C
1	1A	2478	A
1	1A	2491	U
1	1A	2502	G
1	1A	2505	G
1	1A	2506	U
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	2602	A
1	1A	2603	G
1	1A	2609	U
1	1A	2611	U
1	1A	2612	C
1	1A	2630	G
1	1A	2654	A
1	1A	2689	U
1	1A	2690	C
1	1A	2702	U
1	1A	2703	C
1	1A	2712(A)	A
1	1A	2713	A
1	1A	2714	G
1	1A	2726	U
1	1A	2733	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2758	A
1	1A	2761	G
1	1A	2765	A
1	1A	2766	G
1	1A	2778	A
1	1A	2789	C
1	1A	2790	A
1	1A	2791	C
1	1A	2802	G
1	1A	2807	G
1	1A	2818	G
1	1A	2820	A
1	1A	2821	A
1	1A	2833	G
1	1A	2835	A
1	1A	2872	G
1	1A	2894	G
2	1B	2	C
2	1B	7	G
2	1B	13	A
2	1B	45	A
2	1B	53	A
2	1B	56	G
2	1B	63	G
2	1B	64	C
2	1B	67	G
2	1B	73	A
2	1B	85	G
2	1B	90	A
2	1B	110	G
32	1a	7	G
32	1a	9	G
32	1a	32	A
32	1a	39	G
32	1a	48	C
32	1a	50	A
32	1a	51	A
32	1a	61	G
32	1a	78	G
32	1a	79	G
32	1a	97	G
32	1a	101	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	115	G
32	1a	116	A
32	1a	121	C
32	1a	131	C
32	1a	143	A
32	1a	144	G
32	1a	156	G
32	1a	163	C
32	1a	165	C
32	1a	173	U
32	1a	174	C
32	1a	182	U
32	1a	189(D)	C
32	1a	189(G)	G
32	1a	195	A
32	1a	197	A
32	1a	199	G
32	1a	203	U
32	1a	204	U
32	1a	216	G
32	1a	247	G
32	1a	251	G
32	1a	258	G
32	1a	266	G
32	1a	267	C
32	1a	289	G
32	1a	306	G
32	1a	321	A
32	1a	328	C
32	1a	329	A
32	1a	330	C
32	1a	332	G
32	1a	348	G
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	356	A
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	384	G
32	1a	398	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	406	G
32	1a	412	A
32	1a	413	G
32	1a	423	G
32	1a	424	G
32	1a	429	U
32	1a	430	A
32	1a	439	A
32	1a	442	C
32	1a	452	A
32	1a	458	C
32	1a	461	A
32	1a	470	C
32	1a	484	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	532	A
32	1a	547	A
32	1a	550	G
32	1a	559	A
32	1a	561	U
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	577	G
32	1a	596	C
32	1a	607	A
32	1a	616	G
32	1a	618	C
32	1a	619	U
32	1a	630	G
32	1a	631	G
32	1a	632	A
32	1a	642	A
32	1a	653	A
32	1a	661	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	665	A
32	1a	666	G
32	1a	673	G
32	1a	687	A
32	1a	688	G
32	1a	723	U
32	1a	724	G
32	1a	731	G
32	1a	755	G
32	1a	770	C
32	1a	777	A
32	1a	793	U
32	1a	794	A
32	1a	816	A
32	1a	817	C
32	1a	821	G
32	1a	828	A
32	1a	829	G
32	1a	839	U
32	1a	840	C
32	1a	841	U
32	1a	848	C
32	1a	851	G
32	1a	913	A
32	1a	914	A
32	1a	916	G
32	1a	926	G
32	1a	927	G
32	1a	934	C
32	1a	935	A
32	1a	942	G
32	1a	960	U
32	1a	961	U
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	992	U
32	1a	993	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	994	A
32	1a	998	G
32	1a	999	C
32	1a	1001	A
32	1a	1001(A)	G
32	1a	1006	C
32	1a	1022	G
32	1a	1023	G
32	1a	1024	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(B)	C
32	1a	1030(C)	G
32	1a	1030(D)	A
32	1a	1032	G
32	1a	1033	G
32	1a	1037	C
32	1a	1039	C
32	1a	1042	G
32	1a	1044	A
32	1a	1046	A
32	1a	1053	G
32	1a	1065	U
32	1a	1066	C
32	1a	1067	A
32	1a	1070	U
32	1a	1081	G
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1104	G
32	1a	1121	U
32	1a	1124	G
32	1a	1130	A
32	1a	1132	C
32	1a	1134	G
32	1a	1136	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	1137	C
32	1a	1139	G
32	1a	1140	C
32	1a	1146	A
32	1a	1150	U
32	1a	1152	A
32	1a	1159	U
32	1a	1166	G
32	1a	1168	A
32	1a	1183	A
32	1a	1184	G
32	1a	1196	U
32	1a	1197	G
32	1a	1202	G
32	1a	1212	U
32	1a	1213	A
32	1a	1224	G
32	1a	1227	A
32	1a	1238	A
32	1a	1256	A
32	1a	1257	U
32	1a	1258	G
32	1a	1260	C
32	1a	1270	C
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	1320	C
32	1a	1322	C
32	1a	1340	A
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1364	U
32	1a	1370	G
32	1a	1379	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	1397	C
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1442(B)	A
32	1a	1447	A
32	1a	1452	C
32	1a	1456	G
32	1a	1469	G
32	1a	1487	G
32	1a	1492	A
32	1a	1493	A
32	1a	1497	G
32	1a	1499	A
32	1a	1503	A
32	1a	1504	G
32	1a	1505	G
32	1a	1506	U
32	1a	1517	G
32	1a	1519	MA6
32	1a	1520	G
32	1a	1529	G
32	1a	1530	G
32	1a	1531	A
1	2A	10	G
1	2A	12	U
1	2A	15	G
1	2A	34	C
1	2A	45	C
1	2A	51	G
1	2A	64	A
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	84	A
1	2A	94	C
1	2A	118	A
1	2A	119	A
1	2A	120	U
1	2A	125	G
1	2A	141	A
1	2A	157	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	181	A
1	2A	182	A
1	2A	196	A
1	2A	197	A
1	2A	199	A
1	2A	205	G
1	2A	215	G
1	2A	216	A
1	2A	221	A
1	2A	222	A
1	2A	228	A
1	2A	229	A
1	2A	230	U
1	2A	248	G
1	2A	265	A
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	271(O)	C
1	2A	272(A)	U
1	2A	272(B)	G
1	2A	272(J)	C
1	2A	277	C
1	2A	278	A
1	2A	283	A
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	342	G
1	2A	352	G
1	2A	363	G
1	2A	363(B)	G
1	2A	386	G
1	2A	405	U
1	2A	406	G
1	2A	411	G
1	2A	412	A
1	2A	428	A
1	2A	444	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	451	C
1	2A	455	C
1	2A	457	A
1	2A	470	A
1	2A	481	G
1	2A	504	U
1	2A	505	A
1	2A	509	C
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	545	G
1	2A	563	G
1	2A	573	G
1	2A	575	A
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	614(B)	G
1	2A	615	G
1	2A	616	G
1	2A	627	A
1	2A	634	C
1	2A	637	A
1	2A	645	C
1	2A	646	A
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	653	A
1	2A	669	G
1	2A	686	G
1	2A	717	G
1	2A	730	C
1	2A	740	U
1	2A	752	A
1	2A	753	C
1	2A	764	A
1	2A	765	G
1	2A	775	G
1	2A	776	G
1	2A	782	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	827	U
1	2A	828	U
1	2A	857	C
1	2A	859	G
1	2A	866	A
1	2A	869	G
1	2A	878	A
1	2A	880	G
1	2A	881	G
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	890	A
1	2A	893	C
1	2A	896	A
1	2A	897	C
1	2A	900	A
1	2A	901	A
1	2A	910	A
1	2A	914	C
1	2A	915	C
1	2A	917	A
1	2A	932	G
1	2A	938	G
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	953	A
1	2A	961	C
1	2A	963	U
1	2A	974	G
1	2A	975	C
1	2A	983	A
1	2A	996	A
1	2A	1006	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1012	U
1	2A	1013	C
1	2A	1033	U
1	2A	1038	C
1	2A	1041	C
1	2A	1044	G
1	2A	1045	A
1	2A	1046	A
1	2A	1047	G
1	2A	1048	A
1	2A	1053	C
1	2A	1054	A
1	2A	1058	G
1	2A	1060	U
1	2A	1064	C
1	2A	1065	U
1	2A	1066	U
1	2A	1067	A
1	2A	1068	G
1	2A	1070	A
1	2A	1071	G
1	2A	1072	C
1	2A	1073	A
1	2A	1074	G
1	2A	1076	C
1	2A	1077	A
1	2A	1078	U
1	2A	1079	C
1	2A	1082	U
1	2A	1083	U
1	2A	1084	A
1	2A	1085	A
1	2A	1086	A
1	2A	1088	A
1	2A	1090	U
1	2A	1091	G
1	2A	1092	C
1	2A	1093	G
1	2A	1094	U
1	2A	1095	A
1	2A	1096	A
1	2A	1098	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1105	U
1	2A	1108	U
1	2A	1109	C
1	2A	1110	G
1	2A	1111	A
1	2A	1112	G
1	2A	1117	G
1	2A	1128	A
1	2A	1129	A
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1171	G
1	2A	1195	G
1	2A	1211	U
1	2A	1212	G
1	2A	1220	A
1	2A	1230	C
1	2A	1236	G
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1300	U
1	2A	1301	A
1	2A	1303	G
1	2A	1314	C
1	2A	1319	G
1	2A	1321	A
1	2A	1342	A
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1368	G
1	2A	1370	C
1	2A	1384	A
1	2A	1385	G
1	2A	1386	C
1	2A	1416	G
1	2A	1417	C
1	2A	1420	U
1	2A	1421	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1428	C
1	2A	1445	A
1	2A	1450	G
1	2A	1455	G
1	2A	1459	G
1	2A	1467	C
1	2A	1471	A
1	2A	1482	G
1	2A	1493	C
1	2A	1497	U
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1531	C
1	2A	1533	G
1	2A	1537	G
1	2A	1542	A
1	2A	1543	C
1	2A	1547	C
1	2A	1558	A
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1580	A
1	2A	1584	C
1	2A	1586	A
1	2A	1593	G
1	2A	1595	G
1	2A	1608	A
1	2A	1609	A
1	2A	1610	A
1	2A	1640	C
1	2A	1648	C
1	2A	1664	A
1	2A	1674	G
1	2A	1696	G
1	2A	1700	A
1	2A	1701	A
1	2A	1721	G
1	2A	1722	A
1	2A	1756	G
1	2A	1763	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1764	G
1	2A	1773	A
1	2A	1780	A
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1816	G
1	2A	1828	G
1	2A	1839	G
1	2A	1847	A
1	2A	1848	A
1	2A	1858	G
1	2A	1877	A
1	2A	1878	G
1	2A	1889	A
1	2A	1900	A
1	2A	1906	G
1	2A	1913	A
1	2A	1914	C
1	2A	1927	A
1	2A	1929	G
1	2A	1930	G
1	2A	1937	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	1984	G
1	2A	1993	U
1	2A	1997	G
1	2A	2020	A
1	2A	2023	G
1	2A	2031	A
1	2A	2032	G
1	2A	2033	A
1	2A	2043	C
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2061	G
1	2A	2069	G
1	2A	2096	U
1	2A	2103	C
1	2A	2104	G
1	2A	2105	C
1	2A	2107	C
1	2A	2108	C
1	2A	2109	U
1	2A	2110	G
1	2A	2111	C
1	2A	2113	U
1	2A	2114	A
1	2A	2115	G
1	2A	2116	G
1	2A	2117	A
1	2A	2118	U
1	2A	2119	A
1	2A	2120	G
1	2A	2123	G
1	2A	2126	A
1	2A	2127	G
1	2A	2129	C
1	2A	2131	G
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2136	C
1	2A	2145	C
1	2A	2146	C
1	2A	2147	G
1	2A	2148	G
1	2A	2150	U
1	2A	2151	G
1	2A	2157	G
1	2A	2158	A
1	2A	2159	G
1	2A	2160	G
1	2A	2161	C
1	2A	2163	C
1	2A	2164	C
1	2A	2165	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2166	G
1	2A	2170	A
1	2A	2172	U
1	2A	2173	A
1	2A	2176	A
1	2A	2178	C
1	2A	2180	U
1	2A	2184	G
1	2A	2186	G
1	2A	2189	U
1	2A	2190	G
1	2A	2192	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2218	U
1	2A	2219	G
1	2A	2225	A
1	2A	2239	G
1	2A	2269	A
1	2A	2275	C
1	2A	2280	G
1	2A	2283	C
1	2A	2287	A
1	2A	2289	G
1	2A	2292	C
1	2A	2305	A
1	2A	2308	G
1	2A	2312	U
1	2A	2316	C
1	2A	2320	A
1	2A	2321	G
1	2A	2322	A
1	2A	2325	G
1	2A	2334	G
1	2A	2335	A
1	2A	2336	A
1	2A	2343	C
1	2A	2347	C
1	2A	2350	C
1	2A	2383	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2385	C
1	2A	2406	U
1	2A	2407	G
1	2A	2410	G
1	2A	2414	G
1	2A	2422	A
1	2A	2423	U
1	2A	2425	A
1	2A	2429	G
1	2A	2430	A
1	2A	2435	A
1	2A	2439	A
1	2A	2440	C
1	2A	2441	C
1	2A	2448	A
1	2A	2468	G
1	2A	2473	U
1	2A	2474	C
1	2A	2476	A
1	2A	2491	U
1	2A	2492	U
1	2A	2494	G
1	2A	2502	G
1	2A	2505	G
1	2A	2506	U
1	2A	2518	A
1	2A	2529	G
1	2A	2554	U
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2602	A
1	2A	2603	G
1	2A	2609	U
1	2A	2611	U
1	2A	2612	C
1	2A	2615	U
1	2A	2629	A
1	2A	2630	G
1	2A	2654	A
1	2A	2663	G
1	2A	2682	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	2726	U
1	2A	2733	A
1	2A	2757	A
1	2A	2764	A
1	2A	2765	A
1	2A	2778	A
1	2A	2793	G
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2835	A
1	2A	2872	G
1	2A	2873	A
1	2A	2880	C
1	2A	2891	G
1	2A	2894	G
1	2A	2896	C
1	2A	2897	U
2	2B	2	C
2	2B	7	G
2	2B	8	U
2	2B	13	A
2	2B	30	C
2	2B	31	C
2	2B	33	G
2	2B	34	U
2	2B	35	U
2	2B	41	U
2	2B	42	C
2	2B	45	A
2	2B	51	G
2	2B	56	G
2	2B	73	A
2	2B	84	C
2	2B	110	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	5	U
32	2a	9	G
32	2a	22	G
32	2a	32	A
32	2a	39	G
32	2a	44	G
32	2a	47	C
32	2a	48	C
32	2a	50	A
32	2a	51	A
32	2a	61	G
32	2a	65	U
32	2a	66	G
32	2a	89	C
32	2a	101	A
32	2a	116	A
32	2a	121	C
32	2a	129(A)	G
32	2a	131	C
32	2a	142	G
32	2a	163	C
32	2a	173	U
32	2a	174	C
32	2a	182	U
32	2a	189(C)	C
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	220	G
32	2a	227	G
32	2a	231	G
32	2a	240	C
32	2a	247	G
32	2a	251	G
32	2a	258	G
32	2a	266	G
32	2a	267	C
32	2a	289	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	298	A
32	2a	321	A
32	2a	328	C
32	2a	329	A
32	2a	332	G
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	397	A
32	2a	398	C
32	2a	406	G
32	2a	411	A
32	2a	412	A
32	2a	413	G
32	2a	421	U
32	2a	429	U
32	2a	430	A
32	2a	439	A
32	2a	442	C
32	2a	446	G
32	2a	452	A
32	2a	461	A
32	2a	470	C
32	2a	471	G
32	2a	476	G
32	2a	482	A
32	2a	484	G
32	2a	485	G
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	506	G
32	2a	509	A
32	2a	510	A
32	2a	511	C
32	2a	518	C
32	2a	527	G7M
32	2a	532	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	533	A
32	2a	547	A
32	2a	559	A
32	2a	561	U
32	2a	564	C
32	2a	572	A
32	2a	573	A
32	2a	576	G
32	2a	589	C
32	2a	596	C
32	2a	630	G
32	2a	631	G
32	2a	650	G
32	2a	653	A
32	2a	661	G
32	2a	665	A
32	2a	666	G
32	2a	687	A
32	2a	688	G
32	2a	690	G
32	2a	695	A
32	2a	723	U
32	2a	731	G
32	2a	735	C
32	2a	749	C
32	2a	753	A
32	2a	755	G
32	2a	773	G
32	2a	774	G
32	2a	777	A
32	2a	793	U
32	2a	794	A
32	2a	815	A
32	2a	817	C
32	2a	821	G
32	2a	827	U
32	2a	828	A
32	2a	829	G
32	2a	840	C
32	2a	841	U
32	2a	851	G
32	2a	859	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	874	G
32	2a	902	G
32	2a	914	A
32	2a	919	A
32	2a	926	G
32	2a	927	G
32	2a	932	C
32	2a	934	C
32	2a	960	U
32	2a	961	U
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	972	C
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	989	C
32	2a	990	C
32	2a	992	U
32	2a	993	G
32	2a	994	A
32	2a	997	U
32	2a	999	C
32	2a	1004	A
32	2a	1005	A
32	2a	1006	C
32	2a	1009	G
32	2a	1017	G
32	2a	1020	U
32	2a	1025	U
32	2a	1026	G
32	2a	1027	C
32	2a	1028	C
32	2a	1029	C
32	2a	1030(A)	G
32	2a	1030(B)	C
32	2a	1030(C)	G
32	2a	1030(D)	A
32	2a	1033	G
32	2a	1041	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1043	C
32	2a	1044	A
32	2a	1053	G
32	2a	1054	C
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1081	G
32	2a	1093	A
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A
32	2a	1117	G
32	2a	1122	U
32	2a	1123	A
32	2a	1125	U
32	2a	1127	G
32	2a	1129	C
32	2a	1130	A
32	2a	1134	G
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1140	C
32	2a	1146	A
32	2a	1147	C
32	2a	1152	A
32	2a	1154	G
32	2a	1157	A
32	2a	1159	U
32	2a	1183	A
32	2a	1184	G
32	2a	1196	U
32	2a	1197	G
32	2a	1202	G
32	2a	1213	A
32	2a	1214	C
32	2a	1224	G
32	2a	1227	A
32	2a	1238	A
32	2a	1247	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1248	A
32	2a	1256	A
32	2a	1257	U
32	2a	1258	G
32	2a	1270	C
32	2a	1278	U
32	2a	1279	A
32	2a	1281	U
32	2a	1282	C
32	2a	1285	A
32	2a	1286	A
32	2a	1287	A
32	2a	1300	G
32	2a	1302	U
32	2a	1303	C
32	2a	1305	G
32	2a	1306	A
32	2a	1315	U
32	2a	1319	A
32	2a	1320	C
32	2a	1323	G
32	2a	1340	A
32	2a	1346	A
32	2a	1347	G
32	2a	1353	G
32	2a	1363	C
32	2a	1364	U
32	2a	1370	G
32	2a	1397	C
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1442(B)	A
32	2a	1446	U
32	2a	1447	A
32	2a	1456	G
32	2a	1492	A
32	2a	1494	G
32	2a	1497	G
32	2a	1499	A
32	2a	1503	A
32	2a	1504	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1506	U
32	2a	1517	G
32	2a	1519	MA6
32	2a	1520	G
32	2a	1528	U
32	2a	1529	G
32	2a	1530	G

All (72) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	196	A
1	1A	199	A
1	1A	266	G
1	1A	271(K)	U
1	1A	278	A
1	1A	746	A
1	1A	764	A
1	1A	774	A
1	1A	827	U
1	1A	839	U
1	1A	840	C
1	1A	888	C
1	1A	895	U
1	1A	974	G
1	1A	1047	G
1	1A	1065	U
1	1A	1175	U
1	1A	1176	G
1	1A	1210	A
1	1A	1300	U
1	1A	1301	A
1	1A	1442	G
1	1A	1608	A
1	1A	1653	G
1	1A	1762	A
1	1A	2111	C
1	1A	2126	A
1	1A	2238	G
1	1A	2406	U
1	1A	2422	A
1	1A	2430	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2439	A
1	1A	2602	A
1	1A	2689	U
1	1A	2893	G
1	2A	9	U
1	2A	195	A
1	2A	196	A
1	2A	266	G
1	2A	271(M)	G
1	2A	277	C
1	2A	746	A
1	2A	752	A
1	2A	764	A
1	2A	827	U
1	2A	840	C
1	2A	856	C
1	2A	900	A
1	2A	1053	C
1	2A	1057	A
1	2A	1065	U
1	2A	1067	A
1	2A	1073	A
1	2A	1076	C
1	2A	1210	A
1	2A	1420	U
1	2A	1442	G
1	2A	1491	G
1	2A	1608	A
1	2A	1992	G
1	2A	2126	A
1	2A	2171	A
1	2A	2172	U
1	2A	2288	A
1	2A	2321	G
1	2A	2406	U
1	2A	2422	A
1	2A	2439	A
1	2A	2601	C
1	2A	2602	A
1	2A	2689	U
1	2A	2756	U

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

48 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	1.36	2 (11%)	21,30,33	2.03	4 (19%)
1	2MA	1A	2503	1,54	22,25,26	1.48	6 (27%)	32,37,40	2.42	9 (28%)
1	OMG	1A	2251	1,54	23,26,27	1.23	3 (13%)	32,38,41	2.05	7 (21%)
1	5MU	2A	1939	1	19,22,23	1.50	6 (31%)	27,32,35	2.28	8 (29%)
32	4OC	2a	1402	32	20,23,24	0.76	0	25,32,35	0.93	1 (4%)
1	5MC	1A	1962	1,54	19,22,23	1.74	3 (15%)	26,32,35	1.19	4 (15%)
32	PSU	1a	516	32,54	18,21,22	1.37	2 (11%)	21,30,33	2.00	4 (19%)
32	M2G	2a	966	32	24,27,28	1.33	4 (16%)	33,40,43	1.84	5 (15%)
1	5MU	1A	1939	1,54	19,22,23	1.36	4 (21%)	27,32,35	2.27	6 (22%)
32	UR3	2a	1498	32	19,22,23	1.04	2 (10%)	26,32,35	1.70	3 (11%)
1	5MC	1A	1942	1,54	19,22,23	1.41	3 (15%)	26,32,35	1.10	2 (7%)
32	2MG	2a	1207	32	23,26,27	1.28	4 (17%)	33,38,41	2.06	5 (15%)
32	MA6	2a	1519	32	23,26,27	0.43	0	33,38,41	2.15	9 (27%)
1	OMG	2A	2251	1,54	23,26,27	1.20	3 (13%)	32,38,41	2.03	6 (18%)
32	MA6	1a	1518	32	23,26,27	0.39	0	33,38,41	1.89	8 (24%)
1	5MC	2A	1962	1	19,22,23	1.61	3 (15%)	26,32,35	1.12	2 (7%)
1	PSU	1A	1917	1,54	18,21,22	1.40	2 (11%)	21,30,33	2.02	3 (14%)
32	5MC	2a	1404	32	19,22,23	1.72	3 (15%)	26,32,35	1.17	3 (11%)
43	0TD	2l	92	43	8,9,10	4.34	1 (12%)	6,11,13	1.92	3 (50%)
1	5MU	1A	1915	1,54	19,22,23	1.49	5 (26%)	27,32,35	2.25	9 (33%)
32	G7M	1a	527	32,54	23,26,27	2.32	5 (21%)	34,39,42	2.95	10 (29%)
1	2MU	1A	2552	1,54	19,22,24	1.26	3 (15%)	25,31,36	1.75	6 (24%)
32	5MC	2a	1400	32	19,22,23	1.64	3 (15%)	26,32,35	1.20	2 (7%)
1	PSU	2A	1911	1	18,21,22	1.38	2 (11%)	21,30,33	2.07	4 (19%)
1	2MU	2A	2552	1,54	19,22,24	1.26	3 (15%)	25,31,36	1.88	6 (24%)
32	5MC	2a	967	32	19,22,23	1.87	2 (10%)	26,32,35	1.10	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	PSU	2A	1917	1	18,21,22	1.37	2 (11%)	21,30,33	2.07	3 (14%)
32	PSU	2a	516	32,54	18,21,22	1.36	3 (16%)	21,30,33	2.01	5 (23%)
1	PSU	1A	2605	1	18,21,22	1.46	3 (16%)	21,30,33	2.16	5 (23%)
1	2MA	2A	2503	1,54	22,25,26	1.45	4 (18%)	32,37,40	2.35	8 (25%)
32	MA6	1a	1519	32	23,26,27	0.42	0	33,38,41	1.98	9 (27%)
32	MA6	2a	1518	32	23,26,27	0.40	0	33,38,41	2.02	9 (27%)
32	4OC	1a	1402	32	20,23,24	0.72	0	25,32,35	0.96	1 (4%)
43	0TD	1l	92	43	8,9,10	4.65	1 (12%)	6,11,13	2.13	3 (50%)
1	OMC	1A	1920	1,54	19,22,23	0.80	0	25,31,34	0.87	1 (4%)
32	UR3	1a	1498	32	19,22,23	0.92	0	26,32,35	1.82	3 (11%)
32	5MC	2a	1407	32	19,22,23	1.64	3 (15%)	26,32,35	1.19	3 (11%)
32	G7M	2a	527	32,54	23,26,27	2.36	5 (21%)	34,39,42	3.04	10 (29%)
32	5MC	1a	967	32	19,22,23	1.52	3 (15%)	26,32,35	1.03	2 (7%)
1	OMC	2A	1920	1	19,22,23	0.78	0	25,31,34	0.95	1 (4%)
32	5MC	1a	1400	32	19,22,23	1.73	3 (15%)	26,32,35	1.22	2 (7%)
1	5MC	2A	1942	1	19,22,23	1.80	3 (15%)	26,32,35	1.25	3 (11%)
32	2MG	1a	1207	32	23,26,27	1.22	2 (8%)	33,38,41	2.23	8 (24%)
1	PSU	2A	2605	1	18,21,22	1.42	3 (16%)	21,30,33	2.14	5 (23%)
32	M2G	1a	966	32	24,27,28	1.29	5 (20%)	33,40,43	1.81	6 (18%)
32	5MC	1a	1407	32	19,22,23	1.52	3 (15%)	26,32,35	1.20	3 (11%)
32	5MC	1a	1404	32	19,22,23	1.54	2 (10%)	26,32,35	1.04	2 (7%)
1	5MU	2A	1915	1	19,22,23	1.49	4 (21%)	27,32,35	2.24	9 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
1	2MA	1A	2503	1,54	-	1/7/25/26	0/3/3/3
1	OMG	1A	2251	1,54	-	0/9/27/28	0/3/3/3
1	5MU	2A	1939	1	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32	-	2/9/29/30	0/2/2/2
1	5MC	1A	1962	1,54	-	2/7/25/26	0/2/2/2
32	PSU	1a	516	32,54	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MU	1A	1939	1,54	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
1	5MC	1A	1942	1,54	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	0/9/27/28	0/3/3/3
32	MA6	2a	1519	32	-	2/11/29/30	0/3/3/3
1	OMG	2A	2251	1,54	-	0/9/27/28	0/3/3/3
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3
1	5MC	2A	1962	1	-	2/7/25/26	0/2/2/2
1	PSU	1A	1917	1,54	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	1/7/12/14	-
1	5MU	1A	1915	1,54	-	2/7/25/26	0/2/2/2
32	G7M	1a	527	32,54	-	1/7/25/26	0/3/3/3
1	2MU	1A	2552	1,54	-	0/9/27/28	0/2/2/2
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
1	2MU	2A	2552	1,54	-	2/9/27/28	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32,54	-	1/7/25/26	0/2/2/2
1	PSU	1A	2605	1	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	1,54	-	0/7/25/26	0/3/3/3
32	MA6	1a	1519	32	-	2/11/29/30	0/3/3/3
32	MA6	2a	1518	32	-	0/11/29/30	0/3/3/3
32	4OC	1a	1402	32	-	0/9/29/30	0/2/2/2
43	0TD	1l	92	43	-	3/7/12/14	-
1	OMC	1A	1920	1,54	-	1/9/27/28	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
32	G7M	2a	527	32,54	-	2/7/25/26	0/3/3/3
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	2/9/27/28	0/2/2/2
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/9/27/28	0/3/3/3
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	2/7/25/26	0/2/2/2

All (123) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-12.75	1.69	1.82
43	2l	92	0TD	CB-SB	-11.92	1.70	1.82
32	2a	527	G7M	C8-N7	7.55	1.45	1.33
32	1a	527	G7M	C8-N7	7.38	1.45	1.33
32	2a	967	5MC	C5-C4	7.00	1.49	1.44
1	2A	1942	5MC	C5-C4	6.66	1.49	1.44
32	2a	1404	5MC	C5-C4	6.33	1.48	1.44
1	1A	1962	5MC	C5-C4	6.20	1.48	1.44
32	1a	1400	5MC	C5-C4	6.11	1.48	1.44
1	2A	1962	5MC	C5-C4	5.88	1.48	1.44
32	2a	1400	5MC	C5-C4	5.85	1.48	1.44
32	2a	1407	5MC	C5-C4	5.80	1.48	1.44
32	1a	1404	5MC	C5-C4	5.40	1.48	1.44
32	1a	1407	5MC	C5-C4	5.39	1.48	1.44
32	1a	967	5MC	C5-C4	5.30	1.48	1.44
32	1a	527	G7M	C5-N7	-4.67	1.33	1.39
1	1A	1942	5MC	C5-C4	4.63	1.47	1.44
32	2a	527	G7M	C5-N7	-4.53	1.34	1.39
1	2A	2503	2MA	C5-C4	4.42	1.47	1.39
32	2a	527	G7M	C8-N9	4.26	1.47	1.35
32	1a	527	G7M	C8-N9	4.15	1.46	1.35
1	1A	2503	2MA	C5-C4	3.78	1.45	1.39
32	2a	527	G7M	C5-C4	3.74	1.47	1.38
1	2A	2605	PSU	C6-C5	3.66	1.39	1.35
32	1a	527	G7M	C5-C4	3.63	1.47	1.38
1	2A	1911	PSU	C6-C5	3.54	1.39	1.35
1	1A	1917	PSU	C6-C5	3.54	1.39	1.35
1	1A	1911	PSU	C6-C5	3.52	1.39	1.35
32	1a	516	PSU	C6-C5	3.42	1.39	1.35
1	2A	1917	PSU	C6-C5	3.39	1.39	1.35
32	2a	516	PSU	C6-C5	3.36	1.39	1.35
32	2a	1207	2MG	C5-C4	3.34	1.47	1.38
1	1A	2605	PSU	C4-N3	-3.33	1.32	1.38
32	2a	966	M2G	C5-C4	3.30	1.47	1.38
32	1a	1400	5MC	C6-C5	3.28	1.40	1.34
1	1A	1915	5MU	C2-N1	3.13	1.43	1.38
32	1a	966	M2G	C5-C4	3.08	1.47	1.38
32	1a	1404	5MC	C6-C5	3.07	1.39	1.34
1	2A	1915	5MU	C2-N1	3.05	1.43	1.38
1	2A	2251	OMG	C5-C4	3.05	1.47	1.38
32	2a	966	M2G	C2-N2	3.04	1.40	1.35
1	2A	1915	5MU	C6-C5	3.03	1.39	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	1939	5MU	C4-C5	2.96	1.49	1.44
1	2A	1939	5MU	C6-C5	2.96	1.39	1.34
32	2a	1407	5MC	C6-C5	2.95	1.39	1.34
1	1A	2605	PSU	C6-C5	2.94	1.38	1.35
32	2a	967	5MC	C6-C5	2.94	1.39	1.34
1	1A	2503	2MA	C5-N7	-2.89	1.33	1.39
32	1a	1207	2MG	C5-C4	2.89	1.46	1.38
1	1A	2251	OMG	C6-N1	-2.87	1.33	1.38
1	1A	1939	5MU	C6-C5	2.86	1.39	1.34
1	2A	1939	5MU	C4-N3	-2.85	1.33	1.38
1	1A	1915	5MU	C4-N3	-2.84	1.33	1.38
1	1A	2251	OMG	C5-C4	2.82	1.46	1.38
1	2A	2552	2MU	C4-N3	-2.80	1.33	1.38
1	1A	2552	2MU	C4-N3	-2.77	1.33	1.38
32	2a	1404	5MC	C6-C5	2.75	1.39	1.34
1	1A	1939	5MU	C4-N3	-2.75	1.33	1.38
1	1A	1915	5MU	C6-C5	2.74	1.39	1.34
1	1A	1962	5MC	C6-N1	-2.72	1.33	1.38
32	1a	966	M2G	C6-N1	-2.71	1.33	1.38
32	2a	1400	5MC	C6-C5	2.70	1.39	1.34
1	2A	1942	5MC	C6-C5	2.69	1.39	1.34
1	1A	1942	5MC	C6-C5	2.68	1.39	1.34
32	1a	1407	5MC	C6-C5	2.66	1.38	1.34
32	1a	967	5MC	C6-C5	2.65	1.38	1.34
32	1a	966	M2G	C2-N2	2.61	1.39	1.35
1	2A	2605	PSU	C4-N3	-2.61	1.34	1.38
1	2A	1911	PSU	C4-N3	-2.60	1.34	1.38
1	1A	1917	PSU	C4-N3	-2.56	1.34	1.38
1	2A	1915	5MU	C4-N3	-2.54	1.34	1.38
32	2a	527	G7M	C6-N1	-2.53	1.34	1.38
1	2A	1962	5MC	C6-C5	2.52	1.38	1.34
1	2A	1917	PSU	C4-N3	-2.52	1.34	1.38
1	2A	1915	5MU	C4-C5	2.51	1.48	1.44
1	1A	2503	2MA	C8-N9	-2.50	1.33	1.37
1	2A	2503	2MA	C5-C6	2.50	1.47	1.41
1	1A	1939	5MU	C6-N1	-2.50	1.33	1.38
32	2a	516	PSU	C4-N3	-2.50	1.34	1.38
1	1A	1962	5MC	C6-C5	2.49	1.38	1.34
1	1A	1911	PSU	C4-N3	-2.48	1.34	1.38
32	2a	966	M2G	C6-N1	-2.44	1.34	1.38
1	2A	2251	OMG	C6-N1	-2.44	1.34	1.38
1	2A	1942	5MC	C6-N1	-2.43	1.33	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1a	1207	2MG	C6-N1	-2.43	1.34	1.38
32	2a	1207	2MG	C6-N1	-2.42	1.34	1.38
1	1A	1915	5MU	C4-C5	2.41	1.48	1.44
1	2A	1939	5MU	C6-N1	-2.40	1.33	1.38
32	2a	1400	5MC	C6-N1	-2.40	1.33	1.38
1	1A	2503	2MA	C5-C6	2.39	1.47	1.41
1	1A	1942	5MC	C6-N1	-2.38	1.34	1.38
1	2A	2605	PSU	C2-N3	-2.36	1.33	1.37
32	1a	516	PSU	C4-N3	-2.36	1.34	1.38
1	2A	1962	5MC	C6-N1	-2.36	1.34	1.38
1	1A	1939	5MU	C2-N3	-2.29	1.34	1.38
32	1a	527	G7M	C6-N1	-2.29	1.34	1.38
1	2A	2251	OMG	C5-N7	-2.26	1.34	1.39
32	2a	1207	2MG	C2-N3	2.25	1.36	1.32
32	2a	1498	UR3	C2-N1	2.24	1.41	1.38
1	1A	2605	PSU	C2-N3	-2.23	1.33	1.37
1	2A	2552	2MU	C2-N3	-2.22	1.34	1.38
1	1A	2552	2MU	C5-C4	2.22	1.48	1.43
32	1a	967	5MC	C6-N1	-2.21	1.34	1.38
1	1A	2251	OMG	C5-N7	-2.21	1.34	1.39
1	2A	1939	5MU	C2-N3	-2.20	1.34	1.38
1	1A	2503	2MA	C4-N9	-2.20	1.33	1.37
1	2A	2503	2MA	C5-N7	-2.19	1.35	1.39
32	2a	1498	UR3	C6-C5	2.19	1.40	1.35
1	1A	2552	2MU	C2-N3	-2.17	1.34	1.38
1	2A	2503	2MA	C8-N7	2.16	1.35	1.31
1	1A	1915	5MU	C2-N3	-2.16	1.34	1.38
32	1a	1400	5MC	C6-N1	-2.15	1.34	1.38
32	2a	1404	5MC	C6-N1	-2.15	1.34	1.38
32	2a	1407	5MC	C6-N1	-2.11	1.34	1.38
1	2A	2552	2MU	C5-C4	2.10	1.48	1.43
32	1a	1407	5MC	C6-N1	-2.04	1.34	1.38
1	1A	2503	2MA	C8-N7	2.04	1.35	1.31
32	2a	966	M2G	C5-N7	-2.03	1.35	1.39
32	2a	516	PSU	O4'-C1'	-2.01	1.41	1.43
32	1a	966	M2G	C4-N9	-2.01	1.32	1.38
1	2A	1939	5MU	C2-N1	2.01	1.41	1.38
32	2a	1207	2MG	C5-N7	-2.01	1.35	1.39
32	1a	966	M2G	C5-N7	-2.01	1.35	1.39

