Full wwPDB X-ray Structure Validation Report (i)

Mar 9, 2026 – 01:46 AM UTC

PDB ID	:	7U2H / pdb_00007u2h
Title	:	Crystal structure of the Thermus thermophilus 70S ribosome in complex with mRNA, aminoacylated A-site Gly-NH-tRNAgly, aminoacylated P-site fMet-NH-tRNAmet, and deacylated E-site tRNAgly at 2.55A resolution
Authors	:	Syroegin, E.A.; Aleksandrova, E.V.; Polikanov, Y.S.
Deposited on	:	2022-02-24
Resolution	:	2.55 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 (i) 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 (i)) were used in the production of this report:

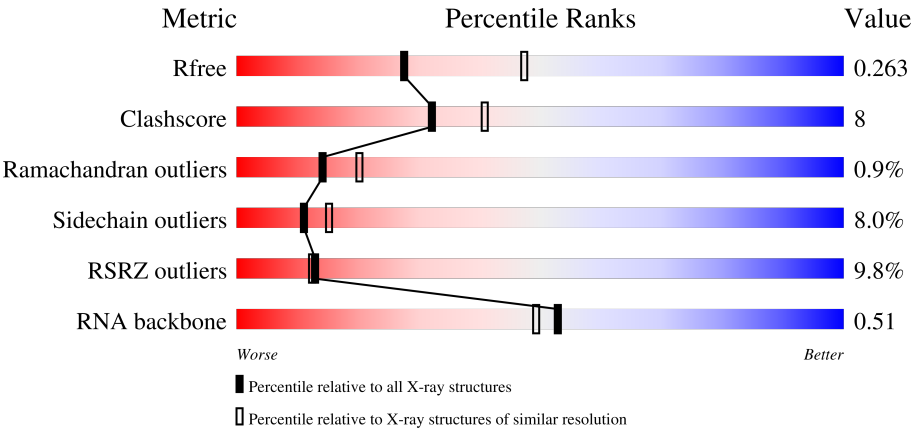
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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.



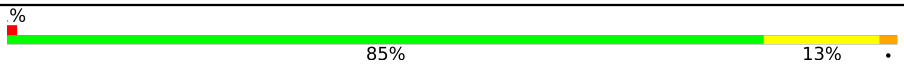
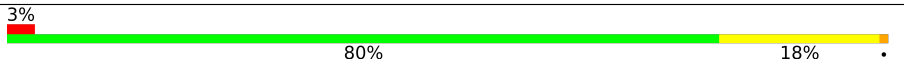
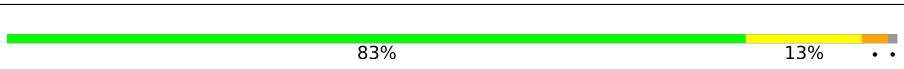
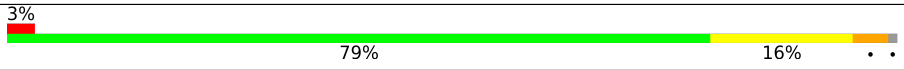
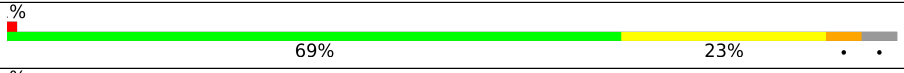
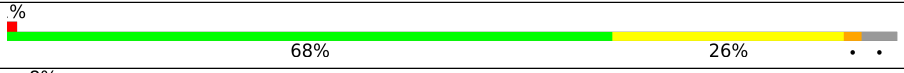
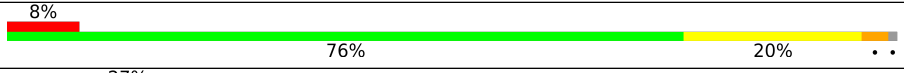
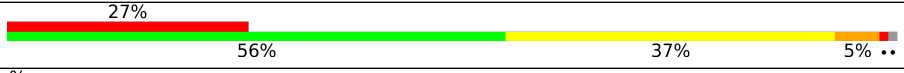
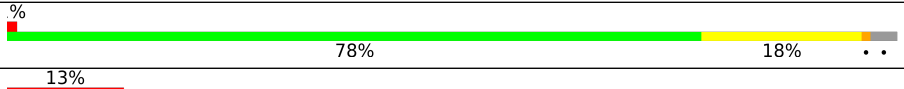
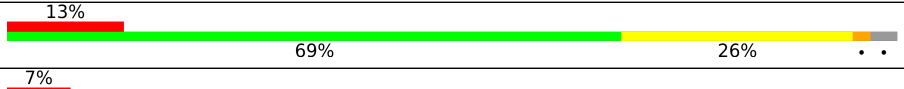
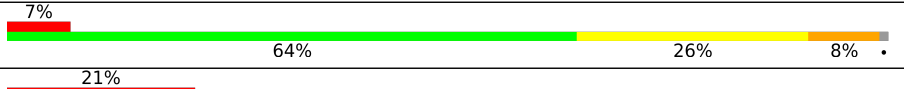
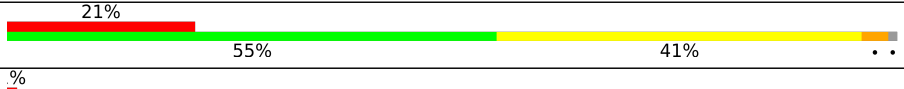
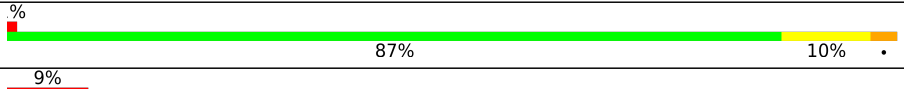
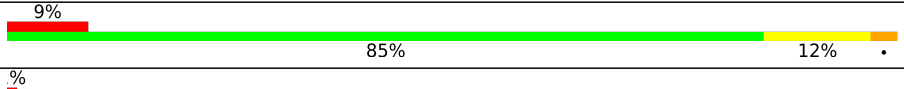
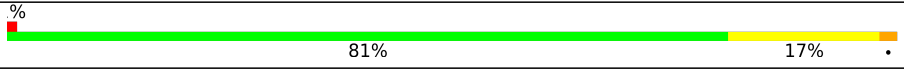
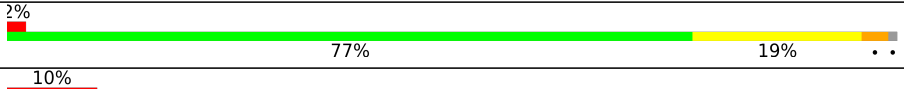
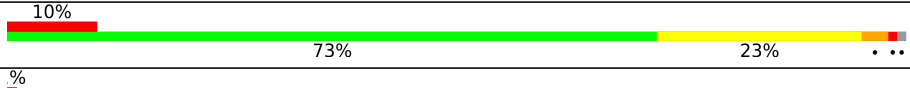
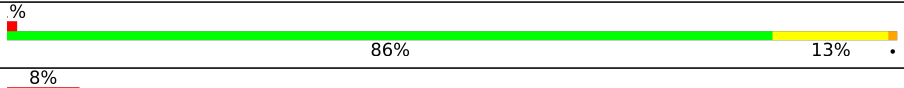
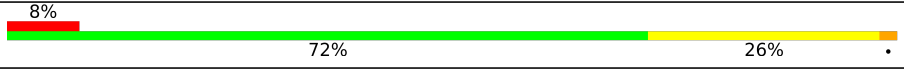
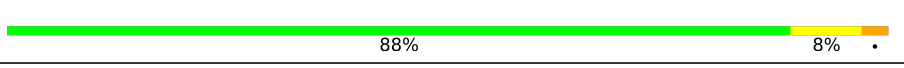
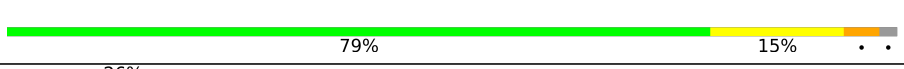
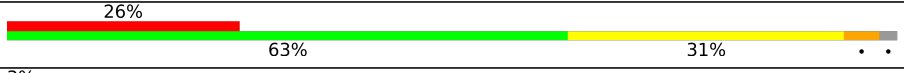
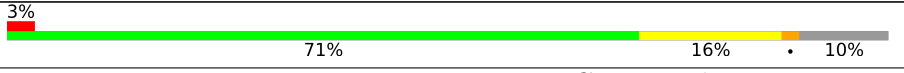
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)
RNA backbone	3983	1112 (2.80-2.28)

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	5% 69% 23% 6% ·
1	2A	2915	5% 62% 29% 6% ·
2	1B	121	74% 24% ··
2	2B	121	3% 47% 42% 10% ·

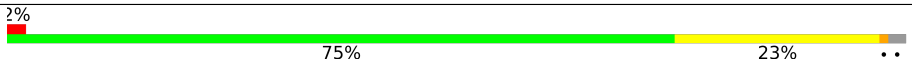
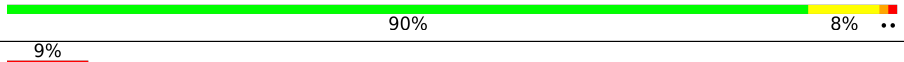
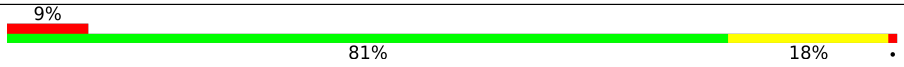
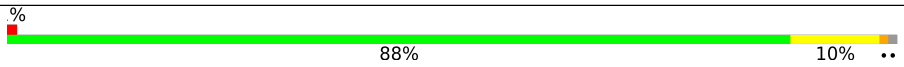
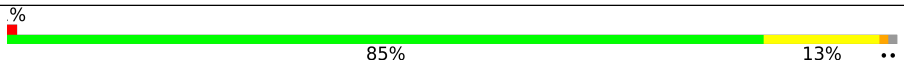
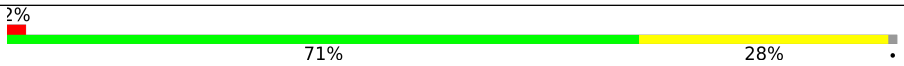
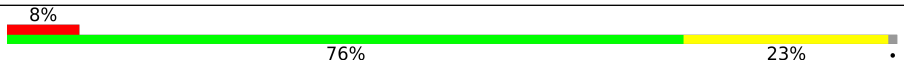
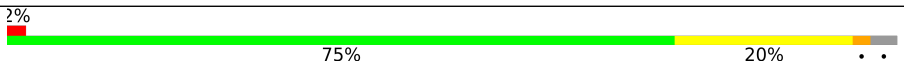
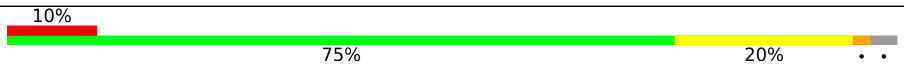
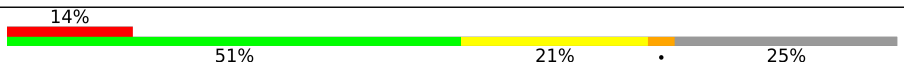
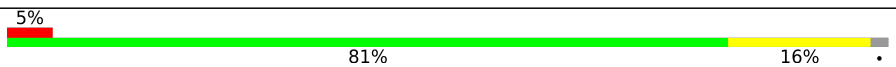
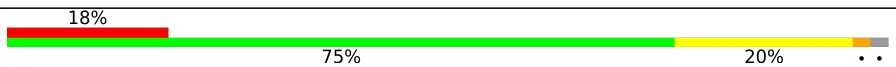
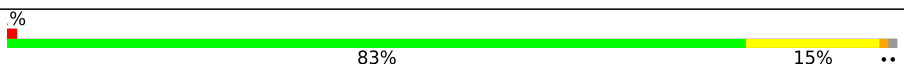
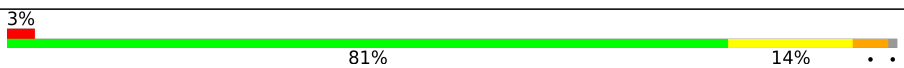
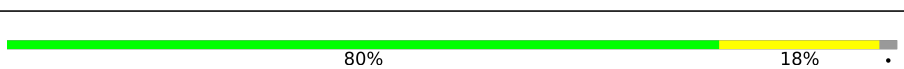
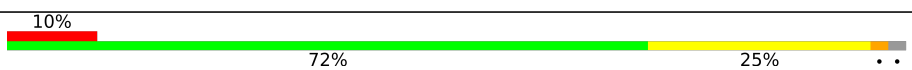
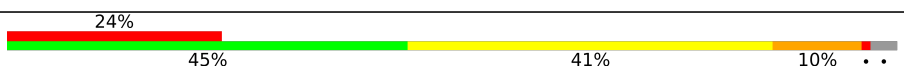
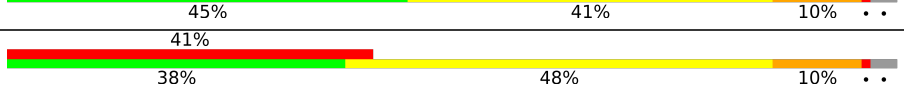
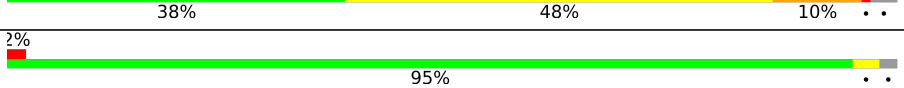
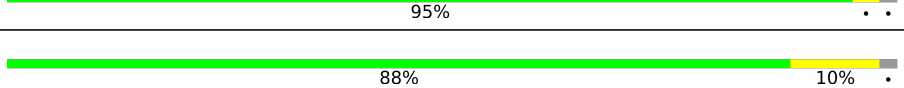
Continued on next page...

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	

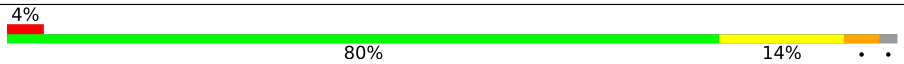
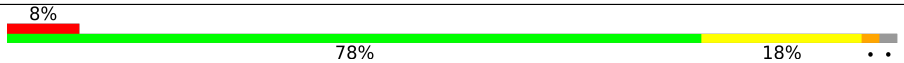
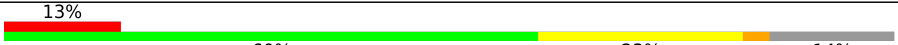
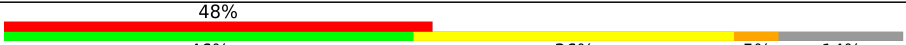
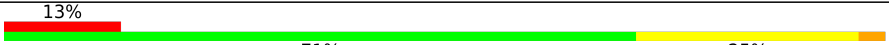
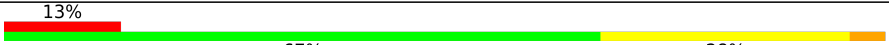
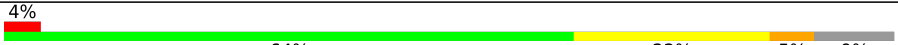
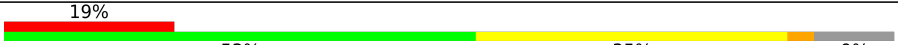
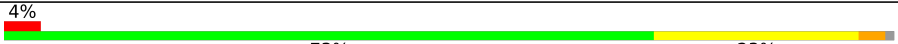
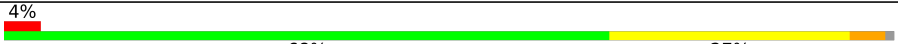
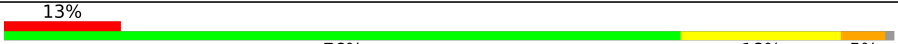
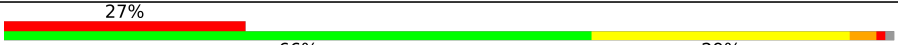
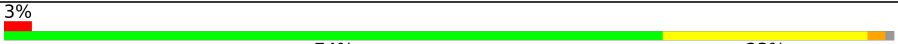
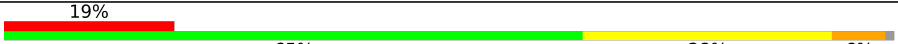
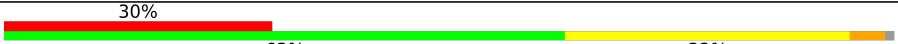
Continued on next page...

Continued from previous page...

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

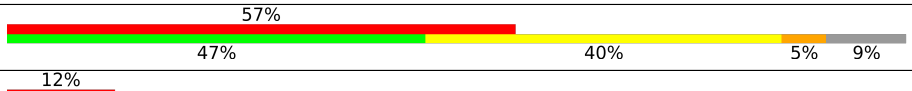
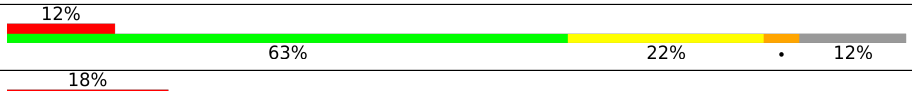
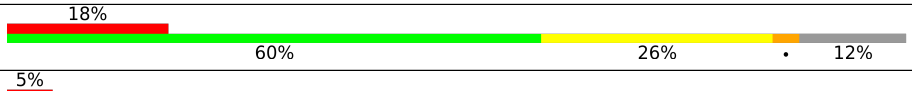
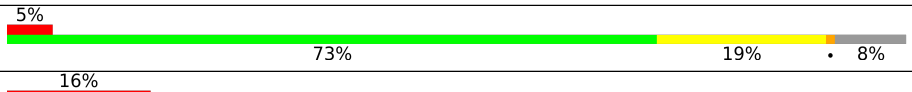
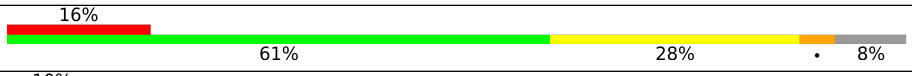
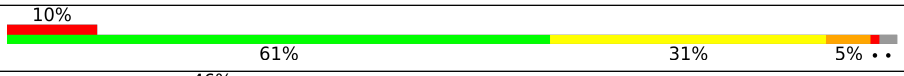
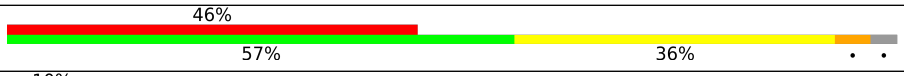
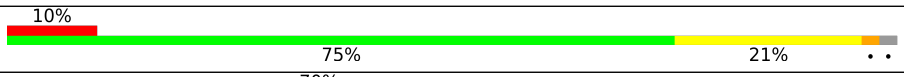
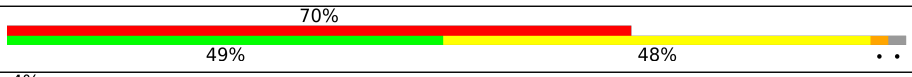
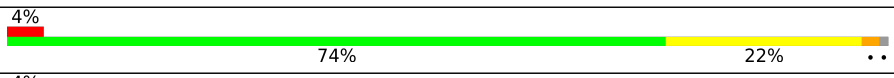
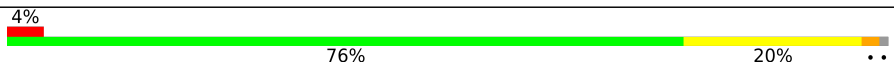
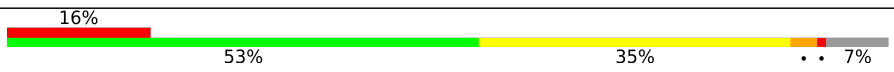
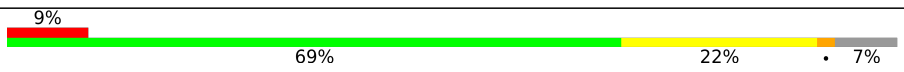
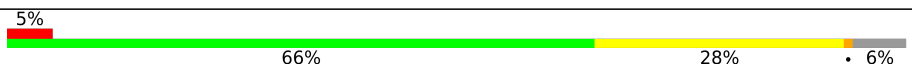
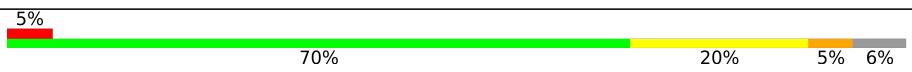
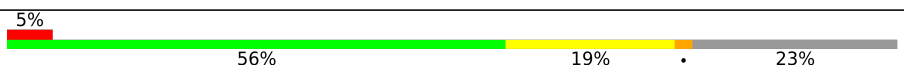
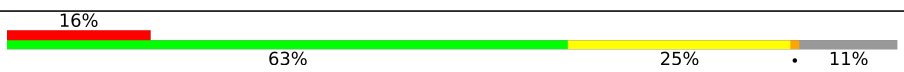
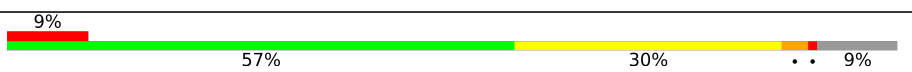
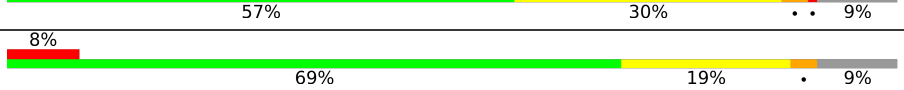
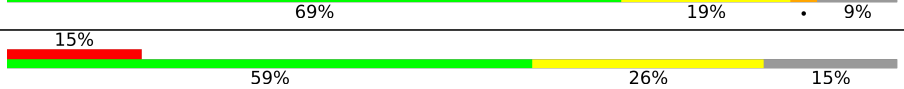
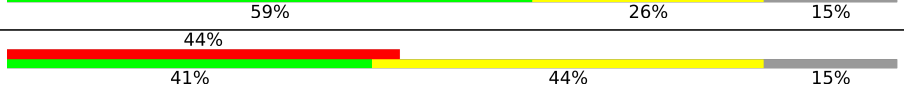
Continued on next page...

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	1v	24	21% 38% 17% 46%
53	2v	24	21% 42% 8% 46%
54	1w	74	27% 28% 45% 26%
54	2w	74	49% 34% 30% 32%
55	1x	77	3% 74% 23%
55	2x	77	4% 71% 25%
56	1y	74	64% 35% 38% 26%
56	2y	74	49% 26% 39% 32%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	2A	3423	-	-	-	X
57	MG	2a	1725	-	-	-	X
57	MG	2a	1743	-	-	-	X

2 Entry composition (i)

There are 61 unique types of molecules in this entry. The entry contains 299852 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	2O	122	Total 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 873	C 550	N 174	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
			771	495	140	135	1			
17	2V	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1v	13	Total	C	N	O	P	0	0	0
			286	128	59	86	13			
53	2v	13	Total	C	N	O	P	0	0	0
			286	128	59	86	13			

- Molecule 54 is a RNA chain called A-site Aminoacyl-tRNA Gly-NH-tRNAgly.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1w	73	Total	C	N	O	P	S	0	0	0
			1556	695	275	512	73	1			
54	2w	72	Total	C	N	O	P	S	0	0	0
			1536	686	273	504	72	1			

- Molecule 55 is a RNA chain called P-site Aminoacyl-tRNA fMet-NH-tRNAmet.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
55	1x	77	Total	C	N	O	P	S	0	0	0
			1656	740	299	538	77	2			
55	2x	77	Total	C	N	O	P	S	0	0	0
			1656	740	299	538	77	2			

- Molecule 56 is a RNA chain called E-site Deacylated tRNAgly.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
56	1y	73	Total	C	N	O	P	S	0	0	0
			1552	693	273	512	73	1			
56	2y	73	Total	C	N	O	P	S	0	0	0
			1552	693	273	512	73	1			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1A	1096	Total	Mg	0	0
			1096	1096		
57	1B	36	Total	Mg	0	0
			36	36		
57	1D	12	Total	Mg	0	0
			12	12		
57	1E	16	Total	Mg	0	0
			16	16		
57	1F	15	Total	Mg	0	0
			15	15		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	1G	4	Total Mg 4 4	0	0
57	1I	1	Total Mg 1 1	0	0
57	1N	6	Total Mg 6 6	0	0
57	1O	5	Total Mg 5 5	0	0
57	1P	6	Total Mg 6 6	0	0
57	1Q	7	Total Mg 7 7	0	0
57	1R	6	Total Mg 6 6	0	0
57	1S	3	Total Mg 3 3	0	0
57	1T	2	Total Mg 2 2	0	0
57	1U	9	Total Mg 9 9	0	0
57	1V	7	Total Mg 7 7	0	0
57	1W	7	Total Mg 7 7	0	0
57	1X	6	Total Mg 6 6	0	0
57	1Y	2	Total Mg 2 2	0	0
57	1Z	2	Total Mg 2 2	0	0
57	10	9	Total Mg 9 9	0	0
57	11	2	Total Mg 2 2	0	0
57	12	1	Total Mg 1 1	0	0
57	13	5	Total Mg 5 5	0	0
57	14	1	Total Mg 1 1	0	0
57	15	7	Total Mg 7 7	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	16	3	Total Mg 3 3	0	0
57	17	5	Total Mg 5 5	0	0
57	18	6	Total Mg 6 6	0	0
57	19	1	Total Mg 1 1	0	0
57	1a	224	Total Mg 224 224	0	0
57	1b	2	Total Mg 2 2	0	0
57	1e	2	Total Mg 2 2	0	0
57	1f	1	Total Mg 1 1	0	0
57	1h	1	Total Mg 1 1	0	0
57	1l	2	Total Mg 2 2	0	0
57	1m	2	Total Mg 2 2	0	0
57	1n	2	Total Mg 2 2	0	0
57	1r	1	Total Mg 1 1	0	0
57	1t	1	Total Mg 1 1	0	0
57	1w	9	Total Mg 9 9	0	0
57	1x	12	Total Mg 12 12	0	0
57	2A	861	Total Mg 861 861	0	0
57	2B	18	Total Mg 18 18	0	0
57	2D	7	Total Mg 7 7	0	0
57	2E	9	Total Mg 9 9	0	0
57	2F	6	Total Mg 6 6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	2G	1	Total Mg 1 1	0	0
57	2N	1	Total Mg 1 1	0	0
57	2O	1	Total Mg 1 1	0	0
57	2P	2	Total Mg 2 2	0	0
57	2Q	4	Total Mg 4 4	0	0
57	2R	2	Total Mg 2 2	0	0
57	2T	3	Total Mg 3 3	0	0
57	2U	2	Total Mg 2 2	0	0
57	2V	3	Total Mg 3 3	0	0
57	2W	2	Total Mg 2 2	0	0
57	2X	2	Total Mg 2 2	0	0
57	2Y	1	Total Mg 1 1	0	0
57	2Z	1	Total Mg 1 1	0	0
57	20	2	Total Mg 2 2	0	0
57	21	2	Total Mg 2 2	0	0
57	23	3	Total Mg 3 3	0	0
57	25	5	Total Mg 5 5	0	0
57	26	1	Total Mg 1 1	0	0
57	27	2	Total Mg 2 2	0	0
57	28	3	Total Mg 3 3	0	0
57	2a	226	Total Mg 226 226	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	2d	2	Total Mg 2 2	0	0
57	2e	1	Total Mg 1 1	0	0
57	2f	1	Total Mg 1 1	0	0
57	2g	1	Total Mg 1 1	0	0
57	2i	1	Total Mg 1 1	0	0
57	2j	2	Total Mg 2 2	0	0
57	2k	1	Total Mg 1 1	0	0
57	2l	3	Total Mg 3 3	0	0
57	2q	2	Total Mg 2 2	0	0
57	2r	2	Total Mg 2 2	0	0
57	2t	1	Total Mg 1 1	0	0
57	2v	2	Total Mg 2 2	0	0
57	2w	4	Total Mg 4 4	0	0
57	2x	6	Total Mg 6 6	0	0

- Molecule 58 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	1A	1	Total K 1 1	0	0
58	2A	1	Total K 1 1	0	0

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

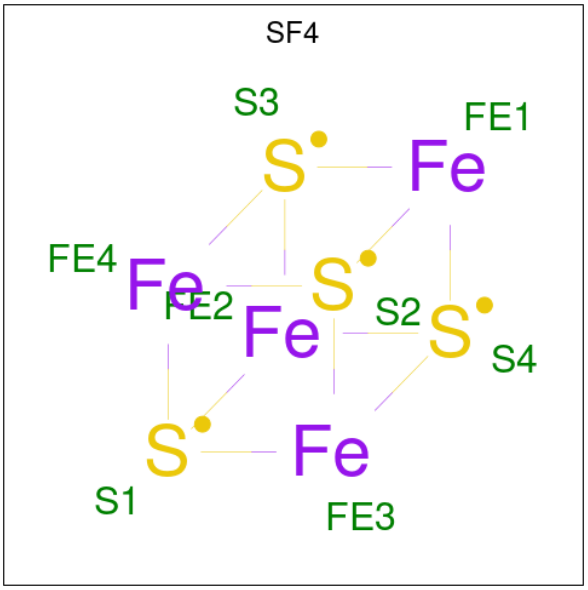
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	1Y	1	Total Zn 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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
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	1984	Total O 1984 1984	0	0
61	1B	63	Total O 63 63	0	0
61	1D	27	Total O 27 27	0	0
61	1E	27	Total O 27 27	0	0
61	1F	17	Total O 17 17	0	0
61	1G	4	Total O 4 4	0	0
61	1H	2	Total O 2 2	0	0
61	1I	1	Total O 1 1	0	0
61	1N	4	Total O 4 4	0	0
61	1O	5	Total O 5 5	0	0
61	1P	17	Total O 17 17	0	0
61	1Q	8	Total O 8 8	0	0
61	1R	6	Total O 6 6	0	0
61	1S	2	Total O 2 2	0	0
61	1T	9	Total O 9 9	0	0
61	1U	10	Total O 10 10	0	0
61	1V	11	Total O 11 11	0	0
61	1W	9	Total O 9 9	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1X	6	Total O 6 6	0	0
61	1Y	4	Total O 4 4	0	0
61	10	12	Total O 12 12	0	0
61	11	8	Total O 8 8	0	0
61	12	3	Total O 3 3	0	0
61	13	6	Total O 6 6	0	0
61	15	7	Total O 7 7	0	0
61	16	4	Total O 4 4	0	0
61	17	9	Total O 9 9	0	0
61	18	12	Total O 12 12	0	0
61	1a	278	Total O 278 278	0	0
61	1b	1	Total O 1 1	0	0
61	1d	1	Total O 1 1	0	0
61	1e	1	Total O 1 1	0	0
61	1f	1	Total O 1 1	0	0
61	1i	1	Total O 1 1	0	0
61	1l	6	Total O 6 6	0	0
61	1m	1	Total O 1 1	0	0
61	1o	1	Total O 1 1	0	0
61	1q	3	Total O 3 3	0	0
61	1u	1	Total O 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1v	4	Total O 4 4	0	0
61	1w	7	Total O 7 7	0	0
61	1x	12	Total O 12 12	0	0
61	1y	1	Total O 1 1	0	0
61	2A	1142	Total O 1142 1142	0	0
61	2B	21	Total O 21 21	0	0
61	2D	28	Total O 28 28	0	0
61	2E	12	Total O 12 12	0	0
61	2F	17	Total O 17 17	0	0
61	2I	1	Total O 1 1	0	0
61	2N	1	Total O 1 1	0	0
61	2O	1	Total O 1 1	0	0
61	2P	8	Total O 8 8	0	0
61	2Q	1	Total O 1 1	0	0
61	2R	4	Total O 4 4	0	0
61	2T	5	Total O 5 5	0	0
61	2U	2	Total O 2 2	0	0
61	2W	2	Total O 2 2	0	0
61	2X	3	Total O 3 3	0	0
61	2Y	1	Total O 1 1	0	0
61	2Z	1	Total O 1 1	0	0

Continued on next page...

Continued from previous page...

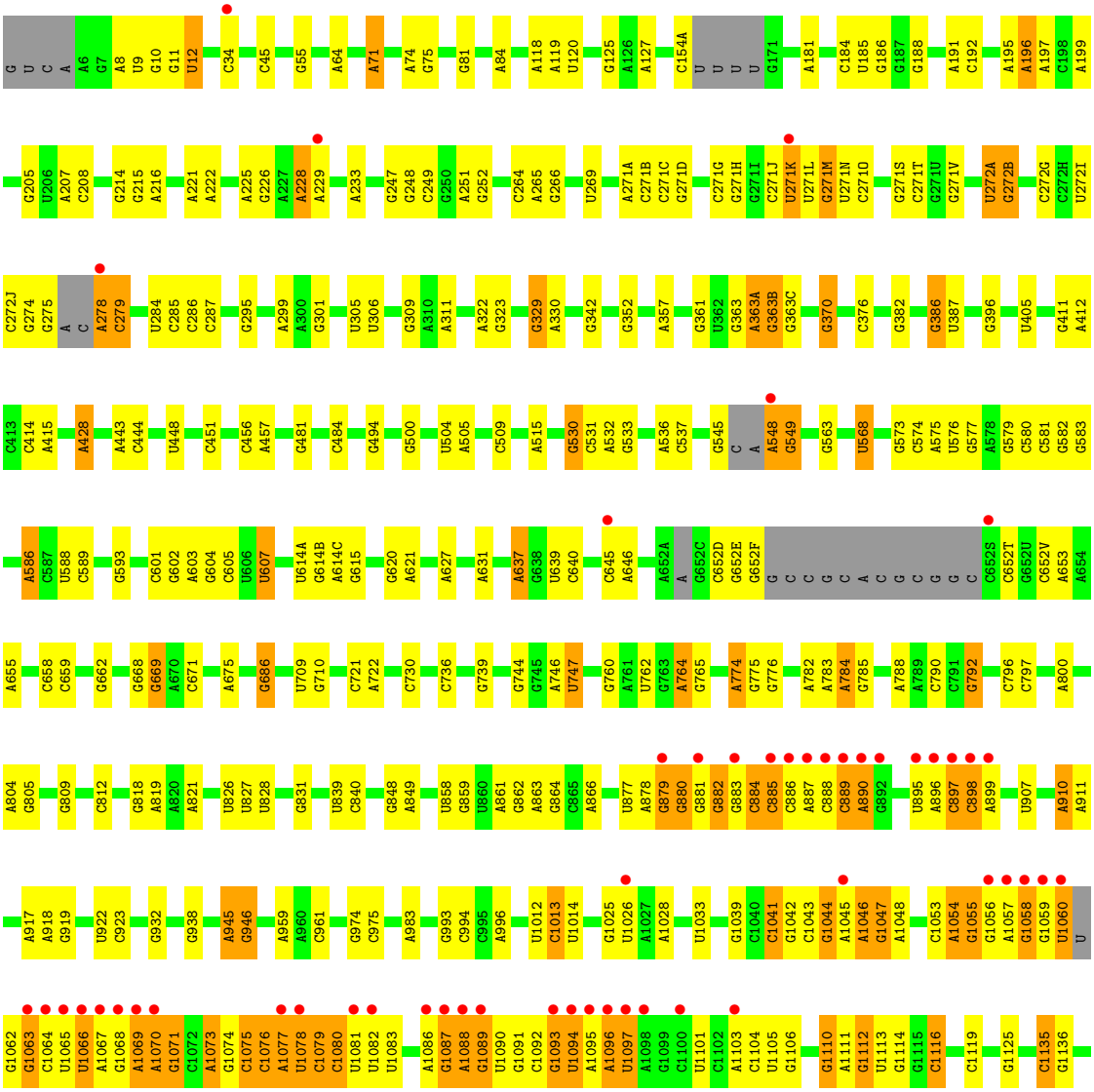
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	20	3	Total O 3 3	0	0
61	21	9	Total O 9 9	0	0
61	23	2	Total O 2 2	0	0
61	25	2	Total O 2 2	0	0
61	27	4	Total O 4 4	0	0
61	28	6	Total O 6 6	0	0
61	29	1	Total O 1 1	0	0
61	2a	210	Total O 210 210	0	0
61	2d	1	Total O 1 1	0	0
61	2g	1	Total O 1 1	0	0
61	2i	1	Total O 1 1	0	0
61	2j	2	Total O 2 2	0	0
61	2l	3	Total O 3 3	0	0
61	2p	1	Total O 1 1	0	0
61	2q	2	Total O 2 2	0	0
61	2r	1	Total O 1 1	0	0
61	2t	3	Total O 3 3	0	0
61	2v	1	Total O 1 1	0	0
61	2w	1	Total O 1 1	0	0
61	2x	3	Total O 3 3	0	0

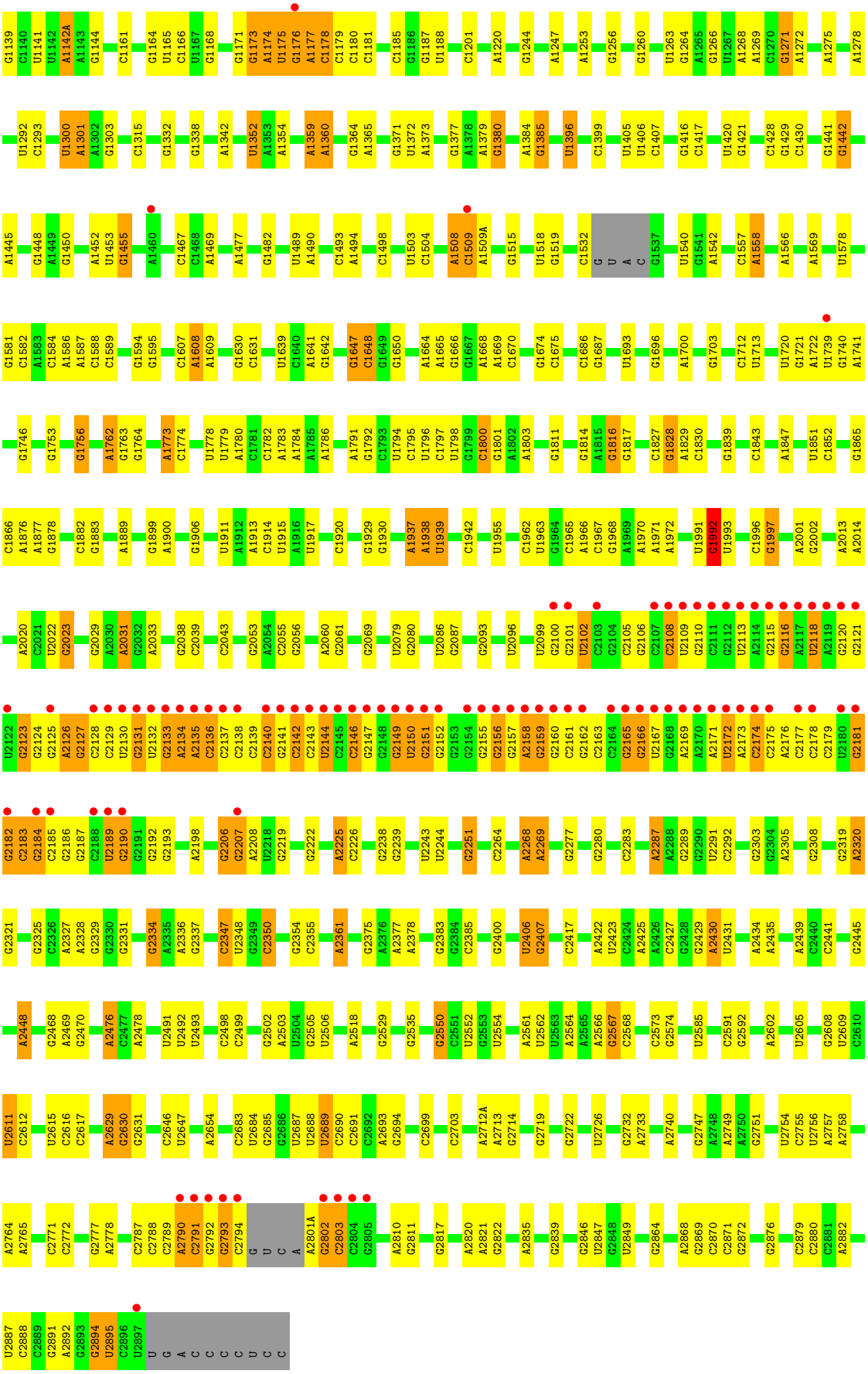
3 Residue-property plots (i)

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

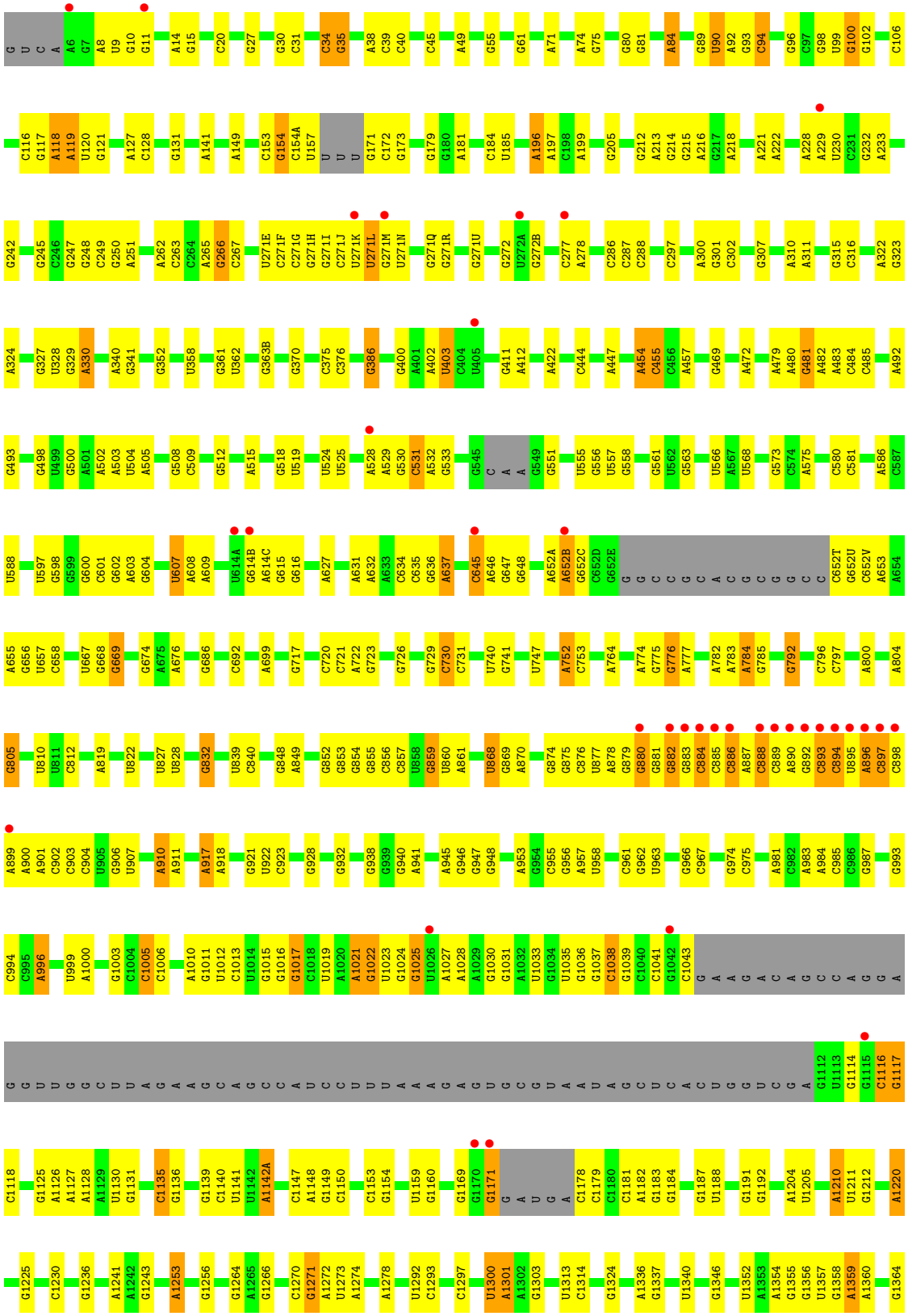
Chain 1A:

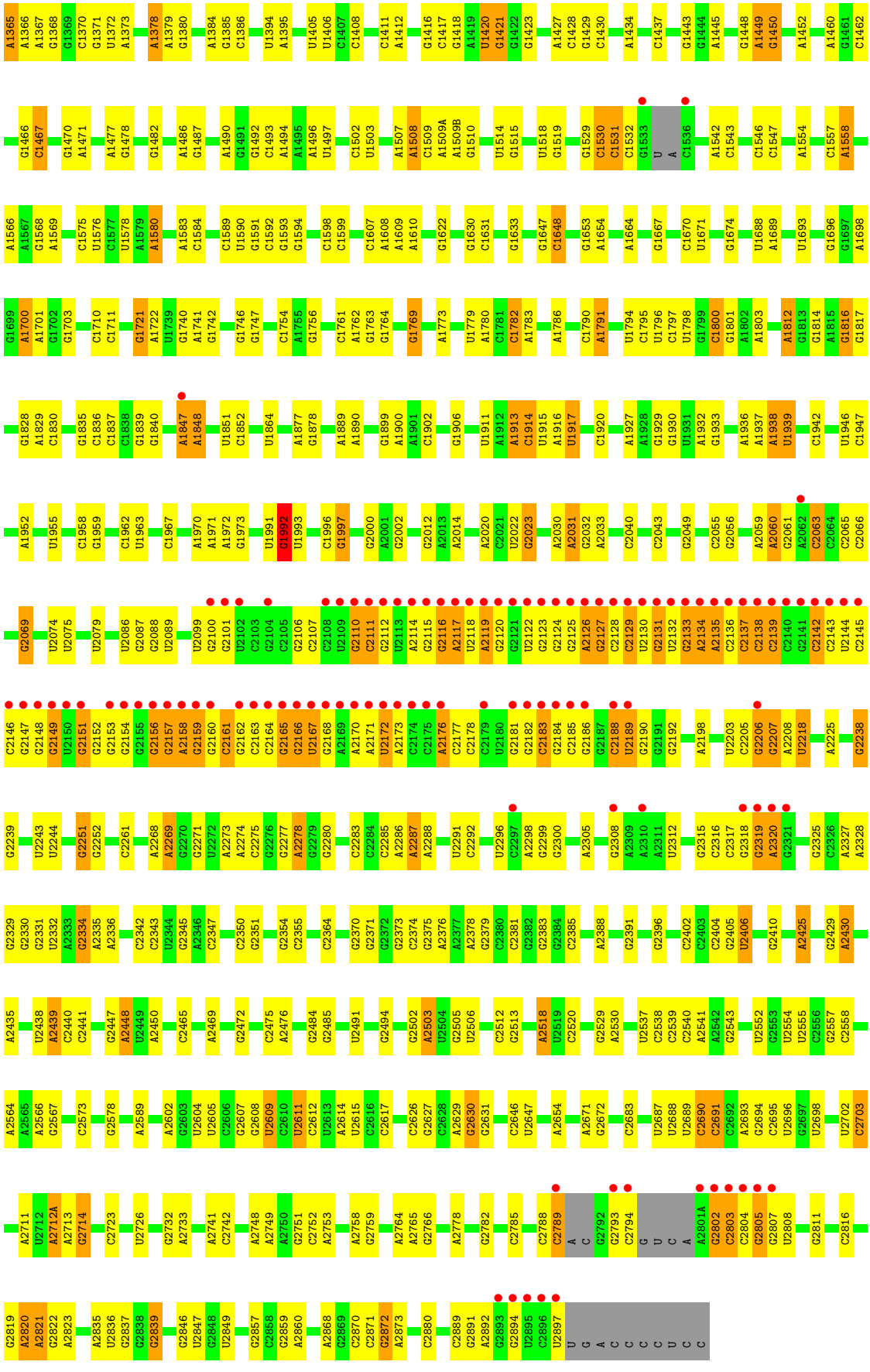



G1139 C1140 U1141 U1142 A1142A A1143 G1144 C1161 G1164 U1165 C1166 U1167 G1168 G1171 G1173 A1174 U1175 G1176 A1177 C1178 C1179 C1180 C1181 C1185 G1186 G1187 U1188 C1201 A1220 G1244 A1247 A1253 G1256 G1260 U1263 G1264 A1265 G1266 U1267 A1268 A1269 C1270 G1271 A1272 A1275 A1278
U1292 C1293 U1300 A1301 A1302 G1303 C1315 G1332 G1338 A1342 U1352 A1353 A1354 A1359 A1360 G1364 A1365 G1371 U1372 A1373 G1377 A1378 A1379 G1380 A1384 G1385 U1396 C1399 U1405 U1406 C1407 G1416 C1417 U1420 G1421 C1428 G1429 C1430 G1441 G1442
A1445 G1448 A1449 G1450 A1452 U1453 G1455 A1460 C1467 C1468 A1469 A1477 G1482 U1489 A1490 C1493 A1494 C1498 U1503 C1504 A1508 C1509 A1509A G1515 U1518 G1519 C1532 G U A C G1537 U1540 G1541 A1542 C1557 A1558 A1566 A1569 U1578
G1581 C1582 A1583 C1584 A1586 A1587 C1588 C1589 G1594 G1595 C1607 A1608 A1609 G1630 C1631 U1639 C1640 A1641 G1642 G1647 C1648 G1649 G1650 A1664 A1665 G1666 G1667 A1668 A1669 C1670 G1674 C1675 C1686 G1687 U1693 G1696 A1700 G1703 C1712 U1713 U1720 G1721 A1722 G1739 G1740 A1741
G1746 G1753 G1756 A1762 G1763 G1764 A1773 C1774 U1778 U1779 A1780 C1781 C1782 A1783 A1784 A1785 A1786 A1791 G1792 C1793 U1794 C1795 U1796 C1797 U1798 G1799 C1800 G1801 A1802 A1803 G1811 G1814 A1815 G1816 G1817 C1827 G1828 A1829 C1830 G1839 C1843 A1847 U1851 C1852 G1865
C1866 A1876 A1877 G1878 C1882 G1883 A1889 G1899 A1900 G1906 U1911 A1912 A1913 C1914 U1915 A1916 U1917 C1920 G1929 G1930 A1937 A1938 U1939 C1942 U1955 C1962 U1963 G1964 C1965 A1966 C1967 G1968 A1969 A1970 A1971 A1972 U1991 G1992 U1993 C1996 G1997 A2001 G2002 A2013 A2014
A2020 C2021 U2022 G2023 G2029 A2030 A2031 G2032 A2033 G2038 C2039 C2043 C2053 A2054 C2055 G2056 A2060 G2061 G2069 U2079 G2080 U2086 G2087 G2093 U2096 U2099 G2100 G2101 U2102 C2103 G2104 C2105 G2106 C2107 C2108 U2109 G2110 C2111 G2112 U2113 A2114 G2115 G2116 A2117 U2118 A2119 G2120 G2121
U2122 G2123 G2124 G2125 A2126 G2127 C2128 C2129 U2130 G2131 U2132 G2133 A2134 A2135 C2136 C2137 C2138 C2139 C2140 G2141 C2142 C2143 U2144 C2145 C2146 G2147 G2148 G2149 U2150 G2151 G2152 G2153 G2154 G2155 G2156 G2157 A2158 G2159 G2160 C2161 G2162 C2163 C2164 G2165 G2166 U2167 G2168 A2169 A2170 A2171 U2172 A2173 C2174 C2175 A2176 C2177 C2178 C2179 U2180 G2181
G2182 C2183 G2184 C2185 G2186 G2187 C2188 U2189 C2190 G2191 G2192 G2193 A2198 G2206 G2207 A2208 U2218 G2219 G2222 A2225 C2226 G2238 G2239 U2243 U2244 G2251 C2264 A2268 A2269 G2277 G2280 C2283 A2287 A2288 G2289 G2290 U2291 C2292 G2303 G2304 A2305 G2308 G2319 A2320
G2321 G2325 C2326 A2327 A2328 G2329 G2330 C2331 G2334 A2335 A2336 G2337 C2347 U2348 G2349 C2350 G2354 C2355 A2361 G2375 A2376 A2377 A2378 G2383 G2384 C2385 G2400 U2406 G2407 C2417 A2422 U2423 C2424 A2425 A2426 C2427 G2428 G2429 A2430 U2431 A2434 A2435 A2439 C2440 C2441 G2445
A2448 G2468 A2469 G2470 A2476 C2477 A2478 U2491 U2492 U2493 C2498 C2499 G2502 A2503 U2504 G2505 U2506 A2518 G2529 G2535 G2550 C2551 U2552 G2553 U2554 A2561 U2562 U2563 A2564 A2565 A2566 G2567 C2568 C2573 G2574 U2585 C2591 G2592 A2602 U2605 G2608 U2609 C2610
U2611 C2612 U2615 C2616 C2617 A2629 G2630 G2631 C2646 U2647 A2654 C2683 U2684 G2685 G2686 U2687 U2688 U2689 C2690 C2691 C2692 A2693 G2694 C2699 C2703 A2712A A2713 G2714 G2719 G2722 U2726 G2732 A2733 A2740 G2747 A2748 A2749 A2750 G2751 U2754 C2755 U2756 A2757 A2758
A2764 A2765 C2771 C2772 G2777 A2778 C2787 C2788 C2789 A2790 C2791 G2792 G2793 C2794 G U C C A2801A G2802 C2803 C2804 G2805 A2810 G2811 G2817 A2820 A2821 G2822 A2835 G2839 G2846 U2847 G2848 U2849 G2864 A2868 G2869 C2870 C2871 A2872 G2876 C2879 C2880 C2881 A2882
U2887 C2888 C2889 G2891 A2892 G2893 G2894 U2895 C2896 U2897 U G A C C C C U C C

• Molecule 1: 23S Ribosomal RNA

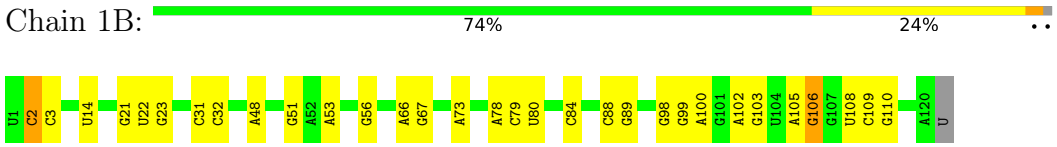
Chain 2A:




A1366 A1366 A1367 G1368 G1369 C1370 G1371 U1372 A1373 A1378 A1379 G1380 A1384 G1385 C1386 U1394 A1395 U1405 U1406 C1407 C1408 C1411 A1412 G1416 C1417 G1418 A1419 U1420 G1421 G1422 G1423 A1427 C1428 G1429 C1430 A1434 C1437 G1443 G1444 A1445 G1448 A1449 G1450 A1452 A1460 G1461 C1462
G1466 C1467 G1470 A1471 A1477 G1478 G1482 A1486 G1487 A1490 G1491 G1492 C1493 A1494 A1495 A1496 U1497 C1502 U1503 A1507 A1508 C1509 A1509A A1509B G1510 U1514 G1515 U1518 G1519 G1529 C1530 C1531 C1532 G1533 U A C1536 A1542 C1543 C1546 C1547 A1554 C1557 A1558
A1566 A1567 G1568 A1569 C1575 U1576 C1577 U1578 A1579 A1580 A1583 C1584 C1589 U1590 G1591 C1592 G1593 G1594 C1598 C1599 C1607 A1608 A1609 A1610 G1622 G1630 C1631 G1633 G1647 C1648 G1653 A1654 A1664 G1667 C1670 U1671 G1674 U1688 A1689 U1693 G1696 G1697 A1698
G1699 A1700 A1701 G1702 G1703 C1710 C1711 G1721 A1722 U1739 G1740 A1741 G1742 G1746 G1747 C1754 A1755 G1756 C1761 A1762 G1763 G1764 G1769 A1773 U1779 A1780 C1781 C1782 A1783 A1786 C1790 A1791 U1794 C1795 U1796 C1797 U1798 G1799 C1800 G1801 A1802 A1803 A1812 G1813 G1814 A1815 G1816 G1817
G1828 A1829 C1830 G1835 C1836 C1837 C1838 G1839 G1840 A1847 A1848 U1851 C1852 U1864 A1877 G1878 A1889 A1890 G1899 A1900 A1901 C1902 G1906 U1911 A1912 A1913 C1914 U1915 A1916 U1917 C1920 A1927 A1928 G1929 G1930 U1931 A1932 G1933 A1936 A1937 A1938 U1939 C1942 U1946 C1947
A1952 U1955 C1958 G1959 C1962 U1963 C1967 A1970 A1971 A1972 G1973 U1991 G1992 U1993 C1996 G1997 G2000 A2001 G2002 G2012 A2013 A2014 A2020 C2021 U2022 G2023 A2030 A2031 G2032 A2033 C2040 C2043 G2049 C2055 G2056 A2059 A2060 G2061 A2062 C2063 C2064 C2065 C2066
U2099 G2100 G2101 U2102 C2103 G2104 C2105 G2106 C2107 C2108 U2109 G2110 C2111 G2112 U2113 A2114 C2115 G2116 A2117 U2118 A2119 G2120 G2121 U2122 G2123 G2124 G2125 A2126 G2127 C2128 C2129 U2130 G2131 U2132 G2133 A2134 A2135 C2136 C2137 C2138 C2139 C2140 G2141 C2142 C2143 U2144 C2145 G2069 U2074 U2075 U2079 U2086 G2087 G2088 U2089
C2146 G2147 G2148 G2149 U2150 G2151 G2152 G2153 G2154 G2155 G2156 G2157 A2158 G2159 G2160 C2161 G2162 C2163 C2164 G2165 G2166 U2167 G2168 A2169 A2170 A2171 U2172 A2173 A2174 C2175 A2176 C2177 C2178 C2179 U2180 G2181 G2182 C2183 G2184 C2185 C2186 G2187 C2188 U2189 G2190 G2191 G2192 A2198 U2203 C2205 G2206 G2207 A2208 U2218 A2225 G2238
G2239 U2243 U2244 G2251 G2252 C2261 A2268 A2269 G2270 G2271 U2272 A2273 A2274 C2275 G2276 G2277 A2278 G2279 G2280 C2283 C2284 C2285 A2286 A2287 A2288 U2291 C2292 U2296 C2297 A2298 G2299 G2300 A2305 G2308 A2309 A2310 A2311 U2312 G2315 C2316 C2317 G2318 G2319 A2320 G2321 G2325 C2326 A2327 A2328
G2329 G2330 G2331 U2332 A2333 G2334 A2335 A2336 C2342 C2343 U2344 G2345 A2346 C2347 C2350 G2351 G2354 C2355 C2364 G2370 G2371 G2372 G2373 C2374 G2375 A2376 A2377 A2378 G2379 C2380 C2381 G2382 G2383 G2384 C2385 A2388 G2391 G2396 C2402 C2403 C2404 G2405 U2406 G2410 A2425 G2429 A2430
A2435 U2438 A2439 C2440 C2441 G2447 A2448 U2449 A2450 C2465 A2469 G2472 C2475 A2476 G2484 G2485 U2491 C2494 G2502 A2503 U2504 G2505 U2506 C2512 G2513 A2518 U2519 C2520 G2529 A2530 U2537 C2538 C2539 C2540 A2541 A2542 G2543 U2552 G2553 U2554 U2555 C2556 G2557 C2558
A2564 A2565 A2566 G2567 C2573 G2578 A2589 A2602 G2603 U2604 U2605 C2606 G2607 G2608 U2609 C2610 U2611 C2612 U2613 A2614 U2615 C2616 C2617 C2626 G2627 C2628 A2629 G2630 G2631 C2646 U2647 A2654 A2671 G2672 C2683 U2687 U2688 U2689 C2690 C2691 C2692 A2693 G2694 C2695 U2696 G2697 U2698 U2702 C2703
A2711 U2712 A2712A A2713 G2714 C2723 U2726 G2732 A2733 A2741 C2742 A2748 A2749 A2750 G2751 C2752 A2753 A2758 G2759 A2764 A2765 G2766 A2778 G2782 C2785 C2788 C2789 A C G2792 G2793 C2794 G U C A A2801A G2802 C2803 C2804 G2805 G2807 U2808 G2811 C2816
G2819 A2820 A2821 G2822 A2823 A2835 U2836 C2837 G2838 G2839 G2846 U2847 C2848 U2849 C2857 C2858 G2859 A2860 A2868 C2869 C2870 C2871 G2872 A2873 C2880 C2889 G2891 A2892 G2893 C2894 U2895 C2896 U2897 U G G A C C C C U C C

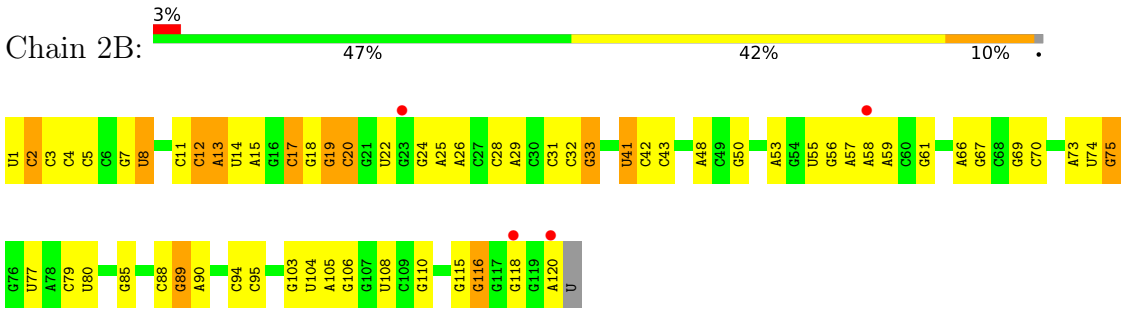
• Molecule 2: 5S Ribosomal RNA

Chain 1B:



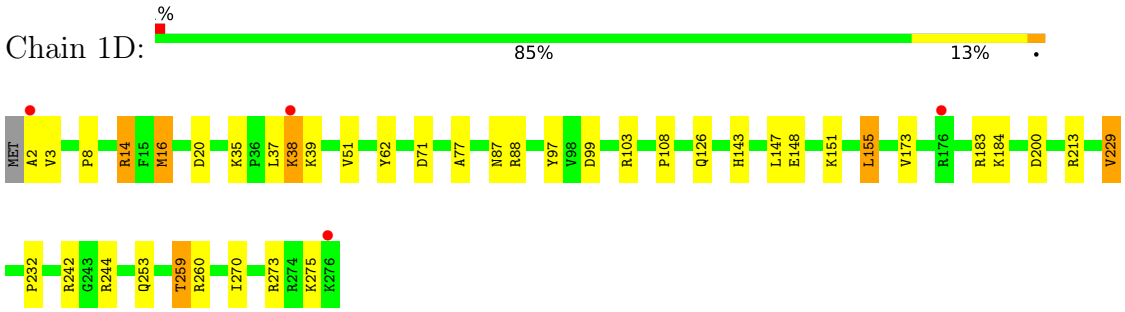
• Molecule 2: 5S Ribosomal RNA

Chain 2B:



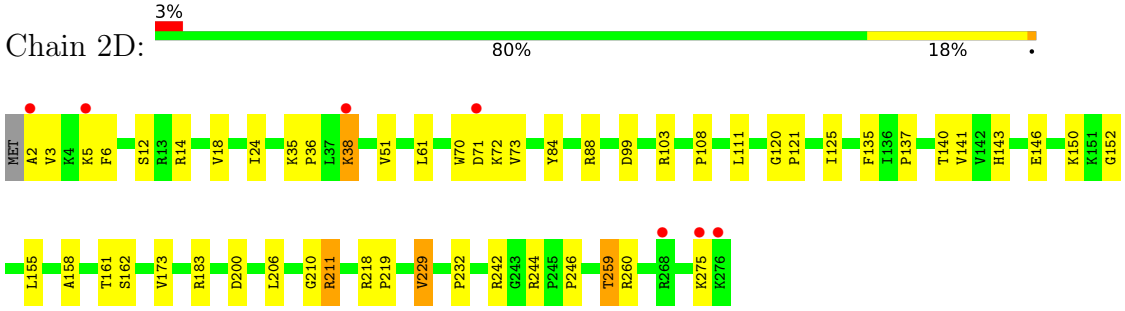
• Molecule 3: 50S ribosomal protein L2

Chain 1D:



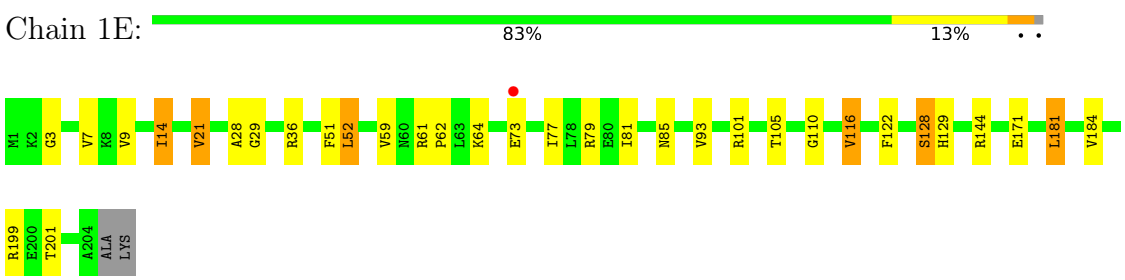
• Molecule 3: 50S ribosomal protein L2

Chain 2D:



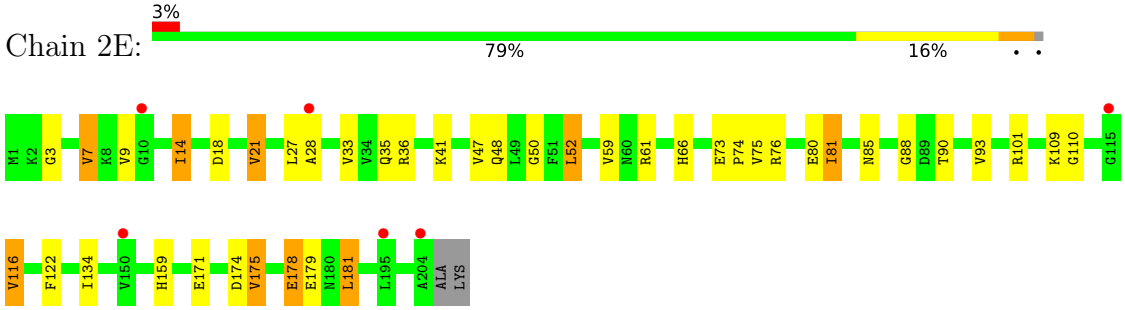
• Molecule 4: 50S ribosomal protein L3

Chain 1E:



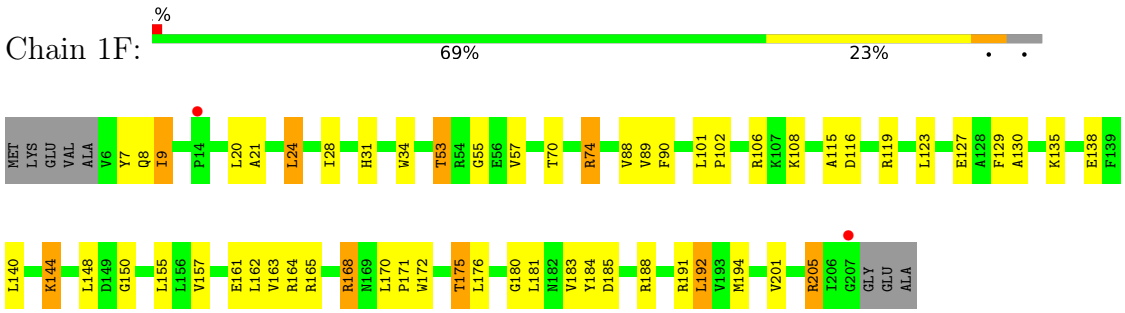
• Molecule 4: 50S ribosomal protein L3

Chain 2E:



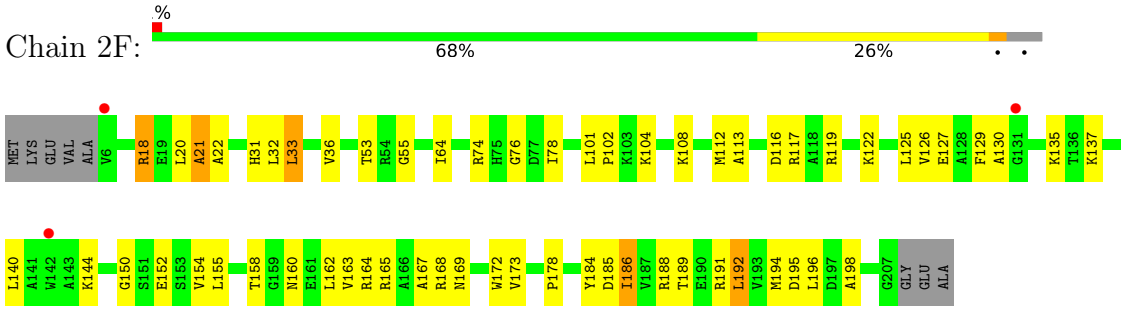
• Molecule 5: 50S ribosomal protein L4

Chain 1F:



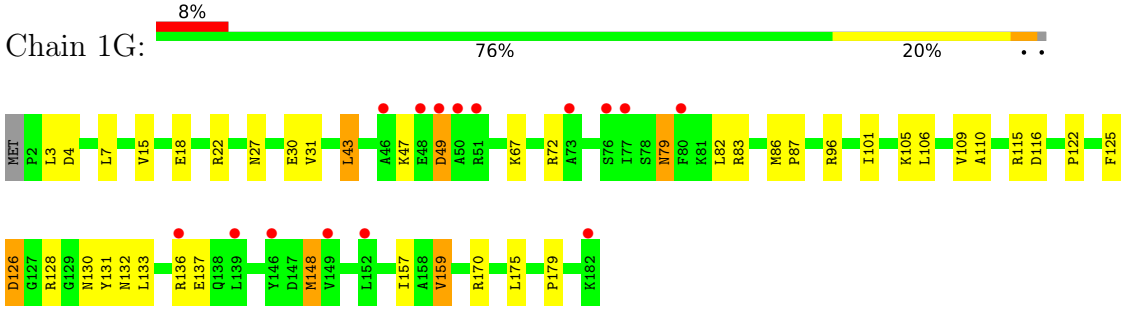
• Molecule 5: 50S ribosomal protein L4

Chain 2F:



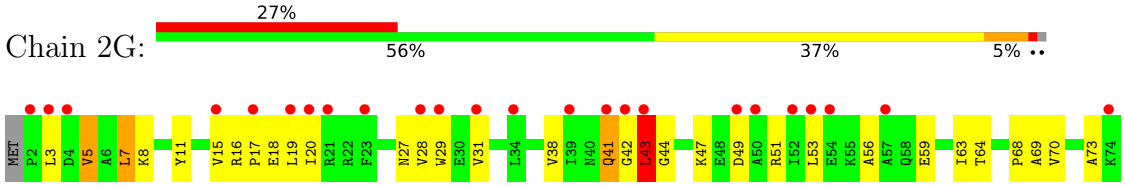
• Molecule 6: 50S ribosomal protein L5

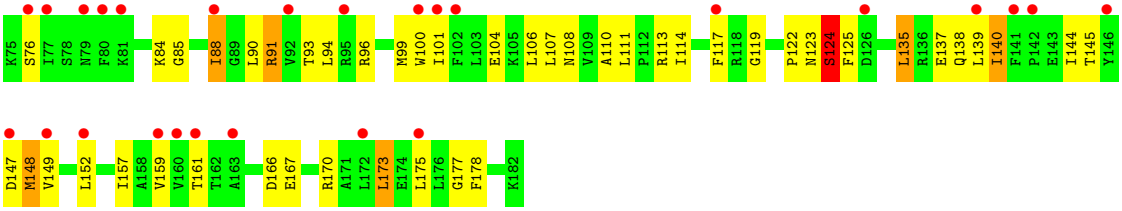
Chain 1G:



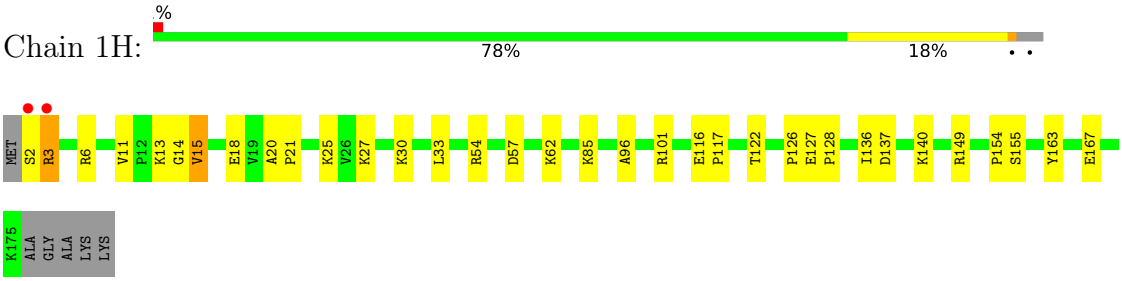
• Molecule 6: 50S ribosomal protein L5

Chain 2G:

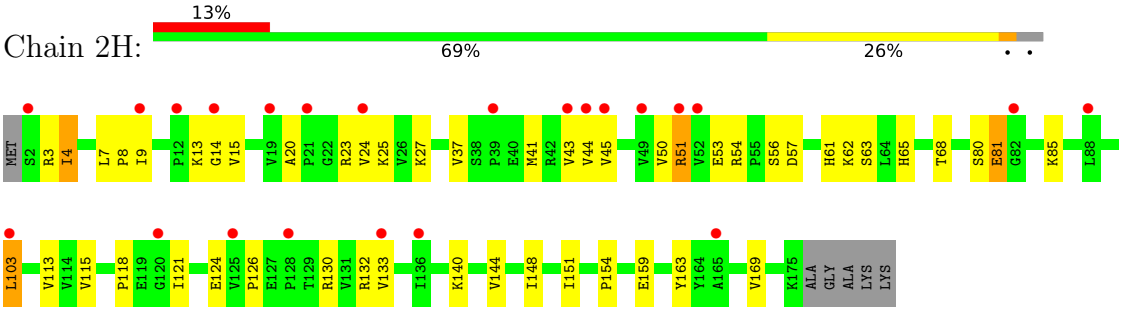




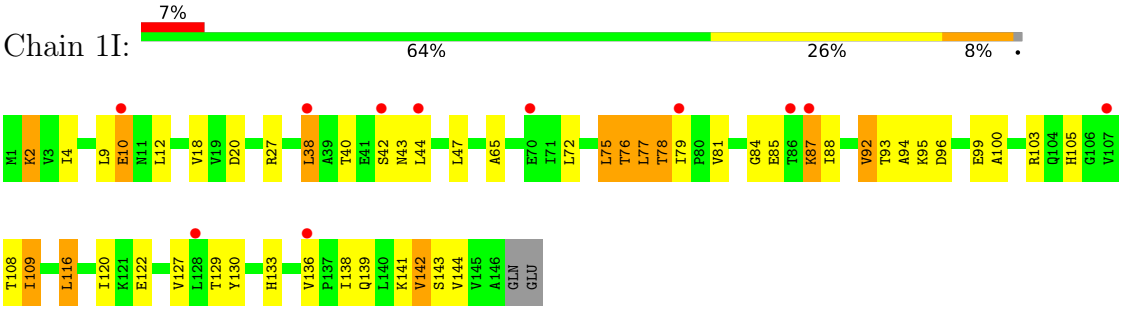
• Molecule 7: 50S ribosomal protein L6



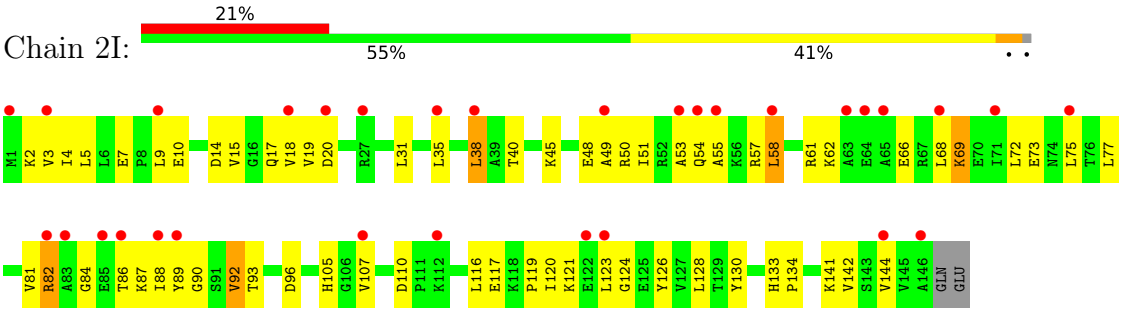
• Molecule 7: 50S ribosomal protein L6



• Molecule 8: 50S ribosomal protein L9

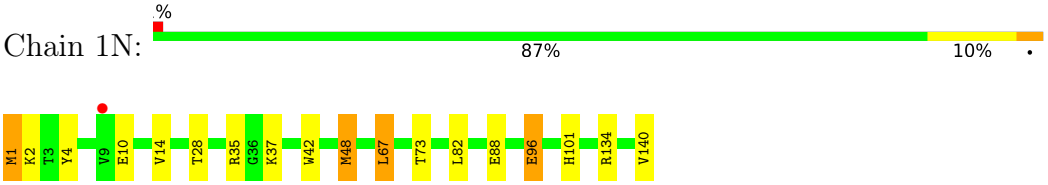


• Molecule 8: 50S ribosomal protein L9



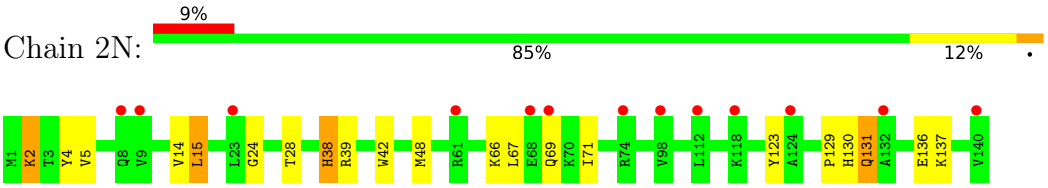
• Molecule 9: 50S ribosomal protein L13

Chain 1N:



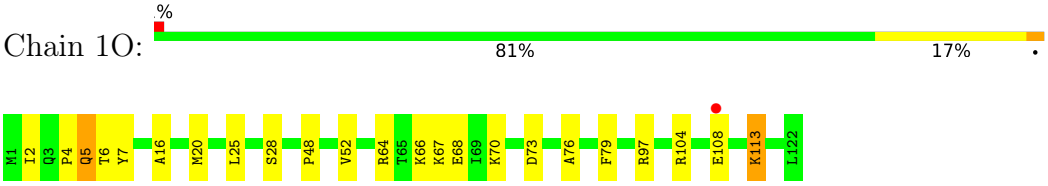
• Molecule 9: 50S ribosomal protein L13

Chain 2N:



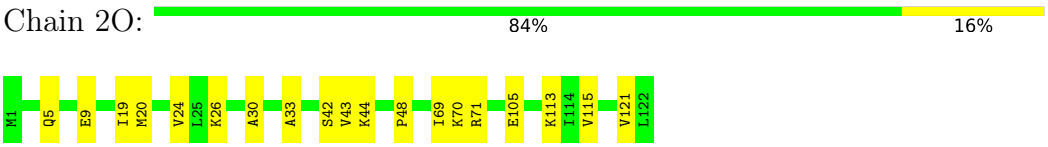
• Molecule 10: 50S ribosomal protein L14

Chain 1O:



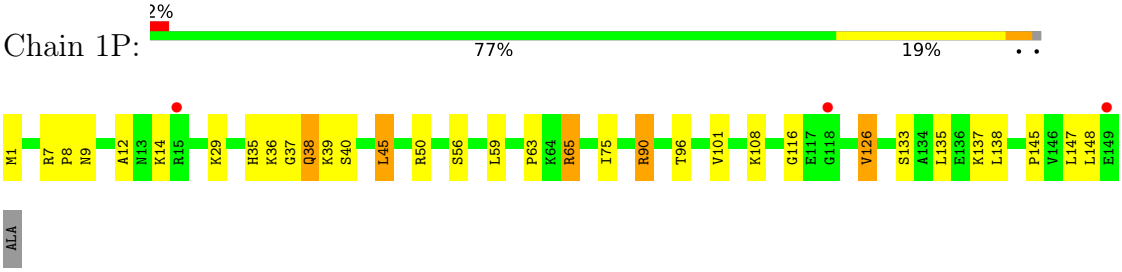
• Molecule 10: 50S ribosomal protein L14

Chain 2O:



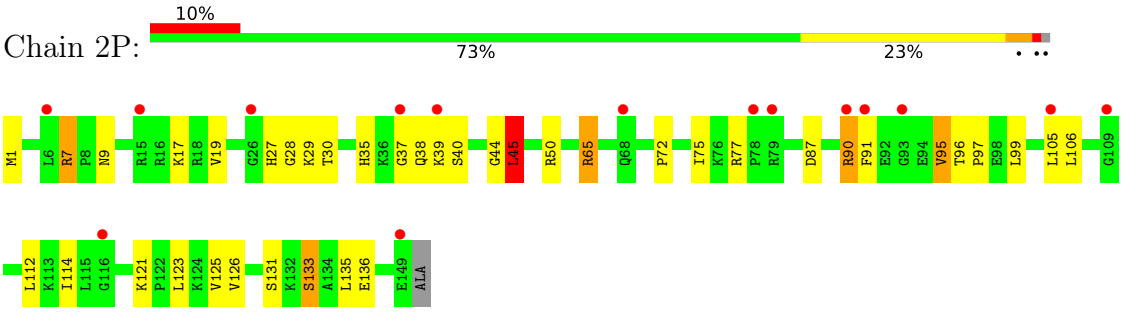
• Molecule 11: 50S ribosomal protein L15

Chain 1P:



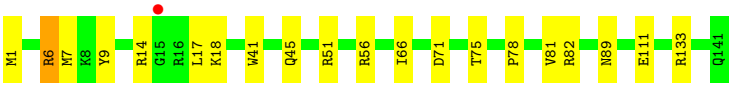
• Molecule 11: 50S ribosomal protein L15

Chain 2P:



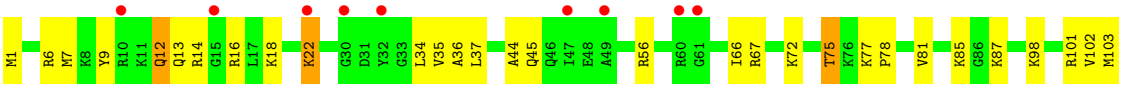
• Molecule 12: 50S ribosomal protein L16

Chain 1Q:



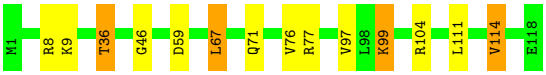
• Molecule 12: 50S ribosomal protein L16

Chain 2Q:



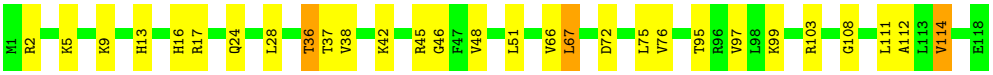
• Molecule 13: 50S ribosomal protein L17

Chain 1R:



• Molecule 13: 50S ribosomal protein L17

Chain 2R:

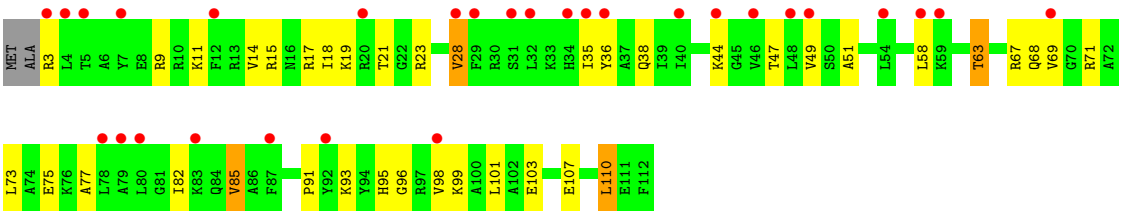


• Molecule 14: 50S ribosomal protein L18

Chain 1S:

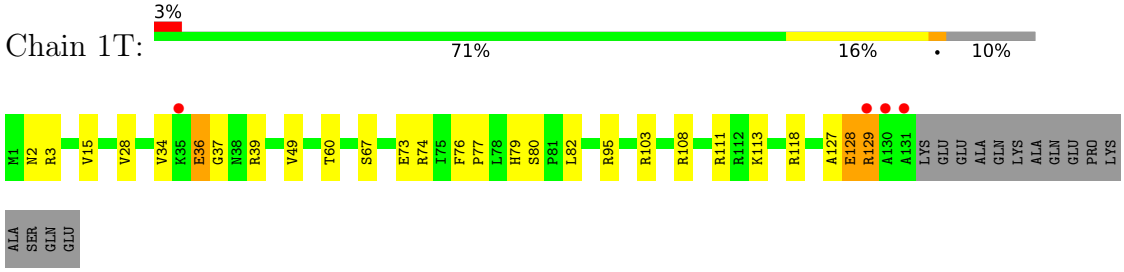
• Molecule 14: 50S ribosomal protein L18

Chain 2S:



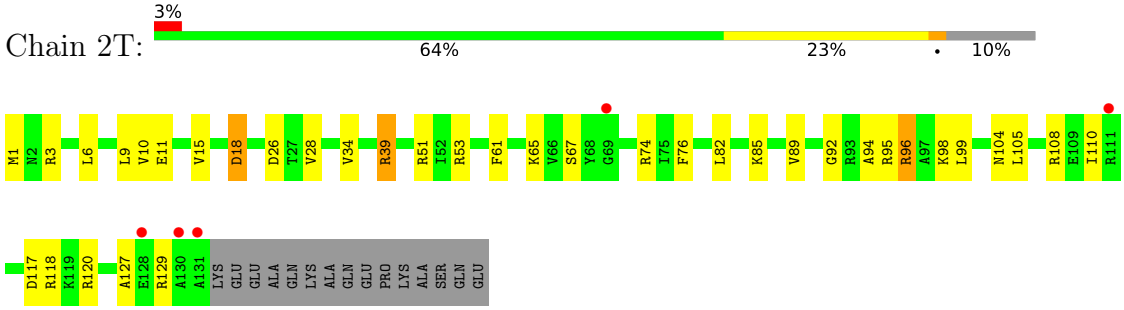
• Molecule 15: 50S ribosomal protein L19

Chain 1T:



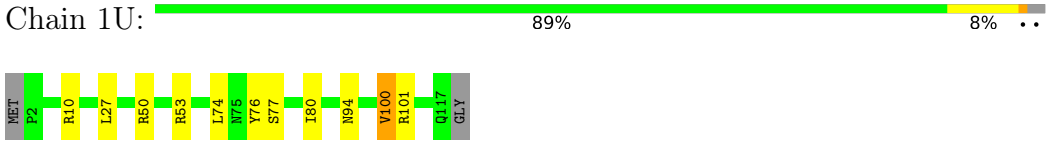
• Molecule 15: 50S ribosomal protein L19

Chain 2T:



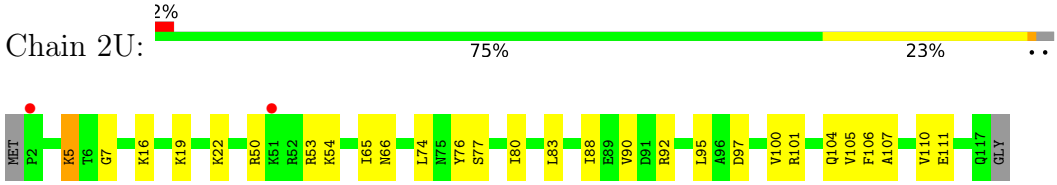
• Molecule 16: 50S ribosomal protein L20

Chain 1U:



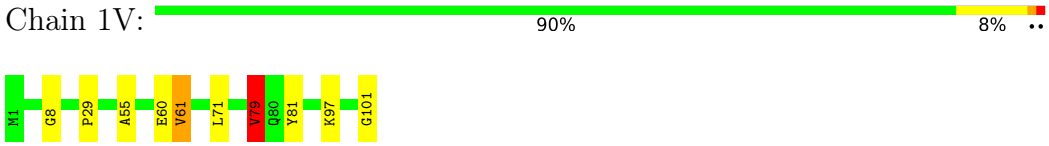
• Molecule 16: 50S ribosomal protein L20

Chain 2U:



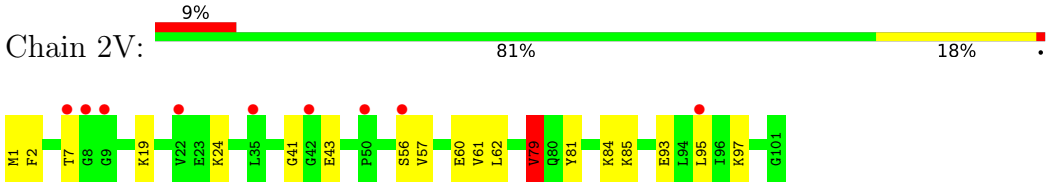
• Molecule 17: 50S ribosomal protein L21

Chain 1V:



• Molecule 17: 50S ribosomal protein L21

Chain 2V:

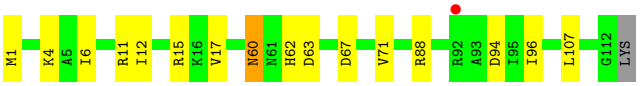


• Molecule 18: 50S ribosomal protein L22

Chain 1W:

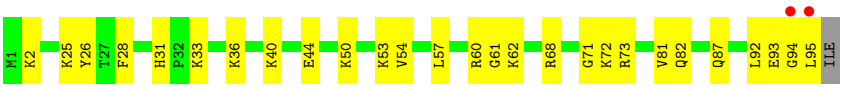
• Molecule 18: 50S ribosomal protein L22

Chain 2W:



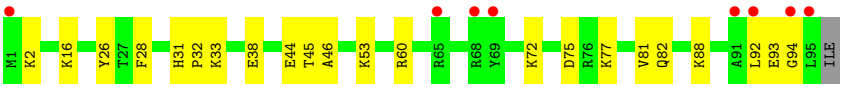
• Molecule 19: 50S ribosomal protein L23

Chain 1X:



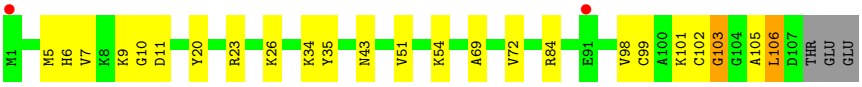
• Molecule 19: 50S ribosomal protein L23

Chain 2X:



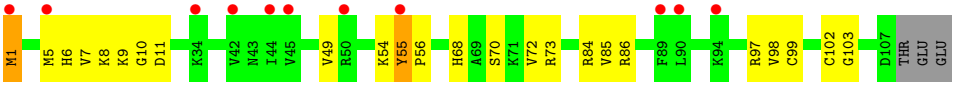
• Molecule 20: 50S ribosomal protein L24

Chain 1Y:



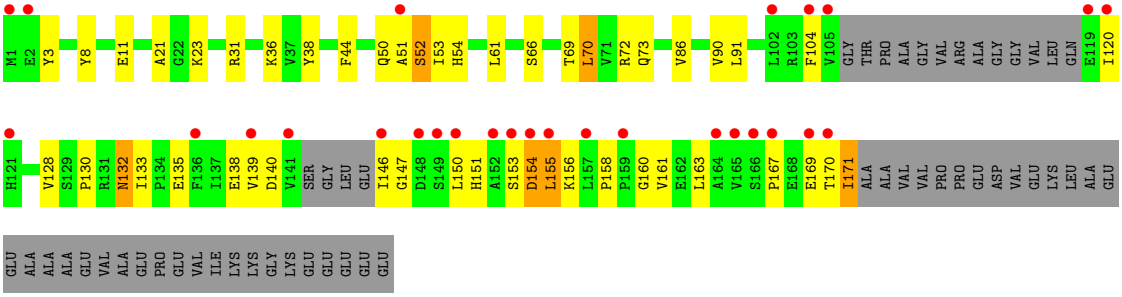
• Molecule 20: 50S ribosomal protein L24

Chain 2Y:



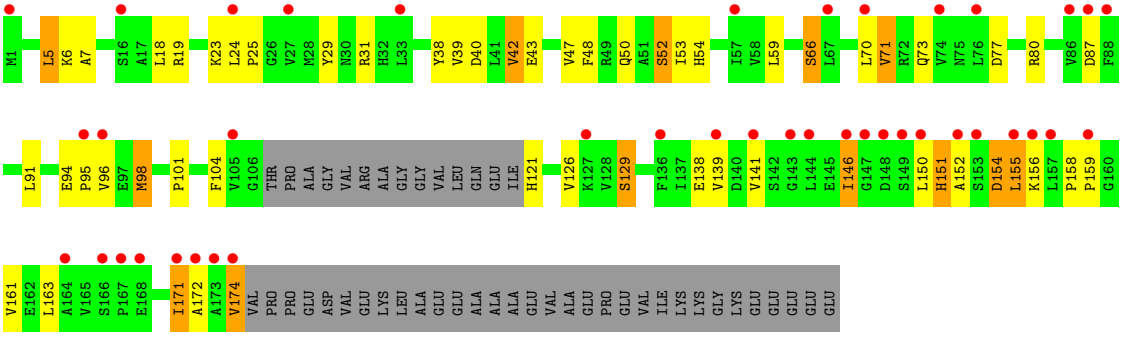
• Molecule 21: 50S ribosomal protein L25

Chain 1Z:



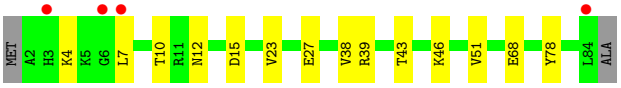
• Molecule 21: 50S ribosomal protein L25

Chain 2Z:



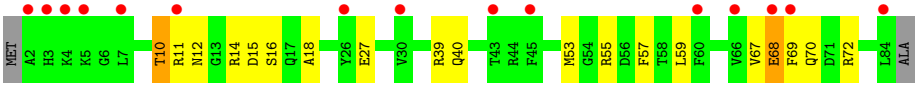
• Molecule 22: 50S ribosomal protein L27

Chain 10:



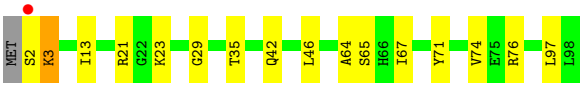
• Molecule 22: 50S ribosomal protein L27

Chain 20:



• Molecule 23: 50S ribosomal protein L28

Chain 11:

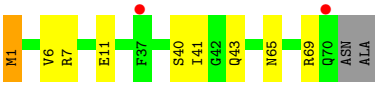


• Molecule 23: 50S ribosomal protein L28

Chain 21:

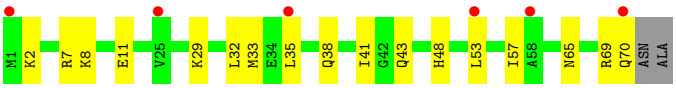
• Molecule 24: 50S ribosomal protein L29

Chain 12:



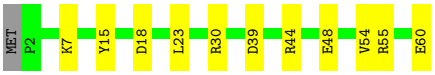
• Molecule 24: 50S ribosomal protein L29

Chain 22:



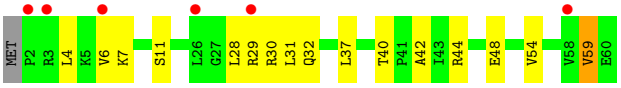
• Molecule 25: 50S ribosomal protein L30

Chain 13:



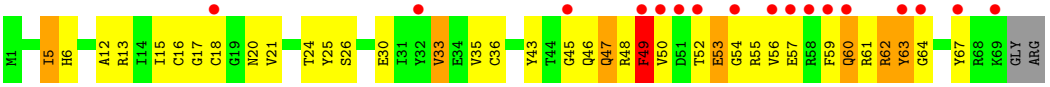
• Molecule 25: 50S ribosomal protein L30

Chain 23:



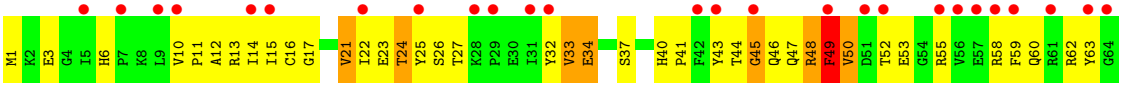
• Molecule 26: 50S ribosomal protein L31

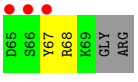
Chain 14:



• Molecule 26: 50S ribosomal protein L31

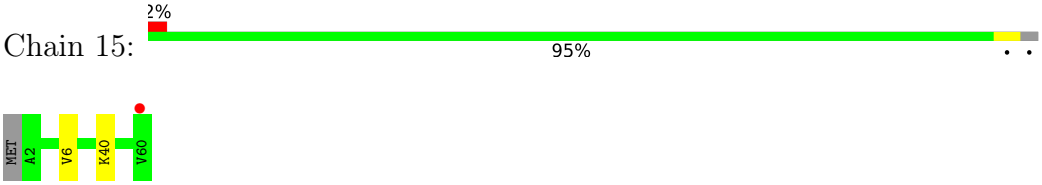
Chain 24:





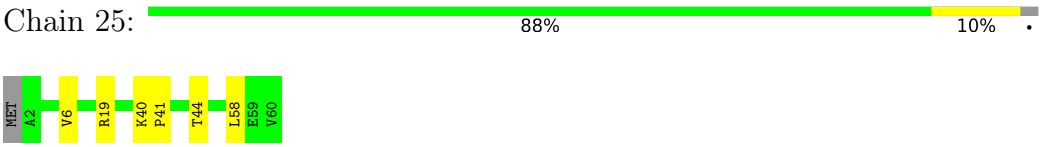
• Molecule 27: 50S ribosomal protein L32

Chain 15:



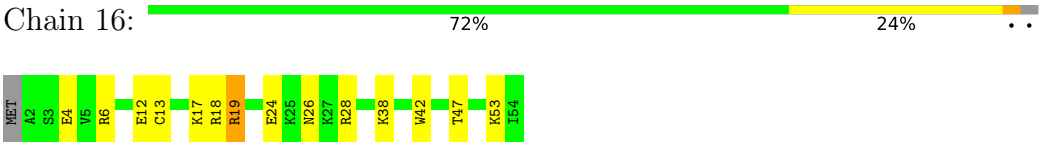
• Molecule 27: 50S ribosomal protein L32

Chain 25:



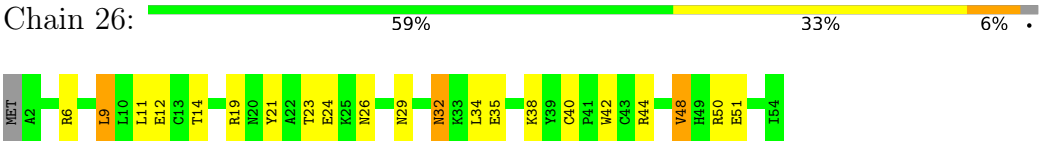
• Molecule 28: 50S ribosomal protein L33

Chain 16:



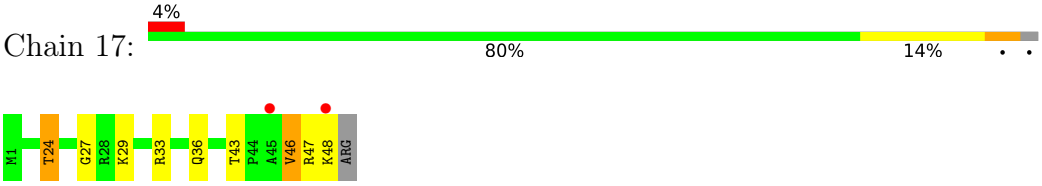
• Molecule 28: 50S ribosomal protein L33

Chain 26:



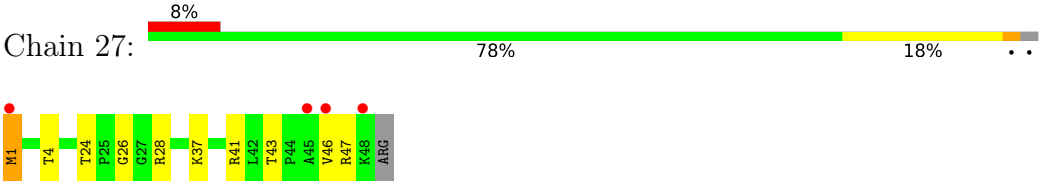
• Molecule 29: 50S ribosomal protein L34

Chain 17:



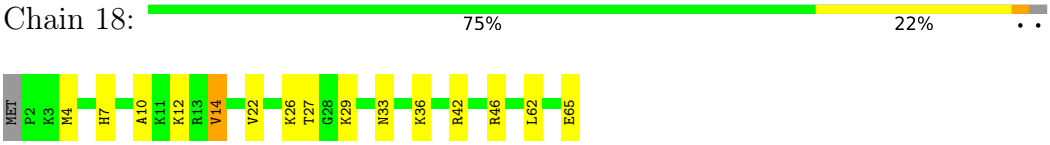
• Molecule 29: 50S ribosomal protein L34

Chain 27:



• Molecule 30: 50S ribosomal protein L35

Chain 18:

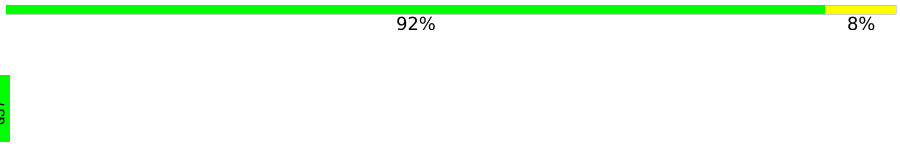


• Molecule 30: 50S ribosomal protein L35

Chain 28:

• Molecule 31: 50S ribosomal protein L36

Chain 19:

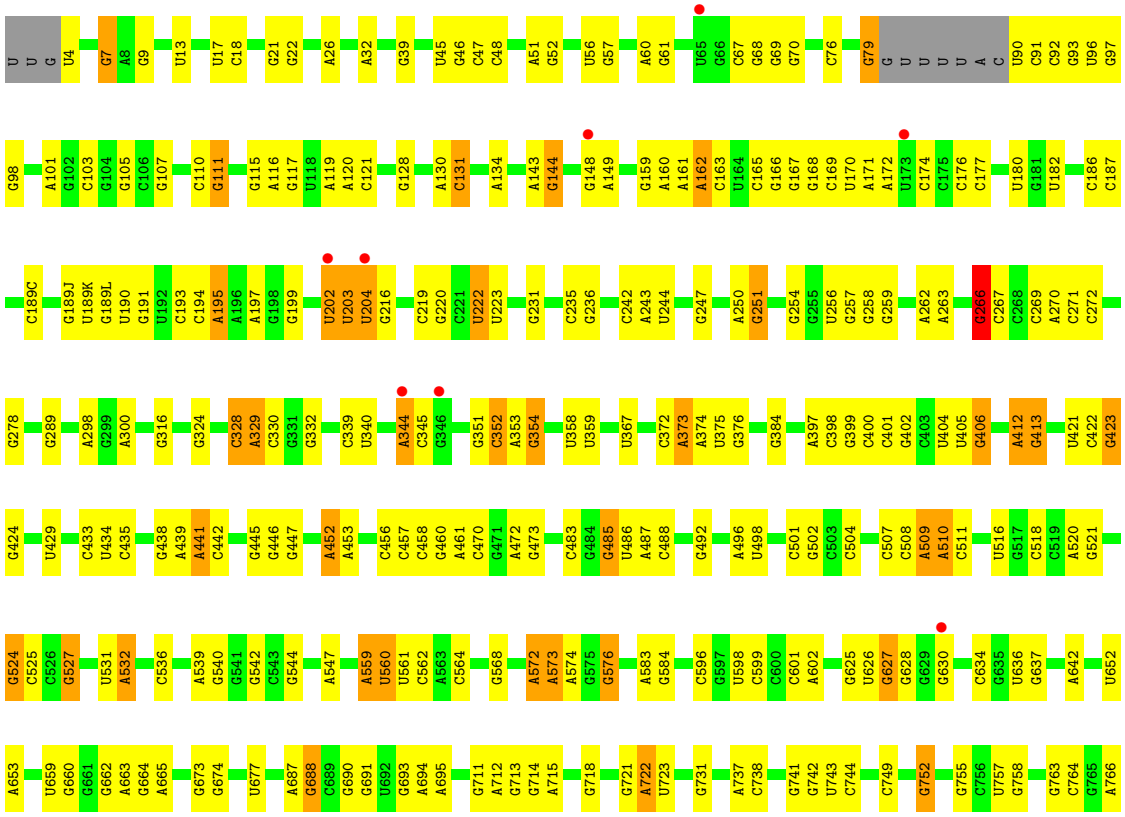


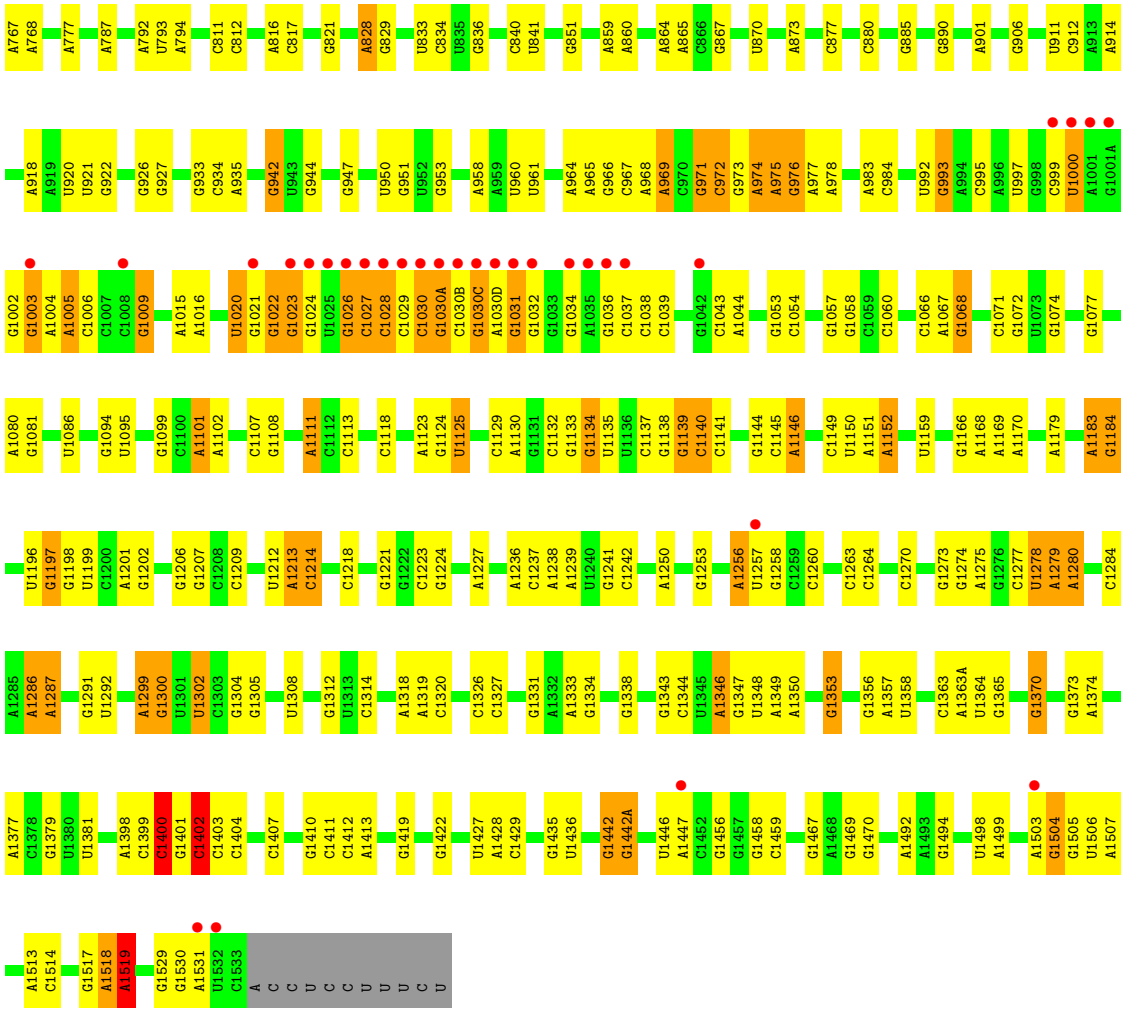
• Molecule 31: 50S ribosomal protein L36

Chain 29:

• Molecule 32: 16S Ribosomal RNA

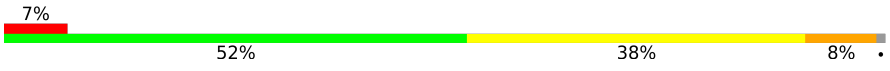
Chain 1a:

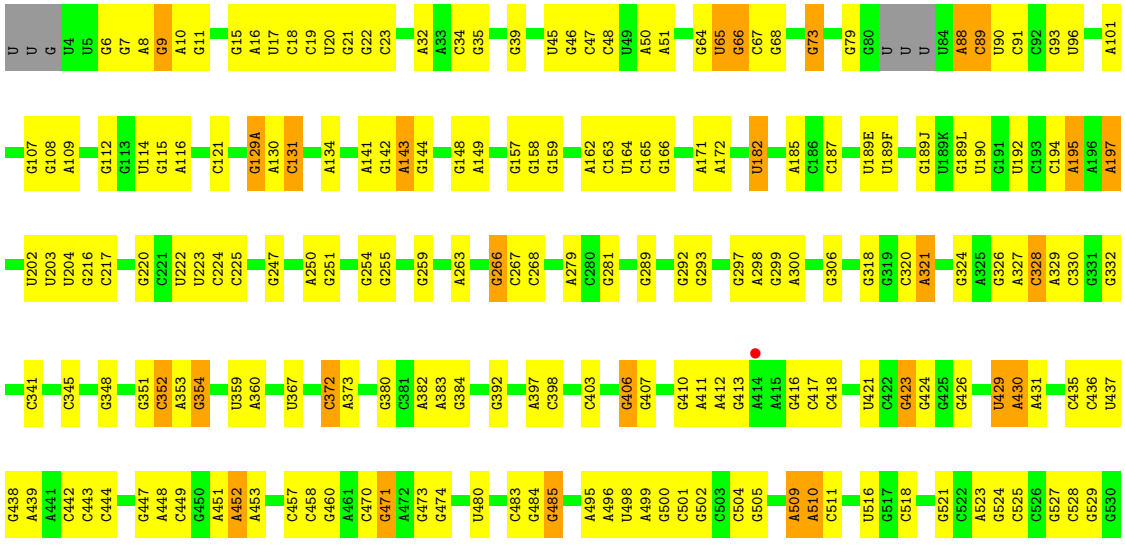


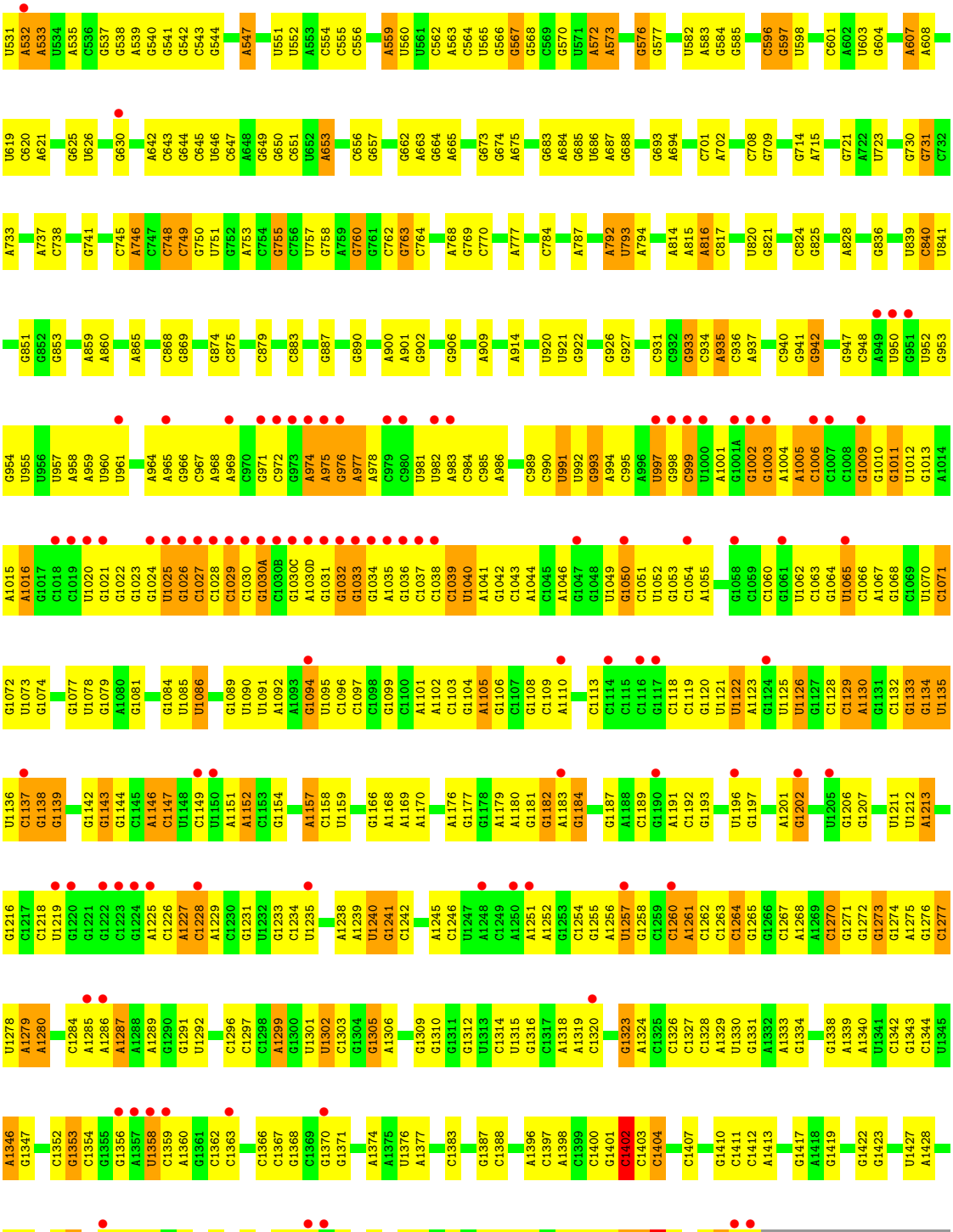


• Molecule 32: 16S Ribosomal RNA

Chain 2a:

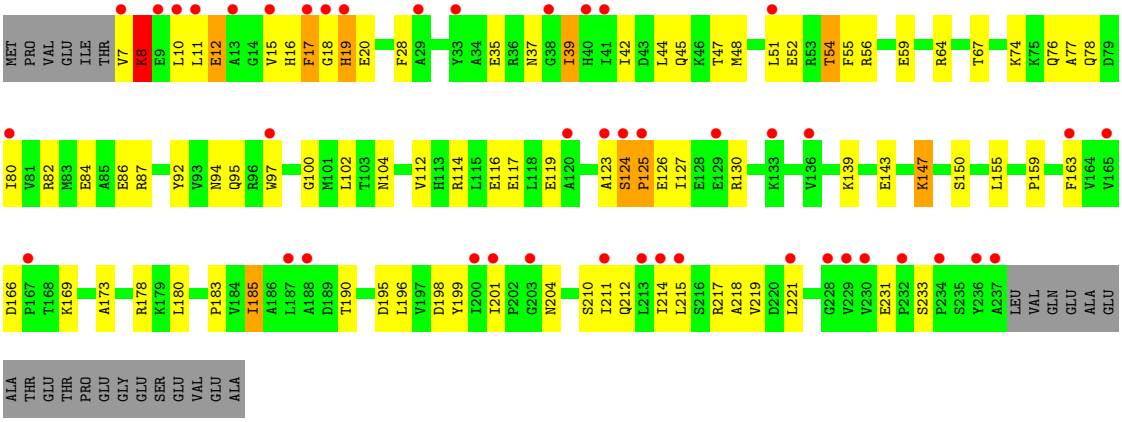






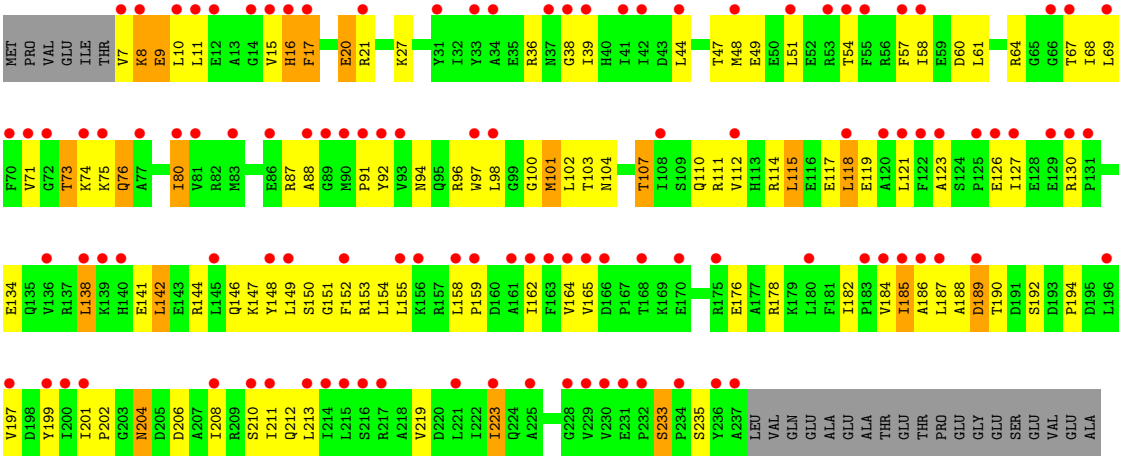
• Molecule 33: 30S ribosomal protein S2

Chain 1b:



