Full wwPDB X-ray Structure Validation Report (i)

Mar 5, 2026 – 10:08 AM UTC

PDB ID	:	8G29 / pdb_00008g29
Title	:	Crystal structure of the A2503-C2,C8-dimethylated Thermus thermophilus 70S ribosome in complex with mRNA, aminoacylated A-site Phe-tRNAphe, aminoacylated P-site fMet-tRNAmet, and deacylated E-site tRNAphe at 2.55A resolution
Authors	:	Aleksandrova, E.V.; Wu, K.J.Y.; Tresco, B.I.C.; Syroegin, E.A.; Killeavy, E.E.; Balasanyants, S.M.; Svetlov, M.S.; Gregory, S.T.; Atkinson, G.C.; Myers, A.G.; Polikanov, Y.S.
Deposited on	:	2023-02-03
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 (1)) were used in the production of this report:

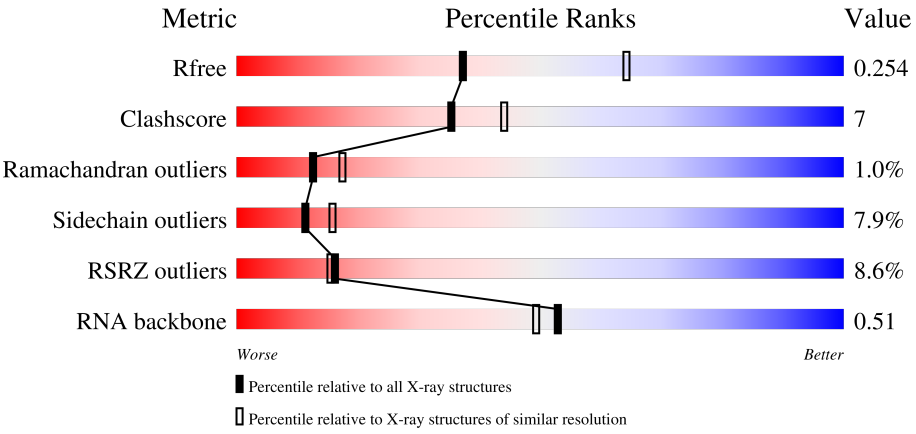
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)

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	6% 69% 23% 6% ·
1	2A	2915	5% 60% 30% 6% ·

Continued on next page...

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

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	1B	121	79% 17%
2	2B	121	2% 60% 34% 5%
3	1D	276	% 82% 17%
3	2D	276	% 80% 17%
4	1E	206	77% 18%
4	2E	206	2% 73% 24%
5	1F	210	2% 72% 20%
5	2F	210	3% 63% 31%
6	1G	182	5% 69% 26%
6	2G	182	10% 69% 28%
7	1H	180	2% 72% 23%
7	2H	180	49% 60% 34%
8	1I	148	6% 65% 30%
8	2I	148	15% 70% 26%
9	1N	140	% 82% 16%
9	2N	140	6% 72% 26%
10	1O	122	% 82% 18%
10	2O	122	% 78% 20%
11	1P	150	3% 81% 16%
11	2P	150	3% 78% 20%
12	1Q	141	% 76% 21%
12	2Q	141	11% 70% 28%
13	1R	118	81% 16%
13	2R	118	2% 72% 25%
14	1S	112	% 79% 18%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
14	2S	112	4% 57% 39%
15	1T	146	3% 72% 17% 10%
15	2T	146	8% 69% 18% 10%
16	1U	118	% 83% 14%
16	2U	118	6% 86% 12%
17	1V	101	88% 9%
17	2V	101	6% 81% 17%
18	1W	113	% 90% 7%
18	2W	113	3% 78% 20%
19	1X	96	3% 82% 16%
19	2X	96	7% 80% 17%
20	1Y	110	3% 73% 21%
20	2Y	110	21% 72% 22%
21	1Z	206	8% 50% 21% 25%
21	2Z	206	21% 34% 35% 7% 22%
22	10	85	% 86% 12%
22	20	85	7% 80% 18%
23	11	98	3% 87% 11%
23	21	98	4% 80% 18%
24	12	72	3% 83% 12%
24	22	72	6% 65% 32%
25	13	60	3% 77% 20%
25	23	60	5% 63% 33%
26	14	71	20% 52% 37%
26	24	71	20% 46% 42% 8%

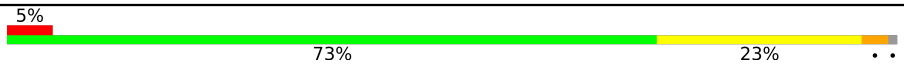
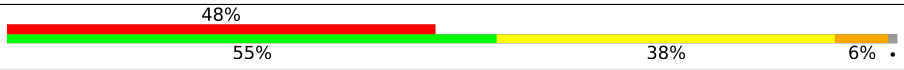
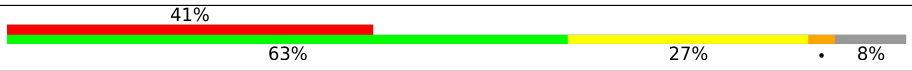
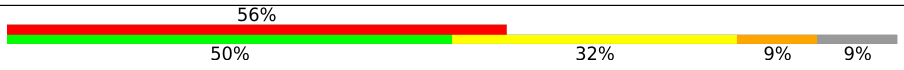
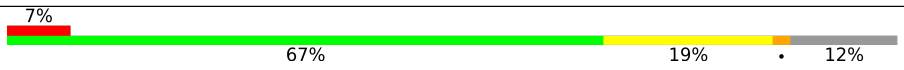
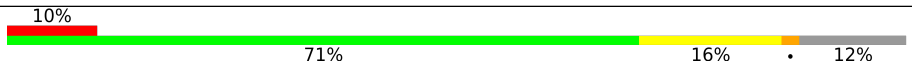
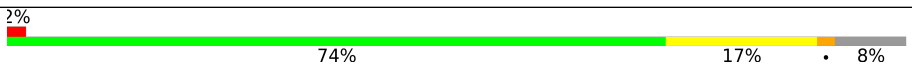
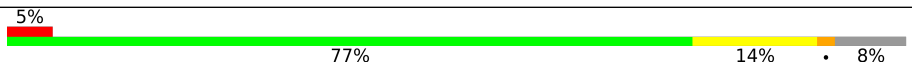
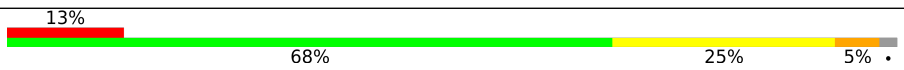
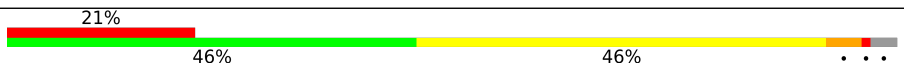
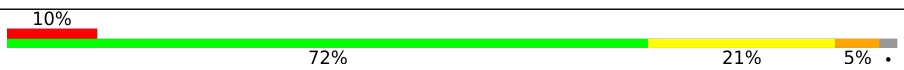
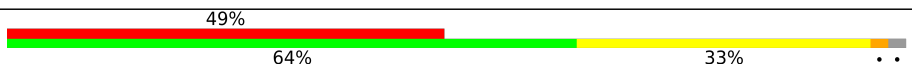
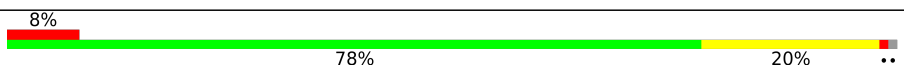
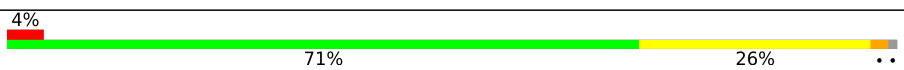
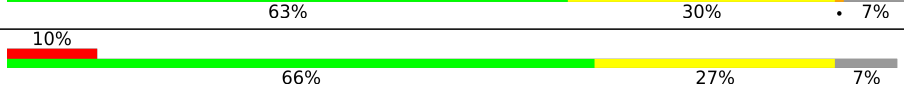
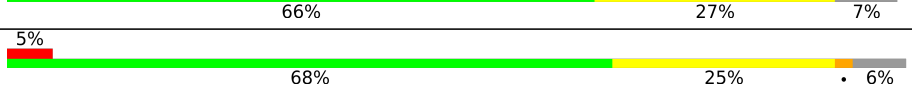
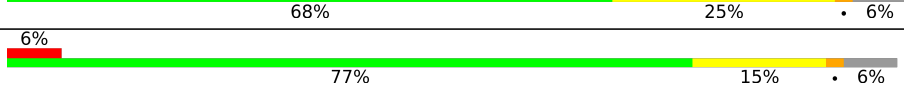
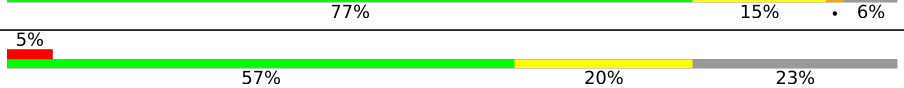
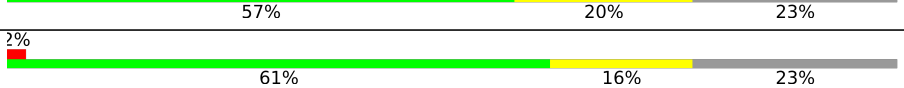
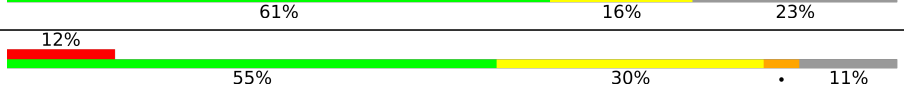
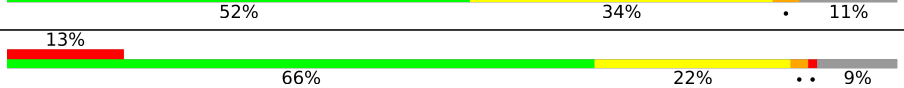
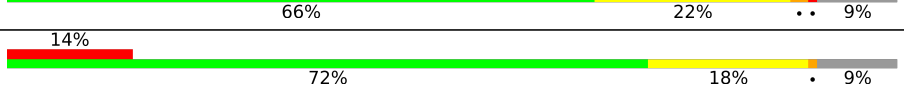
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
27	15	60	87% 10%
27	25	60	2% 82% 15%
28	16	54	2% 74% 19% 6%
28	26	54	2% 76% 20%
29	17	49	8% 80% 16%
29	27	49	10% 71% 20% 6%
30	18	65	75% 23%
30	28	65	80% 17%
31	19	37	86% 14%
31	29	37	19% 59% 38%
32	1a	1521	4% 59% 34% 6%
32	2a	1521	5% 58% 35% 6%
33	1b	256	24% 47% 36% 7% 10%
33	2b	256	32% 54% 24% 12% 10%
34	1c	239	9% 64% 21% 14%
34	2c	239	29% 59% 26% 14%
35	1d	209	10% 69% 27%
35	2d	209	5% 68% 27%
36	1e	162	4% 59% 30% 9%
36	2e	162	4% 51% 36% 9%
37	1f	101	5% 67% 29%
37	2f	101	2% 80% 17%
38	1g	156	12% 73% 23%
38	2g	156	15% 73% 25%
39	1h	138	% 75% 22%

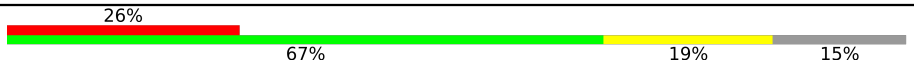
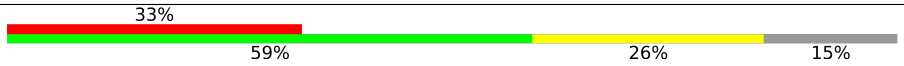
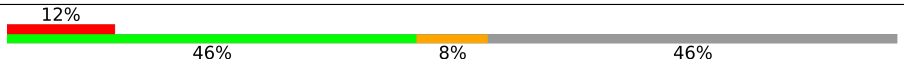
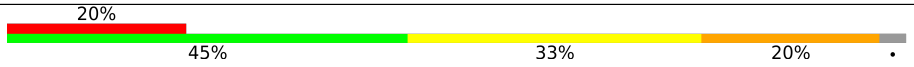
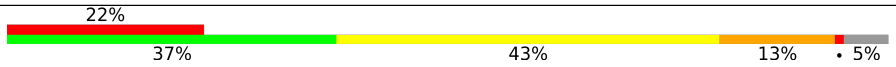
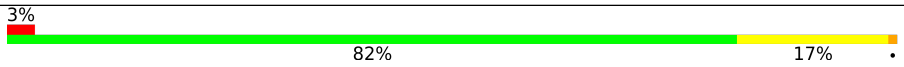
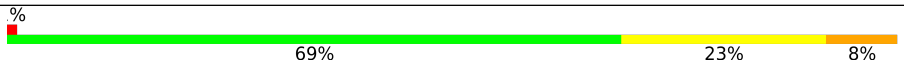
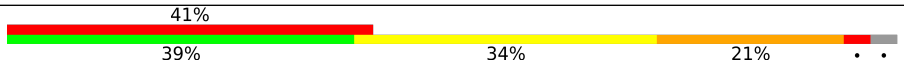
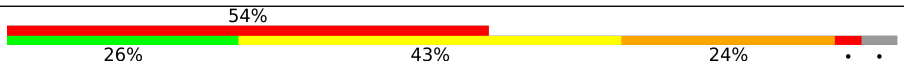
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
39	2h	138	
40	1i	128	
40	2i	128	
41	1j	105	
41	2j	105	
42	1k	129	
42	2k	129	
43	1l	132	
43	2l	132	
44	1m	126	
44	2m	126	
45	1n	61	
45	2n	61	
46	1o	89	
46	2o	89	
47	1p	88	
47	2p	88	
48	1q	105	
48	2q	105	
49	1r	88	
49	2r	88	
50	1s	93	
50	2s	93	
51	1t	106	
51	2t	106	

Continued on next page...

Continued from previous page...

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	15	108	-	-	-	X
57	MG	1a	1659	-	-	-	X
57	MG	2A	3318	-	-	-	X

2 Entry composition (i)

There are 61 unique types of molecules in this entry. The entry contains 299618 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
			61853	27532	11572	19878	2871			
1	2A	2800	Total	C	N	O	P	0	0	0
			60323	26849	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 MF-mRNA.

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

- Molecule 54 is a RNA chain called A-site Aminoacylated Phe-tRNAphe.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1w	74	Total	C	N	O	P	S	0	0	0
			1603	722	287	518	74	2			
54	2w	72	Total	C	N	O	P	S	0	0	0
			1555	699	280	502	72	2			

- Molecule 55 is a RNA chain called P-site Aminoacylated fMet-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 tRNAphe.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	1A	1113	Total	Mg	0	0
			1113	1113		
57	1B	38	Total	Mg	0	0
			38	38		
57	1D	12	Total	Mg	0	0
			12	12		
57	1E	14	Total	Mg	0	0
			14	14		
57	1F	13	Total	Mg	0	0
			13	13		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	1G	5	Total Mg 5 5	0	0
57	1H	1	Total Mg 1 1	0	0
57	1N	6	Total Mg 6 6	0	0
57	1O	4	Total Mg 4 4	0	0
57	1P	5	Total Mg 5 5	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	3	Total Mg 3 3	0	0
57	1U	6	Total Mg 6 6	0	0
57	1V	7	Total Mg 7 7	0	0
57	1W	6	Total Mg 6 6	0	0
57	1X	7	Total Mg 7 7	0	0
57	1Y	2	Total Mg 2 2	0	0
57	1Z	3	Total Mg 3 3	0	0
57	10	7	Total Mg 7 7	0	0
57	11	6	Total Mg 6 6	0	0
57	12	2	Total Mg 2 2	0	0
57	13	3	Total Mg 3 3	0	0
57	14	1	Total Mg 1 1	0	0
57	15	8	Total Mg 8 8	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	16	2	Total Mg 2 2	0	0
57	17	6	Total Mg 6 6	0	0
57	18	5	Total Mg 5 5	0	0
57	19	1	Total Mg 1 1	0	0
57	1a	220	Total Mg 220 220	0	0
57	1b	1	Total Mg 1 1	0	0
57	1d	1	Total Mg 1 1	0	0
57	1e	2	Total Mg 2 2	0	0
57	1f	2	Total Mg 2 2	0	0
57	1l	2	Total Mg 2 2	0	0
57	1m	1	Total Mg 1 1	0	0
57	1n	1	Total Mg 1 1	0	0
57	1p	1	Total Mg 1 1	0	0
57	1q	1	Total Mg 1 1	0	0
57	1t	1	Total Mg 1 1	0	0
57	1v	1	Total Mg 1 1	0	0
57	1w	9	Total Mg 9 9	0	0
57	1x	14	Total Mg 14 14	0	0
57	2A	804	Total Mg 804 804	0	0
57	2B	16	Total Mg 16 16	0	0
57	2D	6	Total Mg 6 6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	2E	7	Total Mg 7 7	0	0
57	2F	6	Total Mg 6 6	0	0
57	2G	1	Total Mg 1 1	0	0
57	2O	1	Total Mg 1 1	0	0
57	2P	1	Total Mg 1 1	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	3	Total Mg 3 3	0	0
57	2V	1	Total Mg 1 1	0	0
57	2W	3	Total Mg 3 3	0	0
57	2X	2	Total Mg 2 2	0	0
57	2Z	1	Total Mg 1 1	0	0
57	20	2	Total Mg 2 2	0	0
57	21	3	Total Mg 3 3	0	0
57	23	2	Total Mg 2 2	0	0
57	25	3	Total Mg 3 3	0	0
57	27	2	Total Mg 2 2	0	0
57	28	2	Total Mg 2 2	0	0
57	2a	2	Total Mg 2 2	0	0
57	2w	6	Total Mg 6 6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	2x	7	Total Mg 7 7	0	0
57	2y	7	Total Mg 7 7	0	0

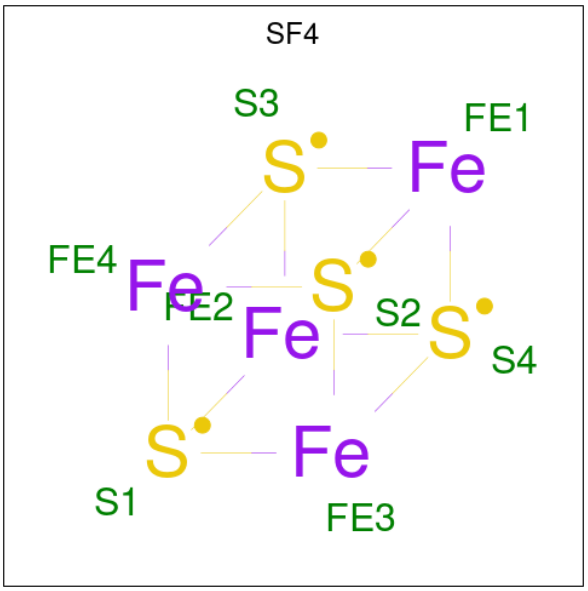
- Molecule 58 is POTASSIUM ION (CCD ID: K) (formula: K).

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
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	2067	Total O 2067 2067	0	0
61	1B	61	Total O 61 61	0	0
61	1D	32	Total O 32 32	0	0
61	1E	26	Total O 26 26	0	0
61	1F	20	Total O 20 20	0	0
61	1G	1	Total O 1 1	0	0
61	1H	2	Total O 2 2	0	0
61	1N	6	Total O 6 6	0	0
61	1O	6	Total O 6 6	0	0
61	1P	21	Total O 21 21	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1Q	7	Total O 7 7	0	0
61	1R	7	Total O 7 7	0	0
61	1S	5	Total O 5 5	0	0
61	1T	9	Total O 9 9	0	0
61	1U	14	Total O 14 14	0	0
61	1V	7	Total O 7 7	0	0
61	1W	6	Total O 6 6	0	0
61	1X	5	Total O 5 5	0	0
61	1Y	3	Total O 3 3	0	0
61	1Z	1	Total O 1 1	0	0
61	10	12	Total O 12 12	0	0
61	11	7	Total O 7 7	0	0
61	12	4	Total O 4 4	0	0
61	13	4	Total O 4 4	0	0
61	14	1	Total O 1 1	0	0
61	15	10	Total O 10 10	0	0
61	16	5	Total O 5 5	0	0
61	17	10	Total O 10 10	0	0
61	18	10	Total O 10 10	0	0
61	1a	425	Total O 425 425	0	0
61	1b	1	Total O 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1f	1	Total O 1 1	0	0
61	1i	1	Total O 1 1	0	0
61	1l	8	Total O 8 8	0	0
61	1m	2	Total O 2 2	0	0
61	1n	1	Total O 1 1	0	0
61	1o	3	Total O 3 3	0	0
61	1p	1	Total O 1 1	0	0
61	1q	2	Total O 2 2	0	0
61	1r	2	Total O 2 2	0	0
61	1u	2	Total O 2 2	0	0
61	1v	4	Total O 4 4	0	0
61	1w	12	Total O 12 12	0	0
61	1x	17	Total O 17 17	0	0
61	1y	1	Total O 1 1	0	0
61	2A	1094	Total O 1094 1094	0	0
61	2B	18	Total O 18 18	0	0
61	2D	22	Total O 22 22	0	0
61	2E	9	Total O 9 9	0	0
61	2F	11	Total O 11 11	0	0
61	2I	3	Total O 3 3	0	0
61	2N	1	Total O 1 1	0	0

Continued on next page...

Continued from previous page...

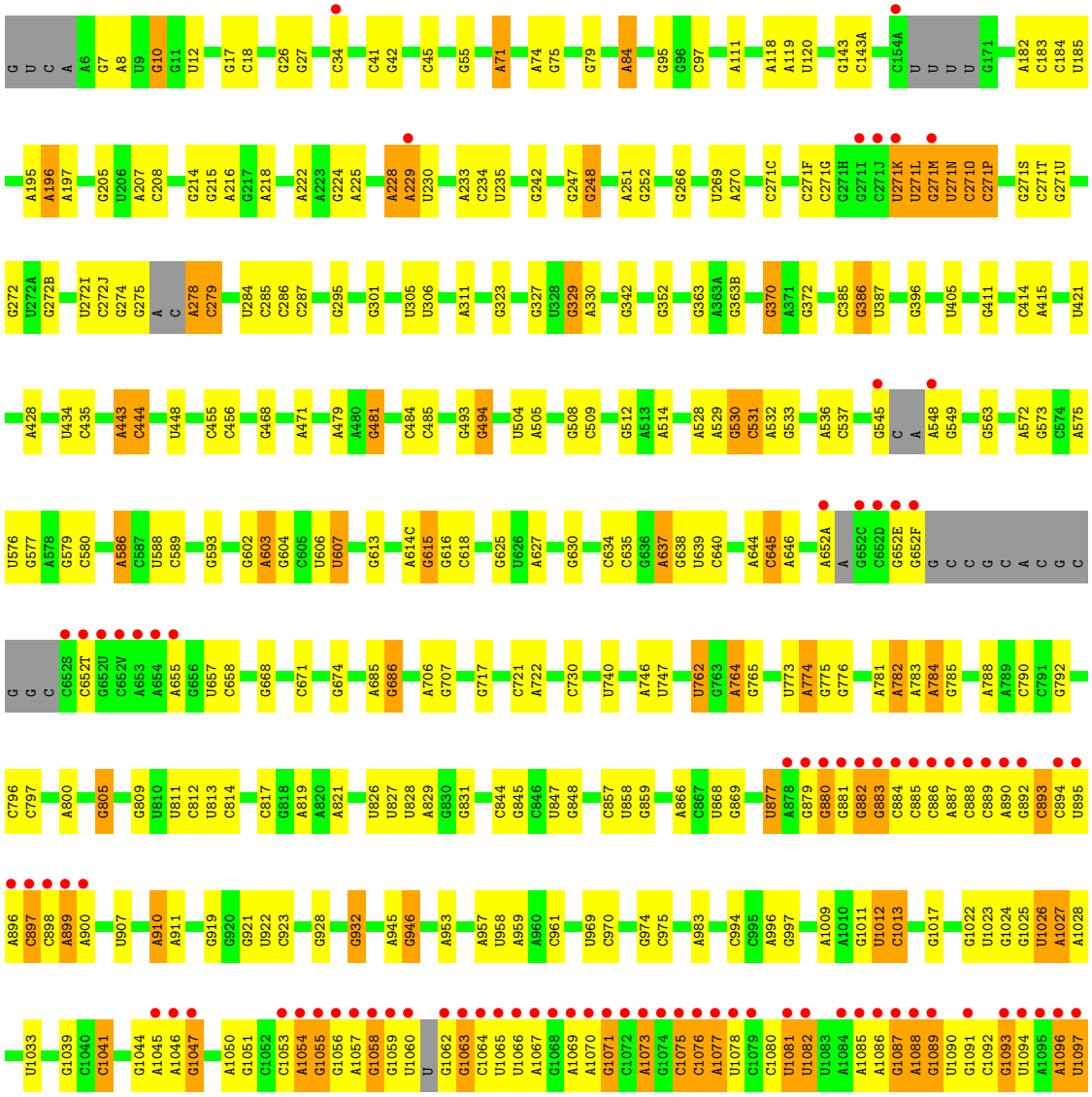
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2O	1	Total O 1 1	0	0
61	2P	9	Total O 9 9	0	0
61	2Q	1	Total O 1 1	0	0
61	2R	1	Total O 1 1	0	0
61	2T	5	Total O 5 5	0	0
61	2U	3	Total O 3 3	0	0
61	2W	3	Total O 3 3	0	0
61	2X	2	Total O 2 2	0	0
61	20	1	Total O 1 1	0	0
61	21	6	Total O 6 6	0	0
61	23	2	Total O 2 2	0	0
61	27	5	Total O 5 5	0	0
61	28	4	Total O 4 4	0	0
61	29	1	Total O 1 1	0	0
61	2w	1	Total O 1 1	0	0
61	2x	6	Total O 6 6	0	0
61	2y	2	Total O 2 2	0	0

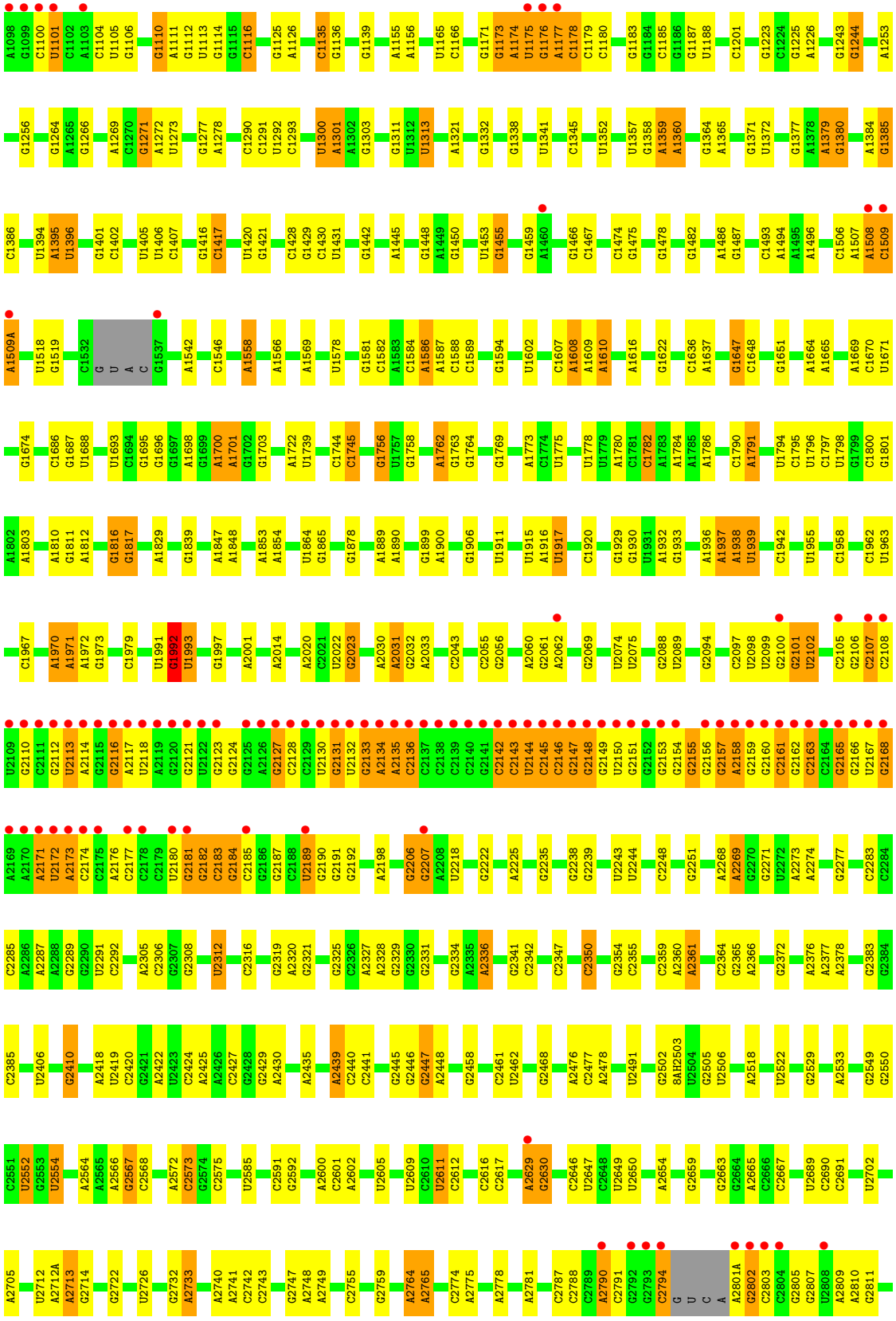
3 Residue-property plots (i)

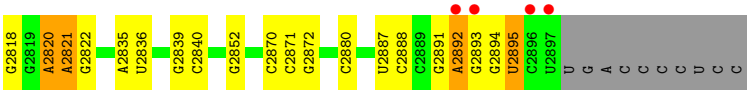
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

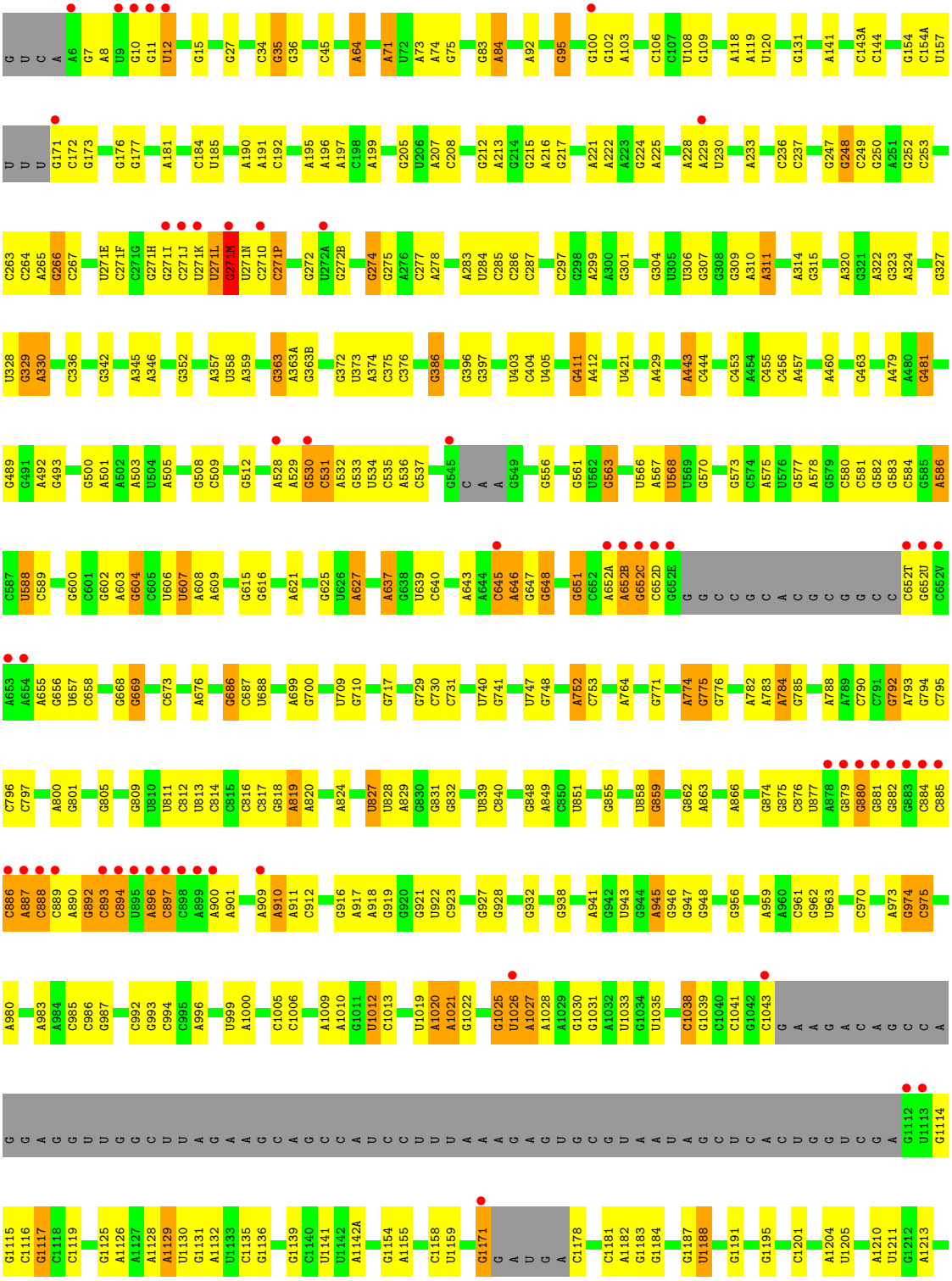


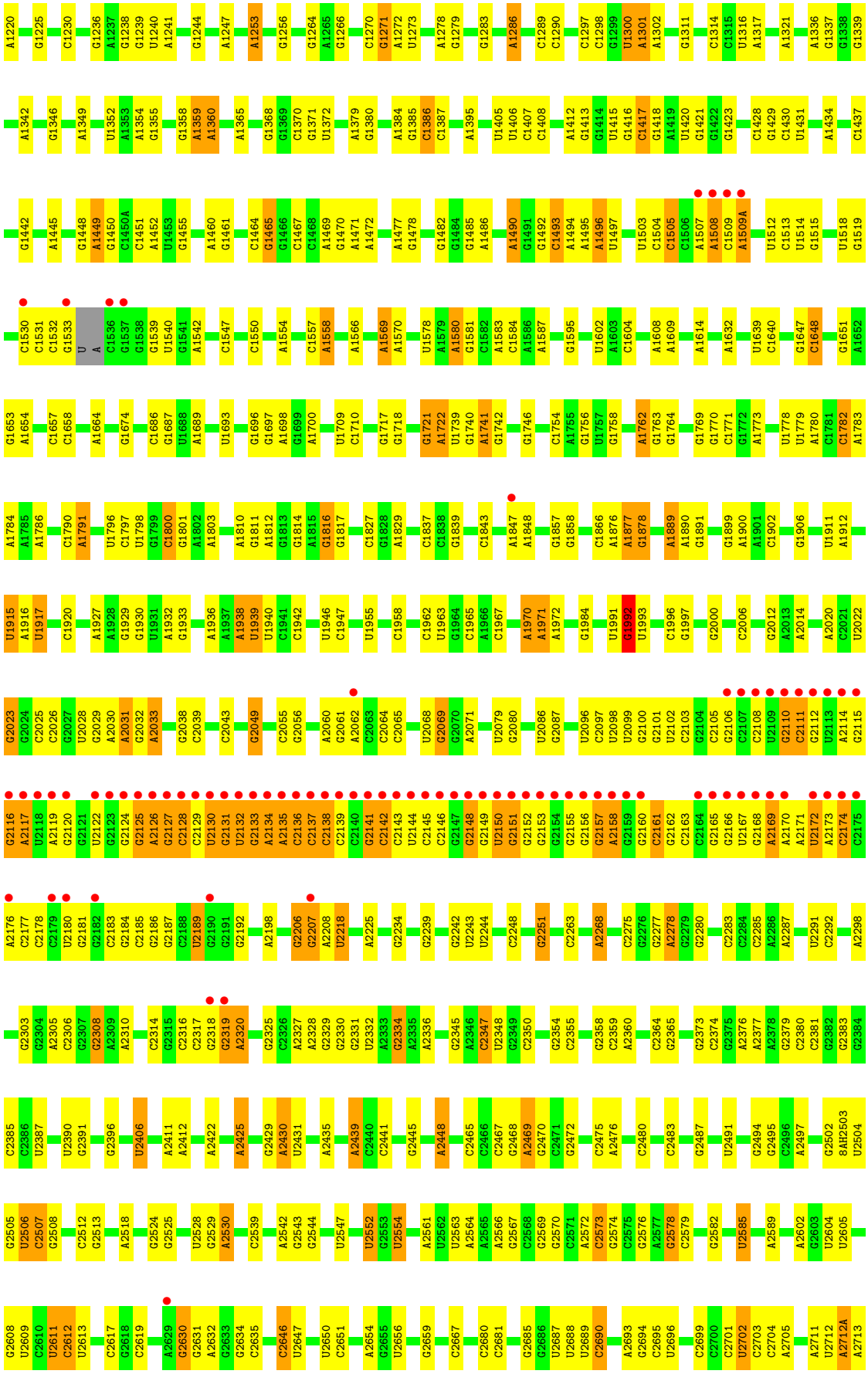

A1098 G1099 C1100 U1101 C1102 A1103 C1104 U1105 G1106 G1110 A1111 G1112 U1113 G1114 G1115 C1116 G1125 A1126 C1135 G1136 G1139 A1155 A1156 U1165 C1166 G1171 G1173 A1174 U1175 G1176 A1177 C1178 C1179 C1180 G1183 G1184 C1185 G1186 G1187 U1188 C1201 G1223 C1224 G1225 A1226 G1243 G1244 A1253
G1256 G1264 A1265 G1266 A1269 C1270 G1271 A1272 U1273 G1277 A1278 C1290 C1291 U1292 C1293 U1300 A1301 A1302 G1303 G1311 U1312 U1313 A1321 G1332 G1338 U1341 C1345 U1352 U1357 G1358 A1359 A1360 G1364 A1365 G1371 U1372 G1377 A1378 A1379 G1380 A1384 G1385
C1386 U1394 A1396 U1396 G1401 C1402 U1405 U1406 C1407 G1416 C1417 U1420 G1421 C1428 G1429 C1430 U1431 G1442 A1445 G1448 A1449 G1450 U1453 G1455 G1459 A1460 G1466 C1467 C1474 G1475 G1478 G1482 A1486 G1487 C1493 A1494 A1495 A1496 C1506 A1507 A1508 C1509
A1509A U1518 G1519 C1532 G U A C G1537 A1542 C1546 A1558 A1566 A1569 U1578 G1581 C1582 A1583 C1584 A1586 A1587 C1588 C1589 G1594 U1602 C1607 A1608 A1609 A1610 A1616 G1622 C1636 A1637 G1647 C1648 G1651 A1664 A1665 A1669 C1670 U1671
G1674 C1686 G1687 U1688 U1693 C1694 G1695 G1696 G1697 A1698 G1699 A1700 A1701 G1702 G1703 A1722 U1739 C1744 C1745 G1756 U1757 G1758 A1762 G1763 G1764 G1769 A1773 C1774 U1775 U1778 U1779 A1780 C1781 C1782 A1783 A1784 A1785 A1786 C1790 A1791 U1794 C1795 U1796 C1797 U1798 G1799 C1800 G1801
A1802 A1803 A1810 G1811 A1812 G1816 G1817 A1829 G1839 A1847 A1848 A1853 A1854 U1864 G1865 G1878 A1889 A1890 G1899 A1900 G1906 U1911 U1915 A1916 U1917 C1920 G1929 G1930 U1931 A1932 G1933 A1936 A1937 A1938 U1939 C1942 U1965 C1958 C1962 U1963
C1967 A1970 A1971 A1972 G1973 C1979 U1991 G1992 U1993 G1997 A2001 A2014 A2020 C2021 U2022 G2023 A2030 A2031 G2032 A2033 C2043 C2055 G2056 A2060 G2061 A2062 G2069 U2074 U2075 G2088 U2089 G2094 C2097 U2098 U2099 G2100 G2101 U2102 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 G2190 G2191 G2192 A2198 G2206 G2207 A2208 U2218 G2222 A2225 G2235 G2238 G2239 U2243 U2244 C2248 G2251 A2268 A2269 G2270 G2271 U2272 A2273 A2274 G2277 C2283 C2284
C2285 A2286 A2287 A2288 G2289 G2290 U2291 C2292 A2305 C2306 G2307 G2308 U2312 C2316 G2319 A2320 G2321 G2325 G2326 A2327 A2328 G2329 G2330 G2331 G2334 A2335 A2336 G2341 C2342 C2347 C2350 G2354 C2355 C2359 A2360 A2361 C2364 G2365 A2366 G2372 A2376 A2377 A2378 G2383 G2384
C2385 U2406 G2410 A2418 U2419 C2420 G2421 A2422 U2423 C2424 A2425 A2426 C2427 G2428 G2429 A2430 A2435 A2439 C2440 C2441 G2445 G2446 G2447 A2448 G2458 C2461 U2462 G2468 A2476 C2477 A2478 U2491 G2502 8AH2503 U2504 G2505 U2506 A2518 U2522 G2529 A2533 G2549 G2550
C2551 U2552 G2553 U2554 A2564 A2565 A2566 G2567 C2568 A2572 C2573 G2574 C2575 U2585 C2591 G2592 A2600 C2601 A2602 U2605 U2609 C2610 U2611 C2612 C2616 C2617 A2629 G2630 C2646 U2647 C2648 U2649 U2650 A2654 G2659 G2663 G2664 A2665 C2666 C2667 U2689 C2690 C2691 U2702
A2705 U2712 A2712A A2713 G2714 G2722 U2726 G2732 A2733 A2740 A2741 C2742 C2743 G2747 A2748 A2749 C2755 G2759 A2764 A2765 C2774 A2775 A2778 A2781 C2787 C2788 C2789 A2790 C2791 G2792 G2793 C2794 G U C A A2801A G2802 C2803 C2804 G2805 G2807 U2808 A2809 A2810 G2811

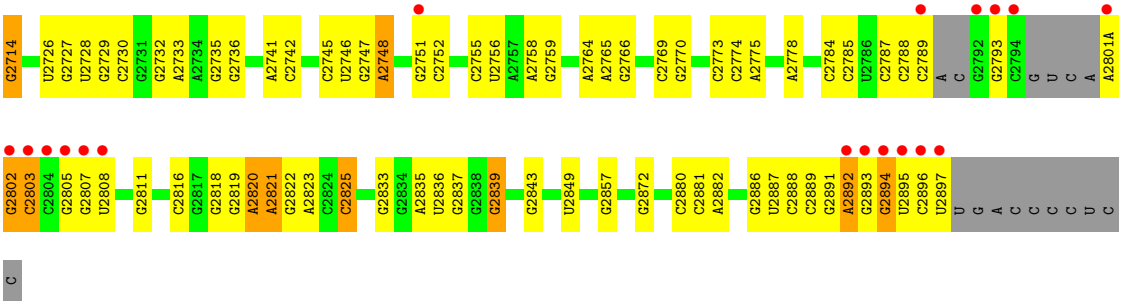


• Molecule 1: 23S Ribosomal RNA

Chain 2A:




A1220 G1225 C1230 G1236 A1237 G1238 G1239 U1240 A1241 G1244 A1247 A1253 G1256 G1264 A1265 G1266 C1270 G1271 A1272 U1273 A1278 G1279 G1283 A1286 C1289 C1290 C1297 C1298 G1299 U1300 A1301 A1302 G1311 C1314 C1315 U1316 A1317 A1321 A1336 G1337 G1338 G1339
A1342 G1346 A1349 U1352 A1353 A1354 G1355 G1358 A1359 A1360 A1365 G1368 G1369 C1370 G1371 U1372 A1379 G1380 A1384 G1385 C1386 C1387 A1395 U1405 U1406 C1407 C1408 A1412 G1413 G1414 U1415 G1416 C1417 G1418 A1419 U1420 G1421 G1422 G1423 C1428 G1429 C1430 U1431 A1434 C1437
G1442 A1445 G1448 A1449 G1450 C1450A C1451 A1452 U1453 G1455 A1460 G1461 C1464 G1465 G1466 C1467 C1468 A1469 G1470 A1471 A1472 A1477 G1478 G1482 G1484 G1485 A1486 A1490 G1491 G1492 C1493 A1494 A1495 A1496 U1497 U1503 C1504 C1505 C1506 A1507 A1508 C1509 A1509A U1512 C1513 U1514 G1515 U1518 G1519
C1530 C1531 C1532 G1533 U A C1536 G1537 G1538 G1539 U1540 G1541 A1542 C1547 C1550 A1554 C1557 A1558 A1566 A1569 A1570 U1578 A1579 A1580 G1581 C1582 A1583 C1584 A1586 A1587 G1595 U1602 A1603 C1604 A1608 A1609 A1614 A1632 U1639 C1640 G1647 C1648 G1651 A1652
G1653 A1654 C1657 C1658 A1664 G1674 C1686 G1687 U1688 A1689 U1693 G1696 G1697 A1698 G1699 A1700 U1709 C1710 G1717 G1718 G1721 A1722 U1739 G1740 A1741 G1742 G1746 C1754 A1755 G1756 U1757 G1758 A1762 G1763 G1764 G1769 G1770 C1771 G1772 A1773 U1778 U1779 A1780 C1781 C1782 A1783
A1784 A1785 A1786 C1790 A1791 U1796 C1797 U1798 G1799 C1800 G1801 A1802 A1803 A1810 G1811 A1812 G1813 G1814 A1815 G1816 G1817 C1827 G1828 A1829 C1837 C1838 G1839 C1843 A1847 A1848 G1857 G1858 C1866 A1876 A1877 G1878 A1889 A1890 G1891 G1899 A1900 A1901 C1902 G1906 U1911 A1912
U1915 A1916 U1917 C1920 A1927 A1928 G1929 G1930 U1931 A1932 G1933 A1936 A1937 A1938 U1939 U1940 C1941 C1942 U1946 C1947 U1955 C1958 C1962 U1963 G1964 C1965 A1966 C1967 A1970 A1971 A1972 G1984 U1991 G1992 U1993 C1996 G1997 G2000 C2006 G2012 A2013 A2014 A2020 C2021 U2022
G2023 G2024 C2025 C2026 G2027 U2028 G2029 A2030 A2031 G2032 A2033 G2038 C2039 C2043 G2049 C2055 G2056 A2060 G2061 A2062 C2063 C2064 C2065 U2068 G2069 G2070 A2071 U2079 G2080 U2086 G2087 U2096 C2097 U2098 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 G2164 G2165 G2166 U2167 G2168 G2169 A2170 A2171 U2172 A2173 C2174 C2175
A2176 C2177 C2178 C2179 U2180 G2181 G2182 C2183 G2184 C2185 G2186 G2187 C2188 U2189 G2190 G2191 G2192 A2198 G2206 G2207 A2208 U2218 A2225 G2234 G2239 G2242 U2243 U2244 C2248 G2251 C2263 A2268 C2275 G2276 G2277 A2278 G2279 G2280 C2283 C2284 C2285 A2286 A2287 U2291 C2292 A2298
G2303 G2304 A2305 C2306 G2307 G2308 A2309 A2310 C2314 G2315 C2316 C2317 G2318 G2319 A2320 G2325 C2326 A2327 A2328 G2329 G2330 G2331 U2332 A2333 G2334 A2335 A2336 G2345 A2346 C2347 U2348 G2349 C2350 G2354 C2355 G2358 C2359 A2360 C2364 G2365 G2373 C2374 G2375 A2376 A2377 A2378 G2379 C2380 C2381 G2382 G2383 G2384
C2385 C2386 U2387 U2390 G2391 G2396 U2406 A2411 A2412 A2422 A2425 G2429 A2430 U2431 A2435 A2439 C2440 C2441 G2445 A2448 C2465 C2466 C2467 G2468 A2469 G2470 C2471 G2472 C2475 A2476 C2480 C2483 G2487 U2491 G2494 G2495 C2496 A2497 G2502 8AH2503 U2504
G2505 U2506 C2507 G2508 C2512 G2513 A2518 G2524 G2525 U2528 G2529 A2530 C2539 A2542 G2543 G2544 U2547 U2552 G2553 U2554 A2561 U2562 U2563 A2564 A2565 A2566 G2567 C2568 G2569 G2570 C2571 A2572 C2573 G2574 C2575 G2576 A2577 G2578 C2579 G2582 U2585 A2589 A2602 G2603 U2604 U2605
G2608 U2609 C2610 U2611 C2612 U2613 C2617 G2618 C2619 A2629 G2630 G2631 A2632 G2633 G2634 C2635 C2646 U2647 U2650 C2651 A2654 G2655 U2656 G2659 C2667 C2680 C2681 G2685 G2686 U2687 U2688 U2689 C2690 A2693 G2694 C2695 U2696 C2699 C2700 C2701 U2702 C2703 C2704 A2705 A2711 U2712 A2712A A2713

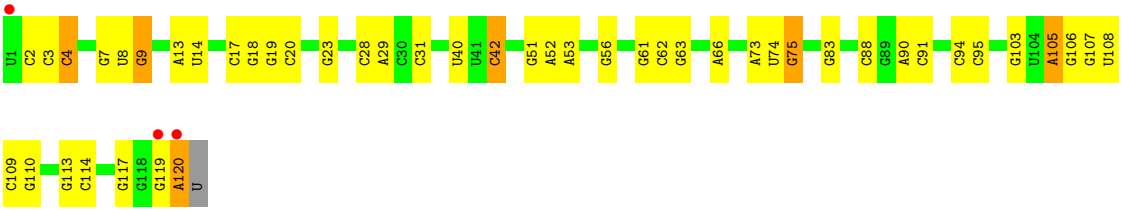


• Molecule 2: 5S Ribosomal RNA

Chain 1B:

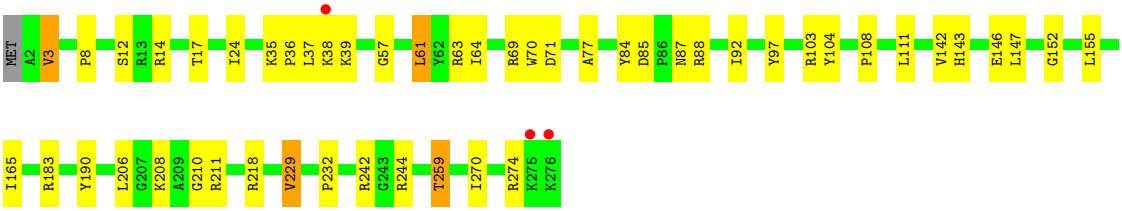
• Molecule 2: 5S Ribosomal RNA

Chain 2B:



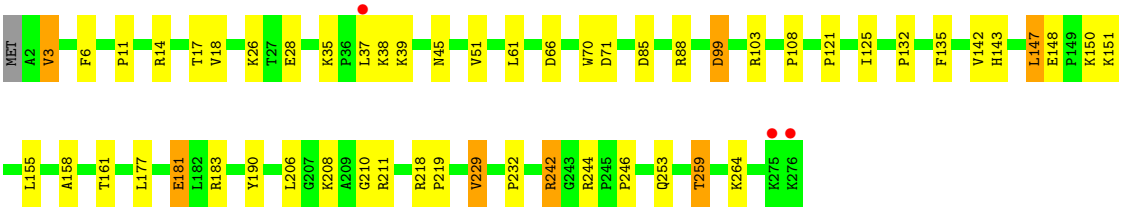
• Molecule 3: 50S ribosomal protein L2

Chain 1D:



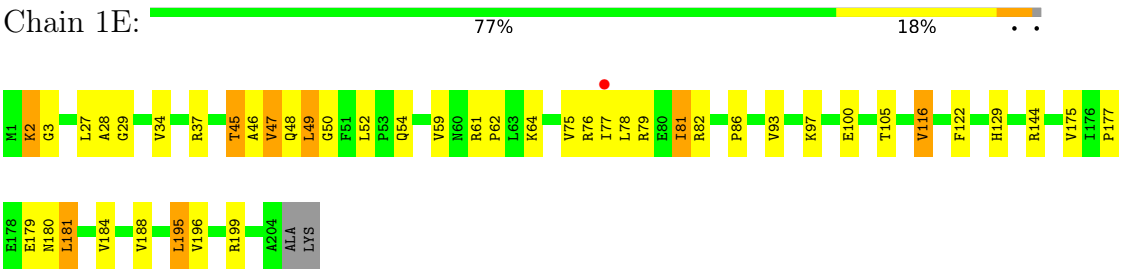
• Molecule 3: 50S ribosomal protein L2

Chain 2D:



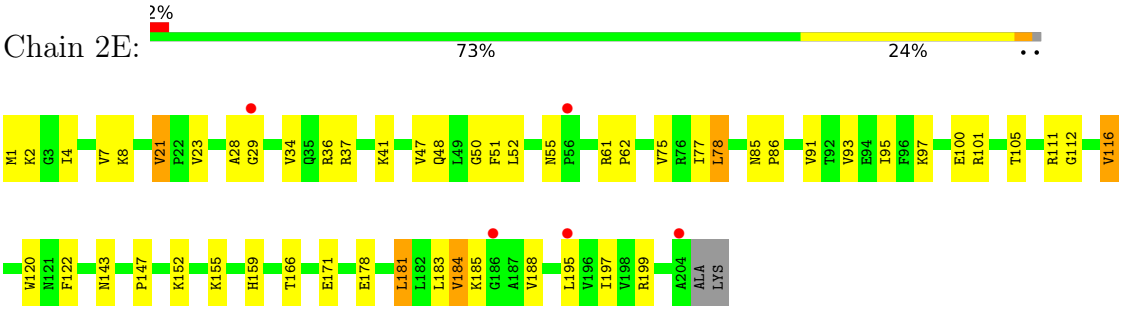
• Molecule 4: 50S ribosomal protein L3

Chain 1E:



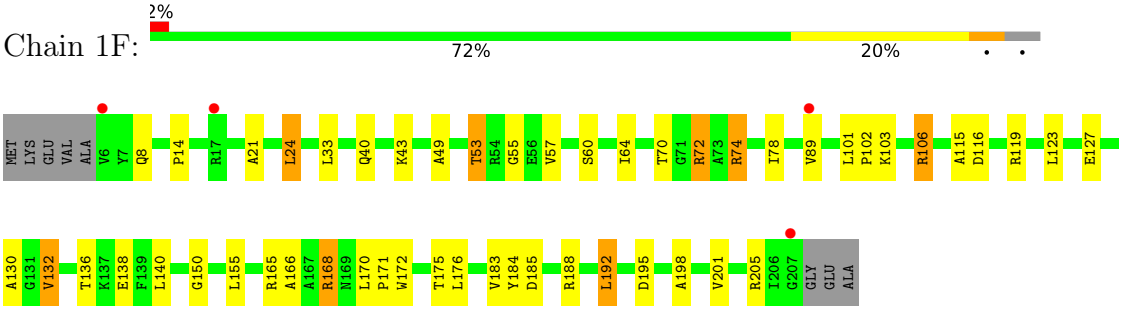
• Molecule 4: 50S ribosomal protein L3

Chain 2E:



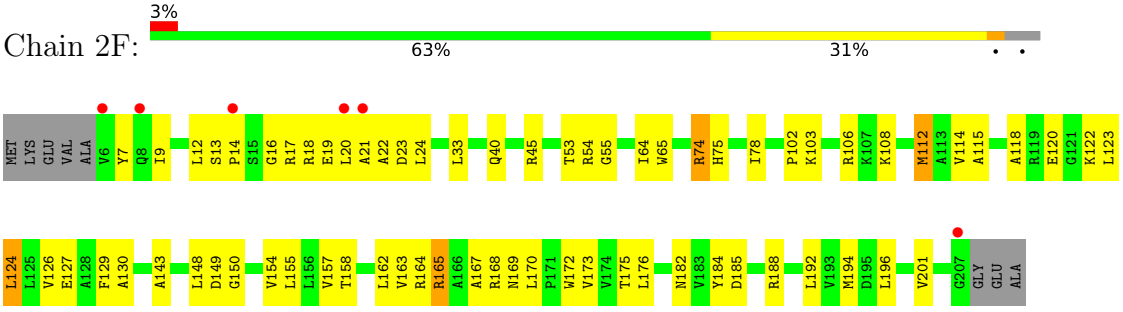
• Molecule 5: 50S ribosomal protein L4

Chain 1F:



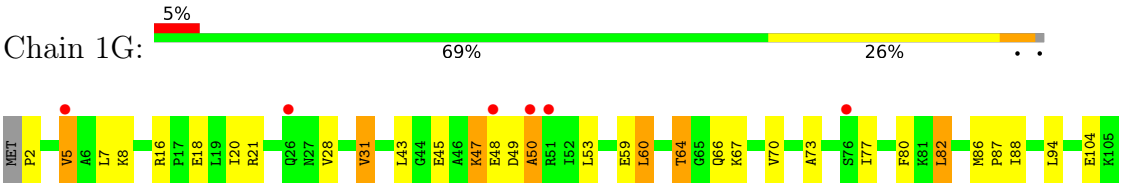
• Molecule 5: 50S ribosomal protein L4

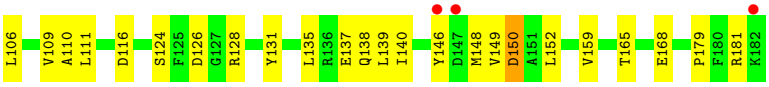
Chain 2F:



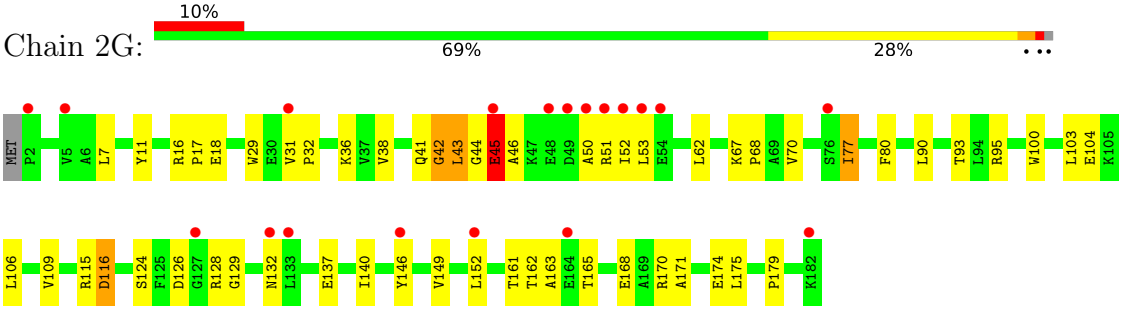
• Molecule 6: 50S ribosomal protein L5

Chain 1G:

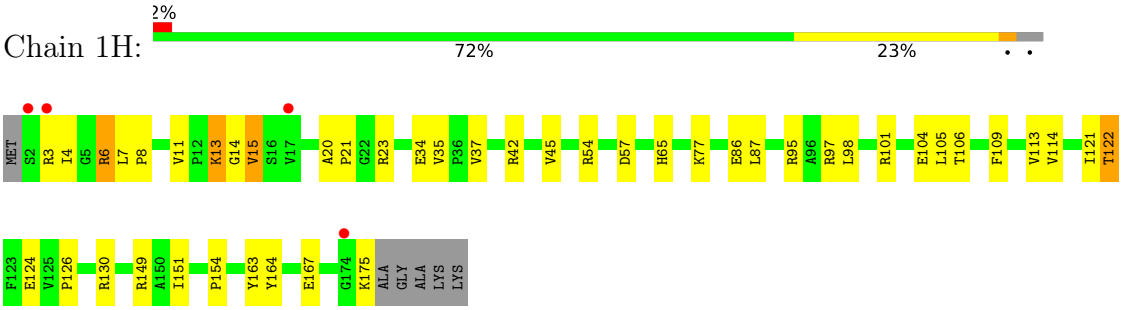




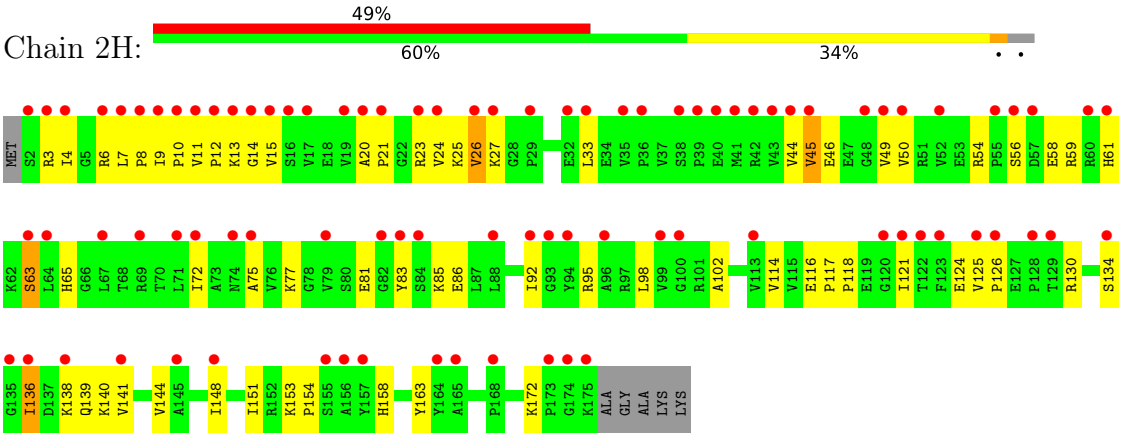
• Molecule 6: 50S ribosomal protein L5



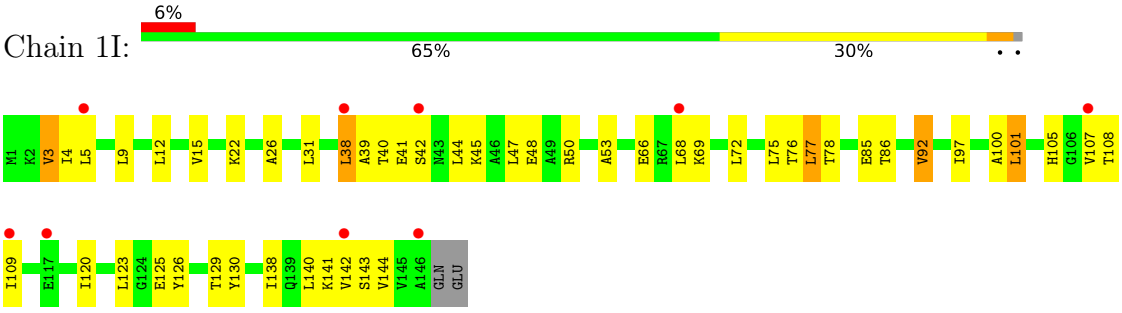
• Molecule 7: 50S ribosomal protein L6



• Molecule 7: 50S ribosomal protein L6

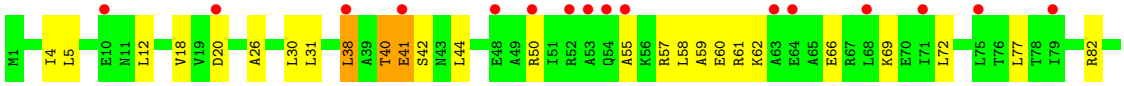


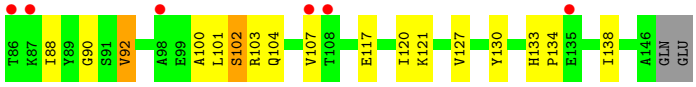
• Molecule 8: 50S ribosomal protein L9



• Molecule 8: 50S ribosomal protein L9

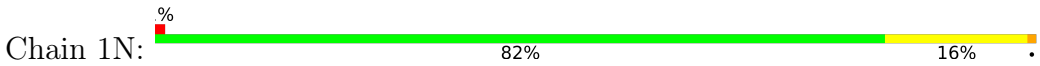
Chain 2I:

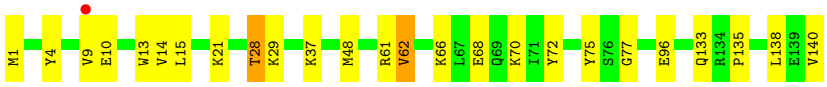




• Molecule 9: 50S ribosomal protein L13

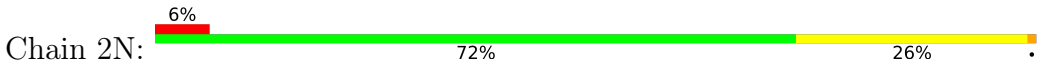
Chain 1N:

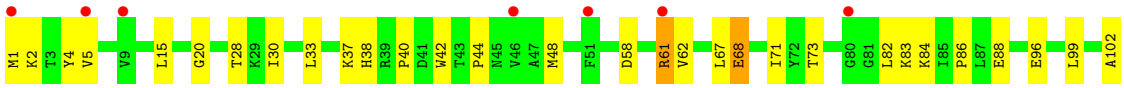




• Molecule 9: 50S ribosomal protein L13

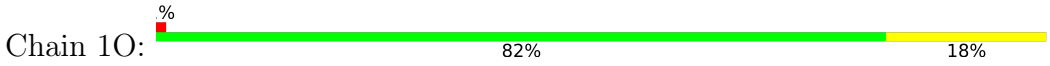
Chain 2N:

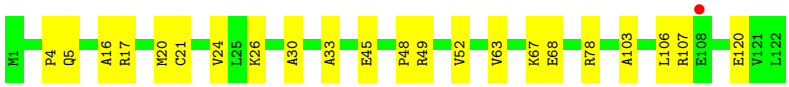




• Molecule 10: 50S ribosomal protein L14

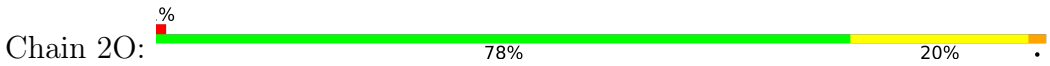
Chain 1O:

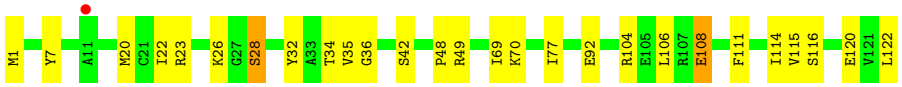




• Molecule 10: 50S ribosomal protein L14

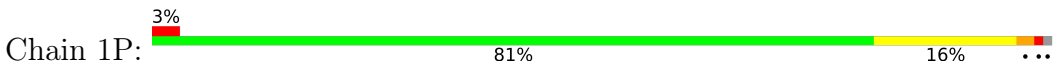
Chain 2O:

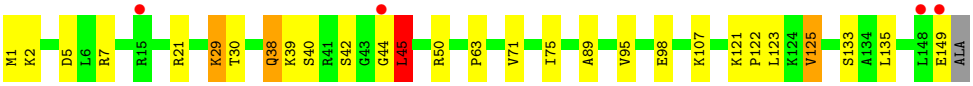




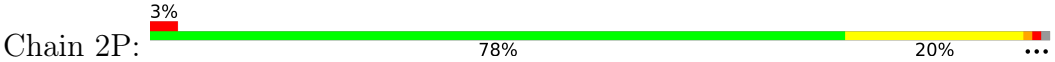
• Molecule 11: 50S ribosomal protein L15

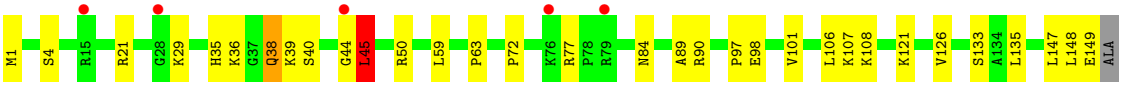
Chain 1P:



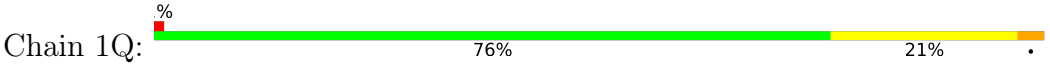


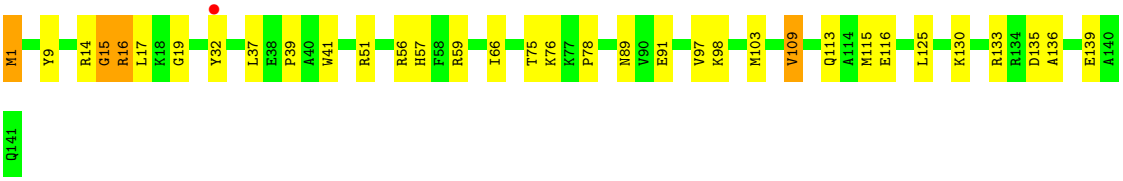
• Molecule 11: 50S ribosomal protein L15



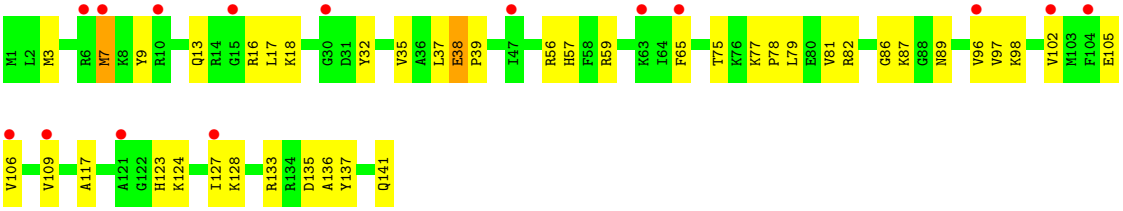


• Molecule 12: 50S ribosomal protein L16

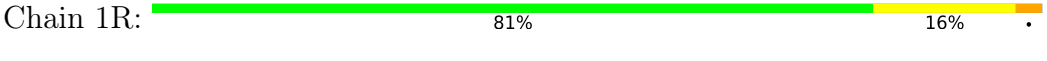




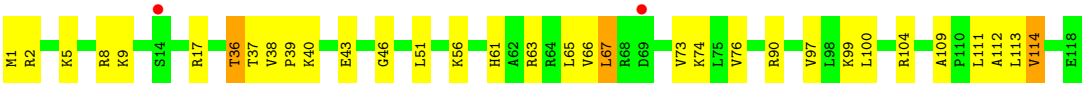
• Molecule 12: 50S ribosomal protein L16



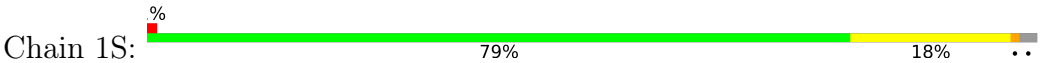
• Molecule 13: 50S ribosomal protein L17

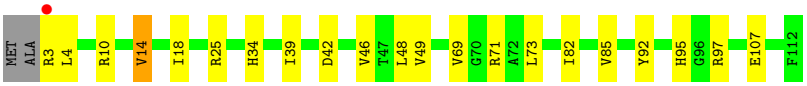


• Molecule 13: 50S ribosomal protein L17



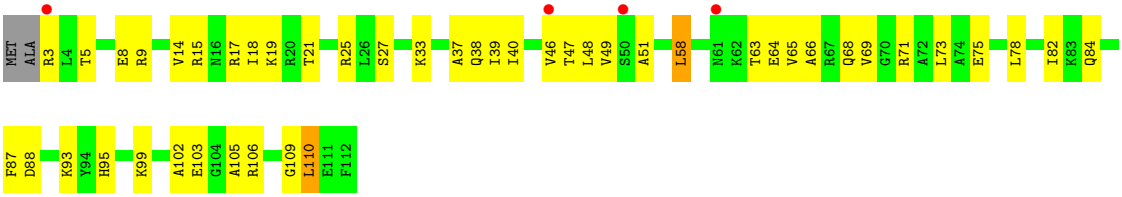
• Molecule 14: 50S ribosomal protein L18





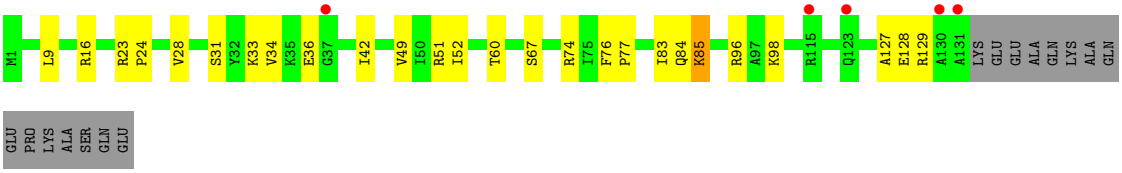
• Molecule 14: 50S ribosomal protein L18

Chain 2S:



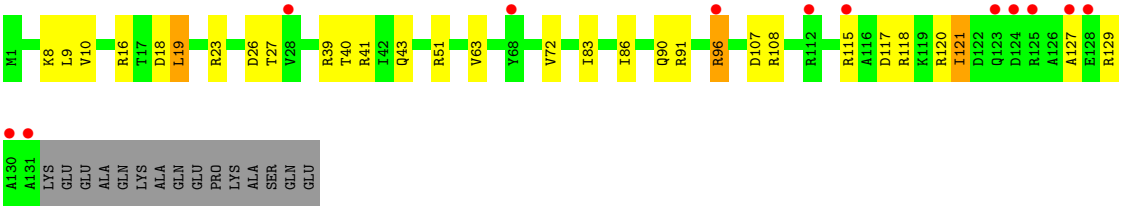
• Molecule 15: 50S ribosomal protein L19

Chain 1T:



• Molecule 15: 50S ribosomal protein L19

Chain 2T:

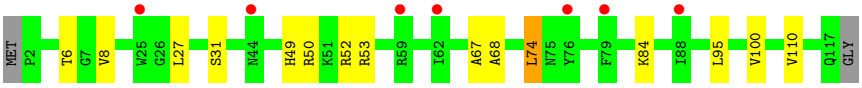


• Molecule 16: 50S ribosomal protein L20

Chain 1U:

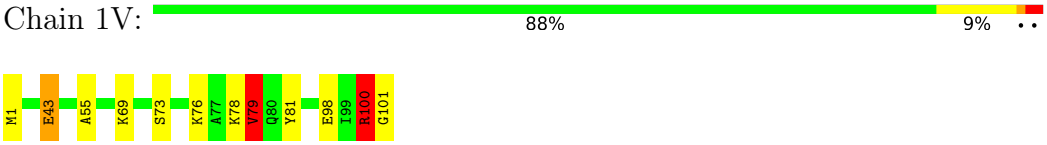
• Molecule 16: 50S ribosomal protein L20

Chain 2U:



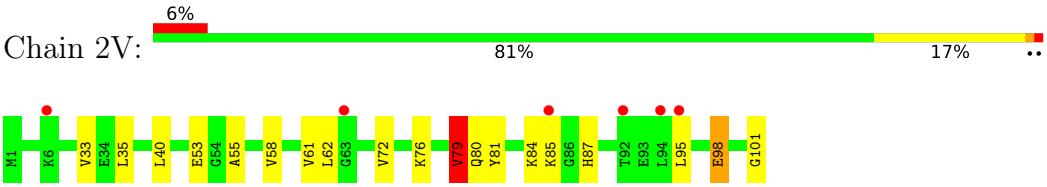
• Molecule 17: 50S ribosomal protein L21

Chain 1V:



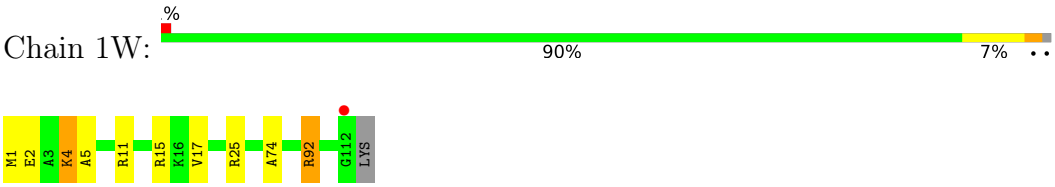
• Molecule 17: 50S ribosomal protein L21

Chain 2V:



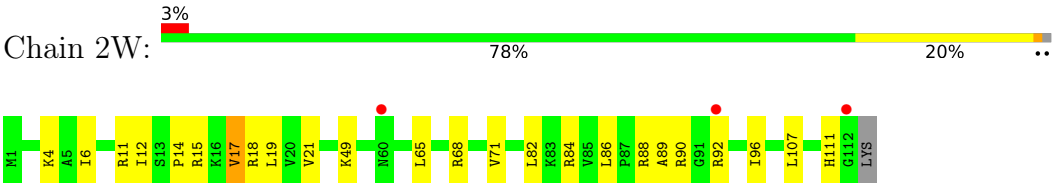
• Molecule 18: 50S ribosomal protein L22

Chain 1W:



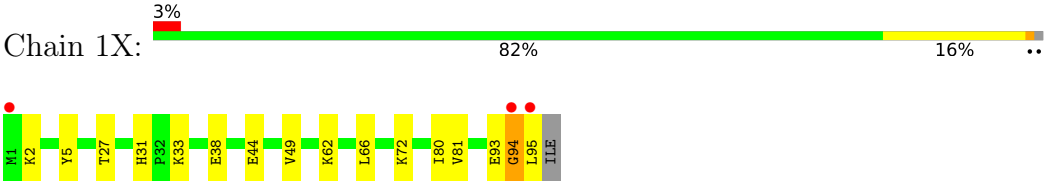
• Molecule 18: 50S ribosomal protein L22

Chain 2W:



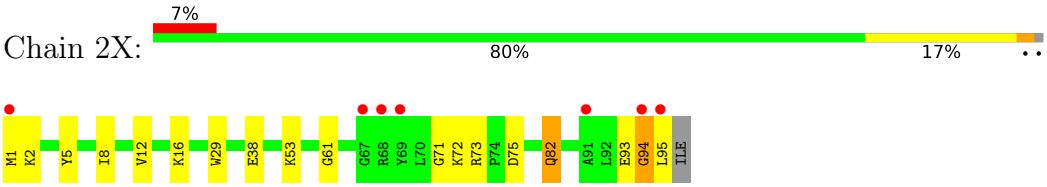
• Molecule 19: 50S ribosomal protein L23

Chain 1X:



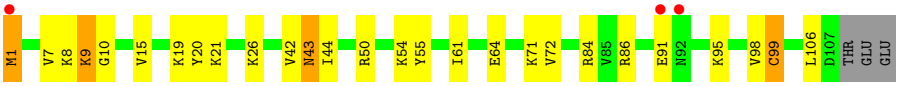
• Molecule 19: 50S ribosomal protein L23

Chain 2X:



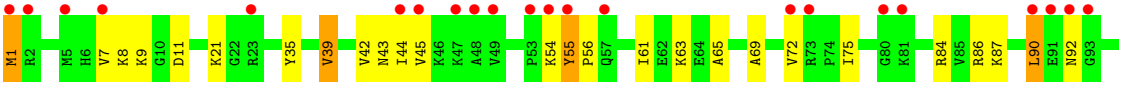
• Molecule 20: 50S ribosomal protein L24

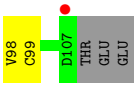
Chain 1Y:



• Molecule 20: 50S ribosomal protein L24

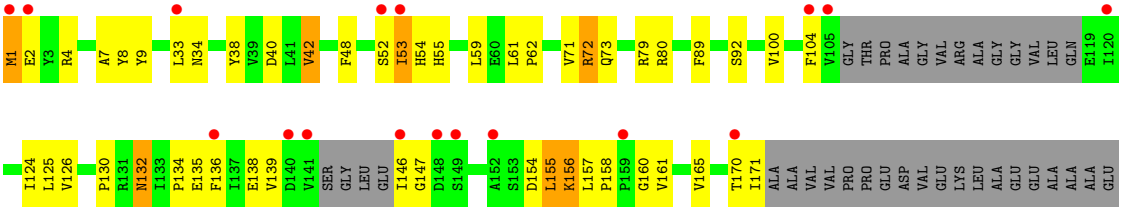
Chain 2Y:





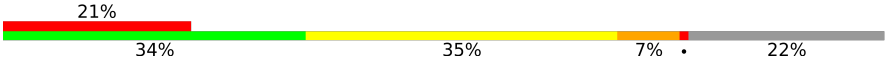
• Molecule 21: 50S ribosomal protein L25

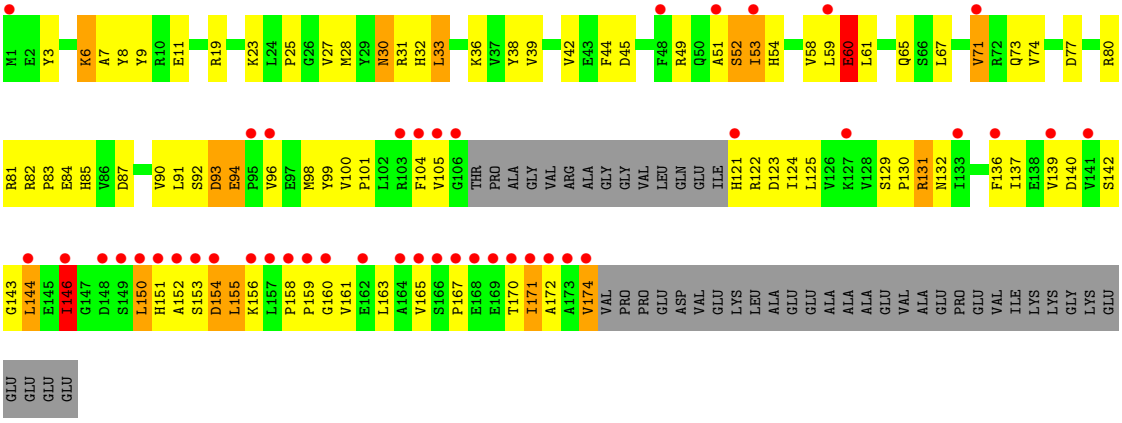
Chain 1Z:



• Molecule 21: 50S ribosomal protein L25

Chain 2Z:



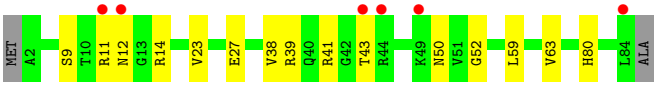


• Molecule 22: 50S ribosomal protein L27

Chain 10:

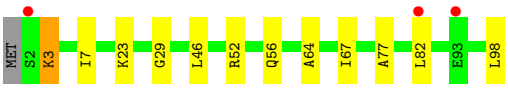
• Molecule 22: 50S ribosomal protein L27

Chain 20:



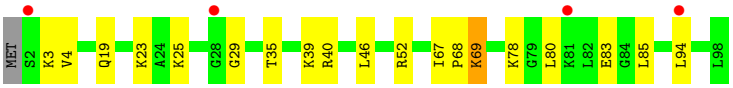
• Molecule 23: 50S ribosomal protein L28

Chain 11:



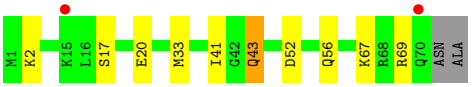
• Molecule 23: 50S ribosomal protein L28

Chain 21:



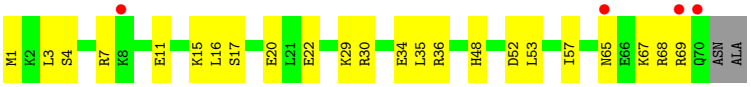
• Molecule 24: 50S ribosomal protein L29

Chain 12:



• Molecule 24: 50S ribosomal protein L29

Chain 22:

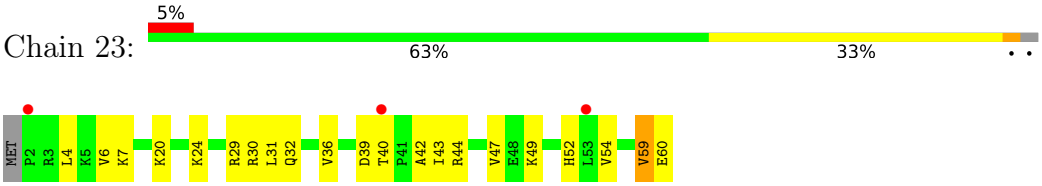


• Molecule 25: 50S ribosomal protein L30

Chain 13:

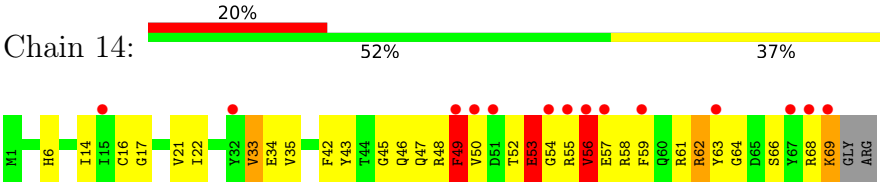
• Molecule 25: 50S ribosomal protein L30

Chain 23:



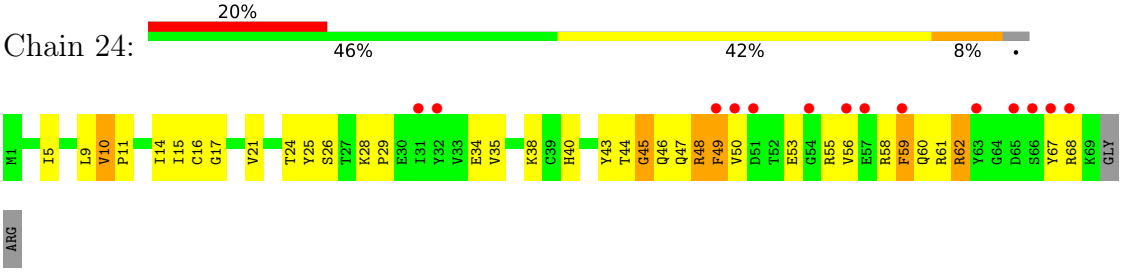
• Molecule 26: 50S ribosomal protein L31

Chain 14:



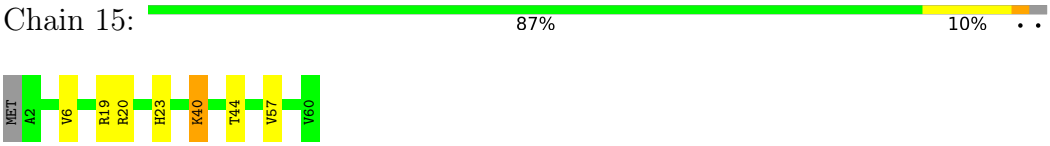
• Molecule 26: 50S ribosomal protein L31

Chain 24:



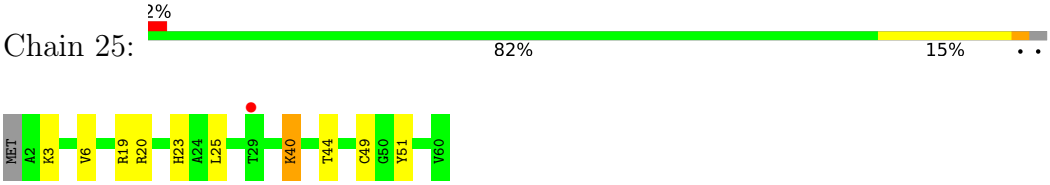
• Molecule 27: 50S ribosomal protein L32

Chain 15:



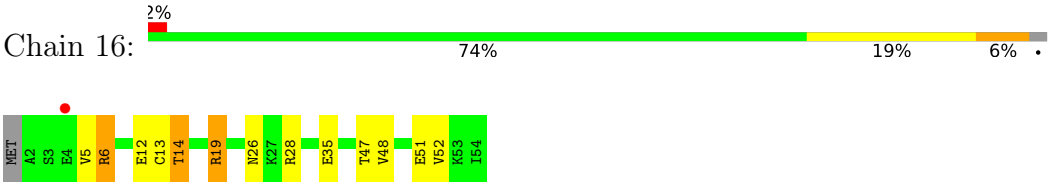
• Molecule 27: 50S ribosomal protein L32

Chain 25:



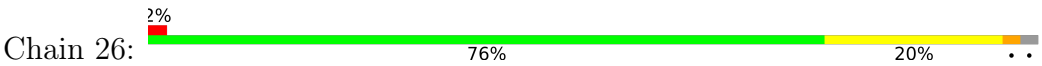
• Molecule 28: 50S ribosomal protein L33

Chain 16:

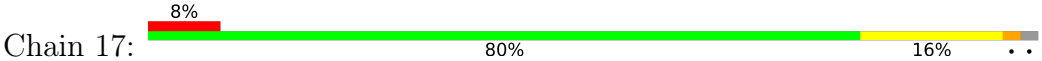


• Molecule 28: 50S ribosomal protein L33

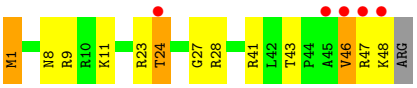
Chain 26:



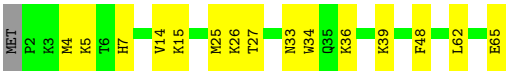
• Molecule 29: 50S ribosomal protein L34



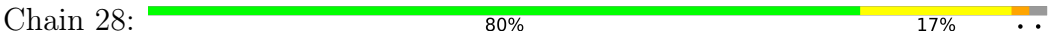
• Molecule 29: 50S ribosomal protein L34

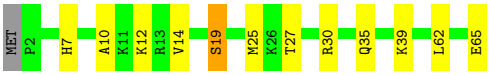


• Molecule 30: 50S ribosomal protein L35

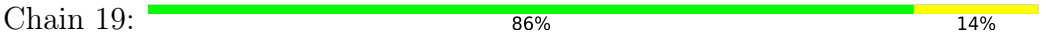


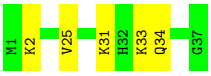
• Molecule 30: 50S ribosomal protein L35



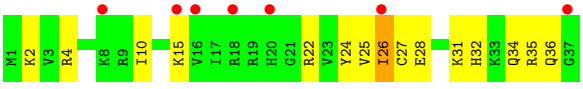


• Molecule 31: 50S ribosomal protein L36

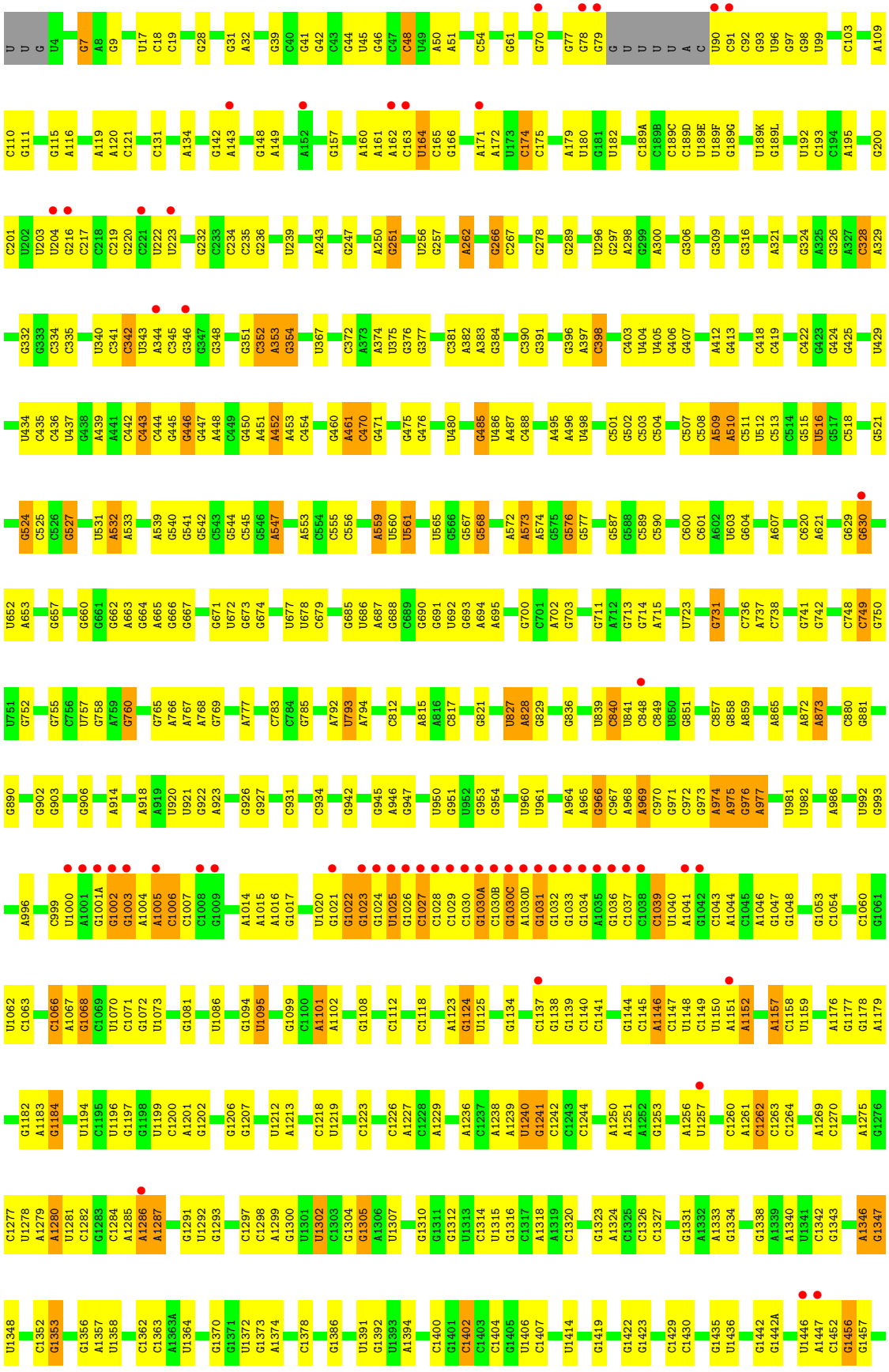


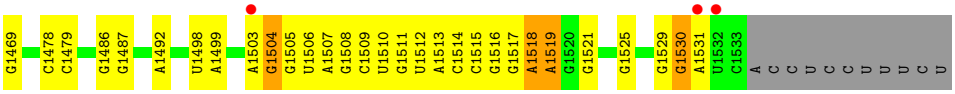


• Molecule 31: 50S ribosomal protein L36



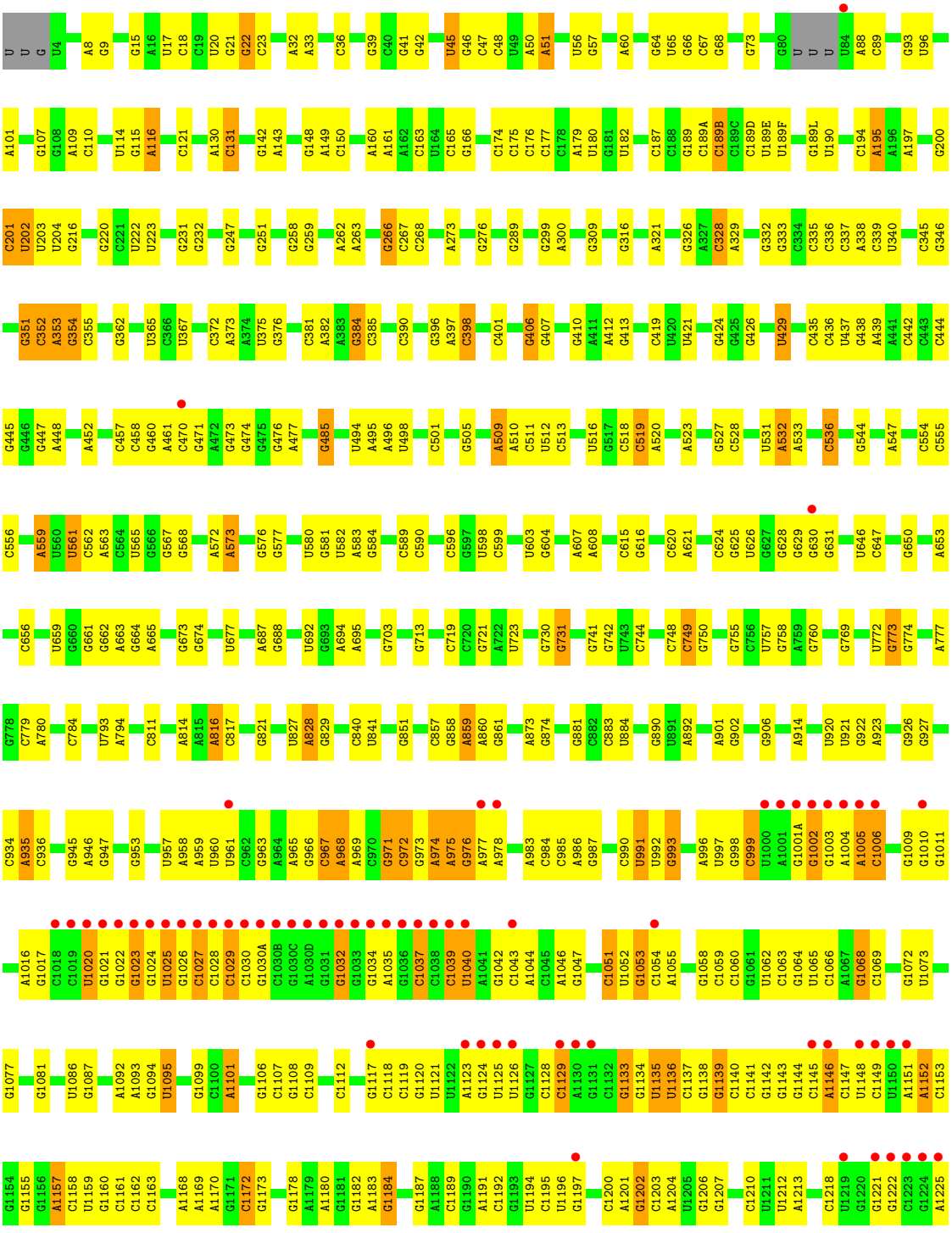
• Molecule 32: 16S Ribosomal RNA

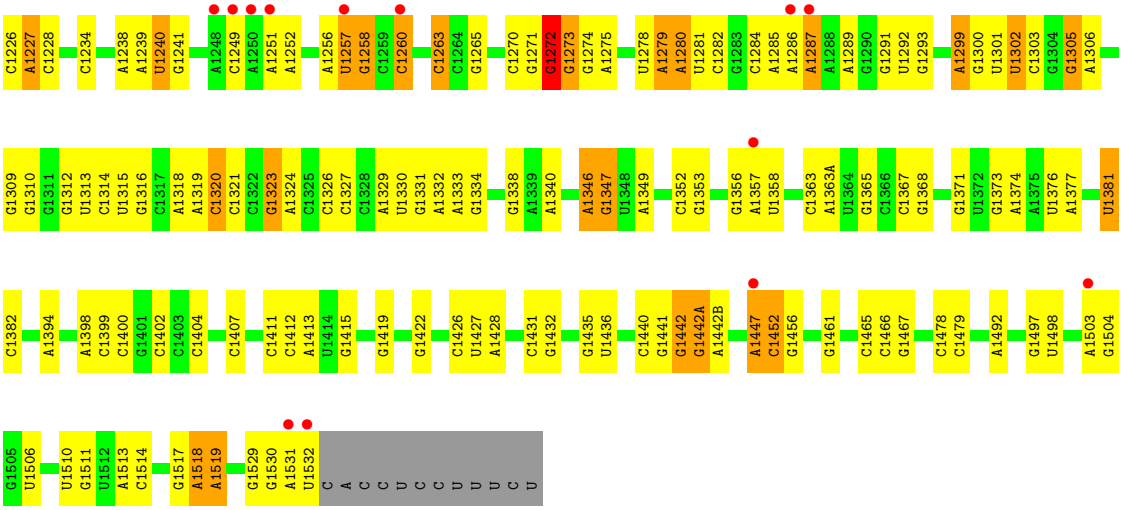

U U G U4 G7 A8 G9 U17 C18 C19 G28 G31 A32 G39 C40 G41 G42 C43 G44 U45 G46 C47 C48 U49 A50 A51 C54 G61 G70 G77 G78 G79 G U U U A C U90 C91 C92 G93 U96 G97 G98 U99 C103 A109
C110 G111 G115 A116 A119 A120 C121 C131 A134 G142 A143 G148 A149 A152 G157 A160 A161 A162 C163 U164 C165 G166 A171 A172 U173 C174 C175 A179 U180 G181 U182 C189A C189B C189C C189D U189E U189F G189G U189K G189L U192 C193 C194 A195 G200
C201 U202 U203 U204 G216 C217 C218 C219 C220 C221 U222 U223 G232 C233 C234 C235 C236 U239 A243 G247 A250 G251 U256 C257 A262 G266 C267 G278 G289 U296 G297 A298 G299 A300 G306 G309 G316 A321 G324 A325 G326 A327 C328 A329
G332 G333 C334 C335 U340 C341 C342 U343 A344 C345 G346 G347 G348 G351 C352 A353 G354 U367 C372 A373 A374 U375 G376 G377 C381 A382 A383 G384 C390 G391 G396 A397 C398 C403 U404 U405 G406 G407 A412 G413 C418 C419 C422 G423 G424 G425 U429
U434 C435 C436 U437 G438 A439 A441 C442 C443 C444 G445 G446 G447 A448 C449 G450 A451 A452 A453 C454 G460 A461 C470 G471 G475 G476 U480 G485 U486 A487 C488 A495 A496 U498 C501 G502 C503 C504 C507 C508 A509 A510 C511 U512 C513 C514 G515 U516 G517 C518 G521
G524 C525 C526 G527 U531 A532 A533 A539 G540 G541 G542 C543 G544 C545 G546 A547 A553 C554 C555 C556 A559 U560 U561 U565 G566 G567 G568 A572 A573 A574 G575 G576 G577 G587 G588 C589 C590 C600 C601 A602 U603 G604 A607 C620 A621 G629 G630
U652 A653 G657 G660 G661 G662 A663 G664 A665 G666 G667 G671 U672 G673 G674 U677 U678 C679 G685 U686 A687 G688 C689 G690 G691 U692 G693 A694 A695 G700 C701 A702 G703 G711 A712 G713 G714 A715 U723 G731 C736 A737 C738 G741 G742 C748 C749 G750
U751 G752 G755 C756 U757 G758 A759 G760 G765 A766 A767 A768 G769 A777 C783 C784 G785 A792 U793 A794 C812 A815 A816 C817 G821 U827 A828 G829 G836 U839 C840 U841 C848 C849 U850 G851 C857 G858 A859 A865 A872 A873 C880 G881
G890 G902 G903 G906 A914 A918 A919 U920 U921 G922 A923 G926 G927 C931 C934 G942 G945 A946 G947 U950 G951 U952 G953 G954 U960 U961 A964 A965 G966 C967 A968 A969 C970 G971 C972 G973 A974 A975 G976 A977 U981 U982 A986 U992 G993
A996 C999 U1000 A1001 G1001A G1002 G1003 A1004 A1005 C1006 C1007 C1008 G1009 A1014 A1015 A1016 G1017 U1020 G1021 G1022 G1023 G1024 U1025 G1026 C1027 C1028 C1029 C1030 G1030A C1030B A1030C A1030D G1031 G1032 G1033 G1034 A1035 G1036 C1037 C1038 C1039 U1040 A1041 G1042 C1043 A1044 C1045 A1046 G1047 G1048 G1053 C1054 C1060 G1061
U1062 C1063 C1066 A1067 G1068 C1069 U1070 C1071 G1072 U1073 G1081 U1086 G1094 U1095 G1099 C1100 A1101 A1102 G1108 C1112 C1118 A1123 G1124 U1125 G1134 C1137 G1138 G1139 C1140 C1141 G1144 C1145 A1146 C1147 U1148 C1149 U1150 A1151 A1152 A1157 C1158 U1159 A1176 G1177 G1178 A1179
G1182 A1183 G1184 U1194 C1195 U1196 G1197 G1198 U1199 C1200 A1201 G1202 G1206 G1207 U1212 A1213 C1218 U1219 C1223 C1226 A1227 C1228 A1229 A1236 C1237 A1238 A1239 U1240 G1241 C1242 C1243 C1244 A1250 A1251 A1252 G1253 A1256 U1257 C1260 A1261 C1262 C1263 C1264 A1269 C1270 A1275 G1276
C1277 U1278 A1279 A1280 U1281 C1282 G1283 C1284 A1285 A1286 A1287 G1291 U1292 G1293 C1297 C1298 A1299 G1300 U1301 U1302 C1303 G1304 G1305 A1306 U1307 G1310 C1311 G1312 U1313 C1314 U1315 G1316 C1317 A1318 A1319 C1320 G1323 A1324 C1325 C1326 C1327 G1331 A1332 A1333 G1334 G1338 A1339 A1340 U1341 C1342 G1343 A1346 G1347
U1348 C1352 G1353 G1356 A1357 U1358 C1362 C1363 A1363A U1364 G1370 G1371 U1372 C1373 A1374 C1378 G1386 U1391 G1392 U1393 A1394 C1400 G1401 C1402 C1403 C1404 G1405 U1406 C1407 U1414 G1419 G1422 G1423 C1429 C1430 G1435 U1436 G1442 G1442A U1446 A1447 C1452 G1456 G1457



• Molecule 32: 16S Ribosomal RNA

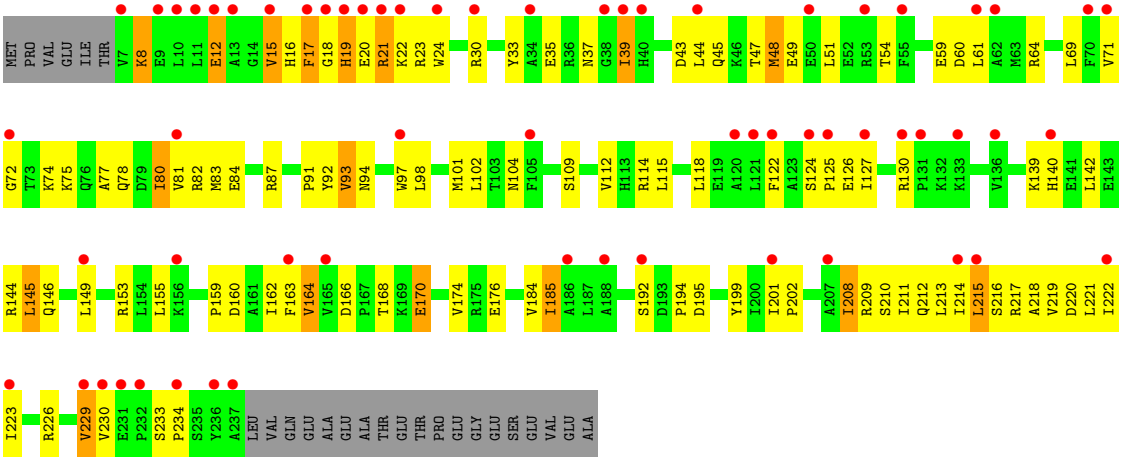
Chain 2a:





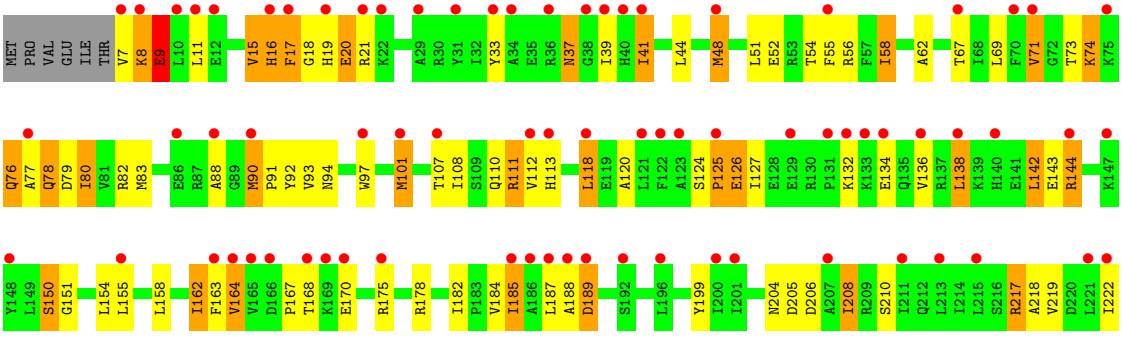
• Molecule 33: 30S ribosomal protein S2

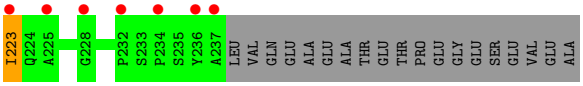
Chain 1b:



• Molecule 33: 30S ribosomal protein S2

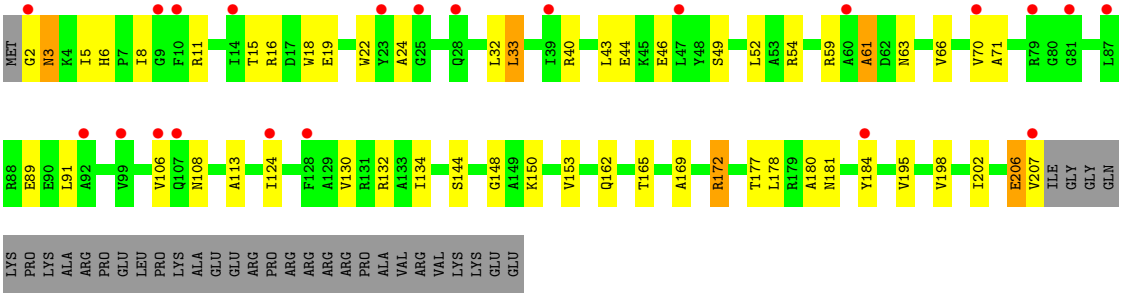
Chain 2b:





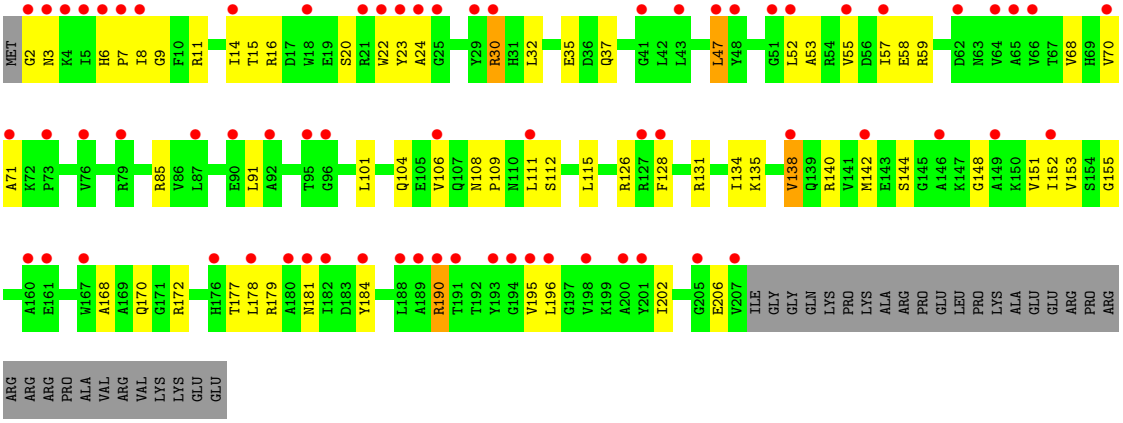
• Molecule 34: 30S ribosomal protein S3

Chain 1c:



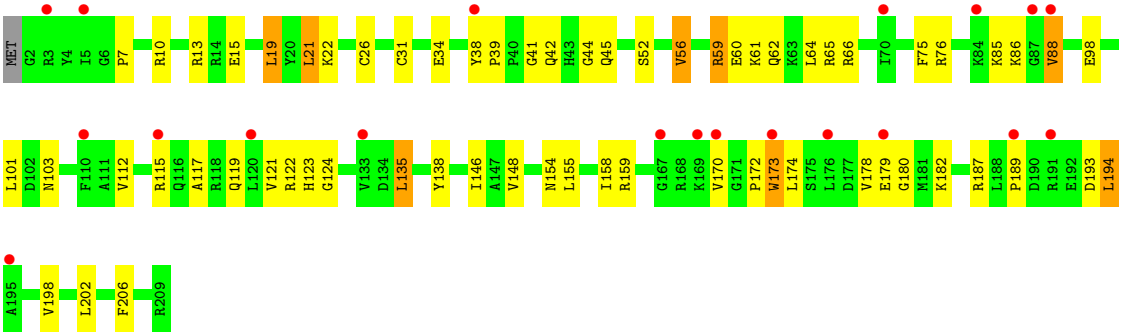
• Molecule 34: 30S ribosomal protein S3

Chain 2c:



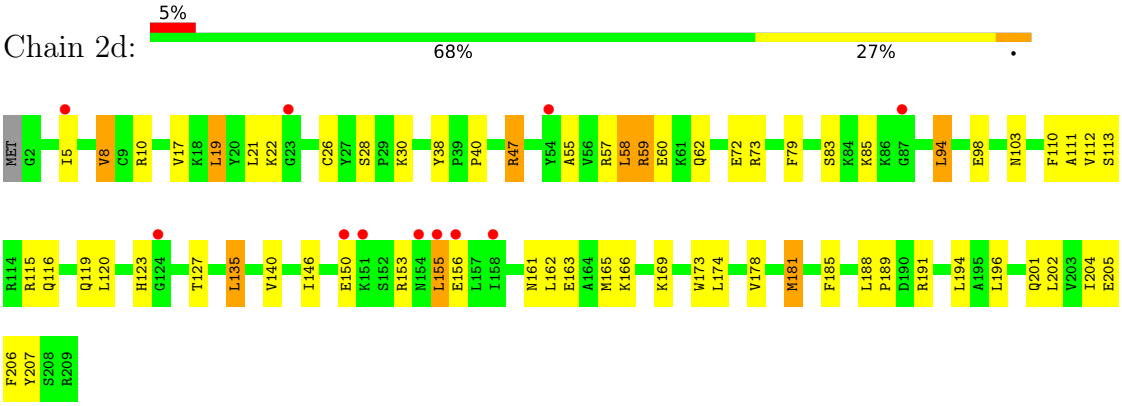
• Molecule 35: 30S ribosomal protein S4

Chain 1d:



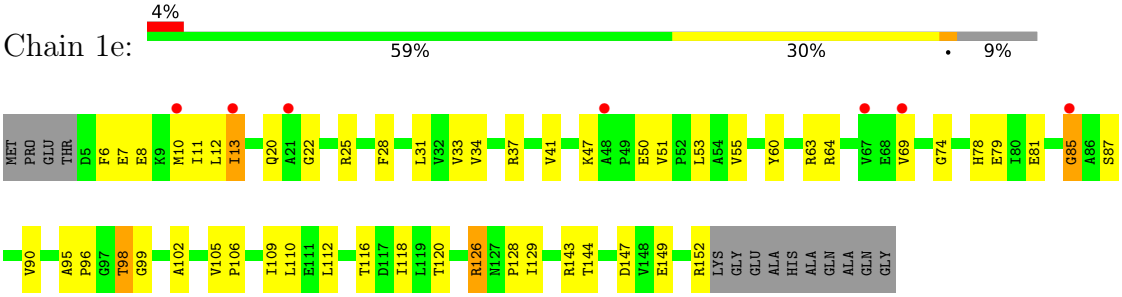
• Molecule 35: 30S ribosomal protein S4

Chain 2d:



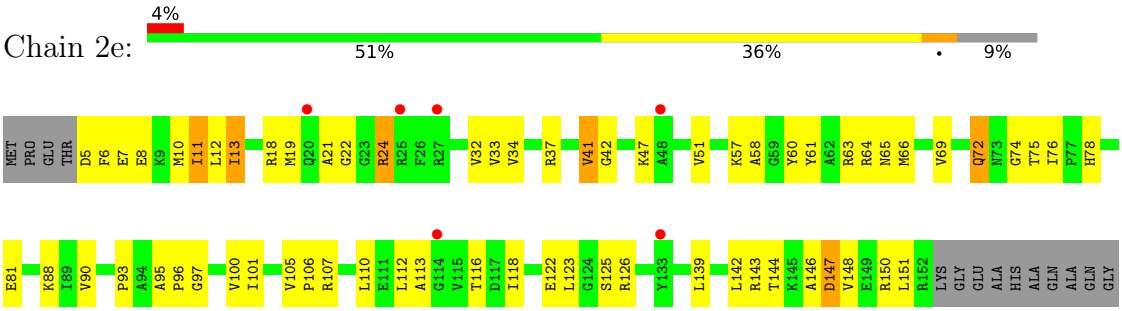
• Molecule 36: 30S ribosomal protein S5

Chain 1e:



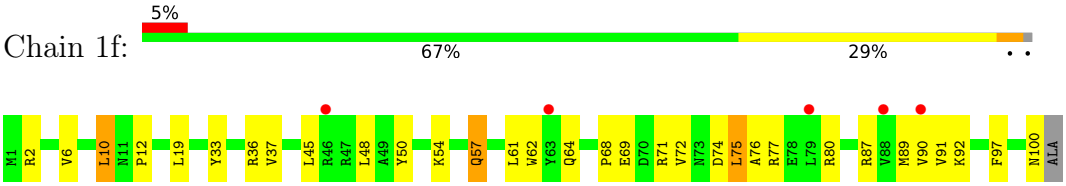
• Molecule 36: 30S ribosomal protein S5

Chain 2e:



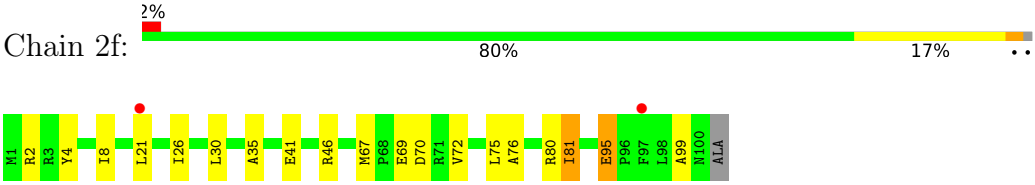
• Molecule 37: 30S ribosomal protein S6

Chain 1f:



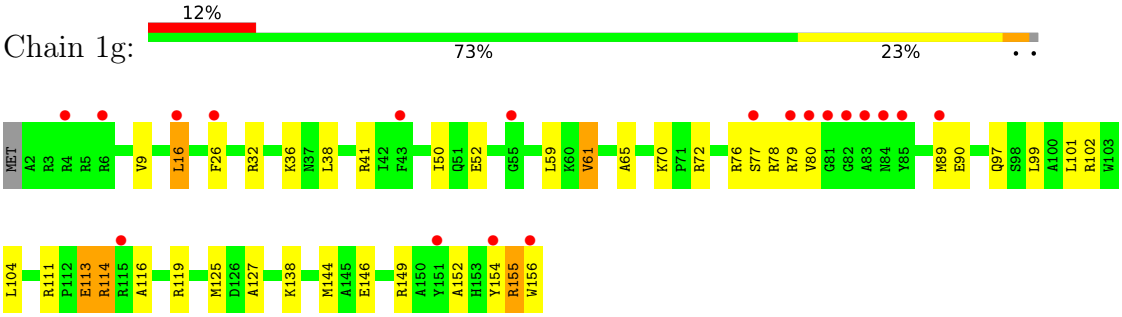
• Molecule 37: 30S ribosomal protein S6

Chain 2f:



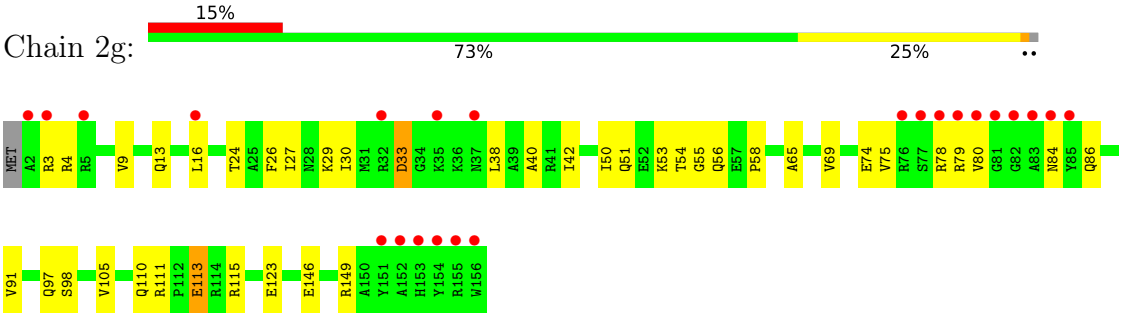
• Molecule 38: 30S ribosomal protein S7

Chain 1g:



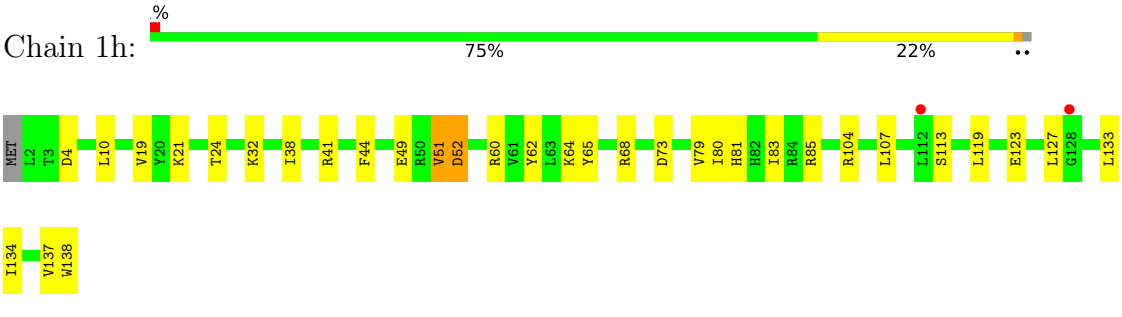
• Molecule 38: 30S ribosomal protein S7

Chain 2g:



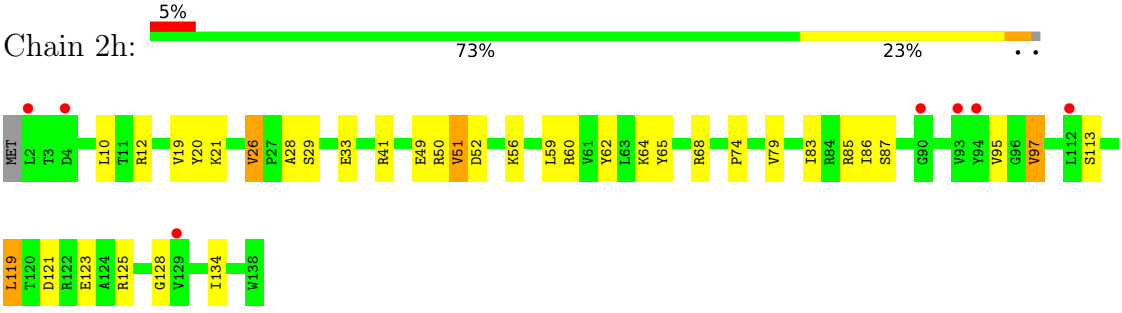
• Molecule 39: 30S ribosomal protein S8

Chain 1h:



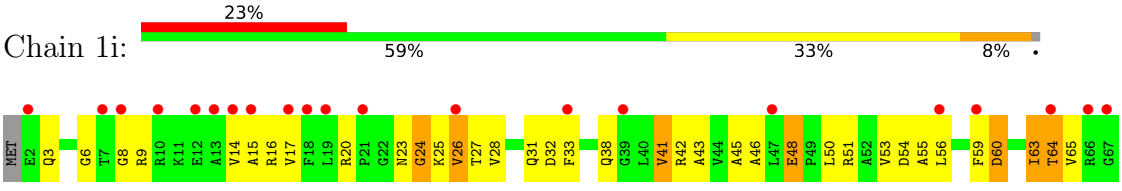
• Molecule 39: 30S ribosomal protein S8

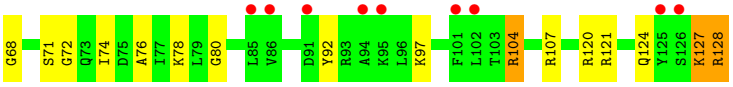
Chain 2h:



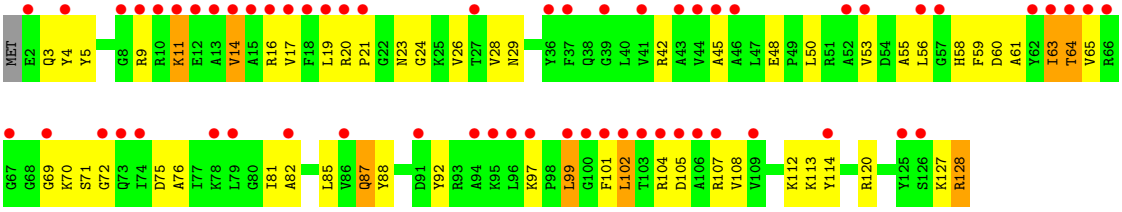
• Molecule 40: 30S ribosomal protein S9

Chain 1i:

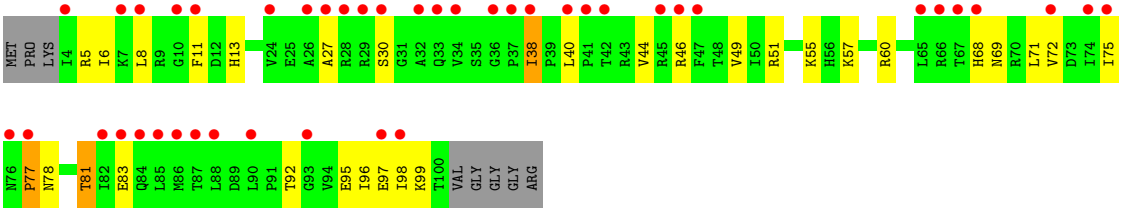




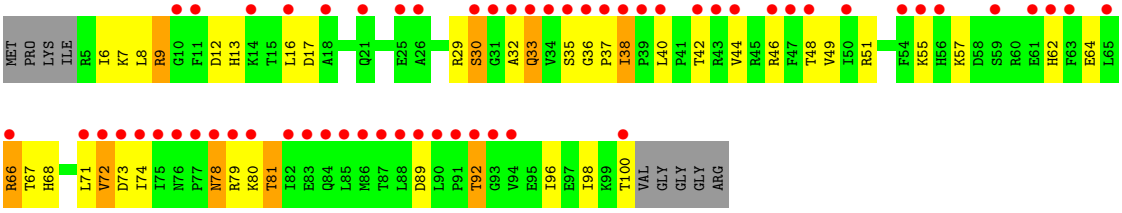
• Molecule 40: 30S ribosomal protein S9



• Molecule 41: 30S ribosomal protein S10



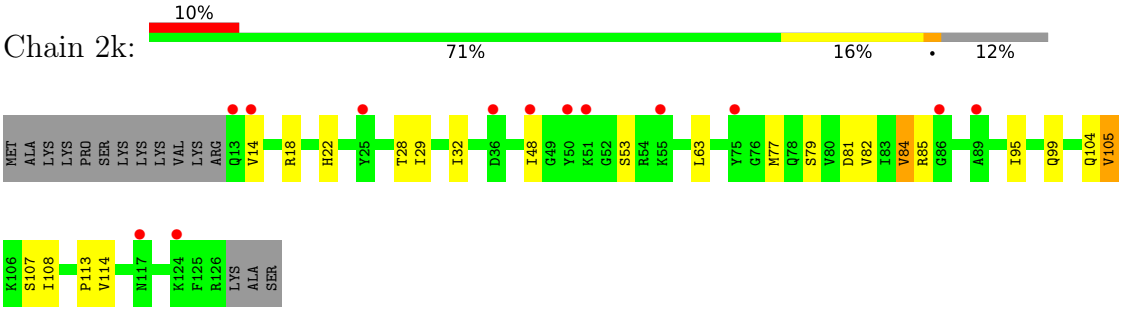
• Molecule 41: 30S ribosomal protein S10



• Molecule 42: 30S ribosomal protein S11

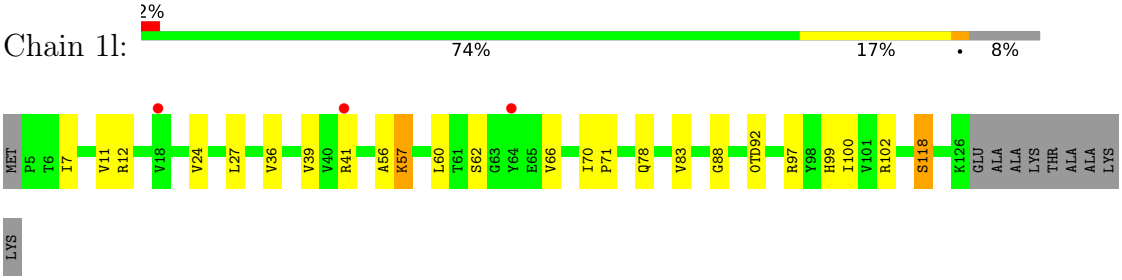
• Molecule 42: 30S ribosomal protein S11

Chain 2k:



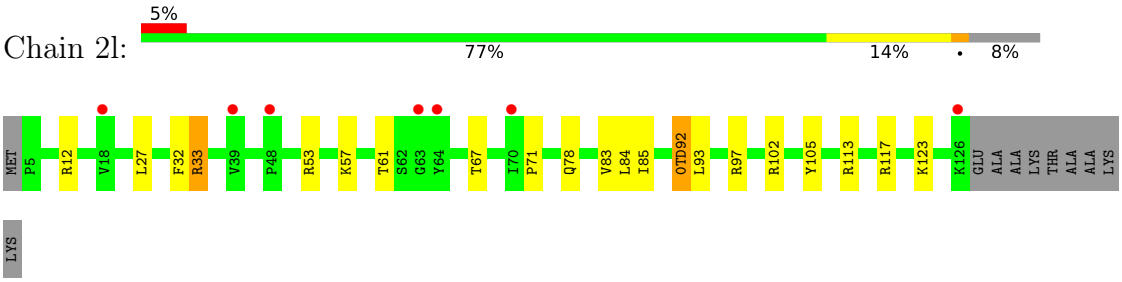
• Molecule 43: 30S ribosomal protein S12

Chain 1l:



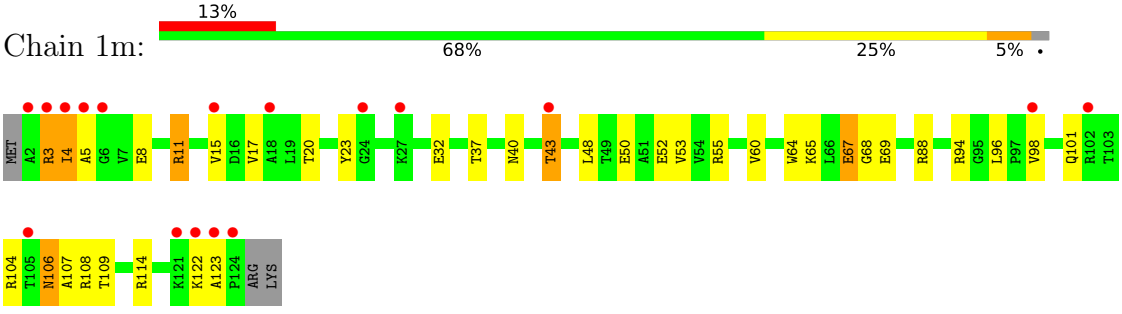
• Molecule 43: 30S ribosomal protein S12

Chain 2l:



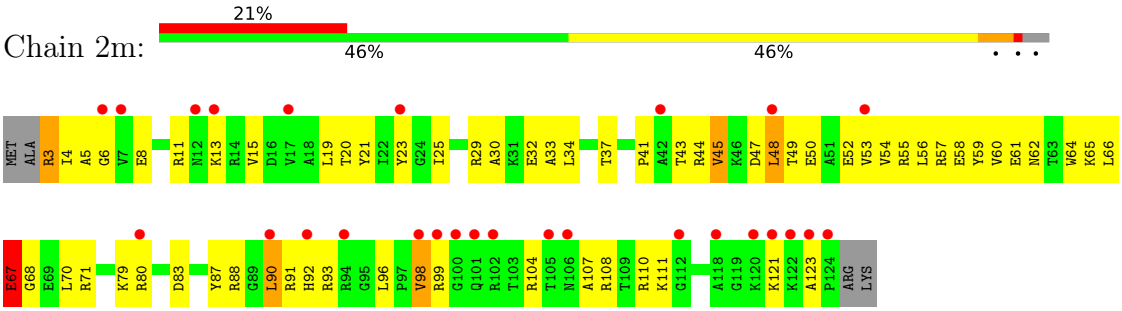
• Molecule 44: 30S ribosomal protein S13

Chain 1m:



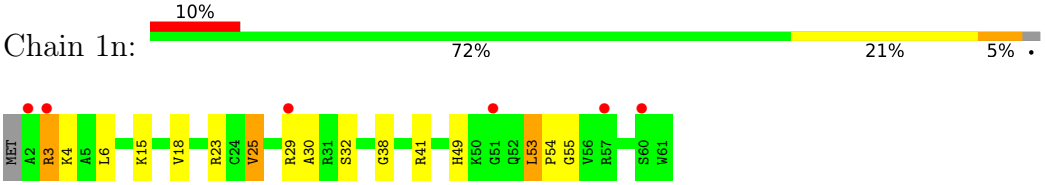
• Molecule 44: 30S ribosomal protein S13

Chain 2m:



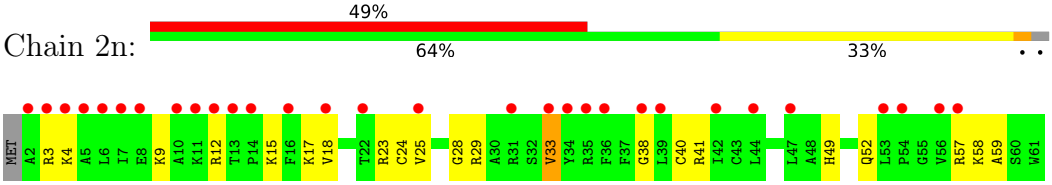
• Molecule 45: 30S ribosomal protein S14 type Z

Chain 1n:



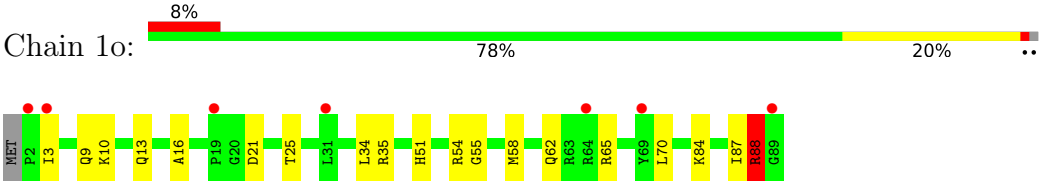
• Molecule 45: 30S ribosomal protein S14 type Z

Chain 2n:



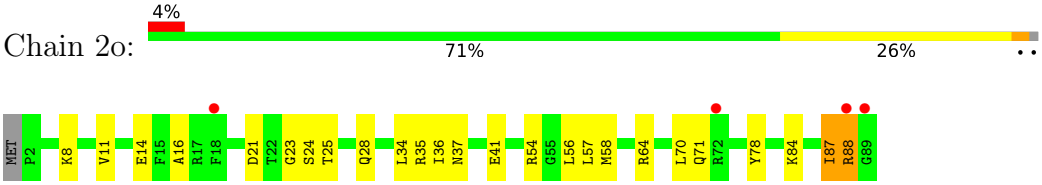
• Molecule 46: 30S ribosomal protein S15

Chain 1o:



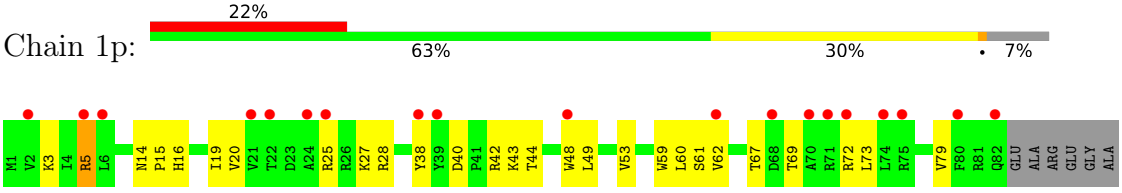
• Molecule 46: 30S ribosomal protein S15

Chain 2o:



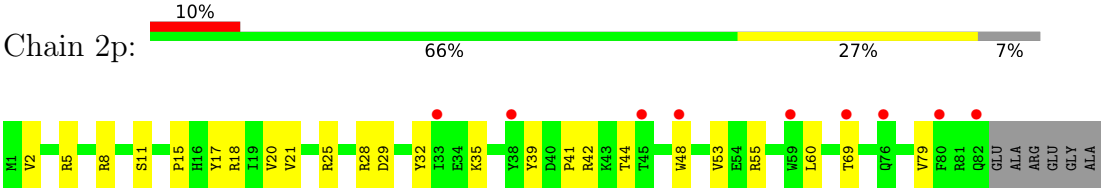
• Molecule 47: 30S ribosomal protein S16

Chain 1p:



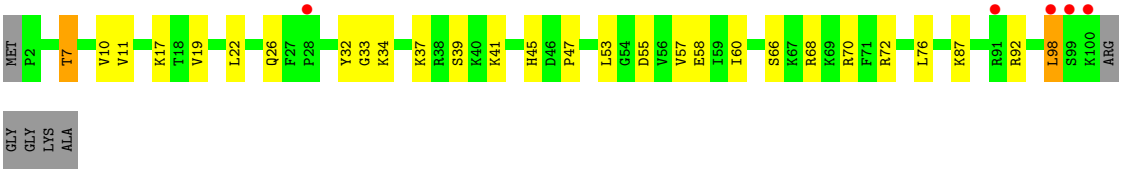
• Molecule 47: 30S ribosomal protein S16

Chain 2p:

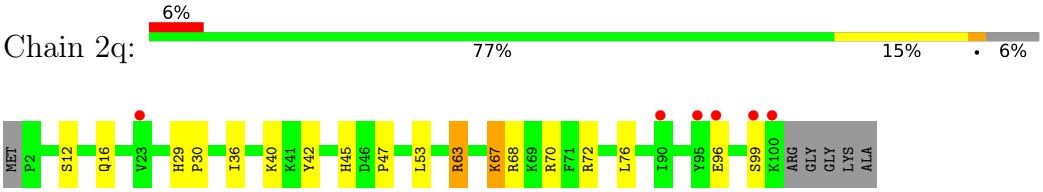


• Molecule 48: 30S ribosomal protein S17

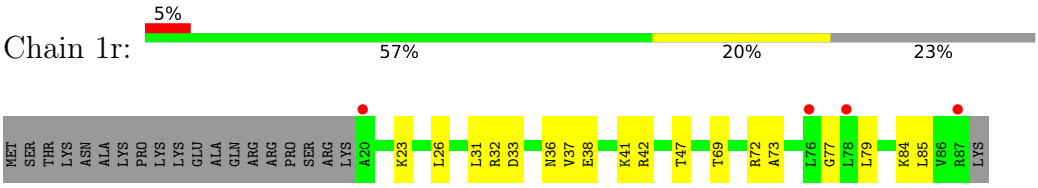
Chain 1q:



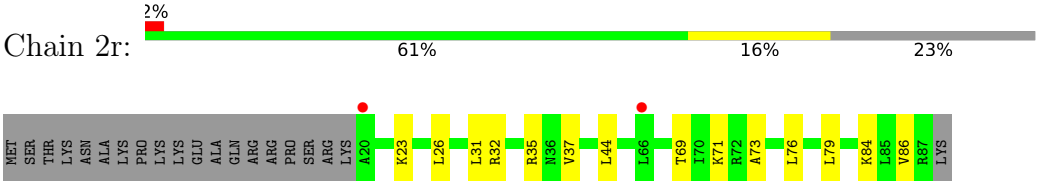
• Molecule 48: 30S ribosomal protein S17



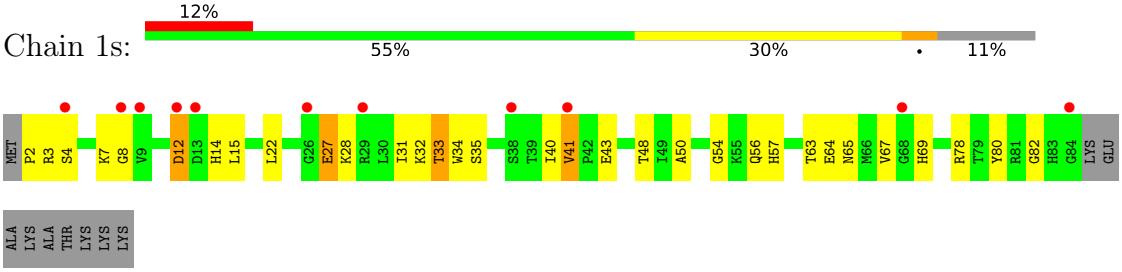
• Molecule 49: 30S ribosomal protein S18



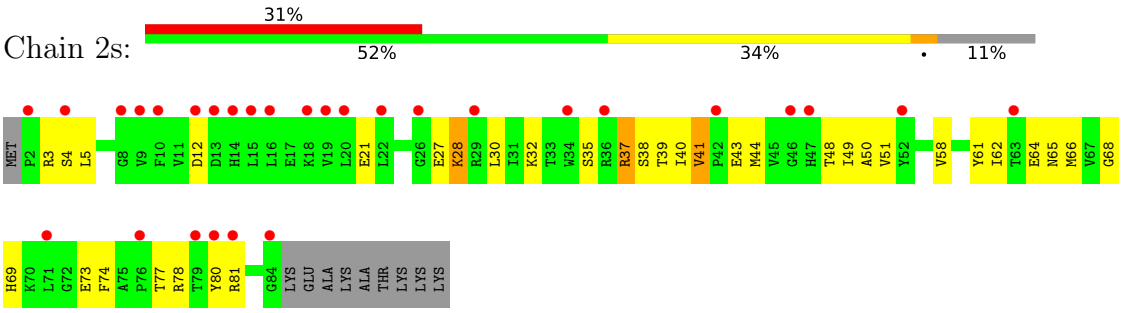
• Molecule 49: 30S ribosomal protein S18



• Molecule 50: 30S ribosomal protein S19

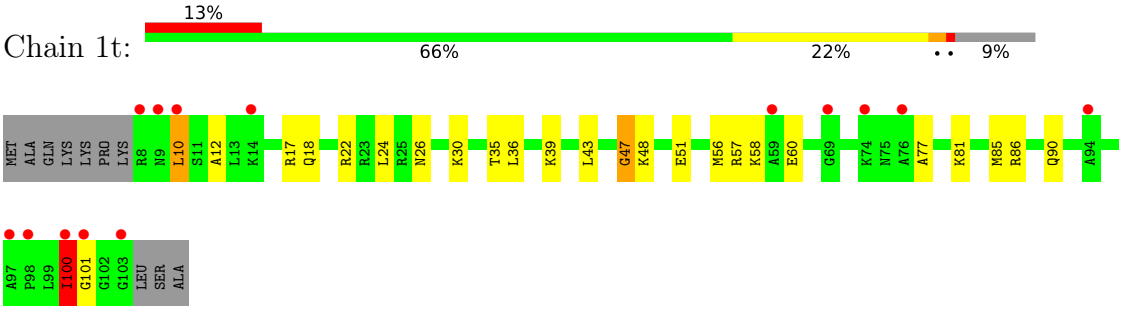


• Molecule 50: 30S ribosomal protein S19



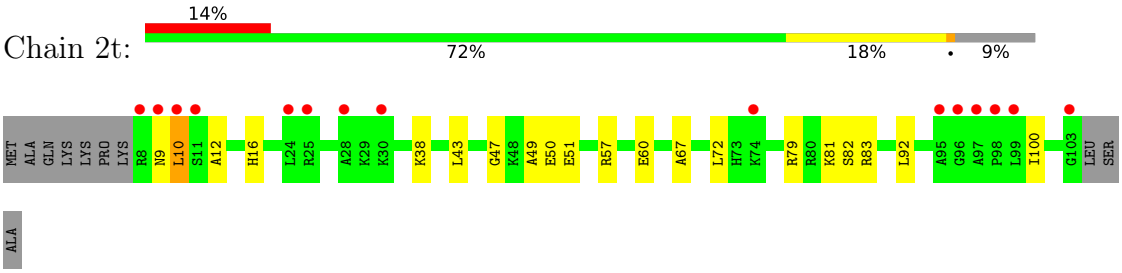
• Molecule 51: 30S ribosomal protein S20

Chain 1t:



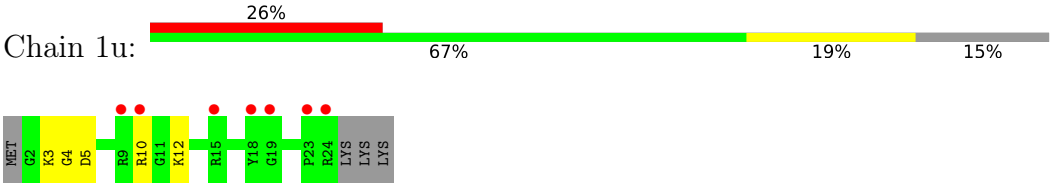
• Molecule 51: 30S ribosomal protein S20

Chain 2t:



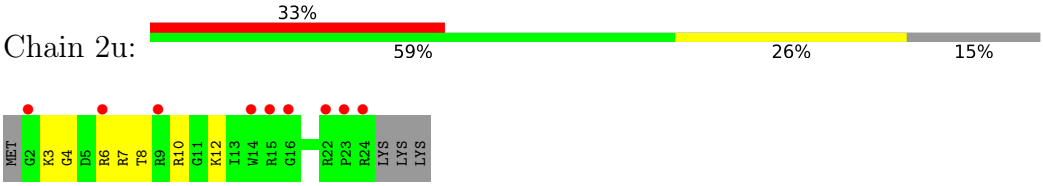
• Molecule 52: 30S ribosomal protein Thx

Chain 1u:



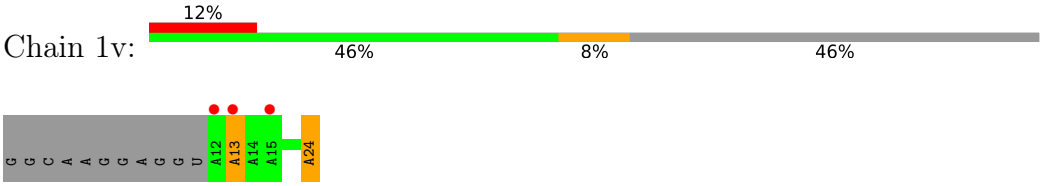
• Molecule 52: 30S ribosomal protein Thx

Chain 2u:



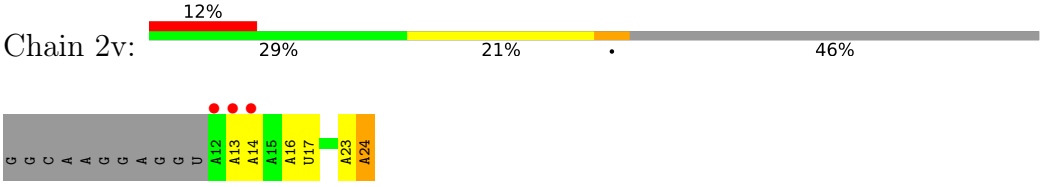
• Molecule 53: MF-mRNA

Chain 1v:



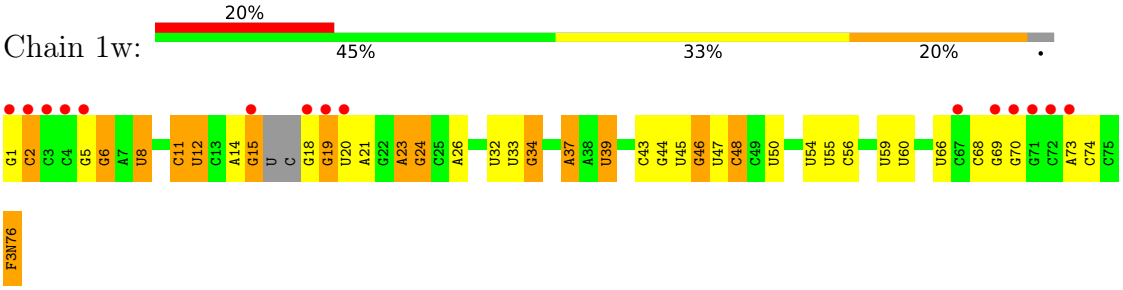
• Molecule 53: MF-mRNA

Chain 2v:



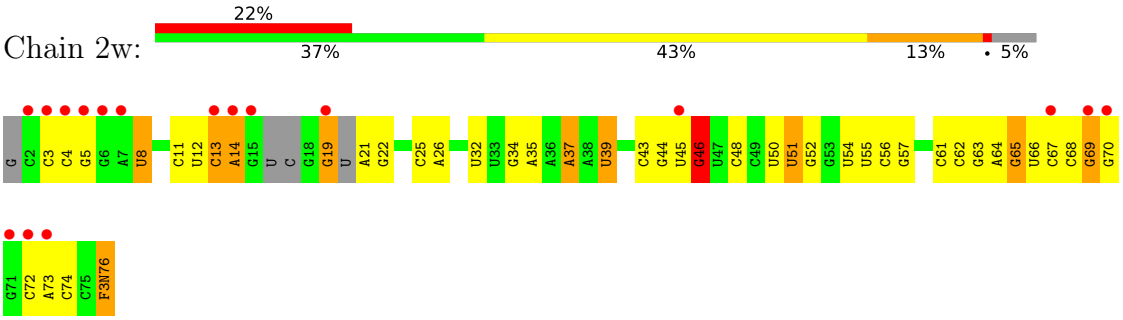
• Molecule 54: A-site Aminoacylated Phe-tRNAphe

Chain 1w:



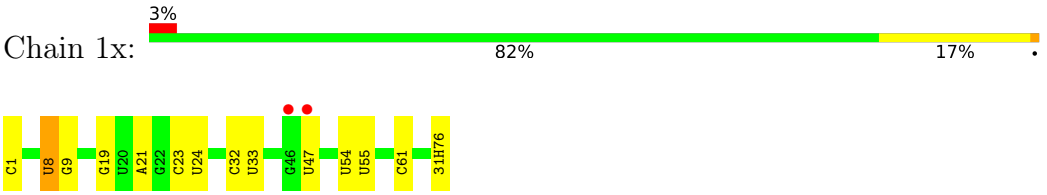
• Molecule 54: A-site Aminoacylated Phe-tRNAphe

Chain 2w:



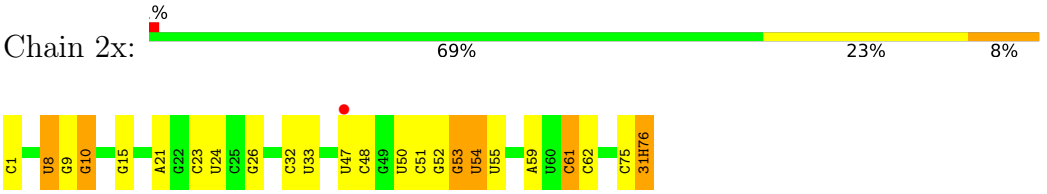
• Molecule 55: P-site Aminoacylated fMet-tRNAmet

Chain 1x:



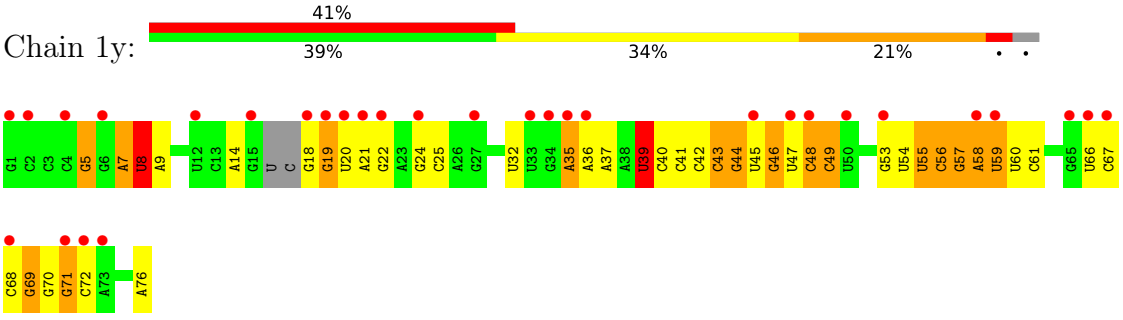
• Molecule 55: P-site Aminoacylated fMet-tRNAmet

Chain 2x:



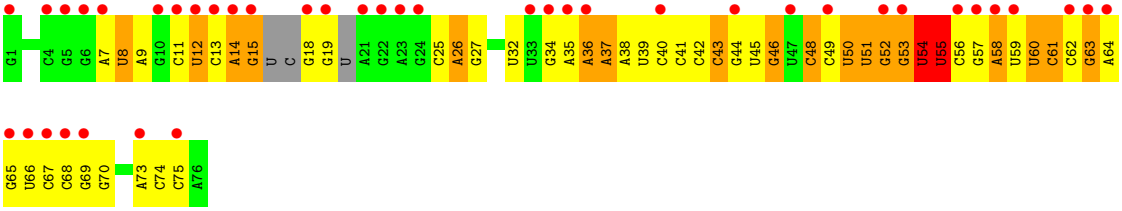
• Molecule 56: E-site Deacylated tRNAphe

Chain 1y:



• Molecule 56: E-site Deacylated tRNAphe

Chain 2y:


G1
C4
G5
G6
A7
U8
A9
G10
C11
U12
C13
A14
G15
U
C
G18
G19
U
A21
G22
A23
G24
C25
A26
G27
U32
U33
G34
A35
A36
A37
A38
U39
C40
C41
C42
C43
G44
U45
G46
U47
C48
C49
U50
U51
G52
G53
U54
U55
C56
G57
A58
U59
U60
C61
C62
G63
A64
G65
U66
C67
C68
G69
G70
A73
C74
C75
A76

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	210.09Å 449.74Å 625.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	153.52 – 2.55 153.52 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.0 (153.52-2.55) 99.1 (153.52-2.55)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.28 (at 2.55Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.213 , 0.252 0.216 , 0.254	Depositor DCC
R_{free} test set	94286 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	54.5	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 50.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	299618	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% 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: ZN, MG, MIA, 4SU, 5MU, SF4, 31H, UR3, F3N, 2MU, OMC, 2MG, 5MC, K, 4OC, 0TD, G7M, PSU, 8AH, OMG, MA6, M2G

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	0/69010	0.46	2/107716 (0.0%)
1	2A	0.21	0/67294	0.40	3/105038 (0.0%)
2	1B	0.21	0/2882	0.40	0/4494
2	2B	0.18	0/2879	0.35	0/4487
3	1D	0.26	0/2186	0.51	0/2944
3	2D	0.22	0/2186	0.45	0/2944
4	1E	0.26	0/1592	0.49	0/2149
4	2E	0.19	0/1592	0.42	0/2149
5	1F	0.25	0/1618	0.50	0/2191
5	2F	0.20	0/1614	0.45	0/2186
6	1G	0.22	0/1448	0.45	0/1957
6	2G	0.19	0/1453	0.39	0/1963
7	1H	0.23	0/1356	0.44	0/1834
7	2H	0.19	0/1356	0.39	0/1834
8	1I	0.19	0/1112	0.44	0/1514
8	2I	0.19	0/1079	0.40	0/1475
9	1N	0.25	0/1144	0.48	0/1543
9	2N	0.18	0/1144	0.39	0/1543
10	1O	0.25	0/943	0.46	0/1269
10	2O	0.19	0/943	0.42	0/1269
11	1P	0.24	0/1152	0.54	0/1533
11	2P	0.20	0/1152	0.49	0/1533
12	1Q	0.26	0/1143	0.46	0/1527
12	2Q	0.19	0/1143	0.41	0/1527
13	1R	0.27	0/982	0.51	0/1312
13	2R	0.19	0/982	0.45	0/1312
14	1S	0.23	0/883	0.46	0/1176
14	2S	0.19	0/880	0.44	0/1172
15	1T	0.24	0/1105	0.44	0/1477
15	2T	0.20	0/1097	0.42	0/1468
16	1U	0.27	0/977	0.46	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	2U	0.19	0/977	0.38	0/1301
17	1V	0.26	0/782	0.47	0/1049
17	2V	0.17	0/782	0.38	0/1049
18	1W	0.28	0/897	0.46	0/1205
18	2W	0.21	0/897	0.40	0/1205
19	1X	0.24	0/764	0.50	2/1025 (0.2%)
19	2X	0.22	0/764	0.48	2/1025 (0.2%)
20	1Y	0.23	0/819	0.50	0/1095
20	2Y	0.20	0/819	0.46	0/1095
21	1Z	0.22	0/1267	0.45	0/1717
21	2Z	0.23	0/1299	0.44	0/1763
22	10	0.25	0/662	0.50	0/881
22	20	0.18	0/662	0.41	0/881
23	11	0.25	0/762	0.46	0/1014
23	21	0.22	0/762	0.40	0/1014
24	12	0.30	0/590	0.50	0/781
24	22	0.19	0/590	0.36	0/781
25	13	0.27	0/474	0.47	0/635
25	23	0.18	0/469	0.41	0/630
26	14	0.24	0/565	0.56	0/761
26	24	0.25	0/545	0.54	0/737
27	15	0.27	0/469	0.46	0/635
27	25	0.20	0/469	0.40	0/635
28	16	0.26	0/460	0.47	0/613
28	26	0.21	0/456	0.45	0/608
29	17	0.31	0/426	0.51	0/561
29	27	0.25	0/426	0.50	0/561
30	18	0.24	0/525	0.45	0/691
30	28	0.20	0/525	0.38	0/691
31	19	0.29	0/310	0.52	0/407
31	29	0.18	0/310	0.41	0/407
32	1a	0.20	0/35795	0.39	0/55864
32	2a	0.19	1/35886 (0.0%)	0.38	3/56005 (0.0%)
33	1b	0.21	0/1881	0.47	0/2542
33	2b	0.21	0/1860	0.45	0/2518
34	1c	0.19	0/1572	0.39	0/2126
34	2c	0.20	0/1566	0.40	0/2119
35	1d	0.19	0/1685	0.44	0/2262
35	2d	0.19	0/1704	0.43	0/2284
36	1e	0.20	0/1145	0.47	0/1543
36	2e	0.21	0/1149	0.44	0/1548
37	1f	0.18	0/823	0.39	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	0.18	0/1250	0.39	0/1679
38	2g	0.20	0/1254	0.41	0/1683
39	1h	0.19	0/1108	0.41	0/1494
39	2h	0.17	0/1108	0.39	0/1494
40	1i	0.19	0/1002	0.48	0/1346
40	2i	0.20	0/997	0.49	0/1343
41	1j	0.20	0/722	0.40	0/982
41	2j	0.20	0/727	0.46	0/988
42	1k	0.18	0/844	0.41	0/1145
42	2k	0.18	0/848	0.41	0/1149
43	1l	0.21	0/937	0.40	0/1260
43	2l	0.18	0/937	0.39	0/1260
44	1m	0.19	0/969	0.51	0/1302
44	2m	0.20	0/961	0.45	0/1291
45	1n	0.19	0/501	0.43	0/664
45	2n	0.20	0/501	0.41	0/664
46	1o	0.19	0/739	0.38	0/985
46	2o	0.18	0/739	0.33	0/985
47	1p	0.21	0/697	0.52	0/939
47	2p	0.19	0/693	0.43	0/935
48	1q	0.20	0/836	0.47	0/1117
48	2q	0.18	0/836	0.42	0/1117
49	1r	0.20	0/560	0.38	0/746
49	2r	0.18	0/560	0.39	0/746
50	1s	0.20	0/667	0.50	0/900
50	2s	0.22	0/661	0.50	0/893
51	1t	0.20	0/730	0.47	0/965
51	2t	0.20	0/729	0.47	0/965
52	1u	0.18	0/203	0.43	0/266
52	2u	0.19	0/203	0.42	0/266
53	1v	0.23	0/310	0.40	0/480
53	2v	0.22	0/310	0.46	0/480
54	1w	0.29	1/1581 (0.1%)	0.41	0/2458
54	2w	0.30	1/1531 (0.1%)	0.39	0/2379
55	1x	0.27	1/1723 (0.1%)	0.42	0/2684
55	2x	0.25	0/1723	0.38	0/2684
56	1y	0.31	2/1606 (0.1%)	0.38	0/2497
56	2y	0.31	1/1583 (0.1%)	0.40	0/2459
All	All	0.23	7/316632 (0.0%)	0.42	12/474029 (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
21	1Z	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	46	G7M	O3'-P	5.64	1.61	1.56
54	2w	46	G7M	O3'-P	5.55	1.61	1.56
56	1y	46	G7M	O3'-P	5.46	1.61	1.56
56	2y	46	G7M	O3'-P	5.31	1.61	1.56
55	1x	8	4SU	O3'-P	5.22	1.61	1.56
56	1y	8	4SU	O3'-P	5.10	1.61	1.56
32	2a	527	G7M	O3'-P	5.05	1.61	1.56

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1992	G	C2'-C3'-O3'	6.63	119.45	109.50
32	2a	1272	G	N1-C2-N2	-6.41	96.97	116.20
32	2a	1263	C	N1-C2-O2	5.80	136.31	118.90
32	2a	1272	G	N3-C2-N2	5.75	137.14	119.90
1	2A	271(M)	G	P-O3'-C3'	5.32	126.08	119.70
1	2A	1992	G	C2'-C3'-O3'	5.27	117.40	109.50
1	2A	271(M)	G	OP1-P-O3'	5.19	116.62	105.20
19	2X	94	GLY	CA-C-N	5.16	130.99	121.70
19	2X	94	GLY	C-N-CA	5.16	130.99	121.70
1	1A	512	G	O4'-C1'-N9	5.09	115.84	108.20
19	1X	94	GLY	CA-C-N	5.07	130.82	121.70
19	1X	94	GLY	C-N-CA	5.07	130.82	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	1Z	136	PHE	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	61853	0	31183	477	0
1	2A	60323	0	30412	625	0
2	1B	2577	0	1305	20	0
2	2B	2575	0	1303	28	0
3	1D	2136	0	2218	35	0
3	2D	2136	0	2218	38	0
4	1E	1559	0	1618	28	0
4	2E	1559	0	1618	37	0
5	1F	1583	0	1625	31	0
5	2F	1579	0	1619	44	0
6	1G	1423	0	1436	34	0
6	2G	1428	0	1438	40	0
7	1H	1330	0	1407	27	0
7	2H	1330	0	1407	39	0
8	1I	1097	0	1140	31	0
8	2I	1064	0	1082	27	0
9	1N	1117	0	1184	13	0
9	2N	1117	0	1184	25	0
10	1O	933	0	996	17	0
10	2O	933	0	996	15	0
11	1P	1135	0	1212	22	0
11	2P	1135	0	1212	22	0
12	1Q	1122	0	1179	23	0
12	2Q	1122	0	1179	34	0
13	1R	968	0	1033	16	0
13	2R	968	0	1033	26	0
14	1S	873	0	927	14	0
14	2S	870	0	923	33	0
15	1T	1091	0	1151	15	0
15	2T	1083	0	1136	19	0
16	1U	959	0	1019	11	0
16	2U	959	0	1019	10	0
17	1V	771	0	830	10	0
17	2V	771	0	830	13	0
18	1W	886	0	940	5	0
18	2W	886	0	940	16	0
19	1X	750	0	814	11	0
19	2X	750	0	814	16	0
20	1Y	806	0	881	12	0
20	2Y	806	0	881	14	0
21	1Z	1240	0	1240	35	0
21	2Z	1271	0	1273	63	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	10	653	0	674	9	0
22	20	653	0	674	9	0
23	11	755	0	826	6	0
23	21	755	0	826	12	0
24	12	588	0	643	7	0
24	22	588	0	643	15	0
25	13	469	0	518	5	0
25	23	464	0	514	10	0
26	14	552	0	533	25	0
26	24	532	0	503	27	0
27	15	455	0	465	4	0
27	25	455	0	465	6	0
28	16	453	0	473	7	0
28	26	449	0	469	8	0
29	17	418	0	467	5	0
29	27	418	0	467	8	0
30	18	517	0	582	11	0
30	28	517	0	582	9	0
31	19	307	0	335	4	0
31	29	307	0	335	9	0
32	1a	32246	0	16295	373	0
32	2a	32327	0	16338	376	0
33	1b	1846	0	1867	65	0
33	2b	1825	0	1828	64	0
34	1c	1548	0	1535	32	0
34	2c	1542	0	1517	37	0
35	1d	1655	0	1672	43	0
35	2d	1674	0	1714	40	0
36	1e	1129	0	1185	33	0
36	2e	1133	0	1191	42	0
37	1f	810	0	804	16	0
37	2f	816	0	808	13	0
38	1g	1231	0	1238	27	0
38	2g	1235	0	1249	20	0
39	1h	1088	0	1126	18	0
39	2h	1088	0	1126	21	0
40	1i	983	0	986	36	0
40	2i	978	0	966	40	0
41	1j	709	0	650	19	0
41	2j	714	0	672	30	0
42	1k	829	0	825	17	0
42	2k	833	0	836	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	1l	932	0	981	13	0
43	2l	932	0	981	14	0
44	1m	958	0	1002	28	0
44	2m	950	0	988	48	0
45	1n	492	0	529	12	0
45	2n	492	0	529	16	0
46	1o	728	0	760	13	0
46	2o	728	0	760	14	0
47	1p	681	0	697	18	0
47	2p	677	0	686	16	0
48	1q	823	0	891	17	0
48	2q	823	0	891	10	0
49	1r	555	0	618	11	0
49	2r	555	0	618	10	0
50	1s	652	0	662	24	0
50	2s	646	0	644	25	0
51	1t	728	0	798	21	0
51	2t	727	0	796	13	0
52	1u	199	0	208	5	0
52	2u	199	0	208	7	0
53	1v	277	0	140	2	0
53	2v	277	0	140	3	0
54	1w	1603	0	828	21	0
54	2w	1555	0	797	20	0
55	1x	1656	0	849	7	0
55	2x	1656	0	849	16	0
56	1y	1585	0	803	26	0
56	2y	1565	0	794	34	0
57	10	7	0	0	0	0
57	11	6	0	0	0	0
57	12	2	0	0	0	0
57	13	3	0	0	0	0
57	14	1	0	0	0	0
57	15	8	0	0	0	0
57	16	2	0	0	0	0
57	17	6	0	0	0	0
57	18	5	0	0	0	0
57	19	1	0	0	0	0
57	1A	1113	0	0	0	0
57	1B	38	0	0	0	0
57	1D	12	0	0	0	0
57	1E	14	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	1F	13	0	0	0	0
57	1G	5	0	0	0	0
57	1H	1	0	0	0	0
57	1N	6	0	0	0	0
57	1O	4	0	0	0	0
57	1P	5	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	3	0	0	0	0
57	1U	6	0	0	0	0
57	1V	7	0	0	0	0
57	1W	6	0	0	0	0
57	1X	7	0	0	0	0
57	1Y	2	0	0	0	0
57	1Z	3	0	0	0	0
57	1a	220	0	0	0	0
57	1b	1	0	0	0	0
57	1d	1	0	0	0	0
57	1e	2	0	0	0	0
57	1f	2	0	0	0	0
57	1l	2	0	0	0	0
57	1m	1	0	0	0	0
57	1n	1	0	0	0	0
57	1p	1	0	0	0	0
57	1q	1	0	0	0	0
57	1t	1	0	0	0	0
57	1v	1	0	0	0	0
57	1w	9	0	0	0	0
57	1x	14	0	0	0	0
57	20	2	0	0	0	0
57	21	3	0	0	0	0
57	23	2	0	0	0	0
57	25	3	0	0	0	0
57	27	2	0	0	0	0
57	28	2	0	0	0	0
57	2A	804	0	0	0	0
57	2B	16	0	0	0	0
57	2D	6	0	0	0	0
57	2E	7	0	0	0	0
57	2F	6	0	0	0	0
57	2G	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	2O	1	0	0	0	0
57	2P	1	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	3	0	0	0	0
57	2V	1	0	0	0	0
57	2W	3	0	0	0	0
57	2X	2	0	0	0	0
57	2Z	1	0	0	0	0
57	2a	2	0	0	0	0
57	2w	6	0	0	0	0
57	2x	7	0	0	0	0
57	2y	7	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	0	0
60	2d	8	0	0	0	0
61	10	12	0	0	1	0
61	11	7	0	0	0	0
61	12	4	0	0	0	0
61	13	4	0	0	0	0
61	14	1	0	0	0	0
61	15	10	0	0	0	0
61	16	5	0	0	0	0
61	17	10	0	0	1	0
61	18	10	0	0	0	0
61	1A	2067	0	0	62	0
61	1B	61	0	0	2	0
61	1D	32	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	1E	26	0	0	1	0
61	1F	20	0	0	1	0
61	1G	1	0	0	0	0
61	1H	2	0	0	0	0
61	1N	6	0	0	0	0
61	1O	6	0	0	0	0
61	1P	21	0	0	2	0
61	1Q	7	0	0	0	0
61	1R	7	0	0	1	0
61	1S	5	0	0	1	0
61	1T	9	0	0	0	0
61	1U	14	0	0	1	0
61	1V	7	0	0	0	0
61	1W	6	0	0	1	0
61	1X	5	0	0	0	0
61	1Y	3	0	0	0	0
61	1Z	1	0	0	1	0
61	1a	425	0	0	25	0
61	1b	1	0	0	0	0
61	1f	1	0	0	0	0
61	1i	1	0	0	0	0
61	1l	8	0	0	0	0
61	1m	2	0	0	1	0
61	1n	1	0	0	0	0
61	1o	3	0	0	0	0
61	1p	1	0	0	0	0
61	1q	2	0	0	0	0
61	1r	2	0	0	0	0
61	1u	2	0	0	1	0
61	1v	4	0	0	0	0
61	1w	12	0	0	1	0
61	1x	17	0	0	0	0
61	1y	1	0	0	0	0
61	20	1	0	0	0	0
61	21	6	0	0	0	0
61	23	2	0	0	0	0
61	27	5	0	0	0	0
61	28	4	0	0	1	0
61	29	1	0	0	0	0
61	2A	1094	0	0	79	0
61	2B	18	0	0	0	0
61	2D	22	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	2E	9	0	0	0	0
61	2F	11	0	0	0	0
61	2I	3	0	0	0	0
61	2N	1	0	0	0	0
61	2O	1	0	0	0	0
61	2P	9	0	0	1	0
61	2Q	1	0	0	0	0
61	2R	1	0	0	0	0
61	2T	5	0	0	0	0
61	2U	3	0	0	0	0
61	2W	3	0	0	0	0
61	2X	2	0	0	0	0
61	2w	1	0	0	0	0
61	2x	6	0	0	1	0
61	2y	2	0	0	0	0
All	All	299618	0	196724	3553	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 7.