All (232) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	527	G7M	CN7-N7-C8	-8.36	112.13	124.79
1	1A	2503	2MA	C5-C4-N3	-8.28	118.46	127.18
1	2A	2503	2MA	C5-C4-N3	-8.12	118.63	127.18
32	1a	527	G7M	CN7-N7-C8	-8.08	112.55	124.79
32	1a	1498	UR3	C4-N3-C2	-7.34	118.67	124.58
32	1a	1207	2MG	C2-N3-C4	7.10	120.89	112.00
1	1A	2605	PSU	N1-C2-N3	6.93	122.48	115.17
32	1a	527	G7M	N9-C8-N7	-6.82	95.93	112.48
1	2A	2503	2MA	N3-C4-N9	6.81	135.63	126.99
32	2a	527	G7M	N9-C8-N7	-6.80	95.96	112.48
1	2A	2605	PSU	N1-C2-N3	6.74	122.27	115.17
32	2a	1207	2MG	C2-N3-C4	6.72	120.40	112.00
32	2a	1498	UR3	C4-N3-C2	-6.59	119.28	124.58
1	2A	1911	PSU	N1-C2-N3	6.56	122.08	115.17
1	2A	1917	PSU	N1-C2-N3	6.54	122.06	115.17
32	2a	527	G7M	C8-N7-C5	6.47	115.88	107.78
1	1A	2503	2MA	N3-C4-N9	6.36	135.06	126.99
1	1A	1917	PSU	N1-C2-N3	6.35	121.86	115.17
32	2a	527	G7M	N9-C4-N3	6.26	138.47	125.95
1	2A	2251	OMG	C5-C4-N3	-6.23	118.48	128.39
32	1a	527	G7M	C8-N7-C5	6.20	115.53	107.78
1	1A	1911	PSU	N1-C2-N3	6.19	121.69	115.17
32	2a	516	PSU	N1-C2-N3	6.15	121.65	115.17
32	2a	966	M2G	C5-C4-N3	-6.08	118.72	128.39
32	1a	527	G7M	N9-C4-N3	5.99	137.94	125.95
32	1a	516	PSU	N1-C2-N3	5.97	121.46	115.17
1	1A	2251	OMG	C5-C4-N3	-5.94	118.94	128.39
32	2a	1207	2MG	C5-C4-N3	-5.88	119.03	128.39
1	2A	1939	5MU	N3-C2-N1	5.81	122.46	114.89
1	2A	1939	5MU	C4-N3-C2	-5.71	119.85	127.34
32	1a	966	M2G	C5-C4-N3	-5.69	119.34	128.39
32	1a	1207	2MG	C5-C4-N3	-5.68	119.35	128.39
1	1A	1915	5MU	N3-C2-N1	5.62	122.21	114.89
1	1A	1939	5MU	C4-N3-C2	-5.60	120.00	127.34
1	1A	1939	5MU	N3-C2-N1	5.38	121.89	114.89
32	2a	527	G7M	C5-C4-N3	-5.33	118.09	128.15
1	2A	1915	5MU	N3-C2-N1	5.30	121.79	114.89
1	1A	2251	OMG	C2-N3-C4	5.19	121.24	112.30
1	2A	2251	OMG	C2-N3-C4	5.03	120.96	112.30
32	1a	527	G7M	C5-C4-N3	-4.91	118.87	128.15
1	2A	2552	2MU	N3-C2-N1	4.90	121.27	114.89
1	1A	1915	5MU	C4-N3-C2	-4.90	120.92	127.34
32	2a	1519	MA6	C5-C4-N3	-4.89	119.98	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2A	2251	OMG	N9-C4-N3	4.81	135.57	125.95
1	1A	1939	5MU	C5-C4-N3	4.81	119.50	115.32
32	2a	1519	MA6	N1-C2-N3	-4.80	121.31	128.58
1	1A	2552	2MU	N3-C2-N1	4.76	121.08	114.89
1	2A	1915	5MU	C4-N3-C2	-4.74	121.13	127.34
32	2a	1518	MA6	N1-C2-N3	-4.70	121.47	128.58
32	1a	1519	MA6	N1-C2-N3	-4.57	121.66	128.58
1	2A	1939	5MU	C5-C4-N3	4.53	119.26	115.32
32	2a	966	M2G	C2-N3-C4	4.53	120.89	112.51
1	1A	2251	OMG	N9-C4-N3	4.52	135.00	125.95
32	2a	1518	MA6	C5-C4-N3	-4.51	120.50	126.72
1	2A	2605	PSU	C4-N3-C2	-4.50	120.18	126.37
32	1a	527	G7M	C8-N9-C4	4.46	118.14	107.09
32	2a	1207	2MG	N9-C4-N3	4.42	134.79	125.95
32	2a	527	G7M	C2-N3-C4	4.41	119.90	112.30
1	1A	2605	PSU	C4-N3-C2	-4.40	120.30	126.37
32	1a	1518	MA6	N1-C2-N3	-4.37	121.96	128.58
32	2a	966	M2G	N9-C4-N3	4.37	134.69	125.95
32	1a	1519	MA6	C5-C4-N3	-4.34	120.74	126.72
32	2a	527	G7M	C8-N9-C4	4.32	117.78	107.09
1	1A	1939	5MU	O4-C4-C5	-4.31	119.98	124.92
1	2A	2552	2MU	C4-N3-C2	-4.27	121.31	126.61
32	1a	966	M2G	C2-N3-C4	4.23	120.34	112.51
32	1a	966	M2G	N9-C4-N3	4.22	134.39	125.95
32	2a	527	G7M	CN7-N7-C5	4.17	131.99	126.80
1	2A	1911	PSU	C4-N3-C2	-4.16	120.64	126.37
1	2A	1917	PSU	O2-C2-N1	-4.16	118.50	122.79
1	1A	1915	5MU	C5-C4-N3	4.14	118.92	115.32
32	2a	516	PSU	C4-N3-C2	-4.12	120.69	126.37
32	1a	527	G7M	CN7-N7-C5	4.11	131.92	126.80
1	1A	1911	PSU	C4-N3-C2	-4.11	120.71	126.37
32	1a	527	G7M	C2-N3-C4	4.10	119.36	112.30
32	2a	1519	MA6	C4-C5-N7	-4.08	105.92	110.58
32	1a	516	PSU	C4-N3-C2	-4.08	120.76	126.37
32	2a	1519	MA6	C5-N7-C8	4.07	109.84	103.45
1	1A	2552	2MU	C4-N3-C2	-4.06	121.57	126.61
32	2a	1518	MA6	C2-N1-C6	4.06	121.76	111.83
1	2A	1942	5MC	C5-C6-N1	-4.04	118.92	123.31
1	2A	1939	5MU	C5-C6-N1	-4.03	118.94	123.31
1	2A	1915	5MU	C1'-N1-C2	4.03	124.83	117.59
32	1a	1519	MA6	C2-N1-C6	3.99	121.58	111.83
1	1A	1939	5MU	C5-C6-N1	-3.97	119.00	123.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2A	1917	PSU	C4-N3-C2	-3.95	120.92	126.37
32	1a	1518	MA6	C2-N1-C6	3.94	121.47	111.83
32	1a	1400	5MC	C5-C6-N1	-3.94	119.04	123.31
32	1a	1207	2MG	N9-C4-N3	3.93	133.82	125.95
1	1A	1917	PSU	C4-N3-C2	-3.93	120.96	126.37
1	2A	1915	5MU	C5-C4-N3	3.90	118.71	115.32
1	1A	2503	2MA	N6-C6-N1	3.88	122.26	117.03
32	2a	1519	MA6	C2-N1-C6	3.86	121.25	111.83
1	1A	1915	5MU	C1'-N1-C2	3.83	124.48	117.59
32	2a	1518	MA6	C4-C5-N7	-3.79	106.25	110.58
32	1a	1518	MA6	C5-N7-C8	3.78	109.38	103.45
1	1A	2503	2MA	C4-C5-N7	-3.77	106.27	110.58
32	1a	1518	MA6	C4-C5-N7	-3.76	106.28	110.58
32	2a	527	G7M	C1'-N9-C8	-3.75	114.08	126.74
32	1a	1519	MA6	C4-C5-N7	-3.74	106.30	110.58
32	2a	1400	5MC	C5-C6-N1	-3.74	119.25	123.31
1	1A	1911	PSU	O2-C2-N1	-3.74	118.94	122.79
32	2a	1518	MA6	C5-N7-C8	3.73	109.31	103.45
1	2A	2552	2MU	C2'-C1'-N1	-3.71	107.21	114.24
1	2A	1915	5MU	O4-C4-C5	-3.70	120.68	124.92
32	1a	1207	2MG	C6-C5-N7	3.70	137.02	130.29
1	1A	1917	PSU	O2-C2-N1	-3.69	118.98	122.79
32	1a	1518	MA6	C5-C4-N3	-3.68	121.64	126.72
1	1A	2251	OMG	C6-C5-N7	3.68	136.99	130.29
32	1a	1519	MA6	C5-N7-C8	3.64	109.16	103.45
1	1A	1939	5MU	O2-C2-N1	-3.63	118.07	122.80
32	2a	967	5MC	C5-C6-N1	-3.61	119.39	123.31
32	1a	516	PSU	O2-C2-N1	-3.60	119.07	122.79
1	2A	1911	PSU	O2-C2-N1	-3.60	119.08	122.79
32	2a	1519	MA6	N9-C8-N7	-3.58	108.86	113.94
32	2a	1519	MA6	C2-N3-C4	3.57	120.55	111.83
32	1a	527	G7M	C1'-N9-C8	-3.54	114.78	126.74
1	2A	1962	5MC	C5-C6-N1	-3.48	119.53	123.31
1	1A	1942	5MC	C5-C6-N1	-3.43	119.59	123.31
1	1A	2552	2MU	O2-C2-N1	-3.41	118.36	122.80
32	1a	966	M2G	C6-C5-N7	3.39	136.45	130.29
43	1l	92	0TD	OD2-CG-CB	3.38	120.44	113.15
1	1A	1915	5MU	O4-C4-C5	-3.37	121.06	124.92
32	1a	1498	UR3	C5-C4-N3	3.34	119.43	115.04
32	2a	1518	MA6	C2-N3-C4	3.32	119.93	111.83
32	1a	1518	MA6	N9-C8-N7	-3.29	109.27	113.94
32	1a	1400	5MC	C5-C4-N3	-3.28	118.39	121.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2A	2503	2MA	N6-C6-N1	3.27	121.44	117.03
32	2a	966	M2G	C6-C5-N7	3.26	136.21	130.29
1	2A	2503	2MA	C4-N9-C8	3.25	109.15	105.74
32	2a	1404	5MC	C5-C4-N3	-3.24	118.43	121.75
1	2A	2503	2MA	C4-C5-N7	-3.23	106.88	110.58
32	1a	1519	MA6	C2-N3-C4	3.22	119.69	111.83
43	2l	92	0TD	OD2-CG-CB	3.22	120.10	113.15
1	2A	1939	5MU	O4-C4-C5	-3.20	121.25	124.92
32	2a	1404	5MC	C5-C6-N1	-3.20	119.84	123.31
32	2a	1518	MA6	N9-C8-N7	-3.19	109.41	113.94
1	2A	1915	5MU	C1'-N1-C6	-3.16	115.95	121.15
32	2a	1407	5MC	C5-C4-N3	-3.15	118.53	121.75
1	2A	2251	OMG	C6-C5-N7	3.13	135.99	130.29
32	2a	1207	2MG	C6-C5-N7	3.12	135.96	130.29
32	1a	1404	5MC	C5-C6-N1	-3.11	119.93	123.31
32	2a	1407	5MC	C5-C6-N1	-3.11	119.94	123.31
1	1A	1915	5MU	O2-C2-N3	-3.08	115.80	121.49
32	1a	1207	2MG	N1-C2-N2	3.07	119.69	116.56
32	1a	1519	MA6	N9-C8-N7	-3.06	109.59	113.94
1	2A	1939	5MU	O2-C2-N1	-3.06	118.81	122.80
1	1A	1962	5MC	C5-C4-N3	-3.01	118.67	121.75
32	2a	516	PSU	O2-C2-N1	-2.99	119.70	122.79
32	2a	1498	UR3	C5-C4-N3	2.98	118.97	115.04
32	2a	1519	MA6	N3-C4-N9	2.96	132.21	127.17
32	1a	1518	MA6	C2-N3-C4	2.91	118.95	111.83
32	1a	967	5MC	C5-C6-N1	-2.91	120.16	123.31
1	2A	2552	2MU	C5-C4-N3	2.90	118.86	114.80
1	1A	2503	2MA	C4-N9-C8	2.87	108.75	105.74
1	1A	2605	PSU	O2-C2-N1	-2.85	119.85	122.79
1	2A	2605	PSU	O2-C2-N1	-2.84	119.86	122.79
1	1A	2503	2MA	C5-N7-C8	2.81	107.86	103.45
32	1a	1407	5MC	C5-C6-N1	-2.80	120.28	123.31
1	2A	2552	2MU	O2-C2-N1	-2.77	119.19	122.80
43	1l	92	0TD	CSB-SB-CB	2.77	107.35	102.36
32	2a	1518	MA6	C4-C5-C6	2.77	118.77	115.91
32	2a	1519	MA6	C4-C5-C6	2.77	118.77	115.91
32	1a	1407	5MC	C5-C4-N3	-2.74	118.95	121.75
32	1a	1207	2MG	C4-C5-N7	-2.73	106.34	110.67
1	2A	1942	5MC	C5-C4-N3	-2.73	118.96	121.75
1	1A	2552	2MU	C2'-C1'-N1	-2.72	109.07	114.24
1	1A	2605	PSU	C5-C6-N1	-2.72	118.36	122.14
1	1A	1915	5MU	C1'-N1-C6	-2.70	116.70	121.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	1a	527	G7M	O6-C6-C5	-2.69	122.01	128.01
32	2a	1518	MA6	N3-C4-N9	2.68	131.73	127.17
1	2A	2503	2MA	C5-N7-C8	2.64	107.59	103.45
1	2A	1962	5MC	C5-C4-N3	-2.63	119.06	121.75
1	1A	2503	2MA	C2-N1-C6	2.61	122.12	118.10
1	1A	1915	5MU	C5-C6-N1	-2.60	120.48	123.31
1	1A	1942	5MC	C5-C4-N3	-2.60	119.09	121.75
32	2a	966	M2G	C4-C5-N7	-2.58	106.58	110.67
1	2A	1915	5MU	O2-C2-N3	-2.58	116.73	121.49
32	1a	1519	MA6	C4-C5-C6	2.58	118.57	115.91
1	2A	1915	5MU	C5-C6-N1	-2.55	120.54	123.31
1	1A	2552	2MU	C5-C4-N3	2.53	118.34	114.80
32	2a	1207	2MG	C4-C5-N7	-2.50	106.72	110.67
32	1a	1519	MA6	N3-C4-N9	2.49	131.41	127.17
32	2a	1407	5MC	O2-C2-N3	-2.49	118.40	122.33
1	1A	2552	2MU	O4-C4-C5	-2.49	120.86	125.16
1	1A	1915	5MU	C6-N1-C2	-2.49	118.82	121.30
1	2A	2605	PSU	C5-C6-N1	-2.49	118.68	122.14
1	1A	2251	OMG	C4-C5-N7	-2.49	106.72	110.67
32	2a	527	G7M	O6-C6-C5	-2.48	122.47	128.01
1	2A	2251	OMG	C4-C5-N7	-2.47	106.75	110.67
32	1a	1407	5MC	O2-C2-N3	-2.46	118.46	122.33
32	1a	1404	5MC	C5-C4-N3	-2.45	119.24	121.75
32	1a	1498	UR3	C3U-N3-C2	2.45	121.60	117.33
1	2A	2503	2MA	C2-N1-C6	2.43	121.83	118.10
32	2a	1400	5MC	C5-C4-N3	-2.43	119.27	121.75
32	1a	966	M2G	C4-C5-N7	-2.42	106.83	110.67
32	1a	967	5MC	C5-C4-N3	-2.42	119.28	121.75
1	2A	2552	2MU	O4-C4-C5	-2.41	121.01	125.16
1	2A	1920	OMC	O2-C2-N3	-2.40	118.55	122.33
1	2A	1939	5MU	C5M-C5-C4	2.39	121.34	118.78
32	2a	516	PSU	O4'-C1'-C2'	2.39	108.46	105.15
1	1A	1962	5MC	CM5-C5-C6	-2.39	119.62	122.85
1	1A	2251	OMG	O6-C6-C5	-2.36	120.31	126.53
1	1A	2605	PSU	O2-C2-N3	-2.36	117.67	121.86
32	2a	967	5MC	C5-C4-N3	-2.36	119.34	121.75
32	2a	1498	UR3	C6-N1-C2	-2.35	119.87	121.80
43	2l	92	0TD	OD1-CG-CB	-2.34	117.54	122.44
32	1a	1402	4OC	C6-C5-C4	2.34	119.82	117.00
1	2A	2503	2MA	N9-C8-N7	-2.33	110.63	113.94
1	1A	2503	2MA	N9-C8-N7	-2.33	110.63	113.94
1	1A	1962	5MC	C1'-N1-C6	-2.32	117.34	121.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2A	2251	OMG	O6-C6-C5	-2.29	120.48	126.53
1	2A	1942	5MC	CM5-C5-C6	-2.29	119.76	122.85
1	1A	2251	OMG	C5-C6-N1	2.28	119.07	113.25
1	2A	2605	PSU	O2-C2-N3	-2.25	117.86	121.86
32	2a	516	PSU	C5-C6-N1	-2.22	119.06	122.14
1	1A	2503	2MA	CM2-C2-N1	2.21	120.44	117.13
1	2A	1939	5MU	C5M-C5-C6	-2.17	119.92	122.85
1	1A	1962	5MC	C5-C6-N1	-2.15	120.98	123.31
32	1a	1207	2MG	N2-C2-N3	-2.15	117.78	120.51
32	1a	1207	2MG	O6-C6-C5	-2.13	120.92	126.53
43	1l	92	0TD	OD1-CG-CB	-2.10	118.04	122.44
1	2A	1915	5MU	C6-N1-C2	-2.10	119.21	121.30
32	1a	516	PSU	O4'-C1'-C2'	2.07	108.02	105.15
32	2a	1402	4OC	C6-C5-C4	2.07	119.49	117.00
32	2a	1404	5MC	O2-C2-N3	-2.07	119.07	122.33
32	1a	966	M2G	O6-C6-C5	-2.06	121.08	126.53
32	1a	1518	MA6	N3-C4-N9	2.05	130.65	127.17
1	2A	1911	PSU	C5-C6-N1	-2.04	119.31	122.14
1	1A	1920	OMC	O2-C2-N3	-2.03	119.12	122.33
43	2l	92	0TD	CSB-SB-CB	-2.03	98.72	102.36
1	1A	1911	PSU	O4'-C1'-C2'	2.01	107.94	105.15

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	1915	5MU	O4'-C1'-N1-C2
1	1A	1915	5MU	O4'-C1'-N1-C6
43	1l	92	0TD	O-C-CA-CB
43	1l	92	0TD	CG-CB-SB-CSB
1	2A	1915	5MU	O4'-C1'-N1-C2
1	2A	1915	5MU	O4'-C1'-N1-C6
32	2a	527	G7M	C3'-C4'-C5'-O5'
32	2a	1519	MA6	O4'-C4'-C5'-O5'
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	527	G7M	O4'-C4'-C5'-O5'
32	2a	1402	4OC	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
43	2l	92	0TD	CG-CB-SB-CSB
32	1a	527	G7M	C3'-C4'-C5'-O5'
1	2A	1962	5MC	C2'-C1'-N1-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	2a	516	PSU	O4'-C1'-C5-C4
32	2a	1402	4OC	C3'-C4'-C5'-O5'
1	2A	2552	2MU	C3'-C2'-O2'-C6'
1	1A	2503	2MA	C4'-C5'-O5'-P
1	2A	1962	5MC	O4'-C1'-N1-C6
43	1l	92	0TD	CA-CB-SB-CSB
1	2A	2552	2MU	C1'-C2'-O2'-C6'
1	2A	1920	OMC	C3'-C2'-O2'-CM2
1	1A	1962	5MC	C2'-C1'-N1-C6
1	1A	1962	5MC	O4'-C1'-N1-C6
1	1A	1920	OMC	C2'-C1'-N1-C2
1	2A	1920	OMC	C2'-C1'-N1-C2

There are no ring outliers.

19 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2A	1939	5MU	1	0
32	2a	1402	4OC	1	0
32	2a	966	M2G	1	0
1	1A	1939	5MU	2	0
32	2a	1207	2MG	2	0
32	2a	1519	MA6	3	0
1	2A	2251	OMG	1	0
32	1a	1518	MA6	2	0
43	2l	92	0TD	3	0
1	1A	2552	2MU	1	0
32	2a	1400	5MC	1	0
32	2a	967	5MC	1	0
1	2A	1917	PSU	1	0
32	1a	1519	MA6	2	0
32	2a	1518	MA6	1	0
43	1l	92	0TD	1	0
1	1A	1920	OMC	1	0
1	2A	1920	OMC	1	0
32	1a	1400	5MC	2	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2534 ligands modelled in this entry, 2519 are monoatomic - leaving 15 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
58	ARG	1F	319	-	10,11,11	0.73	1 (10%)	9,13,13	0.88	1 (11%)
57	MPD	1T	206	-	7,7,7	0.37	0	9,10,10	0.23	0
57	MPD	18	103	-	7,7,7	0.32	0	9,10,10	0.40	0
56	ERY	1A	4042	-	53,53,53	0.94	2 (3%)	82,82,82	1.31	10 (12%)
57	MPD	2A	3733	-	7,7,7	0.39	0	9,10,10	0.49	0
57	MPD	2A	3734	-	7,7,7	0.32	0	9,10,10	0.19	0
55	HGR	1A	4041	-	39,39,39	2.39	8 (20%)	48,58,58	1.82	13 (27%)
57	MPD	1A	4043	-	7,7,7	0.34	0	9,10,10	0.22	0
57	MPD	2B	219	-	7,7,7	0.33	0	9,10,10	0.19	0
58	ARG	1B	230	54	10,11,11	0.79	1 (10%)	9,13,13	0.96	1 (11%)
60	SF4	1d	306	35	0,12,12	-	-	-		
56	ERY	2A	3732	-	53,53,53	0.96	2 (3%)	82,82,82	1.39	11 (13%)
57	MPD	1a	1880	32	7,7,7	0.45	0	9,10,10	0.58	0
60	SF4	2d	501	35	0,12,12	-	-	-		
55	HGR	2A	3731	-	39,39,39	2.42	9 (23%)	48,58,58	1.68	13 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	ARG	1F	319	-	-	3/11/11/11	-
57	MPD	1T	206	-	-	0/5/5/5	-
57	MPD	18	103	-	-	2/5/5/5	-
56	ERY	1A	4042	-	-	0/72/107/107	0/3/3/3
57	MPD	2A	3733	-	-	0/5/5/5	-
57	MPD	2A	3734	-	-	1/5/5/5	-
55	HGR	1A	4041	-	-	5/20/79/79	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	MPD	1A	4043	-	-	2/5/5/5	-
57	MPD	2B	219	-	-	1/5/5/5	-
58	ARG	1B	230	54	-	0/11/11/11	-
60	SF4	1d	306	35	-	-	0/6/5/5
56	ERY	2A	3732	-	-	4/72/107/107	0/3/3/3
57	MPD	1a	1880	32	-	5/5/5/5	-
60	SF4	2d	501	35	-	-	0/6/5/5
55	HGR	2A	3731	-	-	5/20/79/79	0/4/4/4

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	2A	3731	HGR	C12-C14	9.37	1.55	1.33
55	1A	4041	HGR	C12-C14	8.86	1.54	1.33
55	1A	4041	HGR	C5-C4	-5.62	1.39	1.49
55	2A	3731	HGR	C5-C4	-5.47	1.39	1.49
55	1A	4041	HGR	C5-C6	-5.24	1.39	1.50
55	2A	3731	HGR	C5-C6	-5.18	1.39	1.50
56	2A	3732	ERY	O2-C1	5.03	1.45	1.34
55	2A	3731	HGR	C3-C2	-4.86	1.39	1.48
56	1A	4042	ERY	O2-C1	4.83	1.45	1.34
55	1A	4041	HGR	C3-C2	-4.71	1.39	1.48
55	2A	3731	HGR	O4-C2	4.34	1.36	1.24
55	1A	4041	HGR	O4-C2	4.24	1.35	1.24
56	1A	4042	ERY	O2-C13	-2.84	1.41	1.46
55	2A	3731	HGR	O8-C23	2.51	1.45	1.41
55	1A	4041	HGR	O8-C23	2.49	1.45	1.41
55	1A	4041	HGR	O1-C10	2.32	1.45	1.41
56	2A	3732	ERY	O2-C13	-2.26	1.42	1.46
58	1B	230	ARG	OXT-C	-2.19	1.23	1.30
55	2A	3731	HGR	C1-C2	-2.11	1.39	1.44
55	2A	3731	HGR	O1-C10	2.06	1.45	1.41
55	1A	4041	HGR	C1-C2	-2.04	1.39	1.44
58	1F	319	ARG	OXT-C	-2.02	1.24	1.30
55	2A	3731	HGR	O9-C23	2.01	1.44	1.41

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	2A	3731	HGR	C4-C5-C6	4.72	122.42	112.35
55	1A	4041	HGR	C4-C5-C6	4.56	122.08	112.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	2A	3732	ERY	O5-C16-C17	3.90	109.51	103.86
56	2A	3732	ERY	C13-O2-C1	-3.73	111.68	118.20
55	1A	4041	HGR	O9-C22-C18	-3.70	98.20	106.03
55	1A	4041	HGR	C4-C3-C2	-3.62	118.69	121.81
56	1A	4042	ERY	O7-C5-C6	3.56	110.64	106.40
55	1A	4041	HGR	O1-C10-C9	-3.49	100.54	104.98
56	2A	3732	ERY	C6-C5-C4	-3.44	108.89	113.89
56	1A	4042	ERY	O7-C5-C4	-3.38	106.69	111.58
56	1A	4042	ERY	O2-C1-C2	3.29	118.56	111.53
56	2A	3732	ERY	O5-C16-C15	-3.27	107.91	112.95
55	1A	4041	HGR	C12-C6-C1	-3.24	115.74	119.35
56	2A	3732	ERY	O2-C1-C2	3.23	118.43	111.53
55	2A	3731	HGR	O1-C10-C9	-3.20	100.91	104.98
55	2A	3731	HGR	O8-C18-C22	-3.19	99.30	106.03
55	2A	3731	HGR	O4-C2-C3	-3.17	116.51	121.28
55	1A	4041	HGR	O8-C18-C22	-3.15	99.37	106.03
55	1A	4041	HGR	O3-C10-C9	3.04	111.63	106.69
55	2A	3731	HGR	C4-C3-C2	-3.03	119.20	121.81
55	1A	4041	HGR	C23-O9-C22	-2.99	101.75	106.31
56	2A	3732	ERY	O3-C3-C4	2.98	111.75	108.23
56	1A	4042	ERY	O5-C16-C15	-2.91	108.47	112.95
56	1A	4042	ERY	O5-C16-C17	2.86	108.00	103.86
55	2A	3731	HGR	C12-C6-C1	-2.85	116.17	119.35
56	1A	4042	ERY	C6-C5-C4	-2.81	109.81	113.89
55	1A	4041	HGR	C1-C2-C3	2.80	121.33	116.06
55	1A	4041	HGR	O3-C3-C2	2.80	117.60	112.51
55	2A	3731	HGR	C1-C2-C3	2.76	121.26	116.06
56	1A	4042	ERY	C13-O2-C1	-2.76	113.38	118.20
55	2A	3731	HGR	O9-C22-C18	-2.70	100.32	106.03
56	1A	4042	ERY	C32-C6-C5	2.67	114.69	110.13
55	2A	3731	HGR	C23-O9-C22	-2.62	102.32	106.31
55	2A	3731	HGR	C10-C9-C8	-2.56	99.10	102.29
55	1A	4041	HGR	C10-C9-C8	-2.50	99.18	102.29
55	1A	4041	HGR	O4-C2-C3	-2.46	117.58	121.28
58	1F	319	ARG	OXT-C-O	-2.46	118.50	124.08
56	2A	3732	ERY	C2-C3-C4	-2.45	105.86	112.91
58	1B	230	ARG	OXT-C-O	-2.43	118.56	124.08
55	2A	3731	HGR	O3-C10-C9	2.43	110.64	106.69
55	2A	3731	HGR	O3-C3-C2	2.19	116.49	112.51
56	2A	3732	ERY	C6-C7-C8	-2.18	111.25	115.61
55	2A	3731	HGR	C19-C17-N1	2.17	114.62	110.62
55	1A	4041	HGR	C19-C17-N1	2.12	114.51	110.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	2A	3732	ERY	C27-C26-C25	-2.09	110.11	113.27
56	1A	4042	ERY	C2-C3-C4	-2.05	107.00	112.91
56	1A	4042	ERY	O12-C11-C10	-2.05	107.87	110.77
56	2A	3732	ERY	C20-O5-C16	2.03	121.65	117.51
56	2A	3732	ERY	C35-C12-C13	-2.01	108.54	111.26

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	2A	3732	ERY	C15-C16-O5-C20
56	2A	3732	ERY	C19-C16-O5-C20
57	18	103	MPD	C2-C3-C4-O4
57	18	103	MPD	C2-C3-C4-C5
57	2B	219	MPD	C2-C3-C4-O4
56	2A	3732	ERY	C17-C16-O5-C20
55	1A	4041	HGR	C12-C14-C15-O7
55	2A	3731	HGR	C12-C14-C15-O7
55	2A	3731	HGR	C12-C14-C15-N1
58	1F	319	ARG	OXT-C-CA-CB
55	1A	4041	HGR	C2-C3-O3-C10
55	2A	3731	HGR	C2-C3-O3-C10
57	1a	1880	MPD	C1-C2-C3-C4
57	1a	1880	MPD	C2-C3-C4-C5
55	1A	4041	HGR	C12-C14-C15-N1
58	1F	319	ARG	O-C-CA-CB
55	1A	4041	HGR	C16-C14-C15-O7
55	2A	3731	HGR	C16-C14-C15-O7
56	2A	3732	ERY	C32-C6-C7-C8
55	2A	3731	HGR	C16-C14-C15-N1
57	1A	4043	MPD	O2-C2-C3-C4
57	1a	1880	MPD	O2-C2-C3-C4
57	1A	4043	MPD	C2-C3-C4-O4
57	1a	1880	MPD	C2-C3-C4-O4
57	1a	1880	MPD	CM-C2-C3-C4
57	2A	3734	MPD	CM-C2-C3-C4
58	1F	319	ARG	O-C-CA-N
55	1A	4041	HGR	C16-C14-C15-N1

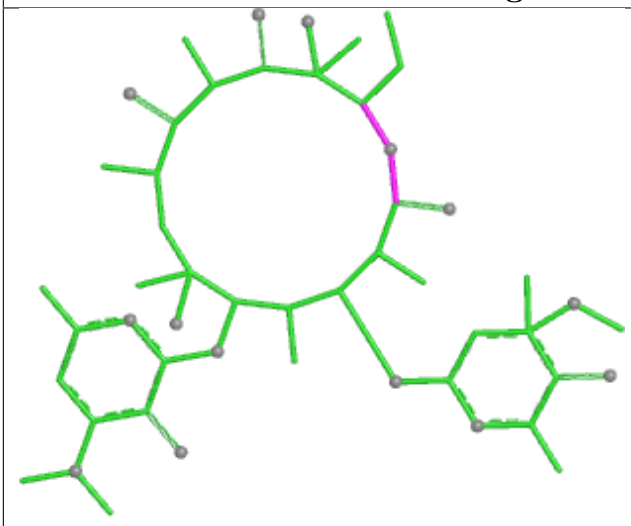
There are no ring outliers.

8 monomers are involved in 15 short contacts:

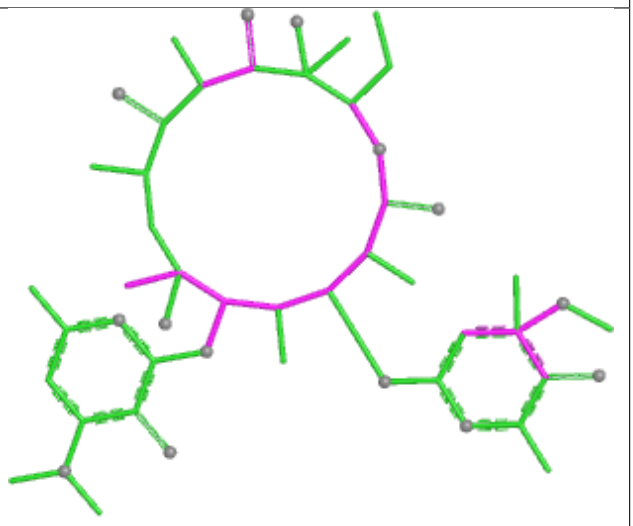
Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	1F	319	ARG	1	0
57	18	103	MPD	3	0
55	1A	4041	HGR	1	0
57	1A	4043	MPD	1	0
56	2A	3732	ERY	1	0
57	1a	1880	MPD	6	0
60	2d	501	SF4	1	0
55	2A	3731	HGR	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

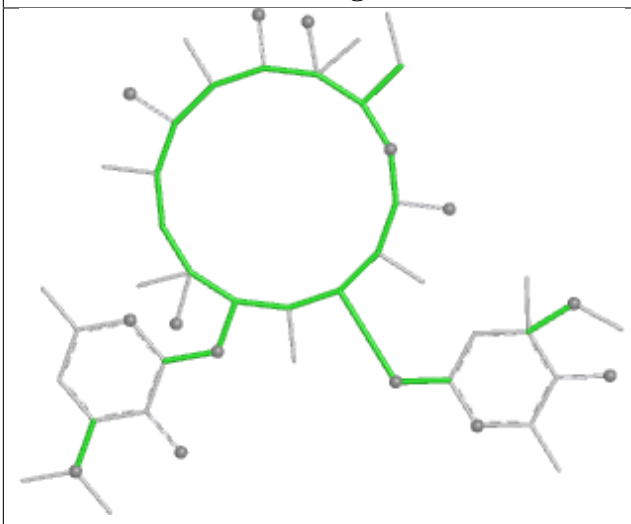
Ligand ERY 1A 4042



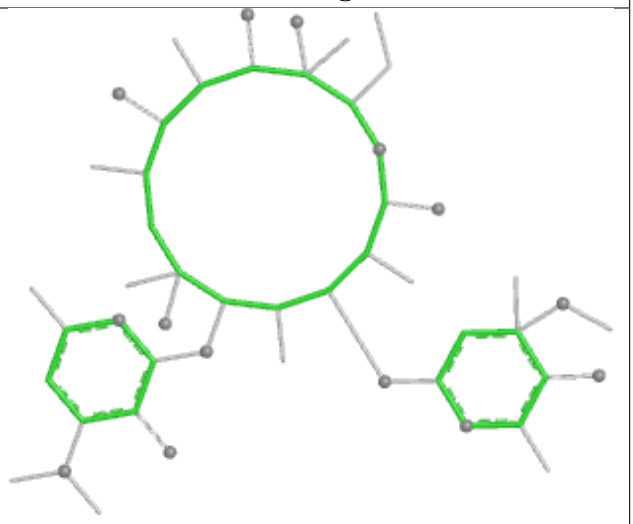
Bond lengths



Bond angles

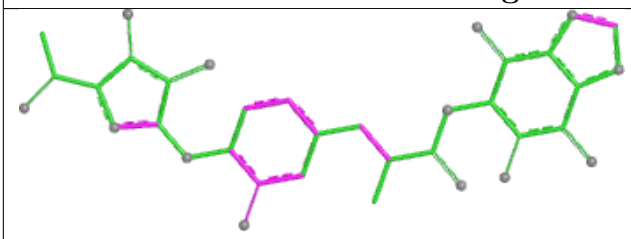


Torsions

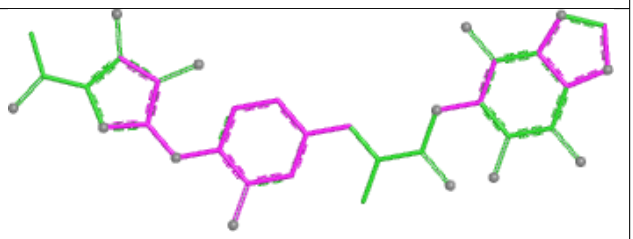


Rings

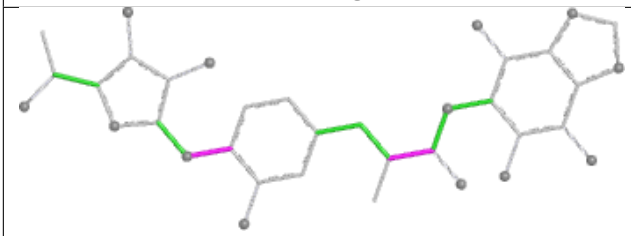
Ligand HGR 1A 4041



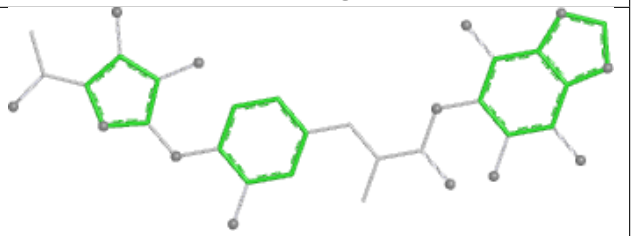
Bond lengths



Bond angles

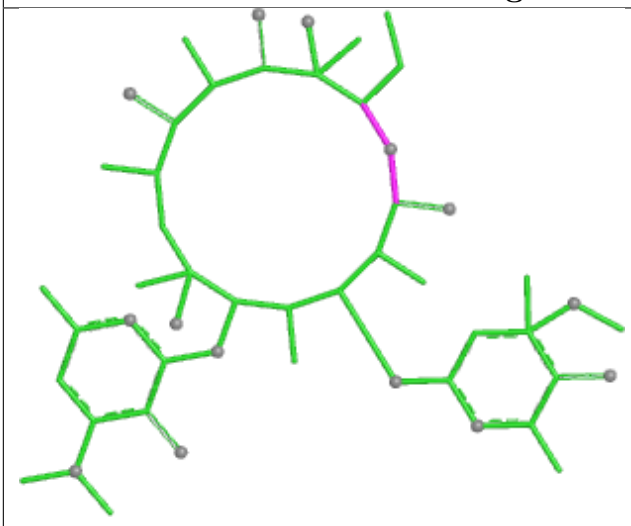


Torsions

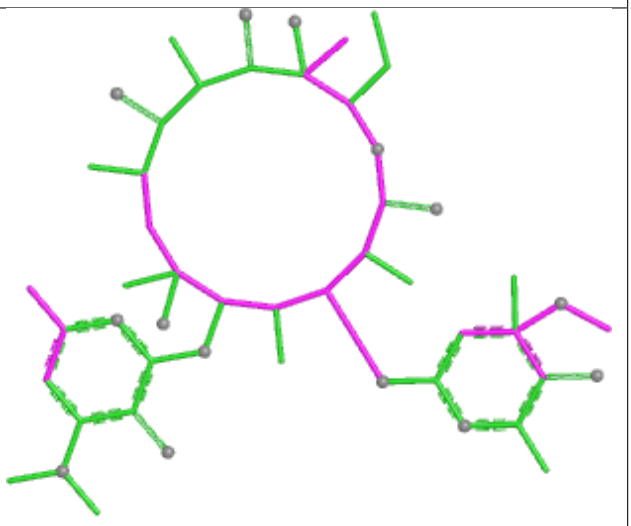


Rings

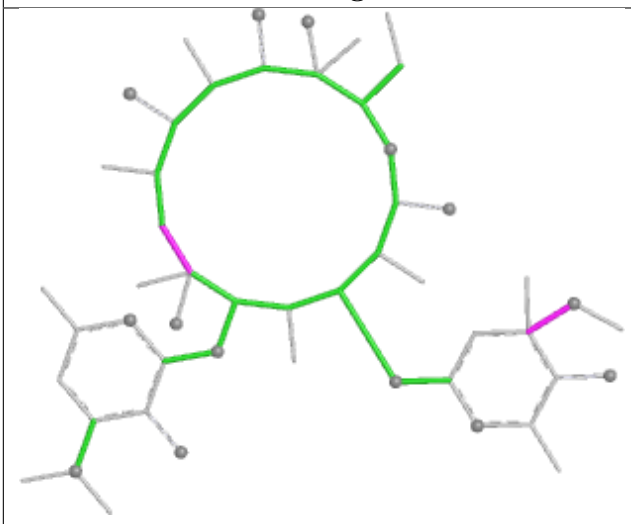
Ligand ERY 2A 3732



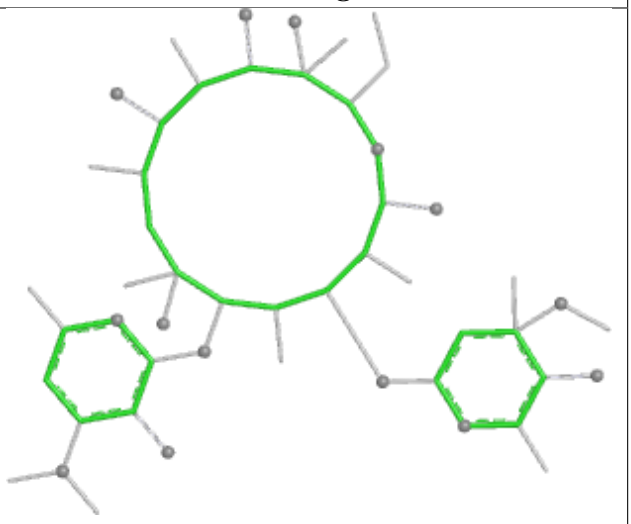
Bond lengths



Bond angles

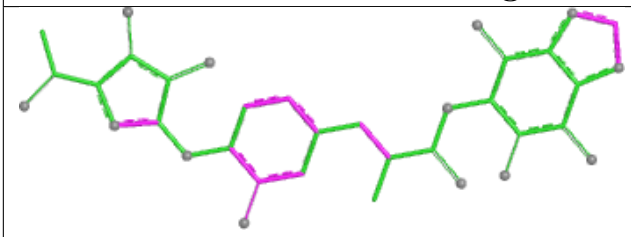


Torsions

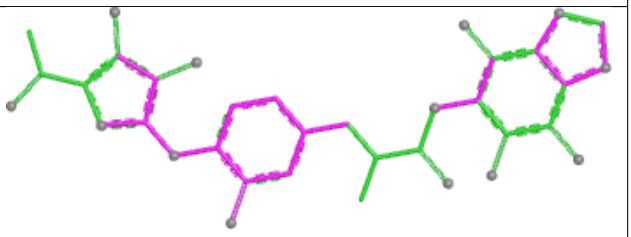


Rings

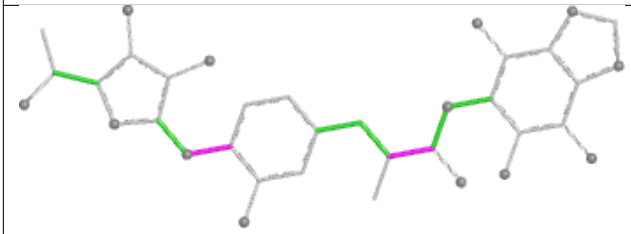
Ligand HGR 2A 3731



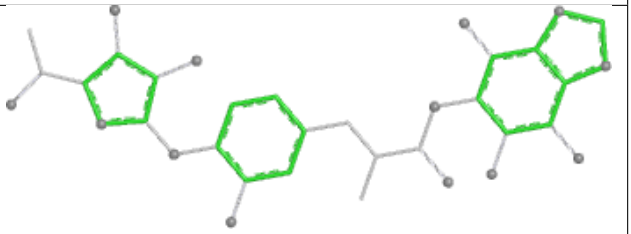
Bond lengths



Bond angles



Torsions



Rings

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	2861/2915 (98%)	-0.51	90 (3%) 51 47	26, 43, 97, 110	0
1	2A	2856/2915 (97%)	-0.04	117 (4%) 41 37	39, 63, 100, 111	0
2	1B	120/121 (99%)	-0.36	1 (0%) 82 80	37, 55, 69, 84	0
2	2B	120/121 (99%)	0.98	6 (5%) 34 30	68, 88, 96, 98	0
3	1D	275/276 (99%)	-0.03	4 (1%) 72 68	27, 43, 56, 79	0
3	2D	275/276 (99%)	0.40	10 (3%) 46 41	36, 56, 68, 82	0
4	1E	204/206 (99%)	0.11	4 (1%) 65 61	26, 46, 64, 79	0
4	2E	204/206 (99%)	0.42	5 (2%) 58 54	38, 62, 75, 85	0
5	1F	203/210 (96%)	0.02	1 (0%) 87 85	24, 48, 72, 87	0
5	2F	203/210 (96%)	0.65	4 (1%) 65 61	41, 73, 83, 92	0
6	1G	181/182 (99%)	0.69	8 (4%) 39 34	52, 68, 81, 90	0
6	2G	181/182 (99%)	2.34	112 (61%) 0 0	81, 89, 94, 97	0
7	1H	174/180 (96%)	0.37	2 (1%) 78 75	43, 58, 70, 79	0
7	2H	173/180 (96%)	1.43	34 (19%) 3 2	74, 84, 90, 94	0
8	1I	147/148 (99%)	0.91	9 (6%) 27 23	48, 76, 85, 87	0
8	2I	146/148 (98%)	1.04	12 (8%) 17 15	58, 78, 87, 91	0
9	1N	140/140 (100%)	0.01	0 100 100	33, 44, 65, 80	0
9	2N	140/140 (100%)	0.80	5 (3%) 46 41	50, 69, 81, 84	0
10	1O	122/122 (100%)	0.14	1 (0%) 82 80	37, 45, 65, 68	0
10	2O	122/122 (100%)	0.44	2 (1%) 70 67	50, 60, 72, 78	0
11	1P	149/150 (99%)	0.05	1 (0%) 84 81	26, 50, 71, 83	0
11	2P	149/150 (99%)	0.53	4 (2%) 56 51	43, 71, 86, 90	0
12	1Q	141/141 (100%)	-0.06	0 100 100	33, 45, 59, 72	0
12	2Q	141/141 (100%)	0.95	9 (6%) 25 22	52, 71, 79, 87	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%)	-0.10	0 100 100	33, 42, 58, 65	0
13	2R	118/118 (100%)	0.23	0 100 100	45, 57, 67, 74	0
14	1S	110/112 (98%)	0.26	1 (0%) 81 78	45, 55, 66, 70	0
14	2S	110/112 (98%)	1.74	43 (39%) 1 0	72, 82, 86, 90	0
15	1T	131/146 (89%)	0.38	7 (5%) 32 28	40, 50, 72, 83	0
15	2T	131/146 (89%)	0.49	3 (2%) 61 57	52, 63, 79, 86	0
16	1U	116/118 (98%)	-0.17	1 (0%) 81 78	28, 38, 50, 69	0
16	2U	116/118 (98%)	0.53	0 100 100	47, 66, 78, 86	0
17	1V	101/101 (100%)	-0.06	1 (0%) 79 76	29, 46, 62, 72	0
17	2V	101/101 (100%)	0.82	3 (2%) 52 48	49, 76, 82, 89	0
18	1W	112/113 (99%)	-0.10	2 (1%) 67 64	31, 38, 58, 86	0
18	2W	112/113 (99%)	0.41	4 (3%) 46 41	46, 56, 74, 87	0
19	1X	95/96 (98%)	0.15	3 (3%) 50 46	32, 43, 64, 79	0
19	2X	95/96 (98%)	0.81	4 (4%) 40 36	55, 66, 79, 86	0
20	1Y	107/110 (97%)	0.42	3 (2%) 55 50	40, 54, 72, 82	0
20	2Y	107/110 (97%)	1.28	16 (14%) 5 4	65, 75, 83, 89	0
21	1Z	203/206 (98%)	0.50	9 (4%) 39 34	45, 62, 77, 87	0
21	2Z	201/206 (97%)	1.50	38 (18%) 3 2	73, 82, 88, 90	0
22	10	77/85 (90%)	0.05	2 (2%) 57 52	35, 43, 60, 68	0
22	20	77/85 (90%)	1.07	7 (9%) 15 13	59, 69, 78, 83	0
23	11	97/98 (98%)	0.27	1 (1%) 79 76	34, 49, 71, 84	0
23	21	97/98 (98%)	0.68	2 (2%) 63 59	47, 61, 79, 86	0
24	12	70/72 (97%)	0.31	2 (2%) 53 49	42, 55, 65, 84	0
24	22	70/72 (97%)	0.67	1 (1%) 73 70	67, 75, 82, 83	0
25	13	59/60 (98%)	-0.12	1 (1%) 69 65	30, 42, 63, 76	0
25	23	59/60 (98%)	0.60	3 (5%) 33 29	57, 67, 82, 93	0
26	14	69/71 (97%)	1.14	14 (20%) 3 2	61, 77, 92, 96	0
26	24	69/71 (97%)	2.35	46 (66%) 0 0	83, 93, 99, 100	0
27	15	59/60 (98%)	-0.21	0 100 100	28, 40, 58, 64	0
27	25	59/60 (98%)	0.25	1 (1%) 69 65	41, 56, 70, 75	0
28	16	53/54 (98%)	-0.09	0 100 100	39, 47, 61, 67	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	26	53/54 (98%)	0.67	2 (3%) 44 39	60, 67, 74, 79	0
29	17	48/49 (97%)	0.07	5 (10%) 11 10	28, 35, 59, 71	0
29	27	48/49 (97%)	0.38	4 (8%) 17 15	39, 48, 70, 78	0
30	18	64/65 (98%)	-0.16	1 (1%) 70 67	35, 40, 47, 59	0
30	28	64/65 (98%)	0.55	2 (3%) 51 47	54, 62, 68, 71	0
31	19	37/37 (100%)	0.05	0 100 100	37, 46, 61, 67	0
31	29	37/37 (100%)	1.08	4 (10%) 11 9	61, 72, 80, 82	0
32	1a	1488/1521 (97%)	0.13	29 (1%) 66 62	41, 73, 96, 110	0
32	2a	1492/1521 (98%)	0.49	56 (3%) 44 39	53, 81, 100, 110	0
33	1b	231/256 (90%)	1.34	48 (20%) 2 2	68, 82, 90, 94	0
33	2b	231/256 (90%)	1.65	65 (28%) 1 1	80, 88, 94, 97	0
34	1c	206/239 (86%)	0.98	18 (8%) 16 14	64, 76, 87, 91	0
34	2c	206/239 (86%)	1.59	54 (26%) 1 1	79, 88, 93, 95	0
35	1d	208/209 (99%)	1.07	23 (11%) 10 8	62, 76, 85, 88	0
35	2d	208/209 (99%)	1.19	18 (8%) 16 14	66, 76, 84, 87	0
36	1e	148/162 (91%)	0.58	4 (2%) 56 51	52, 70, 78, 91	0
36	2e	148/162 (91%)	1.17	19 (12%) 7 6	66, 78, 86, 93	0
37	1f	100/101 (99%)	0.70	2 (2%) 65 61	59, 70, 78, 82	0
37	2f	100/101 (99%)	0.79	3 (3%) 52 48	63, 74, 83, 86	0
38	1g	155/156 (99%)	0.61	4 (2%) 57 52	68, 76, 83, 89	0
38	2g	155/156 (99%)	1.56	41 (26%) 1 1	81, 86, 91, 95	0
39	1h	137/138 (99%)	0.80	6 (4%) 39 34	63, 71, 78, 83	0
39	2h	137/138 (99%)	1.07	9 (6%) 24 21	69, 79, 84, 88	0
40	1i	127/128 (99%)	1.32	20 (15%) 5 4	65, 82, 89, 91	0
40	2i	126/128 (98%)	2.12	65 (51%) 0 0	81, 90, 95, 96	0
41	1j	97/105 (92%)	1.60	28 (28%) 1 1	64, 83, 91, 93	0
41	2j	96/105 (91%)	1.96	46 (47%) 0 0	83, 90, 94, 98	0
42	1k	114/129 (88%)	0.68	6 (5%) 32 28	48, 68, 78, 83	0
42	2k	114/129 (88%)	1.24	16 (14%) 6 5	66, 78, 85, 87	0
43	1l	121/132 (91%)	0.74	7 (5%) 29 25	53, 64, 75, 81	0
43	2l	121/132 (91%)	0.85	9 (7%) 20 18	64, 73, 78, 85	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	1m	116/126 (92%)	0.93	10 (8%) 16 14	64, 78, 83, 88	0
44	2m	114/126 (90%)	1.83	41 (35%) 1 1	84, 89, 93, 95	0
45	1n	60/61 (98%)	0.85	2 (3%) 49 45	68, 75, 81, 83	0
45	2n	60/61 (98%)	2.05	27 (45%) 0 0	83, 88, 93, 95	0
46	1o	88/89 (98%)	0.72	3 (3%) 48 43	51, 69, 79, 84	0
46	2o	88/89 (98%)	0.92	6 (6%) 23 20	64, 77, 83, 89	0
47	1p	82/88 (93%)	1.33	14 (17%) 4 3	69, 77, 85, 89	0
47	2p	82/88 (93%)	1.25	12 (14%) 6 4	66, 75, 83, 91	0
48	1q	99/105 (94%)	0.95	5 (5%) 33 29	59, 72, 82, 84	0
48	2q	99/105 (94%)	0.96	7 (7%) 22 19	63, 75, 82, 85	0
49	1r	68/88 (77%)	0.60	0 100 100	59, 68, 80, 85	0
49	2r	68/88 (77%)	0.97	3 (4%) 39 34	70, 77, 84, 89	0
50	1s	83/93 (89%)	0.97	4 (4%) 35 31	70, 80, 86, 93	0
50	2s	83/93 (89%)	2.05	45 (54%) 0 0	82, 91, 95, 98	0
51	1t	96/106 (90%)	1.19	15 (15%) 5 4	68, 76, 85, 86	0
51	2t	98/106 (92%)	0.88	6 (6%) 27 23	65, 75, 85, 88	0
52	1u	23/27 (85%)	1.22	5 (21%) 2 2	70, 74, 79, 79	0
52	2u	23/27 (85%)	2.29	12 (52%) 0 0	84, 89, 91, 93	0
53	1y	97/113 (85%)	0.93	7 (7%) 21 19	57, 67, 79, 82	0
53	2y	96/113 (84%)	2.01	47 (48%) 0 0	76, 84, 90, 93	0
All	All	20766/21468 (96%)	0.43	1544 (7%) 20 18	24, 69, 93, 111	0