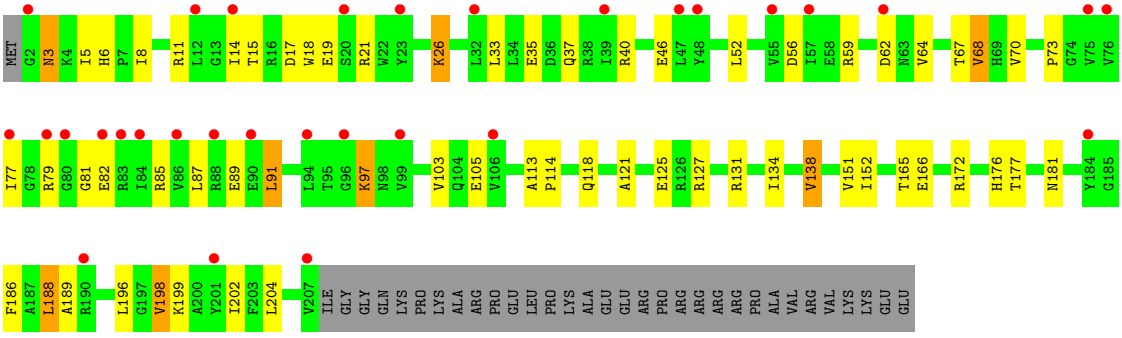
• Molecule 33: 30S ribosomal protein S2

Chain 2b:



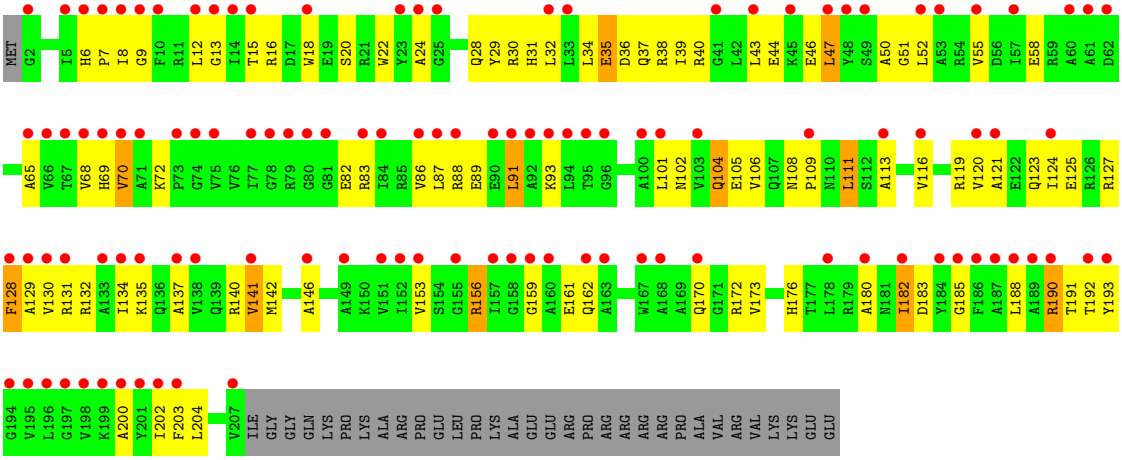
• Molecule 34: 30S ribosomal protein S3

Chain 1c:



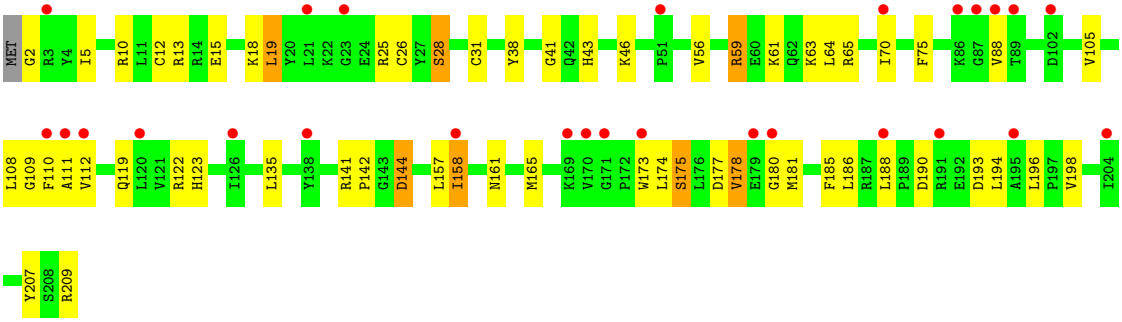
• Molecule 34: 30S ribosomal protein S3

Chain 2c:



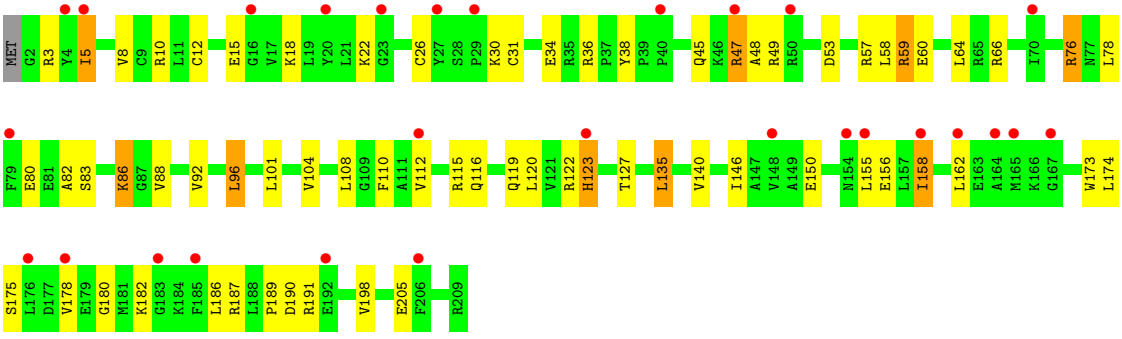
• Molecule 35: 30S ribosomal protein S4

Chain 1d:



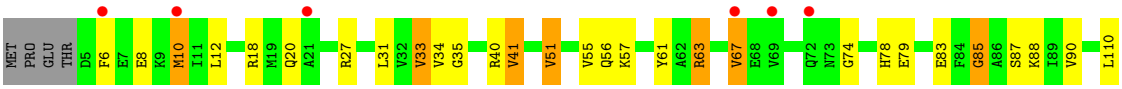
• Molecule 35: 30S ribosomal protein S4

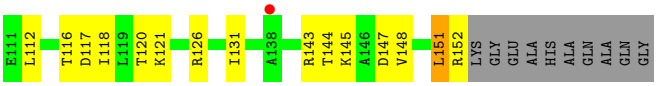
Chain 2d:



• Molecule 36: 30S ribosomal protein S5

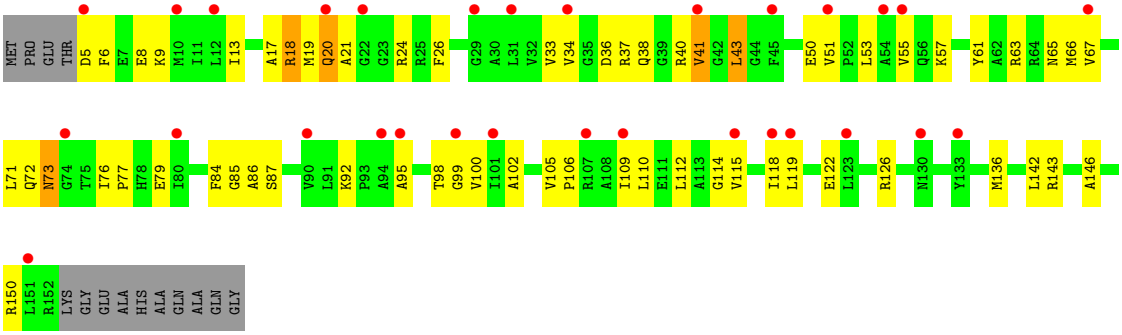
Chain 1e:





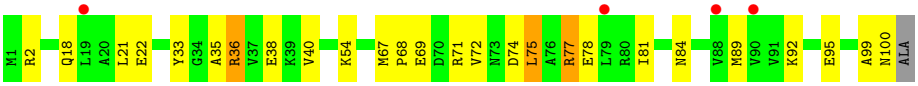
• Molecule 36: 30S ribosomal protein S5

Chain 2e:



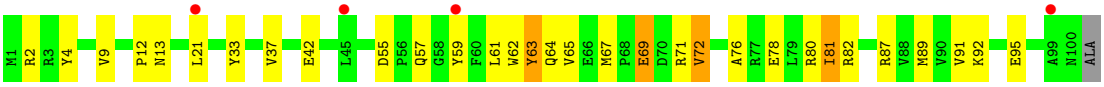
• Molecule 37: 30S ribosomal protein S6

Chain 1f:



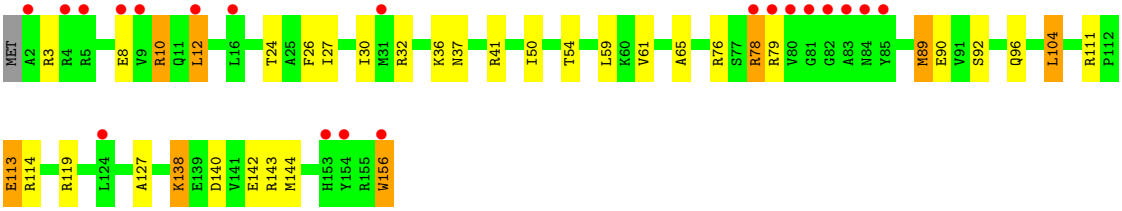
• Molecule 37: 30S ribosomal protein S6

Chain 2f:



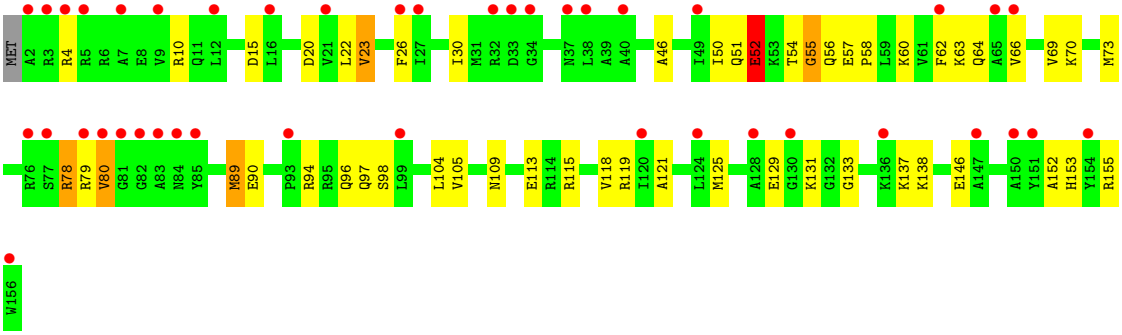
• Molecule 38: 30S ribosomal protein S7

Chain 1g:



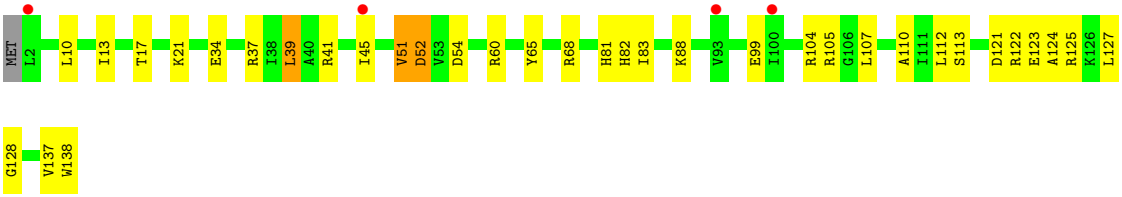
• Molecule 38: 30S ribosomal protein S7

Chain 2g:



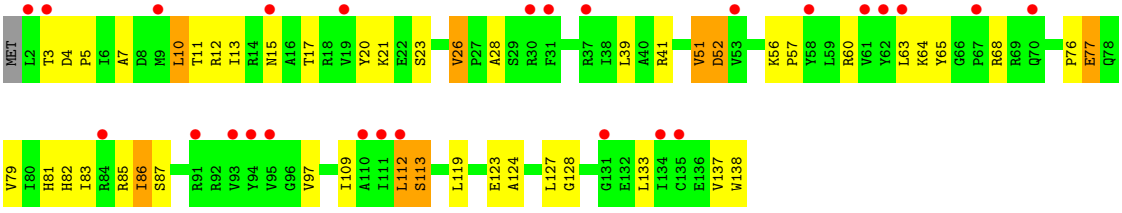
• Molecule 39: 30S ribosomal protein S8

Chain 1h:



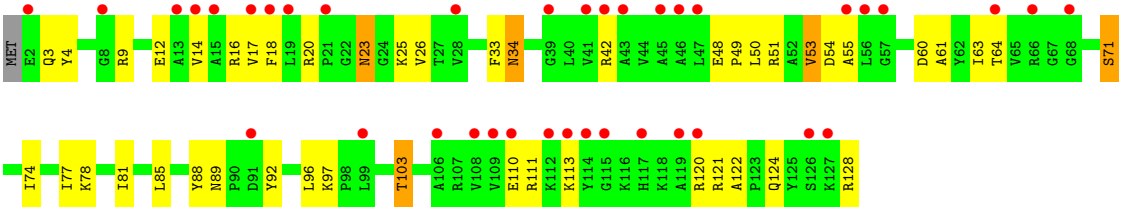
• Molecule 39: 30S ribosomal protein S8

Chain 2h:



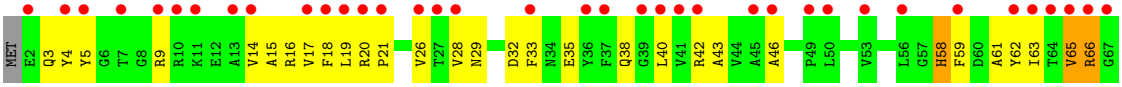
• Molecule 40: 30S ribosomal protein S9

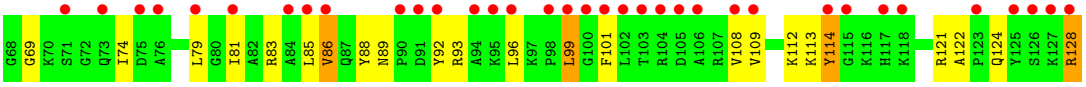
Chain 1i:



• Molecule 40: 30S ribosomal protein S9

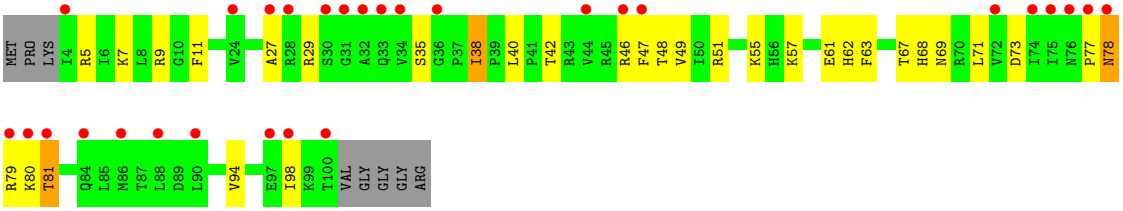
Chain 2i:





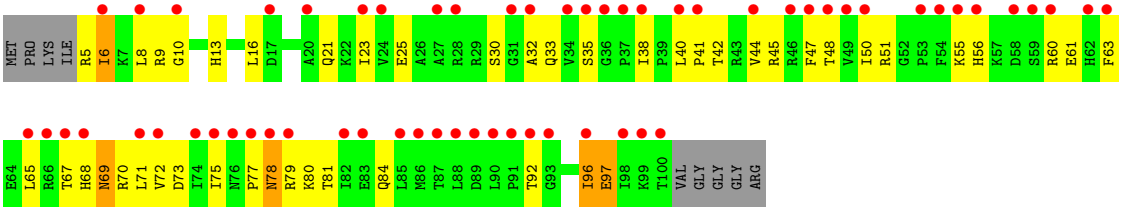
• Molecule 41: 30S ribosomal protein S10

Chain 1j:



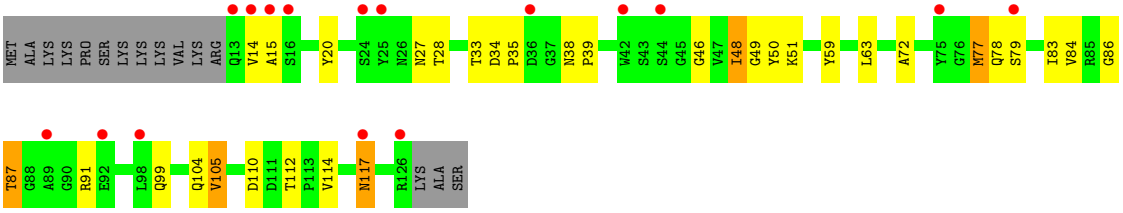
• Molecule 41: 30S ribosomal protein S10

Chain 2j:



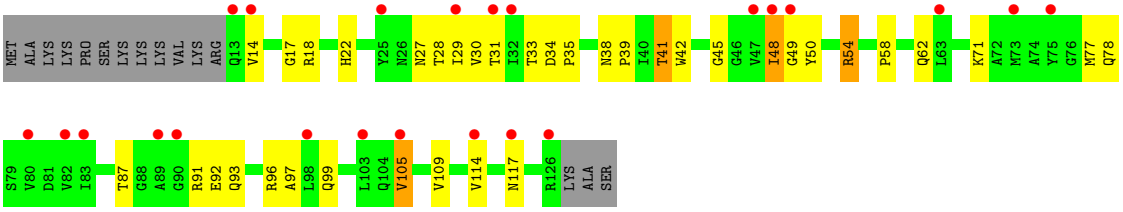
• Molecule 42: 30S ribosomal protein S11

Chain 1k:



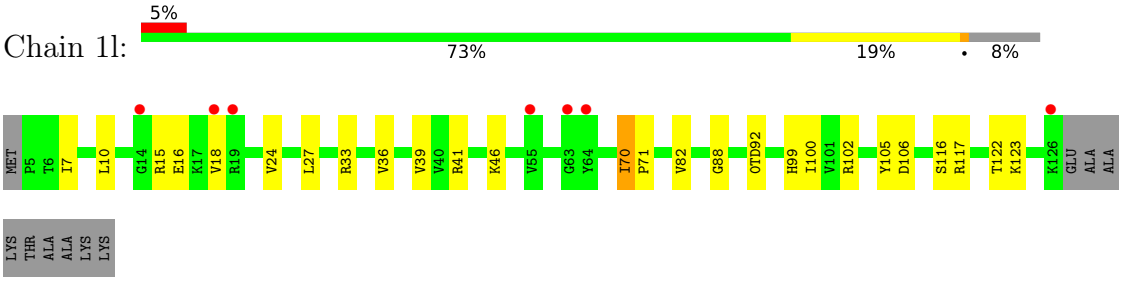
• Molecule 42: 30S ribosomal protein S11

Chain 2k:



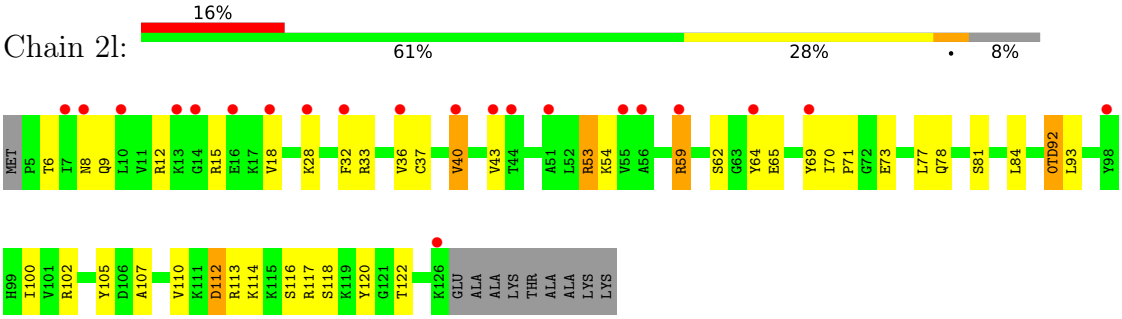
• Molecule 43: 30S ribosomal protein S12

Chain 1l:



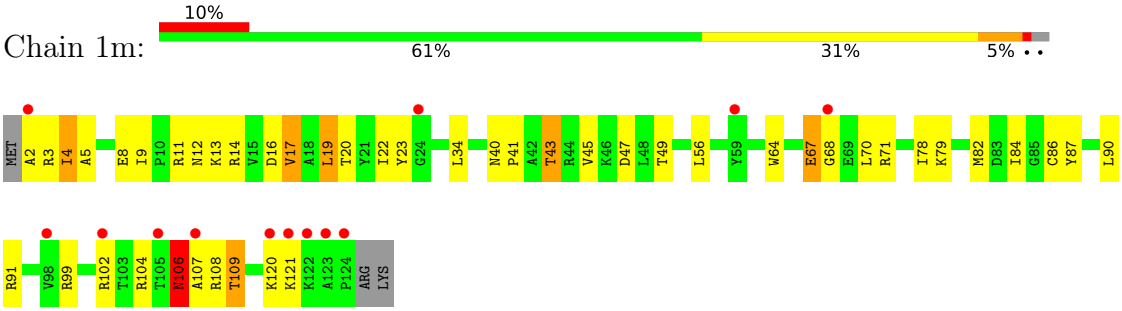
• Molecule 43: 30S ribosomal protein S12

Chain 2l:



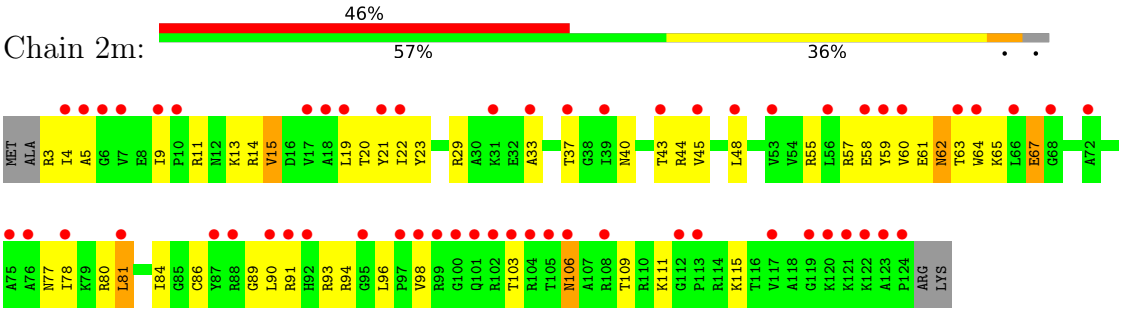
• Molecule 44: 30S ribosomal protein S13

Chain 1m:



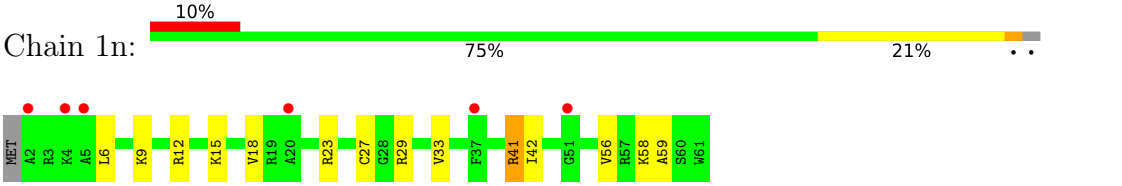
• Molecule 44: 30S ribosomal protein S13

Chain 2m:



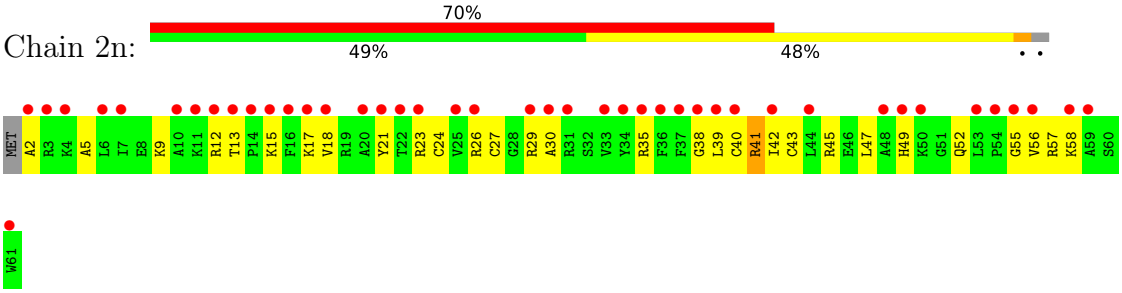
• Molecule 45: 30S ribosomal protein S14 type Z

Chain 1n:



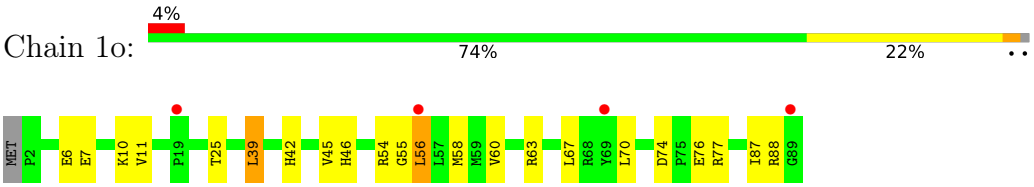
• Molecule 45: 30S ribosomal protein S14 type Z

Chain 2n:



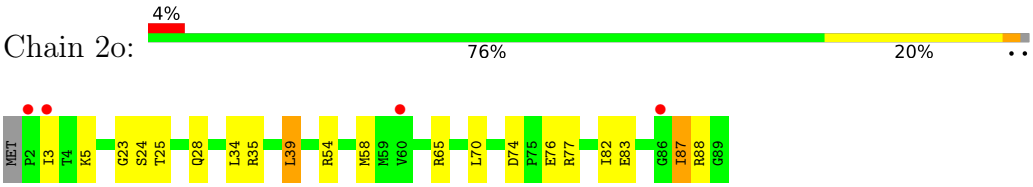
• Molecule 46: 30S ribosomal protein S15

Chain 1o:



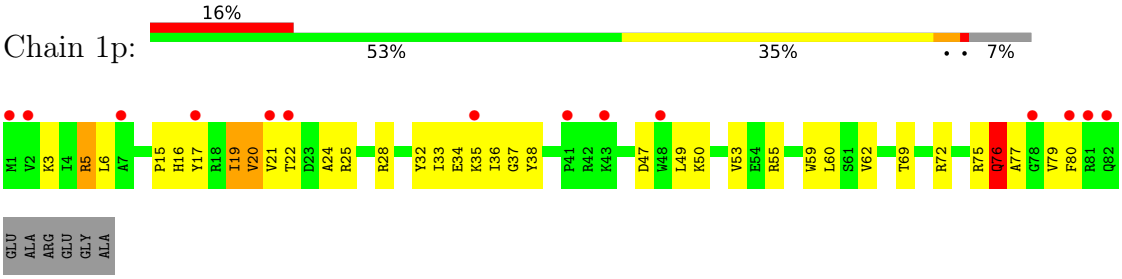
• Molecule 46: 30S ribosomal protein S15

Chain 2o:



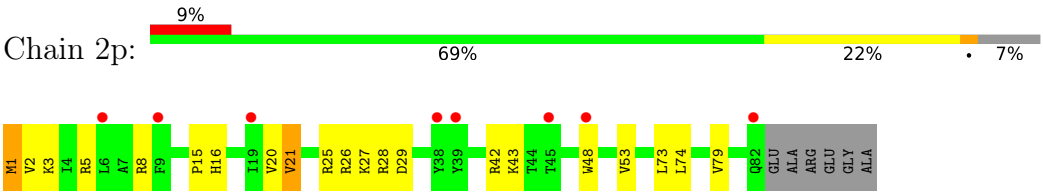
• Molecule 47: 30S ribosomal protein S16

Chain 1p:



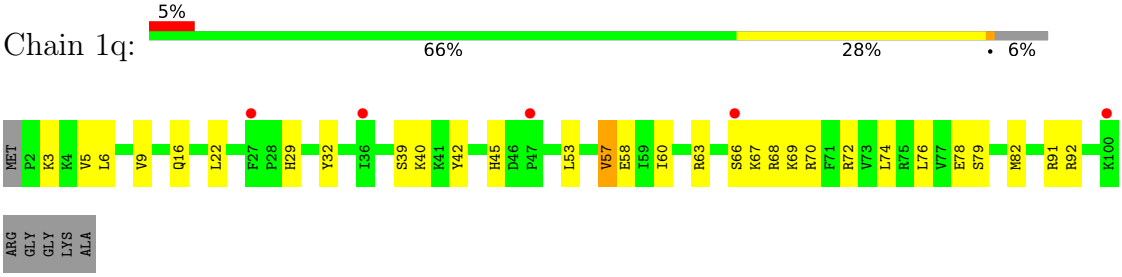
• Molecule 47: 30S ribosomal protein S16

Chain 2p:



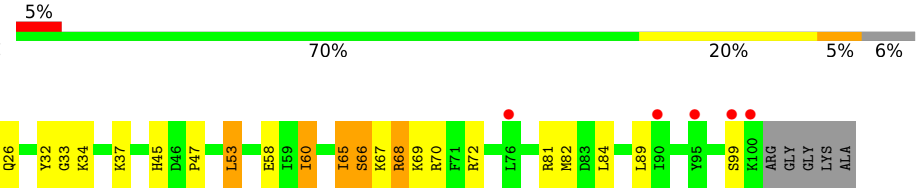
• Molecule 48: 30S ribosomal protein S17

Chain 1q:



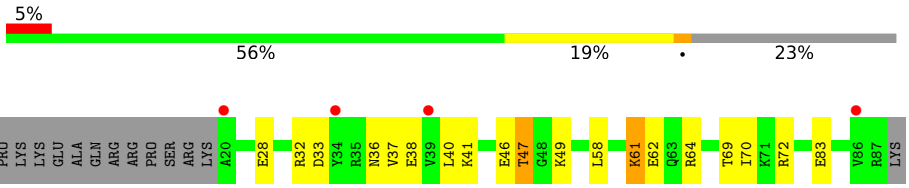
• Molecule 48: 30S ribosomal protein S17

Chain 2q:



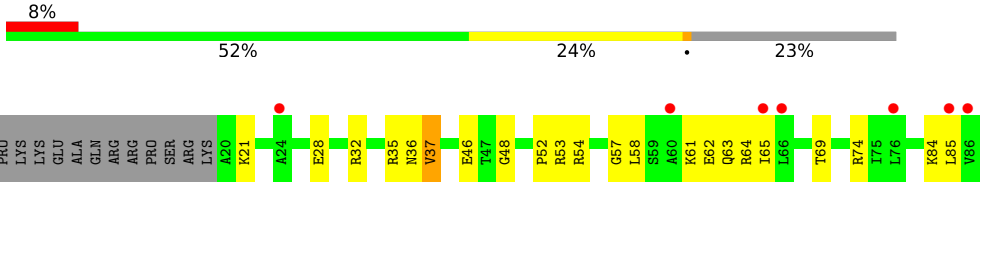
• Molecule 49: 30S ribosomal protein S18

Chain 1r:



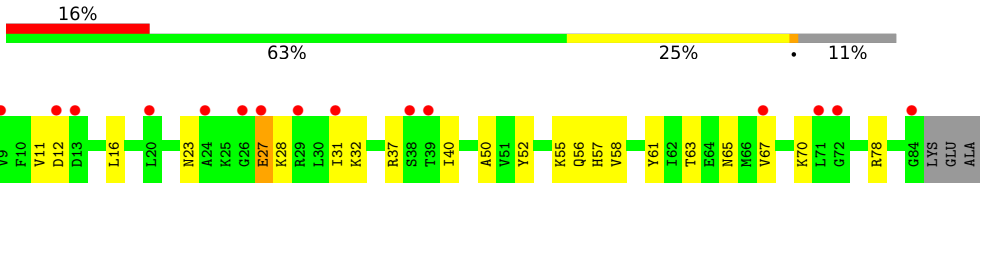
• Molecule 49: 30S ribosomal protein S18

Chain 2r:



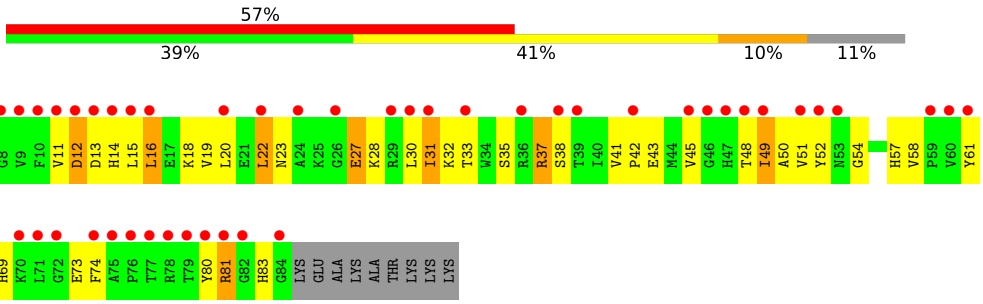
• Molecule 50: 30S ribosomal protein S19

Chain 1s:



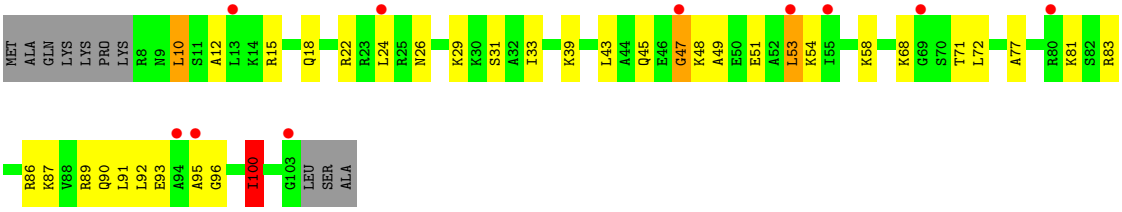
• Molecule 50: 30S ribosomal protein S19

Chain 2s:

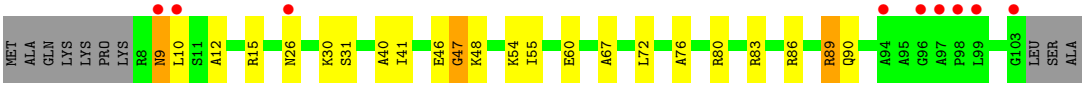


• Molecule 51: 30S ribosomal protein S20

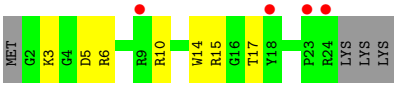
Chain 1t:



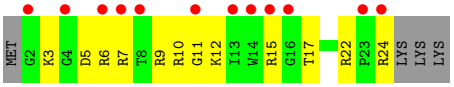
• Molecule 51: 30S ribosomal protein S20



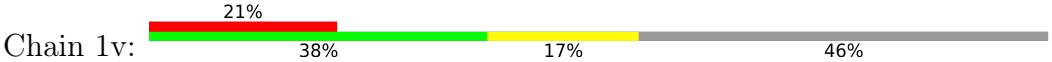
• Molecule 52: 30S ribosomal protein Thx

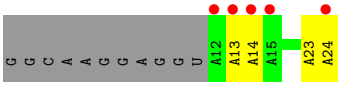


• Molecule 52: 30S ribosomal protein Thx

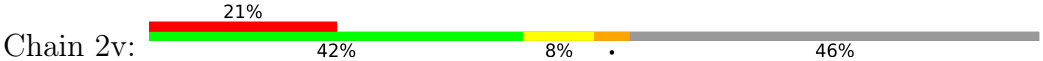


• Molecule 53: MG-mRNA

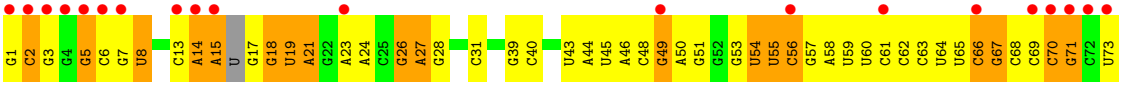




• Molecule 53: MG-mRNA

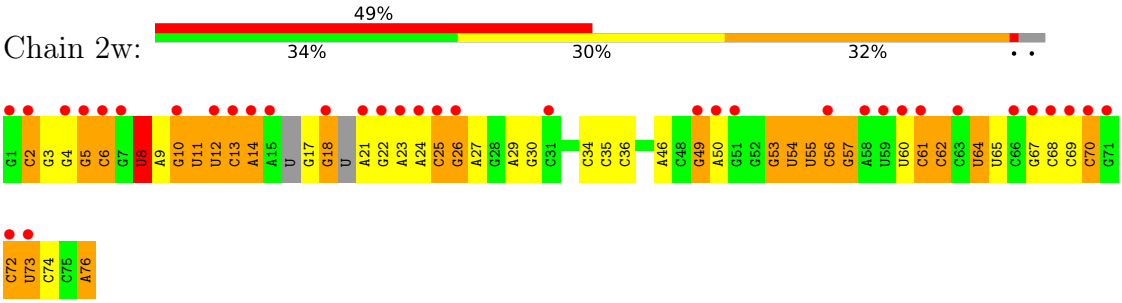


• Molecule 54: A-site Aminoacyl-tRNA Gly-NH-tRNAgly



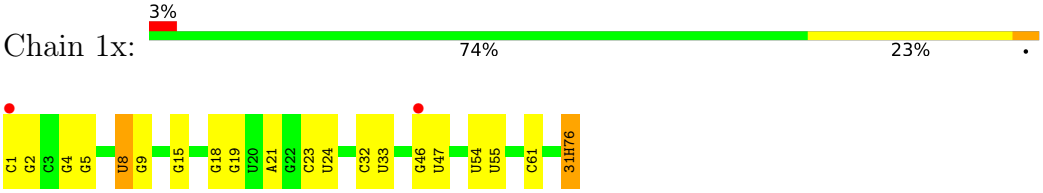
• Molecule 54: A-site Aminoacyl-tRNA Gly-NH-tRNAgly

Chain 2w:



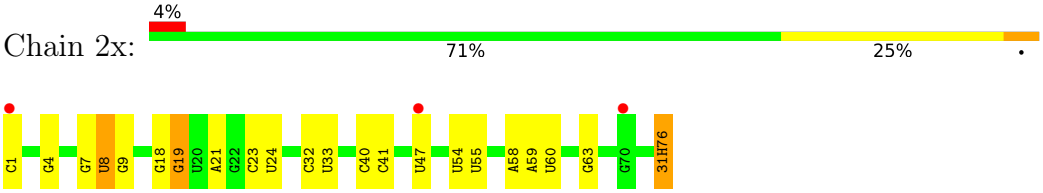
• Molecule 55: P-site Aminoacyl-tRNA fMet-NH-tRNAmet

Chain 1x:



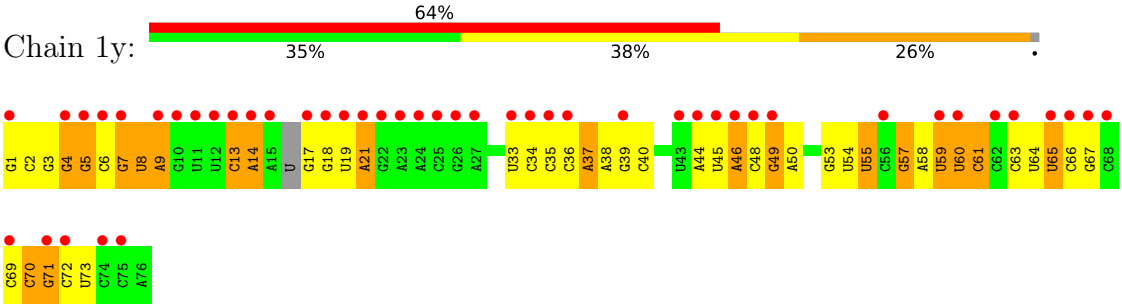
• Molecule 55: P-site Aminoacyl-tRNA fMet-NH-tRNAmet

Chain 2x:



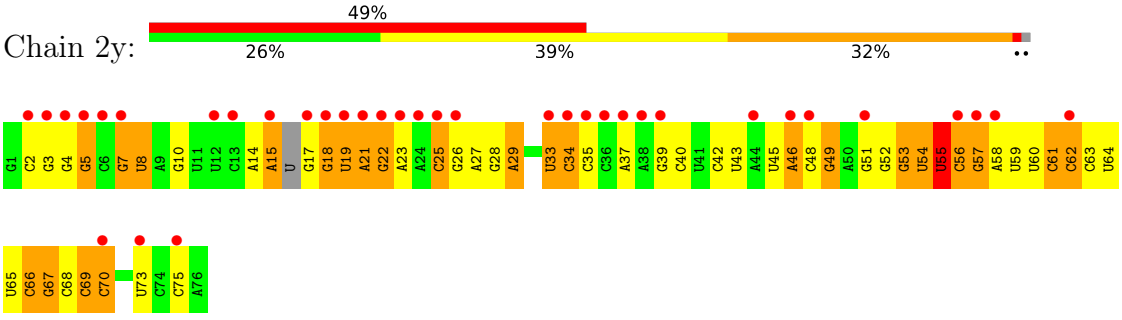
• Molecule 56: E-site Deacylated tRNAgly

Chain 1y:



• Molecule 56: E-site Deacylated tRNAgly

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	210.61Å 451.44Å 624.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	146.30 – 2.55 146.30 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.4 (146.30-2.55) 99.4 (146.30-2.55)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.23 (at 2.55Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.220 , 0.263 0.221 , 0.263	Depositor DCC
R_{free} test set	95245 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	50.7	Xtriage
Anisotropy	0.191	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 59.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	299852	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.62% 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: K, OMG, 31H, 5MC, G7M, MG, 4OC, ZN, L3X, 4SU, M2G, 0TD, OMU, 2MG, SF4, UR3, PSU, 5MU, 2MA, OMC, MA6

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	0.27	0/69011	0.47	3/107720 (0.0%)
1	2A	0.21	0/67295	0.41	1/105042 (0.0%)
2	1B	0.21	0/2882	0.40	0/4494
2	2B	0.19	0/2879	0.35	0/4487
3	1D	0.27	0/2186	0.49	0/2944
3	2D	0.21	0/2186	0.44	0/2944
4	1E	0.26	0/1592	0.51	0/2149
4	2E	0.20	0/1592	0.43	0/2149
5	1F	0.26	0/1618	0.48	0/2191
5	2F	0.20	0/1614	0.45	2/2186 (0.1%)
6	1G	0.21	0/1448	0.45	0/1957
6	2G	0.20	0/1453	0.42	0/1963
7	1H	0.21	0/1356	0.42	0/1834
7	2H	0.18	0/1356	0.38	0/1834
8	1I	0.19	0/1112	0.39	0/1514
8	2I	0.19	0/1079	0.41	0/1475
9	1N	0.25	0/1144	0.48	0/1543
9	2N	0.19	0/1144	0.38	0/1543
10	1O	0.25	0/943	0.45	0/1269
10	2O	0.19	0/943	0.41	0/1269
11	1P	0.25	0/1152	0.53	0/1533
11	2P	0.22	0/1152	0.50	0/1533
12	1Q	0.27	0/1143	0.46	0/1527
12	2Q	0.20	0/1143	0.43	0/1527
13	1R	0.28	0/982	0.48	0/1312
13	2R	0.20	0/982	0.46	0/1312
14	1S	0.21	0/883	0.47	0/1176
14	2S	0.21	0/880	0.45	0/1172
15	1T	0.25	0/1105	0.50	1/1477 (0.1%)
15	2T	0.19	0/1097	0.41	0/1468
16	1U	0.27	0/977	0.45	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	0/782	0.49	0/1049
17	2V	0.18	0/782	0.38	0/1049
18	1W	0.29	0/897	0.45	0/1205
18	2W	0.22	0/897	0.40	0/1205
19	1X	0.26	0/764	0.52	0/1025
19	2X	0.19	0/764	0.45	2/1025 (0.2%)
20	1Y	0.21	0/819	0.46	0/1095
20	2Y	0.19	0/819	0.45	0/1095
21	1Z	0.22	0/1267	0.45	0/1717
21	2Z	0.24	0/1299	0.42	0/1763
22	10	0.27	0/662	0.48	0/881
22	20	0.20	0/662	0.47	0/881
23	11	0.25	0/762	0.47	0/1014
23	21	0.22	0/762	0.40	0/1014
24	12	0.26	0/590	0.44	0/781
24	22	0.18	0/590	0.37	0/781
25	13	0.25	0/474	0.47	0/635
25	23	0.18	0/469	0.40	0/630
26	14	0.25	0/565	0.59	0/761
26	24	0.26	0/545	0.47	0/737
27	15	0.26	0/469	0.49	0/635
27	25	0.21	0/469	0.40	0/635
28	16	0.26	0/460	0.44	0/613
28	26	0.22	0/456	0.42	0/608
29	17	0.30	0/426	0.54	0/561
29	27	0.23	0/426	0.48	0/561
30	18	0.24	0/525	0.49	0/691
30	28	0.17	0/525	0.39	0/691
31	19	0.26	0/310	0.50	0/407
31	29	0.19	0/310	0.43	0/407
32	1a	0.20	0/35795	0.40	1/55864 (0.0%)
32	2a	0.19	0/35886	0.37	0/56005
33	1b	0.21	0/1881	0.47	0/2542
33	2b	0.22	0/1860	0.48	0/2518
34	1c	0.20	0/1572	0.40	0/2126
34	2c	0.22	0/1566	0.43	0/2119
35	1d	0.19	0/1685	0.43	0/2262
35	2d	0.19	0/1704	0.44	0/2284
36	1e	0.21	0/1145	0.45	0/1543
36	2e	0.20	0/1149	0.45	0/1548
37	1f	0.20	0/823	0.41	0/1115
37	2f	0.19	0/829	0.40	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	1g	0.19	0/1250	0.40	0/1679
38	2g	0.20	0/1254	0.40	0/1683
39	1h	0.19	0/1108	0.39	0/1494
39	2h	0.18	0/1108	0.38	0/1494
40	1i	0.19	0/1002	0.47	0/1346
40	2i	0.22	0/997	0.47	0/1343
41	1j	0.20	0/722	0.46	0/982
41	2j	0.22	0/727	0.44	0/988
42	1k	0.19	0/844	0.42	0/1145
42	2k	0.18	0/848	0.37	0/1149
43	1l	0.20	0/937	0.41	0/1260
43	2l	0.18	0/937	0.40	0/1260
44	1m	0.21	0/969	0.47	0/1302
44	2m	0.20	0/961	0.47	0/1291
45	1n	0.18	0/501	0.40	0/664
45	2n	0.19	0/501	0.44	0/664
46	1o	0.20	0/739	0.37	0/985
46	2o	0.16	0/739	0.38	0/985
47	1p	0.20	0/697	0.48	0/939
47	2p	0.18	0/693	0.43	0/935
48	1q	0.20	0/836	0.42	0/1117
48	2q	0.19	0/836	0.44	1/1117 (0.1%)
49	1r	0.18	0/560	0.42	0/746
49	2r	0.17	0/560	0.37	0/746
50	1s	0.19	0/667	0.47	0/900
50	2s	0.25	0/661	0.57	0/893
51	1t	0.19	0/730	0.47	0/965
51	2t	0.19	0/729	0.43	0/965
52	1u	0.18	0/203	0.46	0/266
52	2u	0.20	0/203	0.42	0/266
53	1v	0.21	0/322	0.30	0/501
53	2v	0.21	0/322	0.34	0/501
54	1w	0.28	1/1639 (0.1%)	0.42	0/2548
54	2w	0.29	1/1616 (0.1%)	0.42	0/2510
55	1x	0.26	0/1723	0.41	0/2684
55	2x	0.24	0/1723	0.38	0/2684
56	1y	0.29	0/1664	0.43	0/2587
56	2y	0.31	1/1664 (0.1%)	0.46	0/2587
All	All	0.23	3/316940 (0.0%)	0.43	11/474518 (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
11	1P	0	1
11	2P	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	2y	8	4SU	O3'-P	5.61	1.61	1.56
54	1w	8	4SU	O3'-P	5.38	1.61	1.56
54	2w	8	4SU	O3'-P	5.31	1.61	1.56

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1992	G	C2'-C3'-O3'	6.74	119.61	109.50
1	1A	2689	U	C4'-C3'-O3'	6.12	118.58	109.40
1	2A	1992	G	C2'-C3'-O3'	5.92	118.38	109.50
48	2q	65	ILE	N-CA-C	-5.77	107.19	112.96
1	1A	2689	U	P-O3'-C3'	5.57	128.56	120.20
15	1T	129	ARG	N-CA-C	-5.41	107.23	112.97
32	1a	266	G	C2'-C3'-O3'	5.36	117.53	109.50
19	2X	94	GLY	CA-C-N	5.18	131.02	121.70
19	2X	94	GLY	C-N-CA	5.18	131.02	121.70
5	2F	21	ALA	CA-C-N	5.12	130.92	121.70
5	2F	21	ALA	C-N-CA	5.12	130.92	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	1P	35	HIS	Peptide
11	2P	35	HIS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61852	0	31195	508	0
1	2A	60322	0	30427	611	0
2	1B	2577	0	1305	21	0
2	2B	2575	0	1303	50	0
3	1D	2136	0	2218	28	0
3	2D	2136	0	2218	39	0
4	1E	1559	0	1618	22	0
4	2E	1559	0	1618	26	0
5	1F	1583	0	1625	35	0
5	2F	1579	0	1619	45	0
6	1G	1423	0	1436	26	0
6	2G	1428	0	1438	55	0
7	1H	1330	0	1407	19	0
7	2H	1330	0	1407	25	0
8	1I	1097	0	1140	29	0
8	2I	1064	0	1082	42	0
9	1N	1117	0	1184	9	0
9	2N	1117	0	1184	12	0
10	1O	933	0	996	17	0
10	2O	933	0	996	9	0
11	1P	1135	0	1212	24	0
11	2P	1135	0	1212	29	0
12	1Q	1122	0	1179	16	0
12	2Q	1122	0	1179	28	0
13	1R	968	0	1033	8	0
13	2R	968	0	1033	18	0
14	1S	873	0	927	13	0
14	2S	870	0	923	28	0
15	1T	1091	0	1151	20	0
15	2T	1083	0	1136	24	0
16	1U	959	0	1019	7	0
16	2U	959	0	1019	18	0
17	1V	771	0	830	7	0
17	2V	771	0	830	12	0
18	1W	886	0	940	7	0
18	2W	886	0	940	6	0
19	1X	750	0	814	20	0
19	2X	750	0	814	14	0
20	1Y	806	0	881	12	0
20	2Y	806	0	881	15	0
21	1Z	1240	0	1240	34	0
21	2Z	1271	0	1273	42	0
22	10	653	0	674	13	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	20	653	0	674	14	0
23	11	755	0	826	10	0
23	21	755	0	826	15	0
24	12	588	0	643	5	0
24	22	588	0	643	10	0
25	13	469	0	518	5	0
25	23	464	0	514	8	0
26	14	552	0	533	28	0
26	24	532	0	503	33	0
27	15	455	0	465	0	0
27	25	455	0	465	2	0
28	16	453	0	473	8	0
28	26	449	0	469	12	0
29	17	418	0	467	6	0
29	27	418	0	467	7	0
30	18	517	0	582	12	0
30	28	517	0	582	10	0
31	19	307	0	335	2	0
31	29	307	0	335	8	0
32	1a	32246	0	16295	344	0
32	2a	32327	0	16338	482	0
33	1b	1846	0	1867	47	0
33	2b	1825	0	1828	84	0
34	1c	1548	0	1535	37	0
34	2c	1542	0	1517	77	0
35	1d	1655	0	1672	35	0
35	2d	1674	0	1714	48	0
36	1e	1129	0	1185	28	0
36	2e	1133	0	1191	41	0
37	1f	810	0	804	16	0
37	2f	816	0	808	20	0
38	1g	1231	0	1238	20	0
38	2g	1235	0	1249	32	0
39	1h	1088	0	1126	24	0
39	2h	1088	0	1126	37	0
40	1i	983	0	986	26	0
40	2i	978	0	966	45	0
41	1j	709	0	650	21	0
41	2j	714	0	672	35	0
42	1k	829	0	825	19	0
42	2k	833	0	836	22	0
43	1l	932	0	980	13	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	2l	932	0	980	26	0
44	1m	958	0	1002	32	0
44	2m	950	0	988	49	0
45	1n	492	0	529	10	0
45	2n	492	0	529	27	0
46	1o	728	0	760	12	0
46	2o	728	0	760	11	0
47	1p	681	0	697	26	0
47	2p	677	0	686	12	0
48	1q	823	0	891	22	0
48	2q	823	0	891	16	0
49	1r	555	0	618	12	0
49	2r	555	0	618	13	0
50	1s	652	0	662	19	0
50	2s	646	0	644	35	0
51	1t	728	0	798	27	0
51	2t	727	0	796	16	0
52	1u	199	0	208	5	0
52	2u	199	0	208	10	0
53	1v	286	0	142	1	0
53	2v	286	0	142	3	0
54	1w	1556	0	779	42	0
54	2w	1536	0	770	44	0
55	1x	1656	0	849	10	0
55	2x	1656	0	849	11	0
56	1y	1552	0	791	24	0
56	2y	1552	0	791	41	0
57	10	9	0	0	0	0
57	11	2	0	0	0	0
57	12	1	0	0	0	0
57	13	5	0	0	0	0
57	14	1	0	0	0	0
57	15	7	0	0	0	0
57	16	3	0	0	0	0
57	17	5	0	0	0	0
57	18	6	0	0	0	0
57	19	1	0	0	0	0
57	1A	1096	0	0	0	0
57	1B	36	0	0	0	0
57	1D	12	0	0	0	0
57	1E	16	0	0	0	0
57	1F	15	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	1G	4	0	0	0	0
57	1I	1	0	0	0	0
57	1N	6	0	0	0	0
57	1O	5	0	0	0	0
57	1P	6	0	0	0	0
57	1Q	7	0	0	0	0
57	1R	6	0	0	0	0
57	1S	3	0	0	0	0
57	1T	2	0	0	0	0
57	1U	9	0	0	0	0
57	1V	7	0	0	0	0
57	1W	7	0	0	0	0
57	1X	6	0	0	0	0
57	1Y	2	0	0	0	0
57	1Z	2	0	0	0	0
57	1a	224	0	0	0	0
57	1b	2	0	0	0	0
57	1e	2	0	0	0	0
57	1f	1	0	0	0	0
57	1h	1	0	0	0	0
57	1l	2	0	0	0	0
57	1m	2	0	0	0	0
57	1n	2	0	0	0	0
57	1r	1	0	0	0	0
57	1t	1	0	0	0	0
57	1w	9	0	0	0	0
57	1x	12	0	0	0	0
57	20	2	0	0	0	0
57	21	2	0	0	0	0
57	23	3	0	0	0	0
57	25	5	0	0	0	0
57	26	1	0	0	0	0
57	27	2	0	0	0	0
57	28	3	0	0	0	0
57	2A	861	0	0	0	0
57	2B	18	0	0	0	0
57	2D	7	0	0	0	0
57	2E	9	0	0	0	0
57	2F	6	0	0	0	0
57	2G	1	0	0	0	0
57	2N	1	0	0	0	0
57	2O	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	2P	2	0	0	0	0
57	2Q	4	0	0	0	0
57	2R	2	0	0	0	0
57	2T	3	0	0	0	0
57	2U	2	0	0	0	0
57	2V	3	0	0	0	0
57	2W	2	0	0	0	0
57	2X	2	0	0	0	0
57	2Y	1	0	0	0	0
57	2Z	1	0	0	0	0
57	2a	226	0	0	0	0
57	2d	2	0	0	0	0
57	2e	1	0	0	0	0
57	2f	1	0	0	0	0
57	2g	1	0	0	0	0
57	2i	1	0	0	0	0
57	2j	2	0	0	0	0
57	2k	1	0	0	0	0
57	2l	3	0	0	0	0
57	2q	2	0	0	0	0
57	2r	2	0	0	0	0
57	2t	1	0	0	0	0
57	2v	2	0	0	0	0
57	2w	4	0	0	0	0
57	2x	6	0	0	0	0
58	1A	1	0	0	0	0
58	2A	1	0	0	0	0
59	14	1	0	0	0	0
59	15	1	0	0	0	0
59	16	1	0	0	0	0
59	19	1	0	0	0	0
59	1Y	1	0	0	0	0
59	1n	1	0	0	0	0
59	24	1	0	0	0	0
59	25	1	0	0	0	0
59	26	1	0	0	0	0
59	29	1	0	0	0	0
59	2Y	1	0	0	0	0
59	2n	1	0	0	0	0
60	1d	8	0	0	1	0
60	2d	8	0	0	0	0
61	10	12	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	11	8	0	0	0	0
61	12	3	0	0	0	0
61	13	6	0	0	1	0
61	15	7	0	0	0	0
61	16	4	0	0	0	0
61	17	9	0	0	0	0
61	18	12	0	0	1	0
61	1A	1984	0	0	62	0
61	1B	63	0	0	5	0
61	1D	27	0	0	0	0
61	1E	27	0	0	1	0
61	1F	17	0	0	1	0
61	1G	4	0	0	1	0
61	1H	2	0	0	0	0
61	1I	1	0	0	0	0
61	1N	4	0	0	0	0
61	1O	5	0	0	0	0
61	1P	17	0	0	0	0
61	1Q	8	0	0	0	0
61	1R	6	0	0	1	0
61	1S	2	0	0	0	0
61	1T	9	0	0	0	0
61	1U	10	0	0	0	0
61	1V	11	0	0	0	0
61	1W	9	0	0	1	0
61	1X	6	0	0	2	0
61	1Y	4	0	0	1	0
61	1a	278	0	0	18	0
61	1b	1	0	0	0	0
61	1d	1	0	0	0	0
61	1e	1	0	0	0	0
61	1f	1	0	0	0	0
61	1i	1	0	0	0	0
61	1l	6	0	0	0	0
61	1m	1	0	0	0	0
61	1o	1	0	0	0	0
61	1q	3	0	0	0	0
61	1u	1	0	0	1	0
61	1v	4	0	0	0	0
61	1w	7	0	0	0	0
61	1x	12	0	0	0	0
61	1y	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	20	3	0	0	0	0
61	21	9	0	0	0	0
61	23	2	0	0	0	0
61	25	2	0	0	0	0
61	27	4	0	0	0	0
61	28	6	0	0	0	0
61	29	1	0	0	0	0
61	2A	1142	0	0	70	0
61	2B	21	0	0	1	0
61	2D	28	0	0	1	0
61	2E	12	0	0	0	0
61	2F	17	0	0	0	0
61	2I	1	0	0	0	0
61	2N	1	0	0	0	0
61	2O	1	0	0	0	0
61	2P	8	0	0	0	0
61	2Q	1	0	0	0	0
61	2R	4	0	0	1	0
61	2T	5	0	0	0	0
61	2U	2	0	0	0	0
61	2W	2	0	0	0	0
61	2X	3	0	0	1	0
61	2Y	1	0	0	0	0
61	2Z	1	0	0	0	0
61	2a	210	0	0	24	0
61	2d	1	0	0	0	0
61	2g	1	0	0	0	0
61	2i	1	0	0	0	0
61	2j	2	0	0	1	0
61	2l	3	0	0	1	0
61	2p	1	0	0	0	0
61	2q	2	0	0	0	0
61	2r	1	0	0	0	0
61	2t	3	0	0	0	0
61	2v	1	0	0	0	0
61	2w	1	0	0	0	0
61	2x	3	0	0	0	0
All	All	299852	0	196662	3800	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 8.