All (3553) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1082:U:H3	1:1A:1086:A:N6	1.19	1.40
1:1A:1082:U:N3	1:1A:1086:A:N6	2.05	1.05
1:1A:1082:U:O4	1:1A:1086:A:N1	1.94	1.00
1:1A:1798:U:H5'	3:1D:259:THR:HG22	1.50	0.93
26:14:57:GLU:HB3	26:14:58:ARG:HD2	1.53	0.91
1:2A:2714:G:OP2	61:2A:3902:HOH:O	1.88	0.91
1:2A:2298:A:H62	1:2A:2318:G:H8	1.14	0.90
1:2A:2134:A:H62	1:2A:2157:G:H4'	1.35	0.90
1:2A:1689:A:H62	1:2A:1698:A:H2	1.20	0.89
6:2G:161:THR:HG22	6:2G:163:ALA:H	1.37	0.88
32:1a:1002:G:H3'	32:1a:1003:G:H4'	1.54	0.87
1:1A:1082:U:H3	1:1A:1086:A:H61	0.89	0.86
1:1A:2427:C:OP1	61:1A:4203:HOH:O	1.92	0.86
29:17:24:THR:HG22	29:17:27:GLY:H	1.41	0.86
1:2A:500:G:H22	1:2A:503:A:H5'	1.40	0.86
1:2A:2711:A:OP2	61:2A:3902:HOH:O	1.92	0.86
50:1s:27:GLU:HB2	50:1s:28:LYS:HA	1.56	0.85
32:2a:1086:U:H3	32:2a:1099:G:H22	1.24	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:2b:185:ILE:HG22	33:2b:199:TYR:HB2	1.57	0.85
1:1A:1602:U:O4	61:1A:4204:HOH:O	1.93	0.84
32:2a:559:A:OP1	36:2e:126:ARG:NH2	2.10	0.84
1:1A:1271:G:OP2	61:1A:4205:HOH:O	1.94	0.84
29:27:24:THR:HG22	29:27:27:GLY:H	1.40	0.84
33:1b:185:ILE:HG22	33:1b:199:TYR:HB2	1.58	0.84
1:1A:1054:A:H61	1:1A:1105:U:H3	1.25	0.83
32:1a:1086:U:H3	32:1a:1099:G:H22	1.27	0.83
1:1A:1647:G:OP1	61:1A:4205:HOH:O	1.96	0.83
19:1X:31:HIS:HD2	19:1X:33:LYS:H	1.26	0.83
1:1A:1970:A:OP1	61:1A:4206:HOH:O	1.96	0.82
32:2a:1029:C:C4	32:2a:1032:G:N1	2.46	0.82
56:2y:18:G:H22	56:2y:55:PSU:HN3	1.26	0.82
32:2a:975:A:H4'	32:2a:976:G:H5"	1.59	0.82
46:2o:54:ARG:HG2	46:2o:58:MET:HE2	1.61	0.82
1:2A:890:A:H2'	1:2A:892:G:H8	1.45	0.82
49:2r:32:ARG:HA	49:2r:69:THR:HG21	1.61	0.82
1:2A:1604:C:OP2	61:2A:3903:HOH:O	1.97	0.81
40:1i:128:ARG:NH2	55:1x:33:U:OP2	2.13	0.81
32:2a:406:G:H21	35:2d:119:GLN:HE22	1.28	0.81
1:2A:1798:U:H5'	3:2D:259:THR:HG22	1.63	0.81
2:2B:7:G:H21	14:2S:38:GLN:HE22	1.28	0.80
32:2a:1271:G:N2	32:2a:1272:G:N7	2.30	0.80
1:2A:2162:G:H4'	1:2A:2172:U:H2'	1.64	0.80
32:1a:1027:C:C2	32:1a:1034:G:N2	2.47	0.79
21:1Z:132:ASN:HD22	21:1Z:160:GLY:HA3	1.47	0.79
49:1r:32:ARG:HA	49:1r:69:THR:HG21	1.65	0.79
44:2m:34:LEU:HD13	44:2m:41:PRO:HB3	1.65	0.79
1:1A:1890:A:OP2	61:1A:4207:HOH:O	2.01	0.79
1:2A:792:G:O6	61:2A:3905:HOH:O	2.01	0.79
1:2A:962:G:OP1	61:2A:3904:HOH:O	2.00	0.78
33:1b:21:ARG:O	33:1b:23:ARG:N	2.17	0.78
32:2a:266:G:H5"	32:2a:268:C:H41	1.48	0.78
41:2j:49:VAL:HG23	45:2n:41:ARG:HB2	1.64	0.78
32:1a:134:A:H61	47:1p:25:ARG:HH12	1.32	0.78
32:2a:1286:A:H8	32:2a:1287:A:H4'	1.47	0.77
1:1A:2206:G:H3'	1:1A:2207:G:C8	2.18	0.77
1:1A:1058:G:N2	1:1A:1081:U:O2	2.17	0.77
17:1V:55:ALA:HA	17:1V:101:GLY:HA2	1.64	0.77
1:2A:892:G:H3'	1:2A:893:C:H4'	1.65	0.77
2:2B:103:G:H21	21:2Z:73:GLN:HE22	1.30	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1253:A:OP1	61:2A:3907:HOH:O	2.03	0.77
1:1A:602:G:O2'	1:1A:655:A:N6	2.17	0.77
1:1A:773:U:OP1	61:1A:4208:HOH:O	2.03	0.77
2:2B:66:A:H61	2:2B:109:C:H5'	1.48	0.76
1:1A:2128:C:H42	1:1A:2160:G:H1	1.30	0.76
1:2A:2712(A):A:OP2	61:2A:3902:HOH:O	2.03	0.76
17:1V:98:GLU:OE2	17:1V:100:ARG:NH1	2.19	0.76
1:2A:2028:U:O4	61:2A:3906:HOH:O	2.02	0.75
34:2c:47:LEU:HD12	34:2c:68:VAL:HG11	1.66	0.75
32:2a:953:G:H5'	32:2a:965:A:H61	1.51	0.75
32:2a:1316:G:H22	32:2a:1319:A:H5"	1.49	0.75
1:2A:2448:A:OP1	61:2A:3909:HOH:O	2.05	0.75
3:1D:147:LEU:HD13	3:1D:155:LEU:HD11	1.66	0.75
24:22:22:GLU:OE2	24:22:68:ARG:NH2	2.20	0.75
32:1a:1505:G:OP2	61:1a:1905:HOH:O	2.04	0.75
32:2a:407:G:OP1	35:2d:115:ARG:NH2	2.20	0.74
1:2A:994:C:OP1	16:2U:53:ARG:NH2	2.19	0.74
10:1O:48:PRO:HB3	32:1a:1422:G:H5"	1.70	0.74
21:1Z:156:LYS:HE3	21:1Z:158:PRO:HD3	1.68	0.74
5:2F:53:THR:HG23	5:2F:55:GLY:H	1.52	0.74
37:2f:46:ARG:HH22	49:2r:37:VAL:HG11	1.53	0.74
1:1A:2350:C:OP2	61:1A:4209:HOH:O	2.03	0.74
2:1B:33:G:H5'	6:1G:2:PRO:HD3	1.69	0.74
1:2A:832:G:OP1	61:2A:3908:HOH:O	2.04	0.74
1:2A:921:G:O6	61:2A:3911:HOH:O	2.06	0.74
1:2A:2138:C:H42	1:2A:2153:G:H1	1.35	0.74
11:2P:35:HIS:O	61:2P:301:HOH:O	2.05	0.74
1:2A:1812:A:OP2	61:2A:3910:HOH:O	2.05	0.74
44:2m:15:VAL:HG22	44:2m:45:VAL:HG12	1.70	0.74
43:2l:71:PRO:O	43:2l:102:ARG:NH1	2.20	0.74
1:1A:2550:G:OP1	61:1A:4210:HOH:O	2.04	0.74
1:1A:2788:C:OP1	4:1E:61:ARG:NH2	2.21	0.74
1:2A:2130:U:H2'	1:2A:2158:A:H61	1.53	0.73
21:2Z:19:ARG:NH1	21:2Z:84:GLU:O	2.20	0.73
36:2e:122:GLU:O	36:2e:126:ARG:NH1	2.21	0.73
40:1i:48:GLU:HA	40:1i:51:ARG:HD3	1.69	0.73
10:2O:48:PRO:HB3	32:2a:1422:G:H5"	1.70	0.73
32:2a:1272:G:N2	32:2a:1273:G:N7	2.36	0.73
35:2d:150:GLU:HA	35:2d:153:ARG:HD2	1.70	0.73
1:2A:307:G:H21	1:2A:330:A:H62	1.37	0.73
1:1A:826:U:OP1	61:1A:4203:HOH:O	2.05	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2F:21:ALA:HB3	5:2F:22:ALA:HA	1.70	0.73
12:1Q:56:ARG:HH22	12:1Q:59:ARG:HH21	1.36	0.73
50:2s:49:ILE:HG22	50:2s:62:ILE:HD11	1.70	0.73
1:1A:2822:G:OP2	61:1A:4213:HOH:O	2.07	0.73
56:2y:55:PSU:HN1	56:2y:57:G:H5"	1.54	0.73
1:2A:1264:G:OP1	27:25:19:ARG:NH2	2.21	0.73
32:2a:677:U:H3	32:2a:713:G:H22	1.36	0.73
32:2a:1002:G:C2	32:2a:1003:G:H1'	2.24	0.73
1:1A:1622:G:OP2	61:1A:4211:HOH:O	2.06	0.72
32:1a:975:A:H4'	32:1a:976:G:H5"	1.70	0.72
32:1a:1518:MA6:H93	32:1a:1519:MA6:H92	1.69	0.72
1:2A:783:A:OP2	61:2A:3915:HOH:O	2.08	0.72
26:24:44:THR:O	26:24:46:GLN:N	2.22	0.72
1:1A:1669:A:OP2	61:1A:4210:HOH:O	2.08	0.72
1:1A:884:C:H42	1:1A:892:G:H1	1.34	0.72
1:2A:1762:A:N1	61:2A:3960:HOH:O	2.22	0.72
15:2T:39:ARG:NH2	32:2a:345:C:OP2	2.22	0.72
1:2A:2319:G:H22	14:2S:3:ARG:HH11	1.35	0.72
41:1j:8:LEU:HD22	41:1j:96:ILE:HG22	1.71	0.72
1:2A:1010:A:OP2	61:2A:3914:HOH:O	2.07	0.72
1:1A:2821:A:OP2	61:1A:4213:HOH:O	2.08	0.72
28:16:12:GLU:OE1	28:16:19:ARG:NH1	2.23	0.72
32:1a:700:G:N7	61:1a:1918:HOH:O	2.22	0.72
24:22:65:ASN:OD1	24:22:69:ARG:NH1	2.23	0.72
1:1A:1060:U:H3	1:1A:1088:A:H8	1.37	0.71
32:1a:148:G:H2'	32:1a:149:A:H8	1.55	0.71
32:1a:812:C:N3	61:1a:1921:HOH:O	2.23	0.71
8:2I:92:VAL:HG13	8:2I:120:ILE:HB	1.70	0.71
44:2m:23:TYR:HB3	44:2m:67:GLU:HA	1.70	0.71
1:1A:1013:C:OP2	61:1A:4212:HOH:O	2.07	0.71
1:2A:304:G:O6	61:2A:3912:HOH:O	2.06	0.71
1:2A:2506:U:H1'	54:2w:76:F3N:HD2	1.71	0.71
32:2a:1286:A:C8	32:2a:1287:A:H4'	2.24	0.71
1:1A:1266:G:O5'	18:1W:15:ARG:NH2	2.24	0.71
32:1a:297:G:O2'	61:1a:1906:HOH:O	2.07	0.71
1:2A:2431:U:OP2	61:2A:3916:HOH:O	2.09	0.71
32:1a:1508:G:OP1	61:1a:1907:HOH:O	2.09	0.71
1:2A:794:G:OP2	61:2A:3917:HOH:O	2.09	0.71
1:2A:890:A:H2'	1:2A:892:G:C8	2.23	0.71
12:2Q:135:ASP:OD2	21:2Z:81:ARG:NH1	2.23	0.71
33:2b:88:ALA:HB2	33:2b:219:VAL:HG13	1.72	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:2m:80:ARG:HH22	50:2s:69:HIS:HE1	1.39	0.71
1:1A:530:G:N1	1:1A:2023:G:OP1	2.22	0.71
1:2A:731:C:OP2	61:2A:3913:HOH:O	2.06	0.71
32:2a:1346:A:OP1	40:2i:120:ARG:NH1	2.22	0.71
31:29:25:VAL:HB	31:29:34:GLN:HB2	1.72	0.71
34:2c:112:SER:HB3	34:2c:115:LEU:HD22	1.71	0.71
1:1A:2183:C:H2'	1:1A:2184:G:H8	1.56	0.71
33:2b:91:PRO:HG3	33:2b:154:LEU:HB2	1.72	0.71
1:2A:1021:A:H62	1:2A:1141:U:H3	1.37	0.71
1:1A:301:G:OP2	20:1Y:84:ARG:NH2	2.24	0.70
1:1A:1332:G:OP1	61:1A:4215:HOH:O	2.09	0.70
38:1g:50:ILE:HG12	38:1g:61:VAL:HG11	1.72	0.70
1:2A:2314:C:H5'	6:2G:38:VAL:HG21	1.72	0.70
8:2I:59:ALA:HA	8:2I:62:LYS:HG2	1.72	0.70
14:2S:58:LEU:HD13	14:2S:65:VAL:HB	1.73	0.70
39:1h:41:ARG:NH2	39:1h:123:GLU:OE2	2.24	0.70
42:1k:99:GLN:HG2	42:1k:105:VAL:HG21	1.73	0.70
1:2A:1395:A:OP1	61:2A:3903:HOH:O	2.08	0.70
32:2a:664:G:H22	32:2a:741:G:H1	1.39	0.70
1:1A:2235:G:N7	61:1A:4251:HOH:O	2.23	0.70
1:1A:1693:U:O2'	3:1D:14:ARG:NH2	2.25	0.70
35:1d:7:PRO:HB2	35:1d:10:ARG:HD2	1.72	0.70
2:1B:8:U:O3'	14:1S:25:ARG:NH2	2.24	0.70
1:2A:1970:A:OP1	61:2A:3920:HOH:O	2.10	0.69
35:2d:79:PHE:HE1	35:2d:204:ILE:HD13	1.57	0.69
41:2j:6:ILE:HB	41:2j:72:VAL:HG13	1.73	0.69
56:2y:18:G:N2	56:2y:55:PSU:N3	2.34	0.69
1:2A:143(A):C:O2'	19:2X:2:LYS:NZ	2.25	0.69
4:2E:2:LYS:HB2	4:2E:95:ILE:HD12	1.73	0.69
1:1A:2222:G:OP2	61:1A:4214:HOH:O	2.09	0.69
1:2A:948:G:OP1	61:2A:3904:HOH:O	2.10	0.69
1:2A:2445:G:OP1	5:2F:74:ARG:NH2	2.26	0.69
1:2A:141:A:H8	1:2A:1408:C:HO2'	1.38	0.69
14:2S:48:LEU:HD23	14:2S:82:ILE:HD11	1.74	0.69
1:1A:1024:G:OP2	61:1A:4217:HOH:O	2.10	0.69
1:1A:2319:G:H22	14:1S:3:ARG:HD3	1.56	0.69
56:1y:7:A:H3'	56:1y:8:4SU:H6	1.73	0.69
13:2R:56:LYS:NZ	13:2R:90:ARG:O	2.26	0.69
36:2e:100:VAL:O	36:2e:107:ARG:NH2	2.24	0.69
7:2H:56:SER:OG	7:2H:61:HIS:ND1	2.26	0.69
1:2A:106:C:H1'	20:2Y:1:MET:HE2	1.75	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:570:G:O6	61:2A:3909:HOH:O	2.08	0.69
34:2c:58:GLU:HB3	41:2j:92:THR:HG21	1.74	0.69
1:2A:2430:A:OP2	61:2A:3921:HOH:O	2.10	0.69
1:2A:987:G:O2'	1:2A:1000:A:N3	2.26	0.69
12:2Q:77:LYS:NZ	12:2Q:86:GLY:O	2.25	0.69
1:1A:1023:U:OP2	61:1A:4217:HOH:O	2.11	0.68
1:1A:1062:G:H22	1:1A:1077:A:H61	1.40	0.68
1:2A:217:G:OP2	61:2A:3919:HOH:O	2.10	0.68
1:2A:975:C:OP1	61:2A:3923:HOH:O	2.11	0.68
1:1A:2447:G:OP1	61:1A:4216:HOH:O	2.09	0.68
32:1a:1314:C:OP2	50:1s:4:SER:OG	2.09	0.68
14:2S:78:LEU:HD11	14:2S:109:GLY:HA3	1.72	0.68
20:2Y:90:LEU:HD12	20:2Y:92:ASN:HB3	1.74	0.68
1:1A:1865:G:OP1	61:1A:4219:HOH:O	2.11	0.68
32:1a:542:G:OP1	35:1d:10:ARG:NH2	2.27	0.68
1:1A:2321:G:OP2	61:1A:4218:HOH:O	2.11	0.68
32:2a:1314:C:OP2	50:2s:4:SER:OG	2.07	0.68
1:2A:2306:C:N4	6:2G:42:GLY:O	2.23	0.68
1:2A:973:A:OP2	61:2A:3918:HOH:O	2.09	0.68
1:1A:1594:G:N7	61:1A:4264:HOH:O	2.27	0.68
1:2A:253:C:O2'	61:2A:3924:HOH:O	2.12	0.68
1:1A:1371:G:N7	61:1A:4262:HOH:O	2.26	0.68
1:2A:2839:G:H5'	13:2R:46:GLY:HA2	1.76	0.68
33:2b:69:LEU:HB3	33:2b:162:ILE:HG22	1.76	0.68
34:2c:179:ARG:NH1	34:2c:206:GLU:OE1	2.27	0.68
38:2g:146:GLU:OE1	38:2g:149:ARG:NE	2.26	0.68
1:1A:2629:A:O2'	1:1A:2630:G:OP2	2.12	0.67
1:1A:1026:U:OP1	61:1A:4217:HOH:O	2.11	0.67
38:2g:111:ARG:NH1	38:2g:113:GLU:OE2	2.26	0.67
39:2h:64:LYS:HG2	39:2h:79:VAL:HG21	1.76	0.67
21:1Z:52:SER:O	21:1Z:54:HIS:N	2.27	0.67
1:2A:1006:C:OP2	61:2A:3922:HOH:O	2.11	0.67
32:2a:1279:A:OP2	41:2j:9:ARG:NH2	2.28	0.67
36:1e:144:THR:H	36:1e:147:ASP:HB2	1.60	0.67
1:2A:1754:C:OP1	15:2T:96:ARG:NH1	2.28	0.67
44:1m:17:VAL:O	44:1m:20:THR:OG1	2.13	0.67
4:2E:28:ALA:HB3	4:2E:93:VAL:HG12	1.76	0.67
50:2s:27:GLU:HB3	50:2s:28:LYS:HG3	1.76	0.67
1:2A:963:U:OP2	61:2A:3904:HOH:O	2.12	0.67
32:2a:259:G:OP2	51:2t:83:ARG:NH1	2.27	0.67
32:2a:1129:C:H2'	32:2a:1139:G:N7	2.10	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:471:A:OP1	61:1A:4221:HOH:O	2.13	0.66
1:2A:851:U:H5'	25:23:49:LYS:HD2	1.77	0.66
33:2b:15:VAL:HG22	33:2b:16:HIS:HB3	1.77	0.66
8:1I:4:ILE:HD11	8:1I:44:LEU:HD12	1.77	0.66
1:2A:1025:G:O2'	61:2A:3925:HOH:O	2.12	0.66
1:2A:1784:A:O2'	61:2A:3927:HOH:O	2.13	0.66
1:2A:2524:G:N7	61:2A:3982:HOH:O	2.27	0.66
32:1a:702:A:OP2	61:1a:1908:HOH:O	2.11	0.66
1:2A:1119:C:N4	61:2A:3986:HOH:O	2.27	0.66
1:2A:2112:G:N7	1:2A:2169:A:N6	2.44	0.66
40:2i:128:ARG:NH2	55:2x:33:U:OP2	2.28	0.66
32:1a:165:C:H2'	32:1a:166:G:H8	1.60	0.66
36:1e:8:GLU:OE2	36:1e:63:ARG:NH2	2.29	0.66
1:2A:637:A:OP1	11:2P:133:SER:OG	2.12	0.66
7:2H:98:LEU:HG	7:2H:125:VAL:HG23	1.76	0.66
32:2a:624:C:H2'	32:2a:625:G:H8	1.60	0.66
1:1A:1054:A:N6	1:1A:1105:U:H3	1.94	0.66
5:2F:185:ASP:HA	5:2F:188:ARG:HD3	1.78	0.66
14:2S:99:LYS:NZ	14:2S:103:GLU:OE2	2.26	0.66
5:1F:116:ASP:OD1	5:1F:119:ARG:NH2	2.29	0.66
26:14:55:ARG:N	26:14:56:VAL:HA	2.11	0.66
32:2a:316:G:OP2	32:2a:351:G:O2'	2.10	0.66
40:2i:50:LEU:HD13	40:2i:56:LEU:HA	1.78	0.66
26:24:40:HIS:HB3	26:24:43:TYR:HB2	1.78	0.66
8:1I:101:LEU:HD12	8:1I:107:VAL:HB	1.77	0.66
13:1R:97:VAL:HG22	13:1R:114:VAL:HG13	1.78	0.66
32:1a:375:U:OP1	47:1p:69:THR:OG1	2.11	0.66
32:1a:1414:U:H3	32:1a:1486:G:H1	1.43	0.66
1:2A:500:G:N1	1:2A:503:A:OP2	2.28	0.66
43:2l:57:LYS:HG2	43:2l:67:THR:HG22	1.75	0.66
27:15:40:LYS:NZ	27:15:44:THR:O	2.29	0.66
33:1b:91:PRO:HG2	33:1b:155:LEU:HD13	1.78	0.66
1:2A:2206:G:H3'	1:2A:2207:G:C8	2.31	0.66
46:2o:25:THR:HG21	46:2o:70:LEU:HB2	1.76	0.66
8:1I:92:VAL:HG11	8:1I:144:VAL:HG11	1.76	0.65
32:1a:966:M2G:O2'	40:1i:127:LYS:O	2.13	0.65
35:1d:60:GLU:HG3	35:1d:202:LEU:HD12	1.77	0.65
13:2R:67:LEU:HD13	13:2R:76:VAL:HG21	1.76	0.65
1:1A:2573:C:OP1	61:1A:4223:HOH:O	2.14	0.65
32:1a:515:G:N7	61:1a:1936:HOH:O	2.29	0.65
54:1w:26:A:H61	54:1w:44:G:H1	1.44	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1648:C:OP1	61:2A:3926:HOH:O	2.13	0.65
1:1A:1185:C:OP2	61:1A:4220:HOH:O	2.13	0.65
31:19:25:VAL:HB	31:19:34:GLN:HB2	1.79	0.65
21:2Z:153:SER:HB3	21:2Z:167:PRO:HB3	1.77	0.65
44:2m:80:ARG:NH2	50:2s:65:ASN:O	2.29	0.65
1:1A:2316:C:O2'	6:1G:128:ARG:NH2	2.30	0.65
12:2Q:56:ARG:HH22	12:2Q:59:ARG:HH21	1.42	0.65
39:2h:41:ARG:NH2	39:2h:123:GLU:OE2	2.29	0.65
1:1A:2136:C:N3	1:1A:2155:G:C2	2.64	0.65
14:1S:71:ARG:NH1	14:1S:107:GLU:OE1	2.29	0.65
32:2a:8:A:H5'	36:2e:101:ILE:HG22	1.79	0.65
5:2F:12:LEU:HG	5:2F:124:LEU:HD11	1.77	0.65
5:1F:89:VAL:O	61:1F:401:HOH:O	2.14	0.65
26:14:50:VAL:HG21	44:1m:65:LYS:HA	1.79	0.65
15:1T:74:ARG:HG2	15:1T:76:PHE:CZ	2.32	0.65
32:1a:559:A:OP1	36:1e:126:ARG:NH2	2.26	0.65
1:2A:2332:U:O4	61:2A:3929:HOH:O	2.13	0.65
33:1b:30:ARG:HH21	33:1b:194:PRO:HB2	1.62	0.65
33:1b:122:PHE:HE2	33:1b:139:LYS:HB2	1.61	0.65
34:1c:6:HIS:CD2	34:1c:8:ILE:H	2.14	0.65
40:1i:53:VAL:O	40:1i:55:ALA:N	2.29	0.65
1:2A:453:C:OP1	61:2A:3928:HOH:O	2.13	0.65
2:1B:42:C:OP1	6:1G:67:LYS:NZ	2.31	0.64
34:1c:3:ASN:OD1	34:1c:3:ASN:N	2.30	0.64
32:2a:1029:C:N3	32:2a:1032:G:N2	2.45	0.64
32:1a:544:G:OP1	35:1d:59:ARG:NH2	2.28	0.64
1:2A:2150:U:H2'	1:2A:2151:G:H8	1.61	0.64
1:2A:2646:C:OP2	1:2A:2732:G:O2'	2.15	0.64
3:2D:147:LEU:HD13	3:2D:155:LEU:HD11	1.79	0.64
40:2i:16:ARG:HB2	40:2i:64:THR:HG22	1.79	0.64
56:2y:46:G7M:O2'	56:2y:48:C:OP2	2.15	0.64
1:2A:397:G:N7	61:2A:3995:HOH:O	2.30	0.64
26:14:55:ARG:H	26:14:56:VAL:HA	1.62	0.64
32:1a:1152:A:OP1	41:1j:68:HIS:ND1	2.31	0.64
1:2A:2816:C:O3'	13:2R:99:LYS:NZ	2.30	0.64
32:2a:656:C:O2'	46:2o:28:GLN:OE1	2.12	0.64
32:1a:664:G:H22	32:1a:741:G:H1	1.44	0.64
32:1a:785:G:N7	61:1a:1937:HOH:O	2.29	0.64
1:2A:463:G:OP2	61:2A:3932:HOH:O	2.14	0.64
32:1a:1386:G:N7	61:1a:1940:HOH:O	2.30	0.64
34:1c:150:LYS:HG3	34:1c:169:ALA:HB2	1.79	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1971:A:OP1	61:2A:3920:HOH:O	2.15	0.64
1:2A:2285:C:OP2	28:26:6:ARG:NH1	2.31	0.64
26:14:46:GLN:O	26:14:48:ARG:N	2.30	0.64
1:2A:144:C:H5'	19:2X:2:LYS:HZ2	1.61	0.64
1:2A:1204:A:H2	1:2A:1241:A:H62	1.46	0.64
1:2A:2379:G:O2'	14:2S:17:ARG:NH1	2.31	0.64
32:2a:673:G:H2'	32:2a:674:G:C8	2.33	0.64
43:2l:32:PHE:HB3	43:2l:84:LEU:HD11	1.79	0.64
1:1A:1405:U:H2'	1:1A:1406:U:C6	2.33	0.64
1:1A:2133:G:O2'	1:1A:2157:G:N2	2.31	0.64
19:1X:94:GLY:H	19:1X:95:LEU:HB2	1.62	0.64
32:1a:970:C:OP2	61:1a:1910:HOH:O	2.15	0.64
46:1o:54:ARG:HG2	46:1o:58:MET:HE2	1.80	0.64
1:2A:2268:A:OP1	61:2A:3930:HOH:O	2.14	0.64
11:2P:63:PRO:HD3	30:28:27:THR:HG22	1.79	0.64
56:2y:58:A:O2'	56:2y:60:U:OP2	2.16	0.64
1:1A:1058:G:H1	1:1A:1080:C:H42	1.45	0.64
1:1A:2446:G:OP1	61:1A:4224:HOH:O	2.15	0.64
18:1W:92:ARG:NH1	61:1W:301:HOH:O	2.30	0.64
32:2a:976:G:H5'	32:2a:1358:U:O2'	1.97	0.64
32:1a:504:C:OP1	61:1a:1912:HOH:O	2.15	0.64
1:2A:2857:G:N7	61:2A:3999:HOH:O	2.30	0.64
4:2E:47:VAL:HG11	4:2E:86:PRO:HD2	1.80	0.64
1:1A:2099:U:H3	1:1A:2190:G:H1	1.44	0.63
32:2a:1128:C:H1'	32:2a:1147:C:H42	1.61	0.63
41:2j:6:ILE:HG12	41:2j:98:ILE:HG12	1.80	0.63
1:1A:2291:U:H2'	1:1A:2292:C:C6	2.33	0.63
1:2A:1800:C:OP2	3:2D:183:ARG:NH2	2.31	0.63
36:2e:144:THR:OG1	36:2e:147:ASP:OD1	2.15	0.63
5:1F:184:TYR:CE2	5:1F:188:ARG:HD2	2.33	0.63
1:2A:2100:G:H1	1:2A:2189:U:H3	1.43	0.63
3:2D:206:LEU:HD22	3:2D:211:ARG:HG2	1.80	0.63
10:1O:120:GLU:OE1	15:1T:67:SER:OG	2.16	0.63
52:1u:5:ASP:OD2	61:1u:101:HOH:O	2.15	0.63
8:1I:92:VAL:HG13	8:1I:120:ILE:HB	1.80	0.63
32:1a:316:G:OP2	32:1a:351:G:O2'	2.17	0.63
38:1g:89:MET:SD	38:1g:155:ARG:HB2	2.38	0.63
1:2A:1154:G:N7	61:2A:3997:HOH:O	2.30	0.63
13:2R:100:LEU:HD21	13:2R:113:LEU:HD23	1.80	0.63
32:2a:1099:G:OP2	33:2b:144:ARG:NH2	2.31	0.63
39:2h:51:VAL:HG21	39:2h:60:ARG:HB2	1.81	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1D:206:LEU:HD22	3:1D:211:ARG:HG2	1.80	0.63
1:2A:2327:A:H2'	1:2A:2328:A:C8	2.32	0.63
4:2E:36:ARG:NH1	4:2E:85:ASN:OD1	2.31	0.63
26:24:16:CYS:SG	26:24:17:GLY:N	2.72	0.63
1:1A:1264:G:OP1	27:15:19:ARG:NH2	2.19	0.63
15:1T:127:ALA:C	15:1T:129:ARG:H	2.07	0.63
34:1c:43:LEU:HD21	34:1c:91:LEU:HD11	1.80	0.63
32:1a:677:U:H3	32:1a:713:G:H22	1.47	0.63
5:2F:167:ALA:HB1	5:2F:173:VAL:HG11	1.81	0.63
7:2H:26:VAL:HG21	7:2H:75:ALA:HB1	1.81	0.63
12:2Q:32:TYR:OH	12:2Q:133:ARG:NH2	2.31	0.63
21:2Z:144:LEU:HD11	21:2Z:150:LEU:HD13	1.81	0.63
5:1F:185:ASP:OD1	5:1F:188:ARG:NH1	2.29	0.63
38:1g:111:ARG:NE	38:1g:113:GLU:OE2	2.28	0.63
49:1r:26:LEU:HD21	49:1r:42:ARG:HD3	1.81	0.63
6:1G:64:THR:HB	6:1G:94:LEU:HD11	1.80	0.62
21:1Z:138:GLU:H	21:1Z:156:LYS:HZ3	1.45	0.62
35:1d:173:TRP:CD1	35:1d:173:TRP:H	2.14	0.62
1:2A:2319:G:H22	14:2S:3:ARG:HD2	1.63	0.62
35:2d:8:VAL:HG22	35:2d:21:LEU:HD13	1.81	0.62
56:2y:51:U:H3	56:2y:63:G:H1	1.46	0.62
1:1A:1105:U:H2'	1:1A:1106:G:H8	1.63	0.62
4:1E:28:ALA:HB3	4:1E:93:VAL:HG12	1.81	0.62
33:1b:59:GLU:HB3	33:1b:221:LEU:HD11	1.80	0.62
37:1f:74:ASP:OD1	37:1f:77:ARG:NH2	2.32	0.62
1:2A:2136:C:HO2'	1:2A:2137:C:P	2.21	0.62
6:2G:16:ARG:HB2	6:2G:17:PRO:HD3	1.81	0.62
32:2a:1029:C:N4	32:2a:1032:G:N1	2.46	0.62
41:2j:38:ILE:HG13	41:2j:71:LEU:HB3	1.81	0.62
32:2a:975:A:N1	41:2j:48:THR:HB	2.14	0.62
32:2a:1239:A:H62	32:2a:1299:A:H62	1.46	0.62
32:1a:1456:G:O3'	51:1t:39:LYS:NZ	2.33	0.62
32:2a:396:G:O2'	32:2a:398:C:OP1	2.10	0.62
1:1A:2646:C:OP2	1:1A:2732:G:O2'	2.15	0.62
7:1H:86:GLU:OE1	7:1H:130:ARG:NH1	2.31	0.62
13:1R:56:LYS:NZ	13:1R:87:TYR:O	2.31	0.62
56:1y:55:PSU:C4	56:1y:57:G:H5'	2.33	0.62
1:2A:2483:C:N3	12:2Q:124:LYS:NZ	2.46	0.62
21:1Z:52:SER:C	21:1Z:54:HIS:H	2.07	0.62
32:1a:189(K):U:H2'	32:1a:189(L):G:C8	2.34	0.62
32:1a:1318:A:H5"	50:1s:3:ARG:HH12	1.64	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:2e:147:ASP:OD1	36:2e:147:ASP:N	2.32	0.62
45:2n:23:ARG:NH1	45:2n:28:GLY:O	2.32	0.62
18:1W:25:ARG:NH2	18:1W:74:ALA:O	2.31	0.62
32:1a:945:G:OP1	61:1a:1914:HOH:O	2.16	0.62
32:1a:1047:G:H5"	45:1n:4:LYS:HD3	1.82	0.62
7:1H:3:ARG:HG2	7:1H:6:ARG:HG2	1.82	0.62
32:1a:1435:G:H2'	32:1a:1436:U:C6	2.35	0.62
29:17:33:ARG:NH2	61:17:201:HOH:O	2.33	0.62
32:1a:1378:C:O2	38:1g:76:ARG:NH1	2.26	0.62
32:1a:1530:G:H2'	32:1a:1531:A:C8	2.35	0.62
1:2A:309:G:N3	1:2A:329:G:O2'	2.32	0.62
1:2A:602:G:O2'	1:2A:655:A:N6	2.32	0.62
32:1a:407:G:OP1	35:1d:115:ARG:NH2	2.33	0.62
32:2a:64:G:H4'	32:2a:65:U:H3'	1.82	0.62
40:2i:28:VAL:HG12	40:2i:63:ILE:HB	1.80	0.62
44:2m:67:GLU:HG3	44:2m:71:ARG:HH22	1.65	0.62
1:2A:2690:C:OP1	13:2R:17:ARG:NH2	2.33	0.61
1:1A:2023:G:H5'	1:1A:2617:C:H4'	1.82	0.61
50:1s:22:LEU:HB3	50:1s:27:GLU:HB3	1.82	0.61
32:2a:1183:A:O2'	32:2a:1184:G:OP1	2.18	0.61
39:1h:83:ILE:HG13	39:1h:137:VAL:HG22	1.81	0.61
47:1p:53:VAL:HG13	47:1p:79:VAL:HG22	1.81	0.61
1:2A:2822:G:O2'	1:2A:2825:C:N4	2.34	0.61
8:2I:130:TYR:HB3	8:2I:138:ILE:HB	1.81	0.61
40:2i:72:GLY:O	40:2i:76:ALA:N	2.31	0.61
25:23:59:VAL:HG12	25:23:60:GLU:H	1.65	0.61
42:2k:99:GLN:HG2	42:2k:105:VAL:HG21	1.81	0.61
56:2y:13:C:H2'	56:2y:14:A:H5"	1.81	0.61
32:1a:953:G:H5'	32:1a:965:A:H61	1.64	0.61
44:2m:37:THR:HB	44:2m:55:ARG:HD2	1.83	0.61
44:2m:58:GLU:O	44:2m:62:ASN:ND2	2.33	0.61
56:2y:8:4SU:H1'	56:2y:48:C:H1'	1.83	0.61
1:1A:762:U:OP1	61:1A:4225:HOH:O	2.16	0.61
4:1E:3:GLY:HA3	4:1E:81:ILE:HD12	1.83	0.61
7:1H:101:ARG:HH22	7:1H:122:THR:HA	1.65	0.61
9:1N:13:TRP:CE2	9:1N:133:GLN:HG2	2.36	0.61
33:2b:73:THR:OG1	33:2b:170:GLU:OE2	2.18	0.61
13:1R:104:ARG:HG3	13:1R:111:LEU:HD21	1.83	0.61
1:2A:10:G:O2'	1:2A:2801(A):A:N7	2.34	0.61
41:2j:12:ASP:OD1	41:2j:13:HIS:N	2.33	0.61
1:1A:1188:U:H4'	17:1V:79:VAL:HG22	1.81	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1G:126:ASP:HB3	6:1G:128:ARG:H	1.65	0.61
32:1a:450:G:OP1	47:1p:43:LYS:NZ	2.33	0.61
1:2A:639:U:H2'	1:2A:640:C:C6	2.36	0.61
35:2d:153:ARG:HG2	35:2d:181:MET:HE2	1.83	0.61
53:2v:23:A:H4'	53:2v:24:A:H5'	1.83	0.61
1:1A:1379:A:H4'	1:1A:1380:G:OP2	2.01	0.61
61:1A:4222:HOH:O	6:1G:45:GLU:OE2	2.16	0.61
32:1a:532:A:N6	32:1a:1206:G:O2'	2.34	0.61
34:1c:11:ARG:NH2	34:1c:177:THR:O	2.29	0.61
17:2V:76:LYS:HB2	17:2V:81:TYR:HB3	1.82	0.61
49:2r:73:ALA:HB3	49:2r:79:LEU:HD12	1.82	0.61
1:2A:271(M):G:OP1	8:2I:57:ARG:NH1	2.34	0.61
1:2A:2218:U:O2	23:21:52:ARG:NH1	2.34	0.61
12:2Q:18:LYS:O	12:2Q:98:LYS:NZ	2.25	0.61
1:1A:911:A:H2'	12:1Q:9:TYR:OH	2.01	0.60
32:1a:903:G:OP1	61:1a:1913:HOH:O	2.16	0.60
41:1j:38:ILE:HD11	41:1j:71:LEU:HD23	1.82	0.60
1:2A:652(B):A:N6	1:2A:655:A:O2'	2.30	0.60
1:2A:1271:G:OP2	61:2A:3926:HOH:O	2.16	0.60
1:1A:2136:C:N4	1:1A:2155:G:C6	2.69	0.60
32:1a:1108:G:O6	61:1a:1911:HOH:O	2.15	0.60
33:1b:82:ARG:NE	33:1b:92:TYR:OH	2.34	0.60
32:2a:448:A:P	32:2a:485:G:H22	2.23	0.60
1:1A:1062:G:H22	1:1A:1077:A:N6	1.98	0.60
1:1A:1385:G:O2'	1:1A:1396:U:O2	2.15	0.60
1:1A:1671:U:O4	61:1A:4210:HOH:O	2.15	0.60
32:1a:545:C:OP1	35:1d:61:LYS:NZ	2.31	0.60
1:2A:84:A:H5"	20:2Y:8:LYS:HE3	1.83	0.60
1:2A:2298:A:N6	1:2A:2318:G:H8	1.92	0.60
7:2H:11:VAL:HG13	7:2H:15:VAL:HG23	1.82	0.60
19:2X:53:LYS:HB3	19:2X:82:GLN:HB3	1.82	0.60
1:1A:2306:C:O2	61:1A:4222:HOH:O	2.14	0.60
11:1P:39:LYS:HB2	11:1P:45:LEU:HD13	1.82	0.60
32:1a:486:U:H2'	32:1a:487:A:H8	1.66	0.60
1:1A:1466:G:HO2'	1:1A:1546:C:HO2'	1.34	0.60
1:1A:2100:G:H1	1:1A:2189:U:H3	1.48	0.60
11:1P:39:LYS:HG3	11:1P:45:LEU:HD22	1.82	0.60
50:1s:3:ARG:NE	50:1s:8:GLY:O	2.34	0.60
34:1c:24:ALA:HB2	34:1c:32:LEU:HD12	1.83	0.60
7:2H:59:ARG:O	7:2H:63:SER:OG	2.18	0.60
35:2d:72:GLU:OE2	35:2d:207:TYR:OH	2.19	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:2i:50:LEU:HA	40:2i:53:VAL:HG22	1.84	0.60
1:1A:1174:A:H4'	1:1A:1175:U:OP1	2.01	0.60
32:1a:148:G:H2'	32:1a:149:A:C8	2.37	0.60
1:2A:880:G:H1	1:2A:897:C:H42	1.50	0.60
1:2A:884:C:H3'	1:2A:885:C:C6	2.37	0.60
32:2a:947:G:H1	32:2a:1234:C:H42	1.48	0.60
38:1g:50:ILE:HD13	38:1g:125:MET:HG2	1.84	0.60
1:2A:1786:A:H1'	1:2A:1938:A:N6	2.16	0.60
7:2H:33:LEU:HD21	7:2H:136:ILE:HB	1.84	0.60
32:2a:179:A:H2'	32:2a:180:U:C6	2.37	0.60
44:2m:90:LEU:HA	44:2m:93:ARG:HD2	1.83	0.60
51:2t:9:ASN:O	51:2t:10:LEU:HB2	1.99	0.60
1:2A:2693:A:H2'	1:2A:2694:G:H8	1.66	0.60
1:2A:2819:G:O6	61:2A:3931:HOH:O	2.14	0.60
3:2D:148:GLU:HB2	3:2D:151:LYS:HD2	1.83	0.60
40:2i:26:VAL:HG22	40:2i:61:ALA:HB3	1.83	0.60
1:1A:1803:A:O2'	3:1D:259:THR:HG21	2.02	0.60
1:1A:2171:A:O2'	1:1A:2172:U:H5"	2.02	0.60
1:1A:2759:G:N7	61:1A:4284:HOH:O	2.31	0.60
32:1a:1149:C:P	40:1i:9:ARG:HH21	2.24	0.60
1:2A:1116:C:H2'	1:2A:1117:G:C8	2.37	0.60
32:2a:222:U:H2'	32:2a:223:U:C6	2.37	0.60
32:2a:999:C:H42	32:2a:1042:G:H1	1.49	0.60
35:2d:111:ALA:HB2	35:2d:120:LEU:HD12	1.84	0.60
51:2t:60:GLU:HG3	51:2t:81:LYS:HD2	1.82	0.60
26:14:16:CYS:SG	26:14:17:GLY:N	2.75	0.59
30:18:33:ASN:HA	30:18:36:LYS:HD2	1.84	0.59
8:2I:31:LEU:HD21	8:2I:38:LEU:HG	1.82	0.59
12:2Q:38:GLU:HG3	12:2Q:127:ILE:HB	1.84	0.59
32:2a:1119:C:H2'	32:2a:1120:G:H8	1.66	0.59
32:2a:1202:G:O4'	45:2n:29:ARG:NH1	2.34	0.59
32:2a:1305:G:N2	32:2a:1331:G:H1'	2.17	0.59
3:1D:3:VAL:HG13	3:1D:17:THR:HB	1.84	0.59
35:1d:15:GLU:OE2	35:1d:66:ARG:NH1	2.35	0.59
1:2A:668:G:H5'	1:2A:669:G:OP2	2.01	0.59
1:2A:2033:A:OP1	61:2A:3906:HOH:O	2.17	0.59
32:2a:1106:G:H5"	34:2c:172:ARG:HG2	1.84	0.59
32:2a:1144:G:N2	32:2a:1146:A:H62	2.00	0.59
11:1P:29:LYS:HG3	11:1P:30:THR:N	2.17	0.59
1:2A:489:G:N7	18:2W:49:LYS:NZ	2.50	0.59
1:2A:1225:G:H4'	17:2V:84:LYS:HG2	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2G:137:GLU:HG2	6:2G:152:LEU:HD23	1.85	0.59
21:2Z:11:GLU:O	21:2Z:36:LYS:NZ	2.35	0.59
32:2a:1029:C:N4	32:2a:1032:G:C6	2.69	0.59
47:2p:53:VAL:HG13	47:2p:79:VAL:HG22	1.85	0.59
4:1E:54:GLN:NE2	4:1E:76:ARG:HG2	2.17	0.59
1:2A:625:G:O6	11:2P:107:LYS:NZ	2.35	0.59
1:2A:2619:C:OP1	4:2E:152:LYS:NZ	2.33	0.59
14:2S:15:ARG:O	14:2S:19:LYS:HG2	2.02	0.59
15:2T:108:ARG:NH2	32:2a:1465:C:OP2	2.35	0.59
32:1a:501:C:H2'	32:1a:502:G:H8	1.68	0.59
32:2a:1272:G:N2	32:2a:1273:G:C8	2.71	0.59
38:2g:27:ILE:HD13	38:2g:40:ALA:HA	1.83	0.59
8:1I:3:VAL:HG12	8:1I:38:LEU:HA	1.84	0.59
34:1c:33:LEU:HD21	45:1n:53:LEU:HD22	1.85	0.59
42:1k:87:THR:O	42:1k:87:THR:OG1	2.16	0.59
1:1A:588:U:H2'	1:1A:589:C:C6	2.37	0.59
1:2A:2133:G:O2'	1:2A:2157:G:N2	2.36	0.59
8:2I:4:ILE:HG12	8:2I:18:VAL:HG12	1.83	0.59
36:2e:41:VAL:HG23	36:2e:69:VAL:HG21	1.84	0.59
47:2p:15:PRO:HD2	47:2p:42:ARG:HD3	1.85	0.59
1:1A:1062:G:C4	1:1A:1088:A:H2'	2.38	0.59
1:1A:1187:G:H5"	17:1V:81:TYR:CE1	2.37	0.59
32:1a:1006:C:H42	32:1a:1023:G:H1	1.50	0.59
32:2a:1347:G:N2	32:2a:1373:G:H2'	2.16	0.59
33:2b:8:LYS:HG2	33:2b:9:GLU:H	1.67	0.59
1:2A:1508:A:H4'	1:2A:1509(A):A:C5	2.38	0.59
33:2b:74:LYS:NZ	33:2b:205:ASP:O	2.35	0.59
1:1A:1817:G:OP1	3:1D:88:ARG:NH2	2.36	0.59
1:1A:2591:C:H2'	1:1A:2592:G:C8	2.37	0.59
3:1D:71:ASP:HB3	3:1D:103:ARG:HH12	1.68	0.59
1:2A:2000:G:OP1	13:2R:5:LYS:NZ	2.36	0.59
1:2A:2576:G:O2'	1:2A:2579:C:OP2	2.17	0.59
1:2A:2849:U:O4	15:2T:23:ARG:NH2	2.33	0.59
6:2G:32:PRO:HB3	6:2G:163:ALA:HB2	1.84	0.59
32:2a:110:C:O2'	47:2p:25:ARG:O	2.19	0.59
32:2a:1051:C:H2'	32:2a:1052:U:H6	1.67	0.59
6:1G:47:LYS:HG3	6:1G:48:GLU:H	1.67	0.58
1:2A:775:G:O2'	61:2A:3917:HOH:O	2.16	0.58
5:2F:120:GLU:HG3	5:2F:122:LYS:HG2	1.85	0.58
8:2I:41:GLU:HA	8:2I:44:LEU:HB3	1.85	0.58
11:2P:89:ALA:O	11:2P:121:LYS:NZ	2.32	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:2Y:45:VAL:HG23	20:2Y:63:LYS:HB3	1.85	0.58
34:2c:134:ILE:HG23	34:2c:151:VAL:HB	1.85	0.58
1:1A:2128:C:N4	1:1A:2160:G:H1	1.99	0.58
1:1A:2131:G:N2	1:1A:2158:A:N1	2.51	0.58
4:1E:179:GLU:HG3	15:1T:9:LEU:HD21	1.86	0.58
32:1a:17:U:H2'	32:1a:18:C:C6	2.38	0.58
1:2A:563:G:OP2	61:2A:3937:HOH:O	2.17	0.58
1:2A:1026:U:OP1	61:2A:3925:HOH:O	2.17	0.58
1:2A:2206:G:H3'	1:2A:2207:G:H8	1.68	0.58
1:2A:2784:C:H1'	4:2E:37:ARG:HH12	1.69	0.58
32:2a:165:C:H2'	32:2a:166:G:H8	1.67	0.58
33:2b:16:HIS:HB2	33:2b:204:ASN:HB2	1.85	0.58
1:1A:2319:G:N1	14:1S:3:ARG:HA	2.18	0.58
33:1b:33:TYR:HB2	33:1b:43:ASP:HB2	1.85	0.58
1:2A:1778:U:OP1	61:2A:3934:HOH:O	2.16	0.58
1:1A:1176:G:H21	1:1A:1178:C:P	2.26	0.58
4:1E:29:GLY:HA3	61:1E:403:HOH:O	2.03	0.58
6:2G:7:LEU:HD13	6:2G:104:GLU:HA	1.84	0.58
54:2w:37:MIA:H8	54:2w:37:MIA:O5'	2.04	0.58
1:1A:1057:A:N6	1:1A:1087:G:OP2	2.37	0.58
15:1T:60:THR:HG22	15:1T:77:PRO:HA	1.86	0.58
33:1b:208:ILE:HD13	33:1b:208:ILE:H	1.68	0.58
34:1c:6:HIS:HD2	34:1c:8:ILE:H	1.50	0.58
1:1A:387:U:O4	61:1A:4226:HOH:O	2.17	0.58
1:1A:994:C:OP1	16:1U:53:ARG:NH2	2.36	0.58
32:1a:1023:G:H3'	32:1a:1024:G:H8	1.69	0.58
32:1a:1297:C:O2'	38:1g:114:ARG:NH2	2.36	0.58
32:1a:1525:G:OP1	42:1k:120:ARG:NH2	2.36	0.58
32:2a:165:C:H2'	32:2a:166:G:C8	2.38	0.58
1:1A:1292:U:H2'	1:1A:1293:C:C6	2.39	0.58
5:1F:53:THR:HG22	5:1F:55:GLY:H	1.68	0.58
32:1a:1030(D):A:H2'	32:1a:1031:G:H4'	1.84	0.58
1:2A:2022:U:O2'	1:2A:2617:C:H5'	2.04	0.58
4:2E:183:LEU:HD21	15:2T:10:VAL:HG11	1.86	0.58
1:1A:2794:C:N4	1:1A:2802:G:H22	2.00	0.58
32:1a:757:U:H2'	32:1a:758:G:O4'	2.04	0.58
36:1e:78:HIS:HE1	36:1e:143:ARG:H	1.51	0.58
1:2A:2552:2MU:H6	1:2A:2552:2MU:O5'	2.03	0.58
21:2Z:105:VAL:N	21:2Z:139:VAL:O	2.37	0.58
32:2a:1279:A:O2'	32:2a:1281:U:OP2	2.14	0.58
36:2e:24:ARG:NH1	53:2v:24:A:OP2	2.37	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:2e:88:LYS:HB3	36:2e:123:LEU:HB2	1.86	0.58
54:2w:14:A:H61	54:2w:21:A:H2	1.50	0.58
13:1R:118:GLU:H	13:1R:118:GLU:CD	2.12	0.58
15:1T:84:GLN:HG2	15:1T:85:LYS:HD3	1.85	0.58
20:1Y:15:VAL:HG21	20:1Y:42:VAL:HG11	1.85	0.58
1:2A:1651:G:OP1	13:2R:40:LYS:NZ	2.36	0.58
1:2A:2317:C:H2'	1:2A:2318:G:H5'	1.86	0.58
1:2A:2319:G:N2	14:2S:3:ARG:HD2	2.18	0.58
6:2G:67:LYS:HD3	26:24:5:ILE:HD12	1.86	0.58
26:24:59:PHE:CE2	50:2s:64:GLU:HG2	2.39	0.58
32:2a:1263:C:N3	32:2a:1272:G:O6	2.37	0.58
11:1P:50:ARG:HD3	30:18:7:HIS:CD2	2.39	0.58
25:13:11:SER:HA	25:13:31:LEU:HD11	1.86	0.58
1:2A:1019:U:HO2'	1:2A:1021:A:H2	1.52	0.58
1:2A:2328:A:H2'	1:2A:2329:G:C8	2.39	0.58
1:2A:2589:A:OP1	61:2A:3915:HOH:O	2.16	0.58
6:2G:16:ARG:HE	6:2G:31:VAL:HG11	1.69	0.58
13:2R:51:LEU:HD22	13:2R:66:VAL:HG13	1.84	0.58
1:1A:1075:C:H2'	1:1A:1076:C:H2'	1.86	0.57
36:1e:6:PHE:HB3	36:1e:34:VAL:HG22	1.86	0.57
1:2A:621:A:OP2	11:2P:108:LYS:NZ	2.36	0.57
1:2A:1693:U:O2'	3:2D:14:ARG:NH2	2.36	0.57
33:2b:48:MET:HA	33:2b:51:LEU:HD12	1.86	0.57
38:2g:54:THR:O	38:2g:56:GLN:N	2.35	0.57
32:1a:324:G:N7	61:1a:1944:HOH:O	2.32	0.57
39:1h:44:PHE:HB3	39:1h:80:ILE:HG12	1.86	0.57
1:2A:896:A:H1'	54:2w:56:C:H5'	1.86	0.57
1:2A:2143:C:H42	1:2A:2148:G:H1	1.51	0.57
1:2A:2735:G:H2'	1:2A:2736:G:H8	1.69	0.57
1:2A:2805:G:H2'	1:2A:2807:G:C8	2.40	0.57
9:2N:15:LEU:HB2	9:2N:135:PRO:HB2	1.85	0.57
24:22:1:MET:N	24:22:52:ASP:OD2	2.37	0.57
32:2a:620:C:C2	35:2d:135:LEU:HG	2.39	0.57
1:1A:1105:U:H2'	1:1A:1106:G:C8	2.38	0.57
19:1X:27:THR:HG23	19:1X:80:ILE:HG13	1.86	0.57
32:1a:1305:G:N2	32:1a:1331:G:H1'	2.18	0.57
4:2E:7:VAL:HG23	4:2E:51:PHE:HE2	1.68	0.57
32:2a:1016:A:H2'	32:2a:1017:G:O4'	2.04	0.57
1:1A:1429:G:H2'	1:1A:1430:C:C6	2.39	0.57
32:1a:972:C:O2'	41:1j:55:LYS:O	2.21	0.57
1:2A:2023:G:H5'	1:2A:2617:C:H4'	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2B:83:G:H5”	25:23:52:HIS:CD2	2.40	0.57
32:2a:407:G:H5”	35:2d:115:ARG:HB3	1.86	0.57
32:2a:1263:C:H1’	32:2a:1273:G:N2	2.18	0.57
32:2a:1271:G:C2	32:2a:1272:G:N7	2.73	0.57
34:2c:20:SER:HB3	34:2c:22:TRP:HE1	1.68	0.57
3:1D:183:ARG:HG3	3:1D:270:ILE:HD13	1.86	0.57
1:2A:1816:G:O6	3:2D:35:LYS:NZ	2.26	0.57
1:2A:2504:U:OP2	61:2A:3939:HOH:O	2.17	0.57
1:2A:2659:G:P	7:2H:158:HIS:HE2	2.26	0.57
39:2h:113:SER:HB2	39:2h:134:ILE:HD11	1.85	0.57
1:1A:1076:C:O2’	1:1A:1077:A:N7	2.35	0.57
1:1A:2659:G:O2’	7:1H:175:LYS:NZ	2.35	0.57
32:1a:662:G:H2’	32:1a:663:A:C8	2.38	0.57
32:1a:1240:U:OP2	38:1g:116:ALA:N	2.37	0.57
37:2f:35:ALA:HA	37:2f:67:MET:HB3	1.86	0.57
40:2i:4:TYR:CE1	40:2i:88:TYR:HA	2.39	0.57
14:1S:39:ILE:HB	14:1S:49:VAL:HG12	1.87	0.57
32:1a:1250:A:H4’	40:1i:68:GLY:N	2.19	0.57
33:1b:87:ARG:NH2	33:1b:220:ASP:OD1	2.34	0.57
38:1g:78:ARG:HG2	38:1g:79:ARG:H	1.69	0.57
7:2H:9:ILE:HB	7:2H:50:VAL:HB	1.86	0.57
7:2H:144:VAL:HG12	7:2H:148:ILE:HD11	1.87	0.57
21:2Z:52:SER:C	21:2Z:54:HIS:H	2.12	0.57
32:2a:142:G:H2’	32:2a:143:A:C8	2.39	0.57
32:2a:624:C:H2’	32:2a:625:G:C8	2.40	0.57
39:2h:119:LEU:HB3	39:2h:123:GLU:HB2	1.86	0.57
32:1a:964:A:N3	32:1a:969:A:O2’	2.35	0.57
35:2d:60:GLU:HG3	35:2d:202:LEU:HD12	1.86	0.57
32:2a:189(F):U:O2	48:2q:63:ARG:NH2	2.38	0.57
32:2a:920:U:H2’	32:2a:921:U:C6	2.39	0.57
1:1A:1017:G:N7	61:1A:4292:HOH:O	2.32	0.57
35:1d:154:ASN:HA	35:1d:159:ARG:HH21	1.70	0.57
1:2A:184:C:H2’	1:2A:185:U:C6	2.40	0.57
1:2A:2138:C:N4	1:2A:2153:G:H1	2.01	0.57
3:1D:108:PRO:HB3	3:1D:143:HIS:CE1	2.40	0.56
37:1f:12:PRO:HG3	37:1f:57:GLN:HB2	1.87	0.56
15:2T:41:ARG:NH2	32:2a:346:G:OP1	2.32	0.56
26:24:53:GLU:HG2	26:24:55:ARG:H	1.69	0.56
34:2c:37:GLN:NE2	45:2n:52:GLN:OE1	2.38	0.56
48:2q:45:HIS:HB3	48:2q:72:ARG:HG2	1.85	0.56
1:1A:1225:G:OP1	17:1V:69:LYS:NZ	2.36	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:256:U:OP1	48:1q:17:LYS:NZ	2.33	0.56
32:1a:731:G:H5'	32:1a:766:A:H4'	1.86	0.56
32:1a:1053:G:N7	32:1a:1200:C:H5"	2.19	0.56
46:1o:55:GLY:HA2	46:1o:58:MET:HE3	1.87	0.56
1:2A:1311:G:H2'	29:27:47:ARG:NH2	2.20	0.56
18:2W:4:LYS:HD2	18:2W:6:ILE:HD11	1.86	0.56
32:2a:1226:C:OP2	44:2m:91:ARG:NH1	2.31	0.56
1:1A:1165:U:H2'	1:1A:1166:C:C6	2.40	0.56
1:1A:1769:G:O2'	1:1A:1958:C:OP1	2.21	0.56
22:10:46:LYS:NZ	22:10:75:LEU:O	2.34	0.56
32:1a:1505:G:O2'	53:1v:13:A:O2'	2.23	0.56
40:1i:43:ALA:HA	40:1i:74:ILE:HD13	1.85	0.56
1:2A:492:A:H2'	1:2A:493:G:O4'	2.06	0.56
1:2A:1434:A:H61	1:2A:1558:A:H62	1.51	0.56
1:2A:1912:A:OP1	61:2A:3941:HOH:O	2.18	0.56
1:2A:2136:C:H42	1:2A:2155:G:H1	1.53	0.56
5:2F:184:TYR:CE2	5:2F:188:ARG:HD2	2.40	0.56
12:2Q:57:HIS:HD2	12:2Q:117:ALA:HB2	1.69	0.56
21:2Z:30:ASN:HD21	21:2Z:32:HIS:HD2	1.54	0.56
42:2k:48:ILE:HG21	42:2k:63:LEU:HB3	1.86	0.56
50:2s:32:LYS:HA	50:2s:50:ALA:HB3	1.86	0.56
1:1A:295:G:H4'	20:1Y:1:MET:HE3	1.85	0.56
2:1B:105:A:OP1	21:1Z:72:ARG:NH1	2.33	0.56
32:1a:96:U:H2'	32:1a:97:G:H8	1.70	0.56
32:1a:1183:A:O2'	32:1a:1184:G:OP1	2.23	0.56
33:1b:21:ARG:NH2	33:1b:23:ARG:HH11	2.03	0.56
39:1h:119:LEU:HB3	39:1h:123:GLU:HB2	1.87	0.56
32:2a:1119:C:H2'	32:2a:1120:G:C8	2.41	0.56
32:2a:1272:G:N2	32:2a:1273:G:C5	2.74	0.56
33:2b:76:GLN:HB2	33:2b:208:ILE:HG13	1.86	0.56
1:1A:1062:G:H8	1:1A:1070:A:H4'	1.70	0.56
32:1a:222:U:H2'	32:1a:223:U:C6	2.41	0.56
35:1d:22:LYS:HB2	35:1d:26:CYS:SG	2.45	0.56
54:1w:43:C:H2'	54:1w:44:G:C8	2.40	0.56
1:2A:752:A:H3'	29:27:1:MET:HE1	1.87	0.56
1:2A:2115:G:O2'	1:2A:2117:A:N7	2.28	0.56
7:2H:86:GLU:OE1	7:2H:130:ARG:NH1	2.38	0.56
1:1A:1359:A:H2'	1:1A:1360:A:H5'	1.88	0.56
1:1A:2611:U:H5'	1:1A:2611:U:H6	1.70	0.56
26:14:34:GLU:HG2	26:14:35:VAL:HG12	1.88	0.56
32:1a:1314:C:N4	50:1s:2:PRO:O	2.38	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:1m:40:ASN:O	44:1m:43:THR:OG1	2.24	0.56
48:1q:66:SER:O	48:1q:70:ARG:NH1	2.39	0.56
50:1s:63:THR:OG1	50:1s:65:ASN:OD1	2.20	0.56
1:2A:1507:A:O2'	1:2A:1508:A:O5'	2.23	0.56
1:1A:639:U:H2'	1:1A:640:C:C6	2.41	0.56
1:1A:1156:A:OP2	61:1A:4229:HOH:O	2.18	0.56
14:2S:66:ALA:HA	14:2S:69:VAL:HG12	1.87	0.56
26:24:60:GLN:O	26:24:62:ARG:NH1	2.39	0.56
32:2a:1221:G:OP1	32:2a:1320:C:N4	2.38	0.56
32:2a:1301:U:O2'	32:2a:1302:U:H5'	2.06	0.56
36:2e:105:VAL:HB	36:2e:106:PRO:HD3	1.87	0.56
18:1W:1:MET:HE3	18:1W:2:GLU:H	1.69	0.56
36:1e:11:ILE:HD13	36:1e:105:VAL:HG13	1.88	0.56
44:1m:65:LYS:HG3	44:1m:69:GLU:HG3	1.88	0.56
1:2A:1181:C:H2'	1:2A:1182:A:C8	2.41	0.56
1:2A:2507:C:H2'	1:2A:2508:G:O4'	2.06	0.56
1:2A:2570:G:O6	61:2A:3935:HOH:O	2.16	0.56
1:2A:2576:G:N7	61:2A:4025:HOH:O	2.33	0.56
1:2A:2727:G:O2'	10:2O:70:LYS:NZ	2.39	0.56
5:2F:170:LEU:HB2	5:2F:173:VAL:HB	1.86	0.56
11:2P:63:PRO:HG2	30:28:25:MET:HB2	1.88	0.56
32:2a:460:G:N2	32:2a:471:G:N7	2.54	0.56
54:2w:13:C:O2'	54:2w:14:A:O5'	2.22	0.56
1:1A:2870:C:H2'	1:1A:2871:C:O4'	2.06	0.56
5:1F:185:ASP:HA	5:1F:188:ARG:HD3	1.86	0.56
6:1G:150:ASP:N	6:1G:150:ASP:OD1	2.39	0.56
14:1S:92:TYR:OH	61:1S:301:HOH:O	2.18	0.56
5:2F:53:THR:HG23	5:2F:55:GLY:N	2.20	0.56
34:2c:131:ARG:HE	34:2c:135:LYS:HE3	1.69	0.56
37:2f:67:MET:HE3	37:2f:72:VAL:HG22	1.88	0.56
41:2j:44:VAL:HG22	41:2j:66:ARG:HB3	1.88	0.56
1:2A:888:C:OP1	44:2m:93:ARG:NH1	2.39	0.56
32:2a:1518:MA6:H93	32:2a:1519:MA6:H92	1.88	0.56
1:1A:248:G:OP1	61:1A:4228:HOH:O	2.18	0.55
32:1a:96:U:H2'	32:1a:97:G:C8	2.41	0.55
32:1a:134:A:H61	47:1p:25:ARG:NH1	2.03	0.55
32:1a:974:A:H8	32:1a:974:A:OP1	1.89	0.55
4:2E:21:VAL:HG13	4:2E:185:LYS:HG3	1.87	0.55
15:2T:39:ARG:HH21	15:2T:41:ARG:HD3	1.71	0.55
32:2a:435:C:H2'	32:2a:436:C:H6	1.71	0.55
32:2a:1027:C:O2'	32:2a:1034:G:N2	2.33	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1239:A:H4'	32:2a:1240:U:H5"	1.87	0.55
34:2c:7:PRO:HG2	34:2c:184:TYR:HB2	1.87	0.55
40:2i:42:ARG:NH2	40:2i:71:SER:OG	2.33	0.55
1:1A:2336:A:H61	22:10:43:THR:HG22	1.71	0.55
5:2F:157:VAL:HB	5:2F:194:MET:HG2	1.88	0.55
6:2G:44:GLY:C	6:2G:46:ALA:H	2.14	0.55
1:1A:615:G:OP1	5:1F:40:GLN:NE2	2.37	0.55
1:1A:1405:U:H2'	1:1A:1406:U:H6	1.69	0.55
1:1A:2154:G:C2	1:1A:2155:G:H1'	2.42	0.55
32:1a:542:G:H5'	35:1d:41:GLY:HA3	1.89	0.55
37:1f:2:ARG:HD2	37:1f:69:GLU:HB3	1.89	0.55
42:1k:48:ILE:O	42:1k:50:TYR:N	2.34	0.55
1:2A:2787:C:H1'	4:2E:62:PRO:HG3	1.86	0.55
6:2G:124:SER:O	6:2G:124:SER:OG	2.21	0.55
26:24:46:GLN:NE2	26:24:48:ARG:HD3	2.21	0.55
44:2m:37:THR:HG21	44:2m:56:LEU:HA	1.88	0.55
7:1H:105:LEU:HD12	7:1H:151:ILE:HD12	1.88	0.55
11:1P:63:PRO:HD3	30:18:27:THR:HG22	1.88	0.55
32:1a:1036:G:H5"	32:1a:1037:C:C5	2.41	0.55
1:2A:1495:A:H2'	1:2A:1496:A:C8	2.42	0.55
5:2F:155:LEU:HD11	5:2F:176:LEU:HD12	1.87	0.55
7:2H:45:VAL:HG23	7:2H:50:VAL:HG22	1.87	0.55
32:2a:957:U:O2'	32:2a:959:A:N7	2.32	0.55
1:1A:2123:G:H2'	1:1A:2124:G:C8	2.42	0.55
32:1a:502:G:OP1	43:1l:118:SER:HB3	2.07	0.55
1:2A:652(T):C:H2'	1:2A:652(U):G:C8	2.41	0.55
1:2A:1796:U:H2'	1:2A:1797:C:C6	2.41	0.55
1:1A:271(K):U:O2	8:1I:50:ARG:HD3	2.07	0.55
1:1A:2163:C:OP1	1:1A:2165:G:N2	2.39	0.55
3:1D:8:PRO:HB3	3:1D:14:ARG:HG2	1.88	0.55
32:1a:1250:A:H4'	40:1i:68:GLY:H	1.72	0.55
35:1d:98:GLU:OE1	35:1d:103:ASN:ND2	2.38	0.55
54:1w:37:MIA:H153	54:1w:37:MIA:HN6	1.71	0.55
1:2A:1028:A:N6	1:2A:1125:G:H2'	2.22	0.55
9:2N:40:PRO:HB3	16:2U:68:ALA:HB2	1.87	0.55
32:2a:1051:C:H2'	32:2a:1052:U:C6	2.41	0.55
44:2m:20:THR:HA	44:2m:25:ILE:HG22	1.88	0.55
1:1A:882:G:H4'	54:1w:19:G:O6	2.06	0.55
1:1A:1139:G:OP2	9:1N:70:LYS:NZ	2.37	0.55
1:1A:2366:A:OP1	61:1A:4231:HOH:O	2.18	0.55
32:1a:403:C:O2'	35:1d:122:ARG:NH1	2.39	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:1f:10:LEU:HD11	37:1f:61:LEU:HD22	1.89	0.55
49:1r:38:GLU:OE1	49:1r:41:LYS:NZ	2.31	0.55
1:2A:2334:G:H5'	14:2S:9:ARG:HG2	1.89	0.55
33:2b:118:LEU:HD23	33:2b:142:LEU:HB2	1.89	0.55
46:2o:16:ALA:HB1	46:2o:21:ASP:HB3	1.87	0.55
46:2o:87:ILE:HG22	46:2o:88:ARG:H	1.72	0.55
1:1A:2243:U:H2'	1:1A:2244:U:C6	2.41	0.55
1:1A:2445:G:OP1	5:1F:74:ARG:NH2	2.38	0.55
3:1D:39:LYS:NZ	3:1D:57:GLY:O	2.40	0.55
1:2A:1991:U:H2'	1:2A:1992:G:H5"	1.88	0.55
1:1A:897:C:H5'	54:1w:56:C:OP1	2.06	0.55
3:1D:69:ARG:C	3:1D:71:ASP:H	2.14	0.55
32:1a:553:A:H5"	43:1l:24:VAL:HG21	1.89	0.55
26:24:58:ARG:HD2	50:2s:68:GLY:H	1.72	0.55
1:1A:2130:U:H2'	1:1A:2158:A:H61	1.72	0.55
32:1a:501:C:H2'	32:1a:502:G:C8	2.42	0.55
32:1a:1286:A:H2'	32:1a:1287:A:H4'	1.89	0.55
33:1b:115:LEU:HD11	33:1b:146:GLN:HG3	1.88	0.55
38:1g:152:ALA:O	38:1g:155:ARG:HB3	2.07	0.55
51:1t:36:LEU:HD13	51:1t:58:LYS:HG3	1.89	0.55
1:2A:247:G:H4'	1:2A:386:G:C5	2.42	0.55
4:2E:101:ARG:CZ	4:2E:171:GLU:HB2	2.37	0.55
13:2R:2:ARG:NH1	13:2R:5:LYS:O	2.40	0.55
15:2T:117:ASP:OD2	15:2T:120:ARG:NE	2.26	0.55
33:2b:93:VAL:HG11	33:2b:97:TRP:HE3	1.71	0.55
43:2l:33:ARG:NH1	43:2l:61:THR:OG1	2.40	0.55
1:1A:2533:A:OP1	1:1A:2665:A:O2'	2.23	0.54
21:1Z:92:SER:O	21:1Z:130:PRO:HG2	2.07	0.54
32:1a:1030(A):G:H1'	32:1a:1031:G:H22	1.73	0.54
34:1c:19:GLU:O	34:1c:40:ARG:NH2	2.40	0.54
2:2B:66:A:N6	2:2B:109:C:H5'	2.21	0.54
14:2S:18:ILE:O	14:2S:21:THR:OG1	2.24	0.54
21:2Z:150:LEU:H	21:2Z:171:ILE:HD11	1.72	0.54
32:2a:1381:U:H1'	38:2g:79:ARG:HG3	1.88	0.54
35:2d:173:TRP:CD2	35:2d:189:PRO:HB3	2.42	0.54
1:1A:1864:U:OP1	1:1A:2410:G:O2'	2.24	0.54
11:1P:29:LYS:HG3	11:1P:30:THR:H	1.72	0.54
32:1a:977:A:O2'	32:1a:981:U:N3	2.37	0.54
41:1j:40:LEU:HB2	41:1j:69:ASN:HB2	1.89	0.54
1:2A:7:G:H2'	1:2A:8:A:C8	2.43	0.54
1:2A:801:G:O6	5:2F:53:THR:OG1	2.26	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1278:A:OP1	13:2R:36:THR:HG23	2.07	0.54
1:2A:2802:G:C4	1:2A:2803:C:H1'	2.42	0.54
32:2a:1251:A:H2'	32:2a:1252:A:C8	2.41	0.54
1:1A:1173:G:OP2	1:1A:1173:G:H2'	2.07	0.54
7:1H:20:ALA:HB1	7:1H:21:PRO:HD2	1.90	0.54
23:11:64:ALA:HA	23:11:67:ILE:HG13	1.88	0.54
35:1d:178:VAL:C	35:1d:180:GLY:H	2.16	0.54
1:2A:1770:G:O6	61:2A:3933:HOH:O	2.16	0.54
4:2E:105:THR:HG1	4:2E:199:ARG:HH21	1.55	0.54
6:2G:38:VAL:HG12	6:2G:93:THR:HA	1.88	0.54
18:2W:12:ILE:HD13	18:2W:17:VAL:HG13	1.88	0.54
21:2Z:31:ARG:HG3	21:2Z:32:HIS:CD2	2.42	0.54
32:2a:36:C:OP1	43:2l:123:LYS:NZ	2.34	0.54
32:2a:1228:C:P	44:2m:108:ARG:HH22	2.30	0.54
33:2b:120:ALA:O	33:2b:125:PRO:HD2	2.08	0.54
34:2c:52:LEU:HD12	34:2c:53:ALA:H	1.72	0.54
1:1A:1278:A:OP1	13:1R:36:THR:HG23	2.07	0.54
1:1A:1991:U:H2'	1:1A:1992:G:H5"	1.89	0.54
24:12:41:ILE:HG13	24:12:43:GLN:HG3	1.89	0.54
26:14:59:PHE:CE2	50:1s:64:GLU:HB3	2.42	0.54
36:1e:152:ARG:NH2	39:1h:107:LEU:O	2.35	0.54
1:2A:1721:G:H8	1:2A:1741:A:H62	1.54	0.54
32:2a:935:A:N6	38:2g:3:ARG:HG3	2.22	0.54
1:1A:1058:G:H1	1:1A:1080:C:N4	2.05	0.54
33:1b:163:PHE:HD1	33:1b:185:ILE:HG13	1.71	0.54
42:1k:62:GLN:OE1	42:1k:93:GLN:NE2	2.40	0.54
1:2A:607:U:OP1	5:2F:102:PRO:HA	2.07	0.54
15:2T:127:ALA:C	15:2T:129:ARG:H	2.16	0.54
44:2m:107:ALA:HB3	44:2m:111:LYS:HE2	1.89	0.54
51:2t:79:ARG:HD2	51:2t:83:ARG:HH21	1.71	0.54
56:2y:14:A:O2'	56:2y:15:G:OP1	2.23	0.54
1:1A:1025:G:C4	1:1A:1135:C:H1'	2.43	0.54
1:2A:2530:A:N7	7:2H:172:LYS:NZ	2.42	0.54
32:2a:1435:G:H2'	32:2a:1436:U:C6	2.41	0.54
33:2b:178:ARG:HH22	39:2h:68:ARG:HH12	1.54	0.54
40:2i:21:PRO:HA	40:2i:59:PHE:HA	1.88	0.54
1:1A:2794:C:H42	1:1A:2802:G:H22	1.55	0.54
32:1a:1030(B):C:H2'	32:1a:1030(C):G:H5'	1.89	0.54
44:1m:23:TYR:HB3	44:1m:67:GLU:HG2	1.88	0.54
48:1q:7:THR:HG23	48:1q:58:GLU:HG2	1.90	0.54
1:2A:811:U:H2'	11:2P:21:ARG:HA	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:2V:55:ALA:HA	17:2V:101:GLY:HA2	1.88	0.54
26:24:34:GLU:HG2	26:24:35:VAL:HG23	1.90	0.54
32:2a:860:A:H2'	32:2a:861:G:O4'	2.07	0.54
1:1A:1069:A:H2'	1:1A:1073:A:N7	2.23	0.54
32:1a:848:C:H2'	32:1a:849:C:C6	2.43	0.54
32:1a:1148:U:H2'	32:1a:1149:C:O4'	2.08	0.54
33:1b:195:ASP:O	39:1h:68:ARG:NH2	2.41	0.54
1:2A:1406:U:H2'	1:2A:1407:C:C6	2.42	0.54
1:2A:2823:A:OP1	4:2E:159:HIS:NE2	2.38	0.54
4:2E:1:MET:HE1	4:2E:199:ARG:HB3	1.90	0.54
31:29:10:ILE:HD12	31:29:32:HIS:HA	1.89	0.54
32:2a:646:U:H2'	32:2a:647:C:C6	2.42	0.54
38:2g:111:ARG:HD2	38:2g:123:GLU:HB2	1.90	0.54
40:2i:85:LEU:HB3	40:2i:92:TYR:HD2	1.71	0.54
41:2j:35:SER:HB3	41:2j:73:ASP:H	1.72	0.54
50:2s:66:MET:HB2	50:2s:74:PHE:CZ	2.43	0.54
56:2y:18:G:N2	56:2y:55:PSU:HN3	2.00	0.54
1:1A:1300:U:H4'	1:1A:1301:A:H5"	1.90	0.54
4:1E:175:VAL:O	4:1E:177:PRO:HD3	2.08	0.54
32:1a:475:G:H2'	32:1a:476:G:H8	1.73	0.54
32:1a:560:U:O2'	32:1a:561:U:OP2	2.24	0.54
1:2A:190:A:OP2	23:21:39:LYS:HE3	2.07	0.54
1:2A:2126:A:N6	1:2A:2162:G:O2'	2.36	0.54
5:2F:18:ARG:NH1	5:2F:127:GLU:OE1	2.40	0.54
36:2e:78:HIS:HE1	36:2e:143:ARG:H	1.56	0.54
40:2i:105:ASP:HB2	40:2i:107:ARG:HG3	1.89	0.54
1:1A:1092:C:H2'	1:1A:1093:G:H5'	1.90	0.54
1:2A:284:U:H2'	1:2A:285:C:C6	2.43	0.54
1:2A:1188:U:H4'	17:2V:79:VAL:HG22	1.89	0.54
1:2A:1405:U:H2'	1:2A:1406:U:C6	2.43	0.54
1:2A:2785:C:OP1	4:2E:41:LYS:NZ	2.40	0.54
6:2G:115:ARG:NH1	6:2G:137:GLU:OE1	2.36	0.54
32:2a:1068:G:N2	32:2a:1191:A:N3	2.47	0.54
39:2h:49:GLU:HG2	39:2h:62:TYR:HE2	1.72	0.54
1:1A:2787:C:H1'	4:1E:62:PRO:HG3	1.90	0.53
6:1G:106:LEU:HA	6:1G:110:ALA:HB3	1.89	0.53
21:1Z:48:PHE:CE1	21:1Z:52:SER:HA	2.43	0.53
32:1a:486:U:H2'	32:1a:487:A:C8	2.43	0.53
32:1a:827:U:H5"	32:1a:828:A:OP2	2.09	0.53
32:1a:1005:A:H1'	32:1a:1036:G:O6	2.08	0.53
32:1a:1014:A:H4'	50:1s:14:HIS:CE1	2.43	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1025:U:O2	32:1a:1036:G:O6	2.26	0.53
1:2A:2685:G:O6	61:2A:3938:HOH:O	2.17	0.53
5:2F:108:LYS:HG2	5:2F:112:MET:HE2	1.90	0.53
1:1A:71:A:N7	19:1X:31:HIS:HE1	2.06	0.53
10:1O:17:ARG:HB2	10:1O:45:GLU:HG2	1.90	0.53
34:1c:124:ILE:HG22	34:1c:130:VAL:HG22	1.89	0.53
2:2B:17:C:H2'	2:2B:18:G:O4'	2.08	0.53
17:2V:62:LEU:HD11	17:2V:95:LEU:HB2	1.89	0.53
32:2a:750:G:N3	46:2o:23:GLY:HA3	2.23	0.53
1:1A:800:A:H8	1:1A:800:A:OP1	1.92	0.53
1:1A:1113:U:H2'	1:1A:1114:G:C8	2.43	0.53
6:1G:116:ASP:OD2	44:1m:68:GLY:HA3	2.08	0.53
33:1b:17:PHE:HA	33:1b:44:LEU:HD21	1.90	0.53
1:2A:1355:G:OP1	3:2D:38:LYS:NZ	2.37	0.53
1:2A:1507:A:O2'	1:2A:1508:A:O4'	2.26	0.53
7:2H:6:ARG:HH22	7:2H:54:ARG:HH22	1.56	0.53
32:2a:1313:U:OP1	50:2s:5:LEU:HB2	2.08	0.53
32:2a:1316:G:N2	32:2a:1318:A:H3'	2.23	0.53
1:1A:607:U:OP1	5:1F:102:PRO:HA	2.07	0.53
1:1A:2839:G:H5'	13:1R:46:GLY:HA2	1.90	0.53
32:1a:1182:G:H5'	32:1a:1184:G:H5'	1.90	0.53
35:1d:148:VAL:HG11	35:1d:158:ILE:HG21	1.90	0.53
50:1s:50:ALA:HB1	50:1s:57:HIS:HB3	1.91	0.53
1:2A:1493:C:N4	1:2A:2206:G:O2'	2.41	0.53
1:2A:2110:G:H3'	1:2A:2111:C:H5'	1.89	0.53
30:28:62:LEU:HB3	30:28:65:GLU:HG2	1.90	0.53
32:2a:438:G:N1	32:2a:495:A:OP2	2.40	0.53