All (1544) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	1H	2	SER	6.7
45	2n	2	ALA	6.4
53	2y	98	ALA	6.1
1	1A	1087	G	6.0
1	2A	2602	A	5.7
26	24	56	VAL	5.7
50	2s	2	PRO	5.6
23	21	2	SER	5.5
53	1y	98	ALA	5.4
26	24	49	PHE	5.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
40	2i	2	GLU	5.2
33	2b	237	ALA	5.1
51	1t	103	GLY	5.1
6	2G	20	ILE	5.0
1	1A	1089	G	5.0
6	2G	28	VAL	4.9
8	2I	146	ALA	4.8
6	2G	90	LEU	4.8
1	1A	1102	C	4.8
1	1A	1090	U	4.7
21	2Z	1	MET	4.7
1	1A	1076	C	4.7
44	2m	102	ARG	4.7
33	2b	236	TYR	4.6
20	2Y	1	MET	4.6
3	1D	275	LYS	4.6
40	1i	127	LYS	4.6
1	2A	2147	G	4.6
3	1D	276	LYS	4.6
6	2G	87	PRO	4.5
41	2j	37	PRO	4.5
15	1T	131	ALA	4.5
47	2p	82	GLN	4.5
1	1A	2602	A	4.5
19	1X	95	LEU	4.5
40	2i	102	LEU	4.5
32	2a	1030(A)	G	4.4
1	1A	1064	C	4.4
48	1q	100	LYS	4.4
1	1A	1077	A	4.3
7	2H	45	VAL	4.3
26	14	56	VAL	4.3
12	2Q	104	PHE	4.3
38	2g	5	ARG	4.3
1	1A	1088	A	4.3
40	2i	96	LEU	4.3
26	24	52	THR	4.3
7	2H	136	ILE	4.3
45	2n	18	VAL	4.3
40	2i	101	PHE	4.3
6	2G	139	LEU	4.3
40	1i	128	ARG	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
6	2G	29	TRP	4.3
51	2t	6	PRO	4.3
50	1s	84	GLY	4.3
34	2c	2	GLY	4.2
1	1A	1081	U	4.2
15	1T	130	ALA	4.2
45	1n	2	ALA	4.2
1	1A	1080	C	4.2
34	2c	207	VAL	4.2
44	2m	116	THR	4.2
53	2y	9	GLN	4.1
21	1Z	192	ALA	4.1
40	2i	109	VAL	4.1
1	1A	1103	A	4.1
32	2a	1030(B)	C	4.1
35	1d	167	GLY	4.1
40	2i	125	TYR	4.1
22	10	84	LEU	4.1
39	2h	2	LEU	4.1
1	1A	1078	U	4.0
29	27	48	LYS	4.0
32	2a	1202	G	4.0
33	2b	15	VAL	4.0
1	1A	1104	C	4.0
6	2G	53	LEU	4.0
40	1i	125	TYR	4.0
38	2g	80	VAL	4.0
1	2A	2116	G	4.0
1	1A	1075	C	4.0
1	2A	2140	C	4.0
40	2i	126	SER	4.0
40	2i	59	PHE	4.0
1	1A	1067	A	4.0
6	2G	39	ILE	4.0
41	1j	74	ILE	4.0
52	2u	14	TRP	4.0
14	2S	35	ILE	3.9
6	2G	146	TYR	3.9
41	1j	4	ILE	3.9
1	1A	1086	A	3.9
33	1b	97	TRP	3.9
1	1A	1072	C	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
26	14	50	VAL	3.9
26	24	30	GLU	3.9
50	2s	9	VAL	3.9
53	1y	94	ALA	3.9
41	2j	34	VAL	3.9
14	2S	29	PHE	3.8
51	2t	103	GLY	3.8
21	2Z	191	VAL	3.8
3	2D	276	LYS	3.8
52	2u	6	ARG	3.8
15	2T	130	ALA	3.7
41	1j	32	ALA	3.7
6	2G	88	ILE	3.7
14	2S	61	ASN	3.7
18	2W	60	ASN	3.7
38	2g	85	TYR	3.7
1	1A	1091	G	3.7
53	2y	97	ALA	3.7
6	2G	102	PHE	3.7
26	14	49	PHE	3.7
46	2o	86	GLY	3.7
38	2g	154	TYR	3.7
21	1Z	1	MET	3.7
1	1A	1079	C	3.7
6	2G	70	VAL	3.7
26	14	59	PHE	3.7
15	1T	37	GLY	3.7
33	2b	38	GLY	3.7
6	2G	52	ILE	3.7
1	1A	1026	U	3.7
14	2S	33	LYS	3.7
6	2G	76	SER	3.7
44	1m	2	ALA	3.7
26	24	9	LEU	3.7
46	1o	3	ILE	3.7
52	2u	13	ILE	3.7
53	1y	95	ARG	3.7
6	2G	12	TYR	3.7
1	2A	2169	A	3.6
6	2G	15	VAL	3.6
26	24	50	VAL	3.6
44	1m	117	VAL	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	34	C	3.6
14	2S	54	LEU	3.6
50	2s	16	LEU	3.6
26	24	29	PRO	3.6
42	2k	31	THR	3.6
40	2i	11	LYS	3.6
40	2i	127	LYS	3.6
14	2S	58	LEU	3.6
51	1t	10	LEU	3.6
33	1b	236	TYR	3.6
38	2g	9	VAL	3.6
41	1j	87	THR	3.6
53	2y	8	LYS	3.6
6	2G	151	ALA	3.6
6	2G	152	LEU	3.6
8	1I	147	GLN	3.6
45	2n	30	ALA	3.6
1	2A	2146	C	3.6
1	1A	1066	U	3.6
23	11	2	SER	3.6
4	2E	204	ALA	3.6
21	2Z	192	ALA	3.6
24	12	70	GLN	3.6
38	2g	16	LEU	3.6
25	13	2	PRO	3.6
40	2i	123	PRO	3.6
1	2A	2139	C	3.5
40	2i	36	TYR	3.5
14	2S	32	LEU	3.5
33	2b	10	LEU	3.5
40	1i	106	ALA	3.5
6	2G	2	PRO	3.5
33	2b	208	ILE	3.5
1	2A	1536	C	3.5
33	2b	7	VAL	3.5
41	2j	72	VAL	3.5
15	2T	131	ALA	3.5
38	2g	83	ALA	3.5
1	2A	1046	A	3.5
1	2A	2148	G	3.5
53	2y	38	HIS	3.5
6	2G	137	GLU	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
20	1Y	1	MET	3.5
41	1j	75	ILE	3.5
41	2j	47	PHE	3.5
1	1A	2147	G	3.5
2	1B	1	U	3.5
6	2G	19	LEU	3.5
40	2i	99	LEU	3.5
40	2i	43	ALA	3.5
41	2j	6	ILE	3.5
6	2G	80	PHE	3.5
26	24	28	LYS	3.5
50	2s	69	HIS	3.5
1	2A	2162	G	3.4
33	1b	7	VAL	3.4
33	2b	230	VAL	3.4
44	1m	116	THR	3.4
1	2A	2174	C	3.4
41	2j	98	ILE	3.4
1	2A	2153	G	3.4
1	2A	2168	G	3.4
32	2a	1036	G	3.4
33	2b	232	PRO	3.4
44	2m	113	PRO	3.4
1	1A	1065	U	3.4
6	2G	78	SER	3.4
34	2c	3	ASN	3.4
33	1b	11	LEU	3.4
33	2b	11	LEU	3.4
41	2j	65	LEU	3.4
33	1b	237	ALA	3.4
41	1j	98	ILE	3.4
44	2m	9	ILE	3.4
21	2Z	201	LYS	3.4
1	2A	2173	A	3.4
40	2i	86	VAL	3.4
6	2G	32	PRO	3.4
6	2G	50	ALA	3.4
6	2G	140	ILE	3.4
40	2i	10	ARG	3.4
12	2Q	65	PHE	3.3
1	2A	2145	C	3.3
52	2u	2	GLY	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
29	27	45	ALA	3.3
33	1b	127	ILE	3.3
42	1k	25	TYR	3.3
43	1l	64	TYR	3.3
1	2A	2125	G	3.3
1	1A	2143	C	3.3
1	2A	1509	C	3.3
21	2Z	76	LEU	3.3
33	2b	136	VAL	3.3
34	1c	207	VAL	3.3
33	2b	16	HIS	3.3
51	2t	100	ILE	3.3
1	1A	1073	A	3.3
1	2A	2138	C	3.3
7	2H	21	PRO	3.3
6	2G	77	ILE	3.3
6	2G	163	ALA	3.3
34	2c	124	ILE	3.3
36	2e	10	MET	3.3
38	2g	42	ILE	3.3
44	1m	4	ILE	3.3
43	1l	126	LYS	3.3
6	2G	34	LEU	3.3
44	1m	113	PRO	3.3
50	2s	71	LEU	3.3
32	1a	1036	G	3.3
33	1b	12	GLU	3.3
49	2r	20	ALA	3.3
1	2A	2119	A	3.2
32	1a	1001	A	3.2
22	20	84	LEU	3.2
35	1d	179	GLU	3.2
6	2G	149	VAL	3.2
6	2G	155	MET	3.2
34	1c	2	GLY	3.2
43	2l	17	LYS	3.2
1	1A	34	C	3.2
1	1A	1092	C	3.2
1	2A	2124	G	3.2
1	2A	2133	G	3.2
19	2X	95	LEU	3.2
34	1c	90	GLU	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	1101	U	3.2
1	2A	2118	U	3.2
40	2i	17	VAL	3.2
52	2u	11	GLY	3.2
35	2d	5	ILE	3.2
1	1A	1176	G	3.2
1	2A	2155	G	3.2
2	2B	118	G	3.2
21	2Z	136	PHE	3.2
33	2b	21	ARG	3.2
38	2g	84	ASN	3.2
45	2n	6	LEU	3.2
14	2S	92	TYR	3.2
47	2p	38	TYR	3.2
41	2j	79	ARG	3.2
45	2n	61	TRP	3.2
1	2A	2107	C	3.2
1	2A	2142	C	3.2
14	2S	59	LYS	3.2
53	2y	37	PRO	3.2
1	2A	2167	U	3.2
2	2B	1	U	3.2
33	1b	200	ILE	3.2
53	1y	2	THR	3.2
45	2n	59	ALA	3.1
50	2s	24	ALA	3.1
6	2G	17	PRO	3.1
25	23	60	GLU	3.1
33	2b	133	LYS	3.1
33	1b	10	LEU	3.1
35	1d	155	LEU	3.1
35	1d	194	LEU	3.1
39	1h	2	LEU	3.1
1	1A	1074	G	3.1
32	2a	1353	G	3.1
6	1G	146	TYR	3.1
26	24	5	ILE	3.1
33	1b	188	ALA	3.1
34	2c	129	ALA	3.1
36	1e	21	ALA	3.1
53	1y	97	ALA	3.1
26	24	65	ASP	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
42	2k	117	ASN	3.1
18	1W	112	GLY	3.1
1	1A	1093	G	3.1
33	1b	229	VAL	3.1
50	1s	9	VAL	3.1
1	2A	229	A	3.1
1	2A	1067	A	3.1
1	2A	1084	A	3.1
53	2y	54	ILE	3.1
6	2G	35	GLU	3.1
41	1j	76	ASN	3.1
32	1a	1030(B)	C	3.1
6	2G	136	ARG	3.1
14	2S	46	VAL	3.1
52	2u	15	ARG	3.1
52	2u	24	ARG	3.1
33	2b	214	ILE	3.1
6	2G	25	TYR	3.1
40	2i	7	THR	3.1
45	2n	21	TYR	3.1
45	2n	34	TYR	3.1
1	1A	1068	G	3.1
4	1E	204	ALA	3.1
6	2G	179	PRO	3.1
41	1j	77	PRO	3.1
6	2G	62	LEU	3.1
33	2b	97	TRP	3.1
41	1j	78	ASN	3.1
41	2j	76	ASN	3.1
35	1d	153	ARG	3.1
6	2G	160	VAL	3.1
8	2I	3	VAL	3.1
9	2N	9	VAL	3.1
14	2S	65	VAL	3.1
44	2m	4	ILE	3.1
22	20	43	THR	3.0
26	24	44	THR	3.0
41	2j	42	THR	3.0
6	1G	50	ALA	3.0
33	2b	123	ALA	3.0
1	1A	2117	A	3.0
1	2A	2172	U	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	2152	G	3.0
40	2i	98	PRO	3.0
50	2s	30	LEU	3.0
50	1s	13	ASP	3.0
51	2t	102	GLY	3.0
34	2c	77	ILE	3.0
45	2n	13	THR	3.0
1	1A	2139	C	3.0
1	2A	2136	C	3.0
40	2i	106	ALA	3.0
32	2a	1257	U	3.0
50	2s	59	PRO	3.0
52	2u	23	PRO	3.0
21	2Z	91	LEU	3.0
38	1g	16	LEU	3.0
40	2i	56	LEU	3.0
6	2G	33	ARG	3.0
32	1a	1026	G	3.0
53	2y	4	ASN	3.0
53	2y	55	ASN	3.0
33	2b	165	VAL	3.0
36	2e	13	ILE	3.0
42	2k	13	GLN	3.0
50	2s	60	VAL	3.0
6	2G	145	THR	3.0
3	1D	2	ALA	3.0
40	2i	119	ALA	3.0
26	24	41	PRO	3.0
6	2G	43	LEU	3.0
35	1d	157	LEU	3.0
1	1A	548	A	3.0
6	2G	126	ASP	3.0
53	2y	48	PHE	3.0
29	17	48	LYS	3.0
32	1a	1030(A)	G	3.0
32	2a	1001(A)	G	3.0
53	2y	92	GLY	3.0
6	2G	157	ILE	3.0
35	1d	173	TRP	3.0
38	2g	2	ALA	3.0
14	2S	7	TYR	3.0
21	2Z	99	TYR	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
6	2G	82	LEU	3.0
33	2b	22	LYS	3.0
1	2A	2150	U	3.0
41	2j	54	PHE	3.0
26	24	54	GLY	3.0
6	2G	37	VAL	2.9
33	1b	165	VAL	2.9
33	2b	164	VAL	2.9
44	2m	7	VAL	2.9
45	2n	33	VAL	2.9
40	1i	64	THR	2.9
6	2G	158	ALA	2.9
40	2i	55	ALA	2.9
50	2s	34	TRP	2.9
20	1Y	23	ARG	2.9
26	24	7	PRO	2.9
35	2d	50	ARG	2.9
38	2g	79	ARG	2.9
21	2Z	33	LEU	2.9
26	24	63	TYR	2.9
26	24	67	TYR	2.9
33	1b	33	TYR	2.9
40	1i	56	LEU	2.9
1	2A	2143	C	2.9
1	1A	1105	U	2.9
32	1a	1257	U	2.9
1	1A	1057	A	2.9
40	1i	126	SER	2.9
6	2G	132	ASN	2.9
38	1g	84	ASN	2.9
33	2b	127	ILE	2.9
25	23	59	VAL	2.9
50	2s	41	VAL	2.9
50	2s	63	THR	2.9
21	1Z	51	ALA	2.9
1	1A	1058	G	2.9
1	2A	2104	G	2.9
53	2y	57	PRO	2.9
34	2c	33	LEU	2.9
53	2y	61	LEU	2.9
40	2i	92	TYR	2.9
22	20	69	PHE	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	2144	U	2.9
7	2H	120	GLY	2.9
1	1A	1085	A	2.9
1	2A	1096	A	2.9
4	1E	163	GLU	2.9
26	24	18	CYS	2.9
41	2j	23	ILE	2.9
46	2o	3	ILE	2.9
39	1h	93	VAL	2.9
44	2m	54	VAL	2.9
41	1j	46	ARG	2.9
6	2G	46	ALA	2.9
35	2d	164	ALA	2.9
44	2m	66	LEU	2.9
32	2a	1034	G	2.9
44	2m	87	TYR	2.9
34	1c	107	GLN	2.9
35	1d	2	GLY	2.9
40	2i	30	GLY	2.9
1	1A	1061	U	2.9
1	2A	1083	U	2.9
47	1p	19	ILE	2.9
53	2y	35	ILE	2.9
52	2u	9	ARG	2.9
41	2j	55	LYS	2.9
44	2m	105	THR	2.9
34	2c	160	ALA	2.9
40	1i	15	ALA	2.9
44	2m	76	ALA	2.9
53	2y	52	ALA	2.9
6	2G	175	LEU	2.9
48	2q	98	LEU	2.9
1	2A	1091	G	2.9
32	2a	1190	G	2.9
33	2b	122	PHE	2.9
34	1c	193	TYR	2.9
40	2i	18	PHE	2.9
51	1t	96	GLY	2.9
45	2n	3	ARG	2.8
6	2G	105	LYS	2.8
53	2y	5	ILE	2.8
53	2y	40	ILE	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
41	1j	34	VAL	2.8
44	2m	17	VAL	2.8
1	1A	1053	C	2.8
1	2A	1076	C	2.8
32	2a	1030	C	2.8
9	2N	73	THR	2.8
3	2D	2	ALA	2.8
6	2G	110	ALA	2.8
14	2S	78	LEU	2.8
41	1j	86	MET	2.8
41	1j	54	PHE	2.8
29	17	47	ARG	2.8
33	2b	72	GLY	2.8
46	2o	88	ARG	2.8
1	1A	1063	G	2.8
1	1A	1071	G	2.8
1	2A	2154	G	2.8
34	2c	8	ILE	2.8
35	1d	70	ILE	2.8
50	2s	62	ILE	2.8
1	2A	2113	U	2.8
44	2m	15	VAL	2.8
45	2n	25	VAL	2.8
1	1A	2142	C	2.8
1	2A	2111	C	2.8
34	1c	60	ALA	2.8
34	2c	60	ALA	2.8
1	2A	1085	A	2.8
39	1h	133	LEU	2.8
6	1G	48	GLU	2.8
6	2G	45	GLU	2.8
6	1G	182	LYS	2.8
33	1b	17	PHE	2.8
38	2g	76	ARG	2.8
50	2s	29	ARG	2.8
51	1t	8	ARG	2.8
22	20	8	GLY	2.8
40	2i	88	TYR	2.8
53	2y	7	SER	2.8
33	2b	234	PRO	2.8
50	2s	67	VAL	2.8
1	1A	1062	G	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	2106	G	2.8
33	2b	67	THR	2.8
33	2b	121	LEU	2.8
34	2c	65	ALA	2.8
40	2i	82	ALA	2.8
41	2j	88	LEU	2.8
44	2m	51	ALA	2.8
50	2s	79	THR	2.8
6	2G	172	LEU	2.8
40	2i	85	LEU	2.8
1	1A	888	C	2.8
32	2a	1027	C	2.8
32	2a	1357	A	2.8
6	2G	72	ARG	2.8
21	2Z	198	LYS	2.8
6	2G	42	GLY	2.8
26	24	45	GLY	2.8
50	2s	26	GLY	2.8
41	2j	75	ILE	2.8
42	2k	75	TYR	2.8
47	1p	17	TYR	2.8
53	2y	39	ILE	2.8
40	2i	53	VAL	2.8
14	2S	110	LEU	2.8
33	2b	13	ALA	2.8
34	2c	168	ALA	2.8
34	2c	192	THR	2.8
40	2i	46	ALA	2.8
41	1j	88	LEU	2.8
1	2A	2165	G	2.8
44	2m	110	ARG	2.8
40	2i	105	ASP	2.8
40	2i	115	GLY	2.7
41	2j	63	PHE	2.8
3	2D	106	ILE	2.7
20	2Y	44	ILE	2.7
33	2b	201	ILE	2.7
44	2m	39	ILE	2.7
7	2H	118	PRO	2.7
42	2k	25	TYR	2.7
8	1I	136	VAL	2.7
21	2Z	58	VAL	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	2c	86	VAL	2.7
35	2d	8	VAL	2.7
41	2j	44	VAL	2.7
8	1I	38	LEU	2.7
26	14	52	THR	2.7
33	1b	213	LEU	2.7
36	2e	12	LEU	2.7
40	1i	19	LEU	2.7
1	2A	1089	G	2.7
1	2A	2166	G	2.7
1	1A	2107	C	2.7
32	2a	1286	A	2.7
42	2k	36	ASP	2.7
53	2y	33	HIS	2.7
50	2s	68	GLY	2.7
6	2G	101	ILE	2.7
33	1b	214	ILE	2.7
6	2G	68	PRO	2.7
44	2m	64	TRP	2.7
34	2c	195	VAL	2.7
44	2m	74	VAL	2.7
33	2b	213	LEU	2.7
41	2j	32	ALA	2.7
42	2k	124	LYS	2.7
44	2m	18	ALA	2.7
45	2n	17	LYS	2.7
12	2Q	59	ARG	2.7
39	2h	30	ARG	2.7
6	2G	138	GLN	2.7
26	24	40	HIS	2.7
6	2G	147	ASP	2.7
40	2i	91	ASP	2.7
1	1A	2141	G	2.7
6	2G	89	GLY	2.7
1	2A	2135	A	2.7
21	2Z	88	PHE	2.7
6	1G	52	ILE	2.7
26	24	14	ILE	2.7
32	2a	1397	C	2.7
33	2b	200	ILE	2.7
35	2d	158	ILE	2.7
41	2j	77	PRO	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
6	2G	38	VAL	2.7
6	2G	81	LYS	2.7
6	2G	159	VAL	2.7
35	1d	170	VAL	2.7
44	2m	45	VAL	2.7
26	14	63	TYR	2.7
33	2b	44	LEU	2.7
33	2b	148	TYR	2.7
34	2c	175	LEU	2.7
6	2G	69	ALA	2.7
19	2X	68	ARG	2.7
41	2j	46	ARG	2.7
45	2n	5	ALA	2.7
1	2A	1097	U	2.7
38	2g	33	ASP	2.7
26	24	31	ILE	2.7
35	1d	110	PHE	2.7
38	2g	120	ILE	2.7
45	2n	7	ILE	2.7
1	2A	2160	G	2.7
1	2A	2318	G	2.7
32	2a	630	G	2.7
6	2G	31	VAL	2.7
20	2Y	90	LEU	2.7
33	1b	230	VAL	2.7
44	2m	34	LEU	2.7
34	2c	90	GLU	2.7
47	1p	82	GLN	2.7
7	2H	13	LYS	2.6
8	1I	138	ILE	2.6
12	2Q	29	PHE	2.6
33	2b	75	LYS	2.6
53	2y	14	PRO	2.6
53	2y	3	MET	2.6
1	1A	1045	A	2.6
6	2G	133	LEU	2.6
32	1a	1286	A	2.6
41	1j	44	VAL	2.6
41	2j	24	VAL	2.6
41	2j	71	LEU	2.6
1	2A	2110	G	2.6
1	2A	2141	G	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	1a	1033	G	2.6
32	2a	1373	G	2.6
26	24	32	TYR	2.6
36	2e	21	ALA	2.6
45	1n	13	THR	2.6
34	2c	167	TRP	2.6
38	2g	156	TRP	2.6
1	1A	2144	U	2.6
6	2G	129	GLY	2.6
42	2k	125	PHE	2.6
47	2p	19	ILE	2.6
6	2G	95	ARG	2.6
11	2P	15	ARG	2.6
44	1m	102	ARG	2.6
48	1q	63	ARG	2.6
7	2H	7	LEU	2.6
3	2D	28	GLU	2.6
26	24	35	VAL	2.6
1	1A	1084	A	2.6
41	2j	59	SER	2.6
1	2A	2179	C	2.6
1	2A	2789	C	2.6
10	2O	51	ALA	2.6
32	1a	1030	C	2.6
38	2g	128	ALA	2.6
1	2A	2159	G	2.6
32	1a	1031	G	2.6
32	2a	1026	G	2.6
18	2W	112	GLY	2.6
40	2i	6	GLY	2.6
1	2A	2109	U	2.6
6	2G	142	PRO	2.6
15	1T	108	ARG	2.6
25	23	2	PRO	2.6
44	2m	3	ARG	2.6
44	2m	84	ILE	2.6
33	2b	57	PHE	2.6
23	21	83	GLU	2.6
33	1b	126	GLU	2.6
34	2c	94	LEU	2.6
44	2m	56	LEU	2.6
7	2H	79	VAL	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
40	2i	41	VAL	2.6
41	1j	33	GLN	2.6
6	2G	57	ALA	2.6
6	2G	71	THR	2.6
14	2S	47	THR	2.6
40	2i	94	ALA	2.6
50	2s	25	LYS	2.6
1	1A	2153	G	2.6
1	2A	1533	G	2.6
1	2A	2131	G	2.6
32	2a	1031	G	2.6
32	2a	1033	G	2.6
7	2H	10	PRO	2.6
34	2c	159	GLY	2.6
47	1p	46	PRO	2.6
50	2s	31	ILE	2.6
53	2y	12	ILE	2.6
1	1A	1082	U	2.6
1	1A	1083	U	2.6
34	1c	10	PHE	2.6
33	2b	86	GLU	2.6
40	2i	47	LEU	2.6
41	2j	90	LEU	2.6
21	1Z	191	VAL	2.6
21	1Z	188	ALA	2.6
3	2D	275	LYS	2.6
33	2b	132	LYS	2.6
1	2A	1073	A	2.6
1	2A	2171	A	2.6
40	2i	5	TYR	2.6
1	2A	2103	C	2.5
14	2S	3	ARG	2.5
53	2y	83	ARG	2.5
45	2n	38	GLY	2.5
47	1p	1	MET	2.5
47	2p	48	TRP	2.5
17	1V	101	GLY	2.5
33	1b	228	GLY	2.5
40	2i	49	PRO	2.5
1	1A	2112	G	2.5
1	1A	2159	G	2.5
32	2a	1224	G	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
50	2s	49	ILE	2.5
33	2b	152	PHE	2.5
6	2G	107	LEU	2.5
11	2P	6	LEU	2.5
39	1h	112	LEU	2.5
6	2G	5	VAL	2.5
9	2N	140	VAL	2.5
15	1T	104	ASN	2.5
21	2Z	96	VAL	2.5
26	24	21	VAL	2.5
33	1b	136	VAL	2.5
36	2e	20	GLN	2.5
40	2i	108	VAL	2.5
41	1j	24	VAL	2.5
41	1j	69	ASN	2.5
42	1k	14	VAL	2.5
42	2k	30	VAL	2.5
41	2j	62	HIS	2.5
21	2Z	113	ALA	2.5
33	1b	22	LYS	2.5
45	2n	10	ALA	2.5
6	2G	83	ARG	2.5
14	2S	20	ARG	2.5
37	2f	71	ARG	2.5
1	2A	652(B)	A	2.5
1	2A	2126	A	2.5
1	2A	2134	A	2.5
2	2B	53	A	2.5
26	24	25	TYR	2.5
32	1a	1447	A	2.5
32	1a	1493	A	2.5
8	1I	134	PRO	2.5
44	2m	41	PRO	2.5
6	2G	4	ASP	2.5
50	2s	82	GLY	2.5
39	1h	86	ILE	2.5
8	2I	10	GLU	2.5
26	24	57	GLU	2.5
40	2i	110	GLU	2.5
43	2l	16	GLU	2.5
14	2S	48	LEU	2.5
32	1a	1034	G	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	2a	1030(C)	G	2.5
1	2A	2130	U	2.5
1	2A	2132	U	2.5
7	2H	15	VAL	2.5
7	2H	17	VAL	2.5
14	2S	28	VAL	2.5
21	2Z	199	LYS	2.5
33	2b	37	ASN	2.5
36	1e	67	VAL	2.5
40	2i	117	HIS	2.5
44	2m	106	ASN	2.5
47	2p	2	VAL	2.5
7	2H	165	ALA	2.5
21	2Z	189	ALA	2.5
44	2m	72	ALA	2.5
44	2m	37	THR	2.5
45	2n	22	THR	2.5
26	24	58	ARG	2.5
29	27	47	ARG	2.5
50	2s	3	ARG	2.5
5	2F	14	PRO	2.5
34	2c	184	TYR	2.5
1	1A	2158	A	2.5
43	1l	63	GLY	2.5
14	2S	40	ILE	2.5
21	2Z	171	ILE	2.5
1	2A	645	C	2.5
1	2A	1064	C	2.5
19	2X	92	LEU	2.5
33	2b	17	PHE	2.5
47	1p	49	LEU	2.5
20	2Y	94	LYS	2.5
26	14	46	GLN	2.5
1	1A	2167	U	2.5
1	2A	1026	U	2.5
14	2S	69	VAL	2.5
35	2d	88	VAL	2.5
38	2g	21	VAL	2.5
40	2i	29	ASN	2.5
53	2y	60	VAL	2.5
1	1A	1056	G	2.5
1	2A	171	G	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	2127	G	2.5
40	2i	52	ALA	2.5
41	2j	26	ALA	2.5
6	2G	64	THR	2.5
7	2H	106	THR	2.5
53	2y	6	THR	2.5
53	2y	45	PRO	2.5
7	2H	164	TYR	2.5
33	2b	92	TYR	2.5
34	2c	57	ILE	2.5
1	1A	1095	A	2.5
35	2d	108	LEU	2.5
35	2d	166	LYS	2.5
40	2i	19	LEU	2.5
1	2A	1072	C	2.5
1	2A	2105	C	2.5
32	1a	63	C	2.5
33	1b	19	HIS	2.5
33	2b	19	HIS	2.5
45	2n	49	HIS	2.5
21	2Z	196	VAL	2.5
34	2c	75	VAL	2.5
24	12	69	ARG	2.5
33	1b	130	ARG	2.5
26	24	12	ALA	2.5
53	2y	63	ALA	2.5
47	2p	69	THR	2.5
1	2A	2112	G	2.5
32	2a	951	G	2.5
32	2a	1003	G	2.5
50	2s	35	SER	2.5
33	1b	125	PRO	2.4
33	1b	14	GLY	2.4
33	1b	18	GLY	2.4
33	1b	129	GLU	2.4
33	2b	12	GLU	2.4
33	2b	228	GLY	2.4
34	2c	197	GLY	2.4
46	2o	89	GLY	2.4
20	2Y	54	LYS	2.4
34	2c	5	ILE	2.4
35	1d	169	LYS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
36	2e	5	ASP	2.4
43	1l	7	ILE	2.4
43	2l	23	LYS	2.4
5	2F	181	LEU	2.4
50	2s	15	LEU	2.4
51	1t	13	LEU	2.4
1	2A	2320	A	2.4
18	1W	111	HIS	2.4
8	2I	18	VAL	2.4
1	2A	2180	U	2.4
41	2j	92	THR	2.4
35	1d	150	GLU	2.4
48	2q	49	GLU	2.4
26	14	54	GLY	2.4
34	2c	80	GLY	2.4
35	1d	180	GLY	2.4
40	2i	97	LYS	2.4
41	2j	36	GLY	2.4
43	2l	13	LYS	2.4
51	1t	74	LYS	2.4
38	2g	27	ILE	2.4
7	2H	88	LEU	2.4
20	2Y	55	TYR	2.4
24	22	70	GLN	2.4
34	1c	47	LEU	2.4
34	1c	52	LEU	2.4
41	2j	33	GLN	2.4
44	2m	59	TYR	2.4
44	2m	90	LEU	2.4
47	1p	38	TYR	2.4
51	1t	99	LEU	2.4
53	2y	81	LEU	2.4
33	1b	140	HIS	2.4
6	2G	91	ARG	2.4
6	2G	118	ARG	2.4
14	2S	12	PHE	2.4
40	1i	18	PHE	2.4
40	1i	42	ARG	2.4
45	2n	29	ARG	2.4
1	2A	887	A	2.4
1	2A	1070	A	2.4
32	2a	1035	A	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
6	2G	109	VAL	2.4
8	2I	92	VAL	2.4
47	1p	59	TRP	2.4
50	2s	53	ASN	2.4
1	1A	2145	C	2.4
8	2I	55	ALA	2.4
32	2a	1028	C	2.4
1	1A	12	U	2.4
1	1A	1094	U	2.4
1	2A	271(K)	U	2.4
3	2D	38	LYS	2.4
20	2Y	29	GLU	2.4
33	2b	131	PRO	2.4
6	2G	127	GLY	2.4
6	2G	63	ILE	2.4
31	29	12	ASP	2.4
38	2g	50	ILE	2.4
1	1A	1055	G	2.4
1	1A	2116	G	2.4
8	2I	5	LEU	2.4
6	2G	16	ARG	2.4
34	2c	6	HIS	2.4
34	2c	190	ARG	2.4
44	2m	23	TYR	2.4
34	2c	128	PHE	2.4
47	2p	9	PHE	2.4
6	2G	148	MET	2.4
7	2H	43	VAL	2.4
21	2Z	42	VAL	2.4
33	2b	229	VAL	2.4
34	1c	86	VAL	2.4
35	2d	165	MET	2.4
43	2l	18	VAL	2.4
1	2A	2117	A	2.4
6	2G	27	ASN	2.4
32	2a	532	A	2.4
33	1b	37	ASN	2.4
27	25	14	ALA	2.4
38	2g	7	ALA	2.4
38	2g	147	ALA	2.4
6	2G	161	THR	2.4
14	2S	5	THR	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	2H	8	PRO	2.4
20	2Y	4	LYS	2.4
36	2e	9	LYS	2.4
32	1a	1027	C	2.4
32	1a	1029	C	2.4
32	2a	1116	C	2.4
40	2i	90	PRO	2.4
41	2j	91	PRO	2.4
22	20	76	GLY	2.4
33	2b	227	GLY	2.4
8	2I	4	ILE	2.4
41	2j	38	ILE	2.4
3	2D	182	LEU	2.4
6	2G	3	LEU	2.4
11	2P	99	LEU	2.4
15	1T	129	ARG	2.4
15	2T	111	ARG	2.4
37	2f	16	GLN	2.4
38	2g	6	ARG	2.4
47	2p	25	ARG	2.4
51	2t	10	LEU	2.4
53	2y	96	ARG	2.4
1	2A	2151	G	2.4
6	2G	11	TYR	2.4
20	2Y	89	PHE	2.4
32	2a	1032	G	2.4
33	2b	163	PHE	2.4
40	2i	114	TYR	2.4
36	2e	55	VAL	2.4
41	2j	78	ASN	2.4
6	2G	100	TRP	2.4
26	14	53	GLU	2.4
32	2a	1001	A	2.4
32	2a	1030(D)	A	2.4
34	2c	187	ALA	2.4
21	2Z	167	PRO	2.3
41	1j	100	THR	2.3
1	1A	2174	C	2.3
1	2A	2161	C	2.3
1	2A	2183	C	2.3
36	1e	22	GLY	2.3
40	2i	69	GLY	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
6	2G	41	GLN	2.3
21	2Z	41	LEU	2.3
21	2Z	197	ILE	2.3
33	2b	42	ILE	2.3
36	2e	101	ILE	2.3
49	2r	87	ARG	2.3
28	26	11	LEU	2.3
26	24	39	CYS	2.3
38	2g	125	MET	2.3
6	2G	23	PHE	2.3
14	2S	36	TYR	2.3
12	2Q	18	LYS	2.3
17	2V	47	VAL	2.3
21	2Z	71	VAL	2.3
34	2c	64	VAL	2.3
34	2c	66	VAL	2.3
32	1a	1030(C)	G	2.3
33	1b	13	ALA	2.3
53	2y	44	GLU	2.3
45	2n	14	PRO	2.3
46	2o	75	PRO	2.3
6	2G	93	THR	2.3
1	2A	2170	A	2.3
32	1a	1492	A	2.3
32	2a	1092	A	2.3
41	2j	30	SER	2.3
41	2j	45	ARG	2.3
41	2j	93	GLY	2.3
6	2G	26	GLN	2.3
8	2I	38	LEU	2.3
14	2S	4	LEU	2.3
14	2S	56	LEU	2.3
35	1d	158	ILE	2.3
44	2m	22	ILE	2.3
1	2A	2129	C	2.3
6	2G	75	LYS	2.3
14	2S	11	LYS	2.3
38	2g	36	LYS	2.3
43	2l	28	LYS	2.3
44	2m	31	LYS	2.3
53	2y	26	LYS	2.3
35	1d	112	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
40	1i	17	VAL	2.3
43	2l	64	TYR	2.3
38	2g	28	ASN	2.3
4	2E	114	ALA	2.3
29	17	45	ALA	2.3
40	2i	122	ALA	2.3
44	1m	5	ALA	2.3
51	1t	66	ALA	2.3
1	2A	1171	G	2.3
1	2A	2207	G	2.3
8	1I	108	THR	2.3
26	24	27	THR	2.3
12	2Q	60	ARG	2.3
32	2a	973	G	2.3
40	2i	103	THR	2.3
47	1p	22	THR	2.3
52	2u	17	THR	2.3
34	2c	79	ARG	2.3
45	2n	12	ARG	2.3
52	1u	24	ARG	2.3
1	2A	6	A	2.3
32	2a	1183	A	2.3
33	1b	38	GLY	2.3
51	1t	11	SER	2.3
14	2S	80	LEU	2.3
21	2Z	117	LEU	2.3
36	2e	11	ILE	2.3
41	2j	8	LEU	2.3
51	1t	72	LEU	2.3
32	2a	1235	U	2.3
20	2Y	5	MET	2.3
26	14	51	ASP	2.3
1	1A	2138	C	2.3
1	2A	888	C	2.3
26	24	8	LYS	2.3
48	2q	100	LYS	2.3
3	2D	15	PHE	2.3
19	2X	28	PHE	2.3
35	2d	79	PHE	2.3
7	2H	83	TYR	2.3
29	27	46	VAL	2.3
37	1f	90	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	1b	232	PRO	2.3
41	2j	27	ALA	2.3
26	24	55	ARG	2.3
26	24	61	ARG	2.3
6	2G	165	THR	2.3
35	2d	87	GLY	2.3
35	2d	160	GLN	2.3
36	1e	97	GLY	2.3
39	2h	131	GLY	2.3
41	2j	56	HIS	2.3
53	2y	46	GLN	2.3
1	2A	2319	G	2.3
26	24	66	SER	2.3
4	2E	182	LEU	2.3
32	1a	1001(A)	G	2.3
32	2a	1347	G	2.3
45	2n	53	LEU	2.3
1	2A	1086	A	2.3
2	2B	26	A	2.3
32	1a	1035	A	2.3
7	2H	85	LYS	2.3
9	2N	83	LYS	2.3
21	2Z	179	ASP	2.3
33	2b	79	ASP	2.3
40	2i	95	LYS	2.3
32	2a	1150	U	2.3
32	2a	1532	U	2.3
6	2G	92	VAL	2.3
7	2H	49	VAL	2.3
21	2Z	86	VAL	2.3
33	1b	15	VAL	2.3
33	1b	81	VAL	2.3
34	2c	153	VAL	2.3
7	2H	39	PRO	2.3
19	1X	68	ARG	2.3
37	2f	47	ARG	2.3
38	2g	32	ARG	2.3
40	2i	21	PRO	2.3
50	2s	76	PRO	2.3
5	2F	21	ALA	2.2
6	2G	169	ALA	2.2
21	1Z	187	ALA	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
21	2Z	188	ALA	2.2
38	2g	25	ALA	2.2
51	1t	76	ALA	2.2
7	2H	129	THR	2.2
41	2j	100	THR	2.2
47	1p	44	THR	2.2
7	2H	48	GLY	2.2
14	2S	45	GLY	2.2
20	2Y	57	GLN	2.2
44	2m	6	GLY	2.2
44	2m	100	GLY	2.2
53	2y	67	HIS	2.2
11	1P	99	LEU	2.2
14	2S	73	LEU	2.2
20	2Y	34	LYS	2.2
21	2Z	5	LEU	2.2
26	14	69	LYS	2.2
29	17	1	MET	2.2
35	1d	181	MET	2.2
38	2g	77	SER	2.2
41	2j	35	SER	2.2
44	1m	56	LEU	2.2
48	1q	90	ILE	2.2
53	2y	88	LEU	2.2
1	2A	2801(A)	A	2.2
33	2b	166	ASP	2.2
34	1c	62	ASP	2.2
1	1A	2166	G	2.2
1	1A	2132	U	2.2
1	2A	1090	U	2.2
2	2B	55	U	2.2
32	1a	1025	U	2.2
21	1Z	203	GLU	2.2
53	2y	68	GLU	2.2
22	20	45	PHE	2.2
33	1b	28	PHE	2.2
36	2e	45	PHE	2.2
50	2s	10	PHE	2.2
4	2E	59	VAL	2.2
12	2Q	35	VAL	2.2
20	2Y	49	VAL	2.2
26	24	11	PRO	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
31	29	16	VAL	2.2
32	2a	1354	C	2.2
35	2d	92	VAL	2.2
38	2g	14	PRO	2.2
38	2g	93	PRO	2.2
40	2i	14	VAL	2.2
50	2s	42	PRO	2.2
14	2S	51	ALA	2.2
36	2e	130	ASN	2.2
38	2g	100	ALA	2.2
50	2s	65	ASN	2.2
6	2G	131	TYR	2.2
17	2V	81	TYR	2.2
26	14	67	TYR	2.2
26	24	43	TYR	2.2
40	1i	114	TYR	2.2
40	2i	62	TYR	2.2
53	1y	71	TYR	2.2
14	2S	38	GLN	2.2
34	2c	191	THR	2.2
4	1E	1	MET	2.2
6	2G	85	GLY	2.2
14	2S	60	GLY	2.2
33	2b	99	GLY	2.2
34	1c	159	GLY	2.2
45	2n	50	LYS	2.2
42	2k	103	LEU	2.2
6	1G	88	ILE	2.2
48	2q	99	SER	2.2
50	2s	4	SER	2.2
6	2G	97	ASP	2.2
42	2k	42	TRP	2.2
6	2G	59	GLU	2.2
32	1a	841	U	2.2
32	2a	1351	U	2.2
1	1A	2157	G	2.2
1	2A	1071	G	2.2
18	2W	92	ARG	2.2
45	2n	16	PHE	2.2
8	1I	107	VAL	2.2
10	2O	62	VAL	2.2
14	2S	14	VAL	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	2146	C	2.2
6	2G	6	ALA	2.2
32	1a	1037	C	2.2
33	1b	94	ASN	2.2
41	1j	26	ALA	2.2
47	1p	7	ALA	2.2
51	1t	94	ALA	2.2
14	2S	34	HIS	2.2
14	2S	93	LYS	2.2
16	1U	117	GLN	2.2
42	1k	75	TYR	2.2
43	1l	91	LYS	2.2
48	2q	93	GLN	2.2
50	2s	77	THR	2.2
8	2I	16	GLY	2.2
20	2Y	93	GLY	2.2
21	2Z	125	LEU	2.2
26	14	64	GLY	2.2
33	1b	154	LEU	2.2
36	2e	85	GLY	2.2
39	2h	112	LEU	2.2
53	2y	77	LEU	2.2
34	2c	152	ILE	2.2
42	2k	40	ILE	2.2
40	1i	105	ASP	2.2
41	1j	97	GLU	2.2
6	2G	113	ARG	2.2
7	2H	3	ARG	2.2
34	2c	22	TRP	2.2
38	2g	78	ARG	2.2
47	2p	81	ARG	2.2
1	1A	887	A	2.2
1	1A	2130	U	2.2
26	24	59	PHE	2.2
34	2c	10	PHE	2.2
47	2p	80	PHE	2.2
33	2b	219	VAL	2.2
1	2A	2120	G	2.2
1	2A	2186	G	2.2
32	1a	1002	G	2.2
21	2Z	7	ALA	2.2
28	26	22	ALA	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	2b	40	HIS	2.2
34	1c	92	ALA	2.2
40	2i	45	ALA	2.2
42	2k	15	ALA	2.2
53	2y	58	ASN	2.2
33	2b	83	MET	2.2
34	2c	107	GLN	2.2
53	2y	89	GLN	2.2
1	1A	2140	C	2.2
33	1b	187	LEU	2.2
33	2b	145	LEU	2.2
34	1c	42	LEU	2.2
34	1c	201	TYR	2.2
40	2i	27	THR	2.2
6	1G	43	LEU	2.2
7	2H	103	LEU	2.2
34	2c	87	LEU	2.2
41	1j	85	LEU	2.2
46	1o	89	GLY	2.2
50	2s	5	LEU	2.2
52	1u	2	GLY	2.2
53	2y	41	LEU	2.2
33	2b	68	ILE	2.2
39	2h	109	ILE	2.2
41	1j	38	ILE	2.2
26	24	26	SER	2.2
48	1q	99	SER	2.2
53	2y	64	SER	2.2
14	2S	64	GLU	2.2
21	1Z	135	GLU	2.2
6	2G	153	ARG	2.2
43	1l	19	ARG	2.2
5	1F	14	PRO	2.2
38	2g	103	TRP	2.2
1	1A	229	A	2.1
1	1A	2118	U	2.2
41	2j	80	LYS	2.2
48	2q	71	PHE	2.2
1	2A	1095	A	2.1
1	2A	2114	A	2.1
5	2F	6	VAL	2.1
21	2Z	165	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	2a	1363(A)	A	2.1
32	2a	1493	A	2.1
34	2c	55	VAL	2.1
33	1b	34	ALA	2.1
33	2b	101	MET	2.1
34	2c	92	ALA	2.1
36	2e	94	ALA	2.1
40	1i	43	ALA	2.1
50	2s	14	HIS	2.1
1	1A	1099	G	2.1
1	1A	2155	G	2.1