All (3800) 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:1054:A:N6	1:1A:1105:U:H3	1.39	1.20
1:1A:1082:U:H3	1:1A:1086:A:N6	1.42	1.17
1:1A:1055:G:H1	1:1A:1104:C:H42	1.07	1.00
32:2a:1025:U:H3	32:2a:1036:G:H1	1.10	0.96
1:1A:1082:U:O4	1:1A:1086:A:N1	2.00	0.94
1:1A:1069:A:H5'	1:1A:1070:A:H8	1.31	0.94
1:1A:2499:C:OP1	61:1A:4101:HOH:O	1.85	0.94
1:2A:2138:C:H42	1:2A:2153:G:H1	0.97	0.94
2:2B:7:G:H21	14:2S:38:GLN:HE22	1.13	0.94
1:1A:1082:U:N3	1:1A:1086:A:N6	2.08	0.92
1:2A:2138:C:N4	1:2A:2153:G:H1	1.67	0.92
1:2A:2711:A:OP2	61:2A:3902:HOH:O	1.88	0.92
1:1A:1058:G:H1	1:1A:1080:C:N4	1.69	0.91
1:1A:2427:C:OP1	61:1A:4103:HOH:O	1.90	0.90
32:2a:1286:A:H8	32:2a:1287:A:H4'	1.33	0.90
1:2A:1798:U:H5'	3:2D:259:THR:HG22	1.55	0.89
1:1A:1798:U:H5'	3:1D:259:THR:HG22	1.54	0.89
1:1A:2822:G:OP2	61:1A:4102:HOH:O	1.89	0.89
1:2A:1689:A:H62	1:2A:1698:A:H2	1.19	0.89
10:2O:48:PRO:HB3	32:2a:1422:G:H5"	1.55	0.88
1:1A:2139:C:H42	1:1A:2152:G:H1	1.19	0.88
1:2A:2714:G:OP2	61:2A:3902:HOH:O	1.91	0.87
54:1w:50:A:H61	54:1w:64:U:H3	1.18	0.87
1:1A:2136:C:N3	1:1A:2155:G:C2	2.42	0.87
34:2c:120:VAL:HG11	34:2c:137:ALA:HB2	1.58	0.86
1:1A:2550:G:OP1	61:1A:4104:HOH:O	1.93	0.86
1:1A:1058:G:H1	1:1A:1080:C:H42	1.16	0.86
1:1A:1058:G:N2	1:1A:1080:C:N3	2.23	0.86
10:1O:2:ILE:HD12	10:1O:6:THR:HG21	1.57	0.85
1:1A:2099:U:H3	1:1A:2190:G:H1	1.21	0.85
5:1F:53:THR:HG22	5:1F:55:GLY:H	1.41	0.85
1:1A:1065:U:O2	1:1A:1073:A:N6	2.08	0.85
32:2a:922:G:H4'	36:2e:20:GLN:HA	1.57	0.85
1:1A:2100:G:H1	1:1A:2189:U:H3	0.85	0.85
33:1b:48:MET:HA	33:1b:51:LEU:HB2	1.58	0.84
54:2w:14:A:N6	54:2w:21:A:C2	2.46	0.84
19:2X:53:LYS:HB3	19:2X:82:GLN:HB3	1.58	0.84
1:2A:1204:A:H2	1:2A:1241:A:H62	1.25	0.83
32:1a:405:U:O4	35:1d:2:GLY:N	2.11	0.83
1:1A:2163:C:OP1	1:1A:2165:G:N2	2.11	0.83
1:2A:2143:C:H42	1:2A:2148:G:H1	1.23	0.83
22:10:10:THR:HG22	22:10:12:ASN:H	1.41	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1T:77:PRO:HG2	15:1T:80:SER:HB2	1.59	0.82
32:1a:1505:G:OP2	61:1a:1902:HOH:O	1.95	0.82
54:2w:8:4SU:HN3	54:2w:14:A:H62	1.27	0.82
56:2y:18:G:C2	56:2y:56:C:N3	2.47	0.82
40:1i:128:ARG:NH2	55:1x:33:U:OP2	2.13	0.82
50:2s:49:ILE:HG22	50:2s:62:ILE:HD11	1.60	0.82
19:2X:60:ARG:HH22	29:27:47:ARG:HH22	1.25	0.82
1:1A:1041:C:H42	1:1A:1114:G:H1	1.27	0.81
29:17:24:THR:HG22	29:17:27:GLY:H	1.45	0.81
26:24:16:CYS:HA	26:24:33:VAL:HG12	1.60	0.81
32:2a:999:C:H42	32:2a:1042:G:H1	1.25	0.81
38:2g:115:ARG:HG2	38:2g:118:VAL:HG22	1.59	0.81
1:2A:2206:G:H3'	1:2A:2207:G:C8	2.15	0.81
1:2A:2698:U:O4	61:2A:3904:HOH:O	1.98	0.81
42:1k:48:ILE:HD12	42:1k:63:LEU:HB2	1.60	0.81
45:2n:29:ARG:HH21	45:2n:42:ILE:HD11	1.46	0.81
36:2e:122:GLU:O	36:2e:126:ARG:NH1	2.14	0.81
1:2A:1271:G:OP2	61:2A:3903:HOH:O	1.98	0.81
1:1A:2128:C:N3	1:1A:2160:G:N2	2.30	0.80
1:2A:2134:A:H62	1:2A:2157:G:H4'	1.44	0.80
8:2I:82:ARG:H	8:2I:82:ARG:HD3	1.44	0.80
20:1Y:102:CYS:SG	20:1Y:103:GLY:N	2.55	0.80
32:1a:975:A:H4'	32:1a:976:G:H5"	1.64	0.80
1:2A:2712(A):A:OP2	61:2A:3902:HOH:O	2.00	0.80
41:2j:40:LEU:HB2	41:2j:69:ASN:HB2	1.63	0.79
32:2a:1286:A:C8	32:2a:1287:A:H4'	2.17	0.79
50:2s:13:ASP:HA	50:2s:16:LEU:HB3	1.64	0.79
1:1A:1779:U:OP2	61:1A:4105:HOH:O	2.00	0.79
32:2a:975:A:H4'	32:2a:976:G:H5"	1.65	0.79
1:1A:1055:G:H1	1:1A:1104:C:N4	1.79	0.78
33:2b:114:ARG:HA	33:2b:117:GLU:HB2	1.66	0.78
1:1A:2128:C:N4	1:1A:2160:G:N1	2.30	0.78
32:2a:1029:C:C4	32:2a:1032:G:N1	2.52	0.78
1:2A:2748:A:H5'	7:2H:4:ILE:HD12	1.65	0.78
26:14:16:CYS:SG	26:14:17:GLY:N	2.52	0.78
32:1a:376:G:H5"	47:1p:5:ARG:HB3	1.64	0.78
1:1A:1064:C:N3	1:1A:1074:G:O6	2.17	0.78
1:2A:805:G:OP1	61:2A:3905:HOH:O	2.01	0.78
33:2b:16:HIS:HB2	33:2b:204:ASN:HB3	1.66	0.78
32:2a:596:C:OP2	61:2a:1901:HOH:O	2.01	0.77
1:2A:1352:U:OP2	61:2A:3906:HOH:O	2.02	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:826:U:OP1	61:1A:4103:HOH:O	2.02	0.77
32:2a:573:A:OP2	61:2a:1902:HOH:O	2.02	0.77
1:1A:1670:C:OP2	61:1A:4104:HOH:O	2.03	0.77
34:2c:58:GLU:HB3	41:2j:92:THR:HG21	1.64	0.77
2:2B:22:U:H3	2:2B:61:G:H1	1.32	0.77
36:2e:43:LEU:HD22	36:2e:136:MET:HG3	1.66	0.77
1:2A:878:A:N6	1:2A:899:A:O2'	2.18	0.77
54:2w:14:A:N6	54:2w:21:A:H2	1.80	0.77
1:1A:1664:A:OP1	61:1A:4106:HOH:O	2.03	0.77
32:2a:953:G:H5'	32:2a:965:A:H61	1.48	0.77
1:2A:2319:G:H22	14:2S:3:ARG:HH11	1.33	0.77
32:1a:1009:G:O6	32:1a:1020:U:O2	2.03	0.76
32:2a:1310:G:H5'	44:2m:77:ASN:HD21	1.49	0.76
49:1r:38:GLU:HA	49:1r:41:LYS:HD3	1.68	0.76
5:1F:140:LEU:HD11	5:1F:170:LEU:HD21	1.68	0.76
1:2A:804:A:OP1	61:2A:3905:HOH:O	2.03	0.76
40:2i:86:VAL:HG11	40:2i:93:ARG:HE	1.50	0.76
1:2A:2049:G:N7	61:2A:3932:HOH:O	2.17	0.76
1:2A:994:C:OP1	16:2U:53:ARG:NH2	2.18	0.76
40:2i:46:ALA:HB2	40:2i:74:ILE:HG23	1.66	0.76
44:2m:23:TYR:HB3	44:2m:67:GLU:HA	1.68	0.76
34:2c:70:VAL:HG12	34:2c:72:LYS:H	1.51	0.76
44:2m:13:LYS:HA	44:2m:44:ARG:HH11	1.50	0.76
32:1a:1314:C:OP2	50:1s:4:SER:OG	2.04	0.76
32:2a:562:C:H1'	43:2l:15:ARG:HB3	1.68	0.75
1:1A:2128:C:N4	1:1A:2160:G:H1	1.82	0.75
1:2A:955:C:OP1	12:2Q:87:LYS:NZ	2.17	0.75
32:2a:860:A:OP2	61:2a:1903:HOH:O	2.03	0.75
40:2i:121:ARG:NH1	40:2i:122:ALA:O	2.19	0.75
7:2H:159:GLU:HG3	7:2H:169:VAL:HG11	1.68	0.75
36:1e:78:HIS:HE1	36:1e:143:ARG:H	1.33	0.75
1:2A:870:A:OP1	12:2Q:6:ARG:NH1	2.20	0.75
20:1Y:34:LYS:NZ	61:1Y:301:HOH:O	2.18	0.75
41:1j:27:ALA:HA	41:1j:81:THR:HG21	1.69	0.75
1:1A:1062:G:H1	1:1A:1077:A:H61	1.34	0.75
1:2A:921:G:O6	61:2A:3907:HOH:O	2.03	0.75
34:2c:88:ARG:HA	34:2c:91:LEU:HD13	1.68	0.74
13:1R:67:LEU:HD13	13:1R:76:VAL:HG21	1.67	0.74
34:1c:134:ILE:HG23	34:1c:151:VAL:HG13	1.70	0.74
1:2A:1648:C:OP1	61:2A:3903:HOH:O	2.05	0.74
32:1a:1129:C:O2	32:1a:1130:A:N6	2.19	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:2H:51:ARG:NH2	7:2H:53:GLU:OE1	2.19	0.74
1:1A:792:G:O6	61:1A:4108:HOH:O	2.05	0.74
1:1A:2407:G:OP1	61:1A:4111:HOH:O	2.06	0.74
46:1o:87:ILE:HG22	46:1o:88:ARG:H	1.52	0.74
25:13:39:ASP:OD1	25:13:44:ARG:NH1	2.20	0.74
1:2A:2049:G:OP2	61:2A:3908:HOH:O	2.05	0.74
1:1A:739:G:OP1	61:1A:4107:HOH:O	2.05	0.73
1:1A:1054:A:H61	1:1A:1105:U:H3	0.76	0.73
54:2w:49:G:N2	54:2w:65:U:O2	2.19	0.73
36:1e:78:HIS:HD2	39:1h:104:ARG:HD2	1.53	0.73
44:1m:19:LEU:HD21	44:1m:56:LEU:HD21	1.70	0.73
1:2A:2110:G:OP1	1:2A:2118:U:N3	2.14	0.73
32:2a:572:A:OP1	61:2a:1904:HOH:O	2.06	0.73
14:2S:38:GLN:NE2	14:2S:47:THR:OG1	2.20	0.73
1:1A:1185:C:OP2	61:1A:4109:HOH:O	2.05	0.73
1:1A:1811:G:N7	61:1A:4145:HOH:O	2.21	0.73
1:2A:1443:G:N7	61:2A:3946:HOH:O	2.21	0.73
1:1A:1469:A:OP2	61:1A:4110:HOH:O	2.06	0.73
1:2A:89:G:H3'	1:2A:90:U:H5"	1.69	0.73
34:1c:56:ASP:HB2	34:1c:67:THR:HB	1.70	0.73
32:2a:1270:C:OP2	52:2u:24:ARG:NH2	2.21	0.73
1:1A:1452:A:OP2	61:1A:4114:HOH:O	2.07	0.72
1:1A:2222:G:OP2	61:1A:4113:HOH:O	2.07	0.72
1:2A:2296:U:OP2	14:2S:9:ARG:NH2	2.22	0.72
1:1A:671:C:N4	61:1A:4150:HOH:O	2.23	0.72
6:1G:126:ASP:HB3	6:1G:128:ARG:H	1.52	0.72
9:2N:123:TYR:HH	9:2N:130:HIS:HE2	1.32	0.72
33:2b:69:LEU:HB3	33:2b:162:ILE:HG22	1.70	0.72
54:2w:8:4SU:HN3	54:2w:14:A:N6	1.87	0.72
7:2H:118:PRO:HD2	7:2H:121:ILE:HB	1.70	0.72
1:2A:631:A:OP1	11:2P:65:ARG:NH1	2.22	0.72
1:1A:1332:G:OP1	61:1A:4112:HOH:O	2.06	0.72
1:2A:948:G:OP1	61:2A:3909:HOH:O	2.07	0.72
32:2a:559:A:OP1	36:2e:126:ARG:NH2	2.23	0.72
32:1a:79:G:C6	32:1a:90:U:O2	2.43	0.72
1:1A:631:A:OP1	11:1P:65:ARG:NH1	2.22	0.72
44:1m:3:ARG:HD2	44:1m:9:ILE:HG12	1.70	0.72
1:2A:1647:G:OP1	61:2A:3903:HOH:O	2.07	0.72
54:2w:6:C:N4	54:2w:67:G:N1	2.37	0.72
1:1A:1669:A:OP2	61:1A:4104:HOH:O	2.08	0.72
32:1a:573:A:OP2	61:1a:1903:HOH:O	2.07	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:2k:54:ARG:HH22	56:2y:39:G:H4'	1.52	0.71
40:1i:42:ARG:NH1	40:1i:71:SER:OG	2.23	0.71
1:2A:1420:U:O2'	1:2A:1421:G:OP1	2.08	0.71
48:2q:66:SER:O	48:2q:70:ARG:NH1	2.23	0.71
52:1u:5:ASP:OD2	61:1u:101:HOH:O	2.08	0.71
1:2A:1830:C:OP2	61:2A:3912:HOH:O	2.08	0.71
32:1a:501:C:OP1	43:1l:117:ARG:NH2	2.24	0.71
56:1y:8:4SU:O2'	56:1y:21:A:N1	2.23	0.71
1:2A:271(U):G:N7	61:2A:3959:HOH:O	2.24	0.71
5:2F:122:LYS:NZ	5:2F:152:GLU:OE2	2.22	0.71
13:2R:97:VAL:HG22	13:2R:114:VAL:HG13	1.71	0.71
44:2m:37:THR:O	44:2m:55:ARG:NH1	2.23	0.71
14:1S:25:ARG:NH1	14:1S:42:ASP:OD1	2.23	0.71
1:2A:2839:G:H5'	13:2R:46:GLY:HA2	1.71	0.71
5:2F:21:ALA:HB3	5:2F:22:ALA:HA	1.73	0.71
1:1A:2136:C:N4	1:1A:2155:G:C6	2.58	0.71
1:2A:981:A:OP1	61:2A:3911:HOH:O	2.08	0.71
32:1a:1027:C:C2	32:1a:1034:G:N2	2.58	0.71
10:1O:48:PRO:HB3	32:1a:1422:G:H5"	1.73	0.71
54:1w:60:U:H5"	54:1w:61:C:H5	1.56	0.71
1:1A:192:C:OP1	61:1A:4115:HOH:O	2.08	0.71
1:1A:1271:G:OP2	61:1A:4116:HOH:O	2.09	0.71
54:1w:49:G:N1	54:1w:65:U:N3	2.33	0.71
10:2O:20:MET:HE3	10:2O:44:LYS:HE3	1.72	0.71
1:1A:736:C:OP1	61:1A:4117:HOH:O	2.09	0.70
54:1w:50:A:N6	54:1w:64:U:H3	1.89	0.70
32:2a:1396:A:OP2	61:2a:1905:HOH:O	2.09	0.70
56:2y:18:G:N2	56:2y:56:C:C2	2.59	0.70
1:1A:1075:C:H2'	1:1A:1076:C:H5'	1.72	0.70
1:2A:2143:C:N3	1:2A:2148:G:N2	2.38	0.70
32:2a:673:G:H2'	32:2a:674:G:C8	2.25	0.70
1:1A:2139:C:N4	1:1A:2152:G:H1	1.89	0.70
1:2A:2143:C:N4	1:2A:2148:G:H1	1.89	0.70
1:2A:2156:G:H2'	1:2A:2157:G:C2	2.27	0.70
17:2V:43:GLU:OE1	17:2V:43:GLU:N	2.24	0.70
32:1a:574:A:OP2	61:1a:1903:HOH:O	2.08	0.70
1:2A:568:U:O4	61:2A:3910:HOH:O	2.07	0.70
15:2T:18:ASP:OD1	15:2T:18:ASP:N	2.23	0.70
1:1A:2608:G:N7	61:1A:4153:HOH:O	2.24	0.70
8:1I:92:VAL:HG13	8:1I:120:ILE:HB	1.72	0.70
1:2A:1022:G:H22	1:2A:1142(A):A:H2	1.38	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:473:G:H2'	32:2a:474:G:H8	1.56	0.70
8:1I:40:THR:O	8:1I:44:LEU:HB2	1.91	0.70
8:1I:130:TYR:HB3	8:1I:138:ILE:HB	1.72	0.70
21:1Z:156:LYS:HD2	21:1Z:158:PRO:HD3	1.74	0.70
26:24:40:HIS:HB3	26:24:43:TYR:HB2	1.72	0.70
1:1A:11:G:H2'	1:1A:12:U:H5'	1.74	0.70
32:2a:1105:A:H2'	32:2a:1106:G:H8	1.56	0.70
48:1q:53:LEU:HD23	48:1q:82:MET:HE1	1.74	0.70
1:2A:2166:G:O6	1:2A:2171:A:N6	2.24	0.70
6:2G:123:ASN:O	6:2G:125:PHE:N	2.25	0.70
42:2k:62:GLN:HE21	42:2k:97:ALA:HB2	1.56	0.70
46:2o:87:ILE:HG22	46:2o:88:ARG:H	1.56	0.70
32:1a:236:G:OP1	48:1q:40:LYS:NZ	2.25	0.70
1:2A:962:G:OP1	61:2A:3909:HOH:O	2.10	0.69
32:2a:372:C:O2	61:2a:1906:HOH:O	2.10	0.69
32:2a:597:G:OP2	61:2a:1901:HOH:O	2.10	0.69
6:2G:114:ILE:HA	6:2G:140:ILE:HD11	1.73	0.69
32:1a:664:G:H22	32:1a:741:G:H1	1.37	0.69
1:2A:2343:C:HO2'	1:2A:2373:G:HO2'	1.39	0.69
32:2a:1346:A:H61	32:2a:1374:A:H3'	1.57	0.69
32:1a:1499:A:OP2	61:1a:1902:HOH:O	2.09	0.69
15:1T:39:ARG:HH21	32:1a:345:C:H5"	1.56	0.69
33:1b:8:LYS:O	33:1b:217:ARG:NH1	2.25	0.69
1:2A:2518:A:OP2	61:2A:3913:HOH:O	2.09	0.69
1:1A:1648:C:OP1	61:1A:4116:HOH:O	2.11	0.69
32:2a:504:C:OP1	61:2a:1907:HOH:O	2.10	0.69
35:2d:82:ALA:HB1	35:2d:92:VAL:HG13	1.73	0.69
1:1A:376:C:OP1	61:1A:4118:HOH:O	2.10	0.69
1:1A:1069:A:H5'	1:1A:1070:A:C8	2.22	0.69
1:1A:2303:G:O6	61:1A:4119:HOH:O	2.10	0.69
32:1a:504:C:OP1	61:1a:1904:HOH:O	2.09	0.69
32:1a:972:C:O2'	41:1j:55:LYS:O	2.11	0.69
32:2a:73:G:H1	32:2a:96:U:H3	1.39	0.69
1:1A:2183:C:H2'	1:1A:2184:G:H8	1.56	0.69
34:1c:6:HIS:HD2	34:1c:8:ILE:H	1.39	0.69
46:1o:74:ASP:HB3	46:1o:77:ARG:HB2	1.74	0.69
1:2A:1812:A:OP2	61:2A:3914:HOH:O	2.11	0.69
1:1A:1693:U:O2'	3:1D:14:ARG:NH2	2.25	0.69
38:2g:73:MET:HE3	38:2g:90:GLU:HG3	1.75	0.69
32:1a:1518:MA6:H93	32:1a:1519:MA6:H92	1.75	0.68
31:29:25:VAL:HB	31:29:34:GLN:HB2	1.74	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1F:89:VAL:O	61:1F:401:HOH:O	2.11	0.68
47:1p:72:ARG:HA	47:1p:75:ARG:HB3	1.74	0.68
6:2G:41:GLN:HG2	6:2G:43:LEU:HD12	1.75	0.68
32:1a:642:A:N3	39:1h:113:SER:OG	2.25	0.68
1:1A:2629:A:O2'	1:1A:2630:G:OP2	2.12	0.68
2:1B:102:A:N7	61:1B:304:HOH:O	2.26	0.68
56:1y:13:C:H2'	56:1y:14:A:H5"	1.75	0.68
32:2a:598:U:O4	61:2a:1901:HOH:O	2.07	0.68
39:1h:51:VAL:HG12	39:1h:52:ASP:H	1.59	0.68
54:1w:15:A:H2	54:1w:21:A:H1'	1.59	0.68
39:2h:41:ARG:NH2	39:2h:123:GLU:OE2	2.26	0.68
7:2H:41:MET:HG3	7:2H:68:THR:HG21	1.74	0.68
1:1A:2141:G:O6	1:1A:2150:U:O2	2.12	0.68
32:2a:1129:C:OP1	40:2i:66:ARG:NH1	2.26	0.68
50:1s:27:GLU:HB2	50:1s:28:LYS:HA	1.76	0.68
1:2A:2805:G:H2'	1:2A:2807:G:C8	2.28	0.68
33:2b:189:ASP:OD1	33:2b:189:ASP:N	2.23	0.68
1:1A:1315:C:OP2	61:1A:4112:HOH:O	2.11	0.68
1:2A:400:G:N7	61:2A:3970:HOH:O	2.25	0.68
1:2A:2123:G:H2'	1:2A:2124:G:H8	1.59	0.68
1:2A:2183:C:H2'	1:2A:2184:G:H8	1.59	0.67
33:2b:48:MET:HA	33:2b:51:LEU:HB2	1.74	0.67
50:2s:33:THR:HG22	50:2s:35:SER:H	1.58	0.67
1:2A:2379:G:O2'	14:2S:17:ARG:NH1	2.23	0.67
49:2r:52:PRO:HB2	49:2r:54:ARG:HG2	1.76	0.67
41:1j:38:ILE:HG13	41:1j:71:LEU:HB3	1.77	0.67
34:2c:50:ALA:HB1	34:2c:70:VAL:HG11	1.77	0.67
10:2O:115:VAL:HG13	10:2O:121:VAL:HG21	1.75	0.67
39:2h:86:ILE:HG21	39:2h:133:LEU:HD23	1.75	0.67
40:2i:128:ARG:NH2	55:2x:33:U:OP2	2.28	0.67
1:1A:744:G:OP1	61:1A:4121:HOH:O	2.11	0.67
1:1A:760:G:OP1	61:1A:4122:HOH:O	2.12	0.67
36:1e:110:LEU:HD13	36:1e:118:ILE:HG21	1.75	0.67
51:1t:10:LEU:HB3	51:1t:12:ALA:H	1.58	0.67
1:2A:2131:G:OP2	1:2A:2131:G:N2	2.25	0.67
32:1a:1402:4OC:HM22	32:1a:1403:C:H5'	1.77	0.67
1:2A:301:G:OP2	20:2Y:84:ARG:NH2	2.26	0.67
32:2a:1166:G:N2	32:2a:1170:A:OP2	2.28	0.67
33:1b:10:LEU:HD23	33:1b:48:MET:HE1	1.77	0.67
41:1j:35:SER:HB3	41:1j:73:ASP:HB2	1.77	0.67
1:2A:2114:A:H2	1:2A:2171:A:H61	1.41	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:1k:91:ARG:NH2	42:1k:110:ASP:OD1	2.27	0.67
32:1a:159:G:O2'	32:1a:161:A:N7	2.27	0.67
32:1a:446:G:O6	61:1a:1905:HOH:O	2.11	0.67
54:2w:6:C:N3	54:2w:67:G:N2	2.42	0.67
1:1A:2754:U:OP1	61:1A:4120:HOH:O	2.11	0.67
32:1a:1224:G:OP1	61:1a:1906:HOH:O	2.13	0.67
1:1A:1014:U:OP2	61:1A:4124:HOH:O	2.12	0.66
1:2A:2589:A:OP1	61:2A:3916:HOH:O	2.12	0.66
33:2b:92:TYR:N	33:2b:151:GLY:O	2.21	0.66
4:1E:105:THR:OG1	4:1E:199:ARG:NH2	2.29	0.66
32:1a:673:G:H2'	32:1a:674:G:C8	2.30	0.66
1:2A:1125:G:H5'	31:29:37:GLY:HA2	1.76	0.66
1:2A:2206:G:H5"	1:2A:2207:G:N7	2.10	0.66
1:2A:1816:G:O6	3:2D:35:LYS:NZ	2.23	0.66
5:2F:192:LEU:HD13	5:2F:194:MET:HE2	1.78	0.66
1:2A:1264:G:OP1	27:25:19:ARG:NH2	2.28	0.66
1:2A:2448:A:OP1	61:2A:3917:HOH:O	2.12	0.66
5:2F:53:THR:HG23	5:2F:55:GLY:H	1.60	0.66
1:2A:1890:A:OP2	61:2A:3915:HOH:O	2.12	0.66
32:2a:1089:G:H1	32:2a:1096:C:H42	1.44	0.66
1:2A:1030:G:OP2	12:2Q:128:LYS:NZ	2.29	0.66
42:2k:48:ILE:O	42:2k:50:TYR:N	2.27	0.66
1:1A:2124:G:H1	1:1A:2174:C:H42	1.44	0.66
1:2A:1024:G:OP2	61:2A:3920:HOH:O	2.14	0.66
1:2A:1973:G:OP1	61:2A:3918:HOH:O	2.13	0.66
24:22:29:LYS:HG2	24:22:57:ILE:HD13	1.76	0.66
32:2a:999:C:N4	32:2a:1042:G:H1	1.94	0.66
33:2b:91:PRO:HG3	33:2b:154:LEU:HB2	1.77	0.66
5:2F:185:ASP:HA	5:2F:188:ARG:HD3	1.78	0.66
1:1A:1817:G:OP1	3:1D:88:ARG:NH2	2.29	0.66
1:1A:2849:U:OP2	15:1T:95:ARG:NH1	2.28	0.66
56:1y:70:C:H3'	56:1y:71:G:H8	1.61	0.66
1:2A:832:G:H5'	11:2P:45:LEU:HD11	1.77	0.66
6:2G:3:LEU:O	6:2G:8:LYS:NZ	2.19	0.66
13:2R:103:ARG:NH1	13:2R:108:GLY:O	2.29	0.66
34:2c:70:VAL:O	34:2c:106:VAL:N	2.26	0.66
34:2c:119:ARG:HG2	34:2c:140:ARG:HH22	1.61	0.66
39:2h:12:ARG:HD2	39:2h:26:VAL:HG13	1.78	0.66
1:1A:387:U:O4	61:1A:4123:HOH:O	2.12	0.65
44:1m:79:LYS:HA	44:1m:82:MET:HE3	1.78	0.65
34:2c:20:SER:HB3	34:2c:22:TRP:HE1	1.61	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1324:G:N7	61:2A:3985:HOH:O	2.29	0.65
1:2A:2116:G:N2	1:2A:2162:G:OP1	2.28	0.65
1:2A:2127:G:N2	1:2A:2161:C:N3	2.45	0.65
1:2A:2646:C:OP2	1:2A:2732:G:O2'	2.15	0.65
32:2a:9:G:H2'	32:2a:10:A:H8	1.61	0.65
32:1a:836:G:OP1	49:1r:61:LYS:NZ	2.27	0.65
1:2A:2127:G:N1	1:2A:2161:C:N4	2.44	0.65
32:2a:1176:A:H2'	32:2a:1177:G:C8	2.31	0.65
1:1A:2206:G:H3'	1:1A:2207:G:C8	2.32	0.65
21:1Z:132:ASN:HD22	21:1Z:160:GLY:HA3	1.62	0.65
32:1a:1435:G:H2'	32:1a:1436:U:C6	2.32	0.65
33:1b:82:ARG:NH1	33:1b:86:GLU:OE2	2.30	0.65
1:2A:81:G:N7	61:2A:3993:HOH:O	2.30	0.65
1:2A:2683:C:O2	10:2O:70:LYS:NZ	2.27	0.65
32:2a:662:G:O2'	32:2a:836:G:OP1	2.15	0.65
32:2a:1274:G:N2	32:2a:1275:A:N7	2.43	0.65
1:1A:2142:C:O2	1:1A:2149:G:N1	2.29	0.65
28:16:53:LYS:NZ	56:1y:1:G:OP1	2.28	0.65
1:2A:1449:A:O2'	1:2A:1529:G:N2	2.26	0.65
1:2A:2268:A:OP1	61:2A:3922:HOH:O	2.14	0.65
40:1i:110:GLU:OE2	40:1i:113:LYS:NZ	2.29	0.65
56:1y:37:A:H2'	56:1y:38:A:H8	1.61	0.65
1:2A:370:G:N7	61:2A:3984:HOH:O	2.29	0.65
1:2A:783:A:OP2	61:2A:3916:HOH:O	2.14	0.65
26:24:15:ILE:HG13	26:24:21:VAL:HG13	1.79	0.65
47:2p:53:VAL:HG13	47:2p:79:VAL:HG22	1.78	0.65
36:1e:78:HIS:CE1	36:1e:143:ARG:H	2.13	0.65
1:2A:1313:U:OP1	61:2A:3923:HOH:O	2.15	0.65
32:2a:663:A:O3'	49:2r:64:ARG:NH2	2.28	0.65
34:2c:30:ARG:HH21	45:2n:38:GLY:HA2	1.62	0.65
56:2y:18:G:C6	56:2y:56:C:N4	2.64	0.65
21:1Z:52:SER:O	21:1Z:54:HIS:N	2.29	0.65
1:1A:1937:A:H1'	1:1A:1939:5MU:H72	1.77	0.65
56:1y:66:C:H2'	56:1y:67:G:C8	2.32	0.65
39:2h:7:ALA:HA	39:2h:10:LEU:HD12	1.78	0.65
21:1Z:139:VAL:HG12	21:1Z:140:ASP:H	1.61	0.64
1:2A:896:A:H1'	54:2w:56:C:H5'	1.78	0.64
1:2A:1021:A:H62	1:2A:1141:U:H3	1.44	0.64
40:2i:88:TYR:HD2	40:2i:89:ASN:HB2	1.62	0.64
40:1i:23:ASN:OD1	40:1i:23:ASN:N	2.28	0.64
1:2A:307:G:N7	61:2A:3995:HOH:O	2.30	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:26:35:GLU:HG2	28:26:50:ARG:HD3	1.79	0.64
41:2j:10:GLY:HA3	41:2j:16:LEU:HD21	1.79	0.64
54:2w:6:C:N4	54:2w:67:G:C6	2.66	0.64
1:1A:2810:A:N6	1:1A:2891:G:O2'	2.29	0.64
32:1a:79:G:O6	32:1a:90:U:C2	2.50	0.64
32:1a:1108:G:O6	61:1a:1908:HOH:O	2.13	0.64
2:2B:118:G:OP2	61:2B:301:HOH:O	2.14	0.64
32:2a:299:G:O6	61:2a:1908:HOH:O	2.11	0.64
32:2a:406:G:H21	35:2d:119:GLN:HE22	1.45	0.64
32:2a:1119:C:OP2	40:2i:9:ARG:NH2	2.30	0.64
36:2e:77:PRO:HD2	36:2e:142:LEU:HD13	1.79	0.64
42:2k:41:THR:HG21	42:2k:71:LYS:HB2	1.78	0.64
32:1a:1125:U:H4'	41:1j:5:ARG:NH2	2.12	0.64
32:1a:1381:U:H1'	38:1g:79:ARG:HG2	1.80	0.64
19:2X:44:GLU:OE2	61:2X:201:HOH:O	2.14	0.64
33:2b:74:LYS:NZ	33:2b:206:ASP:OD1	2.29	0.64
32:1a:693:G:OP2	61:1a:1909:HOH:O	2.15	0.64
44:1m:17:VAL:O	44:1m:20:THR:OG1	2.13	0.64
1:2A:1800:C:OP2	3:2D:183:ARG:NH2	2.30	0.64
39:2h:28:ALA:HB3	39:2h:57:PRO:HB2	1.80	0.64
1:1A:1105:U:H2'	1:1A:1106:G:H8	1.62	0.64
5:1F:53:THR:CG2	5:1F:55:GLY:H	2.11	0.64
10:1O:104:ARG:NE	15:1T:36:GLU:OE2	2.25	0.64
32:1a:718:G:H5'	42:1k:117:ASN:HB2	1.78	0.64
33:1b:195:ASP:O	39:1h:68:ARG:NH2	2.31	0.64
1:1A:880:G:H2'	1:1A:881:G:H8	1.61	0.64
1:1A:2142:C:N3	1:1A:2149:G:O6	2.30	0.64
2:1B:99:G:OP2	61:1B:302:HOH:O	2.15	0.64
5:1F:157:VAL:HB	5:1F:194:MET:HG2	1.80	0.64
1:2A:1355:G:O6	61:2A:3919:HOH:O	2.13	0.64
52:2u:6:ARG:HG2	52:2u:15:ARG:HD2	1.79	0.64
1:1A:1060:U:H3	1:1A:1088:A:H8	1.46	0.64
40:1i:9:ARG:HG2	40:1i:14:VAL:HG12	1.78	0.64
46:1o:39:LEU:HD13	46:1o:56:LEU:HB2	1.79	0.64
47:1p:19:ILE:HD12	47:1p:36:ILE:HG13	1.80	0.64
1:2A:2125:G:H1	1:2A:2172:U:P	2.21	0.64
1:2A:2364:C:OP1	22:20:55:ARG:NH1	2.31	0.64
50:2s:51:VAL:O	50:2s:58:VAL:N	2.30	0.64
32:1a:1456:G:O3'	51:1t:39:LYS:NZ	2.30	0.64
46:1o:25:THR:HG21	46:1o:70:LEU:HB2	1.80	0.64
1:2A:297:C:OP2	61:2A:3924:HOH:O	2.15	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2060:A:N3	61:2A:3998:HOH:O	2.30	0.64
1:2A:2819:G:N7	61:2A:3992:HOH:O	2.30	0.63
32:2a:438:G:N1	32:2a:495:A:OP2	2.21	0.63
32:2a:1469:G:N7	61:2a:1926:HOH:O	2.30	0.63
38:2g:105:VAL:O	38:2g:109:ASN:ND2	2.27	0.63
1:1A:1650:G:OP2	61:1A:4126:HOH:O	2.15	0.63
1:1A:2777:G:O6	61:1A:4125:HOH:O	2.15	0.63
15:1T:127:ALA:C	15:1T:129:ARG:H	2.05	0.63
32:1a:1086:U:H3	32:1a:1099:G:H22	1.45	0.63
1:2A:2130:U:H2'	1:2A:2158:A:H61	1.63	0.63
32:2a:1189:C:OP1	41:2j:51:ARG:NH2	2.31	0.63
41:2j:47:PHE:HB2	41:2j:63:PHE:HB2	1.80	0.63
52:1u:6:ARG:HG2	52:1u:15:ARG:HD2	1.81	0.63
8:2I:4:ILE:HG12	8:2I:18:VAL:HG22	1.81	0.63
32:2a:769:G:H4'	32:2a:1513:A:H4'	1.80	0.63
40:2i:9:ARG:HG2	40:2i:14:VAL:HG12	1.80	0.63
49:2r:48:GLY:O	49:2r:74:ARG:NH2	2.31	0.63
17:1V:55:ALA:HA	17:1V:101:GLY:HA2	1.81	0.63
32:2a:770:C:OP1	61:2a:1911:HOH:O	2.16	0.63
32:2a:947:G:O3'	44:2m:109:THR:OG1	2.16	0.63
32:2a:1412:C:H2'	32:2a:1413:A:C8	2.33	0.63
50:2s:11:VAL:O	50:2s:13:ASP:N	2.31	0.63
1:1A:428:A:OP1	61:1A:4127:HOH:O	2.15	0.63
32:1a:1031:G:H2'	32:1a:1032:G:C8	2.34	0.63
1:2A:2133:G:O2'	1:2A:2157:G:N2	2.32	0.63
2:2B:48:A:H4'	14:2S:95:HIS:HD2	1.62	0.63
1:1A:1069:A:O4'	1:1A:1096:A:O2'	2.16	0.63
21:1Z:150:LEU:HD21	21:1Z:154:ASP:HB2	1.81	0.63
1:2A:652(T):C:H2'	1:2A:652(U):G:C8	2.34	0.63
1:2A:2788:C:OP1	4:2E:61:ARG:NH2	2.31	0.63
32:2a:1376:U:OP1	38:2g:98:SER:OG	2.14	0.63
42:2k:62:GLN:OE1	42:2k:93:GLN:NE2	2.31	0.63
32:2a:976:G:H5'	32:2a:1358:U:O2'	1.98	0.63
33:2b:58:ILE:HA	33:2b:61:LEU:HB3	1.79	0.63
34:2c:119:ARG:HG3	34:2c:123:GLN:HE21	1.64	0.63
45:2n:9:LYS:HG3	45:2n:12:ARG:HH21	1.64	0.63
2:1B:23:G:O6	61:1B:301:HOH:O	2.14	0.63
6:1G:15:VAL:HG22	6:1G:175:LEU:HB3	1.79	0.63
35:1d:15:GLU:OE2	35:1d:59:ARG:NH1	2.31	0.63
14:2S:15:ARG:O	14:2S:19:LYS:HG2	1.99	0.63
44:1m:14:ARG:NH2	44:1m:16:ASP:OD2	2.32	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:1w:27:A:H2'	54:1w:28:G:C8	2.34	0.63
18:2W:88:ARG:NH1	18:2W:94:ASP:OD2	2.32	0.63
34:2c:52:LEU:HD13	34:2c:68:VAL:HG13	1.79	0.63
54:2w:50:A:H61	54:2w:64:U:H3	1.44	0.63
1:1A:1119:C:N4	61:1A:4163:HOH:O	2.32	0.62
44:2m:78:ILE:HA	44:2m:81:LEU:HD12	1.81	0.62
1:1A:249:C:O2	30:18:12:LYS:NZ	2.30	0.62
1:1A:1453:U:OP1	13:1R:77:ARG:NH1	2.28	0.62
12:1Q:111:GLU:OE2	12:1Q:133:ARG:NH1	2.30	0.62
32:1a:67:C:H2'	32:1a:68:G:C8	2.33	0.62
1:2A:531:C:OP1	1:2A:561:G:N1	2.32	0.62
1:2A:1721:G:H8	1:2A:1741:A:H62	1.47	0.62
32:2a:157:G:H1	32:2a:164:U:H3	1.46	0.62
54:2w:6:C:C4	54:2w:67:G:N1	2.66	0.62
1:2A:2100:G:H1	1:2A:2189:U:H3	1.48	0.62
8:2I:88:ILE:HG22	8:2I:90:GLY:H	1.64	0.62
56:2y:65:U:H2'	56:2y:66:C:C6	2.35	0.62
1:1A:1053:C:H42	1:1A:1106:G:H1	1.47	0.62
8:1I:94:ALA:H	8:1I:116:LEU:HD22	1.64	0.62
1:2A:1568:G:N7	61:2A:4000:HOH:O	2.31	0.62
33:1b:127:ILE:HG21	33:1b:130:ARG:HD3	1.80	0.62
1:2A:2126:A:N6	1:2A:2163:C:O4'	2.32	0.62
32:2a:1030(A):G:N2	32:2a:1030(D):A:OP2	2.30	0.62
32:1a:1166:G:N2	32:1a:1170:A:OP2	2.32	0.62
32:2a:890:G:O2'	32:2a:906:G:O6	2.15	0.62
1:2A:1783:A:HO2'	1:2A:2607:G:HO2'	1.46	0.62
32:2a:1417:G:O6	61:2a:1909:HOH:O	2.12	0.62
1:1A:2879:C:OP2	61:1A:4128:HOH:O	2.16	0.62
4:1E:29:GLY:HA3	61:1E:404:HOH:O	2.00	0.62
6:1G:126:ASP:HB2	6:1G:130:ASN:H	1.65	0.62
19:1X:31:HIS:HD2	19:1X:33:LYS:H	1.45	0.62
21:2Z:5:LEU:HB2	21:2Z:47:VAL:HG21	1.82	0.62
34:2c:127:ARG:NH2	34:2c:192:THR:OG1	2.32	0.62
1:2A:1959:G:N7	61:2A:4002:HOH:O	2.31	0.62
8:2I:72:LEU:HD21	8:2I:107:VAL:HG11	1.81	0.62
14:2S:23:ARG:NH2	14:2S:85:VAL:O	2.33	0.62
32:2a:1086:U:H3	32:2a:1099:G:H22	1.48	0.62
34:1c:17:ASP:OD2	34:1c:21:ARG:NH2	2.33	0.62
38:1g:89:MET:HE2	38:1g:89:MET:HA	1.81	0.62
39:1h:34:GLU:OE1	39:1h:37:ARG:NH1	2.32	0.62
1:2A:2138:C:N3	1:2A:2153:G:N2	2.42	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:2I:5:LEU:HD11	8:2I:19:VAL:HG22	1.82	0.62
36:2e:57:LYS:HG2	36:2e:61:TYR:HE2	1.65	0.62
1:1A:2361:A:OP1	30:18:27:THR:OG1	2.13	0.61
1:2A:2079:U:O3'	23:21:35:THR:OG1	2.18	0.61
36:2e:20:GLN:NE2	36:2e:21:ALA:O	2.31	0.61
43:2l:32:PHE:HB3	43:2l:84:LEU:HD11	1.80	0.61
1:1A:878:A:N6	1:1A:899:A:O2'	2.29	0.61
21:1Z:120:ILE:N	21:1Z:171:ILE:O	2.28	0.61
7:2H:8:PRO:HB3	7:2H:51:ARG:HG2	1.81	0.61
32:2a:352:C:O2'	32:2a:354:G:OP1	2.17	0.61
1:1A:1054:A:N1	1:1A:1105:U:O2	2.34	0.61
43:1l:70:ILE:HG12	43:1l:100:ILE:HD12	1.82	0.61
5:2F:137:LYS:HA	5:2F:140:LEU:HD12	1.82	0.61
6:2G:108:ASN:HA	26:24:37:SER:HB3	1.83	0.61
32:2a:1142:G:H3'	32:2a:1143:G:H8	1.65	0.61
1:1A:1176:G:H1'	1:1A:1177:A:H5"	1.83	0.61
5:2F:116:ASP:OD2	11:2P:1:MET:N	2.33	0.61
32:2a:820:U:OP1	61:2a:1913:HOH:O	2.16	0.61
52:2u:17:THR:O	52:2u:22:ARG:NH1	2.34	0.61
4:1E:28:ALA:HB3	4:1E:93:VAL:HG12	1.81	0.61
32:1a:1021:G:O2'	32:1a:1022:G:O5'	2.13	0.61
36:1e:78:HIS:CD2	39:1h:104:ARG:HD2	2.34	0.61
1:2A:2110:G:H3'	1:2A:2111:C:H5'	1.82	0.61
8:2I:38:LEU:H	8:2I:38:LEU:HD12	1.64	0.61
32:2a:576:G:OP1	61:2a:1912:HOH:O	2.16	0.61
32:2a:708:C:H2'	32:2a:709:G:H8	1.64	0.61
32:2a:1134:G:C2	32:2a:1135:U:H1'	2.35	0.61
1:1A:2102:U:H3	1:1A:2187:G:H1	1.48	0.61
15:1T:60:THR:HG22	15:1T:77:PRO:HA	1.83	0.61
19:1X:54:VAL:HG22	19:1X:81:VAL:HG12	1.83	0.61
34:2c:108:ASN:HB3	34:2c:111:LEU:HB2	1.83	0.61
1:2A:1670:C:OP1	61:2A:3926:HOH:O	2.16	0.61
33:2b:88:ALA:HB2	33:2b:219:VAL:HG13	1.81	0.61
35:2d:175:SER:HB3	35:2d:186:LEU:HD11	1.82	0.61
11:1P:90:ARG:HG2	11:1P:90:ARG:HH11	1.65	0.61
42:1k:87:THR:O	42:1k:87:THR:OG1	2.14	0.61
54:1w:27:A:H2'	54:1w:28:G:H8	1.66	0.61
54:1w:58:A:O2'	54:1w:61:C:N4	2.34	0.61
1:2A:956:G:H5"	12:2Q:77:LYS:HD2	1.83	0.61
1:2A:2318:G:H21	14:2S:3:ARG:NE	1.98	0.61
34:2c:91:LEU:HD21	34:2c:101:LEU:HD12	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1c:62:ASP:HA	34:1c:97:LYS:HG2	1.81	0.61
1:2A:307:G:N1	1:2A:310:A:OP2	2.33	0.61
1:2A:2125:G:N3	1:2A:2173:A:N6	2.45	0.61
5:2F:155:LEU:HB2	5:2F:189:THR:HG21	1.83	0.61
12:2Q:16:ARG:HG2	12:2Q:18:LYS:HE2	1.83	0.61
21:2Z:171:ILE:HD12	21:2Z:172:ALA:H	1.66	0.61
23:21:52:ARG:HH21	23:21:57:GLU:HB2	1.65	0.61
32:1a:17:U:H2'	32:1a:18:C:C6	2.35	0.60
32:1a:79:G:O6	32:1a:90:U:O2	2.19	0.60
1:2A:271(G):C:H2'	1:2A:271(H):G:C8	2.36	0.60
1:2A:852:G:H2'	1:2A:853:G:H8	1.66	0.60
2:2B:7:G:H21	14:2S:38:GLN:NE2	1.93	0.60
8:2I:82:ARG:HG2	8:2I:89:TYR:HD2	1.66	0.60
13:2R:67:LEU:HD13	13:2R:76:VAL:HG21	1.82	0.60
46:2o:25:THR:HG21	46:2o:70:LEU:HB2	1.82	0.60
47:2p:28:ARG:NH1	47:2p:29:ASP:OD1	2.34	0.60
1:1A:2002:G:OP2	13:1R:9:LYS:NZ	2.30	0.60
3:1D:183:ARG:HG3	3:1D:270:ILE:HD13	1.82	0.60
10:1O:97:ARG:NH1	32:1a:339:C:OP2	2.33	0.60
32:1a:193:C:H2'	32:1a:194:C:H6	1.67	0.60
32:1a:1531:A:H8	32:1a:1531:A:O5'	1.83	0.60
1:2A:1365:A:O2'	23:21:11:ARG:NH1	2.34	0.60
1:1A:1013:C:OP2	61:1A:4124:HOH:O	2.17	0.60
21:1Z:52:SER:C	21:1Z:54:HIS:H	2.08	0.60
1:2A:1693:U:O2'	3:2D:14:ARG:NH2	2.34	0.60
33:2b:21:ARG:HA	33:2b:39:ILE:HA	1.83	0.60
43:2l:53:ARG:HG3	43:2l:93:LEU:HD21	1.82	0.60
50:2s:19:VAL:O	50:2s:23:ASN:ND2	2.34	0.60
32:1a:421:U:O2'	32:1a:423:G:N7	2.35	0.60
1:2A:800:A:H8	1:2A:800:A:OP1	1.85	0.60
1:2A:1278:A:OP1	13:2R:36:THR:HG23	2.00	0.60
21:2Z:152:ALA:HB1	21:2Z:163:LEU:HD11	1.84	0.60
4:2E:3:GLY:HA3	4:2E:81:ILE:HD12	1.83	0.60
14:2S:67:ARG:HG2	14:2S:71:ARG:HD2	1.84	0.60
40:2i:85:LEU:HB3	40:2i:92:TYR:HD2	1.67	0.60
32:1a:973:G:OP1	41:1j:57:LYS:NZ	2.31	0.60
1:2A:2251:OMG:HM22	1:2A:2252:G:H5'	1.82	0.60
54:2w:17:G:O2'	54:2w:57:G:N2	2.34	0.60
1:1A:1054:A:N6	1:1A:1105:U:N3	2.22	0.60
1:1A:2144:U:H3	1:1A:2147:G:H22	1.50	0.60
49:1r:32:ARG:HA	49:1r:69:THR:HG21	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1062:U:H2'	32:2a:1063:C:C6	2.36	0.60
56:2y:15:A:H61	56:2y:48:C:H42	1.47	0.60
1:1A:1087:G:H2'	1:1A:1089:G:C8	2.37	0.60
8:1I:77:LEU:HB3	8:1I:142:VAL:HG12	1.84	0.60
32:1a:13:U:O2'	61:1a:1907:HOH:O	2.13	0.60
32:1a:165:C:H2'	32:1a:166:G:H8	1.65	0.60
1:2A:883:G:N2	1:2A:894:C:O2	2.34	0.60
1:2A:2396:G:OP1	23:21:25:LYS:NZ	2.27	0.60
32:1a:324:G:N7	61:1a:1929:HOH:O	2.31	0.60
33:1b:77:ALA:HB2	33:1b:211:ILE:HD13	1.84	0.60
44:1m:3:ARG:HG2	44:1m:8:GLU:HA	1.84	0.60
54:1w:26:G:O6	54:1w:44:A:N1	2.35	0.60
32:2a:1402:4OC:HM22	32:2a:1403:C:H5'	1.82	0.60
43:2l:40:VAL:HG21	43:2l:78:GLN:HA	1.84	0.60
1:1A:1359:A:H2'	1:1A:1360:A:H5'	1.83	0.59
32:1a:1239:A:H62	32:1a:1299:A:N6	2.00	0.59
54:1w:17:G:O2'	54:1w:57:G:N2	2.23	0.59
5:2F:18:ARG:NH1	5:2F:127:GLU:OE2	2.35	0.59
7:2H:3:ARG:NH1	7:2H:4:ILE:H	2.00	0.59
14:2S:99:LYS:NZ	14:2S:103:GLU:OE2	2.23	0.59
26:24:53:GLU:HG2	26:24:55:ARG:H	1.66	0.59
32:2a:1065:U:H3	32:2a:1109:C:H5"	1.67	0.59
1:1A:301:G:OP2	20:1Y:84:ARG:NH2	2.32	0.59
1:1A:1996:C:H4'	1:1A:1997:G:OP1	2.02	0.59
1:1A:2788:C:OP1	4:1E:61:ARG:NH2	2.34	0.59
32:1a:26:A:O2'	35:1d:209:ARG:NH2	2.36	0.59
32:1a:812:C:N3	61:1a:1928:HOH:O	2.31	0.59
46:1o:54:ARG:HG2	46:1o:58:MET:HE2	1.84	0.59
17:2V:60:GLU:HB2	17:2V:97:LYS:HE2	1.84	0.59
1:1A:588:U:H2'	1:1A:589:C:C6	2.36	0.59
1:1A:602:G:O2'	1:1A:655:A:N6	2.34	0.59
1:1A:2328:A:H2'	1:1A:2329:G:C8	2.37	0.59
1:2A:1147:C:H2'	1:2A:1148:A:H8	1.65	0.59
1:2A:2327:A:H2'	1:2A:2328:A:C8	2.37	0.59
21:2Z:138:GLU:HG2	21:2Z:156:LYS:HE2	1.83	0.59
32:2a:539:A:H2'	32:2a:540:G:C8	2.37	0.59
32:2a:1271:G:C2	32:2a:1272:G:N7	2.70	0.59
32:1a:1036:G:H5"	32:1a:1037:C:C5	2.38	0.59
48:1q:66:SER:O	48:1q:70:ARG:NH1	2.36	0.59
6:2G:124:SER:O	6:2G:124:SER:OG	2.16	0.59
12:2Q:111:GLU:O	12:2Q:115:MET:HG2	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1002:G:C6	32:2a:1003:G:H8	2.21	0.59
32:2a:1518:MA6:H93	32:2a:1519:MA6:H92	1.84	0.59
33:2b:16:HIS:HB2	33:2b:204:ASN:HD22	1.67	0.59
33:2b:144:ARG:NH2	33:2b:148:TYR:OH	2.36	0.59
35:2d:57:ARG:NH1	35:2d:205:GLU:OE2	2.35	0.59
50:2s:15:LEU:HD12	50:2s:18:LYS:HD2	1.84	0.59
13:1R:97:VAL:HG22	13:1R:114:VAL:HG13	1.85	0.59
33:1b:185:ILE:HG22	33:1b:199:TYR:HB2	1.84	0.59
36:1e:74:GLY:HA3	36:1e:116:THR:HG22	1.84	0.59
47:1p:22:THR:HA	47:1p:33:ILE:HG13	1.83	0.59
6:2G:59:GLU:OE2	6:2G:138:GLN:NE2	2.36	0.59
54:2w:8:4SU:S4	54:2w:14:A:N7	2.76	0.59
1:1A:2136:C:C2	1:1A:2155:G:N2	2.70	0.59
8:1I:93:THR:H	8:1I:96:ASP:HB2	1.66	0.59
32:1a:757:U:H2'	32:1a:758:G:O4'	2.03	0.59
6:2G:68:PRO:HB2	6:2G:90:LEU:HB3	1.84	0.59
56:2y:19:U:H1'	56:2y:21:A:H5'	1.83	0.59
39:1h:124:ALA:O	39:1h:128:GLY:N	2.36	0.59
40:2i:21:PRO:HA	40:2i:59:PHE:HA	1.85	0.59
1:1A:1796:U:H2'	1:1A:1797:C:C6	2.38	0.59
5:1F:165:ARG:HA	5:1F:168:ARG:HD2	1.84	0.59
24:12:41:ILE:HG13	24:12:43:GLN:HG3	1.85	0.59
1:2A:947:G:O6	61:2A:3925:HOH:O	2.15	0.59
38:2g:50:ILE:HD11	38:2g:58:PRO:HA	1.84	0.59
1:1A:2787:C:H1'	4:1E:62:PRO:HG3	1.85	0.59
36:1e:152:ARG:NH2	39:1h:107:LEU:O	2.36	0.59
54:1w:2:C:H2'	54:1w:3:G:C8	2.37	0.59
32:2a:936:C:H2'	32:2a:937:A:O4'	2.03	0.59
32:2a:950:U:H3	32:2a:1231:G:H1	1.49	0.59
21:1Z:132:ASN:N	21:1Z:132:ASN:OD1	2.36	0.59
1:2A:271(E):U:H2'	1:2A:271(F):C:C6	2.38	0.59
1:2A:322:A:OP2	5:2F:169:ASN:HB2	2.03	0.59
1:2A:2123:G:H2'	1:2A:2124:G:C8	2.37	0.59
1:2A:2206:G:H3'	1:2A:2207:G:H8	1.63	0.59
8:2I:31:LEU:HD21	8:2I:38:LEU:HG	1.84	0.59
13:2R:2:ARG:NH1	13:2R:5:LYS:O	2.36	0.59
32:2a:473:G:H2'	32:2a:474:G:C8	2.37	0.59
32:2a:537:G:H5"	43:2l:113:ARG:NH1	2.18	0.59
32:2a:1060:C:H5"	41:2j:51:ARG:HG2	1.84	0.59
33:2b:178:ARG:HH22	39:2h:68:ARG:HH22	1.49	0.59
40:1i:20:ARG:O	40:1i:60:ASP:N	2.28	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:271(H):G:H2'	1:2A:271(I):G:H8	1.67	0.58
1:2A:884:C:H3'	1:2A:885:C:C6	2.38	0.58
1:2A:2285:C:OP2	28:26:6:ARG:NH1	2.36	0.58
2:2B:41:U:H5	6:2G:70:VAL:H	1.50	0.58
56:2y:18:G:N1	56:2y:56:C:C4	2.71	0.58
26:14:55:ARG:N	26:14:56:VAL:HA	2.18	0.58
32:1a:1027:C:N4	32:1a:1034:G:H1	2.00	0.58
33:1b:18:GLY:HA3	33:1b:42:ILE:HG13	1.84	0.58
36:1e:8:GLU:OE2	36:1e:63:ARG:NH2	2.36	0.58
1:2A:1153:C:OP1	16:2U:92:ARG:NH2	2.35	0.58
1:2A:1742:G:O6	61:2A:3931:HOH:O	2.17	0.58
1:2A:2022:U:O2'	1:2A:2617:C:H5'	2.03	0.58
6:2G:122:PRO:HB3	6:2G:170:ARG:HH21	1.68	0.58
8:2I:82:ARG:HD3	8:2I:82:ARG:N	2.17	0.58
11:2P:50:ARG:HD3	30:28:7:HIS:CD2	2.38	0.58
3:1D:147:LEU:HD13	3:1D:155:LEU:HD21	1.86	0.58
38:2g:22:LEU:HG	38:2g:62:PHE:HE2	1.68	0.58
40:1i:3:GLN:HE21	40:1i:20:ARG:CZ	2.16	0.58
40:1i:121:ARG:NH1	40:1i:122:ALA:O	2.35	0.58
56:1y:37:A:H2'	56:1y:38:A:C8	2.38	0.58
1:2A:822:U:OP2	61:2A:3929:HOH:O	2.17	0.58
1:2A:898:C:H2'	1:2A:899:A:H5'	1.85	0.58
1:2A:1159:U:H2'	1:2A:1160:G:H8	1.68	0.58
1:2A:2691:C:OP2	61:2A:3933:HOH:O	2.17	0.58
12:2Q:35:VAL:HG22	12:2Q:102:VAL:HG22	1.86	0.58
32:2a:1330:U:H4'	44:2m:23:TYR:CZ	2.38	0.58
38:2g:54:THR:O	38:2g:56:GLN:N	2.33	0.58
38:2g:113:GLU:HG2	38:2g:119:ARG:HG2	1.85	0.58
32:1a:167:G:H2'	32:1a:168:G:H8	1.69	0.58
32:1a:542:G:OP1	35:1d:10:ARG:NH2	2.36	0.58
32:1a:1305:G:N2	32:1a:1331:G:H1'	2.17	0.58
1:2A:271(G):C:H2'	1:2A:271(H):G:H8	1.67	0.58
8:2I:62:LYS:HG2	8:2I:133:HIS:CE1	2.38	0.58
21:2Z:23:LYS:HD3	21:2Z:40:ASP:HA	1.86	0.58
25:23:40:THR:HG22	25:23:42:ALA:H	1.67	0.58
32:2a:664:G:H22	32:2a:741:G:H1	1.50	0.58
1:1A:1278:A:OP1	13:1R:36:THR:HG23	2.03	0.58
1:2A:1449:A:HO2'	1:2A:1529:G:H21	1.51	0.58
33:2b:187:LEU:HA	33:2b:201:ILE:HB	1.85	0.58
37:2f:61:LEU:HB3	37:2f:63:TYR:HE2	1.69	0.58
1:1A:1062:G:P	1:1A:1070:A:H1'	2.44	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1F:9:ILE:HG12	5:1F:123:LEU:HD23	1.85	0.58
23:11:2:SER:HB3	23:11:46:LEU:HD12	1.85	0.58
38:1g:78:ARG:HD3	38:1g:79:ARG:H	1.68	0.58
54:1w:49:G:O6	54:1w:65:U:O4	2.22	0.58
1:2A:731:C:OP1	61:2A:3928:HOH:O	2.17	0.58
1:2A:1864:U:OP1	1:2A:2410:G:O2'	2.17	0.58
6:2G:70:VAL:HA	6:2G:90:LEU:HD23	1.86	0.58
12:2Q:78:PRO:HG2	12:2Q:81:VAL:HG11	1.85	0.58
32:2a:1309:G:O3'	44:2m:77:ASN:ND2	2.37	0.58
32:2a:1376:U:H2'	32:2a:1377:A:H8	1.68	0.58
32:1a:56:U:H2'	32:1a:57:G:C8	2.39	0.58
7:2H:56:SER:HB3	7:2H:61:HIS:ND1	2.17	0.58
32:2a:656:C:O2'	46:2o:28:GLN:OE1	2.13	0.58
34:2c:6:HIS:HB3	45:2n:49:HIS:ND1	2.19	0.58
1:1A:2791:C:H2'	1:1A:2792:G:C8	2.38	0.58
11:1P:101:VAL:HG21	11:1P:108:LYS:HG2	1.85	0.58
1:2A:249:C:O2	30:28:12:LYS:NZ	2.33	0.58
32:2a:1004:A:N6	32:2a:1037:C:H1'	2.18	0.58
1:1A:2470:G:O6	1:1A:2476:A:O2'	2.19	0.58
32:1a:890:G:O2'	32:1a:906:G:O6	2.22	0.58
32:1a:958:A:C4	50:1s:55:LYS:HD2	2.39	0.58
1:2A:1418:G:OP2	61:2A:3927:HOH:O	2.16	0.58
1:2A:2065:C:H4'	1:2A:2251:OMG:HM23	1.86	0.58
21:2Z:154:ASP:N	21:2Z:154:ASP:OD1	2.36	0.58
32:2a:1004:A:H5"	32:2a:1024:G:H22	1.68	0.58
1:1A:1105:U:H2'	1:1A:1106:G:C8	2.38	0.57
32:1a:532:A:N6	32:1a:1206:G:O2'	2.37	0.57
54:1w:66:C:H2'	54:1w:67:G:H8	1.67	0.57
33:2b:57:PHE:HD2	33:2b:58:ILE:HG13	1.69	0.57
34:2c:12:LEU:O	45:2n:57:ARG:NH1	2.36	0.57
40:2i:17:VAL:HG11	40:2i:81:ILE:HG12	1.85	0.57
1:2A:2138:C:H2'	1:2A:2139:C:O4'	2.04	0.57
15:2T:108:ARG:NH1	32:2a:1464:G:OP1	2.37	0.57
32:2a:1316:G:H5"	45:2n:17:LYS:HD2	1.84	0.57
32:2a:1404:5MC:O2	32:2a:1519:MA6:O2'	2.19	0.57
44:2m:86:CYS:HB2	50:2s:73:GLU:HG2	1.85	0.57
56:2y:18:G:C2	56:2y:56:C:C2	2.92	0.57
1:1A:607:U:OP1	5:1F:102:PRO:HA	2.03	0.57
1:1A:1300:U:H4'	1:1A:1301:A:H5"	1.84	0.57
1:1A:2183:C:H2'	1:1A:2184:G:C8	2.38	0.57
28:16:13:CYS:SG	28:16:47:THR:HG21	2.44	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2063:C:OP1	61:2A:3930:HOH:O	2.17	0.57
5:2F:184:TYR:CE2	5:2F:188:ARG:HD2	2.40	0.57
26:24:44:THR:O	26:24:46:GLN:N	2.36	0.57
32:2a:426:G:OP1	35:2d:38:TYR:OH	2.19	0.57
32:2a:1108:G:O6	61:2a:1914:HOH:O	2.17	0.57
38:2g:20:ASP:HB3	38:2g:23:VAL:HB	1.86	0.57
32:1a:1458:G:H5"	51:1t:31:SER:HB2	1.86	0.57
1:2A:1664:A:OP1	61:2A:3934:HOH:O	2.18	0.57
1:2A:1889:A:H2'	1:2A:1890:A:C8	2.39	0.57
32:2a:1012:U:H2'	32:2a:1013:G:C8	2.39	0.57
15:2T:39:ARG:NH2	32:2a:345:C:OP2	2.37	0.57
15:2T:117:ASP:OD2	15:2T:120:ARG:NE	2.31	0.57
23:21:76:ARG:NH1	23:21:97:LEU:O	2.38	0.57
26:24:24:THR:OG1	26:24:25:TYR:N	2.27	0.57
32:2a:984:C:H2'	32:2a:985:C:C6	2.39	0.57
32:2a:984:C:H2'	32:2a:985:C:H6	1.68	0.57
37:2f:37:VAL:HA	37:2f:65:VAL:HG12	1.86	0.57
40:2i:3:GLN:HE21	40:2i:20:ARG:HE	1.51	0.57
56:1y:36:C:H2'	56:1y:37:A:O4'	2.04	0.57
1:2A:1192:G:OP2	11:2P:17:LYS:NZ	2.33	0.57
33:2b:158:LEU:HD23	33:2b:182:ILE:HD11	1.86	0.57
42:2k:34:ASP:HB2	42:2k:35:PRO:HD2	1.86	0.57
1:1A:2331:G:O2'	1:1A:2336:A:N1	2.37	0.57
32:1a:1467:G:O6	61:1a:1910:HOH:O	2.17	0.57
34:1c:3:ASN:OD1	34:1c:3:ASN:N	2.37	0.57
37:1f:74:ASP:OD1	37:1f:77:ARG:NH2	2.38	0.57
1:2A:1188:U:H4'	17:2V:79:VAL:HG22	1.86	0.57
6:2G:15:VAL:HG22	6:2G:175:LEU:HB3	1.85	0.57
8:2I:58:LEU:HD11	8:2I:62:LYS:HE3	1.87	0.57
10:2O:24:VAL:HG13	10:2O:33:ALA:HB2	1.86	0.57
11:2P:95:VAL:HG13	11:2P:125:VAL:HA	1.86	0.57
1:1A:2140:C:N3	1:1A:2151:G:O6	2.37	0.57
32:1a:973:G:H3'	32:1a:974:A:H5"	1.87	0.57
32:2a:1144:G:H21	32:2a:1146:A:H62	1.51	0.57
32:2a:1316:G:N7	50:2s:7:LYS:NZ	2.51	0.57
33:2b:149:LEU:HD22	33:2b:152:PHE:CD2	2.40	0.57
34:2c:123:GLN:O	34:2c:128:PHE:HB2	2.04	0.57
35:2d:76:ARG:NE	35:2d:80:GLU:OE2	2.32	0.57
36:2e:33:VAL:HG21	36:2e:109:ILE:HG13	1.86	0.57
1:1A:2206:G:H5"	1:1A:2207:G:C5	2.39	0.57
44:1m:2:ALA:N	44:1m:8:GLU:OE1	2.38	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:2I:82:ARG:HG2	8:2I:89:TYR:CD2	2.39	0.57
32:2a:1119:C:H2'	32:2a:1120:G:C8	2.39	0.57
32:2a:1279:A:H4'	32:2a:1280:A:OP1	2.05	0.57
1:1A:1055:G:N2	1:1A:1104:C:N3	2.47	0.57
1:1A:1266:G:O5'	18:1W:15:ARG:NH2	2.37	0.57
1:1A:2319:G:N1	14:1S:3:ARG:HA	2.19	0.57
32:1a:406:G:H21	35:1d:119:GLN:HE22	1.52	0.57
38:1g:76:ARG:HD3	38:1g:156:TRP:HZ2	1.69	0.57
44:1m:67:GLU:HG3	44:1m:71:ARG:NH2	2.19	0.57
1:2A:2820:A:OP1	13:2R:2:ARG:NH2	2.37	0.57
3:2D:206:LEU:HD22	3:2D:211:ARG:HG2	1.87	0.57
13:2R:28:LEU:HD23	13:2R:48:VAL:HG21	1.87	0.57
32:2a:1004:A:N6	32:2a:1037:C:O2	2.26	0.57
33:2b:104:ASN:OD1	33:2b:107:THR:OG1	2.20	0.57
33:2b:118:LEU:HB3	33:2b:142:LEU:HD12	1.87	0.57
40:2i:58:HIS:H	40:2i:58:HIS:CD2	2.23	0.57
32:1a:562:C:O2	43:1l:16:GLU:N	2.35	0.56
56:1y:8:4SU:O2	56:1y:21:A:H2	1.87	0.56
22:20:15:ASP:OD1	22:20:16:SER:N	2.36	0.56
23:21:23:LYS:HB3	23:21:29:GLY:HA3	1.87	0.56
33:2b:178:ARG:HH22	39:2h:68:ARG:HH12	1.53	0.56
44:2m:29:ARG:HD3	44:2m:64:TRP:CE2	2.40	0.56
54:2w:61:C:H3'	54:2w:62:C:H5"	1.87	0.56
7:1H:20:ALA:HB1	7:1H:21:PRO:HD2	1.88	0.56
12:1Q:78:PRO:HD3	55:1x:1:C:N3	2.19	0.56
21:1Z:150:LEU:HG	21:1Z:151:HIS:H	1.69	0.56
32:1a:976:G:H5'	32:1a:1358:U:O2'	2.04	0.56
1:2A:637:A:OP1	11:2P:133:SER:OG	2.18	0.56
3:2D:71:ASP:HB2	3:2D:103:ARG:HH12	1.69	0.56
32:2a:266:G:H5"	32:2a:268:C:H41	1.69	0.56
32:2a:1010:G:N1	32:2a:1020:U:H1'	2.20	0.56
32:2a:1226:C:OP2	44:2m:91:ARG:NH1	2.38	0.56
1:1A:530:G:N1	1:1A:2023:G:OP1	2.30	0.56
1:1A:621:A:OP2	11:1P:108:LYS:NZ	2.38	0.56
1:1A:1062:G:H22	1:1A:1077:A:H61	1.54	0.56
1:1A:2887:U:H2'	1:1A:2888:C:C6	2.40	0.56
5:1F:135:LYS:HB2	5:1F:138:GLU:HG3	1.87	0.56
9:1N:42:TRP:HA	9:1N:48:MET:HE1	1.87	0.56
21:1Z:138:GLU:H	21:1Z:156:LYS:HE3	1.70	0.56
26:14:15:ILE:HG12	26:14:21:VAL:HG22	1.88	0.56
33:1b:92:TYR:HH	33:1b:150:SER:HG	1.53	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:1k:86:GLY:H	42:1k:112:THR:HG1	1.50	0.56
1:2A:287:C:H2'	1:2A:288:C:H6	1.71	0.56
1:2A:483:A:O2'	20:2Y:49:VAL:O	2.22	0.56
2:2B:3:C:H2'	2:2B:4:C:C6	2.40	0.56
2:2B:75:G:N2	21:2Z:87:ASP:OD1	2.38	0.56
6:2G:7:LEU:HD13	6:2G:104:GLU:HA	1.86	0.56
6:2G:16:ARG:O	6:2G:20:ILE:HG13	2.05	0.56
20:2Y:102:CYS:SG	20:2Y:103:GLY:N	2.78	0.56
21:2Z:104:PHE:HD2	21:2Z:139:VAL:HB	1.70	0.56
32:2a:148:G:H2'	32:2a:149:A:H8	1.70	0.56
32:2a:1297:C:OP2	44:2m:44:ARG:NH2	2.39	0.56
40:2i:14:VAL:HG23	40:2i:66:ARG:HG3	1.86	0.56
44:2m:5:ALA:HB3	44:2m:22:ILE:HD13	1.87	0.56
51:2t:10:LEU:HB3	51:2t:12:ALA:H	1.70	0.56
1:1A:2591:C:H2'	1:1A:2592:G:C8	2.41	0.56
5:1F:185:ASP:HA	5:1F:188:ARG:HD3	1.88	0.56
32:1a:445:G:H2'	32:1a:446:G:C8	2.41	0.56
1:2A:1769:G:O2'	1:2A:1958:C:OP1	2.19	0.56
8:2I:75:LEU:HD13	8:2I:105:HIS:HD2	1.70	0.56
32:2a:1097:C:O2'	32:2a:1169:A:N3	2.36	0.56
1:1A:2139:C:H2'	1:1A:2140:C:O4'	2.06	0.56
11:1P:39:LYS:HB2	11:1P:45:LEU:HD13	1.87	0.56
1:2A:1803:A:O2'	3:2D:259:THR:HG21	2.05	0.56
33:2b:121:LEU:HD21	33:2b:130:ARG:HH12	1.70	0.56
5:1F:164:ARG:HD2	5:1F:175:THR:HG23	1.88	0.56
29:17:46:VAL:HG22	29:17:48:LYS:HG3	1.87	0.56
33:1b:19:HIS:HA	33:1b:39:ILE:HG23	1.87	0.56
34:1c:81:GLY:O	34:1c:85:ARG:HB2	2.05	0.56
1:2A:2162:G:H4'	1:2A:2172:U:H2'	1.88	0.56
22:20:40:GLN:HE21	22:20:57:PHE:HB3	1.70	0.56
32:2a:714:G:H2'	32:2a:715:A:C8	2.40	0.56
36:2e:143:ARG:NE	39:2h:77:GLU:OE2	2.36	0.56
1:2A:1187:G:H5'	17:2V:81:TYR:CE1	2.39	0.56
1:2A:2125:G:N1	1:2A:2172:U:OP1	2.37	0.56
15:2T:127:ALA:C	15:2T:129:ARG:H	2.14	0.56
34:2c:125:GLU:HB2	34:2c:190:ARG:HH21	1.71	0.56
40:2i:4:TYR:HB2	40:2i:19:LEU:HB2	1.88	0.56
1:1A:1800:C:OP1	3:1D:260:ARG:NH2	2.38	0.56
1:1A:2791:C:H2'	1:1A:2792:G:H8	1.71	0.56
2:1B:21:G:N7	61:1B:305:HOH:O	2.33	0.56
55:1x:8:4SU:O5'	55:1x:8:4SU:H6	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:668:G:H5'	1:2A:669:G:OP2	2.06	0.56
1:2A:1507:A:O2'	1:2A:1508:A:O4'	2.23	0.56
1:2A:1507:A:O2'	1:2A:1508:A:O5'	2.23	0.56
5:2F:64:ILE:HG21	5:2F:78:ILE:HG23	1.86	0.56
22:20:11:ARG:O	22:20:14:ARG:NH2	2.38	0.56
32:2a:921:U:O2	36:2e:19:MET:HB2	2.06	0.56
32:2a:1329:A:OP2	52:2u:7:ARG:NH1	2.34	0.56
33:2b:92:TYR:CZ	33:2b:151:GLY:HA3	2.41	0.56
1:1A:279:C:H42	1:1A:361:G:H1	1.54	0.56
32:1a:1320:C:OP1	50:1s:70:LYS:NZ	2.30	0.56
36:1e:145:LYS:HA	36:1e:148:VAL:HG22	1.88	0.56
50:1s:50:ALA:HB1	50:1s:57:HIS:HB3	1.87	0.56
1:2A:848:G:H2'	1:2A:849:A:C8	2.41	0.56
1:2A:1183:G:H5"	25:23:30:ARG:NH2	2.21	0.56
32:2a:547:A:OP1	61:2a:1916:HOH:O	2.18	0.56
32:2a:750:G:N3	46:2o:23:GLY:HA3	2.20	0.56
32:2a:1060:C:HO2'	41:2j:56:HIS:HD1	1.51	0.56
41:2j:65:LEU:HD13	45:2n:56:VAL:HG22	1.87	0.56
1:1A:1405:U:H2'	1:1A:1406:U:C6	2.41	0.56
1:1A:1429:G:H2'	1:1A:1430:C:C6	2.41	0.56
32:1a:110:C:H2'	32:1a:111:G:O4'	2.05	0.56
40:1i:26:VAL:HG13	40:1i:61:ALA:HB3	1.88	0.56
47:1p:47:ASP:OD1	47:1p:47:ASP:N	2.38	0.56
1:2A:2870:C:H2'	1:2A:2871:C:O4'	2.06	0.56
26:24:41:PRO:HG3	26:24:49:PHE:CE1	2.41	0.56
32:2a:662:G:H2'	32:2a:663:A:H8	1.70	0.56
32:2a:839:U:H3'	32:2a:840:C:H5'	1.88	0.56
44:2m:94:ARG:NH2	50:2s:81:ARG:HA	2.21	0.56
1:1A:1385:G:O2'	1:1A:1396:U:O2	2.20	0.55
5:1F:184:TYR:CE2	5:1F:188:ARG:HD2	2.41	0.55
26:14:18:CYS:SG	26:14:20:ASN:HB2	2.46	0.55
32:1a:1504:G:OP1	32:1a:1507:A:H4'	2.05	0.55
43:1l:39:VAL:HG11	43:1l:41:ARG:HH11	1.71	0.55
2:2B:28:C:H2'	2:2B:29:A:C8	2.41	0.55
3:2D:2:ALA:N	3:2D:200:ASP:OD2	2.39	0.55
26:24:60:GLN:O	26:24:62:ARG:NH1	2.39	0.55
32:2a:1010:G:C2	32:2a:1020:U:H1'	2.42	0.55
32:2a:1305:G:N2	32:2a:1331:G:H1'	2.20	0.55
6:1G:136:ARG:HG3	6:1G:137:GLU:HG3	1.89	0.55
32:2a:19:C:H5"	36:2e:86:ALA:HB1	1.88	0.55
32:2a:1225:A:OP1	44:2m:103:THR:OG1	2.23	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:2e:33:VAL:HG13	36:2e:112:LEU:HD22	1.89	0.55
1:1A:2719:G:OP2	61:1A:4129:HOH:O	2.18	0.55
47:1p:72:ARG:O	47:1p:76:GLN:N	2.34	0.55
11:2P:39:LYS:HB2	11:2P:45:LEU:HD13	1.87	0.55
32:2a:88:A:H5"	32:2a:89:C:C6	2.42	0.55
32:2a:701:C:OP1	32:2a:702:A:O2'	2.17	0.55
32:2a:1092:A:H5"	38:2g:4:ARG:NH1	2.21	0.55
33:2b:16:HIS:HB3	33:2b:210:SER:HB2	1.87	0.55
1:1A:1048:A:N1	1:1A:1112:G:O2'	2.33	0.55
1:1A:2749:A:OP1	7:1H:3:ARG:NH1	2.39	0.55
32:2a:297:G:N2	32:2a:300:A:OP2	2.39	0.55
32:2a:653:A:O5'	39:2h:56:LYS:NZ	2.39	0.55
32:2a:1013:G:N2	32:2a:1016:A:OP2	2.40	0.55
34:2c:162:GLN:NE2	53:2v:24:A:O3'	2.38	0.55
1:1A:882:G:H4'	54:1w:18:G:O6	2.06	0.55
1:1A:1058:G:N2	1:1A:1081:U:O2	2.40	0.55
1:1A:1074:G:C6	1:1A:1075:C:H1'	2.42	0.55
1:2A:646:A:H2'	1:2A:647:G:O4'	2.07	0.55
6:2G:42:GLY:O	6:2G:44:GLY:N	2.40	0.55
21:2Z:47:VAL:O	21:2Z:50:GLN:NE2	2.39	0.55
37:2f:13:ASN:ND2	37:2f:55:ASP:OD2	2.40	0.55
1:1A:2793:G:N1	1:1A:2803:C:O2	2.39	0.55
20:1Y:99:CYS:HB2	20:1Y:106:LEU:HD21	1.88	0.55
41:1j:62:HIS:HB3	45:1n:59:ALA:HB3	1.87	0.55
1:2A:906:G:O2'	12:2Q:67:ARG:NH2	2.33	0.55
1:2A:1220:A:OP2	16:2U:19:LYS:NZ	2.36	0.55
5:2F:101:LEU:HD12	5:2F:102:PRO:HD2	1.88	0.55
8:2I:45:LYS:O	8:2I:49:ALA:N	2.31	0.55
8:2I:93:THR:HG22	8:2I:119:PRO:HB3	1.89	0.55
32:2a:1271:G:N1	32:2a:1272:G:N7	2.53	0.55
34:2c:20:SER:HB3	34:2c:22:TRP:NE1	2.20	0.55
1:1A:2870:C:H2'	1:1A:2871:C:O4'	2.06	0.55
18:1W:13:SER:HB3	18:1W:16:LYS:HD2	1.87	0.55
32:1a:1348:U:H4'	40:1i:120:ARG:HD2	1.87	0.55
50:1s:63:THR:OG1	50:1s:65:ASN:OD1	2.23	0.55
54:1w:2:C:H2'	54:1w:3:G:H8	1.70	0.55
1:2A:80:G:H1	1:2A:106:C:H42	1.55	0.55
6:2G:113:ARG:NH2	6:2G:139:LEU:O	2.39	0.55
12:2Q:36:ALA:HB2	12:2Q:103:MET:SD	2.46	0.55
14:2S:11:LYS:HG3	14:2S:91:PRO:HB3	1.88	0.55
19:2X:72:LYS:NZ	19:2X:75:ASP:OD1	2.40	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:814:A:H2'	32:2a:816:A:H5'	1.88	0.55
34:2c:111:LEU:HD21	34:2c:146:ALA:HB2	1.88	0.55
39:2h:97:VAL:HG21	39:2h:128:GLY:HA2	1.89	0.55
54:2w:11:U:H2'	54:2w:12:U:H6	1.72	0.55
8:1I:84:GLY:O	8:1I:87:LYS:NZ	2.38	0.55
32:1a:1015:A:N3	32:1a:1218:C:O2'	2.32	0.55
51:1t:45:GLN:HB2	51:1t:91:LEU:HD13	1.88	0.55
1:2A:852:G:H2'	1:2A:853:G:C8	2.42	0.55
1:2A:2176:A:H2'	1:2A:2177:C:C6	2.41	0.55
48:2q:32:TYR:O	48:2q:34:LYS:N	2.34	0.55
1:1A:2693:A:H2'	1:1A:2694:G:H8	1.72	0.55
1:1A:2722:G:OP2	61:1A:4132:HOH:O	2.18	0.55
32:1a:1346:A:O2'	38:1g:10:ARG:NH2	2.40	0.55
44:1m:87:TYR:O	44:1m:91:ARG:HG2	2.07	0.55
38:2g:26:PHE:O	38:2g:30:ILE:HD12	2.06	0.55
41:2j:21:GLN:HE22	41:2j:25:GLU:HB2	1.71	0.55
50:2s:52:TYR:HB2	50:2s:57:HIS:CE1	2.42	0.55
32:1a:167:G:H2'	32:1a:168:G:C8	2.42	0.55
33:1b:139:LYS:O	33:1b:143:GLU:HG3	2.07	0.55
1:2A:994:C:O2'	1:2A:996:A:OP1	2.22	0.55
1:2A:1017:G:O6	61:2A:3938:HOH:O	2.18	0.55
6:2G:69:ALA:HB3	6:2G:91:ARG:HH21	1.71	0.55
21:2Z:146:ILE:HG12	21:2Z:174:VAL:HG13	1.88	0.55
33:2b:80:ILE:HD13	33:2b:212:GLN:HG2	1.89	0.55
41:2j:6:ILE:HB	41:2j:72:VAL:HB	1.88	0.55
56:2y:8:4SU:H6	56:2y:8:4SU:O5'	2.07	0.55
8:1I:4:ILE:HG12	8:1I:18:VAL:HG12	1.87	0.54
32:1a:877:C:OP1	39:1h:88:LYS:NZ	2.27	0.54
32:1a:1469:G:H2'	32:1a:1470:G:C8	2.42	0.54
1:2A:218:A:OP2	61:2A:3937:HOH:O	2.18	0.54
32:2a:533:A:OP1	61:2a:1915:HOH:O	2.17	0.54
32:2a:1106:G:H5"	34:2c:172:ARG:HB3	1.89	0.54
36:2e:41:VAL:O	36:2e:66:MET:HA	2.07	0.54
37:2f:2:ARG:NE	37:2f:69:GLU:HG2	2.21	0.54
52:2u:5:ASP:O	52:2u:11:GLY:HA3	2.07	0.54
3:1D:108:PRO:HB3	3:1D:143:HIS:CE1	2.42	0.54
4:1E:3:GLY:HA3	4:1E:81:ILE:HD12	1.88	0.54
39:1h:10:LEU:HD22	39:1h:83:ILE:HD11	1.88	0.54
40:1i:48:GLU:HA	40:1i:51:ARG:HD3	1.89	0.54
51:1t:22:ARG:O	51:1t:26:ASN:ND2	2.37	0.54
1:2A:2126:A:N3	1:2A:2127:G:H1'	2.22	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:2y:18:G:C2	56:2y:56:C:C4	2.95	0.54
6:1G:79:ASN:OD1	6:1G:79:ASN:N	2.40	0.54
26:14:46:GLN:O	26:14:48:ARG:N	2.39	0.54
1:2A:1140:C:OP2	9:2N:66:LYS:NZ	2.41	0.54
1:2A:2106:G:H2'	1:2A:2107:C:O4'	2.08	0.54
1:2A:2785:C:OP1	4:2E:41:LYS:NZ	2.39	0.54
17:2V:62:LEU:HD11	17:2V:95:LEU:HB2	1.88	0.54
32:2a:1353:G:OP1	52:2u:10:ARG:NH1	2.41	0.54
33:2b:73:THR:O	33:2b:73:THR:OG1	2.26	0.54
1:1A:1816:G:O6	3:1D:35:LYS:NZ	2.40	0.54
7:1H:18:GLU:HG2	7:1H:25:LYS:HB3	1.89	0.54
32:1a:636:U:H2'	32:1a:637:G:H8	1.72	0.54
33:1b:59:GLU:HB2	33:1b:221:LEU:HD21	1.87	0.54
1:2A:2135:A:N1	1:2A:2156:G:O2'	2.38	0.54
4:2E:28:ALA:HB3	4:2E:93:VAL:HG12	1.89	0.54
38:2g:69:VAL:HG21	38:2g:104:LEU:HD21	1.88	0.54
39:2h:21:LYS:O	39:2h:65:TYR:OH	2.21	0.54
40:2i:5:TYR:HD1	40:2i:18:PHE:HE1	1.54	0.54
1:1A:323:G:C8	5:1F:171:PRO:HG3	2.43	0.54
61:1A:4102:HOH:O	4:1E:110:GLY:O	2.18	0.54
32:1a:330:C:O2	61:1a:1911:HOH:O	2.18	0.54
40:1i:53:VAL:O	40:1i:55:ALA:N	2.40	0.54
1:2A:1178:C:H2'	1:2A:1179:C:H6	1.73	0.54
1:2A:2154:G:N7	1:2A:2156:G:N2	2.55	0.54
44:2m:40:ASN:HD22	44:2m:43:THR:HG23	1.71	0.54
1:1A:1187:G:H5"	17:1V:81:TYR:CE1	2.42	0.54
1:1A:2123:G:H2'	1:1A:2124:G:H8	1.72	0.54
15:1T:73:GLU:OE2	15:1T:103:ARG:NE	2.38	0.54
21:1Z:155:LEU:HD12	21:1Z:156:LYS:H	1.72	0.54
32:1a:1305:G:H22	32:1a:1331:G:H1'	1.73	0.54
32:1a:1412:C:H2'	32:1a:1413:A:C8	2.43	0.54
6:2G:106:LEU:HA	6:2G:110:ALA:HB3	1.88	0.54
14:2S:15:ARG:HB3	14:2S:19:LYS:HE3	1.90	0.54
32:2a:330:C:O2	61:2a:1910:HOH:O	2.13	0.54
32:2a:1071:C:H2'	32:2a:1072:G:H8	1.72	0.54
34:2c:40:ARG:HA	34:2c:43:LEU:HD12	1.89	0.54
41:2j:8:LEU:HG	41:2j:70:ARG:HB2	1.88	0.54
54:2w:76:L3X:N	55:2x:76:31H:N3'	2.55	0.54
1:1A:1406:U:H2'	1:1A:1407:C:C6	2.43	0.54
1:1A:2131:G:N2	1:1A:2158:A:N1	2.54	0.54
35:1d:119:GLN:HG2	35:1d:123:HIS:CD2	2.42	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2023:G:H5'	1:2A:2617:C:H4'	1.89	0.54
32:2a:1376:U:H2'	32:2a:1377:A:C8	2.43	0.54
8:1I:42:SER:OG	8:1I:43:ASN:N	2.41	0.54
32:1a:664:G:N2	32:1a:741:G:H1	2.06	0.54
1:2A:2119:A:N1	1:2A:2170:A:H2'	2.22	0.54
1:2A:2299:G:N1	1:2A:2318:G:N7	2.55	0.54
1:2A:2749:A:O3'	7:2H:62:LYS:NZ	2.40	0.54
21:2Z:7:ALA:HB2	21:2Z:59:LEU:HB3	1.89	0.54
32:2a:1513:A:H2'	32:2a:1514:C:C6	2.43	0.54
33:2b:87:ARG:NE	33:2b:233:SER:HB2	2.23	0.54
1:1A:278:A:O2'	1:1A:279:C:OP1	2.22	0.54
1:1A:821:A:H2'	1:1A:946:G:H5"	1.89	0.54
2:1B:105:A:OP1	21:1Z:72:ARG:NH1	2.41	0.54
26:14:63:TYR:N	26:14:64:GLY:HA2	2.23	0.54
32:1a:958:A:C2	50:1s:55:LYS:HB2	2.43	0.54
32:1a:1291:G:OP1	38:1g:37:ASN:ND2	2.37	0.54
44:2m:57:ARG:O	44:2m:61:GLU:HB2	2.08	0.54
50:2s:27:GLU:HB2	50:2s:28:LYS:HD3	1.89	0.54
1:1A:299:A:OP2	61:1A:4130:HOH:O	2.18	0.54
1:1A:1039:G:H1	1:1A:1116:C:H42	1.56	0.54
1:1A:1082:U:H3	1:1A:1086:A:H61	0.59	0.54
32:1a:953:G:H5'	32:1a:965:A:H61	1.73	0.54
34:1c:121:ALA:HB1	34:1c:189:ALA:HB2	1.90	0.54
1:2A:271(L):U:H5'	8:2I:50:ARG:HH11	1.73	0.54
2:2B:55:U:O3'	6:2G:27:ASN:ND2	2.39	0.54
5:2F:32:LEU:HD22	5:2F:112:MET:HE2	1.89	0.54
11:2P:38:GLN:O	11:2P:39:LYS:HB3	2.08	0.54
32:2a:662:G:H2'	32:2a:663:A:C8	2.43	0.54
32:2a:1459:C:OP1	51:2t:31:SER:OG	2.20	0.54
45:2n:26:ARG:HD3	45:2n:43:CYS:HB3	1.89	0.54
56:2y:53:G:H3'	56:2y:54:5MU:H73	1.90	0.54
1:1A:1058:G:N1	1:1A:1080:C:N4	2.31	0.53
1:1A:1168:G:H1	1:1A:1181:C:H42	1.56	0.53
32:1a:1278:U:H5'	32:1a:1279:A:O4'	2.08	0.53
32:1a:1442:G:H2'	32:1a:1442:G:N3	2.21	0.53
1:2A:1253:A:OP1	61:2A:3936:HOH:O	2.18	0.53
1:2A:1266:G:O2'	1:2A:2012:G:O6	2.23	0.53
1:2A:1502:C:H2'	1:2A:1503:U:H6	1.73	0.53
1:2A:2163:C:H3'	1:2A:2164:C:H6	1.73	0.53
2:2B:75:G:H22	21:2Z:73:GLN:NE2	2.06	0.53
7:2H:24:VAL:HG13	7:2H:37:VAL:HG21	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:2N:38:HIS:CE1	9:2N:39:ARG:HG3	2.44	0.53
21:2Z:91:LEU:HD22	21:2Z:96:VAL:HG11	1.90	0.53
32:2a:1226:C:O2'	44:2m:111:LYS:NZ	2.37	0.53
34:2c:47:LEU:HD13	34:2c:50:ALA:HB3	1.89	0.53
34:2c:82:GLU:O	34:2c:86:VAL:N	2.35	0.53
1:1A:8:A:H2'	1:1A:9:U:C6	2.43	0.53
26:14:54:GLY:N	26:14:55:ARG:HA	2.23	0.53
32:1a:202:U:H3'	32:1a:203:U:C6	2.43	0.53
46:1o:55:GLY:HA2	46:1o:58:MET:HE3	1.89	0.53
17:2V:19:LYS:HE2	17:2V:95:LEU:HD12	1.89	0.53
32:2a:768:A:OP2	61:2a:1917:HOH:O	2.19	0.53
32:2a:1181:G:O2'	32:2a:1182:G:N7	2.41	0.53
34:2c:44:GLU:HA	34:2c:52:LEU:HD23	1.90	0.53
48:2q:45:HIS:HB3	48:2q:72:ARG:HG2	1.89	0.53
1:1A:1364:G:P	23:11:3:LYS:HG3	2.48	0.53
1:1A:1498:C:OP1	61:1A:4131:HOH:O	2.18	0.53
1:1A:2161:C:HO2'	1:1A:2162:G:H8	1.55	0.53
4:1E:128:SER:OG	4:1E:129:HIS:N	2.41	0.53
8:1I:76:THR:HG23	8:1I:141:LYS:HE2	1.89	0.53
32:1a:134:A:H61	47:1p:25:ARG:HH12	1.57	0.53
32:1a:190:U:H2'	32:1a:191:G:H8	1.74	0.53
32:1a:262:A:H2'	32:1a:263:A:C8	2.43	0.53
32:1a:1427:U:H2'	32:1a:1428:A:C8	2.44	0.53
45:1n:29:ARG:HH22	45:1n:41:ARG:NH2	2.06	0.53
32:2a:11:G:H1	32:2a:23:C:H42	1.57	0.53
32:2a:142:G:H2'	32:2a:143:A:C8	2.43	0.53
38:2g:133:GLY:O	38:2g:137:LYS:N	2.34	0.53
39:2h:20:TYR:CE1	39:2h:76:PRO:HG2	2.42	0.53
43:2l:28:LYS:HE2	43:2l:64:TYR:HE2	1.73	0.53
1:1A:882:G:H4'	54:1w:18:G:C6	2.44	0.53
1:1A:889:C:O2'	1:1A:890:A:O4'	2.26	0.53
1:1A:2131:G:H5'	1:1A:2133:G:C8	2.42	0.53
1:1A:2864:G:OP2	61:1A:4134:HOH:O	2.19	0.53
24:22:32:LEU:HD13	24:22:53:LEU:HB3	1.90	0.53
26:24:16:CYS:SG	26:24:17:GLY:N	2.82	0.53
44:2m:94:ARG:HB3	44:2m:96:LEU:HD12	1.91	0.53
50:2s:31:ILE:O	50:2s:50:ALA:N	2.33	0.53
50:2s:32:LYS:HA	50:2s:50:ALA:HB3	1.90	0.53
1:1A:1803:A:O2'	3:1D:259:THR:HG21	2.08	0.53
32:1a:250:A:H4'	32:1a:251:G:O5'	2.09	0.53
32:1a:1456:G:O6	51:1t:54:LYS:NZ	2.28	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:880:G:N2	1:2A:898:C:O2	2.41	0.53
32:2a:1264:C:N4	32:2a:1272:G:O6	2.41	0.53
34:2c:185:GLY:O	34:2c:200:ALA:N	2.41	0.53
23:11:64:ALA:HA	23:11:67:ILE:HG13	1.91	0.53
32:1a:92:C:H2'	32:1a:93:G:C8	2.43	0.53
32:1a:1273:G:C2	32:1a:1274:G:H1'	2.44	0.53
35:1d:105:VAL:HG13	35:1d:110:PHE:HB2	1.89	0.53
1:2A:500:G:N1	1:2A:503:A:OP2	2.42	0.53
22:20:27:GLU:HB2	22:20:69:PHE:HD1	1.74	0.53
32:2a:9:G:H2'	32:2a:10:A:C8	2.43	0.53
32:2a:259:G:OP2	51:2t:83:ARG:NH1	2.40	0.53
32:2a:1239:A:H62	32:2a:1299:A:N6	2.07	0.53
33:2b:150:SER:OG	33:2b:151:GLY:N	2.41	0.53
1:1A:2243:U:H2'	1:1A:2244:U:C6	2.43	0.53
4:1E:36:ARG:NH1	4:1E:85:ASN:OD1	2.42	0.53
24:12:65:ASN:OD1	24:12:69:ARG:NH1	2.41	0.53
40:1i:17:VAL:HG23	40:1i:63:ILE:HG12	1.91	0.53
6:2G:18:GLU:HG2	6:2G:175:LEU:HD21	1.90	0.53
30:28:26:LYS:HD2	30:28:48:PHE:CD2	2.44	0.53
32:2a:35:G:O2'	43:2l:118:SER:O	2.25	0.53
32:2a:1346:A:N1	32:2a:1374:A:H5"	2.24	0.53
39:2h:17:THR:HG22	39:2h:63:LEU:HD22	1.91	0.53
7:1H:11:VAL:HG13	7:1H:15:VAL:HG22	1.89	0.53
44:1m:78:ILE:HG22	44:1m:82:MET:HE2	1.90	0.53
50:1s:31:ILE:O	50:1s:50:ALA:N	2.34	0.53
33:2b:92:TYR:CE2	33:2b:151:GLY:HA3	2.43	0.53
34:2c:47:LEU:HB3	34:2c:52:LEU:HB2	1.91	0.53
56:2y:2:C:H2'	56:2y:3:G:C8	2.44	0.53
1:1A:2123:G:H2'	1:1A:2124:G:C8	2.43	0.53
32:1a:1125:U:H4'	41:1j:5:ARG:HH22	1.73	0.53
34:1c:11:ARG:NH2	34:1c:177:THR:O	2.35	0.53
36:1e:41:VAL:HG23	36:1e:67:VAL:HG13	1.89	0.53
1:2A:1434:A:H61	1:2A:1558:A:H62	1.56	0.53
1:2A:2690:C:OP1	13:2R:17:ARG:NH2	2.41	0.53
5:2F:117:ARG:HH12	11:2P:1:MET:H3	1.56	0.53
12:2Q:34:LEU:HB2	12:2Q:118:LEU:HD22	1.89	0.53
16:2U:104:GLN:NE2	16:2U:105:VAL:HG23	2.24	0.53
32:2a:664:G:P	49:2r:64:ARG:HH21	2.32	0.53
32:2a:1133:G:H2'	32:2a:1134:G:H8	1.73	0.53
35:2d:64:LEU:HB2	35:2d:198:VAL:HG11	1.91	0.53
8:1I:38:LEU:HD23	8:1I:38:LEU:H	1.74	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:1P:63:PRO:HD3	30:18:27:THR:HG22	1.89	0.53
26:14:63:TYR:N	26:14:63:TYR:CD1	2.77	0.53
37:1f:2:ARG:HD2	37:1f:69:GLU:HB3	1.91	0.53
4:2E:52:LEU:O	4:2E:76:ARG:N	2.41	0.53
5:2F:129:PHE:CD2	5:2F:163:VAL:HG21	2.43	0.53
7:1H:33:LEU:HD21	7:1H:136:ILE:HG13	1.91	0.52
21:1Z:153:SER:HA	21:1Z:167:PRO:HB3	1.89	0.52
32:1a:1256:A:OP2	34:1c:26:LYS:NZ	2.42	0.52
1:2A:1159:U:H2'	1:2A:1160:G:C8	2.44	0.52
1:2A:2811:G:N2	1:2A:2891:G:H1'	2.24	0.52
5:2F:20:LEU:HD12	5:2F:125:LEU:HD13	1.91	0.52
32:2a:501:C:H2'	32:2a:502:G:H8	1.73	0.52
37:2f:95:GLU:O	49:2r:32:ARG:NH1	2.40	0.52
40:2i:99:LEU:HB3	40:2i:101:PHE:CE2	2.43	0.52
1:1A:993:G:OP1	16:1U:50:ARG:NH2	2.42	0.52
1:1A:1056:G:H1'	1:1A:1103:A:H61	1.74	0.52
1:1A:2350:C:OP2	61:1A:4133:HOH:O	2.19	0.52
3:1D:8:PRO:HB3	3:1D:14:ARG:HG2	1.91	0.52
33:1b:166:ASP:HB3	33:1b:169:LYS:HB3	1.91	0.52
1:2A:330:A:H2	1:2A:1210:A:HO2'	1.57	0.52
1:2A:2129:C:N3	1:2A:2159:G:N2	2.55	0.52
12:2Q:75:THR:HG21	12:2Q:87:LYS:HE3	1.92	0.52
14:2S:14:VAL:O	14:2S:18:ILE:HG12	2.09	0.52
32:2a:34:C:H2'	32:2a:35:G:H8	1.74	0.52
32:2a:141:A:H1'	32:2a:182:U:O2	2.08	0.52
32:2a:1245:A:H2'	32:2a:1246:C:O4'	2.10	0.52
48:2q:4:LYS:HE2	48:2q:6:LEU:HD21	1.91	0.52
1:1A:71:A:N7	19:1X:31:HIS:HE1	2.07	0.52
1:1A:184:C:H2'	1:1A:185:U:C6	2.44	0.52
1:1A:1803:A:H4'	3:1D:259:THR:HG23	1.91	0.52
25:13:30:ARG:NH2	61:13:201:HOH:O	2.19	0.52
32:1a:447:G:O6	32:1a:485:G:O2'	2.22	0.52
8:2I:92:VAL:HG23	8:2I:96:ASP:HB2	1.91	0.52
32:2a:1272:G:N2	32:2a:1273:G:C8	2.75	0.52
33:2b:54:THR:HG23	33:2b:199:TYR:HB3	1.92	0.52
35:2d:15:GLU:OE2	35:2d:66:ARG:NH1	2.42	0.52
44:2m:15:VAL:O	44:2m:19:LEU:HG	2.09	0.52
56:2y:22:G:C8	56:2y:46:A:N6	2.77	0.52
1:1A:2079:U:OP1	23:11:21:ARG:NH2	2.30	0.52
4:1E:116:VAL:HG13	4:1E:122:PHE:HB2	1.91	0.52
21:1Z:151:HIS:HB3	21:1Z:169:GLU:O	2.08	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:1e:6:PHE:HB3	36:1e:34:VAL:HG22	1.91	0.52
40:1i:77:ILE:O	40:1i:81:ILE:HG22	2.08	0.52
1:2A:890:A:H2'	1:2A:892:G:H8	1.74	0.52
1:2A:1147:C:H2'	1:2A:1148:A:C8	2.44	0.52
4:2E:9:VAL:HG13	15:2T:3:ARG:HG2	1.91	0.52
4:2E:36:ARG:NH2	4:2E:88:GLY:O	2.41	0.52
19:2X:32:PRO:HA	19:2X:77:LYS:HB2	1.91	0.52
19:2X:60:ARG:HH22	29:27:47:ARG:NH2	2.02	0.52
32:2a:560:U:H5'	32:2a:566:G:N2	2.24	0.52
38:2g:79:ARG:NH2	38:2g:80:VAL:HA	2.24	0.52
1:1A:2124:G:H1	1:1A:2174:C:N4	2.06	0.52
1:1A:2611:U:H5'	1:1A:2611:U:H6	1.75	0.52
33:1b:12:GLU:O	33:1b:15:VAL:HG22	2.10	0.52
33:1b:97:TRP:CH2	33:1b:173:ALA:HA	2.44	0.52
1:2A:839:U:H2'	1:2A:840:C:C6	2.44	0.52
1:2A:2115:G:O2'	1:2A:2117:A:N7	2.39	0.52
14:2S:77:ALA:HB1	14:2S:82:ILE:HB	1.91	0.52
44:2m:58:GLU:O	44:2m:62:ASN:ND2	2.43	0.52
49:2r:21:LYS:NZ	49:2r:54:ARG:O	2.28	0.52
1:1A:2155:G:H2'	1:1A:2155:G:N3	2.25	0.52
21:1Z:70:LEU:HG	21:1Z:91:LEU:HD11	1.92	0.52
32:1a:258:G:H2'	32:1a:259:G:H8	1.74	0.52
32:1a:1140:C:H2'	32:1a:1141:C:H6	1.75	0.52
39:1h:81:HIS:N	39:1h:138:TRP:O	2.43	0.52
26:24:12:ALA:HB3	26:24:26:SER:HB3	1.90	0.52
32:2a:17:U:H2'	32:2a:18:C:C6	2.44	0.52
32:2a:1510:U:H2'	32:2a:1511:G:C8	2.45	0.52
33:2b:107:THR:O	33:2b:110:GLN:HB3	2.09	0.52
41:2j:51:ARG:O	45:2n:45:ARG:NH1	2.43	0.52
1:1A:64:A:O3'	19:1X:71:GLY:HA3	2.09	0.52
1:1A:286:C:H2'	1:1A:287:C:C6	2.45	0.52
1:1A:593:G:H4'	30:18:4:MET:HE2	1.91	0.52
1:1A:1025:G:C4	1:1A:1135:C:H1'	2.45	0.52
1:1A:1028:A:N6	1:1A:1125:G:H2'	2.25	0.52
1:1A:1062:G:H22	1:1A:1077:A:N6	2.07	0.52
1:1A:1174:A:H4'	1:1A:1175:U:OP1	2.10	0.52
32:1a:186:C:H2'	32:1a:187:C:C6	2.45	0.52
6:2G:73:ALA:HB3	6:2G:85:GLY:H	1.73	0.52
21:2Z:52:SER:OG	21:2Z:53:ILE:N	2.41	0.52
32:2a:64:G:H4'	32:2a:65:U:H3'	1.91	0.52
1:1A:2336:A:H61	22:10:43:THR:CG2	2.22	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1144:G:N2	32:1a:1146:A:H62	2.08	0.52
32:1a:1286:A:H2'	32:1a:1287:A:H4'	1.90	0.52
39:1h:110:ALA:HB3	39:1h:121:ASP:HB3	1.92	0.52
43:1l:39:VAL:HG11	43:1l:41:ARG:NH1	2.25	0.52
1:2A:601:C:O2'	5:2F:104:LYS:NZ	2.41	0.52
1:2A:652(A):A:H3'	1:2A:652(B):A:H5"	1.92	0.52
4:2E:174:ASP:OD1	4:2E:175:VAL:N	2.42	0.52
21:2Z:6:LYS:NZ	21:2Z:43:GLU:OE2	2.39	0.52
32:2a:142:G:H2'	32:2a:143:A:H8	1.75	0.52
32:2a:187:C:O2'	51:2t:89:ARG:NH2	2.40	0.52
32:2a:757:U:H2'	32:2a:758:G:O4'	2.09	0.52
32:2a:1005:A:H3'	32:2a:1006:C:C6	2.45	0.52
39:2h:20:TYR:HA	39:2h:65:TYR:CZ	2.45	0.52
42:2k:31:THR:HG23	42:2k:42:TRP:HB3	1.91	0.52
1:1A:579:G:H2'	1:1A:580:C:C6	2.45	0.52
6:1G:101:ILE:HD13	26:14:25:TYR:HB2	1.92	0.52
9:1N:67:LEU:O	9:1N:88:GLU:HG3	2.09	0.52
12:1Q:51:ARG:HD3	12:1Q:66:ILE:HD11	1.91	0.52
32:1a:1118:C:H1'	32:1a:1179:A:C4	2.45	0.52
32:1a:1353:G:OP1	52:1u:10:ARG:NH1	2.43	0.52
1:2A:1023:U:OP2	61:2A:3920:HOH:O	2.19	0.52
2:2B:19:G:H2'	2:2B:20:C:O4'	2.09	0.52
3:2D:108:PRO:HB3	3:2D:143:HIS:CE1	2.45	0.52
5:2F:178:PRO:HB3	5:2F:198:ALA:HA	1.92	0.52
34:2c:124:ILE:HG21	34:2c:130:VAL:HG13	1.91	0.52
42:2k:27:ASN:OD1	42:2k:28:THR:N	2.42	0.52
45:2n:24:CYS:HB2	45:2n:40:CYS:HB3	1.92	0.52
1:1A:2751:G:C2	7:1H:2:SER:HB3	2.45	0.52
9:1N:4:TYR:CD2	16:1U:100:VAL:HG11	2.45	0.52
47:1p:20:VAL:HG21	47:1p:32:TYR:CD2	2.45	0.52
54:1w:1:G:H2'	54:1w:2:C:C6	2.45	0.52
54:1w:15:A:H61	54:1w:59:U:H1'	1.74	0.52
1:2A:271(H):G:H2'	1:2A:271(I):G:C8	2.44	0.52
2:2B:77:U:OP1	21:2Z:19:ARG:NH2	2.42	0.52
3:2D:36:PRO:HA	3:2D:61:LEU:HD23	1.92	0.52
32:2a:1129:C:O2'	32:2a:1130:A:N7	2.43	0.52
32:2a:1228:C:OP1	44:2m:115:LYS:N	2.37	0.52
36:2e:6:PHE:HB3	36:2e:34:VAL:HG22	1.92	0.52
41:2j:78:ASN:O	41:2j:81:THR:N	2.39	0.52
48:2q:3:LYS:HD3	48:2q:60:ILE:HD11	1.91	0.52
1:1A:1364:G:OP2	23:11:3:LYS:HG3	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1356:G:H2'	32:1a:1357:A:C8	2.45	0.51
39:1h:39:LEU:HB3	39:1h:45:ILE:HG12	1.91	0.51
1:2A:179:G:N7	61:2A:4015:HOH:O	2.34	0.51
1:2A:247:G:H4'	1:2A:386:G:C5	2.45	0.51
1:2A:2127:G:H1	1:2A:2161:C:N4	2.08	0.51
1:2A:2133:G:HO2'	1:2A:2157:G:N2	2.07	0.51
8:2I:14:ASP:O	8:2I:17:GLN:HB2	2.09	0.51
19:2X:46:ALA:HB1	24:22:33:MET:HE1	1.92	0.51
32:2a:34:C:H2'	32:2a:35:G:C8	2.45	0.51
32:2a:45:U:H2'	32:2a:46:G:C8	2.45	0.51
32:2a:403:C:O2'	35:2d:122:ARG:NH2	2.42	0.51
36:2e:63:ARG:HA	36:2e:66:MET:HE1	1.90	0.51
56:2y:8:4SU:H1'	56:2y:48:C:C2	2.46	0.51
1:1A:2430:A:N3	1:1A:2430:A:H2'	2.26	0.51
7:1H:149:ARG:NH1	7:1H:167:GLU:OE2	2.43	0.51
34:1c:138:VAL:HG23	34:1c:151:VAL:HG12	1.91	0.51
48:1q:57:VAL:HG12	48:1q:76:LEU:HA	1.92	0.51
1:2A:810:U:C4	11:2P:29:LYS:O	2.63	0.51
1:2A:2137:C:H42	1:2A:2154:G:H1	1.57	0.51
4:2E:116:VAL:HG13	4:2E:122:PHE:HB2	1.91	0.51
12:2Q:45:GLN:OE1	12:2Q:45:GLN:N	2.38	0.51
32:2a:1212:U:H5'	32:2a:1213:A:C8	2.46	0.51
32:2a:1327:C:OP2	52:2u:12:LYS:NZ	2.43	0.51
48:2q:45:HIS:CD2	48:2q:47:PRO:HG3	2.45	0.51
51:2t:9:ASN:OD1	51:2t:9:ASN:N	2.41	0.51
1:1A:2165:G:N1	1:1A:2171:A:H8	2.08	0.51
3:1D:37:LEU:HD13	3:1D:87:ASN:ND2	2.25	0.51
12:1Q:89:ASN:HB2	55:1x:1:C:C4	2.44	0.51
19:1X:72:LYS:HE3	19:1X:73:ARG:O	2.10	0.51
32:1a:171:A:H2'	32:1a:172:A:C8	2.46	0.51
32:1a:219:C:H2'	32:1a:220:G:O4'	2.10	0.51
32:1a:412:A:H4'	32:1a:413:G:H5'	1.92	0.51
32:1a:1074:G:O2'	32:1a:1101:A:N1	2.36	0.51
34:1c:114:PRO:O	34:1c:118:GLN:NE2	2.43	0.51
1:2A:197:A:N6	1:2A:2430:A:H2'	2.26	0.51
1:2A:2127:G:N2	1:2A:2161:C:C2	2.78	0.51
3:2D:218:ARG:HB3	3:2D:219:PRO:HD2	1.91	0.51
5:2F:165:ARG:HG2	5:2F:168:ARG:NH2	2.24	0.51
6:2G:63:ILE:HD11	6:2G:144:ILE:HD11	1.93	0.51
8:2I:48:GLU:HA	8:2I:51:ILE:HG22	1.92	0.51
32:2a:380:G:N7	61:2a:1931:HOH:O	2.33	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:2w:2:C:H2'	54:2w:3:G:C8	2.45	0.51
56:2y:21:A:N6	56:2y:46:A:O2'	2.43	0.51
1:1A:484:C:OP1	20:1Y:51:VAL:HG22	2.10	0.51
32:1a:1469:G:H2'	32:1a:1470:G:H8	1.75	0.51
37:1f:36:ARG:HH21	37:1f:38:GLU:HG2	1.75	0.51
54:1w:49:G:N2	54:1w:65:U:O2	2.43	0.51
1:2A:2137:C:N4	1:2A:2154:G:H1	2.08	0.51
9:2N:15:LEU:HD23	9:2N:137:LYS:HD2	1.92	0.51
16:2U:90:VAL:HG12	16:2U:95:LEU:HG	1.92	0.51
1:1A:271(J):C:O3'	1:1A:271(K):U:H3'	2.11	0.51
1:1A:2176:A:H2'	1:1A:2177:C:C6	2.45	0.51
3:1D:2:ALA:N	3:1D:200:ASP:OD2	2.43	0.51
33:1b:52:GLU:OE2	33:1b:56:ARG:NH2	2.44	0.51
33:1b:178:ARG:HH22	39:1h:68:ARG:HH12	1.59	0.51
52:1u:3:LYS:HB3	52:1u:14:TRP:CD1	2.45	0.51
1:2A:2291:U:H2'	1:2A:2292:C:C6	2.46	0.51
16:2U:5:LYS:HG2	16:2U:7:GLY:H	1.76	0.51
32:2a:1139:G:N2	32:2a:1142:G:O6	2.31	0.51
41:2j:5:ARG:N	61:2j:301:HOH:O	2.43	0.51
41:2j:9:ARG:HH12	41:2j:69:ASN:HB3	1.74	0.51
1:1A:2136:C:C4	1:1A:2155:G:C2	2.99	0.51
2:1B:48:A:H4'	14:1S:95:HIS:HD2	1.76	0.51
35:1d:173:TRP:O	35:1d:186:LEU:HB2	2.09	0.51
56:1y:2:C:H2'	56:1y:3:G:C8	2.46	0.51
1:2A:657:U:H2'	1:2A:658:C:C6	2.45	0.51
1:2A:1019:U:H3	1:2A:1142(A):A:H62	1.58	0.51
1:2A:2135:A:C8	1:2A:2136:C:H5	2.29	0.51
32:2a:1003:G:H2'	32:2a:1004:A:O4'	2.11	0.51
36:2e:98:THR:OG1	36:2e:99:GLY:N	2.44	0.51
1:1A:686:G:N2	1:1A:788:A:H61	2.08	0.51
1:1A:880:G:H2'	1:1A:881:G:C8	2.45	0.51
1:1A:2022:U:O2'	1:1A:2617:C:H5'	2.11	0.51
13:1R:71:GLN:NE2	61:1R:301:HOH:O	2.43	0.51
23:11:76:ARG:HB2	23:11:97:LEU:HD13	1.92	0.51
32:1a:1318:A:H1'	50:1s:37:ARG:HH11	1.76	0.51
1:2A:580:C:H2'	1:2A:581:C:C6	2.46	0.51
1:2A:1025:G:C4	1:2A:1135:C:H1'	2.46	0.51
13:2R:51:LEU:HD22	13:2R:66:VAL:HG13	1.93	0.51
32:2a:1027:C:H2'	32:2a:1034:G:H22	1.73	0.51
32:2a:1352:C:H2'	32:2a:1353:G:C8	2.45	0.51
33:2b:17:PHE:HA	33:2b:44:LEU:HD11	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2226:C:OP2	61:1A:4138:HOH:O	2.20	0.51
6:1G:115:ARG:HG2	6:1G:136:ARG:NH2	2.26	0.51
32:1a:501:C:H2'	32:1a:502:G:C8	2.46	0.51
32:1a:583:A:N6	32:1a:758:G:O2'	2.44	0.51
32:1a:1077:G:N2	32:1a:1080:A:OP2	2.36	0.51
33:1b:116:GLU:HA	33:1b:119:GLU:HB2	1.91	0.51
34:1c:79:ARG:O	34:1c:82:GLU:HG2	2.10	0.51
35:1d:64:LEU:HB2	35:1d:198:VAL:HG11	1.93	0.51
37:1f:89:MET:HE1	49:1r:72:ARG:HB3	1.92	0.51
38:1g:138:LYS:HE2	38:1g:142:GLU:CD	2.36	0.51
32:2a:1010:G:H2'	32:2a:1011:G:H8	1.75	0.51
1:1A:1587:A:H2'	1:1A:1588:C:C6	2.46	0.51
1:2A:2320:A:N3	1:2A:2320:A:H2'	2.26	0.51
5:2F:108:LYS:O	5:2F:112:MET:HG3	2.10	0.51
13:2R:38:VAL:HG22	13:2R:112:ALA:HB2	1.93	0.51
19:2X:2:LYS:NZ	19:2X:38:GLU:OE2	2.42	0.51
24:22:65:ASN:OD1	24:22:69:ARG:NH1	2.43	0.51
32:2a:7:G:H5'	32:2a:298:A:O4'	2.11	0.51
54:2w:50:A:N6	54:2w:64:U:H3	2.07	0.51
1:1A:1354:A:H5"	3:1D:38:LYS:HD3	1.93	0.51
32:1a:536:C:OP2	61:1a:1912:HOH:O	2.18	0.51
34:1c:5:ILE:HD11	45:1n:58:LYS:HE3	1.93	0.51
1:2A:1796:U:H2'	1:2A:1797:C:C6	2.46	0.51
14:2S:69:VAL:HG13	14:2S:101:LEU:HD12	1.93	0.51
32:2a:108:G:C6	51:2t:15:ARG:HG2	2.46	0.51
32:2a:165:C:H2'	32:2a:166:G:H8	1.76	0.51
50:2s:66:MET:HB2	50:2s:74:PHE:CZ	2.46	0.51
1:1A:1441:G:H2'	1:1A:1442:G:H8	1.76	0.50
1:1A:2124:G:H3'	1:1A:2125:G:C8	2.45	0.50
1:1A:2406:U:OP1	61:1A:4137:HOH:O	2.19	0.50
8:1I:129:THR:HG22	8:1I:139:GLN:HE22	1.76	0.50
32:1a:1149:C:O2'	32:1a:1280:A:N1	2.39	0.50
32:1a:1277:C:O2'	32:1a:1279:A:H1'	2.11	0.50
50:1s:40:ILE:HB	50:1s:67:VAL:O	2.11	0.50
1:2A:300:A:P	20:2Y:86:ARG:HH12	2.33	0.50
1:2A:648:G:O2'	1:2A:2351:G:OP1	2.18	0.50
1:2A:1015:G:H2'	1:2A:1016:G:H8	1.75	0.50
1:2A:1688:U:O2	1:2A:1700:A:H5'	2.10	0.50
2:2B:115:G:H2'	2:2B:116:G:O4'	2.11	0.50
6:2G:117:PHE:CE2	6:2G:119:GLY:HA2	2.46	0.50
8:2I:92:VAL:HG13	8:2I:120:ILE:HB	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2Z:48:PHE:CE1	21:2Z:52:SER:HA	2.46	0.50
28:26:9:LEU:HD13	28:26:51:GLU:HG3	1.93	0.50
28:26:40:CYS:O	28:26:44:ARG:N	2.42	0.50
32:2a:1272:G:N2	32:2a:1273:G:C5	2.79	0.50
43:2l:59:ARG:HG3	43:2l:65:GLU:HB2	1.92	0.50
1:1A:994:C:OP1	16:1U:53:ARG:NH2	2.44	0.50
1:1A:1113:U:H2'	1:1A:1114:G:C8	2.46	0.50
1:1A:2337:G:OP1	61:1A:4135:HOH:O	2.19	0.50
26:14:63:TYR:N	26:14:63:TYR:HD1	2.09	0.50
32:1a:458:C:H2'	32:1a:460:G:O4'	2.12	0.50
40:1i:16:ARG:HB2	40:1i:64:THR:HG22	1.92	0.50
54:1w:63:C:H2'	54:1w:64:U:C6	2.47	0.50
1:2A:918:A:C2	2:2B:80:U:H4'	2.46	0.50
1:2A:987:G:O2'	1:2A:1000:A:N3	2.37	0.50
1:2A:1005:C:H2'	1:2A:1006:C:C6	2.46	0.50
1:2A:1557:C:OP2	1:2A:1558:A:O2'	2.18	0.50
6:2G:11:TYR:CZ	6:2G:16:ARG:HD3	2.46	0.50
11:2P:37:GLY:O	11:2P:40:SER:OG	2.28	0.50
14:2S:68:GLN:HA	14:2S:71:ARG:HD3	1.93	0.50
32:2a:1039:C:C2	32:2a:1040:U:H1'	2.47	0.50
8:1I:75:LEU:HD22	8:1I:105:HIS:CD2	2.46	0.50
32:1a:1263:C:H2'	32:1a:1264:C:C6	2.46	0.50
33:1b:95:GLN:HE22	33:1b:147:LYS:NZ	2.09	0.50
41:1j:7:LYS:HE3	41:1j:9:ARG:NH1	2.26	0.50
1:2A:854:G:H2'	1:2A:855:G:H8	1.76	0.50
1:2A:884:C:H3'	1:2A:885:C:H6	1.76	0.50
1:2A:2127:G:N1	1:2A:2160:G:O6	2.43	0.50
29:27:24:THR:HG22	29:27:26:GLY:N	2.26	0.50
32:2a:429:U:H1'	32:2a:430:A:H5"	1.94	0.50
32:2a:1149:C:O2'	32:2a:1280:A:N1	2.35	0.50
32:2a:1427:U:H2'	32:2a:1428:A:C8	2.46	0.50
36:2e:79:GLU:OE1	36:2e:79:GLU:N	2.43	0.50
1:1A:1379:A:H4'	1:1A:1380:G:OP2	2.12	0.50
32:1a:1410:G:H2'	32:1a:1411:C:C6	2.46	0.50
56:1y:38:A:H2'	56:1y:39:G:O4'	2.12	0.50
56:1y:53:G:H1	56:1y:61:C:H42	1.59	0.50
1:2A:667:U:O2	30:28:2:PRO:HD2	2.11	0.50
1:2A:2328:A:H2'	1:2A:2329:G:C8	2.46	0.50
32:2a:1289:A:H5'	52:2u:10:ARG:HH22	1.76	0.50
42:2k:99:GLN:HG2	42:2k:105:VAL:HG21	1.92	0.50
54:2w:49:G:H1	54:2w:65:U:H3	0.71	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:2y:8:4SU:H2'	56:2y:46:A:C2	2.46	0.50
1:1A:2629:A:HO2'	1:1A:2630:G:P	2.33	0.50
32:1a:864:A:H2'	32:1a:865:A:C8	2.46	0.50
35:1d:173:TRP:CD1	35:1d:173:TRP:H	2.30	0.50
54:1w:66:C:H2'	54:1w:67:G:C8	2.45	0.50
1:2A:963:U:OP2	61:2A:3909:HOH:O	2.20	0.50
1:2A:1243:G:O2'	11:2P:7:ARG:NH2	2.44	0.50
8:2I:55:ALA:HA	8:2I:58:LEU:HB3	1.92	0.50
27:25:41:PRO:O	27:25:44:THR:OG1	2.27	0.50
34:2c:39:ILE:HG22	34:2c:43:LEU:HD11	1.92	0.50
35:2d:191:ARG:O	35:2d:191:ARG:NH1	2.42	0.50
41:2j:6:ILE:HD12	41:2j:23:ILE:HG21	1.94	0.50
41:2j:30:SER:O	41:2j:81:THR:OG1	2.24	0.50
1:1A:839:U:H2'	1:1A:840:C:C6	2.47	0.50
1:1A:1740:G:H2'	1:1A:1741:A:C8	2.47	0.50
3:1D:148:GLU:HB2	3:1D:151:LYS:HD2	1.93	0.50
32:1a:193:C:H2'	32:1a:194:C:C6	2.46	0.50
32:1a:352:C:O2'	32:1a:354:G:OP1	2.30	0.50
32:1a:1399:C:H4'	32:1a:1400:5MC:H5"	1.92	0.50
1:2A:2143:C:H2'	1:2A:2144:U:O4'	2.12	0.50
8:2I:110:ASP:N	8:2I:130:TYR:OH	2.39	0.50
40:2i:3:GLN:HE21	40:2i:20:ARG:HH21	1.58	0.50
1:1A:443:A:H1'	1:1A:1201:C:O4'	2.12	0.50
1:1A:1047:G:H2'	1:1A:1110:G:H1	1.76	0.50
1:1A:1865:G:OP1	61:1A:4136:HOH:O	2.19	0.50
1:1A:2134:A:N3	1:1A:2159:G:O2'	2.38	0.50
1:1A:2839:G:H5'	13:1R:46:GLY:HA2	1.92	0.50
21:1Z:104:PHE:HA	21:1Z:139:VAL:HB	1.93	0.50
28:16:12:GLU:OE1	28:16:19:ARG:NH1	2.45	0.50
32:1a:438:G:H4'	35:1d:123:HIS:CE1	2.47	0.50
33:1b:54:THR:HG23	33:1b:199:TYR:HB3	1.94	0.50
36:1e:85:GLY:C	36:1e:87:SER:H	2.20	0.50
1:2A:322:A:OP1	5:2F:168:ARG:HD2	2.11	0.50
1:2A:645:C:H5"	1:2A:646:A:OP2	2.12	0.50
1:2A:839:U:H2'	1:2A:840:C:H6	1.76	0.50
32:2a:222:U:H2'	32:2a:223:U:C6	2.47	0.50
32:2a:521:G:H4'	43:2l:73:GLU:HG2	1.94	0.50
32:2a:538:G:H5"	43:2l:114:LYS:HB2	1.93	0.50
32:2a:933:G:N2	32:2a:935:A:O4'	2.45	0.50
33:2b:219:VAL:O	33:2b:223:ILE:HG12	2.11	0.50
34:2c:180:ALA:HB1	34:2c:203:PHE:HE1	1.76	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:2k:117:ASN:HD22	42:2k:117:ASN:N	2.10	0.50
54:2w:72:C:C4	54:2w:73:U:H5	2.29	0.50
1:1A:9:U:O4	1:1A:2629:A:H2	1.94	0.50
1:1A:2849:U:P	15:1T:95:ARG:HH12	2.34	0.50
5:1F:150:GLY:HA2	5:1F:172:TRP:CD2	2.47	0.50
8:1I:78:THR:HG1	8:1I:143:SER:HG	1.54	0.50
32:1a:316:G:OP2	32:1a:351:G:O2'	2.29	0.50
34:1c:181:ASN:ND2	34:1c:204:LEU:HD12	2.27	0.50
37:1f:18:GLN:HA	37:1f:21:LEU:HD12	1.94	0.50
1:2A:361:G:O2'	1:2A:362:U:H5'	2.11	0.50
1:2A:1803:A:H4'	3:2D:259:THR:HG23	1.94	0.50
1:2A:1817:G:OP1	3:2D:88:ARG:NH2	2.43	0.50
36:2e:24:ARG:HD2	53:2v:24:A:OP2	2.11	0.50
47:2p:5:ARG:HH21	47:2p:28:ARG:HA	1.77	0.50
1:1A:800:A:H8	1:1A:800:A:OP1	1.95	0.50
1:2A:555:U:O2'	1:2A:556:G:N7	2.44	0.50
1:2A:892:G:H3'	1:2A:893:C:H5"	1.94	0.50
1:2A:1028:A:N6	1:2A:1125:G:H2'	2.27	0.50
1:2A:1452:A:OP2	61:2A:3939:HOH:O	2.19	0.50
1:2A:2391:G:O6	1:2A:2425:A:H8	1.94	0.50
1:2A:2630:G:H2'	1:2A:2631:G:H8	1.77	0.50
1:2A:2821:A:H2'	1:2A:2822:G:C8	2.47	0.50
4:2E:7:VAL:HG12	4:2E:27:LEU:HB3	1.94	0.50
32:2a:651:C:N4	32:2a:753:A:OP2	2.39	0.50
32:2a:920:U:H2'	32:2a:921:U:C6	2.47	0.50
32:2a:1130:A:H5"	40:2i:18:PHE:HE2	1.76	0.50
32:2a:1263:C:N3	32:2a:1272:G:O6	2.45	0.50
1:1A:428:A:H8	1:1A:428:A:OP2	1.95	0.49
3:1D:77:ALA:HB2	3:1D:97:TYR:CD1	2.46	0.49
32:1a:1101:A:H4'	32:1a:1102:A:O5'	2.12	0.49
1:2A:286:C:H2'	1:2A:287:C:C6	2.47	0.49
1:2A:607:U:OP1	5:2F:102:PRO:HA	2.12	0.49
1:2A:1378:A:O2'	1:2A:1380:G:N7	2.40	0.49
1:2A:1509(B):A:H2'	1:2A:1510:G:H8	1.77	0.49
1:2A:2156:G:H4'	1:2A:2157:G:OP1	2.11	0.49
2:2B:50:G:OP1	14:2S:63:THR:N	2.43	0.49
19:2X:88:LYS:HE3	19:2X:93:GLU:HG3	1.93	0.49
26:24:46:GLN:HE21	26:24:48:ARG:HB2	1.77	0.49
32:2a:1133:G:H2'	32:2a:1134:G:C8	2.47	0.49
32:2a:1251:A:N1	32:2a:1354:C:O2'	2.42	0.49
33:2b:16:HIS:CG	33:2b:17:PHE:N	2.80	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:2d:18:LYS:NZ	35:2d:31:CYS:SG	2.84	0.49
38:2g:57:GLU:HG3	38:2g:60:LYS:H	1.76	0.49
43:2l:77:LEU:HD21	43:2l:107:ALA:HB2	1.94	0.49
54:2w:6:C:C2	54:2w:67:G:N2	2.80	0.49
1:1A:125:G:H1'	29:17:48:LYS:HD3	1.93	0.49
1:1A:181:A:H5"	29:17:36:GLN:NE2	2.27	0.49
1:1A:1164:G:H2'	1:1A:1165:U:C6	2.47	0.49
1:1A:2115:G:H2'	1:1A:2116:G:H5"	1.94	0.49
11:1P:59:LEU:HD11	30:18:10:ALA:HA	1.94	0.49
32:1a:165:C:H2'	32:1a:166:G:C8	2.46	0.49
37:1f:22:GLU:OE1	37:1f:84:ASN:HB2	2.12	0.49
54:1w:5:G:H2'	54:1w:6:C:C6	2.47	0.49
1:2A:796:C:H2'	1:2A:797:C:C6	2.47	0.49
1:2A:2134:A:H1'	1:2A:2158:A:C6	2.46	0.49
6:2G:173:LEU:HD12	6:2G:178:PHE:CE1	2.47	0.49
9:2N:4:TYR:CD2	16:2U:100:VAL:HG11	2.47	0.49
26:24:40:HIS:CD2	26:24:41:PRO:HD2	2.48	0.49
32:2a:129(A):G:C6	32:2a:189(E):U:H4'	2.47	0.49
32:2a:410:G:OP1	35:2d:30:LYS:NZ	2.39	0.49
32:2a:501:C:H2'	32:2a:502:G:C8	2.46	0.49
32:2a:1005:A:H5"	32:2a:1006:C:H5	1.76	0.49
56:2y:2:C:H2'	56:2y:3:G:H8	1.76	0.49
1:1A:1647:G:OP1	61:1A:4116:HOH:O	2.20	0.49
1:1A:2693:A:H2'	1:1A:2694:G:C8	2.47	0.49
32:1a:269:C:H2'	32:1a:270:A:C8	2.47	0.49
32:1a:721:G:H4'	32:1a:722:A:O4'	2.11	0.49
32:1a:828:A:H2'	32:1a:829:G:O4'	2.12	0.49
32:1a:1030(B):C:O2	32:1a:1030(C):G:H5'	2.12	0.49
45:1n:29:ARG:HH21	45:1n:42:ILE:HD11	1.77	0.49
47:1p:53:VAL:HG13	47:1p:79:VAL:HG22	1.92	0.49
54:1w:26:G:H1	54:1w:44:A:H2	1.60	0.49
1:2A:492:A:H2'	1:2A:493:G:O4'	2.13	0.49
1:2A:1509(B):A:H2'	1:2A:1510:G:C8	2.47	0.49
1:2A:1593:G:H2'	1:2A:1594:G:C8	2.47	0.49
1:2A:1633:G:OP2	61:2A:3941:HOH:O	2.20	0.49
1:2A:1847:A:H4'	1:2A:1848:A:OP2	2.13	0.49
3:2D:108:PRO:HG2	3:2D:111:LEU:HB2	1.94	0.49
4:2E:110:GLY:O	61:2R:301:HOH:O	2.18	0.49
5:2F:113:ALA:HB1	5:2F:186:ILE:HG21	1.93	0.49
5:2F:150:GLY:HA2	5:2F:172:TRP:CD2	2.48	0.49
32:2a:1108:G:H5'	34:2c:176:HIS:NE2	2.27	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1109:C:H2'	32:2a:1110:A:O4'	2.13	0.49
32:2a:1387:G:H2'	32:2a:1388:C:C6	2.46	0.49
1:1A:414:C:H2'	1:1A:415:A:C8	2.47	0.49
1:1A:848:G:H2'	1:1A:849:A:C8	2.47	0.49
1:1A:863:A:H2'	1:1A:864:G:C8	2.47	0.49
1:1A:1074:G:N1	1:1A:1075:C:H1'	2.27	0.49
2:1B:66:A:H61	2:1B:109:C:H5'	1.77	0.49
4:1E:7:VAL:HG23	4:1E:51:PHE:HE2	1.77	0.49
8:1I:78:THR:OG1	8:1I:143:SER:OG	2.22	0.49
32:1a:598:U:H2'	32:1a:599:C:C6	2.47	0.49
39:1h:121:ASP:O	39:1h:125:ARG:HG3	2.13	0.49
45:1n:9:LYS:HG3	45:1n:12:ARG:HH21	1.77	0.49
1:2A:307:G:H21	1:2A:330:A:H62	1.60	0.49
1:2A:892:G:H3'	1:2A:893:C:C5'	2.43	0.49
1:2A:1266:G:O5'	18:2W:15:ARG:NH2	2.44	0.49
1:2A:1598:C:H2'	1:2A:1599:C:H6	1.77	0.49
23:21:86:SER:OG	23:21:89:GLU:OE2	2.21	0.49
26:24:26:SER:OG	26:24:27:THR:N	2.45	0.49
26:24:45:GLY:C	26:24:47:GLN:H	2.20	0.49
32:2a:148:G:H2'	32:2a:149:A:C8	2.48	0.49
32:2a:449:C:O2	47:2p:42:ARG:NH1	2.46	0.49
32:2a:959:A:O2'	32:2a:984:C:O2'	2.27	0.49
33:2b:8:LYS:HE3	33:2b:51:LEU:HD13	1.94	0.49
56:2y:56:C:H2'	56:2y:57:G:H8	1.77	0.49
1:1A:286:C:H2'	1:1A:287:C:H6	1.78	0.49
1:1A:796:C:H2'	1:1A:797:C:C6	2.47	0.49
1:1A:2137:C:H2'	1:1A:2138:C:C6	2.47	0.49
6:1G:116:ASP:OD2	44:1m:68:GLY:HA3	2.12	0.49
32:1a:711:G:OP1	37:1f:54:LYS:NZ	2.30	0.49
32:1a:1023:G:H3'	32:1a:1024:G:C8	2.47	0.49
44:1m:11:ARG:HA	44:1m:45:VAL:HB	1.94	0.49
50:1s:11:VAL:HG11	50:1s:16:LEU:HB2	1.93	0.49
51:1t:47:GLY:N	51:1t:48:LYS:HB2	2.27	0.49
1:2A:1225:G:H4'	17:2V:84:LYS:HG2	1.95	0.49
6:2G:7:LEU:HD11	6:2G:107:LEU:HD12	1.93	0.49
32:2a:642:A:N3	39:2h:113:SER:OG	2.45	0.49
32:2a:1029:C:C2	32:2a:1032:G:N2	2.76	0.49
32:2a:1037:C:H2'	32:2a:1038:C:C6	2.48	0.49
32:2a:1411:C:H2'	32:2a:1412:C:H6	1.77	0.49
54:2w:17:G:H5'	54:2w:60:U:O2'	2.12	0.49
1:1A:762:U:H5"	61:1A:4714:HOH:O	2.11	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2319:G:H1	14:1S:3:ARG:HA	1.77	0.49
32:1a:45:U:H2'	32:1a:46:G:C8	2.48	0.49
34:1c:35:GLU:CD	34:1c:59:ARG:HH22	2.21	0.49
39:1h:121:ASP:HB2	39:1h:125:ARG:NH2	2.27	0.49
1:2A:2646:C:H2'	1:2A:2647:U:O4'	2.12	0.49
7:2H:25:LYS:HE3	7:2H:27:LYS:HE3	1.93	0.49
32:2a:509:A:N3	32:2a:543:C:O2'	2.44	0.49
32:2a:646:U:H2'	32:2a:647:C:C6	2.47	0.49
35:2d:112:VAL:HG22	35:2d:116:GLN:NE2	2.27	0.49
1:1A:500:G:N7	61:1A:4198:HOH:O	2.35	0.49
1:1A:1372:U:H2'	1:1A:1373:A:O4'	2.13	0.49
1:1A:1866:C:H2'	1:1A:1876:A:O4'	2.12	0.49
1:1A:2646:C:H2'	1:1A:2647:U:O4'	2.13	0.49
12:1Q:81:VAL:HB	22:10:7:LEU:HD21	1.94	0.49
18:1W:92:ARG:NH1	61:1W:302:HOH:O	2.45	0.49
21:1Z:132:ASN:ND2	21:1Z:160:GLY:HA3	2.25	0.49
34:1c:131:ARG:HH11	34:1c:166:GLU:HG3	1.77	0.49
56:1y:17:G:O2'	56:1y:57:G:O6	2.28	0.49
1:2A:10:G:N2	1:2A:2629:A:N7	2.60	0.49
1:2A:2114:A:H62	1:2A:2115:G:H21	1.60	0.49
1:2A:2147:G:C6	1:2A:2148:G:H1'	2.47	0.49
1:2A:2857:G:N2	1:2A:2860:A:OP2	2.44	0.49
6:2G:114:ILE:HB	6:2G:117:PHE:HD1	1.78	0.49
6:2G:152:LEU:H	6:2G:152:LEU:HD12	1.78	0.49
23:21:56:GLN:HA	23:21:56:GLN:HE21	1.77	0.49
25:23:7:LYS:HE3	25:23:32:GLN:HE21	1.78	0.49
32:2a:447:G:O6	32:2a:485:G:O2'	2.16	0.49
32:2a:674:G:H2'	32:2a:675:A:H8	1.77	0.49
32:2a:1040:U:H2'	32:2a:1041:A:H8	1.76	0.49
32:2a:1084:G:H5'	32:2a:1102:A:OP2	2.12	0.49
33:2b:147:LYS:HG2	33:2b:148:TYR:CZ	2.47	0.49
40:2i:33:PHE:HE2	40:2i:43:ALA:HB1	1.77	0.49
44:2m:91:ARG:HH12	44:2m:103:THR:HG21	1.77	0.49
55:2x:58:A:H4'	55:2x:59:A:OP1	2.13	0.49
1:1A:1047:G:H2'	1:1A:1110:G:H22	1.77	0.49
1:1A:1070:A:C6	1:1A:1097:U:H4'	2.47	0.49
2:1B:103:G:H21	21:1Z:73:GLN:HE22	1.60	0.49
12:1Q:78:PRO:HG2	12:1Q:81:VAL:HG11	1.95	0.49
32:1a:373:A:H2'	32:1a:374:A:H8	1.76	0.49
1:2A:20:C:OP1	16:2U:22:LYS:NZ	2.41	0.49
1:2A:1630:G:H2'	1:2A:1631:C:C6	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1786:A:H1'	1:2A:1938:A:N6	2.26	0.49
1:2A:2124:G:H1	1:2A:2173:A:N6	2.11	0.49
1:2A:2125:G:H1'	1:2A:2173:A:N6	2.28	0.49
2:2B:13:A:N1	2:2B:69:G:O2'	2.43	0.49
14:2S:67:ARG:NH1	14:2S:107:GLU:OE2	2.46	0.49
21:2Z:141:VAL:HG11	21:2Z:174:VAL:HG21	1.95	0.49
32:2a:1157:A:H5'	32:2a:1158:C:C6	2.47	0.49
34:2c:129:ALA:HB3	34:2c:132:ARG:HB3	1.95	0.49
38:2g:46:ALA:HB1	38:2g:121:ALA:HB2	1.94	0.49
1:1A:583:G:OP2	16:1U:10:ARG:HD2	2.13	0.49
1:1A:2327:A:H2'	1:1A:2328:A:C8	2.47	0.49
1:1A:2887:U:H2'	1:1A:2888:C:H6	1.78	0.49
32:1a:110:C:O2'	47:1p:25:ARG:O	2.26	0.49
32:1a:169:C:H2'	32:1a:170:U:H6	1.78	0.49
32:1a:1107:C:OP1	34:1c:172:ARG:HG3	2.13	0.49
34:1c:186:PHE:HE2	34:1c:188:LEU:HB2	1.77	0.49
39:1h:41:ARG:NH2	39:1h:123:GLU:OE2	2.45	0.49
1:2A:855:G:O2'	22:20:27:GLU:OE2	2.31	0.49
1:2A:1356:G:OP1	61:2A:3940:HOH:O	2.19	0.49
1:2A:2100:G:H2'	1:2A:2101:G:H8	1.78	0.49
2:2B:14:U:OP2	2:2B:70:C:O2'	2.28	0.49
3:2D:158:ALA:O	3:2D:161:THR:OG1	2.27	0.49
32:2a:1326:C:OP1	52:2u:17:THR:OG1	2.27	0.49
34:2c:125:GLU:O	34:2c:190:ARG:NH2	2.46	0.49
51:2t:86:ARG:NH2	51:2t:90:GLN:OE1	2.45	0.49
1:1A:568:U:H5'	1:1A:945:A:N6	2.28	0.49
1:1A:1753:G:N1	1:1A:1756:G:OP2	2.44	0.49
1:1A:2789:C:O2	1:1A:2894:G:N1	2.45	0.49
32:1a:456:C:H2'	32:1a:457:C:C6	2.48	0.49
32:1a:1513:A:H2'	32:1a:1514:C:C6	2.48	0.49
38:1g:26:PHE:CE2	38:1g:30:ILE:HD11	2.47	0.49
1:2A:1477:A:H2'	1:2A:1478:G:O4'	2.12	0.49
1:2A:1996:C:H4'	1:2A:1997:G:OP1	2.12	0.49
1:2A:2278:A:OP2	22:20:12:ASN:ND2	2.46	0.49
5:2F:32:LEU:O	5:2F:36:VAL:HG23	2.13	0.49
13:2R:13:HIS:CE1	13:2R:16:HIS:HB2	2.47	0.49
32:2a:1033:G:H2'	32:2a:1034:G:H8	1.77	0.49
32:2a:1227:A:OP1	50:2s:80:TYR:OH	2.22	0.49
1:1A:897:C:H4'	54:1w:55:PSU:O3'	2.13	0.48
1:1A:2567:G:H2'	1:1A:2568:C:C6	2.48	0.48
12:1Q:82:ARG:NH1	22:10:4:LYS:HE3	2.27	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:161:A:H2'	32:1a:162:A:C8	2.47	0.48
32:1a:947:G:H4'	44:1m:109:THR:HG23	1.95	0.48
32:1a:1071:C:H2'	32:1a:1072:G:H8	1.77	0.48
1:2A:1371:G:N7	61:2A:4020:HOH:O	2.35	0.48
32:2a:865:A:H5'	32:2a:1078:U:C5	2.48	0.48
32:2a:1002:G:C2	32:2a:1003:G:H1'	2.48	0.48
33:2b:9:GLU:O	33:2b:11:LEU:N	2.46	0.48
33:2b:208:ILE:HA	33:2b:211:ILE:HB	1.95	0.48
47:2p:28:ARG:HG2	47:2p:29:ASP:OD1	2.13	0.48
1:1A:81:G:HO2'	1:1A:295:G:HO2'	1.62	0.48
1:1A:2790:A:H3'	1:1A:2790:A:N3	2.28	0.48
19:1X:31:HIS:CD2	19:1X:33:LYS:H	2.28	0.48
32:1a:406:G:N2	35:1d:119:GLN:HE22	2.11	0.48
32:1a:421:U:O4	34:1c:127:ARG:NH2	2.46	0.48
32:1a:584:G:H5'	48:1q:91:ARG:HH22	1.78	0.48
37:1f:69:GLU:H	37:1f:69:GLU:CD	2.21	0.48
41:1j:5:ARG:NH2	41:1j:73:ASP:OD2	2.23	0.48
48:1q:22:LEU:HD11	48:1q:39:SER:HB2	1.95	0.48
54:1w:7:G:O2'	54:1w:49:G:OP2	2.28	0.48
11:2P:19:VAL:HG12	11:2P:27:HIS:HB3	1.95	0.48
26:24:62:ARG:HA	26:24:62:ARG:CZ	2.43	0.48
32:2a:570:G:H1'	32:2a:820:U:C4	2.48	0.48
32:2a:972:C:O2'	41:2j:55:LYS:O	2.31	0.48
33:2b:74:LYS:HG2	33:2b:75:LYS:H	1.79	0.48
33:2b:155:LEU:HD11	33:2b:159:PRO:HG3	1.95	0.48
34:2c:13:GLY:HA3	45:2n:57:ARG:NH2	2.28	0.48
34:2c:183:ASP:HB2	34:2c:204:LEU:HD11	1.94	0.48
35:2d:140:VAL:HG11	35:2d:146:ILE:HD11	1.95	0.48
36:2e:71:LEU:C	36:2e:72:GLN:HE21	2.21	0.48
1:1A:668:G:H5'	1:1A:669:G:OP2	2.13	0.48
32:1a:159:G:N2	32:1a:162:A:OP2	2.46	0.48
51:1t:83:ARG:HG2	51:1t:86:ARG:HH12	1.78	0.48
1:2A:2816:C:O3'	13:2R:99:LYS:NZ	2.47	0.48
21:2Z:5:LEU:O	21:2Z:59:LEU:HA	2.13	0.48
32:2a:948:C:P	44:2m:109:THR:HG1	2.36	0.48
32:2a:1316:G:H22	32:2a:1319:A:H5'	1.77	0.48
33:2b:60:ASP:O	33:2b:64:ARG:HG2	2.13	0.48
33:2b:178:ARG:NH2	39:2h:68:ARG:HH22	2.11	0.48
35:2d:187:ARG:NH1	35:2d:190:ASP:OD1	2.45	0.48
39:2h:85:ARG:NH1	39:2h:87:SER:O	2.46	0.48
2:1B:66:A:H61	2:1B:108:U:H2'	1.79	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1G:122:PRO:HB3	6:1G:170:ARG:HH12	1.78	0.48
6:1G:125:PHE:O	61:1G:301:HOH:O	2.20	0.48
8:1I:9:LEU:HD23	8:1I:12:LEU:HD23	1.94	0.48
15:1T:127:ALA:C	15:1T:129:ARG:N	2.70	0.48
17:1V:29:PRO:HA	17:1V:61:VAL:HG22	1.95	0.48
32:1a:194:C:H2'	32:1a:195:A:H5"	1.96	0.48
32:1a:713:G:H2'	32:1a:714:G:C8	2.48	0.48
32:1a:920:U:H2'	32:1a:921:U:C6	2.49	0.48
32:1a:984:C:H42	32:1a:1221:G:H1	1.61	0.48
32:1a:993:G:H2'	32:1a:995:C:H41	1.77	0.48
36:1e:116:THR:HG23	36:1e:117:ASP:OD2	2.12	0.48
48:1q:67:LYS:HA	48:1q:70:ARG:HH12	1.78	0.48
56:1y:63:C:H2'	56:1y:64:U:O4'	2.13	0.48
1:2A:1420:U:O5'	1:2A:1420:U:H6	1.96	0.48
2:2B:105:A:H5'	2:2B:106:G:OP2	2.13	0.48
7:2H:9:ILE:HB	7:2H:50:VAL:HB	1.94	0.48
8:2I:124:GLY:H	8:2I:144:VAL:HG23	1.78	0.48
10:2O:71:ARG:NE	10:2O:105:GLU:OE2	2.46	0.48
32:2a:620:C:H2'	32:2a:621:A:O4'	2.13	0.48
32:2a:1218:C:H2'	32:2a:1219:U:C6	2.48	0.48
32:2a:1275:A:H2'	32:2a:1276:G:O4'	2.13	0.48
41:2j:78:ASN:O	41:2j:80:LYS:N	2.46	0.48
1:1A:721:C:H2'	1:1A:722:A:C8	2.49	0.48
1:1A:1070:A:N6	1:1A:1097:U:H4'	2.29	0.48
14:1S:14:VAL:O	14:1S:18:ILE:HG12	2.12	0.48
19:1X:28:PHE:CZ	19:1X:92:LEU:HD11	2.49	0.48
32:1a:598:U:H2'	32:1a:599:C:H6	1.77	0.48
32:1a:659:U:H2'	32:1a:660:G:C8	2.49	0.48
33:1b:20:GLU:HB2	33:1b:190:THR:OG1	2.13	0.48
36:1e:12:LEU:HB3	36:1e:31:LEU:HB2	1.96	0.48
48:1q:67:LYS:O	48:1q:68:ARG:HB2	2.13	0.48
1:2A:1591:G:H2'	1:2A:1592:C:C6	2.48	0.48
1:2A:1667:G:O2'	1:2A:1991:U:O4	2.27	0.48
1:2A:2405:G:H5'	11:2P:75:ILE:HD13	1.95	0.48
1:2A:2693:A:H2'	1:2A:2694:G:H8	1.78	0.48
4:2E:59:VAL:HG21	4:2E:74:PRO:HB3	1.95	0.48
32:2a:1278:U:H5'	32:2a:1279:A:H5'	1.95	0.48
32:2a:1302:U:OP2	44:2m:21:TYR:OH	2.20	0.48
34:2c:6:HIS:HD2	34:2c:8:ILE:H	1.62	0.48
34:2c:119:ARG:HG2	34:2c:140:ARG:NH2	2.28	0.48
46:2o:54:ARG:HG2	46:2o:58:MET:HE2	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1E:9:VAL:HG13	15:1T:3:ARG:HG2	1.95	0.48
6:1G:18:GLU:OE2	6:1G:22:ARG:HD2	2.13	0.48
8:1I:100:ALA:HA	8:1I:103:ARG:HG2	1.94	0.48
32:1a:204:U:H4'	32:1a:216:G:H5"	1.96	0.48
32:1a:911:U:H2'	32:1a:912:C:C6	2.48	0.48
32:1a:1108:G:H5'	34:1c:176:HIS:CD2	2.48	0.48
42:1k:72:ALA:HB1	42:1k:77:MET:HG2	1.95	0.48
46:1o:6:GLU:O	46:1o:10:LYS:HG3	2.13	0.48
1:2A:2836:U:H2'	1:2A:2837:G:C8	2.49	0.48
8:2I:50:ARG:O	8:2I:54:GLN:N	2.47	0.48
32:2a:1122:U:N3	32:2a:1123:A:N7	2.61	0.48
32:2a:1251:A:H2'	32:2a:1252:A:C8	2.48	0.48
32:2a:1296:C:H5"	44:2m:44:ARG:NH2	2.28	0.48
32:2a:1343:G:H2'	32:2a:1344:C:C6	2.49	0.48
34:2c:142:MET:HG3	34:2c:170:GLN:HB3	1.95	0.48
1:1A:309:G:N3	1:1A:329:G:O2'	2.39	0.48
1:1A:1518:U:H2'	1:1A:1519:G:O4'	2.13	0.48
9:1N:1:MET:HE1	16:1U:94:ASN:ND2	2.29	0.48
32:1a:942:G:H21	40:1i:124:GLN:NE2	2.12	0.48
34:1c:52:LEU:HD13	34:1c:68:VAL:HG13	1.96	0.48
35:1d:144:ASP:N	35:1d:144:ASP:OD1	2.47	0.48
1:2A:245:G:O6	30:28:8:LYS:NZ	2.43	0.48
1:2A:947:G:H2'	1:2A:948:G:C8	2.49	0.48
1:2A:1364:G:OP2	23:21:3:LYS:HG3	2.14	0.48
1:2A:1530:C:O2'	1:2A:1531:C:O5'	2.25	0.48
1:2A:2059:A:H2'	1:2A:2503:2MA:HM23	1.95	0.48
1:2A:2136:C:O2'	1:2A:2137:C:O5'	2.32	0.48
7:2H:56:SER:OG	7:2H:57:ASP:N	2.45	0.48
26:24:48:ARG:HG2	26:24:52:THR:HG23	1.95	0.48
32:2a:382:A:H2'	32:2a:383:A:C8	2.48	0.48
32:2a:981:U:H5'	45:2n:21:TYR:CE2	2.49	0.48
32:2a:1105:A:H2'	32:2a:1106:G:C8	2.44	0.48
56:2y:5:G:H1	56:2y:68:C:H42	1.60	0.48
1:1A:601:C:OP1	5:1F:108:LYS:HE3	2.14	0.48
1:1A:637:A:OP1	11:1P:133:SER:OG	2.27	0.48
1:1A:1065:U:H5"	1:1A:1066:U:OP2	2.14	0.48
1:1A:1843:C:H5'	3:1D:253:GLN:OE1	2.14	0.48
9:1N:35:ARG:HD3	9:1N:37:LYS:HD2	1.96	0.48
30:18:62:LEU:HB3	30:18:65:GLU:HG3	1.95	0.48
32:1a:202:U:H5"	32:1a:203:U:H5	1.79	0.48
32:1a:328:C:H4'	32:1a:329:A:H5"	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:711:G:H2'	32:1a:712:A:C8	2.49	0.48
41:1j:78:ASN:O	41:1j:80:LYS:N	2.46	0.48
51:1t:87:LYS:O	51:1t:91:LEU:HG	2.13	0.48
1:2A:153:C:H2'	1:2A:154:G:O4'	2.14	0.48
1:2A:1462:C:H4'	1:2A:2703:C:H5'	1.95	0.48
1:2A:1916:A:H2'	1:2A:1917:PSU:O4'	2.13	0.48
32:2a:134:A:H61	47:2p:25:ARG:NH1	2.11	0.48
32:2a:254:G:OP1	48:2q:66:SER:OG	2.31	0.48
32:2a:457:C:H2'	32:2a:458:C:C6	2.49	0.48
32:2a:975:A:N1	41:2j:48:THR:HB	2.29	0.48
32:2a:1002:G:N3	32:2a:1003:G:H1'	2.28	0.48
32:2a:1260:C:O5'	32:2a:1284:C:H4'	2.13	0.48
32:2a:1312:G:H5'	50:2s:5:LEU:HD21	1.96	0.48
34:2c:8:ILE:HG23	34:2c:16:ARG:HG2	1.96	0.48
34:2c:30:ARG:O	34:2c:34:LEU:HB2	2.14	0.48
34:2c:131:ARG:HH21	34:2c:135:LYS:HE3	1.79	0.48
55:2x:40:C:H2'	55:2x:41:C:H6	1.78	0.48
56:2y:42:C:H2'	56:2y:43:U:H6	1.77	0.48
1:1A:918:A:N3	2:1B:80:U:O2'	2.40	0.48
1:1A:2136:C:N4	1:1A:2155:G:N1	2.61	0.48
33:1b:87:ARG:NH1	33:1b:233:SER:OG	2.47	0.48
33:1b:155:LEU:HD11	33:1b:159:PRO:HG3	1.96	0.48
34:1c:6:HIS:CD2	34:1c:8:ILE:H	2.26	0.48
35:1d:108:LEU:HD23	35:1d:174:LEU:HD13	1.94	0.48
43:1l:24:VAL:HB	43:1l:27:LEU:HD12	1.96	0.48
56:1y:6:C:N4	56:1y:7:G:O6	2.47	0.48
1:2A:524:U:H2'	1:2A:525:U:C6	2.49	0.48
1:2A:897:C:H5"	54:2w:56:C:OP1	2.14	0.48
1:2A:1178:C:H2'	1:2A:1179:C:C6	2.49	0.48
1:2A:1580:A:H8	1:2A:1580:A:OP2	1.97	0.48
1:2A:2273:A:H2'	1:2A:2274:A:C8	2.49	0.48
1:2A:2277:G:OP2	22:20:10:THR:HG21	2.13	0.48
6:2G:145:THR:HG22	6:2G:147:ASP:H	1.79	0.48
32:2a:1074:G:H4'	33:2b:103:THR:O	2.14	0.48
33:2b:15:VAL:HG21	33:2b:213:LEU:HD13	1.95	0.48
34:2c:109:PRO:C	34:2c:111:LEU:H	2.22	0.48
36:2e:17:ALA:HB2	36:2e:26:PHE:CD1	2.48	0.48
36:2e:100:VAL:HG22	36:2e:118:ILE:HG22	1.96	0.48
43:2l:113:ARG:NH2	61:2l:302:HOH:O	2.46	0.48
44:2m:14:ARG:HA	44:2m:44:ARG:HA	1.96	0.48
44:2m:20:THR:C	44:2m:22:ILE:H	2.22	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:2w:4:G:C2	54:2w:5:G:H1'	2.48	0.48
1:1A:1477:A:C2	1:1A:1515:G:C2	3.02	0.48
1:1A:2136:C:C4	1:1A:2155:G:N1	2.82	0.48
15:1T:118:ARG:HG2	32:1a:1442(A):G:C8	2.48	0.48
16:1U:76:TYR:CE2	16:1U:80:ILE:HG13	2.49	0.48
31:19:2:LYS:HD3	31:19:4:ARG:NH2	2.29	0.48
39:1h:51:VAL:HG11	39:1h:60:ARG:HH12	1.79	0.48
51:1t:89:ARG:O	51:1t:93:GLU:HG2	2.12	0.48
1:2A:566:U:H5"	11:2P:29:LYS:HE3	1.96	0.48
1:2A:928:G:H8	1:2A:928:G:O5'	1.97	0.48
1:2A:2537:U:H2'	1:2A:2538:C:C6	2.49	0.48
3:2D:108:PRO:HB3	3:2D:143:HIS:HE1	1.78	0.48
4:2E:36:ARG:NH1	4:2E:85:ASN:OD1	2.46	0.48
6:2G:167:GLU:OE1	6:2G:167:GLU:N	2.42	0.48
12:2Q:12:GLN:NE2	12:2Q:72:LYS:HG3	2.29	0.48
14:2S:93:LYS:HB2	14:2S:93:LYS:HE3	1.66	0.48
26:24:1:MET:HE2	26:24:6:HIS:CD2	2.48	0.48
32:2a:266:G:H2'	32:2a:266:G:N3	2.29	0.48
32:2a:299:G:H2'	32:2a:300:A:C8	2.49	0.48
32:2a:1263:C:C4	32:2a:1272:G:O6	2.67	0.48
33:2b:47:THR:O	33:2b:51:LEU:N	2.47	0.48
34:2c:131:ARG:NH2	36:2e:50:GLU:HG3	2.29	0.48
37:2f:12:PRO:HG3	37:2f:57:GLN:O	2.14	0.48
42:2k:54:ARG:NH2	56:2y:39:G:H4'	2.27	0.48
48:2q:81:ARG:HH21	48:2q:84:LEU:HD21	1.79	0.48
54:2w:11:U:H2'	54:2w:12:U:C6	2.48	0.48
32:1a:92:C:H2'	32:1a:93:G:H8	1.78	0.47
43:1l:88:GLY:O	43:1l:99:HIS:HD2	1.97	0.47
48:1q:29:HIS:CE1	48:1q:32:TYR:HD2	2.32	0.47
1:2A:1899:G:H2'	1:2A:1899:G:N3	2.29	0.47
1:2A:2752:C:H2'	1:2A:2753:A:O4'	2.14	0.47
16:2U:107:ALA:O	16:2U:111:GLU:HG2	2.14	0.47
32:2a:1067:A:H8	32:2a:1067:A:O5'	1.96	0.47
32:2a:1070:U:OP1	36:2e:18:ARG:NH2	2.46	0.47
32:2a:1235:U:O2'	32:2a:1305:G:O5'	2.32	0.47
32:2a:1435:G:H2'	32:2a:1436:U:C6	2.49	0.47
33:2b:97:TRP:HH2	33:2b:102:LEU:HG	1.78	0.47
34:2c:119:ARG:O	34:2c:123:GLN:HG3	2.14	0.47
35:2d:173:TRP:CD2	35:2d:189:PRO:HB3	2.49	0.47
39:2h:11:THR:O	39:2h:15:ASN:ND2	2.47	0.47
1:1A:536:A:H2'	1:1A:537:C:C6	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:576:U:H2'	1:1A:577:G:C8	2.49	0.47
1:1A:1093:G:H3'	1:1A:1094:U:H5"	1.95	0.47
1:1A:1453:U:O2'	1:1A:1455:G:N7	2.46	0.47
1:1A:2038:G:O6	61:1A:4140:HOH:O	2.20	0.47
11:1P:90:ARG:HG2	11:1P:90:ARG:NH1	2.29	0.47
1:2A:1671:U:OP2	61:2A:3926:HOH:O	2.19	0.47
3:2D:73:VAL:HG13	3:2D:120:GLY:HA3	1.96	0.47
3:2D:121:PRO:HB3	3:2D:135:PHE:CE2	2.49	0.47
6:2G:38:VAL:HG22	6:2G:93:THR:HG23	1.95	0.47
21:2Z:171:ILE:H	21:2Z:171:ILE:HG13	1.59	0.47
32:2a:67:C:H2'	32:2a:68:G:C8	2.49	0.47
32:2a:537:G:H5"	43:2l:113:ARG:HH12	1.79	0.47
32:2a:952:U:H2'	32:2a:953:G:C8	2.49	0.47
41:2j:50:ILE:HA	41:2j:60:ARG:HD3	1.95	0.47
54:2w:10:G:H2'	54:2w:11:U:C6	2.49	0.47
1:1A:1405:U:H2'	1:1A:1406:U:H6	1.80	0.47
1:1A:2287:A:O2'	1:1A:2289:G:N7	2.44	0.47
3:1D:20:ASP:N	3:1D:20:ASP:OD1	2.44	0.47
5:1F:123:LEU:HD13	5:1F:192:LEU:HD13	1.96	0.47
19:1X:92:LEU:O	19:1X:94:GLY:N	2.47	0.47
24:12:1:MET:HE2	24:12:6:VAL:HG22	1.96	0.47
32:1a:401:C:H2'	32:1a:402:G:C8	2.48	0.47
1:2A:656:G:H2'	1:2A:657:U:O4'	2.14	0.47
1:2A:1181:C:H2'	1:2A:1182:A:H8	1.79	0.47
1:2A:1340:U:OP1	19:2X:16:LYS:NZ	2.47	0.47
1:2A:2074:U:H2'	1:2A:2075:U:C6	2.50	0.47
1:2A:2206:G:H3'	1:2A:2207:G:N7	2.28	0.47
1:2A:2758:A:C2	1:2A:2759:G:H1'	2.49	0.47
13:2R:42:LYS:HB3	13:2R:45:ARG:HH21	1.79	0.47
28:26:23:THR:OG1	28:26:24:GLU:N	2.46	0.47
32:2a:865:A:H5'	32:2a:1078:U:H5	1.78	0.47
32:2a:1002:G:C6	32:2a:1003:G:C8	3.02	0.47
32:2a:1029:C:N4	32:2a:1032:G:C6	2.82	0.47
32:2a:1072:G:H2'	32:2a:1073:U:C6	2.50	0.47
36:2e:106:PRO:O	36:2e:110:LEU:HG	2.14	0.47
1:1A:1075:C:C2'	1:1A:1076:C:H5'	2.44	0.47
1:1A:2023:G:H5'	1:1A:2617:C:H4'	1.96	0.47
12:1Q:14:ARG:HG2	12:1Q:41:TRP:HH2	1.80	0.47
18:1W:18:ARG:HG3	18:1W:76:VAL:HB	1.96	0.47
33:1b:125:PRO:O	33:1b:127:ILE:N	2.48	0.47
40:1i:49:PRO:HG2	40:1i:81:ILE:HG23	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:96:G:H4'	24:22:48:HIS:CD2	2.49	0.47
1:2A:876:C:H2'	1:2A:877:U:H6	1.79	0.47
1:2A:1782:C:H1'	1:2A:2609:U:H5"	1.97	0.47
1:2A:2849:U:OP2	15:2T:95:ARG:NH1	2.47	0.47
19:2X:31:HIS:CD2	19:2X:33:LYS:H	2.32	0.47
32:2a:922:G:N3	32:2a:1398:A:H2	2.12	0.47
32:2a:1309:G:H5'	44:2m:78:ILE:HD11	1.96	0.47
32:2a:1411:C:H2'	32:2a:1412:C:C6	2.48	0.47
48:2q:53:LEU:HD23	48:2q:82:MET:HE1	1.97	0.47
54:2w:3:G:H1	54:2w:70:C:H42	1.62	0.47
1:1A:2080:G:OP1	23:11:35:THR:HG21	2.15	0.47
8:1I:38:LEU:H	8:1I:38:LEU:CD2	2.27	0.47
32:1a:270:A:H2'	32:1a:271:C:C6	2.50	0.47
32:1a:1212:U:H4'	32:1a:1213:A:C8	2.50	0.47
41:1j:7:LYS:HE3	41:1j:9:ARG:HH12	1.78	0.47
42:1k:79:SER:HA	42:1k:104:GLN:HB3	1.95	0.47
54:1w:55:PSU:N3	54:1w:57:G:H5"	2.29	0.47
1:2A:455:C:N3	1:2A:472:A:H2'	2.30	0.47
1:2A:1518:U:H2'	1:2A:1519:G:O4'	2.14	0.47
1:2A:1779:U:H2'	61:2A:4377:HOH:O	2.13	0.47
1:2A:2723:C:OP2	4:2E:109:LYS:NZ	2.48	0.47
9:2N:123:TYR:CZ	9:2N:129:PRO:HD2	2.49	0.47
20:2Y:9:LYS:HA	20:2Y:10:GLY:HA2	1.56	0.47
32:2a:940:C:H2'	32:2a:941:G:C8	2.49	0.47
32:2a:1137:C:O2	32:2a:1138:G:N2	2.47	0.47
32:2a:1257:U:O4	45:2n:17:LYS:NZ	2.47	0.47
39:2h:64:LYS:HD2	39:2h:79:VAL:HG11	1.95	0.47
41:2j:35:SER:HB3	41:2j:73:ASP:HB2	1.95	0.47
43:2l:37:CYS:HB2	43:2l:81:SER:H	1.79	0.47
55:2x:23:C:H2'	55:2x:24:U:C6	2.49	0.47
56:2y:66:C:H2'	56:2y:67:G:O4'	2.15	0.47
1:1A:910:A:N1	1:1A:2277:G:H1'	2.29	0.47
1:1A:1071:G:H1'	1:1A:1089:G:H2'	1.97	0.47
1:1A:1399:C:OP1	19:1X:25:LYS:NZ	2.48	0.47
1:1A:1968:G:OP1	61:1A:4139:HOH:O	2.20	0.47
1:1A:2448:A:OP1	61:1A:4101:HOH:O	2.20	0.47
6:1G:105:LYS:O	6:1G:109:VAL:HG22	2.14	0.47
10:1O:73:ASP:HB2	15:1T:82:LEU:HD13	1.97	0.47
19:1X:44:GLU:OE2	61:1X:201:HOH:O	2.20	0.47
25:13:44:ARG:O	25:13:48:GLU:HG3	2.14	0.47
28:16:26:ASN:HD21	28:16:28:ARG:NH2	2.13	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1d:61:LYS:HD2	35:1d:207:TYR:OH	2.14	0.47
56:1y:59:U:H3'	56:1y:60:U:H6	1.78	0.47
1:2A:340:A:H2'	1:2A:341:G:O4'	2.14	0.47
1:2A:1913:A:OP2	61:2A:3943:HOH:O	2.20	0.47
1:2A:2472:G:H2'	1:2A:2475:C:H42	1.80	0.47
1:2A:2849:U:H4'	1:2A:2868:A:C2	2.48	0.47
2:2B:104:U:O2'	21:2Z:29:TYR:OH	2.27	0.47
6:2G:3:LEU:HD12	6:2G:3:LEU:H	1.80	0.47
16:2U:83:LEU:HD23	16:2U:88:ILE:HD12	1.96	0.47
26:24:15:ILE:HB	26:24:32:TYR:HD1	1.80	0.47
32:2a:20:U:H2'	32:2a:21:G:O4'	2.13	0.47
32:2a:1233:G:H2'	32:2a:1234:C:C6	2.50	0.47
32:2a:1376:U:P	38:2g:94:ARG:HH22	2.37	0.47
32:2a:1387:G:H2'	32:2a:1388:C:H6	1.80	0.47
34:2c:86:VAL:HA	34:2c:89:GLU:HG3	1.96	0.47
35:2d:36:ARG:HD2	35:2d:38:TYR:OH	2.15	0.47
1:1A:251:A:C5	1:1A:252:G:H1'	2.49	0.47
1:1A:271(G):C:H2'	1:1A:271(H):G:H8	1.79	0.47
1:1A:322:A:OP1	5:1F:168:ARG:HD3	2.14	0.47
1:1A:2108:C:H2'	1:1A:2109:U:H6	1.80	0.47
1:1A:2110:G:P	1:1A:2118:U:H3	2.38	0.47
1:1A:2319:G:H22	14:1S:3:ARG:NE	2.13	0.47
1:1A:2336:A:H61	22:10:43:THR:HG22	1.79	0.47
8:1I:27:ARG:HD3	23:11:71:TYR:CE2	2.49	0.47
8:1I:81:VAL:HG21	8:1I:88:ILE:HD13	1.95	0.47
11:1P:126:VAL:HG12	11:1P:148:LEU:HD22	1.95	0.47
19:1X:53:LYS:HB3	19:1X:82:GLN:HB3	1.95	0.47
32:1a:22:G:H4'	32:1a:885:G:C8	2.50	0.47
32:1a:1005:A:OP2	32:1a:1024:G:N2	2.48	0.47
32:1a:1179:A:O3'	40:1i:103:THR:HB	2.15	0.47
32:1a:1456:G:N2	51:1t:51:GLU:OE2	2.46	0.47
33:1b:102:LEU:HB3	33:1b:180:LEU:HD12	1.96	0.47
35:1d:122:ARG:HD2	35:1d:122:ARG:HA	1.66	0.47
47:1p:49:LEU:HD13	47:1p:50:LYS:N	2.29	0.47
1:2A:84:A:N1	1:2A:98:G:O2'	2.36	0.47
1:2A:323:G:O2'	1:2A:1205:U:N3	2.42	0.47
1:2A:2823:A:OP1	4:2E:159:HIS:NE2	2.44	0.47
2:2B:1:U:H2'	2:2B:2:C:C6	2.50	0.47
3:2D:146:GLU:HG2	3:2D:152:GLY:C	2.40	0.47
5:2F:160:ASN:HB3	5:2F:163:VAL:HB	1.96	0.47
6:2G:17:PRO:HA	6:2G:20:ILE:HD12	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2G:101:ILE:HG12	26:24:25:TYR:HB2	1.97	0.47
15:2T:94:ALA:HB1	15:2T:99:LEU:HD21	1.97	0.47
17:2V:1:MET:HG2	17:2V:43:GLU:OE1	2.15	0.47
32:2a:255:G:OP1	48:2q:69:LYS:NZ	2.39	0.47
32:2a:443:C:H2'	32:2a:444:C:H6	1.80	0.47
32:2a:664:G:N2	32:2a:741:G:H1	2.13	0.47
32:2a:685:G:C2	32:2a:686:U:C4	3.03	0.47
32:2a:824:C:H2'	32:2a:825:G:C8	2.50	0.47
32:2a:991:U:C4	32:2a:1212:U:H1'	2.49	0.47
32:2a:1119:C:H2'	32:2a:1120:G:H8	1.80	0.47
32:2a:1128:C:H1'	32:2a:1147:C:H42	1.80	0.47
32:2a:1255:G:OP1	41:2j:45:ARG:NH2	2.41	0.47
33:2b:118:LEU:HD11	33:2b:141:GLU:HB3	1.96	0.47
34:2c:51:GLY:O	34:2c:70:VAL:HG13	2.15	0.47
36:2e:8:GLU:HG2	36:2e:34:VAL:HG23	1.96	0.47
36:2e:105:VAL:HB	36:2e:106:PRO:HD3	1.96	0.47
40:2i:26:VAL:HG13	40:2i:61:ALA:HB3	1.95	0.47
1:1A:370:G:H8	1:1A:370:G:OP2	1.98	0.47
1:1A:639:U:H2'	1:1A:640:C:C6	2.50	0.47
1:1A:1078:U:H5'	1:1A:1079:C:OP1	2.14	0.47
1:1A:1352:U:OP2	61:1A:4141:HOH:O	2.20	0.47
1:1A:1778:U:H2'	1:1A:1784:A:N6	2.30	0.47
4:1E:52:LEU:HD12	4:1E:77:ILE:HD11	1.95	0.47
6:1G:131:TYR:HB3	6:1G:159:VAL:HG13	1.96	0.47
7:1H:13:LYS:HA	7:1H:14:GLY:HA2	1.57	0.47
21:1Z:146:ILE:HA	21:1Z:147:GLY:HA2	1.55	0.47
26:14:24:THR:OG1	26:14:25:TYR:N	2.47	0.47
32:1a:254:G:O2'	48:1q:16:GLN:O	2.31	0.47
32:1a:1237:C:O2'	32:1a:1300:G:N1	2.38	0.47
47:1p:75:ARG:C	47:1p:77:ALA:H	2.22	0.47
1:2A:300:A:OP2	20:2Y:86:ARG:NH1	2.42	0.47
1:2A:1754:C:H5	15:2T:96:ARG:NH2	2.13	0.47
1:2A:1754:C:OP1	15:2T:96:ARG:NH1	2.48	0.47
21:2Z:5:LEU:HD21	21:2Z:39:VAL:HG11	1.97	0.47
40:2i:4:TYR:O	40:2i:18:PHE:HA	2.14	0.47
45:2n:27:CYS:SG	45:2n:29:ARG:HB2	2.55	0.47
49:2r:58:LEU:HD22	49:2r:62:GLU:HB3	1.97	0.47
56:2y:21:A:C6	56:2y:48:C:C5	3.02	0.47
1:1A:1641:A:H2'	1:1A:1642:G:O4'	2.15	0.47
1:1A:1796:U:H2'	1:1A:1797:C:H6	1.79	0.47
19:1X:50:LYS:N	19:1X:87:GLN:OE1	2.44	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:1h:51:VAL:HG11	39:1h:60:ARG:NH1	2.30	0.47
54:1w:67:G:H2'	54:1w:68:C:O4'	2.15	0.47
1:2A:958:U:OP2	12:2Q:14:ARG:NE	2.44	0.47
1:2A:2151:G:H2'	1:2A:2152:G:H8	1.79	0.47
1:2A:2375:G:N2	1:2A:2378:A:OP2	2.43	0.47
5:2F:31:HIS:HB2	11:2P:9:ASN:OD1	2.14	0.47
9:2N:69:GLN:O	9:2N:71:ILE:HG13	2.15	0.47
32:2a:157:G:N2	32:2a:164:U:O2	2.33	0.47
32:2a:171:A:H2'	32:2a:172:A:C8	2.50	0.47
32:2a:359:U:H2'	32:2a:360:A:H8	1.79	0.47
32:2a:1206:G:O2'	34:2c:193:TYR:HA	2.15	0.47
39:2h:51:VAL:HG11	39:2h:60:ARG:NH1	2.30	0.47
40:2i:26:VAL:HG22	40:2i:61:ALA:HB3	1.97	0.47
47:2p:43:LYS:HG2	47:2p:48:TRP:CG	2.50	0.47
1:1A:2031:A:C6	1:1A:2498:C:H1'	2.50	0.47
1:1A:2791:C:OP2	1:1A:2791:C:H6	1.98	0.47
5:1F:181:LEU:HB3	5:1F:205:ARG:NH2	2.30	0.47
7:1H:137:ASP:HB3	7:1H:140:LYS:HB3	1.96	0.47
22:10:27:GLU:HG3	22:10:68:GLU:HA	1.97	0.47
28:16:18:ARG:HD2	28:16:42:TRP:CD1	2.50	0.47
32:1a:134:A:H61	47:1p:25:ARG:NH1	2.13	0.47
32:1a:473:G:OP2	47:1p:75:ARG:NH1	2.47	0.47
32:1a:576:G:O6	32:1a:880:C:O2'	2.30	0.47
37:1f:95:GLU:O	49:1r:32:ARG:NH1	2.48	0.47
1:2A:860:U:C2	1:2A:2268:A:C8	3.03	0.47
1:2A:1371:G:H2'	1:2A:1372:U:H5	1.80	0.47
5:2F:195:ASP:OD1	5:2F:196:LEU:N	2.48	0.47
6:2G:5:VAL:HG23	6:2G:7:LEU:H	1.80	0.47
6:2G:64:THR:HB	6:2G:94:LEU:HD21	1.98	0.47
19:2X:60:ARG:NH2	29:27:47:ARG:HH12	2.13	0.47
21:2Z:66:SER:O	21:2Z:66:SER:OG	2.32	0.47
33:2b:44:LEU:O	33:2b:47:THR:HG22	2.15	0.47
35:2d:104:VAL:HG21	35:2d:140:VAL:HG21	1.95	0.47
40:2i:3:GLN:NE2	40:2i:20:ARG:HE	2.12	0.47
42:2k:33:THR:HG22	42:2k:39:PRO:HA	1.97	0.47
1:1A:911:A:H2'	12:1Q:9:TYR:OH	2.15	0.46
1:1A:1066:U:H2'	1:1A:1068:G:OP2	2.16	0.46
1:1A:1899:G:N3	1:1A:1899:G:H2'	2.30	0.46
1:1A:2126:A:H4'	1:1A:2127:G:OP1	2.14	0.46
4:1E:14:ILE:HG13	4:1E:21:VAL:HG13	1.96	0.46
15:1T:74:ARG:HG2	15:1T:76:PHE:CZ	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:16:17:LYS:HB3	28:16:17:LYS:HE3	1.71	0.46
32:1a:236:G:H5"	48:1q:42:TYR:OH	2.14	0.46
32:1a:452:A:O2'	32:1a:453:A:OP2	2.25	0.46
32:1a:974:A:P	45:1n:41:ARG:HH21	2.37	0.46
41:1j:11:PHE:HE1	41:1j:67:THR:HG22	1.80	0.46
42:1k:27:ASN:OD1	42:1k:28:THR:N	2.46	0.46
1:2A:907:U:O2'	12:2Q:101:ARG:NH2	2.42	0.46
1:2A:1027:A:C6	1:2A:1126:A:C4	3.04	0.46
1:2A:2557:G:H2'	1:2A:2558:C:C6	2.50	0.46
2:2B:1:U:O2'	2:2B:2:C:O5'	2.20	0.46
2:2B:32:C:H2'	2:2B:33:G:O4'	2.14	0.46
2:2B:43:C:H5"	26:24:1:MET:HG2	1.97	0.46
6:2G:111:LEU:HA	6:2G:114:ILE:HD12	1.97	0.46
8:2I:128:LEU:HD23	8:2I:128:LEU:HA	1.81	0.46
26:24:62:ARG:HA	26:24:62:ARG:NE	2.30	0.46
37:2f:61:LEU:HB3	37:2f:63:TYR:CE2	2.50	0.46
39:2h:10:LEU:HD23	39:2h:83:ILE:HD11	1.97	0.46
44:2m:60:VAL:HG13	44:2m:64:TRP:HE3	1.80	0.46
54:2w:6:C:N3	54:2w:67:G:C2	2.83	0.46
1:1A:271(D):G:H1	1:1A:271(T):C:H42	1.63	0.46
24:12:7:ARG:O	24:12:11:GLU:HG3	2.16	0.46
32:1a:244:U:O2	61:1a:1913:HOH:O	2.19	0.46
34:1c:19:GLU:HB3	34:1c:40:ARG:HH21	1.80	0.46
34:1c:73:PRO:O	34:1c:77:ILE:HG13	2.16	0.46
35:1d:25:ARG:HA	35:1d:28:SER:HB3	1.97	0.46
1:2A:30:G:H2'	1:2A:31:C:C6	2.51	0.46
1:2A:882:G:H2'	1:2A:883:G:C8	2.51	0.46
1:2A:1346:G:OP2	61:2A:3942:HOH:O	2.20	0.46
1:2A:2630:G:H2'	1:2A:2631:G:C8	2.50	0.46
5:2F:172:TRP:H	5:2F:172:TRP:CD1	2.33	0.46
15:2T:6:LEU:O	15:2T:10:VAL:HG23	2.15	0.46
20:2Y:55:TYR:N	20:2Y:56:PRO:HD3	2.30	0.46
26:24:14:ILE:HB	26:24:22:ILE:HD13	1.97	0.46
32:2a:1052:U:O2'	32:2a:1055:A:OP2	2.20	0.46
32:2a:1126:U:H3	41:2j:71:LEU:HD22	1.80	0.46
43:2l:6:THR:N	43:2l:9:GLN:OE1	2.44	0.46
48:2q:67:LYS:HA	48:2q:70:ARG:HH12	1.80	0.46
1:1A:1991:U:H2'	1:1A:1992:G:H5"	1.97	0.46
32:1a:4:U:O4	39:1h:105:ARG:HD3	2.15	0.46
32:1a:189(K):U:H2'	32:1a:189(L):G:C8	2.49	0.46
32:1a:524:G:H2'	32:1a:525:C:C6	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:677:U:H3	32:1a:713:G:H22	1.61	0.46
32:1a:811:C:O2'	32:1a:901:A:N1	2.42	0.46
42:1k:48:ILE:O	42:1k:50:TYR:N	2.44	0.46
1:2A:118:A:H5'	1:2A:119:A:H8	1.79	0.46
1:2A:740:U:H2'	1:2A:741:G:C8	2.51	0.46
1:2A:1450:G:H1	1:2A:1462:C:H42	1.62	0.46
1:2A:2749:A:H1'	7:2H:63:SER:HB3	1.97	0.46
2:2B:11:C:H3'	2:2B:12:C:C6	2.50	0.46
32:2a:451:A:N6	32:2a:480:U:H2'	2.30	0.46
32:2a:510:A:N3	32:2a:543:C:H1'	2.31	0.46
54:2w:53:G:H1	54:2w:61:C:H42	1.62	0.46
56:2y:28:G:C2'	56:2y:29:A:H5'	2.45	0.46
1:1A:272(G):C:H42	1:1A:363(C):G:H1	1.64	0.46
1:1A:1779:U:H2'	61:1A:4521:HOH:O	2.15	0.46
5:1F:161:GLU:O	5:1F:165:ARG:HG3	2.15	0.46
14:1S:110:LEU:HD12	14:1S:110:LEU:HA	1.75	0.46
20:1Y:35:TYR:CE2	20:1Y:69:ALA:HB3	2.50	0.46
28:16:6:ARG:HD3	28:16:24:GLU:OE2	2.15	0.46
32:1a:60:A:N1	32:1a:107:G:O2'	2.46	0.46
1:2A:722:A:H2'	1:2A:723:G:C8	2.50	0.46
1:2A:921:G:C6	1:2A:922:U:C4	3.04	0.46
1:2A:1405:U:H2'	1:2A:1406:U:C6	2.51	0.46
1:2A:1790:C:H5"	1:2A:1791:A:OP1	2.15	0.46
1:2A:2129:C:N4	1:2A:2159:G:N1	2.63	0.46
26:24:40:HIS:O	26:24:44:THR:HG22	2.16	0.46
35:2d:158:ILE:O	35:2d:162:LEU:HG	2.16	0.46
38:2g:70:LYS:O	38:2g:138:LYS:HD2	2.15	0.46
40:2i:28:VAL:HG22	40:2i:63:ILE:HB	1.98	0.46
49:2r:35:ARG:O	49:2r:37:VAL:N	2.49	0.46
55:2x:19:G:H5"	55:2x:60:U:O4	2.16	0.46
1:1A:2135:A:H2'	1:1A:2135:A:N3	2.30	0.46
21:1Z:163:LEU:HD23	21:1Z:167:PRO:HG3	1.97	0.46
32:1a:130:A:O2'	32:1a:131:C:O5'	2.30	0.46
32:1a:1263:C:H2'	32:1a:1264:C:H6	1.79	0.46
33:1b:37:ASN:C	33:1b:39:ILE:H	2.21	0.46
34:1c:151:VAL:HA	34:1c:199:LYS:O	2.16	0.46
36:1e:144:THR:H	36:1e:147:ASP:HB2	1.79	0.46
38:1g:92:SER:O	38:1g:96:GLN:HG3	2.15	0.46
48:1q:66:SER:HB3	48:1q:69:LYS:HB2	1.98	0.46
1:2A:287:C:H2'	1:2A:288:C:C6	2.51	0.46
1:2A:469:G:O6	29:27:37:LYS:HE2	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2299:G:H2'	1:2A:2300:G:H8	1.80	0.46
1:2A:2316:C:H2'	1:2A:2317:C:C6	2.51	0.46
1:2A:2693:A:H2'	1:2A:2694:G:C8	2.51	0.46
6:2G:107:LEU:HD21	6:2G:178:PHE:CZ	2.51	0.46
8:2I:84:GLY:C	8:2I:86:THR:H	2.22	0.46
32:2a:6:G:H1	36:2e:98:THR:HG21	1.79	0.46
32:2a:130:A:O2'	32:2a:131:C:O5'	2.30	0.46
33:2b:97:TRP:CH2	33:2b:101:MET:HB2	2.51	0.46
33:2b:100:GLY:H	33:2b:176:GLU:CD	2.23	0.46
40:2i:92:TYR:O	40:2i:96:LEU:HB2	2.16	0.46
44:2m:40:ASN:ND2	44:2m:43:THR:HG23	2.30	0.46
54:2w:13:C:O2'	54:2w:14:A:H8	1.98	0.46
6:1G:67:LYS:H	26:14:6:HIS:CE1	2.32	0.46
32:1a:507:C:OP2	32:1a:508:C:O2'	2.26	0.46
36:1e:79:GLU:H	36:1e:79:GLU:CD	2.23	0.46
38:1g:111:ARG:NE	38:1g:113:GLU:OE2	2.46	0.46
38:1g:113:GLU:HG2	38:1g:119:ARG:HG2	1.98	0.46
44:1m:102:ARG:HH21	44:1m:104:ARG:HB3	1.80	0.46
50:1s:12:ASP:OD1	50:1s:37:ARG:NH2	2.49	0.46
1:2A:1394:U:C4	1:2A:1395:A:C5	3.04	0.46
1:2A:2127:G:N1	1:2A:2161:C:C4	2.83	0.46
13:2R:36:THR:HG22	13:2R:37:THR:H	1.81	0.46
32:2a:551:U:H2'	32:2a:552:U:C6	2.50	0.46
32:2a:1030(A):G:N2	32:2a:1030(C):G:H3'	2.31	0.46
32:2a:1216:G:H5"	45:2n:5:ALA:HB2	1.95	0.46
51:2t:54:LYS:HB3	51:2t:54:LYS:HE2	1.51	0.46
1:1A:1045:A:OP1	1:1A:1046:A:H3'	2.15	0.46
1:1A:1054:A:H3'	1:1A:1055:G:C8	2.50	0.46
1:1A:1178:C:O5'	1:1A:1178:C:H6	1.98	0.46
7:1H:54:ARG:NH2	7:1H:57:ASP:OD2	2.45	0.46
32:1a:222:U:H2'	32:1a:223:U:C6	2.51	0.46
32:1a:1021:G:HO2'	32:1a:1022:G:P	2.38	0.46
32:1a:1152:A:OP1	41:1j:68:HIS:ND1	2.49	0.46
36:1e:35:GLY:HA2	36:1e:40:ARG:O	2.15	0.46
39:1h:82:HIS:O	39:1h:137:VAL:HA	2.16	0.46
41:1j:61:GLU:OE2	45:1n:58:LYS:HE2	2.16	0.46
47:1p:20:VAL:HG22	47:1p:34:GLU:O	2.15	0.46
1:2A:2343:C:O2'	1:2A:2373:G:O2'	2.18	0.46
16:2U:76:TYR:CZ	16:2U:80:ILE:HG13	2.51	0.46
31:29:6:SER:O	31:29:6:SER:OG	2.31	0.46
32:2a:341:C:O2	32:2a:348:G:N2	2.37	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:555:C:H2'	32:2a:556:C:C6	2.51	0.46
32:2a:1089:G:H1	32:2a:1096:C:N4	2.09	0.46
32:2a:1328:C:O2'	44:2m:29:ARG:NH2	2.46	0.46
34:2c:34:LEU:HD22	34:2c:38:ARG:HH21	1.81	0.46
34:2c:35:GLU:O	34:2c:39:ILE:HG12	2.16	0.46
39:2h:127:LEU:HD23	39:2h:127:LEU:HA	1.79	0.46
43:2l:117:ARG:HB3	43:2l:122:THR:HB	1.98	0.46
51:2t:67:ALA:HA	51:2t:72:LEU:O	2.14	0.46
1:1A:1292:U:H2'	1:1A:1293:C:C6	2.50	0.46
1:1A:2161:C:O2'	1:1A:2162:G:H5"	2.15	0.46
12:1Q:1:MET:HB2	12:1Q:1:MET:HE3	1.83	0.46
32:1a:69:G:H2'	32:1a:70:G:C8	2.51	0.46
32:1a:176:C:H2'	32:1a:177:C:H6	1.81	0.46
32:1a:441:A:H8	32:1a:441:A:OP2	1.98	0.46
32:1a:865:A:H2	32:1a:918:A:H4'	1.80	0.46
33:1b:119:GLU:O	33:1b:123:ALA:HB2	2.16	0.46
42:1k:84:VAL:HG11	42:1k:91:ARG:HE	1.80	0.46
50:1s:23:ASN:HA	50:1s:27:GLU:CD	2.41	0.46
1:2A:674:G:H1'	5:2F:74:ARG:HD3	1.98	0.46
1:2A:2243:U:H2'	1:2A:2244:U:C6	2.51	0.46
1:2A:2319:G:H22	14:2S:3:ARG:NH1	2.08	0.46
2:2B:17:C:H2'	2:2B:18:G:O4'	2.16	0.46
11:2P:97:PRO:HG3	11:2P:112:LEU:HD23	1.97	0.46
15:2T:105:LEU:HB2	15:2T:110:ILE:HG13	1.98	0.46
16:2U:106:PHE:O	16:2U:110:VAL:HG23	2.16	0.46
21:2Z:94:GLU:H	21:2Z:94:GLU:CD	2.23	0.46
32:2a:1104:G:H4'	33:2b:111:ARG:HE	1.79	0.46
36:2e:84:PHE:O	36:2e:86:ALA:N	2.49	0.46
44:2m:45:VAL:HA	44:2m:48:LEU:HG	1.97	0.46
1:1A:1094:U:H1'	1:1A:1097:U:C4	2.51	0.46
1:1A:2646:C:OP2	1:1A:2732:G:O2'	2.29	0.46
19:1X:94:GLY:H	19:1X:95:LEU:HB2	1.79	0.46
26:14:55:ARG:H	26:14:56:VAL:HA	1.81	0.46
32:1a:119:A:H4'	32:1a:120:A:C8	2.50	0.46
32:1a:401:C:H2'	32:1a:402:G:H8	1.81	0.46
33:1b:163:PHE:HA	33:1b:185:ILE:HG12	1.98	0.46
38:1g:104:LEU:HD13	38:1g:104:LEU:HA	1.86	0.46
43:1l:117:ARG:HB3	43:1l:122:THR:HB	1.98	0.46
54:1w:76:L3X:N	55:1x:76:31H:O2'	2.49	0.46
1:2A:1292:U:H2'	1:2A:1293:C:C6	2.51	0.46
1:2A:1946:U:H2'	1:2A:1947:C:C6	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2100:G:H2'	1:2A:2101:G:C8	2.51	0.46
1:2A:2134:A:H2'	1:2A:2134:A:N3	2.31	0.46
21:2Z:156:LYS:HB3	21:2Z:156:LYS:HE3	1.81	0.46
22:20:27:GLU:HG3	22:20:68:GLU:HA	1.98	0.46
28:26:12:GLU:OE1	28:26:19:ARG:NH1	2.48	0.46
32:2a:1132:C:H2'	32:2a:1133:G:C8	2.51	0.46
32:2a:1517:G:N7	32:2a:1518:MA6:H103	2.31	0.46
33:2b:118:LEU:HD13	33:2b:142:LEU:HB2	1.98	0.46
34:2c:9:GLY:HA3	45:2n:49:HIS:HA	1.98	0.46
34:2c:13:GLY:HA3	45:2n:57:ARG:HH22	1.81	0.46
35:2d:108:LEU:HD21	35:2d:174:LEU:HB3	1.98	0.46
1:1A:264:C:O2'	1:1A:265:A:H2'	2.16	0.46
1:1A:586:A:N1	1:1A:809:G:O2'	2.42	0.46
2:1B:78:A:C2	2:1B:100:A:C4	3.04	0.46
32:1a:865:A:C2	32:1a:918:A:H4'	2.51	0.46
35:1d:18:LYS:NZ	35:1d:26:CYS:O	2.49	0.46
1:2A:1181:C:H2'	1:2A:1182:A:C8	2.51	0.46
32:2a:359:U:H2'	32:2a:360:A:C8	2.51	0.46
32:2a:603:U:H2'	32:2a:604:G:H8	1.81	0.46
32:2a:1144:G:N2	32:2a:1146:A:H62	2.14	0.46
35:2d:180:GLY:O	35:2d:182:LYS:HG3	2.16	0.46
36:2e:146:ALA:O	36:2e:150:ARG:HG2	2.16	0.46
39:2h:23:SER:OG	39:2h:60:ARG:HG2	2.15	0.46
39:2h:51:VAL:HG12	39:2h:52:ASP:H	1.81	0.46
54:2w:17:G:H4'	54:2w:60:U:C5	2.51	0.46
54:2w:25:C:H3'	54:2w:26:G:H8	1.80	0.46
1:1A:1062:G:H2'	1:1A:1063:G:C8	2.51	0.45
1:1A:2347:C:H2'	1:1A:2348:U:C6	2.51	0.45
2:1B:31:C:O2'	2:1B:53:A:N1	2.44	0.45
7:1H:25:LYS:HE3	7:1H:27:LYS:NZ	2.31	0.45
32:1a:1459:C:OP1	51:1t:31:SER:OG	2.28	0.45
56:1y:55:PSU:C4	56:1y:57:G:H5'	2.51	0.45
1:2A:2118:U:C4	1:2A:2149:G:H1'	2.51	0.45
1:2A:2564:A:C2	1:2A:2647:U:H4'	2.51	0.45
30:28:34:TRP:CG	30:28:35:GLN:N	2.84	0.45
33:2b:16:HIS:CB	33:2b:204:ASN:HB3	2.41	0.45
33:2b:126:GLU:CD	33:2b:126:GLU:H	2.25	0.45
37:2f:62:TRP:CH2	37:2f:64:GLN:HB2	2.51	0.45
56:2y:61:C:H2'	56:2y:62:C:C6	2.51	0.45
8:1I:94:ALA:N	8:1I:116:LEU:HD22	2.30	0.45
32:1a:456:C:H2'	32:1a:457:C:H6	1.80	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1401:G:C2	32:1a:1402:4OC:H1'	2.52	0.45
42:1k:15:ALA:O	42:1k:78:GLN:N	2.42	0.45
11:2P:90:ARG:HD2	11:2P:91:PHE:CZ	2.50	0.45
32:2a:1073:U:H2'	32:2a:1074:G:H8	1.80	0.45
32:2a:1252:A:H61	32:2a:1285:A:H61	1.63	0.45
33:2b:96:ARG:HG2	33:2b:98:LEU:HD12	1.98	0.45
35:2d:96:LEU:HA	35:2d:96:LEU:HD13	1.73	0.45
46:2o:82:ILE:HD12	46:2o:88:ARG:HB2	1.97	0.45
51:2t:72:LEU:HD12	51:2t:72:LEU:HA	1.82	0.45
1:1A:2146:C:H5"	1:1A:2147:G:C8	2.51	0.45
1:1A:2846:G:H2'	1:1A:2847:U:O4'	2.16	0.45
6:1G:49:ASP:N	6:1G:49:ASP:OD1	2.49	0.45
7:1H:116:GLU:HG3	7:1H:117:PRO:HD2	1.97	0.45
32:1a:130:A:H5'	48:1q:63:ARG:HE	1.82	0.45
32:1a:1038:C:H2'	32:1a:1039:C:H6	1.81	0.45
32:1a:1066:C:O2'	32:1a:1067:A:H5'	2.15	0.45
35:1d:142:PRO:HA	35:1d:185:PHE:HD2	1.80	0.45
37:1f:36:ARG:NH2	37:1f:38:GLU:HG2	2.30	0.45
56:1y:4:G:H5'	56:1y:5:G:OP2	2.16	0.45
1:2A:518:G:H2'	1:2A:519:U:C6	2.51	0.45
1:2A:1149:G:H2'	1:2A:1150:C:C6	2.52	0.45
1:2A:1411:C:H2'	1:2A:1412:A:C8	2.50	0.45
1:2A:2872:G:O2'	1:2A:2873:A:H5'	2.17	0.45
2:2B:24:G:N3	2:2B:26:A:N6	2.63	0.45
28:26:11:LEU:HB2	28:26:21:TYR:HB2	1.98	0.45
32:2a:407:G:H5"	35:2d:115:ARG:HB3	1.98	0.45
32:2a:993:G:N3	32:2a:993:G:H2'	2.31	0.45
32:2a:1104:G:H4'	33:2b:111:ARG:HH21	1.82	0.45
34:2c:58:GLU:HB2	34:2c:65:ALA:HB3	1.97	0.45
37:2f:82:ARG:HE	37:2f:82:ARG:HB3	1.55	0.45
50:2s:22:LEU:HG	50:2s:31:ILE:HD11	1.99	0.45
56:2y:7:G:C6	56:2y:49:G:C5	3.04	0.45
1:1A:278:A:P	1:1A:278:A:H8	2.39	0.45
1:1A:1054:A:H3'	1:1A:1055:G:H8	1.82	0.45
1:1A:1814:G:H4'	3:1D:51:VAL:HG21	1.99	0.45
1:1A:2139:C:N3	1:1A:2152:G:N2	2.58	0.45
9:1N:73:THR:HB	9:1N:82:LEU:HD11	1.97	0.45
15:1T:127:ALA:O	15:1T:129:ARG:N	2.45	0.45
32:1a:1197:G:OP2	61:1a:1914:HOH:O	2.20	0.45
32:1a:1442:G:O2'	32:1a:1442(A):G:H5'	2.17	0.45
41:1j:46:ARG:HB2	41:1j:46:ARG:HH11	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:2T:51:ARG:HG3	15:2T:98:LYS:HD2	1.98	0.45
18:2W:12:ILE:HD13	18:2W:17:VAL:HG23	1.98	0.45
21:2Z:53:ILE:HG22	21:2Z:71:VAL:HB	1.97	0.45
32:2a:683:G:H2'	32:2a:684:A:C8	2.51	0.45
32:2a:901:A:O2'	32:2a:1513:A:OP1	2.32	0.45
32:2a:1054:C:C5	54:2w:34:C:H1'	2.52	0.45
32:2a:1129:C:H1'	32:2a:1146:A:H61	1.80	0.45
32:2a:1151:A:O2'	32:2a:1152:A:H8	1.99	0.45
42:2k:41:THR:HG21	42:2k:71:LYS:CB	2.45	0.45
1:1A:1179:C:H2'	1:1A:1180:C:H6	1.81	0.45
1:1A:1882:C:H2'	1:1A:1883:G:O4'	2.17	0.45
1:1A:2136:C:N3	1:1A:2155:G:N2	2.64	0.45
17:1V:71:LEU:HA	17:1V:71:LEU:HD23	1.74	0.45
36:1e:51:VAL:O	36:1e:55:VAL:HG23	2.16	0.45
44:1m:84:ILE:HG13	44:1m:86:CYS:H	1.82	0.45
48:1q:45:HIS:HB3	48:1q:72:ARG:HG2	1.98	0.45
49:1r:58:LEU:HD22	49:1r:62:GLU:HB3	1.97	0.45
55:1x:8:4SU:O2	55:1x:21:A:H2	2.00	0.45
1:2A:98:G:OP2	24:22:2:LYS:HG2	2.17	0.45
1:2A:1607:C:N4	1:2A:1622:G:OP2	2.44	0.45
5:2F:164:ARG:O	5:2F:168:ARG:HB2	2.16	0.45
17:2V:2:PHE:CZ	17:2V:41:GLY:HA3	2.51	0.45
32:2a:957:U:H2'	32:2a:959:A:OP2	2.15	0.45
32:2a:986:A:N3	50:2s:52:TYR:OH	2.40	0.45
32:2a:989:C:H2'	32:2a:990:C:C6	2.51	0.45
33:2b:185:ILE:HB	33:2b:199:TYR:HB2	1.98	0.45
34:2c:116:VAL:HG11	34:2c:141:VAL:HG21	1.99	0.45
39:2h:4:ASP:HB3	39:2h:7:ALA:HB3	1.99	0.45
46:2o:74:ASP:HB3	46:2o:77:ARG:HB2	1.98	0.45
1:1A:1104:C:H2'	1:1A:1105:U:C6	2.51	0.45
1:1A:1359:A:C2	1:1A:1372:U:O4	2.69	0.45
1:1A:2128:C:N4	1:1A:2160:G:C6	2.85	0.45
1:1A:2181:G:O2'	1:1A:2182:G:OP1	2.33	0.45
4:1E:101:ARG:CZ	4:1E:171:GLU:HB2	2.46	0.45
38:1g:65:ALA:HB1	38:1g:127:ALA:HB3	1.99	0.45
54:1w:55:PSU:HN3	54:1w:57:G:H5"	1.81	0.45
1:2A:271(Q):G:H2'	1:2A:271(R):G:C8	2.51	0.45
1:2A:580:C:H2'	1:2A:581:C:H6	1.80	0.45
1:2A:1003:G:O2'	1:2A:1010:A:N1	2.50	0.45
1:2A:1502:C:H2'	1:2A:1503:U:C6	2.51	0.45
2:2B:94:C:H2'	2:2B:95:C:C6	2.52	0.45