32:2a:1279:A:O2'	32:2a:1282:C:N4	2.42	0.53
33:2b:189:ASP:OD1	33:2b:189:ASP:N	2.33	0.53
44:2m:13:LYS:HA	44:2m:44:ARG:HH11	1.73	0.53
6:1G:18:GLU:OE2	6:1G:21:ARG:NH1	2.42	0.53
51:1t:10:LEU:HB3	51:1t:12:ALA:H	1.74	0.53
1:2A:271(H):G:H2'	1:2A:271(I):G:C8	2.43	0.53
13:2R:104:ARG:HD2	13:2R:109:ALA:HB3	1.91	0.53
14:2S:68:GLN:HG3	14:2S:71:ARG:HH21	1.73	0.53
20:2Y:86:ARG:HB2	20:2Y:98:VAL:HG23	1.90	0.53
32:2a:376:G:H5"	47:2p:5:ARG:HB2	1.90	0.53
32:2a:953:G:N7	44:2m:104:ARG:NH2	2.54	0.53
41:2j:30:SER:O	41:2j:81:THR:OG1	2.24	0.53
46:2o:11:VAL:HG21	46:2o:34:LEU:HD22	1.89	0.53
1:2A:568:U:H5'	1:2A:945:A:N1	2.23	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2Z:52:SER:O	21:2Z:54:HIS:N	2.39	0.53
1:1A:881:G:H2'	1:1A:882:G:H5'	1.91	0.53
32:1a:574:A:OP2	61:1a:1916:HOH:O	2.19	0.53
32:1a:736:C:H2'	32:1a:737:A:C8	2.43	0.53
41:1j:30:SER:HB3	41:1j:81:THR:HG23	1.91	0.53
1:2A:1342:A:OP2	61:2A:3943:HOH:O	2.19	0.53
10:2O:111:PHE:HB3	10:2O:114:ILE:HD12	1.91	0.53
32:2a:985:C:H2'	32:2a:986:A:C8	2.44	0.53
32:2a:1123:A:O3'	41:2j:36:GLY:HA3	2.09	0.53
37:2f:30:LEU:HD23	37:2f:75:LEU:HD11	1.91	0.53
32:1a:239:U:O4	61:1a:1909:HOH:O	2.12	0.53
41:1j:5:ARG:O	41:1j:99:LYS:N	2.33	0.53
1:2A:2507:C:H5"	1:2A:2573:C:N4	2.24	0.53
5:2F:24:LEU:HD23	5:2F:115:ALA:HA	1.91	0.53
36:2e:8:GLU:HG2	36:2e:34:VAL:HG23	1.90	0.53
1:1A:603:A:O4'	1:1A:655:A:N6	2.42	0.53
1:1A:1057:A:N7	1:1A:1086:A:H2'	2.24	0.53
1:1A:1377:G:O6	61:1A:4232:HOH:O	2.19	0.53
7:1H:113:VAL:HG11	7:1H:151:ILE:HD13	1.91	0.53
32:1a:1347:G:H5"	40:1i:107:ARG:HB3	1.89	0.53
1:2A:144:C:H5'	19:2X:2:LYS:NZ	2.23	0.53
1:2A:2151:G:H2'	1:2A:2152:G:C8	2.44	0.53
1:2A:2892:A:H2'	1:2A:2893:G:H5'	1.91	0.53
3:2D:108:PRO:HB3	3:2D:143:HIS:CE1	2.43	0.53
28:26:6:ARG:NH1	28:26:26:ASN:HB2	2.24	0.53
34:2c:71:ALA:HA	34:2c:106:VAL:HB	1.91	0.53
32:1a:70:G:H1	32:1a:99:U:H3	1.57	0.53
32:1a:78:G:O6	32:1a:92:C:N4	2.41	0.53
32:1a:1027:C:C4	32:1a:1034:G:N1	2.77	0.53
32:1a:1304:G:OP2	61:1a:1915:HOH:O	2.19	0.53
1:2A:249:C:O2	30:28:12:LYS:NZ	2.39	0.53
1:2A:970:C:OP1	25:23:20:LYS:NZ	2.42	0.53
33:2b:19:HIS:CG	33:2b:20:GLU:H	2.27	0.53
34:2c:20:SER:HB3	34:2c:22:TRP:NE1	2.24	0.53
2:1B:75:G:H22	21:1Z:73:GLN:NE2	2.07	0.52
11:1P:38:GLN:O	11:1P:40:SER:N	2.38	0.52
32:1a:1218:C:H2'	32:1a:1219:U:C6	2.44	0.52
40:1i:42:ARG:NH1	40:1i:71:SER:OG	2.40	0.52
44:1m:88:ARG:HG2	44:1m:98:VAL:HG13	1.91	0.52
55:1x:8:4SU:O5'	55:1x:8:4SU:H6	2.09	0.52
1:2A:2183:C:H2'	1:2A:2184:G:C8	2.44	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2355:C:H1'	22:20:39:ARG:HH21	1.75	0.52
32:2a:339:C:H2'	32:2a:340:U:C6	2.44	0.52
32:2a:1316:G:N2	32:2a:1319:A:H5"	2.21	0.52
34:2c:6:HIS:HD2	34:2c:8:ILE:H	1.57	0.52
34:2c:138:VAL:HG23	34:2c:151:VAL:HG23	1.91	0.52
44:2m:123:ALA:HB2	54:2w:39:PSU:H1'	1.90	0.52
32:1a:749:C:H2'	32:1a:750:G:H8	1.74	0.52
32:1a:1016:A:H2'	32:1a:1017:G:O4'	2.09	0.52
33:1b:77:ALA:HB2	33:1b:211:ILE:HD13	1.90	0.52
33:1b:223:ILE:HA	33:1b:226:ARG:HG2	1.92	0.52
44:1m:3:ARG:HG3	44:1m:4:ILE:H	1.74	0.52
1:2A:141:A:H8	1:2A:1408:C:O2'	1.91	0.52
1:2A:784:A:C6	3:2D:229:VAL:HG11	2.44	0.52
1:2A:1418:G:N7	61:2A:4030:HOH:O	2.34	0.52
1:2A:2242:G:OP1	61:2A:3942:HOH:O	2.19	0.52
21:2Z:73:GLN:O	21:2Z:87:ASP:N	2.34	0.52
32:2a:1148:U:H2'	32:2a:1149:C:O4'	2.09	0.52
32:2a:1513:A:H2'	32:2a:1514:C:C6	2.44	0.52
33:2b:16:HIS:CG	33:2b:17:PHE:N	2.76	0.52
36:2e:110:LEU:HD21	36:2e:139:LEU:HD21	1.90	0.52
1:1A:414:C:H2'	1:1A:415:A:C8	2.44	0.52
2:1B:2:C:H2'	2:1B:3:C:H6	1.74	0.52
51:1t:43:LEU:HD13	51:1t:51:GLU:HG2	1.92	0.52
2:2B:103:G:N2	21:2Z:73:GLN:HE22	2.05	0.52
5:2F:165:ARG:HG2	5:2F:168:ARG:HH21	1.74	0.52
6:2G:146:TYR:HB3	44:2m:11:ARG:HH22	1.74	0.52
20:2Y:44:ILE:HA	20:2Y:63:LYS:O	2.09	0.52
32:2a:972:C:O2'	41:2j:55:LYS:O	2.27	0.52
56:2y:26:A:N1	56:2y:44:G:C6	2.76	0.52
1:1A:2820:A:O2'	1:1A:2821:A:OP1	2.26	0.52
8:1I:72:LEU:HD12	8:1I:138:ILE:HG21	1.92	0.52
33:1b:45:GLN:O	33:1b:49:GLU:HG3	2.08	0.52
54:1w:8:4SU:O5'	54:1w:8:4SU:H6	2.10	0.52
1:2A:992:C:HO2'	17:2V:87:HIS:HD1	1.54	0.52
1:2A:2126:A:N6	1:2A:2163:C:O4'	2.42	0.52
32:2a:401:C:P	35:2d:73:ARG:HH21	2.32	0.52
32:2a:890:G:O2'	32:2a:906:G:O6	2.24	0.52
32:2a:1029:C:C2	32:2a:1032:G:N2	2.74	0.52
1:1A:370:G:H8	1:1A:370:G:OP2	1.93	0.52
1:1A:1506:C:H2'	1:1A:1507:A:H8	1.74	0.52
1:1A:2165:G:H1	1:1A:2171:A:H2'	1.74	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:1w:23:A:H3'	54:1w:24:G:H8	1.75	0.52
21:2Z:28:MET:HE1	21:2Z:61:LEU:HD11	1.92	0.52
32:2a:15:G:H21	36:2e:18:ARG:HA	1.74	0.52
32:2a:1356:G:H2'	32:2a:1357:A:C8	2.44	0.52
4:1E:105:THR:OG1	4:1E:199:ARG:NH2	2.43	0.52
5:1F:155:LEU:HD11	5:1F:176:LEU:HD12	1.91	0.52
9:1N:15:LEU:HB2	9:1N:135:PRO:HB2	1.91	0.52
11:1P:29:LYS:HG3	11:1P:30:THR:HG23	1.91	0.52
32:1a:425:G:O3'	35:1d:45:GLN:NE2	2.42	0.52
1:2A:1030:G:OP2	12:2Q:128:LYS:NZ	2.31	0.52
1:2A:2836:U:H2'	1:2A:2837:G:C8	2.45	0.52
7:2H:83:TYR:CE1	7:2H:138:LYS:HD3	2.45	0.52
32:2a:273:A:H1'	48:2q:16:GLN:HE21	1.75	0.52
32:2a:1053:G:H4'	32:2a:1054:C:H3'	1.91	0.52
32:2a:1278:U:H5'	32:2a:1279:A:H5'	1.91	0.52
32:2a:1329:A:OP2	52:2u:7:ARG:NH1	2.38	0.52
56:2y:55:PSU:N1	56:2y:57:G:H5"	2.24	0.52
32:1a:200:G:H1	32:1a:217:C:H42	1.57	0.52
33:1b:48:MET:HA	33:1b:51:LEU:HD12	1.92	0.52
35:1d:178:VAL:HG12	35:1d:179:GLU:H	1.74	0.52
1:2A:191:A:H2'	1:2A:192:C:C6	2.45	0.52
1:2A:2105:C:H2'	1:2A:2106:G:C8	2.45	0.52
4:2E:116:VAL:HG13	4:2E:122:PHE:HB2	1.91	0.52
6:2G:41:GLN:HB3	6:2G:43:LEU:HD22	1.92	0.52
29:27:46:VAL:HG13	29:27:48:LYS:HZ2	1.75	0.52
31:29:2:LYS:HE2	31:29:31:LYS:O	2.10	0.52
36:2e:74:GLY:HA3	36:2e:116:THR:HG22	1.91	0.52
1:1A:1062:G:N2	1:1A:1077:A:H61	2.08	0.52
1:1A:2336:A:H61	22:10:43:THR:CG2	2.22	0.52
2:1B:48:A:H4'	14:1S:95:HIS:HD2	1.75	0.52
32:1a:1323:G:H2'	32:1a:1324:A:C8	2.44	0.52
42:1k:107:SER:O	42:1k:108:ILE:HG13	2.10	0.52
48:1q:22:LEU:HD11	48:1q:39:SER:HB2	1.92	0.52
1:2A:817:C:OP2	61:2A:3946:HOH:O	2.19	0.52
32:2a:1112:C:N3	34:2c:178:LEU:HD12	2.25	0.52
32:2a:1142:G:H2'	32:2a:1143:G:O4'	2.10	0.52
32:1a:1036:G:H3'	32:1a:1037:C:C6	2.44	0.52
32:1a:1278:U:H5"	32:1a:1279:A:O4'	2.10	0.52
32:1a:1356:G:H2'	32:1a:1357:A:C8	2.45	0.52
32:1a:1391:U:H2'	32:1a:1392:G:C8	2.44	0.52
35:1d:19:LEU:HB2	35:1d:21:LEU:HD11	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:1m:94:ARG:NH1	44:1m:94:ARG:HB2	2.24	0.52
51:1t:26:ASN:O	51:1t:30:LYS:HG3	2.09	0.52
1:2A:531:C:OP1	1:2A:561:G:N1	2.43	0.52
21:2Z:33:LEU:HD21	21:2Z:90:VAL:HG21	1.92	0.52
32:2a:426:G:OP1	35:2d:38:TYR:OH	2.22	0.52
35:2d:22:LYS:HB2	35:2d:26:CYS:SG	2.50	0.52
36:2e:41:VAL:O	36:2e:66:MET:HA	2.10	0.52
42:2k:81:ASP:OD1	42:2k:107:SER:OG	2.24	0.52
47:2p:28:ARG:HG2	47:2p:29:ASP:OD1	2.10	0.52
1:1A:207:A:H2'	1:1A:208:C:O4'	2.08	0.52
32:1a:931:C:H42	32:1a:1386:G:H1	1.57	0.52
1:2A:2143:C:H2'	1:2A:2144:U:O4'	2.10	0.52
6:2G:16:ARG:NE	6:2G:31:VAL:HG11	2.25	0.52
56:2y:57:G:H2'	56:2y:58:A:H5'	1.91	0.52
1:1A:796:C:H2'	1:1A:797:C:C6	2.45	0.51
6:1G:179:PRO:HB2	26:14:42:PHE:HE2	1.75	0.51
32:1a:1124:G:N7	32:1a:1145:C:O2'	2.43	0.51
35:1d:65:ARG:HG3	35:1d:75:PHE:CG	2.45	0.51
40:1i:46:ALA:HA	40:1i:78:LYS:HB2	1.90	0.51
1:2A:2807:G:H22	1:2A:2892:A:N6	2.08	0.51
13:2R:97:VAL:HG22	13:2R:114:VAL:HG13	1.91	0.51
32:2a:811:C:O2'	32:2a:901:A:N1	2.40	0.51
32:2a:1321:C:O2'	50:2s:77:THR:HG21	2.10	0.51
1:1A:2142:C:N3	1:1A:2149:G:O6	2.43	0.51
26:14:50:VAL:HG11	44:1m:64:TRP:C	2.35	0.51
32:1a:235:C:H2'	32:1a:236:G:H8	1.73	0.51
32:1a:1031:G:H2'	32:1a:1032:G:C8	2.45	0.51
48:1q:45:HIS:NE2	48:1q:47:PRO:HG3	2.25	0.51
54:1w:48:C:C2	54:1w:59:U:H1'	2.45	0.51
1:2A:2263:C:OP2	61:2A:3944:HOH:O	2.19	0.51
32:2a:189(D):C:H2'	32:2a:189(E):U:O4'	2.10	0.51
32:2a:985:C:H2'	32:2a:986:A:H8	1.76	0.51
36:2e:11:ILE:HD13	36:2e:105:VAL:HG13	1.91	0.51
44:2m:79:LYS:HG2	44:2m:83:ASP:OD2	2.11	0.51
12:1Q:14:ARG:HG2	12:1Q:41:TRP:HH2	1.76	0.51
32:1a:171:A:H2'	32:1a:172:A:C8	2.45	0.51
32:1a:1244:C:H42	32:1a:1293:G:H1	1.58	0.51
1:2A:307:G:N1	1:2A:310:A:OP2	2.41	0.51
1:2A:1354:A:H2'	1:2A:1355:G:O4'	2.10	0.51
1:2A:1790:C:H5"	1:2A:1791:A:OP1	2.10	0.51
8:2I:5:LEU:HD21	8:2I:12:LEU:HB3	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:381:C:H2'	32:2a:382:A:O4'	2.10	0.51
32:1a:1006:C:H2'	32:1a:1007:C:C6	2.46	0.51
32:1a:1318:A:H5"	50:1s:3:ARG:NH1	2.25	0.51
32:1a:1504:G:OP1	32:1a:1507:A:H4'	2.10	0.51
48:1q:57:VAL:HG12	48:1q:76:LEU:HA	1.92	0.51
51:1t:60:GLU:HG3	51:1t:81:LYS:HD2	1.91	0.51
7:2H:25:LYS:HB3	7:2H:27:LYS:HZ2	1.75	0.51
10:2O:7:TYR:HE2	10:2O:20:MET:HE3	1.76	0.51
32:2a:554:C:H2'	32:2a:555:C:C6	2.46	0.51
1:1A:242:G:C8	30:18:5:LYS:HG2	2.45	0.51
1:1A:1113:U:H2'	1:1A:1114:G:H8	1.75	0.51
32:1a:976:G:H5'	32:1a:1358:U:O2'	2.10	0.51
10:2O:120:GLU:OE2	10:2O:122:LEU:HD21	2.10	0.51
21:2Z:30:ASN:HB3	21:2Z:90:VAL:HB	1.91	0.51
25:23:40:THR:HG22	25:23:42:ALA:H	1.75	0.51
32:2a:1157:A:H5'	32:2a:1158:C:C6	2.46	0.51
41:2j:62:HIS:HB3	45:2n:59:ALA:HB3	1.92	0.51
44:2m:4:ILE:HG23	44:2m:5:ALA:H	1.74	0.51
50:2s:51:VAL:O	50:2s:58:VAL:N	2.44	0.51
54:2w:25:C:H2'	54:2w:26:A:H8	1.76	0.51
2:1B:18:G:N7	61:1B:303:HOH:O	2.35	0.51
32:1a:7:G:H5'	32:1a:298:A:O4'	2.11	0.51
38:1g:65:ALA:HB1	38:1g:127:ALA:HB3	1.91	0.51
1:2A:855:G:O2'	22:20:27:GLU:OE2	2.29	0.51
1:2A:1518:U:H2'	1:2A:1519:G:O4'	2.11	0.51
5:2F:143:ALA:HB1	5:2F:148:LEU:HB2	1.91	0.51
5:2F:150:GLY:HA2	5:2F:172:TRP:CD2	2.45	0.51
32:2a:148:G:H2'	32:2a:149:A:C8	2.45	0.51
32:2a:438:G:H4'	35:2d:123:HIS:CE1	2.46	0.51
44:2m:88:ARG:HG2	44:2m:98:VAL:HG12	1.93	0.51
56:2y:26:A:N1	56:2y:44:G:O6	2.44	0.51
11:1P:63:PRO:HG2	30:18:25:MET:HB2	1.91	0.51
33:1b:74:LYS:HD2	33:1b:166:ASP:HB2	1.93	0.51
34:1c:71:ALA:HA	34:1c:106:VAL:HG12	1.92	0.51
1:2A:1412:A:H2'	1:2A:1413:G:C8	2.45	0.51
1:2A:1580:A:H3'	1:2A:1581:G:H8	1.74	0.51
2:2B:62:C:H2'	2:2B:63:G:H8	1.75	0.51
21:2Z:121:HIS:N	21:2Z:171:ILE:O	2.43	0.51
32:2a:1161:C:H2'	32:2a:1162:C:C6	2.45	0.51
32:2a:1412:C:H2'	32:2a:1413:A:C8	2.46	0.51
39:2h:19:VAL:HG23	39:2h:21:LYS:HG3	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:443:A:H1'	1:1A:1201:C:O4'	2.10	0.51
1:1A:1474:C:H2'	1:1A:1475:G:H8	1.75	0.51
21:1Z:4:ARG:O	61:1Z:401:HOH:O	2.19	0.51
36:1e:81:GLU:HG2	36:1e:90:VAL:HG13	1.91	0.51
7:2H:3:ARG:NH1	7:2H:4:ILE:H	2.09	0.51
15:2T:27:THR:HB	15:2T:90:GLN:HB3	1.92	0.51
24:22:3:LEU:O	24:22:7:ARG:HG3	2.11	0.51
33:2b:55:PHE:HA	33:2b:58:ILE:HD12	1.93	0.51
1:1A:10:G:O2'	1:1A:2801(A):A:N7	2.44	0.51
1:1A:528:A:O2'	1:1A:529:A:H5'	2.10	0.51
1:1A:919:G:N2	1:1A:2269:A:OP2	2.43	0.51
1:1A:1786:A:H1'	1:1A:1938:A:N6	2.26	0.51
1:1A:2134:A:H2'	1:1A:2135:A:C8	2.45	0.51
26:14:16:CYS:HA	26:14:33:VAL:HG12	1.92	0.51
39:1h:64:LYS:HG2	39:1h:79:VAL:HG21	1.92	0.51
44:1m:94:ARG:HB2	44:1m:94:ARG:HH11	1.75	0.51
1:2A:584:C:OP2	16:2U:6:THR:OG1	2.29	0.51
1:2A:1721:G:H3'	1:2A:1722:A:H2'	1.92	0.51
1:2A:2124:G:H1	1:2A:2174:C:H42	1.56	0.51
1:2A:2728:U:H2'	1:2A:2729:G:C8	2.46	0.51
27:25:40:LYS:NZ	27:25:44:THR:O	2.43	0.51
32:2a:501:C:OP1	43:2l:117:ARG:NH2	2.36	0.51
32:2a:772:U:H2'	32:2a:773:G:O4'	2.11	0.51
32:2a:1053:G:N7	32:2a:1200:C:H5'	2.26	0.51
46:2o:36:ILE:HG23	46:2o:56:LEU:HD11	1.93	0.51
56:2y:61:C:H2'	56:2y:62:C:C6	2.46	0.51
1:1A:1009:A:OP2	9:1N:37:LYS:NZ	2.43	0.51
1:1A:2022:U:O2'	1:1A:2617:C:H5'	2.11	0.51
2:1B:88:C:H2'	2:1B:89:G:O4'	2.10	0.51
28:16:19:ARG:NH1	28:16:52:VAL:HG21	2.26	0.51
32:1a:1310:G:OP2	44:1m:88:ARG:NH2	2.44	0.51
34:1c:15:THR:HG21	34:1c:181:ASN:HA	1.93	0.51
34:1c:162:GLN:NE2	53:1v:24:A:O3'	2.43	0.51
36:1e:74:GLY:HA3	36:1e:116:THR:HG22	1.93	0.51
48:1q:45:HIS:HB3	48:1q:72:ARG:HG2	1.92	0.51
1:2A:747:U:O2	1:2A:2014:A:H1'	2.11	0.51
1:2A:748:G:O6	18:2W:90:ARG:NH1	2.44	0.51
1:2A:1019:U:H3	1:2A:1142(A):A:H62	1.58	0.51
1:2A:2788:C:OP1	4:2E:61:ARG:NH2	2.44	0.51
5:2F:118:ALA:HB2	5:2F:123:LEU:HD23	1.92	0.51
22:20:11:ARG:O	22:20:14:ARG:NH1	2.37	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1442:G:H2'	32:2a:1442:G:N3	2.26	0.51
35:2d:140:VAL:HG11	35:2d:146:ILE:HD11	1.91	0.51
1:1A:247:G:H4'	1:1A:386:G:C5	2.46	0.50
1:1A:831:G:O2'	11:1P:38:GLN:OE1	2.28	0.50
1:1A:1041:C:H42	1:1A:1114:G:H1	1.58	0.50
1:1A:1055:G:H3'	1:1A:1056:G:H8	1.75	0.50
1:1A:1816:G:O6	3:1D:35:LYS:NZ	2.40	0.50
42:1k:45:GLY:O	42:1k:50:TYR:HB2	2.10	0.50
54:1w:1:G:OP2	61:1w:201:HOH:O	2.19	0.50
1:2A:748:G:C8	18:2W:89:ALA:HB1	2.45	0.50
1:2A:1266:G:O5'	18:2W:15:ARG:NH2	2.44	0.50
14:2S:14:VAL:O	14:2S:18:ILE:HG12	2.10	0.50
14:2S:37:ALA:HB1	14:2S:73:LEU:HD22	1.94	0.50
32:2a:984:C:H2'	32:2a:985:C:H6	1.75	0.50
34:2c:22:TRP:CH2	34:2c:32:LEU:HB3	2.46	0.50
39:2h:49:GLU:OE2	39:2h:62:TYR:OH	2.16	0.50
32:1a:174:C:H2'	32:1a:175:C:C6	2.47	0.50
1:2A:372:G:OP2	23:21:69:LYS:HE3	2.11	0.50
1:2A:1349:A:OP1	61:2A:3947:HOH:O	2.19	0.50
1:2A:2561:A:H4'	10:2O:22:ILE:HD11	1.93	0.50
1:2A:2572:A:OP1	1:2A:2574:G:O2'	2.28	0.50
2:2B:9:G:P	14:2S:25:ARG:HH22	2.35	0.50
32:2a:1123:A:H4'	41:2j:37:PRO:HD2	1.94	0.50
38:2g:79:ARG:HH21	38:2g:80:VAL:HA	1.76	0.50
40:2i:99:LEU:HB3	40:2i:101:PHE:CE2	2.47	0.50
50:2s:27:GLU:CB	50:2s:28:LYS:HG3	2.41	0.50
54:2w:68:C:H2'	54:2w:69:G:C8	2.46	0.50
55:2x:50:U:H2'	55:2x:51:C:C6	2.46	0.50
1:1A:444:C:H5"	61:1A:5184:HOH:O	2.11	0.50
7:1H:7:LEU:HD12	7:1H:8:PRO:HD2	1.92	0.50
32:1a:353:A:H5'	32:1a:353:A:H8	1.76	0.50
32:1a:567:G:H2'	32:1a:568:G:O4'	2.12	0.50
34:1c:61:ALA:C	34:1c:63:ASN:H	2.20	0.50
1:2A:1503:U:H2'	1:2A:1504:C:C6	2.46	0.50
1:2A:1771:C:OP1	61:2A:3945:HOH:O	2.19	0.50
9:2N:67:LEU:C	9:2N:88:GLU:HG3	2.36	0.50
35:2d:116:GLN:NE2	35:2d:161:ASN:HD21	2.09	0.50
36:2e:63:ARG:C	36:2e:66:MET:HE1	2.36	0.50
55:2x:75:C:OP1	61:2x:201:HOH:O	2.20	0.50
1:1A:1796:U:H2'	1:1A:1797:C:C6	2.46	0.50
1:1A:2646:C:H2'	1:1A:2647:U:O4'	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1I:130:TYR:HB3	8:1I:138:ILE:HB	1.93	0.50
9:1N:75:TYR:CE2	9:1N:77:GLY:HA2	2.47	0.50
32:1a:1101:A:H4'	32:1a:1102:A:O5'	2.12	0.50
45:1n:23:ARG:NH1	45:1n:30:ALA:HB2	2.27	0.50
3:2D:132:PRO:HD3	3:2D:190:TYR:CZ	2.46	0.50
32:2a:935:A:H61	38:2g:3:ARG:HG3	1.75	0.50
1:1A:883:G:O2'	1:1A:884:C:H5	1.95	0.50
1:1A:910:A:N1	1:1A:2277:G:H1'	2.26	0.50
1:1A:1071:G:H1'	1:1A:1089:G:H2'	1.93	0.50
1:1A:2097:C:H2'	1:1A:2098:U:C6	2.47	0.50
8:1I:39:ALA:HB1	8:1I:44:LEU:HD13	1.92	0.50
32:1a:165:C:H2'	32:1a:166:G:C8	2.45	0.50
32:1a:309:G:O2'	32:1a:607:A:N1	2.44	0.50
34:1c:134:ILE:HD11	34:1c:153:VAL:HB	1.94	0.50
36:1e:98:THR:OG1	36:1e:99:GLY:N	2.43	0.50
51:1t:47:GLY:N	51:1t:48:LYS:HB2	2.27	0.50
1:2A:2176:A:H2'	1:2A:2177:C:C6	2.46	0.50
1:2A:2183:C:H2'	1:2A:2184:G:H8	1.76	0.50
5:2F:126:VAL:HG21	5:2F:129:PHE:CZ	2.46	0.50
6:2G:179:PRO:HG3	26:24:43:TYR:CZ	2.47	0.50
9:2N:58:ASP:N	9:2N:58:ASP:OD1	2.41	0.50
26:24:10:VAL:HG22	26:24:11:PRO:HD2	1.93	0.50
26:24:45:GLY:C	26:24:47:GLN:H	2.19	0.50
32:2a:67:C:H2'	32:2a:68:G:C8	2.46	0.50
33:2b:167:PRO:HD3	33:2b:187:LEU:O	2.11	0.50
39:2h:121:ASP:N	39:2h:121:ASP:OD1	2.44	0.50
3:1D:77:ALA:HB2	3:1D:97:TYR:CD1	2.47	0.50
32:1a:1318:A:OP1	50:1s:7:LYS:NZ	2.30	0.50
46:1o:16:ALA:HB1	46:1o:21:ASP:HB3	1.93	0.50
51:1t:43:LEU:O	51:1t:47:GLY:N	2.28	0.50
56:1y:66:U:H2'	56:1y:67:C:C6	2.47	0.50
1:2A:1639:U:H4'	1:2A:2699:C:H4'	1.94	0.50
1:2A:2127:G:N2	1:2A:2161:C:C2	2.79	0.50
32:2a:429:U:O3'	35:2d:22:LYS:NZ	2.44	0.50
35:2d:10:ARG:HB2	35:2d:40:PRO:HG3	1.92	0.50
40:2i:23:ASN:OD1	40:2i:23:ASN:N	2.42	0.50
1:1A:1223:G:N2	1:1A:1226:A:OP2	2.35	0.50
1:1A:1364:G:P	23:11:3:LYS:HG3	2.51	0.50
1:1A:2155:G:H2'	1:1A:2155:G:N3	2.26	0.50
5:1F:170:LEU:HD13	5:1F:172:TRP:CZ2	2.47	0.50
26:14:53:GLU:HB2	26:14:55:ARG:O	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1c:177:THR:HG22	34:1c:180:ALA:H	1.77	0.50
1:2A:1412:A:H2'	1:2A:1413:G:H8	1.77	0.50
7:2H:8:PRO:O	7:2H:10:PRO:HD3	2.11	0.50
21:2Z:121:HIS:N	21:2Z:172:ALA:HB2	2.26	0.50
32:2a:1004:A:N6	32:2a:1037:C:O2	2.34	0.50
1:1A:1359:A:H61	1:1A:1372:U:H3	1.60	0.50
1:1A:2123:G:H2'	1:1A:2124:G:H8	1.77	0.50
4:1E:34:VAL:HB	4:1E:48:GLN:HE21	1.77	0.50
15:1T:31:SER:OG	15:1T:85:LYS:HE3	2.12	0.50
32:1a:673:G:H2'	32:1a:674:G:C8	2.46	0.50
32:1a:1292:U:P	38:1g:41:ARG:HH22	2.35	0.50
38:1g:38:LEU:HA	38:1g:41:ARG:HD2	1.93	0.50
48:1q:26:GLN:HG2	48:1q:37:LYS:HG2	1.94	0.50
1:2A:884:C:H3'	1:2A:885:C:H6	1.77	0.50
1:2A:1019:U:H2'	1:2A:1020:A:C8	2.47	0.50
32:2a:974:A:H8	32:2a:974:A:OP1	1.95	0.50
38:2g:26:PHE:O	38:2g:30:ILE:HD12	2.11	0.50
42:2k:22:HIS:HB3	42:2k:29:ILE:HB	1.93	0.50
47:2p:18:ARG:HD3	47:2p:35:LYS:HD2	1.93	0.50
1:1A:1899:G:N3	1:1A:1899:G:H2'	2.27	0.50
11:1P:38:GLN:HG2	11:1P:45:LEU:H	1.77	0.50
12:1Q:89:ASN:HB2	55:1x:1:C:N3	2.26	0.50
21:1Z:9:TYR:CZ	21:1Z:61:LEU:HD22	2.47	0.50
50:1s:27:GLU:CB	50:1s:28:LYS:HA	2.33	0.50
54:1w:26:A:N6	54:1w:44:G:H1	2.10	0.50
2:2B:119:G:H5'	2:2B:120:A:OP2	2.12	0.50
32:2a:438:G:O2'	32:2a:494:U:O4	2.26	0.50
35:2d:98:GLU:OE1	35:2d:103:ASN:ND2	2.44	0.50
1:1A:7:G:H2'	1:1A:8:A:O4'	2.12	0.49
32:1a:946:A:H2'	32:1a:947:G:C8	2.47	0.49
32:1a:973:G:H3'	32:1a:974:A:H5"	1.93	0.49
40:1i:50:LEU:HD13	40:1i:56:LEU:HA	1.94	0.49
1:2A:831:G:O2'	11:2P:38:GLN:OE1	2.28	0.49
1:2A:2747:G:O6	1:2A:2755:C:H5"	2.12	0.49
1:2A:2773:C:OP1	4:2E:166:THR:OG1	2.30	0.49
28:26:38:LYS:HB2	28:26:49:HIS:CE1	2.47	0.49
32:2a:1060:C:C5	34:2c:2:GLY:HA3	2.47	0.49
34:2c:11:ARG:NH2	34:2c:177:THR:O	2.29	0.49
1:1A:1744:C:H2'	1:1A:1745:C:C6	2.48	0.49
1:1A:2840:C:OP1	61:1A:4235:HOH:O	2.20	0.49
7:1H:154:PRO:HB3	7:1H:163:TYR:CZ	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:407:G:H5”	35:1d:115:ARG:HB3	1.94	0.49
32:1a:1194:U:H4’	36:1e:22:GLY:HA2	1.93	0.49
49:1r:38:GLU:HA	49:1r:41:LYS:HE2	1.94	0.49
1:2A:646:A:H2’	1:2A:647:G:O4’	2.13	0.49
1:2A:2291:U:OP1	1:2A:2380:C:O2’	2.28	0.49
1:2A:2693:A:H2’	1:2A:2694:G:C8	2.45	0.49
1:2A:2741:A:H2’	1:2A:2742:C:O4’	2.12	0.49
3:2D:85:ASP:OD2	3:2D:88:ARG:NH1	2.42	0.49
4:2E:36:ARG:HG2	4:2E:47:VAL:HG12	1.94	0.49
32:2a:1151:A:O2’	32:2a:1152:A:H8	1.95	0.49
36:2e:142:LEU:O	36:2e:143:ARG:NH1	2.35	0.49
41:2j:78:ASN:O	41:2j:80:LYS:N	2.45	0.49
1:1A:2105:C:H2’	1:1A:2106:G:C8	2.47	0.49
6:1G:135:LEU:HD13	6:1G:140:ILE:HD11	1.95	0.49
10:1O:63:VAL:HG12	10:1O:106:LEU:HD21	1.92	0.49
14:1S:14:VAL:O	14:1S:18:ILE:HG12	2.11	0.49
33:1b:218:ALA:O	33:1b:222:ILE:HG13	2.12	0.49
38:1g:16:LEU:HD21	40:1i:45:ALA:HB2	1.93	0.49
1:2A:1181:C:H2’	1:2A:1182:A:H8	1.78	0.49
1:2A:2131:G:H4’	1:2A:2132:U:H3’	1.95	0.49
2:2B:90:A:C5	2:2B:91:C:H1’	2.47	0.49
9:2N:96:GLU:CD	9:2N:96:GLU:H	2.20	0.49
32:2a:921:U:O2	36:2e:19:MET:HB2	2.13	0.49
32:2a:967:5MC:H2’	32:2a:968:A:C8	2.48	0.49
32:2a:984:C:H2’	32:2a:985:C:C6	2.48	0.49
33:2b:82:ARG:HB2	33:2b:92:TYR:CZ	2.47	0.49
39:2h:121:ASP:HB2	39:2h:125:ARG:NH2	2.27	0.49
1:1A:1011:G:OP1	16:1U:77:SER:OG	2.25	0.49
1:1A:1173:G:N2	1:1A:1177:A:OP2	2.43	0.49
4:1E:59:VAL:HB	4:1E:64:LYS:HE3	1.94	0.49
12:1Q:76:LYS:HB3	12:1Q:91:GLU:HG3	1.94	0.49
21:1Z:72:ARG:HG2	21:1Z:89:PHE:HB2	1.94	0.49
33:1b:115:LEU:HD13	33:1b:145:LEU:HB3	1.95	0.49
1:2A:1709:U:H2’	1:2A:1710:C:C6	2.47	0.49
1:2A:1803:A:O2’	3:2D:259:THR:HG21	2.11	0.49
1:2A:2769:C:H2’	1:2A:2770:G:O4’	2.13	0.49
16:2U:74:LEU:HD21	16:2U:110:VAL:HG13	1.94	0.49
45:2n:24:CYS:HB2	45:2n:40:CYS:HB3	1.94	0.49
1:1A:218:A:C2	1:1A:235:U:H4’	2.48	0.49
1:1A:2182:G:H2’	1:1A:2183:C:C6	2.47	0.49
1:1A:2319:G:H1	14:1S:3:ARG:HA	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:1P:121:LYS:O	11:1P:123:LEU:N	2.45	0.49
32:1a:475:G:H2'	32:1a:476:G:C8	2.47	0.49
32:1a:660:G:N7	61:1a:1948:HOH:O	2.35	0.49
32:1a:1027:C:N1	32:1a:1034:G:N2	2.60	0.49
37:1f:6:VAL:HG22	37:1f:90:VAL:HG22	1.95	0.49
43:1l:88:GLY:O	43:1l:99:HIS:HD2	1.95	0.49
44:1m:23:TYR:HB3	44:1m:67:GLU:HA	1.93	0.49
44:1m:37:THR:O	44:1m:55:ARG:NH1	2.43	0.49
56:1y:48:C:OP1	56:1y:48:C:H2'	2.13	0.49
1:2A:1337:G:OP2	19:2X:73:ARG:NH2	2.36	0.49
1:2A:2506:U:O2'	54:2w:76:F3N:H4'	2.12	0.49
2:2B:75:G:H22	21:2Z:73:GLN:HE21	1.60	0.49
6:2G:7:LEU:HD23	6:2G:100:TRP:HE3	1.78	0.49
14:2S:27:SER:HA	14:2S:88:ASP:HB3	1.94	0.49
32:2a:410:G:OP1	35:2d:30:LYS:NZ	2.29	0.49
32:2a:589:C:H2'	32:2a:590:C:H6	1.76	0.49
32:2a:1027:C:C2	32:2a:1034:G:N1	2.81	0.49
32:2a:1047:G:H5"	45:2n:4:LYS:HD3	1.93	0.49
32:2a:1305:G:H22	32:2a:1331:G:H1'	1.76	0.49
39:2h:121:ASP:HB2	39:2h:125:ARG:HH21	1.76	0.49
43:2l:84:LEU:HB2	43:2l:105:TYR:CE2	2.48	0.49
1:1A:1092:C:C2'	1:1A:1093:G:H5'	2.41	0.49
1:1A:1688:U:H1'	1:1A:1701:A:C6	2.48	0.49
32:1a:316:G:H4'	61:1a:2189:HOH:O	2.12	0.49
32:1a:573:A:OP2	61:1a:1916:HOH:O	2.20	0.49
32:1a:1510:U:H2'	32:1a:1511:G:C8	2.48	0.49
40:1i:24:GLY:HA2	40:1i:59:PHE:O	2.13	0.49
40:1i:25:LYS:HB3	40:1i:60:ASP:OD1	2.13	0.49
1:2A:443:A:H1'	1:2A:1201:C:O4'	2.11	0.49
1:2A:2888:C:H2'	1:2A:2889:C:C6	2.48	0.49
4:2E:8:LYS:NZ	4:2E:188:VAL:O	2.45	0.49
7:2H:46:GLU:HB2	7:2H:49:VAL:HB	1.94	0.49
12:2Q:35:VAL:HG22	12:2Q:102:VAL:HG22	1.95	0.49
21:2Z:122:ARG:H	21:2Z:122:ARG:HD2	1.77	0.49
50:2s:77:THR:HG23	50:2s:78:ARG:HG3	1.94	0.49
1:1A:1178:C:H2'	1:1A:1179:C:H6	1.77	0.49
10:1O:16:ALA:HB2	10:1O:52:VAL:HG21	1.94	0.49
33:1b:16:HIS:CG	33:1b:17:PHE:N	2.81	0.49
44:1m:123:ALA:HB2	54:1w:39:PSU:H1'	1.95	0.49
56:1y:5:G:H1'	56:1y:69:G:N2	2.27	0.49
15:2T:26:ASP:OD1	15:2T:120:ARG:NH2	2.44	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1427:U:H2'	32:2a:1428:A:C8	2.48	0.49
33:2b:17:PHE:HA	33:2b:44:LEU:HD21	1.93	0.49
40:2i:20:ARG:O	40:2i:60:ASP:N	2.37	0.49
4:1E:49:LEU:HD22	4:1E:81:ILE:HG13	1.95	0.49
32:1a:1151:A:HO2'	32:1a:1152:A:H8	1.61	0.49
33:1b:87:ARG:NH1	33:1b:233:SER:OG	2.46	0.49
36:1e:78:HIS:CE1	36:1e:143:ARG:H	2.29	0.49
46:1o:62:GLN:NE2	46:1o:65:ARG:HH21	2.11	0.49
1:2A:729:G:C6	3:2D:208:LYS:HB2	2.47	0.49
1:2A:922:U:H2'	1:2A:923:C:C6	2.47	0.49
32:2a:200:G:H2'	32:2a:201:C:O4'	2.12	0.49
32:2a:1279:A:H5"	32:2a:1280:A:OP1	2.13	0.49
47:2p:8:ARG:HB3	47:2p:28:ARG:NH1	2.28	0.49
1:1A:184:C:H2'	1:1A:185:U:C6	2.48	0.49
1:1A:958:U:H4'	61:1A:4460:HOH:O	2.11	0.49
13:1R:64:ARG:NH1	61:1R:301:HOH:O	2.29	0.49
15:1T:51:ARG:HG3	15:1T:98:LYS:HE3	1.94	0.49
32:1a:250:A:H4'	32:1a:251:G:O5'	2.13	0.49
32:1a:1048:G:OP1	45:1n:3:ARG:HB3	2.13	0.49
32:1a:1277:C:O2'	32:1a:1279:A:H1'	2.13	0.49
36:1e:105:VAL:HG21	36:1e:128:PRO:HB3	1.94	0.49
51:1t:18:GLN:O	51:1t:22:ARG:HG3	2.13	0.49
1:2A:709:U:H2'	1:2A:710:G:C8	2.47	0.49
1:2A:731:C:H5"	61:2A:4126:HOH:O	2.12	0.49
1:2A:793:A:OP2	1:2A:2071:A:O2'	2.30	0.49
1:2A:1019:U:OP1	1:2A:1035:U:O2'	2.26	0.49
1:2A:1019:U:O2'	1:2A:1021:A:H2	1.95	0.49
1:2A:1371:G:H2'	1:2A:1372:U:H5	1.78	0.49
1:2A:1915:5MU:H2'	1:2A:1916:A:O4'	2.13	0.49
1:2A:2497:A:H5"	61:2A:4489:HOH:O	2.13	0.49
2:2B:14:U:H1'	2:2B:108:U:O2'	2.13	0.49
12:2Q:136:ALA:HB1	21:2Z:52:SER:HB3	1.94	0.49
19:2X:72:LYS:NZ	19:2X:75:ASP:OD1	2.43	0.49
32:2a:973:G:H3'	32:2a:974:A:H5"	1.95	0.49
32:2a:1055:A:N7	32:2a:1200:C:N4	2.59	0.49
48:2q:45:HIS:CD2	48:2q:47:PRO:HG3	2.48	0.49
50:2s:41:VAL:HG13	50:2s:43:GLU:H	1.78	0.49
1:1A:84:A:OP2	20:1Y:8:LYS:NZ	2.29	0.49
32:1a:390:C:H2'	32:1a:391:G:C8	2.48	0.49
39:1h:113:SER:HB2	39:1h:134:ILE:HD11	1.93	0.49
41:1j:13:HIS:HB3	41:1j:68:HIS:CD2	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:1l:39:VAL:HG11	43:1l:41:ARG:HH11	1.77	0.49
1:2A:299:A:N1	1:2A:322:A:O2'	2.39	0.49
1:2A:1429:G:H2'	1:2A:1430:C:C6	2.48	0.49
1:2A:1803:A:H4'	3:2D:259:THR:HG23	1.95	0.49
1:2A:2635:C:H5"	4:2E:78:LEU:O	2.13	0.49
34:2c:155:GLY:HA3	34:2c:196:LEU:HD22	1.94	0.49
38:2g:33:ASP:N	38:2g:33:ASP:OD1	2.45	0.49
40:2i:82:ALA:HA	40:2i:85:LEU:HD12	1.93	0.49
1:1A:2110:G:P	1:1A:2118:U:H3	2.35	0.48
1:1A:2705:A:O2'	1:1A:2852:G:OP1	2.25	0.48
16:1U:76:TYR:CE2	16:1U:80:ILE:HG13	2.48	0.48
32:1a:92:C:H2'	32:1a:93:G:C8	2.48	0.48
32:1a:192:U:H2'	32:1a:193:C:H6	1.78	0.48
32:1a:1039:C:H2'	32:1a:1040:U:C6	2.47	0.48
1:2A:2758:A:C2	1:2A:2759:G:H1'	2.48	0.48
6:2G:109:VAL:HG11	26:24:14:ILE:HG21	1.95	0.48
28:26:13:CYS:SG	28:26:47:THR:HG21	2.53	0.48
32:2a:620:C:H2'	32:2a:621:A:O4'	2.13	0.48
1:1A:271(T):C:H2'	1:1A:271(U):G:H8	1.77	0.48
1:1A:536:A:H2'	1:1A:537:C:C6	2.48	0.48
1:1A:2176:A:H2'	1:1A:2177:C:C6	2.48	0.48
32:1a:1124:G:N2	32:1a:1125:U:O4	2.43	0.48
37:1f:68:PRO:HG2	37:1f:71:ARG:HD2	1.95	0.48
1:2A:2687:U:H2'	1:2A:2688:U:O4'	2.14	0.48
5:2F:20:LEU:HG	5:2F:21:ALA:H	1.77	0.48
15:2T:91:ARG:HB2	15:2T:121:ILE:HG13	1.95	0.48
21:2Z:105:VAL:O	21:2Z:140:ASP:HA	2.12	0.48
23:21:23:LYS:HB3	23:21:29:GLY:HA3	1.94	0.48
32:2a:1189:C:OP1	41:2j:51:ARG:NH2	2.37	0.48
38:2g:51:GLN:HG2	38:2g:58:PRO:HD3	1.95	0.48
56:2y:50:U:H2'	56:2y:51:U:C6	2.47	0.48
8:1I:40:THR:O	8:1I:44:LEU:HB2	2.13	0.48
13:1R:28:LEU:HD23	13:1R:48:VAL:HG21	1.95	0.48
26:14:58:ARG:HH12	50:1s:69:HIS:CD2	2.31	0.48
54:1w:33:U:O4'	54:1w:37:MIA:H151	2.13	0.48
1:2A:1843:C:H5'	3:2D:253:GLN:OE1	2.13	0.48
1:2A:2243:U:H2'	1:2A:2244:U:C6	2.47	0.48
1:2A:2278:A:OP2	22:20:12:ASN:ND2	2.39	0.48
21:2Z:7:ALA:HB2	21:2Z:59:LEU:HD22	1.95	0.48
32:2a:109:A:C6	32:2a:326:G:C6	3.01	0.48
32:2a:1347:G:H22	32:2a:1373:G:H2'	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:2b:92:TYR:OH	33:2b:150:SER:OG	2.30	0.48
44:2m:67:GLU:HG3	44:2m:71:ARG:NH2	2.27	0.48
48:2q:45:HIS:NE2	48:2q:47:PRO:HG3	2.27	0.48
1:1A:1176:G:N2	1:1A:1178:C:OP2	2.47	0.48
1:1A:2218:U:O4'	23:11:52:ARG:NH2	2.46	0.48
3:1D:85:ASP:OD2	3:1D:88:ARG:NH1	2.37	0.48
9:1N:4:TYR:CD2	16:1U:100:VAL:HG11	2.49	0.48
14:1S:10:ARG:O	14:1S:14:VAL:HG13	2.13	0.48
26:14:63:TYR:N	26:14:64:GLY:HA2	2.27	0.48
32:1a:219:C:H2'	32:1a:220:G:O4'	2.13	0.48
32:1a:300:A:H1'	32:1a:565:U:O2	2.13	0.48
40:1i:3:GLN:OE1	40:1i:20:ARG:NH2	2.37	0.48
43:1l:39:VAL:HB	43:1l:57:LYS:HB2	1.95	0.48
1:2A:699:A:H2'	1:2A:700:G:O4'	2.13	0.48
1:2A:862:G:H2'	1:2A:863:A:O4'	2.12	0.48
1:2A:2135:A:H2'	1:2A:2136:C:C5	2.48	0.48
8:2I:72:LEU:HD11	8:2I:107:VAL:HG11	1.95	0.48
32:2a:337:C:H2'	32:2a:338:A:C8	2.49	0.48
32:2a:1312:G:H5'	50:2s:5:LEU:HD11	1.95	0.48
33:2b:222:ILE:HG13	33:2b:223:ILE:N	2.27	0.48
45:2n:9:LYS:HG3	45:2n:12:ARG:HH22	1.78	0.48
1:1A:674:G:O2'	5:1F:74:ARG:HD3	2.12	0.48
1:1A:1047:G:H2'	1:1A:1110:G:H22	1.78	0.48
1:1A:1778:U:H2'	1:1A:1784:A:N6	2.28	0.48
1:1A:1993:U:OP2	61:1A:4238:HOH:O	2.20	0.48
10:1O:107:ARG:CZ	15:1T:36:GLU:HG2	2.44	0.48
32:1a:1004:A:H5"	32:1a:1025:U:C5	2.47	0.48
32:1a:1343:G:H1'	40:1i:121:ARG:NH1	2.27	0.48
1:2A:774:A:H2'	1:2A:774:A:N3	2.29	0.48
1:2A:1686:C:H2'	1:2A:1687:G:O4'	2.13	0.48
1:2A:1889:A:N1	1:2A:2234:G:H1'	2.29	0.48
1:2A:2376:A:H2'	1:2A:2377:A:O4'	2.13	0.48
21:2Z:99:TYR:HB3	21:2Z:123:ASP:OD1	2.13	0.48
32:2a:1172:C:H2'	32:2a:1173:G:C8	2.49	0.48
32:2a:1289:A:OP1	52:2u:10:ARG:NH2	2.46	0.48
36:2e:60:TYR:O	36:2e:64:ARG:HG3	2.14	0.48
1:1A:1651:G:OP1	13:1R:40:LYS:NZ	2.45	0.48
1:1A:2273:A:H2'	1:1A:2274:A:C8	2.48	0.48
1:1A:2765:A:OP2	61:1A:4234:HOH:O	2.20	0.48
14:1S:34:HIS:O	14:1S:97:ARG:NH2	2.47	0.48
21:1Z:72:ARG:HD3	21:1Z:72:ARG:HA	1.50	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:90:U:O2	32:1a:90:U:H2'	2.13	0.48
32:1a:865:A:H2	32:1a:918:A:H4'	1.78	0.48
33:1b:114:ARG:O	33:1b:118:LEU:HD12	2.13	0.48
33:1b:155:LEU:HD21	33:1b:159:PRO:HG3	1.96	0.48
34:1c:8:ILE:HG12	34:1c:184:TYR:HB3	1.96	0.48
1:2A:271(H):G:H2'	1:2A:271(I):G:H8	1.79	0.48
1:2A:800:A:H8	1:2A:800:A:OP1	1.97	0.48
1:2A:2136:C:N4	1:2A:2155:G:H1	2.10	0.48
43:2l:27:LEU:HD23	43:2l:33:ARG:HB2	1.94	0.48
1:1A:111:A:H4'	24:12:69:ARG:NH1	2.28	0.48
1:1A:899:A:H2'	1:1A:899:A:N3	2.27	0.48
1:1A:2600:A:H2'	1:1A:2601:C:C6	2.49	0.48
1:1A:2743:C:OP1	31:19:33:LYS:NZ	2.35	0.48
20:1Y:86:ARG:HB2	20:1Y:98:VAL:HG23	1.96	0.48
32:1a:953:G:H5'	32:1a:965:A:N6	2.28	0.48
32:1a:1499:A:OP2	61:1a:1905:HOH:O	2.20	0.48
35:1d:13:ARG:HB3	35:1d:38:TYR:O	2.13	0.48
37:1f:33:TYR:CD2	37:1f:75:LEU:HD23	2.49	0.48
56:1y:7:A:O2'	56:1y:49:C:OP2	2.17	0.48
1:2A:274:G:H2'	1:2A:275:G:C8	2.49	0.48
1:2A:2086:U:H2'	1:2A:2087:G:C8	2.48	0.48
1:2A:2889:C:H2'	1:2A:2891:G:O4'	2.13	0.48
6:2G:116:ASP:OD2	44:2m:68:GLY:HA3	2.13	0.48
21:2Z:154:ASP:OD1	21:2Z:154:ASP:N	2.45	0.48
45:2n:9:LYS:HG3	45:2n:12:ARG:NH2	2.28	0.48
1:1A:434:U:H1'	1:1A:435:C:H5	1.79	0.48
1:1A:657:U:H2'	1:1A:658:C:C6	2.49	0.48
33:1b:109:SER:O	33:1b:112:VAL:HG22	2.14	0.48
36:1e:31:LEU:HD11	36:1e:129:ILE:HA	1.96	0.48
1:2A:322:A:OP2	5:2F:169:ASN:HB2	2.13	0.48
1:2A:880:G:H1	1:2A:897:C:N4	2.10	0.48
1:2A:1183:G:H2'	1:2A:1184:G:H8	1.79	0.48
1:2A:1817:G:OP1	3:2D:88:ARG:NH2	2.46	0.48
1:2A:2705:A:OP2	61:2A:3948:HOH:O	2.19	0.48
1:2A:2735:G:H2'	1:2A:2736:G:C8	2.49	0.48
21:2Z:6:LYS:HE3	21:2Z:8:TYR:HE2	1.78	0.48
32:2a:23:C:H5	32:2a:561:U:O4	1.96	0.48
32:2a:1352:C:OP1	52:2u:3:LYS:NZ	2.36	0.48
37:2f:99:ALA:HB1	49:2r:23:LYS:NZ	2.29	0.48
41:2j:7:LYS:HB3	41:2j:71:LEU:HD12	1.95	0.48
1:1A:1341:U:O2	19:1X:80:ILE:HD13	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2461:C:H2'	1:1A:2462:U:C6	2.48	0.48
28:16:26:ASN:HD21	28:16:28:ARG:NH2	2.12	0.48
32:1a:783:C:OP1	32:1a:1515:C:O2'	2.32	0.48
32:1a:1021:G:O2'	32:1a:1022:G:O5'	2.30	0.48
32:1a:1250:A:H2'	32:1a:1251:A:C8	2.49	0.48
32:1a:1402:4OC:O5'	32:1a:1402:4OC:H6	2.13	0.48
32:1a:1513:A:H2'	32:1a:1514:C:C6	2.49	0.48
1:2A:651:G:OP1	30:28:19:SER:HB3	2.14	0.48
1:2A:1031:G:N3	31:29:36:GLN:NE2	2.59	0.48
6:2G:36:LYS:HD3	6:2G:95:ARG:HH12	1.78	0.48
14:2S:39:ILE:HG13	14:2S:73:LEU:HD11	1.95	0.48
32:2a:1145:C:H4'	32:2a:1146:A:H5'	1.95	0.48
32:2a:1265:G:C2	32:2a:1271:G:C2	3.02	0.48
33:2b:88:ALA:HB1	33:2b:222:ILE:HD11	1.96	0.48
35:2d:173:TRP:CD1	35:2d:174:LEU:HG	2.49	0.48
15:1T:127:ALA:C	15:1T:129:ARG:N	2.72	0.48
17:1V:1:MET:HE3	17:1V:43:GLU:HB2	1.95	0.48
17:1V:76:LYS:HB2	17:1V:81:TYR:HB3	1.94	0.48
35:1d:119:GLN:HG2	35:1d:123:HIS:CD2	2.49	0.48
38:1g:144:MET:HB3	38:1g:144:MET:HE2	1.65	0.48
1:2A:1009:A:OP2	9:2N:37:LYS:NZ	2.45	0.48
1:2A:2376:A:N3	14:2S:106:ARG:NH2	2.61	0.48
32:2a:299:G:H2'	32:2a:300:A:C8	2.49	0.48
32:2a:435:C:H2'	32:2a:436:C:C6	2.49	0.48
32:2a:1060:C:H5"	41:2j:51:ARG:HB3	1.95	0.48
33:2b:58:ILE:O	33:2b:62:ALA:N	2.41	0.48
33:2b:93:VAL:HG11	33:2b:97:TRP:CE3	2.48	0.48
1:1A:811:U:H2'	11:1P:21:ARG:HA	1.96	0.47
1:1A:1062:G:P	1:1A:1070:A:H1'	2.54	0.47
8:1I:75:LEU:HD22	8:1I:105:HIS:CD2	2.49	0.47
14:1S:25:ARG:NH1	14:1S:42:ASP:OD1	2.46	0.47
20:1Y:20:TYR:CE2	20:1Y:43:ASN:HA	2.50	0.47
21:1Z:7:ALA:O	21:1Z:62:PRO:HD3	2.13	0.47
32:1a:110:C:H2'	32:1a:111:G:O4'	2.13	0.47
32:1a:1060:C:C5	34:1c:2:GLY:HA3	2.49	0.47
32:1a:1305:G:H22	32:1a:1331:G:H1'	1.78	0.47
34:1c:18:TRP:O	34:1c:54:ARG:NH2	2.47	0.47
36:1e:20:GLN:HG2	36:1e:25:ARG:HD2	1.96	0.47
41:1j:49:VAL:HG13	45:1n:41:ARG:HB2	1.96	0.47
54:1w:18:G:H4'	54:1w:60:U:C5	2.48	0.47
1:2A:1477:A:H2'	1:2A:1478:G:O4'	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2881:C:H2'	1:2A:2882:A:O4'	2.14	0.47
12:2Q:7:MET:HB3	12:2Q:7:MET:HE2	1.83	0.47
32:2a:45:U:H2'	32:2a:46:G:C8	2.49	0.47
32:2a:189(L):G:H2'	32:2a:190:U:C6	2.49	0.47
32:2a:603:U:H2'	32:2a:604:G:H8	1.79	0.47
1:1A:747:U:O2	1:1A:2014:A:H1'	2.14	0.47
32:1a:1068:G:H8	32:1a:1068:G:OP2	1.97	0.47
1:2A:531:C:OP1	1:2A:561:G:N2	2.46	0.47
1:2A:829:A:N7	1:2A:2248:C:H5'	2.29	0.47
1:2A:2134:A:H2'	1:2A:2134:A:N3	2.28	0.47
1:2A:2165:G:H1	1:2A:2171:A:H8	1.61	0.47
32:2a:1260:C:O5'	32:2a:1284:C:H4'	2.14	0.47
32:2a:1318:A:H1'	50:2s:37:ARG:HH21	1.80	0.47
42:2k:84:VAL:HG21	42:2k:95:ILE:HD11	1.96	0.47
4:1E:116:VAL:HG13	4:1E:122:PHE:HB2	1.97	0.47
33:1b:98:LEU:HB2	33:1b:101:MET:HG3	1.96	0.47
37:1f:50:TYR:OH	37:1f:87:ARG:NH2	2.47	0.47
1:2A:652(T):C:H2'	1:2A:652(U):G:H8	1.79	0.47
1:2A:1889:A:H2'	1:2A:1890:A:C8	2.49	0.47
32:2a:1002:G:N2	32:2a:1003:G:O2'	2.48	0.47
32:2a:1249:C:O4'	40:2i:70:LYS:HE2	2.14	0.47
1:1A:2564:A:C2	1:1A:2647:U:H4'	2.50	0.47
1:1A:2741:A:H2'	1:1A:2742:C:O4'	2.14	0.47
2:1B:2:C:H2'	2:1B:3:C:C6	2.49	0.47
5:1F:24:LEU:HD23	5:1F:115:ALA:HA	1.95	0.47
19:1X:31:HIS:CD2	19:1X:33:LYS:H	2.18	0.47
33:1b:97:TRP:CZ2	33:1b:102:LEU:HD13	2.50	0.47
40:1i:46:ALA:HB2	40:1i:74:ILE:HG23	1.95	0.47
1:2A:64:A:O3'	19:2X:71:GLY:HA3	2.14	0.47
1:2A:1019:U:H2'	1:2A:1020:A:H8	1.79	0.47
1:2A:2390:U:P	30:28:35:GLN:HE22	2.37	0.47
1:2A:2528:U:O2'	1:2A:2530:A:OP1	2.27	0.47
1:2A:2886:G:H2'	1:2A:2887:U:H6	1.78	0.47
5:2F:14:PRO:HD2	5:2F:127:GLU:OE2	2.14	0.47
9:2N:73:THR:HB	9:2N:82:LEU:HD11	1.97	0.47
28:26:40:CYS:O	28:26:44:ARG:N	2.45	0.47
32:2a:56:U:H2'	32:2a:57:G:C8	2.49	0.47
32:2a:512:U:H2'	32:2a:513:C:H6	1.80	0.47
32:2a:1323:G:H2'	32:2a:1324:A:C8	2.49	0.47
33:2b:8:LYS:HA	33:2b:217:ARG:HE	1.78	0.47
35:2d:47:ARG:HB2	35:2d:47:ARG:HH11	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1G:16:ARG:O	6:1G:20:ILE:HG13	2.15	0.47
12:1Q:78:PRO:HD3	55:1x:1:C:N3	2.30	0.47
46:1o:87:ILE:HG22	46:1o:88:ARG:H	1.79	0.47
1:2A:1316:U:H2'	1:2A:1317:A:C8	2.50	0.47
1:2A:2108:C:H42	1:2A:2181:G:H1	1.63	0.47
1:2A:2126:A:N3	1:2A:2127:G:H1'	2.29	0.47
1:2A:2320:A:N3	1:2A:2320:A:H2'	2.29	0.47
1:2A:2552:2MU:H6'3	1:2A:2554:U:C6	2.50	0.47
1:2A:2843:G:N7	61:2A:4032:HOH:O	2.35	0.47
12:2Q:18:LYS:HE3	12:2Q:18:LYS:HB2	1.76	0.47
18:2W:82:LEU:HD22	18:2W:84:ARG:HH22	1.79	0.47
32:2a:892:A:O2'	32:2a:1415:G:H4'	2.15	0.47
32:2a:1010:G:N2	32:2a:1020:U:O2'	2.47	0.47
42:2k:85:ARG:HD3	42:2k:113:PRO:HD3	1.97	0.47
1:1A:530:G:H4'	1:1A:531:C:OP1	2.14	0.47
1:1A:1055:G:H1	1:1A:1104:C:H42	1.63	0.47
1:1A:2184:G:H2'	1:1A:2185:C:C6	2.49	0.47
1:1A:2820:A:P	13:1R:2:ARG:HH22	2.37	0.47
3:1D:12:SER:HB3	3:1D:208:LYS:HB3	1.97	0.47
4:1E:27:LEU:HD12	4:1E:180:ASN:O	2.15	0.47
6:1G:67:LYS:H	26:14:6:HIS:CE1	2.33	0.47
11:1P:95:VAL:HB	11:1P:125:VAL:HG12	1.95	0.47
12:1Q:39:PRO:HA	12:1Q:97:VAL:O	2.15	0.47
12:1Q:135:ASP:O	12:1Q:139:GLU:HG2	2.15	0.47
32:1a:974:A:OP2	45:1n:29:ARG:NH2	2.47	0.47
32:1a:1305:G:H5"	52:1u:4:GLY:HA3	1.96	0.47
35:1d:101:LEU:HB2	35:1d:138:TYR:HB3	1.96	0.47
47:1p:59:TRP:HA	47:1p:62:VAL:HG12	1.96	0.47
32:2a:998:G:H1	32:2a:1043:C:H42	1.62	0.47
44:2m:60:VAL:HG12	44:2m:66:LEU:HD11	1.96	0.47
1:1A:706:A:H2'	1:1A:707:G:O4'	2.13	0.47
1:1A:1695:G:H1'	3:1D:8:PRO:O	2.14	0.47
1:1A:2328:A:H2'	1:1A:2329:G:C8	2.49	0.47
1:1A:2341:G:H2'	1:1A:2342:C:C6	2.49	0.47
1:1A:2360:A:H2'	1:1A:2361:A:O4'	2.15	0.47
12:1Q:1:MET:HE3	12:1Q:1:MET:HB2	1.70	0.47
16:1U:43:GLY:HA3	17:1V:73:SER:OG	2.14	0.47
21:1Z:158:PRO:O	21:1Z:161:VAL:HG22	2.15	0.47
25:13:3:ARG:NE	25:13:60:GLU:OE2	2.47	0.47
27:15:20:ARG:HG2	27:15:23:HIS:CE1	2.50	0.47
32:1a:382:A:H2'	32:1a:383:A:C8	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:418:C:H2'	32:1a:419:C:C6	2.50	0.47
32:1a:539:A:H2'	32:1a:540:G:C8	2.50	0.47
33:1b:72:GLY:HA3	33:1b:81:VAL:HG11	1.96	0.47
35:1d:172:PRO:C	35:1d:174:LEU:H	2.23	0.47
36:1e:60:TYR:O	36:1e:64:ARG:HG3	2.15	0.47
38:1g:78:ARG:HB2	38:1g:156:TRP:HZ3	1.80	0.47
38:1g:146:GLU:OE2	38:1g:149:ARG:NE	2.47	0.47
39:1h:4:ASP:OD2	39:1h:85:ARG:NE	2.40	0.47
1:2A:1899:G:H2'	1:2A:1899:G:N3	2.30	0.47
1:2A:2150:U:H2'	1:2A:2151:G:C8	2.46	0.47
5:2F:65:TRP:CZ2	5:2F:75:HIS:HD2	2.32	0.47
10:2O:104:ARG:HH12	15:2T:43:GLN:HE22	1.63	0.47
11:2P:39:LYS:HB2	11:2P:45:LEU:HD13	1.95	0.47
12:2Q:17:LEU:HB3	12:2Q:39:PRO:HB2	1.97	0.47
15:2T:16:ARG:NH2	15:2T:18:ASP:OD2	2.48	0.47
21:2Z:142:SER:OG	21:2Z:143:GLY:N	2.47	0.47
26:24:15:ILE:HG13	26:24:21:VAL:HG23	1.96	0.47
32:2a:603:U:H2'	32:2a:604:G:C8	2.50	0.47
32:2a:769:G:H4'	32:2a:1513:A:H4'	1.97	0.47
32:2a:1095:U:H5"	32:2a:1109:C:O2	2.14	0.47
32:2a:1178:G:N2	32:2a:1180:A:H3'	2.30	0.47
32:2a:1292:U:H2'	32:2a:1293:G:C8	2.50	0.47
32:2a:1478:C:H2'	32:2a:1479:C:H6	1.80	0.47
36:2e:72:GLN:O	36:2e:75:THR:HG22	2.15	0.47
44:2m:64:TRP:HB2	44:2m:66:LEU:HD21	1.97	0.47
46:2o:84:LYS:O	46:2o:84:LYS:HD3	2.15	0.47
56:2y:52:G:H5'	56:2y:53:G:OP2	2.15	0.47
1:1A:1474:C:H2'	1:1A:1475:G:C8	2.50	0.47
1:1A:2112:G:H1'	56:1y:19:G:O2'	2.15	0.47
1:1A:2522:U:O2'	1:1A:2647:U:OP1	2.29	0.47
2:1B:89:G:H8	2:1B:89:G:OP2	1.97	0.47
22:10:11:ARG:HG2	61:10:209:HOH:O	2.13	0.47
32:1a:1073:U:O2'	33:1b:104:ASN:OD1	2.30	0.47
32:1a:1531:A:H8	32:1a:1531:A:O5'	1.96	0.47
33:1b:80:ILE:HD12	33:1b:212:GLN:HA	1.95	0.47
40:1i:28:VAL:HG22	40:1i:63:ILE:HB	1.96	0.47
41:1j:57:LYS:HE2	41:1j:60:ARG:NH2	2.29	0.47
44:1m:108:ARG:HD3	44:1m:108:ARG:HA	1.63	0.47
50:1s:12:ASP:OD2	50:1s:35:SER:OG	2.22	0.47
1:2A:248:G:OP1	61:2A:3950:HOH:O	2.20	0.47
1:2A:301:G:OP2	20:2Y:84:ARG:NH2	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:839:U:H2'	1:2A:840:C:C6	2.50	0.47
1:2A:839:U:H1'	1:2A:1191:G:H1'	1.95	0.47
1:2A:2291:U:H2'	1:2A:2292:C:C6	2.50	0.47
1:2A:2839:G:H5'	13:2R:46:GLY:CA	2.44	0.47
32:2a:21:G:H2'	32:2a:22:G:C8	2.50	0.47
32:2a:115:G:H4'	32:2a:116:A:O5'	2.15	0.47
32:2a:148:G:H2'	32:2a:149:A:H8	1.80	0.47
32:2a:1440:C:H2'	32:2a:1441:G:O4'	2.15	0.47
33:2b:33:TYR:HB3	33:2b:41:ILE:HD12	1.96	0.47
36:2e:81:GLU:HG2	36:2e:90:VAL:HG22	1.97	0.47
54:2w:45:U:H5"	54:2w:46:G7M:OP2	2.14	0.47
1:1A:1853:A:H2'	1:1A:1854:A:C8	2.49	0.47
1:1A:2145:C:OP2	1:1A:2146:C:N4	2.47	0.47
1:1A:2747:G:O6	1:1A:2755:C:H5"	2.15	0.47
7:1H:3:ARG:NH2	7:1H:65:HIS:HB3	2.30	0.47
21:1Z:1:MET:HG3	21:1Z:135:GLU:OE1	2.15	0.47
32:1a:533:A:OP1	61:1a:1917:HOH:O	2.20	0.47
32:1a:603:U:H2'	32:1a:604:G:H8	1.79	0.47
33:1b:19:HIS:CG	33:1b:20:GLU:N	2.82	0.47
41:1j:81:THR:C	41:1j:83:GLU:H	2.22	0.47
48:1q:55:ASP:O	48:1q:57:VAL:HG13	2.14	0.47
50:1s:80:TYR:CZ	50:1s:82:GLY:HA2	2.50	0.47
1:2A:910:A:C5	12:2Q:13:GLN:HG3	2.49	0.47
1:2A:2141:G:H2'	1:2A:2142:C:O4'	2.15	0.47
1:2A:2318:G:H21	14:2S:3:ARG:HD3	1.80	0.47
1:2A:2895:U:H2'	1:2A:2896:C:O4'	2.15	0.47
5:2F:165:ARG:HG2	5:2F:168:ARG:NH2	2.30	0.47
5:2F:172:TRP:H	5:2F:172:TRP:CD1	2.32	0.47
12:2Q:137:TYR:O	12:2Q:141:GLN:HG2	2.15	0.47
32:2a:473:G:H2'	32:2a:474:G:H8	1.80	0.47
32:2a:1005:A:H8	32:2a:1024:G:H21	1.62	0.47
37:2f:99:ALA:HB2	49:2r:31:LEU:HD11	1.97	0.47
43:2l:53:ARG:HG3	43:2l:93:LEU:HD21	1.96	0.47
1:1A:593:G:H4'	30:18:4:MET:HE2	1.95	0.47
1:1A:1937:A:H1'	1:1A:1939:5MU:H72	1.97	0.47
1:1A:2116:G:H2'	1:1A:2117:A:C5	2.50	0.47
6:1G:137:GLU:HG2	6:1G:152:LEU:HD13	1.97	0.47
10:1O:49:ARG:HH12	32:1a:1423:G:P	2.37	0.47
21:1Z:104:PHE:HA	21:1Z:139:VAL:HG22	1.97	0.47
37:1f:97:PHE:HD2	49:1r:31:LEU:HD13	1.80	0.47
1:2A:322:A:OP1	5:2F:168:ARG:HD2	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1504:C:H2'	1:2A:1505:C:C6	2.50	0.47
1:2A:2611:U:C4	27:25:3:LYS:HG2	2.50	0.47
1:2A:2886:G:H2'	1:2A:2887:U:C6	2.50	0.47
4:2E:4:ILE:HD11	4:2E:29:GLY:HA2	1.97	0.47
7:2H:154:PRO:HB3	7:2H:163:TYR:CE1	2.50	0.47
17:2V:62:LEU:HD21	17:2V:95:LEU:HB3	1.97	0.47
21:2Z:9:TYR:OH	21:2Z:61:LEU:HD13	2.15	0.47
32:2a:563:A:H2'	32:2a:567:G:C8	2.50	0.47
32:2a:659:U:OP2	46:2o:8:LYS:NZ	2.38	0.47
33:2b:52:GLU:HG2	33:2b:56:ARG:HH22	1.80	0.47
36:2e:7:GLU:CD	36:2e:37:ARG:HH21	2.22	0.47
50:2s:48:THR:HG22	50:2s:61:TYR:HB2	1.97	0.47
1:1A:228:A:H2'	1:1A:230:U:O4'	2.15	0.46
1:1A:586:A:N1	1:1A:809:G:O2'	2.39	0.46
1:1A:1058:G:N2	1:1A:1080:C:N3	2.55	0.46
9:1N:28:THR:HG22	9:1N:29:LYS:HG3	1.97	0.46
20:1Y:19:LYS:HE2	20:1Y:20:TYR:CE2	2.50	0.46
23:11:23:LYS:HB3	23:11:29:GLY:HA3	1.96	0.46
24:12:17:SER:HB3	24:12:20:GLU:HG3	1.97	0.46
33:1b:145:LEU:HD23	33:1b:149:LEU:HD12	1.96	0.46
36:1e:7:GLU:OE2	36:1e:37:ARG:NH2	2.48	0.46
49:1r:73:ALA:HB3	49:1r:79:LEU:HD12	1.97	0.46
56:1y:44:G:H8	56:1y:44:G:OP2	1.98	0.46
1:2A:95:G:O2'	24:22:48:HIS:ND1	2.42	0.46
1:2A:602:G:N1	1:2A:655:A:OP2	2.41	0.46
1:2A:645:C:H5"	1:2A:646:A:OP2	2.14	0.46
1:2A:848:G:H2'	1:2A:849:A:C8	2.51	0.46
1:2A:2128:C:H6	1:2A:2128:C:O5'	1.98	0.46
4:2E:120:TRP:CD1	4:2E:155:LYS:HB3	2.51	0.46
7:2H:144:VAL:O	7:2H:148:ILE:HG13	2.16	0.46
32:2a:232:G:H1'	32:2a:262:A:N1	2.30	0.46
32:2a:458:C:H2'	32:2a:460:G:O4'	2.15	0.46
32:2a:1162:C:H2'	32:2a:1163:C:H6	1.80	0.46
32:2a:1442:G:O2'	32:2a:1442(A):G:H5'	2.15	0.46
40:2i:55:ALA:HA	40:2i:58:HIS:CD2	2.50	0.46
54:2w:34:G:H2'	54:2w:35:A:C8	2.50	0.46
1:1A:271(M):G:OP1	8:1I:53:ALA:HB1	2.15	0.46
1:1A:1406:U:H2'	1:1A:1407:C:C6	2.51	0.46
1:1A:1973:G:OP1	61:1A:4236:HOH:O	2.20	0.46
1:1A:2807:G:N2	1:1A:2893:G:O6	2.44	0.46
6:1G:28:VAL:O	6:1G:31:VAL:HG13	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1H:11:VAL:HG13	7:1H:15:VAL:CG2	2.46	0.46
13:1R:67:LEU:HD13	13:1R:76:VAL:HG21	1.96	0.46
33:1b:47:THR:HA	33:1b:202:PRO:HG2	1.97	0.46
34:1c:6:HIS:ND1	45:1n:49:HIS:HB3	2.31	0.46
1:2A:11:G:C2'	1:2A:12:U:H5'	2.45	0.46
1:2A:274:G:H2'	1:2A:275:G:H8	1.80	0.46
1:2A:627:A:N7	11:2P:84:ASN:ND2	2.48	0.46
1:2A:1301:A:O2'	1:2A:1302:A:H3'	2.15	0.46
1:2A:1379:A:H4'	1:2A:1380:G:OP2	2.15	0.46
1:2A:2893:G:H5"	1:2A:2894:G:O4'	2.14	0.46
5:2F:13:SER:OG	5:2F:16:GLY:N	2.48	0.46
9:2N:20:GLY:HA2	9:2N:61:ARG:HE	1.79	0.46
21:2Z:65:GLN:HE21	21:2Z:67:LEU:HD21	1.81	0.46
21:2Z:132:ASN:ND2	21:2Z:160:GLY:H	2.13	0.46
21:2Z:156:LYS:HE2	21:2Z:158:PRO:HB3	1.96	0.46
32:2a:730:G:C5	32:2a:731:G:H1'	2.50	0.46
35:2d:58:LEU:HD22	35:2d:62:GLN:HG2	1.97	0.46
1:1A:1025:G:O2'	61:1A:4217:HOH:O	2.15	0.46
1:1A:2106:G:H2'	1:1A:2107:C:O4'	2.16	0.46
5:1F:14:PRO:HD2	5:1F:127:GLU:OE1	2.16	0.46
6:1G:45:GLU:O	6:1G:49:ASP:HB2	2.15	0.46
32:1a:447:G:H2'	32:1a:485:G:N2	2.31	0.46
32:1a:920:U:H2'	32:1a:921:U:C6	2.50	0.46
32:1a:1521:G:N3	61:1a:1951:HOH:O	2.36	0.46
33:1b:185:ILE:CG2	33:1b:199:TYR:HB2	2.39	0.46
1:2A:2695:C:H2'	1:2A:2696:U:C6	2.51	0.46
2:2B:61:G:C6	2:2B:62:C:C4	3.04	0.46
32:2a:1126:U:H3	41:2j:40:LEU:HD11	1.80	0.46
33:2b:76:GLN:HG3	33:2b:206:ASP:O	2.15	0.46
37:2f:76:ALA:O	37:2f:80:ARG:HG3	2.15	0.46
50:2s:35:SER:OG	50:2s:38:SER:OG	2.26	0.46
55:2x:23:C:H2'	55:2x:24:U:C6	2.50	0.46
1:1A:637:A:H4'	1:1A:638:G:O5'	2.16	0.46
1:1A:1782:C:H1'	1:1A:2609:U:H5"	1.97	0.46
1:1A:2774:C:H2'	1:1A:2775:A:O4'	2.15	0.46
4:1E:2:LYS:NZ	4:1E:100:GLU:OE1	2.49	0.46
5:1F:53:THR:CG2	5:1F:55:GLY:H	2.27	0.46
5:1F:101:LEU:HD12	5:1F:102:PRO:HD2	1.97	0.46
10:1O:68:GLU:HB3	10:1O:78:ARG:HB2	1.97	0.46
32:1a:711:G:OP1	37:1f:54:LYS:NZ	2.40	0.46
47:1p:15:PRO:O	47:1p:16:HIS:ND1	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:323:G:HO2'	1:2A:1205:U:H3	1.61	0.46
1:2A:2439:A:N6	55:2x:76:31H:OP1	2.49	0.46
1:2A:2495:G:H5"	12:2Q:82:ARG:HG2	1.98	0.46
32:2a:60:A:N1	32:2a:107:G:O2'	2.41	0.46
32:2a:828:A:H5"	32:2a:859:A:C2	2.50	0.46
32:2a:1062:U:H2'	32:2a:1063:C:C6	2.50	0.46
32:2a:1257:U:O4	45:2n:17:LYS:NZ	2.46	0.46
46:2o:71:GLN:HB2	46:2o:78:TYR:CD1	2.51	0.46
48:2q:67:LYS:HA	48:2q:70:ARG:HH12	1.81	0.46
1:1A:969:U:H2'	1:1A:970:C:C6	2.51	0.46
7:1H:95:ARG:NH1	7:1H:106:THR:HG21	2.31	0.46
12:1Q:15:GLY:O	12:1Q:16:ARG:HB2	2.16	0.46
32:1a:216:G:H2'	32:1a:217:C:C6	2.51	0.46
32:1a:461:A:O2'	32:1a:470:C:H5'	2.15	0.46
32:1a:767:A:H2'	32:1a:768:A:O4'	2.16	0.46
32:1a:1146:A:H2'	32:1a:1147:C:O4'	2.15	0.46
33:1b:97:TRP:HZ3	33:1b:176:GLU:OE2	1.99	0.46
35:1d:146:ILE:H	35:1d:146:ILE:HD12	1.79	0.46
1:2A:71:A:H5"	1:2A:73:A:C8	2.51	0.46
1:2A:657:U:H2'	1:2A:658:C:C6	2.50	0.46
1:2A:1336:A:H2'	1:2A:1337:G:C8	2.51	0.46
1:2A:1866:C:H2'	1:2A:1876:A:O4'	2.15	0.46
1:2A:2819:G:H2'	1:2A:2821:A:N7	2.31	0.46
7:2H:83:TYR:CD2	7:2H:138:LYS:HB2	2.50	0.46
14:2S:25:ARG:HD3	14:2S:40:ILE:HB	1.97	0.46
22:20:23:VAL:HG22	22:20:38:VAL:HG22	1.97	0.46
33:2b:74:LYS:O	33:2b:78:GLN:HG2	2.14	0.46
39:2h:12:ARG:HD2	39:2h:26:VAL:HG13	1.97	0.46
56:2y:65:G:H2'	56:2y:66:U:C6	2.49	0.46
1:1A:271(M):G:O2'	1:1A:271(N):U:H5"	2.14	0.46
1:1A:484:C:H2'	1:1A:485:C:C6	2.51	0.46
1:1A:764:A:H5'	3:1D:210:GLY:HA2	1.97	0.46
1:1A:2810:A:N6	1:1A:2891:G:O2'	2.43	0.46
32:1a:7:G:O2'	36:1e:120:THR:O	2.33	0.46
32:1a:391:G:P	47:1p:28:ARG:HH12	2.39	0.46
32:1a:828:A:H2'	32:1a:829:G:O4'	2.15	0.46
1:2A:271(E):U:H2'	1:2A:271(F):C:C6	2.50	0.46
1:2A:479:A:N3	1:2A:481:G:H5"	2.31	0.46
1:2A:1604:C:OP1	61:2A:3949:HOH:O	2.20	0.46
12:2Q:78:PRO:HG2	12:2Q:81:VAL:HG11	1.97	0.46
32:2a:692:U:O2'	32:2a:694:A:N7	2.32	0.46