1	2A	2123	G	2.1
1	2A	2149	G	2.1
6	2G	60	LEU	2.1
6	2G	120	LEU	2.1
7	2H	98	LEU	2.1
12	2Q	2	LEU	2.1
26	24	24	THR	2.1
35	2d	21	LEU	2.1
38	2g	124	LEU	2.1
52	2u	16	GLY	2.1
7	2H	89	ILE	2.1
33	2b	41	ILE	2.1
35	2d	54	TYR	2.1
35	2d	70	ILE	2.1
40	2i	4	TYR	2.1
46	1o	78	TYR	2.1
1	1A	2161	C	2.1
1	2A	1092	C	2.1
1	2A	2185	C	2.1
32	2a	1038	C	2.1
34	2c	62	ASP	2.1
35	1d	152	SER	2.1
40	1i	66	ARG	2.1
44	2m	58	GLU	2.1
50	2s	27	GLU	2.1
6	1G	76	SER	2.1
15	1T	107	ASP	2.1
6	2G	122	PRO	2.1
35	1d	29	PRO	2.1
7	2H	123	PHE	2.1
40	1i	101	PHE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
20	2Y	45	VAL	2.1
30	28	14	VAL	2.1
31	29	20	HIS	2.1
35	1d	133	VAL	2.1
40	1i	109	VAL	2.1
40	2i	28	VAL	2.1
40	2i	65	VAL	2.1
50	2s	51	VAL	2.1
20	1Y	57	GLN	2.1
32	2a	1000	U	2.1
32	2a	1205	U	2.1
32	2a	1446	U	2.1
53	1y	70	MET	2.1
4	1E	70	ALA	2.1
32	2a	1492	A	2.1
35	1d	195	ALA	2.1
51	2t	97	ALA	2.1
42	1k	117	ASN	2.1
6	2G	44	GLY	2.1
8	2I	12	LEU	2.1
12	2Q	19	GLY	2.1
22	20	52	GLY	2.1
26	14	45	GLY	2.1
26	24	64	GLY	2.1
33	1b	44	LEU	2.1
33	2b	66	GLY	2.1
34	2c	15	THR	2.1
41	1j	90	LEU	2.1
41	2j	67	THR	2.1
43	1l	61	THR	2.1
44	2m	19	LEU	2.1
47	2p	49	LEU	2.1
33	2b	223	ILE	2.1
34	2c	202	ILE	2.1
41	2j	82	ILE	2.1
14	1S	20	ARG	2.1
33	1b	36	ARG	2.1
42	2k	126	ARG	2.1
47	1p	39	TYR	2.1
48	2q	95	TYR	2.1
1	2A	2157	G	2.1
32	1a	78	G	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	1a	1003	G	2.1
32	2a	1124	G	2.1
1	2A	886	C	2.1
21	2Z	159	PRO	2.1
41	1j	91	PRO	2.1
30	28	25	MET	2.1
40	2i	58	HIS	2.1
7	2H	19	VAL	2.1
34	2c	68	VAL	2.1
39	2h	97	VAL	2.1
40	2i	44	VAL	2.1
42	2k	105	VAL	2.1
50	2s	19	VAL	2.1
50	2s	58	VAL	2.1
51	1t	18	GLN	2.1
1	1A	1175	U	2.1
14	2S	77	ALA	2.1
34	1c	71	ALA	2.1
36	2e	17	ALA	2.1
36	2e	146	ALA	2.1
38	1g	156	TRP	2.1
38	2g	152	ALA	2.1
41	1j	27	ALA	2.1
26	24	20	ASN	2.1
14	2S	101	LEU	2.1
32	2a	1349	A	2.1
32	2a	1447	A	2.1
22	10	8	GLY	2.1
35	2d	174	LEU	2.1
44	2m	48	LEU	2.1
53	2y	34	LEU	2.1
41	2j	87	THR	2.1
6	2G	54	GLU	2.1
40	2i	63	ILE	2.1
50	2s	43	GLU	2.1
19	1X	69	TYR	2.1
38	1g	85	TYR	2.1
53	2y	71	TYR	2.1
38	2g	98	SER	2.1
53	2y	69	ASP	2.1
1	1A	2148	G	2.1
1	1A	2207	G	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	1074	G	2.1
1	2A	1087	G	2.1
32	1a	1032	G	2.1
1	2A	885	C	2.1
1	2A	2108	C	2.1
2	2B	5	C	2.1
32	1a	1007	C	2.1
32	1a	1028	C	2.1
32	2a	1029	C	2.1
46	2o	19	PRO	2.1
52	1u	23	PRO	2.1
47	2p	16	HIS	2.1
50	2s	66	MET	2.1
7	2H	26	VAL	2.1
34	2c	173	VAL	2.1
34	2c	186	PHE	2.1
50	2s	74	PHE	2.1
14	2S	37	ALA	2.1
38	2g	65	ALA	2.1
45	2n	20	ALA	2.1
1	1A	2113	U	2.1
3	1D	37	LEU	2.1
4	2E	121	ASN	2.1
6	2G	103	LEU	2.1
6	2G	111	LEU	2.1
33	1b	175	ARG	2.1
34	2c	131	ARG	2.1
34	2c	178	LEU	2.1
36	2e	119	LEU	2.1
48	1q	98	LEU	2.1
53	2y	79	ASN	2.1
7	2H	6	ARG	2.1
21	2Z	114	GLY	2.1
41	1j	10	GLY	2.1
43	2l	88	GLY	2.1
44	2m	95	GLY	2.1
9	2N	22	THR	2.1
10	1O	108	GLU	2.1
33	1b	9	GLU	2.1
1	1A	6	A	2.1
1	2A	529	A	2.1
14	2S	39	ILE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	1b	80	ILE	2.1
33	1b	208	ILE	2.1
33	2b	211	ILE	2.1
34	1c	182	ILE	2.1
20	2Y	19	LYS	2.1
45	2n	58	LYS	2.1
42	1k	36	ASP	2.1
50	2s	61	TYR	2.1
38	2g	112	PRO	2.1
26	24	1	MET	2.1
1	1A	2108	C	2.1
1	1A	2133	G	2.0
32	2a	1037	C	2.1
32	2a	1362	C	2.1
8	1I	3	VAL	2.0
26	24	33	VAL	2.0
34	2c	103	VAL	2.0
36	2e	82	VAL	2.0
43	2l	96	VAL	2.0
50	2s	45	VAL	2.0
7	1H	3	ARG	2.0
11	2P	89	ALA	2.0
21	2Z	173	ALA	2.0
26	24	13	ARG	2.0
30	18	46	ARG	2.0
35	1d	132	ARG	2.0
35	1d	168	ARG	2.0
52	1u	6	ARG	2.0
52	1u	15	ARG	2.0
33	2b	215	LEU	2.0
37	1f	21	LEU	2.0
38	2g	99	LEU	2.0
50	1s	23	ASN	2.0
6	2G	24	GLY	2.0
7	2H	14	GLY	2.0
17	2V	63	GLY	2.0
21	1Z	202	GLU	2.0
31	29	21	GLY	2.0
34	2c	185	GLY	2.0
34	2c	194	GLY	2.0
32	2a	1025	U	2.0
26	24	22	ILE	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	1b	8	LYS	2.0
33	2b	8	LYS	2.0
40	1i	95	LYS	2.0
47	1p	69	THR	2.0
49	2r	47	THR	2.0
50	2s	48	THR	2.0
51	1t	100	ILE	2.0
32	2a	1531	A	2.0
39	1h	94	TYR	2.0
39	2h	4	ASP	2.0
39	2h	52	ASP	2.0
21	2Z	68	PRO	2.0
39	2h	94	TYR	2.0
21	2Z	28	MET	2.0
21	2Z	98	MET	2.0
33	2b	124	SER	2.0
33	1b	40	HIS	2.0
8	1I	139	GLN	2.0
26	24	46	GLN	2.0
1	2A	1075	C	2.0
1	2A	2175	C	2.0
3	2D	262	ARG	2.0
7	2H	52	VAL	2.0
14	2S	97	ARG	2.0
29	17	41	ARG	2.0
33	2b	217	ARG	2.0
40	2i	93	ARG	2.0
41	1j	79	ARG	2.0
41	2j	49	VAL	2.0
44	2m	114	ARG	2.0
47	1p	81	ARG	2.0
1	1A	2152	G	2.0
1	2A	2121	G	2.0
6	2G	106	LEU	2.0
8	2I	35	LEU	2.0
33	1b	123	ALA	2.0
34	2c	52	LEU	2.0
40	1i	102	LEU	2.0
41	2j	40	LEU	2.0
44	2m	81	LEU	2.0
51	1t	97	ALA	2.0
7	2H	82	GLY	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
44	1m	115	LYS	2.0
52	2u	20	LYS	2.0
53	2y	66	LYS	2.0
3	2D	259	THR	2.0
44	1m	9	ILE	2.0
53	2y	78	ILE	2.0
1	1A	2150	U	2.0
32	2a	950	U	2.0
32	2a	1040	U	2.0
42	1k	42	TRP	2.0
1	1A	2790	A	2.0
1	2A	1077	A	2.0
21	2Z	83	PRO	2.0
34	1c	73	PRO	2.0
42	2k	115	PRO	2.0
14	2S	53	SER	2.0
18	2W	111	HIS	2.0
35	2d	20	TYR	2.0
36	2e	60	TYR	2.0
38	2g	92	SER	2.0
38	2g	153	HIS	2.0
50	2s	47	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(Å^2)	Q<0.9
1	5MU	2A	1915	21/22	0.83	0.12	85,90,94,108	0
32	2MG	2a	1207	24/25	0.84	0.13	87,93,99,103	0
32	5MC	2a	967	21/22	0.86	0.14	75,80,86,92	0
1	5MU	1A	1915	21/22	0.86	0.13	75,82,90,93	0
32	M2G	2a	966	25/26	0.88	0.14	70,75,90,97	0
32	G7M	2a	527	24/25	0.89	0.13	75,77,79,84	0
1	PSU	2A	1917	20/21	0.89	0.09	80,85,95,100	0
43	0TD	1l	92	10/11	0.91	0.12	59,62,66,79	0
43	0TD	2l	92	10/11	0.91	0.11	68,72,75,85	0
1	PSU	1A	1917	20/21	0.92	0.09	66,75,86,86	0
1	PSU	1A	1911	20/21	0.92	0.10	64,73,76,86	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	PSU	2a	516	20/21	0.92	0.09	77,81,88,88	0
1	PSU	2A	1911	20/21	0.92	0.10	72,75,83,91	0
32	2MG	1a	1207	24/25	0.93	0.09	73,78,81,83	0
32	4OC	2a	1402	22/23	0.93	0.11	68,72,77,81	0
1	OMC	2A	1920	21/22	0.93	0.11	70,74,81,84	0
32	5MC	1a	967	21/22	0.94	0.12	63,69,77,82	0
32	5MC	2a	1404	21/22	0.94	0.09	65,72,77,79	0
32	UR3	2a	1498	21/22	0.94	0.10	64,70,75,78	0
32	MA6	2a	1519	24/25	0.94	0.13	64,74,78,79	0
32	5MC	2a	1400	21/22	0.94	0.13	73,80,82,85	0
32	5MC	2a	1407	21/22	0.95	0.09	63,72,76,82	0
32	G7M	1a	527	24/25	0.95	0.09	51,57,62,65	0
32	MA6	2a	1518	24/25	0.95	0.11	66,73,78,78	0
32	5MC	1a	1407	21/22	0.95	0.11	56,61,66,72	0
32	PSU	1a	516	20/21	0.95	0.08	65,69,73,75	0
32	4OC	1a	1402	22/23	0.96	0.10	51,60,65,67	0
32	M2G	1a	966	25/26	0.96	0.09	49,62,70,80	0
32	UR3	1a	1498	21/22	0.96	0.10	52,57,60,70	0
32	MA6	1a	1518	24/25	0.96	0.10	47,53,57,58	0
1	5MC	2A	1942	21/22	0.96	0.09	53,59,62,75	0
32	5MC	1a	1400	21/22	0.96	0.09	49,57,63,63	0
1	5MC	2A	1962	21/22	0.97	0.07	45,52,59,65	0
1	OMG	2A	2251	24/25	0.97	0.09	43,47,50,51	0
1	2MA	2A	2503	23/24	0.97	0.08	35,43,47,49	0
32	5MC	1a	1404	21/22	0.97	0.08	50,54,57,61	0
32	MA6	1a	1519	24/25	0.97	0.09	49,54,59,61	0
1	PSU	1A	2605	20/21	0.97	0.08	29,34,37,38	0
1	5MU	2A	1939	21/22	0.97	0.07	38,45,49,51	0
1	OMC	1A	1920	21/22	0.97	0.08	56,64,67,69	0
1	2MA	1A	2503	23/24	0.98	0.05	24,28,32,33	0
1	2MU	2A	2552	21/23	0.98	0.07	41,45,50,54	0
1	PSU	2A	2605	20/21	0.98	0.06	37,45,51,51	0
1	2MU	1A	2552	21/23	0.98	0.08	29,36,38,45	0
1	5MU	1A	1939	21/22	0.98	0.06	30,35,38,41	0
1	5MC	1A	1942	21/22	0.98	0.07	39,43,47,49	0
1	5MC	1A	1962	21/22	0.98	0.06	34,42,47,51	0
1	OMG	1A	2251	24/25	0.98	0.07	26,32,35,37	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3769	1/1	0.42	0.24	73,73,73,73	0
54	MG	2a	3049	1/1	0.43	0.25	86,86,86,86	0
54	MG	2O	202	1/1	0.46	0.23	87,87,87,87	0
54	MG	1a	1772	1/1	0.46	0.18	92,92,92,92	0
54	MG	2a	3010	1/1	0.49	0.40	92,92,92,92	0
54	MG	1A	3719	1/1	0.51	0.24	82,82,82,82	0
54	MG	1a	1680	1/1	0.53	0.32	87,87,87,87	0
54	MG	1A	3458	1/1	0.54	0.22	56,56,56,56	0
54	MG	2A	3270	1/1	0.58	0.34	88,88,88,88	0
54	MG	2A	3724	1/1	0.59	0.16	88,88,88,88	0
54	MG	1a	1797	1/1	0.59	0.22	95,95,95,95	0
54	MG	2B	211	1/1	0.60	0.21	86,86,86,86	0
54	MG	1A	3384	1/1	0.60	0.26	63,63,63,63	0
54	MG	2A	3478	1/1	0.60	0.23	77,77,77,77	0
54	MG	1a	1867	1/1	0.60	0.26	89,89,89,89	0
54	MG	2A	3521	1/1	0.61	0.23	77,77,77,77	0
54	MG	1A	3723	1/1	0.61	0.32	71,71,71,71	0
54	MG	1A	4001	1/1	0.61	0.17	85,85,85,85	0
54	MG	1a	1869	1/1	0.62	0.14	85,85,85,85	0
54	MG	1a	1774	1/1	0.62	0.18	87,87,87,87	0
54	MG	2B	213	1/1	0.62	0.14	84,84,84,84	0
54	MG	1a	1704	1/1	0.63	0.24	81,81,81,81	0
54	MG	2a	3175	1/1	0.63	0.27	91,91,91,91	0
54	MG	1a	1665	1/1	0.64	0.21	86,86,86,86	0
54	MG	1A	3661	1/1	0.65	0.33	43,43,43,43	0
54	MG	2A	3635	1/1	0.67	0.37	69,69,69,69	0
54	MG	1A	3805	1/1	0.67	0.25	47,47,47,47	0
54	MG	1A	3697	1/1	0.68	0.20	68,68,68,68	0
54	MG	1B	206	1/1	0.68	0.39	81,81,81,81	0
54	MG	1a	1635	1/1	0.68	0.24	82,82,82,82	0
54	MG	1A	3844	1/1	0.68	0.31	47,47,47,47	0
54	MG	2A	3477	1/1	0.68	0.26	83,83,83,83	0
54	MG	1a	1874	1/1	0.69	0.20	86,86,86,86	0
54	MG	1a	1611	1/1	0.69	0.27	88,88,88,88	0
54	MG	1a	1821	1/1	0.69	0.27	86,86,86,86	0
54	MG	2a	3106	1/1	0.69	0.40	86,86,86,86	0
54	MG	2a	3118	1/1	0.69	0.23	82,82,82,82	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2B	214	1/1	0.69	0.12	95,95,95,95	0
54	MG	2A	3321	1/1	0.70	0.29	73,73,73,73	0
54	MG	2A	3441	1/1	0.70	0.14	77,77,77,77	0
54	MG	1A	3294	1/1	0.70	0.22	83,83,83,83	0
54	MG	2G	201	1/1	0.70	0.22	86,86,86,86	0
54	MG	1A	3668	1/1	0.70	0.17	70,70,70,70	0
54	MG	2A	3500	1/1	0.70	0.21	85,85,85,85	0
54	MG	2A	3090	1/1	0.70	0.16	75,75,75,75	0
54	MG	2A	3094	1/1	0.70	0.39	89,89,89,89	0
54	MG	1a	1696	1/1	0.70	0.24	86,86,86,86	0
54	MG	2a	3139	1/1	0.70	0.24	84,84,84,84	0
54	MG	2B	204	1/1	0.70	0.16	84,84,84,84	0
54	MG	2r	102	1/1	0.70	0.21	78,78,78,78	0
54	MG	1a	1604	1/1	0.71	0.24	77,77,77,77	0
54	MG	2A	3542	1/1	0.71	0.20	83,83,83,83	0
54	MG	1A	3541	1/1	0.71	0.14	65,65,65,65	0
54	MG	1a	1878	1/1	0.71	0.12	93,93,93,93	0
54	MG	2A	3468	1/1	0.71	0.20	82,82,82,82	0
54	MG	1g	202	1/1	0.71	0.21	83,83,83,83	0
54	MG	1a	1841	1/1	0.71	0.15	77,77,77,77	0
54	MG	1A	3670	1/1	0.71	0.17	67,67,67,67	0
54	MG	2D	309	1/1	0.71	0.29	88,88,88,88	0
54	MG	1H	201	1/1	0.72	0.27	77,77,77,77	0
54	MG	2A	3634	1/1	0.72	0.15	70,70,70,70	0
54	MG	1a	1803	1/1	0.72	0.25	77,77,77,77	0
54	MG	1b	301	1/1	0.72	0.27	87,87,87,87	0
54	MG	2A	3095	1/1	0.72	0.31	81,81,81,81	0
54	MG	2j	201	1/1	0.72	0.19	84,84,84,84	0
54	MG	2A	3522	1/1	0.72	0.24	85,85,85,85	0
54	MG	10	106	1/1	0.73	0.22	69,69,69,69	0
54	MG	1A	3976	1/1	0.73	0.20	76,76,76,76	0
54	MG	2a	3038	1/1	0.73	0.20	94,94,94,94	0
54	MG	1a	1824	1/1	0.73	0.17	84,84,84,84	0
54	MG	1B	220	1/1	0.73	0.20	53,53,53,53	0
54	MG	1a	1850	1/1	0.73	0.22	72,72,72,72	0
54	MG	1B	226	1/1	0.73	0.15	73,73,73,73	0
54	MG	1A	3907	1/1	0.73	0.18	72,72,72,72	0
54	MG	1a	1666	1/1	0.73	0.35	80,80,80,80	0
54	MG	2A	3543	1/1	0.73	0.14	74,74,74,74	0
54	MG	1T	204	1/1	0.74	0.22	78,78,78,78	0
54	MG	2G	202	1/1	0.74	0.20	91,91,91,91	0
54	MG	1a	1629	1/1	0.74	0.35	76,76,76,76	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3461	1/1	0.74	0.16	75,75,75,75	0
54	MG	1A	3853	1/1	0.74	0.20	64,64,64,64	0
54	MG	1A	3601	1/1	0.74	0.21	58,58,58,58	0
54	MG	2a	3059	1/1	0.74	0.32	91,91,91,91	0
54	MG	2a	3061	1/1	0.74	0.34	84,84,84,84	0
54	MG	2a	3099	1/1	0.74	0.30	77,77,77,77	0
54	MG	2A	3261	1/1	0.74	0.25	81,81,81,81	0
54	MG	2B	209	1/1	0.74	0.32	80,80,80,80	0
54	MG	1a	1852	1/1	0.74	0.23	76,76,76,76	0
54	MG	2A	3506	1/1	0.74	0.24	82,82,82,82	0
54	MG	2A	3298	1/1	0.74	0.21	90,90,90,90	0
54	MG	2A	3320	1/1	0.74	0.17	71,71,71,71	0
54	MG	2A	3630	1/1	0.75	0.11	100,100,100,100	0
54	MG	1a	1610	1/1	0.75	0.29	73,73,73,73	0
54	MG	1A	3674	1/1	0.75	0.20	82,82,82,82	0
54	MG	2A	3366	1/1	0.75	0.22	83,83,83,83	0
54	MG	2I	201	1/1	0.75	0.15	78,78,78,78	0
54	MG	2a	3137	1/1	0.75	0.16	80,80,80,80	0
54	MG	1A	3776	1/1	0.75	0.25	72,72,72,72	0
54	MG	1A	4032	1/1	0.75	0.18	65,65,65,65	0
54	MG	1A	3864	1/1	0.75	0.19	64,64,64,64	0
54	MG	1A	3455	1/1	0.75	0.22	66,66,66,66	0
54	MG	2A	3585	1/1	0.76	0.17	67,67,67,67	0
54	MG	1A	3604	1/1	0.76	0.25	64,64,64,64	0
54	MG	1A	3713	1/1	0.76	0.26	78,78,78,78	0
54	MG	2A	3275	1/1	0.76	0.39	72,72,72,72	0
54	MG	2A	3721	1/1	0.76	0.19	78,78,78,78	0
54	MG	2A	3295	1/1	0.76	0.24	71,71,71,71	0
54	MG	1a	1693	1/1	0.76	0.19	88,88,88,88	0
54	MG	1A	3887	1/1	0.76	0.16	71,71,71,71	0
54	MG	1A	3895	1/1	0.76	0.15	60,60,60,60	0
54	MG	1a	1771	1/1	0.76	0.13	94,94,94,94	0
54	MG	2A	3430	1/1	0.76	0.34	83,83,83,83	0
54	MG	2A	3131	1/1	0.76	0.34	81,81,81,81	0
54	MG	2E	306	1/1	0.76	0.25	79,79,79,79	0
54	MG	2A	3567	1/1	0.76	0.28	87,87,87,87	0
54	MG	2A	3568	1/1	0.76	0.19	82,82,82,82	0
57	MPD	2B	219	8/8	0.76	0.25	72,74,84,90	0
54	MG	1A	3666	1/1	0.77	0.14	70,70,70,70	0
54	MG	1A	3492	1/1	0.77	0.16	64,64,64,64	0
54	MG	1P	204	1/1	0.77	0.26	48,48,48,48	0
54	MG	1A	4015	1/1	0.77	0.27	36,36,36,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2a	3037	1/1	0.77	0.13	85,85,85,85	0
54	MG	1e	203	1/1	0.77	0.12	77,77,77,77	0
54	MG	2A	3452	1/1	0.77	0.17	69,69,69,69	0
54	MG	1A	4030	1/1	0.77	0.17	66,66,66,66	0
54	MG	1a	1681	1/1	0.77	0.14	90,90,90,90	0
54	MG	2a	3085	1/1	0.77	0.27	89,89,89,89	0
54	MG	2A	3725	1/1	0.77	0.21	87,87,87,87	0
54	MG	1a	1692	1/1	0.77	0.25	79,79,79,79	0
54	MG	1a	1829	1/1	0.77	0.19	83,83,83,83	0
54	MG	1A	3477	1/1	0.77	0.17	66,66,66,66	0
54	MG	1A	3828	1/1	0.77	0.17	79,79,79,79	0
54	MG	2a	3148	1/1	0.77	0.15	82,82,82,82	0
54	MG	1A	3561	1/1	0.77	0.23	64,64,64,64	0
54	MG	1a	1863	1/1	0.77	0.21	78,78,78,78	0
54	MG	1a	1769	1/1	0.77	0.25	85,85,85,85	0
54	MG	1a	1868	1/1	0.77	0.16	80,80,80,80	0
54	MG	1A	3445	1/1	0.78	0.19	80,80,80,80	0
54	MG	1a	1877	1/1	0.78	0.41	73,73,73,73	0
54	MG	18	102	1/1	0.78	0.31	52,52,52,52	0
54	MG	1A	3014	1/1	0.78	0.35	70,70,70,70	0
54	MG	1d	303	1/1	0.78	0.21	76,76,76,76	0
54	MG	2a	3024	1/1	0.78	0.33	82,82,82,82	0
54	MG	2A	3323	1/1	0.78	0.18	67,67,67,67	0
54	MG	1A	3829	1/1	0.78	0.24	39,39,39,39	0
54	MG	2A	3378	1/1	0.78	0.28	84,84,84,84	0
54	MG	1a	1703	1/1	0.78	0.30	80,80,80,80	0
54	MG	2A	3689	1/1	0.78	0.14	73,73,73,73	0
54	MG	2A	3437	1/1	0.78	0.12	87,87,87,87	0
54	MG	2a	3087	1/1	0.78	0.25	73,73,73,73	0
54	MG	2A	3022	1/1	0.78	0.40	63,63,63,63	0
54	MG	2A	3052	1/1	0.78	0.21	64,64,64,64	0
54	MG	2A	3728	1/1	0.78	0.24	64,64,64,64	0
54	MG	2A	3058	1/1	0.78	0.20	59,59,59,59	0
54	MG	1A	3906	1/1	0.78	0.15	49,49,49,49	0
54	MG	1A	3197	1/1	0.78	0.30	75,75,75,75	0
54	MG	1A	3969	1/1	0.78	0.22	67,67,67,67	0
54	MG	1A	3848	1/1	0.78	0.23	70,70,70,70	0
54	MG	2n	101	1/1	0.78	0.34	81,81,81,81	0
54	MG	1A	3987	1/1	0.78	0.24	58,58,58,58	0
54	MG	1A	3391	1/1	0.78	0.15	58,58,58,58	0
54	MG	2A	3162	1/1	0.79	0.25	76,76,76,76	0
54	MG	2A	3180	1/1	0.79	0.16	76,76,76,76	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3181	1/1	0.79	0.25	76,76,76,76	0
54	MG	2A	3216	1/1	0.79	0.22	69,69,69,69	0
54	MG	1a	1777	1/1	0.79	0.16	82,82,82,82	0
54	MG	2a	3006	1/1	0.79	0.42	87,87,87,87	0
54	MG	15	107	1/1	0.79	0.21	59,59,59,59	0
54	MG	1A	3480	1/1	0.79	0.17	61,61,61,61	0
54	MG	1A	3730	1/1	0.79	0.20	73,73,73,73	0
54	MG	1A	3488	1/1	0.79	0.16	55,55,55,55	0
54	MG	2a	3044	1/1	0.79	0.17	91,91,91,91	0
54	MG	1B	222	1/1	0.79	0.14	61,61,61,61	0
54	MG	1A	3200	1/1	0.79	0.18	86,86,86,86	0
54	MG	1y	202	1/1	0.79	0.22	73,73,73,73	0
54	MG	1a	1712	1/1	0.79	0.20	76,76,76,76	0
54	MG	2A	3697	1/1	0.79	0.17	62,62,62,62	0
54	MG	2A	3024	1/1	0.79	0.17	67,67,67,67	0
54	MG	2A	3386	1/1	0.79	0.14	68,68,68,68	0
54	MG	2a	3110	1/1	0.79	0.19	74,74,74,74	0
54	MG	2A	3047	1/1	0.79	0.20	74,74,74,74	0
54	MG	1a	1738	1/1	0.79	0.22	72,72,72,72	0
54	MG	1a	1861	1/1	0.79	0.16	84,84,84,84	0
54	MG	2A	3074	1/1	0.79	0.19	67,67,67,67	0
54	MG	1A	3703	1/1	0.79	0.15	71,71,71,71	0
54	MG	2e	201	1/1	0.79	0.29	77,77,77,77	0
54	MG	1A	3312	1/1	0.79	0.21	60,60,60,60	0
54	MG	1A	4017	1/1	0.79	0.17	66,66,66,66	0
54	MG	2B	216	1/1	0.79	0.15	86,86,86,86	0
54	MG	1A	3335	1/1	0.79	0.21	78,78,78,78	0
58	ARG	1F	319	12/12	0.79	0.18	61,72,79,80	0
54	MG	1A	4011	1/1	0.80	0.16	84,84,84,84	0
54	MG	2A	3362	1/1	0.80	0.14	51,51,51,51	0
54	MG	1a	1745	1/1	0.80	0.25	70,70,70,70	0
54	MG	2A	3578	1/1	0.80	0.18	71,71,71,71	0
54	MG	2A	3374	1/1	0.80	0.21	82,82,82,82	0
54	MG	2a	3021	1/1	0.80	0.32	79,79,79,79	0
54	MG	2A	3618	1/1	0.80	0.13	48,48,48,48	0
54	MG	2a	3027	1/1	0.80	0.21	83,83,83,83	0
54	MG	2A	3623	1/1	0.80	0.19	44,44,44,44	0
54	MG	1A	3296	1/1	0.80	0.16	77,77,77,77	0
54	MG	2A	3631	1/1	0.80	0.28	64,64,64,64	0
54	MG	2A	3164	1/1	0.80	0.27	88,88,88,88	0
54	MG	1A	3810	1/1	0.80	0.20	67,67,67,67	0
54	MG	2a	3060	1/1	0.80	0.25	73,73,73,73	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3943	1/1	0.80	0.16	75,75,75,75	0
54	MG	2a	3064	1/1	0.80	0.28	89,89,89,89	0
54	MG	2a	3066	1/1	0.80	0.21	82,82,82,82	0
54	MG	2a	3067	1/1	0.80	0.08	95,95,95,95	0
54	MG	2a	3073	1/1	0.80	0.38	82,82,82,82	0
54	MG	2A	3192	1/1	0.80	0.39	82,82,82,82	0
54	MG	2A	3706	1/1	0.80	0.11	88,88,88,88	0
54	MG	2a	3098	1/1	0.80	0.30	83,83,83,83	0
54	MG	2A	3211	1/1	0.80	0.28	76,76,76,76	0
54	MG	1A	3811	1/1	0.80	0.19	61,61,61,61	0
54	MG	1A	3974	1/1	0.80	0.14	59,59,59,59	0
54	MG	1A	3814	1/1	0.80	0.24	69,69,69,69	0
54	MG	2B	202	1/1	0.80	0.29	82,82,82,82	0
54	MG	2A	3273	1/1	0.80	0.31	80,80,80,80	0
54	MG	1A	3986	1/1	0.80	0.23	59,59,59,59	0
54	MG	1A	3556	1/1	0.80	0.17	67,67,67,67	0
54	MG	2a	3185	1/1	0.80	0.16	83,83,83,83	0
54	MG	2A	3089	1/1	0.80	0.24	78,78,78,78	0
54	MG	1A	3149	1/1	0.80	0.29	66,66,66,66	0
54	MG	2A	3526	1/1	0.80	0.18	47,47,47,47	0
54	MG	2A	3535	1/1	0.80	0.18	73,73,73,73	0
54	MG	2A	3539	1/1	0.80	0.19	90,90,90,90	0
54	MG	1a	1717	1/1	0.80	0.26	71,71,71,71	0
54	MG	2A	3620	1/1	0.81	0.26	79,79,79,79	0
54	MG	1a	1864	1/1	0.81	0.12	95,95,95,95	0
54	MG	1A	3581	1/1	0.81	0.16	62,62,62,62	0
54	MG	1a	1749	1/1	0.81	0.25	77,77,77,77	0
54	MG	2A	3140	1/1	0.81	0.24	80,80,80,80	0
54	MG	1A	3473	1/1	0.81	0.18	63,63,63,63	0
54	MG	1a	1669	1/1	0.81	0.22	76,76,76,76	0
54	MG	2A	3691	1/1	0.81	0.17	66,66,66,66	0
54	MG	2A	3165	1/1	0.81	0.18	61,61,61,61	0
54	MG	2A	3705	1/1	0.81	0.17	65,65,65,65	0
54	MG	2A	3459	1/1	0.81	0.21	73,73,73,73	0
54	MG	2A	3460	1/1	0.81	0.14	79,79,79,79	0
54	MG	2A	3174	1/1	0.81	0.10	79,79,79,79	0
54	MG	1A	3522	1/1	0.81	0.10	67,67,67,67	0
54	MG	2a	3079	1/1	0.81	0.22	83,83,83,83	0
54	MG	1A	3607	1/1	0.81	0.14	62,62,62,62	0
54	MG	2A	3729	1/1	0.81	0.34	74,74,74,74	0
54	MG	2a	3088	1/1	0.81	0.26	81,81,81,81	0
54	MG	1A	3923	1/1	0.81	0.11	30,30,30,30	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1a	1794	1/1	0.81	0.17	78,78,78,78	0
54	MG	1A	3089	1/1	0.81	0.21	67,67,67,67	0
54	MG	1A	3953	1/1	0.81	0.12	55,55,55,55	0
54	MG	1A	3543	1/1	0.81	0.16	64,64,64,64	0
54	MG	1A	3555	1/1	0.81	0.12	59,59,59,59	0
54	MG	2a	3138	1/1	0.81	0.22	75,75,75,75	0
54	MG	1A	3154	1/1	0.81	0.21	77,77,77,77	0
54	MG	2A	3284	1/1	0.81	0.32	64,64,64,64	0
54	MG	2a	3171	1/1	0.81	0.20	84,84,84,84	0
54	MG	2A	3043	1/1	0.81	0.29	76,76,76,76	0
54	MG	1a	1713	1/1	0.81	0.29	77,77,77,77	0
54	MG	1a	1842	1/1	0.81	0.21	87,87,87,87	0
54	MG	1A	3395	1/1	0.81	0.16	70,70,70,70	0
54	MG	1a	1722	1/1	0.81	0.26	76,76,76,76	0
54	MG	2a	3005	1/1	0.81	0.19	66,66,66,66	0
54	MG	1a	1737	1/1	0.81	0.16	82,82,82,82	0
54	MG	1a	1641	1/1	0.81	0.13	79,79,79,79	0
54	MG	1A	3539	1/1	0.82	0.15	79,79,79,79	0
54	MG	2A	3182	1/1	0.82	0.14	72,72,72,72	0
54	MG	2A	3514	1/1	0.82	0.15	76,76,76,76	0
54	MG	2A	3184	1/1	0.82	0.27	80,80,80,80	0
54	MG	2A	3188	1/1	0.82	0.27	66,66,66,66	0
54	MG	1A	3605	1/1	0.82	0.32	46,46,46,46	0
54	MG	2A	3208	1/1	0.82	0.13	68,68,68,68	0
54	MG	1A	3168	1/1	0.82	0.27	70,70,70,70	0
54	MG	1A	3724	1/1	0.82	0.17	52,52,52,52	0
54	MG	2a	3032	1/1	0.82	0.14	91,91,91,91	0
54	MG	2A	3248	1/1	0.82	0.21	63,63,63,63	0
54	MG	1A	3656	1/1	0.82	0.22	77,77,77,77	0
54	MG	2A	3266	1/1	0.82	0.31	82,82,82,82	0
54	MG	1a	1786	1/1	0.82	0.14	77,77,77,77	0
54	MG	1A	3742	1/1	0.82	0.13	50,50,50,50	0
54	MG	1A	4036	1/1	0.82	0.20	73,73,73,73	0
54	MG	1a	1799	1/1	0.82	0.20	80,80,80,80	0
54	MG	2A	3286	1/1	0.82	0.21	70,70,70,70	0
54	MG	2A	3626	1/1	0.82	0.15	82,82,82,82	0
54	MG	2A	3034	1/1	0.82	0.33	81,81,81,81	0
54	MG	1A	3328	1/1	0.82	0.12	70,70,70,70	0
54	MG	1a	1820	1/1	0.82	0.18	84,84,84,84	0
54	MG	1A	3330	1/1	0.82	0.16	64,64,64,64	0
54	MG	2A	3053	1/1	0.82	0.27	74,74,74,74	0
54	MG	2A	3356	1/1	0.82	0.14	74,74,74,74	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3801	1/1	0.82	0.15	39,39,39,39	0
54	MG	1A	3667	1/1	0.82	0.24	73,73,73,73	0
54	MG	1A	3262	1/1	0.82	0.26	71,71,71,71	0
54	MG	1A	3362	1/1	0.82	0.16	76,76,76,76	0
54	MG	2A	3385	1/1	0.82	0.13	70,70,70,70	0
54	MG	2a	3129	1/1	0.82	0.21	70,70,70,70	0
54	MG	2a	3131	1/1	0.82	0.12	83,83,83,83	0
54	MG	1A	3504	1/1	0.82	0.12	33,33,33,33	0
54	MG	1Z	301	1/1	0.82	0.17	73,73,73,73	0
54	MG	2A	3104	1/1	0.82	0.23	65,65,65,65	0
54	MG	2A	3118	1/1	0.82	0.29	74,74,74,74	0
54	MG	2A	3442	1/1	0.82	0.18	73,73,73,73	0
54	MG	2A	3446	1/1	0.82	0.17	65,65,65,65	0
54	MG	1A	3826	1/1	0.82	0.16	65,65,65,65	0
54	MG	1A	3981	1/1	0.82	0.17	58,58,58,58	0
54	MG	1A	3589	1/1	0.82	0.16	68,68,68,68	0
54	MG	1A	3376	1/1	0.82	0.13	65,65,65,65	0
54	MG	1A	3990	1/1	0.82	0.16	61,61,61,61	0
54	MG	1A	3999	1/1	0.82	0.11	75,75,75,75	0
54	MG	1a	1760	1/1	0.82	0.10	64,64,64,64	0
54	MG	1a	1679	1/1	0.83	0.17	66,66,66,66	0
54	MG	1a	1781	1/1	0.83	0.18	89,89,89,89	0
54	MG	1a	1785	1/1	0.83	0.15	73,73,73,73	0
54	MG	1m	202	1/1	0.83	0.23	79,79,79,79	0
54	MG	2A	3501	1/1	0.83	0.12	75,75,75,75	0
54	MG	1O	201	1/1	0.83	0.17	57,57,57,57	0
54	MG	2A	3511	1/1	0.83	0.20	77,77,77,77	0
54	MG	2A	3213	1/1	0.83	0.18	72,72,72,72	0
54	MG	1A	3546	1/1	0.83	0.20	66,66,66,66	0
54	MG	2a	3016	1/1	0.83	0.16	79,79,79,79	0
54	MG	2a	3019	1/1	0.83	0.23	80,80,80,80	0
54	MG	2A	3219	1/1	0.83	0.11	62,62,62,62	0
54	MG	2A	3230	1/1	0.83	0.26	72,72,72,72	0
54	MG	1R	205	1/1	0.83	0.23	61,61,61,61	0
54	MG	1A	3893	1/1	0.83	0.20	39,39,39,39	0
54	MG	2a	3036	1/1	0.83	0.22	78,78,78,78	0
54	MG	2A	3262	1/1	0.83	0.14	65,65,65,65	0
54	MG	2A	3037	1/1	0.83	0.30	74,74,74,74	0
54	MG	2a	3041	1/1	0.83	0.27	80,80,80,80	0
54	MG	1W	201	1/1	0.83	0.25	57,57,57,57	0
54	MG	1A	3456	1/1	0.83	0.14	41,41,41,41	0
54	MG	2a	3050	1/1	0.83	0.36	87,87,87,87	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3048	1/1	0.83	0.17	73,73,73,73	0
54	MG	1A	3639	1/1	0.83	0.21	64,64,64,64	0
54	MG	1A	3167	1/1	0.83	0.27	77,77,77,77	0
54	MG	1A	3464	1/1	0.83	0.23	66,66,66,66	0
54	MG	1a	1835	1/1	0.83	0.23	78,78,78,78	0
54	MG	2A	3087	1/1	0.83	0.23	90,90,90,90	0
54	MG	2a	3071	1/1	0.83	0.26	69,69,69,69	0
54	MG	1a	1716	1/1	0.83	0.27	71,71,71,71	0
54	MG	1A	3472	1/1	0.83	0.22	69,69,69,69	0
54	MG	2A	3335	1/1	0.83	0.23	71,71,71,71	0
54	MG	1a	1718	1/1	0.83	0.17	67,67,67,67	0
54	MG	2A	3673	1/1	0.83	0.10	76,76,76,76	0
54	MG	2A	3685	1/1	0.83	0.19	74,74,74,74	0
54	MG	1A	3583	1/1	0.83	0.11	53,53,53,53	0
54	MG	2A	3102	1/1	0.83	0.35	70,70,70,70	0
54	MG	2A	3368	1/1	0.83	0.15	78,78,78,78	0
54	MG	1a	1860	1/1	0.83	0.12	90,90,90,90	0
54	MG	1A	3437	1/1	0.83	0.18	66,66,66,66	0
54	MG	2A	3707	1/1	0.83	0.18	75,75,75,75	0
54	MG	2a	3136	1/1	0.83	0.23	76,76,76,76	0
54	MG	1A	3669	1/1	0.83	0.30	44,44,44,44	0
54	MG	2A	3722	1/1	0.83	0.25	76,76,76,76	0
54	MG	1B	216	1/1	0.83	0.17	51,51,51,51	0
54	MG	2a	3143	1/1	0.83	0.21	73,73,73,73	0
54	MG	2A	3142	1/1	0.83	0.16	76,76,76,76	0
54	MG	2a	3170	1/1	0.83	0.24	68,68,68,68	0
54	MG	1a	1638	1/1	0.83	0.20	71,71,71,71	0
54	MG	2A	3163	1/1	0.83	0.11	67,67,67,67	0
54	MG	2a	3179	1/1	0.83	0.19	67,67,67,67	0
54	MG	1a	1758	1/1	0.83	0.19	76,76,76,76	0
54	MG	1A	3278	1/1	0.83	0.34	75,75,75,75	0
54	MG	1a	1642	1/1	0.83	0.15	65,65,65,65	0
54	MG	1A	3861	1/1	0.83	0.22	68,68,68,68	0
54	MG	1A	3225	1/1	0.83	0.12	77,77,77,77	0
54	MG	2y	3200	1/1	0.83	0.13	74,74,74,74	0
54	MG	1A	3871	1/1	0.83	0.11	66,66,66,66	0
54	MG	2A	3466	1/1	0.83	0.34	68,68,68,68	0
54	MG	1a	1646	1/1	0.84	0.22	76,76,76,76	0
54	MG	1e	201	1/1	0.84	0.29	71,71,71,71	0
54	MG	2a	3026	1/1	0.84	0.23	75,75,75,75	0
54	MG	2A	3607	1/1	0.84	0.12	74,74,74,74	0
54	MG	1a	1656	1/1	0.84	0.16	73,73,73,73	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1a	1805	1/1	0.84	0.31	83,83,83,83	0
54	MG	2A	3622	1/1	0.84	0.23	85,85,85,85	0