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	2.30	0.45
7:2H:103:LEU:O	7:2H:115:VAL:N	2.48	0.45
12:2Q:22:LYS:HE2	12:2Q:22:LYS:HB3	1.72	0.45
15:2T:118:ARG:HG2	32:2a:1442(A):G:C8	2.51	0.45
31:29:8:LYS:O	31:29:34:GLN:NE2	2.39	0.45
32:2a:1401:G:C2	32:2a:1402:4OC:H1'	2.51	0.45
38:2g:78:ARG:HD3	38:2g:79:ARG:HG3	1.98	0.45
1:1A:2053:G:OP1	4:1E:144:ARG:HG3	2.16	0.45
1:1A:2562:U:H4'	10:1O:25:LEU:HD21	1.99	0.45
1:1A:2630:G:H2'	1:1A:2631:G:C8	2.52	0.45
2:1B:84:C:OP1	25:13:15:TYR:OH	2.27	0.45
21:1Z:69:THR:HG22	21:1Z:90:VAL:HG22	1.97	0.45
32:1a:627:G:H2'	32:1a:628:G:H8	1.82	0.45
32:1a:1030(D):A:C8	32:1a:1031:G:H1'	2.51	0.45
41:1j:40:LEU:HB2	41:1j:69:ASN:HB2	1.98	0.45
1:2A:2404:C:O3'	11:2P:77:ARG:NH2	2.50	0.45
1:2A:2484:G:C2	1:2A:2485:G:C8	3.04	0.45
2:2B:106:G:H5'	21:2Z:31:ARG:HG2	1.98	0.45
7:2H:144:VAL:O	7:2H:148:ILE:HG13	2.17	0.45
8:2I:126:TYR:O	8:2I:141:LYS:HA	2.17	0.45
11:2P:121:LYS:O	11:2P:123:LEU:N	2.50	0.45
21:2Z:40:ASP:OD2	21:2Z:42:VAL:HG13	2.15	0.45
32:2a:324:G:N1	32:2a:327:A:OP2	2.48	0.45
32:2a:328:C:H4'	32:2a:329:A:H5'	1.98	0.45
33:2b:27:LYS:HB2	33:2b:194:PRO:HD2	1.99	0.45
40:2i:99:LEU:HB3	40:2i:101:PHE:CD2	2.52	0.45
42:2k:92:GLU:O	42:2k:96:ARG:HG2	2.16	0.45
54:2w:54:5MU:C4	54:2w:55:PSU:C2	3.05	0.45
56:2y:8:4SU:HN3	56:2y:14:A:H62	1.64	0.45
32:1a:572:A:H5'	32:1a:573:A:OP2	2.17	0.45
32:1a:859:A:H2'	32:1a:860:A:O4'	2.16	0.45
44:1m:23:TYR:HB3	44:1m:67:GLU:HA	1.98	0.45
49:1r:47:THR:O	49:1r:83:GLU:N	2.39	0.45
1:2A:93:G:H2'	1:2A:94:C:C6	2.52	0.45
1:2A:1021:A:H3'	1:2A:1021:A:C8	2.52	0.45
1:2A:1470:G:O6	61:2A:3944:HOH:O	2.20	0.45
1:2A:1794:U:H2'	1:2A:1795:C:C6	2.52	0.45
2:2B:1:U:H2'	2:2B:2:C:H6	1.81	0.45
3:2D:24:ILE:HD13	3:2D:84:TYR:HB2	1.99	0.45
4:2E:14:ILE:HG13	4:2E:21:VAL:HG13	1.99	0.45
33:2b:16:HIS:CB	33:2b:210:SER:HB2	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:2d:18:LYS:NZ	35:2d:26:CYS:O	2.40	0.45
42:2k:54:ARG:HE	42:2k:54:ARG:HB2	1.48	0.45
1:1A:879:G:N1	1:1A:899:A:H1'	2.32	0.45
1:1A:1076:C:O2'	1:1A:1077:A:N7	2.50	0.45
1:1A:1588:C:H2'	1:1A:1589:C:H6	1.82	0.45
1:1A:2629:A:H1'	1:1A:2630:G:H5"	1.98	0.45
14:1S:10:ARG:O	14:1S:14:VAL:HG13	2.17	0.45
22:10:10:THR:HG22	22:10:12:ASN:N	2.22	0.45
35:1d:65:ARG:HG3	35:1d:75:PHE:CD1	2.52	0.45
56:1y:49:G:H1	56:1y:65:U:H3	1.65	0.45
1:2A:515:A:H1'	1:2A:581:C:H1'	1.98	0.45
1:2A:859:G:N2	1:2A:917:A:OP2	2.45	0.45
1:2A:2127:G:C6	1:2A:2161:C:N4	2.85	0.45
2:2B:28:C:H2'	2:2B:29:A:H8	1.82	0.45
6:2G:44:GLY:HA2	6:2G:88:ILE:HG22	1.98	0.45
8:2I:66:GLU:HA	8:2I:69:LYS:HB3	1.98	0.45
32:2a:1183:A:H3'	32:2a:1184:G:C5'	2.47	0.45
32:2a:1273:G:H3'	32:2a:1274:G:H8	1.81	0.45
32:2a:1301:U:O2'	32:2a:1302:U:H5'	2.17	0.45
35:2d:22:LYS:HB2	35:2d:26:CYS:SG	2.57	0.45
35:2d:101:LEU:HA	35:2d:104:VAL:HG22	1.99	0.45
35:2d:112:VAL:H	35:2d:116:GLN:NE2	2.15	0.45
47:2p:3:LYS:O	47:2p:21:VAL:HA	2.17	0.45
1:1A:582:G:H2'	1:1A:583:G:C8	2.52	0.45
1:1A:1053:C:N4	1:1A:1106:G:H1	2.13	0.45
1:1A:2175:C:H2'	1:1A:2176:A:O4'	2.16	0.45
1:1A:2801(A):A:H5"	1:1A:2802:G:C8	2.51	0.45
14:1S:20:ARG:NH2	22:10:51:VAL:O	2.48	0.45
14:1S:65:VAL:O	14:1S:69:VAL:HG12	2.17	0.45
32:1a:7:G:H5'	32:1a:298:A:O4'	2.17	0.45
32:1a:202:U:H3'	32:1a:203:U:H6	1.81	0.45
32:1a:266:G:N3	32:1a:266:G:H5"	2.32	0.45
32:1a:971:G:N2	32:1a:1363(A):A:OP2	2.42	0.45
32:1a:974:A:OP2	45:1n:41:ARG:NH2	2.46	0.45
37:1f:33:TYR:CD2	37:1f:75:LEU:HD23	2.52	0.45
41:1j:7:LYS:HD3	41:1j:71:LEU:HD13	1.98	0.45
49:1r:33:ASP:OD2	49:1r:36:ASN:HB2	2.17	0.45
1:2A:479:A:H4'	1:2A:480:A:OP1	2.17	0.45
1:2A:861:A:N3	2:2B:79:C:O2'	2.45	0.45
1:2A:1364:G:P	23:21:3:LYS:HG3	2.56	0.45
4:2E:7:VAL:HG11	15:2T:1:MET:HE1	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2G:53:LEU:HB3	6:2G:56:ALA:HB3	1.98	0.45
8:2I:133:HIS:HD2	8:2I:134:PRO:HD2	1.82	0.45
13:2R:72:ASP:HB3	13:2R:75:LEU:HB3	1.98	0.45
32:2a:868:C:H2'	32:2a:869:G:O4'	2.16	0.45
32:2a:1118:C:H1'	32:2a:1179:A:C4	2.51	0.45
32:2a:1151:A:O2'	32:2a:1152:A:O5'	2.26	0.45
40:2i:28:VAL:HG13	40:2i:63:ILE:HB	1.98	0.45
42:2k:34:ASP:OD2	42:2k:38:ASN:HB2	2.16	0.45
55:2x:40:C:H2'	55:2x:41:C:C6	2.52	0.45
56:2y:19:U:O2	56:2y:21:A:H4'	2.17	0.45
1:1A:1044:G:H5'	1:1A:1045:A:OP2	2.17	0.44
1:1A:2320:A:H2'	1:1A:2320:A:N3	2.32	0.44
5:1F:129:PHE:CD2	5:1F:163:VAL:HG21	2.51	0.44
21:1Z:158:PRO:O	21:1Z:161:VAL:HG22	2.17	0.44
26:14:33:VAL:HG13	26:14:35:VAL:H	1.82	0.44
26:14:50:VAL:HG21	44:1m:64:TRP:C	2.42	0.44
32:1a:1308:U:OP2	44:1m:99:ARG:HD2	2.17	0.44
42:1k:59:TYR:CE2	42:1k:63:LEU:HD11	2.52	0.44
46:1o:56:LEU:O	46:1o:60:VAL:HG23	2.17	0.44
1:2A:910:A:N1	1:2A:2277:G:H1'	2.32	0.44
1:2A:2683:C:OP1	15:2T:53:ARG:NH2	2.47	0.44
5:2F:137:LYS:HE2	5:2F:137:LYS:HB3	1.71	0.44
6:2G:5:VAL:HG21	6:2G:100:TRP:HB3	1.98	0.44
6:2G:145:THR:O	6:2G:148:MET:HG2	2.17	0.44
12:2Q:37:LEU:HD21	12:2Q:130:LYS:HE2	1.99	0.44
20:2Y:8:LYS:HD3	20:2Y:97:ARG:NH1	2.32	0.44
32:2a:523:A:H61	43:2l:92:0TD:CG	2.29	0.44
32:2a:1085:U:H3'	32:2a:1086:U:C6	2.51	0.44
32:2a:1134:G:N1	32:2a:1135:U:H1'	2.32	0.44
32:2a:1255:G:O3'	32:2a:1258:G:H1'	2.17	0.44
34:2c:121:ALA:HB1	34:2c:188:LEU:O	2.17	0.44
35:2d:47:ARG:NH1	35:2d:48:ALA:O	2.47	0.44
35:2d:88:VAL:O	35:2d:92:VAL:HG12	2.17	0.44
38:2g:63:LYS:HE3	38:2g:63:LYS:HB2	1.86	0.44
49:2r:53:ARG:O	49:2r:57:GLY:N	2.48	0.44
1:1A:1712:C:H2'	1:1A:1713:U:O4'	2.17	0.44
1:1A:2788:C:P	4:1E:61:ARG:HH21	2.40	0.44
32:1a:542:G:H5'	35:1d:41:GLY:HA3	1.99	0.44
33:1b:28:PHE:CD2	33:1b:190:THR:HA	2.52	0.44
35:1d:190:ASP:H	35:1d:193:ASP:HB2	1.82	0.44
50:1s:50:ALA:HA	50:1s:58:VAL:O	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2188:C:H5'	1:2A:2189:U:OP2	2.17	0.44
1:2A:2218:U:H1'	23:21:52:ARG:HH12	1.83	0.44
1:2A:2406:U:C2	11:2P:72:PRO:HG2	2.53	0.44
6:2G:7:LEU:HD22	6:2G:104:GLU:N	2.33	0.44
8:2I:5:LEU:HB3	8:2I:7:GLU:O	2.17	0.44
32:2a:1004:A:N3	32:2a:1038:C:C2	2.85	0.44
32:2a:1026:G:H5'	32:2a:1027:C:O5'	2.17	0.44
32:2a:1279:A:H3'	32:2a:1279:A:N3	2.32	0.44
32:2a:1367:C:P	40:2i:112:LYS:HZ1	2.40	0.44
32:2a:1518:MA6:H93	32:2a:1519:MA6:C9	2.47	0.44
33:2b:87:ARG:HH11	33:2b:219:VAL:HG12	1.82	0.44
33:2b:119:GLU:CD	33:2b:153:ARG:HH12	2.25	0.44
40:2i:85:LEU:HD22	40:2i:92:TYR:HE2	1.82	0.44
49:2r:32:ARG:HA	49:2r:69:THR:HG21	1.99	0.44
50:2s:30:LEU:HD11	50:2s:50:ALA:HB2	1.99	0.44
56:2y:14:A:H3'	56:2y:15:A:H5"	1.99	0.44
1:1A:284:U:H2'	1:1A:285:C:C6	2.52	0.44
1:1A:1055:G:H2'	1:1A:1056:G:O4'	2.16	0.44
1:1A:2167:U:O2	1:1A:2167:U:H2'	2.16	0.44
10:1O:48:PRO:CB	32:1a:1422:G:H5"	2.46	0.44
32:1a:664:G:P	49:1r:64:ARG:HH21	2.40	0.44
33:1b:114:ARG:NH1	33:1b:117:GLU:OE1	2.47	0.44
36:1e:31:LEU:HD23	36:1e:31:LEU:HA	1.84	0.44
37:1f:99:ALA:O	49:1r:28:GLU:HA	2.17	0.44
46:1o:63:ARG:HG2	46:1o:67:LEU:HD12	1.98	0.44
54:1w:53:G:H2'	54:1w:54:5MU:C6	2.52	0.44
56:1y:4:G:C2	56:1y:5:G:H1'	2.52	0.44
1:2A:674:G:H5"	5:2F:76:GLY:H	1.82	0.44
1:2A:764:A:H5"	3:2D:210:GLY:CA	2.47	0.44
1:2A:776:G:H4'	1:2A:777:A:O5'	2.17	0.44
1:2A:1021:A:H3'	1:2A:1021:A:H8	1.81	0.44
1:2A:2030:A:H4'	1:2A:2031:A:C8	2.53	0.44
1:2A:2782:G:OP2	61:2A:3945:HOH:O	2.21	0.44
7:2H:140:LYS:HE3	7:2H:140:LYS:HB2	1.78	0.44
8:2I:3:VAL:O	8:2I:18:VAL:HA	2.17	0.44
21:2Z:98:MET:O	21:2Z:126:VAL:N	2.43	0.44
32:2a:417:C:H2'	32:2a:418:C:C6	2.53	0.44
32:2a:429:U:O3'	35:2d:22:LYS:NZ	2.50	0.44
32:2a:431:A:OP1	61:2a:1918:HOH:O	2.21	0.44
32:2a:645:C:OP2	61:2a:1919:HOH:O	2.21	0.44
32:2a:693:G:H2'	32:2a:694:A:C8	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1314:C:H2'	32:2a:1315:U:H6	1.83	0.44
32:2a:1530:G:OP1	32:2a:1530:G:H4'	2.17	0.44
33:2b:115:LEU:HD13	33:2b:153:ARG:CZ	2.48	0.44
54:2w:5:G:H1	54:2w:68:C:H42	1.65	0.44
1:1A:271(M):G:O2'	1:1A:271(N):U:H5"	2.17	0.44
1:1A:658:C:H2'	1:1A:659:C:C6	2.52	0.44
1:1A:1047:G:H2'	1:1A:1110:G:N2	2.33	0.44
1:1A:1786:A:H1'	1:1A:1938:A:N6	2.32	0.44
1:1A:1913:A:H4'	1:1A:1914:C:H5"	2.00	0.44
1:1A:2291:U:H2'	1:1A:2292:C:C6	2.53	0.44
10:1O:76:ALA:O	15:1T:74:ARG:NH1	2.49	0.44
11:1P:38:GLN:O	11:1P:39:LYS:HB3	2.17	0.44
11:1P:50:ARG:HD3	30:18:7:HIS:CD2	2.52	0.44
23:11:23:LYS:HB3	23:11:29:GLY:HA3	2.00	0.44
32:1a:964:A:N3	32:1a:969:A:O2'	2.48	0.44
43:1l:82:VAL:O	43:1l:106:ASP:HB2	2.16	0.44
46:1o:7:GLU:O	46:1o:11:VAL:HG23	2.17	0.44
51:1t:18:GLN:O	51:1t:22:ARG:HG3	2.16	0.44
55:1x:15:G:N2	55:1x:21:A:N3	2.66	0.44
1:2A:2125:G:H1'	1:2A:2173:A:H61	1.83	0.44
1:2A:2135:A:H2'	1:2A:2136:C:C5	2.52	0.44
3:2D:70:TRP:CE2	3:2D:150:LYS:HD3	2.53	0.44
11:2P:106:LEU:HD22	11:2P:112:LEU:HB2	1.98	0.44
20:2Y:5:MET:HB2	20:2Y:5:MET:HE2	1.63	0.44
21:2Z:138:GLU:CG	21:2Z:156:LYS:HE2	2.47	0.44
23:21:35:THR:OG1	23:21:35:THR:O	2.33	0.44
24:22:8:LYS:HD2	24:22:8:LYS:HA	1.67	0.44
26:24:58:ARG:HG3	50:2s:65:ASN:O	2.17	0.44
32:2a:1010:G:H2'	32:2a:1011:G:C8	2.52	0.44
32:2a:1092:A:N3	32:2a:1183:A:N6	2.65	0.44
32:2a:1261:A:H3'	32:2a:1262:C:C6	2.52	0.44
34:2c:30:ARG:HH21	45:2n:38:GLY:CA	2.29	0.44
34:2c:131:ARG:NH2	34:2c:135:LYS:HE3	2.33	0.44
37:2f:76:ALA:O	37:2f:80:ARG:HG3	2.18	0.44
48:2q:67:LYS:O	48:2q:68:ARG:HB2	2.18	0.44
1:1A:2086:U:H2'	1:1A:2087:G:C8	2.52	0.44
1:1A:2093:G:C6	1:1A:2225:A:C8	3.06	0.44
1:1A:2771:C:H2'	1:1A:2772:C:C6	2.51	0.44
4:1E:79:ARG:HD3	4:1E:79:ARG:HA	1.81	0.44
6:1G:148:MET:HE2	6:1G:148:MET:HB2	1.81	0.44
26:14:13:ARG:HB3	26:14:30:GLU:HG2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:663:A:H2'	32:1a:664:G:O4'	2.18	0.44
36:1e:10:MET:H	36:1e:10:MET:HG2	1.58	0.44
40:1i:85:LEU:HD22	40:1i:92:TYR:HE2	1.82	0.44
1:2A:90:U:H1'	1:2A:92:A:C8	2.53	0.44
1:2A:984:A:H5"	1:2A:985:C:H5	1.82	0.44
1:2A:1037:G:H2'	1:2A:1038:C:O4'	2.18	0.44
1:2A:1357:U:H2'	1:2A:1358:G:O4'	2.18	0.44
1:2A:1448:G:H4'	1:2A:1542:A:OP1	2.18	0.44
1:2A:1486:A:H2'	1:2A:1487:G:C8	2.51	0.44
1:2A:2261:C:H1'	1:2A:2388:A:N3	2.32	0.44
1:2A:2741:A:H2'	1:2A:2742:C:O4'	2.18	0.44
6:2G:96:ARG:N	6:2G:99:MET:HE2	2.32	0.44
11:2P:87:ASP:O	11:2P:90:ARG:NH1	2.51	0.44
28:26:32:ASN:OD1	28:26:32:ASN:N	2.39	0.44
32:2a:532:A:N6	32:2a:1206:G:O2'	2.50	0.44
32:2a:1002:G:C5	32:2a:1003:G:H8	2.36	0.44
35:2d:59:ARG:NH1	35:2d:59:ARG:HA	2.32	0.44
42:2k:22:HIS:HB3	42:2k:29:ILE:HB	1.99	0.44
56:2y:10:G:H1	56:2y:25:C:H42	1.66	0.44
56:2y:69:C:H2'	56:2y:70:C:O4'	2.18	0.44
1:1A:620:G:N3	1:1A:620:G:H5'	2.32	0.44
5:1F:53:THR:HG22	5:1F:55:GLY:N	2.22	0.44
10:1O:7:TYR:HE2	10:1O:20:MET:HE3	1.81	0.44
20:1Y:5:MET:HE2	20:1Y:5:MET:HB2	1.89	0.44
32:1a:21:G:H2'	32:1a:22:G:C8	2.53	0.44
32:1a:128:G:O2'	48:1q:3:LYS:NZ	2.43	0.44
32:1a:743:U:H2'	32:1a:744:C:C6	2.52	0.44
34:1c:113:ALA:HB3	34:1c:114:PRO:HD3	1.98	0.44
1:2A:692:C:O2'	3:2D:38:LYS:NZ	2.47	0.44
1:2A:784:A:C6	3:2D:229:VAL:HG11	2.53	0.44
1:2A:1598:C:H2'	1:2A:1599:C:C6	2.53	0.44
1:2A:2802:G:C4	1:2A:2803:C:H1'	2.52	0.44
2:2B:57:A:N3	6:2G:29:TRP:HB3	2.33	0.44
2:2B:75:G:H22	21:2Z:73:GLN:HE21	1.66	0.44
21:2Z:54:HIS:CD2	21:2Z:101:PRO:HG3	2.53	0.44
24:22:7:ARG:O	24:22:11:GLU:HG3	2.17	0.44
24:22:38:GLN:HG3	24:22:43:GLN:HB2	2.00	0.44
32:2a:165:C:H2'	32:2a:166:G:C8	2.52	0.44
32:2a:921:U:O2'	36:2e:19:MET:O	2.29	0.44
32:2a:1318:A:O2'	50:2s:37:ARG:HB3	2.17	0.44
33:2b:188:ALA:HB1	33:2b:192:SER:HB2	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:2w:17:G:O2'	54:2w:18:G:OP2	2.33	0.44
1:1A:774:A:N3	1:1A:774:A:H2'	2.32	0.44
1:1A:2251:OMG:HM23	1:1A:2251:OMG:H1'	1.85	0.44
2:1B:51:G:OP2	61:1B:303:HOH:O	2.21	0.44
5:1F:34:TRP:CE2	11:1P:8:PRO:HD3	2.52	0.44
10:1O:64:ARG:HD3	10:1O:79:PHE:CD1	2.53	0.44
26:14:48:ARG:HA	26:14:48:ARG:HD3	1.88	0.44
28:16:38:LYS:HB3	28:16:38:LYS:HE3	1.81	0.44
32:1a:933:G:OP2	38:1g:3:ARG:HB2	2.18	0.44
32:1a:1260:C:O5'	32:1a:1284:C:H4'	2.18	0.44
34:1c:91:LEU:HD12	34:1c:91:LEU:HA	1.78	0.44
44:1m:108:ARG:HD3	44:1m:108:ARG:HA	1.70	0.44
56:1y:7:G:C2	56:1y:67:G:C2	3.06	0.44
1:2A:271(L):U:H5'	8:2I:50:ARG:NH1	2.32	0.44
1:2A:2626:C:H2'	1:2A:2627:G:O4'	2.17	0.44
1:2A:2759:G:OP2	61:2A:3947:HOH:O	2.21	0.44
3:2D:6:PHE:HE2	3:2D:18:VAL:HG13	1.83	0.44
7:2H:113:VAL:HG11	7:2H:151:ILE:HG21	1.99	0.44
32:2a:109:A:H2'	32:2a:326:G:N2	2.32	0.44
32:2a:114:U:O2'	32:2a:115:G:H5'	2.18	0.44
32:2a:197:A:O2'	32:2a:220:G:N2	2.51	0.44
32:2a:986:A:H1'	50:2s:54:GLY:O	2.18	0.44
32:2a:1182:G:H4'	32:2a:1183:A:H5"	2.00	0.44
32:2a:1371:G:O3'	40:2i:69:GLY:HA3	2.17	0.44
39:2h:64:LYS:HG2	39:2h:79:VAL:HG21	2.00	0.44
50:2s:20:LEU:HD23	50:2s:20:LEU:HA	1.84	0.44
1:1A:1338:G:N7	19:1X:62:LYS:NZ	2.64	0.44
1:1A:2137:C:H2'	1:1A:2138:C:H6	1.83	0.44
1:1A:2629:A:H1'	1:1A:2630:G:C5'	2.48	0.44
18:1W:17:VAL:HG13	18:1W:76:VAL:HG21	2.00	0.44
32:1a:1002:G:C5	32:1a:1003:G:H1'	2.53	0.44
32:1a:1037:C:H2'	32:1a:1038:C:H6	1.82	0.44
34:1c:121:ALA:O	34:1c:125:GLU:HG3	2.18	0.44
47:1p:55:ARG:HH21	47:1p:59:TRP:NE1	2.16	0.44
50:1s:32:LYS:HA	50:1s:50:ALA:HB3	1.99	0.44
54:1w:1:G:H2'	54:1w:2:C:C5	2.53	0.44
54:1w:39:G:H2'	54:1w:40:C:C6	2.53	0.44
1:2A:652(T):C:H2'	1:2A:652(U):G:H8	1.83	0.44
1:2A:764:A:H5"	3:2D:210:GLY:HA2	1.99	0.44
2:2B:14:U:O3'	2:2B:108:U:O2'	2.35	0.44
2:2B:31:C:H4'	6:2G:29:TRP:CZ2	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:26:38:LYS:HB3	28:26:38:LYS:HE3	1.82	0.44
32:2a:90:U:H2'	32:2a:91:C:C6	2.52	0.44
32:2a:457:C:H2'	32:2a:458:C:H6	1.83	0.44
32:2a:533:A:O2'	32:2a:535:A:OP2	2.30	0.44
32:2a:815:A:N7	32:2a:1509:C:O2'	2.44	0.44
33:2b:186:ALA:HB3	33:2b:197:VAL:HG13	2.00	0.44
34:2c:34:LEU:HD22	34:2c:38:ARG:NH2	2.32	0.44
35:2d:3:ARG:NH1	35:2d:5:ILE:HG13	2.33	0.44
36:2e:95:ALA:O	36:2e:98:THR:HG23	2.17	0.44
39:2h:17:THR:HA	39:2h:65:TYR:HE1	1.83	0.44
40:2i:18:PHE:HD2	40:2i:62:TYR:HD2	1.66	0.44
41:2j:30:SER:OG	41:2j:84:GLN:OE1	2.31	0.44
43:2l:59:ARG:HA	43:2l:65:GLU:HA	1.99	0.44
43:2l:112:ASP:N	43:2l:112:ASP:OD1	2.51	0.44
44:2m:84:ILE:HG13	44:2m:86:CYS:H	1.82	0.44
47:2p:15:PRO:O	47:2p:16:HIS:ND1	2.50	0.44
50:2s:27:GLU:CB	50:2s:28:LYS:HD3	2.48	0.44
56:2y:19:U:P	56:2y:19:U:H3'	2.58	0.44
1:1A:207:A:H2'	1:1A:208:C:O4'	2.17	0.44
1:1A:593:G:C4'	30:18:4:MET:HE2	2.48	0.44
1:1A:1173:G:N1	1:1A:1176:G:OP2	2.47	0.44
1:1A:1762:A:H2'	61:1A:5797:HOH:O	2.17	0.44
32:1a:130:A:N3	32:1a:263:A:O2'	2.47	0.44
32:1a:693:G:H2'	32:1a:694:A:C8	2.53	0.44
32:1a:1134:G:N3	32:1a:1134:G:H2'	2.33	0.44
32:1a:1302:U:H5	44:1m:17:VAL:HG21	1.82	0.44
33:1b:100:GLY:O	33:1b:104:ASN:N	2.48	0.44
34:1c:152:ILE:O	34:1c:198:VAL:HA	2.18	0.44
43:1l:7:ILE:HD13	43:1l:10:LEU:HD12	1.99	0.44
48:1q:66:SER:OG	48:1q:67:LYS:N	2.51	0.44
56:1y:9:A:H5'	56:1y:46:A:N3	2.33	0.44
1:2A:910:A:H2'	1:2A:911:A:C8	2.53	0.44
3:2D:108:PRO:HD2	3:2D:111:LEU:HD22	1.99	0.44
7:2H:80:SER:OG	7:2H:81:GLU:HG3	2.18	0.44
11:2P:114:ILE:HG13	11:2P:125:VAL:HG11	1.99	0.44
32:2a:224:C:H2'	32:2a:225:C:C6	2.53	0.44
32:2a:738:C:OP1	37:2f:2:ARG:NH1	2.51	0.44
32:2a:997:U:H3	32:2a:1044:A:H61	1.65	0.44
32:2a:1265:G:C4	32:2a:1271:G:N2	2.85	0.44
35:2d:76:ARG:O	35:2d:80:GLU:HG2	2.18	0.44
36:2e:43:LEU:H	36:2e:65:ASN:HB3	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:2m:58:GLU:C	44:2m:62:ASN:HD21	2.25	0.44
1:1A:305:U:H2'	1:1A:306:U:C6	2.53	0.43
1:1A:1064:C:N3	1:1A:1074:G:C6	2.86	0.43
1:1A:1965:C:OP1	1:1A:1966:A:O2'	2.33	0.43
1:1A:2086:U:H2'	1:1A:2087:G:H8	1.83	0.43
8:1I:95:LYS:NZ	8:1I:99:GLU:OE2	2.36	0.43
21:1Z:44:PHE:CZ	21:1Z:86:VAL:HG11	2.53	0.43
26:14:49:PHE:HB3	26:14:50:VAL:H	1.42	0.43
32:1a:256:U:H2'	32:1a:257:G:O4'	2.18	0.43
32:1a:737:A:H2'	32:1a:738:C:C6	2.53	0.43
32:1a:1149:C:H2'	32:1a:1150:U:C6	2.52	0.43
51:1t:29:LYS:O	51:1t:33:ILE:HG13	2.17	0.43
51:1t:71:THR:HG22	51:1t:72:LEU:HG	2.00	0.43
55:1x:23:C:H2'	55:1x:24:U:C6	2.53	0.43
1:2A:903:C:H2'	1:2A:904:C:C6	2.52	0.43
1:2A:910:A:C5	12:2Q:13:GLN:HG3	2.53	0.43
1:2A:1851:U:H2'	1:2A:1852:C:O4'	2.18	0.43
6:2G:107:LEU:HD13	6:2G:177:GLY:O	2.18	0.43
7:2H:13:LYS:HA	7:2H:14:GLY:HA2	1.46	0.43
15:2T:11:GLU:O	15:2T:15:VAL:HG23	2.17	0.43
30:28:32:LEU:O	30:28:36:LYS:HE3	2.17	0.43
32:2a:448:A:P	32:2a:485:G:H22	2.41	0.43
32:2a:643:C:H2'	32:2a:644:G:H8	1.83	0.43
32:2a:1490:C:H2'	32:2a:1491:G:O4'	2.18	0.43
42:2k:18:ARG:NH2	42:2k:35:PRO:O	2.51	0.43
42:2k:87:THR:HA	42:2k:91:ARG:NH1	2.33	0.43
47:2p:1:MET:HE2	47:2p:1:MET:N	2.33	0.43
1:1A:548:A:H1'	1:1A:549:G:OP1	2.18	0.43
1:1A:652(V):C:H2'	1:1A:653:A:O4'	2.18	0.43
1:1A:1173:G:OP2	1:1A:1173:G:H2'	2.18	0.43
1:1A:1639:U:O2'	1:1A:2699:C:H4'	2.18	0.43
1:1A:2685:G:H5'	10:1O:68:GLU:OE2	2.19	0.43
1:1A:2740:A:C6	1:1A:2764:A:C8	3.07	0.43
11:1P:37:GLY:C	11:1P:38:GLN:O	2.61	0.43
15:1T:15:VAL:HG13	15:1T:79:HIS:CE1	2.53	0.43
25:13:18:ASP:OD1	25:13:18:ASP:N	2.50	0.43
31:19:2:LYS:HE2	31:19:31:LYS:O	2.19	0.43
32:1a:501:C:H2'	32:1a:502:G:H8	1.82	0.43
32:1a:625:G:H2'	32:1a:626:U:H6	1.83	0.43
32:1a:1151:A:O2'	32:1a:1152:A:H8	2.00	0.43
32:1a:1286:A:C8	32:1a:1287:A:H4'	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1373:G:H5"	38:1g:36:LYS:HE2	2.00	0.43
34:1c:131:ARG:NH1	34:1c:166:GLU:HG3	2.33	0.43
36:1e:57:LYS:HG2	36:1e:61:TYR:CE2	2.53	0.43
46:1o:39:LEU:HB3	46:1o:56:LEU:HD12	2.00	0.43
51:1t:10:LEU:HD22	51:1t:10:LEU:HA	1.86	0.43
1:2A:141:A:H8	1:2A:1408:C:HO2'	1.58	0.43
1:2A:1131:G:O6	1:2A:2040:C:H1'	2.18	0.43
1:2A:2540:C:H2'	1:2A:2541:A:O4'	2.18	0.43
1:2A:2695:C:H2'	1:2A:2696:U:C6	2.53	0.43
3:2D:125:ILE:HB	37:2f:81:ILE:HD11	2.00	0.43
5:2F:33:LEU:HD22	5:2F:112:MET:HE3	2.00	0.43
6:2G:125:PHE:HB3	6:2G:166:ASP:CG	2.43	0.43
15:2T:74:ARG:HG2	15:2T:76:PHE:CZ	2.53	0.43
25:23:11:SER:HA	25:23:31:LEU:HD11	1.99	0.43
26:24:41:PRO:HG3	26:24:49:PHE:CZ	2.52	0.43
26:24:50:VAL:HG21	44:2m:65:LYS:N	2.34	0.43
32:2a:554:C:H2'	32:2a:555:C:C6	2.53	0.43
32:2a:755:G:OP2	46:2o:65:ARG:HD2	2.18	0.43
32:2a:1094:G:O2'	32:2a:1108:G:N1	2.50	0.43
32:2a:1216:G:OP1	45:2n:2:ALA:HA	2.19	0.43
32:2a:1241:G:H2'	32:2a:1242:C:C6	2.53	0.43
32:2a:1273:G:N7	32:2a:1274:G:C5	2.86	0.43
32:2a:1276:G:C2'	32:2a:1277:C:H5'	2.49	0.43
34:2c:69:HIS:CD2	34:2c:104:GLN:HG2	2.54	0.43
35:2d:158:ILE:H	35:2d:158:ILE:HG12	1.32	0.43
40:2i:114:TYR:CD2	41:2j:60:ARG:HB2	2.53	0.43
1:1A:515:A:H2	1:1A:1260:G:N3	2.16	0.43
1:1A:1489:U:HO2'	1:1A:1490:A:H8	1.65	0.43
1:1A:1665:A:H4'	10:1O:67:LYS:HB2	2.00	0.43
8:1I:109:ILE:HD12	8:1I:130:TYR:OH	2.18	0.43
9:1N:96:GLU:H	9:1N:96:GLU:CD	2.26	0.43
19:1X:60:ARG:HH22	29:17:47:ARG:HH22	1.66	0.43
32:1a:96:U:H2'	32:1a:97:G:C8	2.53	0.43
32:1a:1003:G:H2'	32:1a:1004:A:N3	2.34	0.43
1:2A:1031:G:N3	31:29:36:GLN:NE2	2.63	0.43
1:2A:1140:C:H5'	9:2N:24:GLY:HA3	2.00	0.43
1:2A:1300:U:H4'	1:2A:1301:A:H5'	2.00	0.43
1:2A:1423:G:OP1	1:2A:1492:G:O2'	2.36	0.43
1:2A:1837:C:OP1	32:2a:784:C:H4'	2.18	0.43
1:2A:1939:5MU:OP1	1:2A:2604:U:O2'	2.33	0.43
1:2A:2129:C:N4	1:2A:2159:G:H1	2.15	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2D:72:LYS:NZ	3:2D:99:ASP:OD2	2.41	0.43
3:2D:232:PRO:O	61:2D:401:HOH:O	2.21	0.43
7:2H:154:PRO:HB3	7:2H:163:TYR:CE1	2.54	0.43
26:24:15:ILE:O	26:24:33:VAL:N	2.52	0.43
32:2a:524:G:H2'	32:2a:525:C:C6	2.52	0.43
32:2a:528:C:H5'	32:2a:529:G:OP2	2.18	0.43
32:2a:585:G:O2'	32:2a:879:C:OP1	2.25	0.43
32:2a:1314:C:H2'	32:2a:1315:U:C6	2.53	0.43
33:2b:92:TYR:CE1	33:2b:94:ASN:HB2	2.53	0.43
33:2b:104:ASN:CG	33:2b:107:THR:HG1	2.22	0.43
36:2e:40:ARG:HD3	36:2e:67:VAL:O	2.18	0.43
37:2f:4:TYR:CE1	37:2f:92:LYS:HG3	2.53	0.43
39:2h:112:LEU:HD11	39:2h:124:ALA:HB2	2.00	0.43
42:2k:45:GLY:O	42:2k:50:TYR:HB2	2.19	0.43
1:1A:747:U:O2	1:1A:2014:A:H1'	2.18	0.43
1:1A:1165:U:H2'	1:1A:1166:C:C6	2.53	0.43
1:1A:1371:G:H2'	1:1A:1372:U:H5	1.82	0.43
1:1A:2105:C:H2'	1:1A:2106:G:H8	1.83	0.43
1:1A:2206:G:OP2	1:1A:2206:G:H4'	2.17	0.43
1:1A:2811:G:N2	1:1A:2891:G:H1'	2.33	0.43
6:1G:179:PRO:HG3	26:14:43:TYR:OH	2.18	0.43
10:1O:4:PRO:O	10:1O:5:GLN:HB2	2.18	0.43
11:1P:116:GLY:O	11:1P:137:LYS:NZ	2.33	0.43
32:1a:160:A:H1'	32:1a:344:A:C5	2.54	0.43
32:1a:452:A:H4'	47:1p:72:ARG:NH1	2.33	0.43
32:1a:1168:A:H2'	32:1a:1169:A:C8	2.54	0.43
40:1i:34:ASN:HD22	40:1i:34:ASN:N	2.16	0.43
44:1m:4:ILE:HA	44:1m:5:ALA:HA	1.75	0.43
54:1w:13:C:H2'	54:1w:14:A:H5"	1.99	0.43
1:2A:116:C:H2'	1:2A:117:G:O4'	2.19	0.43
1:2A:557:U:H2'	1:2A:558:G:C8	2.54	0.43
1:2A:602:G:O2'	1:2A:655:A:N6	2.51	0.43
1:2A:2107:C:N3	1:2A:2182:G:O6	2.51	0.43
5:2F:150:GLY:HA2	5:2F:172:TRP:CE3	2.52	0.43
9:2N:42:TRP:HA	9:2N:48:MET:SD	2.59	0.43
32:2a:452:A:O2'	32:2a:453:A:OP2	2.29	0.43
32:2a:565:U:OP2	32:2a:566:G:O2'	2.21	0.43
32:2a:1179:A:H2'	32:2a:1180:A:O4'	2.18	0.43
43:2l:8:ASN:O	43:2l:12:ARG:HG3	2.18	0.43
50:2s:61:TYR:CE2	50:2s:63:THR:HG22	2.53	0.43
50:2s:64:GLU:OE2	50:2s:65:ASN:ND2	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:272(A):U:O2'	1:1A:272(B):G:O5'	2.23	0.43
1:1A:884:C:C4	1:1A:885:C:H1'	2.53	0.43
1:1A:1047:G:H2'	1:1A:1110:G:N1	2.33	0.43
11:1P:38:GLN:O	11:1P:40:SER:N	2.45	0.43
18:1W:62:HIS:O	18:1W:64:MET:HG3	2.19	0.43
21:1Z:8:TYR:HB2	21:1Z:38:TYR:CE2	2.54	0.43
26:14:16:CYS:HB2	26:14:36:CYS:HB3	2.01	0.43
32:1a:1002:G:H3'	32:1a:1003:G:C4'	2.48	0.43
32:1a:1002:G:H3'	32:1a:1003:G:H4'	1.99	0.43
32:1a:1140:C:H2'	32:1a:1141:C:C6	2.52	0.43
33:1b:183:PRO:HA	33:1b:198:ASP:OD2	2.18	0.43
44:1m:3:ARG:HG3	44:1m:4:ILE:H	1.83	0.43
44:1m:45:VAL:C	44:1m:47:ASP:H	2.25	0.43
49:1r:40:LEU:HD22	49:1r:70:ILE:HG12	2.00	0.43
1:2A:557:U:H2'	1:2A:558:G:H8	1.82	0.43
1:2A:868:U:C4	1:2A:869:G:N7	2.87	0.43
1:2A:894:C:O2'	1:2A:895:U:H5"	2.19	0.43
1:2A:1359:A:C2	1:2A:1372:U:O4	2.71	0.43
1:2A:2142:C:H2'	1:2A:2143:C:C6	2.53	0.43
1:2A:2319:G:N2	14:2S:3:ARG:HD2	2.34	0.43
1:2A:2439:A:N6	55:2x:76:31H:OP1	2.51	0.43
1:2A:2889:C:H2'	1:2A:2891:G:O4'	2.18	0.43
12:2Q:78:PRO:HD3	55:2x:1:C:N3	2.34	0.43
21:2Z:77:ASP:CG	21:2Z:80:ARG:HH11	2.26	0.43
28:26:6:ARG:NH1	28:26:26:ASN:HB2	2.33	0.43
31:29:17:ILE:HG13	31:29:24:TYR:HB2	2.00	0.43
32:2a:532:A:N1	34:2c:156:ARG:NH1	2.55	0.43
32:2a:1103:C:C2	32:2a:1104:G:C8	3.06	0.43
33:2b:235:SER:O	33:2b:235:SER:OG	2.30	0.43
34:2c:18:TRP:CD1	45:2n:55:GLY:H	2.37	0.43
40:2i:88:TYR:CD2	40:2i:89:ASN:HB2	2.50	0.43
50:2s:27:GLU:HB3	50:2s:28:LYS:HA	2.01	0.43
1:1A:271(G):C:H2'	1:1A:271(H):G:C8	2.53	0.43
1:1A:2155:G:H3'	1:1A:2156:G:H5'	1.99	0.43
1:1A:2165:G:H2'	1:1A:2166:G:C5	2.54	0.43
1:1A:2331:G:O2'	22:10:43:THR:HG22	2.18	0.43
1:1A:2375:G:O2'	1:1A:2377:A:N7	2.44	0.43
5:1F:89:VAL:HG12	5:1F:90:PHE:CD2	2.53	0.43
26:14:12:ALA:CB	26:14:26:SER:HB3	2.49	0.43
32:1a:7:G:H21	36:1e:121:LYS:HG2	1.83	0.43
32:1a:148:G:H2'	32:1a:149:A:H8	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:601:C:H2'	32:1a:602:A:C8	2.54	0.43
32:1a:659:U:H2'	32:1a:660:G:H8	1.84	0.43
32:1a:690:G:C6	32:1a:691:G:C6	3.06	0.43
37:1f:100:ASN:HB2	49:1r:28:GLU:HA	2.00	0.43
41:1j:47:PHE:N	41:1j:63:PHE:O	2.44	0.43
55:1x:4:G:H2'	55:1x:5:G:C8	2.54	0.43
1:2A:8:A:H2'	1:2A:9:U:C6	2.54	0.43
1:2A:1514:U:H2'	1:2A:1515:G:C8	2.54	0.43
1:2A:1589:C:H2'	1:2A:1590:U:C6	2.54	0.43
1:2A:1913:A:H4'	1:2A:1914:C:O5'	2.19	0.43
1:2A:2127:G:C2	1:2A:2161:C:N3	2.86	0.43
3:2D:5:LYS:HE3	3:2D:5:LYS:HB3	1.87	0.43
6:2G:135:LEU:HD11	6:2G:157:ILE:HD11	1.99	0.43
9:2N:2:LYS:HA	9:2N:2:LYS:HD2	1.90	0.43
25:23:4:LEU:N	25:23:37:LEU:O	2.52	0.43
32:2a:8:A:N6	35:2d:205:GLU:O	2.49	0.43
32:2a:983:A:O2'	32:2a:1050:G:OP2	2.36	0.43
32:2a:1027:C:C2'	32:2a:1034:G:H22	2.32	0.43
32:2a:1152:A:H5'	41:2j:13:HIS:CD2	2.54	0.43
49:2r:63:GLN:HE21	49:2r:63:GLN:HB2	1.70	0.43
1:1A:709:U:H2'	1:1A:710:G:C8	2.54	0.43
1:1A:919:G:N2	1:1A:2269:A:OP2	2.49	0.43
1:1A:2869:G:H2'	1:1A:2870:C:O4'	2.18	0.43
5:1F:155:LEU:HD11	5:1F:176:LEU:HD12	2.00	0.43
12:1Q:71:ASP:OD1	12:1Q:71:ASP:N	2.50	0.43
32:1a:652:U:O4	32:1a:752:G:O2'	2.28	0.43
32:1a:833:U:H2'	32:1a:834:C:H6	1.84	0.43
32:1a:1028:C:H2'	32:1a:1029:C:O4'	2.19	0.43
37:1f:35:ALA:HA	37:1f:67:MET:HB3	2.01	0.43
47:1p:38:TYR:O	47:1p:49:LEU:HD22	2.19	0.43
48:1q:5:VAL:O	48:1q:6:LEU:HD23	2.19	0.43
50:1s:52:TYR:HB2	50:1s:57:HIS:CE1	2.54	0.43
51:1t:77:ALA:O	51:1t:81:LYS:HG3	2.19	0.43
1:2A:171:G:H2'	1:2A:172:C:C6	2.53	0.43
1:2A:212:G:H2'	1:2A:213:A:O4'	2.18	0.43
1:2A:878:A:H61	1:2A:899:A:H1'	1.83	0.43
1:2A:2183:C:H2'	1:2A:2184:G:C8	2.45	0.43
1:2A:2334:G:H5'	14:2S:9:ARG:HG2	2.00	0.43
1:2A:2543:G:H21	1:2A:2646:C:H5"	1.84	0.43
4:2E:101:ARG:CZ	4:2E:171:GLU:HB2	2.49	0.43
7:2H:20:ALA:HB3	7:2H:23:ARG:HG3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:2I:53:ALA:O	8:2I:57:ARG:HG2	2.19	0.43
24:22:41:ILE:HG13	24:22:43:GLN:HG2	2.01	0.43
32:2a:745:C:H2'	32:2a:746:A:C8	2.54	0.43
32:2a:1280:A:H5'	41:2j:40:LEU:HD22	2.00	0.43
37:2f:33:TYR:HA	37:2f:71:ARG:HH21	1.84	0.43
38:2g:78:ARG:HD3	38:2g:79:ARG:H	1.84	0.43
38:2g:125:MET:O	38:2g:129:GLU:HG3	2.19	0.43
40:2i:3:GLN:NE2	40:2i:20:ARG:HH21	2.15	0.43
43:2l:70:ILE:HG12	43:2l:100:ILE:HD12	2.00	0.43
44:2m:89:GLY:O	44:2m:93:ARG:HG2	2.19	0.43
1:1A:278:A:H2'	1:1A:279:C:C6	2.53	0.43
1:1A:382:G:O6	61:1A:4142:HOH:O	2.21	0.43
1:1A:1057:A:C8	1:1A:1086:A:C8	3.07	0.43
1:1A:2001:A:H2'	1:1A:2002:G:C8	2.53	0.43
1:1A:2178:C:H2'	1:1A:2179:C:H6	1.84	0.43
1:1A:2185:C:H2'	1:1A:2186:G:C8	2.53	0.43
6:1G:83:ARG:O	6:1G:86:MET:HG3	2.19	0.43
8:1I:79:ILE:HB	8:1I:144:VAL:HG12	2.00	0.43
29:17:29:LYS:O	29:17:33:ARG:HB2	2.19	0.43
32:1a:1273:G:H3'	32:1a:1274:G:H8	1.84	0.43
32:1a:1518:MA6:H93	32:1a:1519:MA6:C9	2.46	0.43
54:1w:18:G:H4'	54:1w:19:U:OP2	2.11	0.43
1:2A:250:G:H2'	1:2A:251:A:C8	2.54	0.43
1:2A:1839:G:C8	1:2A:1927:A:H1'	2.53	0.43
2:2B:88:C:H2'	2:2B:89:G:O4'	2.19	0.43
12:2Q:36:ALA:HB1	12:2Q:127:ILE:HD12	2.00	0.43
15:2T:65:LYS:HE3	15:2T:67:SER:HB2	2.00	0.43
21:2Z:23:LYS:HB3	21:2Z:38:TYR:CD1	2.54	0.43
32:2a:10:A:OP2	36:2e:126:ARG:HD2	2.19	0.43
32:2a:416:G:C5	32:2a:417:C:C4	3.07	0.43
32:2a:974:A:P	45:2n:41:ARG:HH21	2.41	0.43
32:2a:1120:G:C6	32:2a:1121:U:C4	3.07	0.43
32:2a:1191:A:H8	32:2a:1191:A:O5'	2.02	0.43
32:2a:1291:G:C6	32:2a:1292:U:C4	3.07	0.43
32:2a:1360:A:OP2	45:2n:35:ARG:NH2	2.51	0.43
36:2e:102:ALA:HB1	36:2e:106:PRO:HB2	1.99	0.43
1:1A:247:G:H4'	1:1A:386:G:C5	2.53	0.43
1:1A:1827:C:C2'	1:1A:1828:G:H5'	2.49	0.43
1:1A:1913:A:H4'	1:1A:1914:C:C5'	2.49	0.43
1:1A:2102:U:O2	1:1A:2187:G:N2	2.48	0.43
1:1A:2165:G:H2'	1:1A:2166:G:C4	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2377:A:H2'	1:1A:2378:A:C8	2.54	0.43
1:1A:2591:C:H2'	1:1A:2592:G:H8	1.82	0.43
3:1D:71:ASP:HB2	3:1D:103:ARG:HH12	1.84	0.43
5:1F:144:LYS:NZ	5:1F:144:LYS:HB3	2.34	0.43
11:1P:8:PRO:HB2	11:1P:12:ALA:HB3	2.00	0.43
32:1a:195:A:OP1	51:1t:68:LYS:NZ	2.49	0.43
32:1a:1343:G:H2'	32:1a:1344:C:C6	2.54	0.43
33:1b:155:LEU:HD12	33:1b:155:LEU:HA	1.88	0.43
1:2A:38:A:H2'	1:2A:39:C:C6	2.54	0.43
1:2A:121:G:H4'	1:2A:149:A:H5'	2.01	0.43
1:2A:302:C:OP2	20:2Y:73:ARG:NH1	2.48	0.43
1:2A:676:A:H2	1:2A:2069:G:N3	2.16	0.43
1:2A:2065:C:H2'	1:2A:2066:C:C6	2.53	0.43
1:2A:2115:G:H4'	1:2A:2167:U:C4	2.54	0.43
1:2A:2238:G:H2'	1:2A:2238:G:N3	2.33	0.43
17:2V:24:LYS:HB3	17:2V:24:LYS:HE2	1.67	0.43
18:2W:71:VAL:HA	18:2W:107:LEU:HD23	2.01	0.43
21:2Z:95:PRO:HA	21:2Z:129:SER:HA	2.01	0.43
21:2Z:151:HIS:HB3	21:2Z:152:ALA:H	1.62	0.43
32:2a:320:C:H2'	32:2a:321:A:O4'	2.17	0.43
32:2a:1323:G:H2'	32:2a:1324:A:C8	2.54	0.43
33:2b:165:VAL:HG23	33:2b:187:LEU:HD22	2.01	0.43
34:2c:101:LEU:HD23	34:2c:102:ASN:N	2.34	0.43
38:2g:66:VAL:O	38:2g:70:LYS:HG3	2.18	0.43
39:2h:51:VAL:HG21	39:2h:60:ARG:HH11	1.84	0.43
51:2t:47:GLY:HA2	51:2t:48:LYS:C	2.44	0.43
56:2y:34:C:H2'	56:2y:35:C:O4'	2.19	0.43
1:1A:271(B):C:H42	1:1A:271(V):G:H1	1.67	0.43
1:1A:601:C:O2'	1:1A:605:C:H5"	2.18	0.43
1:1A:1359:A:H2	1:1A:1372:U:O4	2.01	0.43
1:1A:1851:U:H2'	1:1A:1852:C:O4'	2.18	0.43
1:1A:2130:U:H1'	1:1A:2159:G:N2	2.34	0.43
1:1A:2469:A:O3'	12:1Q:56:ARG:NH1	2.51	0.43
1:1A:2817:G:OP1	13:1R:99:LYS:HE2	2.19	0.43
2:1B:88:C:H2'	2:1B:89:G:O4'	2.19	0.43
18:1W:58:ALA:HB1	18:1W:64:MET:HB2	2.01	0.43
19:1X:57:LEU:HA	61:1X:203:HOH:O	2.18	0.43
20:1Y:9:LYS:HA	20:1Y:10:GLY:HA2	1.63	0.43
30:18:42:ARG:HD2	61:18:201:HOH:O	2.18	0.43
32:1a:143:A:O2'	32:1a:144:G:OP2	2.32	0.43
32:1a:1292:U:OP2	38:1g:41:ARG:NH2	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:1h:127:LEU:HA	39:1h:127:LEU:HD23	1.81	0.43
43:1l:7:ILE:HD13	43:1l:7:ILE:HA	1.88	0.43
44:1m:106:ASN:HB2	44:1m:107:ALA:H	1.47	0.43
51:1t:49:ALA:O	51:1t:53:LEU:HD12	2.19	0.43
51:1t:100:ILE:H	51:1t:100:ILE:HG12	1.55	0.43
1:2A:699:A:H4'	1:2A:1554:A:N6	2.34	0.43
1:2A:1005:C:H2'	1:2A:1006:C:H6	1.84	0.43
1:2A:1116:C:H2'	1:2A:1117:G:C8	2.54	0.43
1:2A:2162:G:H2'	1:2A:2163:C:C6	2.54	0.43
14:2S:28:VAL:HG11	14:2S:98:VAL:HG13	2.01	0.43
21:2Z:24:LEU:HD12	21:2Z:25:PRO:HD2	2.00	0.43
32:2a:15:G:H2'	32:2a:16:A:H8	1.84	0.43
32:2a:292:G:N7	32:2a:293:G:H1'	2.33	0.43
32:2a:435:C:H2'	32:2a:436:C:H6	1.84	0.43
32:2a:1055:A:C6	32:2a:1206:G:C5	3.07	0.43
33:2b:98:LEU:HB2	33:2b:101:MET:SD	2.59	0.43
33:2b:188:ALA:HB1	33:2b:192:SER:CB	2.49	0.43
38:2g:51:GLN:O	38:2g:55:GLY:HA2	2.19	0.43
46:2o:3:ILE:HD13	46:2o:34:LEU:HD23	2.01	0.43
54:2w:17:G:N2	54:2w:57:G:H2'	2.34	0.43
54:2w:34:C:H2'	54:2w:35:C:C6	2.54	0.43
1:1A:191:A:H2'	1:1A:192:C:C6	2.54	0.42
1:1A:863:A:H2'	1:1A:864:G:H8	1.82	0.42
1:1A:1095:A:N6	1:1A:1097:U:O2	2.52	0.42
1:1A:1188:U:H5'	17:1V:79:VAL:HG13	2.01	0.42
1:1A:2100:G:H2'	1:1A:2101:G:C8	2.54	0.42
6:1G:47:LYS:O	6:1G:86:MET:HE2	2.19	0.42
7:1H:25:LYS:HE3	7:1H:27:LYS:HZ2	1.83	0.42
7:1H:154:PRO:HB3	7:1H:163:TYR:CE1	2.54	0.42
21:1Z:150:LEU:HG	21:1Z:151:HIS:N	2.34	0.42
22:10:46:LYS:HD2	22:10:78:TYR:CZ	2.54	0.42
32:1a:1326:C:H2'	32:1a:1327:C:C6	2.54	0.42
32:1a:1333:A:H2'	32:1a:1334:G:O4'	2.19	0.42
32:1a:1428:A:H2'	32:1a:1429:C:C6	2.54	0.42
34:1c:6:HIS:CD2	34:1c:8:ILE:HB	2.54	0.42
44:1m:20:THR:C	44:1m:22:ILE:H	2.27	0.42
51:1t:90:GLN:HA	51:1t:93:GLU:HG2	2.01	0.42
1:2A:35:G:H1'	1:2A:454:A:C4	2.54	0.42
1:2A:1336:A:H2'	1:2A:1337:G:C8	2.53	0.42
1:2A:2000:G:OP1	13:2R:5:LYS:NZ	2.45	0.42
1:2A:2345:G:N3	1:2A:2381:C:H2'	2.33	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2370:G:C6	1:2A:2371:G:C6	3.07	0.42
1:2A:2805:G:H2'	1:2A:2807:G:H8	1.78	0.42
5:2F:192:LEU:HD22	5:2F:194:MET:HG3	2.00	0.42
8:2I:50:ARG:HA	8:2I:53:ALA:HB3	2.00	0.42
19:2X:28:PHE:CZ	19:2X:92:LEU:HD11	2.54	0.42
31:29:27:CYS:SG	31:29:28:GLU:N	2.91	0.42
32:2a:563:A:N7	32:2a:567:G:H1'	2.34	0.42
32:2a:1187:G:OP1	40:2i:113:LYS:HE2	2.19	0.42
32:2a:1333:A:H2'	32:2a:1334:G:O4'	2.19	0.42
41:2j:51:ARG:H	41:2j:60:ARG:HA	1.83	0.42
44:2m:33:ALA:HB1	44:2m:59:TYR:HE2	1.84	0.42
1:1A:818:G:H5'	1:1A:839:U:OP1	2.19	0.42
1:1A:1042:G:H2'	1:1A:1043:C:O4'	2.20	0.42
1:1A:1059:G:H2'	1:1A:1060:U:C5	2.54	0.42
1:1A:1113:U:H2'	1:1A:1114:G:H8	1.84	0.42
1:1A:1508:A:O2'	1:1A:1509:C:H5"	2.18	0.42
3:1D:232:PRO:HB3	3:1D:244:ARG:CZ	2.49	0.42
6:1G:115:ARG:HG2	6:1G:136:ARG:HH22	1.85	0.42
6:1G:126:ASP:CG	6:1G:130:ASN:HB2	2.44	0.42
32:1a:399:G:H2'	32:1a:400:C:C6	2.54	0.42
32:1a:520:A:N1	32:1a:536:C:H1'	2.35	0.42
32:1a:999:C:H2'	32:1a:1000:U:O4'	2.18	0.42
33:1b:16:HIS:HB2	33:1b:204:ASN:CB	2.49	0.42
50:1s:61:TYR:CE2	50:1s:63:THR:HG22	2.54	0.42
1:2A:635:C:H2'	1:2A:636:G:O4'	2.19	0.42
1:2A:784:A:C8	1:2A:792:G:C5	3.07	0.42
1:2A:1782:C:O2	1:2A:2608:G:O2'	2.31	0.42
1:2A:2100:G:C6	1:2A:2190:G:C6	3.08	0.42
1:2A:2218:U:N3	23:21:55:GLY:O	2.52	0.42
26:24:13:ARG:HG3	26:24:23:GLU:HA	2.01	0.42
32:2a:66:G:H8	32:2a:66:G:OP1	2.02	0.42
32:2a:79:G:H1	32:2a:90:U:H3	1.67	0.42
32:2a:607:A:H2'	32:2a:608:A:O4'	2.19	0.42
32:2a:673:G:O3'	37:2f:87:ARG:NH2	2.52	0.42
32:2a:748:C:H4'	32:2a:749:C:O5'	2.19	0.42
48:2q:81:ARG:NH2	48:2q:84:LEU:HD21	2.34	0.42
54:2w:18:G:N2	54:2w:57:G:H1'	2.34	0.42
56:2y:60:U:P	56:2y:61:C:H41	2.41	0.42
1:1A:897:C:H1'	54:1w:56:C:H5	1.84	0.42
1:1A:2801(A):A:H1'	1:1A:2895:U:H1'	2.00	0.42
6:1G:132:ASN:HA	6:1G:157:ILE:O	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1Q:6:ARG:C	12:1Q:7:MET:HG2	2.44	0.42
32:1a:433:C:H2'	32:1a:434:U:C6	2.55	0.42
32:1a:601:C:H2'	32:1a:602:A:H8	1.82	0.42
32:1a:1030(C):G:H8	32:1a:1030(D):A:C8	2.38	0.42
32:1a:1302:U:OP1	44:1m:13:LYS:HE3	2.19	0.42
32:1a:1349:A:C2	32:1a:1374:A:C4	3.07	0.42
33:1b:19:HIS:HA	33:1b:39:ILE:CG2	2.49	0.42
33:1b:124:SER:HA	33:1b:125:PRO:HA	1.64	0.42
38:1g:26:PHE:O	38:1g:30:ILE:HG13	2.19	0.42
50:1s:52:TYR:HA	50:1s:56:GLN:O	2.20	0.42
54:1w:70:C:H2'	54:1w:71:G:O4'	2.19	0.42
1:2A:1171:G:H8	1:2A:1171:G:O5'	2.02	0.42
30:28:28:GLY:HA3	30:28:44:LYS:HE2	2.01	0.42
32:2a:410:G:H5"	35:2d:30:LYS:NZ	2.34	0.42
34:2c:83:ARG:O	34:2c:87:LEU:HB2	2.19	0.42
40:2i:79:LEU:HG	40:2i:83:ARG:HD2	2.01	0.42
40:2i:112:LYS:NZ	40:2i:113:LYS:O	2.51	0.42
54:2w:11:U:O2'	54:2w:12:U:H5'	2.19	0.42
1:1A:1268:A:C2	1:1A:2013:A:C4	3.08	0.42
1:1A:2417:C:OP1	11:1P:65:ARG:NH2	2.52	0.42
1:1A:2849:U:H4'	1:1A:2868:A:C2	2.54	0.42
1:1A:2876:G:H4'	15:1T:2:ASN:ND2	2.35	0.42
6:1G:27:ASN:HB3	6:1G:30:GLU:HG3	2.01	0.42
19:1X:26:TYR:CD1	19:1X:92:LEU:HD13	2.55	0.42
32:1a:1030(B):C:O2	32:1a:1030(B):C:H2'	2.18	0.42
33:1b:16:HIS:ND1	33:1b:210:SER:OG	2.53	0.42
33:1b:74:LYS:O	33:1b:78:GLN:HG3	2.20	0.42
47:1p:15:PRO:O	47:1p:16:HIS:ND1	2.52	0.42
48:1q:58:GLU:O	48:1q:74:LEU:N	2.37	0.42
51:1t:58:LYS:HA	51:1t:58:LYS:HD2	1.71	0.42
54:1w:15:A:C2	54:1w:21:A:H1'	2.46	0.42
1:2A:328:U:H4'	20:2Y:68:HIS:CD2	2.54	0.42
1:2A:730:C:H3'	61:2A:4019:HOH:O	2.18	0.42
1:2A:1420:U:HO2'	1:2A:1421:G:P	2.39	0.42
2:2B:94:C:H2'	2:2B:95:C:H6	1.84	0.42
16:2U:16:LYS:HB3	16:2U:16:LYS:HE2	1.78	0.42
32:2a:109:A:C6	32:2a:326:G:C6	3.08	0.42
32:2a:762:C:H2'	32:2a:763:G:H8	1.84	0.42
32:2a:1239:A:H4'	32:2a:1240:U:H5'	2.00	0.42
34:2c:159:GLY:HA2	34:2c:193:TYR:CE1	2.54	0.42
37:2f:89:MET:HG2	37:2f:91:VAL:HG23	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:2x:7:G:H5”	55:2x:8:4SU:H5	2.00	0.42
1:1A:185:U:H2’	1:1A:186:G:C8	2.55	0.42
1:1A:2615:U:H2’	1:1A:2616:C:H6	1.84	0.42
1:1A:2683:C:O2	10:1O:70:LYS:NZ	2.43	0.42
32:1a:434:U:H2’	32:1a:435:C:C6	2.55	0.42
32:1a:487:A:H2’	32:1a:488:C:O4’	2.18	0.42
32:1a:1037:C:H2’	32:1a:1038:C:C6	2.53	0.42
32:1a:1129:C:O2’	32:1a:1139:G:N7	2.43	0.42
34:1c:18:TRP:H	34:1c:18:TRP:HE3	1.67	0.42
35:1d:108:LEU:HD21	35:1d:174:LEU:HD22	2.02	0.42
36:1e:18:ARG:HH11	36:1e:27:ARG:HH12	1.66	0.42
40:1i:33:PHE:HD2	40:1i:34:ASN:HD22	1.67	0.42
41:1j:47:PHE:HB2	41:1j:63:PHE:HB2	2.02	0.42
42:1k:99:GLN:HG3	42:1k:105:VAL:HG21	2.00	0.42
51:1t:86:ARG:O	51:1t:90:GLN:NE2	2.52	0.42
54:1w:43:U:H2’	54:1w:44:A:O4’	2.20	0.42
1:2A:500:G:N2	1:2A:502:A:H3’	2.35	0.42
1:2A:631:A:H2’	1:2A:632:A:O4’	2.19	0.42
1:2A:911:A:H2’	12:2Q:9:TYR:OH	2.18	0.42
1:2A:993:G:OP1	16:2U:50:ARG:HD2	2.19	0.42
1:2A:1913:A:H4’	1:2A:1914:C:C5’	2.48	0.42
1:2A:2846:G:H2’	1:2A:2847:U:O4’	2.20	0.42
2:2B:24:G:H4’	2:2B:25:A:C8	2.54	0.42
8:2I:90:GLY:O	8:2I:121:LYS:HE3	2.18	0.42
12:2Q:18:LYS:O	12:2Q:98:LYS:NZ	2.34	0.42
15:2T:92:GLY:O	15:2T:120:ARG:NH2	2.52	0.42
32:2a:1254:C:O4’	32:2a:1356:G:H5”	2.19	0.42
32:2a:1515:C:H2’	32:2a:1516:G:H8	1.85	0.42
36:2e:92:LYS:HB3	36:2e:119:LEU:HB2	2.01	0.42
44:2m:60:VAL:HG13	44:2m:64:TRP:CE3	2.54	0.42
46:2o:39:LEU:HD23	46:2o:39:LEU:HA	1.83	0.42
51:2t:86:ARG:O	51:2t:90:GLN:HG3	2.20	0.42
56:2y:17:G:O6	56:2y:55:PSU:H1’	2.19	0.42
1:1A:1139:G:OP1	9:1N:101:HIS:ND1	2.44	0.42
1:1A:1342:A:OP1	19:1X:36:LYS:NZ	2.39	0.42
1:1A:2105:C:H2’	1:1A:2106:G:C8	2.55	0.42
8:1I:72:LEU:HA	8:1I:75:LEU:HD11	2.01	0.42
32:1a:1277:C:O2’	32:1a:1279:A:H8	2.03	0.42
40:1i:49:PRO:HD3	40:1i:78:LYS:HG3	2.02	0.42
51:1t:92:LEU:O	51:1t:96:GLY:HA2	2.19	0.42
1:2A:1902:C:H5’	3:2D:246:PRO:HD3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1932:A:H2'	1:2A:1933:G:O4'	2.20	0.42
1:2A:2184:G:H2'	1:2A:2185:C:C6	2.54	0.42
4:2E:33:VAL:HG13	4:2E:47:VAL:HG23	2.01	0.42
10:2O:26:LYS:O	10:2O:30:ALA:HB2	2.20	0.42
18:2W:1:MET:HE2	18:2W:62:HIS:HB3	2.00	0.42
28:26:40:CYS:SG	28:26:42:TRP:HB2	2.60	0.42
32:2a:406:G:H21	35:2d:119:GLN:NE2	2.12	0.42
32:2a:1327:C:H2'	32:2a:1328:C:C6	2.55	0.42
32:2a:1359:C:H1'	32:2a:1362:C:H41	1.83	0.42
32:2a:1427:U:H2'	32:2a:1428:A:H8	1.84	0.42
33:2b:36:ARG:C	33:2b:38:GLY:H	2.27	0.42
39:2h:3:THR:O	39:2h:5:PRO:HD3	2.19	0.42
39:2h:13:ILE:O	39:2h:17:THR:HG23	2.19	0.42
39:2h:82:HIS:CD2	39:2h:82:HIS:C	2.97	0.42
41:2j:32:ALA:HA	41:2j:33:GLN:HA	1.66	0.42
1:1A:55:G:O2'	1:1A:127:A:N1	2.45	0.42
1:1A:784:A:C5	3:1D:229:VAL:HG21	2.54	0.42
1:1A:1142(A):A:C4	1:1A:1144:G:N7	2.88	0.42
1:1A:2334:G:H5'	14:1S:9:ARG:HG2	2.02	0.42
1:1A:2506:U:C2	1:1A:2585:U:O4	2.73	0.42
3:1D:37:LEU:HD12	3:1D:62:TYR:HB2	2.01	0.42
21:1Z:158:PRO:HD2	21:1Z:161:VAL:HG21	2.01	0.42
22:10:23:VAL:HG22	22:10:38:VAL:HG22	2.01	0.42
30:18:26:LYS:HG2	30:18:46:ARG:O	2.20	0.42
32:1a:539:A:H2'	32:1a:540:G:C8	2.54	0.42
32:1a:1026:G:H3'	32:1a:1027:C:C6	2.55	0.42
32:1a:1346:A:N1	32:1a:1374:A:H5"	2.35	0.42
33:1b:16:HIS:CG	33:1b:17:PHE:N	2.87	0.42
40:1i:4:TYR:CZ	40:1i:88:TYR:HD1	2.38	0.42
1:2A:10:G:H2'	1:2A:11:G:C8	2.55	0.42
1:2A:265:A:H1'	1:2A:266:G:O4'	2.20	0.42
1:2A:747:U:O2	1:2A:2014:A:H1'	2.19	0.42
1:2A:881:G:C2	1:2A:897:C:C2	3.07	0.42
1:2A:902:C:H2'	1:2A:903:C:H6	1.85	0.42
1:2A:918:A:N3	2:2B:80:U:O2'	2.51	0.42
1:2A:921:G:H4'	1:2A:2269:A:C5	2.55	0.42
1:2A:947:G:H2'	1:2A:948:G:H8	1.84	0.42
1:2A:1274:A:N3	1:2A:1297:C:H1'	2.34	0.42
1:2A:1429:G:H2'	1:2A:1430:C:C6	2.54	0.42
1:2A:1467:C:C5	1:2A:1546:C:H2'	2.54	0.42
1:2A:2614:A:OP1	61:2A:3949:HOH:O	2.22	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2G:117:PHE:HB3	26:24:40:HIS:HE1	1.83	0.42
8:2I:2:LYS:HA	8:2I:19:VAL:O	2.19	0.42
12:2Q:85:LYS:HD2	12:2Q:85:LYS:N	2.35	0.42
18:2W:4:LYS:HD3	18:2W:6:ILE:HD11	2.01	0.42
26:24:47:GLN:O	26:24:48:ARG:C	2.63	0.42
32:2a:189(L):G:H2'	32:2a:190:U:H6	1.85	0.42
32:2a:1508:G:H2'	32:2a:1509:C:C6	2.55	0.42
33:2b:15:VAL:O	33:2b:17:PHE:N	2.49	0.42
34:2c:28:GLN:HG2	34:2c:31:HIS:ND1	2.35	0.42
44:2m:3:ARG:HB3	44:2m:9:ILE:H	1.83	0.42
47:2p:8:ARG:HB3	47:2p:28:ARG:NH1	2.34	0.42
1:1A:897:C:N3	1:1A:898:C:N4	2.68	0.42
1:1A:2355:C:H1'	22:10:39:ARG:HH21	1.84	0.42
5:1F:101:LEU:HD12	5:1F:102:PRO:HD2	2.00	0.42
6:1G:72:ARG:NH1	6:1G:87:PRO:HG3	2.35	0.42
32:1a:103:C:O2'	32:1a:172:A:N1	2.51	0.42
32:1a:833:U:H2'	32:1a:834:C:C6	2.54	0.42
32:1a:1111:A:N1	34:1c:177:THR:OG1	2.46	0.42
35:1d:43:HIS:HB3	35:1d:46:LYS:HG3	2.02	0.42
44:1m:34:LEU:HD13	44:1m:41:PRO:HA	2.02	0.42
44:1m:40:ASN:O	44:1m:43:THR:OG1	2.35	0.42
51:1t:71:THR:O	51:1t:72:LEU:HD23	2.20	0.42
1:2A:197:A:H62	1:2A:2430:A:H2'	1.85	0.42
1:2A:482:A:H1'	1:2A:498:G:N2	2.34	0.42
1:2A:608:A:H2'	1:2A:609:A:C8	2.54	0.42
2:2B:31:C:H4'	6:2G:29:TRP:HZ2	1.83	0.42
2:2B:103:G:H21	21:2Z:73:GLN:HE22	1.68	0.42
8:2I:69:LYS:HG2	8:2I:73:GLU:HG3	2.00	0.42
32:2a:192:U:O2'	51:2t:60:GLU:OE1	2.32	0.42
32:2a:224:C:H2'	32:2a:225:C:H6	1.84	0.42
32:2a:942:G:C2	32:2a:1342:C:C2	3.08	0.42
35:2d:110:PHE:N	35:2d:110:PHE:CD1	2.88	0.42
38:2g:10:ARG:HA	38:2g:10:ARG:HD2	1.87	0.42
40:2i:93:ARG:HD3	40:2i:93:ARG:HA	1.79	0.42
43:2l:71:PRO:O	43:2l:102:ARG:NH1	2.51	0.42
51:2t:76:ALA:O	51:2t:80:ARG:HG3	2.19	0.42
1:1A:1607:C:H4'	1:1A:1608:A:O5'	2.19	0.42
1:1A:2096:U:H3	1:1A:2193:G:H1	1.68	0.42
1:1A:2445:G:OP1	5:1F:74:ARG:NH2	2.52	0.42
3:1D:16:MET:HE2	3:1D:16:MET:HB2	1.78	0.42
32:1a:107:G:N7	51:1t:15:ARG:NH2	2.68	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1057:G:H2'	32:1a:1058:G:O4'	2.20	0.42
32:1a:1060:C:H5"	41:1j:51:ARG:HG2	2.01	0.42
35:1d:59:ARG:HD3	35:1d:59:ARG:HA	1.74	0.42
36:1e:33:VAL:HG22	36:1e:112:LEU:HD12	2.02	0.42
54:1w:15:A:N6	54:1w:59:U:H1'	2.35	0.42
1:2A:1127:A:C2'	1:2A:1128:A:H5"	2.49	0.42
1:2A:1688:U:H2'	1:2A:1698:A:N6	2.34	0.42
1:2A:2406:U:H6	1:2A:2406:U:H2'	1.74	0.42
2:2B:103:G:H21	21:2Z:73:GLN:NE2	2.18	0.42
8:2I:77:LEU:HB3	8:2I:142:VAL:HG13	2.02	0.42
12:2Q:1:MET:HG2	12:2Q:44:ALA:HB1	2.02	0.42
29:27:24:THR:O	29:27:28:ARG:HG3	2.20	0.42
32:2a:130:A:N3	32:2a:263:A:O2'	2.45	0.42
32:2a:935:A:O2'	32:2a:1383:C:N3	2.53	0.42
32:2a:1122:U:C4	32:2a:1123:A:N7	2.88	0.42
33:2b:178:ARG:NH2	39:2h:68:ARG:HH12	2.17	0.42
34:2c:39:ILE:O	34:2c:43:LEU:HG	2.19	0.42
40:2i:40:LEU:HD23	40:2i:42:ARG:H	1.84	0.42
1:1A:1092:C:C2'	1:1A:1093:G:H5'	2.50	0.42
1:1A:1630:G:H2'	1:1A:1631:C:C6	2.55	0.42
1:1A:2406:U:H6	1:1A:2406:U:H2'	1.67	0.42
1:1A:2747:G:O6	1:1A:2755:C:H5"	2.20	0.42
11:1P:138:LEU:HD23	11:1P:145:PRO:HB3	2.01	0.42
12:1Q:1:MET:SD	12:1Q:45:GLN:HG3	2.60	0.42
12:1Q:18:LYS:HE3	12:1Q:18:LYS:HB2	1.78	0.42
14:1S:4:LEU:HD22	14:1S:8:GLU:HB3	2.02	0.42
15:1T:113:LYS:HA	15:1T:113:LYS:HD3	1.76	0.42
21:1Z:130:PRO:HA	21:1Z:133:ILE:HD11	2.01	0.42
32:1a:375:U:OP1	47:1p:69:THR:OG1	2.27	0.42
32:1a:741:G:H2'	32:1a:742:G:O4'	2.20	0.42
32:1a:1304:G:C6	32:1a:1305:G:N1	2.88	0.42
33:1b:44:LEU:O	33:1b:47:THR:HB	2.20	0.42
35:1d:12:CYS:SG	35:1d:19:LEU:N	2.86	0.42
39:1h:13:ILE:O	39:1h:17:THR:HG23	2.20	0.42
1:2A:479:A:N3	1:2A:481:G:H5"	2.34	0.42
1:2A:2286:A:H4'	1:2A:2287:A:O4'	2.19	0.42
5:2F:116:ASP:OD1	5:2F:119:ARG:NH2	2.50	0.42
6:2G:41:GLN:O	6:2G:43:LEU:HB2	2.19	0.42
7:2H:140:LYS:O	7:2H:144:VAL:HG23	2.20	0.42
8:2I:9:LEU:HD21	8:2I:35:LEU:HD13	2.01	0.42
9:2N:131:GLN:H	9:2N:131:GLN:HG2	1.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:2Q:66:ILE:HG12	12:2Q:104:PHE:CD1	2.55	0.42
21:2Z:73:GLN:O	21:2Z:87:ASP:N	2.48	0.42
32:2a:93:G:C6	32:2a:96:U:C4	3.08	0.42
32:2a:540:G:H2'	32:2a:541:G:H8	1.85	0.42
32:2a:952:U:H4'	32:2a:964:A:H61	1.85	0.42
32:2a:1296:C:H5"	44:2m:44:ARG:HH22	1.84	0.42
32:2a:1352:C:OP1	52:2u:3:LYS:NZ	2.51	0.42
35:2d:86:LYS:H	35:2d:86:LYS:HD2	1.84	0.42
36:2e:36:ASP:C	36:2e:38:GLN:H	2.27	0.42
41:2j:77:PRO:O	41:2j:81:THR:HB	2.20	0.42
1:1A:764:A:O4'	3:1D:213:ARG:HG3	2.20	0.41
1:1A:861:A:H2'	1:1A:862:G:O4'	2.19	0.41
1:1A:2110:G:C2	1:1A:2120:G:H1'	2.55	0.41
1:1A:2125:G:N1	1:1A:2172:U:OP1	2.35	0.41
1:1A:2161:C:O2'	1:1A:2162:G:H8	2.02	0.41
6:1G:106:LEU:HA	6:1G:110:ALA:HB3	2.02	0.41
11:1P:1:MET:HE3	11:1P:1:MET:HB2	1.71	0.41
20:1Y:20:TYR:CE2	20:1Y:43:ASN:HA	2.54	0.41
21:1Z:11:GLU:O	21:1Z:36:LYS:NZ	2.29	0.41
21:1Z:150:LEU:O	21:1Z:171:ILE:HG12	2.20	0.41
26:14:49:PHE:HD1	26:14:49:PHE:HA	1.75	0.41
26:14:53:GLU:H	26:14:53:GLU:HG3	1.43	0.41
32:1a:339:C:H2'	32:1a:340:U:C6	2.55	0.41
32:1a:562:C:H1'	43:1l:15:ARG:HB3	2.01	0.41
32:1a:688:G:H5'	42:1k:46:GLY:C	2.45	0.41
32:1a:1183:A:O2'	32:1a:1184:G:OP1	2.36	0.41
33:1b:201:ILE:HG21	33:1b:214:ILE:HG21	2.02	0.41
43:1l:71:PRO:O	43:1l:102:ARG:NH1	2.53	0.41
47:1p:6:LEU:HB3	47:1p:17:TYR:CD1	2.55	0.41
1:2A:127:A:H5"	1:2A:128:C:C6	2.55	0.41
1:2A:196:A:N3	1:2A:196:A:H2'	2.35	0.41
1:2A:752:A:H3'	29:27:1:MET:HE1	2.01	0.41
1:2A:854:G:H2'	1:2A:855:G:C8	2.54	0.41
1:2A:1037:G:H1	1:2A:1118:C:H42	1.68	0.41
1:2A:2088:G:H2'	1:2A:2089:U:O4'	2.20	0.41
1:2A:2164:C:C4	1:2A:2165:G:H1'	2.55	0.41
1:2A:2271:G:OP1	22:20:18:ALA:HB1	2.20	0.41
1:2A:2611:U:H5'	1:2A:2611:U:H6	1.85	0.41
5:2F:154:VAL:HG22	5:2F:191:ARG:HB2	2.02	0.41
8:2I:123:LEU:HA	8:2I:144:VAL:HG23	2.02	0.41
10:2O:19:ILE:HG22	10:2O:43:VAL:HA	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:2Y:1:MET:O	20:2Y:1:MET:HG2	2.20	0.41
22:20:70:GLN:HG2	22:20:72:ARG:HG3	2.01	0.41
32:2a:194:C:H2'	32:2a:195:A:H5"	2.00	0.41
32:2a:423:G:H3'	32:2a:423:G:N3	2.35	0.41
32:2a:437:U:O2'	35:2d:123:HIS:HD2	2.02	0.41
32:2a:1013:G:O2'	32:2a:1015:A:N7	2.47	0.41
32:2a:1329:A:H5'	44:2m:29:ARG:NE	2.35	0.41
32:2a:1503:A:N3	53:2v:13:A:N6	2.67	0.41
33:2b:76:GLN:NE2	33:2b:76:GLN:H	2.18	0.41
34:2c:7:PRO:HB2	34:2c:182:ILE:HD11	2.02	0.41
44:2m:3:ARG:HH12	44:2m:11:ARG:HE	1.68	0.41
45:2n:39:LEU:HD11	45:2n:47:LEU:HD12	2.02	0.41
54:2w:67:G:H2'	54:2w:68:C:C6	2.54	0.41
1:1A:196:A:H2'	1:1A:196:A:N3	2.36	0.41
1:1A:2264:C:N4	22:10:15:ASP:OD2	2.46	0.41
11:1P:39:LYS:HG3	11:1P:45:LEU:HD22	2.03	0.41
20:1Y:6:HIS:H	20:1Y:6:HIS:CD2	2.38	0.41
32:1a:258:G:H2'	32:1a:259:G:C8	2.55	0.41
32:1a:509:A:HO2'	32:1a:510:A:P	2.40	0.41
32:1a:944:G:OP1	61:1a:1915:HOH:O	2.21	0.41
34:1c:33:LEU:O	34:1c:37:GLN:HG2	2.20	0.41
44:1m:11:ARG:O	44:1m:12:ASN:HB2	2.20	0.41
56:1y:72:C:H2'	56:1y:73:U:O4'	2.20	0.41
1:2A:720:C:H2'	1:2A:721:C:C6	2.55	0.41
1:2A:1184:G:H5'	25:23:29:ARG:HH11	1.85	0.41
1:2A:1270:C:H5"	1:2A:1271:G:O5'	2.20	0.41
1:2A:2788:C:C4	1:2A:2789:C:N4	2.89	0.41
2:2B:11:C:OP2	2:2B:12:C:N4	2.47	0.41
4:2E:35:GLN:OE1	4:2E:66:HIS:HE1	2.04	0.41
12:2Q:103:MET:HE1	12:2Q:125:LEU:HD13	2.01	0.41
17:2V:62:LEU:HD12	17:2V:93:GLU:HG2	2.01	0.41
32:2a:392:G:O2'	32:2a:483:C:O2'	2.26	0.41
32:2a:625:G:H2'	32:2a:626:U:H6	1.85	0.41
32:2a:649:G:H2'	32:2a:650:G:O4'	2.20	0.41
32:2a:1033:G:H2'	32:2a:1034:G:C8	2.53	0.41
33:2b:47:THR:HB	33:2b:202:PRO:HG2	2.01	0.41
34:2c:119:ARG:HG3	34:2c:123:GLN:NE2	2.31	0.41
36:2e:53:LEU:HD12	36:2e:53:LEU:H	1.84	0.41
38:2g:89:MET:HE3	38:2g:89:MET:HB3	1.96	0.41
42:2k:17:GLY:HA3	42:2k:77:MET:HE1	2.01	0.41
51:2t:40:ALA:HB2	51:2t:55:ILE:HB	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:2y:42:C:H2'	56:2y:43:U:C6	2.55	0.41
56:2y:63:C:H2'	56:2y:64:U:C6	2.55	0.41
1:1A:568:U:OP1	1:1A:945:A:N6	2.49	0.41
1:1A:1074:G:C2	1:1A:1075:C:H1'	2.55	0.41
1:1A:1077:A:H2'	1:1A:1078:U:H4'	2.01	0.41
1:1A:1377:G:H2'	61:1A:5180:HOH:O	2.20	0.41
1:1A:1594:G:H2'	1:1A:1595:G:O4'	2.20	0.41
1:1A:1783:A:H5'	1:1A:2608:G:H4'	2.01	0.41
1:1A:2178:C:H2'	1:1A:2179:C:C6	2.55	0.41
3:1D:183:ARG:HG2	3:1D:184:LYS:N	2.35	0.41
15:1T:39:ARG:NH2	32:1a:345:C:H5"	2.32	0.41
20:1Y:11:ASP:O	20:1Y:26:LYS:HD3	2.19	0.41
21:1Z:3:TYR:CD2	21:1Z:51:ALA:HB2	2.55	0.41
23:11:13:ILE:HD11	23:11:42:GLN:OE1	2.20	0.41
26:14:56:VAL:HG22	26:14:60:GLN:HG3	2.02	0.41
32:1a:271:C:H2'	32:1a:272:C:C6	2.55	0.41
32:1a:1198:G:H2'	32:1a:1199:U:C6	2.56	0.41
32:1a:1370:G:H5"	40:1i:12:GLU:HG3	2.03	0.41
34:1c:87:LEU:O	34:1c:91:LEU:HB2	2.20	0.41
38:1g:12:LEU:HD12	38:1g:12:LEU:H	1.84	0.41
1:2A:888:C:OP1	44:2m:93:ARG:HD3	2.20	0.41
1:2A:1800:C:OP1	3:2D:260:ARG:NH2	2.54	0.41
1:2A:1991:U:H2'	1:2A:1992:G:H5"	2.03	0.41
1:2A:2330:G:H2'	1:2A:2331:G:O4'	2.21	0.41
6:2G:3:LEU:HD23	26:24:25:TYR:CE1	2.55	0.41
8:2I:87:LYS:HG2	8:2I:121:LYS:O	2.20	0.41
9:2N:15:LEU:N	9:2N:136:GLU:O	2.50	0.41
14:2S:51:ALA:HB3	14:2S:73:LEU:HB2	2.02	0.41
23:21:3:LYS:HB2	23:21:61:ARG:HH22	1.85	0.41
32:2a:573:A:N3	32:2a:883:C:O2'	2.52	0.41
32:2a:900:A:H2'	32:2a:901:A:C8	2.55	0.41
32:2a:1515:C:H2'	32:2a:1516:G:C8	2.54	0.41
33:2b:134:GLU:O	33:2b:138:LEU:HD22	2.19	0.41
47:2p:26:ARG:HG3	47:2p:27:LYS:N	2.34	0.41
1:1A:1503:U:H2'	1:1A:1504:C:C6	2.55	0.41
1:1A:2029:G:H2'	1:1A:2031:A:OP1	2.20	0.41
1:1A:2684:U:O2'	10:1O:68:GLU:OE2	2.32	0.41
4:1E:101:ARG:HB2	4:1E:201:THR:HG21	2.02	0.41
7:1H:101:ARG:NH1	7:1H:122:THR:HG22	2.34	0.41
17:1V:60:GLU:HB2	17:1V:97:LYS:HE2	2.01	0.41
21:1Z:70:LEU:HD23	21:1Z:70:LEU:HA	1.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:14:15:ILE:O	26:14:33:VAL:N	2.54	0.41
32:1a:404:U:H2'	32:1a:405:U:C6	2.55	0.41
32:1a:1326:C:OP1	52:1u:17:THR:OG1	2.24	0.41
33:1b:84:GLU:OE1	33:1b:87:ARG:NH1	2.52	0.41
38:1g:144:MET:HE2	38:1g:144:MET:HB3	1.99	0.41
40:1i:33:PHE:HD2	40:1i:34:ASN:ND2	2.17	0.41
53:1v:23:A:H4'	53:1v:24:A:H5'	2.02	0.41
1:2A:402:A:C2'	1:2A:403:U:H5'	2.50	0.41
1:2A:958:U:O2	2:2B:90:A:O2'	2.27	0.41
1:2A:1354:A:H5"	3:2D:38:LYS:HD3	2.02	0.41
1:2A:2171:A:C4	1:2A:2172:U:C4	3.09	0.41
1:2A:2538:C:H2'	1:2A:2539:C:H6	1.86	0.41
32:2a:158:G:H2'	32:2a:159:G:O4'	2.21	0.41
32:2a:540:G:H2'	32:2a:541:G:C8	2.55	0.41
32:2a:544:G:OP1	35:2d:59:ARG:NH2	2.45	0.41
32:2a:959:A:HO2'	32:2a:984:C:HO2'	1.57	0.41
32:2a:1366:C:H2'	32:2a:1367:C:C6	2.56	0.41
39:2h:81:HIS:N	39:2h:138:TRP:O	2.52	0.41
48:2q:89:LEU:HD23	48:2q:89:LEU:HA	1.89	0.41
54:2w:29:A:H2'	54:2w:30:G:C8	2.55	0.41
56:2y:14:A:H61	56:2y:21:A:H2	1.65	0.41
1:1A:858:U:O2	1:1A:2268:A:H2'	2.21	0.41
1:1A:922:U:H2'	1:1A:923:C:C6	2.56	0.41
1:1A:1665:A:H2'	1:1A:1666:G:O4'	2.20	0.41
1:1A:1668:A:H4'	1:1A:1669:A:O5'	2.21	0.41
1:1A:2134:A:O2'	1:1A:2135:A:OP1	2.25	0.41
8:1I:65:ALA:HB1	8:1I:136:VAL:HG11	2.01	0.41
32:1a:1030:C:N4	32:1a:1030(A):G:N3	2.68	0.41
35:1d:111:ALA:HA	35:1d:161:ASN:ND2	2.35	0.41
44:1m:87:TYR:HA	44:1m:90:LEU:HD12	2.02	0.41
45:1n:6:LEU:HB3	45:1n:23:ARG:NH2	2.35	0.41
47:1p:5:ARG:HH21	47:1p:28:ARG:HA	1.86	0.41
54:1w:54:5MU:C4	54:1w:55:PSU:C2	3.08	0.41
1:2A:315:G:H2'	1:2A:316:C:C6	2.55	0.41
1:2A:597:U:H2'	1:2A:598:G:H8	1.85	0.41
1:2A:885:C:H2'	1:2A:886:C:H4'	2.02	0.41
1:2A:1761:C:H2'	1:2A:1762:A:H5"	2.02	0.41
1:2A:2171:A:H1'	1:2A:2172:U:C6	2.56	0.41
1:2A:2273:A:O2'	1:2A:2274:A:H5'	2.20	0.41
1:2A:2811:G:H22	1:2A:2891:G:H1'	1.85	0.41
2:2B:66:A:N6	2:2B:108:U:H3'	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2G:76:SER:N	6:2G:84:LYS:HB2	2.36	0.41
7:2H:124:GLU:OE1	7:2H:132:ARG:HG2	2.20	0.41
11:2P:90:ARG:NH1	11:2P:105:LEU:HD11	2.35	0.41
31:29:2:LYS:NZ	31:29:31:LYS:O	2.44	0.41
32:2a:619:U:C4	35:2d:135:LEU:HD11	2.55	0.41
32:2a:1004:A:C6	32:2a:1037:C:H1'	2.56	0.41
32:2a:1009:G:H2'	32:2a:1010:G:H5'	2.03	0.41
32:2a:1147:C:O2'	40:2i:16:ARG:NE	2.54	0.41
32:2a:1168:A:C6	32:2a:1169:A:C6	3.08	0.41
48:2q:6:LEU:O	48:2q:58:GLU:HA	2.21	0.41
2:1B:2:C:H2'	2:1B:3:C:C6	2.56	0.41
2:1B:21:G:H2'	2:1B:22:U:O4'	2.21	0.41
2:1B:106:G:H5'	21:1Z:31:ARG:HG2	2.01	0.41
26:14:61:ARG:O	26:14:62:ARG:C	2.63	0.41
32:1a:235:C:H5'	48:1q:70:ARG:HG3	2.02	0.41
32:1a:300:A:O2'	32:1a:564:C:N3	2.51	0.41
32:1a:867:G:O2'	32:1a:873:A:N1	2.50	0.41
32:1a:1068:G:H8	32:1a:1068:G:OP2	2.02	0.41
32:1a:1223:C:P	50:1s:78:ARG:HH21	2.43	0.41
33:1b:84:GLU:HB3	33:1b:219:VAL:HG21	2.02	0.41
33:1b:196:LEU:HD23	33:1b:196:LEU:HA	1.90	0.41
54:1w:60:U:H5"	54:1w:61:C:C5	2.45	0.41
1:2A:93:G:H2'	1:2A:94:C:H6	1.85	0.41
1:2A:484:C:H2'	1:2A:485:C:C6	2.56	0.41
1:2A:729:G:OP1	3:2D:12:SER:HB2	2.21	0.41
1:2A:940:G:N3	1:2A:1191:G:H4'	2.36	0.41
1:2A:2332:U:O2'	1:2A:2335:A:N3	2.52	0.41
11:2P:97:PRO:HD3	11:2P:126:VAL:O	2.21	0.41
21:2Z:158:PRO:HA	21:2Z:159:PRO:HD3	1.95	0.41
32:2a:955:U:O2'	50:2s:83:HIS:HD2	2.04	0.41
33:2b:97:TRP:CH2	33:2b:102:LEU:HG	2.54	0.41
33:2b:178:ARG:HH22	39:2h:68:ARG:NH2	2.16	0.41
36:2e:73:ASN:OD1	36:2e:73:ASN:N	2.54	0.41
38:2g:89:MET:SD	38:2g:155:ARG:HB2	2.60	0.41
38:2g:152:ALA:O	38:2g:155:ARG:HD3	2.21	0.41
40:2i:3:GLN:HG3	40:2i:20:ARG:HE	1.85	0.41
41:2j:42:THR:O	41:2j:44:VAL:HG23	2.21	0.41
44:2m:29:ARG:HD3	44:2m:64:TRP:CD2	2.56	0.41
55:2x:8:4SU:O5'	55:2x:8:4SU:H6	2.21	0.41
1:1A:762:U:OP1	61:1A:4143:HOH:O	2.21	0.41
1:1A:897:C:H4'	54:1w:56:C:P	2.61	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1056:G:H5”	1:1A:1057:A:O4’	2.20	0.41
1:1A:1161:C:O2’	17:1V:8:GLY:HA2	2.21	0.41
1:1A:1773:A:H2’	1:1A:1774:C:O4’	2.21	0.41
12:1Q:17:LEU:HD23	12:1Q:17:LEU:HA	1.78	0.41
21:1Z:151:HIS:HA	21:1Z:171:ILE:HG23	2.03	0.41
32:1a:763:G:H2’	32:1a:764:C:H6	1.85	0.41
35:1d:158:ILE:H	35:1d:158:ILE:HG13	1.54	0.41
38:1g:90:GLU:CD	38:1g:90:GLU:H	2.28	0.41
56:1y:60:U:O2’	56:1y:61:C:H5’	2.20	0.41
1:2A:27:G:N2	1:2A:512:G:H1’	2.34	0.41
1:2A:184:C:H2’	1:2A:185:U:C6	2.56	0.41
1:2A:922:U:H2’	1:2A:923:C:C6	2.56	0.41
1:2A:994:C:OP2	16:2U:54:LYS:NZ	2.52	0.41
1:2A:2512:C:H2’	1:2A:2513:G:O4’	2.20	0.41
5:2F:21:ALA:CB	5:2F:22:ALA:HA	2.47	0.41
14:2S:110:LEU:HD12	14:2S:110:LEU:HA	1.92	0.41
21:2Z:155:LEU:HB3	21:2Z:156:LYS:H	1.72	0.41
30:28:26:LYS:HB2	30:28:44:LYS:O	2.20	0.41
32:2a:460:G:N2	32:2a:471:G:N7	2.69	0.41
32:2a:954:G:H2’	32:2a:955:U:O4’	2.21	0.41
32:2a:1142:G:H2’	32:2a:1143:G:O4’	2.21	0.41
32:2a:1226:C:H4’	50:2s:80:TYR:CZ	2.56	0.41
37:2f:42:GLU:OE2	37:2f:59:TYR:OH	2.39	0.41
40:2i:15:ALA:HB2	40:2i:65:VAL:HG23	2.03	0.41
1:1A:614(C):A:C4	5:1F:180:GLY:HA2	2.56	0.41
1:1A:1268:A:H2’	1:1A:1269:A:O4’	2.21	0.41
1:1A:1448:G:H4’	1:1A:1542:A:OP1	2.21	0.41
1:1A:1792:G:O2’	1:1A:1830:C:OP1	2.34	0.41
6:1G:67:LYS:HD3	26:14:5:ILE:HD12	2.02	0.41
32:1a:159:G:H2’	32:1a:161:A:OP2	2.21	0.41
32:1a:375:U:C2	32:1a:376:G:C8	3.08	0.41
32:1a:737:A:H5”	37:1f:92:LYS:HG3	2.03	0.41
35:1d:13:ARG:HB3	35:1d:38:TYR:O	2.20	0.41
35:1d:63:LYS:HE3	35:1d:63:LYS:HB2	1.87	0.41
36:1e:83:GLU:HG2	36:1e:88:LYS:HG3	2.02	0.41
36:1e:147:ASP:O	36:1e:151:LEU:HB2	2.20	0.41
47:1p:3:LYS:HG3	47:1p:24:ALA:HB2	2.01	0.41
51:1t:39:LYS:O	51:1t:43:LEU:HG	2.21	0.41
1:2A:1011:G:OP2	16:2U:66:ASN:ND2	2.50	0.41
1:2A:2086:U:H2’	1:2A:2087:G:C8	2.56	0.41
1:2A:2438:U:O2’	1:2A:2440:C:OP1	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:2E:178:GLU:CD	4:2E:178:GLU:H	2.28	0.41
16:2U:97:ASP:OD1	16:2U:101:ARG:HD2	2.20	0.41
32:2a:730:G:C5	32:2a:731:G:H1'	2.56	0.41
32:2a:1049:U:C5	32:2a:1201:A:H5'	2.56	0.41
32:2a:1085:U:H3'	32:2a:1086:U:C5	2.56	0.41
32:2a:1410:G:H2'	32:2a:1411:C:C6	2.56	0.41
34:2c:37:GLN:NE2	45:2n:52:GLN:OE1	2.36	0.41
38:2g:22:LEU:HD13	38:2g:97:GLN:CD	2.46	0.41
38:2g:52:GLU:H	38:2g:52:GLU:HG2	1.69	0.41
40:2i:18:PHE:O	40:2i:61:ALA:HA	2.20	0.41
41:2j:96:ILE:HG22	41:2j:97:GLU:H	1.86	0.41
44:2m:80:ARG:HH22	50:2s:69:HIS:HE1	1.67	0.41
48:2q:26:GLN:HG2	48:2q:37:LYS:HG2	2.03	0.41
50:2s:27:GLU:H	50:2s:27:GLU:HG3	1.52	0.41
1:1A:11:G:C2'	1:1A:12:U:H5'	2.47	0.41
1:1A:662:G:H5'	11:1P:14:LYS:O	2.20	0.41
1:1A:831:G:O2'	11:1P:38:GLN:OE1	2.33	0.41
1:1A:879:G:H8	1:1A:879:G:O5'	2.04	0.41
1:1A:1263:U:H2'	1:1A:1264:G:C8	2.56	0.41
1:1A:1675:C:N3	4:1E:128:SER:OG	2.52	0.41
1:1A:1720:U:H2'	1:1A:1721:G:O4'	2.21	0.41
1:1A:2492:U:H2'	1:1A:2493:U:C6	2.56	0.41
1:1A:2561:A:H2'	1:1A:2562:U:O4'	2.21	0.41
2:1B:78:A:H2'	2:1B:79:C:O4'	2.21	0.41
3:1D:38:LYS:NZ	3:1D:39:LYS:O	2.36	0.41
3:1D:71:ASP:CB	3:1D:103:ARG:HH12	2.34	0.41
5:1F:7:TYR:CD2	5:1F:24:LEU:HB2	2.56	0.41
5:1F:8:GLN:NE2	5:1F:21:ALA:HB2	2.36	0.41
5:1F:31:HIS:HB2	11:1P:9:ASN:OD1	2.21	0.41
5:1F:148:LEU:HD23	5:1F:191:ARG:HH11	1.84	0.41
7:1H:3:ARG:HD2	7:1H:3:ARG:HA	1.52	0.41
8:1I:10:GLU:H	8:1I:10:GLU:HG3	1.59	0.41
10:1O:113:LYS:HD3	10:1O:113:LYS:HA	1.91	0.41
20:1Y:98:VAL:HG12	20:1Y:105:ALA:HA	2.01	0.41
30:18:33:ASN:HA	30:18:36:LYS:HD2	2.03	0.41
32:1a:148:G:H2'	32:1a:149:A:C8	2.55	0.41
32:1a:271:C:H2'	32:1a:272:C:H6	1.86	0.41
32:1a:472:A:H5"	47:1p:80:PHE:HB3	2.02	0.41
32:1a:485:G:O2'	32:1a:486:U:OP2	2.38	0.41
32:1a:1053:G:O5'	32:1a:1054:C:H3'	2.21	0.41
33:1b:92:TYR:CE1	33:1b:94:ASN:HB2	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:1e:90:VAL:O	36:1e:120:THR:HA	2.21	0.41
39:1h:21:LYS:O	39:1h:65:TYR:OH	2.35	0.41
42:1k:20:TYR:CZ	42:1k:83:ILE:HD12	2.56	0.41
42:1k:38:ASN:HA	42:1k:39:PRO:HD3	1.94	0.41
42:1k:51:LYS:HE3	42:1k:51:LYS:HB3	1.91	0.41
42:1k:59:TYR:CZ	42:1k:63:LEU:HD21	2.56	0.41
44:1m:40:ASN:HB3	44:1m:43:THR:OG1	2.21	0.41
1:2A:55:G:O2'	1:2A:127:A:N1	2.47	0.41
1:2A:171:G:H2'	1:2A:172:C:H6	1.85	0.41
1:2A:956:G:H2'	1:2A:957:A:H2'	2.02	0.41
1:2A:1364:G:N7	23:21:3:LYS:HD2	2.35	0.41
1:2A:2143:C:N4	1:2A:2148:G:N1	2.46	0.41
1:2A:2280:G:O6	22:20:14:ARG:HD2	2.20	0.41
1:2A:2315:G:H2'	1:2A:2316:C:C6	2.55	0.41
2:2B:7:G:H2'	2:2B:8:U:O4'	2.21	0.41
2:2B:11:C:H3'	2:2B:12:C:H6	1.86	0.41
3:2D:206:LEU:HD23	3:2D:206:LEU:HA	1.85	0.41
3:2D:232:PRO:HB3	3:2D:244:ARG:CZ	2.50	0.41
4:2E:18:ASP:HB3	15:2T:82:LEU:HD21	2.02	0.41
4:2E:48:GLN:HA	4:2E:80:GLU:HA	2.02	0.41
4:2E:181:LEU:HD12	4:2E:181:LEU:HA	1.79	0.41
5:2F:167:ALA:HB1	5:2F:173:VAL:HG11	2.03	0.41
6:2G:11:TYR:OH	6:2G:16:ARG:HD3	2.20	0.41
22:20:53:MET:HG3	22:20:59:LEU:HD23	2.03	0.41
25:23:6:VAL:HG22	25:23:28:LEU:HD11	2.01	0.41
28:26:14:THR:OG1	28:26:48:VAL:HG13	2.21	0.41
32:2a:330:C:H5"	61:2a:2035:HOH:O	2.21	0.41
32:2a:583:A:H2'	32:2a:584:G:O4'	2.20	0.41
32:2a:737:A:H2'	32:2a:738:C:C6	2.56	0.41
32:2a:909:A:N3	32:2a:1413:A:O2'	2.43	0.41
32:2a:977:A:H2'	32:2a:978:A:H5"	2.02	0.41
32:2a:1090:U:H2'	32:2a:1091:U:C6	2.56	0.41
32:2a:1129:C:H2'	32:2a:1139:G:O6	2.21	0.41
32:2a:1152:A:H4'	41:2j:13:HIS:HD2	1.86	0.41
32:2a:1228:C:H2'	32:2a:1229:A:H8	1.85	0.41
32:2a:1305:G:H22	32:2a:1331:G:H1'	1.85	0.41
33:2b:20:GLU:HB2	33:2b:190:THR:OG1	2.21	0.41
33:2b:146:GLN:HE21	33:2b:146:GLN:HB3	1.78	0.41
34:2c:6:HIS:ND1	45:2n:49:HIS:HB3	2.35	0.41
34:2c:91:LEU:C	34:2c:93:LYS:H	2.29	0.41
34:2c:130:VAL:O	34:2c:134:ILE:HG12	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:2e:84:PHE:N	36:2e:87:SER:O	2.53	0.41
37:2f:67:MET:HE3	37:2f:72:VAL:HB	2.03	0.41
38:2g:153:HIS:CE1	42:2k:58:PRO:HD2	2.56	0.41
49:2r:61:LYS:O	49:2r:65:ILE:HG12	2.21	0.41
1:1A:226:G:N2	1:1A:228:A:H62	2.18	0.41
1:1A:272(J):C:H2'	1:1A:274:G:C8	2.56	0.41
1:1A:1557:C:H5"	1:1A:1558:A:OP2	2.21	0.41
5:1F:24:LEU:HB3	5:1F:115:ALA:HB2	2.02	0.41
5:1F:116:ASP:OD1	5:1F:119:ARG:NH2	2.53	0.41
7:1H:96:ALA:N	7:1H:128:PRO:O	2.53	0.41
32:1a:202:U:H3'	32:1a:203:U:C5	2.56	0.41
32:1a:242:C:H2'	32:1a:243:A:H5'	2.03	0.41
32:1a:559:A:H4'	32:1a:560:U:H3'	2.03	0.41
32:1a:767:A:H2'	32:1a:768:A:O4'	2.21	0.41
32:1a:1209:C:O2'	32:1a:1214:C:N4	2.51	0.41
35:1d:178:VAL:O	35:1d:180:GLY:N	2.43	0.41
35:1d:196:LEU:O	35:1d:198:VAL:N	2.48	0.41
46:1o:42:HIS:CE1	46:1o:46:HIS:CD2	3.09	0.41
1:2A:242:G:C8	30:28:5:LYS:HG2	2.56	0.41
1:2A:262:A:H2'	1:2A:263:C:O4'	2.21	0.41
1:2A:1127:A:H2'	1:2A:1128:A:H5"	2.03	0.41
1:2A:1153:C:H2'	1:2A:1154:G:O4'	2.21	0.41
1:2A:1786:A:C4	1:2A:1938:A:C6	3.09	0.41
1:2A:1952:A:OP1	10:2O:42:SER:OG	2.39	0.41
1:2A:2002:G:OP2	13:2R:9:LYS:NZ	2.53	0.41
1:2A:2286:A:H4'	1:2A:2287:A:O5'	2.20	0.41
1:2A:2447:G:N2	1:2A:2450:A:OP2	2.54	0.41
2:2B:58:A:H2'	2:2B:59:A:O4'	2.21	0.41
3:2D:137:PRO:O	3:2D:140:THR:OG1	2.37	0.41
4:2E:50:GLY:HA3	4:2E:75:VAL:HG21	2.03	0.41
11:2P:7:ARG:HB3	11:2P:7:ARG:HH21	1.84	0.41
15:2T:26:ASP:OD1	15:2T:120:ARG:NH2	2.45	0.41
32:2a:107:G:H2'	32:2a:108:G:O4'	2.21	0.41
34:2c:24:ALA:HB3	34:2c:29:TYR:CD1	2.56	0.41
37:2f:9:VAL:HB	37:2f:87:ARG:HB2	2.02	0.41
43:2l:110:VAL:HG23	43:2l:120:TYR:HB3	2.03	0.41
49:2r:84:LYS:N	49:2r:84:LYS:HD2	2.36	0.41
54:2w:10:G:N2	54:2w:11:U:C2	2.89	0.41
56:2y:33:U:H2'	56:2y:35:C:OP2	2.21	0.41
1:1A:675:A:C8	1:1A:804:A:C6	3.09	0.40
1:1A:1062:G:N2	1:1A:1088:A:C6	2.89	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1686:C:H2'	1:1A:1687:G:O4'	2.21	0.40
1:1A:2564:A:C2	1:1A:2647:U:H4'	2.56	0.40
1:1A:2751:G:OP2	7:1H:2:SER:HB2	2.22	0.40
2:1B:14:U:O2	2:1B:108:U:H4'	2.21	0.40
4:1E:181:LEU:HD12	4:1E:181:LEU:HA	1.79	0.40
32:1a:278:G:OP2	48:1q:92:ARG:NH2	2.54	0.40
33:1b:55:PHE:CE1	33:1b:218:ALA:HA	2.56	0.40
36:1e:131:ILE:HD13	36:1e:131:ILE:HA	1.97	0.40
40:1i:18:PHE:O	40:1i:61:ALA:HA	2.21	0.40
1:2A:634:C:H2'	1:2A:635:C:C6	2.55	0.40
1:2A:1710:C:H2'	1:2A:1711:C:C6	2.56	0.40
1:2A:2161:C:H2'	1:2A:2162:G:O4'	2.21	0.40
1:2A:2355:C:H1'	22:20:39:ARG:HH21	1.86	0.40
8:2I:58:LEU:O	8:2I:62:LYS:HG3	2.21	0.40
20:2Y:55:TYR:H	20:2Y:56:PRO:HD3	1.85	0.40
32:2a:406:G:H5'	35:2d:5:ILE:HG12	2.02	0.40
32:2a:952:U:H2'	32:2a:953:G:H8	1.85	0.40
32:2a:1108:G:H5'	34:2c:176:HIS:CD2	2.56	0.40
32:2a:1201:A:H1'	32:2a:1202:G:OP2	2.21	0.40
34:2c:32:LEU:O	34:2c:36:ASP:HB2	2.21	0.40
35:2d:47:ARG:NH1	35:2d:49:ARG:HA	2.36	0.40
36:2e:37:ARG:HB3	36:2e:114:GLY:HA2	2.02	0.40
39:2h:39:LEU:HD12	39:2h:39:LEU:HA	1.91	0.40
39:2h:119:LEU:HB3	39:2h:123:GLU:HB2	2.03	0.40
1:1A:363(A):A:H2'	1:1A:363(B):G:C8	2.56	0.40
1:1A:1794:U:H2'	1:1A:1795:C:C6	2.56	0.40
61:1A:4283:HOH:O	19:1X:40:LYS:HE2	2.21	0.40
10:1O:16:ALA:HB2	10:1O:52:VAL:HG21	2.03	0.40
14:1S:84:GLN:HA	14:1S:111:GLU:HB2	2.03	0.40
15:1T:108:ARG:HA	15:1T:111:ARG:NH1	2.37	0.40
32:1a:950:U:H2'	32:1a:951:G:C8	2.56	0.40
32:1a:1237:C:HO2'	32:1a:1300:G:H1	1.66	0.40
32:1a:1241:G:H2'	32:1a:1242:C:C6	2.56	0.40
32:1a:1302:U:C5	44:1m:17:VAL:HG21	2.56	0.40
35:1d:18:LYS:HD2	60:1d:501:SF4:S1	2.62	0.40
35:1d:109:GLY:HA3	35:1d:165:MET:SD	2.62	0.40
47:1p:34:GLU:HG2	47:1p:35:LYS:N	2.36	0.40
1:2A:84:A:H5"	20:2Y:8:LYS:HE3	2.04	0.40
1:2A:93:G:O2'	1:2A:94:C:H5'	2.21	0.40
1:2A:652(U):G:H2'	1:2A:652(V):C:O4'	2.22	0.40
1:2A:966:G:H2'	1:2A:967:C:C6	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1015:G:H2'	1:2A:1016:G:C8	2.53	0.40
1:2A:1814:G:H4'	3:2D:51:VAL:HG21	2.03	0.40
2:2B:25:A:H2'	2:2B:26:A:C8	2.57	0.40
4:2E:179:GLU:HG3	15:2T:9:LEU:HD21	2.04	0.40
5:2F:126:VAL:HG21	5:2F:129:PHE:CZ	2.56	0.40
5:2F:126:VAL:HG21	5:2F:129:PHE:CE1	2.56	0.40
14:2S:19:LYS:C	14:2S:21:THR:H	2.28	0.40
20:2Y:6:HIS:CD2	20:2Y:7:VAL:HG23	2.56	0.40
32:2a:683:G:H2'	32:2a:684:A:H8	1.87	0.40
32:2a:751:U:H4'	46:2o:24:SER:HA	2.03	0.40
32:2a:1181:G:O2'	32:2a:1182:G:C5	2.74	0.40
32:2a:1183:A:H3'	32:2a:1184:G:H5"	2.04	0.40
32:2a:1342:C:H1'	40:2i:124:GLN:OE1	2.21	0.40
33:2b:92:TYR:CD1	33:2b:94:ASN:HB2	2.56	0.40
33:2b:110:GLN:HB3	33:2b:110:GLN:HE21	1.71	0.40
34:2c:113:ALA:HB2	34:2c:202:ILE:HG13	2.02	0.40
35:2d:3:ARG:HH12	35:2d:5:ILE:HG13	1.86	0.40
35:2d:38:TYR:CE1	35:2d:45:GLN:HG3	2.56	0.40
35:2d:112:VAL:HG22	35:2d:116:GLN:CD	2.46	0.40
41:2j:69:ASN:OD1	41:2j:69:ASN:N	2.53	0.40
44:2m:90:LEU:O	44:2m:94:ARG:HB2	2.22	0.40
45:2n:9:LYS:CG	45:2n:12:ARG:HH21	2.33	0.40
45:2n:23:ARG:NH1	45:2n:30:ALA:HB2	2.36	0.40
50:2s:12:ASP:HB2	50:2s:38:SER:OG	2.21	0.40
50:2s:41:VAL:HG23	50:2s:42:PRO:HD2	2.03	0.40
1:1A:586:A:H5'	5:1F:89:VAL:HG21	2.03	0.40
1:1A:1039:G:H1	1:1A:1116:C:N4	2.20	0.40
26:14:47:GLN:HE22	26:14:49:PHE:HE1	1.69	0.40
32:1a:358:U:H2'	32:1a:359:U:C6	2.56	0.40
32:1a:922:G:N3	32:1a:1398:A:H2	2.19	0.40
55:1x:23:C:H2'	55:1x:24:U:H6	1.85	0.40
1:2A:99:U:H4'	1:2A:100:G:H5'	2.04	0.40
1:2A:375:C:H2'	1:2A:376:C:C6	2.57	0.40
1:2A:2342:C:O2'	1:2A:2374:C:OP1	2.35	0.40
1:2A:2671:A:H2'	1:2A:2672:G:O4'	2.22	0.40
1:2A:2687:U:H2'	1:2A:2688:U:O4'	2.21	0.40
15:2T:61:PHE:CE2	15:2T:76:PHE:HB2	2.56	0.40
16:2U:104:GLN:OE1	16:2U:104:GLN:N	2.53	0.40
19:2X:26:TYR:HB3	19:2X:92:LEU:HD13	2.02	0.40
25:23:44:ARG:O	25:23:48:GLU:HG3	2.20	0.40
26:24:34:GLU:CB	44:2m:57:ARG:HH21	2.35	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:382:A:H2'	32:2a:383:A:H8	1.87	0.40
32:2a:499:A:H4'	32:2a:500:G:OP1	2.20	0.40
32:2a:582:U:C2	32:2a:760:G:C6	3.09	0.40
34:2c:6:HIS:CD2	34:2c:8:ILE:H	2.38	0.40
43:2l:28:LYS:HE2	43:2l:64:TYR:CE2	2.54	0.40
43:2l:69:TYR:HE2	43:2l:71:PRO:HA	1.87	0.40
54:2w:17:G:H4'	54:2w:60:U:C6	2.56	0.40
1:1A:918:A:H5"	2:1B:98:G:O2'	2.21	0.40
1:1A:1071:G:H3'	1:1A:1071:G:OP1	2.21	0.40
19:1X:61:GLY:HA3	19:1X:73:ARG:O	2.22	0.40
21:1Z:21:ALA:O	21:1Z:23:LYS:NZ	2.54	0.40
30:18:14:VAL:HG13	30:18:22:VAL:HG13	2.03	0.40
32:1a:1038:C:H2'	32:1a:1039:C:C6	2.56	0.40
37:1f:68:PRO:HG2	37:1f:71:ARG:HD2	2.03	0.40
42:1k:34:ASP:HB2	42:1k:35:PRO:HD2	2.03	0.40
45:1n:27:CYS:SG	45:1n:29:ARG:HB2	2.61	0.40
48:1q:69:LYS:O	48:1q:70:ARG:HD3	2.21	0.40
1:2A:597:U:H2'	1:2A:598:G:C8	2.56	0.40
1:2A:1188:U:C4'	17:2V:79:VAL:HG22	2.49	0.40
1:2A:1366:A:H2'	1:2A:1367:A:O4'	2.21	0.40
1:2A:1514:U:H2'	1:2A:1515:G:H8	1.87	0.40
1:2A:1710:C:H5'	1:2A:2859:G:H1'	2.02	0.40
1:2A:1840:G:OP2	61:2A:3952:HOH:O	2.22	0.40
1:2A:2131:G:C8	1:2A:2133:G:C2	3.10	0.40
1:2A:2203:U:H2'	1:2A:2205:C:C6	2.56	0.40
11:2P:28:GLY:O	11:2P:30:THR:N	2.52	0.40
32:2a:542:G:P	35:2d:10:ARG:HH22	2.45	0.40
32:2a:981:U:H2'	32:2a:982:U:C5	2.57	0.40
32:2a:1318:A:H5"	50:2s:3:ARG:NH2	2.37	0.40
32:2a:1422:G:H2'	32:2a:1423:G:H8	1.87	0.40
43:2l:54:LYS:HD2	43:2l:54:LYS:N	2.37	0.40
51:2t:26:ASN:O	51:2t:30:LYS:HE2	2.21	0.40
56:2y:51:G:N2	56:2y:64:U:O2	2.55	0.40
1:1A:580:C:H2'	1:1A:581:C:C6	2.56	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:O4'	2.21	0.40
1:1A:2158:A:H1'	1:1A:2159:G:O4'	2.22	0.40
1:1A:2687:U:H2'	1:1A:2688:U:O4'	2.20	0.40
4:1E:59:VAL:O	4:1E:64:LYS:HE3	2.22	0.40
7:1H:6:ARG:NH2	7:1H:54:ARG:HH22	2.20	0.40
8:1I:2:LYS:HB2	8:1I:2:LYS:NZ	2.36	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1I:38:LEU:HD23	8:1I:38:LEU:N	2.36	0.40
9:1N:4:TYR:HB2	16:1U:101:ARG:NH1	2.37	0.40
24:12:65:ASN:O	24:12:69:ARG:HB2	2.22	0.40
32:1a:266:G:O3'	48:1q:67:LYS:HB2	2.20	0.40
32:1a:544:G:OP1	35:1d:59:ARG:NH2	2.43	0.40
32:1a:714:G:H2'	32:1a:715:A:C8	2.57	0.40
32:1a:1023:G:H3'	32:1a:1024:G:H8	1.87	0.40
32:1a:1113:C:O2'	34:1c:14:ILE:HD11	2.21	0.40
32:1a:1145:C:H4'	32:1a:1146:A:H5'	2.02	0.40
47:1p:19:ILE:HG13	47:1p:37:GLY:C	2.47	0.40
1:2A:34:C:N4	1:2A:447:A:H61	2.19	0.40
1:2A:39:C:H2'	1:2A:40:C:C6	2.57	0.40
1:2A:141:A:C8	1:2A:1408:C:O2'	2.69	0.40
1:2A:600:G:O3'	5:2F:108:LYS:HE3	2.21	0.40
1:2A:875:G:C2	1:2A:903:C:C2	3.10	0.40
1:2A:1035:U:H2'	1:2A:1036:G:C8	2.56	0.40
1:2A:1575:C:H2'	1:2A:1576:U:C6	2.57	0.40
1:2A:2111:C:N4	1:2A:2144:U:O2'	2.52	0.40
1:2A:2808:U:H5"	1:2A:2891:G:O6	2.20	0.40
7:2H:54:ARG:HB3	7:2H:65:HIS:CD2	2.56	0.40
12:2Q:18:LYS:HE3	12:2Q:18:LYS:HB2	1.94	0.40
32:2a:792:A:H4'	32:2a:793:U:H5"	2.04	0.40
33:2b:114:ARG:O	33:2b:118:LEU:HB2	2.21	0.40
33:2b:147:LYS:HG2	33:2b:148:TYR:CE1	2.56	0.40
37:2f:33:TYR:HE2	37:2f:78:GLU:HG2	1.86	0.40
38:2g:70:LYS:HD3	38:2g:96:GLN:HB3	2.03	0.40
44:2m:22:ILE:HG23	44:2m:67:GLU:HG3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	1D	273/276 (99%)	258 (94%)	15 (6%)	0	100 100
3	2D	273/276 (99%)	256 (94%)	17 (6%)	0	100 100
4	1E	202/206 (98%)	190 (94%)	11 (5%)	1 (0%)	24 34
4	2E	202/206 (98%)	192 (95%)	9 (4%)	1 (0%)	24 34
5	1F	200/210 (95%)	194 (97%)	5 (2%)	1 (0%)	24 34
5	2F	200/210 (95%)	188 (94%)	10 (5%)	2 (1%)	12 17
6	1G	179/182 (98%)	161 (90%)	16 (9%)	2 (1%)	11 15
6	2G	179/182 (98%)	157 (88%)	19 (11%)	3 (2%)	7 8
7	1H	172/180 (96%)	160 (93%)	11 (6%)	1 (1%)	21 29
7	2H	172/180 (96%)	157 (91%)	14 (8%)	1 (1%)	21 29
8	1I	144/148 (97%)	129 (90%)	15 (10%)	0	100 100
8	2I	144/148 (97%)	126 (88%)	17 (12%)	1 (1%)	18 25
9	1N	138/140 (99%)	130 (94%)	7 (5%)	1 (1%)	18 25
9	2N	138/140 (99%)	129 (94%)	8 (6%)	1 (1%)	18 25
10	1O	120/122 (98%)	113 (94%)	6 (5%)	1 (1%)	16 22
10	2O	120/122 (98%)	115 (96%)	4 (3%)	1 (1%)	16 22
11	1P	147/150 (98%)	136 (92%)	9 (6%)	2 (1%)	9 11
11	2P	147/150 (98%)	132 (90%)	13 (9%)	2 (1%)	9 11
12	1Q	139/141 (99%)	132 (95%)	7 (5%)	0	100 100
12	2Q	139/141 (99%)	131 (94%)	8 (6%)	0	100 100
13	1R	116/118 (98%)	111 (96%)	5 (4%)	0	100 100
13	2R	116/118 (98%)	113 (97%)	3 (3%)	0	100 100
14	1S	108/112 (96%)	104 (96%)	4 (4%)	0	100 100
14	2S	108/112 (96%)	100 (93%)	7 (6%)	1 (1%)	14 20
15	1T	129/146 (88%)	120 (93%)	7 (5%)	2 (2%)	7 9
15	2T	129/146 (88%)	124 (96%)	5 (4%)	0	100 100
16	1U	114/118 (97%)	114 (100%)	0	0	100 100
16	2U	114/118 (97%)	113 (99%)	1 (1%)	0	100 100
17	1V	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	12 17
17	2V	99/101 (98%)	93 (94%)	5 (5%)	1 (1%)	12 17
18	1W	110/113 (97%)	110 (100%)	0	0	100 100
18	2W	110/113 (97%)	108 (98%)	1 (1%)	1 (1%)	14 20