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"	1.96	0.46
32:2a:953:G:H5'	32:2a:965:A:N6	2.27	0.46
32:2a:1292:U:H2'	32:2a:1293:G:H8	1.80	0.46
56:2y:9:A:H4'	56:2y:46:G7M:H5'	1.98	0.46
56:2y:63:G:H2'	56:2y:64:A:H8	1.81	0.46
1:1A:1063:G:C6	1:1A:1064:C:N4	2.84	0.46
26:14:63:TYR:N	26:14:63:TYR:CD1	2.83	0.46
32:1a:278:G:OP2	48:1q:92:ARG:NH2	2.49	0.46
32:1a:404:U:H2'	32:1a:405:U:H6	1.81	0.46
37:1f:48:LEU:HD22	49:1r:77:GLY:HA3	1.98	0.46
1:2A:530:G:C5	1:2A:2022:U:H5"	2.50	0.46
1:2A:600:G:O3'	5:2F:108:LYS:HE3	2.15	0.46
1:2A:1550:C:H5'	1:2A:1742:G:N2	2.31	0.46
1:2A:2134:A:N6	1:2A:2157:G:H4'	2.17	0.46
1:2A:2406:U:C2	11:2P:72:PRO:HG2	2.51	0.46
14:2S:38:GLN:NE2	14:2S:47:THR:OG1	2.49	0.46
19:2X:94:GLY:H	19:2X:95:LEU:HB2	1.80	0.46
31:29:15:LYS:HB3	31:29:26:ILE:HD12	1.98	0.46
32:2a:335:C:H2'	32:2a:336:C:C6	2.51	0.46
32:2a:628:G:H2'	32:2a:629:G:C8	2.51	0.46
32:2a:828:A:H2'	32:2a:829:G:O4'	2.15	0.46
32:2a:1274:G:N2	32:2a:1275:A:N7	2.63	0.46
32:2a:1441:G:H1'	32:2a:1461:G:N2	2.30	0.46
36:2e:146:ALA:O	36:2e:150:ARG:HG2	2.16	0.46
42:2k:79:SER:HB3	42:2k:104:GLN:HE21	1.80	0.46
51:2t:43:LEU:HD13	51:2t:51:GLU:HB3	1.96	0.46
1:1A:572:A:OP2	17:1V:78:LYS:NZ	2.47	0.46
1:1A:847:U:OP2	61:1A:4239:HOH:O	2.21	0.46
1:1A:1936:A:OP1	1:1A:1937:A:H5'	2.16	0.46
1:1A:2206:G:H5"	1:1A:2207:G:N7	2.31	0.46
12:1Q:115:MET:HE3	12:1Q:115:MET:HB3	1.80	0.46
21:1Z:100:VAL:HG11	21:1Z:134:PRO:HG2	1.98	0.46
32:1a:235:C:H2'	32:1a:236:G:C8	2.50	0.46
32:1a:1095:U:P	32:1a:1108:G:H1	2.39	0.46
32:1a:1140:C:H2'	32:1a:1141:C:H6	1.81	0.46
32:1a:1145:C:H4'	32:1a:1146:A:H5'	1.98	0.46
32:1a:1157:A:H4'	32:1a:1158:C:O5'	2.15	0.46
32:1a:1229:A:OP2	44:1m:114:ARG:HD3	2.16	0.46
34:1c:71:ALA:HA	34:1c:106:VAL:CG1	2.46	0.46
34:1c:108:ASN:ND2	34:1c:144:SER:HB3	2.30	0.46
1:2A:832:G:H5'	11:2P:45:LEU:HD11	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1359:A:H2	1:2A:1372:U:O4	1.98	0.46
1:2A:2331:G:O2'	22:20:43:THR:HG22	2.16	0.46
1:2A:2364:C:H2'	1:2A:2365:G:O4'	2.15	0.46
8:2I:26:ALA:HA	8:2I:30:LEU:HB2	1.97	0.46
32:2a:333:G:H4'	51:2t:16:HIS:CE1	2.51	0.46
44:2m:87:TYR:N	50:2s:73:GLU:O	2.45	0.46
56:2y:42:C:H2'	56:2y:43:C:C6	2.50	0.46
1:1A:251:A:C5	1:1A:252:G:H1'	2.51	0.46
1:1A:2887:U:H2'	1:1A:2888:C:C6	2.50	0.46
4:1E:181:LEU:HD12	4:1E:181:LEU:HA	1.84	0.46
32:1a:445:G:H2'	32:1a:446:G:O4'	2.16	0.46
32:1a:512:U:H2'	32:1a:513:C:C6	2.51	0.46
32:1a:1062:U:H2'	32:1a:1063:C:C6	2.50	0.46
39:1h:51:VAL:HG12	39:1h:52:ASP:H	1.81	0.46
40:1i:16:ARG:HB2	40:1i:64:THR:HB	1.98	0.46
43:1l:60:LEU:HD11	43:1l:66:VAL:HG22	1.98	0.46
44:1m:15:VAL:HG11	44:1m:48:LEU:HD21	1.97	0.46
1:2A:171:G:H2'	1:2A:172:C:C6	2.51	0.46
1:2A:265:A:C8	1:2A:266:G:H1'	2.51	0.46
1:2A:286:C:H2'	1:2A:287:C:C6	2.51	0.46
1:2A:1508:A:H4'	1:2A:1509(A):A:N7	2.30	0.46
1:2A:2472:G:H2'	1:2A:2475:C:H42	1.81	0.46
9:2N:4:TYR:CD2	16:2U:100:VAL:HG11	2.51	0.46
9:2N:30:ILE:HA	9:2N:33:LEU:HD12	1.98	0.46
9:2N:42:TRP:CH2	9:2N:44:PRO:HB3	2.51	0.46
32:2a:1218:C:OP2	45:2n:9:LYS:NZ	2.49	0.46
56:2y:55:PSU:O2	56:2y:57:G:H3'	2.16	0.46
1:1A:2105:C:H2'	1:1A:2106:G:H8	1.80	0.46
1:1A:2285:C:OP2	28:16:6:ARG:NH1	2.47	0.46
1:1A:2788:C:O2'	1:1A:2809:A:N3	2.45	0.46
32:1a:111:G:H5"	47:1p:27:LYS:HB3	1.96	0.46
32:1a:179:A:H2'	32:1a:180:U:C6	2.51	0.46
32:1a:328:C:H4'	32:1a:329:A:H5'	1.98	0.46
32:1a:600:C:H2'	32:1a:601:C:C6	2.51	0.46
32:1a:950:U:H2'	32:1a:951:G:C8	2.51	0.46
32:1a:1262:C:H2'	32:1a:1263:C:H6	1.80	0.46
1:2A:320:A:H4'	1:2A:322:A:N7	2.31	0.46
1:2A:570:G:H2'	1:2A:2030:A:C5	2.50	0.46
1:2A:881:G:H3'	1:2A:882:G:C8	2.51	0.46
1:2A:1038:C:H42	1:2A:1117:G:H1	1.64	0.46
1:2A:1769:G:O2'	1:2A:1958:C:OP1	2.29	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2186:G:H2'	1:2A:2187:G:C8	2.51	0.46
1:2A:2314:C:C5'	6:2G:38:VAL:HG21	2.42	0.46
13:2R:61:HIS:O	13:2R:65:LEU:HG	2.14	0.46
32:2a:130:A:H1'	32:2a:263:A:O2'	2.16	0.46
34:2c:148:GLY:HA3	34:2c:172:ARG:O	2.15	0.46
54:2w:25:C:H2'	54:2w:26:A:C8	2.52	0.46
56:2y:37:MIA:H2'	56:2y:38:A:O4'	2.16	0.46
1:1A:579:G:H2'	1:1A:580:C:C6	2.51	0.45
1:1A:721:C:H2'	1:1A:722:A:C8	2.51	0.45
1:1A:1453:U:O2'	1:1A:1455:G:N7	2.44	0.45
1:1A:1665:A:H4'	10:1O:67:LYS:HB2	1.97	0.45
1:1A:1794:U:H2'	1:1A:1795:C:C6	2.51	0.45
1:1A:2364:C:H2'	1:1A:2365:G:O4'	2.16	0.45
1:1A:2790:A:H3'	1:1A:2790:A:N3	2.31	0.45
21:1Z:132:ASN:N	21:1Z:132:ASN:OD1	2.47	0.45
32:1a:377:G:OP1	47:1p:3:LYS:HD3	2.16	0.45
32:1a:975:A:H5'	32:1a:975:A:H8	1.81	0.45
32:1a:1239:A:H62	32:1a:1299:A:H62	1.64	0.45
35:1d:189:PRO:HB2	35:1d:194:LEU:HD21	1.97	0.45
1:2A:740:U:H2'	1:2A:741:G:C8	2.51	0.45
1:2A:921:G:H2'	1:2A:922:U:C6	2.50	0.45
1:2A:1187:G:O6	61:2A:3951:HOH:O	2.21	0.45
1:2A:1800:C:OP1	3:2D:264:LYS:NZ	2.42	0.45
6:2G:50:ALA:O	6:2G:52:ILE:N	2.49	0.45
7:2H:24:VAL:HG21	7:2H:72:ILE:HG12	1.98	0.45
12:2Q:137:TYR:CE1	21:2Z:83:PRO:HG3	2.51	0.45
21:2Z:158:PRO:O	21:2Z:161:VAL:HG12	2.17	0.45
31:29:27:CYS:SG	31:29:28:GLU:N	2.89	0.45
32:2a:266:G:H2'	32:2a:266:G:N3	2.31	0.45
32:2a:375:U:OP1	47:2p:69:THR:HG21	2.15	0.45
39:2h:10:LEU:HD22	39:2h:83:ILE:HD11	1.98	0.45
47:2p:20:VAL:HG23	47:2p:35:LYS:HA	1.98	0.45
56:2y:62:C:H2'	56:2y:63:G:C8	2.50	0.45
1:1A:1012:U:C5	9:1N:28:THR:HG21	2.51	0.45
1:1A:1607:C:H4'	1:1A:1608:A:O5'	2.16	0.45
3:1D:35:LYS:HE2	3:1D:64:ILE:HG12	1.97	0.45
5:1F:8:GLN:HE22	5:1F:21:ALA:HB2	1.79	0.45
32:1a:160:A:H1'	32:1a:344:A:C5	2.51	0.45
32:1a:589:C:H2'	32:1a:590:C:H6	1.80	0.45
32:1a:1002:G:H3'	32:1a:1003:G:C4'	2.38	0.45
32:1a:1021:G:O2'	32:1a:1022:G:O4'	2.34	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:1b:83:MET:HB3	33:1b:234:PRO:HG3	1.98	0.45
36:1e:95:ALA:HB1	36:1e:96:PRO:HD2	1.97	0.45
1:2A:999:U:H5"	1:2A:1154:G:O6	2.16	0.45
1:2A:1857:G:C6	1:2A:1858:G:N1	2.84	0.45
1:2A:2102:U:H2'	1:2A:2103:C:C6	2.51	0.45
1:2A:2345:G:N3	1:2A:2381:C:H2'	2.32	0.45
1:2A:2396:G:OP1	23:21:25:LYS:NZ	2.40	0.45
2:2B:4:C:H42	2:2B:117:G:H1	1.64	0.45
8:2I:102:SER:OG	8:2I:103:ARG:N	2.49	0.45
32:2a:41:G:H2'	32:2a:42:G:H8	1.81	0.45
34:2c:126:ARG:HB3	34:2c:128:PHE:CE2	2.51	0.45
42:2k:82:VAL:HB	42:2k:108:ILE:HD13	1.98	0.45
54:2w:51:U:H2'	54:2w:52:G:C8	2.52	0.45
36:1e:85:GLY:C	36:1e:87:SER:H	2.24	0.45
1:2A:588:U:H2'	1:2A:589:C:C6	2.51	0.45
1:2A:1512:U:H2'	1:2A:1513:C:C6	2.51	0.45
1:2A:1939:5MU:OP1	1:2A:2604:U:O2'	2.32	0.45
2:2B:103:G:H21	21:2Z:73:GLN:NE2	2.05	0.45
9:2N:38:HIS:O	16:2U:67:ALA:HB1	2.16	0.45
13:2R:38:VAL:HG22	13:2R:112:ALA:HB2	1.98	0.45
14:2S:93:LYS:HE2	14:2S:93:LYS:HB2	1.81	0.45
38:2g:16:LEU:HD21	40:2i:45:ALA:HB2	1.98	0.45
56:2y:40:C:H2'	56:2y:41:C:C6	2.52	0.45
1:1A:479:A:N3	1:1A:481:G:H5"	2.32	0.45
1:1A:1448:G:H4'	1:1A:1542:A:OP1	2.16	0.45
1:1A:2377:A:H2'	1:1A:2378:A:C8	2.51	0.45
1:1A:2478:A:OP2	31:19:2:LYS:NZ	2.40	0.45
38:1g:50:ILE:HD13	38:1g:125:MET:CG	2.47	0.45
56:1y:57:G:H2'	56:1y:58:A:C5'	2.46	0.45
1:2A:460:A:P	29:27:41:ARG:HH22	2.39	0.45
1:2A:927:G:H2'	1:2A:928:G:O4'	2.16	0.45
1:2A:1916:A:H2'	1:2A:1917:PSU:O4'	2.16	0.45
1:2A:2049:G:N7	61:2A:4035:HOH:O	2.35	0.45
1:2A:2542:A:H4'	1:2A:2543:G:C8	2.52	0.45
1:2A:2630:G:H2'	1:2A:2631:G:H8	1.81	0.45
19:2X:5:TYR:CE2	24:22:30:ARG:HB2	2.51	0.45
21:2Z:92:SER:O	21:2Z:94:GLU:N	2.49	0.45
22:20:52:GLY:O	22:20:59:LEU:HA	2.16	0.45
32:2a:390:C:H4'	47:2p:28:ARG:HH21	1.80	0.45
33:2b:219:VAL:O	33:2b:223:ILE:HG12	2.17	0.45
35:2d:110:PHE:N	35:2d:110:PHE:CD1	2.84	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:2e:5:ASP:CG	36:2e:6:PHE:H	2.23	0.45
36:2e:42:GLY:HA2	36:2e:65:ASN:O	2.17	0.45
40:2i:3:GLN:HE21	40:2i:20:ARG:HE	1.65	0.45
1:1A:1269:A:N7	61:1A:4328:HOH:O	2.36	0.45
7:1H:23:ARG:HE	7:1H:34:GLU:CD	2.25	0.45
26:14:69:LYS:HA	26:14:69:LYS:HD2	1.62	0.45
32:1a:748:C:H4'	32:1a:749:C:O5'	2.17	0.45
32:1a:1002:G:N7	32:1a:1003:G:H1'	2.32	0.45
33:1b:166:ASP:O	33:1b:170:GLU:HB2	2.17	0.45
1:2A:2748:A:C2	7:2H:63:SER:HB3	2.50	0.45
5:2F:40:GLN:NE2	5:2F:182:ASN:HB2	2.32	0.45
10:2O:49:ARG:NH1	32:2a:1422:G:O3'	2.49	0.45
19:2X:1:MET:HE1	24:22:22:GLU:HG2	1.98	0.45
21:2Z:53:ILE:HG22	21:2Z:71:VAL:O	2.17	0.45
21:2Z:60:GLU:H	21:2Z:60:GLU:HG2	1.36	0.45
32:2a:149:A:H2'	32:2a:150:C:C6	2.50	0.45
33:2b:110:GLN:HA	33:2b:113:HIS:CD2	2.51	0.45
36:2e:57:LYS:HG2	36:2e:61:TYR:CE2	2.51	0.45
37:2f:4:TYR:CZ	37:2f:72:VAL:HG21	2.51	0.45
44:2m:3:ARG:NH1	44:2m:8:GLU:OE2	2.50	0.45
1:1A:880:G:H8	1:1A:880:G:OP2	1.99	0.45
1:1A:1155:A:OP1	16:1U:55:ARG:HD2	2.17	0.45
1:1A:1698:A:C8	1:1A:1700:A:O4'	2.69	0.45
1:1A:2439:A:H5'	1:1A:2439:A:C8	2.52	0.45
1:1A:2748:A:H5'	7:1H:4:ILE:HD13	1.99	0.45
5:1F:165:ARG:HA	5:1F:168:ARG:HD2	1.98	0.45
10:1O:16:ALA:HB2	10:1O:52:VAL:CG2	2.46	0.45
20:1Y:9:LYS:HA	20:1Y:10:GLY:HA2	1.57	0.45
32:1a:142:G:H2'	32:1a:143:A:H8	1.82	0.45
32:1a:418:C:H1'	32:1a:540:G:O2'	2.16	0.45
33:1b:60:ASP:O	33:1b:64:ARG:HG2	2.16	0.45
35:1d:173:TRP:CE3	35:1d:189:PRO:HG3	2.51	0.45
40:1i:56:LEU:H	40:1i:56:LEU:HD12	1.82	0.45
44:1m:3:ARG:HG2	44:1m:8:GLU:HA	1.99	0.45
54:1w:1:G:H2'	54:1w:2:C:C6	2.50	0.45
4:2E:143:ASN:HD22	4:2E:147:PRO:HD3	1.82	0.45
7:2H:102:ALA:HB2	7:2H:116:GLU:CD	2.41	0.45
8:2I:60:GLU:O	8:2I:61:ARG:HD3	2.16	0.45
18:2W:86:LEU:HD22	18:2W:96:ILE:HD11	1.97	0.45
25:23:43:ILE:O	25:23:47:VAL:HG23	2.17	0.45
33:2b:8:LYS:O	33:2b:9:GLU:HB2	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:2b:58:ILE:H	33:2b:58:ILE:HG13	1.57	0.45
36:2e:47:LYS:HE2	36:2e:47:LYS:HB2	1.76	0.45
1:1A:305:U:H2'	1:1A:306:U:C6	2.52	0.45
1:1A:1775:U:OP1	1:1A:1979:C:O2'	2.24	0.45
2:1B:74:U:H2'	2:1B:75:G:O4'	2.17	0.45
3:1D:274:ARG:NH1	61:1D:402:HOH:O	2.47	0.45
11:1P:5:ASP:OD1	61:1P:301:HOH:O	2.21	0.45
12:1Q:17:LEU:HB3	12:1Q:39:PRO:HB2	1.97	0.45
32:1a:436:C:H2'	32:1a:437:U:C6	2.52	0.45
32:1a:1223:C:P	50:1s:78:ARG:HH21	2.39	0.45
32:1a:1302:U:C5	44:1m:17:VAL:HG11	2.51	0.45
34:1c:172:ARG:NH2	34:1c:206:GLU:OE2	2.49	0.45
44:1m:50:GLU:HA	44:1m:53:VAL:HG22	1.99	0.45
50:1s:22:LEU:HD12	50:1s:31:ILE:HD11	1.98	0.45
56:1y:57:G:H2'	56:1y:58:A:H5"	1.98	0.45
1:2A:184:C:H2'	1:2A:185:U:H6	1.82	0.45
1:2A:909:A:C6	1:2A:912:C:C2	3.04	0.45
1:2A:1346:G:OP2	61:2A:3952:HOH:O	2.21	0.45
4:2E:34:VAL:HB	4:2E:48:GLN:HE21	1.81	0.45
7:2H:6:ARG:HG2	7:2H:65:HIS:HE1	1.81	0.45
10:2O:108:GLU:H	10:2O:108:GLU:HG3	1.53	0.45
12:2Q:89:ASN:HB2	55:2x:1:C:C4	2.51	0.45
21:2Z:45:ASP:O	21:2Z:49:ARG:HG3	2.17	0.45
32:2a:983:A:N1	32:2a:1222:G:N2	2.62	0.45
40:2i:4:TYR:CE2	40:2i:88:TYR:HD1	2.35	0.45
1:1A:2133:G:N2	1:1A:2157:G:H1'	2.32	0.45
32:1a:487:A:H2'	32:1a:488:C:O4'	2.16	0.45
32:1a:1040:U:H2'	32:1a:1041:A:C8	2.52	0.45
32:1a:1066:C:O2'	32:1a:1067:A:H5'	2.16	0.45
35:1d:59:ARG:HH12	35:1d:62:GLN:HB2	1.82	0.45
38:1g:70:LYS:O	38:1g:138:LYS:HE3	2.17	0.45
45:1n:25:VAL:HG13	45:1n:38:GLY:O	2.17	0.45
1:2A:207:A:H2'	1:2A:208:C:O4'	2.17	0.45
1:2A:608:A:H2'	1:2A:609:A:C8	2.52	0.45
1:2A:1359:A:C2	1:2A:1372:U:O4	2.70	0.45
1:2A:1485:G:H2'	1:2A:1486:A:H8	1.82	0.45
1:2A:1902:C:H5'	3:2D:246:PRO:HD3	1.99	0.45
1:2A:2373:G:H2'	1:2A:2374:C:C6	2.52	0.45
1:2A:2805:G:H2'	1:2A:2807:G:H8	1.80	0.45
21:2Z:146:ILE:HG22	21:2Z:174:VAL:O	2.17	0.45
26:24:53:GLU:HG2	26:24:55:ARG:N	2.30	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:509:A:H5"	35:2d:55:ALA:HB2	1.97	0.45
32:2a:1005:A:H5"	32:2a:1006:C:H5	1.82	0.45
32:2a:1411:C:H2'	32:2a:1412:C:C6	2.52	0.45
35:2d:163:GLU:C	35:2d:165:MET:H	2.25	0.45
38:2g:78:ARG:O	38:2g:84:ASN:HA	2.17	0.45
40:2i:99:LEU:HB3	40:2i:101:PHE:CD2	2.52	0.45
1:1A:185:U:H4'	1:1A:218:A:H4'	1.99	0.45
1:1A:323:G:C8	5:1F:171:PRO:HG3	2.51	0.45
1:1A:2355:C:H1'	22:10:39:ARG:HH21	1.81	0.45
4:1E:77:ILE:HD13	4:1E:195:LEU:HD13	1.99	0.45
5:1F:64:ILE:HG21	5:1F:78:ILE:HG23	1.99	0.45
8:1I:69:LYS:HA	8:1I:138:ILE:HG12	1.98	0.45
32:1a:119:A:H4'	32:1a:120:A:C8	2.52	0.45
32:1a:451:A:N6	32:1a:480:U:H2'	2.32	0.45
54:1w:11:C:H2'	54:1w:12:U:C6	2.51	0.45
1:2A:985:C:H2'	1:2A:986:C:H6	1.82	0.45
1:2A:2143:C:N4	1:2A:2148:G:H1	2.15	0.45
6:2G:11:TYR:O	6:2G:16:ARG:HG2	2.16	0.45
8:2I:38:LEU:H	8:2I:38:LEU:HD12	1.82	0.45
9:2N:102:ALA:O	9:2N:106:MET:HG3	2.16	0.45
12:2Q:56:ARG:HB3	12:2Q:56:ARG:HH11	1.81	0.45
13:2R:8:ARG:HE	13:2R:43:GLU:HG2	1.81	0.45
15:2T:118:ARG:HD3	15:2T:118:ARG:HA	1.78	0.45
21:2Z:159:PRO:HA	21:2Z:160:GLY:HA2	1.60	0.45
32:2a:1023:G:H3'	32:2a:1024:G:H8	1.82	0.45
33:2b:124:SER:HB3	33:2b:125:PRO:HD3	1.99	0.45
33:2b:132:LYS:O	33:2b:136:VAL:HG22	2.17	0.45
34:2c:142:MET:HG3	34:2c:170:GLN:HB3	1.98	0.45
55:2x:61:C:H2'	55:2x:62:C:H6	1.81	0.45
1:1A:848:G:O6	1:1A:928:G:H2'	2.17	0.45
1:1A:893:C:H2'	1:1A:894:C:C6	2.52	0.45
1:1A:1056:G:O2'	1:1A:1086:A:H1'	2.17	0.45
1:1A:1178:C:H2'	1:1A:1179:C:C6	2.52	0.45
1:1A:2271:G:OP1	22:10:18:ALA:HB1	2.16	0.45
3:1D:71:ASP:CB	3:1D:103:ARG:HH12	2.30	0.45
6:1G:59:GLU:OE2	6:1G:138:GLN:NE2	2.37	0.45
28:16:14:THR:HB	28:16:48:VAL:O	2.17	0.45
32:1a:1118:C:H1'	32:1a:1179:A:C4	2.52	0.45
32:1a:1178:G:OP2	40:1i:97:LYS:NZ	2.49	0.45
32:1a:1239:A:H4'	32:1a:1240:U:H5"	1.98	0.45
33:1b:69:LEU:HB3	33:1b:162:ILE:HG22	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:1h:21:LYS:O	39:1h:65:TYR:OH	2.34	0.45
1:2A:686:G:N2	1:2A:788:A:H61	2.15	0.45
1:2A:849:A:H2	25:23:24:LYS:HG2	1.81	0.45
1:2A:886:C:H2'	1:2A:887:A:O4'	2.17	0.45
1:2A:1116:C:H2'	1:2A:1117:G:H8	1.81	0.45
1:2A:1504:C:O2'	1:2A:1505:C:H5'	2.16	0.45
11:2P:59:LEU:HD11	30:28:10:ALA:HA	1.99	0.45
15:2T:83:ILE:HD13	15:2T:86:ILE:HD11	1.99	0.45
32:2a:1291:G:C6	32:2a:1292:U:C4	3.04	0.45
48:2q:29:HIS:CD2	48:2q:30:PRO:HD2	2.52	0.45
1:1A:671:C:N4	61:1A:4471:HOH:O	2.50	0.44
1:1A:1104:C:H2'	1:1A:1105:U:C6	2.52	0.44
6:1G:179:PRO:HG3	26:14:43:TYR:CZ	2.52	0.44
32:1a:44:G:H2'	32:1a:45:U:O4'	2.17	0.44
35:1d:85:LYS:HG3	35:1d:86:LYS:N	2.31	0.44
35:1d:187:ARG:HH22	35:1d:193:ASP:CG	2.25	0.44
50:1s:40:ILE:HB	50:1s:67:VAL:O	2.17	0.44
54:1w:14:A:H5'	54:1w:15:G:OP2	2.17	0.44
1:2A:224:G:H2'	1:2A:225:A:O4'	2.17	0.44
1:2A:363:G:H2'	1:2A:363(A):A:H8	1.83	0.44
1:2A:656:G:H2'	1:2A:657:U:O4'	2.16	0.44
1:2A:729:G:O5'	3:2D:208:LYS:NZ	2.48	0.44
1:2A:1827:C:O2'	1:2A:1970:A:N3	2.48	0.44
1:2A:1839:G:C8	1:2A:1927:A:H1'	2.52	0.44
1:2A:2134:A:H1'	1:2A:2158:A:C6	2.51	0.44
1:2A:2161:C:H2'	1:2A:2162:G:O4'	2.16	0.44
1:2A:2206:G:H5"	1:2A:2207:G:N7	2.32	0.44
2:2B:94:C:H2'	2:2B:95:C:H6	1.80	0.44
14:2S:87:PHE:CE1	14:2S:102:ALA:HB2	2.52	0.44
32:2a:447:G:O6	32:2a:485:G:O2'	2.28	0.44
32:2a:544:G:P	35:2d:59:ARG:HH22	2.39	0.44
32:2a:946:A:H2'	32:2a:947:G:C8	2.52	0.44
32:2a:973:G:OP1	41:2j:57:LYS:NZ	2.46	0.44
32:2a:1152:A:H2'	32:2a:1153:C:C6	2.51	0.44
32:2a:1162:C:H2'	32:2a:1163:C:C6	2.52	0.44
33:2b:178:ARG:NH2	39:2h:74:PRO:HB3	2.32	0.44
41:2j:9:ARG:O	41:2j:16:LEU:HD11	2.17	0.44
53:2v:16:A:H2'	53:2v:17:U:O4'	2.16	0.44
1:1A:615:G:OP2	5:1F:43:LYS:NZ	2.40	0.44
1:1A:1062:G:C8	1:1A:1070:A:H4'	2.52	0.44
1:1A:2101:G:H2'	1:1A:2102:U:C6	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1G:82:LEU:HD21	6:1G:88:ILE:HG21	1.99	0.44
10:1O:48:PRO:CB	32:1a:1422:G:H5"	2.45	0.44
16:1U:69:CYS:HB3	16:1U:74:LEU:HD13	1.99	0.44
21:1Z:125:LEU:HB3	21:1Z:165:VAL:HG13	2.00	0.44
32:1a:18:C:H2'	32:1a:19:C:O4'	2.16	0.44
41:1j:6:ILE:HA	41:1j:97:GLU:O	2.18	0.44
44:1m:96:LEU:HD23	44:1m:96:LEU:HA	1.86	0.44
47:1p:40:ASP:OD2	47:1p:44:THR:OG1	2.24	0.44
1:2A:212:G:H2'	1:2A:213:A:O4'	2.17	0.44
1:2A:443:A:N7	5:2F:45:ARG:HG2	2.33	0.44
1:2A:1469:A:H2'	1:2A:1470:G:O4'	2.18	0.44
1:2A:1539:G:H2'	1:2A:1540:U:O4'	2.18	0.44
2:2B:28:C:H2'	2:2B:29:A:C8	2.52	0.44
4:2E:181:LEU:HD12	4:2E:181:LEU:HA	1.83	0.44
17:2V:58:VAL:HB	17:2V:98:GLU:HG3	1.99	0.44
20:2Y:55:TYR:CZ	20:2Y:61:ILE:HG21	2.53	0.44
32:2a:1058:G:H2'	32:2a:1059:C:O4'	2.17	0.44
34:2c:108:ASN:HB3	34:2c:111:LEU:HD12	1.99	0.44
38:2g:50:ILE:HD11	38:2g:58:PRO:HB3	1.99	0.44
47:2p:17:TYR:HE2	47:2p:41:PRO:HG3	1.82	0.44
1:1A:41:C:H2'	1:1A:42:G:O4'	2.16	0.44
1:1A:278:A:O2'	1:1A:279:C:OP1	2.26	0.44
1:1A:613:G:O2'	1:1A:614(C):A:N1	2.47	0.44
1:1A:829:A:N7	1:1A:2248:C:H5'	2.33	0.44
1:1A:1096:A:N6	1:1A:1097:U:O2	2.51	0.44
1:1A:2629:A:HO2'	1:1A:2630:G:P	2.38	0.44
2:1B:103:G:H21	21:1Z:73:GLN:HE22	1.65	0.44
8:1I:109:ILE:HG23	8:1I:130:TYR:CZ	2.52	0.44
12:1Q:32:TYR:CE1	12:1Q:133:ARG:HB3	2.53	0.44
32:1a:555:C:H2'	32:1a:556:C:C6	2.52	0.44
42:1k:89:ALA:C	42:1k:91:ARG:H	2.25	0.44
43:1l:24:VAL:HB	43:1l:27:LEU:HG	1.99	0.44
51:1t:100:ILE:H	51:1t:100:ILE:HG12	1.62	0.44
1:2A:265:A:H1'	1:2A:266:G:O4'	2.17	0.44
1:2A:403:U:H4'	1:2A:404:C:H5'	1.99	0.44
1:2A:884:C:H2'	1:2A:885:C:O4'	2.17	0.44
1:2A:2151:G:H2'	1:2A:2152:G:H8	1.82	0.44
5:2F:7:TYR:O	5:2F:22:ALA:N	2.50	0.44
5:2F:20:LEU:HD12	5:2F:20:LEU:HA	1.83	0.44
9:2N:123:TYR:OH	9:2N:130:HIS:NE2	2.40	0.44
10:2O:36:GLY:HA2	10:2O:106:LEU:HD23	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:2R:36:THR:HG22	13:2R:37:THR:H	1.82	0.44
23:21:19:GLN:O	23:21:35:THR:HG22	2.18	0.44
23:21:83:GLU:OE1	23:21:83:GLU:N	2.50	0.44
24:22:35:LEU:HD12	24:22:53:LEU:HD23	1.99	0.44
24:22:53:LEU:O	24:22:57:ILE:HG13	2.17	0.44
26:24:24:THR:OG1	26:24:25:TYR:N	2.44	0.44
32:2a:986:A:H2'	32:2a:987:G:O4'	2.16	0.44
33:2b:134:GLU:O	33:2b:138:LEU:HD22	2.17	0.44
1:1A:1055:G:H3'	1:1A:1056:G:C8	2.53	0.44
1:1A:2630:G:N7	61:1A:4325:HOH:O	2.36	0.44
21:1Z:1:MET:HG2	21:1Z:55:HIS:ND1	2.32	0.44
32:1a:547:A:H5'	61:1a:1950:HOH:O	2.16	0.44
32:1a:690:G:C6	32:1a:691:G:C6	3.06	0.44
32:1a:1004:A:H5"	32:1a:1025:U:H5	1.81	0.44
32:1a:1032:G:H2'	32:1a:1033:G:O4'	2.18	0.44
32:1a:1054:C:C5	54:1w:34:G:H1'	2.52	0.44
39:1h:19:VAL:HG23	39:1h:21:LYS:HG2	1.98	0.44
1:2A:892:G:H2'	1:2A:894:C:OP2	2.17	0.44
1:2A:1602:U:O4	61:2A:3943:HOH:O	2.20	0.44
8:2I:90:GLY:O	8:2I:121:LYS:HE3	2.18	0.44
19:2X:12:VAL:HG22	19:2X:29:TRP:CE2	2.52	0.44
20:2Y:43:ASN:CG	20:2Y:65:ALA:HB3	2.43	0.44
21:2Z:98:MET:O	21:2Z:125:LEU:HD12	2.17	0.44
32:2a:130:A:O2'	32:2a:131:C:O5'	2.32	0.44
32:2a:999:C:N4	32:2a:1042:G:H1	2.15	0.44
34:2c:30:ARG:HH21	45:2n:38:GLY:HA2	1.82	0.44
40:2i:112:LYS:NZ	40:2i:113:LYS:O	2.47	0.44
1:1A:1588:C:H2'	1:1A:1589:C:C6	2.52	0.44
1:1A:1803:A:H4'	3:1D:259:THR:HG23	1.99	0.44
5:1F:72:ARG:HE	5:1F:72:ARG:HB3	1.59	0.44
10:1O:24:VAL:HG13	10:1O:33:ALA:HB2	1.99	0.44
18:1W:4:LYS:HG2	18:1W:5:ALA:N	2.33	0.44
21:1Z:1:MET:SD	21:1Z:135:GLU:HG2	2.57	0.44
26:14:68:ARG:HD3	26:14:69:LYS:H	1.82	0.44
32:1a:714:G:H2'	32:1a:715:A:C8	2.53	0.44
32:1a:1226:C:H4'	50:1s:80:TYR:CZ	2.52	0.44
32:1a:1262:C:H2'	32:1a:1263:C:C6	2.53	0.44
32:1a:1263:C:H2'	32:1a:1264:C:C6	2.53	0.44
33:1b:127:ILE:HD13	33:1b:130:ARG:NH2	2.32	0.44
36:1e:33:VAL:HG21	36:1e:109:ILE:HA	1.99	0.44
37:1f:89:MET:HE1	49:1r:72:ARG:HB3	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:236:C:H2'	1:2A:237:C:C6	2.53	0.44
1:2A:881:G:H3'	1:2A:882:G:H8	1.82	0.44
1:2A:1877:A:H5'	1:2A:1878:G:OP2	2.17	0.44
1:2A:2347:C:H2'	1:2A:2348:U:C6	2.53	0.44
1:2A:2646:C:H2'	1:2A:2647:U:O4'	2.18	0.44
1:2A:2701:C:H2'	1:2A:2702:U:H2'	2.00	0.44
2:2B:114:C:H4'	14:2S:46:VAL:HG22	1.98	0.44
3:2D:11:PRO:O	3:2D:14:ARG:HG3	2.17	0.44
12:2Q:37:LEU:HD12	12:2Q:128:LYS:HB3	1.98	0.44
12:2Q:56:ARG:HH22	12:2Q:59:ARG:NH2	2.13	0.44
17:2V:85:LYS:HB2	17:2V:85:LYS:HE3	1.81	0.44
18:2W:68:ARG:HH11	18:2W:111:HIS:HA	1.82	0.44
32:2a:476:G:H2'	32:2a:477:A:C8	2.52	0.44
32:2a:923:A:OP1	36:2e:21:ALA:HB2	2.18	0.44
32:2a:1005:A:H5"	32:2a:1006:C:C5	2.53	0.44
32:2a:1152:A:OP1	41:2j:68:HIS:ND1	2.47	0.44
32:2a:1302:U:OP1	44:2m:13:LYS:NZ	2.46	0.44
32:2a:1305:G:H5'	52:2u:4:GLY:HA3	1.99	0.44
34:2c:35:GLU:HG2	34:2c:59:ARG:HH22	1.81	0.44
37:2f:41:GLU:CD	49:2r:35:ARG:HH22	2.26	0.44
54:2w:68:C:H2'	54:2w:69:G:H8	1.82	0.44
56:2y:58:A:H1'	56:2y:60:U:N3	2.33	0.44
1:1A:1688:U:O2	1:1A:1700:A:H5'	2.17	0.44
19:1X:2:LYS:HA	19:1X:2:LYS:HD2	1.77	0.44
24:12:67:LYS:C	24:12:69:ARG:H	2.25	0.44
32:1a:109:A:C6	32:1a:326:G:C6	3.05	0.44
35:1d:61:LYS:HD3	35:1d:206:PHE:CE2	2.53	0.44
35:1d:117:ALA:O	35:1d:121:VAL:HG23	2.17	0.44
44:1m:104:ARG:NH2	61:1m:3101:HOH:O	2.50	0.44
48:1q:32:TYR:O	48:1q:34:LYS:N	2.43	0.44
51:1t:56:MET:HE3	51:1t:85:MET:HG2	1.99	0.44
1:2A:358:U:H2'	1:2A:359:A:C8	2.53	0.44
4:2E:178:GLU:CD	4:2E:178:GLU:H	2.25	0.44
16:2U:50:ARG:HH22	17:2V:72:VAL:HG22	1.83	0.44
26:24:68:ARG:NH1	26:24:68:ARG:HA	2.32	0.44
32:2a:437:U:H5"	35:2d:155:LEU:HD11	2.00	0.44
32:2a:1005:A:H3'	32:2a:1006:C:C6	2.52	0.44
32:2a:1318:A:OP1	50:2s:3:ARG:NH2	2.42	0.44
32:2a:1346:A:N1	32:2a:1374:A:H5"	2.32	0.44
34:2c:8:ILE:HG23	34:2c:16:ARG:HG2	1.98	0.44
34:2c:109:PRO:HA	34:2c:115:LEU:HD23	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:2h:20:TYR:HA	39:2h:65:TYR:CE1	2.53	0.44
1:1A:468:G:N7	29:17:39:ARG:NH2	2.57	0.44
1:1A:821:A:H2'	1:1A:946:G:H5"	1.99	0.44
1:1A:1636:C:H2'	1:1A:1637:A:C8	2.52	0.44
1:1A:1810:A:H2'	1:1A:1811:G:O4'	2.18	0.44
8:1I:77:LEU:HD11	8:1I:100:ALA:HB3	2.00	0.44
12:1Q:51:ARG:HD3	12:1Q:66:ILE:HD11	2.00	0.44
20:1Y:99:CYS:HB2	20:1Y:106:LEU:HD21	1.99	0.44
32:1a:448:A:P	32:1a:485:G:H22	2.41	0.44
32:1a:1140:C:H2'	32:1a:1141:C:C6	2.53	0.44
32:1a:1429:C:H2'	32:1a:1430:C:C6	2.53	0.44
38:1g:26:PHE:HD1	38:1g:101:LEU:HD22	1.82	0.44
38:1g:113:GLU:HG2	38:1g:119:ARG:HG2	1.98	0.44
42:1k:54:ARG:NH1	56:1y:39:PSU:O2'	2.51	0.44
56:1y:41:C:H2'	56:1y:42:C:C6	2.52	0.44
6:2G:70:VAL:HA	6:2G:90:LEU:HD23	1.99	0.44
10:2O:111:PHE:O	10:2O:115:VAL:HG23	2.17	0.44
16:2U:49:HIS:HA	16:2U:52:ARG:HB2	2.00	0.44
23:21:94:LEU:HA	23:21:94:LEU:HD23	1.85	0.44
24:22:16:LEU:O	24:22:67:LYS:NZ	2.48	0.44
25:23:7:LYS:HE3	25:23:32:GLN:HE21	1.81	0.44
32:2a:923:A:O2'	32:2a:1399:C:OP2	2.34	0.44
32:2a:1101:A:H62	33:2b:175:ARG:HH21	1.66	0.44
1:1A:228:A:H3'	1:1A:229:A:C5'	2.48	0.44
1:1A:1290:C:H2'	1:1A:1291:C:H6	1.83	0.44
1:1A:2420:C:OP1	30:18:34:TRP:HB3	2.18	0.44
1:1A:2781:A:O2'	61:1A:4233:HOH:O	2.19	0.44
1:1A:2790:A:H4'	1:1A:2893:G:H21	1.82	0.44
4:1E:97:LYS:N	4:1E:100:GLU:OE2	2.48	0.44
7:1H:35:VAL:O	7:1H:37:VAL:HG23	2.18	0.44
21:1Z:1:MET:HA	21:1Z:2:GLU:HA	1.73	0.44
32:1a:103:C:P	51:1t:17:ARG:HH21	2.40	0.44
32:1a:620:C:C2	35:1d:135:LEU:HG	2.52	0.44
32:1a:1006:C:N4	32:1a:1023:G:H1	2.13	0.44
32:1a:1280:A:O2'	32:1a:1281:U:H5'	2.18	0.44
32:1a:1530:G:H4'	32:1a:1530:G:OP1	2.18	0.44
33:1b:219:VAL:HA	33:1b:222:ILE:HD12	2.00	0.44
43:1l:7:ILE:O	43:1l:11:VAL:HG23	2.18	0.44
1:2A:141:A:C8	1:2A:1408:C:O2'	2.65	0.44
1:2A:176:G:O2'	1:2A:177:G:H5'	2.18	0.44
1:2A:885:C:H2'	1:2A:886:C:O4'	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1550:C:H5'	1:2A:1742:G:H22	1.82	0.44
1:2A:1932:A:H2'	1:2A:1933:G:O4'	2.18	0.44
6:2G:43:LEU:HD13	6:2G:43:LEU:HA	1.70	0.44
6:2G:171:ALA:O	6:2G:175:LEU:HG	2.18	0.44
9:2N:73:THR:HG22	9:2N:84:LYS:HG2	2.00	0.44
15:2T:8:LYS:HD3	15:2T:8:LYS:HA	1.86	0.44
22:20:50:ASN:HB3	22:20:63:VAL:HG22	1.99	0.44
32:2a:160:A:H2'	32:2a:161:A:O4'	2.18	0.44
32:2a:187:C:OP1	51:2t:82:SER:OG	2.28	0.44
32:2a:194:C:H2'	32:2a:195:A:H5"	1.99	0.44
32:2a:881:G:P	43:2l:12:ARG:HH22	2.41	0.44
32:2a:945:G:C2	32:2a:946:A:C8	3.06	0.44
32:2a:1280:A:O2'	32:2a:1281:U:H5'	2.18	0.44
32:2a:1333:A:H2'	32:2a:1334:G:O4'	2.18	0.44
32:2a:1349:A:H1'	32:2a:1374:A:N6	2.33	0.44
33:2b:90:MET:HE2	33:2b:91:PRO:HD3	2.00	0.44
36:2e:78:HIS:CE1	36:2e:143:ARG:H	2.36	0.44
50:2s:80:TYR:O	50:2s:81:ARG:HG2	2.18	0.44
56:2y:50:U:H2'	56:2y:51:U:H6	1.83	0.44
8:1I:72:LEU:HD21	8:1I:107:VAL:HG11	2.00	0.44
12:1Q:109:VAL:HG22	12:1Q:113:GLN:OE1	2.18	0.44
14:1S:48:LEU:HD23	14:1S:82:ILE:HD11	1.99	0.44
16:1U:27:LEU:HB3	16:1U:31:SER:HB3	2.00	0.44
32:1a:161:A:H2'	32:1a:162:A:C8	2.53	0.44
32:1a:189(D):C:H2'	32:1a:189(E):U:O4'	2.17	0.44
32:1a:1015:A:H2'	32:1a:1016:A:C8	2.53	0.44
32:1a:1261:A:H3'	32:1a:1262:C:H6	1.82	0.44
35:1d:173:TRP:CE3	35:1d:174:LEU:HG	2.53	0.44
36:1e:106:PRO:O	36:1e:110:LEU:HG	2.18	0.44
37:1f:62:TRP:CH2	37:1f:64:GLN:HB2	2.52	0.44
39:1h:49:GLU:HG2	39:1h:62:TYR:HE2	1.81	0.44
56:1y:56:C:H2'	56:1y:57:G:O4'	2.18	0.44
1:2A:1115:G:H2'	1:2A:1116:C:C6	2.53	0.44
1:2A:1415:U:O2'	1:2A:1417:C:OP1	2.30	0.44
1:2A:1514:U:H2'	1:2A:1515:G:H8	1.83	0.44
1:2A:2807:G:C2	1:2A:2808:U:H1'	2.53	0.44
1:2A:2888:C:H2'	1:2A:2889:C:H6	1.83	0.44
4:2E:197:ILE:HG22	4:2E:199:ARG:HG3	2.00	0.44
9:2N:71:ILE:HA	9:2N:86:PRO:HA	1.99	0.44
19:2X:8:ILE:O	24:22:36:ARG:NH2	2.50	0.44
21:2Z:124:ILE:HD11	21:2Z:165:VAL:HG21	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:23:39:ASP:OD1	25:23:44:ARG:NH1	2.46	0.44
32:2a:142:G:H2'	32:2a:143:A:H8	1.79	0.44
32:2a:628:G:H2'	32:2a:629:G:H8	1.83	0.44
32:2a:748:C:H4'	32:2a:749:C:O5'	2.18	0.44
32:2a:1146:A:H2'	32:2a:1147:C:O4'	2.17	0.44
33:2b:111:ARG:HH11	33:2b:111:ARG:HA	1.83	0.44
36:2e:33:VAL:HG13	36:2e:112:LEU:HD12	1.98	0.44
41:2j:8:LEU:HG	41:2j:96:ILE:HG23	1.99	0.44
41:2j:38:ILE:HD11	41:2j:71:LEU:HD23	2.00	0.44
54:2w:19:G:N2	54:2w:57:G:H1'	2.33	0.44
1:1A:79:G:OP1	61:1A:4241:HOH:O	2.21	0.43
1:1A:271(O):C:H2'	1:1A:271(P):C:C6	2.53	0.43
1:1A:484:C:H2'	1:1A:485:C:H6	1.83	0.43
1:1A:877:U:O2'	1:1A:900:A:N6	2.51	0.43
1:1A:1183:G:O2'	25:13:29:ARG:NH1	2.51	0.43
1:1A:1292:U:H2'	1:1A:1293:C:H6	1.83	0.43
1:1A:1478:G:O2'	1:1A:1558:A:N7	2.50	0.43
4:1E:47:VAL:HG11	4:1E:86:PRO:HD2	1.99	0.43
5:1F:136:THR:HA	5:1F:166:ALA:O	2.18	0.43
32:1a:769:G:H4'	32:1a:1513:A:H4'	1.99	0.43
32:1a:1291:G:O2'	40:1i:38:GLN:OE1	2.32	0.43
38:1g:78:ARG:HD2	38:1g:156:TRP:HE3	1.83	0.43
39:1h:81:HIS:ND1	39:1h:138:TRP:OXT	2.41	0.43
48:1q:22:LEU:HD13	48:1q:41:LYS:HG2	2.00	0.43
1:2A:373:U:H2'	1:2A:374:A:H8	1.83	0.43
1:2A:1266:G:O2'	1:2A:2012:G:O6	2.36	0.43
1:2A:1779:U:OP2	61:2A:3953:HOH:O	2.21	0.43
1:2A:2127:G:H22	1:2A:2160:G:H1	1.66	0.43
9:2N:61:ARG:HD3	9:2N:61:ARG:HA	1.65	0.43
9:2N:67:LEU:O	9:2N:88:GLU:HG3	2.18	0.43
32:2a:1203:C:H2'	32:2a:1204:A:O4'	2.18	0.43
39:2h:85:ARG:NH1	39:2h:87:SER:O	2.51	0.43
44:2m:108:ARG:HD3	44:2m:108:ARG:HA	1.55	0.43
47:2p:20:VAL:HG21	47:2p:32:TYR:CG	2.53	0.43
1:1A:2160:G:C6	1:1A:2161:C:N4	2.86	0.43
1:1A:2740:A:C6	1:1A:2764:A:C8	3.06	0.43
1:1A:2788:C:P	4:1E:61:ARG:HH21	2.41	0.43
2:1B:23:G:O6	61:1B:301:HOH:O	2.21	0.43
3:1D:69:ARG:C	3:1D:71:ASP:N	2.75	0.43
3:1D:70:TRP:HB3	3:1D:190:TYR:CE2	2.52	0.43
7:1H:101:ARG:NH2	7:1H:122:THR:HA	2.31	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:1N:61:ARG:HA	9:1N:61:ARG:HD3	1.80	0.43
32:1a:524:G:H2'	32:1a:525:C:C6	2.53	0.43
43:1l:39:VAL:HG11	43:1l:41:ARG:NH1	2.33	0.43
1:2A:816:C:OP2	61:2A:3955:HOH:O	2.21	0.43
1:2A:910:A:N1	1:2A:2277:G:H1'	2.32	0.43
1:2A:2079:U:O3'	23:21:35:THR:OG1	2.36	0.43
7:2H:121:ILE:HD11	7:2H:140:LYS:HG2	1.99	0.43
13:2R:38:VAL:HB	13:2R:39:PRO:HD3	2.00	0.43
32:2a:580:U:H2'	32:2a:581:G:O4'	2.18	0.43
32:2a:983:A:H3'	32:2a:983:A:N3	2.33	0.43
39:2h:97:VAL:HG21	39:2h:128:GLY:HA2	1.98	0.43
40:2i:9:ARG:HG2	40:2i:14:VAL:HG13	1.99	0.43
1:1A:71:A:OP2	61:1A:4237:HOH:O	2.20	0.43
1:1A:644:A:H4'	1:1A:645:C:H5	1.83	0.43
8:1I:26:ALA:O	8:1I:31:LEU:HB2	2.19	0.43
17:1V:55:ALA:CA	17:1V:101:GLY:HA2	2.41	0.43
32:1a:404:U:H2'	32:1a:405:U:C6	2.53	0.43
32:1a:443:C:H2'	32:1a:444:C:H6	1.83	0.43
32:1a:977:A:H1'	32:1a:982:U:O4	2.18	0.43
32:1a:1149:C:H2'	32:1a:1150:U:C6	2.53	0.43
43:1l:71:PRO:O	43:1l:102:ARG:NH1	2.51	0.43
47:1p:48:TRP:CE3	47:1p:49:LEU:HB2	2.53	0.43
48:1q:72:ARG:HE	48:1q:72:ARG:HB2	1.61	0.43
1:2A:2096:U:H2'	1:2A:2097:C:C6	2.54	0.43
2:2B:3:C:H2'	2:2B:4:C:C6	2.54	0.43
3:2D:158:ALA:O	3:2D:161:THR:OG1	2.31	0.43
4:2E:23:VAL:HA	4:2E:184:VAL:O	2.18	0.43
21:2Z:93:ASP:HB3	21:2Z:131:ARG:HH22	1.83	0.43
29:27:24:THR:O	29:27:28:ARG:HG3	2.18	0.43
32:2a:17:U:H2'	32:2a:18:C:C6	2.53	0.43
32:2a:149:A:H2'	32:2a:150:C:H6	1.82	0.43
33:2b:163:PHE:CD1	33:2b:185:ILE:HG13	2.53	0.43
33:2b:223:ILE:HG12	33:2b:223:ILE:H	1.62	0.43
1:1A:606:U:H4'	1:1A:658:C:H4'	2.00	0.43
3:1D:92:ILE:HD12	3:1D:104:TYR:CD1	2.54	0.43
6:1G:70:VAL:HG11	6:1G:87:PRO:HB3	2.00	0.43
7:1H:11:VAL:HG13	7:1H:15:VAL:HG22	2.00	0.43
13:1R:96:ARG:HD2	13:1R:115:GLU:OE2	2.18	0.43
32:1a:376:G:H5"	47:1p:5:ARG:HB3	1.99	0.43
32:1a:460:G:N2	32:1a:471:G:N7	2.66	0.43
32:1a:693:G:H2'	32:1a:694:A:C8	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:848:C:H2'	32:1a:849:C:H6	1.80	0.43
35:1d:52:SER:O	35:1d:56:VAL:HG13	2.19	0.43
1:2A:2506:U:C2	1:2A:2585:U:O4	2.71	0.43
6:2G:44:GLY:C	6:2G:46:ALA:N	2.76	0.43
21:2Z:153:SER:O	21:2Z:155:LEU:N	2.52	0.43
32:2a:779:C:H2'	32:2a:780:A:O4'	2.18	0.43
32:2a:971:G:H1'	32:2a:1365:G:O2'	2.19	0.43
35:2d:57:ARG:NE	35:2d:205:GLU:OE2	2.50	0.43
45:2n:57:ARG:HG2	45:2n:58:LYS:H	1.82	0.43
1:1A:603:A:N1	1:1A:625:G:O2'	2.52	0.43
1:1A:897:C:N3	1:1A:898:C:N4	2.67	0.43
7:1H:6:ARG:HH22	7:1H:54:ARG:NH2	2.17	0.43
12:1Q:89:ASN:HB2	55:1x:1:C:C4	2.53	0.43
15:1T:127:ALA:O	15:1T:128:GLU:HB3	2.17	0.43
21:1Z:40:ASP:OD2	21:1Z:42:VAL:HG12	2.18	0.43
21:1Z:53:ILE:HG22	21:1Z:71:VAL:HG12	1.99	0.43
26:14:58:ARG:O	26:14:61:ARG:HB3	2.18	0.43
32:1a:966:M2G:HM11	40:1i:127:LYS:HE2	2.00	0.43
33:1b:37:ASN:C	33:1b:39:ILE:H	2.27	0.43
40:1i:8:GLY:HA3	40:1i:76:ALA:O	2.18	0.43
56:1y:8:4SU:H4'	56:1y:48:C:H4'	2.00	0.43
1:2A:796:C:H2'	1:2A:797:C:C6	2.54	0.43
1:2A:1490:A:O2'	3:2D:99:ASP:OD1	2.36	0.43
1:2A:2685:G:P	15:2T:51:ARG:HH12	2.42	0.43
1:2A:2704:C:H2'	1:2A:2705:A:O4'	2.18	0.43
1:2A:2811:G:N2	1:2A:2891:G:H1'	2.33	0.43
3:2D:66:ASP:OD2	3:2D:103:ARG:NH1	2.51	0.43
8:2I:40:THR:OG1	8:2I:41:GLU:N	2.44	0.43
9:2N:68:GLU:H	9:2N:68:GLU:HG2	1.62	0.43
17:2V:40:LEU:HD11	17:2V:101:GLY:HA3	2.00	0.43
18:2W:14:PRO:O	18:2W:18:ARG:HG3	2.19	0.43
23:21:67:ILE:N	23:21:68:PRO:HD2	2.34	0.43
32:2a:1003:G:H2'	32:2a:1004:A:O4'	2.18	0.43
32:2a:1310:G:H1	32:2a:1327:C:H42	1.67	0.43
36:2e:110:LEU:HD13	36:2e:118:ILE:HD13	2.00	0.43
44:2m:57:ARG:HG2	44:2m:61:GLU:CD	2.44	0.43
54:2w:43:C:H2'	54:2w:44:G:C8	2.53	0.43
1:1A:444:C:H4'	5:1F:49:ALA:HB2	2.00	0.43
1:1A:1173:G:N1	1:1A:1176:G:OP2	2.45	0.43
1:1A:1508:A:O2'	1:1A:1509:C:OP1	2.31	0.43
1:1A:2181:G:O2'	1:1A:2182:G:OP1	2.31	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:1A:4778:HOH:O	5:1F:74:ARG:HD2	2.18	0.43
3:1D:24:ILE:HD13	3:1D:84:TYR:HB2	1.99	0.43
7:1H:13:LYS:HA	7:1H:14:GLY:HA2	1.58	0.43
10:1O:26:LYS:O	10:1O:30:ALA:HB2	2.18	0.43
32:1a:41:G:H2'	32:1a:42:G:C8	2.53	0.43
32:1a:453:A:C5	32:1a:454:C:C4	3.07	0.43
32:1a:953:G:H2'	32:1a:954:G:O4'	2.19	0.43
32:1a:1347:G:O2'	32:1a:1373:G:O6	2.33	0.43
33:1b:12:GLU:O	33:1b:15:VAL:HG22	2.17	0.43
40:1i:20:ARG:O	40:1i:60:ASP:N	2.36	0.43
46:1o:3:ILE:HG21	46:1o:34:LEU:HD21	1.99	0.43
56:1y:59:U:H3'	56:1y:60:U:H6	1.84	0.43
1:2A:947:G:H2'	1:2A:948:G:C8	2.53	0.43
1:2A:1300:U:H4'	1:2A:1301:A:H5"	2.01	0.43
1:2A:1451:C:H4'	1:2A:1452:A:C8	2.53	0.43
1:2A:2114:A:H2'	1:2A:2114:A:N3	2.34	0.43
1:2A:2359:C:H2'	1:2A:2360:A:O4'	2.18	0.43
1:2A:2784:C:H1'	4:2E:37:ARG:NH1	2.32	0.43
5:2F:21:ALA:CB	5:2F:22:ALA:HA	2.45	0.43
5:2F:129:PHE:CD2	5:2F:163:VAL:HG21	2.54	0.43
7:2H:13:LYS:HA	7:2H:14:GLY:HA2	1.59	0.43
8:2I:66:GLU:OE1	8:2I:69:LYS:HD2	2.18	0.43
11:2P:97:PRO:HD3	11:2P:126:VAL:O	2.18	0.43
32:2a:335:C:H2'	32:2a:336:C:H6	1.84	0.43
32:2a:1072:G:H2'	32:2a:1073:U:C6	2.53	0.43
32:2a:1431:C:H2'	32:2a:1432:G:O4'	2.18	0.43
32:2a:1510:U:H2'	32:2a:1511:G:C8	2.54	0.43
33:2b:150:SER:OG	33:2b:151:GLY:N	2.52	0.43
33:2b:187:LEU:HD23	33:2b:188:ALA:N	2.33	0.43
38:2g:74:GLU:HG2	38:2g:91:VAL:HG22	2.00	0.43
47:2p:28:ARG:NH1	47:2p:29:ASP:OD1	2.51	0.43
1:1A:97:C:OP1	24:12:2:LYS:HE2	2.19	0.43
1:1A:1290:C:H2'	1:1A:1291:C:C6	2.54	0.43
1:1A:2567:G:H2'	1:1A:2568:C:C6	2.54	0.43
3:1D:37:LEU:HD22	3:1D:87:ASN:ND2	2.34	0.43
6:1G:5:VAL:HG13	6:1G:8:LYS:HE2	2.01	0.43
8:1I:77:LEU:HD23	8:1I:77:LEU:HA	1.82	0.43
26:14:59:PHE:C	26:14:61:ARG:H	2.27	0.43
32:1a:600:C:H2'	32:1a:601:C:H6	1.84	0.43
32:1a:1261:A:H3'	32:1a:1262:C:C6	2.53	0.43
33:1b:15:VAL:HB	33:1b:209:ARG:HG3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1d:31:CYS:HB3	35:1d:34:GLU:HG3	2.01	0.43
35:1d:173:TRP:CD2	35:1d:189:PRO:HG3	2.53	0.43
36:1e:102:ALA:HB1	36:1e:106:PRO:HB2	2.00	0.43
36:1e:110:LEU:HD13	36:1e:118:ILE:HG21	2.00	0.43
42:1k:20:TYR:CE1	42:1k:83:ILE:HD12	2.53	0.43
46:1o:87:ILE:HG22	46:1o:88:ARG:N	2.33	0.43
1:2A:27:G:N2	1:2A:512:G:H1'	2.33	0.43
1:2A:566:U:P	17:2V:80:GLN:HE21	2.41	0.43
1:2A:1339:G:H5"	19:2X:16:LYS:HD3	2.00	0.43
1:2A:1430:C:H2'	1:2A:1431:U:C6	2.53	0.43
1:2A:1697:G:OP2	1:2A:1698:A:O2'	2.30	0.43
1:2A:2303:G:O2'	6:2G:132:ASN:HB2	2.18	0.43
1:2A:2391:G:O2'	1:2A:2422:A:N7	2.52	0.43
1:2A:2411:A:H2'	1:2A:2412:A:H8	1.84	0.43
1:2A:2650:U:H2'	1:2A:2651:C:C6	2.54	0.43
29:27:9:ARG:HG2	29:27:46:VAL:HG23	2.01	0.43
32:2a:176:C:H2'	32:2a:177:C:C6	2.54	0.43
32:2a:947:G:H1	32:2a:1234:C:N4	2.15	0.43
32:2a:1320:C:H2'	32:2a:1321:C:O4'	2.18	0.43
32:2a:1381:U:H2'	32:2a:1382:C:H6	1.82	0.43
34:2c:134:ILE:HD11	34:2c:153:VAL:HG23	2.00	0.43
35:2d:57:ARG:HB3	35:2d:206:PHE:HB2	2.00	0.43
37:2f:95:GLU:O	49:2r:32:ARG:NH1	2.52	0.43
44:2m:49:THR:OG1	44:2m:52:GLU:HG3	2.18	0.43
48:2q:40:LYS:HD3	48:2q:42:TYR:CZ	2.53	0.43
54:2w:64:A:C2'	54:2w:65:G:H5'	2.48	0.43
1:1A:625:G:N7	11:1P:107:LYS:NZ	2.65	0.43
1:1A:1179:C:H2'	1:1A:1180:C:H6	1.84	0.43
2:1B:24:G:N7	2:1B:56:G:H2'	2.34	0.43
6:1G:60:LEU:HD12	6:1G:60:LEU:HA	1.80	0.43
6:1G:165:THR:OG1	6:1G:168:GLU:HG3	2.19	0.43
22:10:70:GLN:HB3	22:10:80:HIS:HE2	1.83	0.43
28:16:6:ARG:NH1	28:16:26:ASN:HB2	2.34	0.43
30:18:62:LEU:HB3	30:18:65:GLU:HG2	2.00	0.43
32:1a:345:C:H5'	32:1a:346:G:C5	2.53	0.43
32:1a:1326:C:OP1	52:1u:12:LYS:NZ	2.34	0.43
32:1a:1353:G:OP1	52:1u:10:ARG:NH1	2.52	0.43
33:1b:24:TRP:CD1	33:1b:24:TRP:H	2.37	0.43
36:1e:12:LEU:HB3	36:1e:31:LEU:HB2	2.01	0.43
36:1e:33:VAL:HG13	36:1e:112:LEU:HD12	2.01	0.43
1:2A:252:G:OP1	11:2P:50:ARG:NH1	2.39	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:813:U:H2'	1:2A:814:C:C6	2.53	0.43
1:2A:858:U:O2	1:2A:2268:A:H2'	2.18	0.43
1:2A:1239:G:H2'	1:2A:1240:U:O4'	2.19	0.43
1:2A:1283:G:N2	1:2A:1286:A:OP2	2.49	0.43
1:2A:2512:C:H2'	1:2A:2513:G:O4'	2.19	0.43
32:2a:352:C:O2'	32:2a:354:G:OP1	2.29	0.43
32:2a:362:G:N1	32:2a:365:U:OP2	2.52	0.43
32:2a:1299:A:H2'	32:2a:1299:A:N3	2.32	0.43
39:2h:20:TYR:HA	39:2h:65:TYR:CZ	2.54	0.43
40:2i:24:GLY:N	40:2i:60:ASP:OD1	2.51	0.43
41:2j:46:ARG:HG2	41:2j:64:GLU:HB3	2.00	0.43
44:2m:29:ARG:HD3	44:2m:64:TRP:CE2	2.54	0.43
44:2m:96:LEU:C	44:2m:110:ARG:HG2	2.44	0.43
54:2w:51:U:H2'	54:2w:52:G:H8	1.84	0.43
55:2x:53:G:H2'	55:2x:54:5MU:C6	2.53	0.43
1:1A:286:C:H2'	1:1A:287:C:H6	1.84	0.43
1:1A:1394:U:H2'	1:1A:1395:A:O4'	2.18	0.43
1:1A:1686:C:H2'	1:1A:1687:G:O4'	2.19	0.43
1:1A:2331:G:O2'	22:10:43:THR:HG22	2.19	0.43
1:1A:2749:A:OP1	7:1H:3:ARG:NH1	2.51	0.43
1:1A:2801(A):A:H1'	1:1A:2895:U:H1'	2.00	0.43
2:1B:48:A:H2'	2:1B:49:C:C6	2.54	0.43
6:1G:53:LEU:HD11	6:1G:87:PRO:HB2	2.01	0.43
7:1H:164:TYR:HB2	7:1H:167:GLU:HB2	2.00	0.43
12:1Q:136:ALA:HB1	21:1Z:52:SER:HB2	2.01	0.43
29:17:9:ARG:CZ	29:17:47:ARG:HG3	2.48	0.43
32:1a:266:G:N3	32:1a:266:G:H5"	2.34	0.43
32:1a:434:U:H2'	32:1a:435:C:C6	2.53	0.43
32:1a:502:G:H2'	32:1a:503:C:O4'	2.19	0.43
32:1a:507:C:OP2	32:1a:508:C:O2'	2.26	0.43
32:1a:857:C:H2'	32:1a:858:G:O4'	2.18	0.43
32:1a:1036:G:H3'	32:1a:1037:C:H6	1.83	0.43
32:1a:1118:C:P	40:1i:104:ARG:HH11	2.41	0.43
32:1a:1241:G:H2'	32:1a:1242:C:C6	2.54	0.43
33:1b:201:ILE:HG21	33:1b:214:ILE:HG21	2.00	0.43
34:1c:22:TRP:CE2	34:1c:59:ARG:HD2	2.54	0.43
35:1d:39:PRO:O	35:1d:44:GLY:HA3	2.19	0.43
36:1e:78:HIS:CD2	39:1h:104:ARG:HD2	2.54	0.43
42:1k:59:TYR:CZ	42:1k:63:LEU:HD11	2.54	0.43
47:1p:72:ARG:HD2	47:1p:73:LEU:HD23	2.01	0.43
56:1y:24:G:H2'	56:1y:25:C:O4'	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:271(M):G:H21	8:2I:50:ARG:HD2	1.83	0.43
1:2A:345:A:N3	1:2A:346:A:N6	2.66	0.43
1:2A:652(C):G:H2'	1:2A:652(D):C:C6	2.54	0.43
1:2A:1814:G:H4'	3:2D:51:VAL:HG21	2.01	0.43
3:2D:218:ARG:HB3	3:2D:219:PRO:HD2	2.00	0.43
6:2G:77:ILE:HG22	6:2G:80:PHE:H	1.83	0.43
8:2I:57:ARG:HB2	8:2I:61:ARG:HH21	1.83	0.43
11:2P:38:GLN:O	11:2P:40:SER:N	2.46	0.43
23:21:3:LYS:HB3	23:21:4:VAL:H	1.63	0.43
32:2a:201:C:H5'	32:2a:202:U:OP2	2.19	0.43
41:2j:16:LEU:HD12	41:2j:16:LEU:HA	1.64	0.43
49:2r:73:ALA:HA	49:2r:76:LEU:HD12	2.00	0.43
1:1A:196:A:O2'	1:1A:805:G:O6	2.31	0.43
1:1A:284:U:H2'	1:1A:285:C:C6	2.54	0.43
1:1A:813:U:H2'	1:1A:814:C:C6	2.54	0.43
1:1A:1069:A:H1'	1:1A:1096:A:H4'	2.01	0.43
1:1A:2667:C:H1'	7:1H:109:PHE:CD1	2.54	0.43
1:1A:2722:G:OP2	61:1A:4242:HOH:O	2.21	0.43
4:1E:46:ALA:HB2	4:1E:82:ARG:HA	2.01	0.43
15:1T:33:LYS:HA	15:1T:42:ILE:HD13	2.01	0.43
32:1a:922:G:C6	32:1a:923:A:C6	3.07	0.43
32:1a:1302:U:C6	44:1m:17:VAL:HG11	2.53	0.43
39:1h:10:LEU:HD22	39:1h:83:ILE:HD11	2.01	0.43
41:1j:55:LYS:HE3	41:1j:55:LYS:HB3	1.87	0.43
50:1s:41:VAL:HG13	50:1s:43:GLU:OE1	2.18	0.43
56:1y:71:G:H2'	56:1y:72:C:C6	2.53	0.43
1:2A:314:A:H2'	1:2A:315:G:C8	2.54	0.43
1:2A:688:U:O4	61:2A:3956:HOH:O	2.21	0.43
4:2E:97:LYS:N	4:2E:100:GLU:OE2	2.39	0.43
5:2F:23:ASP:O	5:2F:24:LEU:HD12	2.18	0.43
6:2G:68:PRO:HB2	6:2G:90:LEU:HD22	2.01	0.43
9:2N:111:PRO:HA	9:2N:114:ARG:NH1	2.34	0.43
20:2Y:55:TYR:N	20:2Y:56:PRO:HD3	2.34	0.43
26:24:47:GLN:O	26:24:48:ARG:C	2.62	0.43
32:2a:583:A:H2'	32:2a:584:G:O4'	2.19	0.43
32:2a:1128:C:H4'	32:2a:1129:C:OP1	2.19	0.43
32:2a:1327:C:OP2	52:2u:12:LYS:NZ	2.52	0.43
32:2a:1330:U:H4'	44:2m:23:TYR:CE1	2.53	0.43
36:2e:60:TYR:OH	36:2e:64:ARG:NH1	2.52	0.43
38:2g:29:LYS:HB2	38:2g:105:VAL:HG21	2.01	0.43
42:2k:18:ARG:O	42:2k:32:ILE:HA	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:2t:67:ALA:HA	51:2t:72:LEU:HB3	2.01	0.43
1:1A:634:C:H2'	1:1A:635:C:C6	2.54	0.42
1:1A:784:A:C6	3:1D:229:VAL:HG11	2.53	0.42
1:1A:2113:U:H2'	1:1A:2114:A:H5'	2.01	0.42
26:14:54:GLY:N	26:14:55:ARG:HA	2.34	0.42
32:1a:157:G:H1	32:1a:164:U:H3	1.66	0.42
32:1a:1125:U:H4'	41:1j:5:ARG:NH2	2.34	0.42
33:1b:84:GLU:OE1	33:1b:216:SER:HA	2.19	0.42
34:1c:22:TRP:CZ2	45:1n:54:PRO:HG2	2.54	0.42
40:1i:26:VAL:HB	40:1i:33:PHE:HB2	2.01	0.42
44:1m:11:ARG:H	44:1m:11:ARG:HG2	1.66	0.42
51:1t:10:LEU:HD22	51:1t:10:LEU:HA	1.78	0.42
1:2A:604:G:OP2	11:2P:90:ARG:NH1	2.52	0.42
1:2A:1012:U:C5	9:2N:28:THR:HG21	2.54	0.42
1:2A:2116:G:N1	1:2A:2162:G:OP1	2.52	0.42
1:2A:2329:G:H2'	1:2A:2330:G:C8	2.54	0.42
1:2A:2547:U:O2	10:2O:23:ARG:NH2	2.52	0.42
1:2A:2774:C:H2'	1:2A:2775:A:O4'	2.18	0.42
3:2D:70:TRP:CE2	3:2D:150:LYS:HD3	2.54	0.42
7:2H:46:GLU:N	7:2H:49:VAL:O	2.51	0.42
32:2a:1133:G:H1	32:2a:1141:C:H42	1.66	0.42
32:2a:1326:C:OP1	52:2u:12:LYS:NZ	2.51	0.42
32:2a:1466:C:H2'	32:2a:1467:G:O4'	2.18	0.42
33:2b:101:MET:HA	33:2b:108:ILE:HD12	2.01	0.42
40:2i:5:TYR:N	40:2i:87:GLN:OE1	2.32	0.42
1:1A:17:G:H2'	1:1A:18:C:C6	2.54	0.42
1:1A:143:G:H2'	1:1A:143(A):C:C6	2.54	0.42
1:1A:271(L):U:O2'	1:1A:271(M):G:OP2	2.31	0.42
1:1A:271(T):C:H2'	1:1A:271(U):G:C8	2.53	0.42
1:1A:329:G:OP2	20:1Y:71:LYS:HD2	2.19	0.42
1:1A:385:C:O2	11:1P:71:VAL:HG21	2.18	0.42
1:1A:2327:A:H2'	1:1A:2328:A:C8	2.53	0.42
1:1A:2616:C:O2	61:1A:4230:HOH:O	2.18	0.42
1:1A:2811:G:N2	1:1A:2891:G:H1'	2.34	0.42
2:1B:42:C:O2'	6:1G:66:GLN:HG2	2.18	0.42
8:1I:42:SER:O	8:1I:45:LYS:HG2	2.18	0.42
10:1O:4:PRO:HA	10:1O:21:CYS:O	2.19	0.42
1:2A:271(M):G:N2	8:2I:50:ARG:HD2	2.34	0.42
1:2A:336:C:O2'	20:2Y:35:TYR:OH	2.35	0.42
1:2A:577:G:C6	1:2A:578:A:C6	3.08	0.42
1:2A:859:G:O2'	1:2A:916:G:O6	2.35	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1289:C:H2'	1:2A:1290:C:H6	1.83	0.42
1:2A:1810:A:H2'	1:2A:1811:G:O4'	2.19	0.42
1:2A:1812:A:O2'	3:2D:45:ASN:N	2.49	0.42
1:2A:2745:C:C4	1:2A:2746:U:C4	3.08	0.42
2:2B:8:U:H3	2:2B:113:G:H1	1.67	0.42
4:2E:120:TRP:CG	4:2E:155:LYS:HB3	2.54	0.42
9:2N:15:LEU:N	9:2N:136:GLU:O	2.43	0.42
12:2Q:75:THR:HG21	12:2Q:87:LYS:NZ	2.33	0.42
14:2S:5:THR:OG1	14:2S:8:GLU:HG3	2.19	0.42
26:24:68:ARG:HA	26:24:68:ARG:CZ	2.49	0.42
32:2a:1133:G:C4	32:2a:1134:G:C8	3.07	0.42
32:2a:1169:A:C6	32:2a:1170:A:C6	3.07	0.42
44:2m:33:ALA:HA	44:2m:59:TYR:CE2	2.54	0.42
1:1A:271(F):C:H2'	1:1A:271(G):C:C6	2.54	0.42
1:1A:278:A:P	1:1A:278:A:H8	2.41	0.42
1:1A:2153:G:H2'	1:1A:2154:G:H8	1.85	0.42
1:1A:2361:A:H5'	30:18:27:THR:OG1	2.19	0.42
8:1I:76:THR:HG22	8:1I:141:LYS:HE2	2.00	0.42
8:1I:109:ILE:HD12	8:1I:130:TYR:CE2	2.54	0.42
9:1N:21:LYS:NZ	9:1N:140:VAL:HG23	2.35	0.42
23:11:7:ILE:HG23	23:11:98:LEU:HD11	2.00	0.42
32:1a:192:U:H2'	32:1a:193:C:C6	2.55	0.42
32:1a:515:G:H2'	32:1a:516:PSU:O4'	2.18	0.42
32:1a:1348:U:H4'	40:1i:120:ARG:HD2	2.01	0.42
41:1j:75:ILE:O	41:1j:77:PRO:HD3	2.19	0.42
43:1l:56:ALA:HB2	43:1l:70:ILE:HD11	2.01	0.42
54:1w:8:4SU:H4'	54:1w:48:C:H4'	2.00	0.42
56:1y:71:G:H2'	56:1y:72:C:H6	1.84	0.42
1:2A:567:A:OP2	11:2P:29:LYS:NZ	2.44	0.42
1:2A:2632:A:O2'	1:2A:2811:G:O2'	2.14	0.42
2:2B:52:A:N6	14:2S:33:LYS:HG2	2.33	0.42
7:2H:138:LYS:HA	7:2H:141:VAL:HB	2.01	0.42
9:2N:99:LEU:O	9:2N:103:VAL:HG23	2.19	0.42
12:2Q:78:PRO:HD3	55:2x:1:C:N3	2.34	0.42
21:2Z:104:PHE:HA	21:2Z:139:VAL:HB	2.00	0.42
21:2Z:171:ILE:HD12	21:2Z:172:ALA:H	1.84	0.42
24:22:11:GLU:O	24:22:15:LYS:HG2	2.19	0.42
32:2a:562:C:H4'	32:2a:563:A:O5'	2.19	0.42
32:2a:976:G:C8	32:2a:1358:U:C2	3.08	0.42
32:2a:1106:G:H2'	32:2a:1107:C:C6	2.54	0.42
35:2d:94:LEU:HD12	35:2d:94:LEU:HA	1.87	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:2l:85:ILE:O	43:2l:85:ILE:HG13	2.19	0.42
44:2m:15:VAL:HG23	44:2m:43:THR:O	2.20	0.42
1:1A:270:A:H1'	1:1A:370:G:C2	2.54	0.42
1:1A:997:G:OP1	16:1U:92:ARG:HD2	2.19	0.42
1:1A:1176:G:N2	1:1A:1178:C:O5'	2.49	0.42
1:1A:1430:C:H2'	1:1A:1431:U:C6	2.54	0.42
1:1A:2206:G:H3'	1:1A:2207:G:H8	1.78	0.42
2:1B:73:A:N1	21:1Z:34:ASN:ND2	2.68	0.42
12:1Q:103:MET:HE1	12:1Q:125:LEU:HD13	2.00	0.42
32:1a:31:G:O2'	32:1a:48:C:N4	2.53	0.42
32:1a:341:C:H2'	32:1a:342:C:C6	2.54	0.42
33:1b:16:HIS:HB3	33:1b:210:SER:HB2	2.02	0.42
33:1b:140:HIS:O	33:1b:144:ARG:HG3	2.19	0.42
36:1e:28:PHE:O	36:1e:47:LYS:HA	2.20	0.42
1:2A:271(L):U:H5'	8:2I:50:ARG:NH1	2.34	0.42
1:2A:536:A:H2'	1:2A:537:C:C6	2.55	0.42
1:2A:581:C:H2'	1:2A:582:G:C8	2.54	0.42
1:2A:2142:C:H2'	1:2A:2143:C:C6	2.54	0.42
3:2D:125:ILE:HB	37:2f:81:ILE:HD11	2.01	0.42
5:2F:24:LEU:HD21	5:2F:114:VAL:HG12	2.00	0.42
19:2X:1:MET:N	24:22:29:LYS:HE3	2.34	0.42
21:2Z:27:VAL:HG12	21:2Z:85:HIS:CE1	2.55	0.42
32:2a:384:G:H2'	32:2a:385:C:C6	2.54	0.42
32:2a:523:A:N1	43:2l:92:0TD:H6	2.35	0.42
32:2a:719:C:N4	49:2r:71:LYS:HE2	2.34	0.42
32:2a:974:A:OP2	45:2n:29:ARG:NH2	2.40	0.42
32:2a:1148:U:O3'	40:2i:14:VAL:HG11	2.19	0.42
35:2d:22:LYS:O	35:2d:113:SER:HB3	2.19	0.42
1:1A:26:G:C6	1:1A:27:G:N1	2.87	0.42
1:1A:272(J):C:H2'	1:1A:274:G:H8	1.84	0.42
1:1A:880:G:H2'	1:1A:881:G:C8	2.54	0.42
1:1A:1028:A:N6	1:1A:1125:G:H2'	2.34	0.42
1:1A:1313:U:H2'	1:1A:1610:A:C2	2.55	0.42
3:1D:232:PRO:HB3	3:1D:244:ARG:CZ	2.49	0.42
6:1G:124:SER:HB2	6:1G:131:TYR:CE1	2.54	0.42
11:1P:89:ALA:HA	11:1P:121:LYS:HD3	2.00	0.42
13:1R:36:THR:HG22	13:1R:37:THR:H	1.85	0.42
26:14:49:PHE:HB3	26:14:50:VAL:H	1.49	0.42
32:1a:1346:A:N1	32:1a:1374:A:H5"	2.35	0.42
33:1b:12:GLU:HB2	33:1b:213:LEU:CD2	2.50	0.42
36:1e:12:LEU:HD23	36:1e:13:ILE:N	2.35	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:1f:76:ALA:O	37:1f:80:ARG:HG3	2.20	0.42
37:1f:100:ASN:HD21	49:1r:23:LYS:HE3	1.85	0.42
39:1h:51:VAL:HG21	39:1h:60:ARG:HB2	2.02	0.42
1:2A:271(P):C:O3'	8:2I:42:SER:OG	2.32	0.42
1:2A:2097:C:H2'	1:2A:2098:U:O4'	2.20	0.42
1:2A:2543:G:H2'	1:2A:2544:G:C8	2.55	0.42
12:2Q:39:PRO:HA	12:2Q:97:VAL:O	2.20	0.42
32:2a:662:G:H2'	32:2a:663:A:C8	2.55	0.42
32:2a:1376:U:H2'	32:2a:1377:A:C8	2.54	0.42
34:2c:3:ASN:N	34:2c:3:ASN:OD1	2.51	0.42
34:2c:131:ARG:NE	34:2c:135:LYS:HE3	2.35	0.42
35:2d:174:LEU:HD23	35:2d:185:PHE:HA	2.02	0.42
37:2f:2:ARG:NE	37:2f:69:GLU:HG2	2.34	0.42
40:2i:45:ALA:O	40:2i:48:GLU:HB2	2.19	0.42
49:2r:44:LEU:HD11	49:2r:79:LEU:HD22	2.02	0.42
55:2x:61:C:H2'	55:2x:62:C:C6	2.55	0.42
1:1A:2110:G:OP1	1:1A:2118:U:N3	2.51	0.42
1:1A:2892:A:N6	1:1A:2893:G:C6	2.87	0.42
3:1D:70:TRP:HB3	3:1D:190:TYR:CZ	2.54	0.42
7:1H:97:ARG:NE	7:1H:104:GLU:OE1	2.51	0.42
14:1S:3:ARG:HD2	14:1S:4:LEU:O	2.20	0.42
20:1Y:95:LYS:HB3	20:1Y:95:LYS:HE2	1.77	0.42
32:1a:381:C:H2'	32:1a:382:A:O4'	2.19	0.42
32:1a:541:G:HO2'	35:1d:42:GLN:H	1.66	0.42
32:1a:685:G:O2'	32:1a:686:U:H5'	2.19	0.42
32:1a:1053:G:N7	32:1a:1199:U:H3'	2.34	0.42
50:1s:32:LYS:HE2	50:1s:32:LYS:HB3	1.71	0.42
1:2A:306:U:H2'	1:2A:307:G:O4'	2.20	0.42
1:2A:1891:G:O6	61:2A:3936:HOH:O	2.17	0.42
13:2R:97:VAL:CG2	13:2R:114:VAL:HG13	2.49	0.42
14:2S:93:LYS:HG2	14:2S:95:HIS:HB2	2.01	0.42
32:2a:519:C:H2'	32:2a:520:A:O4'	2.19	0.42
32:2a:555:C:H2'	32:2a:556:C:C6	2.55	0.42
32:2a:1226:C:H4'	32:2a:1227:A:OP1	2.19	0.42
34:2c:23:TYR:CG	34:2c:24:ALA:N	2.87	0.42
41:2j:17:ASP:OD1	41:2j:17:ASP:N	2.53	0.42
44:2m:13:LYS:NZ	44:2m:21:TYR:OH	2.53	0.42
52:2u:6:ARG:C	52:2u:8:THR:H	2.27	0.42
1:1A:1486:A:H2'	1:1A:1487:G:H8	1.84	0.42
1:1A:2712:U:O2'	1:1A:2713:A:H5'	2.20	0.42
6:1G:106:LEU:O	6:1G:111:LEU:HG	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1I:77:LEU:HB3	8:1I:142:VAL:HG12	2.02	0.42
21:1Z:52:SER:C	21:1Z:54:HIS:N	2.72	0.42
21:1Z:157:LEU:HG	21:1Z:161:VAL:HG23	2.00	0.42
32:1a:792:A:H4'	32:1a:793:U:O5'	2.19	0.42
32:1a:1072:G:H2'	32:1a:1073:U:C6	2.54	0.42
32:1a:1260:C:O5'	32:1a:1284:C:H4'	2.19	0.42
32:1a:1269:A:H2	32:1a:1312:G:N3	2.17	0.42
32:1a:1478:C:H2'	32:1a:1479:C:C6	2.54	0.42
33:1b:16:HIS:C	33:1b:18:GLY:H	2.27	0.42
36:1e:50:GLU:HB2	36:1e:53:LEU:HD13	2.01	0.42
40:1i:32:ASP:OD1	40:1i:33:PHE:N	2.52	0.42
42:1k:81:ASP:OD1	42:1k:107:SER:HB3	2.20	0.42
46:1o:10:LYS:HE3	46:1o:10:LYS:HB2	1.64	0.42
56:1y:55:PSU:N3	56:1y:57:G:H5'	2.35	0.42
1:2A:35:G:H2'	1:2A:36:G:O4'	2.19	0.42
1:2A:818:G:OP2	61:2A:3951:HOH:O	2.22	0.42
1:2A:1129:A:N1	1:2A:2569:G:O2'	2.50	0.42
1:2A:1297:C:H2'	1:2A:1298:C:H6	1.84	0.42
1:2A:1580:A:H3'	1:2A:1581:G:C8	2.52	0.42
3:2D:147:LEU:HD22	3:2D:155:LEU:HD21	2.01	0.42
18:2W:88:ARG:HA	18:2W:88:ARG:HD2	1.84	0.42
32:2a:174:C:H2'	32:2a:175:C:H6	1.85	0.42
33:2b:16:HIS:HB3	33:2b:210:SER:HB2	2.02	0.42
1:1A:1338:G:N7	19:1X:62:LYS:NZ	2.58	0.42
1:1A:1417:C:H3'	61:1A:4376:HOH:O	2.19	0.42
1:1A:1586:A:H8	1:1A:1586:A:O5'	2.02	0.42
32:1a:342:C:H2'	32:1a:343:U:O4'	2.20	0.42
32:1a:1511:G:H2'	32:1a:1512:U:O4'	2.20	0.42
33:1b:118:LEU:HB3	33:1b:142:LEU:HD12	2.02	0.42
34:1c:130:VAL:HG11	34:1c:153:VAL:HG11	2.02	0.42
37:1f:91:VAL:HG11	49:1r:72:ARG:NH1	2.35	0.42
40:1i:31:GLN:HE21	40:1i:31:GLN:HB3	1.65	0.42
41:1j:11:PHE:HB3	45:1n:55:GLY:HA3	2.02	0.42
41:1j:38:ILE:HG13	41:1j:71:LEU:HB3	2.02	0.42
42:1k:51:LYS:HA	42:1k:51:LYS:HD3	1.77	0.42
1:2A:534:U:H2'	1:2A:535:C:C6	2.55	0.42
1:2A:700:G:O2'	1:2A:1632:A:N3	2.38	0.42
1:2A:2029:G:H2'	1:2A:2031:A:OP1	2.20	0.42
1:2A:2251:OMG:HM23	1:2A:2251:OMG:H1'	1.88	0.42
3:2D:121:PRO:HB3	3:2D:135:PHE:CE2	2.55	0.42
4:2E:7:VAL:HG23	4:2E:51:PHE:CE2	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2F:64:ILE:HG21	5:2F:78:ILE:HG23	2.02	0.42
8:2I:82:ARG:O	8:2I:88:ILE:HG23	2.20	0.42
9:2N:71:ILE:HG21	9:2N:84:LYS:HB3	2.02	0.42
13:2R:8:ARG:O	13:2R:17:ARG:HD2	2.20	0.42
32:2a:309:G:H1'	32:2a:608:A:C2	2.55	0.42
32:2a:1087:G:N2	32:2a:1099:G:H1'	2.34	0.42
36:2e:10:MET:H	36:2e:10:MET:HG2	1.73	0.42
39:2h:33:GLU:CD	39:2h:50:ARG:HE	2.28	0.42
44:2m:37:THR:O	44:2m:55:ARG:NH1	2.39	0.42
56:2y:63:G:H2'	56:2y:64:A:C8	2.54	0.42
1:1A:1044:G:H5'	1:1A:1045:A:OP2	2.19	0.42
1:1A:1053:C:H42	1:1A:1106:G:H1	1.68	0.42
1:1A:1054:A:C6	1:1A:1055:G:C6	3.08	0.42
1:1A:2143:C:H2'	1:1A:2144:U:O4'	2.19	0.42
1:1A:2667:C:H1'	7:1H:109:PHE:HD1	1.84	0.42
2:1B:66:A:H61	2:1B:109:C:H5'	1.85	0.42
4:1E:50:GLY:HA3	4:1E:75:VAL:HG21	2.02	0.42
10:1O:107:ARG:NH2	32:1a:346:G:OP2	2.53	0.42
12:1Q:37:LEU:HD21	12:1Q:130:LYS:HE2	2.02	0.42
12:1Q:56:ARG:NH2	12:1Q:59:ARG:HH21	2.11	0.42
15:1T:127:ALA:O	15:1T:129:ARG:N	2.53	0.42
21:1Z:79:ARG:HD2	21:1Z:80:ARG:HH12	1.84	0.42
32:1a:352:C:H4'	32:1a:354:G:OP1	2.19	0.42
32:1a:390:C:O3'	47:1p:28:ARG:NH1	2.50	0.42
32:1a:1284:C:H3'	32:1a:1285:A:H8	1.85	0.42
32:1a:1324:A:O4'	32:1a:1362:C:H4'	2.20	0.42
32:1a:1525:G:P	42:1k:120:ARG:HH22	2.42	0.42
42:1k:95:ILE:H	42:1k:95:ILE:HG13	1.64	0.42
43:1l:7:ILE:HD13	43:1l:7:ILE:HA	1.93	0.42
1:2A:108:U:H2'	1:2A:109:G:C8	2.55	0.42
1:2A:827:U:O2'	1:2A:2068:U:C2	2.68	0.42
1:2A:2006:C:O2'	1:2A:2823:A:N3	2.48	0.42
25:23:4:LEU:O	25:23:36:VAL:HA	2.20	0.42
26:24:59:PHE:CD2	50:2s:64:GLU:HG2	2.54	0.42
29:27:8:ASN:HB3	29:27:11:LYS:HB3	2.02	0.42
31:29:22:ARG:HB2	31:29:24:TYR:CE2	2.55	0.42
32:2a:661:G:H1	32:2a:744:C:H42	1.68	0.42
32:2a:1002:G:OP1	32:2a:1002:G:H4'	2.18	0.42
32:2a:1005:A:OP2	32:2a:1024:G:N2	2.53	0.42
32:2a:1225:A:H2'	32:2a:1226:C:C5	2.55	0.42
33:2b:69:LEU:HD22	33:2b:155:LEU:HD11	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:2y:36:A:H2'	56:2y:37:MIA:O4'	2.18	0.42
1:1A:616:G:H2'	1:1A:618:C:O4'	2.20	0.42
1:1A:1039:G:H1	1:1A:1116:C:H42	1.68	0.42
1:1A:1050:A:H2'	1:1A:1051:G:O4'	2.20	0.42
1:1A:1932:A:H2'	1:1A:1933:G:O4'	2.20	0.42
1:1A:2102:U:H3	1:1A:2187:G:H1	1.68	0.42
8:1I:125:GLU:OE2	8:1I:143:SER:HB2	2.20	0.42
16:1U:93:LYS:HE2	61:1U:303:HOH:O	2.19	0.42
25:13:43:ILE:O	25:13:47:VAL:HG23	2.20	0.42
32:1a:396:G:O2'	32:1a:398:C:OP1	2.25	0.42
32:1a:872:A:H4'	32:1a:873:A:OP1	2.19	0.42
32:1a:1315:U:H2'	32:1a:1316:G:O4'	2.20	0.42
40:1i:15:ALA:HA	40:1i:65:VAL:HG12	2.01	0.42
40:1i:17:VAL:HG11	40:1i:80:GLY:C	2.44	0.42
46:1o:87:ILE:O	46:1o:88:ARG:HB2	2.19	0.42
56:1y:40:C:H2'	56:1y:41:C:C6	2.55	0.42
1:2A:582:G:H2'	1:2A:583:G:C8	2.54	0.42
1:2A:586:A:N1	1:2A:809:G:O2'	2.47	0.42
1:2A:795:C:H2'	1:2A:796:C:C6	2.55	0.42
1:2A:1027:A:C6	1:2A:1126:A:C4	3.08	0.42
1:2A:1187:G:H5'	17:2V:81:TYR:CE1	2.55	0.42
1:2A:2469:A:H5"	1:2A:2470:G:OP2	2.20	0.42
1:2A:2576:G:H5'	1:2A:2578:G:N7	2.34	0.42
3:2D:232:PRO:HB3	3:2D:244:ARG:CZ	2.50	0.42
8:2I:133:HIS:CD2	8:2I:134:PRO:HD2	2.53	0.42
12:2Q:3:MET:HE3	12:2Q:3:MET:HB2	1.91	0.42
12:2Q:65:PHE:HB2	12:2Q:105:GLU:HB2	2.02	0.42
21:2Z:3:TYR:O	21:2Z:58:VAL:HG23	2.20	0.42
32:2a:857:C:H2'	32:2a:858:G:O4'	2.20	0.42
32:2a:920:U:H2'	32:2a:921:U:H6	1.82	0.42
32:2a:1265:G:C4	32:2a:1271:G:N2	2.88	0.42
33:2b:16:HIS:HB2	33:2b:204:ASN:CB	2.49	0.42
40:2i:17:VAL:HG11	40:2i:81:ILE:HA	2.02	0.42
1:1A:657:U:H2'	1:1A:658:C:H6	1.85	0.41
1:1A:1243:G:O2'	11:1P:7:ARG:NH2	2.51	0.41
1:1A:1587:A:H2'	1:1A:1588:C:C6	2.55	0.41
1:1A:2572:A:C8	4:1E:144:ARG:HD3	2.54	0.41
1:1A:2649:U:H2'	1:1A:2650:U:C6	2.54	0.41
24:12:52:ASP:O	24:12:56:GLN:HG3	2.20	0.41
26:14:61:ARG:O	26:14:62:ARG:C	2.63	0.41
30:18:26:LYS:HD2	30:18:48:PHE:CD2	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:234:C:H5"	48:1q:70:ARG:HH21	1.85	0.41
32:1a:881:G:P	43:1l:12:ARG:HH22	2.43	0.41
32:1a:1176:A:H2'	32:1a:1177:G:C8	2.55	0.41
32:1a:1352:C:OP1	52:1u:3:LYS:NZ	2.44	0.41
33:1b:211:ILE:O	33:1b:215:LEU:HB2	2.20	0.41
36:1e:51:VAL:O	36:1e:55:VAL:HG23	2.19	0.41
38:1g:113:GLU:CG	38:1g:119:ARG:HG2	2.50	0.41
42:1k:44:SER:OG	42:1k:47:VAL:HG23	2.20	0.41
51:1t:100:ILE:HB	51:1t:101:GLY:H	1.65	0.41
54:1w:5:G:H2'	54:1w:6:G:C8	2.55	0.41
1:2A:820:A:H1'	1:2A:943:U:H1'	2.02	0.41
1:2A:1171:G:H1	1:2A:1178:C:H42	1.68	0.41
1:2A:1557:C:H5"	1:2A:1558:A:OP2	2.20	0.41
1:2A:1569:A:H2'	1:2A:1570:A:O4'	2.19	0.41
1:2A:2680:C:H2'	1:2A:2681:C:C6	2.55	0.41
4:2E:112:GLY:O	4:2E:159:HIS:HA	2.20	0.41
6:2G:170:ARG:O	6:2G:174:GLU:HB2	2.20	0.41
8:2I:55:ALA:C	8:2I:57:ARG:H	2.27	0.41
18:2W:71:VAL:HA	18:2W:107:LEU:HD23	2.02	0.41
26:24:45:GLY:O	26:24:47:GLN:N	2.45	0.41
28:26:38:LYS:HE3	28:26:38:LYS:HB3	1.77	0.41
30:28:30:ARG:NH1	61:28:202:HOH:O	2.52	0.41
32:2a:1001(A):G:C5	32:2a:1002:G:H1'	2.55	0.41
32:2a:1346:A:H61	32:2a:1374:A:H3'	1.85	0.41
33:2b:71:VAL:HG23	33:2b:164:VAL:HA	2.01	0.41
33:2b:77:ALA:HA	33:2b:80:ILE:HG22	2.01	0.41
35:2d:155:LEU:HD23	35:2d:156:GLU:H	1.84	0.41
40:2i:97:LYS:HA	40:2i:102:LEU:HG	2.01	0.41
41:2j:32:ALA:HA	41:2j:33:GLN:HA	1.77	0.41
41:2j:42:THR:HG23	41:2j:68:HIS:HA	2.01	0.41
51:2t:57:ARG:HH12	51:2t:100:ILE:HD12	1.85	0.41
1:1A:781:A:OP1	3:1D:218:ARG:NH2	2.53	0.41
1:1A:2094:G:P	8:1I:22:LYS:HD2	2.60	0.41
1:1A:2180:U:H2'	1:1A:2181:G:O4'	2.19	0.41
19:1X:44:GLU:HG2	19:1X:49:VAL:O	2.19	0.41
32:1a:374:A:C6	32:1a:375:U:C4	3.07	0.41
32:1a:865:A:C2	32:1a:918:A:H4'	2.55	0.41
32:1a:1070:U:H2'	32:1a:1071:C:C6	2.55	0.41
34:1c:44:GLU:HA	34:1c:52:LEU:HD23	2.02	0.41
48:1q:87:LYS:HA	48:1q:87:LYS:HE2	2.03	0.41
54:1w:5:G:H2'	54:1w:6:G:H8	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:1y:68:C:N3	56:1y:69:G:C8	2.88	0.41
1:2A:263:C:O2'	1:2A:429:A:N3	2.53	0.41
1:2A:956:G:H5"	12:2Q:77:LYS:HE2	2.01	0.41
1:2A:2080:G:OP1	23:21:35:THR:HG21	2.20	0.41
2:2B:9:G:OP1	14:2S:25:ARG:NH2	2.53	0.41
18:2W:19:LEU:HB3	27:25:25:LEU:HG	2.01	0.41
19:2X:61:GLY:HA3	19:2X:73:ARG:O	2.20	0.41
20:2Y:35:TYR:CE2	20:2Y:69:ALA:HB3	2.54	0.41
32:2a:276:G:OP1	48:2q:12:SER:OG	2.27	0.41
32:2a:419:C:OP1	32:2a:513:C:O2'	2.33	0.41
32:2a:1187:G:OP1	40:2i:113:LYS:NZ	2.53	0.41
32:2a:1194:U:H4'	36:2e:22:GLY:HA2	2.01	0.41
33:2b:37:ASN:OD1	33:2b:37:ASN:N	2.53	0.41
33:2b:218:ALA:O	33:2b:222:ILE:HG23	2.20	0.41
38:2g:38:LEU:O	38:2g:42:ILE:HG13	2.20	0.41
50:2s:39:THR:HG22	50:2s:40:ILE:O	2.19	0.41
1:1A:224:G:H2'	1:1A:225:A:O4'	2.19	0.41
1:1A:1062:G:H1	1:1A:1077:A:H61	1.68	0.41
1:1A:2074:U:H2'	1:1A:2075:U:C6	2.55	0.41
11:1P:42:SER:O	61:1P:302:HOH:O	2.22	0.41
21:1Z:146:ILE:HA	21:1Z:147:GLY:HA2	1.71	0.41
28:16:13:CYS:SG	28:16:47:THR:HG21	2.60	0.41
32:1a:1005:A:C2	32:1a:1025:U:H1'	2.55	0.41
32:1a:1326:C:H2'	32:1a:1327:C:C6	2.55	0.41
32:1a:1333:A:H2'	32:1a:1334:G:O4'	2.20	0.41
33:1b:168:THR:HG23	33:1b:192:SER:HB3	2.02	0.41
38:1g:78:ARG:HD2	38:1g:156:TRP:CE3	2.55	0.41
38:1g:78:ARG:NH1	38:1g:154:TYR:O	2.53	0.41
1:2A:263:C:H2'	1:2A:264:C:O4'	2.20	0.41
1:2A:918:A:C5	1:2A:919:G:H1'	2.55	0.41
1:2A:1508:A:H4'	1:2A:1509(A):A:C8	2.55	0.41
1:2A:1657:C:H2'	1:2A:1658:C:C6	2.55	0.41
1:2A:2820:A:O2'	1:2A:2821:A:OP1	2.37	0.41
3:2D:26:LYS:HE2	3:2D:28:GLU:O	2.21	0.41
5:2F:192:LEU:HD21	5:2F:194:MET:HE2	2.03	0.41
6:2G:103:LEU:HD23	6:2G:106:LEU:HD23	2.02	0.41
14:2S:105:ALA:HB1	14:2S:110:LEU:HD23	2.02	0.41
26:24:48:ARG:HA	26:24:48:ARG:HD2	1.82	0.41
32:2a:448:A:O5'	32:2a:485:G:N2	2.53	0.41
32:2a:1309:G:N7	44:2m:99:ARG:NH2	2.68	0.41
36:2e:41:VAL:HG22	36:2e:113:ALA:HA	2.00	0.41