54	MG	1a	1813	1/1	0.84	0.31	78,78,78,78	0
54	MG	1a	1817	1/1	0.84	0.12	75,75,75,75	0
54	MG	1A	3937	1/1	0.84	0.14	35,35,35,35	0
54	MG	1A	3736	1/1	0.84	0.17	37,37,37,37	0
54	MG	2A	3031	1/1	0.84	0.27	84,84,84,84	0
54	MG	1A	3662	1/1	0.84	0.19	66,66,66,66	0
54	MG	1B	221	1/1	0.84	0.19	72,72,72,72	0
54	MG	1a	1751	1/1	0.84	0.18	76,76,76,76	0
54	MG	1a	1756	1/1	0.84	0.25	68,68,68,68	0
54	MG	2A	3210	1/1	0.84	0.17	70,70,70,70	0
54	MG	1A	3325	1/1	0.84	0.19	64,64,64,64	0
54	MG	1A	3606	1/1	0.84	0.35	66,66,66,66	0
54	MG	1a	1761	1/1	0.84	0.20	79,79,79,79	0
54	MG	2A	3054	1/1	0.84	0.19	72,72,72,72	0
54	MG	1a	1690	1/1	0.84	0.33	76,76,76,76	0
54	MG	2a	3086	1/1	0.84	0.15	80,80,80,80	0
54	MG	2A	3231	1/1	0.84	0.43	75,75,75,75	0
54	MG	2A	3474	1/1	0.84	0.11	84,84,84,84	0
54	MG	2A	3069	1/1	0.84	0.28	72,72,72,72	0
54	MG	1F	314	1/1	0.84	0.15	52,52,52,52	0
54	MG	2a	3100	1/1	0.84	0.24	80,80,80,80	0
54	MG	2A	3491	1/1	0.84	0.14	52,52,52,52	0
54	MG	1a	1862	1/1	0.84	0.14	82,82,82,82	0
54	MG	2a	3116	1/1	0.84	0.35	87,87,87,87	0
54	MG	1A	3261	1/1	0.84	0.22	69,69,69,69	0
54	MG	2A	3503	1/1	0.84	0.16	76,76,76,76	0
54	MG	1N	202	1/1	0.84	0.21	66,66,66,66	0
54	MG	1a	1617	1/1	0.84	0.11	70,70,70,70	0
54	MG	1A	3193	1/1	0.84	0.24	77,77,77,77	0
54	MG	2A	3276	1/1	0.84	0.33	70,70,70,70	0
54	MG	2A	3277	1/1	0.84	0.36	70,70,70,70	0
54	MG	2A	3096	1/1	0.84	0.18	64,64,64,64	0
54	MG	1a	1782	1/1	0.84	0.19	79,79,79,79	0
54	MG	2a	3149	1/1	0.84	0.12	71,71,71,71	0
54	MG	2A	3536	1/1	0.84	0.15	68,68,68,68	0
54	MG	2A	3538	1/1	0.84	0.13	75,75,75,75	0
54	MG	1P	203	1/1	0.84	0.25	74,74,74,74	0
54	MG	2U	201	1/1	0.84	0.22	79,79,79,79	0
54	MG	2a	3002	1/1	0.84	0.17	75,75,75,75	0
54	MG	2A	3109	1/1	0.84	0.23	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3310	1/1	0.84	0.17	59,59,59,59	0
54	MG	2a	3008	1/1	0.84	0.20	62,62,62,62	0
54	MG	2A	3555	1/1	0.84	0.10	63,63,63,63	0
54	MG	2a	3013	1/1	0.84	0.34	79,79,79,79	0
57	MPD	1a	1880	8/8	0.84	0.16	60,72,78,78	0
57	MPD	2A	3733	8/8	0.84	0.27	54,60,66,66	0
54	MG	1A	3172	1/1	0.84	0.15	50,50,50,50	0
54	MG	1T	201	1/1	0.84	0.26	62,62,62,62	0
54	MG	1a	1798	1/1	0.85	0.10	83,83,83,83	0
54	MG	2A	3530	1/1	0.85	0.19	63,63,63,63	0
54	MG	1a	1697	1/1	0.85	0.29	63,63,63,63	0
54	MG	2A	3036	1/1	0.85	0.17	66,66,66,66	0
54	MG	1A	3748	1/1	0.85	0.11	39,39,39,39	0
54	MG	1A	4025	1/1	0.85	0.29	44,44,44,44	0
54	MG	1a	1811	1/1	0.85	0.18	85,85,85,85	0
54	MG	2A	3271	1/1	0.85	0.20	63,63,63,63	0
54	MG	1a	1709	1/1	0.85	0.20	73,73,73,73	0
54	MG	1A	4028	1/1	0.85	0.19	66,66,66,66	0
54	MG	18	101	1/1	0.85	0.21	74,74,74,74	0
54	MG	2A	3573	1/1	0.85	0.10	49,49,49,49	0
54	MG	2A	3574	1/1	0.85	0.18	60,60,60,60	0
54	MG	2a	3040	1/1	0.85	0.15	73,73,73,73	0
54	MG	1a	1715	1/1	0.85	0.25	76,76,76,76	0
54	MG	1A	3767	1/1	0.85	0.13	64,64,64,64	0
54	MG	2A	3596	1/1	0.85	0.11	73,73,73,73	0
54	MG	1A	3947	1/1	0.85	0.12	64,64,64,64	0
54	MG	2A	3612	1/1	0.85	0.15	51,51,51,51	0
54	MG	1a	1831	1/1	0.85	0.19	86,86,86,86	0
54	MG	1A	4034	1/1	0.85	0.17	79,79,79,79	0
54	MG	2A	3299	1/1	0.85	0.14	43,43,43,43	0
54	MG	1a	1840	1/1	0.85	0.13	73,73,73,73	0
54	MG	1A	3702	1/1	0.85	0.24	85,85,85,85	0
54	MG	1A	4037	1/1	0.85	0.18	71,71,71,71	0
54	MG	1a	1623	1/1	0.85	0.40	75,75,75,75	0
54	MG	1a	1744	1/1	0.85	0.27	78,78,78,78	0
54	MG	1a	1853	1/1	0.85	0.19	67,67,67,67	0
54	MG	1B	205	1/1	0.85	0.12	61,61,61,61	0
54	MG	1A	3954	1/1	0.85	0.10	55,55,55,55	0
54	MG	2A	3112	1/1	0.85	0.16	78,78,78,78	0
54	MG	2a	3096	1/1	0.85	0.17	73,73,73,73	0
54	MG	2a	3097	1/1	0.85	0.30	84,84,84,84	0
54	MG	2A	3113	1/1	0.85	0.14	76,76,76,76	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3321	1/1	0.85	0.34	56,56,56,56	0
54	MG	2A	3703	1/1	0.85	0.13	68,68,68,68	0
54	MG	2A	3125	1/1	0.85	0.17	66,66,66,66	0
54	MG	2A	3389	1/1	0.85	0.18	49,49,49,49	0
54	MG	1A	3784	1/1	0.85	0.17	58,58,58,58	0
54	MG	1A	3609	1/1	0.85	0.19	72,72,72,72	0
54	MG	1A	3804	1/1	0.85	0.15	50,50,50,50	0
54	MG	1A	3875	1/1	0.85	0.13	73,73,73,73	0
54	MG	1A	3557	1/1	0.85	0.13	40,40,40,40	0
54	MG	1a	1870	1/1	0.85	0.26	75,75,75,75	0
54	MG	1A	3640	1/1	0.85	0.24	56,56,56,56	0
54	MG	1A	3993	1/1	0.85	0.22	61,61,61,61	0
54	MG	1A	3462	1/1	0.85	0.23	74,74,74,74	0
54	MG	1A	3526	1/1	0.85	0.14	60,60,60,60	0
54	MG	1A	4006	1/1	0.85	0.23	54,54,54,54	0
54	MG	2a	3167	1/1	0.85	0.13	75,75,75,75	0
54	MG	2a	3169	1/1	0.85	0.23	76,76,76,76	0
54	MG	1a	1686	1/1	0.85	0.27	82,82,82,82	0
54	MG	1A	3689	1/1	0.85	0.21	65,65,65,65	0
54	MG	1A	4012	1/1	0.85	0.25	88,88,88,88	0
54	MG	2B	217	1/1	0.85	0.10	79,79,79,79	0
54	MG	2a	3181	1/1	0.85	0.17	82,82,82,82	0
54	MG	2A	3485	1/1	0.85	0.20	82,82,82,82	0
54	MG	2a	3188	1/1	0.85	0.18	88,88,88,88	0
54	MG	2A	3205	1/1	0.85	0.36	76,76,76,76	0
54	MG	2A	3207	1/1	0.85	0.15	73,73,73,73	0
54	MG	1h	202	1/1	0.85	0.19	67,67,67,67	0
54	MG	1a	1788	1/1	0.85	0.15	72,72,72,72	0
54	MG	1a	1793	1/1	0.85	0.19	74,74,74,74	0
54	MG	2A	3002	1/1	0.85	0.23	70,70,70,70	0
54	MG	2A	3010	1/1	0.85	0.33	73,73,73,73	0
54	MG	1A	4013	1/1	0.85	0.19	66,66,66,66	0
54	MG	1A	3283	1/1	0.85	0.12	56,56,56,56	0
54	MG	1A	3813	1/1	0.86	0.11	75,75,75,75	0
54	MG	1a	1667	1/1	0.86	0.43	74,74,74,74	0
54	MG	2A	3403	1/1	0.86	0.18	57,57,57,57	0
54	MG	2A	3406	1/1	0.86	0.17	60,60,60,60	0
54	MG	2A	3421	1/1	0.86	0.20	80,80,80,80	0
54	MG	2A	3185	1/1	0.86	0.14	71,71,71,71	0
54	MG	1A	3552	1/1	0.86	0.14	64,64,64,64	0
54	MG	1A	3034	1/1	0.86	0.10	59,59,59,59	0
54	MG	2a	3051	1/1	0.86	0.35	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2a	3053	1/1	0.86	0.32	72,72,72,72	0
54	MG	2A	3636	1/1	0.86	0.14	79,79,79,79	0
54	MG	2A	3653	1/1	0.86	0.10	94,94,94,94	0
54	MG	1A	3379	1/1	0.86	0.08	41,41,41,41	0
54	MG	1A	3273	1/1	0.86	0.27	71,71,71,71	0
54	MG	2A	3450	1/1	0.86	0.17	66,66,66,66	0
54	MG	1a	1682	1/1	0.86	0.15	60,60,60,60	0
54	MG	1A	3833	1/1	0.86	0.14	45,45,45,45	0
54	MG	1A	3635	1/1	0.86	0.24	42,42,42,42	0
54	MG	1a	1775	1/1	0.86	0.20	76,76,76,76	0
54	MG	2a	3082	1/1	0.86	0.41	68,68,68,68	0
54	MG	1A	3959	1/1	0.86	0.13	49,49,49,49	0
54	MG	1a	1780	1/1	0.86	0.12	80,80,80,80	0
54	MG	2A	3714	1/1	0.86	0.11	59,59,59,59	0
54	MG	2A	3083	1/1	0.86	0.21	72,72,72,72	0
54	MG	2a	3092	1/1	0.86	0.40	86,86,86,86	0
54	MG	10	107	1/1	0.86	0.15	70,70,70,70	0
54	MG	2A	3233	1/1	0.86	0.12	60,60,60,60	0
54	MG	1A	3847	1/1	0.86	0.10	60,60,60,60	0
54	MG	2A	3490	1/1	0.86	0.17	71,71,71,71	0
54	MG	1A	3035	1/1	0.86	0.13	55,55,55,55	0
54	MG	2a	3105	1/1	0.86	0.54	83,83,83,83	0
54	MG	2A	3093	1/1	0.86	0.20	82,82,82,82	0
54	MG	2a	3108	1/1	0.86	0.37	71,71,71,71	0
54	MG	1A	3691	1/1	0.86	0.12	66,66,66,66	0
54	MG	2A	3269	1/1	0.86	0.23	60,60,60,60	0
54	MG	1A	3471	1/1	0.86	0.21	71,71,71,71	0
54	MG	2a	3121	1/1	0.86	0.11	81,81,81,81	0
54	MG	2a	3122	1/1	0.86	0.19	67,67,67,67	0
54	MG	1a	1789	1/1	0.86	0.20	64,64,64,64	0
54	MG	1B	210	1/1	0.86	0.23	70,70,70,70	0
54	MG	1A	3652	1/1	0.86	0.14	60,60,60,60	0
54	MG	1A	3038	1/1	0.86	0.27	69,69,69,69	0
54	MG	1d	301	1/1	0.86	0.28	74,74,74,74	0
54	MG	2D	311	1/1	0.86	0.11	36,36,36,36	0
54	MG	2a	3140	1/1	0.86	0.22	72,72,72,72	0
54	MG	2E	303	1/1	0.86	0.14	39,39,39,39	0
54	MG	1A	3704	1/1	0.86	0.10	62,62,62,62	0
54	MG	1A	3877	1/1	0.86	0.11	56,56,56,56	0
54	MG	2a	3153	1/1	0.86	0.13	82,82,82,82	0
54	MG	1A	3033	1/1	0.86	0.15	55,55,55,55	0
54	MG	1B	229	1/1	0.86	0.08	68,68,68,68	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3809	1/1	0.86	0.10	39,39,39,39	0
54	MG	2A	3312	1/1	0.86	0.17	70,70,70,70	0
54	MG	28	102	1/1	0.86	0.20	66,66,66,66	0
54	MG	1F	316	1/1	0.86	0.20	56,56,56,56	0
54	MG	2A	3546	1/1	0.86	0.12	50,50,50,50	0
54	MG	2A	3143	1/1	0.86	0.14	54,54,54,54	0
54	MG	1a	1814	1/1	0.86	0.18	81,81,81,81	0
54	MG	1A	3238	1/1	0.86	0.23	65,65,65,65	0
54	MG	2A	3355	1/1	0.86	0.20	75,75,75,75	0
54	MG	1a	1743	1/1	0.86	0.23	72,72,72,72	0
54	MG	2A	3019	1/1	0.86	0.52	58,58,58,58	0
54	MG	2A	3170	1/1	0.86	0.23	61,61,61,61	0
54	MG	1a	1651	1/1	0.86	0.13	67,67,67,67	0
54	MG	2A	3179	1/1	0.86	0.25	76,76,76,76	0
54	MG	1A	3901	1/1	0.86	0.09	33,33,33,33	0
54	MG	1A	3134	1/1	0.86	0.15	51,51,51,51	0
54	MG	1A	3775	1/1	0.87	0.13	51,51,51,51	0
54	MG	1A	3890	1/1	0.87	0.17	71,71,71,71	0
54	MG	2A	3410	1/1	0.87	0.31	78,78,78,78	0
54	MG	2B	210	1/1	0.87	0.24	77,77,77,77	0
54	MG	11	104	1/1	0.87	0.16	63,63,63,63	0
54	MG	2A	3422	1/1	0.87	0.13	66,66,66,66	0
54	MG	2A	3427	1/1	0.87	0.12	71,71,71,71	0
54	MG	1A	3228	1/1	0.87	0.24	66,66,66,66	0
54	MG	2A	3436	1/1	0.87	0.15	76,76,76,76	0
54	MG	1A	3112	1/1	0.87	0.10	67,67,67,67	0
54	MG	2A	3439	1/1	0.87	0.11	41,41,41,41	0
54	MG	2D	313	1/1	0.87	0.35	70,70,70,70	0
54	MG	1A	3899	1/1	0.87	0.19	75,75,75,75	0
54	MG	1a	1601	1/1	0.87	0.38	78,78,78,78	0
54	MG	1a	1730	1/1	0.87	0.21	75,75,75,75	0
54	MG	2A	3156	1/1	0.87	0.18	72,72,72,72	0
54	MG	1a	1733	1/1	0.87	0.12	72,72,72,72	0
54	MG	1A	3259	1/1	0.87	0.16	45,45,45,45	0
54	MG	1A	3127	1/1	0.87	0.22	58,58,58,58	0
54	MG	21	102	1/1	0.87	0.15	84,84,84,84	0
54	MG	1A	3679	1/1	0.87	0.12	63,63,63,63	0
54	MG	2A	3462	1/1	0.87	0.16	72,72,72,72	0
54	MG	2a	3004	1/1	0.87	0.11	56,56,56,56	0
54	MG	2A	3465	1/1	0.87	0.16	67,67,67,67	0
54	MG	1a	1614	1/1	0.87	0.11	67,67,67,67	0
54	MG	2a	3007	1/1	0.87	0.10	73,73,73,73	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	4035	1/1	0.87	0.21	66,66,66,66	0
54	MG	1A	3204	1/1	0.87	0.15	70,70,70,70	0
54	MG	1a	1750	1/1	0.87	0.17	76,76,76,76	0
54	MG	2a	3015	1/1	0.87	0.18	74,74,74,74	0
54	MG	1A	3690	1/1	0.87	0.21	41,41,41,41	0
54	MG	2a	3018	1/1	0.87	0.25	69,69,69,69	0
54	MG	2A	3479	1/1	0.87	0.17	69,69,69,69	0
54	MG	2A	3481	1/1	0.87	0.16	73,73,73,73	0
54	MG	2A	3483	1/1	0.87	0.10	75,75,75,75	0
54	MG	1A	3401	1/1	0.87	0.13	64,64,64,64	0
54	MG	2A	3486	1/1	0.87	0.10	76,76,76,76	0
54	MG	1a	1757	1/1	0.87	0.16	67,67,67,67	0
54	MG	1A	3693	1/1	0.87	0.10	61,61,61,61	0
54	MG	1A	3610	1/1	0.87	0.14	36,36,36,36	0
54	MG	1A	3612	1/1	0.87	0.12	55,55,55,55	0
54	MG	2a	3039	1/1	0.87	0.14	68,68,68,68	0
54	MG	2A	3197	1/1	0.87	0.26	70,70,70,70	0
54	MG	1a	1765	1/1	0.87	0.20	57,57,57,57	0
54	MG	2A	3206	1/1	0.87	0.16	66,66,66,66	0
54	MG	2a	3046	1/1	0.87	0.17	76,76,76,76	0
54	MG	2a	3048	1/1	0.87	0.21	84,84,84,84	0
54	MG	1a	1645	1/1	0.87	0.24	62,62,62,62	0
54	MG	1A	3958	1/1	0.87	0.09	34,34,34,34	0
54	MG	1l	202	1/1	0.87	0.18	75,75,75,75	0
54	MG	2A	3524	1/1	0.87	0.21	69,69,69,69	0
54	MG	2a	3056	1/1	0.87	0.16	73,73,73,73	0
54	MG	1A	3613	1/1	0.87	0.21	67,67,67,67	0
54	MG	2A	3527	1/1	0.87	0.12	69,69,69,69	0
54	MG	1a	1773	1/1	0.87	0.18	83,83,83,83	0
54	MG	1a	1655	1/1	0.87	0.26	59,59,59,59	0
54	MG	1A	3621	1/1	0.87	0.13	69,69,69,69	0
54	MG	2A	3537	1/1	0.87	0.13	79,79,79,79	0
54	MG	1a	1662	1/1	0.87	0.15	81,81,81,81	0
54	MG	1A	3623	1/1	0.87	0.11	47,47,47,47	0
54	MG	1A	3429	1/1	0.87	0.20	60,60,60,60	0
54	MG	2A	3238	1/1	0.87	0.38	51,51,51,51	0
54	MG	1D	317	1/1	0.87	0.15	76,76,76,76	0
54	MG	1a	1668	1/1	0.87	0.20	73,73,73,73	0
54	MG	1A	3977	1/1	0.87	0.10	59,59,59,59	0
54	MG	2A	3264	1/1	0.87	0.10	73,73,73,73	0
54	MG	2A	3570	1/1	0.87	0.18	57,57,57,57	0
54	MG	2A	3571	1/1	0.87	0.16	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1a	1673	1/1	0.87	0.33	71,71,71,71	0
54	MG	1a	1676	1/1	0.87	0.19	75,75,75,75	0
54	MG	1a	1790	1/1	0.87	0.14	73,73,73,73	0
54	MG	1a	1678	1/1	0.87	0.20	55,55,55,55	0
54	MG	1F	315	1/1	0.87	0.23	72,72,72,72	0
54	MG	2A	3602	1/1	0.87	0.15	71,71,71,71	0
54	MG	1A	3435	1/1	0.87	0.27	60,60,60,60	0
54	MG	1A	3355	1/1	0.87	0.14	54,54,54,54	0
54	MG	2a	3112	1/1	0.87	0.10	84,84,84,84	0
54	MG	2A	3055	1/1	0.87	0.35	80,80,80,80	0
54	MG	2A	3280	1/1	0.87	0.23	65,65,65,65	0
54	MG	2A	3283	1/1	0.87	0.31	73,73,73,73	0
54	MG	1H	202	1/1	0.87	0.15	58,58,58,58	0
54	MG	2a	3124	1/1	0.87	0.14	74,74,74,74	0
54	MG	2A	3060	1/1	0.87	0.18	67,67,67,67	0
54	MG	2A	3294	1/1	0.87	0.17	65,65,65,65	0
54	MG	2a	3134	1/1	0.87	0.12	92,92,92,92	0
54	MG	2A	3068	1/1	0.87	0.21	70,70,70,70	0
54	MG	1A	3852	1/1	0.87	0.10	49,49,49,49	0
54	MG	1a	1804	1/1	0.87	0.28	77,77,77,77	0
54	MG	2A	3077	1/1	0.87	0.20	74,74,74,74	0
54	MG	2A	3081	1/1	0.87	0.23	68,68,68,68	0
54	MG	2A	3661	1/1	0.87	0.12	48,48,48,48	0
54	MG	1A	3047	1/1	0.87	0.24	61,61,61,61	0
54	MG	2A	3680	1/1	0.87	0.13	81,81,81,81	0
54	MG	1A	3449	1/1	0.87	0.17	44,44,44,44	0
54	MG	1A	3373	1/1	0.87	0.14	63,63,63,63	0
54	MG	1a	1694	1/1	0.87	0.24	62,62,62,62	0
54	MG	1A	3866	1/1	0.87	0.12	64,64,64,64	0
54	MG	2A	3699	1/1	0.87	0.15	71,71,71,71	0
54	MG	2A	3702	1/1	0.87	0.14	68,68,68,68	0
54	MG	1A	4004	1/1	0.87	0.23	52,52,52,52	0
54	MG	1a	1700	1/1	0.87	0.28	62,62,62,62	0
54	MG	1A	3510	1/1	0.87	0.10	31,31,31,31	0
54	MG	2A	3097	1/1	0.87	0.18	77,77,77,77	0
54	MG	1A	3520	1/1	0.87	0.20	60,60,60,60	0
54	MG	2e	202	1/1	0.87	0.17	77,77,77,77	0
54	MG	2A	3718	1/1	0.87	0.22	75,75,75,75	0
54	MG	1A	3590	1/1	0.87	0.14	61,61,61,61	0
54	MG	1a	1710	1/1	0.87	0.12	72,72,72,72	0
54	MG	2A	3723	1/1	0.87	0.16	85,85,85,85	0
57	MPD	1T	206	8/8	0.87	0.24	71,73,77,78	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3387	1/1	0.87	0.16	74,74,74,74	0
54	MG	2A	3111	1/1	0.87	0.20	65,65,65,65	0
54	MG	2A	3391	1/1	0.87	0.17	75,75,75,75	0
54	MG	2A	3395	1/1	0.87	0.18	74,74,74,74	0
54	MG	1a	1729	1/1	0.88	0.16	72,72,72,72	0
54	MG	1A	3952	1/1	0.88	0.12	47,47,47,47	0
54	MG	2A	3161	1/1	0.88	0.15	71,71,71,71	0
54	MG	1a	1732	1/1	0.88	0.12	78,78,78,78	0
54	MG	1A	3201	1/1	0.88	0.25	68,68,68,68	0
54	MG	1a	1632	1/1	0.88	0.16	68,68,68,68	0
54	MG	1A	3722	1/1	0.88	0.23	43,43,43,43	0
54	MG	1A	3133	1/1	0.88	0.19	47,47,47,47	0
54	MG	2A	3173	1/1	0.88	0.30	71,71,71,71	0
54	MG	1A	3588	1/1	0.88	0.16	64,64,64,64	0
54	MG	2A	3470	1/1	0.88	0.13	74,74,74,74	0
54	MG	2A	3177	1/1	0.88	0.13	59,59,59,59	0
54	MG	1a	1872	1/1	0.88	0.11	58,58,58,58	0
54	MG	1A	3349	1/1	0.88	0.17	66,66,66,66	0
54	MG	1a	1876	1/1	0.88	0.15	62,62,62,62	0
54	MG	1a	1746	1/1	0.88	0.21	62,62,62,62	0
54	MG	1a	1643	1/1	0.88	0.16	61,61,61,61	0
54	MG	1A	3518	1/1	0.88	0.13	40,40,40,40	0
54	MG	1A	3737	1/1	0.88	0.19	35,35,35,35	0
54	MG	1a	1753	1/1	0.88	0.15	66,66,66,66	0
54	MG	2A	3194	1/1	0.88	0.48	80,80,80,80	0
54	MG	2A	3494	1/1	0.88	0.13	67,67,67,67	0
54	MG	1a	1650	1/1	0.88	0.28	65,65,65,65	0
54	MG	1D	301	1/1	0.88	0.18	50,50,50,50	0
54	MG	1f	201	1/1	0.88	0.21	78,78,78,78	0
54	MG	1a	1652	1/1	0.88	0.29	74,74,74,74	0
54	MG	1D	311	1/1	0.88	0.38	57,57,57,57	0
54	MG	1D	313	1/1	0.88	0.18	53,53,53,53	0
54	MG	1a	1764	1/1	0.88	0.14	72,72,72,72	0
54	MG	1n	101	1/1	0.88	0.38	76,76,76,76	0
54	MG	1A	3850	1/1	0.88	0.11	60,60,60,60	0
54	MG	1a	1663	1/1	0.88	0.20	75,75,75,75	0
54	MG	1a	1664	1/1	0.88	0.10	76,76,76,76	0
54	MG	2A	3528	1/1	0.88	0.14	66,66,66,66	0
54	MG	2a	3042	1/1	0.88	0.22	65,65,65,65	0
54	MG	2a	3043	1/1	0.88	0.12	85,85,85,85	0
54	MG	2A	3017	1/1	0.88	0.14	65,65,65,65	0
54	MG	2a	3045	1/1	0.88	0.24	73,73,73,73	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1F	311	1/1	0.88	0.23	61,61,61,61	0
54	MG	1F	312	1/1	0.88	0.17	45,45,45,45	0
54	MG	2A	3247	1/1	0.88	0.45	81,81,81,81	0
54	MG	1A	3739	1/1	0.88	0.20	59,59,59,59	0
54	MG	2A	3250	1/1	0.88	0.14	67,67,67,67	0
54	MG	2A	3251	1/1	0.88	0.18	51,51,51,51	0
54	MG	1A	3982	1/1	0.88	0.15	70,70,70,70	0
54	MG	1A	3207	1/1	0.88	0.24	67,67,67,67	0
54	MG	1a	1779	1/1	0.88	0.15	79,79,79,79	0
54	MG	1A	3293	1/1	0.88	0.10	74,74,74,74	0
54	MG	2A	3267	1/1	0.88	0.30	64,64,64,64	0
54	MG	2A	3039	1/1	0.88	0.27	77,77,77,77	0
54	MG	2A	3040	1/1	0.88	0.16	59,59,59,59	0
54	MG	2a	3068	1/1	0.88	0.20	78,78,78,78	0
54	MG	1A	3760	1/1	0.88	0.11	53,53,53,53	0
54	MG	1A	3524	1/1	0.88	0.10	46,46,46,46	0
54	MG	2A	3575	1/1	0.88	0.16	64,64,64,64	0
54	MG	2A	3274	1/1	0.88	0.20	60,60,60,60	0
54	MG	1a	1784	1/1	0.88	0.09	83,83,83,83	0
54	MG	2A	3049	1/1	0.88	0.38	82,82,82,82	0
54	MG	2A	3051	1/1	0.88	0.15	55,55,55,55	0
54	MG	2A	3604	1/1	0.88	0.13	51,51,51,51	0
54	MG	1A	3869	1/1	0.88	0.15	55,55,55,55	0
54	MG	2A	3282	1/1	0.88	0.39	73,73,73,73	0
54	MG	2A	3616	1/1	0.88	0.13	40,40,40,40	0
54	MG	1A	3022	1/1	0.88	0.12	47,47,47,47	0
54	MG	1A	3872	1/1	0.88	0.12	69,69,69,69	0
54	MG	2A	3285	1/1	0.88	0.20	61,61,61,61	0
54	MG	2a	3103	1/1	0.88	0.22	65,65,65,65	0
54	MG	1P	205	1/1	0.88	0.28	61,61,61,61	0
54	MG	1a	1684	1/1	0.88	0.26	70,70,70,70	0
54	MG	1a	1685	1/1	0.88	0.37	78,78,78,78	0
54	MG	2a	3109	1/1	0.88	0.33	57,57,57,57	0
54	MG	1A	3536	1/1	0.88	0.09	32,32,32,32	0
54	MG	2A	3633	1/1	0.88	0.18	70,70,70,70	0
54	MG	2a	3113	1/1	0.88	0.28	58,58,58,58	0
54	MG	2a	3114	1/1	0.88	0.37	72,72,72,72	0
54	MG	1a	1688	1/1	0.88	0.10	53,53,53,53	0
54	MG	1A	3188	1/1	0.88	0.16	63,63,63,63	0
54	MG	1A	3780	1/1	0.88	0.18	72,72,72,72	0
54	MG	1A	3115	1/1	0.88	0.11	55,55,55,55	0
54	MG	2A	3322	1/1	0.88	0.14	78,78,78,78	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2a	3127	1/1	0.88	0.23	79,79,79,79	0
54	MG	1A	3792	1/1	0.88	0.09	36,36,36,36	0
54	MG	1A	3797	1/1	0.88	0.10	46,46,46,46	0
54	MG	2A	3350	1/1	0.88	0.11	45,45,45,45	0
54	MG	1A	4018	1/1	0.88	0.15	48,48,48,48	0
54	MG	1a	1699	1/1	0.88	0.24	57,57,57,57	0
54	MG	1A	3027	1/1	0.88	0.26	72,72,72,72	0
54	MG	1A	3388	1/1	0.88	0.11	27,27,27,27	0
54	MG	1A	3905	1/1	0.88	0.12	55,55,55,55	0
54	MG	2a	3141	1/1	0.88	0.21	70,70,70,70	0
54	MG	1a	1706	1/1	0.88	0.35	71,71,71,71	0
54	MG	2a	3144	1/1	0.88	0.12	67,67,67,67	0
54	MG	1A	4031	1/1	0.88	0.10	60,60,60,60	0
54	MG	2A	3098	1/1	0.88	0.12	73,73,73,73	0
54	MG	1a	1826	1/1	0.88	0.11	76,76,76,76	0
54	MG	2a	3166	1/1	0.88	0.14	77,77,77,77	0
54	MG	1A	3617	1/1	0.88	0.13	61,61,61,61	0
54	MG	2A	3716	1/1	0.88	0.17	81,81,81,81	0
54	MG	1a	1602	1/1	0.88	0.21	77,77,77,77	0
54	MG	1A	3315	1/1	0.88	0.19	38,38,38,38	0
54	MG	1a	1609	1/1	0.88	0.32	62,62,62,62	0
54	MG	2a	3177	1/1	0.88	0.18	67,67,67,67	0
54	MG	1A	3199	1/1	0.88	0.11	55,55,55,55	0
54	MG	2A	3116	1/1	0.88	0.22	56,56,56,56	0
54	MG	2A	3408	1/1	0.88	0.14	57,57,57,57	0
54	MG	2a	3186	1/1	0.88	0.16	75,75,75,75	0
54	MG	1A	3128	1/1	0.88	0.31	60,60,60,60	0
54	MG	2A	3121	1/1	0.88	0.15	74,74,74,74	0
54	MG	2A	3124	1/1	0.88	0.12	46,46,46,46	0
54	MG	2A	3426	1/1	0.88	0.14	58,58,58,58	0
54	MG	1A	3407	1/1	0.88	0.17	67,67,67,67	0
54	MG	2A	3126	1/1	0.88	0.14	72,72,72,72	0
54	MG	2A	3432	1/1	0.88	0.23	54,54,54,54	0
54	MG	2A	3129	1/1	0.88	0.13	67,67,67,67	0
54	MG	1A	3266	1/1	0.88	0.10	74,74,74,74	0
54	MG	2A	3138	1/1	0.88	0.17	66,66,66,66	0
54	MG	1a	1723	1/1	0.88	0.14	58,58,58,58	0
54	MG	1a	1727	1/1	0.88	0.11	64,64,64,64	0
54	MG	1B	225	1/1	0.89	0.11	52,52,52,52	0
54	MG	2A	3512	1/1	0.89	0.10	60,60,60,60	0
54	MG	2A	3513	1/1	0.89	0.15	65,65,65,65	0
54	MG	1a	1639	1/1	0.89	0.24	74,74,74,74	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3576	1/1	0.89	0.10	44,44,44,44	0
54	MG	1B	228	1/1	0.89	0.11	76,76,76,76	0
54	MG	2A	3523	1/1	0.89	0.19	71,71,71,71	0
54	MG	1A	3301	1/1	0.89	0.13	66,66,66,66	0
54	MG	1A	3651	1/1	0.89	0.17	69,69,69,69	0
54	MG	1A	3390	1/1	0.89	0.22	78,78,78,78	0
54	MG	1A	3344	1/1	0.89	0.15	59,59,59,59	0
54	MG	1D	316	1/1	0.89	0.16	70,70,70,70	0
54	MG	2A	3533	1/1	0.89	0.10	73,73,73,73	0
54	MG	1a	1747	1/1	0.89	0.31	75,75,75,75	0
54	MG	1a	1748	1/1	0.89	0.19	66,66,66,66	0
54	MG	1A	3657	1/1	0.89	0.11	48,48,48,48	0
54	MG	1A	3248	1/1	0.89	0.11	73,73,73,73	0
54	MG	2a	3031	1/1	0.89	0.17	75,75,75,75	0
54	MG	2A	3115	1/1	0.89	0.24	65,65,65,65	0
54	MG	1A	3352	1/1	0.89	0.14	58,58,58,58	0
54	MG	1a	1657	1/1	0.89	0.13	77,77,77,77	0
54	MG	1A	3663	1/1	0.89	0.21	34,34,34,34	0
54	MG	2A	3551	1/1	0.89	0.09	59,59,59,59	0
54	MG	1A	3854	1/1	0.89	0.11	35,35,35,35	0
54	MG	1A	3744	1/1	0.89	0.13	58,58,58,58	0
54	MG	2A	3309	1/1	0.89	0.13	70,70,70,70	0
54	MG	1F	317	1/1	0.89	0.15	75,75,75,75	0
54	MG	1A	3596	1/1	0.89	0.23	64,64,64,64	0
54	MG	1a	1762	1/1	0.89	0.22	72,72,72,72	0
54	MG	1a	1763	1/1	0.89	0.30	76,76,76,76	0
54	MG	2a	3047	1/1	0.89	0.34	72,72,72,72	0
54	MG	1A	3527	1/1	0.89	0.11	54,54,54,54	0
54	MG	2A	3141	1/1	0.89	0.14	54,54,54,54	0
54	MG	2A	3580	1/1	0.89	0.13	68,68,68,68	0
54	MG	2A	3583	1/1	0.89	0.13	75,75,75,75	0
54	MG	2A	3339	1/1	0.89	0.10	52,52,52,52	0
54	MG	2a	3055	1/1	0.89	0.13	76,76,76,76	0
54	MG	1A	3867	1/1	0.89	0.11	41,41,41,41	0
54	MG	2a	3058	1/1	0.89	0.23	79,79,79,79	0
54	MG	2A	3351	1/1	0.89	0.10	54,54,54,54	0
54	MG	1e	202	1/1	0.89	0.12	62,62,62,62	0
54	MG	2A	3144	1/1	0.89	0.16	60,60,60,60	0
54	MG	2A	3154	1/1	0.89	0.28	64,64,64,64	0
54	MG	2A	3155	1/1	0.89	0.17	70,70,70,70	0
54	MG	1A	3762	1/1	0.89	0.10	62,62,62,62	0
54	MG	2A	3373	1/1	0.89	0.14	59,59,59,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	4005	1/1	0.89	0.15	47,47,47,47	0
54	MG	1A	3250	1/1	0.89	0.33	66,66,66,66	0
54	MG	1A	3280	1/1	0.89	0.24	48,48,48,48	0
54	MG	1A	3430	1/1	0.89	0.15	61,61,61,61	0
54	MG	2a	3083	1/1	0.89	0.33	77,77,77,77	0
54	MG	1A	3673	1/1	0.89	0.14	62,62,62,62	0
54	MG	1T	203	1/1	0.89	0.20	65,65,65,65	0
54	MG	2A	3171	1/1	0.89	0.15	56,56,56,56	0
54	MG	1A	4014	1/1	0.89	0.10	93,93,93,93	0
54	MG	2a	3090	1/1	0.89	0.17	70,70,70,70	0
54	MG	1V	205	1/1	0.89	0.17	72,72,72,72	0
54	MG	2A	3638	1/1	0.89	0.12	70,70,70,70	0
54	MG	1A	3882	1/1	0.89	0.27	43,43,43,43	0
54	MG	2A	3407	1/1	0.89	0.12	68,68,68,68	0
54	MG	2A	3016	1/1	0.89	0.30	77,77,77,77	0
54	MG	2A	3678	1/1	0.89	0.13	73,73,73,73	0
54	MG	1A	3192	1/1	0.89	0.11	53,53,53,53	0
54	MG	2a	3104	1/1	0.89	0.32	71,71,71,71	0
54	MG	2A	3683	1/1	0.89	0.11	50,50,50,50	0
54	MG	1A	3544	1/1	0.89	0.07	28,28,28,28	0
54	MG	1A	3790	1/1	0.89	0.27	73,73,73,73	0
54	MG	2A	3690	1/1	0.89	0.09	57,57,57,57	0
54	MG	11	102	1/1	0.89	0.13	62,62,62,62	0
54	MG	1A	3486	1/1	0.89	0.21	73,73,73,73	0
54	MG	14	101	1/1	0.89	0.08	82,82,82,82	0
54	MG	2A	3190	1/1	0.89	0.20	55,55,55,55	0
54	MG	2A	3191	1/1	0.89	0.31	76,76,76,76	0
54	MG	1A	3375	1/1	0.89	0.15	63,63,63,63	0
54	MG	1A	3198	1/1	0.89	0.12	55,55,55,55	0
54	MG	1A	3904	1/1	0.89	0.10	52,52,52,52	0
54	MG	2A	3709	1/1	0.89	0.14	65,65,65,65	0
54	MG	2A	3198	1/1	0.89	0.41	75,75,75,75	0
54	MG	2A	3200	1/1	0.89	0.26	76,76,76,76	0
54	MG	2a	3130	1/1	0.89	0.12	64,64,64,64	0
54	MG	2A	3448	1/1	0.89	0.20	72,72,72,72	0
54	MG	2A	3720	1/1	0.89	0.14	73,73,73,73	0
54	MG	1A	3616	1/1	0.89	0.11	57,57,57,57	0
54	MG	1A	3696	1/1	0.89	0.10	51,51,51,51	0
54	MG	2A	3458	1/1	0.89	0.11	69,69,69,69	0
54	MG	1a	1603	1/1	0.89	0.15	75,75,75,75	0
54	MG	1A	3499	1/1	0.89	0.09	27,27,27,27	0
54	MG	1A	3699	1/1	0.89	0.10	71,71,71,71	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3067	1/1	0.89	0.13	57,57,57,57	0
54	MG	2B	201	1/1	0.89	0.10	86,86,86,86	0
54	MG	1A	3206	1/1	0.89	0.08	50,50,50,50	0
54	MG	2B	203	1/1	0.89	0.21	79,79,79,79	0
54	MG	1a	1812	1/1	0.89	0.08	78,78,78,78	0
54	MG	2a	3165	1/1	0.89	0.27	79,79,79,79	0
54	MG	1B	207	1/1	0.89	0.43	73,73,73,73	0
54	MG	2A	3226	1/1	0.89	0.26	58,58,58,58	0
54	MG	2A	3229	1/1	0.89	0.11	77,77,77,77	0
54	MG	2A	3476	1/1	0.89	0.12	69,69,69,69	0
54	MG	1a	1714	1/1	0.89	0.16	68,68,68,68	0
54	MG	2a	3172	1/1	0.89	0.10	76,76,76,76	0
54	MG	1A	3624	1/1	0.89	0.09	45,45,45,45	0
54	MG	1A	3821	1/1	0.89	0.12	65,65,65,65	0
54	MG	2A	3066	1/1	0.89	0.07	66,66,66,66	0
54	MG	1a	1625	1/1	0.89	0.12	64,64,64,64	0
54	MG	2D	312	1/1	0.89	0.14	73,73,73,73	0
54	MG	1a	1628	1/1	0.89	0.33	70,70,70,70	0
54	MG	1A	3822	1/1	0.89	0.13	56,56,56,56	0
54	MG	2a	3190	1/1	0.89	0.16	68,68,68,68	0
54	MG	1a	1828	1/1	0.89	0.18	56,56,56,56	0
54	MG	1A	3563	1/1	0.89	0.36	41,41,41,41	0
54	MG	1A	3955	1/1	0.89	0.10	62,62,62,62	0
54	MG	2A	3263	1/1	0.89	0.40	69,69,69,69	0
54	MG	1a	1636	1/1	0.89	0.31	66,66,66,66	0
54	MG	2P	201	1/1	0.89	0.12	71,71,71,71	0
54	MG	2A	3265	1/1	0.89	0.14	74,74,74,74	0
54	MG	2V	202	1/1	0.89	0.24	65,65,65,65	0
54	MG	1a	1837	1/1	0.89	0.23	72,72,72,72	0
54	MG	25	101	1/1	0.89	0.50	57,57,57,57	0
54	MG	25	103	1/1	0.89	0.14	74,74,74,74	0
54	MG	1h	201	1/1	0.90	0.18	59,59,59,59	0
54	MG	2A	3449	1/1	0.90	0.28	47,47,47,47	0
54	MG	1A	3525	1/1	0.90	0.12	61,61,61,61	0
54	MG	1l	201	1/1	0.90	0.30	71,71,71,71	0
54	MG	2A	3187	1/1	0.90	0.22	78,78,78,78	0
54	MG	1B	224	1/1	0.90	0.19	74,74,74,74	0
54	MG	1A	3302	1/1	0.90	0.17	50,50,50,50	0