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
19	1X	93/96 (97%)	89 (96%)	2 (2%)	2 (2%)	5 5
19	2X	93/96 (97%)	88 (95%)	5 (5%)	0	100 100
20	1Y	105/110 (96%)	97 (92%)	6 (6%)	2 (2%)	6 7
20	2Y	105/110 (96%)	95 (90%)	7 (7%)	3 (3%)	3 3
21	1Z	148/206 (72%)	127 (86%)	19 (13%)	2 (1%)	9 11
21	2Z	156/206 (76%)	132 (85%)	22 (14%)	2 (1%)	9 12
22	10	81/85 (95%)	80 (99%)	1 (1%)	0	100 100
22	20	81/85 (95%)	79 (98%)	2 (2%)	0	100 100
23	11	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	11 15
23	21	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	11 15
24	12	68/72 (94%)	65 (96%)	3 (4%)	0	100 100
24	22	68/72 (94%)	67 (98%)	1 (2%)	0	100 100
25	13	57/60 (95%)	55 (96%)	2 (4%)	0	100 100
25	23	57/60 (95%)	54 (95%)	2 (4%)	1 (2%)	6 7
26	14	67/71 (94%)	53 (79%)	9 (13%)	5 (8%)	1 0
26	24	67/71 (94%)	49 (73%)	13 (19%)	5 (8%)	1 0
27	15	57/60 (95%)	57 (100%)	0	0	100 100
27	25	57/60 (95%)	56 (98%)	1 (2%)	0	100 100
28	16	51/54 (94%)	51 (100%)	0	0	100 100
28	26	51/54 (94%)	48 (94%)	3 (6%)	0	100 100
29	17	46/49 (94%)	45 (98%)	1 (2%)	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%)	62 (100%)	0	0	100 100
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%)	192 (84%)	30 (13%)	7 (3%)	3 2
33	2b	229/256 (90%)	181 (79%)	43 (19%)	5 (2%)	5 5
34	1c	204/239 (85%)	184 (90%)	20 (10%)	0	100 100
34	2c	204/239 (85%)	173 (85%)	29 (14%)	2 (1%)	12 17
35	1d	206/209 (99%)	188 (91%)	17 (8%)	1 (0%)	24 34

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
35	2d	206/209 (99%)	186 (90%)	20 (10%)	0	100 100
36	1e	146/162 (90%)	132 (90%)	13 (9%)	1 (1%)	18 25
36	2e	146/162 (90%)	130 (89%)	15 (10%)	1 (1%)	18 25
37	1f	98/101 (97%)	94 (96%)	3 (3%)	1 (1%)	12 17
37	2f	98/101 (97%)	94 (96%)	4 (4%)	0	100 100
38	1g	153/156 (98%)	142 (93%)	9 (6%)	2 (1%)	9 12
38	2g	153/156 (98%)	136 (89%)	14 (9%)	3 (2%)	6 6
39	1h	135/138 (98%)	127 (94%)	8 (6%)	0	100 100
39	2h	135/138 (98%)	125 (93%)	9 (7%)	1 (1%)	18 25
40	1i	125/128 (98%)	114 (91%)	10 (8%)	1 (1%)	16 22
40	2i	125/128 (98%)	102 (82%)	23 (18%)	0	100 100
41	1j	95/105 (90%)	83 (87%)	8 (8%)	4 (4%)	2 1
41	2j	94/105 (90%)	80 (85%)	10 (11%)	4 (4%)	2 1
42	1k	112/129 (87%)	101 (90%)	8 (7%)	3 (3%)	4 3
42	2k	112/129 (87%)	98 (88%)	13 (12%)	1 (1%)	14 20
43	1l	119/132 (90%)	114 (96%)	4 (3%)	1 (1%)	16 22
43	2l	119/132 (90%)	109 (92%)	9 (8%)	1 (1%)	16 22
44	1m	121/126 (96%)	107 (88%)	12 (10%)	2 (2%)	7 8
44	2m	120/126 (95%)	99 (82%)	18 (15%)	3 (2%)	4 4
45	1n	58/61 (95%)	56 (97%)	2 (3%)	0	100 100
45	2n	58/61 (95%)	54 (93%)	4 (7%)	0	100 100
46	1o	86/89 (97%)	81 (94%)	5 (6%)	0	100 100
46	2o	86/89 (97%)	81 (94%)	5 (6%)	0	100 100
47	1p	80/88 (91%)	70 (88%)	9 (11%)	1 (1%)	9 12
47	2p	80/88 (91%)	70 (88%)	10 (12%)	0	100 100
48	1q	97/105 (92%)	90 (93%)	7 (7%)	0	100 100
48	2q	97/105 (92%)	88 (91%)	7 (7%)	2 (2%)	5 5
49	1r	66/88 (75%)	62 (94%)	4 (6%)	0	100 100
49	2r	66/88 (75%)	64 (97%)	1 (2%)	1 (2%)	8 10
50	1s	81/93 (87%)	70 (86%)	10 (12%)	1 (1%)	10 13
50	2s	81/93 (87%)	64 (79%)	15 (18%)	2 (2%)	4 4

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
51	1t	94/106 (89%)	86 (92%)	5 (5%)	3 (3%)	3 2
51	2t	94/106 (89%)	83 (88%)	10 (11%)	1 (1%)	11 15
52	1u	21/27 (78%)	20 (95%)	1 (5%)	0	100 100
52	2u	21/27 (78%)	18 (86%)	3 (14%)	0	100 100
All	All	11368/12128 (94%)	10449 (92%)	813 (7%)	106 (1%)	14 20

All (106) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
21	1Z	53	ILE
26	14	47	GLN
26	14	49	PHE
26	14	62	ARG
33	1b	17	PHE
40	1i	54	ASP
44	1m	67	GLU
5	2F	130	ALA
6	2G	124	SER
33	2b	123	ALA
38	2g	80	VAL
44	2m	67	GLU
50	2s	12	ASP
6	1G	43	LEU
15	1T	37	GLY
19	1X	93	GLU
23	11	3	LYS
33	1b	8	LYS
33	1b	126	GLU
36	1e	85	GLY
41	1j	79	ARG
42	1k	77	MET
42	1k	105	VAL
8	2I	10	GLU
17	2V	79	VAL
20	2Y	55	TYR
26	24	3	GLU
26	24	45	GLY
33	2b	17	PHE
33	2b	20	GLU
34	2c	91	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	2e	85	GLY
38	2g	55	GLY
42	2k	49	GLY
49	2r	36	ASN
6	1G	96	ARG
17	1V	79	VAL
21	1Z	52	SER
33	1b	124	SER
5	2F	18	ARG
6	2G	51	ARG
7	2H	126	PRO
9	2N	2	LYS
11	2P	44	GLY
11	2P	45	LEU
26	24	48	ARG
33	2b	9	GLU
33	2b	10	LEU
41	2j	79	ARG
44	2m	106	ASN
48	2q	33	GLY
4	1E	52	LEU
9	1N	2	LYS
11	1P	29	LYS
11	1P	38	GLN
20	1Y	54	LYS
20	1Y	103	GLY
26	14	57	GLU
38	1g	114	ARG
41	1j	78	ASN
43	1l	105	TYR
51	1t	100	ILE
4	2E	52	LEU
6	2G	43	LEU
23	21	3	LYS
34	2c	156	ARG
43	2l	105	TYR
44	2m	63	THR
50	2s	81	ARG
7	1H	126	PRO
10	1O	5	GLN
15	1T	128	GLU
19	1X	2	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	1b	19	HIS
35	1d	175	SER
41	1j	29	ARG
44	1m	106	ASN
47	1p	76	GLN
51	1t	47	GLY
51	1t	95	ALA
10	2O	5	GLN
14	2S	96	GLY
18	2W	60	ASN
20	2Y	54	LYS
21	2Z	146	ILE
26	24	49	PHE
38	2g	52	GLU
41	2j	75	ILE
41	2j	78	ASN
48	2q	68	ARG
38	1g	54	THR
50	1s	27	GLU
20	2Y	11	ASP
21	2Z	52	SER
26	14	45	GLY
25	23	59	VAL
41	2j	41	PRO
33	1b	231	GLU
42	1k	49	GLY
37	1f	40	VAL
26	24	11	PRO
51	2t	47	GLY
41	1j	77	PRO
39	2h	86	ILE
33	1b	125	PRO

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	215/218 (99%)	202 (94%)	13 (6%)	17 26
3	2D	215/218 (99%)	204 (95%)	11 (5%)	21 33
4	1E	164/166 (99%)	157 (96%)	7 (4%)	26 39
4	2E	164/166 (99%)	153 (93%)	11 (7%)	15 21
5	1F	160/166 (96%)	141 (88%)	19 (12%)	5 5
5	2F	159/166 (96%)	152 (96%)	7 (4%)	25 38
6	1G	143/156 (92%)	131 (92%)	12 (8%)	10 14
6	2G	143/156 (92%)	123 (86%)	20 (14%)	3 3
7	1H	144/148 (97%)	137 (95%)	7 (5%)	22 34
7	2H	144/148 (97%)	132 (92%)	12 (8%)	10 14
8	1I	113/124 (91%)	94 (83%)	19 (17%)	2 2
8	2I	105/124 (85%)	92 (88%)	13 (12%)	4 4
9	1N	118/119 (99%)	109 (92%)	9 (8%)	12 17
9	2N	118/119 (99%)	111 (94%)	7 (6%)	18 27
10	1O	100/100 (100%)	96 (96%)	4 (4%)	28 42
10	2O	100/100 (100%)	97 (97%)	3 (3%)	36 53
11	1P	115/116 (99%)	104 (90%)	11 (10%)	8 9
11	2P	115/116 (99%)	104 (90%)	11 (10%)	8 9
12	1Q	111/111 (100%)	109 (98%)	2 (2%)	51 70
12	2Q	111/111 (100%)	104 (94%)	7 (6%)	16 23
13	1R	101/101 (100%)	93 (92%)	8 (8%)	11 16
13	2R	101/101 (100%)	95 (94%)	6 (6%)	18 27
14	1S	86/88 (98%)	77 (90%)	9 (10%)	6 8
14	2S	85/88 (97%)	75 (88%)	10 (12%)	5 5
15	1T	115/127 (91%)	109 (95%)	6 (5%)	21 32
15	2T	113/127 (89%)	105 (93%)	8 (7%)	13 19
16	1U	93/94 (99%)	89 (96%)	4 (4%)	26 39
16	2U	93/94 (99%)	89 (96%)	4 (4%)	26 39
17	1V	80/82 (98%)	78 (98%)	2 (2%)	42 60
17	2V	80/82 (98%)	74 (92%)	6 (8%)	12 17
18	1W	90/92 (98%)	87 (97%)	3 (3%)	33 50
18	2W	90/92 (98%)	85 (94%)	5 (6%)	19 29

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
19	1X	77/78 (99%)	76 (99%)	1 (1%)	61 76
19	2X	77/78 (99%)	75 (97%)	2 (3%)	40 59
20	1Y	85/91 (93%)	80 (94%)	5 (6%)	18 27
20	2Y	85/91 (93%)	79 (93%)	6 (7%)	13 19
21	1Z	135/179 (75%)	124 (92%)	11 (8%)	11 15
21	2Z	137/179 (76%)	121 (88%)	16 (12%)	5 6
22	10	65/67 (97%)	65 (100%)	0	100 100
22	20	65/67 (97%)	62 (95%)	3 (5%)	24 36
23	11	80/83 (96%)	78 (98%)	2 (2%)	42 60
23	21	80/83 (96%)	74 (92%)	6 (8%)	12 17
24	12	65/67 (97%)	63 (97%)	2 (3%)	35 53
24	22	65/67 (97%)	63 (97%)	2 (3%)	35 53
25	13	51/52 (98%)	46 (90%)	5 (10%)	7 9
25	23	50/52 (96%)	48 (96%)	2 (4%)	28 42
26	14	59/63 (94%)	50 (85%)	9 (15%)	3 2
26	24	53/63 (84%)	42 (79%)	11 (21%)	1 1
27	15	50/52 (96%)	48 (96%)	2 (4%)	28 42
27	25	50/52 (96%)	47 (94%)	3 (6%)	17 26
28	16	51/52 (98%)	49 (96%)	2 (4%)	28 43
28	26	50/52 (96%)	45 (90%)	5 (10%)	7 9
29	17	41/42 (98%)	38 (93%)	3 (7%)	13 18
29	27	41/42 (98%)	36 (88%)	5 (12%)	5 4
30	18	54/55 (98%)	52 (96%)	2 (4%)	30 45
30	28	54/55 (98%)	52 (96%)	2 (4%)	30 45
31	19	34/34 (100%)	34 (100%)	0	100 100
31	29	34/34 (100%)	31 (91%)	3 (9%)	9 12
33	1b	192/220 (87%)	175 (91%)	17 (9%)	9 12
33	2b	187/220 (85%)	162 (87%)	25 (13%)	4 3
34	1c	142/188 (76%)	124 (87%)	18 (13%)	4 4
34	2c	140/188 (74%)	123 (88%)	17 (12%)	5 5
35	1d	169/181 (93%)	149 (88%)	20 (12%)	5 5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
35	2d	173/181 (96%)	150 (87%)	23 (13%)	4 4
36	1e	113/123 (92%)	103 (91%)	10 (9%)	9 12
36	2e	114/123 (93%)	102 (90%)	12 (10%)	6 8
37	1f	84/90 (93%)	78 (93%)	6 (7%)	13 19
37	2f	85/90 (94%)	80 (94%)	5 (6%)	18 27
38	1g	119/127 (94%)	102 (86%)	17 (14%)	3 3
38	2g	120/127 (94%)	112 (93%)	8 (7%)	15 21
39	1h	114/119 (96%)	107 (94%)	7 (6%)	17 25
39	2h	114/119 (96%)	105 (92%)	9 (8%)	11 16
40	1i	90/99 (91%)	78 (87%)	12 (13%)	4 4
40	2i	89/99 (90%)	76 (85%)	13 (15%)	3 2
41	1j	66/92 (72%)	59 (89%)	7 (11%)	6 7
41	2j	69/92 (75%)	61 (88%)	8 (12%)	5 6
42	1k	82/99 (83%)	76 (93%)	6 (7%)	13 18
42	2k	83/99 (84%)	74 (89%)	9 (11%)	6 7
43	1l	96/108 (89%)	89 (93%)	7 (7%)	13 18
43	2l	96/108 (89%)	86 (90%)	10 (10%)	7 8
44	1m	93/101 (92%)	83 (89%)	10 (11%)	6 7
44	2m	92/101 (91%)	86 (94%)	6 (6%)	15 22
45	1n	49/50 (98%)	44 (90%)	5 (10%)	7 8
45	2n	49/50 (98%)	44 (90%)	5 (10%)	7 8
46	1o	78/80 (98%)	74 (95%)	4 (5%)	21 33
46	2o	78/80 (98%)	72 (92%)	6 (8%)	12 17
47	1p	69/74 (93%)	62 (90%)	7 (10%)	7 8
47	2p	68/74 (92%)	62 (91%)	6 (9%)	9 12
48	1q	94/97 (97%)	89 (95%)	5 (5%)	20 31
48	2q	94/97 (97%)	88 (94%)	6 (6%)	16 23
49	1r	59/77 (77%)	54 (92%)	5 (8%)	10 13
49	2r	59/77 (77%)	55 (93%)	4 (7%)	14 20
50	1s	69/80 (86%)	68 (99%)	1 (1%)	59 75
50	2s	67/80 (84%)	56 (84%)	11 (16%)	2 2

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
51	1t	70/82 (85%)	66 (94%)	4 (6%)	18 28
51	2t	70/82 (85%)	66 (94%)	4 (6%)	18 28
52	1u	18/22 (82%)	18 (100%)	0	100 100
52	2u	18/22 (82%)	17 (94%)	1 (6%)	19 29
All	All	9303/10064 (92%)	8561 (92%)	742 (8%)	11 15

All (742) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	3	VAL
3	1D	14	ARG
3	1D	16	MET
3	1D	38	LYS
3	1D	99	ASP
3	1D	126	GLN
3	1D	155	LEU
3	1D	173	VAL
3	1D	229	VAL
3	1D	242	ARG
3	1D	259	THR
3	1D	273	ARG
3	1D	275	LYS
4	1E	14	ILE
4	1E	21	VAL
4	1E	73	GLU
4	1E	116	VAL
4	1E	128	SER
4	1E	181	LEU
4	1E	184	VAL
5	1F	9	ILE
5	1F	20	LEU
5	1F	24	LEU
5	1F	28	ILE
5	1F	53	THR
5	1F	57	VAL
5	1F	70	THR
5	1F	74	ARG
5	1F	88	VAL
5	1F	106	ARG
5	1F	127	GLU
5	1F	144	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	1F	162	LEU
5	1F	168	ARG
5	1F	175	THR
5	1F	183	VAL
5	1F	192	LEU
5	1F	201	VAL
5	1F	205	ARG
6	1G	3	LEU
6	1G	4	ASP
6	1G	7	LEU
6	1G	31	VAL
6	1G	43	LEU
6	1G	49	ASP
6	1G	79	ASN
6	1G	82	LEU
6	1G	126	ASP
6	1G	133	LEU
6	1G	148	MET
6	1G	159	VAL
7	1H	3	ARG
7	1H	15	VAL
7	1H	30	LYS
7	1H	62	LYS
7	1H	85	LYS
7	1H	127	GLU
7	1H	155	SER
8	1I	2	LYS
8	1I	10	GLU
8	1I	20	ASP
8	1I	38	LEU
8	1I	47	LEU
8	1I	75	LEU
8	1I	76	THR
8	1I	77	LEU
8	1I	78	THR
8	1I	85	GLU
8	1I	87	LYS
8	1I	92	VAL
8	1I	108	THR
8	1I	109	ILE
8	1I	116	LEU
8	1I	122	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	1I	127	VAL
8	1I	133	HIS
8	1I	142	VAL
9	1N	1	MET
9	1N	10	GLU
9	1N	14	VAL
9	1N	28	THR
9	1N	48	MET
9	1N	67	LEU
9	1N	96	GLU
9	1N	134	ARG
9	1N	140	VAL
10	1O	28	SER
10	1O	66	LYS
10	1O	108	GLU
10	1O	113	LYS
11	1P	7	ARG
11	1P	36	LYS
11	1P	45	LEU
11	1P	56	SER
11	1P	65	ARG
11	1P	75	ILE
11	1P	90	ARG
11	1P	96	THR
11	1P	126	VAL
11	1P	135	LEU
11	1P	147	LEU
12	1Q	6	ARG
12	1Q	75	THR
13	1R	8	ARG
13	1R	36	THR
13	1R	59	ASP
13	1R	67	LEU
13	1R	99	LYS
13	1R	104	ARG
13	1R	111	LEU
13	1R	114	VAL
14	1S	14	VAL
14	1S	25	ARG
14	1S	33	LYS
14	1S	36	TYR
14	1S	46	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	1S	69	VAL
14	1S	73	LEU
14	1S	85	VAL
14	1S	110	LEU
15	1T	28	VAL
15	1T	34	VAL
15	1T	36	GLU
15	1T	49	VAL
15	1T	67	SER
15	1T	128	GLU
16	1U	27	LEU
16	1U	74	LEU
16	1U	77	SER
16	1U	100	VAL
17	1V	61	VAL
17	1V	79	VAL
18	1W	11	ARG
18	1W	17	VAL
18	1W	63	ASP
19	1X	68	ARG
20	1Y	7	VAL
20	1Y	23	ARG
20	1Y	72	VAL
20	1Y	101	LYS
20	1Y	106	LEU
21	1Z	50	GLN
21	1Z	61	LEU
21	1Z	66	SER
21	1Z	70	LEU
21	1Z	128	VAL
21	1Z	132	ASN
21	1Z	135	GLU
21	1Z	154	ASP
21	1Z	155	LEU
21	1Z	170	THR
21	1Z	171	ILE
23	11	65	SER
23	11	74	VAL
24	12	1	MET
24	12	40	SER
25	13	7	LYS
25	13	23	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	13	54	VAL
25	13	55	ARG
25	13	60	GLU
26	14	5	ILE
26	14	33	VAL
26	14	49	PHE
26	14	52	THR
26	14	53	GLU
26	14	59	PHE
26	14	60	GLN
26	14	63	TYR
26	14	67	TYR
27	15	6	VAL
27	15	40	LYS
28	16	4	GLU
28	16	19	ARG
29	17	24	THR
29	17	43	THR
29	17	46	VAL
30	18	14	VAL
30	18	29	LYS
33	1b	7	VAL
33	1b	8	LYS
33	1b	11	LEU
33	1b	12	GLU
33	1b	35	GLU
33	1b	39	ILE
33	1b	45	GLN
33	1b	54	THR
33	1b	64	ARG
33	1b	67	THR
33	1b	76	GLN
33	1b	80	ILE
33	1b	112	VAL
33	1b	147	LYS
33	1b	185	ILE
33	1b	212	GLN
33	1b	215	LEU
34	1c	3	ASN
34	1c	15	THR
34	1c	26	LYS
34	1c	46	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	1c	64	VAL
34	1c	68	VAL
34	1c	70	VAL
34	1c	89	GLU
34	1c	91	LEU
34	1c	97	LYS
34	1c	103	VAL
34	1c	105	GLU
34	1c	138	VAL
34	1c	165	THR
34	1c	188	LEU
34	1c	196	LEU
34	1c	198	VAL
34	1c	202	ILE
35	1d	5	ILE
35	1d	19	LEU
35	1d	28	SER
35	1d	31	CYS
35	1d	56	VAL
35	1d	59	ARG
35	1d	70	ILE
35	1d	88	VAL
35	1d	112	VAL
35	1d	135	LEU
35	1d	141	ARG
35	1d	144	ASP
35	1d	157	LEU
35	1d	158	ILE
35	1d	175	SER
35	1d	177	ASP
35	1d	178	VAL
35	1d	181	MET
35	1d	188	LEU
35	1d	194	LEU
36	1e	10	MET
36	1e	20	GLN
36	1e	33	VAL
36	1e	41	VAL
36	1e	51	VAL
36	1e	56	GLN
36	1e	63	ARG
36	1e	67	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	1e	126	ARG
36	1e	151	LEU
37	1f	36	ARG
37	1f	72	VAL
37	1f	75	LEU
37	1f	77	ARG
37	1f	78	GLU
37	1f	81	ILE
38	1g	8	GLU
38	1g	10	ARG
38	1g	12	LEU
38	1g	24	THR
38	1g	27	ILE
38	1g	32	ARG
38	1g	50	ILE
38	1g	59	LEU
38	1g	61	VAL
38	1g	78	ARG
38	1g	89	MET
38	1g	104	LEU
38	1g	113	GLU
38	1g	138	LYS
38	1g	140	ASP
38	1g	143	ARG
38	1g	156	TRP
39	1h	39	LEU
39	1h	51	VAL
39	1h	52	ASP
39	1h	54	ASP
39	1h	99	GLU
39	1h	112	LEU
39	1h	122	ARG
40	1i	23	ASN
40	1i	25	LYS
40	1i	34	ASN
40	1i	50	LEU
40	1i	53	VAL
40	1i	71	SER
40	1i	74	ILE
40	1i	89	ASN
40	1i	96	LEU
40	1i	97	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	1i	103	THR
40	1i	111	ARG
41	1j	38	ILE
41	1j	42	THR
41	1j	48	THR
41	1j	49	VAL
41	1j	81	THR
41	1j	94	VAL
41	1j	98	ILE
42	1k	14	VAL
42	1k	33	THR
42	1k	48	ILE
42	1k	87	THR
42	1k	114	VAL
42	1k	117	ASN
43	1l	18	VAL
43	1l	33	ARG
43	1l	36	VAL
43	1l	46	LYS
43	1l	70	ILE
43	1l	116	SER
43	1l	123	LYS
44	1m	4	ILE
44	1m	17	VAL
44	1m	19	LEU
44	1m	43	THR
44	1m	49	THR
44	1m	70	LEU
44	1m	106	ASN
44	1m	109	THR
44	1m	120	LYS
44	1m	121	LYS
45	1n	15	LYS
45	1n	18	VAL
45	1n	33	VAL
45	1n	41	ARG
45	1n	56	VAL
46	1o	39	LEU
46	1o	45	VAL
46	1o	56	LEU
46	1o	76	GLU
47	1p	5	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
47	1p	19	ILE
47	1p	20	VAL
47	1p	21	VAL
47	1p	60	LEU
47	1p	62	VAL
47	1p	76	GLN
48	1q	9	VAL
48	1q	57	VAL
48	1q	60	ILE
48	1q	78	GLU
48	1q	79	SER
49	1r	37	VAL
49	1r	46	GLU
49	1r	47	THR
49	1r	49	LYS
49	1r	61	LYS
50	1s	6	LYS
51	1t	10	LEU
51	1t	24	LEU
51	1t	53	LEU
51	1t	100	ILE
3	2D	3	VAL
3	2D	38	LYS
3	2D	141	VAL
3	2D	155	LEU
3	2D	162	SER
3	2D	173	VAL
3	2D	211	ARG
3	2D	229	VAL
3	2D	242	ARG
3	2D	259	THR
3	2D	275	LYS
4	2E	7	VAL
4	2E	14	ILE
4	2E	21	VAL
4	2E	73	GLU
4	2E	81	ILE
4	2E	90	THR
4	2E	116	VAL
4	2E	134	ILE
4	2E	175	VAL
4	2E	178	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	2E	181	LEU
5	2F	33	LEU
5	2F	135	LYS
5	2F	144	LYS
5	2F	158	THR
5	2F	162	LEU
5	2F	186	ILE
5	2F	192	LEU
6	2G	5	VAL
6	2G	7	LEU
6	2G	19	LEU
6	2G	28	VAL
6	2G	31	VAL
6	2G	41	GLN
6	2G	43	LEU
6	2G	47	LYS
6	2G	49	ASP
6	2G	88	ILE
6	2G	91	ARG
6	2G	124	SER
6	2G	135	LEU
6	2G	137	GLU
6	2G	140	ILE
6	2G	148	MET
6	2G	149	VAL
6	2G	159	VAL
6	2G	161	THR
6	2G	173	LEU
7	2H	4	ILE
7	2H	7	LEU
7	2H	15	VAL
7	2H	43	VAL
7	2H	44	VAL
7	2H	45	VAL
7	2H	51	ARG
7	2H	81	GLU
7	2H	85	LYS
7	2H	103	LEU
7	2H	130	ARG
7	2H	133	VAL
8	2I	15	VAL
8	2I	20	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	2I	38	LEU
8	2I	40	THR
8	2I	58	LEU
8	2I	61	ARG
8	2I	68	LEU
8	2I	69	LYS
8	2I	81	VAL
8	2I	82	ARG
8	2I	92	VAL
8	2I	116	LEU
8	2I	117	GLU
9	2N	5	VAL
9	2N	14	VAL
9	2N	15	LEU
9	2N	28	THR
9	2N	38	HIS
9	2N	67	LEU
9	2N	131	GLN
10	2O	9	GLU
10	2O	69	ILE
10	2O	113	LYS
11	2P	7	ARG
11	2P	45	LEU
11	2P	65	ARG
11	2P	90	ARG
11	2P	95	VAL
11	2P	96	THR
11	2P	99	LEU
11	2P	131	SER
11	2P	133	SER
11	2P	135	LEU
11	2P	136	GLU
12	2Q	7	MET
12	2Q	12	GLN
12	2Q	22	LYS
12	2Q	56	ARG
12	2Q	75	THR
12	2Q	106	VAL
12	2Q	110	THR
13	2R	24	GLN
13	2R	36	THR
13	2R	67	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	2R	95	THR
13	2R	111	LEU
13	2R	114	VAL
14	2S	28	VAL
14	2S	35	ILE
14	2S	36	TYR
14	2S	44	LYS
14	2S	49	VAL
14	2S	58	LEU
14	2S	63	THR
14	2S	75	GLU
14	2S	85	VAL
14	2S	110	LEU
15	2T	18	ASP
15	2T	28	VAL
15	2T	34	VAL
15	2T	39	ARG
15	2T	85	LYS
15	2T	89	VAL
15	2T	96	ARG
15	2T	104	ASN
16	2U	5	LYS
16	2U	65	ILE
16	2U	74	LEU
16	2U	77	SER
17	2V	7	THR
17	2V	56	SER
17	2V	57	VAL
17	2V	61	VAL
17	2V	79	VAL
17	2V	85	LYS
18	2W	11	ARG
18	2W	60	ASN
18	2W	63	ASP
18	2W	67	ASP
18	2W	96	ILE
19	2X	45	THR
19	2X	81	VAL
20	2Y	1	MET
20	2Y	70	SER
20	2Y	72	VAL
20	2Y	85	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	2Y	98	VAL
20	2Y	99	CYS
21	2Z	5	LEU
21	2Z	18	LEU
21	2Z	42	VAL
21	2Z	66	SER
21	2Z	70	LEU
21	2Z	71	VAL
21	2Z	98	MET
21	2Z	121	HIS
21	2Z	129	SER
21	2Z	150	LEU
21	2Z	151	HIS
21	2Z	154	ASP
21	2Z	155	LEU
21	2Z	161	VAL
21	2Z	171	ILE
21	2Z	174	VAL
22	20	10	THR
22	20	67	VAL
22	20	68	GLU
23	21	35	THR
23	21	40	ARG
23	21	46	LEU
23	21	56	GLN
23	21	81	LYS
23	21	89	GLU
24	22	35	LEU
24	22	70	GLN
25	23	54	VAL
25	23	59	VAL
26	24	10	VAL
26	24	21	VAL
26	24	24	THR
26	24	33	VAL
26	24	34	GLU
26	24	49	PHE
26	24	50	VAL
26	24	59	PHE
26	24	63	TYR
26	24	67	TYR
26	24	68	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	25	6	VAL
27	25	40	LYS
27	25	58	LEU
28	26	9	LEU
28	26	29	ASN
28	26	32	ASN
28	26	34	LEU
28	26	48	VAL
29	27	1	MET
29	27	4	THR
29	27	41	ARG
29	27	43	THR
29	27	46	VAL
30	28	14	VAL
30	28	29	LYS
31	29	6	SER
31	29	7	VAL
31	29	14	CYS
33	2b	7	VAL
33	2b	8	LYS
33	2b	16	HIS
33	2b	49	GLU
33	2b	67	THR
33	2b	68	ILE
33	2b	71	VAL
33	2b	73	THR
33	2b	76	GLN
33	2b	80	ILE
33	2b	101	MET
33	2b	107	THR
33	2b	112	VAL
33	2b	115	LEU
33	2b	118	LEU
33	2b	127	ILE
33	2b	138	LEU
33	2b	142	LEU
33	2b	164	VAL
33	2b	184	VAL
33	2b	185	ILE
33	2b	189	ASP
33	2b	204	ASN
33	2b	223	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	2b	233	SER
34	2c	15	THR
34	2c	35	GLU
34	2c	46	GLU
34	2c	47	LEU
34	2c	55	VAL
34	2c	70	VAL
34	2c	104	GLN
34	2c	105	GLU
34	2c	111	LEU
34	2c	128	PHE
34	2c	141	VAL
34	2c	153	VAL
34	2c	161	GLU
34	2c	173	VAL
34	2c	182	ILE
34	2c	190	ARG
34	2c	191	THR
35	2d	5	ILE
35	2d	8	VAL
35	2d	12	CYS
35	2d	34	GLU
35	2d	47	ARG
35	2d	53	ASP
35	2d	58	LEU
35	2d	59	ARG
35	2d	60	GLU
35	2d	76	ARG
35	2d	78	LEU
35	2d	83	SER
35	2d	86	LYS
35	2d	96	LEU
35	2d	120	LEU
35	2d	123	HIS
35	2d	127	THR
35	2d	135	LEU
35	2d	150	GLU
35	2d	155	LEU
35	2d	156	GLU
35	2d	158	ILE
35	2d	178	VAL
36	2e	5	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	2e	9	LYS
36	2e	13	ILE
36	2e	18	ARG
36	2e	20	GLN
36	2e	41	VAL
36	2e	43	LEU
36	2e	51	VAL
36	2e	55	VAL
36	2e	73	ASN
36	2e	76	ILE
36	2e	115	VAL
37	2f	21	LEU
37	2f	63	TYR
37	2f	69	GLU
37	2f	72	VAL
37	2f	81	ILE
38	2g	15	ASP
38	2g	23	VAL
38	2g	52	GLU
38	2g	64	GLN
38	2g	78	ARG
38	2g	89	MET
38	2g	131	LYS
38	2g	146	GLU
39	2h	10	LEU
39	2h	26	VAL
39	2h	51	VAL
39	2h	52	ASP
39	2h	77	GLU
39	2h	109	ILE
39	2h	112	LEU
39	2h	113	SER
39	2h	137	VAL
40	2i	29	ASN
40	2i	32	ASP
40	2i	35	GLU
40	2i	38	GLN
40	2i	58	HIS
40	2i	65	VAL
40	2i	66	ARG
40	2i	86	VAL
40	2i	99	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	2i	108	VAL
40	2i	109	VAL
40	2i	114	TYR
40	2i	128	ARG
41	2j	6	ILE
41	2j	38	ILE
41	2j	61	GLU
41	2j	67	THR
41	2j	68	HIS
41	2j	69	ASN
41	2j	96	ILE
41	2j	97	GLU
42	2k	14	VAL
42	2k	30	VAL
42	2k	41	THR
42	2k	48	ILE
42	2k	54	ARG
42	2k	78	GLN
42	2k	105	VAL
42	2k	109	VAL
42	2k	114	VAL
43	2l	18	VAL
43	2l	33	ARG
43	2l	36	VAL
43	2l	40	VAL
43	2l	43	VAL
43	2l	53	ARG
43	2l	59	ARG
43	2l	62	SER
43	2l	112	ASP
43	2l	116	SER
44	2m	4	ILE
44	2m	15	VAL
44	2m	62	ASN
44	2m	81	LEU
44	2m	98	VAL
44	2m	106	ASN
45	2n	13	THR
45	2n	15	LYS
45	2n	18	VAL
45	2n	41	ARG
45	2n	58	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
46	2o	5	LYS
46	2o	35	ARG
46	2o	39	LEU
46	2o	76	GLU
46	2o	83	GLU
46	2o	87	ILE
47	2p	1	MET
47	2p	2	VAL
47	2p	20	VAL
47	2p	21	VAL
47	2p	73	LEU
47	2p	74	LEU
48	2q	5	VAL
48	2q	53	LEU
48	2q	60	ILE
48	2q	65	ILE
48	2q	66	SER
48	2q	99	SER
49	2r	28	GLU
49	2r	37	VAL
49	2r	46	GLU
49	2r	85	LEU
50	2s	5	LEU
50	2s	14	HIS
50	2s	16	LEU
50	2s	22	LEU
50	2s	27	GLU
50	2s	31	ILE
50	2s	37	ARG
50	2s	43	GLU
50	2s	45	VAL
50	2s	48	THR
50	2s	49	ILE
51	2t	9	ASN
51	2t	41	ILE
51	2t	46	GLU
51	2t	89	ARG
52	2u	9	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (145) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	87	ASN
3	1D	201	HIS
5	1F	8	GLN
5	1F	69	HIS
6	1G	26	GLN
9	1N	94	HIS
9	1N	131	GLN
10	1O	3	GLN
12	1Q	12	GLN
12	1Q	57	HIS
13	1R	71	GLN
14	1S	68	GLN
14	1S	95	HIS
15	1T	84	GLN
16	1U	94	ASN
18	1W	111	HIS
19	1X	31	HIS
19	1X	82	GLN
20	1Y	6	HIS
21	1Z	34	ASN
21	1Z	73	GLN
21	1Z	121	HIS
21	1Z	151	HIS
23	11	56	GLN
24	12	46	GLN
33	1b	40	HIS
33	1b	45	GLN
33	1b	95	GLN
33	1b	212	GLN
34	1c	6	HIS
34	1c	98	ASN
34	1c	118	GLN
34	1c	123	GLN
34	1c	162	GLN
34	1c	170	GLN
34	1c	176	HIS
34	1c	181	ASN
35	1d	77	ASN
35	1d	119	GLN
35	1d	123	HIS
35	1d	160	GLN
35	1d	161	ASN
36	1e	78	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	1f	18	GLN
37	1f	57	GLN
37	1f	100	ASN
38	1g	28	ASN
38	1g	86	GLN
40	1i	3	GLN
40	1i	31	GLN
40	1i	34	ASN
40	1i	58	HIS
40	1i	73	GLN
40	1i	124	GLN
41	1j	56	HIS
43	1l	99	HIS
44	1m	77	ASN
44	1m	106	ASN
46	1o	9	GLN
46	1o	46	HIS
47	1p	13	HIS
48	1q	93	GLN
49	1r	63	GLN
50	1s	23	ASN
50	1s	47	HIS
50	1s	83	HIS
51	1t	90	GLN
3	2D	87	ASN
3	2D	115	GLN
3	2D	166	GLN
4	2E	48	GLN
5	2F	69	HIS
5	2F	160	ASN
6	2G	41	GLN
6	2G	58	GLN
6	2G	132	ASN
7	2H	74	ASN
8	2I	11	ASN
8	2I	74	ASN
8	2I	133	HIS
8	2I	139	GLN
9	2N	94	HIS
9	2N	131	GLN
10	2O	3	GLN
12	2Q	12	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	2R	50	HIS
14	2S	38	GLN
14	2S	84	GLN
15	2T	43	GLN
15	2T	58	ASN
16	2U	72	HIS
16	2U	94	ASN
19	2X	31	HIS
19	2X	82	GLN
21	2Z	73	GLN
22	20	50	ASN
23	21	56	GLN
24	22	70	GLN
25	23	32	GLN
26	24	46	GLN
33	2b	76	GLN
33	2b	110	GLN
33	2b	135	GLN
33	2b	140	HIS
34	2c	6	HIS
34	2c	123	GLN
34	2c	162	GLN
34	2c	181	ASN
35	2d	45	GLN
35	2d	77	ASN
35	2d	116	GLN
35	2d	119	GLN
35	2d	123	HIS
35	2d	125	HIS
36	2e	72	GLN
36	2e	78	HIS
36	2e	141	GLN
37	2f	73	ASN
37	2f	94	GLN
37	2f	100	ASN
38	2g	11	GLN
38	2g	28	ASN
38	2g	86	GLN
40	2i	3	GLN
40	2i	58	HIS
40	2i	73	GLN
41	2j	13	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	2j	21	GLN
41	2j	68	HIS
42	2k	62	GLN
42	2k	93	GLN
42	2k	104	GLN
42	2k	117	ASN
43	2l	99	HIS
44	2m	77	ASN
46	2o	9	GLN
47	2p	16	HIS
48	2q	26	GLN
48	2q	93	GLN
49	2r	63	GLN
50	2s	57	HIS
50	2s	69	HIS
50	2s	83	HIS
51	2t	45	GLN
51	2t	75	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	418 (14%)	32 (1%)
1	2A	2791/2915 (95%)	430 (15%)	25 (0%)
2	1B	119/121 (98%)	7 (5%)	0
2	2B	118/121 (97%)	23 (19%)	0
32	1a	1497/1521 (98%)	234 (15%)	0
32	2a	1501/1521 (98%)	283 (18%)	0
53	1v	12/24 (50%)	2 (16%)	0
53	2v	12/24 (50%)	2 (16%)	0
54	1w	70/74 (94%)	27 (38%)	0
54	2w	68/74 (91%)	31 (45%)	0
55	1x	75/77 (97%)	7 (9%)	0
55	2x	75/77 (97%)	7 (9%)	0
56	1y	71/74 (95%)	29 (40%)	0
56	2y	71/74 (95%)	35 (49%)	0
All	All	9344/9612 (97%)	1535 (16%)	57 (0%)

All (1535) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	10	G
1	1A	12	U
1	1A	34	C
1	1A	45	C
1	1A	71	A
1	1A	74	A
1	1A	75	G
1	1A	84	A
1	1A	118	A
1	1A	119	A
1	1A	120	U
1	1A	154(A)	C
1	1A	188	G
1	1A	196	A
1	1A	197	A
1	1A	199	A
1	1A	205	G
1	1A	214	G
1	1A	215	G
1	1A	216	A
1	1A	221	A
1	1A	222	A
1	1A	225	A
1	1A	228	A
1	1A	229	A
1	1A	233	A
1	1A	248	G
1	1A	269	U
1	1A	271(A)	A
1	1A	271(C)	C
1	1A	271(K)	U
1	1A	271(L)	U
1	1A	271(M)	G
1	1A	271(O)	C
1	1A	271(S)	G
1	1A	272(A)	U
1	1A	272(B)	G
1	1A	272(I)	U
1	1A	275	G
1	1A	279	C
1	1A	311	A
1	1A	329	G
1	1A	330	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	342	G
1	1A	352	G
1	1A	357	A
1	1A	363	G
1	1A	363(A)	A
1	1A	363(B)	G
1	1A	370	G
1	1A	386	G
1	1A	396	G
1	1A	405	U
1	1A	411	G
1	1A	412	A
1	1A	428	A
1	1A	444	C
1	1A	448	U
1	1A	451	C
1	1A	456	C
1	1A	457	A
1	1A	481	G
1	1A	494	G
1	1A	504	U
1	1A	505	A
1	1A	509	C
1	1A	530	G
1	1A	531	C
1	1A	532	A
1	1A	533	G
1	1A	545	G
1	1A	549	G
1	1A	563	G
1	1A	568	U
1	1A	573	G
1	1A	574	C
1	1A	575	A
1	1A	586	A
1	1A	603	A
1	1A	604	G
1	1A	607	U
1	1A	614(A)	U
1	1A	614(B)	G
1	1A	615	G
1	1A	627	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	637	A
1	1A	645	C
1	1A	646	A
1	1A	652(D)	C
1	1A	652(E)	G
1	1A	652(F)	G
1	1A	652(T)	C
1	1A	669	G
1	1A	686	G
1	1A	730	C
1	1A	746	A
1	1A	747	U
1	1A	764	A
1	1A	765	G
1	1A	775	G
1	1A	776	G
1	1A	782	A
1	1A	783	A
1	1A	784	A
1	1A	785	G
1	1A	790	C
1	1A	792	G
1	1A	805	G
1	1A	812	C
1	1A	819	A
1	1A	827	U
1	1A	828	U
1	1A	859	G
1	1A	866	A
1	1A	877	U
1	1A	879	G
1	1A	880	G
1	1A	882	G
1	1A	883	G
1	1A	884	C
1	1A	885	C
1	1A	886	C
1	1A	887	A
1	1A	888	C
1	1A	889	C
1	1A	890	A
1	1A	895	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	896	A
1	1A	897	C
1	1A	898	C
1	1A	907	U
1	1A	910	A
1	1A	932	G
1	1A	938	G
1	1A	945	A
1	1A	946	G
1	1A	959	A
1	1A	961	C
1	1A	974	G
1	1A	975	C
1	1A	983	A
1	1A	996	A
1	1A	1012	U
1	1A	1013	C
1	1A	1026	U
1	1A	1033	U
1	1A	1041	C
1	1A	1044	G
1	1A	1046	A
1	1A	1047	G
1	1A	1054	A
1	1A	1055	G
1	1A	1058	G
1	1A	1060	U
1	1A	1063	G
1	1A	1066	U
1	1A	1069	A
1	1A	1070	A
1	1A	1071	G
1	1A	1073	A
1	1A	1075	C
1	1A	1076	C
1	1A	1077	A
1	1A	1078	U
1	1A	1079	C
1	1A	1080	C
1	1A	1083	U
1	1A	1087	G
1	1A	1088	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1089	G
1	1A	1090	U
1	1A	1091	G
1	1A	1093	G
1	1A	1094	U
1	1A	1096	A
1	1A	1097	U
1	1A	1101	U
1	1A	1110	G
1	1A	1111	A
1	1A	1112	G
1	1A	1116	C
1	1A	1135	C
1	1A	1136	G
1	1A	1141	U
1	1A	1171	G
1	1A	1173	G
1	1A	1174	A
1	1A	1175	U
1	1A	1176	G
1	1A	1177	A
1	1A	1178	C
1	1A	1220	A
1	1A	1244	G
1	1A	1247	A
1	1A	1253	A
1	1A	1256	G
1	1A	1271	G
1	1A	1272	A
1	1A	1275	A
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	1380	G
1	1A	1384	A
1	1A	1385	G
1	1A	1396	U
1	1A	1416	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1417	C
1	1A	1420	U
1	1A	1421	G
1	1A	1428	C
1	1A	1445	A
1	1A	1450	G
1	1A	1455	G
1	1A	1467	C
1	1A	1482	G
1	1A	1493	C
1	1A	1494	A
1	1A	1508	A
1	1A	1509	C
1	1A	1509(A)	A
1	1A	1532	C
1	1A	1540	U
1	1A	1558	A
1	1A	1566	A
1	1A	1569	A
1	1A	1578	U
1	1A	1581	G
1	1A	1582	C
1	1A	1584	C
1	1A	1586	A
1	1A	1608	A
1	1A	1609	A
1	1A	1647	G
1	1A	1648	C
1	1A	1674	G
1	1A	1696	G
1	1A	1700	A
1	1A	1703	G
1	1A	1722	A
1	1A	1739	U
1	1A	1746	G
1	1A	1756	G
1	1A	1763	G
1	1A	1764	G
1	1A	1773	A
1	1A	1780	A
1	1A	1782	C
1	1A	1791	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1800	C
1	1A	1801	G
1	1A	1816	G
1	1A	1828	G
1	1A	1829	A
1	1A	1839	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	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	2039	C
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	2102	U
1	1A	2108	C
1	1A	2113	U
1	1A	2116	G
1	1A	2118	U
1	1A	2121	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2123	G
1	1A	2126	A
1	1A	2127	G
1	1A	2129	C
1	1A	2131	G
1	1A	2132	U
1	1A	2133	G
1	1A	2134	A
1	1A	2135	A
1	1A	2136	C
1	1A	2140	C
1	1A	2142	C
1	1A	2143	C
1	1A	2144	U
1	1A	2146	C
1	1A	2149	G
1	1A	2150	U
1	1A	2151	G
1	1A	2156	G
1	1A	2157	G
1	1A	2158	A
1	1A	2159	G
1	1A	2165	G
1	1A	2166	G
1	1A	2169	A
1	1A	2172	U
1	1A	2173	A
1	1A	2174	C
1	1A	2181	G
1	1A	2182	G
1	1A	2184	G
1	1A	2189	U
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	2219	G
1	1A	2225	A
1	1A	2238	G
1	1A	2239	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2268	A
1	1A	2269	A
1	1A	2280	G
1	1A	2283	C
1	1A	2287	A
1	1A	2305	A
1	1A	2308	G
1	1A	2320	A
1	1A	2321	G
1	1A	2325	G
1	1A	2334	G
1	1A	2347	C
1	1A	2350	C
1	1A	2354	G
1	1A	2361	A
1	1A	2383	G
1	1A	2385	C
1	1A	2400	G
1	1A	2406	U
1	1A	2407	G
1	1A	2422	A
1	1A	2423	U
1	1A	2425	A
1	1A	2429	G
1	1A	2430	A
1	1A	2431	U
1	1A	2434	A
1	1A	2435	A
1	1A	2439	A
1	1A	2441	C
1	1A	2448	A
1	1A	2468	G
1	1A	2476	A
1	1A	2478	A
1	1A	2491	U
1	1A	2502	G
1	1A	2505	G
1	1A	2518	A
1	1A	2529	G
1	1A	2535	G
1	1A	2550	G
1	1A	2554	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2566	A
1	1A	2567	G
1	1A	2573	C
1	1A	2574	G
1	1A	2602	A
1	1A	2609	U
1	1A	2611	U
1	1A	2612	C
1	1A	2629	A
1	1A	2630	G
1	1A	2654	A
1	1A	2689	U
1	1A	2690	C
1	1A	2691	C
1	1A	2703	C
1	1A	2712(A)	A
1	1A	2713	A
1	1A	2714	G
1	1A	2726	U
1	1A	2733	A
1	1A	2757	A
1	1A	2758	A
1	1A	2765	A
1	1A	2778	A
1	1A	2790	A
1	1A	2791	C
1	1A	2793	G
1	1A	2794	C
1	1A	2802	G
1	1A	2803	C
1	1A	2820	A
1	1A	2821	A
1	1A	2835	A
1	1A	2872	G
1	1A	2880	C
1	1A	2882	A
1	1A	2892	A
1	1A	2894	G
1	1A	2895	U
2	1B	2	C
2	1B	32	C
2	1B	56	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	1B	67	G
2	1B	73	A
2	1B	106	G
2	1B	110	G
32	1a	7	G
32	1a	9	G
32	1a	32	A
32	1a	39	G
32	1a	47	C
32	1a	48	C
32	1a	51	A
32	1a	52	G
32	1a	61	G
32	1a	76	C
32	1a	79	G
32	1a	91	C
32	1a	98	G
32	1a	101	A
32	1a	105	G
32	1a	111	G
32	1a	115	G
32	1a	116	A
32	1a	117	G
32	1a	121	C
32	1a	131	C
32	1a	144	G
32	1a	162	A
32	1a	163	C
32	1a	174	C
32	1a	180	U
32	1a	182	U
32	1a	189(C)	C
32	1a	189(J)	G
32	1a	195	A
32	1a	197	A
32	1a	199	G
32	1a	202	U
32	1a	203	U
32	1a	204	U
32	1a	222	U
32	1a	231	G
32	1a	247	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	251	G
32	1a	266	G
32	1a	267	C
32	1a	289	G
32	1a	328	C
32	1a	329	A
32	1a	332	G
32	1a	344	A
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	384	G
32	1a	397	A
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	413	G
32	1a	422	C
32	1a	423	G
32	1a	424	G
32	1a	429	U
32	1a	439	A
32	1a	441	A
32	1a	442	C
32	1a	452	A
32	1a	461	A
32	1a	470	C
32	1a	483	C
32	1a	485	G
32	1a	492	G
32	1a	496	A
32	1a	498	U
32	1a	509	A
32	1a	510	A
32	1a	511	C
32	1a	518	C
32	1a	521	G
32	1a	524	G
32	1a	527	G7M

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	531	U
32	1a	532	A
32	1a	547	A
32	1a	559	A
32	1a	560	U
32	1a	561	U
32	1a	568	G
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	596	C
32	1a	627	G
32	1a	630	G
32	1a	634	C
32	1a	653	A
32	1a	662	G
32	1a	665	A
32	1a	687	A
32	1a	688	G
32	1a	695	A
32	1a	722	A
32	1a	723	U
32	1a	731	G
32	1a	749	C
32	1a	752	G
32	1a	755	G
32	1a	766	A
32	1a	777	A
32	1a	787	A
32	1a	792	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	840	C
32	1a	841	U
32	1a	851	G
32	1a	870	U
32	1a	914	A
32	1a	926	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	927	G
32	1a	934	C
32	1a	935	A
32	1a	942	G
32	1a	960	U
32	1a	961	U
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	972	C
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	978	A
32	1a	983	A
32	1a	992	U
32	1a	993	G
32	1a	997	U
32	1a	1000	U
32	1a	1003	G
32	1a	1005	A
32	1a	1006	C
32	1a	1009	G
32	1a	1016	A
32	1a	1020	U
32	1a	1022	G
32	1a	1023	G
32	1a	1026	G
32	1a	1027	C
32	1a	1028	C
32	1a	1030	C
32	1a	1030(A)	G
32	1a	1030(C)	G
32	1a	1031	G
32	1a	1043	C
32	1a	1044	A
32	1a	1068	G
32	1a	1081	G
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	1111	A
32	1a	1123	A
32	1a	1124	G
32	1a	1125	U
32	1a	1132	C
32	1a	1133	G
32	1a	1134	G
32	1a	1135	U
32	1a	1137	C
32	1a	1138	G
32	1a	1139	G
32	1a	1140	C
32	1a	1146	A
32	1a	1152	A
32	1a	1159	U
32	1a	1183	A
32	1a	1184	G
32	1a	1196	U
32	1a	1197	G
32	1a	1201	A
32	1a	1202	G
32	1a	1213	A
32	1a	1214	C
32	1a	1227	A
32	1a	1236	A
32	1a	1238	A
32	1a	1250	A
32	1a	1253	G
32	1a	1256	A
32	1a	1257	U
32	1a	1258	G
32	1a	1270	C
32	1a	1275	A
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	1312	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	1319	A
32	1a	1338	G
32	1a	1346	A
32	1a	1347	G
32	1a	1350	A
32	1a	1353	G
32	1a	1363	C
32	1a	1364	U
32	1a	1365	G
32	1a	1370	G
32	1a	1377	A
32	1a	1379	G
32	1a	1400	5MC
32	1a	1402	4OC
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1446	U
32	1a	1447	A
32	1a	1492	A
32	1a	1494	G
32	1a	1503	A
32	1a	1504	G
32	1a	1506	U
32	1a	1517	G
32	1a	1519	MA6
32	1a	1529	G
32	1a	1530	G
53	1v	13	A
53	1v	14	A
54	1w	2	C
54	1w	5	G
54	1w	8	4SU
54	1w	14	A
54	1w	15	A
54	1w	18	G
54	1w	19	U
54	1w	21	A
54	1w	23	A
54	1w	24	A
54	1w	26	G
54	1w	27	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	1w	31	C
54	1w	45	U
54	1w	46	A
54	1w	48	C
54	1w	49	G
54	1w	51	G
54	1w	56	C
54	1w	62	C
54	1w	66	C
54	1w	67	G
54	1w	69	C
54	1w	70	C
54	1w	71	G
54	1w	73	U
54	1w	74	C
55	1x	2	G
55	1x	9	G
55	1x	18	G
55	1x	19	G
55	1x	46	G
55	1x	47	U
55	1x	61	C
56	1y	4	G
56	1y	5	G
56	1y	7	G
56	1y	9	A
56	1y	13	C
56	1y	14	A
56	1y	18	G
56	1y	19	U
56	1y	21	A
56	1y	33	U
56	1y	34	C
56	1y	35	C
56	1y	37	A
56	1y	40	C
56	1y	44	A
56	1y	45	U
56	1y	46	A
56	1y	48	C
56	1y	49	G
56	1y	50	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
56	1y	57	G
56	1y	58	A
56	1y	59	U
56	1y	60	U
56	1y	61	C
56	1y	65	U
56	1y	69	C
56	1y	70	C
56	1y	71	G
1	2A	14	A
1	2A	15	G
1	2A	34	C
1	2A	35	G
1	2A	45	C
1	2A	49	A
1	2A	61	G
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	84	A
1	2A	90	U
1	2A	94	C
1	2A	100	G
1	2A	102	G
1	2A	118	A
1	2A	119	A
1	2A	120	U
1	2A	131	G
1	2A	154	G
1	2A	154(A)	C
1	2A	157	U
1	2A	173	G
1	2A	181	A
1	2A	196	A
1	2A	199	A
1	2A	205	G
1	2A	214	G
1	2A	215	G
1	2A	216	A
1	2A	221	A
1	2A	222	A
1	2A	228	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	229	A
1	2A	230	U
1	2A	232	G
1	2A	233	A
1	2A	248	G
1	2A	266	G
1	2A	267	C
1	2A	271(J)	C
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	272	G
1	2A	272(B)	G
1	2A	277	C
1	2A	278	A
1	2A	311	A
1	2A	324	A
1	2A	327	G
1	2A	329	G
1	2A	330	A
1	2A	352	G
1	2A	358	U
1	2A	363(B)	G
1	2A	386	G
1	2A	403	U
1	2A	411	G
1	2A	412	A
1	2A	422	A
1	2A	444	C
1	2A	454	A
1	2A	455	C
1	2A	457	A
1	2A	481	G
1	2A	504	U
1	2A	505	A
1	2A	508	G
1	2A	509	C
1	2A	529	A
1	2A	530	G
1	2A	531	C
1	2A	532	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	533	G
1	2A	551	G
1	2A	563	G
1	2A	573	G
1	2A	575	A
1	2A	586	A
1	2A	588	U
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	614(B)	G
1	2A	614(C)	A
1	2A	615	G
1	2A	616	G
1	2A	627	A
1	2A	637	A
1	2A	645	C
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	726	G
1	2A	730	C
1	2A	752	A
1	2A	753	C
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	792	G
1	2A	805	G
1	2A	812	C
1	2A	819	A
1	2A	827	U
1	2A	828	U
1	2A	832	G
1	2A	857	C
1	2A	859	G
1	2A	868	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	874	G
1	2A	879	G
1	2A	880	G
1	2A	882	G
1	2A	884	C
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	893	C
1	2A	894	C
1	2A	896	A
1	2A	897	C
1	2A	900	A
1	2A	901	A
1	2A	910	A
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	974	G
1	2A	975	C
1	2A	983	A
1	2A	996	A
1	2A	999	U
1	2A	1005	C
1	2A	1012	U
1	2A	1013	C
1	2A	1017	G
1	2A	1021	A
1	2A	1022	G
1	2A	1025	G
1	2A	1033	U
1	2A	1038	C
1	2A	1039	G
1	2A	1041	C
1	2A	1043	C
1	2A	1114	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1116	C
1	2A	1117	G
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1139	G
1	2A	1142(A)	A
1	2A	1169	G
1	2A	1171	G
1	2A	1210	A
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	1273	U
1	2A	1300	U
1	2A	1301	A
1	2A	1303	G
1	2A	1314	C
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1368	G
1	2A	1370	C
1	2A	1373	A
1	2A	1378	A
1	2A	1379	A
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
1	2A	1427	A
1	2A	1428	C
1	2A	1437	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1445	A
1	2A	1449	A
1	2A	1450	G
1	2A	1460	A
1	2A	1466	G
1	2A	1467	C
1	2A	1471	A
1	2A	1482	G
1	2A	1490	A
1	2A	1493	C
1	2A	1494	A
1	2A	1496	A
1	2A	1497	U
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1531	C
1	2A	1532	C
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	1583	A
1	2A	1584	C
1	2A	1608	A
1	2A	1609	A
1	2A	1610	A
1	2A	1648	C
1	2A	1654	A
1	2A	1674	G
1	2A	1696	G
1	2A	1700	A
1	2A	1701	A
1	2A	1703	G
1	2A	1721	G
1	2A	1722	A
1	2A	1740	G
1	2A	1746	G
1	2A	1747	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1756	G
1	2A	1763	G
1	2A	1764	G
1	2A	1769	G
1	2A	1773	A
1	2A	1780	A
1	2A	1782	C
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1812	A
1	2A	1816	G
1	2A	1828	G
1	2A	1829	A
1	2A	1835	G
1	2A	1836	C
1	2A	1847	A
1	2A	1848	A
1	2A	1877	A
1	2A	1878	G
1	2A	1900	A
1	2A	1906	G
1	2A	1913	A
1	2A	1914	C
1	2A	1929	G
1	2A	1930	G
1	2A	1936	A
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	1992	G
1	2A	1993	U
1	2A	1997	G
1	2A	2020	A
1	2A	2023	G
1	2A	2031	A
1	2A	2032	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2033	A
1	2A	2043	C
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2063	C
1	2A	2069	G
1	2A	2099	U
1	2A	2110	G
1	2A	2111	C
1	2A	2112	G
1	2A	2116	G
1	2A	2117	A
1	2A	2120	G
1	2A	2122	U
1	2A	2126	A
1	2A	2127	G
1	2A	2128	C
1	2A	2129	C
1	2A	2131	G
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2135	A
1	2A	2137	C
1	2A	2138	C
1	2A	2139	C
1	2A	2142	C
1	2A	2145	C
1	2A	2146	C
1	2A	2149	G
1	2A	2151	G
1	2A	2156	G
1	2A	2157	G
1	2A	2158	A
1	2A	2159	G
1	2A	2161	C
1	2A	2165	G
1	2A	2166	G
1	2A	2167	U
1	2A	2168	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2172	U
1	2A	2176	A
1	2A	2178	C
1	2A	2181	G
1	2A	2183	C
1	2A	2186	G
1	2A	2188	C
1	2A	2189	U
1	2A	2192	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2218	U
1	2A	2225	A
1	2A	2238	G
1	2A	2239	G
1	2A	2269	A
1	2A	2275	C
1	2A	2278	A
1	2A	2283	C
1	2A	2287	A
1	2A	2288	A
1	2A	2298	A
1	2A	2305	A
1	2A	2308	G
1	2A	2312	U
1	2A	2319	G
1	2A	2320	A
1	2A	2325	G
1	2A	2334	G
1	2A	2336	A
1	2A	2347	C
1	2A	2350	C
1	2A	2354	G
1	2A	2376	A
1	2A	2383	G
1	2A	2385	C
1	2A	2402	C
1	2A	2406	U
1	2A	2425	A
1	2A	2429	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2430	A
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2448	A
1	2A	2465	C
1	2A	2469	A
1	2A	2476	A
1	2A	2491	U
1	2A	2494	G
1	2A	2502	G
1	2A	2505	G
1	2A	2506	U
1	2A	2518	A
1	2A	2520	C
1	2A	2529	G
1	2A	2530	A
1	2A	2554	U
1	2A	2555	U
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2578	G
1	2A	2602	A
1	2A	2609	U
1	2A	2611	U
1	2A	2612	C
1	2A	2615	U
1	2A	2630	G
1	2A	2654	A
1	2A	2689	U
1	2A	2690	C
1	2A	2691	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	2751	G
1	2A	2764	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2765	A
1	2A	2766	G
1	2A	2778	A
1	2A	2789	C
1	2A	2793	G
1	2A	2794	C
1	2A	2802	G
1	2A	2803	C
1	2A	2804	C
1	2A	2805	G
1	2A	2820	A
1	2A	2821	A
1	2A	2835	A
1	2A	2839	G
1	2A	2872	G
1	2A	2880	C
1	2A	2892	A
1	2A	2894	G
1	2A	2897	U
2	2B	2	C
2	2B	5	C
2	2B	8	U
2	2B	12	C
2	2B	13	A
2	2B	15	A
2	2B	17	C
2	2B	19	G
2	2B	20	C
2	2B	33	G
2	2B	41	U
2	2B	42	C
2	2B	53	A
2	2B	56	G
2	2B	67	G
2	2B	73	A
2	2B	74	U
2	2B	75	G
2	2B	85	G
2	2B	89	G
2	2B	110	G
2	2B	116	G
2	2B	120	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	9	G
32	2a	22	G
32	2a	32	A
32	2a	39	G
32	2a	47	C
32	2a	48	C
32	2a	50	A
32	2a	51	A
32	2a	65	U
32	2a	66	G
32	2a	73	G
32	2a	88	A
32	2a	89	C
32	2a	101	A
32	2a	112	G
32	2a	116	A
32	2a	121	C
32	2a	129(A)	G
32	2a	131	C
32	2a	143	A
32	2a	144	G
32	2a	162	A
32	2a	163	C
32	2a	182	U
32	2a	185	A
32	2a	189(F)	U
32	2a	189(J)	G
32	2a	195	A
32	2a	197	A
32	2a	202	U
32	2a	203	U
32	2a	204	U
32	2a	216	G
32	2a	217	C
32	2a	247	G
32	2a	250	A
32	2a	251	G
32	2a	266	G
32	2a	267	C
32	2a	279	A
32	2a	281	G
32	2a	289	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	306	G
32	2a	318	G
32	2a	321	A
32	2a	328	C
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	384	G
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	423	G
32	2a	424	G
32	2a	429	U
32	2a	430	A
32	2a	439	A
32	2a	442	C
32	2a	452	A
32	2a	470	C
32	2a	471	G
32	2a	484	G
32	2a	485	G
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	509	A
32	2a	510	A
32	2a	511	C
32	2a	518	C
32	2a	531	U
32	2a	532	A
32	2a	533	A
32	2a	547	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	559	A
32	2a	564	C
32	2a	567	G
32	2a	568	G
32	2a	572	A
32	2a	573	A
32	2a	576	G
32	2a	577	G
32	2a	596	C
32	2a	597	G
32	2a	601	C
32	2a	607	A
32	2a	630	G
32	2a	653	A
32	2a	657	G
32	2a	665	A
32	2a	687	A
32	2a	688	G
32	2a	721	G
32	2a	723	U
32	2a	731	G
32	2a	733	A
32	2a	746	A
32	2a	748	C
32	2a	749	C
32	2a	755	G
32	2a	760	G
32	2a	763	G
32	2a	764	C
32	2a	777	A
32	2a	787	A
32	2a	792	A
32	2a	793	U
32	2a	794	A
32	2a	816	A
32	2a	817	C
32	2a	821	G
32	2a	828	A
32	2a	840	C
32	2a	841	U
32	2a	851	G
32	2a	853	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	859	A
32	2a	874	G
32	2a	875	C
32	2a	887	G
32	2a	902	G
32	2a	914	A
32	2a	926	G
32	2a	927	G
32	2a	931	C
32	2a	933	G
32	2a	934	C
32	2a	935	A
32	2a	942	G
32	2a	958	A
32	2a	960	U
32	2a	961	U
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	991	U
32	2a	992	U
32	2a	993	G
32	2a	994	A
32	2a	995	C
32	2a	997	U
32	2a	998	G
32	2a	999	C
32	2a	1001	A
32	2a	1002	G
32	2a	1003	G
32	2a	1005	A
32	2a	1006	C
32	2a	1009	G
32	2a	1011	G
32	2a	1016	A
32	2a	1021	G
32	2a	1022	G
32	2a	1023	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1025	U
32	2a	1026	G
32	2a	1027	C
32	2a	1028	C
32	2a	1029	C
32	2a	1030	C
32	2a	1030(A)	G
32	2a	1031	G
32	2a	1032	G
32	2a	1033	G
32	2a	1035	A
32	2a	1039	C
32	2a	1040	U
32	2a	1043	C
32	2a	1046	A
32	2a	1050	G
32	2a	1051	C
32	2a	1053	G
32	2a	1064	G
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1071	C
32	2a	1077	G
32	2a	1079	G
32	2a	1081	G
32	2a	1086	U
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A
32	2a	1105	A
32	2a	1113	C
32	2a	1122	U
32	2a	1125	U
32	2a	1126	U
32	2a	1129	C
32	2a	1130	A
32	2a	1133	G
32	2a	1134	G
32	2a	1135	U
32	2a	1136	U
32	2a	1137	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1138	G
32	2a	1139	G
32	2a	1143	G
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	1182	G
32	2a	1184	G
32	2a	1192	C
32	2a	1193	G
32	2a	1196	U
32	2a	1197	G
32	2a	1202	G
32	2a	1211	U
32	2a	1213	A
32	2a	1227	A
32	2a	1228	C
32	2a	1238	A
32	2a	1240	U
32	2a	1241	G
32	2a	1256	A
32	2a	1257	U
32	2a	1260	C
32	2a	1261	A
32	2a	1264	C
32	2a	1267	C
32	2a	1268	A
32	2a	1270	C
32	2a	1273	G
32	2a	1277	C
32	2a	1279	A
32	2a	1280	A
32	2a	1287	A
32	2a	1299	A
32	2a	1302	U
32	2a	1303	C
32	2a	1305	G
32	2a	1306	A
32	2a	1320	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1323	G
32	2a	1338	G
32	2a	1339	A
32	2a	1340	A
32	2a	1346	A
32	2a	1347	G
32	2a	1353	G
32	2a	1358	U
32	2a	1363	C
32	2a	1368	G
32	2a	1370	G
32	2a	1397	C
32	2a	1402	4OC
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1447	A
32	2a	1452	C
32	2a	1456	G
32	2a	1457	G
32	2a	1492	A
32	2a	1494	G
32	2a	1504	G
32	2a	1506	U
32	2a	1517	G
32	2a	1519	MA6
32	2a	1520	G
32	2a	1529	G
32	2a	1530	G
32	2a	1531	A
32	2a	1532	U
53	2v	13	A
53	2v	14	A
54	2w	2	C
54	2w	5	G
54	2w	6	C
54	2w	8	4SU
54	2w	9	A
54	2w	10	G
54	2w	11	U
54	2w	12	U
54	2w	13	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	2w	14	A
54	2w	18	G
54	2w	22	G
54	2w	23	A
54	2w	24	A
54	2w	25	C
54	2w	26	G
54	2w	27	A
54	2w	36	C
54	2w	46	A
54	2w	49	G
54	2w	53	G
54	2w	56	C
54	2w	57	G
54	2w	61	C
54	2w	62	C
54	2w	64	U
54	2w	69	C
54	2w	70	C
54	2w	72	C
54	2w	73	U
54	2w	74	C
55	2x	4	G
55	2x	9	G
55	2x	18	G
55	2x	19	G
55	2x	21	A
55	2x	47	U
55	2x	63	G
56	2y	4	G
56	2y	5	G
56	2y	7	G
56	2y	15	A
56	2y	18	G
56	2y	19	U
56	2y	21	A
56	2y	22	G
56	2y	23	A
56	2y	25	C
56	2y	26	G
56	2y	27	A
56	2y	29	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
56	2y	33	U
56	2y	34	C
56	2y	37	A
56	2y	40	C
56	2y	45	U
56	2y	46	A
56	2y	49	G
56	2y	52	G
56	2y	53	G
56	2y	55	PSU
56	2y	56	C
56	2y	57	G
56	2y	58	A
56	2y	59	U
56	2y	61	C
56	2y	62	C
56	2y	66	C
56	2y	67	G
56	2y	69	C
56	2y	70	C
56	2y	73	U
56	2y	75	C

All (57) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	195	A
1	1A	196	A
1	1A	266	G
1	1A	271(K)	U
1	1A	278	A
1	1A	548	A
1	1A	573	G
1	1A	746	A
1	1A	764	A
1	1A	774	A
1	1A	827	U
1	1A	974	G
1	1A	1067	A
1	1A	1142(A)	A
1	1A	1174	A
1	1A	1176	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1442	G
1	1A	1508	A
1	1A	1608	A
1	1A	1762	A
1	1A	1992	G
1	1A	2126	A
1	1A	2134	A
1	1A	2181	G
1	1A	2183	C
1	1A	2406	U
1	1A	2422	A
1	1A	2430	A
1	1A	2439	A
1	1A	2629	A
1	1A	2689	U
1	1A	2756	U
1	2A	196	A
1	2A	228	A
1	2A	266	G
1	2A	271(K)	U
1	2A	271(M)	G
1	2A	277	C
1	2A	528	A
1	2A	752	A
1	2A	774	A
1	2A	827	U
1	2A	856	C
1	2A	900	A
1	2A	1210	A
1	2A	1378	A
1	2A	1420	U
1	2A	1530	C
1	2A	1653	G
1	2A	1913	A
1	2A	1992	G
1	2A	2119	A
1	2A	2126	A
1	2A	2156	G
1	2A	2406	U
1	2A	2439	A
1	2A	2689	U

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

72 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	$\#\|Z\| > 2$
32	UR3	2a	1498	32	19,22,23	1.01	2 (10%)	26,32,35	1.78	3 (11%)
1	PSU	1A	1917	1	18,21,22	1.37	2 (11%)	21,30,33	2.00	3 (14%)
56	PSU	2y	55	56	18,21,22	1.42	2 (11%)	21,30,33	2.03	3 (14%)
32	MA6	2a	1519	32	23,26,27	0.42	0	33,38,41	2.08	9 (27%)
54	PSU	2w	55	57,54	18,21,22	1.38	2 (11%)	21,30,33	2.08	3 (14%)
1	OMU	1A	2552	1	19,22,23	1.24	3 (15%)	25,31,34	1.96	6 (24%)
32	2MG	2a	1207	32	23,26,27	1.25	3 (13%)	33,38,41	2.13	6 (18%)
54	L3X	2w	76	1,54	24,28,29	1.44	3 (12%)	27,40,43	2.07	8 (29%)
56	5MU	1y	54	56	19,22,23	1.44	4 (21%)	27,32,35	2.04	6 (22%)
54	4SU	1w	8	54	18,21,22	1.84	5 (27%)	25,30,33	2.11	6 (24%)
1	5MU	1A	1915	1	19,22,23	1.39	6 (31%)	27,32,35	2.05	7 (25%)
1	OMC	1A	1920	1	19,22,23	0.81	0	25,31,34	0.97	1 (4%)
1	PSU	1A	2605	1,57	18,21,22	1.46	3 (16%)	21,30,33	2.01	5 (23%)
55	5MU	1x	54	55,57	19,22,23	1.46	5 (26%)	27,32,35	1.95	5 (18%)
56	4SU	2y	8	56	18,21,22	1.69	4 (22%)	25,30,33	2.08	4 (16%)
32	2MG	1a	1207	32	23,26,27	1.23	3 (13%)	33,38,41	2.26	9 (27%)
32	5MC	1a	967	32	19,22,23	1.58	3 (15%)	26,32,35	1.15	2 (7%)
1	OMU	2A	2552	1,57	19,22,23	1.23	2 (10%)	25,31,34	1.88	5 (20%)
32	G7M	2a	527	32,57	23,26,27	1.49	4 (17%)	34,39,42	1.71	5 (14%)
32	5MC	2a	1404	32	19,22,23	1.66	3 (15%)	26,32,35	1.14	3 (11%)
1	5MC	1A	1942	1	19,22,23	1.55	3 (15%)	26,32,35	1.23	2 (7%)
1	2MA	2A	2503	1,57	22,25,26	1.46	4 (18%)	32,37,40	2.30	9 (28%)
54	5MU	2w	54	54	19,22,23	1.39	4 (21%)	27,32,35	1.67	6 (22%)
54	4SU	2w	8	54	18,21,22	1.73	4 (22%)	25,30,33	2.79	5 (20%)
56	5MU	2y	54	56	19,22,23	1.50	4 (21%)	27,32,35	1.74	8 (29%)
43	0TD	1l	92	43	8,9,10	4.42	1 (12%)	6,11,13	7.30	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	PSU	2A	2605	1	18,21,22	1.32	2 (11%)	21,30,33	1.95	4 (19%)
55	5MC	1x	32	55	19,22,23	1.58	3 (15%)	26,32,35	1.25	2 (7%)
1	PSU	1A	1911	1	18,21,22	1.43	2 (11%)	21,30,33	2.00	4 (19%)
43	0TD	2l	92	43	8,9,10	4.55	1 (12%)	6,11,13	3.19	3 (50%)
1	OMG	2A	2251	1,55	23,26,27	1.23	3 (13%)	32,38,41	1.94	6 (18%)
1	5MC	2A	1962	1,57	19,22,23	1.74	3 (15%)	26,32,35	1.10	2 (7%)
1	PSU	2A	1911	1	18,21,22	1.37	2 (11%)	21,30,33	1.98	3 (14%)
32	G7M	1a	527	32,57	23,26,27	1.54	4 (17%)	34,39,42	1.72	5 (14%)
1	2MA	1A	2503	1,57	22,25,26	1.49	4 (18%)	32,37,40	2.36	8 (25%)
55	PSU	1x	55	55	18,21,22	1.35	2 (11%)	21,30,33	2.06	3 (14%)
55	5MU	2x	54	55	19,22,23	1.40	5 (26%)	27,32,35	1.95	6 (22%)
32	5MC	2a	967	32	19,22,23	1.78	3 (15%)	26,32,35	1.10	3 (11%)
55	5MC	2x	32	55	19,22,23	1.63	3 (15%)	26,32,35	1.19	3 (11%)
32	5MC	1a	1400	32	19,22,23	1.73	3 (15%)	26,32,35	1.18	4 (15%)
1	PSU	2A	1917	1	18,21,22	1.39	2 (11%)	21,30,33	2.05	4 (19%)
1	OMG	1A	2251	1,55,57	23,26,27	1.25	3 (13%)	32,38,41	1.95	7 (21%)
32	4OC	1a	1402	32	20,23,24	0.74	0	25,32,35	0.91	1 (4%)
32	UR3	1a	1498	32	19,22,23	0.97	1 (5%)	26,32,35	1.75	4 (15%)
54	L3X	1w	76	1,54	24,28,29	1.40	3 (12%)	27,40,43	2.10	9 (33%)
32	MA6	1a	1519	32	23,26,27	0.44	0	33,38,41	2.06	9 (27%)
55	4SU	1x	8	55	18,21,22	2.23	6 (33%)	25,30,33	1.68	6 (24%)
32	5MC	2a	1407	32	19,22,23	1.59	3 (15%)	26,32,35	1.25	3 (11%)
55	31H	2x	76	55,57	31,34,35	1.15	3 (9%)	35,47,50	2.38	14 (40%)
32	PSU	1a	516	32	18,21,22	1.42	2 (11%)	21,30,33	1.92	4 (19%)
32	5MC	1a	1404	32	19,22,23	1.85	3 (15%)	26,32,35	1.25	4 (15%)
1	5MU	2A	1939	1,57	19,22,23	1.38	5 (26%)	27,32,35	2.38	6 (22%)
54	5MU	1w	54	54	19,22,23	1.38	4 (21%)	27,32,35	1.79	6 (22%)
55	PSU	2x	55	55	18,21,22	1.36	2 (11%)	21,30,33	2.06	5 (23%)
32	5MC	1a	1407	32	19,22,23	1.54	2 (10%)	26,32,35	1.16	3 (11%)
1	5MU	2A	1915	1	19,22,23	1.46	5 (26%)	27,32,35	2.07	5 (18%)
1	OMC	2A	1920	1	19,22,23	0.80	0	25,31,34	0.99	1 (4%)
32	MA6	2a	1518	32	23,26,27	0.39	0	33,38,41	2.00	9 (27%)
32	M2G	2a	966	32	24,27,28	1.29	4 (16%)	33,40,43	1.89	5 (15%)
55	31H	1x	76	55,57	31,34,35	1.18	3 (9%)	35,47,50	2.05	13 (37%)
1	5MC	2A	1942	1	19,22,23	1.63	3 (15%)	26,32,35	1.12	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	5MC	1A	1962	1	19,22,23	1.85	3 (15%)	26,32,35	1.24	3 (11%)
56	4SU	1y	8	56	18,21,22	1.87	6 (33%)	25,30,33	1.66	5 (20%)
32	MA6	1a	1518	32	23,26,27	0.40	0	33,38,41	2.07	9 (27%)
55	4SU	2x	8	55	18,21,22	1.98	5 (27%)	25,30,33	1.32	4 (16%)
32	M2G	1a	966	32	24,27,28	1.30	4 (16%)	33,40,43	1.89	6 (18%)
54	PSU	1w	55	57,54	18,21,22	1.42	2 (11%)	21,30,33	2.00	3 (14%)
32	PSU	2a	516	32	18,21,22	1.32	2 (11%)	21,30,33	1.94	4 (19%)
1	5MU	1A	1939	1,57	19,22,23	1.47	4 (21%)	27,32,35	2.12	6 (22%)
32	5MC	2a	1400	32	19,22,23	1.58	3 (15%)	26,32,35	1.10	3 (11%)
56	PSU	1y	55	56	18,21,22	1.38	2 (11%)	21,30,33	2.06	3 (14%)
32	4OC	2a	1402	32	20,23,24	0.78	0	25,32,35	1.07	3 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
56	PSU	2y	55	56	-	2/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	3/11/29/30	0/3/3/3
54	PSU	2w	55	57,54	-	0/7/25/26	0/2/2/2
1	OMU	1A	2552	1	-	0/9/27/28	0/2/2/2
32	2MG	2a	1207	32	-	0/9/27/28	0/3/3/3
54	L3X	2w	76	1,54	-	2/13/31/32	0/3/3/3
56	5MU	1y	54	56	-	0/7/25/26	0/2/2/2
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
1	5MU	1A	1915	1	-	0/7/25/26	0/2/2/2
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
1	PSU	1A	2605	1,57	-	0/7/25/26	0/2/2/2
55	5MU	1x	54	55,57	-	0/7/25/26	0/2/2/2
56	4SU	2y	8	56	-	2/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/9/27/28	0/3/3/3
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
1	OMU	2A	2552	1,57	-	0/9/27/28	0/2/2/2
32	G7M	2a	527	32,57	-	1/7/25/26	0/3/3/3
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MA	2A	2503	1,57	-	1/7/25/26	0/3/3/3
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
56	5MU	2y	54	56	-	2/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	1/7/12/14	-
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	1/7/12/14	-
1	OMG	2A	2251	1,55	-	0/9/27/28	0/3/3/3
1	5MC	2A	1962	1,57	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
32	G7M	1a	527	32,57	-	3/7/25/26	0/3/3/3
1	2MA	1A	2503	1,57	-	2/7/25/26	0/3/3/3
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	1/7/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	2/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	1,55,57	-	0/9/27/28	0/3/3/3
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
54	L3X	1w	76	1,54	-	0/13/31/32	0/3/3/3
32	MA6	1a	1519	32	-	3/11/29/30	0/3/3/3
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
55	31H	2x	76	55,57	-	5/22/40/41	0/3/3/3
32	PSU	1a	516	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	1939	1,57	-	0/7/25/26	0/2/2/2
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
32	MA6	2a	1518	32	-	0/11/29/30	0/3/3/3
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
55	31H	1x	76	55,57	-	6/22/40/41	0/3/3/3
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	1A	1962	1	-	0/7/25/26	0/2/2/2
56	4SU	1y	8	56	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3
55	4SU	2x	8	55	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
54	PSU	1w	55	57,54	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	1,57	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
56	PSU	1y	55	56	-	2/7/25/26	0/2/2/2
32	4OC	2a	1402	32	-	2/9/29/30	0/2/2/2