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	2.56	0.41
1:1A:1065:U:H5"	1:1A:1066:U:OP2	2.21	0.41
1:1A:1401:G:H2'	1:1A:1402:C:O4'	2.20	0.41
1:1A:1796:U:H2'	1:1A:1797:C:H6	1.85	0.41
1:1A:2161:C:O2'	1:1A:2162:G:H5"	2.20	0.41
1:1A:2359:C:H2'	1:1A:2360:A:O4'	2.20	0.41
4:1E:195:LEU:HG	4:1E:196:VAL:N	2.36	0.41
5:1F:103:LYS:O	5:1F:106:ARG:HG2	2.21	0.41
7:1H:149:ARG:HH11	7:1H:149:ARG:HD2	1.74	0.41
32:1a:256:U:H2'	32:1a:257:G:C8	2.56	0.41
32:1a:443:C:H2'	32:1a:444:C:C6	2.55	0.41
32:1a:1025:U:C2	32:1a:1036:G:O6	2.74	0.41
32:1a:1277:C:H1'	32:1a:1282:C:O2	2.21	0.41
33:1b:61:LEU:HD21	33:1b:160:ASP:HB2	2.01	0.41
41:1j:27:ALA:HA	41:1j:81:THR:HG21	2.01	0.41
55:1x:23:C:H2'	55:1x:24:U:C6	2.56	0.41
1:2A:297:C:OP1	20:2Y:87:LYS:NZ	2.51	0.41
1:2A:652(A):A:H3'	1:2A:652(B):A:H5"	2.02	0.41
1:2A:676:A:N1	1:2A:2069:G:O2'	2.51	0.41
1:2A:876:C:H2'	1:2A:877:U:C6	2.55	0.41
1:2A:1278:A:H2'	1:2A:1279:G:C8	2.56	0.41
1:2A:1485:G:H2'	1:2A:1486:A:C8	2.55	0.41
1:2A:2125:G:H5"	1:2A:2126:A:OP2	2.21	0.41
13:2R:9:LYS:O	13:2R:17:ARG:HD3	2.20	0.41
19:2X:94:GLY:H	19:2X:95:LEU:C	2.28	0.41
21:2Z:54:HIS:CD2	21:2Z:101:PRO:HG3	2.55	0.41
21:2Z:129:SER:OG	21:2Z:130:PRO:HD2	2.20	0.41
21:2Z:152:ALA:HB1	21:2Z:163:LEU:HD21	2.01	0.41
27:25:49:CYS:SG	27:25:51:TYR:HB2	2.61	0.41
31:29:2:LYS:HD3	31:29:4:ARG:NH2	2.35	0.41
32:2a:20:U:OP2	36:2e:125:SER:HB3	2.21	0.41
32:2a:93:G:H2'	32:2a:96:U:O4'	2.21	0.41
32:2a:457:C:H2'	32:2a:458:C:C6	2.55	0.41
54:2w:8:4SU:S4	54:2w:14:A:N7	2.93	0.41
55:2x:10:G:N2	55:2x:26:G:H1'	2.35	0.41
1:1A:493:G:H2'	1:1A:494:G:O4'	2.20	0.41
2:1B:84:C:OP1	25:13:15:TYR:OH	2.24	0.41
6:1G:77:ILE:HG22	6:1G:80:PHE:H	1.83	0.41
8:1I:5:LEU:H	8:1I:5:LEU:HD12	1.85	0.41
9:1N:96:GLU:H	9:1N:96:GLU:CD	2.28	0.41
32:1a:620:C:H2'	32:1a:621:A:O4'	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:742:G:OP2	46:1o:35:ARG:NH2	2.46	0.41
32:1a:977:A:C8	32:1a:1223:C:N3	2.89	0.41
33:1b:75:LYS:HD3	33:1b:75:LYS:HA	1.67	0.41
34:1c:113:ALA:HB2	34:1c:202:ILE:HG13	2.03	0.41
41:1j:5:ARG:HG3	41:1j:71:LEU:HD11	2.02	0.41
1:2A:10:G:H2'	1:2A:11:G:C8	2.55	0.41
1:2A:580:C:H2'	1:2A:581:C:C6	2.56	0.41
1:2A:673:C:OP1	5:2F:54:ARG:NH1	2.48	0.41
1:2A:974:G:OP1	1:2A:1187:G:O2'	2.27	0.41
1:2A:993:G:OP1	16:2U:50:ARG:NH2	2.53	0.41
1:2A:1717:G:H2'	1:2A:1718:G:H8	1.85	0.41
1:2A:1783:A:H5'	1:2A:2608:G:H4'	2.02	0.41
1:2A:1946:U:H2'	1:2A:1947:C:C6	2.56	0.41
7:2H:9:ILE:N	7:2H:50:VAL:O	2.36	0.41
8:2I:77:LEU:HD21	8:2I:100:ALA:HB3	2.03	0.41
11:2P:101:VAL:HA	11:2P:106:LEU:O	2.20	0.41
13:2R:63:ARG:O	13:2R:67:LEU:HB2	2.21	0.41
24:22:17:SER:HB3	24:22:20:GLU:HG3	2.01	0.41
32:2a:353:A:H5'	32:2a:353:A:H8	1.86	0.41
32:2a:1447:A:H5"	32:2a:1452:C:OP2	2.19	0.41
43:2l:113:ARG:HD2	43:2l:113:ARG:HA	1.88	0.41
44:2m:15:VAL:HG21	44:2m:48:LEU:HD11	2.03	0.41
48:2q:53:LEU:HD12	48:2q:53:LEU:HA	1.94	0.41
51:2t:10:LEU:HG	51:2t:12:ALA:H	1.85	0.41
55:2x:15:G:H2'	55:2x:59:A:N1	2.36	0.41
55:2x:53:G:H2'	55:2x:54:5MU:H6	1.85	0.41
1:1A:817:C:H4'	1:1A:932:G:C5	2.56	0.41
1:1A:1045:A:H1'	1:1A:1047:G:N3	2.35	0.41
1:1A:1518:U:H2'	1:1A:1519:G:O4'	2.21	0.41
1:1A:1790:C:H2'	1:1A:1791:A:C5	2.55	0.41
1:1A:1916:A:H2'	1:1A:1917:PSU:O4'	2.21	0.41
1:1A:2575:C:OP2	61:1A:4223:HOH:O	2.22	0.41
7:1H:121:ILE:HD13	7:1H:121:ILE:HA	1.94	0.41
16:1U:81:HIS:CE1	16:1U:85:LYS:HD2	2.56	0.41
20:1Y:55:TYR:CE1	20:1Y:61:ILE:HG21	2.55	0.41
21:1Z:8:TYR:HB2	21:1Z:38:TYR:CE2	2.56	0.41
32:1a:28:G:O2'	32:1a:296:U:OP1	2.35	0.41
32:1a:334:C:H2'	32:1a:335:C:C6	2.54	0.41
32:1a:340:U:H2'	32:1a:341:C:C6	2.56	0.41
32:1a:950:U:H2'	32:1a:951:G:H8	1.85	0.41
32:1a:1239:A:O2'	38:1g:114:ARG:O	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1509:C:H2'	32:1a:1510:U:O4'	2.21	0.41
33:1b:170:GLU:O	33:1b:174:VAL:HG23	2.21	0.41
47:1p:19:ILE:HD12	47:1p:38:TYR:N	2.35	0.41
51:1t:57:ARG:HH22	51:1t:100:ILE:HD11	1.85	0.41
1:2A:103:A:H5'	24:22:3:LEU:HD11	2.01	0.41
1:2A:687:C:H2'	1:2A:688:U:O4'	2.20	0.41
6:2G:36:LYS:HD3	6:2G:95:ARG:NH1	2.36	0.41
13:2R:2:ARG:HG2	13:2R:5:LYS:HB2	2.02	0.41
20:2Y:39:VAL:HB	20:2Y:42:VAL:HB	2.02	0.41
21:2Z:52:SER:C	21:2Z:54:HIS:N	2.78	0.41
26:24:50:VAL:HG21	44:2m:65:LYS:HA	2.01	0.41
32:2a:532:A:N6	32:2a:1206:G:O2'	2.53	0.41
32:2a:757:U:H2'	32:2a:758:G:O4'	2.20	0.41
32:2a:1039:C:C2	32:2a:1040:U:H1'	2.56	0.41
32:2a:1367:C:H5"	40:2i:114:TYR:CB	2.50	0.41
33:2b:51:LEU:O	33:2b:55:PHE:HB2	2.20	0.41
33:2b:158:LEU:HD23	33:2b:182:ILE:HD11	2.03	0.41
44:2m:50:GLU:O	44:2m:54:VAL:HG22	2.21	0.41
1:1A:1756:G:H4'	1:1A:1758:G:O4'	2.20	0.41
5:1F:150:GLY:HA2	5:1F:172:TRP:CD2	2.55	0.41
8:1I:126:TYR:HB2	8:1I:142:VAL:HG23	2.03	0.41
19:1X:94:GLY:N	19:1X:95:LEU:HB2	2.33	0.41
32:1a:678:U:H2'	32:1a:679:C:C6	2.56	0.41
33:1b:71:VAL:HB	33:1b:164:VAL:HG12	2.02	0.41
34:1c:19:GLU:HG2	34:1c:54:ARG:NH1	2.36	0.41
1:2A:792:G:H5"	1:2A:793:A:H5'	2.03	0.41
1:2A:1359:A:H2'	1:2A:1360:A:H5'	2.01	0.41
1:2A:1514:U:H2'	1:2A:1515:G:C8	2.56	0.41
1:2A:2308:G:O2'	1:2A:2310:A:N7	2.52	0.41
2:2B:62:C:H2'	2:2B:63:G:C8	2.55	0.41
2:2B:105:A:H5'	2:2B:106:G:OP2	2.21	0.41
21:2Z:23:LYS:O	21:2Z:25:PRO:HD3	2.21	0.41
21:2Z:98:MET:HE3	21:2Z:98:MET:HB2	1.97	0.41
32:2a:328:C:H4'	32:2a:329:A:H5'	2.02	0.41
32:2a:512:U:H2'	32:2a:513:C:C6	2.55	0.41
32:2a:991:U:C4	32:2a:1212:U:H1'	2.56	0.41
32:2a:1285:A:H5'	32:2a:1286:A:C2	2.56	0.41
32:2a:1315:U:H2'	32:2a:1316:G:O4'	2.20	0.41
32:2a:1332:A:H2'	32:2a:1333:A:C8	2.56	0.41
32:2a:1518:MA6:H8	32:2a:1518:MA6:O5'	2.21	0.41
34:2c:190:ARG:O	34:2c:190:ARG:NE	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:2g:65:ALA:O	38:2g:69:VAL:HG23	2.21	0.41
56:2y:74:C:H2'	56:2y:75:C:C6	2.56	0.41
1:1A:234:C:H2'	1:1A:235:U:C6	2.56	0.41
1:1A:234:C:H2'	1:1A:235:U:H6	1.86	0.41
1:1A:2127:G:N2	1:1A:2173:A:H1'	2.36	0.41
4:1E:79:ARG:HD3	4:1E:79:ARG:HA	1.85	0.41
12:1Q:19:GLY:O	12:1Q:98:LYS:HE3	2.21	0.41
31:19:2:LYS:HE2	31:19:31:LYS:O	2.21	0.41
32:1a:174:C:H2'	32:1a:175:C:H6	1.86	0.41
32:1a:589:C:H2'	32:1a:590:C:C6	2.56	0.41
32:1a:976:G:OP1	45:1n:32:SER:N	2.52	0.41
32:1a:1456:G:N2	51:1t:51:GLU:OE2	2.49	0.41
35:1d:15:GLU:OE2	35:1d:59:ARG:NH1	2.53	0.41
36:1e:31:LEU:HD23	36:1e:31:LEU:HA	1.91	0.41
51:1t:86:ARG:HB3	51:1t:90:GLN:HE22	1.84	0.41
56:1y:35:A:OP2	56:1y:35:A:H8	2.03	0.41
1:2A:307:G:N2	1:2A:330:A:H62	2.12	0.41
1:2A:824:A:H1'	1:2A:2358:G:N7	2.36	0.41
1:2A:911:A:H2'	12:2Q:9:TYR:OH	2.21	0.41
1:2A:1270:C:H5"	1:2A:1271:G:O5'	2.21	0.41
1:2A:1508:A:H5'	1:2A:1509(A):A:C8	2.55	0.41
1:2A:1647:G:H3'	1:2A:1647:G:OP2	2.20	0.41
5:2F:103:LYS:HA	5:2F:106:ARG:HD3	2.03	0.41
7:2H:3:ARG:HG2	7:2H:6:ARG:HE	1.84	0.41
7:2H:117:PRO:HA	7:2H:118:PRO:HD3	1.90	0.41
11:2P:50:ARG:HH21	30:28:7:HIS:CD2	2.39	0.41
21:2Z:77:ASP:N	21:2Z:84:GLU:HG3	2.35	0.41
32:2a:1002:G:N3	32:2a:1003:G:H1'	2.35	0.41
32:2a:1024:G:H2'	32:2a:1025:U:H5"	2.03	0.41
33:2b:16:HIS:O	33:2b:18:GLY:N	2.54	0.41
34:2c:140:ARG:O	34:2c:144:SER:N	2.54	0.41
40:2i:24:GLY:HA2	40:2i:59:PHE:O	2.20	0.41
44:2m:19:LEU:HD21	44:2m:56:LEU:HD21	2.02	0.41
47:2p:42:ARG:HB3	47:2p:44:THR:HG23	2.02	0.41
1:1A:844:C:C5	1:1A:845:G:C6	3.09	0.41
1:1A:1243:G:H2'	1:1A:1244:G:O4'	2.20	0.41
1:1A:1357:U:H2'	1:1A:1358:G:O4'	2.21	0.41
1:1A:1359:A:N6	1:1A:1372:U:H3	2.18	0.41
1:1A:1486:A:H2'	1:1A:1487:G:C8	2.56	0.41
1:1A:1508:A:H4'	1:1A:1509(A):A:C5	2.55	0.41
1:1A:1762:A:N1	61:1A:4332:HOH:O	2.37	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2418:A:H2'	1:1A:2419:U:C6	2.55	0.41
1:1A:2552:2MU:H2'	1:1A:2554:U:OP2	2.21	0.41
3:1D:35:LYS:HB2	3:1D:36:PRO:HD2	2.01	0.41
5:1F:123:LEU:HD13	5:1F:192:LEU:HD13	2.03	0.41
5:1F:195:ASP:HB3	5:1F:198:ALA:H	1.86	0.41
7:1H:13:LYS:H	7:1H:13:LYS:HG2	1.49	0.41
8:1I:66:GLU:C	8:1I:68:LEU:N	2.78	0.41
8:1I:101:LEU:HD13	8:1I:101:LEU:HA	1.82	0.41
11:1P:135:LEU:HA	11:1P:135:LEU:HD23	1.78	0.41
12:1Q:57:HIS:CE1	12:1Q:116:GLU:HG2	2.56	0.41
12:1Q:78:PRO:HD3	55:1x:1:C:C4	2.56	0.41
15:1T:16:ARG:NH1	15:1T:83:ILE:O	2.44	0.41
21:1Z:7:ALA:HB2	21:1Z:59:LEU:HD22	2.02	0.41
32:1a:232:G:H1'	32:1a:262:A:N1	2.36	0.41
32:1a:452:A:OP1	47:1p:43:LYS:NZ	2.45	0.41
32:1a:629:G:H2'	32:1a:630:G:O4'	2.21	0.41
32:1a:691:G:H2'	32:1a:692:U:C6	2.56	0.41
32:1a:736:C:H2'	32:1a:737:A:H8	1.85	0.41
32:1a:760:G:O2'	48:1q:98:LEU:HD22	2.21	0.41
32:1a:839:U:H3'	32:1a:840:C:H6	1.85	0.41
32:1a:1298:C:H4'	32:1a:1299:A:C4	2.55	0.41
32:1a:1314:C:H2'	32:1a:1315:U:C6	2.55	0.41
32:1a:1457:G:H5"	51:1t:35:THR:HG21	2.03	0.41
32:1a:1516:G:H2'	32:1a:1518:MA6:OP2	2.21	0.41
34:1c:148:GLY:HA3	34:1c:172:ARG:O	2.21	0.41
35:1d:65:ARG:HG3	35:1d:75:PHE:CD1	2.56	0.41
35:1d:155:LEU:HD12	35:1d:155:LEU:HA	1.82	0.41
36:1e:105:VAL:HB	36:1e:106:PRO:HD3	2.03	0.41
44:1m:4:ILE:HA	44:1m:5:ALA:HA	1.93	0.41
45:1n:3:ARG:HA	45:1n:3:ARG:HE	1.86	0.41
50:1s:33:THR:OG1	50:1s:34:TRP:N	2.54	0.41
51:1t:47:GLY:HA2	51:1t:48:LYS:C	2.46	0.41
56:1y:18:G:H4'	56:1y:19:G:OP1	2.21	0.41
56:1y:42:C:H2'	56:1y:43:C:C6	2.55	0.41
1:2A:191:A:H2'	1:2A:192:C:H6	1.86	0.41
1:2A:311:A:C6	1:2A:328:U:C4	3.09	0.41
1:2A:375:C:H2'	1:2A:376:C:C6	2.56	0.41
1:2A:643:A:C8	28:26:44:ARG:NH1	2.89	0.41
1:2A:819:A:OP2	1:2A:1187:G:N2	2.47	0.41
1:2A:985:C:H2'	1:2A:986:C:C6	2.56	0.41
1:2A:1316:U:H2'	1:2A:1317:A:H8	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1464:C:H2'	1:2A:1465:G:C8	2.55	0.41
1:2A:1782:C:O2	1:2A:2608:G:O2'	2.36	0.41
1:2A:2038:G:H2'	1:2A:2039:C:O4'	2.20	0.41
1:2A:2169:A:H2'	1:2A:2170:A:C8	2.56	0.41
1:2A:2391:G:O6	1:2A:2425:A:H8	2.04	0.41
1:2A:2563:U:O2'	10:2O:28:SER:HB2	2.21	0.41
2:2B:66:A:N6	2:2B:108:U:H3'	2.36	0.41
4:2E:111:ARG:HG3	13:2R:1:MET:SD	2.61	0.41
7:2H:3:ARG:HA	7:2H:3:ARG:HD2	1.79	0.41
7:2H:10:PRO:O	7:2H:12:PRO:HD3	2.21	0.41
7:2H:77:LYS:HD2	7:2H:83:TYR:CZ	2.56	0.41
10:2O:1:MET:HE2	10:2O:32:TYR:CE1	2.56	0.41
12:2Q:79:LEU:HD23	12:2Q:79:LEU:HA	1.84	0.41
13:2R:73:VAL:HG23	13:2R:74:LYS:H	1.86	0.41
18:2W:68:ARG:NH1	18:2W:111:HIS:HA	2.36	0.41
21:2Z:80:ARG:HB2	21:2Z:82:ARG:HG2	2.02	0.41
26:24:9:LEU:HA	26:24:9:LEU:HD23	1.82	0.41
32:2a:406:G:H21	35:2d:119:GLN:NE2	2.07	0.41
32:2a:444:C:H2'	32:2a:445:G:H8	1.85	0.41
32:2a:598:U:H2'	32:2a:599:C:C6	2.56	0.41
32:2a:625:G:H2'	32:2a:626:U:C6	2.56	0.41
32:2a:881:G:OP2	43:2l:12:ARG:NH2	2.54	0.41
32:2a:1020:U:H2'	32:2a:1021:G:C8	2.56	0.41
32:2a:1029:C:C4	32:2a:1032:G:C2	3.08	0.41
33:2b:126:GLU:OE1	33:2b:126:GLU:N	2.54	0.41
33:2b:162:ILE:HD11	33:2b:184:VAL:HG22	2.02	0.41
34:2c:52:LEU:HA	34:2c:70:VAL:HG12	2.03	0.41
35:2d:17:VAL:HG13	35:2d:19:LEU:HD13	2.03	0.41
35:2d:112:VAL:HG23	35:2d:116:GLN:HE22	1.85	0.41
35:2d:191:ARG:HA	35:2d:191:ARG:HD2	1.85	0.41
36:2e:12:LEU:HD22	36:2e:13:ILE:H	1.85	0.41
36:2e:32:VAL:HB	36:2e:58:ALA:HB1	2.03	0.41
47:2p:39:TYR:HA	47:2p:48:TRP:O	2.21	0.41
54:2w:76:F3N:N	55:2x:76:31H:O2'	2.53	0.41
1:1A:774:A:H2'	1:1A:774:A:N3	2.36	0.41
1:1A:868:U:C4	1:1A:869:G:N7	2.89	0.41
1:1A:1075:C:C2'	1:1A:1076:C:H5'	2.51	0.41
1:1A:1082:U:O4	1:1A:1086:A:C2	2.70	0.41
1:1A:1173:G:O2'	1:1A:1174:A:O4'	2.38	0.41
8:1I:77:LEU:HD12	8:1I:97:ILE:HG23	2.01	0.41
10:1O:103:ALA:O	10:1O:106:LEU:HD12	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:41:G:H2'	32:1a:42:G:H8	1.86	0.41
32:1a:45:U:H2'	32:1a:46:G:C8	2.56	0.41
33:1b:71:VAL:HG13	33:1b:93:VAL:HG13	2.02	0.41
33:1b:92:TYR:CD1	33:1b:94:ASN:HB2	2.55	0.41
33:1b:155:LEU:HD12	33:1b:155:LEU:HA	1.89	0.41
34:1c:8:ILE:HD12	34:1c:16:ARG:NE	2.36	0.41
42:1k:20:TYR:HB2	42:1k:31:THR:HG23	2.02	0.41
44:1m:15:VAL:HG13	44:1m:43:THR:O	2.20	0.41
56:1y:56:C:C2	56:1y:57:G:C8	3.09	0.41
1:2A:1012:U:O4	9:2N:28:THR:HG21	2.21	0.41
1:2A:1902:C:OP1	3:2D:242:ARG:HD2	2.21	0.41
1:2A:2064:C:H2'	1:2A:2065:C:C6	2.56	0.41
1:2A:2135:A:C8	1:2A:2136:C:H5	2.39	0.41
1:2A:2316:C:O2'	6:2G:128:ARG:NH2	2.54	0.41
1:2A:2387:U:H1'	22:20:41:ARG:HE	1.86	0.41
1:2A:2612:C:H2'	1:2A:2613:U:H5'	2.03	0.41
1:2A:2630:G:H2'	1:2A:2631:G:C8	2.56	0.41
1:2A:2659:G:OP1	7:2H:158:HIS:NE2	2.46	0.41
3:2D:3:VAL:HG13	3:2D:17:THR:HB	2.02	0.41
4:2E:50:GLY:HA3	4:2E:75:VAL:HG21	2.02	0.41
5:2F:164:ARG:O	5:2F:168:ARG:HB2	2.21	0.41
6:2G:45:GLU:H	6:2G:45:GLU:HG2	1.44	0.41
16:2U:27:LEU:HD23	16:2U:27:LEU:HA	1.92	0.41
21:2Z:3:TYR:CG	21:2Z:51:ALA:HB2	2.56	0.41
27:25:20:ARG:HG2	27:25:23:HIS:ND1	2.35	0.41
32:2a:20:U:H2'	32:2a:21:G:O4'	2.21	0.41
32:2a:520:A:N1	32:2a:536:C:H1'	2.36	0.41
32:2a:742:G:OP2	46:2o:35:ARG:NH2	2.37	0.41
32:2a:1069:C:O2'	32:2a:1192:C:H1'	2.20	0.41
36:2e:76:ILE:O	36:2e:93:PRO:HB3	2.21	0.41
44:2m:92:HIS:CE1	44:2m:98:VAL:HG21	2.56	0.41
51:2t:49:ALA:HB2	51:2t:92:LEU:HD22	2.03	0.41
56:2y:34:G:H2'	56:2y:35:A:O4'	2.21	0.41
56:2y:58:A:H1'	56:2y:60:U:H3	1.85	0.41
1:1A:182:A:H2'	1:1A:183:C:O4'	2.20	0.40
1:1A:630:G:OP2	30:18:15:LYS:NZ	2.38	0.40
1:1A:921:G:H4'	1:1A:2269:A:C5	2.56	0.40
1:1A:1277:G:O2'	13:1R:24:GLN:HG2	2.20	0.40
1:1A:1670:C:O2	4:1E:129:HIS:NE2	2.47	0.40
1:1A:2001:A:OP1	13:1R:9:LYS:NZ	2.43	0.40
1:1A:2114:A:H2	1:1A:2168:G:H1'	1.85	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2312:U:OP1	6:1G:73:ALA:HA	2.21	0.40
1:1A:2376:A:H2'	1:1A:2377:A:O4'	2.21	0.40
3:1D:146:GLU:HG2	3:1D:152:GLY:C	2.46	0.40
5:1F:132:VAL:HA	5:1F:138:GLU:HB3	2.03	0.40
8:1I:9:LEU:HD23	8:1I:9:LEU:HA	1.78	0.40
32:1a:189(C):C:H2'	32:1a:189(D):C:O4'	2.21	0.40
33:1b:8:LYS:HE2	33:1b:8:LYS:HB2	1.69	0.40
35:1d:64:LEU:HB2	35:1d:198:VAL:HG11	2.03	0.40
38:1g:99:LEU:HD23	38:1g:102:ARG:NH1	2.36	0.40
39:1h:81:HIS:N	39:1h:138:TRP:O	2.54	0.40
46:1o:25:THR:HG21	46:1o:70:LEU:HB2	2.03	0.40
48:1q:53:LEU:HA	48:1q:53:LEU:HD12	1.85	0.40
1:2A:411:G:C5	11:2P:72:PRO:HB3	2.56	0.40
1:2A:1386:C:H2'	1:2A:1387:C:C6	2.57	0.40
1:2A:1614:A:N6	18:2W:92:ARG:O	2.53	0.40
1:2A:2171:A:H1'	1:2A:2172:U:C6	2.56	0.40
1:2A:2206:G:H5"	1:2A:2207:G:C8	2.56	0.40
1:2A:2712:U:OP1	1:2A:2714:G:H4'	2.21	0.40
2:2B:31:C:H4'	6:2G:29:TRP:CZ2	2.55	0.40
2:2B:42:C:O2	6:2G:93:THR:N	2.52	0.40
10:2O:34:THR:OG1	10:2O:35:VAL:N	2.54	0.40
12:2Q:56:ARG:HB3	12:2Q:56:ARG:NH1	2.36	0.40
15:2T:19:LEU:H	15:2T:19:LEU:HG	1.67	0.40
21:2Z:8:TYR:HB2	21:2Z:38:TYR:CE2	2.56	0.40
26:24:38:LYS:O	26:24:44:THR:HB	2.20	0.40
32:2a:189(A):C:H2'	32:2a:189(B):C:C6	2.57	0.40
32:2a:615:C:H2'	32:2a:616:G:O4'	2.21	0.40
32:2a:922:G:N3	32:2a:1398:A:H2	2.19	0.40
32:2a:1010:G:C2	32:2a:1020:U:H1'	2.56	0.40
32:2a:1029:C:N3	32:2a:1032:G:C2	2.88	0.40
32:2a:1194:U:H2'	32:2a:1195:C:C6	2.56	0.40
33:2b:163:PHE:HA	33:2b:185:ILE:HG12	2.03	0.40
34:2c:134:ILE:HG22	34:2c:168:ALA:HB3	2.03	0.40
37:2f:8:ILE:HD13	37:2f:26:ILE:HD13	2.02	0.40
40:2i:4:TYR:HB2	40:2i:19:LEU:HB2	2.02	0.40
40:2i:11:LYS:HA	40:2i:108:VAL:HG12	2.03	0.40
40:2i:127:LYS:O	40:2i:128:ARG:HB3	2.21	0.40
44:2m:43:THR:OG1	44:2m:48:LEU:HD21	2.21	0.40
45:2n:33:VAL:HA	45:2n:40:CYS:HA	2.03	0.40
55:2x:8:4SU:H6	55:2x:8:4SU:O5'	2.21	0.40
1:1A:272:G:N7	1:1A:421:U:H2'	2.36	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:782:A:H5'	1:1A:783:A:N7	2.36	0.40
1:1A:884:C:N4	1:1A:892:G:H1	2.10	0.40
1:1A:1027:A:C6	1:1A:1126:A:C4	3.09	0.40
1:1A:2190:G:C2	1:1A:2191:G:C8	3.09	0.40
21:1Z:155:LEU:HD12	21:1Z:156:LYS:H	1.86	0.40
32:1a:986:A:H1'	50:1s:54:GLY:O	2.20	0.40
33:1b:174:VAL:HG13	33:1b:184:VAL:HG11	2.03	0.40
40:1i:6:GLY:O	40:1i:17:VAL:HG12	2.21	0.40
47:1p:14:ASN:ND2	47:1p:42:ARG:HH22	2.19	0.40
56:1y:60:U:O2'	56:1y:61:C:H5'	2.21	0.40
1:2A:271(L):U:H5'	8:2I:50:ARG:HH11	1.85	0.40
1:2A:1213:A:N3	1:2A:1238:G:O2'	2.43	0.40
1:2A:1423:G:OP1	1:2A:1492:G:O2'	2.39	0.40
1:2A:2169:A:N7	1:2A:2170:A:N6	2.70	0.40
3:2D:177:LEU:HD12	3:2D:181:GLU:HG2	2.03	0.40
6:2G:163:ALA:HB1	6:2G:168:GLU:HB2	2.04	0.40
21:2Z:59:LEU:HD23	21:2Z:59:LEU:HA	1.91	0.40
26:24:28:LYS:HA	26:24:29:PRO:HD3	1.97	0.40
32:2a:300:A:H1'	32:2a:565:U:O2	2.21	0.40
32:2a:993:G:H2'	32:2a:993:G:N3	2.36	0.40
32:2a:1135:U:H4'	32:2a:1136:U:C5	2.57	0.40
32:2a:1149:C:OP2	40:2i:9:ARG:NH1	2.54	0.40
33:2b:54:THR:O	33:2b:58:ILE:HG13	2.21	0.40
34:2c:9:GLY:HA3	45:2n:49:HIS:HA	2.03	0.40
44:2m:66:LEU:O	44:2m:67:GLU:C	2.65	0.40
47:2p:55:ARG:HD2	47:2p:55:ARG:HA	1.93	0.40
51:2t:50:GLU:HG3	51:2t:100:ILE:HD13	2.03	0.40
1:1A:686:G:N2	1:1A:788:A:H61	2.19	0.40
1:1A:1311:G:H2'	29:17:47:ARG:HH22	1.85	0.40
1:1A:2147:G:C5	1:1A:2148:G:H1'	2.57	0.40
5:1F:116:ASP:OD2	11:1P:1:MET:HB3	2.20	0.40
8:1I:97:ILE:H	8:1I:97:ILE:HG13	1.75	0.40
10:1O:4:PRO:O	10:1O:5:GLN:HB2	2.21	0.40
15:1T:24:PRO:HD3	15:1T:52:ILE:HD12	2.04	0.40
22:10:43:THR:HG23	22:10:43:THR:O	2.21	0.40
23:11:77:ALA:HB1	23:11:82:LEU:HD11	2.02	0.40
32:1a:576:G:O6	32:1a:880:C:O2'	2.35	0.40
32:1a:890:G:O2'	32:1a:906:G:O6	2.24	0.40
32:1a:1112:C:C4	34:1c:178:LEU:HD12	2.56	0.40
1:2A:647:G:H2'	1:2A:648:G:O4'	2.22	0.40
1:2A:1358:G:O2'	1:2A:1359:A:H5"	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1580:A:OP2	1:2A:1580:A:H8	2.04	0.40
1:2A:2467:C:H4'	12:2Q:123:HIS:CD2	2.56	0.40
4:2E:143:ASN:HB2	4:2E:147:PRO:HD2	2.04	0.40
7:2H:20:ALA:HB1	7:2H:21:PRO:HD2	2.03	0.40
18:2W:65:LEU:HD12	18:2W:68:ARG:HE	1.85	0.40
21:2Z:156:LYS:HD3	21:2Z:158:PRO:HD3	2.03	0.40
32:2a:51:A:N7	32:2a:114:U:O2'	2.51	0.40
32:2a:1118:C:P	40:2i:104:ARG:HH11	2.45	0.40
36:2e:95:ALA:C	36:2e:97:GLY:H	2.29	0.40
46:2o:57:LEU:HD23	46:2o:57:LEU:HA	1.91	0.40
51:2t:38:LYS:HD3	51:2t:38:LYS:HA	1.83	0.40
1:1A:652(A):A:H2'	1:1A:652(A):A:N3	2.35	0.40
1:1A:857:C:N4	1:1A:858:U:O4	2.54	0.40
1:1A:922:U:H2'	1:1A:923:C:C6	2.57	0.40
1:1A:1062:G:H2'	1:1A:1063:G:C8	2.56	0.40
1:1A:1100:C:H5'	1:1A:1101:U:OP2	2.22	0.40
1:1A:1506:C:H2'	1:1A:1507:A:C8	2.53	0.40
1:1A:2088:G:C6	1:1A:2089:U:C4	3.09	0.40
1:1A:2732:G:H3'	1:1A:2733:A:O4'	2.21	0.40
3:1D:61:LEU:O	3:1D:63:ARG:NH1	2.54	0.40
6:1G:109:VAL:HG11	26:14:14:ILE:HG21	2.03	0.40
9:1N:62:VAL:HG13	9:1N:66:LYS:HB2	2.03	0.40
9:1N:70:LYS:HE3	9:1N:72:TYR:CZ	2.56	0.40
19:1X:5:TYR:HB3	24:12:33:MET:HB2	2.03	0.40
32:1a:509:A:HO2'	32:1a:510:A:P	2.40	0.40
32:1a:765:G:H5"	32:1a:766:A:OP1	2.21	0.40
32:1a:1307:U:OP1	44:1m:101:GLN:NE2	2.48	0.40
32:1a:1374:A:OP1	38:1g:36:LYS:NZ	2.55	0.40
46:1o:9:GLN:HE21	46:1o:13:GLN:HE22	1.70	0.40
49:1r:33:ASP:OD2	49:1r:36:ASN:HB2	2.21	0.40
1:2A:709:U:H2'	1:2A:710:G:H8	1.86	0.40
1:2A:880:G:H2'	1:2A:881:G:H8	1.86	0.40
1:2A:1158:C:H2'	1:2A:1159:U:H6	1.87	0.40
1:2A:2025:C:H2'	1:2A:2026:C:C6	2.56	0.40
1:2A:2317:C:C2'	1:2A:2318:G:H5'	2.51	0.40
1:2A:2539:C:O2'	31:29:35:ARG:NH2	2.55	0.40
1:2A:2729:G:H2'	1:2A:2730:C:C6	2.57	0.40
3:2D:6:PHE:HE2	3:2D:18:VAL:HG13	1.87	0.40
6:2G:129:GLY:O	6:2G:161:THR:HB	2.21	0.40
7:2H:148:ILE:O	7:2H:151:ILE:HG12	2.21	0.40
14:2S:51:ALA:HB3	14:2S:73:LEU:HB2	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:444:C:H2'	32:2a:445:G:C8	2.56	0.40
32:2a:473:G:C2	32:2a:474:G:C5	3.09	0.40
32:2a:573:A:N3	32:2a:883:C:O2'	2.48	0.40
32:2a:1168:A:H2'	32:2a:1169:A:C8	2.57	0.40
32:2a:1263:C:C4	32:2a:1272:G:O6	2.75	0.40
39:2h:28:ALA:HA	39:2h:59:LEU:HG	2.02	0.40
44:2m:30:ALA:O	44:2m:34:LEU:HG	2.21	0.40
50:2s:40:ILE:HA	50:2s:44:MET:SD	2.62	0.40
56:2y:53:G:H3'	56:2y:54:5MU:H71	2.04	0.40
1:1A:957:A:N1	1:1A:2458:G:H4'	2.36	0.40
1:1A:1971:A:OP1	61:1A:4206:HOH:O	2.22	0.40
1:1A:2030:A:H4'	1:1A:2031:A:C8	2.57	0.40
1:1A:2097:C:H2'	1:1A:2098:U:H6	1.85	0.40
1:1A:2136:C:C2	1:1A:2155:G:N2	2.89	0.40
1:1A:2506:U:O2	54:1w:76:F3N:HD2	2.21	0.40
4:1E:2:LYS:H	4:1E:2:LYS:HG3	1.40	0.40
4:1E:37:ARG:O	4:1E:45:THR:HA	2.21	0.40
6:1G:49:ASP:O	6:1G:50:ALA:HB2	2.20	0.40
6:1G:146:TYR:O	6:1G:149:VAL:HG12	2.22	0.40
13:1R:98:LEU:HD12	27:15:57:VAL:HG11	2.02	0.40
32:1a:192:U:O2'	51:1t:60:GLU:OE1	2.32	0.40
32:1a:652:U:O4	32:1a:752:G:O2'	2.35	0.40
32:1a:667:G:H4'	46:1o:51:HIS:ND1	2.36	0.40
32:1a:737:A:H2'	32:1a:738:C:C6	2.57	0.40
32:1a:1053:G:O6	32:1a:1199:U:H2'	2.21	0.40
32:1a:1342:C:O2'	40:1i:124:GLN:HG3	2.22	0.40
32:1a:1372:U:OP1	40:1i:72:GLY:N	2.49	0.40
51:1t:77:ALA:O	51:1t:81:LYS:HG3	2.21	0.40
1:2A:764:A:H5"	3:2D:210:GLY:CA	2.50	0.40
1:2A:1131:G:C2	1:2A:1132:A:C4	3.10	0.40
1:2A:1448:G:H2'	1:2A:1449:A:C8	2.56	0.40
1:2A:1721:G:H5"	1:2A:1721:G:N3	2.37	0.40
1:2A:1837:C:OP1	32:2a:784:C:H4'	2.22	0.40
1:2A:2755:C:O2'	1:2A:2756:U:H2'	2.22	0.40
7:2H:77:LYS:HE3	7:2H:81:GLU:OE1	2.21	0.40
8:2I:26:ALA:O	8:2I:31:LEU:HB2	2.22	0.40
12:2Q:78:PRO:HD3	55:2x:1:C:C4	2.57	0.40
14:2S:49:VAL:HG12	14:2S:73:LEU:HD12	2.04	0.40
21:2Z:39:VAL:HG21	21:2Z:44:PHE:HB2	2.02	0.40
21:2Z:150:LEU:HD12	21:2Z:150:LEU:HA	1.94	0.40
28:26:11:LEU:HB2	28:26:21:TYR:HB2	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:582:U:C2	32:2a:760:G:C6	3.09	0.40
32:2a:1124:G:O2'	32:2a:1145:C:C4	2.75	0.40
32:2a:1258:G:OP2	32:2a:1258:G:H8	2.04	0.40
32:2a:1371:G:O3'	40:2i:69:GLY:HA3	2.21	0.40
32:2a:1426:C:H2'	32:2a:1427:U:C6	2.57	0.40
33:2b:76:GLN:HB2	33:2b:208:ILE:CG1	2.49	0.40
38:2g:79:ARG:NH2	38:2g:80:VAL:HA	2.36	0.40
46:2o:37:ASN:O	46:2o:41:GLU:HG2	2.22	0.40
56:2y:11:C:H2'	56:2y:12:U:C6	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	1D	273/276 (99%)	256 (94%)	17 (6%)	0	100 100
3	2D	273/276 (99%)	259 (95%)	14 (5%)	0	100 100
4	1E	202/206 (98%)	193 (96%)	8 (4%)	1 (0%)	24 34
4	2E	202/206 (98%)	187 (93%)	14 (7%)	1 (0%)	24 34
5	1F	200/210 (95%)	195 (98%)	4 (2%)	1 (0%)	24 34
5	2F	200/210 (95%)	188 (94%)	11 (6%)	1 (0%)	24 34
6	1G	179/182 (98%)	168 (94%)	10 (6%)	1 (1%)	21 29
6	2G	179/182 (98%)	157 (88%)	19 (11%)	3 (2%)	7 8
7	1H	172/180 (96%)	159 (92%)	12 (7%)	1 (1%)	21 29
7	2H	172/180 (96%)	158 (92%)	13 (8%)	1 (1%)	21 29
8	1I	144/148 (97%)	128 (89%)	16 (11%)	0	100 100
8	2I	144/148 (97%)	128 (89%)	14 (10%)	2 (1%)	9 11
9	1N	138/140 (99%)	133 (96%)	5 (4%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
9	2N	138/140 (99%)	125 (91%)	12 (9%)	1 (1%)	18 25
10	1O	120/122 (98%)	114 (95%)	6 (5%)	0	100 100
10	2O	120/122 (98%)	112 (93%)	7 (6%)	1 (1%)	16 22
11	1P	147/150 (98%)	132 (90%)	10 (7%)	5 (3%)	3 1
11	2P	147/150 (98%)	132 (90%)	11 (8%)	4 (3%)	4 3
12	1Q	139/141 (99%)	134 (96%)	3 (2%)	2 (1%)	9 11
12	2Q	139/141 (99%)	129 (93%)	9 (6%)	1 (1%)	18 25
13	1R	116/118 (98%)	112 (97%)	4 (3%)	0	100 100
13	2R	116/118 (98%)	110 (95%)	6 (5%)	0	100 100
14	1S	108/112 (96%)	103 (95%)	5 (5%)	0	100 100
14	2S	108/112 (96%)	100 (93%)	7 (6%)	1 (1%)	14 20
15	1T	129/146 (88%)	120 (93%)	9 (7%)	0	100 100
15	2T	129/146 (88%)	122 (95%)	7 (5%)	0	100 100
16	1U	114/118 (97%)	113 (99%)	1 (1%)	0	100 100
16	2U	114/118 (97%)	112 (98%)	2 (2%)	0	100 100
17	1V	99/101 (98%)	92 (93%)	4 (4%)	3 (3%)	3 2
17	2V	99/101 (98%)	88 (89%)	10 (10%)	1 (1%)	12 17
18	1W	110/113 (97%)	108 (98%)	2 (2%)	0	100 100
18	2W	110/113 (97%)	108 (98%)	2 (2%)	0	100 100
19	1X	93/96 (97%)	88 (95%)	4 (4%)	1 (1%)	11 15
19	2X	93/96 (97%)	89 (96%)	3 (3%)	1 (1%)	11 15
20	1Y	105/110 (96%)	99 (94%)	5 (5%)	1 (1%)	12 17
20	2Y	105/110 (96%)	96 (91%)	7 (7%)	2 (2%)	6 7
21	1Z	148/206 (72%)	132 (89%)	14 (10%)	2 (1%)	9 11
21	2Z	156/206 (76%)	124 (80%)	25 (16%)	7 (4%)	2 1
22	10	81/85 (95%)	80 (99%)	1 (1%)	0	100 100
22	20	81/85 (95%)	78 (96%)	3 (4%)	0	100 100
23	11	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	11 15
23	21	95/98 (97%)	92 (97%)	3 (3%)	0	100 100
24	12	68/72 (94%)	65 (96%)	3 (4%)	0	100 100
24	22	68/72 (94%)	68 (100%)	0	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
25	13	57/60 (95%)	55 (96%)	2 (4%)	0	100 100
25	23	57/60 (95%)	52 (91%)	5 (9%)	0	100 100
26	14	67/71 (94%)	54 (81%)	6 (9%)	7 (10%)	0 0
26	24	67/71 (94%)	50 (75%)	14 (21%)	3 (4%)	2 1
27	15	57/60 (95%)	55 (96%)	2 (4%)	0	100 100
27	25	57/60 (95%)	54 (95%)	3 (5%)	0	100 100
28	16	51/54 (94%)	49 (96%)	2 (4%)	0	100 100
28	26	51/54 (94%)	48 (94%)	3 (6%)	0	100 100
29	17	46/49 (94%)	46 (100%)	0	0	100 100
29	27	46/49 (94%)	46 (100%)	0	0	100 100
30	18	62/65 (95%)	62 (100%)	0	0	100 100
30	28	62/65 (95%)	60 (97%)	2 (3%)	0	100 100
31	19	35/37 (95%)	35 (100%)	0	0	100 100
31	29	35/37 (95%)	35 (100%)	0	0	100 100
33	1b	229/256 (90%)	197 (86%)	26 (11%)	6 (3%)	4 3
33	2b	229/256 (90%)	185 (81%)	37 (16%)	7 (3%)	3 2
34	1c	204/239 (85%)	188 (92%)	15 (7%)	1 (0%)	24 34
34	2c	204/239 (85%)	185 (91%)	18 (9%)	1 (0%)	24 34
35	1d	206/209 (99%)	193 (94%)	9 (4%)	4 (2%)	6 7
35	2d	206/209 (99%)	197 (96%)	9 (4%)	0	100 100
36	1e	146/162 (90%)	131 (90%)	13 (9%)	2 (1%)	9 11
36	2e	146/162 (90%)	134 (92%)	10 (7%)	2 (1%)	9 11
37	1f	98/101 (97%)	92 (94%)	6 (6%)	0	100 100
37	2f	98/101 (97%)	95 (97%)	3 (3%)	0	100 100
38	1g	153/156 (98%)	147 (96%)	5 (3%)	1 (1%)	18 25
38	2g	153/156 (98%)	140 (92%)	12 (8%)	1 (1%)	18 25
39	1h	135/138 (98%)	127 (94%)	7 (5%)	1 (1%)	18 25
39	2h	135/138 (98%)	128 (95%)	7 (5%)	0	100 100
40	1i	125/128 (98%)	110 (88%)	12 (10%)	3 (2%)	4 4
40	2i	125/128 (98%)	110 (88%)	14 (11%)	1 (1%)	16 22
41	1j	95/105 (90%)	84 (88%)	9 (10%)	2 (2%)	5 5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
41	2j	94/105 (90%)	79 (84%)	12 (13%)	3 (3%)	3 2
42	1k	112/129 (87%)	98 (88%)	13 (12%)	1 (1%)	14 20
42	2k	112/129 (87%)	100 (89%)	11 (10%)	1 (1%)	14 20
43	1l	119/132 (90%)	114 (96%)	5 (4%)	0	100 100
43	2l	119/132 (90%)	111 (93%)	8 (7%)	0	100 100
44	1m	121/126 (96%)	108 (89%)	10 (8%)	3 (2%)	4 4
44	2m	120/126 (95%)	109 (91%)	9 (8%)	2 (2%)	7 8
45	1n	58/61 (95%)	55 (95%)	3 (5%)	0	100 100
45	2n	58/61 (95%)	54 (93%)	4 (7%)	0	100 100
46	1o	86/89 (97%)	82 (95%)	3 (4%)	1 (1%)	10 13
46	2o	86/89 (97%)	83 (96%)	3 (4%)	0	100 100
47	1p	80/88 (91%)	71 (89%)	9 (11%)	0	100 100
47	2p	80/88 (91%)	76 (95%)	4 (5%)	0	100 100
48	1q	97/105 (92%)	89 (92%)	6 (6%)	2 (2%)	5 5
48	2q	97/105 (92%)	90 (93%)	5 (5%)	2 (2%)	5 5
49	1r	66/88 (75%)	62 (94%)	4 (6%)	0	100 100
49	2r	66/88 (75%)	65 (98%)	1 (2%)	0	100 100
50	1s	81/93 (87%)	71 (88%)	9 (11%)	1 (1%)	10 13
50	2s	81/93 (87%)	71 (88%)	10 (12%)	0	100 100
51	1t	94/106 (89%)	87 (93%)	5 (5%)	2 (2%)	5 5
51	2t	94/106 (89%)	86 (92%)	6 (6%)	2 (2%)	5 5
52	1u	21/27 (78%)	20 (95%)	1 (5%)	0	100 100
52	2u	21/27 (78%)	19 (90%)	2 (10%)	0	100 100
All	All	11368/12128 (94%)	10523 (93%)	737 (6%)	108 (1%)	12 17