54	MG	1a	1644	1/1	0.90	0.25	59,59,59,59	0
54	MG	1A	3685	1/1	0.90	0.08	24,24,24,24	0
54	MG	2A	3193	1/1	0.90	0.20	67,67,67,67	0
54	MG	1y	203	1/1	0.90	0.13	90,90,90,90	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1B	227	1/1	0.90	0.19	76,76,76,76	0
54	MG	1A	3808	1/1	0.90	0.10	64,64,64,64	0
54	MG	2T	203	1/1	0.90	0.18	63,63,63,63	0
54	MG	1A	3105	1/1	0.90	0.11	63,63,63,63	0
54	MG	1A	3533	1/1	0.90	0.12	63,63,63,63	0
54	MG	20	101	1/1	0.90	0.12	59,59,59,59	0
54	MG	1A	3110	1/1	0.90	0.15	52,52,52,52	0
54	MG	1A	3211	1/1	0.90	0.27	70,70,70,70	0
54	MG	1D	315	1/1	0.90	0.10	68,68,68,68	0
54	MG	1a	1659	1/1	0.90	0.33	79,79,79,79	0
54	MG	2A	3032	1/1	0.90	0.31	68,68,68,68	0
54	MG	2A	3212	1/1	0.90	0.13	62,62,62,62	0
54	MG	1A	3316	1/1	0.90	0.15	54,54,54,54	0
54	MG	1A	3968	1/1	0.90	0.09	61,61,61,61	0
54	MG	1E	301	1/1	0.90	0.34	52,52,52,52	0
54	MG	2A	3224	1/1	0.90	0.21	66,66,66,66	0
54	MG	2A	3225	1/1	0.90	0.47	57,57,57,57	0
54	MG	1E	303	1/1	0.90	0.30	57,57,57,57	0
54	MG	1A	3277	1/1	0.90	0.14	73,73,73,73	0
54	MG	2A	3505	1/1	0.90	0.10	78,78,78,78	0
54	MG	2A	3041	1/1	0.90	0.14	54,54,54,54	0
54	MG	1A	3620	1/1	0.90	0.10	58,58,58,58	0
54	MG	1A	3823	1/1	0.90	0.26	46,46,46,46	0
54	MG	2A	3234	1/1	0.90	0.14	70,70,70,70	0
54	MG	2A	3235	1/1	0.90	0.15	75,75,75,75	0
54	MG	2A	3518	1/1	0.90	0.14	71,71,71,71	0
54	MG	2a	3029	1/1	0.90	0.20	76,76,76,76	0
54	MG	2a	3030	1/1	0.90	0.19	69,69,69,69	0
54	MG	2A	3519	1/1	0.90	0.11	85,85,85,85	0
54	MG	1A	3322	1/1	0.90	0.31	48,48,48,48	0
54	MG	2a	3033	1/1	0.90	0.28	70,70,70,70	0
54	MG	2A	3239	1/1	0.90	0.35	65,65,65,65	0
54	MG	1A	3980	1/1	0.90	0.17	52,52,52,52	0
54	MG	1A	3031	1/1	0.90	0.08	25,25,25,25	0
54	MG	1a	1677	1/1	0.90	0.16	67,67,67,67	0
54	MG	1A	3327	1/1	0.90	0.14	70,70,70,70	0
54	MG	1A	3984	1/1	0.90	0.12	46,46,46,46	0
54	MG	1A	3630	1/1	0.90	0.09	70,70,70,70	0
54	MG	2A	3056	1/1	0.90	0.22	63,63,63,63	0
54	MG	2A	3534	1/1	0.90	0.12	63,63,63,63	0
54	MG	1A	3843	1/1	0.90	0.09	20,20,20,20	0
54	MG	1A	3152	1/1	0.90	0.15	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3061	1/1	0.90	0.17	76,76,76,76	0
54	MG	2A	3063	1/1	0.90	0.23	61,61,61,61	0
54	MG	2A	3065	1/1	0.90	0.09	51,51,51,51	0
54	MG	1A	3720	1/1	0.90	0.13	56,56,56,56	0
54	MG	1A	3998	1/1	0.90	0.13	55,55,55,55	0
54	MG	1A	3721	1/1	0.90	0.35	49,49,49,49	0
54	MG	1A	3637	1/1	0.90	0.21	42,42,42,42	0
54	MG	1A	3483	1/1	0.90	0.14	48,48,48,48	0
54	MG	1A	3061	1/1	0.90	0.14	56,56,56,56	0
54	MG	1V	204	1/1	0.90	0.13	65,65,65,65	0
54	MG	2A	3085	1/1	0.90	0.46	58,58,58,58	0
54	MG	1A	3644	1/1	0.90	0.11	29,29,29,29	0
54	MG	2a	3062	1/1	0.90	0.15	81,81,81,81	0
54	MG	2a	3063	1/1	0.90	0.24	75,75,75,75	0
54	MG	1A	3732	1/1	0.90	0.13	69,69,69,69	0
54	MG	1A	3647	1/1	0.90	0.12	39,39,39,39	0
54	MG	10	102	1/1	0.90	0.22	46,46,46,46	0
54	MG	2A	3577	1/1	0.90	0.13	64,64,64,64	0
54	MG	1A	3648	1/1	0.90	0.14	69,69,69,69	0
54	MG	1A	3405	1/1	0.90	0.17	58,58,58,58	0
54	MG	2a	3077	1/1	0.90	0.17	66,66,66,66	0
54	MG	1a	1825	1/1	0.90	0.12	79,79,79,79	0
54	MG	1A	3489	1/1	0.90	0.14	64,64,64,64	0
54	MG	2A	3590	1/1	0.90	0.15	58,58,58,58	0
54	MG	2A	3592	1/1	0.90	0.10	56,56,56,56	0
54	MG	1a	1705	1/1	0.90	0.26	62,62,62,62	0
54	MG	2A	3599	1/1	0.90	0.12	75,75,75,75	0
54	MG	2A	3300	1/1	0.90	0.18	67,67,67,67	0
54	MG	1A	3290	1/1	0.90	0.33	51,51,51,51	0
54	MG	2A	3103	1/1	0.90	0.23	64,64,64,64	0
54	MG	2a	3095	1/1	0.90	0.27	79,79,79,79	0
54	MG	2A	3610	1/1	0.90	0.16	49,49,49,49	0
54	MG	2A	3319	1/1	0.90	0.09	44,44,44,44	0
54	MG	11	105	1/1	0.90	0.10	47,47,47,47	0
54	MG	1A	3340	1/1	0.90	0.10	46,46,46,46	0
54	MG	1a	1711	1/1	0.90	0.20	69,69,69,69	0
54	MG	15	103	1/1	0.90	0.26	46,46,46,46	0
54	MG	2A	3326	1/1	0.90	0.26	76,76,76,76	0
54	MG	2A	3624	1/1	0.90	0.15	61,61,61,61	0
54	MG	2A	3328	1/1	0.90	0.25	72,72,72,72	0
54	MG	2A	3332	1/1	0.90	0.15	76,76,76,76	0
54	MG	1A	3658	1/1	0.90	0.18	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3114	1/1	0.90	0.31	70,70,70,70	0
54	MG	2A	3341	1/1	0.90	0.09	45,45,45,45	0
54	MG	2A	3349	1/1	0.90	0.15	67,67,67,67	0
54	MG	17	106	1/1	0.90	0.16	62,62,62,62	0
54	MG	1a	1843	1/1	0.90	0.08	77,77,77,77	0
54	MG	1a	1849	1/1	0.90	0.12	63,63,63,63	0
54	MG	2A	3656	1/1	0.90	0.10	62,62,62,62	0
54	MG	1A	3502	1/1	0.90	0.11	42,42,42,42	0
54	MG	2A	3666	1/1	0.90	0.16	57,57,57,57	0
54	MG	2a	3126	1/1	0.90	0.27	78,78,78,78	0
54	MG	2A	3671	1/1	0.90	0.14	60,60,60,60	0
54	MG	2a	3128	1/1	0.90	0.21	73,73,73,73	0
54	MG	1A	4029	1/1	0.90	0.23	59,59,59,59	0
54	MG	19	102	1/1	0.90	0.14	61,61,61,61	0
54	MG	2A	3679	1/1	0.90	0.16	63,63,63,63	0
54	MG	1A	3160	1/1	0.90	0.69	51,51,51,51	0
54	MG	1A	3886	1/1	0.90	0.14	52,52,52,52	0
54	MG	1A	3768	1/1	0.90	0.23	69,69,69,69	0
54	MG	2A	3375	1/1	0.90	0.30	73,73,73,73	0
54	MG	2A	3376	1/1	0.90	0.12	70,70,70,70	0
54	MG	1A	3889	1/1	0.90	0.10	47,47,47,47	0
54	MG	2A	3694	1/1	0.90	0.15	56,56,56,56	0
54	MG	2A	3696	1/1	0.90	0.08	55,55,55,55	0
54	MG	1a	1607	1/1	0.90	0.18	69,69,69,69	0
54	MG	2a	3145	1/1	0.90	0.20	72,72,72,72	0
54	MG	1A	3506	1/1	0.90	0.12	52,52,52,52	0
54	MG	1A	3664	1/1	0.90	0.15	55,55,55,55	0
54	MG	1A	3036	1/1	0.90	0.10	41,41,41,41	0
54	MG	2a	3156	1/1	0.90	0.23	72,72,72,72	0
54	MG	2a	3160	1/1	0.90	0.19	79,79,79,79	0
54	MG	1a	1735	1/1	0.90	0.13	70,70,70,70	0
54	MG	1B	201	1/1	0.90	0.20	64,64,64,64	0
54	MG	2A	3399	1/1	0.90	0.12	45,45,45,45	0
54	MG	2a	3168	1/1	0.90	0.20	75,75,75,75	0
54	MG	1B	203	1/1	0.90	0.38	77,77,77,77	0
54	MG	2A	3404	1/1	0.90	0.14	54,54,54,54	0
54	MG	2A	3405	1/1	0.90	0.12	57,57,57,57	0
54	MG	1a	1620	1/1	0.90	0.19	71,71,71,71	0
54	MG	1A	3595	1/1	0.90	0.12	48,48,48,48	0
54	MG	2a	3176	1/1	0.90	0.14	72,72,72,72	0
54	MG	1A	3783	1/1	0.90	0.13	66,66,66,66	0
54	MG	1a	1879	1/1	0.90	0.20	75,75,75,75	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3414	1/1	0.90	0.23	66,66,66,66	0
54	MG	1A	3350	1/1	0.90	0.12	63,63,63,63	0
54	MG	1B	209	1/1	0.90	0.11	58,58,58,58	0
54	MG	2A	3727	1/1	0.90	0.13	74,74,74,74	0
54	MG	2A	3167	1/1	0.90	0.24	61,61,61,61	0
54	MG	2A	3169	1/1	0.90	0.15	67,67,67,67	0
54	MG	2A	3428	1/1	0.90	0.23	67,67,67,67	0
54	MG	1d	302	1/1	0.90	0.36	82,82,82,82	0
54	MG	1A	3785	1/1	0.90	0.17	52,52,52,52	0
54	MG	2r	101	1/1	0.90	0.22	80,80,80,80	0
54	MG	1B	211	1/1	0.90	0.29	71,71,71,71	0
54	MG	1A	3032	1/1	0.90	0.15	65,65,65,65	0
54	MG	1A	3130	1/1	0.90	0.16	64,64,64,64	0
54	MG	1A	3450	1/1	0.90	0.09	27,27,27,27	0
54	MG	2B	212	1/1	0.90	0.09	95,95,95,95	0
54	MG	1f	202	1/1	0.90	0.13	55,55,55,55	0
54	MG	1a	1754	1/1	0.90	0.16	77,77,77,77	0
59	ZN	24	501	1/1	0.90	0.09	140,140,140,140	0
54	MG	2A	3520	1/1	0.91	0.16	76,76,76,76	0
54	MG	2A	3110	1/1	0.91	0.12	69,69,69,69	0
54	MG	1A	3222	1/1	0.91	0.20	55,55,55,55	0
54	MG	1A	3945	1/1	0.91	0.10	62,62,62,62	0
54	MG	1A	3571	1/1	0.91	0.12	52,52,52,52	0
54	MG	1a	1739	1/1	0.91	0.16	72,72,72,72	0
54	MG	1a	1740	1/1	0.91	0.21	60,60,60,60	0
54	MG	1a	1871	1/1	0.91	0.27	70,70,70,70	0
54	MG	2A	3289	1/1	0.91	0.20	68,68,68,68	0
54	MG	2A	3531	1/1	0.91	0.34	57,57,57,57	0
54	MG	2A	3532	1/1	0.91	0.12	62,62,62,62	0
54	MG	1A	3385	1/1	0.91	0.12	50,50,50,50	0
54	MG	2A	3120	1/1	0.91	0.20	52,52,52,52	0
54	MG	1A	3706	1/1	0.91	0.10	80,80,80,80	0
54	MG	1a	1875	1/1	0.91	0.32	70,70,70,70	0
54	MG	1A	3709	1/1	0.91	0.09	35,35,35,35	0
54	MG	2A	3308	1/1	0.91	0.19	68,68,68,68	0
54	MG	1A	3819	1/1	0.91	0.10	49,49,49,49	0
54	MG	2A	3540	1/1	0.91	0.26	65,65,65,65	0
54	MG	1a	1640	1/1	0.91	0.21	78,78,78,78	0
54	MG	1A	3712	1/1	0.91	0.11	67,67,67,67	0
54	MG	2a	3025	1/1	0.91	0.27	70,70,70,70	0
54	MG	2A	3544	1/1	0.91	0.11	60,60,60,60	0
54	MG	2A	3132	1/1	0.91	0.14	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3550	1/1	0.91	0.14	65,65,65,65	0
54	MG	2A	3133	1/1	0.91	0.37	72,72,72,72	0
54	MG	1A	3515	1/1	0.91	0.08	74,74,74,74	0
54	MG	2A	3557	1/1	0.91	0.26	59,59,59,59	0
54	MG	2A	3559	1/1	0.91	0.09	64,64,64,64	0
54	MG	1A	3966	1/1	0.91	0.23	33,33,33,33	0
54	MG	1A	3141	1/1	0.91	0.10	57,57,57,57	0
54	MG	1A	3587	1/1	0.91	0.12	61,61,61,61	0
54	MG	1d	304	1/1	0.91	0.28	71,71,71,71	0
54	MG	1A	3827	1/1	0.91	0.27	52,52,52,52	0
54	MG	1A	3049	1/1	0.91	0.28	57,57,57,57	0
54	MG	1E	305	1/1	0.91	0.12	31,31,31,31	0
54	MG	1A	3650	1/1	0.91	0.11	31,31,31,31	0
54	MG	1A	3461	1/1	0.91	0.08	66,66,66,66	0
54	MG	1A	3836	1/1	0.91	0.09	65,65,65,65	0
54	MG	2A	3581	1/1	0.91	0.12	70,70,70,70	0
54	MG	1A	3837	1/1	0.91	0.11	72,72,72,72	0
54	MG	2A	3584	1/1	0.91	0.09	54,54,54,54	0
54	MG	1a	1658	1/1	0.91	0.21	52,52,52,52	0
54	MG	2A	3587	1/1	0.91	0.16	61,61,61,61	0
54	MG	1A	3838	1/1	0.91	0.07	33,33,33,33	0
54	MG	2A	3363	1/1	0.91	0.15	84,84,84,84	0
54	MG	1A	3343	1/1	0.91	0.23	65,65,65,65	0
54	MG	1G	203	1/1	0.91	0.10	57,57,57,57	0
54	MG	2A	3369	1/1	0.91	0.13	51,51,51,51	0
54	MG	1A	3591	1/1	0.91	0.15	53,53,53,53	0
54	MG	1t	201	1/1	0.91	0.10	66,66,66,66	0
54	MG	2A	3172	1/1	0.91	0.15	66,66,66,66	0
54	MG	1A	3593	1/1	0.91	0.16	57,57,57,57	0
54	MG	1A	3311	1/1	0.91	0.27	74,74,74,74	0
54	MG	1A	3995	1/1	0.91	0.11	65,65,65,65	0
54	MG	2a	3065	1/1	0.91	0.30	80,80,80,80	0
54	MG	2A	3178	1/1	0.91	0.11	71,71,71,71	0
54	MG	2A	3005	1/1	0.91	0.10	63,63,63,63	0
54	MG	1A	3470	1/1	0.91	0.21	77,77,77,77	0
54	MG	2a	3070	1/1	0.91	0.08	72,72,72,72	0
54	MG	1a	1776	1/1	0.91	0.16	79,79,79,79	0
54	MG	2A	3625	1/1	0.91	0.10	69,69,69,69	0
54	MG	1A	3738	1/1	0.91	0.11	47,47,47,47	0
54	MG	2A	3627	1/1	0.91	0.14	72,72,72,72	0
54	MG	2A	3628	1/1	0.91	0.09	63,63,63,63	0
54	MG	2A	3396	1/1	0.91	0.11	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1a	1670	1/1	0.91	0.13	66,66,66,66	0
54	MG	2A	3632	1/1	0.91	0.14	64,64,64,64	0
54	MG	2A	3400	1/1	0.91	0.14	60,60,60,60	0
54	MG	1A	3598	1/1	0.91	0.17	71,71,71,71	0
54	MG	2A	3186	1/1	0.91	0.20	70,70,70,70	0
54	MG	2a	3091	1/1	0.91	0.15	70,70,70,70	0
54	MG	2A	3023	1/1	0.91	0.20	74,74,74,74	0
54	MG	1R	202	1/1	0.91	0.15	48,48,48,48	0
54	MG	2A	3639	1/1	0.91	0.12	62,62,62,62	0
54	MG	1A	3231	1/1	0.91	0.22	47,47,47,47	0
54	MG	1A	3529	1/1	0.91	0.09	52,52,52,52	0
54	MG	2A	3657	1/1	0.91	0.12	61,61,61,61	0
54	MG	1A	3531	1/1	0.91	0.17	73,73,73,73	0
54	MG	1A	3759	1/1	0.91	0.09	51,51,51,51	0
54	MG	1A	3314	1/1	0.91	0.17	65,65,65,65	0
54	MG	1A	3004	1/1	0.91	0.11	52,52,52,52	0
54	MG	1A	3766	1/1	0.91	0.15	57,57,57,57	0
54	MG	2a	3107	1/1	0.91	0.41	66,66,66,66	0
54	MG	1A	3537	1/1	0.91	0.07	23,23,23,23	0
54	MG	1A	3208	1/1	0.91	0.08	55,55,55,55	0
54	MG	2A	3044	1/1	0.91	0.11	62,62,62,62	0
54	MG	2a	3111	1/1	0.91	0.43	74,74,74,74	0
54	MG	1A	3611	1/1	0.91	0.11	60,60,60,60	0
54	MG	2A	3433	1/1	0.91	0.12	63,63,63,63	0
54	MG	1A	4019	1/1	0.91	0.10	57,57,57,57	0
54	MG	2A	3209	1/1	0.91	0.33	60,60,60,60	0
54	MG	2a	3117	1/1	0.91	0.14	76,76,76,76	0
54	MG	10	108	1/1	0.91	0.14	69,69,69,69	0
54	MG	2A	3695	1/1	0.91	0.16	74,74,74,74	0
54	MG	1A	3879	1/1	0.91	0.10	50,50,50,50	0
54	MG	1A	3249	1/1	0.91	0.23	70,70,70,70	0
54	MG	1A	3885	1/1	0.91	0.09	41,41,41,41	0
54	MG	1A	3676	1/1	0.91	0.14	56,56,56,56	0
54	MG	2A	3218	1/1	0.91	0.22	73,73,73,73	0
54	MG	1A	3432	1/1	0.91	0.13	71,71,71,71	0
54	MG	2A	3221	1/1	0.91	0.20	67,67,67,67	0
54	MG	2A	3454	1/1	0.91	0.10	58,58,58,58	0
54	MG	2A	3457	1/1	0.91	0.16	62,62,62,62	0
54	MG	2A	3710	1/1	0.91	0.08	70,70,70,70	0
54	MG	15	105	1/1	0.91	0.22	72,72,72,72	0
54	MG	15	106	1/1	0.91	0.23	38,38,38,38	0
54	MG	2A	3717	1/1	0.91	0.09	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3059	1/1	0.91	0.12	54,54,54,54	0
54	MG	2A	3719	1/1	0.91	0.10	79,79,79,79	0
54	MG	2a	3142	1/1	0.91	0.11	82,82,82,82	0
54	MG	1A	3888	1/1	0.91	0.07	50,50,50,50	0
54	MG	1A	3093	1/1	0.91	0.12	52,52,52,52	0
54	MG	1A	3687	1/1	0.91	0.12	33,33,33,33	0
54	MG	1A	3254	1/1	0.91	0.13	55,55,55,55	0
54	MG	1A	3786	1/1	0.91	0.09	36,36,36,36	0
54	MG	1A	4039	1/1	0.91	0.15	66,66,66,66	0
54	MG	2A	3726	1/1	0.91	0.23	69,69,69,69	0
54	MG	2A	3473	1/1	0.91	0.09	79,79,79,79	0
54	MG	2a	3161	1/1	0.91	0.16	78,78,78,78	0
54	MG	1A	3619	1/1	0.91	0.11	42,42,42,42	0
54	MG	1A	3443	1/1	0.91	0.11	71,71,71,71	0
54	MG	2A	3240	1/1	0.91	0.21	68,68,68,68	0
54	MG	2A	3243	1/1	0.91	0.19	62,62,62,62	0
54	MG	2A	3245	1/1	0.91	0.08	66,66,66,66	0
54	MG	1A	3214	1/1	0.91	0.21	56,56,56,56	0
54	MG	2B	205	1/1	0.91	0.34	71,71,71,71	0
54	MG	2B	207	1/1	0.91	0.24	76,76,76,76	0
54	MG	2A	3078	1/1	0.91	0.09	60,60,60,60	0
54	MG	1A	3799	1/1	0.91	0.14	55,55,55,55	0
54	MG	1A	3447	1/1	0.91	0.11	36,36,36,36	0
54	MG	2A	3487	1/1	0.91	0.17	87,87,87,87	0
54	MG	2A	3489	1/1	0.91	0.22	72,72,72,72	0
54	MG	2a	3183	1/1	0.91	0.11	74,74,74,74	0
54	MG	1A	3448	1/1	0.91	0.14	53,53,53,53	0
54	MG	1A	3909	1/1	0.91	0.17	43,43,43,43	0
54	MG	1a	1613	1/1	0.91	0.23	75,75,75,75	0
54	MG	2B	218	1/1	0.91	0.13	79,79,79,79	0
54	MG	2D	302	1/1	0.91	0.16	57,57,57,57	0
54	MG	1A	3915	1/1	0.91	0.08	57,57,57,57	0
54	MG	1a	1725	1/1	0.91	0.20	53,53,53,53	0
54	MG	1a	1726	1/1	0.91	0.14	86,86,86,86	0
54	MG	1A	3698	1/1	0.91	0.18	39,39,39,39	0
54	MG	1A	3924	1/1	0.91	0.15	35,35,35,35	0
54	MG	2A	3508	1/1	0.91	0.16	72,72,72,72	0
57	MPD	1A	4043	8/8	0.91	0.18	56,63,69,69	0
54	MG	1a	1854	1/1	0.91	0.17	74,74,74,74	0
54	MG	1a	1858	1/1	0.91	0.14	86,86,86,86	0
54	MG	1A	3931	1/1	0.91	0.12	31,31,31,31	0
57	MPD	2A	3734	8/8	0.91	0.23	72,77,82,83	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1a	1731	1/1	0.91	0.14	61,61,61,61	0
54	MG	1A	3220	1/1	0.91	0.38	74,74,74,74	0
54	MG	1a	1627	1/1	0.91	0.40	77,77,77,77	0
54	MG	1A	3174	1/1	0.92	0.16	59,59,59,59	0
54	MG	1A	3076	1/1	0.92	0.08	44,44,44,44	0
54	MG	27	101	1/1	0.92	0.34	62,62,62,62	0
54	MG	2A	3134	1/1	0.92	0.32	66,66,66,66	0
54	MG	2A	3314	1/1	0.92	0.10	68,68,68,68	0
54	MG	2a	3003	1/1	0.92	0.10	71,71,71,71	0
54	MG	1A	3281	1/1	0.92	0.14	64,64,64,64	0
54	MG	1A	3324	1/1	0.92	0.23	65,65,65,65	0
54	MG	1a	1661	1/1	0.92	0.16	65,65,65,65	0
54	MG	1A	3868	1/1	0.92	0.11	43,43,43,43	0
54	MG	1N	204	1/1	0.92	0.13	60,60,60,60	0
54	MG	1g	201	1/1	0.92	0.28	74,74,74,74	0
54	MG	2A	3151	1/1	0.92	0.17	65,65,65,65	0
54	MG	1A	3282	1/1	0.92	0.09	60,60,60,60	0
54	MG	1a	1766	1/1	0.92	0.27	70,70,70,70	0
54	MG	2A	3556	1/1	0.92	0.10	76,76,76,76	0
54	MG	2A	3338	1/1	0.92	0.10	41,41,41,41	0
54	MG	1A	3465	1/1	0.92	0.11	56,56,56,56	0
54	MG	2A	3563	1/1	0.92	0.28	67,67,67,67	0
54	MG	2A	3566	1/1	0.92	0.10	74,74,74,74	0
54	MG	2A	3160	1/1	0.92	0.29	50,50,50,50	0
54	MG	2A	3344	1/1	0.92	0.10	46,46,46,46	0
54	MG	1i	201	1/1	0.92	0.21	76,76,76,76	0
54	MG	1A	3469	1/1	0.92	0.14	48,48,48,48	0
54	MG	1A	3011	1/1	0.92	0.22	70,70,70,70	0
54	MG	1A	3683	1/1	0.92	0.07	33,33,33,33	0
54	MG	1A	3119	1/1	0.92	0.32	47,47,47,47	0
54	MG	1n	102	1/1	0.92	0.10	61,61,61,61	0
54	MG	1A	4007	1/1	0.92	0.13	62,62,62,62	0
54	MG	1a	1671	1/1	0.92	0.30	64,64,64,64	0
54	MG	1a	1672	1/1	0.92	0.30	74,74,74,74	0
54	MG	1a	1778	1/1	0.92	0.09	73,73,73,73	0
54	MG	2A	3370	1/1	0.92	0.12	49,49,49,49	0
54	MG	1A	3686	1/1	0.92	0.13	58,58,58,58	0
54	MG	2A	3006	1/1	0.92	0.10	57,57,57,57	0
54	MG	2A	3176	1/1	0.92	0.19	62,62,62,62	0
54	MG	1A	3399	1/1	0.92	0.10	49,49,49,49	0
54	MG	2A	3012	1/1	0.92	0.12	68,68,68,68	0
54	MG	2A	3384	1/1	0.92	0.12	73,73,73,73	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3012	1/1	0.92	0.13	55,55,55,55	0
54	MG	2A	3603	1/1	0.92	0.09	45,45,45,45	0
54	MG	1A	3404	1/1	0.92	0.09	52,52,52,52	0
54	MG	2A	3018	1/1	0.92	0.41	55,55,55,55	0
54	MG	1A	3255	1/1	0.92	0.24	53,53,53,53	0
54	MG	2a	3054	1/1	0.92	0.34	72,72,72,72	0
54	MG	1W	202	1/1	0.92	0.20	61,61,61,61	0
54	MG	1A	3339	1/1	0.92	0.16	62,62,62,62	0
54	MG	1A	3622	1/1	0.92	0.10	57,57,57,57	0
54	MG	2A	3398	1/1	0.92	0.08	40,40,40,40	0
54	MG	2A	3026	1/1	0.92	0.12	62,62,62,62	0
54	MG	1a	1683	1/1	0.92	0.11	66,66,66,66	0
54	MG	2A	3402	1/1	0.92	0.11	51,51,51,51	0
54	MG	2A	3189	1/1	0.92	0.13	70,70,70,70	0
54	MG	1A	3484	1/1	0.92	0.08	30,30,30,30	0
54	MG	2A	3033	1/1	0.92	0.27	57,57,57,57	0
54	MG	1a	1792	1/1	0.92	0.10	76,76,76,76	0
54	MG	1A	3802	1/1	0.92	0.17	48,48,48,48	0
54	MG	1A	3411	1/1	0.92	0.11	29,29,29,29	0
54	MG	1a	1796	1/1	0.92	0.12	65,65,65,65	0
54	MG	1A	3627	1/1	0.92	0.10	66,66,66,66	0
54	MG	2A	3418	1/1	0.92	0.10	57,57,57,57	0
54	MG	2a	3075	1/1	0.92	0.26	72,72,72,72	0
54	MG	2A	3419	1/1	0.92	0.19	75,75,75,75	0
54	MG	1A	3903	1/1	0.92	0.09	45,45,45,45	0
54	MG	2A	3201	1/1	0.92	0.11	58,58,58,58	0
54	MG	2A	3203	1/1	0.92	0.31	76,76,76,76	0
54	MG	2a	3084	1/1	0.92	0.34	72,72,72,72	0
54	MG	1A	3807	1/1	0.92	0.14	60,60,60,60	0
54	MG	1a	1802	1/1	0.92	0.12	75,75,75,75	0
54	MG	1A	3701	1/1	0.92	0.15	62,62,62,62	0
54	MG	2A	3658	1/1	0.92	0.07	86,86,86,86	0
54	MG	2a	3089	1/1	0.92	0.28	62,62,62,62	0
54	MG	2A	3660	1/1	0.92	0.15	44,44,44,44	0
54	MG	1A	4033	1/1	0.92	0.12	62,62,62,62	0
54	MG	1A	3629	1/1	0.92	0.35	40,40,40,40	0
54	MG	2A	3667	1/1	0.92	0.10	77,77,77,77	0
54	MG	1A	3418	1/1	0.92	0.11	31,31,31,31	0
54	MG	1A	3632	1/1	0.92	0.23	41,41,41,41	0
54	MG	2A	3438	1/1	0.92	0.11	64,64,64,64	0
54	MG	17	105	1/1	0.92	0.18	65,65,65,65	0
54	MG	1A	3910	1/1	0.92	0.23	39,39,39,39	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3634	1/1	0.92	0.28	40,40,40,40	0
54	MG	2A	3443	1/1	0.92	0.27	75,75,75,75	0
54	MG	2A	3445	1/1	0.92	0.14	76,76,76,76	0
54	MG	2A	3217	1/1	0.92	0.13	64,64,64,64	0
54	MG	1A	3918	1/1	0.92	0.10	51,51,51,51	0
54	MG	2A	3692	1/1	0.92	0.10	56,56,56,56	0
54	MG	1A	3922	1/1	0.92	0.10	55,55,55,55	0
54	MG	1a	1823	1/1	0.92	0.13	76,76,76,76	0
54	MG	1A	3295	1/1	0.92	0.11	49,49,49,49	0
54	MG	1A	3257	1/1	0.92	0.31	51,51,51,51	0
54	MG	2A	3455	1/1	0.92	0.14	69,69,69,69	0
54	MG	2A	3701	1/1	0.92	0.11	64,64,64,64	0
54	MG	1A	3930	1/1	0.92	0.09	51,51,51,51	0
54	MG	1A	3575	1/1	0.92	0.27	40,40,40,40	0
54	MG	1A	3297	1/1	0.92	0.12	71,71,71,71	0
54	MG	1A	3300	1/1	0.92	0.20	52,52,52,52	0
54	MG	1a	1832	1/1	0.92	0.13	76,76,76,76	0
54	MG	1a	1834	1/1	0.92	0.16	69,69,69,69	0
54	MG	2a	3125	1/1	0.92	0.16	65,65,65,65	0
54	MG	1B	215	1/1	0.92	0.08	65,65,65,65	0
54	MG	2A	3712	1/1	0.92	0.09	49,49,49,49	0
54	MG	1A	3582	1/1	0.92	0.15	65,65,65,65	0
54	MG	1a	1838	1/1	0.92	0.13	73,73,73,73	0
54	MG	1a	1612	1/1	0.92	0.11	36,36,36,36	0
54	MG	2A	3241	1/1	0.92	0.26	51,51,51,51	0
54	MG	1B	218	1/1	0.92	0.08	46,46,46,46	0
54	MG	1A	3215	1/1	0.92	0.20	46,46,46,46	0
54	MG	1A	3949	1/1	0.92	0.09	59,59,59,59	0
54	MG	1A	3950	1/1	0.92	0.09	65,65,65,65	0
54	MG	2A	3092	1/1	0.92	0.18	61,61,61,61	0
54	MG	2A	3480	1/1	0.92	0.09	68,68,68,68	0
54	MG	1A	3951	1/1	0.92	0.08	70,70,70,70	0
54	MG	2A	3482	1/1	0.92	0.10	61,61,61,61	0
54	MG	2A	3253	1/1	0.92	0.20	65,65,65,65	0
54	MG	2A	3256	1/1	0.92	0.16	56,56,56,56	0
54	MG	2A	3258	1/1	0.92	0.27	50,50,50,50	0
54	MG	2a	3147	1/1	0.92	0.19	81,81,81,81	0
54	MG	1A	3441	1/1	0.92	0.11	33,33,33,33	0
54	MG	2A	3488	1/1	0.92	0.14	68,68,68,68	0
54	MG	1A	3507	1/1	0.92	0.09	33,33,33,33	0
54	MG	1A	3351	1/1	0.92	0.14	38,38,38,38	0
54	MG	2a	3158	1/1	0.92	0.10	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3511	1/1	0.92	0.14	71,71,71,71	0
54	MG	2B	206	1/1	0.92	0.25	73,73,73,73	0
54	MG	1a	1631	1/1	0.92	0.27	71,71,71,71	0
54	MG	1A	3155	1/1	0.92	0.16	57,57,57,57	0
54	MG	1a	1634	1/1	0.92	0.11	56,56,56,56	0
54	MG	1A	3099	1/1	0.92	0.12	59,59,59,59	0
54	MG	1A	3839	1/1	0.92	0.18	37,37,37,37	0
54	MG	1A	3967	1/1	0.92	0.08	34,34,34,34	0
54	MG	1D	314	1/1	0.92	0.26	49,49,49,49	0
54	MG	2B	215	1/1	0.92	0.17	77,77,77,77	0
54	MG	2a	3173	1/1	0.92	0.18	63,63,63,63	0
54	MG	1A	3659	1/1	0.92	0.15	53,53,53,53	0
54	MG	1A	3263	1/1	0.92	0.14	53,53,53,53	0
54	MG	1A	3970	1/1	0.92	0.18	60,60,60,60	0
54	MG	2D	301	1/1	0.92	0.23	53,53,53,53	0
54	MG	1A	3971	1/1	0.92	0.12	73,73,73,73	0
54	MG	2D	307	1/1	0.92	0.28	60,60,60,60	0
54	MG	2D	308	1/1	0.92	0.24	50,50,50,50	0
54	MG	2A	3278	1/1	0.92	0.19	53,53,53,53	0
54	MG	2A	3279	1/1	0.92	0.30	66,66,66,66	0
54	MG	2a	3189	1/1	0.92	0.30	65,65,65,65	0
54	MG	1A	3002	1/1	0.92	0.09	49,49,49,49	0
54	MG	2A	3117	1/1	0.92	0.18	63,63,63,63	0
54	MG	1A	3597	1/1	0.92	0.09	46,46,46,46	0
54	MG	1A	3849	1/1	0.92	0.10	64,64,64,64	0
54	MG	2F	302	1/1	0.92	0.10	55,55,55,55	0
54	MG	1a	1647	1/1	0.92	0.23	63,63,63,63	0
54	MG	1A	3106	1/1	0.92	0.21	37,37,37,37	0
54	MG	1A	3751	1/1	0.92	0.16	65,65,65,65	0
54	MG	2A	3291	1/1	0.92	0.30	78,78,78,78	0
54	MG	2A	3529	1/1	0.92	0.08	46,46,46,46	0
54	MG	1A	3756	1/1	0.92	0.11	66,66,66,66	0
54	MG	2A	3128	1/1	0.92	0.24	46,46,46,46	0
54	MG	1a	1755	1/1	0.92	0.18	65,65,65,65	0
54	MG	2A	3130	1/1	0.92	0.25	61,61,61,61	0
54	MG	21	101	1/1	0.92	0.14	59,59,59,59	0
54	MG	1A	3039	1/1	0.92	0.12	56,56,56,56	0
54	MG	1A	3270	1/1	0.93	0.22	49,49,49,49	0
54	MG	2F	301	1/1	0.93	0.34	48,48,48,48	0
54	MG	11	101	1/1	0.93	0.24	50,50,50,50	0
54	MG	1A	3272	1/1	0.93	0.12	68,68,68,68	0
54	MG	2A	3272	1/1	0.93	0.34	72,72,72,72	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	11	103	1/1	0.93	0.11	58,58,58,58	0
54	MG	2O	201	1/1	0.93	0.14	79,79,79,79	0
54	MG	2A	3517	1/1	0.93	0.07	81,81,81,81	0
54	MG	1a	1708	1/1	0.93	0.14	64,64,64,64	0
54	MG	2R	203	1/1	0.93	0.15	56,56,56,56	0
54	MG	1A	3066	1/1	0.93	0.15	72,72,72,72	0
54	MG	1A	4009	1/1	0.93	0.12	84,84,84,84	0
54	MG	2V	201	1/1	0.93	0.22	59,59,59,59	0
54	MG	1A	3860	1/1	0.93	0.24	60,60,60,60	0
54	MG	2W	201	1/1	0.93	0.23	70,70,70,70	0
54	MG	2A	3105	1/1	0.93	0.08	73,73,73,73	0
54	MG	2A	3106	1/1	0.93	0.20	53,53,53,53	0
54	MG	1A	3010	1/1	0.93	0.15	61,61,61,61	0
54	MG	1A	3158	1/1	0.93	0.07	53,53,53,53	0
54	MG	25	102	1/1	0.93	0.20	50,50,50,50	0
54	MG	1A	3628	1/1	0.93	0.13	45,45,45,45	0
54	MG	1A	3213	1/1	0.93	0.21	45,45,45,45	0
54	MG	1A	3345	1/1	0.93	0.28	46,46,46,46	0
54	MG	1a	1856	1/1	0.93	0.10	70,70,70,70	0
54	MG	1A	3348	1/1	0.93	0.17	46,46,46,46	0
54	MG	2A	3290	1/1	0.93	0.27	52,52,52,52	0
54	MG	1A	3068	1/1	0.93	0.25	51,51,51,51	0
54	MG	1a	1720	1/1	0.93	0.21	63,63,63,63	0
54	MG	1A	3020	1/1	0.93	0.33	43,43,43,43	0
54	MG	2A	3297	1/1	0.93	0.14	65,65,65,65	0
54	MG	2a	3009	1/1	0.93	0.13	76,76,76,76	0
54	MG	19	101	1/1	0.93	0.21	65,65,65,65	0
54	MG	2a	3011	1/1	0.93	0.12	74,74,74,74	0
54	MG	1A	3740	1/1	0.93	0.32	43,43,43,43	0
54	MG	1A	3125	1/1	0.93	0.09	44,44,44,44	0
54	MG	2A	3305	1/1	0.93	0.14	45,45,45,45	0
54	MG	1A	3084	1/1	0.93	0.17	54,54,54,54	0
54	MG	1A	3553	1/1	0.93	0.17	61,61,61,61	0
54	MG	2A	3311	1/1	0.93	0.22	72,72,72,72	0
54	MG	1A	3086	1/1	0.93	0.30	50,50,50,50	0
54	MG	1a	1605	1/1	0.93	0.24	63,63,63,63	0
54	MG	2A	3318	1/1	0.93	0.09	43,43,43,43	0
54	MG	2A	3554	1/1	0.93	0.08	74,74,74,74	0
54	MG	1A	3754	1/1	0.93	0.08	39,39,39,39	0
54	MG	1a	1873	1/1	0.93	0.22	64,64,64,64	0
54	MG	1A	3645	1/1	0.93	0.08	31,31,31,31	0
54	MG	1A	3757	1/1	0.93	0.09	61,61,61,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3561	1/1	0.93	0.09	71,71,71,71	0
54	MG	1A	3358	1/1	0.93	0.05	34,34,34,34	0
54	MG	2A	3565	1/1	0.93	0.08	83,83,83,83	0
54	MG	1A	3227	1/1	0.93	0.13	41,41,41,41	0
54	MG	2A	3139	1/1	0.93	0.10	56,56,56,56	0
54	MG	2A	3331	1/1	0.93	0.10	58,58,58,58	0
54	MG	1A	3761	1/1	0.93	0.09	41,41,41,41	0
54	MG	1A	3649	1/1	0.93	0.14	57,57,57,57	0
54	MG	1a	1741	1/1	0.93	0.13	71,71,71,71	0
54	MG	1a	1615	1/1	0.93	0.17	76,76,76,76	0
54	MG	1a	1616	1/1	0.93	0.11	76,76,76,76	0
54	MG	2A	3342	1/1	0.93	0.09	65,65,65,65	0
54	MG	2A	3148	1/1	0.93	0.14	54,54,54,54	0
54	MG	2A	3346	1/1	0.93	0.11	45,45,45,45	0
54	MG	1A	3897	1/1	0.93	0.09	40,40,40,40	0
54	MG	1A	3764	1/1	0.93	0.07	50,50,50,50	0
54	MG	1A	3558	1/1	0.93	0.08	49,49,49,49	0
54	MG	2A	3353	1/1	0.93	0.09	42,42,42,42	0
54	MG	1A	3560	1/1	0.93	0.08	69,69,69,69	0
54	MG	2A	3157	1/1	0.93	0.15	63,63,63,63	0
54	MG	1A	3364	1/1	0.93	0.09	48,48,48,48	0
54	MG	2A	3595	1/1	0.93	0.09	72,72,72,72	0
54	MG	1A	3466	1/1	0.93	0.09	51,51,51,51	0
54	MG	2A	3364	1/1	0.93	0.14	56,56,56,56	0
54	MG	1A	3774	1/1	0.93	0.20	49,49,49,49	0
54	MG	1B	212	1/1	0.93	0.07	55,55,55,55	0
54	MG	1A	3565	1/1	0.93	0.07	36,36,36,36	0
54	MG	1A	3569	1/1	0.93	0.09	54,54,54,54	0
54	MG	2A	3609	1/1	0.93	0.07	50,50,50,50	0
54	MG	2A	3166	1/1	0.93	0.17	68,68,68,68	0
54	MG	1A	3777	1/1	0.93	0.12	50,50,50,50	0
54	MG	2A	3168	1/1	0.93	0.14	53,53,53,53	0