All (204) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.44	1.69	1.82
43	1l	92	0TD	CB-SB	-11.93	1.70	1.82
32	1a	1404	5MC	C5-C4	6.93	1.49	1.44
1	1A	1962	5MC	C5-C4	6.90	1.49	1.44
32	2a	967	5MC	C5-C4	6.66	1.49	1.44
1	2A	1962	5MC	C5-C4	6.49	1.49	1.44
32	1a	1400	5MC	C5-C4	6.36	1.48	1.44
32	2a	1404	5MC	C5-C4	6.04	1.48	1.44
55	2x	32	5MC	C5-C4	5.86	1.48	1.44
1	2A	1942	5MC	C5-C4	5.80	1.48	1.44
32	2a	1407	5MC	C5-C4	5.67	1.48	1.44
32	1a	967	5MC	C5-C4	5.65	1.48	1.44
32	1a	1407	5MC	C5-C4	5.61	1.48	1.44
32	2a	1400	5MC	C5-C4	5.61	1.48	1.44
55	1x	32	5MC	C5-C4	5.60	1.48	1.44
1	1A	1942	5MC	C5-C4	5.37	1.48	1.44
55	1x	8	4SU	C4-N3	-5.19	1.32	1.37
32	1a	527	G7M	C5-N7	-4.89	1.33	1.39
54	1w	8	4SU	C4-S4	-4.88	1.60	1.68
56	1y	8	4SU	C4-S4	-4.71	1.60	1.68
54	2w	8	4SU	C4-S4	-4.70	1.60	1.68
55	1x	8	4SU	C4-S4	-4.66	1.60	1.68
55	2x	8	4SU	C4-N3	-4.56	1.32	1.37
56	2y	8	4SU	C4-S4	-4.49	1.60	1.68
1	1A	2503	2MA	C5-C4	4.46	1.47	1.39
32	2a	527	G7M	C5-N7	-4.35	1.34	1.39
1	2A	2503	2MA	C5-C4	4.32	1.46	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	2x	8	4SU	C4-S4	-4.28	1.61	1.68
54	1w	55	PSU	C6-C5	4.21	1.40	1.35
56	2y	55	PSU	C6-C5	4.16	1.39	1.35
55	1x	8	4SU	C2-N3	-4.02	1.31	1.38
54	2w	76	L3X	C5-N7	-3.94	1.31	1.39
54	2w	55	PSU	C6-C5	3.94	1.39	1.35
54	1w	76	L3X	C5-N7	-3.90	1.32	1.39
55	1x	76	31H	C5-N7	-3.86	1.32	1.39
56	1y	55	PSU	C6-C5	3.85	1.39	1.35
1	1A	1917	PSU	C6-C5	3.85	1.39	1.35
55	2x	76	31H	C5-N7	-3.82	1.32	1.39
1	1A	1911	PSU	C6-C5	3.76	1.39	1.35
32	1a	516	PSU	C6-C5	3.70	1.39	1.35
55	2x	55	PSU	C6-C5	3.68	1.39	1.35
1	2A	1917	PSU	C6-C5	3.60	1.39	1.35
32	2a	516	PSU	C6-C5	3.55	1.39	1.35
55	1x	8	4SU	C5-C4	-3.53	1.38	1.42
1	2A	1911	PSU	C6-C5	3.47	1.39	1.35
56	1y	8	4SU	C4-N3	-3.38	1.34	1.37
1	2A	2251	OMG	C5-C4	3.33	1.47	1.38
55	1x	55	PSU	C6-C5	3.33	1.39	1.35
32	2a	1207	2MG	C5-C4	3.32	1.47	1.38
1	1A	2605	PSU	C4-N3	-3.31	1.32	1.38
1	2A	2605	PSU	C6-C5	3.28	1.38	1.35
32	2a	527	G7M	C5-C4	3.23	1.46	1.38
54	2w	76	L3X	C5-C4	-3.22	1.33	1.39
32	1a	527	G7M	C5-C4	3.22	1.46	1.38
1	1A	2251	OMG	C5-C4	3.22	1.47	1.38
32	2a	966	M2G	C5-C4	3.21	1.47	1.38
56	2y	54	5MU	C6-C5	3.12	1.39	1.34
56	1y	54	5MU	C6-C5	3.12	1.39	1.34
55	2x	8	4SU	C2-N3	-3.11	1.32	1.38
56	2y	54	5MU	C2-N1	3.10	1.43	1.38
55	2x	76	31H	C5-C4	-3.10	1.33	1.39
32	1a	966	M2G	C5-C4	3.09	1.47	1.38
54	1w	76	L3X	C5-C4	-3.09	1.33	1.39
55	1x	76	31H	C5-C4	-3.09	1.33	1.39
54	2w	8	4SU	C2-N1	3.08	1.43	1.38
32	1a	1207	2MG	C5-C4	3.03	1.47	1.38
1	1A	1939	5MU	C4-N3	-3.00	1.33	1.38
1	2A	1915	5MU	C6-C5	2.99	1.39	1.34
54	1w	8	4SU	C5-C4	-2.97	1.38	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1a	1404	5MC	C6-C5	2.96	1.39	1.34
1	2A	1939	5MU	C6-C5	2.93	1.39	1.34
1	2A	1942	5MC	C6-C5	2.92	1.39	1.34
55	1x	54	5MU	C6-C5	2.91	1.39	1.34
55	2x	54	5MU	C6-C5	2.89	1.39	1.34
54	1w	54	5MU	C6-C5	2.89	1.39	1.34
54	2w	54	5MU	C6-C5	2.86	1.39	1.34
32	2a	1404	5MC	C6-C5	2.86	1.39	1.34
1	1A	2605	PSU	C6-C5	2.85	1.38	1.35
32	1a	966	M2G	C2-N2	2.85	1.40	1.35
32	2a	1400	5MC	C6-C5	2.84	1.39	1.34
55	2x	8	4SU	C5-C4	-2.84	1.39	1.42
1	1A	1942	5MC	C6-C5	2.84	1.39	1.34
32	1a	1400	5MC	C6-C5	2.83	1.39	1.34
32	2a	966	M2G	C2-N2	2.83	1.40	1.35
1	1A	1911	PSU	C4-N3	-2.82	1.33	1.38
1	2A	1939	5MU	C4-N3	-2.80	1.33	1.38
32	2a	967	5MC	C6-C5	2.80	1.39	1.34
54	1w	8	4SU	C2-N1	2.79	1.42	1.38
1	1A	1939	5MU	C6-N1	-2.78	1.33	1.38
56	1y	54	5MU	C4-C5	2.75	1.49	1.44
1	1A	1962	5MC	C6-N1	-2.74	1.33	1.38
1	1A	1939	5MU	C2-N3	-2.73	1.33	1.38
55	2x	32	5MC	C6-C5	2.72	1.39	1.34
54	2w	8	4SU	O2-C2	2.71	1.27	1.23
55	1x	54	5MU	C2-N1	2.70	1.42	1.38
1	2A	1915	5MU	C2-N1	2.69	1.42	1.38
1	2A	1962	5MC	C6-C5	2.68	1.39	1.34
54	1w	8	4SU	C4-N3	-2.68	1.34	1.37
32	1a	516	PSU	C4-N3	-2.68	1.33	1.38
1	1A	2552	OMU	C4-N3	-2.68	1.34	1.38
55	1x	32	5MC	C6-C5	2.66	1.39	1.34
1	2A	1915	5MU	C4-C5	2.64	1.49	1.44
1	1A	1915	5MU	C6-C5	2.64	1.38	1.34
55	1x	54	5MU	C4-N3	-2.64	1.33	1.38
55	1x	76	31H	C5-C6	-2.63	1.33	1.41
1	1A	1915	5MU	C4-N3	-2.62	1.33	1.38
1	2A	2503	2MA	C5-C6	2.60	1.48	1.41
1	1A	2251	OMG	C6-N1	-2.60	1.34	1.38
56	2y	8	4SU	C2-N1	2.60	1.42	1.38
1	1A	1939	5MU	C6-C5	2.58	1.38	1.34
56	1y	8	4SU	C5-C4	-2.58	1.39	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1a	1407	5MC	C6-C5	2.57	1.38	1.34
56	2y	8	4SU	C5-C4	-2.57	1.39	1.42
55	2x	54	5MU	C4-N3	-2.56	1.34	1.38
56	2y	54	5MU	C4-N3	-2.56	1.34	1.38
55	2x	76	31H	C5-C6	-2.55	1.33	1.41
1	1A	2503	2MA	C5-N7	-2.55	1.34	1.39
32	2a	1407	5MC	C6-C5	2.52	1.38	1.34
32	1a	966	M2G	C6-N1	-2.51	1.34	1.38
1	2A	1917	PSU	C4-N3	-2.48	1.34	1.38
54	1w	76	L3X	C5-C6	-2.47	1.34	1.41
32	2a	527	G7M	C6-N1	-2.45	1.34	1.38
55	2x	55	PSU	C4-N3	-2.45	1.34	1.38
1	2A	2552	OMU	C4-N3	-2.45	1.34	1.38
54	2w	54	5MU	C4-N3	-2.44	1.34	1.38
32	1a	967	5MC	C6-C5	2.44	1.38	1.34
55	1x	55	PSU	C4-N3	-2.44	1.34	1.38
54	1w	54	5MU	C4-C5	2.44	1.48	1.44
1	2A	1911	PSU	C4-N3	-2.43	1.34	1.38
54	1w	55	PSU	C4-N3	-2.43	1.34	1.38
56	1y	8	4SU	C2-N1	2.43	1.42	1.38
54	2w	54	5MU	C2-N1	2.43	1.42	1.38
32	1a	1207	2MG	C6-N1	-2.43	1.34	1.38
56	2y	8	4SU	C4-N3	-2.42	1.35	1.37
32	1a	967	5MC	C6-N1	-2.42	1.33	1.38
1	1A	1962	5MC	C6-C5	2.41	1.38	1.34
1	2A	1915	5MU	C4-N3	-2.41	1.34	1.38
56	1y	8	4SU	C2-N3	-2.40	1.33	1.38
1	2A	2605	PSU	C4-N3	-2.40	1.34	1.38
54	1w	54	5MU	C4-N3	-2.40	1.34	1.38
1	1A	2605	PSU	C2-N3	-2.40	1.33	1.37
55	2x	54	5MU	C4-C5	2.39	1.48	1.44
32	2a	1207	2MG	C6-N1	-2.38	1.34	1.38
54	2w	76	L3X	C5-C6	-2.38	1.34	1.41
55	1x	32	5MC	C6-N1	-2.38	1.34	1.38
32	1a	527	G7M	C6-N1	-2.38	1.34	1.38
54	2w	55	PSU	C4-N3	-2.37	1.34	1.38
56	1y	55	PSU	C4-N3	-2.35	1.34	1.38
1	1A	1915	5MU	C2-N1	2.33	1.42	1.38
56	1y	54	5MU	C2-N1	2.33	1.42	1.38
54	2w	54	5MU	C4-C5	2.33	1.48	1.44
56	1y	54	5MU	C4-N3	-2.33	1.34	1.38
1	1A	2503	2MA	C8-N7	2.32	1.36	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	8	4SU	O2-C2	2.32	1.27	1.23
32	1a	1400	5MC	C6-N1	-2.31	1.34	1.38
32	2a	966	M2G	C6-N1	-2.31	1.34	1.38
1	2A	1962	5MC	C6-N1	-2.30	1.34	1.38
32	2a	1407	5MC	C6-N1	-2.30	1.34	1.38
54	2w	8	4SU	C5-C4	-2.29	1.39	1.42
55	1x	54	5MU	C4-C5	2.29	1.48	1.44
1	1A	1917	PSU	C4-N3	-2.29	1.34	1.38
1	1A	1942	5MC	C6-N1	-2.29	1.34	1.38
1	1A	2503	2MA	C5-C6	2.28	1.47	1.41
54	1w	54	5MU	C2-N1	2.28	1.42	1.38
1	2A	2552	OMU	C5-C4	2.27	1.48	1.43
32	2a	516	PSU	C4-N3	-2.26	1.34	1.38
1	2A	2251	OMG	C5-N7	-2.25	1.34	1.39
1	1A	1915	5MU	C4-C5	2.25	1.48	1.44
1	2A	2251	OMG	C6-N1	-2.24	1.34	1.38
1	2A	1939	5MU	C2-N3	-2.24	1.34	1.38
32	2a	1498	UR3	C2-N1	2.23	1.41	1.38
1	2A	2503	2MA	C8-N7	2.22	1.36	1.31
1	2A	1939	5MU	C4-C5	2.22	1.48	1.44
1	2A	2503	2MA	C5-N7	-2.21	1.35	1.39
55	2x	54	5MU	C2-N3	-2.20	1.34	1.38
55	2x	32	5MC	C6-N1	-2.19	1.34	1.38
55	1x	8	4SU	O2-C2	2.17	1.26	1.23
56	2y	54	5MU	C4-C5	2.17	1.48	1.44
55	2x	8	4SU	O2-C2	2.17	1.26	1.23
32	1a	1498	UR3	C2-N1	2.17	1.41	1.38
32	1a	527	G7M	C4-N9	-2.15	1.32	1.38
32	1a	1404	5MC	C6-N1	-2.14	1.34	1.38
55	2x	54	5MU	C2-N1	2.13	1.41	1.38
1	1A	2251	OMG	C5-N7	-2.12	1.34	1.39
1	2A	1942	5MC	C6-N1	-2.12	1.34	1.38
32	2a	1207	2MG	C2-N3	2.12	1.36	1.32
32	2a	527	G7M	C5-C6	2.09	1.49	1.43
56	2y	55	PSU	C4-N3	-2.09	1.34	1.38
32	1a	966	M2G	C5-N7	-2.08	1.34	1.39
32	2a	1498	UR3	C6-C5	2.07	1.39	1.35
32	2a	967	5MC	C6-N1	-2.07	1.34	1.38
1	2A	1915	5MU	C6-N1	-2.07	1.34	1.38
56	1y	8	4SU	O2-C2	2.05	1.26	1.23
1	2A	1939	5MU	C6-N1	-2.05	1.34	1.38
32	2a	1404	5MC	C6-N1	-2.04	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1x	8	4SU	C6-C5	2.04	1.39	1.35
55	1x	54	5MU	C2-N3	-2.04	1.34	1.38
1	1A	2552	OMU	C5-C4	2.03	1.48	1.43
32	2a	966	M2G	C5-N7	-2.03	1.35	1.39
32	2a	1400	5MC	C6-N1	-2.03	1.34	1.38
1	1A	2552	OMU	C2-N1	2.02	1.41	1.38
1	1A	1915	5MU	C6-N1	-2.02	1.34	1.38
32	1a	1207	2MG	C5-N7	-2.01	1.35	1.39
1	1A	1915	5MU	C2-N3	-2.00	1.34	1.38

All (356) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	1l	92	0TD	CSB-SB-CB	-17.50	70.91	102.36
54	2w	8	4SU	C4-N3-C2	-8.54	119.13	127.31
1	2A	2503	2MA	C5-C4-N3	-8.31	118.43	127.18
1	1A	2503	2MA	C5-C4-N3	-8.01	118.75	127.18
32	2a	1498	UR3	C4-N3-C2	-7.02	118.93	124.58
32	1a	1207	2MG	C2-N3-C4	6.96	120.71	112.00
32	1a	1498	UR3	C4-N3-C2	-6.81	119.10	124.58
32	2a	1207	2MG	C2-N3-C4	6.76	120.45	112.00
43	2l	92	0TD	CSB-SB-CB	-6.73	90.27	102.36
1	1A	2503	2MA	N3-C4-N9	6.73	135.53	126.99
54	2w	8	4SU	C5-C4-N3	6.59	120.88	114.75
1	2A	1917	PSU	N1-C2-N3	6.50	122.03	115.17
55	2x	76	31H	O4'-C1'-N9	-6.49	95.62	108.09
55	1x	55	PSU	N1-C2-N3	6.45	121.98	115.17
55	2x	55	PSU	N1-C2-N3	6.45	121.97	115.17
56	1y	55	PSU	N1-C2-N3	6.42	121.94	115.17
1	2A	2503	2MA	N3-C4-N9	6.40	135.12	126.99
56	2y	55	PSU	N1-C2-N3	6.36	121.88	115.17
54	2w	55	PSU	N1-C2-N3	6.36	121.88	115.17
54	1w	55	PSU	N1-C2-N3	6.27	121.78	115.17
32	2a	966	M2G	C5-C4-N3	-6.25	118.44	128.39
1	1A	2605	PSU	N1-C2-N3	6.22	121.73	115.17
32	1a	966	M2G	C5-C4-N3	-6.17	118.56	128.39
1	2A	1911	PSU	N1-C2-N3	6.17	121.67	115.17
1	1A	1917	PSU	N1-C2-N3	6.16	121.66	115.17
1	1A	1911	PSU	N1-C2-N3	6.14	121.65	115.17
32	2a	1207	2MG	C5-C4-N3	-6.12	118.64	128.39
1	2A	2251	OMG	C5-C4-N3	-6.09	118.70	128.39
32	1a	516	PSU	N1-C2-N3	6.06	121.56	115.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2A	2605	PSU	N1-C2-N3	6.00	121.50	115.17
54	2w	8	4SU	C5-C4-S4	-5.97	117.49	124.31
32	2a	516	PSU	N1-C2-N3	5.95	121.45	115.17
1	1A	2251	OMG	C5-C4-N3	-5.90	119.00	128.39
1	2A	1939	5MU	C4-N3-C2	-5.88	119.63	127.34
32	1a	1207	2MG	C5-C4-N3	-5.82	119.14	128.39
55	2x	76	31H	N1-C2-N3	-5.78	119.83	128.58
55	1x	76	31H	N1-C2-N3	-5.76	119.87	128.58
54	1w	8	4SU	C5-C4-N3	5.72	120.07	114.75
56	2y	8	4SU	C4-N3-C2	-5.71	121.84	127.31
54	1w	76	L3X	N1-C2-N3	-5.70	119.95	128.58
54	2w	76	L3X	N1-C2-N3	-5.67	120.00	128.58
1	2A	1939	5MU	N3-C2-N1	5.48	122.02	114.89
1	1A	2552	OMU	N3-C2-N1	5.46	122.00	114.89
32	2a	527	G7M	C5-C4-N3	-5.34	118.05	128.15
32	1a	527	G7M	N9-C4-N3	5.32	136.59	125.95
32	2a	527	G7M	N9-C4-N3	5.27	136.49	125.95
56	1y	54	5MU	N3-C2-N1	5.23	121.69	114.89
1	2A	2552	OMU	N3-C2-N1	5.21	121.67	114.89
1	2A	1939	5MU	C5-C4-N3	5.21	119.85	115.32
54	1w	8	4SU	C4-N3-C2	-5.20	122.33	127.31
55	2x	76	31H	C5-C4-N3	-5.09	119.70	126.72
56	2y	8	4SU	C5-C4-N3	5.09	119.48	114.75
32	1a	1519	MA6	N1-C2-N3	-5.08	120.89	128.58
1	2A	1915	5MU	N3-C2-N1	5.06	121.48	114.89
1	1A	1939	5MU	C4-N3-C2	-5.05	120.72	127.34
1	2A	1915	5MU	C4-N3-C2	-5.03	120.74	127.34
56	1y	54	5MU	C4-N3-C2	-5.03	120.75	127.34
1	1A	2251	OMG	C2-N3-C4	5.02	120.95	112.30
1	1A	1939	5MU	C5-C4-N3	5.00	119.67	115.32
32	1a	527	G7M	C5-C4-N3	-4.99	118.72	128.15
32	2a	1518	MA6	N1-C2-N3	-4.99	121.03	128.58
55	1x	76	31H	C5-C4-N3	-4.97	119.87	126.72
32	1a	1518	MA6	N1-C2-N3	-4.95	121.08	128.58
54	1w	76	L3X	C5-C4-N3	-4.93	119.92	126.72
55	1x	54	5MU	N3-C2-N1	4.93	121.31	114.89
56	1y	8	4SU	C5-C4-N3	4.91	119.32	114.75
1	1A	1915	5MU	C4-N3-C2	-4.88	120.94	127.34
55	2x	54	5MU	N3-C2-N1	4.87	121.23	114.89
1	1A	1915	5MU	N3-C2-N1	4.86	121.22	114.89
1	2A	2251	OMG	N9-C4-N3	4.81	135.56	125.95
54	1w	8	4SU	C5-C4-S4	-4.81	118.82	124.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	1519	MA6	N1-C2-N3	-4.80	121.31	128.58
54	2w	76	L3X	C5-C4-N3	-4.80	120.11	126.72
32	2a	527	G7M	C2-N3-C4	4.80	120.57	112.30
1	2A	2552	OMU	C4-N3-C2	-4.78	120.68	126.61
1	1A	2552	OMU	C4-N3-C2	-4.77	120.69	126.61
1	2A	1939	5MU	O4-C4-C5	-4.71	119.53	124.92
32	1a	966	M2G	N9-C4-N3	4.70	135.35	125.95
1	1A	2251	OMG	N9-C4-N3	4.70	135.34	125.95
1	2A	1939	5MU	C5-C6-N1	-4.66	118.25	123.31
55	2x	54	5MU	C4-N3-C2	-4.61	121.30	127.34
55	1x	54	5MU	C4-N3-C2	-4.61	121.30	127.34
32	2a	966	M2G	C2-N3-C4	4.59	121.00	112.51
32	2a	1519	MA6	C5-C4-N3	-4.55	120.45	126.72
32	2a	1518	MA6	C5-C4-N3	-4.54	120.46	126.72
1	2A	2251	OMG	C2-N3-C4	4.54	120.13	112.30
1	1A	1915	5MU	C5-C4-N3	4.53	119.26	115.32
32	2a	966	M2G	N9-C4-N3	4.52	134.99	125.95
55	1x	8	4SU	C6-C5-C4	-4.51	116.05	119.95
32	1a	966	M2G	C2-N3-C4	4.48	120.79	112.51
54	2w	55	PSU	O2-C2-N1	-4.43	118.22	122.79
1	1A	1939	5MU	C5-C6-N1	-4.36	118.57	123.31
1	1A	1939	5MU	N3-C2-N1	4.33	120.53	114.89
32	1a	527	G7M	C2-N3-C4	4.32	119.75	112.30
56	2y	55	PSU	O2-C2-N1	-4.31	118.34	122.79
56	2y	8	4SU	C5-C4-S4	-4.29	119.41	124.31
32	1a	1519	MA6	C5-C4-N3	-4.29	120.81	126.72
1	1A	1939	5MU	O4-C4-C5	-4.26	120.04	124.92
55	2x	55	PSU	C4-N3-C2	-4.23	120.54	126.37
1	1A	2605	PSU	C4-N3-C2	-4.22	120.56	126.37
32	1a	1518	MA6	C2-N1-C6	4.21	122.10	111.83
54	1w	54	5MU	N3-C2-N1	4.19	120.34	114.89
56	1y	55	PSU	O2-C2-N1	-4.18	118.47	122.79
32	2a	1207	2MG	N9-C4-N3	4.17	134.30	125.95
32	1a	1519	MA6	C2-N1-C6	4.17	122.02	111.83
32	1a	1518	MA6	C5-N7-C8	4.15	109.97	103.45
1	2A	2605	PSU	C4-N3-C2	-4.14	120.67	126.37
56	1y	54	5MU	C5-C4-N3	4.11	118.90	115.32
1	2A	1915	5MU	C5-C4-N3	4.10	118.88	115.32
1	1A	1911	PSU	C4-N3-C2	-4.09	120.74	126.37
54	1w	54	5MU	C4-N3-C2	-4.08	121.98	127.34
55	2x	54	5MU	C5-C4-N3	4.08	118.87	115.32
54	2w	8	4SU	N3-C2-N1	4.05	120.16	114.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1917	PSU	C4-N3-C2	-4.03	120.81	126.37
1	2A	1911	PSU	C4-N3-C2	-4.03	120.82	126.37
54	2w	8	4SU	O2-C2-N1	-3.97	117.63	122.80
54	1w	54	5MU	O4-C4-C5	-3.96	120.38	124.92
1	2A	1917	PSU	C4-N3-C2	-3.96	120.92	126.37
55	1x	55	PSU	C4-N3-C2	-3.96	120.92	126.37
54	1w	54	5MU	C5-C4-N3	3.95	118.75	115.32
32	1a	1518	MA6	C4-C5-N7	-3.94	106.08	110.58
55	1x	32	5MC	C5-C6-N1	-3.94	119.03	123.31
32	2a	1518	MA6	C2-N1-C6	3.94	121.45	111.83
55	1x	54	5MU	C5-C4-N3	3.93	118.74	115.32
32	1a	1207	2MG	N9-C4-N3	3.92	133.80	125.95
56	1y	8	4SU	C4-N3-C2	-3.91	123.56	127.31
32	2a	1519	MA6	C4-C5-N7	-3.90	106.12	110.58
32	2a	1519	MA6	C2-N1-C6	3.88	121.30	111.83
32	1a	1207	2MG	C6-C5-N7	3.88	137.34	130.29
1	2A	1915	5MU	O4-C4-C5	-3.88	120.48	124.92
32	2a	1519	MA6	C5-N7-C8	3.88	109.54	103.45
55	1x	55	PSU	O2-C2-N1	-3.87	118.80	122.79
32	2a	516	PSU	C4-N3-C2	-3.87	121.05	126.37
32	1a	1518	MA6	C5-C4-N3	-3.85	121.42	126.72
32	1a	1518	MA6	N9-C8-N7	-3.84	108.49	113.94
54	2w	55	PSU	C4-N3-C2	-3.83	121.09	126.37
32	1a	516	PSU	C4-N3-C2	-3.83	121.09	126.37
55	2x	54	5MU	O4-C4-C5	-3.82	120.55	124.92
1	2A	1917	PSU	O2-C2-N1	-3.81	118.86	122.79
1	1A	1915	5MU	O4-C4-C5	-3.79	120.59	124.92
56	1y	55	PSU	C4-N3-C2	-3.78	121.16	126.37
32	1a	1404	5MC	C5-C6-N1	-3.78	119.20	123.31
54	2w	54	5MU	N3-C2-N1	3.77	119.80	114.89
32	1a	1519	MA6	C5-N7-C8	3.77	109.37	103.45
1	1A	1942	5MC	C5-C6-N1	-3.77	119.22	123.31
1	1A	2503	2MA	N6-C6-N1	3.76	122.10	117.03
56	2y	8	4SU	N3-C2-N1	3.76	119.78	114.89
54	1w	55	PSU	C4-N3-C2	-3.71	121.26	126.37
32	1a	1519	MA6	C4-C5-N7	-3.71	106.34	110.58
55	1x	54	5MU	O4-C4-C5	-3.70	120.68	124.92
56	2y	54	5MU	N3-C2-N1	3.69	119.69	114.89
54	2w	54	5MU	C5-C4-N3	3.65	118.50	115.32
1	2A	1962	5MC	C5-C6-N1	-3.65	119.35	123.31
54	2w	54	5MU	O4-C4-C5	-3.64	120.75	124.92
56	2y	55	PSU	C4-N3-C2	-3.61	121.40	126.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	2y	54	5MU	O4-C4-C5	-3.59	120.81	124.92
56	1y	54	5MU	O4-C4-C5	-3.57	120.83	124.92
56	2y	54	5MU	C5-C4-N3	3.56	118.42	115.32
1	2A	2503	2MA	C4-C5-N7	-3.56	106.52	110.58
32	2a	1518	MA6	C2-N3-C4	3.55	120.50	111.83
32	2a	1518	MA6	C5-N7-C8	3.53	109.00	103.45
54	1w	55	PSU	O2-C2-N1	-3.53	119.15	122.79
32	2a	1518	MA6	C4-C5-N7	-3.49	106.60	110.58
1	2A	1915	5MU	C5-C6-N1	-3.48	119.53	123.31
55	1x	8	4SU	O2-C2-N1	3.47	127.31	122.80
54	2w	54	5MU	C4-N3-C2	-3.47	122.80	127.34
55	2x	76	31H	N9-C8-N7	-3.46	109.03	113.94
32	2a	1519	MA6	C2-N3-C4	3.46	120.28	111.83
1	2A	2552	OMU	O2-C2-N1	-3.46	118.30	122.80
32	2a	1207	2MG	C6-C5-N7	3.45	136.58	130.29
1	2A	1942	5MC	C5-C6-N1	-3.45	119.56	123.31
54	1w	8	4SU	C1'-N1-C2	3.44	123.77	117.59
54	1w	76	L3X	N9-C8-N7	-3.43	109.07	113.94
55	2x	76	31H	C2-N3-C4	3.43	120.20	111.83
32	1a	1519	MA6	C2-N3-C4	3.42	120.18	111.83
55	1x	76	31H	N9-C8-N7	-3.42	109.09	113.94
1	2A	1911	PSU	O2-C2-N1	-3.40	119.28	122.79
32	2a	1519	MA6	N9-C8-N7	-3.39	109.13	113.94
55	1x	76	31H	C2-N3-C4	3.36	120.03	111.83
32	1a	1400	5MC	C5-C6-N1	-3.35	119.67	123.31
1	1A	2552	OMU	O2-C2-N1	-3.35	118.43	122.80
1	2A	1939	5MU	O2-C2-N1	-3.34	118.45	122.80
54	1w	76	L3X	C2-N3-C4	3.34	119.98	111.83
1	1A	1917	PSU	O2-C2-N1	-3.33	119.35	122.79
32	1a	1519	MA6	N9-C8-N7	-3.33	109.21	113.94
56	1y	54	5MU	C5-C6-N1	-3.32	119.71	123.31
54	2w	76	L3X	N9-C8-N7	-3.31	109.25	113.94
32	2a	516	PSU	O2-C2-N1	-3.31	119.38	122.79
55	2x	76	31H	C4'-O4'-C1'	-3.29	102.21	109.47
54	2w	76	L3X	C2-N3-C4	3.27	119.82	111.83
32	2a	1407	5MC	C5-C6-N1	-3.26	119.77	123.31
32	2a	1498	UR3	C5-C4-N3	3.25	119.32	115.04
1	1A	1962	5MC	CM5-C5-C6	-3.22	118.49	122.85
56	2y	54	5MU	C4-N3-C2	-3.22	123.12	127.34
32	2a	1400	5MC	C5-C6-N1	-3.21	119.83	123.31
55	1x	54	5MU	C5-C6-N1	-3.21	119.83	123.31
32	1a	1518	MA6	C2-N3-C4	3.21	119.67	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	1a	1407	5MC	C5-C6-N1	-3.20	119.83	123.31
1	1A	1962	5MC	C5-C6-N1	-3.20	119.84	123.31
55	2x	8	4SU	C5-C4-N3	3.20	117.72	114.75
1	1A	1911	PSU	O2-C2-N1	-3.20	119.49	122.79
32	2a	1407	5MC	C5-C4-N3	-3.19	118.48	121.75
55	2x	54	5MU	C5-C6-N1	-3.19	119.84	123.31
32	2a	966	M2G	C6-C5-N7	3.16	136.04	130.29
55	2x	32	5MC	C5-C6-N1	-3.16	119.88	123.31
55	2x	55	PSU	O2-C2-N1	-3.15	119.54	122.79
1	1A	2503	2MA	C4-N9-C8	3.15	109.04	105.74
55	1x	8	4SU	C5-C4-N3	3.12	117.66	114.75
32	1a	1207	2MG	C4-C5-N7	-3.12	105.73	110.67
32	2a	967	5MC	C5-C6-N1	-3.11	119.94	123.31
55	1x	8	4SU	S4-C4-N3	-3.10	116.96	120.20
1	1A	2503	2MA	C4-C5-N7	-3.10	107.04	110.58
32	1a	967	5MC	C5-C6-N1	-3.07	119.97	123.31
32	1a	1400	5MC	C5-C4-N3	-3.07	118.61	121.75
1	1A	2251	OMG	C6-C5-N7	3.07	135.88	130.29
54	1w	76	L3X	C5-N7-C8	3.07	108.27	103.45
55	1x	76	31H	C5-N7-C8	3.06	108.27	103.45
43	2l	92	0TD	OD2-CG-CB	3.06	119.77	113.15
32	2a	1518	MA6	N9-C8-N7	-3.06	109.60	113.94
55	2x	76	31H	C5-N7-C8	3.06	108.25	103.45
56	2y	54	5MU	C1'-N1-C2	3.05	123.07	117.59
32	1a	966	M2G	C6-C5-N7	3.05	135.84	130.29
32	2a	1404	5MC	C5-C6-N1	-3.05	120.00	123.31
32	1a	1207	2MG	N1-C2-N2	3.03	119.66	116.56
32	1a	1498	UR3	C5-C4-N3	3.00	119.00	115.04
32	2a	1207	2MG	C4-C5-N7	-2.97	105.96	110.67
1	2A	2552	OMU	C5-C4-N3	2.91	118.87	114.80
54	2w	76	L3X	C5-N7-C8	2.90	108.01	103.45
55	1x	32	5MC	C5-C4-N3	-2.90	118.79	121.75
1	1A	1915	5MU	C5-C6-N1	-2.86	120.21	123.31
32	2a	1518	MA6	N3-C4-N9	2.82	131.97	127.17
32	1a	527	G7M	O6-C6-C5	-2.80	121.75	128.01
55	2x	8	4SU	C6-C5-C4	-2.76	117.56	119.95
1	2A	2251	OMG	C6-C5-N7	2.76	135.31	130.29
1	1A	2552	OMU	O4-C4-C5	-2.76	120.41	125.16
55	2x	32	5MC	C5-C4-N3	-2.76	118.93	121.75
55	2x	76	31H	C5-C4-N9	2.75	108.81	105.81
43	1l	92	0TD	OD2-CG-CB	2.74	119.07	113.15
1	2A	1942	5MC	C5-C4-N3	-2.73	118.96	121.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	1a	516	PSU	O2-C2-N1	-2.72	119.98	122.79
32	1a	1407	5MC	O2-C2-N3	-2.72	118.05	122.33
1	2A	2552	OMU	O4-C4-C5	-2.71	120.49	125.16
32	2a	1519	MA6	N3-C4-N9	2.71	131.77	127.17
56	1y	54	5MU	O2-C2-N1	-2.70	119.28	122.80
1	2A	2605	PSU	O2-C2-N1	-2.69	120.01	122.79
32	2a	966	M2G	C4-C5-N7	-2.68	106.42	110.67
1	1A	1942	5MC	C5-C4-N3	-2.67	119.02	121.75
1	1A	2605	PSU	C5-C6-N1	-2.66	118.44	122.14
1	2A	2503	2MA	C4-N9-C8	2.66	108.53	105.74
32	1a	1404	5MC	C5-C4-N3	-2.65	119.03	121.75
32	1a	1519	MA6	N3-C4-N9	2.65	131.67	127.17
55	1x	76	31H	C5-C4-N9	2.64	108.69	105.81
54	1w	76	L3X	C5-C4-N9	2.64	108.69	105.81
32	1a	1404	5MC	O2-C2-N3	-2.63	118.18	122.33
32	1a	1207	2MG	N2-C2-N3	-2.62	117.17	120.51
55	2x	8	4SU	C1'-N1-C2	2.61	122.28	117.59
1	1A	2552	OMU	C5-C4-N3	2.61	118.45	114.80
1	2A	2503	2MA	C5-N7-C8	2.59	107.53	103.45
32	2a	1404	5MC	C5-C4-N3	-2.59	119.10	121.75
1	1A	2503	2MA	C5-N7-C8	2.58	107.51	103.45
1	1A	1962	5MC	C5-C4-N3	-2.56	119.13	121.75
1	1A	2503	2MA	C2-N1-C6	2.55	122.02	118.10
54	2w	76	L3X	C5-C4-N9	2.55	108.59	105.81
55	2x	76	31H	N3-C4-N9	2.54	131.49	127.17
56	2y	54	5MU	C1'-N1-C6	-2.53	116.98	121.15
1	2A	1920	OMC	O2-C2-N3	-2.52	118.35	122.33
55	2x	32	5MC	O2-C2-N3	-2.51	118.38	122.33
55	1x	76	31H	N3-C4-N9	2.50	131.43	127.17
54	1w	54	5MU	C5-C6-N1	-2.50	120.60	123.31
55	2x	55	PSU	C5-C6-N1	-2.49	118.68	122.14
1	2A	2503	2MA	N6-C6-N1	2.49	120.39	117.03
54	1w	76	L3X	N3-C4-N9	2.48	131.38	127.17
56	1y	8	4SU	N3-C2-N1	2.47	118.11	114.89
54	1w	8	4SU	N3-C2-N1	2.46	118.10	114.89
32	2a	967	5MC	C5-C4-N3	-2.45	119.24	121.75
1	1A	1915	5MU	O2-C2-N1	-2.45	119.61	122.80
32	1a	1407	5MC	C5-C4-N3	-2.44	119.25	121.75
1	1A	2552	OMU	C2'-C1'-N1	-2.44	109.62	114.24
1	1A	1915	5MU	C5M-C5-C4	2.44	121.38	118.78
1	2A	2251	OMG	O6-C6-C5	-2.44	120.10	126.53
54	2w	76	L3X	N3-C4-N9	2.43	131.30	127.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	1y	8	4SU	C1'-N1-C2	2.43	121.95	117.59
1	1A	2251	OMG	O6-C6-C5	-2.43	120.13	126.53
32	1a	967	5MC	C5-C4-N3	-2.42	119.27	121.75
32	1a	1498	UR3	C6-N1-C2	-2.42	119.82	121.80
55	2x	76	31H	CA-N-CN	-2.42	119.11	122.82
56	1y	8	4SU	C5-C4-S4	-2.42	121.55	124.31
32	2a	1407	5MC	O2-C2-N3	-2.38	118.58	122.33
32	1a	966	M2G	C4-C5-N7	-2.38	106.90	110.67
32	1a	1402	4OC	C6-C5-C4	2.36	119.85	117.00
32	1a	1518	MA6	N3-C4-N9	2.36	131.17	127.17
32	2a	1519	MA6	C4-C5-C6	2.35	118.34	115.91
32	2a	1400	5MC	C5-C4-N3	-2.35	119.34	121.75
32	1a	1207	2MG	CM2-N2-C2	-2.35	118.60	123.65
32	2a	527	G7M	C5-C6-N1	2.35	116.69	111.84
1	2A	2503	2MA	C2-N1-C6	2.34	121.70	118.10
1	2A	2251	OMG	C4-C5-N7	-2.34	106.96	110.67
56	2y	54	5MU	O2-C2-N3	-2.33	117.19	121.49
55	2x	76	31H	O4'-C1'-C2'	-2.33	101.64	106.62
55	2x	54	5MU	O2-C2-N1	-2.32	119.78	122.80
1	2A	1962	5MC	C5-C4-N3	-2.31	119.38	121.75
32	2a	1498	UR3	C3U-N3-C4	2.31	121.07	117.87
55	1x	76	31H	CA-N-CN	-2.31	119.28	122.82
32	2a	1402	4OC	O2-C2-N3	-2.30	118.70	122.33
1	1A	2503	2MA	N9-C8-N7	-2.29	110.68	113.94
1	1A	2605	PSU	O2-C2-N1	-2.29	120.43	122.79
55	2x	76	31H	C6-C5-C4	2.28	120.29	117.18
55	2x	76	31H	C4-C5-N7	-2.27	107.99	110.58
1	1A	2605	PSU	O2-C2-N3	-2.26	117.84	121.86
32	2a	1404	5MC	O2-C2-N3	-2.26	118.77	122.33
55	2x	76	31H	OCN-CN-N	-2.26	119.49	125.32
55	1x	76	31H	OCN-CN-N	-2.25	119.50	125.32
1	2A	2605	PSU	C5-C6-N1	-2.24	119.03	122.14
32	1a	1519	MA6	C4-C5-C6	2.23	118.22	115.91
54	1w	54	5MU	O2-C2-N1	-2.23	119.89	122.80
32	1a	966	M2G	O6-C6-C5	-2.23	120.66	126.53
32	1a	1404	5MC	CM5-C5-C6	-2.22	119.84	122.85
32	1a	1400	5MC	O2-C2-N3	-2.22	118.84	122.33
32	1a	1207	2MG	C8-N7-C5	2.21	108.20	104.26
55	1x	76	31H	C4-C5-N7	-2.21	108.06	110.58
54	2w	54	5MU	C5M-C5-C4	2.20	121.14	118.78
32	2a	1402	4OC	CM4-N4-C4	-2.20	118.16	122.45
1	1A	1939	5MU	O2-C2-N1	-2.20	119.94	122.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	1a	1518	MA6	C4-N9-C8	2.19	108.04	105.74
1	1A	1920	OMC	O2-C2-N3	-2.19	118.88	122.33
55	2x	8	4SU	O2-C2-N1	2.19	125.64	122.80
32	2a	1518	MA6	C4-C5-C6	2.18	118.17	115.91
1	2A	2503	2MA	C6-C5-N7	2.17	136.28	132.09
56	2y	54	5MU	C5-C6-N1	-2.17	120.96	123.31
55	1x	76	31H	C6-C5-C4	2.17	120.14	117.18
54	1w	76	L3X	C6-C5-C4	2.15	120.12	117.18
54	2w	76	L3X	C6-C5-C4	2.15	120.11	117.18
32	2a	1207	2MG	C2-N1-C6	-2.14	121.96	124.55
54	1w	76	L3X	C4-C5-N7	-2.13	108.15	110.58
32	1a	1400	5MC	CM5-C5-C6	-2.13	119.97	122.85
32	2a	527	G7M	O6-C6-C5	-2.13	123.26	128.01
32	1a	516	PSU	O4'-C1'-C2'	2.13	108.09	105.15
32	2a	1402	4OC	C6-C5-C4	2.12	119.56	117.00
32	2a	516	PSU	O4'-C1'-C2'	2.12	108.09	105.15
1	2A	2503	2MA	N9-C8-N7	-2.09	110.97	113.94
55	1x	8	4SU	O2-C2-N3	-2.09	117.63	121.49
55	1x	76	31H	O2'-C2'-C3'	2.09	116.28	111.16
55	1x	76	31H	C4'-O4'-C1'	-2.08	104.88	109.47
32	2a	967	5MC	O2-C2-N3	-2.08	119.06	122.33
43	2l	92	0TD	OD1-CG-CB	-2.07	118.10	122.44
32	1a	527	G7M	C5-C6-N1	2.07	116.12	111.84
54	1w	8	4SU	C1'-N1-C6	-2.07	116.36	120.78
32	2a	1400	5MC	O2-C2-N3	-2.06	119.08	122.33
1	1A	1911	PSU	C6-C5-C4	-2.06	116.78	118.17
54	2w	54	5MU	C5-C6-N1	-2.04	121.10	123.31
32	1a	1498	UR3	C3U-N3-C4	2.03	120.69	117.87
1	1A	2251	OMG	C5-C6-N1	2.03	118.43	113.25
55	1x	8	4SU	C1'-N1-C2	2.02	121.21	117.59
1	1A	2251	OMG	C4-C5-N7	-2.01	107.48	110.67
1	2A	1917	PSU	C5-C6-N1	-2.01	119.35	122.14
55	2x	55	PSU	O4'-C1'-C2'	2.00	107.92	105.15

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	1400	5MC	O4'-C4'-C5'-O5'
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1519	MA6	O4'-C4'-C5'-O5'
54	2w	76	L3X	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
55	1x	76	31H	C3'-C4'-C5'-O5'
55	1x	76	31H	N-CA-CB-CG
55	2x	76	31H	C3'-C4'-C5'-O5'
55	2x	76	31H	O4'-C4'-C5'-O5'
56	2y	55	PSU	O4'-C4'-C5'-O5'
54	2w	76	L3X	C3'-C4'-C5'-O5'
32	1a	1402	4OC	O4'-C4'-C5'-O5'
32	2a	1402	4OC	O4'-C4'-C5'-O5'
56	2y	8	4SU	O4'-C4'-C5'-O5'
56	2y	55	PSU	C3'-C4'-C5'-O5'
32	1a	527	G7M	C3'-C4'-C5'-O5'
55	1x	76	31H	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
55	2x	76	31H	N-CA-CB-CG
32	1a	1400	5MC	C3'-C4'-C5'-O5'
32	1a	1402	4OC	C3'-C4'-C5'-O5'
32	2a	1402	4OC	C3'-C4'-C5'-O5'
55	1x	76	31H	C4'-C5'-O5'-P
32	1a	527	G7M	O4'-C4'-C5'-O5'
55	1x	76	31H	C-CA-CB-CG
55	2x	76	31H	C-CA-CB-CG
56	2y	8	4SU	C3'-C4'-C5'-O5'
55	1x	76	31H	CB-CG-SD-CE
32	2a	527	G7M	C3'-C4'-C5'-O5'
43	2l	92	0TD	CG-CB-SB-CSB
56	1y	55	PSU	O4'-C1'-C5-C4
32	1a	1519	MA6	C4'-C5'-O5'-P
32	2a	1519	MA6	C4'-C5'-O5'-P
1	2A	2503	2MA	O4'-C4'-C5'-O5'
56	2y	54	5MU	O4'-C4'-C5'-O5'
56	2y	54	5MU	C2'-C1'-N1-C6
56	1y	55	PSU	O4'-C1'-C5-C6
32	2a	967	5MC	O4'-C4'-C5'-O5'
43	1l	92	0TD	CG-CB-SB-CSB
1	1A	2503	2MA	O4'-C4'-C5'-O5'
32	1a	527	G7M	C4'-C5'-O5'-P
55	2x	76	31H	C4'-C5'-O5'-P
1	1A	2503	2MA	C4'-C5'-O5'-P
1	1A	1920	OMC	C2'-C1'-N1-C2

There are no ring outliers.

31 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	2y	55	PSU	1	0
32	2a	1519	MA6	3	0
54	2w	55	PSU	1	0
54	2w	76	L3X	1	0
56	2y	8	4SU	4	0
32	2a	1404	5MC	1	0
1	2A	2503	2MA	1	0
54	2w	54	5MU	1	0
54	2w	8	4SU	3	0
56	2y	54	5MU	1	0
43	2l	92	0TD	1	0
1	2A	2251	OMG	2	0
32	1a	1400	5MC	1	0
1	2A	1917	PSU	1	0
1	1A	2251	OMG	1	0
32	1a	1402	4OC	2	0
54	1w	76	L3X	1	0
32	1a	1519	MA6	2	0
55	1x	8	4SU	2	0
55	2x	76	31H	2	0
1	2A	1939	5MU	1	0
54	1w	54	5MU	2	0
32	2a	1518	MA6	3	0
55	1x	76	31H	1	0
56	1y	8	4SU	2	0
32	1a	1518	MA6	2	0
55	2x	8	4SU	2	0
54	1w	55	PSU	4	0
1	1A	1939	5MU	1	0
56	1y	55	PSU	1	0
32	2a	1402	4OC	2	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2762 ligands modelled in this entry, 2760 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
60	SF4	1d	501	35	0,12,12	-	-	-		
60	SF4	2d	303	35	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	SF4	1d	501	35	-	-	0/6/5/5
60	SF4	2d	303	35	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	1d	501	SF4	1	0

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	1A	2860/2915 (98%)	-0.51	143 (5%) 34 33	17, 34, 92, 102	0
1	2A	2789/2915 (95%)	0.03	141 (5%) 33 33	32, 55, 90, 102	0
2	1B	120/121 (99%)	-0.36	0 100 100	29, 49, 63, 84	0
2	2B	120/121 (99%)	0.93	4 (3%) 49 50	61, 77, 85, 93	0
3	1D	275/276 (99%)	-0.07	4 (1%) 72 73	18, 35, 48, 70	0
3	2D	275/276 (99%)	0.42	7 (2%) 58 59	30, 49, 61, 78	0
4	1E	204/206 (99%)	-0.10	1 (0%) 87 89	17, 37, 57, 72	0
4	2E	204/206 (99%)	0.49	6 (2%) 53 55	32, 55, 67, 79	0
5	1F	202/210 (96%)	-0.13	2 (0%) 79 80	17, 40, 63, 81	0
5	2F	202/210 (96%)	0.48	3 (1%) 72 73	33, 65, 75, 80	0
6	1G	181/182 (99%)	0.67	15 (8%) 17 17	38, 58, 70, 80	0
6	2G	181/182 (99%)	1.60	50 (27%) 1 1	67, 77, 82, 88	0
7	1H	174/180 (96%)	0.24	2 (1%) 78 79	34, 50, 61, 64	0
7	2H	174/180 (96%)	1.31	23 (13%) 7 6	66, 78, 85, 88	0
8	1I	146/148 (98%)	0.99	11 (7%) 20 19	45, 70, 78, 83	0
8	2I	146/148 (98%)	1.40	31 (21%) 2 2	54, 71, 79, 81	0
9	1N	140/140 (100%)	-0.08	1 (0%) 84 86	24, 36, 57, 70	0
9	2N	140/140 (100%)	1.11	13 (9%) 14 13	44, 63, 75, 81	0
10	1O	122/122 (100%)	-0.09	1 (0%) 82 84	28, 38, 55, 63	0
10	2O	122/122 (100%)	0.42	0 100 100	42, 54, 68, 72	0
11	1P	149/150 (99%)	0.17	3 (2%) 65 65	18, 43, 63, 70	0
11	2P	149/150 (99%)	0.90	15 (10%) 12 11	39, 64, 77, 87	0
12	1Q	141/141 (100%)	-0.02	1 (0%) 84 86	25, 39, 52, 70	0
12	2Q	141/141 (100%)	0.95	11 (7%) 19 18	45, 63, 72, 79	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%)	-0.27	0 100 100	23, 32, 46, 56	0
13	2R	118/118 (100%)	0.17	0 100 100	38, 49, 58, 65	0
14	1S	110/112 (98%)	0.10	0 100 100	36, 49, 58, 66	0
14	2S	110/112 (98%)	1.52	29 (26%) 1 1	61, 72, 79, 83	0
15	1T	131/146 (89%)	0.23	4 (3%) 51 52	32, 43, 67, 76	0
15	2T	131/146 (89%)	0.55	5 (3%) 44 45	46, 57, 72, 77	0
16	1U	116/118 (98%)	-0.41	0 100 100	19, 27, 44, 61	0
16	2U	116/118 (98%)	0.75	2 (1%) 69 69	43, 60, 72, 77	0
17	1V	101/101 (100%)	-0.33	0 100 100	20, 35, 50, 63	0
17	2V	101/101 (100%)	1.16	9 (8%) 15 14	42, 69, 76, 79	0
18	1W	112/113 (99%)	-0.22	1 (0%) 81 83	22, 30, 49, 71	0
18	2W	112/113 (99%)	0.29	1 (0%) 81 83	38, 47, 65, 78	0
19	1X	95/96 (98%)	0.01	2 (2%) 63 64	25, 37, 57, 75	0
19	2X	95/96 (98%)	0.84	8 (8%) 17 16	45, 57, 73, 82	0
20	1Y	107/110 (97%)	0.19	2 (1%) 66 66	34, 47, 64, 75	0
20	2Y	107/110 (97%)	1.20	11 (10%) 12 11	55, 67, 77, 86	0
21	1Z	154/206 (74%)	1.06	28 (18%) 3 3	39, 61, 83, 86	0
21	2Z	160/206 (77%)	1.64	41 (25%) 1 1	62, 78, 87, 91	0
22	10	83/85 (97%)	0.12	4 (4%) 35 35	27, 36, 51, 64	0
22	20	83/85 (97%)	1.25	15 (18%) 3 3	43, 63, 71, 77	0
23	11	97/98 (98%)	0.26	1 (1%) 79 80	25, 44, 65, 69	0
23	21	97/98 (98%)	0.72	3 (3%) 51 52	39, 54, 71, 76	0
24	12	70/72 (97%)	0.20	2 (2%) 53 55	33, 46, 57, 72	0
24	22	70/72 (97%)	0.95	6 (8%) 16 15	58, 67, 76, 79	0
25	13	59/60 (98%)	-0.20	0 100 100	26, 33, 55, 70	0
25	23	59/60 (98%)	0.95	6 (10%) 12 11	52, 64, 72, 78	0
26	14	69/71 (97%)	1.32	17 (24%) 2 1	51, 72, 85, 89	0
26	24	69/71 (97%)	1.92	29 (42%) 0 0	74, 83, 89, 93	0
27	15	59/60 (98%)	-0.39	1 (1%) 69 69	18, 28, 49, 59	0
27	25	59/60 (98%)	0.19	0 100 100	33, 48, 62, 75	0
28	16	53/54 (98%)	-0.20	0 100 100	30, 40, 55, 59	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%)	0.76	0 100 100	54, 60, 66, 71	0
29	17	48/49 (97%)	-0.29	2 (4%) 40 41	19, 26, 51, 58	0
29	27	48/49 (97%)	0.25	4 (8%) 17 17	32, 39, 65, 70	0
30	18	64/65 (98%)	-0.28	0 100 100	24, 31, 39, 53	0
30	28	64/65 (98%)	0.56	0 100 100	44, 56, 63, 65	0
31	19	37/37 (100%)	-0.06	0 100 100	29, 37, 53, 55	0
31	29	37/37 (100%)	0.98	1 (2%) 56 57	58, 63, 75, 76	0
32	1a	1488/1521 (97%)	0.31	39 (2%) 57 58	33, 66, 89, 100	0
32	2a	1491/1521 (98%)	0.66	99 (6%) 24 24	48, 75, 92, 102	0
33	1b	231/256 (90%)	1.31	44 (19%) 3 2	59, 74, 82, 88	0
33	2b	231/256 (90%)	2.14	112 (48%) 0 0	73, 82, 87, 92	0
34	1c	206/239 (86%)	1.19	31 (15%) 5 5	58, 70, 78, 85	0
34	2c	206/239 (86%)	2.22	114 (55%) 0 0	70, 82, 86, 89	0
35	1d	208/209 (99%)	1.23	27 (12%) 7 6	53, 68, 76, 82	0
35	2d	208/209 (99%)	1.28	28 (13%) 7 5	60, 70, 77, 81	0
36	1e	148/162 (91%)	0.77	7 (4%) 36 36	46, 62, 71, 76	0
36	2e	148/162 (91%)	1.50	30 (20%) 3 2	67, 74, 81, 83	0
37	1f	100/101 (99%)	1.02	4 (4%) 42 43	55, 65, 73, 76	0
37	2f	100/101 (99%)	0.95	4 (4%) 42 43	59, 67, 75, 78	0
38	1g	155/156 (99%)	1.16	20 (12%) 7 6	58, 69, 81, 85	0
38	2g	155/156 (99%)	1.62	42 (27%) 1 1	69, 77, 84, 88	0
39	1h	137/138 (99%)	0.76	4 (2%) 53 55	51, 63, 70, 74	0
39	2h	137/138 (99%)	1.48	26 (18%) 3 2	65, 74, 79, 82	0
40	1i	127/128 (99%)	1.57	38 (29%) 1 1	51, 73, 78, 82	0
40	2i	127/128 (99%)	2.20	72 (56%) 0 0	73, 82, 86, 88	0
41	1j	97/105 (92%)	1.58	29 (29%) 1 1	57, 74, 81, 87	0
41	2j	96/105 (91%)	2.36	60 (62%) 0 0	75, 83, 87, 89	0
42	1k	114/129 (88%)	1.22	16 (14%) 6 5	41, 64, 74, 80	0
42	2k	114/129 (88%)	1.47	23 (20%) 3 2	56, 72, 78, 81	0
43	1l	121/132 (91%)	0.73	7 (5%) 29 28	42, 55, 65, 77	0
43	2l	121/132 (91%)	1.26	21 (17%) 4 3	59, 70, 77, 80	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	1m	123/126 (97%)	1.28	13 (10%) 11 11	57, 68, 76, 87	0
44	2m	122/126 (96%)	2.24	58 (47%) 0 0	71, 80, 84, 91	0
45	1n	60/61 (98%)	1.14	6 (10%) 12 12	61, 66, 72, 76	0
45	2n	60/61 (98%)	2.75	43 (71%) 0 0	77, 82, 85, 87	0
46	1o	88/89 (98%)	0.93	4 (4%) 38 38	46, 62, 72, 74	0
46	2o	88/89 (98%)	0.97	4 (4%) 38 38	59, 70, 78, 82	0
47	1p	82/88 (93%)	1.45	14 (17%) 4 3	55, 69, 75, 82	0
47	2p	82/88 (93%)	1.16	8 (9%) 13 12	57, 67, 74, 78	0
48	1q	99/105 (94%)	1.08	5 (5%) 33 33	51, 64, 71, 73	0
48	2q	99/105 (94%)	0.99	5 (5%) 33 33	58, 70, 77, 80	0
49	1r	68/88 (77%)	0.89	4 (5%) 28 27	54, 64, 72, 76	0
49	2r	68/88 (77%)	1.10	7 (10%) 12 11	63, 71, 78, 79	0
50	1s	83/93 (89%)	1.44	15 (18%) 3 3	63, 73, 78, 82	0
50	2s	83/93 (89%)	2.47	53 (63%) 0 0	76, 82, 86, 88	0
51	1t	96/106 (90%)	1.20	10 (10%) 11 11	60, 68, 75, 79	0
51	2t	96/106 (90%)	0.95	9 (9%) 14 13	56, 67, 76, 80	0
52	1u	23/27 (85%)	1.14	4 (17%) 4 3	62, 66, 72, 74	0
52	2u	23/27 (85%)	2.29	12 (52%) 0 0	74, 79, 81, 82	0
53	1v	13/24 (54%)	1.19	5 (38%) 1 0	49, 67, 89, 95	0
53	2v	13/24 (54%)	1.79	5 (38%) 1 0	71, 83, 96, 97	0
54	1w	69/74 (93%)	1.62	20 (28%) 1 1	49, 91, 97, 99	0
54	2w	68/74 (91%)	2.02	36 (52%) 0 0	62, 95, 98, 99	0
55	1x	72/77 (93%)	0.39	2 (2%) 55 56	29, 63, 78, 88	0
55	2x	72/77 (93%)	0.84	3 (4%) 40 41	49, 80, 88, 94	0
56	1y	70/74 (94%)	2.30	47 (67%) 0 0	54, 95, 99, 100	0
56	2y	70/74 (94%)	2.18	36 (51%) 0 0	66, 97, 100, 103	0
All	All	20885/21740 (96%)	0.52	2047 (9%) 13 12	17, 62, 87, 103	0