54	MG	2A	3617	1/1	0.93	0.07	69,69,69,69	0
54	MG	1A	3467	1/1	0.93	0.10	63,63,63,63	0
54	MG	2A	3619	1/1	0.93	0.11	66,66,66,66	0
54	MG	1A	3574	1/1	0.93	0.23	73,73,73,73	0
54	MG	2a	3076	1/1	0.93	0.13	74,74,74,74	0
54	MG	2A	3621	1/1	0.93	0.12	68,68,68,68	0
54	MG	1a	1759	1/1	0.93	0.16	70,70,70,70	0
54	MG	2a	3080	1/1	0.93	0.18	61,61,61,61	0
54	MG	2a	3081	1/1	0.93	0.26	76,76,76,76	0
54	MG	1A	3919	1/1	0.93	0.09	72,72,72,72	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3369	1/1	0.93	0.13	60,60,60,60	0
54	MG	1A	3372	1/1	0.93	0.08	55,55,55,55	0
54	MG	1A	3580	1/1	0.93	0.09	44,44,44,44	0
54	MG	1A	3927	1/1	0.93	0.09	32,32,32,32	0
54	MG	1A	3665	1/1	0.93	0.30	45,45,45,45	0
54	MG	2A	3629	1/1	0.93	0.14	73,73,73,73	0
54	MG	2A	3001	1/1	0.93	0.37	66,66,66,66	0
54	MG	1A	3177	1/1	0.93	0.23	47,47,47,47	0
54	MG	2A	3003	1/1	0.93	0.11	66,66,66,66	0
54	MG	2A	3004	1/1	0.93	0.09	47,47,47,47	0
54	MG	2A	3401	1/1	0.93	0.11	82,82,82,82	0
54	MG	1a	1768	1/1	0.93	0.09	77,77,77,77	0
54	MG	1A	3087	1/1	0.93	0.26	47,47,47,47	0
54	MG	1a	1770	1/1	0.93	0.10	75,75,75,75	0
54	MG	1D	305	1/1	0.93	0.22	50,50,50,50	0
54	MG	2A	3652	1/1	0.93	0.07	71,71,71,71	0
54	MG	2a	3102	1/1	0.93	0.33	62,62,62,62	0
54	MG	1D	309	1/1	0.93	0.13	64,64,64,64	0
54	MG	1A	3232	1/1	0.93	0.11	44,44,44,44	0
54	MG	1A	3586	1/1	0.93	0.07	66,66,66,66	0
54	MG	1A	3377	1/1	0.93	0.07	41,41,41,41	0
54	MG	1A	3233	1/1	0.93	0.28	41,41,41,41	0
54	MG	2A	3416	1/1	0.93	0.17	66,66,66,66	0
54	MG	2A	3662	1/1	0.93	0.08	56,56,56,56	0
54	MG	2A	3417	1/1	0.93	0.11	46,46,46,46	0
54	MG	1A	3190	1/1	0.93	0.25	48,48,48,48	0
54	MG	1A	3239	1/1	0.93	0.21	41,41,41,41	0
54	MG	2A	3195	1/1	0.93	0.07	65,65,65,65	0
54	MG	2A	3025	1/1	0.93	0.10	54,54,54,54	0
54	MG	2a	3115	1/1	0.93	0.33	68,68,68,68	0
54	MG	2A	3423	1/1	0.93	0.07	47,47,47,47	0
54	MG	2A	3424	1/1	0.93	0.07	47,47,47,47	0
54	MG	1A	3677	1/1	0.93	0.24	65,65,65,65	0
54	MG	2a	3120	1/1	0.93	0.15	70,70,70,70	0
54	MG	2A	3684	1/1	0.93	0.09	71,71,71,71	0
54	MG	1A	3305	1/1	0.93	0.11	45,45,45,45	0
54	MG	1A	3132	1/1	0.93	0.07	40,40,40,40	0
54	MG	2A	3202	1/1	0.93	0.23	53,53,53,53	0
54	MG	1E	307	1/1	0.93	0.14	32,32,32,32	0
54	MG	2A	3204	1/1	0.93	0.34	73,73,73,73	0
54	MG	2A	3435	1/1	0.93	0.09	58,58,58,58	0
54	MG	1a	1783	1/1	0.93	0.13	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3684	1/1	0.93	0.09	64,64,64,64	0
54	MG	1A	3058	1/1	0.93	0.17	58,58,58,58	0
54	MG	1A	3392	1/1	0.93	0.09	39,39,39,39	0
54	MG	1A	3962	1/1	0.93	0.10	51,51,51,51	0
54	MG	1A	3816	1/1	0.93	0.17	69,69,69,69	0
54	MG	1A	3498	1/1	0.93	0.13	60,60,60,60	0
54	MG	1A	3194	1/1	0.93	0.27	44,44,44,44	0
54	MG	2A	3045	1/1	0.93	0.18	76,76,76,76	0
54	MG	1A	3599	1/1	0.93	0.09	66,66,66,66	0
54	MG	1A	3501	1/1	0.93	0.07	27,27,27,27	0
54	MG	1A	3196	1/1	0.93	0.28	53,53,53,53	0
54	MG	2A	3711	1/1	0.93	0.12	62,62,62,62	0
54	MG	2A	3451	1/1	0.93	0.10	59,59,59,59	0
54	MG	1a	1675	1/1	0.93	0.32	69,69,69,69	0
54	MG	1A	3972	1/1	0.93	0.08	64,64,64,64	0
54	MG	2A	3222	1/1	0.93	0.16	70,70,70,70	0
54	MG	2A	3456	1/1	0.93	0.09	68,68,68,68	0
54	MG	2a	3154	1/1	0.93	0.09	80,80,80,80	0
54	MG	1A	3695	1/1	0.93	0.14	53,53,53,53	0
54	MG	1A	3060	1/1	0.93	0.08	58,58,58,58	0
54	MG	1A	3135	1/1	0.93	0.23	49,49,49,49	0
54	MG	1A	3831	1/1	0.93	0.10	39,39,39,39	0
54	MG	2a	3162	1/1	0.93	0.10	74,74,74,74	0
54	MG	1A	3320	1/1	0.93	0.18	47,47,47,47	0
54	MG	1a	1809	1/1	0.93	0.10	76,76,76,76	0
54	MG	2A	3463	1/1	0.93	0.13	59,59,59,59	0
54	MG	1a	1810	1/1	0.93	0.07	76,76,76,76	0
54	MG	1R	203	1/1	0.93	0.12	52,52,52,52	0
54	MG	2A	3467	1/1	0.93	0.08	73,73,73,73	0
54	MG	2A	3062	1/1	0.93	0.10	50,50,50,50	0
54	MG	1A	3138	1/1	0.93	0.07	59,59,59,59	0
54	MG	2A	3064	1/1	0.93	0.10	63,63,63,63	0
54	MG	1A	3260	1/1	0.93	0.11	59,59,59,59	0
54	MG	2A	3475	1/1	0.93	0.14	63,63,63,63	0
54	MG	1A	3041	1/1	0.93	0.14	61,61,61,61	0
54	MG	2A	3242	1/1	0.93	0.11	69,69,69,69	0
54	MG	1a	1816	1/1	0.93	0.15	75,75,75,75	0
54	MG	1A	3424	1/1	0.93	0.05	30,30,30,30	0
54	MG	2a	3184	1/1	0.93	0.12	73,73,73,73	0
54	MG	1A	3425	1/1	0.93	0.10	32,32,32,32	0
54	MG	1a	1689	1/1	0.93	0.13	68,68,68,68	0
54	MG	2a	3187	1/1	0.93	0.11	74,74,74,74	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3614	1/1	0.93	0.11	57,57,57,57	0
54	MG	2A	3080	1/1	0.93	0.13	63,63,63,63	0
54	MG	2A	3252	1/1	0.93	0.12	47,47,47,47	0
54	MG	1A	3845	1/1	0.93	0.08	40,40,40,40	0
54	MG	2A	3255	1/1	0.93	0.41	48,48,48,48	0
54	MG	2f	201	1/1	0.93	0.11	57,57,57,57	0
54	MG	2A	3082	1/1	0.93	0.16	65,65,65,65	0
54	MG	2A	3257	1/1	0.93	0.13	40,40,40,40	0
54	MG	1A	3143	1/1	0.93	0.34	50,50,50,50	0
54	MG	1A	3062	1/1	0.93	0.22	50,50,50,50	0
54	MG	2t	201	1/1	0.93	0.16	53,53,53,53	0
54	MG	2D	303	1/1	0.93	0.33	50,50,50,50	0
54	MG	2D	304	1/1	0.93	0.28	60,60,60,60	0
54	MG	1A	3065	1/1	0.93	0.08	41,41,41,41	0
54	MG	2A	3499	1/1	0.93	0.11	69,69,69,69	0
54	MG	10	103	1/1	0.93	0.09	52,52,52,52	0
54	MG	1a	1830	1/1	0.93	0.11	79,79,79,79	0
54	MG	2A	3091	1/1	0.93	0.15	57,57,57,57	0
54	MG	1A	4002	1/1	0.93	0.07	52,52,52,52	0
54	MG	1A	3434	1/1	0.93	0.09	46,46,46,46	0
54	MG	1A	3008	1/1	0.94	0.06	46,46,46,46	0
54	MG	1A	3478	1/1	0.94	0.08	66,66,66,66	0
54	MG	2A	3560	1/1	0.94	0.10	45,45,45,45	0
54	MG	1B	202	1/1	0.94	0.25	70,70,70,70	0
54	MG	1A	3169	1/1	0.94	0.06	36,36,36,36	0
54	MG	1a	1752	1/1	0.94	0.07	71,71,71,71	0
54	MG	1k	201	1/1	0.94	0.12	54,54,54,54	0
54	MG	1A	3579	1/1	0.94	0.14	61,61,61,61	0
54	MG	1A	3170	1/1	0.94	0.16	54,54,54,54	0
54	MG	1m	201	1/1	0.94	0.07	76,76,76,76	0
54	MG	2A	3365	1/1	0.94	0.10	46,46,46,46	0
54	MG	1A	3210	1/1	0.94	0.18	50,50,50,50	0
54	MG	1A	3778	1/1	0.94	0.06	55,55,55,55	0
54	MG	1A	3397	1/1	0.94	0.15	51,51,51,51	0
54	MG	2a	3017	1/1	0.94	0.10	57,57,57,57	0
54	MG	1A	3025	1/1	0.94	0.45	43,43,43,43	0
54	MG	1A	3265	1/1	0.94	0.09	53,53,53,53	0
54	MG	2a	3020	1/1	0.94	0.08	66,66,66,66	0
54	MG	1A	3107	1/1	0.94	0.45	42,42,42,42	0
54	MG	2a	3023	1/1	0.94	0.41	76,76,76,76	0
54	MG	2A	3175	1/1	0.94	0.06	58,58,58,58	0
54	MG	1A	3497	1/1	0.94	0.10	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3787	1/1	0.94	0.09	61,61,61,61	0
54	MG	1A	3920	1/1	0.94	0.07	64,64,64,64	0
54	MG	2a	3028	1/1	0.94	0.10	66,66,66,66	0
54	MG	1A	3921	1/1	0.94	0.07	60,60,60,60	0
54	MG	1A	3326	1/1	0.94	0.12	59,59,59,59	0
54	MG	1A	3671	1/1	0.94	0.15	48,48,48,48	0
54	MG	2A	3388	1/1	0.94	0.10	63,63,63,63	0
54	MG	1A	3796	1/1	0.94	0.10	57,57,57,57	0
54	MG	2a	3034	1/1	0.94	0.21	66,66,66,66	0
54	MG	2A	3390	1/1	0.94	0.14	70,70,70,70	0
54	MG	1A	3268	1/1	0.94	0.11	52,52,52,52	0
54	MG	2A	3015	1/1	0.94	0.21	48,48,48,48	0
54	MG	1A	3409	1/1	0.94	0.07	37,37,37,37	0
54	MG	2A	3605	1/1	0.94	0.09	51,51,51,51	0
54	MG	1A	3592	1/1	0.94	0.09	27,27,27,27	0
54	MG	1A	3410	1/1	0.94	0.09	32,32,32,32	0
54	MG	1A	3175	1/1	0.94	0.23	60,60,60,60	0
54	MG	1D	303	1/1	0.94	0.13	46,46,46,46	0
54	MG	1A	3271	1/1	0.94	0.16	36,36,36,36	0
54	MG	1D	307	1/1	0.94	0.09	47,47,47,47	0
54	MG	1A	3419	1/1	0.94	0.09	37,37,37,37	0
54	MG	1A	3333	1/1	0.94	0.13	57,57,57,57	0
54	MG	2A	3030	1/1	0.94	0.20	42,42,42,42	0
54	MG	1A	3334	1/1	0.94	0.08	51,51,51,51	0
54	MG	1A	3600	1/1	0.94	0.11	33,33,33,33	0
54	MG	1A	3109	1/1	0.94	0.14	38,38,38,38	0
54	MG	2A	3411	1/1	0.94	0.18	67,67,67,67	0
54	MG	1A	3217	1/1	0.94	0.13	52,52,52,52	0
54	MG	2A	3035	1/1	0.94	0.21	68,68,68,68	0
54	MG	1A	3218	1/1	0.94	0.10	51,51,51,51	0
54	MG	1A	3521	1/1	0.94	0.10	30,30,30,30	0
54	MG	2A	3038	1/1	0.94	0.13	58,58,58,58	0
54	MG	1A	3341	1/1	0.94	0.12	61,61,61,61	0
54	MG	1A	3219	1/1	0.94	0.33	46,46,46,46	0
54	MG	1a	1787	1/1	0.94	0.09	68,68,68,68	0
54	MG	1A	3279	1/1	0.94	0.23	55,55,55,55	0
54	MG	1E	308	1/1	0.94	0.19	75,75,75,75	0
54	MG	1A	3964	1/1	0.94	0.09	24,24,24,24	0
54	MG	2A	3046	1/1	0.94	0.21	76,76,76,76	0
54	MG	1A	3178	1/1	0.94	0.12	57,57,57,57	0
54	MG	2A	3431	1/1	0.94	0.12	67,67,67,67	0
54	MG	2A	3646	1/1	0.94	0.09	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1F	313	1/1	0.94	0.27	48,48,48,48	0
54	MG	2a	3074	1/1	0.94	0.28	56,56,56,56	0
54	MG	1A	3442	1/1	0.94	0.13	35,35,35,35	0
54	MG	2A	3434	1/1	0.94	0.21	63,63,63,63	0
54	MG	1a	1795	1/1	0.94	0.10	78,78,78,78	0
54	MG	1A	3528	1/1	0.94	0.09	52,52,52,52	0
54	MG	2A	3220	1/1	0.94	0.10	57,57,57,57	0
54	MG	1A	3221	1/1	0.94	0.44	44,44,44,44	0
54	MG	1A	3615	1/1	0.94	0.09	33,33,33,33	0
54	MG	2A	3665	1/1	0.94	0.07	81,81,81,81	0
54	MG	1G	202	1/1	0.94	0.25	63,63,63,63	0
54	MG	1a	1800	1/1	0.94	0.10	58,58,58,58	0
54	MG	2A	3668	1/1	0.94	0.08	76,76,76,76	0
54	MG	2A	3057	1/1	0.94	0.09	51,51,51,51	0
54	MG	2A	3672	1/1	0.94	0.08	47,47,47,47	0
54	MG	2A	3444	1/1	0.94	0.10	48,48,48,48	0
54	MG	2A	3677	1/1	0.94	0.17	74,74,74,74	0
54	MG	1A	3530	1/1	0.94	0.08	31,31,31,31	0
54	MG	1A	3705	1/1	0.94	0.06	74,74,74,74	0
54	MG	1A	3973	1/1	0.94	0.09	68,68,68,68	0
54	MG	2A	3682	1/1	0.94	0.08	60,60,60,60	0
54	MG	1A	3184	1/1	0.94	0.41	46,46,46,46	0
54	MG	1N	203	1/1	0.94	0.14	47,47,47,47	0
54	MG	1A	3045	1/1	0.94	0.17	39,39,39,39	0
54	MG	2A	3236	1/1	0.94	0.07	63,63,63,63	0
54	MG	2A	3453	1/1	0.94	0.07	59,59,59,59	0
54	MG	1A	3286	1/1	0.94	0.19	60,60,60,60	0
54	MG	1A	3226	1/1	0.94	0.10	62,62,62,62	0
54	MG	1A	3716	1/1	0.94	0.13	66,66,66,66	0
54	MG	2A	3067	1/1	0.94	0.16	57,57,57,57	0
54	MG	1A	3353	1/1	0.94	0.10	33,33,33,33	0
54	MG	1a	1815	1/1	0.94	0.11	66,66,66,66	0
54	MG	1Q	203	1/1	0.94	0.10	51,51,51,51	0
54	MG	2A	3075	1/1	0.94	0.39	60,60,60,60	0
54	MG	1Q	204	1/1	0.94	0.13	47,47,47,47	0
54	MG	1a	1819	1/1	0.94	0.07	72,72,72,72	0
54	MG	2A	3079	1/1	0.94	0.12	59,59,59,59	0
54	MG	1A	3453	1/1	0.94	0.07	21,21,21,21	0
54	MG	1a	1687	1/1	0.94	0.15	56,56,56,56	0
54	MG	1A	3291	1/1	0.94	0.10	58,58,58,58	0
54	MG	1R	204	1/1	0.94	0.12	48,48,48,48	0
54	MG	2A	3472	1/1	0.94	0.12	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3625	1/1	0.94	0.12	48,48,48,48	0
54	MG	1a	1691	1/1	0.94	0.14	65,65,65,65	0
54	MG	2A	3715	1/1	0.94	0.13	71,71,71,71	0
54	MG	1a	1827	1/1	0.94	0.09	56,56,56,56	0
54	MG	1A	3003	1/1	0.94	0.07	36,36,36,36	0
54	MG	1A	3991	1/1	0.94	0.10	62,62,62,62	0
54	MG	1A	3545	1/1	0.94	0.19	48,48,48,48	0
54	MG	1a	1695	1/1	0.94	0.16	52,52,52,52	0
54	MG	1U	206	1/1	0.94	0.28	44,44,44,44	0
54	MG	1V	203	1/1	0.94	0.10	46,46,46,46	0
54	MG	1A	3994	1/1	0.94	0.09	71,71,71,71	0
54	MG	2a	3132	1/1	0.94	0.11	71,71,71,71	0
54	MG	1A	3191	1/1	0.94	0.07	58,58,58,58	0
54	MG	1A	3997	1/1	0.94	0.08	32,32,32,32	0
54	MG	1a	1839	1/1	0.94	0.08	51,51,51,51	0
54	MG	1A	3019	1/1	0.94	0.37	34,34,34,34	0
54	MG	1Y	201	1/1	0.94	0.12	55,55,55,55	0
54	MG	1A	3631	1/1	0.94	0.11	64,64,64,64	0
54	MG	2A	3730	1/1	0.94	0.08	68,68,68,68	0
54	MG	10	101	1/1	0.94	0.17	43,43,43,43	0
54	MG	1A	4000	1/1	0.94	0.11	50,50,50,50	0
54	MG	1A	3855	1/1	0.94	0.06	46,46,46,46	0
54	MG	2A	3495	1/1	0.94	0.19	57,57,57,57	0
54	MG	2A	3497	1/1	0.94	0.19	73,73,73,73	0
54	MG	1A	3116	1/1	0.94	0.18	44,44,44,44	0
54	MG	1A	3633	1/1	0.94	0.30	37,37,37,37	0
54	MG	2a	3151	1/1	0.94	0.16	80,80,80,80	0
54	MG	2B	208	1/1	0.94	0.24	71,71,71,71	0
54	MG	2A	3281	1/1	0.94	0.34	74,74,74,74	0
54	MG	1A	3091	1/1	0.94	0.08	42,42,42,42	0
54	MG	1A	3865	1/1	0.94	0.07	48,48,48,48	0
54	MG	1A	3153	1/1	0.94	0.11	52,52,52,52	0
54	MG	1A	4008	1/1	0.94	0.20	41,41,41,41	0
54	MG	2A	3510	1/1	0.94	0.11	66,66,66,66	0
54	MG	2a	3164	1/1	0.94	0.14	76,76,76,76	0
54	MG	1A	3741	1/1	0.94	0.17	43,43,43,43	0
54	MG	2A	3287	1/1	0.94	0.11	64,64,64,64	0
54	MG	1A	3092	1/1	0.94	0.16	44,44,44,44	0
54	MG	2A	3119	1/1	0.94	0.09	57,57,57,57	0
54	MG	1a	1719	1/1	0.94	0.20	63,63,63,63	0
54	MG	13	102	1/1	0.94	0.15	72,72,72,72	0
54	MG	2A	3122	1/1	0.94	0.10	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3123	1/1	0.94	0.14	49,49,49,49	0
54	MG	2D	305	1/1	0.94	0.44	49,49,49,49	0
54	MG	1a	1721	1/1	0.94	0.11	56,56,56,56	0
54	MG	1A	3126	1/1	0.94	0.09	40,40,40,40	0
54	MG	15	102	1/1	0.94	0.26	39,39,39,39	0
54	MG	1A	3054	1/1	0.94	0.20	34,34,34,34	0
54	MG	2a	3180	1/1	0.94	0.09	59,59,59,59	0
54	MG	2A	3307	1/1	0.94	0.15	62,62,62,62	0
54	MG	1A	3749	1/1	0.94	0.10	59,59,59,59	0
54	MG	1A	3874	1/1	0.94	0.15	32,32,32,32	0
54	MG	1A	3643	1/1	0.94	0.07	50,50,50,50	0
54	MG	1A	3001	1/1	0.94	0.06	39,39,39,39	0
54	MG	1A	3878	1/1	0.94	0.06	58,58,58,58	0
54	MG	2A	3317	1/1	0.94	0.07	54,54,54,54	0
54	MG	1A	4022	1/1	0.94	0.14	64,64,64,64	0
54	MG	1A	3562	1/1	0.94	0.14	58,58,58,58	0
54	MG	1A	4026	1/1	0.94	0.08	66,66,66,66	0
54	MG	1A	3164	1/1	0.94	0.30	41,41,41,41	0
54	MG	1A	3883	1/1	0.94	0.08	68,68,68,68	0
54	MG	1A	3758	1/1	0.94	0.18	37,37,37,37	0
54	MG	1A	3101	1/1	0.94	0.11	46,46,46,46	0
54	MG	1A	3566	1/1	0.94	0.08	44,44,44,44	0
54	MG	2A	3541	1/1	0.94	0.16	60,60,60,60	0
54	MG	2A	3146	1/1	0.94	0.27	60,60,60,60	0
54	MG	1a	1742	1/1	0.94	0.12	44,44,44,44	0
54	MG	1A	3567	1/1	0.94	0.08	43,43,43,43	0
54	MG	2A	3152	1/1	0.94	0.10	48,48,48,48	0
54	MG	1A	3205	1/1	0.94	0.10	60,60,60,60	0
54	MG	1A	3474	1/1	0.94	0.12	53,53,53,53	0
54	MG	1A	3572	1/1	0.94	0.19	48,48,48,48	0
54	MG	1A	3573	1/1	0.94	0.10	57,57,57,57	0
58	ARG	1B	230	12/12	0.94	0.09	32,44,59,61	0
54	MG	2A	3158	1/1	0.94	0.15	76,76,76,76	0
54	MG	28	101	1/1	0.94	0.10	68,68,68,68	0
54	MG	1A	3415	1/1	0.95	0.09	37,37,37,37	0
54	MG	1A	3798	1/1	0.95	0.11	30,30,30,30	0
54	MG	2A	3586	1/1	0.95	0.09	67,67,67,67	0
54	MG	2A	3397	1/1	0.95	0.08	61,61,61,61	0
54	MG	2A	3589	1/1	0.95	0.08	60,60,60,60	0
54	MG	1A	3416	1/1	0.95	0.07	35,35,35,35	0
54	MG	2a	3014	1/1	0.95	0.19	63,63,63,63	0
54	MG	2A	3591	1/1	0.95	0.07	52,52,52,52	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1a	1818	1/1	0.95	0.11	72,72,72,72	0
54	MG	2A	3593	1/1	0.95	0.06	58,58,58,58	0
54	MG	1A	3108	1/1	0.95	0.19	40,40,40,40	0
54	MG	10	105	1/1	0.95	0.07	55,55,55,55	0
54	MG	1A	3908	1/1	0.95	0.10	61,61,61,61	0
54	MG	1A	3485	1/1	0.95	0.16	52,52,52,52	0
54	MG	1a	1698	1/1	0.95	0.30	74,74,74,74	0
54	MG	1A	3803	1/1	0.95	0.08	42,42,42,42	0
54	MG	2A	3214	1/1	0.95	0.24	60,60,60,60	0
54	MG	2A	3215	1/1	0.95	0.13	65,65,65,65	0
54	MG	1A	3304	1/1	0.95	0.06	45,45,45,45	0
54	MG	2A	3409	1/1	0.95	0.12	51,51,51,51	0
54	MG	1a	1702	1/1	0.95	0.20	61,61,61,61	0
54	MG	2A	3613	1/1	0.95	0.09	56,56,56,56	0
54	MG	2A	3615	1/1	0.95	0.05	29,29,29,29	0
54	MG	1A	3223	1/1	0.95	0.15	36,36,36,36	0
54	MG	1A	3564	1/1	0.95	0.07	29,29,29,29	0
54	MG	1A	3057	1/1	0.95	0.15	54,54,54,54	0
54	MG	1A	3490	1/1	0.95	0.10	57,57,57,57	0
54	MG	1a	1707	1/1	0.95	0.29	60,60,60,60	0
54	MG	2A	3223	1/1	0.95	0.11	55,55,55,55	0
54	MG	1A	4040	1/1	0.95	0.08	61,61,61,61	0
54	MG	1A	3017	1/1	0.95	0.19	36,36,36,36	0
54	MG	1A	3495	1/1	0.95	0.05	34,34,34,34	0
54	MG	2A	3228	1/1	0.95	0.21	60,60,60,60	0
54	MG	1A	3812	1/1	0.95	0.06	38,38,38,38	0
54	MG	15	104	1/1	0.95	0.10	43,43,43,43	0
54	MG	1A	3496	1/1	0.95	0.09	61,61,61,61	0
54	MG	2A	3232	1/1	0.95	0.10	63,63,63,63	0
54	MG	1A	3202	1/1	0.95	0.15	42,42,42,42	0
54	MG	1A	3636	1/1	0.95	0.14	44,44,44,44	0
54	MG	2A	3086	1/1	0.95	0.07	45,45,45,45	0
54	MG	15	108	1/1	0.95	0.07	56,56,56,56	0
54	MG	1a	1847	1/1	0.95	0.11	73,73,73,73	0
54	MG	2a	3052	1/1	0.95	0.14	55,55,55,55	0
54	MG	17	101	1/1	0.95	0.08	38,38,38,38	0
54	MG	17	102	1/1	0.95	0.10	48,48,48,48	0
54	MG	17	104	1/1	0.95	0.17	43,43,43,43	0
54	MG	1B	208	1/1	0.95	0.06	56,56,56,56	0
54	MG	2A	3640	1/1	0.95	0.08	69,69,69,69	0
54	MG	1A	3714	1/1	0.95	0.11	67,67,67,67	0
54	MG	2A	3649	1/1	0.95	0.06	69,69,69,69	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3820	1/1	0.95	0.13	36,36,36,36	0
54	MG	1A	3015	1/1	0.95	0.18	32,32,32,32	0
54	MG	1A	3040	1/1	0.95	0.14	42,42,42,42	0
54	MG	2A	3249	1/1	0.95	0.13	69,69,69,69	0
54	MG	1A	3948	1/1	0.95	0.11	50,50,50,50	0
54	MG	1A	3366	1/1	0.95	0.12	37,37,37,37	0
54	MG	1B	217	1/1	0.95	0.09	58,58,58,58	0
54	MG	1A	3825	1/1	0.95	0.09	57,57,57,57	0
54	MG	2a	3069	1/1	0.95	0.19	74,74,74,74	0
54	MG	1a	1866	1/1	0.95	0.15	67,67,67,67	0
54	MG	1B	219	1/1	0.95	0.07	38,38,38,38	0
54	MG	2A	3108	1/1	0.95	0.09	74,74,74,74	0
54	MG	1A	3642	1/1	0.95	0.13	63,63,63,63	0
54	MG	2A	3259	1/1	0.95	0.05	70,70,70,70	0
54	MG	2A	3260	1/1	0.95	0.29	73,73,73,73	0
54	MG	1A	3080	1/1	0.95	0.23	53,53,53,53	0
54	MG	2A	3675	1/1	0.95	0.07	49,49,49,49	0
54	MG	2A	3676	1/1	0.95	0.06	47,47,47,47	0
54	MG	1A	3439	1/1	0.95	0.07	48,48,48,48	0
54	MG	1A	3505	1/1	0.95	0.09	32,32,32,32	0
54	MG	1A	3727	1/1	0.95	0.15	51,51,51,51	0
54	MG	1A	3957	1/1	0.95	0.06	36,36,36,36	0
54	MG	2A	3681	1/1	0.95	0.05	76,76,76,76	0
54	MG	1A	3440	1/1	0.95	0.08	34,34,34,34	0
54	MG	1A	3319	1/1	0.95	0.21	40,40,40,40	0
54	MG	2A	3464	1/1	0.95	0.09	53,53,53,53	0
54	MG	1A	3733	1/1	0.95	0.08	53,53,53,53	0
54	MG	2A	3686	1/1	0.95	0.09	41,41,41,41	0
54	MG	1A	3734	1/1	0.95	0.14	51,51,51,51	0
54	MG	1A	3965	1/1	0.95	0.05	32,32,32,32	0
54	MG	2a	3094	1/1	0.95	0.27	59,59,59,59	0
54	MG	1a	1619	1/1	0.95	0.11	70,70,70,70	0
54	MG	1A	3144	1/1	0.95	0.14	47,47,47,47	0
54	MG	1A	3585	1/1	0.95	0.09	51,51,51,51	0
54	MG	1A	3236	1/1	0.95	0.15	44,44,44,44	0
54	MG	1A	3444	1/1	0.95	0.08	35,35,35,35	0
54	MG	1D	312	1/1	0.95	0.17	37,37,37,37	0
54	MG	1A	3655	1/1	0.95	0.07	30,30,30,30	0
54	MG	1A	3148	1/1	0.95	0.14	38,38,38,38	0
54	MG	1A	3323	1/1	0.95	0.16	46,46,46,46	0
54	MG	1a	1633	1/1	0.95	0.08	42,42,42,42	0
54	MG	1A	3209	1/1	0.95	0.29	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3241	1/1	0.95	0.30	45,45,45,45	0
54	MG	1A	3975	1/1	0.95	0.09	68,68,68,68	0
54	MG	1A	3660	1/1	0.95	0.16	50,50,50,50	0
54	MG	2A	3484	1/1	0.95	0.08	38,38,38,38	0
54	MG	2A	3136	1/1	0.95	0.12	72,72,72,72	0
54	MG	2A	3137	1/1	0.95	0.22	72,72,72,72	0
54	MG	2A	3713	1/1	0.95	0.25	71,71,71,71	0
54	MG	2A	3288	1/1	0.95	0.14	65,65,65,65	0
54	MG	1A	3243	1/1	0.95	0.29	51,51,51,51	0
54	MG	1A	3752	1/1	0.95	0.07	35,35,35,35	0
54	MG	1A	3452	1/1	0.95	0.06	32,32,32,32	0
54	MG	1F	306	1/1	0.95	0.17	42,42,42,42	0
54	MG	1A	3387	1/1	0.95	0.06	39,39,39,39	0
54	MG	1A	3863	1/1	0.95	0.10	55,55,55,55	0
54	MG	2A	3496	1/1	0.95	0.12	48,48,48,48	0
54	MG	1A	3100	1/1	0.95	0.06	55,55,55,55	0
54	MG	1A	3284	1/1	0.95	0.39	49,49,49,49	0
54	MG	2A	3147	1/1	0.95	0.13	67,67,67,67	0
54	MG	1A	3120	1/1	0.95	0.14	51,51,51,51	0
54	MG	2A	3150	1/1	0.95	0.08	52,52,52,52	0
54	MG	1A	3289	1/1	0.95	0.16	40,40,40,40	0
54	MG	1A	3992	1/1	0.95	0.07	63,63,63,63	0
54	MG	2A	3153	1/1	0.95	0.13	63,63,63,63	0
54	MG	1F	318	1/1	0.95	0.06	55,55,55,55	0
54	MG	1a	1653	1/1	0.95	0.07	48,48,48,48	0
54	MG	2a	3135	1/1	0.95	0.17	71,71,71,71	0
54	MG	2A	3316	1/1	0.95	0.06	41,41,41,41	0
54	MG	1a	1654	1/1	0.95	0.21	66,66,66,66	0
54	MG	1G	201	1/1	0.95	0.16	66,66,66,66	0
54	MG	2A	3515	1/1	0.95	0.07	45,45,45,45	0
54	MG	1A	3052	1/1	0.95	0.23	42,42,42,42	0
54	MG	1A	3396	1/1	0.95	0.06	58,58,58,58	0
54	MG	1G	204	1/1	0.95	0.11	51,51,51,51	0
54	MG	2A	3008	1/1	0.95	0.09	51,51,51,51	0
54	MG	1A	3870	1/1	0.95	0.08	47,47,47,47	0
54	MG	2A	3324	1/1	0.95	0.07	47,47,47,47	0
54	MG	2a	3146	1/1	0.95	0.13	68,68,68,68	0
54	MG	2A	3011	1/1	0.95	0.07	47,47,47,47	0
54	MG	1a	1660	1/1	0.95	0.10	74,74,74,74	0
54	MG	2A	3329	1/1	0.95	0.15	45,45,45,45	0
54	MG	1A	3996	1/1	0.95	0.06	65,65,65,65	0
54	MG	1N	201	1/1	0.95	0.13	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3333	1/1	0.95	0.19	65,65,65,65	0
54	MG	1A	3102	1/1	0.95	0.12	45,45,45,45	0
54	MG	1A	3292	1/1	0.95	0.13	52,52,52,52	0
54	MG	1A	3538	1/1	0.95	0.06	42,42,42,42	0
54	MG	1A	3103	1/1	0.95	0.26	50,50,50,50	0
54	MG	1P	202	1/1	0.95	0.22	36,36,36,36	0
54	MG	1A	3675	1/1	0.95	0.10	35,35,35,35	0
54	MG	1A	3064	1/1	0.95	0.07	44,44,44,44	0
54	MG	1A	3542	1/1	0.95	0.05	61,61,61,61	0
54	MG	2A	3028	1/1	0.95	0.09	56,56,56,56	0
54	MG	2A	3029	1/1	0.95	0.08	52,52,52,52	0
54	MG	1Q	201	1/1	0.95	0.12	40,40,40,40	0
54	MG	1A	3258	1/1	0.95	0.17	47,47,47,47	0
54	MG	1A	3681	1/1	0.95	0.10	38,38,38,38	0
54	MG	2A	3357	1/1	0.95	0.12	43,43,43,43	0
54	MG	2A	3360	1/1	0.95	0.23	72,72,72,72	0
54	MG	1a	1674	1/1	0.95	0.18	75,75,75,75	0
54	MG	2F	303	1/1	0.95	0.14	66,66,66,66	0
54	MG	2A	3547	1/1	0.95	0.07	56,56,56,56	0
54	MG	2a	3178	1/1	0.95	0.10	82,82,82,82	0
54	MG	1A	3682	1/1	0.95	0.06	46,46,46,46	0
54	MG	1A	3779	1/1	0.95	0.06	49,49,49,49	0
54	MG	2A	3553	1/1	0.95	0.07	66,66,66,66	0
54	MG	1A	3129	1/1	0.95	0.11	54,54,54,54	0
54	MG	1A	3162	1/1	0.95	0.22	45,45,45,45	0
54	MG	2R	202	1/1	0.95	0.09	48,48,48,48	0
54	MG	2A	3367	1/1	0.95	0.07	44,44,44,44	0
54	MG	2T	201	1/1	0.95	0.22	71,71,71,71	0
54	MG	2T	202	1/1	0.95	0.19	72,72,72,72	0
54	MG	1A	3030	1/1	0.95	0.06	33,33,33,33	0
54	MG	1A	3548	1/1	0.95	0.07	53,53,53,53	0
54	MG	1a	1801	1/1	0.95	0.05	76,76,76,76	0
54	MG	2A	3371	1/1	0.95	0.06	48,48,48,48	0
54	MG	1A	3891	1/1	0.95	0.05	30,30,30,30	0
54	MG	1U	201	1/1	0.95	0.17	42,42,42,42	0
54	MG	1A	3551	1/1	0.95	0.39	37,37,37,37	0
54	MG	1U	207	1/1	0.95	0.17	40,40,40,40	0
54	MG	1a	1806	1/1	0.95	0.11	65,65,65,65	0
54	MG	2A	3383	1/1	0.95	0.26	60,60,60,60	0
54	MG	1a	1808	1/1	0.95	0.07	61,61,61,61	0
55	HGR	2A	3731	36/36	0.95	0.11	36,44,52,57	0
54	MG	1A	4016	1/1	0.95	0.09	19,19,19,19	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	27	102	1/1	0.95	0.23	47,47,47,47	0
57	MPD	18	103	8/8	0.95	0.12	36,41,45,49	0
54	MG	1A	3088	1/1	0.95	0.41	46,46,46,46	0
54	MG	2A	3199	1/1	0.95	0.10	58,58,58,58	0
54	MG	1A	3412	1/1	0.95	0.06	38,38,38,38	0
54	MG	1A	3791	1/1	0.95	0.12	62,62,62,62	0
54	MG	1A	3413	1/1	0.95	0.08	42,42,42,42	0
54	MG	1A	3479	1/1	0.95	0.09	58,58,58,58	0
54	MG	2A	3393	1/1	0.95	0.13	71,71,71,71	0
54	MG	1D	308	1/1	0.96	0.19	39,39,39,39	0
54	MG	1A	3694	1/1	0.96	0.12	52,52,52,52	0
54	MG	1D	310	1/1	0.96	0.10	55,55,55,55	0
54	MG	2A	3572	1/1	0.96	0.08	73,73,73,73	0
54	MG	1A	3298	1/1	0.96	0.10	31,31,31,31	0
54	MG	1a	1637	1/1	0.96	0.06	45,45,45,45	0
54	MG	2a	3001	1/1	0.96	0.07	54,54,54,54	0
54	MG	1A	3361	1/1	0.96	0.16	43,43,43,43	0
54	MG	1A	3171	1/1	0.96	0.04	32,32,32,32	0
54	MG	2A	3382	1/1	0.96	0.07	64,64,64,64	0
54	MG	1A	3094	1/1	0.96	0.28	42,42,42,42	0
54	MG	1A	3532	1/1	0.96	0.07	53,53,53,53	0
54	MG	1A	3700	1/1	0.96	0.08	66,66,66,66	0
54	MG	1A	3173	1/1	0.96	0.30	46,46,46,46	0
54	MG	1A	3303	1/1	0.96	0.14	39,39,39,39	0
54	MG	1A	3142	1/1	0.96	0.07	50,50,50,50	0
54	MG	1A	3095	1/1	0.96	0.18	40,40,40,40	0
54	MG	2a	3012	1/1	0.96	0.07	60,60,60,60	0
54	MG	2A	3588	1/1	0.96	0.07	57,57,57,57	0
54	MG	1A	3817	1/1	0.96	0.11	62,62,62,62	0
54	MG	1a	1648	1/1	0.96	0.12	49,49,49,49	0
54	MG	1A	3818	1/1	0.96	0.06	81,81,81,81	0
54	MG	2A	3394	1/1	0.96	0.06	72,72,72,72	0
54	MG	1F	304	1/1	0.96	0.21	39,39,39,39	0
54	MG	1A	3176	1/1	0.96	0.06	41,41,41,41	0
54	MG	1F	307	1/1	0.96	0.27	33,33,33,33	0
54	MG	2A	3597	1/1	0.96	0.10	72,72,72,72	0
54	MG	2A	3598	1/1	0.96	0.09	71,71,71,71	0
54	MG	1F	309	1/1	0.96	0.24	59,59,59,59	0
54	MG	1A	3960	1/1	0.96	0.15	60,60,60,60	0
54	MG	1A	3059	1/1	0.96	0.13	29,29,29,29	0
54	MG	1A	3708	1/1	0.96	0.14	59,59,59,59	0
54	MG	1A	3457	1/1	0.96	0.06	43,43,43,43	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3606	1/1	0.96	0.09	66,66,66,66	0
54	MG	1A	3146	1/1	0.96	0.15	48,48,48,48	0
54	MG	1A	3824	1/1	0.96	0.10	74,74,74,74	0
54	MG	1A	3459	1/1	0.96	0.09	62,62,62,62	0
54	MG	1A	3460	1/1	0.96	0.17	62,62,62,62	0
54	MG	1A	3313	1/1	0.96	0.34	41,41,41,41	0
54	MG	2A	3614	1/1	0.96	0.07	61,61,61,61	0
54	MG	1A	3717	1/1	0.96	0.06	51,51,51,51	0
54	MG	1A	3718	1/1	0.96	0.17	48,48,48,48	0
54	MG	1A	3830	1/1	0.96	0.09	52,52,52,52	0
54	MG	1A	3383	1/1	0.96	0.07	58,58,58,58	0
54	MG	2A	3413	1/1	0.96	0.07	42,42,42,42	0
54	MG	1A	3179	1/1	0.96	0.15	37,37,37,37	0
54	MG	1A	3834	1/1	0.96	0.09	43,43,43,43	0
54	MG	1A	3267	1/1	0.96	0.10	54,54,54,54	0
54	MG	1A	3181	1/1	0.96	0.15	61,61,61,61	0
54	MG	1A	3317	1/1	0.96	0.05	21,21,21,21	0
54	MG	2A	3420	1/1	0.96	0.07	39,39,39,39	0
54	MG	1A	3389	1/1	0.96	0.06	22,22,22,22	0
54	MG	1A	3841	1/1	0.96	0.22	42,42,42,42	0
54	MG	1A	3842	1/1	0.96	0.10	70,70,70,70	0
54	MG	1A	3725	1/1	0.96	0.17	46,46,46,46	0
54	MG	2A	3425	1/1	0.96	0.10	65,65,65,65	0
54	MG	1A	3269	1/1	0.96	0.29	36,36,36,36	0
54	MG	1A	3729	1/1	0.96	0.09	64,64,64,64	0
54	MG	2A	3071	1/1	0.96	0.12	61,61,61,61	0
54	MG	2A	3072	1/1	0.96	0.06	34,34,34,34	0