All (2047) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	2m	124	PRO	12.6
44	2m	123	ALA	10.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
44	1m	123	ALA	8.4
44	1m	124	PRO	7.3
1	2A	2111	C	6.9
44	2m	102	ARG	6.9
38	1g	80	VAL	6.7
1	2A	2145	C	6.6
1	1A	2115	G	6.4
1	2A	2112	G	6.4
44	2m	122	LYS	6.4
33	2b	165	VAL	6.3
23	11	2	SER	6.3
7	1H	2	SER	6.2
41	2j	65	LEU	6.2
1	2A	2113	U	6.1
1	1A	2145	C	6.0
45	1n	2	ALA	6.0
41	2j	47	PHE	6.0
1	1A	2112	G	5.9
23	21	2	SER	5.8
45	2n	34	TYR	5.8
34	2c	87	LEU	5.7
1	2A	2146	C	5.7
33	2b	237	ALA	5.7
38	1g	79	ARG	5.7
45	2n	25	VAL	5.6
50	2s	80	TYR	5.5
21	1Z	146	ILE	5.5
1	1A	2113	U	5.5
1	1A	2159	G	5.5
40	2i	102	LEU	5.5
38	2g	83	ALA	5.5
41	1j	32	ALA	5.5
1	2A	2115	G	5.4
1	2A	2144	U	5.4
34	2c	158	GLY	5.4
21	1Z	141	VAL	5.4
33	2b	71	VAL	5.3
1	1A	2111	C	5.3
19	1X	95	LEU	5.3
1	2A	2170	A	5.2
44	1m	122	LYS	5.2
1	1A	2146	C	5.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
45	2n	39	LEU	5.2
45	2n	2	ALA	5.1
1	1A	2114	A	5.1
1	2A	2147	G	5.1
44	1m	2	ALA	5.0
15	1T	130	ALA	5.0
1	2A	2143	C	5.0
21	1Z	150	LEU	5.0
34	2c	129	ALA	4.9
38	1g	4	ARG	4.9
1	2A	2167	U	4.9
40	2i	14	VAL	4.9
33	2b	236	TYR	4.9
26	14	56	VAL	4.9
1	2A	2138	C	4.9
1	2A	2166	G	4.9
1	1A	2147	G	4.8
38	2g	80	VAL	4.8
45	2n	38	GLY	4.8
50	2s	79	THR	4.8
32	2a	1033	G	4.7
19	1X	94	GLY	4.7
34	2c	2	GLY	4.7
50	1s	13	ASP	4.6
44	2m	6	GLY	4.6
38	2g	82	GLY	4.6
34	2c	77	ILE	4.6
1	2A	2802	G	4.6
33	2b	70	PHE	4.5
9	2N	9	VAL	4.5
6	1G	146	TYR	4.5
1	1A	2803	C	4.5
26	24	51	ASP	4.5
44	2m	90	LEU	4.5
34	1c	2	GLY	4.5
33	2b	152	PHE	4.5
45	2n	30	ALA	4.5
45	2n	29	ARG	4.4
1	2A	2155	G	4.4
1	2A	2803	C	4.4
1	2A	2117	A	4.4
51	1t	103	GLY	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	2a	1034	G	4.4
21	1Z	120	ILE	4.4
33	2b	185	ILE	4.4
44	1m	121	LYS	4.4
34	2c	78	GLY	4.4
33	1b	17	PHE	4.4
41	2j	32	ALA	4.3
1	2A	2109	U	4.3
21	2Z	174	VAL	4.3
33	2b	122	PHE	4.3
54	2w	71	G	4.3
26	24	65	ASP	4.3
40	2i	9	ARG	4.3
1	1A	2119	A	4.3
1	2A	2169	A	4.3
15	1T	131	ALA	4.3
45	2n	6	LEU	4.3
1	2A	2123	G	4.2
41	1j	76	ASN	4.2
20	2Y	1	MET	4.2
34	2c	73	PRO	4.2
44	2m	121	LYS	4.2
1	1A	2144	U	4.2
1	2A	2142	C	4.2
54	1w	72	C	4.2
40	1i	113	LYS	4.2
56	1y	15	A	4.2
44	2m	78	ILE	4.2
19	2X	92	LEU	4.2
21	2Z	144	LEU	4.2
33	1b	237	ALA	4.2
40	2i	103	THR	4.1
35	2d	112	VAL	4.1
50	2s	22	LEU	4.1
21	1Z	1	MET	4.1
40	2i	125	TYR	4.1
1	1A	2804	C	4.1
1	2A	2119	A	4.1
42	1k	14	VAL	4.1
38	2g	32	ARG	4.1
40	2i	11	LYS	4.1
1	1A	2117	A	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	2136	C	4.1
56	2y	34	C	4.1
34	2c	189	ALA	4.1
22	10	6	GLY	4.1
21	2Z	146	ILE	4.1
1	1A	2160	G	4.1
33	1b	11	LEU	4.1
38	2g	5	ARG	4.0
37	2f	21	LEU	4.0
1	2A	2182	G	4.0
26	24	56	VAL	4.0
1	2A	2114	A	4.0
1	1A	889	C	4.0
42	2k	29	ILE	4.0
40	2i	5	TYR	4.0
43	2l	18	VAL	4.0
45	2n	33	VAL	4.0
33	2b	34	ALA	4.0
52	2u	14	TRP	4.0
33	2b	187	LEU	4.0
45	2n	21	TYR	4.0
47	2p	82	GLN	4.0
21	1Z	104	PHE	4.0
35	1d	169	LYS	4.0
1	1A	1057	A	4.0
54	2w	72	C	4.0
34	2c	33	LEU	4.0
6	2G	28	VAL	4.0
34	2c	68	VAL	4.0
40	1i	8	GLY	3.9
22	10	7	LEU	3.9
38	2g	84	ASN	3.9
35	1d	87	GLY	3.9
1	1A	2165	G	3.9
1	2A	2154	G	3.9
1	1A	888	C	3.9
40	1i	2	GLU	3.9
42	1k	75	TYR	3.9
45	2n	7	ILE	3.9
1	1A	2130	U	3.9
1	1A	2141	G	3.9
1	1A	2166	G	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	2c	55	VAL	3.9
1	1A	2140	C	3.9
26	14	63	TYR	3.9
44	2m	87	TYR	3.9
41	2j	78	ASN	3.9
41	2j	91	PRO	3.9
33	1b	229	VAL	3.9
54	2w	15	A	3.9
1	1A	2143	C	3.8
21	2Z	173	ALA	3.8
26	24	66	SER	3.8
45	2n	20	ALA	3.8
1	2A	2159	G	3.8
1	2A	2805	G	3.8
33	2b	91	PRO	3.8
50	2s	2	PRO	3.8
32	2a	1532	U	3.8
1	1A	1096	A	3.8
33	2b	123	ALA	3.8
51	1t	47	GLY	3.8
1	2A	2110	G	3.8
32	2a	1202	G	3.8
41	2j	88	LEU	3.8
26	24	49	PHE	3.8
32	1a	204	U	3.8
38	1g	153	HIS	3.8
45	2n	16	PHE	3.8
34	2c	124	ILE	3.8
1	1A	1064	C	3.8
1	2A	2165	G	3.8
50	2s	4	SER	3.7
3	1D	276	LYS	3.7
34	2c	128	PHE	3.7
34	2c	159	GLY	3.7
1	1A	2133	G	3.7
12	2Q	10	ARG	3.7
22	20	2	ALA	3.7
1	1A	1078	U	3.7
1	2A	2135	A	3.7
32	1a	1531	A	3.7
38	2g	85	TYR	3.7
1	2A	2137	C	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	1b	7	VAL	3.7
33	2b	229	VAL	3.7
38	1g	82	GLY	3.7
39	1h	2	LEU	3.7
41	1j	4	ILE	3.7
50	1s	71	LEU	3.7
35	2d	154	ASN	3.7
42	1k	25	TYR	3.7
52	2u	24	ARG	3.7
50	2s	77	THR	3.7
56	2y	13	C	3.7
40	2i	45	ALA	3.7
1	2A	2127	G	3.7
33	2b	80	ILE	3.7
34	2c	196	LEU	3.7
38	2g	154	TYR	3.7
38	1g	156	TRP	3.6
21	2Z	141	VAL	3.6
1	1A	2142	C	3.6
38	2g	81	GLY	3.6
50	2s	68	GLY	3.6
50	2s	84	GLY	3.6
45	2n	14	PRO	3.6
1	2A	2141	G	3.6
50	2s	13	ASP	3.6
1	1A	1081	U	3.6
56	2y	19	U	3.6
33	2b	93	VAL	3.6
15	2T	130	ALA	3.6
26	14	59	PHE	3.6
33	2b	121	LEU	3.6
56	1y	19	U	3.6
1	1A	2805	G	3.6
22	20	30	VAL	3.6
41	2j	34	VAL	3.6
50	2s	9	VAL	3.6
35	2d	164	ALA	3.6
38	2g	2	ALA	3.6
40	1i	106	ALA	3.6
1	2A	2804	C	3.6
43	2l	64	TYR	3.6
34	2c	207	VAL	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
42	2k	31	THR	3.6
21	1Z	149	SER	3.6
4	2E	204	ALA	3.6
21	2Z	143	GLY	3.6
14	2S	35	ILE	3.6
1	1A	2109	U	3.5
6	2G	146	TYR	3.5
34	2c	48	TYR	3.5
42	2k	25	TYR	3.5
44	2m	103	THR	3.5
50	2s	52	TYR	3.5
41	2j	79	ARG	3.5
1	2A	2116	G	3.5
41	2j	90	LEU	3.5
42	2k	89	ALA	3.5
56	2y	17	G	3.5
40	2i	67	GLY	3.5
1	1A	2158	A	3.5
34	2c	157	ILE	3.5
42	2k	48	ILE	3.5
50	2s	53	ASN	3.5
1	1A	2161	C	3.5
1	1A	2167	U	3.5
56	2y	33	U	3.5
40	2i	36	TYR	3.5
40	2i	62	TYR	3.5
38	2g	16	LEU	3.5
1	2A	2168	G	3.5
54	1w	1	G	3.5
56	1y	13	C	3.5
50	2s	71	LEU	3.5
8	2I	53	ALA	3.5
51	2t	97	ALA	3.5
1	2A	2126	A	3.5
1	2A	2120	G	3.5
33	1b	230	VAL	3.5
33	2b	15	VAL	3.5
33	1b	10	LEU	3.5
33	2b	225	ALA	3.5
41	2j	75	ILE	3.5
1	1A	2135	A	3.4
1	1A	2169	A	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
45	2n	3	ARG	3.4
1	2A	2149	G	3.4
32	2a	1030(A)	G	3.4
32	2a	1032	G	3.4
44	2m	7	VAL	3.4
41	2j	40	LEU	3.4
1	1A	2138	C	3.4
34	2c	13	GLY	3.4
55	2x	1	C	3.4
6	2G	29	TRP	3.4
36	2e	10	MET	3.4
33	2b	81	VAL	3.4
33	2b	230	VAL	3.4
47	1p	21	VAL	3.4
40	2i	13	ALA	3.4
52	2u	13	ILE	3.4
1	2A	2134	A	3.4
50	2s	16	LEU	3.4
25	23	2	PRO	3.4
33	2b	234	PRO	3.4
36	2e	29	GLY	3.4
38	1g	81	GLY	3.4
1	1A	1087	G	3.4
1	2A	2181	G	3.4
40	2i	10	ARG	3.4
56	1y	35	C	3.4
34	2c	62	ASP	3.4
38	2g	156	TRP	3.4
6	2G	3	LEU	3.4
33	2b	213	LEU	3.4
40	2i	96	LEU	3.4
41	2j	87	THR	3.4
39	2h	131	GLY	3.4
41	2j	93	GLY	3.4
6	2G	20	ILE	3.4
8	2I	82	ARG	3.4
33	2b	200	ILE	3.4
11	2P	149	GLU	3.4
1	1A	1066	U	3.3
1	2A	2189	U	3.3
38	1g	85	TYR	3.3
48	2q	95	TYR	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
40	2i	127	LYS	3.3
19	2X	95	LEU	3.3
40	2i	40	LEU	3.3
41	2j	37	PRO	3.3
43	2l	43	VAL	3.3
34	2c	6	HIS	3.3
6	2G	50	ALA	3.3
6	2G	52	ILE	3.3
33	2b	201	ILE	3.3
45	2n	37	PHE	3.3
1	1A	2132	U	3.3
1	1A	2120	G	3.3
1	2A	2319	G	3.3
32	2a	1220	G	3.3
54	2w	18	G	3.3
41	2j	76	ASN	3.3
35	1d	173	TRP	3.3
45	2n	53	LEU	3.3
33	2b	136	VAL	3.3
34	2c	80	GLY	3.3
34	2c	185	GLY	3.3
21	2Z	171	ILE	3.3
21	2Z	149	SER	3.3
1	1A	1094	U	3.3
36	2e	20	GLN	3.3
56	2y	18	G	3.3
32	2a	1030	C	3.3
32	2a	1030(B)	C	3.3
34	2c	188	LEU	3.3
50	2s	76	PRO	3.3
34	2c	75	VAL	3.3
35	1d	23	GLY	3.3
50	2s	82	GLY	3.3
44	2m	33	ALA	3.3
26	14	69	LYS	3.3
32	2a	1035	A	3.3
40	2i	59	PHE	3.3
47	1p	17	TYR	3.3
1	2A	2122	U	3.3
54	1w	73	U	3.3
41	1j	77	PRO	3.3
41	2j	8	LEU	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
44	2m	113	PRO	3.3
32	2a	1036	G	3.3
52	2u	16	GLY	3.3
56	1y	34	C	3.3
56	1y	36	C	3.3
36	1e	10	MET	3.3
34	2c	84	ILE	3.3
44	1m	120	LYS	3.3
45	1n	5	ALA	3.3
51	2t	94	ALA	3.3
1	2A	2801(A)	A	3.2
41	2j	63	PHE	3.2
42	2k	75	TYR	3.2
8	1I	38	LEU	3.2
32	1a	1532	U	3.2
40	1i	14	VAL	3.2
45	2n	13	THR	3.2
51	2t	103	GLY	3.2
6	1G	182	LYS	3.2
1	1A	1068	G	3.2
1	1A	2110	G	3.2
1	1A	2121	G	3.2
1	1A	2157	G	3.2
1	2A	1536	C	3.2
33	2b	186	ALA	3.2
34	2c	92	ALA	3.2
50	2s	24	ALA	3.2
54	1w	70	C	3.2
56	1y	18	G	3.2
56	2y	36	C	3.2
33	2b	55	PHE	3.2
33	2b	57	PHE	3.2
33	2b	163	PHE	3.2
1	2A	229	A	3.2
11	2P	15	ARG	3.2
40	2i	19	LEU	3.2
22	20	3	HIS	3.2
42	1k	92	GLU	3.2
44	2m	58	GLU	3.2
20	2Y	5	MET	3.2
33	1b	15	VAL	3.2
33	2b	197	VAL	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
41	2j	10	GLY	3.2
8	1I	79	ILE	3.2
43	2l	56	ALA	3.2
1	2A	2140	C	3.2
1	2A	2174	C	3.2
32	2a	1031	G	3.2
36	1e	6	PHE	3.2
40	1i	126	SER	3.2
40	2i	37	PHE	3.2
41	1j	79	ARG	3.2
1	1A	2170	A	3.2
39	2h	2	LEU	3.2
39	2h	9	MET	3.2
1	1A	2189	U	3.2
34	1c	86	VAL	3.2
34	2c	41	GLY	3.2
44	2m	37	THR	3.2
45	2n	22	THR	3.2
3	1D	2	ALA	3.2
44	2m	76	ALA	3.2
51	1t	94	ALA	3.2
6	1G	136	ARG	3.2
14	2S	20	ARG	3.2
34	2c	167	TRP	3.2
38	2g	4	ARG	3.2
1	1A	2174	C	3.2
6	2G	102	PHE	3.2
32	2a	1223	C	3.2
33	1b	124	SER	3.2
56	2y	4	G	3.2
29	27	48	LYS	3.2
34	2c	47	LEU	3.2
34	2c	109	PRO	3.2
53	2v	13	A	3.2
34	2c	201	TYR	3.2
43	1l	64	TYR	3.2
33	2b	89	GLY	3.2
34	2c	74	GLY	3.2
34	2c	195	VAL	3.2
40	1i	41	VAL	3.2
44	2m	100	GLY	3.2
50	2s	46	GLY	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	2118	U	3.2
33	2b	211	ILE	3.2
52	2u	8	THR	3.2
7	2H	165	ALA	3.1
44	2m	104	ARG	3.1
40	2i	126	SER	3.1
1	1A	2129	C	3.1
1	2A	2297	C	3.1
22	10	3	HIS	3.1
1	2A	2125	G	3.1
7	2H	45	VAL	3.1
34	2c	198	VAL	3.1
36	2e	90	VAL	3.1
44	2m	117	VAL	3.1
52	2u	4	GLY	3.1
53	2v	12	A	3.1
56	2y	46	A	3.1
55	2x	47	U	3.1
21	2Z	172	ALA	3.1
34	2c	83	ARG	3.1
33	2b	12	GLU	3.1
33	1b	97	TRP	3.1
40	2i	91	ASP	3.1
51	2t	98	PRO	3.1
6	2G	139	LEU	3.1
40	1i	56	LEU	3.1
50	2s	30	LEU	3.1
42	2k	117	ASN	3.1
56	1y	75	C	3.1
1	2A	2121	G	3.1
1	2A	2793	G	3.1
9	2N	140	VAL	3.1
11	2P	109	GLY	3.1
35	2d	183	GLY	3.1
1	2A	2310	A	3.1
33	2b	33	TYR	3.1
33	2b	214	ILE	3.1
3	2D	276	LYS	3.1
45	2n	4	LYS	3.1
8	2I	68	LEU	3.1
50	2s	15	LEU	3.1
1	1A	885	C	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	2c	194	GLY	3.1
36	2e	74	GLY	3.1
41	1j	74	ILE	3.1
26	24	67	TYR	3.1
38	1g	154	TYR	3.1
1	1A	2156	G	3.1
1	1A	2181	G	3.1
1	2A	883	G	3.1
1	2A	896	A	3.1
1	2A	2157	G	3.1
22	20	5	LYS	3.1
34	2c	45	LYS	3.1
34	2c	168	ALA	3.1
38	2g	65	ALA	3.1
45	2n	48	ALA	3.1
53	1v	13	A	3.1
56	2y	38	A	3.1
56	1y	12	U	3.1
26	24	57	GLU	3.1
6	2G	175	LEU	3.1
22	20	7	LEU	3.1
26	14	49	PHE	3.1
41	2j	59	SER	3.1
35	1d	191	ARG	3.1
1	2A	886	C	3.1
33	2b	208	ILE	3.1
41	1j	24	VAL	3.1
45	2n	18	VAL	3.1
34	2c	67	THR	3.0
6	1G	73	ALA	3.0
21	2Z	164	ALA	3.0
34	1c	184	TYR	3.0
34	2c	65	ALA	3.0
34	2c	184	TYR	3.0
34	2c	187	ALA	3.0
44	2m	72	ALA	3.0
45	2n	10	ALA	3.0
33	2b	86	GLU	3.0
53	2v	14	A	3.0
53	2v	24	A	3.0
1	1A	1056	G	3.0
1	1A	2792	G	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	2148	G	3.0
1	2A	2162	G	3.0
33	1b	125	PRO	3.0
33	2b	11	LEU	3.0
36	2e	123	LEU	3.0
26	14	51	ASP	3.0
50	1s	12	ASP	3.0
45	2n	31	ARG	3.0
41	2j	55	LYS	3.0
36	1e	72	GLN	3.0
41	1j	75	ILE	3.0
44	2m	101	GLN	3.0
47	2p	19	ILE	3.0
34	2c	15	THR	3.0
1	1A	2108	C	3.0
1	2A	2164	C	3.0
34	2c	60	ALA	3.0
41	2j	27	ALA	3.0
19	2X	69	TYR	3.0
40	1i	114	TYR	3.0
54	2w	24	A	3.0
56	2y	15	A	3.0
1	1A	1058	G	3.0
14	2S	3	ARG	3.0
32	1a	1001(A)	G	3.0
32	2a	973	G	3.0
50	2s	38	SER	3.0
51	1t	69	GLY	3.0
21	1Z	139	VAL	3.0
33	2b	108	ILE	3.0
44	2m	53	VAL	3.0
47	2p	48	TRP	3.0
26	14	52	THR	3.0
15	2T	128	GLU	3.0
33	1b	9	GLU	3.0
33	2b	77	ALA	3.0
34	2c	53	ALA	3.0
35	1d	111	ALA	3.0
40	1i	15	ALA	3.0
1	2A	2188	C	3.0
32	2a	1027	C	3.0
34	2c	193	TYR	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
56	2y	6	C	3.0
14	2S	48	LEU	3.0
21	2Z	155	LEU	3.0
40	2i	99	LEU	3.0
1	1A	1082	U	3.0
33	2b	8	LYS	3.0
1	1A	2131	G	3.0
32	2a	1002	G	3.0
32	2a	1356	G	3.0
34	2c	197	GLY	3.0
44	2m	112	GLY	3.0
7	2H	136	ILE	3.0
41	1j	34	VAL	3.0
44	2m	105	THR	3.0
34	2c	133	ALA	3.0
40	2i	49	PRO	3.0
34	1c	201	TYR	3.0
40	2i	114	TYR	3.0
1	1A	2188	C	3.0
33	2b	10	LEU	3.0
33	2b	221	LEU	3.0
34	1c	79	ARG	3.0
35	1d	188	LEU	3.0
36	2e	12	LEU	3.0
56	1y	48	C	3.0
1	1A	1065	U	3.0
14	2S	29	PHE	3.0
50	2s	12	ASP	3.0
32	2a	969	A	3.0
56	1y	24	A	3.0
6	2G	41	GLN	3.0
41	1j	31	GLY	3.0
52	2u	11	GLY	3.0
34	2c	130	VAL	2.9
40	2i	108	VAL	2.9
40	2i	109	VAL	2.9
1	2A	2160	G	2.9
32	1a	1036	G	2.9
56	1y	1	G	2.9
11	2P	78	PRO	2.9
6	2G	74	LYS	2.9
14	2S	80	LEU	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
14	2S	92	TYR	2.9
46	1o	69	TYR	2.9
1	1A	2794	C	2.9
1	2A	888	C	2.9
54	2w	13	C	2.9
54	2w	25	C	2.9
1	1A	1060	U	2.9
33	2b	216	SER	2.9
56	1y	27	A	2.9
35	2d	16	GLY	2.9
33	2b	223	ILE	2.9
36	2e	80	ILE	2.9
8	2I	107	VAL	2.9
14	2S	46	VAL	2.9
39	2h	95	VAL	2.9
1	1A	2116	G	2.9
1	2A	2100	G	2.9
1	2A	2104	G	2.9
1	2A	2133	G	2.9
32	1a	1024	G	2.9
33	2b	21	ARG	2.9
34	2c	160	ALA	2.9
33	2b	131	PRO	2.9
45	2n	17	LYS	2.9
42	1k	36	ASP	2.9
32	2a	1257	U	2.9
54	2w	2	C	2.9
54	2w	70	C	2.9
34	2c	81	GLY	2.9
36	2e	130	ASN	2.9
1	1A	899	A	2.9
32	1a	1447	A	2.9
34	2c	90	GLU	2.9
41	2j	38	ILE	2.9
21	2Z	139	VAL	2.9
40	1i	17	VAL	2.9
50	2s	11	VAL	2.9
33	2b	130	ARG	2.9
40	2i	66	ARG	2.9
7	2H	21	PRO	2.9
8	2I	146	ALA	2.9
33	1b	188	ALA	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	1b	232	PRO	2.9
1	1A	2125	G	2.9
1	2A	882	G	2.9
1	2A	2156	G	2.9
56	1y	5	G	2.9
56	1y	17	G	2.9
56	2y	57	G	2.9
38	2g	26	PHE	2.9
33	2b	90	MET	2.9
21	2Z	147	GLY	2.9
33	2b	14	GLY	2.9
43	1l	63	GLY	2.9
56	1y	33	U	2.9
1	1A	2164	C	2.9
32	2a	1228	C	2.9
50	2s	31	ILE	2.9
1	1A	1095	A	2.9
33	1b	123	ALA	2.9
33	2b	161	ALA	2.9
33	2b	44	LEU	2.9
40	1i	47	LEU	2.9
1	2A	271(M)	G	2.9
1	2A	2894	G	2.9
21	2Z	136	PHE	2.9
33	2b	31	TYR	2.9
42	1k	13	GLN	2.9
15	2T	69	GLY	2.9
26	14	45	GLY	2.9
34	1c	80	GLY	2.9
46	1o	89	GLY	2.9
34	2c	182	ILE	2.8
43	1l	19	ARG	2.8
48	1q	36	ILE	2.8
48	1q	100	LYS	2.8
56	1y	45	U	2.8
34	2c	153	VAL	2.8
39	2h	61	VAL	2.8
50	1s	9	VAL	2.8
1	1A	1086	A	2.8
15	2T	131	ALA	2.8
36	1e	21	ALA	2.8
6	2G	19	LEU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
14	2S	87	PHE	2.8
33	2b	148	TYR	2.8
6	2G	81	LYS	2.8
11	2P	90	ARG	2.8
33	1b	228	GLY	2.8
34	2c	155	GLY	2.8
44	2m	108	ARG	2.8
50	2s	36	ARG	2.8
1	1A	2162	G	2.8
32	1a	630	G	2.8
32	1a	1030(A)	G	2.8
32	1a	1034	G	2.8
33	1b	19	HIS	2.8
33	2b	39	ILE	2.8
50	2s	49	ILE	2.8
7	2H	52	VAL	2.8
32	1a	1257	U	2.8
43	2l	55	VAL	2.8
50	2s	51	VAL	2.8
21	1Z	159	PRO	2.8
33	2b	159	PRO	2.8
35	2d	29	PRO	2.8
38	2g	93	PRO	2.8
41	2j	41	PRO	2.8
47	2p	45	THR	2.8
32	2a	1114	C	2.8
32	2a	1286	A	2.8
34	1c	94	LEU	2.8
34	2c	52	LEU	2.8
34	2c	94	LEU	2.8
54	2w	23	A	2.8
26	24	59	PHE	2.8
33	2b	17	PHE	2.8
50	1s	29	ARG	2.8
50	2s	74	PHE	2.8
36	2e	22	GLY	2.8
45	1n	51	GLY	2.8
34	1c	106	VAL	2.8
40	2i	21	PRO	2.8
40	2i	41	VAL	2.8
49	1r	86	VAL	2.8
1	1A	1059	G	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	2101	G	2.8
1	2A	2153	G	2.8
54	1w	3	G	2.8
54	2w	1	G	2.8
41	1j	27	ALA	2.8
41	2j	71	LEU	2.8
47	1p	7	ALA	2.8
32	2a	1116	C	2.8
56	2y	48	C	2.8
1	1A	887	A	2.8
1	2A	2171	A	2.8
8	2I	1	MET	2.8
32	2a	983	A	2.8
3	2D	275	LYS	2.8
14	2S	59	LYS	2.8
33	2b	175	ARG	2.8
34	2c	79	ARG	2.8
41	2j	89	ASP	2.8
50	2s	78	ARG	2.8
35	2d	167	GLY	2.8
50	1s	26	GLY	2.8
20	2Y	55	TYR	2.8
26	24	63	TYR	2.8
34	2c	5	ILE	2.8
41	2j	35	SER	2.8
43	2l	8	ASN	2.8
6	2G	159	VAL	2.8
33	1b	136	VAL	2.8
35	1d	170	VAL	2.8
42	2k	80	VAL	2.8
1	2A	614(A)	U	2.8
14	2S	58	LEU	2.8
22	20	84	LEU	2.8
56	1y	11	U	2.8
1	2A	1533	G	2.8
54	2w	22	G	2.8
1	2A	885	C	2.8
1	2A	894	C	2.8
1	2A	2129	C	2.8
1	2A	2139	C	2.8
33	2b	231	GLU	2.8
41	2j	58	ASP	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
14	2S	34	HIS	2.8
33	1b	214	ILE	2.7
34	1c	77	ILE	2.7
34	2c	14	ILE	2.7
45	2n	42	ILE	2.7
51	1t	55	ILE	2.7
14	2S	36	TYR	2.7
33	1b	236	TYR	2.7
33	2b	92	TYR	2.7
44	2m	21	TYR	2.7
39	2h	93	VAL	2.7
40	2i	17	VAL	2.7
43	1l	18	VAL	2.7
50	2s	67	VAL	2.7
12	2Q	121	ALA	2.7
21	1Z	170	THR	2.7
33	2b	98	LEU	2.7
29	27	45	ALA	2.7
37	2f	99	ALA	2.7
38	2g	40	ALA	2.7
38	2g	150	ALA	2.7
40	2i	64	THR	2.7
18	2W	92	ARG	2.7
36	2e	107	ARG	2.7
47	1p	81	ARG	2.7
1	1A	2793	G	2.7
1	2A	1170	G	2.7
32	1a	1030(C)	G	2.7
32	2a	1224	G	2.7
56	2y	26	G	2.7
45	2n	40	CYS	2.7
1	1A	2136	C	2.7
1	2A	2183	C	2.7
32	1a	999	C	2.7
32	1a	1503	A	2.7
32	2a	1028	C	2.7
56	1y	14	A	2.7
56	2y	37	A	2.7
12	2Q	104	PHE	2.7
6	1G	77	ILE	2.7
34	2c	57	ILE	2.7
7	2H	133	VAL	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	1c	75	VAL	2.7
40	2i	65	VAL	2.7
40	2i	92	TYR	2.7
41	2j	72	VAL	2.7
44	2m	98	VAL	2.7
33	2b	149	LEU	2.7
40	2i	79	LEU	2.7
3	2D	38	LYS	2.7
33	2b	168	THR	2.7
35	1d	195	ALA	2.7
36	2e	94	ALA	2.7
40	2i	94	ALA	2.7
9	2N	61	ARG	2.7
22	20	11	ARG	2.7
44	1m	102	ARG	2.7
6	1G	48	GLU	2.7
26	14	57	GLU	2.7
1	2A	2897	U	2.7
9	2N	69	GLN	2.7
34	2c	162	GLN	2.7
23	21	28	GLY	2.7
32	2a	1026	G	2.7
42	2k	90	GLY	2.7
32	1a	344	A	2.7
32	1a	1028	C	2.7
33	2b	162	ILE	2.7
41	2j	23	ILE	2.7
54	2w	56	C	2.7
56	1y	25	C	2.7
6	2G	160	VAL	2.7
9	2N	118	LYS	2.7
21	2Z	86	VAL	2.7
14	2S	7	TYR	2.7
14	2S	31	SER	2.7
35	1d	138	TYR	2.7
37	1f	19	LEU	2.7
39	2h	112	LEU	2.7
40	2i	95	LYS	2.7
50	2s	45	VAL	2.7
21	2Z	150	LEU	2.7
43	2l	10	LEU	2.7
8	2I	83	ALA	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
17	2V	7	THR	2.7
21	1Z	51	ALA	2.7
22	20	43	THR	2.7
41	2j	48	THR	2.7
50	2s	29	ARG	2.7
1	2A	2102	U	2.7
32	2a	950	U	2.7
41	2j	56	HIS	2.7
21	2Z	148	ASP	2.7
34	2c	9	GLY	2.7
34	2c	134	ILE	2.7
35	1d	70	ILE	2.7
45	2n	36	PHE	2.7
1	1A	1176	G	2.7
1	2A	899	A	2.7
1	2A	2893	G	2.7
32	1a	1021	G	2.7
32	2a	1001(A)	G	2.7
32	2a	980	C	2.7
53	1v	12	A	2.7
3	2D	268	ARG	2.7
19	2X	68	ARG	2.7
20	2Y	90	LEU	2.7
21	2Z	153	SER	2.7
33	2b	210	SER	2.7
34	2c	190	ARG	2.7
36	2e	67	VAL	2.7
36	2e	115	VAL	2.7
38	2g	76	ARG	2.7
41	1j	90	LEU	2.7
44	2m	60	VAL	2.7
50	2s	20	LEU	2.7
21	1Z	119	GLU	2.7
34	2c	24	ALA	2.7
41	2j	83	GLU	2.7
32	2a	1020	U	2.7
32	2a	1219	U	2.7
33	2b	228	GLY	2.6
14	2S	40	ILE	2.6
33	2b	75	LYS	2.6
35	2d	206	PHE	2.6
43	1l	126	LYS	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
46	2o	3	ILE	2.6
48	1q	27	PHE	2.6
20	1Y	1	MET	2.6
34	2c	131	ARG	2.6
52	2u	6	ARG	2.6
1	1A	2790	A	2.6
1	2A	1847	A	2.6
6	2G	152	LEU	2.6
32	2a	965	A	2.6
33	2b	158	LEU	2.6
1	1A	2137	C	2.6
1	1A	2185	C	2.6
8	2I	144	VAL	2.6
34	2c	43	LEU	2.6
34	2c	116	VAL	2.6
35	2d	155	LEU	2.6
1	1A	2802	G	2.6
1	2A	2163	C	2.6
38	2g	9	VAL	2.6
42	1k	24	SER	2.6
42	1k	79	SER	2.6
56	1y	49	G	2.6
8	2I	49	ALA	2.6
21	1Z	164	ALA	2.6
41	1j	33	GLN	2.6
41	2j	20	ALA	2.6
47	1p	22	THR	2.6
1	2A	2118	U	2.6
11	2P	93	GLY	2.6
19	2X	94	GLY	2.6
26	24	45	GLY	2.6
42	2k	49	GLY	2.6
21	2Z	159	PRO	2.6
26	24	14	ILE	2.6
34	2c	202	ILE	2.6
46	1o	19	PRO	2.6
50	2s	42	PRO	2.6
25	23	29	ARG	2.6
26	24	58	ARG	2.6
44	2m	99	ARG	2.6
14	2S	54	LEU	2.6
21	1Z	102	LEU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
25	23	26	LEU	2.6
33	2b	112	VAL	2.6
35	2d	192	GLU	2.6
39	2h	53	VAL	2.6
21	1Z	166	SER	2.6
32	1a	1030(D)	A	2.6
56	1y	44	A	2.6
56	1y	46	A	2.6
1	1A	2175	C	2.6
1	2A	2108	C	2.6
1	2A	2128	C	2.6
32	2a	1037	C	2.6
32	2a	1054	C	2.6
38	1g	83	ALA	2.6
40	1i	43	ALA	2.6
1	2A	11	G	2.6
32	1a	1042	G	2.6
32	2a	1190	G	2.6
54	1w	7	G	2.6
33	2b	97	TRP	2.6
33	2b	139	LYS	2.6
5	2F	131	GLY	2.6
7	2H	82	GLY	2.6
11	2P	37	GLY	2.6
1	2A	1026	U	2.6
17	2V	50	PRO	2.6
45	2n	54	PRO	2.6
47	1p	41	PRO	2.6
8	2I	88	ILE	2.6
26	24	31	ILE	2.6
38	2g	27	ILE	2.6
41	2j	6	ILE	2.6
49	2r	65	ILE	2.6
50	2s	62	ILE	2.6
39	2h	31	PHE	2.6
26	24	9	LEU	2.6
33	1b	187	LEU	2.6
33	2b	69	LEU	2.6
35	2d	162	LEU	2.6
26	24	10	VAL	2.6
34	2c	66	VAL	2.6
34	2c	151	VAL	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
37	1f	90	VAL	2.6
40	2i	28	VAL	2.6
34	2c	137	ALA	2.6
40	2i	27	THR	2.6
45	2n	59	ALA	2.6
1	1A	229	A	2.6
32	2a	1531	A	2.6
32	1a	1029	C	2.6
32	2a	1029	C	2.6
54	1w	69	C	2.6
1	1A	2151	G	2.6
1	2A	614(B)	G	2.6
1	2A	2151	G	2.6
32	1a	1031	G	2.6
32	2a	951	G	2.6
32	2a	976	G	2.6
33	2b	232	PRO	2.6
34	2c	7	PRO	2.6
44	2m	68	GLY	2.6
41	1j	86	MET	2.6
33	2b	127	ILE	2.6
34	2c	152	ILE	2.6
41	2j	82	ILE	2.6
1	1A	2897	U	2.6
26	24	42	PHE	2.6
8	2I	75	LEU	2.6
21	2Z	33	LEU	2.6
47	2p	6	LEU	2.6
21	2Z	96	VAL	2.6
35	1d	112	VAL	2.6
38	1g	84	ASN	2.6
42	2k	114	VAL	2.6
26	14	18	CYS	2.6
33	2b	120	ALA	2.6
34	2c	71	ALA	2.6
39	2h	110	ALA	2.6
40	2i	106	ALA	2.6
41	2j	68	HIS	2.6
50	2s	48	THR	2.6
43	2l	126	LYS	2.6
1	2A	2173	A	2.6
39	2h	58	TYR	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
39	2h	94	TYR	2.6
1	1A	886	C	2.5
26	24	55	ARG	2.5
32	1a	1027	C	2.5
41	2j	28	ARG	2.5
50	2s	81	ARG	2.5
54	1w	2	C	2.5
41	2j	86	MET	2.5
44	2m	64	TRP	2.5
6	2G	147	ASP	2.5
21	2Z	87	ASP	2.5
26	14	64	GLY	2.5
50	2s	26	GLY	2.5
1	2A	1171	G	2.5
32	1a	1023	G	2.5
32	2a	630	G	2.5
34	2c	8	ILE	2.5
56	2y	5	G	2.5
22	20	69	PHE	2.5
38	1g	8	GLU	2.5
40	2i	18	PHE	2.5
41	2j	54	PHE	2.5
1	2A	2132	U	2.5
11	2P	6	LEU	2.5
32	1a	1025	U	2.5
33	2b	145	LEU	2.5
38	1g	12	LEU	2.5
38	2g	12	LEU	2.5
51	2t	99	LEU	2.5
56	2y	12	U	2.5
9	2N	98	VAL	2.5
26	14	50	VAL	2.5
38	1g	9	VAL	2.5
38	2g	66	VAL	2.5
41	2j	44	VAL	2.5
42	2k	13	GLN	2.5
44	2m	92	HIS	2.5
6	2G	57	ALA	2.5
22	20	4	LYS	2.5
36	2e	95	ALA	2.5
40	2i	84	ALA	2.5
35	1d	89	THR	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
48	2q	99	SER	2.5
35	1d	3	ARG	2.5
40	2i	104	ARG	2.5
33	2b	199	TYR	2.5
38	2g	151	TYR	2.5
47	1p	1	MET	2.5
56	2y	23	A	2.5
1	1A	898	C	2.5
1	1A	2107	C	2.5
1	1A	2128	C	2.5
1	1A	2178	C	2.5
1	2A	884	C	2.5
1	2A	897	C	2.5
1	2A	2896	C	2.5
6	2G	126	ASP	2.5
32	1a	1030(B)	C	2.5
33	1b	38	GLY	2.5
42	1k	42	TRP	2.5
54	1w	66	C	2.5
56	2y	35	C	2.5
26	24	15	ILE	2.5
40	2i	63	ILE	2.5
1	2A	2318	G	2.5
33	2b	118	LEU	2.5
37	1f	79	LEU	2.5
40	1i	19	LEU	2.5
40	2i	56	LEU	2.5
50	2s	10	PHE	2.5
54	2w	7	G	2.5
54	2w	67	G	2.5
56	2y	51	G	2.5
9	2N	8	GLN	2.5
54	2w	60	U	2.5
3	2D	5	LYS	2.5
34	2c	138	VAL	2.5
36	2e	41	VAL	2.5
40	1i	109	VAL	2.5
45	2n	56	VAL	2.5
49	2r	86	VAL	2.5
33	2b	88	ALA	2.5
38	2g	147	ALA	2.5
44	1m	107	ALA	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
44	2m	75	ALA	2.5
33	2b	67	THR	2.5
34	2c	95	THR	2.5
41	2j	67	THR	2.5
6	1G	51	ARG	2.5
26	14	58	ARG	2.5
26	24	61	ARG	2.5
41	2j	66	ARG	2.5
21	1Z	167	PRO	2.5
21	2Z	95	PRO	2.5
33	1b	33	TYR	2.5
33	2b	125	PRO	2.5
1	1A	890	A	2.5
32	2a	1447	A	2.5
56	1y	21	A	2.5
26	24	5	ILE	2.5
54	2w	68	C	2.5
9	2N	23	LEU	2.5
14	2S	12	PHE	2.5
33	2b	180	LEU	2.5
34	2c	91	LEU	2.5
36	2e	151	LEU	2.5
40	2i	101	PHE	2.5
12	2Q	22	LYS	2.5
6	2G	92	VAL	2.5
17	2V	22	VAL	2.5
20	2Y	42	VAL	2.5
25	23	6	VAL	2.5
41	2j	49	VAL	2.5
45	2n	49	HIS	2.5
50	2s	14	HIS	2.5
1	1A	2182	G	2.5
9	2N	132	ALA	2.5
40	1i	13	ALA	2.5
41	2j	100	THR	2.5
50	2s	33	THR	2.5
8	1I	10	GLU	2.5
22	20	68	GLU	2.5
41	2j	36	GLY	2.5
45	2n	55	GLY	2.5
38	2g	33	ASP	2.5
47	2p	38	TYR	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	1b	211	ILE	2.5
39	2h	134	ILE	2.5
1	2A	2158	A	2.5
32	2a	1030(D)	A	2.5
32	2a	1357	A	2.5
54	1w	15	A	2.5
14	2S	32	LEU	2.5
33	1b	221	LEU	2.5
33	2b	196	LEU	2.5
36	2e	119	LEU	2.5
38	2g	38	LEU	2.5
40	1i	99	LEU	2.5
24	22	70	GLN	2.5
38	2g	62	PHE	2.5
1	1A	897	C	2.5
1	2A	2175	C	2.5
32	2a	999	C	2.5
56	2y	70	C	2.5
8	2I	3	VAL	2.5
19	2X	65	ARG	2.5
33	2b	37	ASN	2.5
33	2b	184	VAL	2.5
35	1d	88	VAL	2.5
40	2i	26	VAL	2.5
35	2d	47	ARG	2.5
34	2c	121	ALA	2.5
40	2i	7	THR	2.5
50	2s	39	THR	2.5
1	2A	880	G	2.5
1	2A	2131	G	2.5
1	2A	2321	G	2.5
6	2G	42	GLY	2.4
17	2V	42	GLY	2.4
34	1c	96	GLY	2.4
35	2d	23	GLY	2.4
36	2e	99	GLY	2.4
3	1D	38	LYS	2.4
26	14	32	TYR	2.4
33	2b	42	ILE	2.4
33	2b	156	LYS	2.4
34	2c	135	LYS	2.4
42	2k	83	ILE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
45	2n	58	LYS	2.4
33	1b	215	LEU	2.4
42	2k	103	LEU	2.4
47	1p	82	GLN	2.4
33	1b	163	PHE	2.4
34	2c	69	HIS	2.4
41	1j	47	PHE	2.4
41	2j	62	HIS	2.4
53	2v	15	A	2.4
6	2G	100	TRP	2.4
41	2j	60	ARG	2.4
1	1A	34	C	2.4
1	2A	2789	C	2.4
33	1b	165	VAL	2.4
34	2c	103	VAL	2.4
35	2d	178	VAL	2.4
37	1f	88	VAL	2.4
39	2h	15	ASN	2.4
47	1p	2	VAL	2.4
56	2y	75	C	2.4
1	2A	2130	U	2.4
8	2I	55	ALA	2.4
35	2d	165	MET	2.4
43	2l	51	ALA	2.4
50	2s	66	MET	2.4
56	1y	59	U	2.4
40	1i	21	PRO	2.4
50	2s	59	PRO	2.4
52	2u	23	PRO	2.4
4	1E	73	GLU	2.4
8	2I	112	LYS	2.4
17	2V	9	GLY	2.4
34	2c	93	LYS	2.4
46	2o	86	GLY	2.4
6	1G	49	ASP	2.4
7	2H	9	ILE	2.4
8	2I	71	ILE	2.4
34	1c	57	ILE	2.4
36	2e	118	ILE	2.4
44	2m	4	ILE	2.4
44	2m	39	ILE	2.4
6	2G	43	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
8	2I	35	LEU	2.4
8	2I	54	GLN	2.4
24	22	35	LEU	2.4
26	14	67	TYR	2.4
39	2h	62	TYR	2.4
33	2b	217	ARG	2.4
35	1d	110	PHE	2.4
52	2u	7	ARG	2.4
1	1A	548	A	2.4
1	1A	2134	A	2.4
1	2A	652(B)	A	2.4
32	2a	414	A	2.4
32	2a	1225	A	2.4
32	2a	1492	A	2.4
53	1v	14	A	2.4
53	1v	15	A	2.4
27	15	60	VAL	2.4
47	1p	48	TRP	2.4
1	1A	1509	C	2.4
32	2a	1260	C	2.4
33	1b	29	ALA	2.4
44	2m	18	ALA	2.4
54	1w	13	C	2.4
55	1x	1	C	2.4
1	1A	2122	U	2.4
1	2A	895	U	2.4
41	2j	92	THR	2.4
50	2s	63	THR	2.4
6	2G	76	SER	2.4
7	2H	128	PRO	2.4
10	1O	108	GLU	2.4
21	1Z	153	SER	2.4
33	2b	183	PRO	2.4
41	1j	30	SER	2.4
41	2j	77	PRO	2.4
44	2m	120	LYS	2.4
45	2n	50	LYS	2.4
3	2D	71	ASP	2.4
33	1b	41	ILE	2.4
39	1h	45	ILE	2.4
1	1A	881	G	2.4
1	1A	1093	G	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	2807	G	2.4
6	2G	53	LEU	2.4
7	2H	88	LEU	2.4
21	1Z	157	LEU	2.4
32	2a	1030(C)	G	2.4
33	2b	138	LEU	2.4
40	2i	73	GLN	2.4
41	1j	84	GLN	2.4
54	2w	10	G	2.4
56	1y	22	G	2.4
39	2h	91	ARG	2.4
45	2n	23	ARG	2.4
26	24	25	TYR	2.4
6	1G	80	PHE	2.4
21	2Z	88	PHE	2.4
34	2c	203	PHE	2.4
43	2l	32	PHE	2.4
7	2H	44	VAL	2.4
8	1I	136	VAL	2.4
14	2S	49	VAL	2.4
19	2X	1	MET	2.4
40	1i	28	VAL	2.4
50	1s	67	VAL	2.4
32	2a	1110	A	2.4
42	1k	117	ASN	2.4
34	2c	149	ALA	2.4
40	2i	76	ALA	2.4
8	2I	86	THR	2.4
34	2c	192	THR	2.4
44	2m	43	THR	2.4
50	1s	39	THR	2.4
6	2G	142	PRO	2.4
41	2j	53	PRO	2.4
1	1A	1026	U	2.4
48	1q	66	SER	2.4
56	1y	69	C	2.4
4	2E	10	GLY	2.4
38	2g	34	GLY	2.4
34	1c	190	ARG	2.4
36	2e	5	ASP	2.4
1	1A	2149	G	2.4
1	2A	2184	G	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
26	24	32	TYR	2.4
32	2a	1222	G	2.4
40	2i	4	TYR	2.4
42	2k	73	MET	2.4
56	1y	7	G	2.4
4	2E	150	VAL	2.4
42	2k	47	VAL	2.4
44	1m	98	VAL	2.4
33	2b	74	LYS	2.4
35	1d	86	LYS	2.4
1	1A	2171	A	2.4
1	2A	890	A	2.4
32	2a	975	A	2.4
38	1g	2	ALA	2.4
42	1k	89	ALA	2.4
50	2s	75	ALA	2.4
51	1t	95	ALA	2.4
33	2b	129	GLU	2.4
54	2w	21	A	2.4
56	1y	23	A	2.4
56	2y	24	A	2.4
40	2i	123	PRO	2.3
41	1j	100	THR	2.3
44	2m	10	PRO	2.3
32	1a	1000	U	2.3
40	1i	57	GLY	2.3
44	1m	68	GLY	2.3
56	1y	6	C	2.3
56	2y	2	C	2.3
56	2y	56	C	2.3
8	2I	123	LEU	2.3
21	2Z	57	ILE	2.3
41	1j	46	ARG	2.3
35	1d	102	ASP	2.3
40	1i	91	ASP	2.3
40	2i	75	ASP	2.3
40	2i	105	ASP	2.3
51	1t	24	LEU	2.3
24	22	1	MET	2.3
43	2l	98	TYR	2.3
44	1m	59	TYR	2.3
50	2s	61	TYR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
21	2Z	27	VAL	2.3
21	2Z	156	LYS	2.3
26	24	28	LYS	2.3
29	27	46	VAL	2.3
41	2j	24	VAL	2.3
2	2B	23	G	2.3
32	1a	346	G	2.3
54	1w	5	G	2.3
54	1w	49	G	2.3
54	1w	71	G	2.3
56	1y	10	G	2.3
8	2I	122	GLU	2.3
49	2r	60	ALA	2.3
39	2h	67	PRO	2.3
39	2h	3	THR	2.3
1	1A	1088	A	2.3
1	1A	1098	A	2.3
1	2A	2062	A	2.3
32	1a	1001	A	2.3
32	2a	1250	A	2.3
56	1y	9	A	2.3
7	2H	51	ARG	2.3
33	2b	38	GLY	2.3
43	2l	59	ARG	2.3
52	2u	2	GLY	2.3
6	2G	101	ILE	2.3
21	1Z	121	HIS	2.3
22	10	84	LEU	2.3
40	2i	81	ILE	2.3
44	2m	56	LEU	2.3
1	2A	277	C	2.3
56	1y	63	C	2.3
56	1y	66	C	2.3
56	1y	68	C	2.3
56	2y	25	C	2.3
33	2b	83	MET	2.3
6	2G	80	PHE	2.3
11	2P	91	PHE	2.3
22	20	60	PHE	2.3
40	1i	127	LYS	2.3
7	2H	19	VAL	2.3
8	1I	107	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	2b	7	VAL	2.3
49	1r	39	VAL	2.3
8	2I	85	GLU	2.3
41	1j	97	GLU	2.3
51	2t	26	ASN	2.3
6	2G	2	PRO	2.3
6	2G	163	ALA	2.3
8	2I	63	ALA	2.3
29	17	45	ALA	2.3
33	1b	13	ALA	2.3
34	2c	100	ALA	2.3
34	2c	146	ALA	2.3
34	2c	163	ALA	2.3
49	2r	24	ALA	2.3
41	1j	81	THR	2.3
15	2T	111	ARG	2.3
33	2b	53	ARG	2.3
35	2d	50	ARG	2.3
39	2h	30	ARG	2.3
56	2y	3	G	2.3
1	1A	896	A	2.3
1	2A	6	A	2.3
17	2V	56	SER	2.3
32	2a	1248	A	2.3
33	1b	18	GLY	2.3
38	2g	130	GLY	2.3
6	2G	77	ILE	2.3
8	2I	38	LEU	2.3
20	2Y	44	ILE	2.3
33	1b	201	ILE	2.3
34	1c	12	LEU	2.3
36	2e	101	ILE	2.3
38	1g	16	LEU	2.3
38	2g	124	LEU	2.3
44	2m	22	ILE	2.3
50	1s	31	ILE	2.3
51	1t	13	LEU	2.3
1	1A	2172	U	2.3
32	2a	961	U	2.3
32	2a	1358	U	2.3
54	2w	73	U	2.3
8	2I	20	ASP	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	2a	1137	C	2.3
34	2c	199	LYS	2.3
54	2w	69	C	2.3
56	2y	62	C	2.3
6	2G	23	PHE	2.3
35	2d	79	PHE	2.3
40	1i	18	PHE	2.3
6	2G	15	VAL	2.3
7	2H	24	VAL	2.3
34	1c	99	VAL	2.3
34	1c	207	VAL	2.3
34	2c	141	VAL	2.3
36	2e	34	VAL	2.3
40	1i	110	GLU	2.3
40	2i	2	GLU	2.3
8	2I	89	TYR	2.3
36	2e	133	TYR	2.3
40	2i	53	VAL	2.3
6	1G	50	ALA	2.3
7	2H	12	PRO	2.3
26	24	29	PRO	2.3
38	2g	7	ALA	2.3
41	1j	78	ASN	2.3
45	1n	20	ALA	2.3
49	1r	20	ALA	2.3
38	1g	78	ARG	2.3
38	2g	79	ARG	2.3
40	2i	128	ARG	2.3
43	2l	44	THR	2.3
44	2m	63	THR	2.3
11	2P	26	GLY	2.3
11	2P	116	GLY	2.3
1	2A	2186	G	2.3
21	2Z	16	SER	2.3
33	2b	140	HIS	2.3
44	2m	119	GLY	2.3
50	1s	38	SER	2.3
6	2G	172	LEU	2.3
21	1Z	155	LEU	2.3
33	2b	155	LEU	2.3
35	1d	126	ILE	2.3
38	2g	120	ILE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
39	2h	63	LEU	2.3
44	2m	19	LEU	2.3
44	2m	81	LEU	2.3
54	2w	4	G	2.3
56	1y	71	G	2.3
2	2B	58	A	2.3
32	2a	532	A	2.3
53	1v	24	A	2.3
41	2j	99	LYS	2.3
44	2m	31	LYS	2.3
1	2A	271(K)	U	2.3
1	2A	2150	U	2.3
32	1a	202	U	2.3
24	12	37	PHE	2.3
34	1c	90	GLU	2.3
56	1y	62	C	2.3
5	2F	6	VAL	2.3
21	1Z	165	VAL	2.3
34	1c	55	VAL	2.3
46	2o	60	VAL	2.3
12	2Q	60	ARG	2.3
16	2U	2	PRO	2.3
35	1d	51	PRO	2.3
3	2D	2	ALA	2.2
6	1G	46	ALA	2.2
6	2G	79	ASN	2.2
9	2N	124	ALA	2.2
14	2S	79	ALA	2.2
22	20	26	TYR	2.3
34	1c	23	TYR	2.3
35	2d	4	TYR	2.3
38	2g	37	ASN	2.2
40	1i	66	ARG	2.3
52	2u	15	ARG	2.3
40	1i	45	ALA	2.2
44	2m	5	ALA	2.2
40	1i	117	HIS	2.2
43	1l	14	GLY	2.2
4	2E	195	LEU	2.2
26	24	22	ILE	2.2
33	1b	200	ILE	2.2
34	1c	14	ILE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	2c	12	LEU	2.2
34	2c	178	LEU	2.2
35	2d	158	ILE	2.2
37	2f	45	LEU	2.2
41	1j	88	LEU	2.2
41	2j	50	ILE	2.2
42	1k	16	SER	2.2
43	2l	7	ILE	2.2
47	1p	43	LYS	2.2
51	1t	53	LEU	2.2
1	1A	1103	A	2.2
1	2A	2320	A	2.2
6	2G	4	ASP	2.2
54	2w	14	A	2.2
56	2y	21	A	2.2
1	1A	2207	G	2.2
32	1a	1003	G	2.2
32	2a	1021	G	2.2
54	1w	4	G	2.2
56	1y	4	G	2.2
1	1A	1739	U	2.2
21	1Z	2	GLU	2.2
6	2G	141	PHE	2.2
20	2Y	89	PHE	2.2
1	1A	1100	C	2.2
1	1A	2177	C	2.2
1	1A	2791	C	2.2
1	2A	2179	C	2.2
6	2G	31	VAL	2.2
8	2I	18	VAL	2.2
9	2N	74	ARG	2.2
25	23	58	VAL	2.2
34	1c	88	ARG	2.2
36	2e	51	VAL	2.2
40	1i	108	VAL	2.2
41	1j	44	VAL	2.2
42	2k	14	VAL	2.2
42	2k	82	VAL	2.2
44	2m	88	ARG	2.2
32	2a	979	C	2.2
52	1u	23	PRO	2.2
54	2w	31	C	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	2c	61	ALA	2.2
40	1i	119	ALA	2.2
44	1m	105	THR	2.2
17	2V	8	GLY	2.2
40	1i	112	LYS	2.2
40	1i	115	GLY	2.2
50	2s	72	GLY	2.2
33	2b	51	LEU	2.2
35	1d	21	LEU	2.2
42	1k	98	LEU	2.2
42	2k	63	LEU	2.2
49	2r	76	LEU	2.2
50	1s	20	LEU	2.2
6	1G	76	SER	2.2
42	1k	44	SER	2.2
45	2n	61	TRP	2.2
1	1A	278	A	2.2
1	1A	1067	A	2.2
8	1I	70	GLU	2.2
8	2I	64	GLU	2.2
32	1a	1035	A	2.2
33	2b	126	GLU	2.2
1	1A	271(K)	U	2.2
32	2a	1065	U	2.2
56	1y	43	U	2.2
1	2A	1115	G	2.2
6	2G	95	ARG	2.2
32	1a	1032	G	2.2
32	2a	1117	G	2.2
52	1u	24	ARG	2.2
54	2w	26	G	2.2
6	2G	17	PRO	2.2
20	2Y	45	VAL	2.2
21	2Z	74	VAL	2.2
26	24	7	PRO	2.2
33	2b	164	VAL	2.2
35	2d	148	VAL	2.2
43	2l	36	VAL	2.2
43	2l	40	VAL	2.2
1	2A	898	C	2.2
1	2A	2794	C	2.2
32	1a	1008	C	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	1a	1037	C	2.2
32	2a	972	C	2.2
36	1e	138	ALA	2.2
38	2g	128	ALA	2.2
50	1s	24	ALA	2.2
11	2P	39	LYS	2.2
34	2c	170	GLN	2.2
33	2b	48	MET	2.2
8	1I	44	LEU	2.2
33	2b	72	GLY	2.2
34	2c	96	GLY	2.2
35	1d	180	GLY	2.2
40	2i	100	GLY	2.2
41	2j	31	GLY	2.2
43	2l	14	GLY	2.2
49	2r	66	LEU	2.2
51	2t	96	GLY	2.2
6	2G	88	ILE	2.2
33	1b	80	ILE	2.2
39	1h	100	ILE	2.2
6	2G	49	ASP	2.2
21	1Z	154	ASP	2.2
33	2b	166	ASP	2.2
21	1Z	169	GLU	2.2
6	2G	21	ARG	2.2
15	1T	129	ARG	2.2
39	2h	84	ARG	2.2
41	2j	46	ARG	2.2
42	2k	126	ARG	2.2
45	2n	26	ARG	2.2
45	2n	35	ARG	2.2
1	1A	2150	U	2.2
1	1A	2180	U	2.2
32	2a	1000	U	2.2
32	2a	1251	A	2.2
33	1b	234	PRO	2.2
56	1y	60	U	2.2
6	1G	149	VAL	2.2
9	1N	9	VAL	2.2
34	2c	120	VAL	2.2
40	2i	86	VAL	2.2
42	2k	105	VAL	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	1042	G	2.2
16	2U	51	LYS	2.2
20	2Y	34	LYS	2.2
34	2c	180	ALA	2.2
34	2c	200	ALA	2.2
45	2n	11	LYS	2.2
40	2i	117	HIS	2.2
44	2m	106	ASN	2.2
26	24	52	THR	2.2
12	2Q	15	GLY	2.2
12	2Q	30	GLY	2.2
32	2a	1007	C	2.2
33	2b	66	GLY	2.2
33	2b	215	LEU	2.2
35	2d	20	TYR	2.2
35	2d	27	TYR	2.2
36	2e	31	LEU	2.2
40	2i	39	GLY	2.2
48	2q	76	LEU	2.2
50	1s	72	GLY	2.2
6	2G	39	ILE	2.2
39	2h	111	ILE	2.2
8	1I	42	SER	2.2
40	2i	71	SER	2.2
21	1Z	148	ASP	2.2
21	2Z	168	GLU	2.2
50	1s	27	GLU	2.2
8	2I	27	ARG	2.2
34	2c	88	ARG	2.2
38	1g	5	ARG	2.2
40	1i	120	ARG	2.2
40	2i	20	ARG	2.2
44	2m	91	ARG	2.2
45	2n	12	ARG	2.2
7	2H	39	PRO	2.2
40	2i	98	PRO	2.2
1	2A	528	A	2.1
14	2S	83	LYS	2.2
22	20	45	PHE	2.2
40	2i	33	PHE	2.2
7	2H	125	VAL	2.1
14	2S	69	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	2a	1183	A	2.1
32	2a	1285	A	2.1
41	1j	80	LYS	2.2
34	2c	70	VAL	2.1
43	1l	55	VAL	2.1
54	1w	14	A	2.1
54	2w	59	U	2.2
51	2t	9	ASN	2.1
1	1A	883	G	2.1
1	1A	1063	G	2.1
1	2A	892	G	2.1
1	2A	2101	G	2.1
1	2A	2308	G	2.1
6	1G	139	LEU	2.1
6	2G	34	LEU	2.1
8	1I	128	LEU	2.1
11	1P	118	GLY	2.1
14	2S	4	LEU	2.1
21	2Z	157	LEU	2.1
31	29	37	GLY	2.1
32	2a	1003	G	2.1
32	2a	1061	G	2.1
34	2c	25	GLY	2.1
38	1g	124	LEU	2.1
40	2i	50	LEU	2.1
41	1j	36	GLY	2.1
44	1m	24	GLY	2.1
55	1x	46	G	2.1
56	1y	26	G	2.1
56	1y	67	G	2.1
33	2b	58	ILE	2.1
37	2f	59	TYR	2.1
47	2p	39	TYR	2.1
48	2q	90	ILE	2.1
1	1A	652(S)	C	2.1
32	2a	1149	C	2.1
54	2w	6	C	2.1
54	2w	61	C	2.1
56	1y	72	C	2.1
6	2G	54	GLU	2.1
21	2Z	166	SER	2.1
25	23	3	ARG	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	1c	82	GLU	2.1
34	2c	49	SER	2.1
38	2g	77	SER	2.1
41	1j	28	ARG	2.1
14	2S	44	LYS	2.1
33	1b	133	LYS	2.1
38	2g	136	LYS	2.1
48	2q	100	LYS	2.1
34	2c	18	TRP	2.1
34	2c	186	PHE	2.1
34	2c	86	VAL	2.1
36	2e	55	VAL	2.1
38	2g	21	VAL	2.1
39	2h	19	VAL	2.1
41	1j	72	VAL	2.1
1	1A	895	U	2.1
1	2A	272(A)	U	2.1
1	2A	405	U	2.1
32	2a	982	U	2.1
32	2a	997	U	2.1
2	2B	120	A	2.1
21	1Z	152	ALA	2.1
32	2a	974	A	2.1
39	2h	70	GLN	2.1
40	1i	46	ALA	2.1
54	1w	23	A	2.1
12	1Q	15	GLY	2.1
17	2V	35	LEU	2.1
21	2Z	24	LEU	2.1
26	24	64	GLY	2.1
33	1b	213	LEU	2.1
47	1p	78	GLY	2.1
49	2r	85	LEU	2.1
51	2t	10	LEU	2.1
35	1d	204	ILE	2.1
36	2e	109	ILE	2.1
41	1j	98	ILE	2.1
42	2k	32	ILE	2.1
11	1P	15	ARG	2.1
12	2Q	32	TYR	2.1
20	2Y	50	ARG	2.1
1	1A	2148	G	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	2206	G	2.1
32	1a	148	G	2.1
32	2a	1050	G	2.1
32	2a	1370	G	2.1
33	1b	129	GLU	2.1
38	2g	3	ARG	2.1
44	2m	59	TYR	2.1
55	2x	70	G	2.1
56	1y	39	G	2.1
39	2h	135	CYS	2.1
1	2A	2185	C	2.1
32	2a	1038	C	2.1
32	2a	1363	C	2.1
34	1c	20	SER	2.1
34	1c	62	ASP	2.1
54	1w	6	C	2.1
54	1w	56	C	2.1
56	1y	56	C	2.1
21	2Z	127	LYS	2.1
29	17	48	LYS	2.1
45	1n	4	LYS	2.1
33	2b	16	HIS	2.1
35	2d	123	HIS	2.1
35	2d	185	PHE	2.1
14	2S	28	VAL	2.1
14	2S	98	VAL	2.1
21	2Z	105	VAL	2.1
22	20	66	VAL	2.1
24	22	25	VAL	2.1
34	1c	76	VAL	2.1
36	1e	69	VAL	2.1
5	2F	142	TRP	2.1
1	2A	2172	U	2.1
19	2X	91	ALA	2.1
32	1a	65	U	2.1
32	2a	1235	U	2.1
34	2c	113	ALA	2.1
56	2y	73	U	2.1
6	1G	152	LEU	2.1
17	2V	95	LEU	2.1
21	2Z	70	LEU	2.1
21	2Z	76	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	2a	949	A	2.1
32	2a	1493	A	2.1
42	2k	98	LEU	2.1
46	1o	56	LEU	2.1
54	2w	50	A	2.1
56	2y	44	A	2.1
6	2G	161	THR	2.1
7	2H	14	GLY	2.1
12	2Q	61	GLY	2.1
23	21	29	GLY	2.1
33	2b	54	THR	2.1
40	1i	64	THR	2.1
40	2i	115	GLY	2.1
7	1H	3	ARG	2.1
39	2h	37	ARG	2.1
9	2N	68	GLU	2.1
33	2b	170	GLU	2.1
34	1c	39	ILE	2.1
34	1c	84	ILE	2.1
35	2d	5	ILE	2.1
38	2g	49	ILE	2.1
43	2l	16	GLU	2.1
44	2m	9	ILE	2.1
43	2l	69	TYR	2.1
8	1I	87	LYS	2.1
33	2b	189	ASP	2.1
45	2n	15	LYS	2.1
47	1p	35	LYS	2.1
1	1A	892	G	2.1
1	1A	2152	G	2.1
1	1A	2154	G	2.1
54	2w	5	G	2.1
56	2y	22	G	2.1
5	1F	14	PRO	2.1
21	2Z	167	PRO	2.1
32	2a	1018	C	2.1
32	2a	1320	C	2.1
33	1b	167	PRO	2.1
35	2d	40	PRO	2.1
40	2i	90	PRO	2.1
46	2o	2	PRO	2.1
54	1w	61	C	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	2H	49	VAL	2.1
44	2m	17	VAL	2.1
47	2p	9	PHE	2.1
50	2s	60	VAL	2.1
21	2Z	152	ALA	2.1
24	22	58	ALA	2.1
36	2e	54	ALA	2.1
40	2i	46	ALA	2.1
42	1k	15	ALA	2.1
8	2I	58	LEU	2.1
9	2N	112	LEU	2.1
32	2a	1196	U	2.1
5	1F	207	GLY	2.1
11	2P	79	ARG	2.1
56	1y	65	U	2.1
18	1W	112	GLY	2.1
33	1b	203	GLY	2.1
50	1s	84	GLY	2.1
50	2s	3	ARG	2.1
52	1u	9	ARG	2.1
8	1I	86	THR	2.1
14	2S	5	THR	2.1
1	1A	2173	A	2.1
12	2Q	47	ILE	2.1
41	2j	96	ILE	2.1
34	2c	23	TYR	2.1
41	2j	17	ASP	2.1
7	2H	2	SER	2.1
44	2m	97	PRO	2.1
48	1q	47	PRO	2.1
21	2Z	1	MET	2.1
1	1A	645	C	2.1
1	1A	879	G	2.0
1	1A	1089	G	2.0
1	1A	2155	G	2.0
1	1A	2168	G	2.0
1	2A	645	C	2.1
1	2A	893	C	2.1
2	2B	118	G	2.0
32	2a	998	G	2.0
32	2a	1019	C	2.1
32	2a	1047	G	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	2a	1359	C	2.1
50	2s	47	HIS	2.1
54	2w	49	G	2.0
54	2w	63	C	2.1
56	1y	74	C	2.1
56	2y	39	G	2.0
6	2G	149	VAL	2.0
21	1Z	105	VAL	2.0
39	1h	93	VAL	2.0
4	2E	28	ALA	2.0
8	2I	65	ALA	2.0
33	1b	120	ALA	2.0
34	1c	83	ARG	2.0
40	1i	42	ARG	2.0
40	1i	55	ALA	2.0
40	2i	42	ARG	2.0
42	1k	126	ARG	2.0
51	1t	80	ARG	2.0
7	2H	103	LEU	2.0
8	2I	9	LEU	2.0
11	2P	105	LEU	2.0
24	22	53	LEU	2.0
34	2c	101	LEU	2.0
38	2g	99	LEU	2.0
44	2m	48	LEU	2.0
7	2H	120	GLY	2.0
11	1P	149	GLU	2.0
20	1Y	91	GLU	2.0
35	1d	171	GLY	2.0
35	1d	179	GLU	2.0
40	1i	39	GLY	2.0
50	2s	8	GLY	2.0
1	1A	1097	U	2.0
1	2A	2895	U	2.0
15	1T	35	LYS	2.0
32	1a	173	U	2.0
32	2a	1025	U	2.0
32	2a	1150	U	2.0
32	2a	1205	U	2.0
33	2b	41	ILE	2.0
35	1d	158	ILE	2.0
35	2d	70	ILE	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
40	2i	118	LYS	2.0
43	2l	13	LYS	2.0
1	1A	1045	A	2.0
1	1A	1069	A	2.0
1	1A	1460	A	2.0
1	2A	2176	A	2.0
54	2w	58	A	2.0
34	1c	48	TYR	2.0
29	27	1	MET	2.0
38	1g	31	MET	2.0
33	1b	40	HIS	2.0
11	2P	68	GLN	2.0
24	12	70	GLN	2.0
26	14	60	GLN	2.0
1	1A	2103	C	2.0
1	2A	889	C	2.0
3	1D	176	ARG	2.0
6	2G	117	PHE	2.0
7	2H	43	VAL	2.0
21	1Z	136	PHE	2.0
32	1a	1030	C	2.0
32	2a	1006	C	2.0
34	2c	10	PHE	2.0
36	1e	67	VAL	2.0
36	2e	45	PHE	2.0
44	2m	45	VAL	2.0
45	1n	37	PHE	2.0
47	1p	80	PHE	2.0
54	2w	66	C	2.0
1	1A	2100	G	2.0
1	1A	2184	G	2.0
1	1A	2190	G	2.0
1	2A	2124	G	2.0
12	2Q	49	ALA	2.0
32	1a	1026	G	2.0
32	2a	971	G	2.0
32	2a	1009	G	2.0
32	2a	1024	G	2.0
32	2a	1058	G	2.0
32	2a	1094	G	2.0
32	2a	1124	G	2.0
54	2w	51	G	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
56	2y	7	G	2.0
14	2S	78	LEU	2.0
21	2Z	67	LEU	2.0
33	1b	51	LEU	2.0
34	1c	32	LEU	2.0
34	1c	47	LEU	2.0
34	2c	32	LEU	2.0
35	1d	120	LEU	2.0
35	2d	176	LEU	2.0
40	2i	85	LEU	2.0
41	2j	85	LEU	2.0
44	2m	66	LEU	2.0
45	2n	44	LEU	2.0
4	2E	115	GLY	2.0
20	2Y	94	LYS	2.0
26	14	54	GLY	2.0
40	1i	68	GLY	2.0
43	2l	28	LYS	2.0
44	2m	95	GLY	2.0
50	2s	70	LYS	2.0
41	2j	74	ILE	2.0
41	2j	98	ILE	2.0
54	2w	12	U	2.0
1	1A	1070	A	2.0
1	1A	1077	A	2.0
56	2y	58	A	2.0
26	24	43	TYR	2.0
49	1r	34	TYR	2.0
52	1u	18	TYR	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, 95^{th} 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	4SU	2w	8	20/21	0.39	0.18	89,95,110,110	0
56	4SU	2y	8	20/21	0.40	0.18	90,98,104,115	0
56	PSU	2y	55	20/21	0.42	0.18	93,99,107,111	0
54	PSU	2w	55	20/21	0.52	0.17	87,94,102,114	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	5MU	2y	54	21/22	0.55	0.17	88,95,99,117	0
56	5MU	1y	54	21/22	0.55	0.16	86,90,94,107	0
56	4SU	1y	8	20/21	0.57	0.16	90,95,100,115	0
54	5MU	2w	54	21/22	0.59	0.16	83,91,97,101	0
56	PSU	1y	55	20/21	0.60	0.16	88,93,98,104	0
54	4SU	1w	8	20/21	0.68	0.15	87,93,103,113	0
54	PSU	1w	55	20/21	0.69	0.16	81,89,98,101	0
54	5MU	1w	54	21/22	0.78	0.14	67,82,88,91	0
32	2MG	2a	1207	24/25	0.79	0.15	81,85,92,101	0
1	5MU	2A	1915	21/22	0.80	0.16	74,78,82,92	0
55	4SU	2x	8	20/21	0.82	0.13	75,78,83,86	0
55	PSU	2x	55	20/21	0.82	0.12	73,78,87,92	0
55	5MU	2x	54	21/22	0.83	0.13	74,82,88,92	0
1	PSU	2A	1917	20/21	0.87	0.12	58,71,80,82	0
32	G7M	2a	527	24/25	0.88	0.12	67,70,74,82	0
32	PSU	2a	516	20/21	0.88	0.12	73,79,84,84	0
43	0TD	2l	92	10/11	0.88	0.14	67,71,78,82	0
32	M2G	2a	966	25/26	0.89	0.16	62,68,83,90	0
32	5MC	2a	1404	21/22	0.90	0.12	54,60,69,71	0
55	5MU	1x	54	21/22	0.90	0.11	60,68,70,74	0
32	2MG	1a	1207	24/25	0.90	0.12	68,72,77,77	0
43	0TD	1l	92	10/11	0.90	0.12	44,53,59,67	0
32	5MC	2a	1400	21/22	0.90	0.18	68,74,78,82	0
54	L3X	2w	76	26/27	0.91	0.13	45,57,62,63	0
32	5MC	2a	967	21/22	0.91	0.13	66,69,78,82	0
55	5MC	2x	32	21/22	0.91	0.12	66,73,76,80	0
32	4OC	2a	1402	22/23	0.91	0.13	52,66,68,73	0
55	PSU	1x	55	20/21	0.92	0.10	53,62,69,73	0
1	PSU	2A	1911	20/21	0.92	0.10	58,63,68,70	0
55	4SU	1x	8	20/21	0.92	0.11	51,61,66,67	0
1	5MU	1A	1915	21/22	0.92	0.11	49,61,65,74	0
55	5MC	1x	32	21/22	0.93	0.12	51,56,61,64	0
32	PSU	1a	516	20/21	0.93	0.09	60,63,66,72	0
32	M2G	1a	966	25/26	0.94	0.11	44,52,60,65	0
1	PSU	1A	1917	20/21	0.94	0.10	42,54,60,61	0
32	5MC	2a	1407	21/22	0.94	0.11	45,57,65,68	0
32	MA6	2a	1519	24/25	0.94	0.13	54,64,68,68	0
1	OMC	2A	1920	21/22	0.94	0.10	57,63,66,68	0
55	31H	2x	76	32/33	0.94	0.12	46,53,59,61	0
32	5MC	1a	1400	21/22	0.95	0.10	38,49,54,58	0
1	5MC	1A	1942	21/22	0.95	0.10	31,41,46,55	0
32	G7M	1a	527	24/25	0.95	0.10	43,48,54,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MA6	2a	1518	24/25	0.95	0.11	47,62,70,71	0
55	31H	1x	76	32/33	0.95	0.10	21,31,39,51	10
54	L3X	1w	76	26/27	0.95	0.09	31,42,47,48	0
32	UR3	2a	1498	21/22	0.96	0.10	54,59,65,68	0
1	5MC	2A	1962	21/22	0.96	0.09	36,45,56,57	0
1	OMG	2A	2251	24/25	0.96	0.09	37,42,44,51	0
1	PSU	2A	2605	20/21	0.96	0.08	35,40,45,46	0
32	MA6	1a	1519	24/25	0.96	0.09	35,40,44,46	0
32	5MC	1a	967	21/22	0.96	0.10	49,54,59,60	0
32	5MC	1a	1404	21/22	0.96	0.09	30,37,41,43	0
1	2MA	2A	2503	23/24	0.97	0.09	30,36,40,43	0
1	OMU	2A	2552	21/22	0.97	0.07	32,39,42,47	0
1	PSU	1A	1911	20/21	0.97	0.09	39,47,52,52	0
32	4OC	1a	1402	22/23	0.97	0.07	37,46,50,58	0
1	5MU	2A	1939	21/22	0.97	0.08	30,35,40,47	0
1	5MC	2A	1942	21/22	0.97	0.08	43,53,57,61	0
1	OMC	1A	1920	21/22	0.97	0.09	34,45,48,50	0
32	5MC	1a	1407	21/22	0.97	0.08	36,41,44,48	0
1	PSU	1A	2605	20/21	0.98	0.06	23,26,32,32	0
1	5MU	1A	1939	21/22	0.98	0.06	24,27,30,32	0
32	UR3	1a	1498	21/22	0.98	0.07	32,39,43,46	0
32	MA6	1a	1518	24/25	0.98	0.09	34,38,46,50	0
1	5MC	1A	1962	21/22	0.98	0.06	23,32,37,41	0
1	OMU	1A	2552	21/22	0.98	0.07	22,28,31,33	0
1	2MA	1A	2503	23/24	0.99	0.05	17,22,25,28	0
1	OMG	1A	2251	24/25	0.99	0.05	22,25,26,27	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	4071	1/1	0.40	0.21	73,73,73,73	0
57	MG	2A	3089	1/1	0.49	0.17	86,86,86,86	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3325	1/1	0.57	0.28	80,80,80,80	0
57	MG	2v	101	1/1	0.57	0.24	83,83,83,83	0
57	MG	2a	1806	1/1	0.60	0.20	79,79,79,79	0
57	MG	1E	313	1/1	0.60	0.24	68,68,68,68	0
57	MG	1B	229	1/1	0.62	0.25	84,84,84,84	0
57	MG	2a	1812	1/1	0.64	0.23	76,76,76,76	0
57	MG	1A	3101	1/1	0.65	0.27	74,74,74,74	0
57	MG	1B	230	1/1	0.66	0.19	71,71,71,71	0
57	MG	2j	202	1/1	0.67	0.13	85,85,85,85	0
57	MG	2B	216	1/1	0.67	0.20	77,77,77,77	0
57	MG	2a	1649	1/1	0.69	0.18	80,80,80,80	0
57	MG	1a	1633	1/1	0.69	0.18	69,69,69,69	0
57	MG	2A	3524	1/1	0.69	0.32	71,71,71,71	0
57	MG	2A	3678	1/1	0.69	0.20	68,68,68,68	0
57	MG	2A	3109	1/1	0.69	0.24	66,66,66,66	0
57	MG	2A	3609	1/1	0.70	0.22	62,62,62,62	0
57	MG	2A	3423	1/1	0.70	0.42	84,84,84,84	0
57	MG	2a	1817	1/1	0.71	0.15	77,77,77,77	0
57	MG	1x	110	1/1	0.72	0.23	70,70,70,70	0
57	MG	1A	3704	1/1	0.72	0.12	72,72,72,72	0
57	MG	2a	1743	1/1	0.72	0.46	84,84,84,84	0
57	MG	2A	3763	1/1	0.72	0.24	50,50,50,50	0
57	MG	2a	1805	1/1	0.73	0.16	82,82,82,82	0
57	MG	1A	3743	1/1	0.73	0.16	61,61,61,61	0
57	MG	2A	3342	1/1	0.73	0.24	62,62,62,62	0
57	MG	2A	3229	1/1	0.73	0.21	67,67,67,67	0
57	MG	2a	1742	1/1	0.73	0.31	79,79,79,79	0
57	MG	2A	3742	1/1	0.73	0.17	41,41,41,41	0
57	MG	2A	3561	1/1	0.74	0.15	40,40,40,40	0
57	MG	2A	3098	1/1	0.74	0.31	82,82,82,82	0
57	MG	1A	3883	1/1	0.74	0.13	36,36,36,36	0
57	MG	1B	207	1/1	0.74	0.25	76,76,76,76	0
57	MG	2A	3298	1/1	0.74	0.32	67,67,67,67	0
57	MG	2a	1710	1/1	0.75	0.26	75,75,75,75	0
57	MG	2a	1714	1/1	0.75	0.30	77,77,77,77	0
57	MG	1w	101	1/1	0.75	0.16	84,84,84,84	0
57	MG	1x	103	1/1	0.75	0.28	76,76,76,76	0
57	MG	2A	3662	1/1	0.75	0.13	68,68,68,68	0
57	MG	1A	3644	1/1	0.75	0.19	58,58,58,58	0
57	MG	1A	4036	1/1	0.75	0.17	61,61,61,61	0
57	MG	1A	3818	1/1	0.75	0.12	53,53,53,53	0
57	MG	1A	3863	1/1	0.75	0.16	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
57	MG	2A	3531	1/1	0.75	0.24	77,77,77,77	0
57	MG	2a	1707	1/1	0.76	0.28	76,76,76,76	0
57	MG	1A	3477	1/1	0.76	0.16	70,70,70,70	0
57	MG	1B	234	1/1	0.76	0.29	75,75,75,75	0
57	MG	2a	1740	1/1	0.76	0.23	74,74,74,74	0
57	MG	2A	3318	1/1	0.76	0.29	62,62,62,62	0
57	MG	1A	3826	1/1	0.76	0.18	55,55,55,55	0
57	MG	2a	1768	1/1	0.76	0.12	82,82,82,82	0
57	MG	2A	3738	1/1	0.76	0.26	60,60,60,60	0
57	MG	1A	3480	1/1	0.76	0.15	68,68,68,68	0
57	MG	1A	3535	1/1	0.76	0.29	57,57,57,57	0
57	MG	2A	3793	1/1	0.76	0.13	56,56,56,56	0
57	MG	2A	3169	1/1	0.76	0.24	79,79,79,79	0
57	MG	2A	3194	1/1	0.76	0.22	64,64,64,64	0
57	MG	1a	1677	1/1	0.77	0.26	74,74,74,74	0
57	MG	2A	3622	1/1	0.77	0.18	61,61,61,61	0
57	MG	1A	3197	1/1	0.77	0.25	55,55,55,55	0
57	MG	2A	3361	1/1	0.77	0.17	75,75,75,75	0
57	MG	2A	3708	1/1	0.77	0.20	66,66,66,66	0
57	MG	1E	309	1/1	0.77	0.23	68,68,68,68	0
57	MG	1A	3366	1/1	0.77	0.20	76,76,76,76	0
57	MG	2A	3748	1/1	0.77	0.15	43,43,43,43	0
57	MG	2a	1802	1/1	0.77	0.15	74,74,74,74	0
57	MG	13	104	1/1	0.77	0.20	54,54,54,54	0
57	MG	2A	3792	1/1	0.77	0.21	86,86,86,86	0
57	MG	1A	4090	1/1	0.77	0.15	58,58,58,58	0
57	MG	2A	3862	1/1	0.77	0.15	73,73,73,73	0
57	MG	2A	3574	1/1	0.77	0.12	67,67,67,67	0
57	MG	2a	1615	1/1	0.77	0.21	73,73,73,73	0
57	MG	2A	3613	1/1	0.78	0.19	56,56,56,56	0
57	MG	1r	101	1/1	0.78	0.26	72,72,72,72	0
57	MG	2A	3204	1/1	0.78	0.17	75,75,75,75	0
57	MG	2B	209	1/1	0.78	0.30	75,75,75,75	0
57	MG	1D	311	1/1	0.78	0.38	77,77,77,77	0
57	MG	2a	1603	1/1	0.78	0.16	72,72,72,72	0
57	MG	2A	3296	1/1	0.78	0.23	68,68,68,68	0
57	MG	1A	3855	1/1	0.78	0.15	51,51,51,51	0
57	MG	2A	3167	1/1	0.78	0.21	76,76,76,76	0
57	MG	1a	1721	1/1	0.78	0.29	63,63,63,63	0
57	MG	2A	3333	1/1	0.78	0.14	74,74,74,74	0
57	MG	26	101	1/1	0.79	0.16	64,64,64,64	0
57	MG	2A	3328	1/1	0.79	0.18	80,80,80,80	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2a	1614	1/1	0.79	0.26	78,78,78,78	0
57	MG	1A	3026	1/1	0.79	0.28	66,66,66,66	0
57	MG	2a	1617	1/1	0.79	0.35	77,77,77,77	0
57	MG	1A	3266	1/1	0.79	0.22	70,70,70,70	0
57	MG	2a	1702	1/1	0.79	0.27	80,80,80,80	0
57	MG	2A	3188	1/1	0.79	0.16	59,59,59,59	0
57	MG	2A	3732	1/1	0.79	0.23	70,70,70,70	0
57	MG	2A	3734	1/1	0.79	0.16	72,72,72,72	0
57	MG	2a	1725	1/1	0.79	0.45	78,78,78,78	0
57	MG	2a	1729	1/1	0.79	0.23	87,87,87,87	0
57	MG	2A	3362	1/1	0.79	0.20	70,70,70,70	0
57	MG	1A	3567	1/1	0.79	0.17	71,71,71,71	0
57	MG	1w	105	1/1	0.79	0.17	77,77,77,77	0
57	MG	2A	3526	1/1	0.79	0.18	69,69,69,69	0
57	MG	2A	3779	1/1	0.79	0.19	81,81,81,81	0
57	MG	1A	3619	1/1	0.79	0.16	50,50,50,50	0
57	MG	1S	203	1/1	0.79	0.13	75,75,75,75	0
57	MG	2A	3812	1/1	0.79	0.14	48,48,48,48	0
57	MG	1B	228	1/1	0.79	0.20	81,81,81,81	0
57	MG	1A	3895	1/1	0.79	0.23	61,61,61,61	0
57	MG	1A	3984	1/1	0.79	0.19	67,67,67,67	0
57	MG	1A	3899	1/1	0.80	0.20	30,30,30,30	0
57	MG	2N	201	1/1	0.80	0.21	71,71,71,71	0
57	MG	1a	1789	1/1	0.80	0.14	70,70,70,70	0
57	MG	2A	3249	1/1	0.80	0.32	65,65,65,65	0
57	MG	2A	3286	1/1	0.80	0.14	63,63,63,63	0
57	MG	1A	3907	1/1	0.80	0.17	45,45,45,45	0
57	MG	2A	3629	1/1	0.80	0.20	52,52,52,52	0
57	MG	2a	1621	1/1	0.80	0.35	75,75,75,75	0
57	MG	2a	1627	1/1	0.80	0.20	68,68,68,68	0
57	MG	2a	1637	1/1	0.80	0.38	83,83,83,83	0
57	MG	1A	3518	1/1	0.80	0.17	66,66,66,66	0
57	MG	2A	3666	1/1	0.80	0.20	68,68,68,68	0
57	MG	1A	4033	1/1	0.80	0.26	69,69,69,69	0
57	MG	2A	3680	1/1	0.80	0.23	76,76,76,76	0
57	MG	2a	1713	1/1	0.80	0.16	79,79,79,79	0
57	MG	1A	3360	1/1	0.80	0.14	61,61,61,61	0
57	MG	2A	3730	1/1	0.80	0.18	65,65,65,65	0
57	MG	1A	4059	1/1	0.80	0.17	63,63,63,63	0
57	MG	1A	3248	1/1	0.80	0.28	66,66,66,66	0
57	MG	1A	3732	1/1	0.80	0.18	62,62,62,62	0
57	MG	1A	3618	1/1	0.80	0.19	65,65,65,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	1668	1/1	0.80	0.26	65,65,65,65	0
57	MG	2A	3379	1/1	0.80	0.21	64,64,64,64	0
57	MG	1A	3765	1/1	0.80	0.17	61,61,61,61	0
57	MG	2A	3483	1/1	0.80	0.24	64,64,64,64	0
57	MG	2A	3505	1/1	0.80	0.29	72,72,72,72	0
57	MG	2A	3186	1/1	0.80	0.26	72,72,72,72	0
57	MG	1a	1678	1/1	0.80	0.22	66,66,66,66	0
57	MG	1a	1687	1/1	0.80	0.13	72,72,72,72	0
57	MG	2w	103	1/1	0.80	0.22	79,79,79,79	0
57	MG	1a	1692	1/1	0.81	0.18	70,70,70,70	0
57	MG	2A	3513	1/1	0.81	0.13	71,71,71,71	0
57	MG	1a	1707	1/1	0.81	0.17	63,63,63,63	0
57	MG	1a	1712	1/1	0.81	0.16	61,61,61,61	0
57	MG	1A	3666	1/1	0.81	0.13	63,63,63,63	0
57	MG	2Q	203	1/1	0.81	0.16	72,72,72,72	0
57	MG	1A	3088	1/1	0.81	0.12	46,46,46,46	0
57	MG	28	103	1/1	0.81	0.11	88,88,88,88	0
57	MG	2A	3565	1/1	0.81	0.24	77,77,77,77	0
57	MG	2A	3255	1/1	0.81	0.15	62,62,62,62	0
57	MG	2A	3601	1/1	0.81	0.25	64,64,64,64	0
57	MG	1A	3898	1/1	0.81	0.20	59,59,59,59	0
57	MG	1A	4082	1/1	0.81	0.16	34,34,34,34	0
57	MG	1A	3264	1/1	0.81	0.23	69,69,69,69	0
57	MG	2A	3309	1/1	0.81	0.19	62,62,62,62	0
57	MG	1a	1607	1/1	0.81	0.36	74,74,74,74	0
57	MG	2a	1701	1/1	0.81	0.32	75,75,75,75	0
57	MG	1A	3854	1/1	0.81	0.22	67,67,67,67	0
57	MG	2A	3672	1/1	0.81	0.15	55,55,55,55	0
57	MG	2A	3674	1/1	0.81	0.15	65,65,65,65	0
57	MG	2A	3677	1/1	0.81	0.13	58,58,58,58	0
57	MG	1a	1645	1/1	0.81	0.18	75,75,75,75	0
57	MG	2A	3332	1/1	0.81	0.15	74,74,74,74	0
57	MG	2A	3694	1/1	0.81	0.17	69,69,69,69	0
57	MG	2A	3094	1/1	0.81	0.13	72,72,72,72	0
57	MG	1a	1665	1/1	0.81	0.15	71,71,71,71	0
57	MG	1A	3610	1/1	0.81	0.34	61,61,61,61	0
57	MG	2A	3111	1/1	0.81	0.29	71,71,71,71	0
57	MG	2a	1785	1/1	0.81	0.17	66,66,66,66	0
57	MG	1A	4001	1/1	0.81	0.13	31,31,31,31	0
57	MG	2A	3417	1/1	0.81	0.33	59,59,59,59	0
57	MG	1A	4007	1/1	0.81	0.12	82,82,82,82	0
57	MG	2A	3426	1/1	0.81	0.28	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
57	MG	1A	3751	1/1	0.81	0.17	60,60,60,60	0
57	MG	2A	3791	1/1	0.81	0.15	66,66,66,66	0
57	MG	2A	3487	1/1	0.81	0.15	61,61,61,61	0
57	MG	2A	3504	1/1	0.81	0.26	64,64,64,64	0
57	MG	2R	201	1/1	0.82	0.25	68,68,68,68	0
57	MG	20	102	1/1	0.82	0.18	71,71,71,71	0
57	MG	1a	1639	1/1	0.82	0.19	65,65,65,65	0
57	MG	2A	3649	1/1	0.82	0.12	73,73,73,73	0
57	MG	2a	1601	1/1	0.82	0.11	61,61,61,61	0
57	MG	1A	3595	1/1	0.82	0.15	57,57,57,57	0
57	MG	2A	3334	1/1	0.82	0.15	73,73,73,73	0
57	MG	2A	3341	1/1	0.82	0.27	64,64,64,64	0
57	MG	1A	3460	1/1	0.82	0.29	73,73,73,73	0
57	MG	2a	1620	1/1	0.82	0.25	74,74,74,74	0
57	MG	2A	3106	1/1	0.82	0.18	76,76,76,76	0
57	MG	1A	3530	1/1	0.82	0.20	73,73,73,73	0
57	MG	1a	1676	1/1	0.82	0.17	69,69,69,69	0
57	MG	1A	3320	1/1	0.82	0.14	44,44,44,44	0
57	MG	1A	3996	1/1	0.82	0.11	31,31,31,31	0
57	MG	1a	1682	1/1	0.82	0.13	75,75,75,75	0
57	MG	1A	3620	1/1	0.82	0.17	47,47,47,47	0
57	MG	1A	3870	1/1	0.82	0.16	62,62,62,62	0
57	MG	1A	4022	1/1	0.82	0.11	68,68,68,68	0
57	MG	1A	3879	1/1	0.82	0.15	51,51,51,51	0
57	MG	1A	3882	1/1	0.82	0.15	47,47,47,47	0
57	MG	2A	3759	1/1	0.82	0.16	57,57,57,57	0
57	MG	1R	205	1/1	0.82	0.20	43,43,43,43	0
57	MG	1a	1809	1/1	0.82	0.12	71,71,71,71	0
57	MG	2A	3788	1/1	0.82	0.18	53,53,53,53	0
57	MG	1a	1822	1/1	0.82	0.15	67,67,67,67	0
57	MG	1A	4043	1/1	0.82	0.12	56,56,56,56	0
57	MG	2a	1786	1/1	0.82	0.21	72,72,72,72	0
57	MG	1A	4045	1/1	0.82	0.16	58,58,58,58	0
57	MG	2A	3568	1/1	0.82	0.13	45,45,45,45	0
57	MG	1A	3382	1/1	0.82	0.21	57,57,57,57	0
57	MG	2B	201	1/1	0.82	0.40	79,79,79,79	0
57	MG	2a	1814	1/1	0.82	0.14	78,78,78,78	0
57	MG	2a	1816	1/1	0.82	0.18	66,66,66,66	0
57	MG	2A	3323	1/1	0.82	0.15	74,74,74,74	0
57	MG	2g	201	1/1	0.82	0.18	81,81,81,81	0
57	MG	1a	1628	1/1	0.82	0.26	61,61,61,61	0
57	MG	2r	102	1/1	0.82	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
57	MG	1A	3776	1/1	0.82	0.09	15,15,15,15	0
57	MG	2A	3331	1/1	0.82	0.31	75,75,75,75	0
57	MG	2A	3438	1/1	0.83	0.21	74,74,74,74	0
57	MG	10	108	1/1	0.83	0.18	60,60,60,60	0
57	MG	2A	3268	1/1	0.83	0.40	75,75,75,75	0
57	MG	1B	221	1/1	0.83	0.21	62,62,62,62	0
57	MG	1A	3399	1/1	0.83	0.13	51,51,51,51	0
57	MG	2A	3062	1/1	0.83	0.14	58,58,58,58	0
57	MG	2A	3063	1/1	0.83	0.18	74,74,74,74	0
57	MG	2a	1644	1/1	0.83	0.19	70,70,70,70	0
57	MG	2A	3739	1/1	0.83	0.19	75,75,75,75	0
57	MG	2a	1698	1/1	0.83	0.17	64,64,64,64	0
57	MG	2A	3071	1/1	0.83	0.14	50,50,50,50	0
57	MG	1A	3972	1/1	0.83	0.09	29,29,29,29	0
57	MG	1A	3061	1/1	0.83	0.23	65,65,65,65	0
57	MG	1A	3829	1/1	0.83	0.13	46,46,46,46	0
57	MG	1A	3849	1/1	0.83	0.15	59,59,59,59	0
57	MG	2A	3783	1/1	0.83	0.12	53,53,53,53	0
57	MG	2A	3786	1/1	0.83	0.15	58,58,58,58	0
57	MG	1a	1782	1/1	0.83	0.22	75,75,75,75	0
57	MG	1a	1783	1/1	0.83	0.11	75,75,75,75	0
57	MG	2a	1741	1/1	0.83	0.21	70,70,70,70	0
57	MG	2A	3165	1/1	0.83	0.17	68,68,68,68	0
57	MG	1A	4080	1/1	0.83	0.11	52,52,52,52	0
57	MG	2A	3614	1/1	0.83	0.21	65,65,65,65	0
57	MG	2A	3619	1/1	0.83	0.20	72,72,72,72	0
57	MG	1a	1666	1/1	0.83	0.09	66,66,66,66	0
57	MG	2B	203	1/1	0.83	0.13	71,71,71,71	0
57	MG	2A	3357	1/1	0.83	0.25	54,54,54,54	0
57	MG	1a	1813	1/1	0.83	0.13	61,61,61,61	0
57	MG	2B	217	1/1	0.83	0.14	63,63,63,63	0
57	MG	2A	3654	1/1	0.83	0.22	67,67,67,67	0
57	MG	1a	1814	1/1	0.83	0.31	76,76,76,76	0
57	MG	2A	3665	1/1	0.83	0.14	52,52,52,52	0
57	MG	2a	1819	1/1	0.83	0.21	82,82,82,82	0
57	MG	1a	1817	1/1	0.83	0.31	64,64,64,64	0
57	MG	2j	201	1/1	0.83	0.18	73,73,73,73	0
57	MG	2A	3411	1/1	0.83	0.20	61,61,61,61	0
57	MG	1A	3724	1/1	0.83	0.14	26,26,26,26	0
57	MG	1A	3470	1/1	0.83	0.23	63,63,63,63	0
57	MG	1A	3788	1/1	0.83	0.10	15,15,15,15	0
57	MG	2A	3090	1/1	0.84	0.22	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
57	MG	1A	3424	1/1	0.84	0.11	55,55,55,55	0
57	MG	1A	3902	1/1	0.84	0.14	32,32,32,32	0
57	MG	2A	3102	1/1	0.84	0.23	77,77,77,77	0
57	MG	2a	1604	1/1	0.84	0.31	71,71,71,71	0
57	MG	1a	1748	1/1	0.84	0.19	66,66,66,66	0
57	MG	1a	1763	1/1	0.84	0.19	65,65,65,65	0
57	MG	1a	1774	1/1	0.84	0.15	70,70,70,70	0
57	MG	2a	1619	1/1	0.84	0.24	78,78,78,78	0
57	MG	2A	3371	1/1	0.84	0.28	71,71,71,71	0
57	MG	2A	3373	1/1	0.84	0.15	70,70,70,70	0
57	MG	2a	1624	1/1	0.84	0.11	66,66,66,66	0
57	MG	2A	3148	1/1	0.84	0.18	73,73,73,73	0
57	MG	14	101	1/1	0.84	0.28	74,74,74,74	0
57	MG	2a	1640	1/1	0.84	0.13	74,74,74,74	0
57	MG	1A	3722	1/1	0.84	0.17	52,52,52,52	0
57	MG	1a	1627	1/1	0.84	0.25	64,64,64,64	0
57	MG	2a	1671	1/1	0.84	0.23	62,62,62,62	0
57	MG	2a	1695	1/1	0.84	0.21	80,80,80,80	0
57	MG	1A	3922	1/1	0.84	0.11	47,47,47,47	0
57	MG	1A	4087	1/1	0.84	0.15	64,64,64,64	0
57	MG	2A	3446	1/1	0.84	0.11	65,65,65,65	0
57	MG	2A	3193	1/1	0.84	0.21	63,63,63,63	0
57	MG	2A	3743	1/1	0.84	0.14	60,60,60,60	0
57	MG	1A	3926	1/1	0.84	0.19	60,60,60,60	0
57	MG	2A	3755	1/1	0.84	0.11	65,65,65,65	0
57	MG	2a	1716	1/1	0.84	0.32	77,77,77,77	0
57	MG	2a	1721	1/1	0.84	0.12	68,68,68,68	0
57	MG	2A	3198	1/1	0.84	0.16	69,69,69,69	0
57	MG	1A	3517	1/1	0.84	0.20	57,57,57,57	0
57	MG	1A	3458	1/1	0.84	0.21	59,59,59,59	0
57	MG	2A	3238	1/1	0.84	0.11	63,63,63,63	0
57	MG	1A	3024	1/1	0.84	0.25	60,60,60,60	0
57	MG	1A	3354	1/1	0.84	0.17	54,54,54,54	0
57	MG	1w	103	1/1	0.84	0.20	74,74,74,74	0
57	MG	2a	1769	1/1	0.84	0.12	76,76,76,76	0
57	MG	2A	3283	1/1	0.84	0.35	68,68,68,68	0
57	MG	1A	3627	1/1	0.84	0.14	52,52,52,52	0
57	MG	1w	109	1/1	0.84	0.29	71,71,71,71	0
57	MG	2A	3855	1/1	0.84	0.22	63,63,63,63	0
57	MG	2A	3598	1/1	0.84	0.19	58,58,58,58	0
57	MG	1A	3774	1/1	0.84	0.18	52,52,52,52	0
57	MG	1A	4024	1/1	0.84	0.13	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
57	MG	2A	3043	1/1	0.84	0.15	68,68,68,68	0
57	MG	1A	3552	1/1	0.84	0.14	59,59,59,59	0
57	MG	1A	3651	1/1	0.84	0.09	22,22,22,22	0
57	MG	1A	3816	1/1	0.84	0.10	36,36,36,36	0
57	MG	2A	3087	1/1	0.84	0.30	75,75,75,75	0
57	MG	2A	3636	1/1	0.84	0.14	36,36,36,36	0
57	MG	2l	203	1/1	0.84	0.13	73,73,73,73	0
57	MG	2Z	301	1/1	0.84	0.15	74,74,74,74	0
57	MG	1A	3157	1/1	0.84	0.12	29,29,29,29	0
57	MG	21	102	1/1	0.84	0.41	52,52,52,52	0
57	MG	2x	105	1/1	0.84	0.14	75,75,75,75	0
57	MG	2a	1605	1/1	0.85	0.18	73,73,73,73	0
57	MG	1B	212	1/1	0.85	0.20	63,63,63,63	0
57	MG	2A	3686	1/1	0.85	0.12	70,70,70,70	0
57	MG	1a	1719	1/1	0.85	0.16	62,62,62,62	0
57	MG	2A	3211	1/1	0.85	0.29	70,70,70,70	0
57	MG	2A	3712	1/1	0.85	0.10	56,56,56,56	0
57	MG	2A	3212	1/1	0.85	0.19	66,66,66,66	0
57	MG	2A	3031	1/1	0.85	0.12	56,56,56,56	0
57	MG	2A	3042	1/1	0.85	0.21	59,59,59,59	0
57	MG	2a	1629	1/1	0.85	0.21	76,76,76,76	0
57	MG	2a	1633	1/1	0.85	0.29	69,69,69,69	0
57	MG	1A	3333	1/1	0.85	0.26	58,58,58,58	0
57	MG	2A	3054	1/1	0.85	0.16	70,70,70,70	0
57	MG	2A	3265	1/1	0.85	0.14	67,67,67,67	0
57	MG	2a	1648	1/1	0.85	0.20	73,73,73,73	0
57	MG	2A	3266	1/1	0.85	0.13	69,69,69,69	0
57	MG	2a	1657	1/1	0.85	0.17	87,87,87,87	0
57	MG	2A	3746	1/1	0.85	0.19	66,66,66,66	0
57	MG	2a	1680	1/1	0.85	0.20	73,73,73,73	0
57	MG	1a	1738	1/1	0.85	0.14	76,76,76,76	0
57	MG	2a	1697	1/1	0.85	0.20	70,70,70,70	0
57	MG	1A	3942	1/1	0.85	0.11	27,27,27,27	0
57	MG	2A	3529	1/1	0.85	0.17	46,46,46,46	0
57	MG	1a	1629	1/1	0.85	0.13	57,57,57,57	0
57	MG	2A	3540	1/1	0.85	0.14	52,52,52,52	0
57	MG	2A	3288	1/1	0.85	0.22	65,65,65,65	0
57	MG	1A	3697	1/1	0.85	0.17	55,55,55,55	0
57	MG	1A	3834	1/1	0.85	0.18	59,59,59,59	0
57	MG	2A	3789	1/1	0.85	0.10	90,90,90,90	0
57	MG	1A	4060	1/1	0.85	0.08	15,15,15,15	0
57	MG	1A	4069	1/1	0.85	0.17	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
57	MG	1a	1793	1/1	0.85	0.15	70,70,70,70	0
57	MG	2A	3604	1/1	0.85	0.16	57,57,57,57	0
57	MG	2A	3827	1/1	0.85	0.13	48,48,48,48	0
57	MG	2A	3842	1/1	0.85	0.13	56,56,56,56	0
57	MG	2A	3101	1/1	0.85	0.33	72,72,72,72	0
57	MG	2a	1750	1/1	0.85	0.21	82,82,82,82	0
57	MG	1A	3444	1/1	0.85	0.23	61,61,61,61	0
57	MG	1a	1811	1/1	0.85	0.19	70,70,70,70	0
57	MG	2a	1778	1/1	0.85	0.10	80,80,80,80	0
57	MG	1A	4074	1/1	0.85	0.20	39,39,39,39	0
57	MG	2B	204	1/1	0.85	0.21	70,70,70,70	0
57	MG	2B	208	1/1	0.85	0.12	70,70,70,70	0
57	MG	1A	3451	1/1	0.85	0.21	46,46,46,46	0
57	MG	2A	3118	1/1	0.85	0.15	60,60,60,60	0
57	MG	1A	3510	1/1	0.85	0.14	69,69,69,69	0
57	MG	2A	3154	1/1	0.85	0.23	66,66,66,66	0
57	MG	2Q	202	1/1	0.85	0.26	58,58,58,58	0
57	MG	1T	201	1/1	0.85	0.19	56,56,56,56	0
57	MG	2A	3661	1/1	0.85	0.20	64,64,64,64	0
57	MG	2a	1820	1/1	0.85	0.20	67,67,67,67	0
57	MG	2a	1822	1/1	0.85	0.23	62,62,62,62	0
57	MG	1n	102	1/1	0.85	0.14	62,62,62,62	0
57	MG	10	106	1/1	0.85	0.11	51,51,51,51	0
57	MG	1a	1683	1/1	0.85	0.13	55,55,55,55	0
57	MG	2A	3671	1/1	0.85	0.14	64,64,64,64	0
57	MG	1A	3861	1/1	0.85	0.18	56,56,56,56	0
57	MG	1A	3079	1/1	0.85	0.17	53,53,53,53	0
57	MG	2A	3381	1/1	0.85	0.28	65,65,65,65	0
57	MG	2w	104	1/1	0.85	0.25	72,72,72,72	0
57	MG	1A	3415	1/1	0.85	0.19	42,42,42,42	0
57	MG	1a	1625	1/1	0.86	0.27	55,55,55,55	0
57	MG	2A	3174	1/1	0.86	0.15	52,52,52,52	0
57	MG	1A	3946	1/1	0.86	0.10	42,42,42,42	0
57	MG	2E	303	1/1	0.86	0.27	62,62,62,62	0
57	MG	1A	3949	1/1	0.86	0.13	56,56,56,56	0
57	MG	1A	3958	1/1	0.86	0.13	31,31,31,31	0
57	MG	1a	1816	1/1	0.86	0.13	64,64,64,64	0
57	MG	2A	3196	1/1	0.86	0.11	54,54,54,54	0
57	MG	1a	1632	1/1	0.86	0.31	60,60,60,60	0
57	MG	2A	3548	1/1	0.86	0.13	71,71,71,71	0
57	MG	1A	3736	1/1	0.86	0.15	50,50,50,50	0
57	MG	1A	3974	1/1	0.86	0.09	22,22,22,22	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3980	1/1	0.86	0.11	47,47,47,47	0
57	MG	1A	3165	1/1	0.86	0.13	36,36,36,36	0
57	MG	2A	3575	1/1	0.86	0.15	69,69,69,69	0
57	MG	2A	3233	1/1	0.86	0.27	57,57,57,57	0
57	MG	2A	3599	1/1	0.86	0.14	62,62,62,62	0
57	MG	2a	1613	1/1	0.86	0.17	57,57,57,57	0
57	MG	1A	3417	1/1	0.86	0.36	66,66,66,66	0
57	MG	2A	3240	1/1	0.86	0.29	69,69,69,69	0
57	MG	1B	225	1/1	0.86	0.13	63,63,63,63	0
57	MG	2a	1618	1/1	0.86	0.15	70,70,70,70	0
57	MG	1a	1672	1/1	0.86	0.20	60,60,60,60	0
57	MG	1x	101	1/1	0.86	0.19	70,70,70,70	0
57	MG	1B	226	1/1	0.86	0.14	65,65,65,65	0
57	MG	1x	104	1/1	0.86	0.21	68,68,68,68	0
57	MG	2a	1625	1/1	0.86	0.22	67,67,67,67	0
57	MG	2A	3269	1/1	0.86	0.13	72,72,72,72	0
57	MG	2A	3270	1/1	0.86	0.13	63,63,63,63	0
57	MG	2A	3278	1/1	0.86	0.23	67,67,67,67	0
57	MG	2A	3281	1/1	0.86	0.27	67,67,67,67	0
57	MG	2A	3655	1/1	0.86	0.15	68,68,68,68	0
57	MG	2A	3659	1/1	0.86	0.14	51,51,51,51	0
57	MG	2a	1646	1/1	0.86	0.23	73,73,73,73	0
57	MG	2a	1647	1/1	0.86	0.21	69,69,69,69	0
57	MG	1x	106	1/1	0.86	0.18	62,62,62,62	0
57	MG	1A	3628	1/1	0.86	0.13	32,32,32,32	0
57	MG	2A	3008	1/1	0.86	0.15	61,61,61,61	0
57	MG	2a	1660	1/1	0.86	0.14	64,64,64,64	0
57	MG	2A	3291	1/1	0.86	0.19	81,81,81,81	0
57	MG	2A	3295	1/1	0.86	0.20	59,59,59,59	0
57	MG	2a	1689	1/1	0.86	0.24	79,79,79,79	0
57	MG	2A	3024	1/1	0.86	0.11	52,52,52,52	0
57	MG	1A	3554	1/1	0.86	0.19	57,57,57,57	0
57	MG	2A	3301	1/1	0.86	0.16	67,67,67,67	0
57	MG	1A	3302	1/1	0.86	0.34	71,71,71,71	0
57	MG	2A	3312	1/1	0.86	0.14	60,60,60,60	0
57	MG	2a	1703	1/1	0.86	0.11	79,79,79,79	0
57	MG	1A	3652	1/1	0.86	0.15	63,63,63,63	0
57	MG	2A	3053	1/1	0.86	0.20	71,71,71,71	0
57	MG	1A	4027	1/1	0.86	0.16	52,52,52,52	0
57	MG	2A	3055	1/1	0.86	0.20	58,58,58,58	0
57	MG	2A	3715	1/1	0.86	0.12	72,72,72,72	0
57	MG	2A	3330	1/1	0.86	0.19	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
57	MG	1A	3808	1/1	0.86	0.19	80,80,80,80	0
57	MG	1a	1702	1/1	0.86	0.24	61,61,61,61	0
57	MG	1A	3256	1/1	0.86	0.12	61,61,61,61	0
57	MG	2A	3081	1/1	0.86	0.17	58,58,58,58	0
57	MG	1A	3601	1/1	0.86	0.38	67,67,67,67	0
57	MG	1A	3702	1/1	0.86	0.10	40,40,40,40	0
57	MG	1A	4051	1/1	0.86	0.12	31,31,31,31	0
57	MG	1U	203	1/1	0.86	0.15	56,56,56,56	0
57	MG	2A	3751	1/1	0.86	0.21	58,58,58,58	0
57	MG	1A	3368	1/1	0.86	0.17	57,57,57,57	0
57	MG	2A	3364	1/1	0.86	0.16	64,64,64,64	0
57	MG	1a	1759	1/1	0.86	0.24	76,76,76,76	0
57	MG	2a	1787	1/1	0.86	0.16	82,82,82,82	0
57	MG	2a	1799	1/1	0.86	0.17	56,56,56,56	0
57	MG	2A	3764	1/1	0.86	0.15	79,79,79,79	0
57	MG	1A	3611	1/1	0.86	0.15	50,50,50,50	0
57	MG	2A	3378	1/1	0.86	0.30	75,75,75,75	0
57	MG	1A	4065	1/1	0.86	0.16	40,40,40,40	0
57	MG	1A	3027	1/1	0.86	0.27	70,70,70,70	0
57	MG	2A	3389	1/1	0.86	0.11	65,65,65,65	0
57	MG	1a	1601	1/1	0.86	0.22	68,68,68,68	0
57	MG	1a	1605	1/1	0.86	0.10	68,68,68,68	0
57	MG	2A	3130	1/1	0.86	0.12	48,48,48,48	0
57	MG	1a	1791	1/1	0.86	0.16	52,52,52,52	0
57	MG	2A	3432	1/1	0.86	0.14	66,66,66,66	0
57	MG	2A	3839	1/1	0.86	0.14	69,69,69,69	0
57	MG	1A	3344	1/1	0.86	0.35	69,69,69,69	0
57	MG	1a	1794	1/1	0.86	0.16	50,50,50,50	0
57	MG	2A	3453	1/1	0.86	0.22	71,71,71,71	0
57	MG	2A	3166	1/1	0.86	0.23	67,67,67,67	0
57	MG	2w	101	1/1	0.86	0.16	70,70,70,70	0
57	MG	1a	1795	1/1	0.86	0.13	62,62,62,62	0
57	MG	2A	3499	1/1	0.86	0.13	52,52,52,52	0
57	MG	2A	3502	1/1	0.86	0.15	59,59,59,59	0
57	MG	1A	3832	1/1	0.87	0.18	63,63,63,63	0
57	MG	2A	3583	1/1	0.87	0.11	69,69,69,69	0
57	MG	2A	3590	1/1	0.87	0.16	68,68,68,68	0
57	MG	1A	4097	1/1	0.87	0.12	58,58,58,58	0
57	MG	20	101	1/1	0.87	0.21	64,64,64,64	0
57	MG	1A	3343	1/1	0.87	0.14	60,60,60,60	0
57	MG	2A	3304	1/1	0.87	0.10	62,62,62,62	0
57	MG	2A	3602	1/1	0.87	0.10	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3457	1/1	0.87	0.11	54,54,54,54	0
57	MG	1A	3981	1/1	0.87	0.26	49,49,49,49	0
57	MG	2A	3611	1/1	0.87	0.18	42,42,42,42	0
57	MG	2A	3316	1/1	0.87	0.12	68,68,68,68	0
57	MG	1A	3418	1/1	0.87	0.10	48,48,48,48	0
57	MG	2a	1609	1/1	0.87	0.34	75,75,75,75	0
57	MG	2a	1610	1/1	0.87	0.30	67,67,67,67	0
57	MG	2A	3319	1/1	0.87	0.17	59,59,59,59	0
57	MG	1a	1812	1/1	0.87	0.29	67,67,67,67	0
57	MG	1A	3727	1/1	0.87	0.14	41,41,41,41	0
57	MG	2A	3327	1/1	0.87	0.12	51,51,51,51	0
57	MG	2A	3127	1/1	0.87	0.11	69,69,69,69	0
57	MG	2A	3651	1/1	0.87	0.12	55,55,55,55	0
57	MG	1A	3207	1/1	0.87	0.20	60,60,60,60	0
57	MG	1A	3431	1/1	0.87	0.15	56,56,56,56	0
57	MG	1A	3742	1/1	0.87	0.12	43,43,43,43	0
57	MG	1a	1820	1/1	0.87	0.27	61,61,61,61	0
57	MG	1A	3546	1/1	0.87	0.28	61,61,61,61	0
57	MG	2A	3336	1/1	0.87	0.14	67,67,67,67	0
57	MG	1A	3550	1/1	0.87	0.16	59,59,59,59	0
57	MG	1A	3630	1/1	0.87	0.11	35,35,35,35	0
57	MG	1A	3438	1/1	0.87	0.15	60,60,60,60	0
57	MG	1R	204	1/1	0.87	0.15	37,37,37,37	0
57	MG	2a	1645	1/1	0.87	0.10	65,65,65,65	0
57	MG	2A	3676	1/1	0.87	0.16	61,61,61,61	0
57	MG	1A	3478	1/1	0.87	0.18	56,56,56,56	0
57	MG	2A	3192	1/1	0.87	0.14	67,67,67,67	0
57	MG	2A	3370	1/1	0.87	0.37	65,65,65,65	0
57	MG	1A	3783	1/1	0.87	0.10	24,24,24,24	0
57	MG	2A	3692	1/1	0.87	0.15	64,64,64,64	0
57	MG	2a	1662	1/1	0.87	0.13	67,67,67,67	0
57	MG	2a	1667	1/1	0.87	0.15	64,64,64,64	0
57	MG	1a	1696	1/1	0.87	0.08	59,59,59,59	0
57	MG	2A	3195	1/1	0.87	0.23	63,63,63,63	0
57	MG	2a	1686	1/1	0.87	0.12	80,80,80,80	0
57	MG	2a	1688	1/1	0.87	0.29	65,65,65,65	0
57	MG	1a	1700	1/1	0.87	0.25	59,59,59,59	0
57	MG	2A	3380	1/1	0.87	0.23	51,51,51,51	0
57	MG	2A	3720	1/1	0.87	0.11	60,60,60,60	0
57	MG	1A	3338	1/1	0.87	0.12	42,42,42,42	0
57	MG	1a	1705	1/1	0.87	0.27	71,71,71,71	0
57	MG	2A	3404	1/1	0.87	0.25	40,40,40,40	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	1706	1/1	0.87	0.31	64,64,64,64	0
57	MG	2a	1705	1/1	0.87	0.16	77,77,77,77	0
57	MG	1A	3500	1/1	0.87	0.11	55,55,55,55	0
57	MG	2A	3216	1/1	0.87	0.15	57,57,57,57	0
57	MG	2A	3023	1/1	0.87	0.28	67,67,67,67	0
57	MG	2A	3230	1/1	0.87	0.19	62,62,62,62	0
57	MG	1A	3673	1/1	0.87	0.12	38,38,38,38	0
57	MG	2A	3235	1/1	0.87	0.14	63,63,63,63	0
57	MG	2a	1724	1/1	0.87	0.24	67,67,67,67	0
57	MG	1A	3599	1/1	0.87	0.26	64,64,64,64	0
57	MG	2A	3462	1/1	0.87	0.16	65,65,65,65	0
57	MG	2a	1731	1/1	0.87	0.12	80,80,80,80	0
57	MG	2A	3464	1/1	0.87	0.11	56,56,56,56	0
57	MG	2A	3478	1/1	0.87	0.09	64,64,64,64	0
57	MG	1A	3820	1/1	0.87	0.15	51,51,51,51	0
57	MG	2A	3782	1/1	0.87	0.13	61,61,61,61	0
57	MG	2A	3244	1/1	0.87	0.22	69,69,69,69	0
57	MG	2A	3488	1/1	0.87	0.27	58,58,58,58	0
57	MG	2A	3491	1/1	0.87	0.24	71,71,71,71	0
57	MG	2a	1771	1/1	0.87	0.11	75,75,75,75	0
57	MG	2A	3493	1/1	0.87	0.35	57,57,57,57	0
57	MG	1a	1736	1/1	0.87	0.14	67,67,67,67	0
57	MG	2A	3050	1/1	0.87	0.23	61,61,61,61	0
57	MG	1A	3943	1/1	0.87	0.10	45,45,45,45	0
57	MG	2a	1797	1/1	0.87	0.12	74,74,74,74	0
57	MG	2A	3811	1/1	0.87	0.14	56,56,56,56	0
57	MG	16	103	1/1	0.87	0.26	52,52,52,52	0
57	MG	1a	1757	1/1	0.87	0.14	56,56,56,56	0
57	MG	1A	3700	1/1	0.87	0.15	54,54,54,54	0
57	MG	1a	1603	1/1	0.87	0.20	57,57,57,57	0
57	MG	2A	3852	1/1	0.87	0.12	65,65,65,65	0
57	MG	2A	3527	1/1	0.87	0.25	65,65,65,65	0
57	MG	2A	3858	1/1	0.87	0.16	64,64,64,64	0
57	MG	2A	3066	1/1	0.87	0.33	68,68,68,68	0
57	MG	1a	1767	1/1	0.87	0.12	60,60,60,60	0
57	MG	2A	3282	1/1	0.87	0.14	65,65,65,65	0
57	MG	2a	1823	1/1	0.87	0.16	78,78,78,78	0
57	MG	2d	302	1/1	0.87	0.09	68,68,68,68	0
57	MG	2e	201	1/1	0.87	0.12	74,74,74,74	0
57	MG	2A	3072	1/1	0.87	0.10	51,51,51,51	0
57	MG	2i	201	1/1	0.87	0.15	65,65,65,65	0
57	MG	2A	3551	1/1	0.87	0.19	44,44,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3554	1/1	0.87	0.15	44,44,44,44	0
57	MG	2B	211	1/1	0.87	0.17	61,61,61,61	0
57	MG	2B	215	1/1	0.87	0.27	73,73,73,73	0
57	MG	1A	4079	1/1	0.87	0.16	49,49,49,49	0
57	MG	1A	3827	1/1	0.87	0.15	48,48,48,48	0
57	MG	1A	3509	1/1	0.87	0.25	71,71,71,71	0
57	MG	1A	3968	1/1	0.87	0.17	53,53,53,53	0
57	MG	2x	103	1/1	0.87	0.15	74,74,74,74	0
57	MG	2x	104	1/1	0.87	0.24	64,64,64,64	0
57	MG	2P	201	1/1	0.87	0.23	68,68,68,68	0
57	MG	1A	3350	1/1	0.88	0.17	54,54,54,54	0
57	MG	1A	4064	1/1	0.88	0.11	54,54,54,54	0
57	MG	2A	3016	1/1	0.88	0.16	68,68,68,68	0
57	MG	2A	3223	1/1	0.88	0.15	50,50,50,50	0
57	MG	2A	3224	1/1	0.88	0.16	57,57,57,57	0
57	MG	1a	1709	1/1	0.88	0.20	62,62,62,62	0
57	MG	11	102	1/1	0.88	0.11	75,75,75,75	0
57	MG	2A	3695	1/1	0.88	0.15	63,63,63,63	0
57	MG	2A	3700	1/1	0.88	0.16	71,71,71,71	0
57	MG	1A	3845	1/1	0.88	0.15	46,46,46,46	0
57	MG	2A	3710	1/1	0.88	0.11	64,64,64,64	0
57	MG	1A	3049	1/1	0.88	0.10	33,33,33,33	0
57	MG	2a	1628	1/1	0.88	0.07	78,78,78,78	0
57	MG	1A	3534	1/1	0.88	0.20	52,52,52,52	0
57	MG	2a	1632	1/1	0.88	0.30	62,62,62,62	0
57	MG	2A	3717	1/1	0.88	0.14	51,51,51,51	0
57	MG	2a	1634	1/1	0.88	0.22	64,64,64,64	0
57	MG	2A	3044	1/1	0.88	0.15	55,55,55,55	0
57	MG	2A	3727	1/1	0.88	0.14	59,59,59,59	0
57	MG	1A	3960	1/1	0.88	0.15	64,64,64,64	0
57	MG	1A	3605	1/1	0.88	0.32	64,64,64,64	0
57	MG	2A	3252	1/1	0.88	0.13	54,54,54,54	0
57	MG	1A	3767	1/1	0.88	0.11	40,40,40,40	0
57	MG	1a	1758	1/1	0.88	0.11	57,57,57,57	0
57	MG	1A	3606	1/1	0.88	0.15	66,66,66,66	0
57	MG	2a	1651	1/1	0.88	0.14	63,63,63,63	0
57	MG	1A	3869	1/1	0.88	0.14	66,66,66,66	0
57	MG	2A	3745	1/1	0.88	0.09	34,34,34,34	0
57	MG	1A	3684	1/1	0.88	0.11	27,27,27,27	0
57	MG	1A	4093	1/1	0.88	0.19	64,64,64,64	0
57	MG	2A	3750	1/1	0.88	0.10	74,74,74,74	0
57	MG	2a	1675	1/1	0.88	0.11	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
57	MG	2A	3503	1/1	0.88	0.15	34,34,34,34	0
57	MG	2a	1681	1/1	0.88	0.13	62,62,62,62	0
57	MG	1A	3874	1/1	0.88	0.25	34,34,34,34	0
57	MG	2A	3756	1/1	0.88	0.19	69,69,69,69	0
57	MG	2A	3758	1/1	0.88	0.22	66,66,66,66	0
57	MG	2a	1693	1/1	0.88	0.17	62,62,62,62	0
57	MG	1A	3985	1/1	0.88	0.12	48,48,48,48	0
57	MG	1A	3169	1/1	0.88	0.25	65,65,65,65	0
57	MG	1a	1636	1/1	0.88	0.21	72,72,72,72	0
57	MG	2A	3766	1/1	0.88	0.15	73,73,73,73	0
57	MG	1A	3998	1/1	0.88	0.14	43,43,43,43	0
57	MG	2A	3287	1/1	0.88	0.24	67,67,67,67	0
57	MG	1B	223	1/1	0.88	0.13	55,55,55,55	0
57	MG	1a	1664	1/1	0.88	0.19	55,55,55,55	0
57	MG	2A	3536	1/1	0.88	0.13	35,35,35,35	0
57	MG	2A	3099	1/1	0.88	0.22	65,65,65,65	0
57	MG	1a	1799	1/1	0.88	0.14	79,79,79,79	0
57	MG	1a	1806	1/1	0.88	0.11	64,64,64,64	0
57	MG	2a	1720	1/1	0.88	0.20	67,67,67,67	0
57	MG	1A	3880	1/1	0.88	0.14	66,66,66,66	0
57	MG	2A	3800	1/1	0.88	0.08	44,44,44,44	0
57	MG	2A	3804	1/1	0.88	0.09	69,69,69,69	0
57	MG	1A	3539	1/1	0.88	0.10	63,63,63,63	0
57	MG	1A	4009	1/1	0.88	0.09	60,60,60,60	0
57	MG	2a	1736	1/1	0.88	0.28	66,66,66,66	0
57	MG	2a	1737	1/1	0.88	0.17	70,70,70,70	0
57	MG	2a	1739	1/1	0.88	0.41	75,75,75,75	0
57	MG	2A	3117	1/1	0.88	0.19	70,70,70,70	0
57	MG	1a	1670	1/1	0.88	0.11	49,49,49,49	0
57	MG	2A	3124	1/1	0.88	0.19	70,70,70,70	0
57	MG	2A	3847	1/1	0.88	0.14	51,51,51,51	0
57	MG	2A	3579	1/1	0.88	0.15	69,69,69,69	0
57	MG	1a	1671	1/1	0.88	0.17	62,62,62,62	0
57	MG	1A	3806	1/1	0.88	0.09	39,39,39,39	0
57	MG	2A	3861	1/1	0.88	0.34	73,73,73,73	0
57	MG	2a	1777	1/1	0.88	0.12	66,66,66,66	0
57	MG	1A	3295	1/1	0.88	0.09	39,39,39,39	0
57	MG	1A	3507	1/1	0.88	0.10	56,56,56,56	0
57	MG	1A	3421	1/1	0.88	0.17	62,62,62,62	0
57	MG	2A	3329	1/1	0.88	0.14	75,75,75,75	0
57	MG	2a	1788	1/1	0.88	0.13	69,69,69,69	0
57	MG	2a	1792	1/1	0.88	0.20	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
57	MG	2a	1794	1/1	0.88	0.17	61,61,61,61	0
57	MG	2B	206	1/1	0.88	0.15	60,60,60,60	0
57	MG	2B	207	1/1	0.88	0.27	67,67,67,67	0
57	MG	1n	101	1/1	0.88	0.33	67,67,67,67	0
57	MG	2A	3605	1/1	0.88	0.19	68,68,68,68	0
57	MG	1a	1680	1/1	0.88	0.23	77,77,77,77	0
57	MG	2B	214	1/1	0.88	0.28	68,68,68,68	0
57	MG	1A	3623	1/1	0.88	0.13	51,51,51,51	0
57	MG	2A	3170	1/1	0.88	0.23	64,64,64,64	0
57	MG	1A	3164	1/1	0.88	0.28	59,59,59,59	0
57	MG	2A	3175	1/1	0.88	0.26	68,68,68,68	0
57	MG	2F	302	1/1	0.88	0.12	64,64,64,64	0
57	MG	1w	102	1/1	0.88	0.09	57,57,57,57	0
57	MG	1F	315	1/1	0.88	0.21	55,55,55,55	0
57	MG	2a	1826	1/1	0.88	0.29	60,60,60,60	0
57	MG	2A	3343	1/1	0.88	0.14	70,70,70,70	0
57	MG	2A	3640	1/1	0.88	0.14	57,57,57,57	0
57	MG	2A	3189	1/1	0.88	0.33	64,64,64,64	0
57	MG	1A	3559	1/1	0.88	0.13	60,60,60,60	0
57	MG	1w	108	1/1	0.88	0.12	64,64,64,64	0
57	MG	1a	1694	1/1	0.88	0.18	59,59,59,59	0
57	MG	1A	4046	1/1	0.88	0.10	50,50,50,50	0
57	MG	1A	4048	1/1	0.88	0.19	49,49,49,49	0
57	MG	1A	3314	1/1	0.88	0.19	55,55,55,55	0
57	MG	2A	3201	1/1	0.88	0.17	66,66,66,66	0
57	MG	1A	3737	1/1	0.88	0.21	54,54,54,54	0
57	MG	2A	3207	1/1	0.88	0.25	70,70,70,70	0
57	MG	2A	3210	1/1	0.88	0.13	60,60,60,60	0
57	MG	2a	1606	1/1	0.88	0.36	77,77,77,77	0
57	MG	2A	3388	1/1	0.88	0.14	73,73,73,73	0
57	MG	1a	1739	1/1	0.89	0.27	58,58,58,58	0
57	MG	2G	201	1/1	0.89	0.22	75,75,75,75	0
57	MG	1a	1740	1/1	0.89	0.25	66,66,66,66	0
57	MG	1A	3916	1/1	0.89	0.09	43,43,43,43	0
57	MG	2A	3083	1/1	0.89	0.12	55,55,55,55	0
57	MG	2A	3084	1/1	0.89	0.11	52,52,52,52	0
57	MG	2A	3293	1/1	0.89	0.13	66,66,66,66	0
57	MG	1A	3920	1/1	0.89	0.14	36,36,36,36	0
57	MG	1A	3087	1/1	0.89	0.13	29,29,29,29	0
57	MG	1A	4062	1/1	0.89	0.13	58,58,58,58	0
57	MG	1A	3688	1/1	0.89	0.09	38,38,38,38	0
57	MG	1A	3935	1/1	0.89	0.11	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3307	1/1	0.89	0.29	75,75,75,75	0
57	MG	1A	3209	1/1	0.89	0.09	48,48,48,48	0
57	MG	2A	3615	1/1	0.89	0.13	60,60,60,60	0
57	MG	2A	3310	1/1	0.89	0.13	64,64,64,64	0
57	MG	1a	1778	1/1	0.89	0.11	68,68,68,68	0
57	MG	1a	1779	1/1	0.89	0.12	49,49,49,49	0
57	MG	1a	1612	1/1	0.89	0.11	65,65,65,65	0
57	MG	2A	3637	1/1	0.89	0.12	49,49,49,49	0
57	MG	1a	1615	1/1	0.89	0.10	67,67,67,67	0
57	MG	1A	3341	1/1	0.89	0.12	54,54,54,54	0
57	MG	1A	3271	1/1	0.89	0.12	44,44,44,44	0
57	MG	1A	3469	1/1	0.89	0.16	65,65,65,65	0
57	MG	1A	3831	1/1	0.89	0.12	57,57,57,57	0
57	MG	1A	3959	1/1	0.89	0.11	26,26,26,26	0
57	MG	1A	3709	1/1	0.89	0.10	23,23,23,23	0
57	MG	2A	3147	1/1	0.89	0.23	63,63,63,63	0
57	MG	1A	4089	1/1	0.89	0.10	47,47,47,47	0
57	MG	2A	3151	1/1	0.89	0.14	57,57,57,57	0
57	MG	2a	1626	1/1	0.89	0.17	60,60,60,60	0
57	MG	2A	3669	1/1	0.89	0.10	52,52,52,52	0
57	MG	1a	1637	1/1	0.89	0.33	78,78,78,78	0
57	MG	2A	3335	1/1	0.89	0.07	69,69,69,69	0
57	MG	2A	3155	1/1	0.89	0.13	65,65,65,65	0
57	MG	1A	3612	1/1	0.89	0.18	63,63,63,63	0
57	MG	1A	3210	1/1	0.89	0.09	65,65,65,65	0
57	MG	2a	1635	1/1	0.89	0.21	66,66,66,66	0
57	MG	2a	1636	1/1	0.89	0.22	65,65,65,65	0
57	MG	1a	1646	1/1	0.89	0.15	62,62,62,62	0
57	MG	2A	3679	1/1	0.89	0.10	61,61,61,61	0
57	MG	2A	3351	1/1	0.89	0.17	76,76,76,76	0
57	MG	2A	3683	1/1	0.89	0.12	51,51,51,51	0
57	MG	2A	3684	1/1	0.89	0.14	59,59,59,59	0
57	MG	2A	3355	1/1	0.89	0.13	66,66,66,66	0
57	MG	2A	3356	1/1	0.89	0.21	53,53,53,53	0
57	MG	2A	3168	1/1	0.89	0.17	63,63,63,63	0
57	MG	1a	1647	1/1	0.89	0.14	60,60,60,60	0
57	MG	2a	1654	1/1	0.89	0.14	85,85,85,85	0
57	MG	1a	1657	1/1	0.89	0.09	43,43,43,43	0
57	MG	1a	1660	1/1	0.89	0.14	73,73,73,73	0
57	MG	1a	1661	1/1	0.89	0.13	65,65,65,65	0
57	MG	2A	3176	1/1	0.89	0.18	64,64,64,64	0
57	MG	2A	3372	1/1	0.89	0.21	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
57	MG	1a	1821	1/1	0.89	0.21	65,65,65,65	0
57	MG	1A	3297	1/1	0.89	0.18	60,60,60,60	0
57	MG	2A	3724	1/1	0.89	0.11	57,57,57,57	0
57	MG	1b	302	1/1	0.89	0.16	77,77,77,77	0
57	MG	2A	3729	1/1	0.89	0.11	69,69,69,69	0
57	MG	2A	3190	1/1	0.89	0.14	72,72,72,72	0
57	MG	1A	3851	1/1	0.89	0.08	34,34,34,34	0
57	MG	2A	3387	1/1	0.89	0.13	69,69,69,69	0
57	MG	2a	1696	1/1	0.89	0.21	61,61,61,61	0
57	MG	1A	3090	1/1	0.89	0.09	40,40,40,40	0
57	MG	1A	3734	1/1	0.89	0.13	57,57,57,57	0
57	MG	2A	3740	1/1	0.89	0.12	65,65,65,65	0
57	MG	2A	3390	1/1	0.89	0.15	76,76,76,76	0
57	MG	2A	3398	1/1	0.89	0.19	64,64,64,64	0
57	MG	1t	201	1/1	0.89	0.16	57,57,57,57	0
57	MG	1A	3093	1/1	0.89	0.11	50,50,50,50	0
57	MG	2A	3416	1/1	0.89	0.26	64,64,64,64	0
57	MG	2a	1712	1/1	0.89	0.16	61,61,61,61	0
57	MG	1A	3994	1/1	0.89	0.12	22,22,22,22	0
57	MG	2A	3421	1/1	0.89	0.25	60,60,60,60	0
57	MG	1A	3488	1/1	0.89	0.10	59,59,59,59	0
57	MG	2A	3203	1/1	0.89	0.14	64,64,64,64	0
57	MG	1A	3489	1/1	0.89	0.15	54,54,54,54	0
57	MG	1A	3556	1/1	0.89	0.12	68,68,68,68	0
57	MG	1A	3558	1/1	0.89	0.13	65,65,65,65	0
57	MG	1A	3499	1/1	0.89	0.15	41,41,41,41	0
57	MG	2A	3456	1/1	0.89	0.12	68,68,68,68	0
57	MG	1A	4013	1/1	0.89	0.12	37,37,37,37	0
57	MG	2A	3213	1/1	0.89	0.34	63,63,63,63	0
57	MG	2A	3472	1/1	0.89	0.16	69,69,69,69	0
57	MG	1E	301	1/1	0.89	0.13	30,30,30,30	0
57	MG	2A	3221	1/1	0.89	0.21	57,57,57,57	0
57	MG	1E	306	1/1	0.89	0.14	52,52,52,52	0
57	MG	1A	4019	1/1	0.89	0.09	48,48,48,48	0
57	MG	1x	112	1/1	0.89	0.21	68,68,68,68	0
57	MG	2a	1764	1/1	0.89	0.09	68,68,68,68	0
57	MG	1a	1693	1/1	0.89	0.20	68,68,68,68	0
57	MG	2A	3799	1/1	0.89	0.14	49,49,49,49	0
57	MG	2A	3231	1/1	0.89	0.14	70,70,70,70	0
57	MG	1E	311	1/1	0.89	0.10	26,26,26,26	0
57	MG	1a	1695	1/1	0.89	0.26	70,70,70,70	0
57	MG	2a	1781	1/1	0.89	0.17	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
57	MG	2A	3236	1/1	0.89	0.15	61,61,61,61	0
57	MG	2A	3822	1/1	0.89	0.17	66,66,66,66	0
57	MG	2A	3823	1/1	0.89	0.13	36,36,36,36	0
57	MG	2A	3824	1/1	0.89	0.13	50,50,50,50	0
57	MG	1A	4021	1/1	0.89	0.18	63,63,63,63	0
57	MG	2a	1793	1/1	0.89	0.23	66,66,66,66	0
57	MG	2A	3830	1/1	0.89	0.08	60,60,60,60	0
57	MG	2A	3833	1/1	0.89	0.11	61,61,61,61	0
57	MG	2A	3838	1/1	0.89	0.12	59,59,59,59	0
57	MG	2A	3507	1/1	0.89	0.15	57,57,57,57	0
57	MG	2A	3239	1/1	0.89	0.11	51,51,51,51	0
57	MG	2A	3029	1/1	0.89	0.20	55,55,55,55	0
57	MG	1E	315	1/1	0.89	0.20	55,55,55,55	0
57	MG	2a	1813	1/1	0.89	0.13	83,83,83,83	0
57	MG	1A	3434	1/1	0.89	0.13	42,42,42,42	0
57	MG	2A	3857	1/1	0.89	0.12	73,73,73,73	0
57	MG	1A	3881	1/1	0.89	0.08	22,22,22,22	0
57	MG	2a	1818	1/1	0.89	0.19	61,61,61,61	0
57	MG	2A	3530	1/1	0.89	0.14	52,52,52,52	0
57	MG	1A	3656	1/1	0.89	0.14	52,52,52,52	0
57	MG	2A	3258	1/1	0.89	0.15	56,56,56,56	0
57	MG	2B	202	1/1	0.89	0.35	76,76,76,76	0
57	MG	2A	3047	1/1	0.89	0.25	71,71,71,71	0
57	MG	1A	3660	1/1	0.89	0.15	66,66,66,66	0
57	MG	1A	3263	1/1	0.89	0.26	66,66,66,66	0
57	MG	1A	3330	1/1	0.89	0.11	47,47,47,47	0
57	MG	2A	3556	1/1	0.89	0.11	59,59,59,59	0
57	MG	1V	205	1/1	0.89	0.14	51,51,51,51	0
57	MG	1A	3681	1/1	0.89	0.09	52,52,52,52	0
57	MG	2A	3279	1/1	0.89	0.09	62,62,62,62	0
57	MG	2q	202	1/1	0.89	0.14	76,76,76,76	0
57	MG	2A	3572	1/1	0.89	0.18	52,52,52,52	0
57	MG	1A	3682	1/1	0.89	0.12	43,43,43,43	0
57	MG	1A	3809	1/1	0.89	0.13	51,51,51,51	0
57	MG	2D	303	1/1	0.89	0.33	68,68,68,68	0
57	MG	2D	307	1/1	0.89	0.13	62,62,62,62	0
57	MG	2E	301	1/1	0.89	0.12	57,57,57,57	0
57	MG	2A	3577	1/1	0.89	0.16	64,64,64,64	0
57	MG	2E	307	1/1	0.89	0.15	55,55,55,55	0
57	MG	2A	3033	1/1	0.90	0.14	57,57,57,57	0
57	MG	2A	3272	1/1	0.90	0.30	70,70,70,70	0
57	MG	2A	3275	1/1	0.90	0.11	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
57	MG	2A	3277	1/1	0.90	0.12	59,59,59,59	0
57	MG	2E	305	1/1	0.90	0.12	56,56,56,56	0
57	MG	2E	306	1/1	0.90	0.11	31,31,31,31	0
57	MG	1A	3094	1/1	0.90	0.16	51,51,51,51	0
57	MG	2E	309	1/1	0.90	0.20	58,58,58,58	0
57	MG	2A	3578	1/1	0.90	0.18	62,62,62,62	0
57	MG	1A	3370	1/1	0.90	0.12	51,51,51,51	0
57	MG	2A	3581	1/1	0.90	0.20	59,59,59,59	0
57	MG	1A	3379	1/1	0.90	0.19	47,47,47,47	0
57	MG	2A	3585	1/1	0.90	0.14	61,61,61,61	0
57	MG	2A	3045	1/1	0.90	0.17	70,70,70,70	0
57	MG	2Q	204	1/1	0.90	0.15	56,56,56,56	0
57	MG	1B	203	1/1	0.90	0.07	34,34,34,34	0
57	MG	2R	202	1/1	0.90	0.09	54,54,54,54	0
57	MG	2X	101	1/1	0.90	0.19	65,65,65,65	0
57	MG	2A	3285	1/1	0.90	0.30	57,57,57,57	0
57	MG	1A	3381	1/1	0.90	0.34	61,61,61,61	0
57	MG	1B	210	1/1	0.90	0.12	52,52,52,52	0
57	MG	1A	3945	1/1	0.90	0.07	49,49,49,49	0
57	MG	23	102	1/1	0.90	0.13	60,60,60,60	0
57	MG	2A	3289	1/1	0.90	0.10	65,65,65,65	0
57	MG	2A	3606	1/1	0.90	0.17	65,65,65,65	0
57	MG	2A	3607	1/1	0.90	0.09	31,31,31,31	0
57	MG	1a	1691	1/1	0.90	0.27	74,74,74,74	0
57	MG	2A	3058	1/1	0.90	0.20	65,65,65,65	0
57	MG	1B	215	1/1	0.90	0.10	63,63,63,63	0
57	MG	1A	3492	1/1	0.90	0.15	44,44,44,44	0
57	MG	1A	3784	1/1	0.90	0.15	30,30,30,30	0
57	MG	1B	224	1/1	0.90	0.09	55,55,55,55	0
57	MG	1A	3315	1/1	0.90	0.13	56,56,56,56	0
57	MG	1A	3384	1/1	0.90	0.28	43,43,43,43	0
57	MG	1A	3392	1/1	0.90	0.12	50,50,50,50	0
57	MG	1A	3961	1/1	0.90	0.12	62,62,62,62	0
57	MG	2A	3311	1/1	0.90	0.10	51,51,51,51	0
57	MG	2A	3642	1/1	0.90	0.18	73,73,73,73	0
57	MG	2A	3648	1/1	0.90	0.14	64,64,64,64	0
57	MG	1A	3966	1/1	0.90	0.13	47,47,47,47	0
57	MG	1A	3316	1/1	0.90	0.25	54,54,54,54	0
57	MG	1A	3814	1/1	0.90	0.10	27,27,27,27	0
57	MG	1a	1710	1/1	0.90	0.27	60,60,60,60	0
57	MG	2A	3657	1/1	0.90	0.17	68,68,68,68	0
57	MG	1A	3411	1/1	0.90	0.11	41,41,41,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3660	1/1	0.90	0.11	50,50,50,50	0
57	MG	2A	3324	1/1	0.90	0.28	62,62,62,62	0
57	MG	1a	1716	1/1	0.90	0.26	68,68,68,68	0
57	MG	1a	1717	1/1	0.90	0.20	53,53,53,53	0
57	MG	1A	3414	1/1	0.90	0.15	39,39,39,39	0
57	MG	1A	3319	1/1	0.90	0.21	54,54,54,54	0
57	MG	1A	3416	1/1	0.90	0.27	69,69,69,69	0
57	MG	1A	3659	1/1	0.90	0.16	57,57,57,57	0
57	MG	2A	3673	1/1	0.90	0.11	72,72,72,72	0
57	MG	1E	314	1/1	0.90	0.20	45,45,45,45	0
57	MG	1A	3986	1/1	0.90	0.15	59,59,59,59	0
57	MG	1A	3989	1/1	0.90	0.15	65,65,65,65	0
57	MG	1Q	204	1/1	0.90	0.15	61,61,61,61	0
57	MG	1A	3992	1/1	0.90	0.09	30,30,30,30	0
57	MG	2a	1650	1/1	0.90	0.13	69,69,69,69	0
57	MG	2A	3134	1/1	0.90	0.20	62,62,62,62	0
57	MG	2a	1653	1/1	0.90	0.31	62,62,62,62	0
57	MG	2A	3145	1/1	0.90	0.14	55,55,55,55	0
57	MG	2a	1656	1/1	0.90	0.21	76,76,76,76	0
57	MG	1A	3068	1/1	0.90	0.11	57,57,57,57	0
57	MG	2A	3344	1/1	0.90	0.16	66,66,66,66	0
57	MG	2A	3691	1/1	0.90	0.11	54,54,54,54	0
57	MG	2A	3350	1/1	0.90	0.17	70,70,70,70	0
57	MG	2a	1669	1/1	0.90	0.26	66,66,66,66	0
57	MG	1A	3329	1/1	0.90	0.17	55,55,55,55	0
57	MG	2a	1674	1/1	0.90	0.18	65,65,65,65	0
57	MG	2A	3354	1/1	0.90	0.09	64,64,64,64	0
57	MG	2A	3697	1/1	0.90	0.11	60,60,60,60	0
57	MG	2A	3150	1/1	0.90	0.16	66,66,66,66	0
57	MG	2a	1682	1/1	0.90	0.14	71,71,71,71	0
57	MG	1A	3058	1/1	0.90	0.09	42,42,42,42	0
57	MG	1A	3678	1/1	0.90	0.08	24,24,24,24	0
57	MG	2A	3359	1/1	0.90	0.08	69,69,69,69	0
57	MG	2A	3360	1/1	0.90	0.17	48,48,48,48	0
57	MG	1A	3542	1/1	0.90	0.27	53,53,53,53	0
57	MG	2A	3159	1/1	0.90	0.23	58,58,58,58	0
57	MG	2A	3721	1/1	0.90	0.17	63,63,63,63	0
57	MG	2A	3363	1/1	0.90	0.30	62,62,62,62	0
57	MG	2a	1700	1/1	0.90	0.13	62,62,62,62	0
57	MG	2A	3725	1/1	0.90	0.10	65,65,65,65	0
57	MG	1A	3265	1/1	0.90	0.11	41,41,41,41	0
57	MG	1a	1781	1/1	0.90	0.17	65,65,65,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3425	1/1	0.90	0.19	63,63,63,63	0
57	MG	2A	3731	1/1	0.90	0.16	52,52,52,52	0
57	MG	2a	1708	1/1	0.90	0.23	71,71,71,71	0
57	MG	10	109	1/1	0.90	0.09	43,43,43,43	0
57	MG	1a	1787	1/1	0.90	0.07	77,77,77,77	0
57	MG	2A	3737	1/1	0.90	0.08	59,59,59,59	0
57	MG	1A	3853	1/1	0.90	0.14	65,65,65,65	0
57	MG	1A	3551	1/1	0.90	0.11	55,55,55,55	0
57	MG	2a	1717	1/1	0.90	0.17	66,66,66,66	0
57	MG	2a	1719	1/1	0.90	0.10	64,64,64,64	0
57	MG	13	105	1/1	0.90	0.11	53,53,53,53	0
57	MG	1A	3336	1/1	0.90	0.33	67,67,67,67	0
57	MG	2a	1722	1/1	0.90	0.13	69,69,69,69	0
57	MG	2A	3385	1/1	0.90	0.10	67,67,67,67	0
57	MG	2A	3178	1/1	0.90	0.15	51,51,51,51	0
57	MG	2A	3184	1/1	0.90	0.11	57,57,57,57	0
57	MG	15	107	1/1	0.90	0.11	54,54,54,54	0
57	MG	2a	1734	1/1	0.90	0.31	60,60,60,60	0
57	MG	1A	3181	1/1	0.90	0.30	56,56,56,56	0
57	MG	1A	3437	1/1	0.90	0.33	73,73,73,73	0
57	MG	2A	3403	1/1	0.90	0.27	50,50,50,50	0
57	MG	1A	4029	1/1	0.90	0.08	58,58,58,58	0
57	MG	1A	4032	1/1	0.90	0.17	52,52,52,52	0
57	MG	1A	3864	1/1	0.90	0.19	52,52,52,52	0
57	MG	1A	3270	1/1	0.90	0.16	47,47,47,47	0
57	MG	2a	1744	1/1	0.90	0.18	78,78,78,78	0
57	MG	2a	1749	1/1	0.90	0.11	71,71,71,71	0
57	MG	1A	3707	1/1	0.90	0.11	39,39,39,39	0
57	MG	2a	1751	1/1	0.90	0.17	73,73,73,73	0
57	MG	2a	1761	1/1	0.90	0.10	67,67,67,67	0