54	MG	1Q	202	1/1	0.96	0.06	35,35,35,35	0
54	MG	1A	3846	1/1	0.96	0.05	25,25,25,25	0
54	MG	1A	3183	1/1	0.96	0.11	53,53,53,53	0
54	MG	1Q	205	1/1	0.96	0.12	62,62,62,62	0
54	MG	1A	3028	1/1	0.96	0.24	41,41,41,41	0
54	MG	2A	3641	1/1	0.96	0.05	65,65,65,65	0
54	MG	2A	3645	1/1	0.96	0.06	70,70,70,70	0
54	MG	1A	3393	1/1	0.96	0.05	30,30,30,30	0
54	MG	1A	3081	1/1	0.96	0.31	44,44,44,44	0
54	MG	2A	3651	1/1	0.96	0.10	60,60,60,60	0
54	MG	1A	3150	1/1	0.96	0.08	42,42,42,42	0
54	MG	1A	3274	1/1	0.96	0.13	50,50,50,50	0
54	MG	2A	3655	1/1	0.96	0.08	69,69,69,69	0
54	MG	2A	3440	1/1	0.96	0.08	59,59,59,59	0
54	MG	2a	3072	1/1	0.96	0.06	63,63,63,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3084	1/1	0.96	0.13	51,51,51,51	0
54	MG	1T	202	1/1	0.96	0.09	68,68,68,68	0
54	MG	2A	3246	1/1	0.96	0.10	56,56,56,56	0
54	MG	1A	3276	1/1	0.96	0.18	33,33,33,33	0
54	MG	1A	3151	1/1	0.96	0.29	41,41,41,41	0
54	MG	2A	3664	1/1	0.96	0.06	35,35,35,35	0
54	MG	1A	3856	1/1	0.96	0.15	50,50,50,50	0
54	MG	1a	1833	1/1	0.96	0.09	68,68,68,68	0
54	MG	1U	202	1/1	0.96	0.16	40,40,40,40	0
54	MG	1U	204	1/1	0.96	0.27	65,65,65,65	0
54	MG	2A	3669	1/1	0.96	0.13	78,78,78,78	0
54	MG	1U	205	1/1	0.96	0.30	35,35,35,35	0
54	MG	1A	3402	1/1	0.96	0.08	40,40,40,40	0
54	MG	1A	4003	1/1	0.96	0.06	28,28,28,28	0
54	MG	1A	3051	1/1	0.96	0.31	52,52,52,52	0
54	MG	1A	3570	1/1	0.96	0.06	30,30,30,30	0
54	MG	1A	3085	1/1	0.96	0.37	40,40,40,40	0
54	MG	2A	3099	1/1	0.96	0.16	65,65,65,65	0
54	MG	2A	3101	1/1	0.96	0.14	58,58,58,58	0
54	MG	2a	3093	1/1	0.96	0.30	63,63,63,63	0
54	MG	1V	206	1/1	0.96	0.07	61,61,61,61	0
54	MG	1A	3745	1/1	0.96	0.06	40,40,40,40	0
54	MG	1A	3406	1/1	0.96	0.15	62,62,62,62	0
54	MG	1A	3487	1/1	0.96	0.10	59,59,59,59	0
54	MG	1A	3750	1/1	0.96	0.13	48,48,48,48	0
54	MG	2A	3107	1/1	0.96	0.05	35,35,35,35	0
54	MG	2A	3268	1/1	0.96	0.10	60,60,60,60	0
54	MG	2A	3688	1/1	0.96	0.09	72,72,72,72	0
54	MG	1A	3654	1/1	0.96	0.06	44,44,44,44	0
54	MG	1A	3329	1/1	0.96	0.05	43,43,43,43	0
54	MG	1A	3753	1/1	0.96	0.07	58,58,58,58	0
54	MG	10	104	1/1	0.96	0.08	64,64,64,64	0
54	MG	1A	3026	1/1	0.96	0.25	40,40,40,40	0
54	MG	1A	3873	1/1	0.96	0.14	43,43,43,43	0
54	MG	1A	3755	1/1	0.96	0.08	37,37,37,37	0
54	MG	1A	3332	1/1	0.96	0.10	29,29,29,29	0
54	MG	2A	3698	1/1	0.96	0.05	75,75,75,75	0
54	MG	1A	3577	1/1	0.96	0.07	57,57,57,57	0
54	MG	1A	3063	1/1	0.96	0.06	38,38,38,38	0
54	MG	1A	3157	1/1	0.96	0.15	46,46,46,46	0
54	MG	1A	3069	1/1	0.96	0.10	42,42,42,42	0
54	MG	1A	3414	1/1	0.96	0.07	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3337	1/1	0.96	0.05	34,34,34,34	0
54	MG	1A	3584	1/1	0.96	0.10	45,45,45,45	0
54	MG	2A	3708	1/1	0.96	0.07	80,80,80,80	0
54	MG	1A	3159	1/1	0.96	0.28	49,49,49,49	0
54	MG	1A	3285	1/1	0.96	0.07	49,49,49,49	0
54	MG	1A	3131	1/1	0.96	0.09	64,64,64,64	0
54	MG	1a	1724	1/1	0.96	0.06	43,43,43,43	0
54	MG	1A	3420	1/1	0.96	0.06	45,45,45,45	0
54	MG	1A	3770	1/1	0.96	0.14	52,52,52,52	0
54	MG	1A	3892	1/1	0.96	0.04	56,56,56,56	0
54	MG	1a	1728	1/1	0.96	0.12	46,46,46,46	0
54	MG	2A	3292	1/1	0.96	0.18	74,74,74,74	0
54	MG	1A	3287	1/1	0.96	0.07	39,39,39,39	0
54	MG	1A	4038	1/1	0.96	0.14	57,57,57,57	0
54	MG	2a	3133	1/1	0.96	0.10	64,64,64,64	0
54	MG	1A	3070	1/1	0.96	0.23	45,45,45,45	0
54	MG	17	103	1/1	0.96	0.24	41,41,41,41	0
54	MG	1A	3072	1/1	0.96	0.27	39,39,39,39	0
54	MG	1A	3508	1/1	0.96	0.13	40,40,40,40	0
54	MG	2A	3301	1/1	0.96	0.06	38,38,38,38	0
54	MG	2A	3502	1/1	0.96	0.07	47,47,47,47	0
54	MG	2A	3302	1/1	0.96	0.07	57,57,57,57	0
54	MG	2A	3303	1/1	0.96	0.10	29,29,29,29	0
54	MG	1A	3346	1/1	0.96	0.07	31,31,31,31	0
54	MG	1A	3347	1/1	0.96	0.08	42,42,42,42	0
54	MG	1B	204	1/1	0.96	0.07	51,51,51,51	0
54	MG	1A	3513	1/1	0.96	0.08	29,29,29,29	0
54	MG	1A	3781	1/1	0.96	0.08	51,51,51,51	0
54	MG	1A	3433	1/1	0.96	0.06	26,26,26,26	0
54	MG	2A	3145	1/1	0.96	0.08	44,44,44,44	0
54	MG	1A	3165	1/1	0.96	0.17	42,42,42,42	0
54	MG	2a	3150	1/1	0.96	0.11	73,73,73,73	0
54	MG	2A	3516	1/1	0.96	0.09	68,68,68,68	0
54	MG	1A	3680	1/1	0.96	0.20	55,55,55,55	0
54	MG	1A	3519	1/1	0.96	0.07	58,58,58,58	0
54	MG	2a	3155	1/1	0.96	0.09	81,81,81,81	0
54	MG	2A	3149	1/1	0.96	0.12	60,60,60,60	0
54	MG	1A	3073	1/1	0.96	0.06	47,47,47,47	0
54	MG	1a	1606	1/1	0.96	0.10	72,72,72,72	0
54	MG	1A	3911	1/1	0.96	0.09	63,63,63,63	0
54	MG	1a	1608	1/1	0.96	0.07	63,63,63,63	0
54	MG	1A	3913	1/1	0.96	0.10	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3325	1/1	0.96	0.06	36,36,36,36	0
54	MG	1A	3788	1/1	0.96	0.06	49,49,49,49	0
54	MG	2A	3327	1/1	0.96	0.16	70,70,70,70	0
54	MG	1A	3111	1/1	0.96	0.14	49,49,49,49	0
54	MG	1o	101	1/1	0.96	0.14	53,53,53,53	0
54	MG	1A	3603	1/1	0.96	0.11	36,36,36,36	0
54	MG	2A	3159	1/1	0.96	0.33	55,55,55,55	0
54	MG	1y	201	1/1	0.96	0.07	72,72,72,72	0
54	MG	1A	3253	1/1	0.96	0.28	40,40,40,40	0
54	MG	2D	306	1/1	0.96	0.08	48,48,48,48	0
54	MG	2A	3336	1/1	0.96	0.06	51,51,51,51	0
54	MG	1A	3795	1/1	0.96	0.06	36,36,36,36	0
54	MG	1A	3523	1/1	0.96	0.08	46,46,46,46	0
54	MG	2D	310	1/1	0.96	0.09	61,61,61,61	0
54	MG	2A	3340	1/1	0.96	0.10	59,59,59,59	0
54	MG	1A	3136	1/1	0.96	0.20	39,39,39,39	0
54	MG	1A	3074	1/1	0.96	0.12	32,32,32,32	0
54	MG	2A	3343	1/1	0.96	0.08	68,68,68,68	0
54	MG	1A	3925	1/1	0.96	0.07	34,34,34,34	0
54	MG	1A	3608	1/1	0.96	0.10	44,44,44,44	0
54	MG	1a	1622	1/1	0.96	0.09	55,55,55,55	0
54	MG	2A	3007	1/1	0.96	0.08	49,49,49,49	0
54	MG	1A	3929	1/1	0.96	0.08	27,27,27,27	0
54	MG	2A	3548	1/1	0.96	0.08	44,44,44,44	0
54	MG	2A	3549	1/1	0.96	0.14	39,39,39,39	0
54	MG	2A	3352	1/1	0.96	0.09	55,55,55,55	0
54	MG	2A	3009	1/1	0.96	0.07	49,49,49,49	0
54	MG	2A	3552	1/1	0.96	0.06	88,88,88,88	0
54	MG	2k	201	1/1	0.96	0.12	69,69,69,69	0
54	MG	2R	201	1/1	0.96	0.24	55,55,55,55	0
54	MG	1a	1624	1/1	0.96	0.10	54,54,54,54	0
54	MG	1A	3354	1/1	0.96	0.10	26,26,26,26	0
54	MG	1A	3692	1/1	0.96	0.07	58,58,58,58	0
54	MG	2A	3013	1/1	0.96	0.07	28,28,28,28	0
55	HGR	1A	4041	36/36	0.96	0.08	21,29,35,39	0
54	MG	2A	3014	1/1	0.96	0.09	55,55,55,55	0
54	MG	2A	3558	1/1	0.96	0.07	65,65,65,65	0
54	MG	1A	3256	1/1	0.96	0.19	43,43,43,43	0
54	MG	1A	3938	1/1	0.96	0.08	46,46,46,46	0
54	MG	1a	1630	1/1	0.96	0.11	50,50,50,50	0
54	MG	2Y	201	1/1	0.96	0.14	59,59,59,59	0
54	MG	1A	3939	1/1	0.96	0.07	69,69,69,69	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3942	1/1	0.96	0.05	60,60,60,60	0
54	MG	2A	3021	1/1	0.96	0.06	52,52,52,52	0
54	MG	23	101	1/1	0.96	0.12	62,62,62,62	0
54	MG	2A	3183	1/1	0.96	0.08	55,55,55,55	0
59	ZN	2n	102	1/1	0.96	0.07	108,108,108,108	0
54	MG	1A	3638	1/1	0.97	0.09	45,45,45,45	0
54	MG	1A	3840	1/1	0.97	0.29	39,39,39,39	0
54	MG	1A	3212	1/1	0.97	0.30	46,46,46,46	0
54	MG	1A	3113	1/1	0.97	0.26	36,36,36,36	0
54	MG	2A	3659	1/1	0.97	0.07	48,48,48,48	0
54	MG	2a	3035	1/1	0.97	0.06	46,46,46,46	0
54	MG	1A	3114	1/1	0.97	0.28	42,42,42,42	0
54	MG	2A	3313	1/1	0.97	0.06	51,51,51,51	0
54	MG	1a	1649	1/1	0.97	0.11	53,53,53,53	0
54	MG	2A	3663	1/1	0.97	0.06	43,43,43,43	0
54	MG	2A	3020	1/1	0.97	0.10	50,50,50,50	0
54	MG	1A	3023	1/1	0.97	0.16	40,40,40,40	0
54	MG	1A	3559	1/1	0.97	0.06	57,57,57,57	0
54	MG	1A	3216	1/1	0.97	0.11	53,53,53,53	0
54	MG	1A	3077	1/1	0.97	0.25	45,45,45,45	0
54	MG	1A	3979	1/1	0.97	0.08	81,81,81,81	0
54	MG	2A	3670	1/1	0.97	0.06	72,72,72,72	0
54	MG	1A	3147	1/1	0.97	0.05	37,37,37,37	0
54	MG	2A	3027	1/1	0.97	0.06	41,41,41,41	0
54	MG	1A	3117	1/1	0.97	0.18	36,36,36,36	0
54	MG	1A	3096	1/1	0.97	0.07	43,43,43,43	0
54	MG	2A	3493	1/1	0.97	0.06	57,57,57,57	0
54	MG	1A	3983	1/1	0.97	0.10	51,51,51,51	0
54	MG	1A	3182	1/1	0.97	0.16	35,35,35,35	0
54	MG	1A	3985	1/1	0.97	0.12	59,59,59,59	0
54	MG	1A	3394	1/1	0.97	0.09	35,35,35,35	0
54	MG	1A	3653	1/1	0.97	0.08	36,36,36,36	0
54	MG	1P	201	1/1	0.97	0.34	36,36,36,36	0
54	MG	1A	3988	1/1	0.97	0.04	28,28,28,28	0
54	MG	2A	3334	1/1	0.97	0.08	58,58,58,58	0
54	MG	1A	3098	1/1	0.97	0.03	22,22,22,22	0
54	MG	2A	3504	1/1	0.97	0.09	59,59,59,59	0
54	MG	1A	3122	1/1	0.97	0.33	44,44,44,44	0
54	MG	2A	3337	1/1	0.97	0.06	53,53,53,53	0
54	MG	1A	3858	1/1	0.97	0.06	43,43,43,43	0
54	MG	1A	3859	1/1	0.97	0.06	48,48,48,48	0
54	MG	1A	3185	1/1	0.97	0.17	33,33,33,33	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3187	1/1	0.97	0.27	43,43,43,43	0
54	MG	1A	3481	1/1	0.97	0.06	60,60,60,60	0
54	MG	1A	3400	1/1	0.97	0.06	64,64,64,64	0
54	MG	1A	3124	1/1	0.97	0.09	36,36,36,36	0
54	MG	1A	3331	1/1	0.97	0.07	56,56,56,56	0
54	MG	1A	3403	1/1	0.97	0.06	55,55,55,55	0
54	MG	2A	3700	1/1	0.97	0.06	64,64,64,64	0
54	MG	1A	3189	1/1	0.97	0.28	42,42,42,42	0
54	MG	2A	3050	1/1	0.97	0.15	49,49,49,49	0
54	MG	1A	3578	1/1	0.97	0.11	55,55,55,55	0
54	MG	2a	3078	1/1	0.97	0.08	69,69,69,69	0
54	MG	2A	3704	1/1	0.97	0.05	65,65,65,65	0
54	MG	1A	3229	1/1	0.97	0.16	44,44,44,44	0
54	MG	2A	3354	1/1	0.97	0.06	40,40,40,40	0
54	MG	2A	3196	1/1	0.97	0.07	61,61,61,61	0
54	MG	1A	3763	1/1	0.97	0.05	27,27,27,27	0
54	MG	1A	3079	1/1	0.97	0.17	45,45,45,45	0
54	MG	2A	3359	1/1	0.97	0.09	62,62,62,62	0
54	MG	1A	3765	1/1	0.97	0.08	50,50,50,50	0
54	MG	2A	3361	1/1	0.97	0.08	49,49,49,49	0
54	MG	1A	3053	1/1	0.97	0.11	37,37,37,37	0
54	MG	1U	203	1/1	0.97	0.31	41,41,41,41	0
54	MG	1A	3491	1/1	0.97	0.07	58,58,58,58	0
54	MG	1A	3408	1/1	0.97	0.08	39,39,39,39	0
54	MG	1A	3024	1/1	0.97	0.06	28,28,28,28	0
54	MG	1A	3338	1/1	0.97	0.12	41,41,41,41	0
54	MG	1A	3880	1/1	0.97	0.05	63,63,63,63	0
54	MG	1A	3881	1/1	0.97	0.07	48,48,48,48	0
54	MG	1A	3771	1/1	0.97	0.05	32,32,32,32	0
54	MG	1A	3773	1/1	0.97	0.10	32,32,32,32	0
54	MG	1A	3884	1/1	0.97	0.06	36,36,36,36	0
54	MG	1A	3235	1/1	0.97	0.23	42,42,42,42	0
54	MG	1W	203	1/1	0.97	0.06	56,56,56,56	0
54	MG	2a	3101	1/1	0.97	0.31	61,61,61,61	0
54	MG	1A	3156	1/1	0.97	0.21	38,38,38,38	0
54	MG	2A	3070	1/1	0.97	0.24	49,49,49,49	0
54	MG	2A	3545	1/1	0.97	0.09	59,59,59,59	0
54	MG	1A	3237	1/1	0.97	0.32	36,36,36,36	0
54	MG	1A	3342	1/1	0.97	0.05	29,29,29,29	0
54	MG	2A	3073	1/1	0.97	0.11	53,53,53,53	0
54	MG	1A	3288	1/1	0.97	0.09	37,37,37,37	0
54	MG	1A	4027	1/1	0.97	0.06	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	2A	3076	1/1	0.97	0.09	60,60,60,60	0
54	MG	1A	3678	1/1	0.97	0.07	56,56,56,56	0
54	MG	1a	1701	1/1	0.97	0.10	65,65,65,65	0
54	MG	1A	3083	1/1	0.97	0.14	40,40,40,40	0
54	MG	1A	3417	1/1	0.97	0.06	31,31,31,31	0
54	MG	2A	3392	1/1	0.97	0.12	54,54,54,54	0
54	MG	1A	3782	1/1	0.97	0.14	36,36,36,36	0
54	MG	1A	3055	1/1	0.97	0.23	34,34,34,34	0
54	MG	2A	3227	1/1	0.97	0.12	56,56,56,56	0
54	MG	2a	3119	1/1	0.97	0.05	74,74,74,74	0
54	MG	1A	3594	1/1	0.97	0.06	55,55,55,55	0
54	MG	1A	3898	1/1	0.97	0.06	29,29,29,29	0
54	MG	1A	3104	1/1	0.97	0.20	44,44,44,44	0
54	MG	1A	3242	1/1	0.97	0.27	44,44,44,44	0
54	MG	1A	3422	1/1	0.97	0.07	23,23,23,23	0
54	MG	2A	3088	1/1	0.97	0.07	47,47,47,47	0
54	MG	13	101	1/1	0.97	0.11	43,43,43,43	0
54	MG	2A	3569	1/1	0.97	0.11	73,73,73,73	0
54	MG	1A	3056	1/1	0.97	0.10	39,39,39,39	0
54	MG	1A	3244	1/1	0.97	0.21	45,45,45,45	0
54	MG	2A	3237	1/1	0.97	0.29	44,44,44,44	0
54	MG	15	101	1/1	0.97	0.11	45,45,45,45	0
54	MG	1a	1859	1/1	0.97	0.13	60,60,60,60	0
54	MG	1A	3514	1/1	0.97	0.05	43,43,43,43	0
54	MG	2A	3576	1/1	0.97	0.08	41,41,41,41	0
54	MG	1A	3426	1/1	0.97	0.05	29,29,29,29	0
54	MG	1A	3516	1/1	0.97	0.06	36,36,36,36	0
54	MG	1A	3427	1/1	0.97	0.08	36,36,36,36	0
54	MG	2A	3412	1/1	0.97	0.07	45,45,45,45	0
54	MG	2E	301	1/1	0.97	0.22	54,54,54,54	0
54	MG	1A	3246	1/1	0.97	0.28	38,38,38,38	0
54	MG	2E	305	1/1	0.97	0.07	43,43,43,43	0
54	MG	1a	1865	1/1	0.97	0.05	71,71,71,71	0
54	MG	1A	3161	1/1	0.97	0.15	45,45,45,45	0
54	MG	1A	3018	1/1	0.97	0.19	31,31,31,31	0
54	MG	1A	3800	1/1	0.97	0.06	42,42,42,42	0
54	MG	2F	304	1/1	0.97	0.22	52,52,52,52	0
54	MG	1A	3006	1/1	0.97	0.05	36,36,36,36	0
54	MG	1A	3251	1/1	0.97	0.29	41,41,41,41	0
54	MG	1A	3016	1/1	0.97	0.30	41,41,41,41	0
54	MG	1A	3356	1/1	0.97	0.11	28,28,28,28	0
54	MG	2a	3152	1/1	0.97	0.06	66,66,66,66	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3357	1/1	0.97	0.06	30,30,30,30	0
54	MG	1B	213	1/1	0.97	0.07	52,52,52,52	0
54	MG	2Q	201	1/1	0.97	0.04	58,58,58,58	0
54	MG	1A	3203	1/1	0.97	0.16	51,51,51,51	0
54	MG	2a	3157	1/1	0.97	0.09	75,75,75,75	0
54	MG	1A	3359	1/1	0.97	0.06	15,15,15,15	0
54	MG	1A	3166	1/1	0.97	0.18	41,41,41,41	0
54	MG	1A	3071	1/1	0.97	0.34	34,34,34,34	0
54	MG	1A	3928	1/1	0.97	0.04	35,35,35,35	0
54	MG	2a	3163	1/1	0.97	0.16	65,65,65,65	0
54	MG	2A	3600	1/1	0.97	0.04	50,50,50,50	0
54	MG	1A	3363	1/1	0.97	0.10	30,30,30,30	0
54	MG	1A	3618	1/1	0.97	0.06	44,44,44,44	0
54	MG	1A	3707	1/1	0.97	0.07	55,55,55,55	0
54	MG	1A	3934	1/1	0.97	0.18	48,48,48,48	0
54	MG	2W	202	1/1	0.97	0.07	68,68,68,68	0
54	MG	2X	101	1/1	0.97	0.09	67,67,67,67	0
54	MG	1A	3048	1/1	0.97	0.05	30,30,30,30	0
54	MG	1A	3815	1/1	0.97	0.07	79,79,79,79	0
54	MG	1A	3446	1/1	0.97	0.11	34,34,34,34	0
54	MG	1A	3940	1/1	0.97	0.08	69,69,69,69	0
54	MG	1A	3941	1/1	0.97	0.07	63,63,63,63	0
54	MG	1A	3307	1/1	0.97	0.11	57,57,57,57	0
54	MG	1A	3367	1/1	0.97	0.09	55,55,55,55	0
54	MG	1A	3368	1/1	0.97	0.08	48,48,48,48	0
54	MG	1g	203	1/1	0.97	0.07	65,65,65,65	0
54	MG	1A	3946	1/1	0.97	0.07	58,58,58,58	0
54	MG	1A	3715	1/1	0.97	0.10	46,46,46,46	0
54	MG	1A	3308	1/1	0.97	0.27	48,48,48,48	0
54	MG	1a	1618	1/1	0.97	0.05	53,53,53,53	0
54	MG	1A	3451	1/1	0.97	0.10	34,34,34,34	0
54	MG	1A	3626	1/1	0.97	0.06	56,56,56,56	0
54	MG	1A	3370	1/1	0.97	0.07	58,58,58,58	0
54	MG	1A	3309	1/1	0.97	0.14	41,41,41,41	0
54	MG	1A	3137	1/1	0.97	0.19	39,39,39,39	0
54	MG	1A	3021	1/1	0.97	0.23	45,45,45,45	0
54	MG	1a	1626	1/1	0.97	0.05	59,59,59,59	0
54	MG	1A	3139	1/1	0.97	0.19	33,33,33,33	0
54	MG	1A	3547	1/1	0.97	0.06	24,24,24,24	0
54	MG	1D	318	1/1	0.97	0.11	52,52,52,52	0
54	MG	1A	3140	1/1	0.97	0.25	36,36,36,36	0
54	MG	1A	3726	1/1	0.97	0.09	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3832	1/1	0.97	0.12	53,53,53,53	0
54	MG	1A	3005	1/1	0.97	0.09	30,30,30,30	0
54	MG	1A	3963	1/1	0.97	0.06	70,70,70,70	0
54	MG	1F	301	1/1	0.97	0.11	40,40,40,40	0
54	MG	1A	3380	1/1	0.97	0.08	30,30,30,30	0
56	ERY	1A	4042	51/51	0.97	0.08	20,37,45,53	0
56	ERY	2A	3732	51/51	0.97	0.09	38,48,57,63	0
54	MG	1F	305	1/1	0.97	0.12	46,46,46,46	0
54	MG	1A	3835	1/1	0.97	0.09	55,55,55,55	0
54	MG	1A	3381	1/1	0.97	0.12	41,41,41,41	0
54	MG	2a	3022	1/1	0.97	0.04	54,54,54,54	0
54	MG	2A	3469	1/1	0.97	0.09	42,42,42,42	0
54	MG	1F	308	1/1	0.97	0.13	36,36,36,36	0
54	MG	2A	3471	1/1	0.97	0.05	65,65,65,65	0
54	MG	1A	3731	1/1	0.97	0.07	50,50,50,50	0
54	MG	1F	310	1/1	0.97	0.10	45,45,45,45	0
54	MG	1A	3554	1/1	0.97	0.07	34,34,34,34	0
59	ZN	29	501	1/1	0.97	0.04	77,77,77,77	0
54	MG	2A	3654	1/1	0.97	0.06	52,52,52,52	0
60	SF4	1d	306	8/8	0.97	0.07	68,77,83,90	0
60	SF4	2d	501	8/8	0.97	0.06	74,89,98,98	0
54	MG	1V	202	1/1	0.98	0.20	38,38,38,38	0
54	MG	2E	302	1/1	0.98	0.08	53,53,53,53	0
54	MG	1A	3118	1/1	0.98	0.09	46,46,46,46	0
54	MG	1D	302	1/1	0.98	0.07	57,57,57,57	0
54	MG	2A	3637	1/1	0.98	0.04	83,83,83,83	0
54	MG	1A	3378	1/1	0.98	0.04	28,28,28,28	0
54	MG	1D	304	1/1	0.98	0.04	45,45,45,45	0
54	MG	1A	3746	1/1	0.98	0.04	57,57,57,57	0
54	MG	1A	3747	1/1	0.98	0.05	80,80,80,80	0
54	MG	2A	3643	1/1	0.98	0.07	45,45,45,45	0
54	MG	1A	3641	1/1	0.98	0.14	41,41,41,41	0
54	MG	1A	3932	1/1	0.98	0.05	21,21,21,21	0
54	MG	2A	3647	1/1	0.98	0.06	89,89,89,89	0
54	MG	2A	3648	1/1	0.98	0.06	48,48,48,48	0
54	MG	2A	3293	1/1	0.98	0.06	68,68,68,68	0
54	MG	2A	3650	1/1	0.98	0.13	62,62,62,62	0
54	MG	2A	3100	1/1	0.98	0.09	56,56,56,56	0
54	MG	1A	3933	1/1	0.98	0.07	53,53,53,53	0
54	MG	2A	3296	1/1	0.98	0.08	46,46,46,46	0
54	MG	2A	3525	1/1	0.98	0.06	62,62,62,62	0
54	MG	1A	3264	1/1	0.98	0.23	36,36,36,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3935	1/1	0.98	0.04	52,52,52,52	0
54	MG	1a	1734	1/1	0.98	0.06	46,46,46,46	0
54	MG	1A	3936	1/1	0.98	0.06	63,63,63,63	0
54	MG	1A	3240	1/1	0.98	0.17	33,33,33,33	0
54	MG	2A	3415	1/1	0.98	0.04	43,43,43,43	0
54	MG	1A	3318	1/1	0.98	0.16	44,44,44,44	0
54	MG	1A	3503	1/1	0.98	0.05	29,29,29,29	0
54	MG	1A	3382	1/1	0.98	0.05	31,31,31,31	0
54	MG	2A	3306	1/1	0.98	0.05	43,43,43,43	0
54	MG	1A	4010	1/1	0.98	0.06	57,57,57,57	0
54	MG	1A	3186	1/1	0.98	0.10	38,38,38,38	0
54	MG	1E	302	1/1	0.98	0.13	35,35,35,35	0
54	MG	1A	3078	1/1	0.98	0.26	37,37,37,37	0
54	MG	1A	3145	1/1	0.98	0.12	27,27,27,27	0
54	MG	2a	3123	1/1	0.98	0.06	61,61,61,61	0
54	MG	1A	3602	1/1	0.98	0.06	24,24,24,24	0
54	MG	1A	3421	1/1	0.98	0.07	46,46,46,46	0
54	MG	2A	3315	1/1	0.98	0.05	44,44,44,44	0
54	MG	1A	3876	1/1	0.98	0.04	39,39,39,39	0
54	MG	2A	3429	1/1	0.98	0.04	55,55,55,55	0
54	MG	13	103	1/1	0.98	0.14	45,45,45,45	0
54	MG	1F	302	1/1	0.98	0.11	39,39,39,39	0
54	MG	1F	303	1/1	0.98	0.14	38,38,38,38	0
54	MG	1A	3509	1/1	0.98	0.05	37,37,37,37	0
54	MG	1A	3463	1/1	0.98	0.05	18,18,18,18	0
54	MG	1A	3042	1/1	0.98	0.04	35,35,35,35	0
54	MG	1a	1845	1/1	0.98	0.06	70,70,70,70	0
54	MG	1A	4020	1/1	0.98	0.04	42,42,42,42	0
54	MG	1a	1848	1/1	0.98	0.06	62,62,62,62	0
54	MG	2A	3127	1/1	0.98	0.22	47,47,47,47	0
54	MG	1A	4021	1/1	0.98	0.04	54,54,54,54	0
54	MG	2A	3687	1/1	0.98	0.05	52,52,52,52	0
54	MG	1A	3512	1/1	0.98	0.12	28,28,28,28	0
54	MG	1a	1851	1/1	0.98	0.09	65,65,65,65	0
54	MG	2A	3330	1/1	0.98	0.11	63,63,63,63	0
54	MG	1A	4023	1/1	0.98	0.10	46,46,46,46	0
54	MG	1A	3423	1/1	0.98	0.11	29,29,29,29	0
54	MG	2A	3693	1/1	0.98	0.08	49,49,49,49	0
54	MG	2A	3562	1/1	0.98	0.05	30,30,30,30	0
54	MG	1A	3245	1/1	0.98	0.12	36,36,36,36	0
54	MG	2A	3564	1/1	0.98	0.06	64,64,64,64	0
54	MG	2A	3447	1/1	0.98	0.06	47,47,47,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1a	1855	1/1	0.98	0.08	39,39,39,39	0
54	MG	1A	3224	1/1	0.98	0.14	29,29,29,29	0
54	MG	1a	1857	1/1	0.98	0.05	58,58,58,58	0
54	MG	2A	3042	1/1	0.98	0.09	40,40,40,40	0
54	MG	1A	3710	1/1	0.98	0.05	51,51,51,51	0
54	MG	1A	3956	1/1	0.98	0.04	62,62,62,62	0
54	MG	1A	3468	1/1	0.98	0.04	27,27,27,27	0
54	MG	1A	3517	1/1	0.98	0.07	32,32,32,32	0
54	MG	1A	3050	1/1	0.98	0.18	39,39,39,39	0
54	MG	1a	1767	1/1	0.98	0.05	80,80,80,80	0
54	MG	1A	3123	1/1	0.98	0.04	22,22,22,22	0
54	MG	2A	3345	1/1	0.98	0.07	58,58,58,58	0
54	MG	1A	3961	1/1	0.98	0.05	48,48,48,48	0
54	MG	2A	3347	1/1	0.98	0.06	35,35,35,35	0
54	MG	2A	3348	1/1	0.98	0.09	38,38,38,38	0
54	MG	1A	3568	1/1	0.98	0.06	35,35,35,35	0
54	MG	1A	3299	1/1	0.98	0.09	22,22,22,22	0
54	MG	2A	3244	1/1	0.98	0.13	56,56,56,56	0
54	MG	1A	3090	1/1	0.98	0.10	47,47,47,47	0
54	MG	1A	3431	1/1	0.98	0.06	33,33,33,33	0
54	MG	1A	3275	1/1	0.98	0.22	41,41,41,41	0
54	MG	1A	3163	1/1	0.98	0.10	39,39,39,39	0
54	MG	2a	3174	1/1	0.98	0.10	68,68,68,68	0
54	MG	1A	3252	1/1	0.98	0.16	32,32,32,32	0
54	MG	1A	3043	1/1	0.98	0.10	22,22,22,22	0
54	MG	2A	3358	1/1	0.98	0.06	39,39,39,39	0
54	MG	1A	3672	1/1	0.98	0.11	47,47,47,47	0
54	MG	1A	3398	1/1	0.98	0.04	30,30,30,30	0
54	MG	1A	3902	1/1	0.98	0.05	67,67,67,67	0
54	MG	2A	3254	1/1	0.98	0.11	27,27,27,27	0
54	MG	1A	3230	1/1	0.98	0.05	50,50,50,50	0
54	MG	1A	3306	1/1	0.98	0.10	50,50,50,50	0
54	MG	1A	3365	1/1	0.98	0.05	38,38,38,38	0
54	MG	1A	3195	1/1	0.98	0.14	45,45,45,45	0
54	MG	1A	3336	1/1	0.98	0.10	38,38,38,38	0
54	MG	2a	3057	1/1	0.98	0.13	66,66,66,66	0
54	MG	1A	3978	1/1	0.98	0.08	56,56,56,56	0
54	MG	1A	3082	1/1	0.98	0.07	48,48,48,48	0
54	MG	1A	3534	1/1	0.98	0.04	31,31,31,31	0
54	MG	1d	305	1/1	0.98	0.04	74,74,74,74	0
54	MG	2A	3608	1/1	0.98	0.06	54,54,54,54	0
54	MG	2A	3372	1/1	0.98	0.09	35,35,35,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1R	201	1/1	0.98	0.10	44,44,44,44	0
54	MG	2A	3611	1/1	0.98	0.04	73,73,73,73	0
54	MG	1a	1621	1/1	0.98	0.04	55,55,55,55	0
54	MG	1B	214	1/1	0.98	0.05	46,46,46,46	0
54	MG	1A	3180	1/1	0.98	0.20	34,34,34,34	0
54	MG	1A	3735	1/1	0.98	0.04	43,43,43,43	0
54	MG	2A	3379	1/1	0.98	0.05	59,59,59,59	0
54	MG	1A	3912	1/1	0.98	0.03	35,35,35,35	0
54	MG	1A	3234	1/1	0.98	0.20	39,39,39,39	0
54	MG	1A	3793	1/1	0.98	0.04	45,45,45,45	0
54	MG	1A	3371	1/1	0.98	0.08	31,31,31,31	0
54	MG	2A	3498	1/1	0.98	0.04	65,65,65,65	0
54	MG	1A	3044	1/1	0.98	0.15	40,40,40,40	0
54	MG	1T	205	1/1	0.98	0.10	54,54,54,54	0
54	MG	1A	3540	1/1	0.98	0.05	27,27,27,27	0
54	MG	1A	3007	1/1	0.98	0.08	42,42,42,42	0
54	MG	1A	3037	1/1	0.98	0.09	47,47,47,47	0
54	MG	1A	3857	1/1	0.98	0.05	42,42,42,42	0
54	MG	1A	3029	1/1	0.98	0.10	48,48,48,48	0
59	ZN	15	109	1/1	0.98	0.03	46,46,46,46	0
59	ZN	2Y	202	1/1	0.98	0.05	94,94,94,94	0
54	MG	1A	3743	1/1	0.98	0.04	35,35,35,35	0
59	ZN	26	501	1/1	0.98	0.05	75,75,75,75	0
54	MG	1a	1807	1/1	0.98	0.04	83,83,83,83	0
54	MG	2A	3509	1/1	0.98	0.07	49,49,49,49	0
54	MG	1A	3926	1/1	0.98	0.04	53,53,53,53	0
54	MG	1V	201	1/1	0.98	0.20	35,35,35,35	0
54	MG	1A	3989	1/1	0.99	0.07	40,40,40,40	0
54	MG	1A	3013	1/1	0.99	0.03	23,23,23,23	0
54	MG	2A	3579	1/1	0.99	0.04	59,59,59,59	0
54	MG	2a	3159	1/1	0.99	0.06	51,51,51,51	0
54	MG	1a	1844	1/1	0.99	0.04	61,61,61,61	0
54	MG	1A	3097	1/1	0.99	0.19	38,38,38,38	0
54	MG	2A	3644	1/1	0.99	0.06	49,49,49,49	0
54	MG	2A	3582	1/1	0.99	0.05	56,56,56,56	0
54	MG	1a	1846	1/1	0.99	0.03	61,61,61,61	0
54	MG	1D	306	1/1	0.99	0.04	20,20,20,20	0
54	MG	1A	3549	1/1	0.99	0.03	49,49,49,49	0
54	MG	1A	3914	1/1	0.99	0.08	44,44,44,44	0
54	MG	1A	3550	1/1	0.99	0.06	37,37,37,37	0
54	MG	2A	3304	1/1	0.99	0.05	69,69,69,69	0
54	MG	1A	3916	1/1	0.99	0.03	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3917	1/1	0.99	0.07	39,39,39,39	0
54	MG	1A	3046	1/1	0.99	0.05	14,14,14,14	0
54	MG	1A	3789	1/1	0.99	0.03	36,36,36,36	0
54	MG	1A	3009	1/1	0.99	0.10	33,33,33,33	0
54	MG	2A	3594	1/1	0.99	0.05	43,43,43,43	0
54	MG	2A	3310	1/1	0.99	0.10	50,50,50,50	0
54	MG	1A	3851	1/1	0.99	0.05	50,50,50,50	0
54	MG	1A	3711	1/1	0.99	0.03	37,37,37,37	0
54	MG	1A	3475	1/1	0.99	0.04	34,34,34,34	0
54	MG	1A	3688	1/1	0.99	0.03	50,50,50,50	0
54	MG	1A	3794	1/1	0.99	0.06	47,47,47,47	0
54	MG	2a	3182	1/1	0.99	0.03	68,68,68,68	0
54	MG	2A	3601	1/1	0.99	0.04	42,42,42,42	0
54	MG	1A	3493	1/1	0.99	0.02	44,44,44,44	0
54	MG	1A	3494	1/1	0.99	0.04	35,35,35,35	0
54	MG	1E	304	1/1	0.99	0.14	34,34,34,34	0
54	MG	1A	3476	1/1	0.99	0.04	35,35,35,35	0
54	MG	1E	306	1/1	0.99	0.07	50,50,50,50	0
54	MG	1A	3535	1/1	0.99	0.07	28,28,28,28	0
54	MG	1A	3646	1/1	0.99	0.10	38,38,38,38	0
54	MG	2A	3377	1/1	0.99	0.06	46,46,46,46	0
54	MG	1A	3374	1/1	0.99	0.08	34,34,34,34	0
54	MG	2A	3674	1/1	0.99	0.07	62,62,62,62	0
54	MG	1A	3894	1/1	0.99	0.04	36,36,36,36	0
54	MG	2A	3381	1/1	0.99	0.06	45,45,45,45	0
54	MG	1A	3862	1/1	0.99	0.03	27,27,27,27	0
54	MG	1A	3896	1/1	0.99	0.06	44,44,44,44	0
54	MG	1A	3772	1/1	0.99	0.10	39,39,39,39	0
54	MG	1a	1822	1/1	0.99	0.04	61,61,61,61	0
54	MG	1A	3075	1/1	0.99	0.04	39,39,39,39	0
54	MG	1A	3436	1/1	0.99	0.04	34,34,34,34	0
54	MG	1A	3900	1/1	0.99	0.06	50,50,50,50	0
54	MG	1A	3247	1/1	0.99	0.20	33,33,33,33	0
54	MG	1A	3438	1/1	0.99	0.05	35,35,35,35	0
54	MG	1A	3806	1/1	0.99	0.05	44,44,44,44	0
54	MG	1A	3482	1/1	0.99	0.03	62,62,62,62	0
54	MG	1a	1736	1/1	0.99	0.06	45,45,45,45	0
54	MG	2A	3507	1/1	0.99	0.06	40,40,40,40	0
54	MG	1B	223	1/1	0.99	0.03	55,55,55,55	0
54	MG	1A	3386	1/1	0.99	0.02	19,19,19,19	0
54	MG	1A	3944	1/1	0.99	0.05	56,56,56,56	0
54	MG	1A	4024	1/1	0.99	0.03	69,69,69,69	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	MG	1A	3360	1/1	0.99	0.05	43,43,43,43	0
59	ZN	1Y	202	1/1	0.99	0.06	61,61,61,61	0
59	ZN	14	102	1/1	0.99	0.04	94,94,94,94	0
54	MG	1a	1836	1/1	0.99	0.09	67,67,67,67	0
59	ZN	16	501	1/1	0.99	0.05	49,49,49,49	0
59	ZN	19	103	1/1	0.99	0.04	45,45,45,45	0
59	ZN	1n	103	1/1	0.99	0.03	79,79,79,79	0
54	MG	1A	3454	1/1	0.99	0.04	39,39,39,39	0
54	MG	1A	3728	1/1	0.99	0.03	48,48,48,48	0
59	ZN	25	104	1/1	0.99	0.06	68,68,68,68	0
54	MG	2A	3135	1/1	0.99	0.06	38,38,38,38	0
54	MG	1A	3428	1/1	0.99	0.04	28,28,28,28	0
54	MG	1a	1791	1/1	0.99	0.04	77,77,77,77	0
54	MG	1A	3121	1/1	0.99	0.19	38,38,38,38	0
54	MG	2E	304	1/1	0.99	0.05	62,62,62,62	0
54	MG	2A	3642	1/1	1.00	0.03	62,62,62,62	0
54	MG	2A	3492	1/1	1.00	0.06	42,42,42,42	0
54	MG	2A	3380	1/1	1.00	0.04	40,40,40,40	0
54	MG	1A	3500	1/1	1.00	0.09	51,51,51,51	0

6.5 Other polymers (i)

There are no such residues in this entry.