57	MG	1a	1624	1/1	0.90	0.11	50,50,50,50	0
57	MG	1A	3234	1/1	0.90	0.12	55,55,55,55	0
57	MG	2A	3427	1/1	0.90	0.10	69,69,69,69	0
57	MG	1A	3243	1/1	0.90	0.24	42,42,42,42	0
57	MG	2a	1775	1/1	0.90	0.19	58,58,58,58	0
57	MG	2A	3435	1/1	0.90	0.33	65,65,65,65	0
57	MG	1A	4047	1/1	0.90	0.07	25,25,25,25	0
57	MG	2a	1779	1/1	0.90	0.14	66,66,66,66	0
57	MG	2A	3439	1/1	0.90	0.39	59,59,59,59	0
57	MG	1A	3579	1/1	0.90	0.30	39,39,39,39	0
57	MG	1A	3592	1/1	0.90	0.09	37,37,37,37	0
57	MG	1l	202	1/1	0.90	0.10	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
57	MG	1A	4052	1/1	0.90	0.12	33,33,33,33	0
57	MG	2a	1789	1/1	0.90	0.24	65,65,65,65	0
57	MG	2a	1791	1/1	0.90	0.11	64,64,64,64	0
57	MG	1A	4053	1/1	0.90	0.12	31,31,31,31	0
57	MG	1A	4054	1/1	0.90	0.09	62,62,62,62	0
57	MG	2A	3809	1/1	0.90	0.08	40,40,40,40	0
57	MG	1A	3730	1/1	0.90	0.10	44,44,44,44	0
57	MG	1a	1641	1/1	0.90	0.16	52,52,52,52	0
57	MG	2A	3814	1/1	0.90	0.08	45,45,45,45	0
57	MG	2A	3486	1/1	0.90	0.23	53,53,53,53	0
57	MG	1a	1642	1/1	0.90	0.32	71,71,71,71	0
57	MG	2a	1810	1/1	0.90	0.12	73,73,73,73	0
57	MG	1A	3188	1/1	0.90	0.15	41,41,41,41	0
57	MG	1A	4061	1/1	0.90	0.14	63,63,63,63	0
57	MG	1w	106	1/1	0.90	0.17	71,71,71,71	0
57	MG	2a	1815	1/1	0.90	0.20	67,67,67,67	0
57	MG	1A	3887	1/1	0.90	0.07	26,26,26,26	0
57	MG	1a	1651	1/1	0.90	0.12	67,67,67,67	0
57	MG	1a	1652	1/1	0.90	0.21	66,66,66,66	0
57	MG	1A	3892	1/1	0.90	0.17	51,51,51,51	0
57	MG	1A	3299	1/1	0.90	0.15	51,51,51,51	0
57	MG	1A	3357	1/1	0.90	0.16	57,57,57,57	0
57	MG	2A	3512	1/1	0.90	0.13	65,65,65,65	0
57	MG	2a	1825	1/1	0.90	0.24	64,64,64,64	0
57	MG	1x	107	1/1	0.90	0.17	63,63,63,63	0
57	MG	2A	3520	1/1	0.90	0.10	36,36,36,36	0
57	MG	1x	108	1/1	0.90	0.11	35,35,35,35	0
57	MG	1A	3604	1/1	0.90	0.23	64,64,64,64	0
57	MG	1A	3250	1/1	0.90	0.22	58,58,58,58	0
57	MG	1A	3365	1/1	0.90	0.12	60,60,60,60	0
57	MG	2A	3256	1/1	0.90	0.22	61,61,61,61	0
57	MG	1A	3913	1/1	0.90	0.17	30,30,30,30	0
57	MG	2A	3262	1/1	0.90	0.11	65,65,65,65	0
57	MG	2A	3263	1/1	0.90	0.12	61,61,61,61	0
57	MG	2A	3264	1/1	0.90	0.17	62,62,62,62	0
57	MG	2A	3549	1/1	0.90	0.09	47,47,47,47	0
57	MG	1A	3307	1/1	0.90	0.09	31,31,31,31	0
57	MG	1A	3753	1/1	0.90	0.09	49,49,49,49	0
57	MG	2A	3267	1/1	0.90	0.11	59,59,59,59	0
57	MG	1A	3754	1/1	0.90	0.19	57,57,57,57	0
57	MG	1a	1674	1/1	0.90	0.21	70,70,70,70	0
57	MG	1A	3246	1/1	0.91	0.28	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3626	1/1	0.91	0.08	49,49,49,49	0
57	MG	1A	3450	1/1	0.91	0.14	47,47,47,47	0
57	MG	2A	3634	1/1	0.91	0.12	52,52,52,52	0
57	MG	2A	3182	1/1	0.91	0.10	59,59,59,59	0
57	MG	25	104	1/1	0.91	0.13	53,53,53,53	0
57	MG	2A	3347	1/1	0.91	0.14	62,62,62,62	0
57	MG	27	102	1/1	0.91	0.11	47,47,47,47	0
57	MG	28	102	1/1	0.91	0.13	48,48,48,48	0
57	MG	2A	3348	1/1	0.91	0.13	65,65,65,65	0
57	MG	1A	3755	1/1	0.91	0.07	51,51,51,51	0
57	MG	2a	1602	1/1	0.91	0.28	60,60,60,60	0
57	MG	1A	3275	1/1	0.91	0.08	49,49,49,49	0
57	MG	2A	3352	1/1	0.91	0.17	67,67,67,67	0
57	MG	2A	3353	1/1	0.91	0.13	68,68,68,68	0
57	MG	2A	3187	1/1	0.91	0.18	70,70,70,70	0
57	MG	2a	1607	1/1	0.91	0.19	66,66,66,66	0
57	MG	1A	3331	1/1	0.91	0.30	58,58,58,58	0
57	MG	1A	3247	1/1	0.91	0.12	60,60,60,60	0
57	MG	2a	1611	1/1	0.91	0.21	69,69,69,69	0
57	MG	1A	3296	1/1	0.91	0.23	50,50,50,50	0
57	MG	2A	3358	1/1	0.91	0.09	61,61,61,61	0
57	MG	1A	3657	1/1	0.91	0.07	21,21,21,21	0
57	MG	1a	1686	1/1	0.91	0.15	48,48,48,48	0
57	MG	1F	303	1/1	0.91	0.32	32,32,32,32	0
57	MG	1a	1689	1/1	0.91	0.13	66,66,66,66	0
57	MG	1A	3658	1/1	0.91	0.07	16,16,16,16	0
57	MG	2A	3197	1/1	0.91	0.15	66,66,66,66	0
57	MG	1N	201	1/1	0.91	0.14	56,56,56,56	0
57	MG	1A	3785	1/1	0.91	0.13	31,31,31,31	0
57	MG	1x	105	1/1	0.91	0.17	69,69,69,69	0
57	MG	1A	3911	1/1	0.91	0.17	75,75,75,75	0
57	MG	2A	3374	1/1	0.91	0.13	67,67,67,67	0
57	MG	2A	3206	1/1	0.91	0.17	67,67,67,67	0
57	MG	1A	3463	1/1	0.91	0.09	51,51,51,51	0
57	MG	2A	3208	1/1	0.91	0.19	44,44,44,44	0
57	MG	1A	3801	1/1	0.91	0.08	74,74,74,74	0
57	MG	2A	3382	1/1	0.91	0.08	69,69,69,69	0
57	MG	2A	3685	1/1	0.91	0.14	48,48,48,48	0
57	MG	2A	3384	1/1	0.91	0.16	61,61,61,61	0
57	MG	2A	3690	1/1	0.91	0.15	62,62,62,62	0
57	MG	2a	1641	1/1	0.91	0.19	67,67,67,67	0
57	MG	2a	1643	1/1	0.91	0.09	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
57	MG	1x	109	1/1	0.91	0.10	61,61,61,61	0
57	MG	1a	1699	1/1	0.91	0.27	47,47,47,47	0
57	MG	1A	3468	1/1	0.91	0.16	59,59,59,59	0
57	MG	2A	3001	1/1	0.91	0.33	59,59,59,59	0
57	MG	2A	3218	1/1	0.91	0.32	41,41,41,41	0
57	MG	2A	3393	1/1	0.91	0.24	63,63,63,63	0
57	MG	1A	3089	1/1	0.91	0.08	34,34,34,34	0
57	MG	1A	3200	1/1	0.91	0.12	47,47,47,47	0
57	MG	1A	3931	1/1	0.91	0.10	20,20,20,20	0
57	MG	2A	3408	1/1	0.91	0.34	68,68,68,68	0
57	MG	2A	3409	1/1	0.91	0.18	39,39,39,39	0
57	MG	2A	3718	1/1	0.91	0.09	60,60,60,60	0
57	MG	1A	3933	1/1	0.91	0.16	35,35,35,35	0
57	MG	2A	3415	1/1	0.91	0.27	63,63,63,63	0
57	MG	2A	3723	1/1	0.91	0.11	64,64,64,64	0
57	MG	1A	3934	1/1	0.91	0.19	56,56,56,56	0
57	MG	1A	3472	1/1	0.91	0.24	67,67,67,67	0
57	MG	2a	1672	1/1	0.91	0.28	72,72,72,72	0
57	MG	2a	1673	1/1	0.91	0.13	61,61,61,61	0
57	MG	2A	3420	1/1	0.91	0.36	61,61,61,61	0
57	MG	2A	3728	1/1	0.91	0.16	49,49,49,49	0
57	MG	2a	1679	1/1	0.91	0.19	70,70,70,70	0
57	MG	1a	1711	1/1	0.91	0.18	67,67,67,67	0
57	MG	1A	3052	1/1	0.91	0.08	40,40,40,40	0
57	MG	1a	1715	1/1	0.91	0.11	63,63,63,63	0
57	MG	2a	1683	1/1	0.91	0.14	64,64,64,64	0
57	MG	1A	3257	1/1	0.91	0.13	72,72,72,72	0
57	MG	1A	3568	1/1	0.91	0.11	48,48,48,48	0
57	MG	2A	3433	1/1	0.91	0.23	51,51,51,51	0
57	MG	1A	4063	1/1	0.91	0.08	42,42,42,42	0
57	MG	2a	1694	1/1	0.91	0.15	68,68,68,68	0
57	MG	2A	3436	1/1	0.91	0.36	65,65,65,65	0
57	MG	2A	3243	1/1	0.91	0.39	60,60,60,60	0
57	MG	1A	3123	1/1	0.91	0.09	40,40,40,40	0
57	MG	2A	3441	1/1	0.91	0.13	52,52,52,52	0
57	MG	2A	3051	1/1	0.91	0.14	54,54,54,54	0
57	MG	1a	1724	1/1	0.91	0.11	53,53,53,53	0
57	MG	2A	3254	1/1	0.91	0.31	64,64,64,64	0
57	MG	2A	3457	1/1	0.91	0.17	66,66,66,66	0
57	MG	2A	3461	1/1	0.91	0.10	69,69,69,69	0
57	MG	2A	3754	1/1	0.91	0.13	64,64,64,64	0
57	MG	1a	1727	1/1	0.91	0.24	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
57	MG	1a	1728	1/1	0.91	0.20	50,50,50,50	0
57	MG	2A	3056	1/1	0.91	0.17	64,64,64,64	0
57	MG	2A	3057	1/1	0.91	0.14	55,55,55,55	0
57	MG	1A	3591	1/1	0.91	0.08	33,33,33,33	0
57	MG	1A	3952	1/1	0.91	0.06	26,26,26,26	0
57	MG	2A	3765	1/1	0.91	0.25	68,68,68,68	0
57	MG	1A	3351	1/1	0.91	0.21	39,39,39,39	0
57	MG	1A	3171	1/1	0.91	0.35	41,41,41,41	0
57	MG	2A	3489	1/1	0.91	0.33	63,63,63,63	0
57	MG	1a	1744	1/1	0.91	0.28	56,56,56,56	0
57	MG	2a	1723	1/1	0.91	0.37	71,71,71,71	0
57	MG	2A	3785	1/1	0.91	0.11	56,56,56,56	0
57	MG	1a	1747	1/1	0.91	0.19	60,60,60,60	0
57	MG	2a	1726	1/1	0.91	0.32	63,63,63,63	0
57	MG	2A	3495	1/1	0.91	0.17	64,64,64,64	0
57	MG	2A	3078	1/1	0.91	0.12	47,47,47,47	0
57	MG	2A	3500	1/1	0.91	0.11	74,74,74,74	0
57	MG	2A	3501	1/1	0.91	0.10	64,64,64,64	0
57	MG	1a	1610	1/1	0.91	0.07	66,66,66,66	0
57	MG	1a	1756	1/1	0.91	0.22	64,64,64,64	0
57	MG	1A	3226	1/1	0.91	0.12	51,51,51,51	0
57	MG	1A	3833	1/1	0.91	0.10	31,31,31,31	0
57	MG	2A	3807	1/1	0.91	0.10	55,55,55,55	0
57	MG	1A	4081	1/1	0.91	0.10	21,21,21,21	0
57	MG	2A	3509	1/1	0.91	0.14	46,46,46,46	0
57	MG	2a	1747	1/1	0.91	0.20	77,77,77,77	0
57	MG	2a	1748	1/1	0.91	0.07	68,68,68,68	0
57	MG	1A	3497	1/1	0.91	0.13	44,44,44,44	0
57	MG	1A	3603	1/1	0.91	0.26	44,44,44,44	0
57	MG	2A	3515	1/1	0.91	0.14	58,58,58,58	0
57	MG	2A	3097	1/1	0.91	0.19	64,64,64,64	0
57	MG	2a	1763	1/1	0.91	0.11	69,69,69,69	0
57	MG	1A	3848	1/1	0.91	0.24	53,53,53,53	0
57	MG	2a	1765	1/1	0.91	0.09	55,55,55,55	0
57	MG	1A	3714	1/1	0.91	0.11	33,33,33,33	0
57	MG	1A	3358	1/1	0.91	0.10	42,42,42,42	0
57	MG	1A	3130	1/1	0.91	0.08	64,64,64,64	0
57	MG	2a	1772	1/1	0.91	0.18	69,69,69,69	0
57	MG	2A	3835	1/1	0.91	0.10	70,70,70,70	0
57	MG	1B	202	1/1	0.91	0.24	54,54,54,54	0
57	MG	1A	3982	1/1	0.91	0.17	53,53,53,53	0
57	MG	1a	1786	1/1	0.91	0.15	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
57	MG	1A	3361	1/1	0.91	0.10	57,57,57,57	0
57	MG	2A	3851	1/1	0.91	0.13	64,64,64,64	0
57	MG	1a	1788	1/1	0.91	0.17	65,65,65,65	0
57	MG	1a	1640	1/1	0.91	0.17	56,56,56,56	0
57	MG	1B	208	1/1	0.91	0.26	65,65,65,65	0
57	MG	2A	3300	1/1	0.91	0.12	60,60,60,60	0
57	MG	1A	3364	1/1	0.91	0.12	57,57,57,57	0
57	MG	1a	1643	1/1	0.91	0.18	63,63,63,63	0
57	MG	2A	3563	1/1	0.91	0.09	39,39,39,39	0
57	MG	2A	3306	1/1	0.91	0.11	74,74,74,74	0
57	MG	2a	1796	1/1	0.91	0.11	72,72,72,72	0
57	MG	2A	3136	1/1	0.91	0.20	55,55,55,55	0
57	MG	1A	3433	1/1	0.91	0.09	41,41,41,41	0
57	MG	2B	205	1/1	0.91	0.18	70,70,70,70	0
57	MG	2a	1803	1/1	0.91	0.11	61,61,61,61	0
57	MG	2a	1804	1/1	0.91	0.21	56,56,56,56	0
57	MG	2A	3573	1/1	0.91	0.12	50,50,50,50	0
57	MG	2A	3146	1/1	0.91	0.11	48,48,48,48	0
57	MG	1A	3511	1/1	0.91	0.10	52,52,52,52	0
57	MG	2A	3576	1/1	0.91	0.10	28,28,28,28	0
57	MG	2B	210	1/1	0.91	0.24	68,68,68,68	0
57	MG	1B	219	1/1	0.91	0.12	41,41,41,41	0
57	MG	2A	3315	1/1	0.91	0.13	53,53,53,53	0
57	MG	1A	3065	1/1	0.91	0.16	55,55,55,55	0
57	MG	2A	3317	1/1	0.91	0.37	54,54,54,54	0
57	MG	1A	3866	1/1	0.91	0.18	36,36,36,36	0
57	MG	1A	3325	1/1	0.91	0.12	41,41,41,41	0
57	MG	2A	3586	1/1	0.91	0.07	54,54,54,54	0
57	MG	1a	1659	1/1	0.91	0.19	66,66,66,66	0
57	MG	1A	3527	1/1	0.91	0.24	55,55,55,55	0
57	MG	2A	3161	1/1	0.91	0.23	62,62,62,62	0
57	MG	2A	3162	1/1	0.91	0.24	58,58,58,58	0
57	MG	2A	3163	1/1	0.91	0.11	42,42,42,42	0
57	MG	1A	3529	1/1	0.91	0.24	70,70,70,70	0
57	MG	1A	4003	1/1	0.91	0.19	32,32,32,32	0
57	MG	1A	4006	1/1	0.91	0.11	68,68,68,68	0
57	MG	1A	3745	1/1	0.91	0.14	66,66,66,66	0
57	MG	2A	3608	1/1	0.91	0.10	29,29,29,29	0
57	MG	1B	232	1/1	0.91	0.12	59,59,59,59	0
57	MG	1A	3328	1/1	0.91	0.19	61,61,61,61	0
57	MG	2A	3171	1/1	0.91	0.08	56,56,56,56	0
57	MG	1h	201	1/1	0.91	0.09	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2v	102	1/1	0.91	0.12	61,61,61,61	0
57	MG	2A	3337	1/1	0.91	0.18	61,61,61,61	0
57	MG	2w	102	1/1	0.91	0.12	62,62,62,62	0
57	MG	2U	201	1/1	0.91	0.29	59,59,59,59	0
57	MG	2U	202	1/1	0.91	0.15	51,51,51,51	0
57	MG	2x	101	1/1	0.91	0.23	49,49,49,49	0
57	MG	2V	203	1/1	0.91	0.28	67,67,67,67	0
57	MG	2W	201	1/1	0.91	0.10	64,64,64,64	0
57	MG	1D	309	1/1	0.91	0.12	47,47,47,47	0
57	MG	2x	106	1/1	0.91	0.14	59,59,59,59	0
57	MG	1A	3305	1/1	0.92	0.17	49,49,49,49	0
57	MG	1A	3225	1/1	0.92	0.14	46,46,46,46	0
57	MG	2A	3137	1/1	0.92	0.18	49,49,49,49	0
57	MG	2A	3139	1/1	0.92	0.11	43,43,43,43	0
57	MG	2A	3479	1/1	0.92	0.29	65,65,65,65	0
57	MG	1A	3932	1/1	0.92	0.09	33,33,33,33	0
57	MG	1A	4049	1/1	0.92	0.07	49,49,49,49	0
57	MG	2A	3294	1/1	0.92	0.25	53,53,53,53	0
57	MG	1a	1681	1/1	0.92	0.17	63,63,63,63	0
57	MG	2A	3733	1/1	0.92	0.12	43,43,43,43	0
57	MG	1e	201	1/1	0.92	0.11	70,70,70,70	0
57	MG	2a	1638	1/1	0.92	0.14	52,52,52,52	0
57	MG	2a	1639	1/1	0.92	0.15	62,62,62,62	0
57	MG	1f	201	1/1	0.92	0.17	53,53,53,53	0
57	MG	2A	3299	1/1	0.92	0.12	67,67,67,67	0
57	MG	2a	1642	1/1	0.92	0.09	62,62,62,62	0
57	MG	1N	202	1/1	0.92	0.28	43,43,43,43	0
57	MG	2A	3497	1/1	0.92	0.19	58,58,58,58	0
57	MG	1O	205	1/1	0.92	0.10	67,67,67,67	0
57	MG	2A	3302	1/1	0.92	0.22	51,51,51,51	0
57	MG	1P	206	1/1	0.92	0.22	49,49,49,49	0
57	MG	1A	3277	1/1	0.92	0.13	49,49,49,49	0
57	MG	2A	3747	1/1	0.92	0.20	43,43,43,43	0
57	MG	1A	3828	1/1	0.92	0.08	26,26,26,26	0
57	MG	1A	3719	1/1	0.92	0.11	30,30,30,30	0
57	MG	1A	3291	1/1	0.92	0.08	45,45,45,45	0
57	MG	2A	3752	1/1	0.92	0.10	62,62,62,62	0
57	MG	2a	1655	1/1	0.92	0.08	60,60,60,60	0
57	MG	1A	3617	1/1	0.92	0.10	38,38,38,38	0
57	MG	1A	3342	1/1	0.92	0.08	58,58,58,58	0
57	MG	2a	1658	1/1	0.92	0.21	63,63,63,63	0
57	MG	2A	3314	1/1	0.92	0.27	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
57	MG	2A	3757	1/1	0.92	0.17	63,63,63,63	0
57	MG	2a	1664	1/1	0.92	0.13	68,68,68,68	0
57	MG	1A	3420	1/1	0.92	0.10	35,35,35,35	0
57	MG	1A	3292	1/1	0.92	0.19	53,53,53,53	0
57	MG	2A	3760	1/1	0.92	0.18	63,63,63,63	0
57	MG	1A	3847	1/1	0.92	0.15	65,65,65,65	0
57	MG	2A	3523	1/1	0.92	0.20	67,67,67,67	0
57	MG	1A	3622	1/1	0.92	0.09	31,31,31,31	0
57	MG	1A	3543	1/1	0.92	0.15	36,36,36,36	0
57	MG	2A	3770	1/1	0.92	0.18	68,68,68,68	0
57	MG	2A	3776	1/1	0.92	0.10	55,55,55,55	0
57	MG	2A	3321	1/1	0.92	0.10	57,57,57,57	0
57	MG	2A	3322	1/1	0.92	0.08	44,44,44,44	0
57	MG	1A	4066	1/1	0.92	0.11	53,53,53,53	0
57	MG	2A	3784	1/1	0.92	0.15	73,73,73,73	0
57	MG	2a	1687	1/1	0.92	0.14	58,58,58,58	0
57	MG	1A	3422	1/1	0.92	0.12	47,47,47,47	0
57	MG	2A	3534	1/1	0.92	0.11	60,60,60,60	0
57	MG	1A	3293	1/1	0.92	0.10	55,55,55,55	0
57	MG	2A	3539	1/1	0.92	0.11	49,49,49,49	0
57	MG	1A	3964	1/1	0.92	0.08	61,61,61,61	0
57	MG	16	101	1/1	0.92	0.12	41,41,41,41	0
57	MG	1A	3204	1/1	0.92	0.09	43,43,43,43	0
57	MG	2A	3185	1/1	0.92	0.09	74,74,74,74	0
57	MG	17	105	1/1	0.92	0.15	51,51,51,51	0
57	MG	1a	1713	1/1	0.92	0.11	58,58,58,58	0
57	MG	2A	3806	1/1	0.92	0.08	41,41,41,41	0
57	MG	1x	111	1/1	0.92	0.09	57,57,57,57	0
57	MG	1A	3639	1/1	0.92	0.11	27,27,27,27	0
57	MG	1A	3971	1/1	0.92	0.07	38,38,38,38	0
57	MG	2A	3566	1/1	0.92	0.09	48,48,48,48	0
57	MG	1A	3859	1/1	0.92	0.08	63,63,63,63	0
57	MG	2a	1711	1/1	0.92	0.11	67,67,67,67	0
57	MG	1A	3082	1/1	0.92	0.16	40,40,40,40	0
57	MG	1A	3975	1/1	0.92	0.09	60,60,60,60	0
57	MG	1A	3172	1/1	0.92	0.13	51,51,51,51	0
57	MG	1a	1613	1/1	0.92	0.15	67,67,67,67	0
57	MG	1a	1614	1/1	0.92	0.27	60,60,60,60	0
57	MG	2A	3831	1/1	0.92	0.09	57,57,57,57	0
57	MG	2A	3345	1/1	0.92	0.19	68,68,68,68	0
57	MG	1a	1732	1/1	0.92	0.24	63,63,63,63	0
57	MG	2A	3836	1/1	0.92	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
57	MG	2A	3199	1/1	0.92	0.14	62,62,62,62	0
57	MG	2A	3349	1/1	0.92	0.16	70,70,70,70	0
57	MG	2A	3200	1/1	0.92	0.08	50,50,50,50	0
57	MG	2A	3584	1/1	0.92	0.13	61,61,61,61	0
57	MG	2A	3848	1/1	0.92	0.09	52,52,52,52	0
57	MG	2a	1730	1/1	0.92	0.26	70,70,70,70	0
57	MG	2A	3036	1/1	0.92	0.10	57,57,57,57	0
57	MG	2a	1732	1/1	0.92	0.31	64,64,64,64	0
57	MG	1A	3385	1/1	0.92	0.09	44,44,44,44	0
57	MG	2a	1735	1/1	0.92	0.17	70,70,70,70	0
57	MG	1a	1620	1/1	0.92	0.09	47,47,47,47	0
57	MG	1a	1622	1/1	0.92	0.31	73,73,73,73	0
57	MG	1A	3490	1/1	0.92	0.12	52,52,52,52	0
57	MG	2A	3600	1/1	0.92	0.21	65,65,65,65	0
57	MG	1a	1742	1/1	0.92	0.20	64,64,64,64	0
57	MG	2A	3209	1/1	0.92	0.24	57,57,57,57	0
57	MG	1A	3435	1/1	0.92	0.17	44,44,44,44	0
57	MG	1a	1745	1/1	0.92	0.08	69,69,69,69	0
57	MG	2A	3052	1/1	0.92	0.14	54,54,54,54	0
57	MG	1A	3120	1/1	0.92	0.08	36,36,36,36	0
57	MG	1A	3773	1/1	0.92	0.19	67,67,67,67	0
57	MG	1A	3875	1/1	0.92	0.12	48,48,48,48	0
57	MG	1A	3258	1/1	0.92	0.11	22,22,22,22	0
57	MG	2a	1752	1/1	0.92	0.17	66,66,66,66	0
57	MG	2a	1757	1/1	0.92	0.08	61,61,61,61	0
57	MG	2A	3366	1/1	0.92	0.26	63,63,63,63	0
57	MG	2a	1762	1/1	0.92	0.12	70,70,70,70	0
57	MG	1B	211	1/1	0.92	0.10	48,48,48,48	0
57	MG	1A	3440	1/1	0.92	0.09	44,44,44,44	0
57	MG	2B	213	1/1	0.92	0.15	72,72,72,72	0
57	MG	2A	3616	1/1	0.92	0.19	65,65,65,65	0
57	MG	2A	3226	1/1	0.92	0.21	44,44,44,44	0
57	MG	2A	3620	1/1	0.92	0.09	51,51,51,51	0
57	MG	2A	3228	1/1	0.92	0.14	65,65,65,65	0
57	MG	2A	3059	1/1	0.92	0.15	54,54,54,54	0
57	MG	1B	214	1/1	0.92	0.20	62,62,62,62	0
57	MG	1a	1764	1/1	0.92	0.11	61,61,61,61	0
57	MG	1a	1638	1/1	0.92	0.11	45,45,45,45	0
57	MG	2A	3070	1/1	0.92	0.14	51,51,51,51	0
57	MG	1A	3779	1/1	0.92	0.11	20,20,20,20	0
57	MG	1A	3997	1/1	0.92	0.10	39,39,39,39	0
57	MG	2A	3073	1/1	0.92	0.21	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
57	MG	1A	3580	1/1	0.92	0.11	34,34,34,34	0
57	MG	2F	303	1/1	0.92	0.09	50,50,50,50	0
57	MG	2a	1790	1/1	0.92	0.17	64,64,64,64	0
57	MG	2F	304	1/1	0.92	0.12	60,60,60,60	0
57	MG	1A	3581	1/1	0.92	0.15	52,52,52,52	0
57	MG	1A	3583	1/1	0.92	0.17	62,62,62,62	0
57	MG	2A	3245	1/1	0.92	0.16	63,63,63,63	0
57	MG	2A	3391	1/1	0.92	0.16	61,61,61,61	0
57	MG	2A	3246	1/1	0.92	0.06	60,60,60,60	0
57	MG	1A	3888	1/1	0.92	0.17	32,32,32,32	0
57	MG	2A	3251	1/1	0.92	0.12	64,64,64,64	0
57	MG	1A	3443	1/1	0.92	0.15	44,44,44,44	0
57	MG	2A	3405	1/1	0.92	0.18	50,50,50,50	0
57	MG	2A	3407	1/1	0.92	0.35	59,59,59,59	0
57	MG	1A	3893	1/1	0.92	0.12	33,33,33,33	0
57	MG	2a	1807	1/1	0.92	0.22	56,56,56,56	0
57	MG	2a	1809	1/1	0.92	0.18	68,68,68,68	0
57	MG	1A	3791	1/1	0.92	0.07	21,21,21,21	0
57	MG	2A	3092	1/1	0.92	0.16	50,50,50,50	0
57	MG	2A	3413	1/1	0.92	0.27	67,67,67,67	0
57	MG	2A	3414	1/1	0.92	0.26	64,64,64,64	0
57	MG	1A	3797	1/1	0.92	0.10	36,36,36,36	0
57	MG	2A	3096	1/1	0.92	0.08	45,45,45,45	0
57	MG	1B	231	1/1	0.92	0.09	59,59,59,59	0
57	MG	25	102	1/1	0.92	0.11	50,50,50,50	0
57	MG	1A	3401	1/1	0.92	0.30	42,42,42,42	0
57	MG	1A	3445	1/1	0.92	0.13	41,41,41,41	0
57	MG	1D	305	1/1	0.92	0.09	41,41,41,41	0
57	MG	28	101	1/1	0.92	0.11	54,54,54,54	0
57	MG	1A	3447	1/1	0.92	0.10	62,62,62,62	0
57	MG	1A	3909	1/1	0.92	0.07	29,29,29,29	0
57	MG	2A	3428	1/1	0.92	0.19	56,56,56,56	0
57	MG	2A	3430	1/1	0.92	0.13	41,41,41,41	0
57	MG	2A	3431	1/1	0.92	0.27	49,49,49,49	0
57	MG	1a	1808	1/1	0.92	0.09	46,46,46,46	0
57	MG	2A	3110	1/1	0.92	0.22	61,61,61,61	0
57	MG	1A	3910	1/1	0.92	0.10	21,21,21,21	0
57	MG	2A	3113	1/1	0.92	0.10	45,45,45,45	0
57	MG	2q	201	1/1	0.92	0.10	65,65,65,65	0
57	MG	2a	1608	1/1	0.92	0.10	64,64,64,64	0
57	MG	2A	3114	1/1	0.92	0.10	66,66,66,66	0
57	MG	2A	3702	1/1	0.92	0.10	70,70,70,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3705	1/1	0.92	0.13	33,33,33,33	0
57	MG	1A	3513	1/1	0.92	0.10	52,52,52,52	0
57	MG	2A	3440	1/1	0.92	0.29	59,59,59,59	0
57	MG	1A	3303	1/1	0.92	0.26	33,33,33,33	0
57	MG	2A	3713	1/1	0.92	0.08	51,51,51,51	0
57	MG	2A	3121	1/1	0.92	0.07	57,57,57,57	0
57	MG	2x	102	1/1	0.92	0.17	75,75,75,75	0
57	MG	1A	3815	1/1	0.92	0.13	21,21,21,21	0
57	MG	1A	3412	1/1	0.92	0.12	55,55,55,55	0
57	MG	2A	3284	1/1	0.92	0.17	61,61,61,61	0
57	MG	1A	3526	1/1	0.92	0.20	47,47,47,47	0
59	ZN	24	501	1/1	0.92	0.15	138,138,138,138	0
57	MG	2A	3140	1/1	0.93	0.34	73,73,73,73	0
57	MG	21	101	1/1	0.93	0.19	63,63,63,63	0
57	MG	2A	3623	1/1	0.93	0.16	34,34,34,34	0
57	MG	2A	3624	1/1	0.93	0.15	57,57,57,57	0
57	MG	25	101	1/1	0.93	0.16	56,56,56,56	0
57	MG	2A	3141	1/1	0.93	0.15	58,58,58,58	0
57	MG	1O	204	1/1	0.93	0.09	56,56,56,56	0
57	MG	25	105	1/1	0.93	0.11	58,58,58,58	0
57	MG	1a	1755	1/1	0.93	0.11	56,56,56,56	0
57	MG	2A	3635	1/1	0.93	0.12	64,64,64,64	0
57	MG	1A	3976	1/1	0.93	0.12	60,60,60,60	0
57	MG	1A	3798	1/1	0.93	0.08	43,43,43,43	0
57	MG	1A	3380	1/1	0.93	0.17	51,51,51,51	0
57	MG	1A	3312	1/1	0.93	0.21	53,53,53,53	0
57	MG	2A	3643	1/1	0.93	0.11	39,39,39,39	0
57	MG	2A	3646	1/1	0.93	0.26	64,64,64,64	0
57	MG	2A	3647	1/1	0.93	0.23	62,62,62,62	0
57	MG	1A	3983	1/1	0.93	0.13	59,59,59,59	0
57	MG	1A	3471	1/1	0.93	0.11	31,31,31,31	0
57	MG	2A	3650	1/1	0.93	0.10	43,43,43,43	0
57	MG	1A	3081	1/1	0.93	0.12	36,36,36,36	0
57	MG	1a	1772	1/1	0.93	0.09	54,54,54,54	0
57	MG	1T	202	1/1	0.93	0.14	59,59,59,59	0
57	MG	1A	3095	1/1	0.93	0.14	39,39,39,39	0
57	MG	2a	1612	1/1	0.93	0.14	58,58,58,58	0
57	MG	1U	204	1/1	0.93	0.12	26,26,26,26	0
57	MG	1a	1780	1/1	0.93	0.08	56,56,56,56	0
57	MG	1U	208	1/1	0.93	0.21	39,39,39,39	0
57	MG	1A	3098	1/1	0.93	0.08	41,41,41,41	0
57	MG	1W	202	1/1	0.93	0.23	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
57	MG	1A	3388	1/1	0.93	0.15	58,58,58,58	0
57	MG	1A	3993	1/1	0.93	0.13	39,39,39,39	0
57	MG	2A	3172	1/1	0.93	0.12	63,63,63,63	0
57	MG	1A	3817	1/1	0.93	0.05	38,38,38,38	0
57	MG	1A	3482	1/1	0.93	0.13	61,61,61,61	0
57	MG	1A	3389	1/1	0.93	0.11	55,55,55,55	0
57	MG	2A	3367	1/1	0.93	0.09	52,52,52,52	0
57	MG	2A	3369	1/1	0.93	0.24	49,49,49,49	0
57	MG	1A	3391	1/1	0.93	0.19	43,43,43,43	0
57	MG	2a	1631	1/1	0.93	0.18	59,59,59,59	0
57	MG	1A	3099	1/1	0.93	0.21	65,65,65,65	0
57	MG	2A	3183	1/1	0.93	0.22	55,55,55,55	0
57	MG	2A	3682	1/1	0.93	0.13	61,61,61,61	0
57	MG	1A	3182	1/1	0.93	0.17	38,38,38,38	0
57	MG	1A	3635	1/1	0.93	0.14	10,10,10,10	0
57	MG	2A	3377	1/1	0.93	0.14	61,61,61,61	0
57	MG	1A	3638	1/1	0.93	0.08	56,56,56,56	0
57	MG	1A	3321	1/1	0.93	0.17	52,52,52,52	0
57	MG	18	105	1/1	0.93	0.13	41,41,41,41	0
57	MG	1A	3642	1/1	0.93	0.13	42,42,42,42	0
57	MG	2A	3693	1/1	0.93	0.08	77,77,77,77	0
57	MG	1A	4017	1/1	0.93	0.08	44,44,44,44	0
57	MG	1A	3404	1/1	0.93	0.29	37,37,37,37	0
57	MG	2A	3696	1/1	0.93	0.07	58,58,58,58	0
57	MG	1a	1606	1/1	0.93	0.14	57,57,57,57	0
57	MG	2A	3699	1/1	0.93	0.10	64,64,64,64	0
57	MG	1A	3840	1/1	0.93	0.10	27,27,27,27	0
57	MG	1A	3407	1/1	0.93	0.14	43,43,43,43	0
57	MG	1A	3501	1/1	0.93	0.09	51,51,51,51	0
57	MG	2A	3706	1/1	0.93	0.09	37,37,37,37	0
57	MG	1A	3409	1/1	0.93	0.12	55,55,55,55	0
57	MG	2A	3709	1/1	0.93	0.12	60,60,60,60	0
57	MG	1A	3184	1/1	0.93	0.14	66,66,66,66	0
57	MG	1A	3045	1/1	0.93	0.10	34,34,34,34	0
57	MG	2A	3396	1/1	0.93	0.13	57,57,57,57	0
57	MG	1A	3852	1/1	0.93	0.12	47,47,47,47	0
57	MG	2A	3402	1/1	0.93	0.24	62,62,62,62	0
57	MG	1e	202	1/1	0.93	0.20	52,52,52,52	0
57	MG	1A	3413	1/1	0.93	0.12	35,35,35,35	0
57	MG	2a	1666	1/1	0.93	0.15	62,62,62,62	0
57	MG	1a	1623	1/1	0.93	0.16	70,70,70,70	0
57	MG	2A	3722	1/1	0.93	0.08	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
57	MG	1A	3115	1/1	0.93	0.22	39,39,39,39	0
57	MG	1m	3002	1/1	0.93	0.17	56,56,56,56	0
57	MG	1A	3047	1/1	0.93	0.09	32,32,32,32	0
57	MG	2A	3726	1/1	0.93	0.17	74,74,74,74	0
57	MG	1A	3667	1/1	0.93	0.09	44,44,44,44	0
57	MG	2a	1677	1/1	0.93	0.09	66,66,66,66	0
57	MG	1A	3062	1/1	0.93	0.18	51,51,51,51	0
57	MG	1A	3675	1/1	0.93	0.17	55,55,55,55	0
57	MG	1a	1630	1/1	0.93	0.34	68,68,68,68	0
57	MG	1a	1631	1/1	0.93	0.19	70,70,70,70	0
57	MG	2A	3215	1/1	0.93	0.23	66,66,66,66	0
57	MG	2a	1684	1/1	0.93	0.20	55,55,55,55	0
57	MG	1A	3521	1/1	0.93	0.32	35,35,35,35	0
57	MG	2A	3217	1/1	0.93	0.16	60,60,60,60	0
57	MG	1A	4050	1/1	0.93	0.09	46,46,46,46	0
57	MG	2A	3425	1/1	0.93	0.39	63,63,63,63	0
57	MG	2A	3219	1/1	0.93	0.13	62,62,62,62	0
57	MG	1A	3865	1/1	0.93	0.10	54,54,54,54	0
57	MG	1A	3679	1/1	0.93	0.07	20,20,20,20	0
57	MG	2A	3429	1/1	0.93	0.14	49,49,49,49	0
57	MG	2A	3744	1/1	0.93	0.10	59,59,59,59	0
57	MG	1A	3680	1/1	0.93	0.07	16,16,16,16	0
57	MG	1A	3332	1/1	0.93	0.13	51,51,51,51	0
57	MG	1A	4056	1/1	0.93	0.08	42,42,42,42	0
57	MG	1A	3020	1/1	0.93	0.09	34,34,34,34	0
57	MG	2A	3434	1/1	0.93	0.28	53,53,53,53	0
57	MG	2a	1704	1/1	0.93	0.10	71,71,71,71	0
57	MG	1A	3143	1/1	0.93	0.11	58,58,58,58	0
57	MG	1A	3144	1/1	0.93	0.09	42,42,42,42	0
57	MG	1a	1644	1/1	0.93	0.13	69,69,69,69	0
57	MG	2A	3234	1/1	0.93	0.25	49,49,49,49	0
57	MG	1A	3532	1/1	0.93	0.09	60,60,60,60	0
57	MG	1A	3533	1/1	0.93	0.11	53,53,53,53	0
57	MG	2A	3445	1/1	0.93	0.26	66,66,66,66	0
57	MG	1A	3214	1/1	0.93	0.16	49,49,49,49	0
57	MG	2A	3449	1/1	0.93	0.12	62,62,62,62	0
57	MG	1a	1648	1/1	0.93	0.10	52,52,52,52	0
57	MG	1A	3423	1/1	0.93	0.09	57,57,57,57	0
57	MG	2A	3242	1/1	0.93	0.37	62,62,62,62	0
57	MG	1A	3884	1/1	0.93	0.18	41,41,41,41	0
57	MG	2A	3767	1/1	0.93	0.16	67,67,67,67	0
57	MG	2A	3003	1/1	0.93	0.19	45,45,45,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3288	1/1	0.93	0.13	50,50,50,50	0
57	MG	2A	3467	1/1	0.93	0.14	54,54,54,54	0
57	MG	2A	3010	1/1	0.93	0.09	58,58,58,58	0
57	MG	2A	3476	1/1	0.93	0.19	70,70,70,70	0
57	MG	2A	3247	1/1	0.93	0.06	80,80,80,80	0
57	MG	2A	3248	1/1	0.93	0.14	61,61,61,61	0
57	MG	1A	3289	1/1	0.93	0.20	49,49,49,49	0
57	MG	2A	3484	1/1	0.93	0.28	67,67,67,67	0
57	MG	2A	3250	1/1	0.93	0.11	50,50,50,50	0
57	MG	2A	3018	1/1	0.93	0.16	58,58,58,58	0
57	MG	1A	3889	1/1	0.93	0.13	35,35,35,35	0
57	MG	1A	3712	1/1	0.93	0.11	26,26,26,26	0
57	MG	2A	3798	1/1	0.93	0.07	58,58,58,58	0
57	MG	1a	1663	1/1	0.93	0.07	66,66,66,66	0
57	MG	1A	3429	1/1	0.93	0.09	44,44,44,44	0
57	MG	2A	3257	1/1	0.93	0.14	54,54,54,54	0
57	MG	1A	3715	1/1	0.93	0.10	28,28,28,28	0
57	MG	2A	3261	1/1	0.93	0.08	72,72,72,72	0
57	MG	1A	3222	1/1	0.93	0.07	42,42,42,42	0
57	MG	1A	4086	1/1	0.93	0.23	63,63,63,63	0
57	MG	1A	3720	1/1	0.93	0.05	20,20,20,20	0
57	MG	1A	3548	1/1	0.93	0.08	25,25,25,25	0
57	MG	2A	3816	1/1	0.93	0.13	34,34,34,34	0
57	MG	2a	1756	1/1	0.93	0.06	82,82,82,82	0
57	MG	1A	3348	1/1	0.93	0.16	45,45,45,45	0
57	MG	1A	4092	1/1	0.93	0.08	47,47,47,47	0
57	MG	1A	3726	1/1	0.93	0.12	43,43,43,43	0
57	MG	1A	4094	1/1	0.93	0.12	49,49,49,49	0
57	MG	1A	4096	1/1	0.93	0.12	61,61,61,61	0
57	MG	1a	1679	1/1	0.93	0.21	67,67,67,67	0
57	MG	1A	3148	1/1	0.93	0.40	37,37,37,37	0
57	MG	1A	3152	1/1	0.93	0.19	39,39,39,39	0
57	MG	1A	3228	1/1	0.93	0.10	47,47,47,47	0
57	MG	1A	3914	1/1	0.93	0.10	45,45,45,45	0
57	MG	1A	3233	1/1	0.93	0.15	60,60,60,60	0
57	MG	2A	3840	1/1	0.93	0.12	60,60,60,60	0
57	MG	1A	3917	1/1	0.93	0.18	53,53,53,53	0
57	MG	2A	3844	1/1	0.93	0.10	53,53,53,53	0
57	MG	2A	3060	1/1	0.93	0.21	58,58,58,58	0
57	MG	1A	3557	1/1	0.93	0.07	57,57,57,57	0
57	MG	1A	3439	1/1	0.93	0.07	47,47,47,47	0
57	MG	1A	3924	1/1	0.93	0.09	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
57	MG	1A	3050	1/1	0.93	0.14	27,27,27,27	0
57	MG	1A	3927	1/1	0.93	0.17	39,39,39,39	0
57	MG	1A	3298	1/1	0.93	0.11	58,58,58,58	0
57	MG	2A	3860	1/1	0.93	0.18	57,57,57,57	0
57	MG	2A	3541	1/1	0.93	0.06	45,45,45,45	0
57	MG	1A	3239	1/1	0.93	0.10	43,43,43,43	0
57	MG	1A	3750	1/1	0.93	0.10	59,59,59,59	0
57	MG	2A	3079	1/1	0.93	0.14	59,59,59,59	0
57	MG	1A	3571	1/1	0.93	0.09	51,51,51,51	0
57	MG	1A	3091	1/1	0.93	0.20	55,55,55,55	0
57	MG	2a	1800	1/1	0.93	0.24	77,77,77,77	0
57	MG	1A	3446	1/1	0.93	0.09	54,54,54,54	0
57	MG	1A	3244	1/1	0.93	0.12	48,48,48,48	0
57	MG	1A	3759	1/1	0.93	0.10	19,19,19,19	0
57	MG	1A	3448	1/1	0.93	0.10	37,37,37,37	0
57	MG	1A	3585	1/1	0.93	0.22	56,56,56,56	0
57	MG	2A	3303	1/1	0.93	0.11	53,53,53,53	0
57	MG	2A	3093	1/1	0.93	0.09	40,40,40,40	0
57	MG	1B	233	1/1	0.93	0.12	58,58,58,58	0
57	MG	2a	1811	1/1	0.93	0.10	64,64,64,64	0
57	MG	1A	3304	1/1	0.93	0.21	44,44,44,44	0
57	MG	2A	3308	1/1	0.93	0.10	68,68,68,68	0
57	MG	1B	235	1/1	0.93	0.07	44,44,44,44	0
57	MG	1A	3367	1/1	0.93	0.11	44,44,44,44	0
57	MG	2D	302	1/1	0.93	0.15	56,56,56,56	0
57	MG	1A	3245	1/1	0.93	0.09	46,46,46,46	0
57	MG	2D	306	1/1	0.93	0.16	54,54,54,54	0
57	MG	1A	3777	1/1	0.93	0.12	42,42,42,42	0
57	MG	2A	3313	1/1	0.93	0.09	46,46,46,46	0
57	MG	2a	1821	1/1	0.93	0.11	62,62,62,62	0
57	MG	1a	1718	1/1	0.93	0.12	54,54,54,54	0
57	MG	1A	3040	1/1	0.93	0.18	51,51,51,51	0
57	MG	1A	3371	1/1	0.93	0.11	53,53,53,53	0
57	MG	1A	3375	1/1	0.93	0.32	42,42,42,42	0
57	MG	2d	301	1/1	0.93	0.26	62,62,62,62	0
57	MG	2E	308	1/1	0.93	0.11	32,32,32,32	0
57	MG	2A	3596	1/1	0.93	0.21	66,66,66,66	0
57	MG	1a	1726	1/1	0.93	0.26	43,43,43,43	0
57	MG	1E	310	1/1	0.93	0.23	38,38,38,38	0
57	MG	2A	3320	1/1	0.93	0.14	56,56,56,56	0
57	MG	2F	306	1/1	0.93	0.26	51,51,51,51	0
57	MG	1A	3967	1/1	0.93	0.08	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
57	MG	2A	3116	1/1	0.93	0.14	45,45,45,45	0
57	MG	1A	3464	1/1	0.93	0.09	56,56,56,56	0
57	MG	1A	3970	1/1	0.93	0.14	54,54,54,54	0
57	MG	2t	201	1/1	0.93	0.14	48,48,48,48	0
57	MG	1A	3786	1/1	0.93	0.09	34,34,34,34	0
57	MG	2A	3122	1/1	0.93	0.07	67,67,67,67	0
57	MG	1A	3467	1/1	0.93	0.22	44,44,44,44	0
57	MG	1F	310	1/1	0.93	0.07	47,47,47,47	0
57	MG	2T	3502	1/1	0.93	0.28	59,59,59,59	0
57	MG	2A	3128	1/1	0.93	0.07	47,47,47,47	0
57	MG	1a	1741	1/1	0.93	0.22	58,58,58,58	0
57	MG	2A	3131	1/1	0.93	0.10	44,44,44,44	0
57	MG	1A	3973	1/1	0.93	0.08	55,55,55,55	0
57	MG	2W	202	1/1	0.93	0.18	48,48,48,48	0
57	MG	1A	3308	1/1	0.93	0.16	51,51,51,51	0
57	MG	1A	3607	1/1	0.93	0.24	51,51,51,51	0
58	K	2A	3450	1/1	0.93	0.10	65,65,65,65	0
57	MG	1O	202	1/1	0.93	0.18	51,51,51,51	0
57	MG	1W	207	1/1	0.94	0.13	27,27,27,27	0
57	MG	1X	105	1/1	0.94	0.10	48,48,48,48	0
57	MG	1a	1751	1/1	0.94	0.07	66,66,66,66	0
57	MG	1Y	201	1/1	0.94	0.12	52,52,52,52	0
57	MG	2A	3338	1/1	0.94	0.33	52,52,52,52	0
57	MG	2A	3340	1/1	0.94	0.14	53,53,53,53	0
57	MG	1Y	202	1/1	0.94	0.31	46,46,46,46	0
57	MG	1Z	302	1/1	0.94	0.18	51,51,51,51	0
57	MG	25	103	1/1	0.94	0.22	44,44,44,44	0
57	MG	1A	4034	1/1	0.94	0.08	44,44,44,44	0
57	MG	1A	3613	1/1	0.94	0.19	46,46,46,46	0
57	MG	2A	3638	1/1	0.94	0.10	43,43,43,43	0
57	MG	2A	3142	1/1	0.94	0.17	52,52,52,52	0
57	MG	2A	3641	1/1	0.94	0.07	51,51,51,51	0
57	MG	2A	3143	1/1	0.94	0.23	40,40,40,40	0
57	MG	1A	3885	1/1	0.94	0.06	35,35,35,35	0
57	MG	2A	3644	1/1	0.94	0.07	38,38,38,38	0
57	MG	2A	3645	1/1	0.94	0.16	63,63,63,63	0
57	MG	11	101	1/1	0.94	0.08	43,43,43,43	0
57	MG	1A	4044	1/1	0.94	0.10	49,49,49,49	0
57	MG	1A	3886	1/1	0.94	0.14	33,33,33,33	0
57	MG	1A	3615	1/1	0.94	0.15	60,60,60,60	0
57	MG	1A	3073	1/1	0.94	0.18	51,51,51,51	0
57	MG	1A	3272	1/1	0.94	0.12	39,39,39,39	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3652	1/1	0.94	0.12	63,63,63,63	0
57	MG	1A	3309	1/1	0.94	0.24	53,53,53,53	0
57	MG	2A	3158	1/1	0.94	0.22	62,62,62,62	0
57	MG	1A	3386	1/1	0.94	0.22	42,42,42,42	0
57	MG	1A	3757	1/1	0.94	0.07	55,55,55,55	0
57	MG	18	101	1/1	0.94	0.25	52,52,52,52	0
57	MG	18	104	1/1	0.94	0.11	49,49,49,49	0
57	MG	2a	1616	1/1	0.94	0.07	71,71,71,71	0
57	MG	2A	3164	1/1	0.94	0.14	55,55,55,55	0
57	MG	1A	3896	1/1	0.94	0.11	35,35,35,35	0
57	MG	18	106	1/1	0.94	0.07	47,47,47,47	0
57	MG	2A	3667	1/1	0.94	0.11	49,49,49,49	0
57	MG	1A	3537	1/1	0.94	0.24	30,30,30,30	0
57	MG	2a	1622	1/1	0.94	0.10	58,58,58,58	0
57	MG	2a	1623	1/1	0.94	0.09	65,65,65,65	0
57	MG	1A	3761	1/1	0.94	0.07	33,33,33,33	0
57	MG	1A	3762	1/1	0.94	0.05	14,14,14,14	0
57	MG	1A	3764	1/1	0.94	0.08	57,57,57,57	0
57	MG	1A	3538	1/1	0.94	0.24	47,47,47,47	0
57	MG	1a	1796	1/1	0.94	0.09	66,66,66,66	0
57	MG	1A	3427	1/1	0.94	0.14	55,55,55,55	0
57	MG	2a	1630	1/1	0.94	0.13	54,54,54,54	0
57	MG	1a	1803	1/1	0.94	0.08	66,66,66,66	0
57	MG	1a	1805	1/1	0.94	0.08	54,54,54,54	0
57	MG	2A	3375	1/1	0.94	0.18	70,70,70,70	0
57	MG	2A	3681	1/1	0.94	0.18	67,67,67,67	0
57	MG	1A	3768	1/1	0.94	0.09	53,53,53,53	0
57	MG	2A	3181	1/1	0.94	0.18	59,59,59,59	0
57	MG	1A	3912	1/1	0.94	0.06	37,37,37,37	0
57	MG	1A	3428	1/1	0.94	0.14	57,57,57,57	0
57	MG	1a	1810	1/1	0.94	0.10	67,67,67,67	0
57	MG	1A	3078	1/1	0.94	0.10	25,25,25,25	0
57	MG	1a	1616	1/1	0.94	0.13	58,58,58,58	0
57	MG	1a	1617	1/1	0.94	0.09	62,62,62,62	0
57	MG	2A	3386	1/1	0.94	0.11	61,61,61,61	0
57	MG	1A	3915	1/1	0.94	0.07	32,32,32,32	0
57	MG	1A	3632	1/1	0.94	0.09	48,48,48,48	0
57	MG	1A	3544	1/1	0.94	0.23	47,47,47,47	0
57	MG	2A	3191	1/1	0.94	0.29	63,63,63,63	0
57	MG	1a	1818	1/1	0.94	0.18	53,53,53,53	0
57	MG	2A	3392	1/1	0.94	0.16	53,53,53,53	0
57	MG	1a	1819	1/1	0.94	0.16	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
57	MG	1A	3918	1/1	0.94	0.13	43,43,43,43	0
57	MG	2a	1652	1/1	0.94	0.09	62,62,62,62	0
57	MG	1A	4075	1/1	0.94	0.08	22,22,22,22	0
57	MG	2A	3707	1/1	0.94	0.19	64,64,64,64	0
57	MG	2A	3400	1/1	0.94	0.17	38,38,38,38	0
57	MG	1A	3545	1/1	0.94	0.19	44,44,44,44	0
57	MG	1a	1823	1/1	0.94	0.15	62,62,62,62	0
57	MG	1A	3313	1/1	0.94	0.24	49,49,49,49	0
57	MG	1A	3479	1/1	0.94	0.11	47,47,47,47	0
57	MG	2A	3714	1/1	0.94	0.11	41,41,41,41	0
57	MG	1A	3549	1/1	0.94	0.23	44,44,44,44	0
57	MG	1A	4085	1/1	0.94	0.12	72,72,72,72	0
57	MG	1A	3648	1/1	0.94	0.06	35,35,35,35	0
57	MG	1A	3928	1/1	0.94	0.13	32,32,32,32	0
57	MG	1m	3001	1/1	0.94	0.10	58,58,58,58	0
57	MG	1a	1635	1/1	0.94	0.09	56,56,56,56	0
57	MG	1A	3787	1/1	0.94	0.08	28,28,28,28	0
57	MG	1A	3649	1/1	0.94	0.06	15,15,15,15	0
57	MG	1A	4091	1/1	0.94	0.09	51,51,51,51	0
57	MG	1A	3789	1/1	0.94	0.07	65,65,65,65	0
57	MG	1A	3216	1/1	0.94	0.16	58,58,58,58	0
57	MG	1A	3335	1/1	0.94	0.06	50,50,50,50	0
57	MG	2A	3424	1/1	0.94	0.21	55,55,55,55	0
57	MG	2A	3214	1/1	0.94	0.27	59,59,59,59	0
57	MG	1A	3654	1/1	0.94	0.08	48,48,48,48	0
57	MG	1A	3483	1/1	0.94	0.08	53,53,53,53	0
57	MG	1A	3553	1/1	0.94	0.08	53,53,53,53	0
57	MG	1A	3394	1/1	0.94	0.28	60,60,60,60	0
57	MG	1A	3947	1/1	0.94	0.05	51,51,51,51	0
57	MG	1A	3555	1/1	0.94	0.12	57,57,57,57	0
57	MG	1B	209	1/1	0.94	0.11	41,41,41,41	0
57	MG	1a	1649	1/1	0.94	0.10	49,49,49,49	0
57	MG	1a	1650	1/1	0.94	0.08	54,54,54,54	0
57	MG	1A	3810	1/1	0.94	0.06	44,44,44,44	0
57	MG	1A	3362	1/1	0.94	0.07	49,49,49,49	0
57	MG	1a	1653	1/1	0.94	0.08	53,53,53,53	0
57	MG	1A	3400	1/1	0.94	0.49	46,46,46,46	0
57	MG	2A	3232	1/1	0.94	0.12	57,57,57,57	0
57	MG	1a	1658	1/1	0.94	0.17	59,59,59,59	0
57	MG	2A	3749	1/1	0.94	0.19	67,67,67,67	0
57	MG	1A	3218	1/1	0.94	0.15	39,39,39,39	0
57	MG	1A	3493	1/1	0.94	0.15	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
57	MG	1A	3566	1/1	0.94	0.16	31,31,31,31	0
57	MG	1A	3965	1/1	0.94	0.09	52,52,52,52	0
57	MG	2a	1709	1/1	0.94	0.12	67,67,67,67	0
57	MG	2A	3454	1/1	0.94	0.05	48,48,48,48	0
57	MG	2A	3455	1/1	0.94	0.18	58,58,58,58	0
57	MG	2A	3005	1/1	0.94	0.24	62,62,62,62	0
57	MG	2A	3006	1/1	0.94	0.18	58,58,58,58	0
57	MG	1B	222	1/1	0.94	0.10	48,48,48,48	0
57	MG	2a	1715	1/1	0.94	0.18	59,59,59,59	0
57	MG	1A	3494	1/1	0.94	0.16	52,52,52,52	0
57	MG	1A	3402	1/1	0.94	0.20	55,55,55,55	0
57	MG	2A	3465	1/1	0.94	0.17	55,55,55,55	0
57	MG	1a	1667	1/1	0.94	0.14	68,68,68,68	0
57	MG	2A	3471	1/1	0.94	0.10	54,54,54,54	0
57	MG	1A	3569	1/1	0.94	0.35	54,54,54,54	0
57	MG	2A	3769	1/1	0.94	0.11	57,57,57,57	0
57	MG	2A	3473	1/1	0.94	0.12	62,62,62,62	0
57	MG	2A	3474	1/1	0.94	0.10	54,54,54,54	0
57	MG	2A	3777	1/1	0.94	0.07	37,37,37,37	0
57	MG	1A	3441	1/1	0.94	0.10	52,52,52,52	0
57	MG	1A	3301	1/1	0.94	0.23	51,51,51,51	0
57	MG	1A	3339	1/1	0.94	0.29	58,58,58,58	0
57	MG	2A	3482	1/1	0.94	0.14	61,61,61,61	0
57	MG	2a	1733	1/1	0.94	0.32	65,65,65,65	0
57	MG	2A	3032	1/1	0.94	0.08	44,44,44,44	0
57	MG	1a	1673	1/1	0.94	0.06	59,59,59,59	0
57	MG	2A	3485	1/1	0.94	0.37	73,73,73,73	0
57	MG	1A	3060	1/1	0.94	0.07	30,30,30,30	0
57	MG	2A	3253	1/1	0.94	0.09	58,58,58,58	0
57	MG	2A	3039	1/1	0.94	0.34	72,72,72,72	0
57	MG	2A	3040	1/1	0.94	0.09	54,54,54,54	0
57	MG	2A	3041	1/1	0.94	0.16	56,56,56,56	0
57	MG	1A	3508	1/1	0.94	0.10	50,50,50,50	0
57	MG	1A	3698	1/1	0.94	0.08	51,51,51,51	0
57	MG	2a	1746	1/1	0.94	0.09	62,62,62,62	0
57	MG	2A	3803	1/1	0.94	0.06	39,39,39,39	0
57	MG	2A	3259	1/1	0.94	0.09	54,54,54,54	0
57	MG	2A	3260	1/1	0.94	0.11	65,65,65,65	0
57	MG	1A	3100	1/1	0.94	0.08	38,38,38,38	0
57	MG	1A	3979	1/1	0.94	0.15	39,39,39,39	0
57	MG	2A	3810	1/1	0.94	0.08	54,54,54,54	0
57	MG	1A	3841	1/1	0.94	0.14	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
57	MG	1A	3842	1/1	0.94	0.10	40,40,40,40	0
57	MG	2a	1758	1/1	0.94	0.09	62,62,62,62	0
57	MG	2a	1759	1/1	0.94	0.09	69,69,69,69	0
57	MG	1A	3843	1/1	0.94	0.08	36,36,36,36	0
57	MG	1A	3586	1/1	0.94	0.12	51,51,51,51	0
57	MG	2A	3506	1/1	0.94	0.07	30,30,30,30	0
57	MG	1D	312	1/1	0.94	0.16	30,30,30,30	0
57	MG	1A	3587	1/1	0.94	0.12	41,41,41,41	0
57	MG	1A	3590	1/1	0.94	0.14	42,42,42,42	0
57	MG	1A	3369	1/1	0.94	0.11	52,52,52,52	0
57	MG	1A	3254	1/1	0.94	0.17	52,52,52,52	0
57	MG	2A	3517	1/1	0.94	0.12	59,59,59,59	0
57	MG	2A	3518	1/1	0.94	0.08	35,35,35,35	0
57	MG	2a	1776	1/1	0.94	0.17	50,50,50,50	0
57	MG	1A	3991	1/1	0.94	0.10	20,20,20,20	0
57	MG	2A	3837	1/1	0.94	0.14	37,37,37,37	0
57	MG	1A	3593	1/1	0.94	0.10	23,23,23,23	0
57	MG	1A	3512	1/1	0.94	0.09	40,40,40,40	0
57	MG	2a	1783	1/1	0.94	0.12	64,64,64,64	0
57	MG	1A	3717	1/1	0.94	0.13	27,27,27,27	0
57	MG	1a	1698	1/1	0.94	0.20	49,49,49,49	0
57	MG	1A	3718	1/1	0.94	0.08	54,54,54,54	0
57	MG	2A	3067	1/1	0.94	0.08	48,48,48,48	0
57	MG	1A	3323	1/1	0.94	0.12	36,36,36,36	0
57	MG	1a	1701	1/1	0.94	0.23	47,47,47,47	0
57	MG	1A	3600	1/1	0.94	0.34	52,52,52,52	0
57	MG	1a	1704	1/1	0.94	0.37	58,58,58,58	0
57	MG	1G	202	1/1	0.94	0.17	55,55,55,55	0
57	MG	1G	203	1/1	0.94	0.22	58,58,58,58	0
57	MG	1I	201	1/1	0.94	0.07	62,62,62,62	0
57	MG	1A	3345	1/1	0.94	0.09	56,56,56,56	0
57	MG	2a	1798	1/1	0.94	0.16	70,70,70,70	0
57	MG	2A	3550	1/1	0.94	0.09	38,38,38,38	0
57	MG	1A	4002	1/1	0.94	0.07	15,15,15,15	0
57	MG	2a	1801	1/1	0.94	0.13	61,61,61,61	0
57	MG	2A	3085	1/1	0.94	0.08	58,58,58,58	0
57	MG	1N	206	1/1	0.94	0.13	44,44,44,44	0
57	MG	2A	3557	1/1	0.94	0.07	31,31,31,31	0
57	MG	2A	3297	1/1	0.94	0.06	45,45,45,45	0
57	MG	2A	3088	1/1	0.94	0.09	52,52,52,52	0
57	MG	2A	3564	1/1	0.94	0.14	58,58,58,58	0
57	MG	1A	3602	1/1	0.94	0.18	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
57	MG	1A	3376	1/1	0.94	0.18	40,40,40,40	0
57	MG	2A	3091	1/1	0.94	0.08	40,40,40,40	0
57	MG	2A	3569	1/1	0.94	0.16	51,51,51,51	0
57	MG	2B	212	1/1	0.94	0.09	73,73,73,73	0
57	MG	1A	3520	1/1	0.94	0.29	31,31,31,31	0
57	MG	1A	3377	1/1	0.94	0.12	45,45,45,45	0
57	MG	1A	4011	1/1	0.94	0.07	19,19,19,19	0
57	MG	2A	3305	1/1	0.94	0.20	58,58,58,58	0
57	MG	2A	3095	1/1	0.94	0.13	55,55,55,55	0
57	MG	1R	202	1/1	0.94	0.09	48,48,48,48	0
57	MG	1A	3731	1/1	0.94	0.08	59,59,59,59	0
57	MG	1a	1720	1/1	0.94	0.18	65,65,65,65	0
57	MG	1A	3346	1/1	0.94	0.30	44,44,44,44	0
57	MG	2A	3100	1/1	0.94	0.07	33,33,33,33	0
57	MG	2E	302	1/1	0.94	0.14	65,65,65,65	0
57	MG	1S	202	1/1	0.94	0.10	55,55,55,55	0
57	MG	1A	3255	1/1	0.94	0.18	49,49,49,49	0
57	MG	1A	3876	1/1	0.94	0.11	38,38,38,38	0
57	MG	2A	3587	1/1	0.94	0.20	65,65,65,65	0
57	MG	2A	3107	1/1	0.94	0.17	61,61,61,61	0
57	MG	2A	3594	1/1	0.94	0.17	55,55,55,55	0
57	MG	2A	3595	1/1	0.94	0.08	34,34,34,34	0
57	MG	2A	3108	1/1	0.94	0.16	55,55,55,55	0
57	MG	1A	3878	1/1	0.94	0.09	42,42,42,42	0
57	MG	1a	1730	1/1	0.94	0.19	52,52,52,52	0
57	MG	1a	1731	1/1	0.94	0.11	49,49,49,49	0
57	MG	1A	3609	1/1	0.94	0.30	62,62,62,62	0
57	MG	2O	201	1/1	0.94	0.18	54,54,54,54	0
57	MG	1a	1733	1/1	0.94	0.28	61,61,61,61	0
57	MG	1A	3528	1/1	0.94	0.10	42,42,42,42	0
57	MG	1U	206	1/1	0.94	0.17	27,27,27,27	0
57	MG	1A	3741	1/1	0.94	0.14	64,64,64,64	0
57	MG	2A	3119	1/1	0.94	0.30	65,65,65,65	0
57	MG	2A	3326	1/1	0.94	0.15	56,56,56,56	0
57	MG	2A	3120	1/1	0.94	0.13	57,57,57,57	0
57	MG	1V	202	1/1	0.94	0.37	35,35,35,35	0
57	MG	1A	3349	1/1	0.94	0.09	55,55,55,55	0
57	MG	2V	202	1/1	0.94	0.23	45,45,45,45	0
57	MG	2A	3123	1/1	0.94	0.32	59,59,59,59	0
57	MG	1V	206	1/1	0.94	0.10	54,54,54,54	0
57	MG	1V	207	1/1	0.94	0.08	52,52,52,52	0
57	MG	1A	3466	1/1	0.94	0.19	65,65,65,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3656	1/1	0.95	0.12	55,55,55,55	0
57	MG	1A	3334	1/1	0.95	0.10	43,43,43,43	0
57	MG	1A	3241	1/1	0.95	0.05	32,32,32,32	0
57	MG	1A	3514	1/1	0.95	0.16	28,28,28,28	0
57	MG	1A	3723	1/1	0.95	0.09	28,28,28,28	0
57	MG	2A	3399	1/1	0.95	0.28	47,47,47,47	0
57	MG	1a	1675	1/1	0.95	0.10	65,65,65,65	0
57	MG	2A	3401	1/1	0.95	0.18	47,47,47,47	0
57	MG	1A	3515	1/1	0.95	0.06	49,49,49,49	0
57	MG	2A	3002	1/1	0.95	0.27	58,58,58,58	0
57	MG	1A	3186	1/1	0.95	0.11	45,45,45,45	0
57	MG	1F	311	1/1	0.95	0.05	40,40,40,40	0
57	MG	2A	3406	1/1	0.95	0.31	50,50,50,50	0
57	MG	1F	313	1/1	0.95	0.12	36,36,36,36	0
57	MG	1A	3337	1/1	0.95	0.17	53,53,53,53	0
57	MG	1A	3729	1/1	0.95	0.12	50,50,50,50	0
57	MG	2A	3410	1/1	0.95	0.10	48,48,48,48	0
57	MG	2A	3220	1/1	0.95	0.08	49,49,49,49	0
57	MG	2A	3011	1/1	0.95	0.12	50,50,50,50	0
57	MG	1A	3871	1/1	0.95	0.08	19,19,19,19	0
57	MG	2A	3017	1/1	0.95	0.19	51,51,51,51	0
57	MG	1A	3442	1/1	0.95	0.23	35,35,35,35	0
57	MG	2A	3019	1/1	0.95	0.06	38,38,38,38	0
57	MG	2A	3418	1/1	0.95	0.23	59,59,59,59	0
57	MG	1A	3134	1/1	0.95	0.07	37,37,37,37	0
57	MG	2A	3689	1/1	0.95	0.06	62,62,62,62	0
57	MG	1A	3135	1/1	0.95	0.10	44,44,44,44	0
57	MG	2A	3025	1/1	0.95	0.15	61,61,61,61	0
57	MG	2A	3028	1/1	0.95	0.12	51,51,51,51	0
57	MG	1a	1688	1/1	0.95	0.12	60,60,60,60	0
57	MG	1N	205	1/1	0.95	0.16	43,43,43,43	0
57	MG	1A	3877	1/1	0.95	0.05	38,38,38,38	0
57	MG	1A	3387	1/1	0.95	0.09	54,54,54,54	0
57	MG	2A	3237	1/1	0.95	0.13	52,52,52,52	0
57	MG	2A	3698	1/1	0.95	0.07	24,24,24,24	0
57	MG	1O	203	1/1	0.95	0.11	50,50,50,50	0
57	MG	1A	3340	1/1	0.95	0.32	57,57,57,57	0
57	MG	1A	4020	1/1	0.95	0.08	50,50,50,50	0
57	MG	2A	3703	1/1	0.95	0.08	46,46,46,46	0
57	MG	1A	3199	1/1	0.95	0.21	40,40,40,40	0
57	MG	1A	3016	1/1	0.95	0.18	58,58,58,58	0
57	MG	1A	3531	1/1	0.95	0.13	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
57	MG	1A	4026	1/1	0.95	0.05	45,45,45,45	0
57	MG	1A	3449	1/1	0.95	0.16	41,41,41,41	0
57	MG	2A	3046	1/1	0.95	0.09	56,56,56,56	0
57	MG	1A	3744	1/1	0.95	0.05	50,50,50,50	0
57	MG	1A	4030	1/1	0.95	0.07	45,45,45,45	0
57	MG	2A	3442	1/1	0.95	0.17	37,37,37,37	0
57	MG	1A	3203	1/1	0.95	0.10	30,30,30,30	0
57	MG	1A	3019	1/1	0.95	0.15	50,50,50,50	0
57	MG	1A	3455	1/1	0.95	0.20	30,30,30,30	0
57	MG	1a	1708	1/1	0.95	0.25	70,70,70,70	0
57	MG	1A	3624	1/1	0.95	0.09	24,24,24,24	0
57	MG	1U	205	1/1	0.95	0.24	35,35,35,35	0
57	MG	1A	4038	1/1	0.95	0.06	38,38,38,38	0
57	MG	1U	207	1/1	0.95	0.30	35,35,35,35	0
57	MG	2A	3458	1/1	0.95	0.18	46,46,46,46	0
57	MG	2A	3460	1/1	0.95	0.12	67,67,67,67	0
57	MG	1A	4041	1/1	0.95	0.10	68,68,68,68	0
57	MG	1A	3536	1/1	0.95	0.08	30,30,30,30	0
57	MG	2A	3061	1/1	0.95	0.09	45,45,45,45	0
57	MG	1A	3456	1/1	0.95	0.14	31,31,31,31	0
57	MG	2a	1659	1/1	0.95	0.08	71,71,71,71	0
57	MG	1A	3756	1/1	0.95	0.08	48,48,48,48	0
57	MG	2A	3468	1/1	0.95	0.33	52,52,52,52	0
57	MG	2A	3469	1/1	0.95	0.20	57,57,57,57	0
57	MG	2a	1665	1/1	0.95	0.17	61,61,61,61	0
57	MG	2A	3065	1/1	0.95	0.20	45,45,45,45	0
57	MG	2A	3735	1/1	0.95	0.07	59,59,59,59	0
57	MG	1A	3894	1/1	0.95	0.11	31,31,31,31	0
57	MG	1A	3252	1/1	0.95	0.05	59,59,59,59	0
57	MG	1W	203	1/1	0.95	0.19	62,62,62,62	0
57	MG	2A	3475	1/1	0.95	0.31	61,61,61,61	0
57	MG	2A	3741	1/1	0.95	0.09	59,59,59,59	0
57	MG	1A	3034	1/1	0.95	0.30	34,34,34,34	0
57	MG	2A	3477	1/1	0.95	0.10	41,41,41,41	0
57	MG	1a	1722	1/1	0.95	0.15	48,48,48,48	0
57	MG	1a	1723	1/1	0.95	0.33	61,61,61,61	0
57	MG	2A	3480	1/1	0.95	0.20	60,60,60,60	0
57	MG	2A	3076	1/1	0.95	0.06	40,40,40,40	0
57	MG	2A	3271	1/1	0.95	0.08	58,58,58,58	0
57	MG	1X	103	1/1	0.95	0.14	46,46,46,46	0
57	MG	2a	1685	1/1	0.95	0.29	64,64,64,64	0
57	MG	2A	3274	1/1	0.95	0.23	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
57	MG	1a	1725	1/1	0.95	0.09	49,49,49,49	0
57	MG	2A	3276	1/1	0.95	0.13	49,49,49,49	0
57	MG	1A	3634	1/1	0.95	0.05	32,32,32,32	0
57	MG	2a	1690	1/1	0.95	0.12	52,52,52,52	0
57	MG	1A	3347	1/1	0.95	0.16	43,43,43,43	0
57	MG	1A	3900	1/1	0.95	0.06	28,28,28,28	0
57	MG	2A	3492	1/1	0.95	0.30	56,56,56,56	0
57	MG	1A	3637	1/1	0.95	0.08	31,31,31,31	0
57	MG	10	101	1/1	0.95	0.08	38,38,38,38	0
57	MG	10	105	1/1	0.95	0.22	62,62,62,62	0
57	MG	2A	3498	1/1	0.95	0.17	63,63,63,63	0
57	MG	1A	3903	1/1	0.95	0.09	37,37,37,37	0
57	MG	10	107	1/1	0.95	0.16	56,56,56,56	0
57	MG	1A	3906	1/1	0.95	0.08	23,23,23,23	0
57	MG	1A	3461	1/1	0.95	0.18	45,45,45,45	0
57	MG	1A	3908	1/1	0.95	0.09	22,22,22,22	0
57	MG	1A	3035	1/1	0.95	0.07	44,44,44,44	0
57	MG	2A	3775	1/1	0.95	0.08	52,52,52,52	0
57	MG	2A	3290	1/1	0.95	0.10	56,56,56,56	0
57	MG	12	101	1/1	0.95	0.06	39,39,39,39	0
57	MG	2A	3292	1/1	0.95	0.10	57,57,57,57	0
57	MG	13	103	1/1	0.95	0.09	46,46,46,46	0
57	MG	1A	3102	1/1	0.95	0.10	31,31,31,31	0
57	MG	1a	1746	1/1	0.95	0.12	51,51,51,51	0
57	MG	1A	3465	1/1	0.95	0.10	43,43,43,43	0
57	MG	1A	3647	1/1	0.95	0.05	25,25,25,25	0
57	MG	15	105	1/1	0.95	0.13	31,31,31,31	0
57	MG	2a	1718	1/1	0.95	0.11	61,61,61,61	0
57	MG	1A	3406	1/1	0.95	0.27	34,34,34,34	0
57	MG	2A	3790	1/1	0.95	0.09	58,58,58,58	0
57	MG	2A	3104	1/1	0.95	0.23	52,52,52,52	0
57	MG	2A	3105	1/1	0.95	0.08	43,43,43,43	0
57	MG	1A	3212	1/1	0.95	0.19	43,43,43,43	0
57	MG	2A	3796	1/1	0.95	0.08	52,52,52,52	0
57	MG	2A	3797	1/1	0.95	0.07	62,62,62,62	0
57	MG	1A	3408	1/1	0.95	0.22	45,45,45,45	0
57	MG	2a	1727	1/1	0.95	0.28	69,69,69,69	0
57	MG	2a	1728	1/1	0.95	0.21	61,61,61,61	0
57	MG	17	103	1/1	0.95	0.14	29,29,29,29	0
57	MG	17	104	1/1	0.95	0.08	52,52,52,52	0
57	MG	2A	3801	1/1	0.95	0.07	55,55,55,55	0
57	MG	1A	4068	1/1	0.95	0.07	37,37,37,37	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3158	1/1	0.95	0.07	42,42,42,42	0
57	MG	1a	1765	1/1	0.95	0.08	63,63,63,63	0
57	MG	2A	3538	1/1	0.95	0.10	40,40,40,40	0
57	MG	1A	3410	1/1	0.95	0.14	48,48,48,48	0
57	MG	1a	1768	1/1	0.95	0.05	64,64,64,64	0
57	MG	2a	1738	1/1	0.95	0.10	55,55,55,55	0
57	MG	1A	3260	1/1	0.95	0.06	34,34,34,34	0
57	MG	2A	3542	1/1	0.95	0.06	53,53,53,53	0
57	MG	2A	3543	1/1	0.95	0.10	40,40,40,40	0
57	MG	2A	3544	1/1	0.95	0.14	51,51,51,51	0
57	MG	1a	1773	1/1	0.95	0.19	70,70,70,70	0
57	MG	1A	3108	1/1	0.95	0.18	37,37,37,37	0
57	MG	1a	1777	1/1	0.95	0.18	66,66,66,66	0
57	MG	1A	3921	1/1	0.95	0.16	53,53,53,53	0
57	MG	2A	3553	1/1	0.95	0.08	34,34,34,34	0
57	MG	1a	1602	1/1	0.95	0.14	69,69,69,69	0
57	MG	1A	3054	1/1	0.95	0.09	40,40,40,40	0
57	MG	1a	1604	1/1	0.95	0.10	55,55,55,55	0
57	MG	2A	3558	1/1	0.95	0.10	51,51,51,51	0
57	MG	2a	1753	1/1	0.95	0.10	50,50,50,50	0
57	MG	2A	3125	1/1	0.95	0.07	41,41,41,41	0
57	MG	2A	3126	1/1	0.95	0.08	43,43,43,43	0
57	MG	1A	3359	1/1	0.95	0.06	47,47,47,47	0
57	MG	1A	3219	1/1	0.95	0.06	44,44,44,44	0
57	MG	1a	1785	1/1	0.95	0.07	46,46,46,46	0
57	MG	2A	3843	1/1	0.95	0.07	37,37,37,37	0
57	MG	1A	4083	1/1	0.95	0.19	40,40,40,40	0
57	MG	2A	3846	1/1	0.95	0.07	55,55,55,55	0
57	MG	1A	3663	1/1	0.95	0.05	26,26,26,26	0
57	MG	2a	1766	1/1	0.95	0.05	62,62,62,62	0
57	MG	2a	1767	1/1	0.95	0.09	72,72,72,72	0
57	MG	2A	3570	1/1	0.95	0.05	40,40,40,40	0
57	MG	2A	3849	1/1	0.95	0.13	56,56,56,56	0
57	MG	1a	1611	1/1	0.95	0.05	21,21,21,21	0
57	MG	1A	3793	1/1	0.95	0.06	62,62,62,62	0
57	MG	2A	3138	1/1	0.95	0.11	39,39,39,39	0
57	MG	2A	3856	1/1	0.95	0.07	48,48,48,48	0
57	MG	1A	3665	1/1	0.95	0.07	26,26,26,26	0
57	MG	1A	3221	1/1	0.95	0.14	40,40,40,40	0
57	MG	2A	3859	1/1	0.95	0.10	59,59,59,59	0
57	MG	1A	3481	1/1	0.95	0.11	49,49,49,49	0
57	MG	1A	3672	1/1	0.95	0.09	31,31,31,31	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3807	1/1	0.95	0.07	16,16,16,16	0
57	MG	1a	1797	1/1	0.95	0.12	56,56,56,56	0
57	MG	1a	1798	1/1	0.95	0.06	42,42,42,42	0
57	MG	1A	3936	1/1	0.95	0.05	64,64,64,64	0
57	MG	1a	1800	1/1	0.95	0.14	53,53,53,53	0
57	MG	2A	3149	1/1	0.95	0.09	51,51,51,51	0
57	MG	2A	3339	1/1	0.95	0.28	59,59,59,59	0
57	MG	1A	3269	1/1	0.95	0.12	60,60,60,60	0
57	MG	2A	3592	1/1	0.95	0.12	64,64,64,64	0
57	MG	2A	3593	1/1	0.95	0.16	55,55,55,55	0
57	MG	1A	3004	1/1	0.95	0.05	20,20,20,20	0
57	MG	1A	3676	1/1	0.95	0.12	35,35,35,35	0
57	MG	1a	1807	1/1	0.95	0.16	52,52,52,52	0
57	MG	1A	3487	1/1	0.95	0.13	38,38,38,38	0
57	MG	1A	3224	1/1	0.95	0.25	34,34,34,34	0
57	MG	1A	3322	1/1	0.95	0.16	54,54,54,54	0
57	MG	1A	3574	1/1	0.95	0.17	45,45,45,45	0
57	MG	1A	3956	1/1	0.95	0.08	53,53,53,53	0
57	MG	1A	3042	1/1	0.95	0.15	29,29,29,29	0
57	MG	1A	3126	1/1	0.95	0.27	38,38,38,38	0
57	MG	1a	1815	1/1	0.95	0.10	59,59,59,59	0
57	MG	1A	3685	1/1	0.95	0.05	27,27,27,27	0
57	MG	2a	1808	1/1	0.95	0.16	51,51,51,51	0
57	MG	1A	3327	1/1	0.95	0.07	48,48,48,48	0
57	MG	1A	3689	1/1	0.95	0.06	42,42,42,42	0
57	MG	1B	216	1/1	0.95	0.08	59,59,59,59	0
57	MG	2A	3612	1/1	0.95	0.09	33,33,33,33	0
57	MG	1B	217	1/1	0.95	0.13	46,46,46,46	0
57	MG	1B	218	1/1	0.95	0.06	51,51,51,51	0
57	MG	1A	3690	1/1	0.95	0.05	18,18,18,18	0
57	MG	1A	3692	1/1	0.95	0.04	18,18,18,18	0
57	MG	2F	301	1/1	0.95	0.08	38,38,38,38	0
57	MG	1A	3695	1/1	0.95	0.05	18,18,18,18	0
57	MG	1A	3180	1/1	0.95	0.10	28,28,28,28	0
57	MG	1A	3969	1/1	0.95	0.07	43,43,43,43	0
57	MG	1A	3495	1/1	0.95	0.19	49,49,49,49	0
57	MG	1A	3835	1/1	0.95	0.26	26,26,26,26	0
57	MG	2A	3625	1/1	0.95	0.07	31,31,31,31	0
57	MG	1l	201	1/1	0.95	0.08	59,59,59,59	0
57	MG	2A	3628	1/1	0.95	0.08	35,35,35,35	0
57	MG	1A	3837	1/1	0.95	0.08	39,39,39,39	0
57	MG	2A	3630	1/1	0.95	0.17	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
57	MG	2A	3631	1/1	0.95	0.10	39,39,39,39	0
57	MG	2A	3633	1/1	0.95	0.09	44,44,44,44	0
57	MG	1A	3281	1/1	0.95	0.35	42,42,42,42	0
57	MG	2T	3501	1/1	0.95	0.35	66,66,66,66	0
57	MG	1A	3372	1/1	0.95	0.10	59,59,59,59	0
57	MG	2l	201	1/1	0.95	0.09	54,54,54,54	0
57	MG	1A	3374	1/1	0.95	0.26	45,45,45,45	0
57	MG	1A	3430	1/1	0.95	0.14	49,49,49,49	0
57	MG	1A	3708	1/1	0.95	0.09	19,19,19,19	0
57	MG	1A	3506	1/1	0.95	0.13	39,39,39,39	0
57	MG	1a	1654	1/1	0.95	0.13	48,48,48,48	0
57	MG	1A	3230	1/1	0.95	0.15	27,27,27,27	0
57	MG	1B	236	1/1	0.95	0.07	31,31,31,31	0
57	MG	1w	104	1/1	0.95	0.07	67,67,67,67	0
57	MG	1D	302	1/1	0.95	0.18	43,43,43,43	0
57	MG	1A	3713	1/1	0.95	0.07	48,48,48,48	0
57	MG	1A	3850	1/1	0.95	0.14	36,36,36,36	0
57	MG	1A	3128	1/1	0.95	0.19	56,56,56,56	0
57	MG	1A	3009	1/1	0.95	0.06	24,24,24,24	0
57	MG	1A	3716	1/1	0.95	0.10	36,36,36,36	0
57	MG	1A	3378	1/1	0.95	0.13	40,40,40,40	0
57	MG	1E	308	1/1	0.95	0.10	48,48,48,48	0
57	MG	2A	3653	1/1	0.95	0.10	65,65,65,65	0
58	K	1A	3570	1/1	0.95	0.09	57,57,57,57	0
57	MG	1A	3131	1/1	0.95	0.09	40,40,40,40	0
59	ZN	14	102	1/1	0.95	0.13	114,114,114,114	0
57	MG	1A	3856	1/1	0.95	0.08	33,33,33,33	0
57	MG	1a	1662	1/1	0.96	0.07	56,56,56,56	0
57	MG	2A	3129	1/1	0.96	0.18	45,45,45,45	0
57	MG	1A	3353	1/1	0.96	0.06	36,36,36,36	0
57	MG	1A	3403	1/1	0.96	0.22	55,55,55,55	0
57	MG	2A	3132	1/1	0.96	0.26	48,48,48,48	0
57	MG	1A	3160	1/1	0.96	0.12	25,25,25,25	0
57	MG	1A	3215	1/1	0.96	0.19	50,50,50,50	0
57	MG	2A	3490	1/1	0.96	0.25	47,47,47,47	0
57	MG	1A	3124	1/1	0.96	0.17	33,33,33,33	0
57	MG	1b	301	1/1	0.96	0.05	78,78,78,78	0
57	MG	1A	3594	1/1	0.96	0.07	31,31,31,31	0
57	MG	2A	3494	1/1	0.96	0.06	72,72,72,72	0
57	MG	1a	1669	1/1	0.96	0.07	61,61,61,61	0
57	MG	1A	3318	1/1	0.96	0.13	41,41,41,41	0
57	MG	1A	3006	1/1	0.96	0.19	65,65,65,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1P	203	1/1	0.96	0.22	28,28,28,28	0
57	MG	1A	3166	1/1	0.96	0.17	34,34,34,34	0
57	MG	1A	3799	1/1	0.96	0.09	58,58,58,58	0
57	MG	1A	3686	1/1	0.96	0.05	17,17,17,17	0
57	MG	1A	3523	1/1	0.96	0.14	49,49,49,49	0
57	MG	1A	3028	1/1	0.96	0.24	29,29,29,29	0
57	MG	1R	206	1/1	0.96	0.10	41,41,41,41	0
57	MG	1S	201	1/1	0.96	0.31	41,41,41,41	0
57	MG	1A	3462	1/1	0.96	0.17	44,44,44,44	0
57	MG	1A	3363	1/1	0.96	0.14	39,39,39,39	0
57	MG	2A	3511	1/1	0.96	0.10	56,56,56,56	0
57	MG	1A	3693	1/1	0.96	0.10	19,19,19,19	0
57	MG	1A	3811	1/1	0.96	0.06	46,46,46,46	0
57	MG	2A	3160	1/1	0.96	0.08	35,35,35,35	0
57	MG	2A	3516	1/1	0.96	0.08	44,44,44,44	0
57	MG	1U	202	1/1	0.96	0.24	40,40,40,40	0
57	MG	1A	4055	1/1	0.96	0.04	29,29,29,29	0
57	MG	2A	3519	1/1	0.96	0.08	54,54,54,54	0
57	MG	1A	3812	1/1	0.96	0.05	16,16,16,16	0
57	MG	2A	3522	1/1	0.96	0.08	37,37,37,37	0
57	MG	1w	107	1/1	0.96	0.09	64,64,64,64	0
57	MG	1A	3170	1/1	0.96	0.05	30,30,30,30	0
57	MG	1a	1690	1/1	0.96	0.16	62,62,62,62	0
57	MG	1A	3018	1/1	0.96	0.09	26,26,26,26	0
57	MG	2A	3528	1/1	0.96	0.12	37,37,37,37	0
57	MG	1A	3324	1/1	0.96	0.15	25,25,25,25	0
57	MG	1A	3105	1/1	0.96	0.05	29,29,29,29	0
57	MG	1A	3174	1/1	0.96	0.25	31,31,31,31	0
57	MG	1A	3930	1/1	0.96	0.03	28,28,28,28	0
57	MG	1A	3178	1/1	0.96	0.12	18,18,18,18	0
57	MG	1A	3821	1/1	0.96	0.07	21,21,21,21	0
57	MG	1A	4067	1/1	0.96	0.04	15,15,15,15	0
57	MG	1A	3132	1/1	0.96	0.06	34,34,34,34	0
57	MG	2A	3177	1/1	0.96	0.07	45,45,45,45	0
57	MG	1A	3282	1/1	0.96	0.15	31,31,31,31	0
57	MG	2A	3768	1/1	0.96	0.08	51,51,51,51	0
57	MG	2A	3179	1/1	0.96	0.09	52,52,52,52	0
57	MG	1X	101	1/1	0.96	0.25	32,32,32,32	0
57	MG	2A	3771	1/1	0.96	0.05	51,51,51,51	0
57	MG	2A	3773	1/1	0.96	0.11	51,51,51,51	0
57	MG	1A	4070	1/1	0.96	0.05	34,34,34,34	0
57	MG	2a	1676	1/1	0.96	0.09	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
57	MG	1A	3107	1/1	0.96	0.18	36,36,36,36	0
57	MG	2A	3346	1/1	0.96	0.07	58,58,58,58	0
57	MG	1A	3616	1/1	0.96	0.23	41,41,41,41	0
57	MG	1A	3830	1/1	0.96	0.06	57,57,57,57	0
57	MG	1Z	301	1/1	0.96	0.14	59,59,59,59	0
57	MG	2A	3007	1/1	0.96	0.15	48,48,48,48	0
57	MG	1A	4078	1/1	0.96	0.15	52,52,52,52	0
57	MG	1A	3475	1/1	0.96	0.10	47,47,47,47	0
57	MG	2A	3787	1/1	0.96	0.09	45,45,45,45	0
57	MG	2A	3559	1/1	0.96	0.09	37,37,37,37	0
57	MG	1A	3083	1/1	0.96	0.09	36,36,36,36	0
57	MG	2A	3014	1/1	0.96	0.10	44,44,44,44	0
57	MG	2A	3015	1/1	0.96	0.07	42,42,42,42	0
57	MG	1A	3540	1/1	0.96	0.20	42,42,42,42	0
57	MG	1A	3541	1/1	0.96	0.08	42,42,42,42	0
57	MG	2A	3794	1/1	0.96	0.07	61,61,61,61	0
57	MG	2A	3795	1/1	0.96	0.11	66,66,66,66	0
57	MG	2A	3567	1/1	0.96	0.12	67,67,67,67	0
57	MG	1a	1714	1/1	0.96	0.09	60,60,60,60	0
57	MG	1A	3290	1/1	0.96	0.11	36,36,36,36	0
57	MG	2A	3020	1/1	0.96	0.04	55,55,55,55	0
57	MG	2A	3571	1/1	0.96	0.12	31,31,31,31	0
57	MG	2A	3021	1/1	0.96	0.07	24,24,24,24	0
57	MG	2A	3802	1/1	0.96	0.11	52,52,52,52	0
57	MG	2A	3022	1/1	0.96	0.19	45,45,45,45	0
57	MG	1A	3836	1/1	0.96	0.06	41,41,41,41	0
57	MG	1A	3953	1/1	0.96	0.06	29,29,29,29	0
57	MG	2A	3202	1/1	0.96	0.17	53,53,53,53	0
57	MG	2A	3808	1/1	0.96	0.12	42,42,42,42	0
57	MG	1A	3235	1/1	0.96	0.19	47,47,47,47	0
57	MG	2A	3368	1/1	0.96	0.05	56,56,56,56	0
57	MG	2A	3026	1/1	0.96	0.09	48,48,48,48	0
57	MG	2A	3205	1/1	0.96	0.17	67,67,67,67	0
57	MG	2A	3813	1/1	0.96	0.05	47,47,47,47	0
57	MG	1A	4088	1/1	0.96	0.17	51,51,51,51	0
57	MG	2A	3815	1/1	0.96	0.10	39,39,39,39	0
57	MG	1A	3838	1/1	0.96	0.06	24,24,24,24	0
57	MG	2A	3817	1/1	0.96	0.06	57,57,57,57	0
57	MG	2A	3821	1/1	0.96	0.14	61,61,61,61	0
57	MG	1A	3426	1/1	0.96	0.27	56,56,56,56	0
57	MG	1A	3625	1/1	0.96	0.09	47,47,47,47	0
57	MG	1A	3237	1/1	0.96	0.21	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
57	MG	2A	3376	1/1	0.96	0.18	61,61,61,61	0
57	MG	15	104	1/1	0.96	0.15	33,33,33,33	0
57	MG	1A	3183	1/1	0.96	0.05	52,52,52,52	0
57	MG	1A	3629	1/1	0.96	0.07	46,46,46,46	0
57	MG	1A	3846	1/1	0.96	0.18	41,41,41,41	0
57	MG	16	102	1/1	0.96	0.09	59,59,59,59	0
57	MG	1a	1729	1/1	0.96	0.18	51,51,51,51	0
57	MG	2A	3383	1/1	0.96	0.08	57,57,57,57	0
57	MG	1A	3547	1/1	0.96	0.25	49,49,49,49	0
57	MG	1B	201	1/1	0.96	0.10	53,53,53,53	0
57	MG	2A	3841	1/1	0.96	0.07	38,38,38,38	0
57	MG	1A	3631	1/1	0.96	0.07	38,38,38,38	0
57	MG	2A	3603	1/1	0.96	0.08	35,35,35,35	0
57	MG	1A	3728	1/1	0.96	0.09	55,55,55,55	0
57	MG	1B	205	1/1	0.96	0.08	39,39,39,39	0
57	MG	2A	3222	1/1	0.96	0.12	41,41,41,41	0
57	MG	1a	1737	1/1	0.96	0.17	61,61,61,61	0
57	MG	1B	206	1/1	0.96	0.12	44,44,44,44	0
57	MG	2A	3850	1/1	0.96	0.05	57,57,57,57	0
57	MG	2A	3225	1/1	0.96	0.15	42,42,42,42	0
57	MG	2A	3610	1/1	0.96	0.11	41,41,41,41	0
57	MG	2A	3853	1/1	0.96	0.12	63,63,63,63	0
57	MG	1A	3138	1/1	0.96	0.09	42,42,42,42	0
57	MG	2A	3394	1/1	0.96	0.17	64,64,64,64	0
57	MG	2A	3395	1/1	0.96	0.22	70,70,70,70	0
57	MG	1A	3633	1/1	0.96	0.06	19,19,19,19	0
57	MG	19	101	1/1	0.96	0.19	49,49,49,49	0
57	MG	1A	3486	1/1	0.96	0.13	52,52,52,52	0
57	MG	2A	3617	1/1	0.96	0.08	37,37,37,37	0
57	MG	2a	1755	1/1	0.96	0.09	57,57,57,57	0
57	MG	2A	3618	1/1	0.96	0.07	32,32,32,32	0
57	MG	1a	1743	1/1	0.96	0.23	56,56,56,56	0
57	MG	1A	3139	1/1	0.96	0.08	41,41,41,41	0
57	MG	1A	3142	1/1	0.96	0.10	51,51,51,51	0
57	MG	2a	1760	1/1	0.96	0.12	48,48,48,48	0
57	MG	1A	3735	1/1	0.96	0.08	35,35,35,35	0
57	MG	1A	3195	1/1	0.96	0.20	26,26,26,26	0
57	MG	1A	3977	1/1	0.96	0.12	45,45,45,45	0
57	MG	1A	3978	1/1	0.96	0.07	25,25,25,25	0
57	MG	2A	3064	1/1	0.96	0.18	60,60,60,60	0
57	MG	1a	1608	1/1	0.96	0.16	52,52,52,52	0
57	MG	1A	3857	1/1	0.96	0.21	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
57	MG	1A	3110	1/1	0.96	0.06	39,39,39,39	0
57	MG	2A	3069	1/1	0.96	0.14	57,57,57,57	0
57	MG	2a	1770	1/1	0.96	0.06	74,74,74,74	0
57	MG	2A	3412	1/1	0.96	0.30	49,49,49,49	0
57	MG	1A	3491	1/1	0.96	0.10	36,36,36,36	0
57	MG	2a	1773	1/1	0.96	0.09	61,61,61,61	0
57	MG	2a	1774	1/1	0.96	0.13	59,59,59,59	0
57	MG	1A	3862	1/1	0.96	0.08	49,49,49,49	0
57	MG	1A	3111	1/1	0.96	0.10	35,35,35,35	0
57	MG	1A	3436	1/1	0.96	0.16	46,46,46,46	0
57	MG	1A	3112	1/1	0.96	0.12	27,27,27,27	0
57	MG	2A	3077	1/1	0.96	0.10	25,25,25,25	0
57	MG	2D	305	1/1	0.96	0.33	44,44,44,44	0
57	MG	2a	1782	1/1	0.96	0.07	50,50,50,50	0
57	MG	2A	3419	1/1	0.96	0.26	57,57,57,57	0
57	MG	2a	1784	1/1	0.96	0.07	68,68,68,68	0
57	MG	1a	1766	1/1	0.96	0.06	52,52,52,52	0
57	MG	1A	3149	1/1	0.96	0.28	29,29,29,29	0
57	MG	2A	3422	1/1	0.96	0.18	51,51,51,51	0
57	MG	2A	3080	1/1	0.96	0.09	52,52,52,52	0
57	MG	1a	1618	1/1	0.96	0.06	43,43,43,43	0
57	MG	2A	3082	1/1	0.96	0.16	45,45,45,45	0
57	MG	1a	1771	1/1	0.96	0.09	53,53,53,53	0
57	MG	1A	3650	1/1	0.96	0.05	28,28,28,28	0
57	MG	1A	3150	1/1	0.96	0.27	40,40,40,40	0
57	MG	1A	3752	1/1	0.96	0.06	45,45,45,45	0
57	MG	2a	1795	1/1	0.96	0.14	62,62,62,62	0
57	MG	1A	3873	1/1	0.96	0.06	44,44,44,44	0
57	MG	1A	3498	1/1	0.96	0.06	43,43,43,43	0
57	MG	1A	3995	1/1	0.96	0.08	28,28,28,28	0
57	MG	1A	3653	1/1	0.96	0.08	24,24,24,24	0
57	MG	1A	3253	1/1	0.96	0.08	45,45,45,45	0
57	MG	2A	3658	1/1	0.96	0.06	27,27,27,27	0
57	MG	1A	3056	1/1	0.96	0.15	37,37,37,37	0
57	MG	1A	3208	1/1	0.96	0.12	32,32,32,32	0
57	MG	2A	3437	1/1	0.96	0.34	60,60,60,60	0
57	MG	1a	1784	1/1	0.96	0.06	54,54,54,54	0
57	MG	2A	3664	1/1	0.96	0.08	60,60,60,60	0
57	MG	1A	3502	1/1	0.96	0.16	38,38,38,38	0
57	MG	1A	3760	1/1	0.96	0.10	27,27,27,27	0
57	MG	2T	3500	1/1	0.96	0.07	58,58,58,58	0
57	MG	1A	3503	1/1	0.96	0.14	34,34,34,34	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3668	1/1	0.96	0.22	41,41,41,41	0
57	MG	1A	3575	1/1	0.96	0.27	31,31,31,31	0
57	MG	2A	3443	1/1	0.96	0.07	53,53,53,53	0
57	MG	2V	201	1/1	0.96	0.08	66,66,66,66	0
57	MG	2A	3444	1/1	0.96	0.19	44,44,44,44	0
57	MG	1A	3763	1/1	0.96	0.14	54,54,54,54	0
57	MG	1A	3661	1/1	0.96	0.13	22,22,22,22	0
57	MG	2A	3447	1/1	0.96	0.08	48,48,48,48	0
57	MG	2A	3273	1/1	0.96	0.14	56,56,56,56	0
57	MG	2Y	201	1/1	0.96	0.19	61,61,61,61	0
57	MG	1E	302	1/1	0.96	0.21	45,45,45,45	0
57	MG	2A	3103	1/1	0.96	0.13	44,44,44,44	0
57	MG	1A	3662	1/1	0.96	0.07	31,31,31,31	0
57	MG	2a	1824	1/1	0.96	0.17	61,61,61,61	0
57	MG	1A	4016	1/1	0.96	0.05	41,41,41,41	0
57	MG	1A	3766	1/1	0.96	0.05	36,36,36,36	0
57	MG	23	101	1/1	0.96	0.14	64,64,64,64	0
57	MG	1A	3155	1/1	0.96	0.10	31,31,31,31	0
57	MG	23	103	1/1	0.96	0.06	57,57,57,57	0
57	MG	2f	201	1/1	0.96	0.08	45,45,45,45	0
57	MG	2A	3459	1/1	0.96	0.08	47,47,47,47	0
57	MG	2A	3280	1/1	0.96	0.08	65,65,65,65	0
57	MG	1A	3397	1/1	0.96	0.25	31,31,31,31	0
57	MG	2A	3687	1/1	0.96	0.08	34,34,34,34	0
57	MG	2k	201	1/1	0.96	0.10	67,67,67,67	0
57	MG	1E	312	1/1	0.96	0.09	25,25,25,25	0
57	MG	2l	202	1/1	0.96	0.07	74,74,74,74	0
57	MG	2A	3463	1/1	0.96	0.19	62,62,62,62	0
57	MG	27	101	1/1	0.96	0.27	61,61,61,61	0
57	MG	1A	3398	1/1	0.96	0.20	26,26,26,26	0
57	MG	2r	101	1/1	0.96	0.12	69,69,69,69	0
57	MG	1A	3015	1/1	0.96	0.19	36,36,36,36	0
57	MG	1a	1804	1/1	0.96	0.06	56,56,56,56	0
57	MG	1A	4023	1/1	0.96	0.06	61,61,61,61	0
57	MG	1F	301	1/1	0.96	0.19	38,38,38,38	0
57	MG	2A	3470	1/1	0.96	0.06	56,56,56,56	0
57	MG	1A	3669	1/1	0.96	0.06	36,36,36,36	0
57	MG	1F	306	1/1	0.96	0.06	36,36,36,36	0
57	MG	1A	4025	1/1	0.96	0.07	75,75,75,75	0
57	MG	1A	3670	1/1	0.96	0.13	36,36,36,36	0
57	MG	2A	3701	1/1	0.96	0.07	61,61,61,61	0
57	MG	1A	3036	1/1	0.96	0.08	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
57	MG	1a	1656	1/1	0.96	0.27	66,66,66,66	0
57	MG	1A	3781	1/1	0.96	0.05	23,23,23,23	0
57	MG	1A	3352	1/1	0.96	0.17	37,37,37,37	0
57	MG	1A	4031	1/1	0.96	0.08	67,67,67,67	0
57	MG	1G	204	1/1	0.96	0.08	50,50,50,50	0
57	MG	2A	3481	1/1	0.96	0.09	50,50,50,50	0
59	ZN	2Y	202	1/1	0.96	0.06	94,94,94,94	0
57	MG	1A	3674	1/1	0.96	0.06	38,38,38,38	0
59	ZN	2n	501	1/1	0.96	0.06	91,91,91,91	0
57	MG	1A	3137	1/1	0.97	0.21	32,32,32,32	0
57	MG	1A	3202	1/1	0.97	0.05	38,38,38,38	0
57	MG	2A	3074	1/1	0.97	0.08	47,47,47,47	0
57	MG	1A	3059	1/1	0.97	0.31	57,57,57,57	0
57	MG	1A	3733	1/1	0.97	0.04	12,12,12,12	0
57	MG	1A	4037	1/1	0.97	0.11	56,56,56,56	0
57	MG	1W	201	1/1	0.97	0.05	36,36,36,36	0
57	MG	1A	3273	1/1	0.97	0.18	38,38,38,38	0
57	MG	1A	3014	1/1	0.97	0.05	28,28,28,28	0
57	MG	1a	1735	1/1	0.97	0.34	47,47,47,47	0
57	MG	1A	4042	1/1	0.97	0.07	47,47,47,47	0
57	MG	1A	3276	1/1	0.97	0.22	38,38,38,38	0
57	MG	1A	3205	1/1	0.97	0.10	21,21,21,21	0
57	MG	1X	104	1/1	0.97	0.09	34,34,34,34	0
57	MG	1A	3738	1/1	0.97	0.06	41,41,41,41	0
57	MG	1A	3278	1/1	0.97	0.15	37,37,37,37	0
57	MG	1A	3280	1/1	0.97	0.18	30,30,30,30	0
57	MG	2A	3496	1/1	0.97	0.08	59,59,59,59	0
57	MG	1A	3516	1/1	0.97	0.20	52,52,52,52	0
57	MG	1A	3141	1/1	0.97	0.07	15,15,15,15	0
57	MG	1A	3432	1/1	0.97	0.18	37,37,37,37	0
57	MG	2A	3736	1/1	0.97	0.15	40,40,40,40	0
57	MG	10	103	1/1	0.97	0.11	37,37,37,37	0
57	MG	10	104	1/1	0.97	0.26	32,32,32,32	0
57	MG	1A	3747	1/1	0.97	0.05	47,47,47,47	0
57	MG	1a	1749	1/1	0.97	0.08	53,53,53,53	0
57	MG	1A	3519	1/1	0.97	0.18	29,29,29,29	0
57	MG	1a	1752	1/1	0.97	0.05	34,34,34,34	0
57	MG	1a	1754	1/1	0.97	0.06	39,39,39,39	0
57	MG	1A	3890	1/1	0.97	0.13	32,32,32,32	0
57	MG	2A	3508	1/1	0.97	0.09	26,26,26,26	0
57	MG	1A	3626	1/1	0.97	0.08	20,20,20,20	0
57	MG	1A	3355	1/1	0.97	0.17	27,27,27,27	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3041	1/1	0.97	0.05	28,28,28,28	0
57	MG	1A	3522	1/1	0.97	0.17	37,37,37,37	0
57	MG	2A	3514	1/1	0.97	0.07	40,40,40,40	0
57	MG	1a	1761	1/1	0.97	0.06	36,36,36,36	0
57	MG	1A	3285	1/1	0.97	0.07	49,49,49,49	0
57	MG	13	102	1/1	0.97	0.14	37,37,37,37	0
57	MG	1A	3525	1/1	0.97	0.11	45,45,45,45	0
57	MG	1A	3287	1/1	0.97	0.10	36,36,36,36	0
57	MG	1A	3008	1/1	0.97	0.12	25,25,25,25	0
57	MG	2A	3521	1/1	0.97	0.06	40,40,40,40	0
57	MG	2a	1661	1/1	0.97	0.06	58,58,58,58	0
57	MG	1A	3063	1/1	0.97	0.23	46,46,46,46	0
57	MG	2a	1663	1/1	0.97	0.06	56,56,56,56	0
57	MG	1a	1770	1/1	0.97	0.05	48,48,48,48	0
57	MG	2A	3761	1/1	0.97	0.08	36,36,36,36	0
57	MG	2A	3762	1/1	0.97	0.09	35,35,35,35	0
57	MG	2A	3115	1/1	0.97	0.12	34,34,34,34	0
57	MG	2a	1668	1/1	0.97	0.13	44,44,44,44	0
57	MG	15	101	1/1	0.97	0.23	33,33,33,33	0
57	MG	1A	3145	1/1	0.97	0.20	28,28,28,28	0
57	MG	1A	3905	1/1	0.97	0.04	35,35,35,35	0
57	MG	15	106	1/1	0.97	0.10	37,37,37,37	0
57	MG	1A	3636	1/1	0.97	0.07	35,35,35,35	0
57	MG	1A	3147	1/1	0.97	0.06	30,30,30,30	0
57	MG	1A	3064	1/1	0.97	0.15	31,31,31,31	0
57	MG	1A	3043	1/1	0.97	0.29	30,30,30,30	0
57	MG	2a	1678	1/1	0.97	0.09	67,67,67,67	0
57	MG	17	101	1/1	0.97	0.10	34,34,34,34	0
57	MG	1A	3294	1/1	0.97	0.17	30,30,30,30	0
57	MG	1A	4072	1/1	0.97	0.06	11,11,11,11	0
57	MG	1A	3103	1/1	0.97	0.16	27,27,27,27	0
57	MG	2A	3778	1/1	0.97	0.06	62,62,62,62	0
57	MG	1A	3151	1/1	0.97	0.16	36,36,36,36	0
57	MG	1A	4077	1/1	0.97	0.05	35,35,35,35	0
57	MG	1A	3769	1/1	0.97	0.05	46,46,46,46	0
57	MG	2A	3545	1/1	0.97	0.10	31,31,31,31	0
57	MG	2A	3547	1/1	0.97	0.13	40,40,40,40	0
57	MG	1A	3772	1/1	0.97	0.07	33,33,33,33	0
57	MG	1A	3220	1/1	0.97	0.08	38,38,38,38	0
57	MG	2a	1692	1/1	0.97	0.30	61,61,61,61	0
57	MG	1A	3044	1/1	0.97	0.07	39,39,39,39	0
57	MG	2A	3135	1/1	0.97	0.17	41,41,41,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3552	1/1	0.97	0.08	50,50,50,50	0
57	MG	1a	1792	1/1	0.97	0.08	55,55,55,55	0
57	MG	1A	3775	1/1	0.97	0.08	51,51,51,51	0
57	MG	2A	3555	1/1	0.97	0.12	58,58,58,58	0
57	MG	2a	1699	1/1	0.97	0.10	57,57,57,57	0
57	MG	1A	3001	1/1	0.97	0.10	36,36,36,36	0
57	MG	1A	3300	1/1	0.97	0.06	32,32,32,32	0
57	MG	1A	3373	1/1	0.97	0.16	37,37,37,37	0
57	MG	1A	3223	1/1	0.97	0.06	44,44,44,44	0
57	MG	2A	3560	1/1	0.97	0.08	35,35,35,35	0
57	MG	1A	3782	1/1	0.97	0.06	30,30,30,30	0
57	MG	2A	3562	1/1	0.97	0.10	47,47,47,47	0
57	MG	1A	3925	1/1	0.97	0.08	39,39,39,39	0
57	MG	1a	1609	1/1	0.97	0.28	53,53,53,53	0
57	MG	1A	3452	1/1	0.97	0.12	30,30,30,30	0
57	MG	1A	3655	1/1	0.97	0.08	36,36,36,36	0
57	MG	1A	3075	1/1	0.97	0.07	24,24,24,24	0
57	MG	1A	3109	1/1	0.97	0.21	31,31,31,31	0
57	MG	1A	3077	1/1	0.97	0.11	32,32,32,32	0
57	MG	1A	4095	1/1	0.97	0.14	47,47,47,47	0
57	MG	2A	3152	1/1	0.97	0.18	38,38,38,38	0
57	MG	1A	3227	1/1	0.97	0.11	41,41,41,41	0
57	MG	1A	3162	1/1	0.97	0.33	29,29,29,29	0
57	MG	2A	3157	1/1	0.97	0.18	42,42,42,42	0
57	MG	1A	3046	1/1	0.97	0.07	34,34,34,34	0
57	MG	1a	1619	1/1	0.97	0.05	52,52,52,52	0
57	MG	1A	3232	1/1	0.97	0.09	43,43,43,43	0
57	MG	1a	1621	1/1	0.97	0.04	41,41,41,41	0
57	MG	2A	3819	1/1	0.97	0.07	54,54,54,54	0
57	MG	1A	3794	1/1	0.97	0.05	37,37,37,37	0
57	MG	1B	204	1/1	0.97	0.17	63,63,63,63	0
57	MG	1A	3937	1/1	0.97	0.11	34,34,34,34	0
57	MG	1A	3938	1/1	0.97	0.12	42,42,42,42	0
57	MG	2A	3826	1/1	0.97	0.05	57,57,57,57	0
57	MG	1a	1626	1/1	0.97	0.14	53,53,53,53	0
57	MG	2A	3829	1/1	0.97	0.04	68,68,68,68	0
57	MG	1A	3939	1/1	0.97	0.10	56,56,56,56	0
57	MG	2A	3365	1/1	0.97	0.12	39,39,39,39	0
57	MG	2A	3589	1/1	0.97	0.04	44,44,44,44	0
57	MG	1A	3940	1/1	0.97	0.06	50,50,50,50	0
57	MG	1A	3941	1/1	0.97	0.09	49,49,49,49	0
57	MG	1A	3795	1/1	0.97	0.04	22,22,22,22	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	1824	1/1	0.97	0.07	54,54,54,54	0
57	MG	1A	3310	1/1	0.97	0.10	38,38,38,38	0
57	MG	1A	3944	1/1	0.97	0.09	39,39,39,39	0
57	MG	2A	3597	1/1	0.97	0.05	55,55,55,55	0
57	MG	1A	3664	1/1	0.97	0.08	22,22,22,22	0
57	MG	1A	3383	1/1	0.97	0.07	49,49,49,49	0
57	MG	1A	3800	1/1	0.97	0.06	22,22,22,22	0
57	MG	2A	3845	1/1	0.97	0.16	41,41,41,41	0
57	MG	1A	3948	1/1	0.97	0.04	12,12,12,12	0
57	MG	1A	3311	1/1	0.97	0.04	26,26,26,26	0
57	MG	2A	3180	1/1	0.97	0.08	40,40,40,40	0
57	MG	1A	3802	1/1	0.97	0.07	43,43,43,43	0
57	MG	1B	220	1/1	0.97	0.06	36,36,36,36	0
57	MG	1A	3030	1/1	0.97	0.23	28,28,28,28	0
57	MG	1A	3955	1/1	0.97	0.07	43,43,43,43	0
57	MG	2a	1754	1/1	0.97	0.14	41,41,41,41	0
57	MG	1A	3668	1/1	0.97	0.05	29,29,29,29	0
57	MG	1A	3048	1/1	0.97	0.07	21,21,21,21	0
57	MG	1A	3168	1/1	0.97	0.10	31,31,31,31	0
57	MG	1A	3671	1/1	0.97	0.05	45,45,45,45	0
57	MG	1A	3236	1/1	0.97	0.05	53,53,53,53	0
57	MG	1A	3116	1/1	0.97	0.11	36,36,36,36	0
57	MG	1A	3119	1/1	0.97	0.11	45,45,45,45	0
57	MG	1A	3032	1/1	0.97	0.14	24,24,24,24	0
57	MG	1A	3564	1/1	0.97	0.19	33,33,33,33	0
57	MG	1A	3677	1/1	0.97	0.05	34,34,34,34	0
57	MG	1A	3474	1/1	0.97	0.09	35,35,35,35	0
57	MG	1A	3122	1/1	0.97	0.18	39,39,39,39	0
57	MG	1A	3395	1/1	0.97	0.13	40,40,40,40	0
57	MG	2A	3621	1/1	0.97	0.05	36,36,36,36	0
57	MG	1x	102	1/1	0.97	0.09	52,52,52,52	0
57	MG	1D	301	1/1	0.97	0.07	29,29,29,29	0
57	MG	2A	3397	1/1	0.97	0.13	43,43,43,43	0
57	MG	1A	3825	1/1	0.97	0.23	22,22,22,22	0
57	MG	1A	3033	1/1	0.97	0.29	25,25,25,25	0
57	MG	2A	3627	1/1	0.97	0.15	53,53,53,53	0
57	MG	1D	308	1/1	0.97	0.09	45,45,45,45	0
57	MG	1A	3085	1/1	0.97	0.18	23,23,23,23	0
57	MG	1A	3572	1/1	0.97	0.19	32,32,32,32	0
57	MG	1A	3179	1/1	0.97	0.09	34,34,34,34	0
57	MG	2A	3632	1/1	0.97	0.09	41,41,41,41	0
57	MG	2a	1780	1/1	0.97	0.11	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
57	MG	1A	3051	1/1	0.97	0.13	31,31,31,31	0
57	MG	2B	218	1/1	0.97	0.23	76,76,76,76	0
57	MG	1A	3687	1/1	0.97	0.10	28,28,28,28	0
57	MG	1E	303	1/1	0.97	0.13	27,27,27,27	0
57	MG	2D	304	1/1	0.97	0.05	31,31,31,31	0
57	MG	1A	3576	1/1	0.97	0.20	38,38,38,38	0
57	MG	1A	3127	1/1	0.97	0.21	32,32,32,32	0
57	MG	1A	3022	1/1	0.97	0.04	39,39,39,39	0
57	MG	2A	3004	1/1	0.97	0.32	55,55,55,55	0
57	MG	1A	3484	1/1	0.97	0.08	43,43,43,43	0
57	MG	1A	3485	1/1	0.97	0.15	43,43,43,43	0
57	MG	2E	304	1/1	0.97	0.09	38,38,38,38	0
57	MG	1A	3251	1/1	0.97	0.15	37,37,37,37	0
57	MG	1A	3696	1/1	0.97	0.04	27,27,27,27	0
57	MG	1A	3839	1/1	0.97	0.05	28,28,28,28	0
57	MG	1A	3988	1/1	0.97	0.05	63,63,63,63	0
57	MG	2A	3013	1/1	0.97	0.05	40,40,40,40	0
57	MG	1A	3129	1/1	0.97	0.07	31,31,31,31	0
57	MG	1A	3990	1/1	0.97	0.11	42,42,42,42	0
57	MG	1F	305	1/1	0.97	0.18	30,30,30,30	0
57	MG	1A	3053	1/1	0.97	0.06	48,48,48,48	0
57	MG	2F	305	1/1	0.97	0.17	40,40,40,40	0
57	MG	1F	307	1/1	0.97	0.04	36,36,36,36	0
57	MG	1F	308	1/1	0.97	0.13	21,21,21,21	0
57	MG	1A	3699	1/1	0.97	0.05	26,26,26,26	0
57	MG	2A	3227	1/1	0.97	0.24	42,42,42,42	0
57	MG	1A	3588	1/1	0.97	0.05	37,37,37,37	0
57	MG	2P	202	1/1	0.97	0.06	50,50,50,50	0
57	MG	1a	1685	1/1	0.97	0.15	53,53,53,53	0
57	MG	1F	312	1/1	0.97	0.11	28,28,28,28	0
57	MG	1A	3701	1/1	0.97	0.05	21,21,21,21	0
57	MG	1A	3589	1/1	0.97	0.06	44,44,44,44	0
57	MG	1G	201	1/1	0.97	0.11	35,35,35,35	0
57	MG	2A	3027	1/1	0.97	0.04	42,42,42,42	0
57	MG	1A	3703	1/1	0.97	0.04	26,26,26,26	0
57	MG	1A	3185	1/1	0.97	0.05	36,36,36,36	0
57	MG	1A	3017	1/1	0.97	0.10	57,57,57,57	0
57	MG	1A	3999	1/1	0.97	0.04	44,44,44,44	0
57	MG	1A	4000	1/1	0.97	0.06	48,48,48,48	0
57	MG	2A	3035	1/1	0.97	0.11	37,37,37,37	0
57	MG	2A	3670	1/1	0.97	0.05	54,54,54,54	0
57	MG	2A	3241	1/1	0.97	0.12	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
57	MG	1A	3025	1/1	0.97	0.08	32,32,32,32	0
57	MG	1N	203	1/1	0.97	0.06	40,40,40,40	0
57	MG	1a	1697	1/1	0.97	0.13	43,43,43,43	0
57	MG	2A	3675	1/1	0.97	0.10	38,38,38,38	0
57	MG	1A	3189	1/1	0.97	0.10	40,40,40,40	0
57	MG	1A	3711	1/1	0.97	0.06	63,63,63,63	0
57	MG	1O	201	1/1	0.97	0.22	50,50,50,50	0
57	MG	1A	4004	1/1	0.97	0.07	17,17,17,17	0
57	MG	1A	3190	1/1	0.97	0.15	29,29,29,29	0
57	MG	2A	3448	1/1	0.97	0.29	49,49,49,49	0
57	MG	1a	1703	1/1	0.97	0.17	48,48,48,48	0
57	MG	2A	3451	1/1	0.97	0.17	50,50,50,50	0
57	MG	1A	3259	1/1	0.97	0.06	34,34,34,34	0
57	MG	2A	3048	1/1	0.97	0.10	42,42,42,42	0
57	MG	2A	3049	1/1	0.97	0.12	28,28,28,28	0
57	MG	1A	3597	1/1	0.97	0.17	29,29,29,29	0
57	MG	2A	3688	1/1	0.97	0.05	61,61,61,61	0
57	MG	1A	3598	1/1	0.97	0.20	39,39,39,39	0
57	MG	1P	205	1/1	0.97	0.04	35,35,35,35	0
57	MG	1A	4012	1/1	0.97	0.04	28,28,28,28	0
57	MG	1A	3192	1/1	0.97	0.06	41,41,41,41	0
57	MG	1Q	207	1/1	0.97	0.08	33,33,33,33	0
57	MG	1A	3262	1/1	0.97	0.13	48,48,48,48	0
57	MG	1A	3193	1/1	0.97	0.20	27,27,27,27	0
57	MG	1A	3194	1/1	0.97	0.25	29,29,29,29	0
57	MG	1A	3133	1/1	0.97	0.05	37,37,37,37	0
57	MG	2A	3466	1/1	0.97	0.08	43,43,43,43	0
57	MG	1A	3092	1/1	0.97	0.06	21,21,21,21	0
57	MG	1A	3419	1/1	0.97	0.07	50,50,50,50	0
57	MG	1A	3268	1/1	0.97	0.15	36,36,36,36	0
57	MG	1A	3867	1/1	0.97	0.06	15,15,15,15	0
57	MG	1A	3868	1/1	0.97	0.12	36,36,36,36	0
57	MG	1A	3504	1/1	0.97	0.15	25,25,25,25	0
57	MG	1A	3608	1/1	0.97	0.10	35,35,35,35	0
57	MG	1A	4028	1/1	0.97	0.11	57,57,57,57	0
57	MG	2A	3068	1/1	0.97	0.14	38,38,38,38	0
57	MG	1A	3505	1/1	0.97	0.06	46,46,46,46	0
57	MG	1A	3872	1/1	0.97	0.12	20,20,20,20	0
57	MG	1A	3039	1/1	0.97	0.27	31,31,31,31	0
57	MG	1A	3286	1/1	0.98	0.17	47,47,47,47	0
57	MG	1A	3573	1/1	0.98	0.04	15,15,15,15	0
57	MG	1a	1802	1/1	0.98	0.05	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
57	MG	1A	3390	1/1	0.98	0.07	22,22,22,22	0
57	MG	1A	3191	1/1	0.98	0.23	38,38,38,38	0
57	MG	2a	1670	1/1	0.98	0.08	49,49,49,49	0
57	MG	1A	3037	1/1	0.98	0.12	21,21,21,21	0
57	MG	2A	3820	1/1	0.98	0.05	48,48,48,48	0
57	MG	1A	3577	1/1	0.98	0.20	42,42,42,42	0
57	MG	2A	3112	1/1	0.98	0.24	49,49,49,49	0
57	MG	2A	3452	1/1	0.98	0.12	22,22,22,22	0
57	MG	1A	3578	1/1	0.98	0.19	31,31,31,31	0
57	MG	2A	3825	1/1	0.98	0.04	37,37,37,37	0
57	MG	1A	3393	1/1	0.98	0.08	45,45,45,45	0
57	MG	1N	204	1/1	0.98	0.05	37,37,37,37	0
57	MG	1A	3096	1/1	0.98	0.04	30,30,30,30	0
57	MG	1A	3739	1/1	0.98	0.09	38,38,38,38	0
57	MG	1A	3740	1/1	0.98	0.06	20,20,20,20	0
57	MG	2A	3832	1/1	0.98	0.05	57,57,57,57	0
57	MG	2A	3639	1/1	0.98	0.10	35,35,35,35	0
57	MG	2A	3834	1/1	0.98	0.06	28,28,28,28	0
57	MG	1A	4057	1/1	0.98	0.05	38,38,38,38	0
57	MG	1A	4058	1/1	0.98	0.05	18,18,18,18	0
57	MG	1a	1655	1/1	0.98	0.03	40,40,40,40	0
57	MG	1A	3153	1/1	0.98	0.03	31,31,31,31	0
57	MG	1A	3582	1/1	0.98	0.23	36,36,36,36	0
57	MG	2a	1691	1/1	0.98	0.17	42,42,42,42	0
57	MG	1P	201	1/1	0.98	0.24	26,26,26,26	0
57	MG	1P	202	1/1	0.98	0.14	27,27,27,27	0
57	MG	1A	3396	1/1	0.98	0.20	29,29,29,29	0
57	MG	1A	3844	1/1	0.98	0.09	51,51,51,51	0
57	MG	1A	3584	1/1	0.98	0.15	35,35,35,35	0
57	MG	1Q	201	1/1	0.98	0.25	39,39,39,39	0
57	MG	1Q	202	1/1	0.98	0.05	30,30,30,30	0
57	MG	1Q	203	1/1	0.98	0.05	40,40,40,40	0
57	MG	1A	3154	1/1	0.98	0.05	34,34,34,34	0
57	MG	2A	3133	1/1	0.98	0.08	41,41,41,41	0
57	MG	1Q	205	1/1	0.98	0.05	44,44,44,44	0
57	MG	1A	3746	1/1	0.98	0.04	46,46,46,46	0
57	MG	1R	201	1/1	0.98	0.06	35,35,35,35	0
57	MG	1A	3453	1/1	0.98	0.21	41,41,41,41	0
57	MG	2a	1706	1/1	0.98	0.04	69,69,69,69	0
57	MG	2A	3854	1/1	0.98	0.05	43,43,43,43	0
57	MG	1R	203	1/1	0.98	0.18	37,37,37,37	0
57	MG	1A	3454	1/1	0.98	0.18	28,28,28,28	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3954	1/1	0.98	0.04	40,40,40,40	0
57	MG	1A	3196	1/1	0.98	0.22	29,29,29,29	0
57	MG	2A	3663	1/1	0.98	0.04	39,39,39,39	0
57	MG	1A	3038	1/1	0.98	0.12	25,25,25,25	0
57	MG	1A	3957	1/1	0.98	0.03	38,38,38,38	0
57	MG	1A	3198	1/1	0.98	0.07	41,41,41,41	0
57	MG	1A	3125	1/1	0.98	0.17	28,28,28,28	0
57	MG	1A	3459	1/1	0.98	0.06	38,38,38,38	0
57	MG	1A	3029	1/1	0.98	0.08	29,29,29,29	0
57	MG	1A	3962	1/1	0.98	0.04	47,47,47,47	0
57	MG	1A	3963	1/1	0.98	0.05	39,39,39,39	0
57	MG	1A	3080	1/1	0.98	0.08	33,33,33,33	0
57	MG	1a	1684	1/1	0.98	0.12	48,48,48,48	0
57	MG	2A	3153	1/1	0.98	0.07	56,56,56,56	0
57	MG	1A	3002	1/1	0.98	0.05	46,46,46,46	0
57	MG	1A	3858	1/1	0.98	0.04	33,33,33,33	0
57	MG	2A	3156	1/1	0.98	0.06	54,54,54,54	0
57	MG	1A	3596	1/1	0.98	0.09	24,24,24,24	0
57	MG	1U	209	1/1	0.98	0.21	29,29,29,29	0
57	MG	1V	201	1/1	0.98	0.11	27,27,27,27	0
57	MG	1A	3524	1/1	0.98	0.09	26,26,26,26	0
57	MG	1V	204	1/1	0.98	0.11	28,28,28,28	0
57	MG	1A	3405	1/1	0.98	0.06	34,34,34,34	0
57	MG	1A	3249	1/1	0.98	0.24	33,33,33,33	0
57	MG	1A	3163	1/1	0.98	0.21	46,46,46,46	0
57	MG	1A	3031	1/1	0.98	0.09	28,28,28,28	0
57	MG	1A	3206	1/1	0.98	0.06	34,34,34,34	0
57	MG	1A	3005	1/1	0.98	0.04	32,32,32,32	0
57	MG	1W	204	1/1	0.98	0.19	30,30,30,30	0
57	MG	1W	205	1/1	0.98	0.16	34,34,34,34	0
57	MG	1W	206	1/1	0.98	0.12	37,37,37,37	0
57	MG	1A	3356	1/1	0.98	0.14	36,36,36,36	0
57	MG	1A	3104	1/1	0.98	0.11	46,46,46,46	0
57	MG	1X	102	1/1	0.98	0.07	26,26,26,26	0
57	MG	1A	3770	1/1	0.98	0.04	39,39,39,39	0
57	MG	2a	1745	1/1	0.98	0.08	64,64,64,64	0
57	MG	1A	3167	1/1	0.98	0.07	36,36,36,36	0
57	MG	1A	3683	1/1	0.98	0.08	37,37,37,37	0
57	MG	1X	106	1/1	0.98	0.05	30,30,30,30	0
57	MG	2A	3009	1/1	0.98	0.08	42,42,42,42	0
57	MG	1A	3084	1/1	0.98	0.11	25,25,25,25	0
57	MG	1A	3473	1/1	0.98	0.15	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
57	MG	2A	3012	1/1	0.98	0.04	31,31,31,31	0
57	MG	1A	3211	1/1	0.98	0.04	36,36,36,36	0
57	MG	2A	3704	1/1	0.98	0.05	34,34,34,34	0
57	MG	1A	3010	1/1	0.98	0.04	27,27,27,27	0
57	MG	1A	3476	1/1	0.98	0.05	46,46,46,46	0
57	MG	1A	3780	1/1	0.98	0.04	36,36,36,36	0
57	MG	1A	3213	1/1	0.98	0.13	27,27,27,27	0
57	MG	1A	3987	1/1	0.98	0.04	42,42,42,42	0
57	MG	1A	3086	1/1	0.98	0.16	28,28,28,28	0
57	MG	1A	3691	1/1	0.98	0.09	22,22,22,22	0
57	MG	1A	3614	1/1	0.98	0.15	50,50,50,50	0
57	MG	2A	3532	1/1	0.98	0.08	46,46,46,46	0
57	MG	2A	3533	1/1	0.98	0.05	47,47,47,47	0
57	MG	2A	3716	1/1	0.98	0.05	33,33,33,33	0
57	MG	1A	3261	1/1	0.98	0.09	49,49,49,49	0
57	MG	2A	3535	1/1	0.98	0.06	50,50,50,50	0
57	MG	2A	3719	1/1	0.98	0.10	36,36,36,36	0
57	MG	1A	3066	1/1	0.98	0.11	31,31,31,31	0
57	MG	2A	3537	1/1	0.98	0.06	50,50,50,50	0
57	MG	1A	3136	1/1	0.98	0.10	26,26,26,26	0
57	MG	1A	3217	1/1	0.98	0.14	38,38,38,38	0
57	MG	13	101	1/1	0.98	0.05	32,32,32,32	0
57	MG	1A	3003	1/1	0.98	0.06	23,23,23,23	0
57	MG	1A	3790	1/1	0.98	0.05	15,15,15,15	0
57	MG	1A	3317	1/1	0.98	0.18	49,49,49,49	0
57	MG	2X	102	1/1	0.98	0.08	47,47,47,47	0
57	MG	2A	3030	1/1	0.98	0.06	38,38,38,38	0
57	MG	1A	3792	1/1	0.98	0.09	40,40,40,40	0
57	MG	2A	3546	1/1	0.98	0.09	29,29,29,29	0
57	MG	1A	3891	1/1	0.98	0.18	29,29,29,29	0
57	MG	1A	3621	1/1	0.98	0.07	21,21,21,21	0
57	MG	2A	3034	1/1	0.98	0.06	49,49,49,49	0
57	MG	15	102	1/1	0.98	0.15	32,32,32,32	0
57	MG	15	103	1/1	0.98	0.25	22,22,22,22	0
57	MG	2A	3037	1/1	0.98	0.05	39,39,39,39	0
57	MG	2A	3038	1/1	0.98	0.09	26,26,26,26	0
57	MG	1A	3176	1/1	0.98	0.07	25,25,25,25	0
57	MG	1A	3267	1/1	0.98	0.23	35,35,35,35	0
57	MG	1a	1734	1/1	0.98	0.26	47,47,47,47	0
57	MG	1A	3796	1/1	0.98	0.04	22,22,22,22	0
57	MG	1A	3069	1/1	0.98	0.07	23,23,23,23	0
57	MG	1A	4005	1/1	0.98	0.04	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
57	MG	1B	227	1/1	0.98	0.04	38,38,38,38	0
57	MG	1A	3897	1/1	0.98	0.06	38,38,38,38	0
57	MG	1A	3071	1/1	0.98	0.12	22,22,22,22	0
57	MG	17	102	1/1	0.98	0.17	26,26,26,26	0
57	MG	1A	4008	1/1	0.98	0.04	65,65,65,65	0
57	MG	1A	3113	1/1	0.98	0.07	31,31,31,31	0
57	MG	1A	4010	1/1	0.98	0.06	24,24,24,24	0
57	MG	1A	3114	1/1	0.98	0.04	29,29,29,29	0
57	MG	18	102	1/1	0.98	0.12	36,36,36,36	0
57	MG	2A	3753	1/1	0.98	0.11	51,51,51,51	0
57	MG	18	103	1/1	0.98	0.08	38,38,38,38	0
57	MG	1A	3072	1/1	0.98	0.05	11,11,11,11	0
57	MG	1A	3710	1/1	0.98	0.04	27,27,27,27	0
57	MG	1a	1750	1/1	0.98	0.10	47,47,47,47	0
57	MG	1A	4014	1/1	0.98	0.05	16,16,16,16	0
57	MG	1A	4015	1/1	0.98	0.04	32,32,32,32	0
57	MG	1a	1753	1/1	0.98	0.10	30,30,30,30	0
57	MG	1A	3904	1/1	0.98	0.06	48,48,48,48	0
57	MG	1D	303	1/1	0.98	0.07	31,31,31,31	0
57	MG	1D	304	1/1	0.98	0.06	17,17,17,17	0
57	MG	1A	3803	1/1	0.98	0.04	33,33,33,33	0
57	MG	2A	3580	1/1	0.98	0.08	54,54,54,54	0
57	MG	1D	306	1/1	0.98	0.12	30,30,30,30	0
57	MG	2A	3582	1/1	0.98	0.06	34,34,34,34	0
57	MG	1A	4018	1/1	0.98	0.07	33,33,33,33	0
57	MG	1A	3804	1/1	0.98	0.04	45,45,45,45	0
57	MG	1D	310	1/1	0.98	0.15	26,26,26,26	0
57	MG	1A	3007	1/1	0.98	0.07	35,35,35,35	0
57	MG	2A	3772	1/1	0.98	0.05	64,64,64,64	0
57	MG	1A	3274	1/1	0.98	0.16	33,33,33,33	0
57	MG	1A	3117	1/1	0.98	0.14	25,25,25,25	0
57	MG	1A	3146	1/1	0.98	0.14	29,29,29,29	0
57	MG	2A	3591	1/1	0.98	0.04	37,37,37,37	0
57	MG	1A	3118	1/1	0.98	0.07	35,35,35,35	0
57	MG	1a	1769	1/1	0.98	0.12	34,34,34,34	0
57	MG	2A	3780	1/1	0.98	0.04	37,37,37,37	0
57	MG	2A	3781	1/1	0.98	0.04	51,51,51,51	0
57	MG	2A	3075	1/1	0.98	0.12	40,40,40,40	0
57	MG	1E	304	1/1	0.98	0.13	27,27,27,27	0
57	MG	1E	305	1/1	0.98	0.13	28,28,28,28	0
57	MG	1A	3229	1/1	0.98	0.08	27,27,27,27	0
57	MG	1E	307	1/1	0.98	0.06	26,26,26,26	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3562	1/1	0.98	0.05	48,48,48,48	0
57	MG	1a	1776	1/1	0.98	0.04	43,43,43,43	0
57	MG	1A	3279	1/1	0.98	0.10	21,21,21,21	0
57	MG	1A	3565	1/1	0.98	0.11	28,28,28,28	0
57	MG	1A	3021	1/1	0.98	0.06	22,22,22,22	0
57	MG	1A	3721	1/1	0.98	0.06	14,14,14,14	0
57	MG	2A	3086	1/1	0.98	0.07	47,47,47,47	0
57	MG	1A	3231	1/1	0.98	0.20	29,29,29,29	0
57	MG	1A	3819	1/1	0.98	0.04	48,48,48,48	0
57	MG	1A	3640	1/1	0.98	0.07	31,31,31,31	0
57	MG	1A	3076	1/1	0.98	0.17	42,42,42,42	0
57	MG	1F	302	1/1	0.98	0.12	25,25,25,25	0
57	MG	1A	4035	1/1	0.98	0.04	44,44,44,44	0
57	MG	1F	304	1/1	0.98	0.10	27,27,27,27	0
57	MG	1A	3822	1/1	0.98	0.04	21,21,21,21	0
57	MG	1A	3824	1/1	0.98	0.04	31,31,31,31	0
57	MG	1a	1790	1/1	0.98	0.05	49,49,49,49	0
57	MG	1A	3725	1/1	0.98	0.05	38,38,38,38	0
57	MG	2A	3805	1/1	0.98	0.06	36,36,36,36	0
57	MG	1A	4040	1/1	0.98	0.04	44,44,44,44	0
57	MG	1A	3643	1/1	0.98	0.09	54,54,54,54	0
57	MG	1A	3284	1/1	0.98	0.29	31,31,31,31	0
57	MG	1A	3929	1/1	0.98	0.04	22,22,22,22	0
59	ZN	1n	103	1/1	0.98	0.04	66,66,66,66	0
57	MG	1A	3646	1/1	0.98	0.05	47,47,47,47	0
57	MG	1F	314	1/1	0.98	0.05	42,42,42,42	0
59	ZN	25	106	1/1	0.98	0.07	60,60,60,60	0
59	ZN	26	102	1/1	0.98	0.05	64,64,64,64	0
59	ZN	29	501	1/1	0.98	0.04	71,71,71,71	0
57	MG	1A	3121	1/1	0.98	0.37	46,46,46,46	0
60	SF4	1d	501	8/8	0.98	0.06	60,70,77,81	0
60	SF4	2d	303	8/8	0.98	0.06	69,79,88,91	0
57	MG	1A	3748	1/1	0.99	0.05	18,18,18,18	0
57	MG	1F	309	1/1	0.99	0.11	23,23,23,23	0
57	MG	1A	3749	1/1	0.99	0.04	21,21,21,21	0
57	MG	2Q	201	1/1	0.99	0.04	50,50,50,50	0
57	MG	1A	3306	1/1	0.99	0.10	25,25,25,25	0
57	MG	1A	3919	1/1	0.99	0.04	34,34,34,34	0
57	MG	1A	3560	1/1	0.99	0.24	34,34,34,34	0
57	MG	1A	3561	1/1	0.99	0.08	23,23,23,23	0
57	MG	1A	3283	1/1	0.99	0.17	29,29,29,29	0
57	MG	1A	3923	1/1	0.99	0.07	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
57	MG	1A	3563	1/1	0.99	0.09	28,28,28,28	0
57	MG	1A	3055	1/1	0.99	0.08	30,30,30,30	0
57	MG	1a	1801	1/1	0.99	0.03	44,44,44,44	0
57	MG	1A	3240	1/1	0.99	0.13	35,35,35,35	0
57	MG	1A	3201	1/1	0.99	0.14	22,22,22,22	0
57	MG	1A	4073	1/1	0.99	0.06	23,23,23,23	0
57	MG	2A	3144	1/1	0.99	0.06	26,26,26,26	0
57	MG	1A	3758	1/1	0.99	0.06	41,41,41,41	0
57	MG	1A	3242	1/1	0.99	0.22	30,30,30,30	0
57	MG	1A	4076	1/1	0.99	0.06	37,37,37,37	0
57	MG	1A	3106	1/1	0.99	0.03	23,23,23,23	0
57	MG	2A	3774	1/1	0.99	0.04	47,47,47,47	0
57	MG	1A	3140	1/1	0.99	0.10	26,26,26,26	0
57	MG	1A	3023	1/1	0.99	0.07	13,13,13,13	0
57	MG	1A	3097	1/1	0.99	0.09	15,15,15,15	0
57	MG	1A	3187	1/1	0.99	0.03	36,36,36,36	0
57	MG	10	102	1/1	0.99	0.15	41,41,41,41	0
57	MG	1A	3694	1/1	0.99	0.02	20,20,20,20	0
57	MG	1A	3805	1/1	0.99	0.05	38,38,38,38	0
57	MG	1A	4084	1/1	0.99	0.03	41,41,41,41	0
57	MG	1A	3070	1/1	0.99	0.05	14,14,14,14	0
57	MG	2A	3711	1/1	0.99	0.04	45,45,45,45	0
57	MG	1A	3156	1/1	0.99	0.14	20,20,20,20	0
57	MG	1P	204	1/1	0.99	0.11	29,29,29,29	0
57	MG	1D	307	1/1	0.99	0.15	30,30,30,30	0
57	MG	1A	3057	1/1	0.99	0.04	22,22,22,22	0
57	MG	1A	3173	1/1	0.99	0.06	33,33,33,33	0
57	MG	1A	3496	1/1	0.99	0.10	34,34,34,34	0
57	MG	1a	1634	1/1	0.99	0.03	24,24,24,24	0
57	MG	1A	3771	1/1	0.99	0.06	18,18,18,18	0
57	MG	1a	1760	1/1	0.99	0.09	44,44,44,44	0
57	MG	1A	4039	1/1	0.99	0.02	18,18,18,18	0
57	MG	1a	1762	1/1	0.99	0.07	38,38,38,38	0
57	MG	2A	3510	1/1	0.99	0.07	39,39,39,39	0
57	MG	1A	3011	1/1	0.99	0.12	39,39,39,39	0
57	MG	1Q	206	1/1	0.99	0.20	39,39,39,39	0
57	MG	1A	3813	1/1	0.99	0.07	15,15,15,15	0
57	MG	1A	3175	1/1	0.99	0.12	25,25,25,25	0
57	MG	2A	3173	1/1	0.99	0.14	37,37,37,37	0
57	MG	1A	3159	1/1	0.99	0.10	31,31,31,31	0
57	MG	1A	3901	1/1	0.99	0.07	30,30,30,30	0
57	MG	2A	3588	1/1	0.99	0.06	27,27,27,27	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3177	1/1	0.99	0.07	23,23,23,23	0
57	MG	2D	301	1/1	0.99	0.07	42,42,42,42	0
57	MG	1A	3641	1/1	0.99	0.05	20,20,20,20	0
57	MG	1A	3950	1/1	0.99	0.06	54,54,54,54	0
57	MG	1A	3951	1/1	0.99	0.06	24,24,24,24	0
57	MG	1A	3860	1/1	0.99	0.03	52,52,52,52	0
57	MG	1A	3705	1/1	0.99	0.07	28,28,28,28	0
57	MG	1a	1775	1/1	0.99	0.06	62,62,62,62	0
57	MG	2A	3525	1/1	0.99	0.04	32,32,32,32	0
57	MG	1A	3778	1/1	0.99	0.09	42,42,42,42	0
57	MG	1A	3706	1/1	0.99	0.03	22,22,22,22	0
57	MG	1U	201	1/1	0.99	0.14	30,30,30,30	0
57	MG	1A	3012	1/1	0.99	0.05	34,34,34,34	0
57	MG	1A	3326	1/1	0.99	0.06	30,30,30,30	0
57	MG	2A	3818	1/1	0.99	0.03	54,54,54,54	0
59	ZN	1Y	203	1/1	0.99	0.03	57,57,57,57	0
57	MG	1E	316	1/1	0.99	0.08	41,41,41,41	0
59	ZN	15	108	1/1	0.99	0.04	41,41,41,41	0
59	ZN	16	104	1/1	0.99	0.05	48,48,48,48	0
57	MG	1A	3823	1/1	0.99	0.03	42,42,42,42	0
57	MG	1A	3074	1/1	0.99	0.08	26,26,26,26	0
57	MG	1A	3645	1/1	0.99	0.05	15,15,15,15	0
57	MG	1B	213	1/1	0.99	0.04	30,30,30,30	0
57	MG	1A	3013	1/1	0.99	0.09	24,24,24,24	0
57	MG	1A	3067	1/1	0.99	0.07	28,28,28,28	0
57	MG	1A	3238	1/1	0.99	0.07	30,30,30,30	0
57	MG	1V	203	1/1	0.99	0.14	32,32,32,32	0
57	MG	2A	3828	1/1	0.99	0.04	29,29,29,29	0
59	ZN	19	102	1/1	1.00	0.04	40,40,40,40	0
57	MG	1A	3161	1/1	1.00	0.10	25,25,25,25	0

6.5 Other polymers (i)

There are no such residues in this entry.