All (108) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
11	1P	29	LYS
11	1P	38	GLN
11	1P	44	GLY
17	1V	79	VAL
21	1Z	53	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	14	49	PHE
26	14	62	ARG
33	1b	17	PHE
33	1b	22	LYS
40	1i	54	ASP
44	1m	67	GLU
44	1m	107	ALA
5	2F	130	ALA
8	2I	40	THR
11	2P	36	LYS
21	2Z	154	ASP
26	24	45	GLY
33	2b	9	GLU
33	2b	17	PHE
44	2m	67	GLU
12	1Q	16	ARG
23	11	3	LYS
26	14	45	GLY
26	14	47	GLN
35	1d	88	VAL
38	1g	52	GLU
42	1k	49	GLY
48	1q	68	ARG
6	2G	51	ARG
8	2I	41	GLU
17	2V	79	VAL
19	2X	93	GLU
21	2Z	53	ILE
21	2Z	93	ASP
26	24	48	ARG
33	2b	21	ARG
38	2g	55	GLY
48	2q	68	ARG
51	2t	10	LEU
11	1P	45	LEU
17	1V	100	ARG
20	1Y	54	LYS
26	14	52	THR
33	1b	124	SER
35	1d	173	TRP
36	1e	85	GLY
11	2P	38	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	2Q	16	ARG
14	2S	84	GLN
20	2Y	54	LYS
21	2Z	52	SER
26	24	49	PHE
33	2b	20	GLU
41	2j	79	ARG
4	1E	52	LEU
7	1H	126	PRO
17	1V	43	GLU
19	1X	93	GLU
21	1Z	156	LYS
26	14	53	GLU
33	1b	126	GLU
34	1c	61	ALA
41	1j	78	ASN
44	1m	106	ASN
46	1o	88	ARG
51	1t	100	ILE
4	2E	52	LEU
6	2G	45	GLU
7	2H	126	PRO
9	2N	2	LYS
10	2O	26	LYS
11	2P	44	GLY
21	2Z	60	GLU
21	2Z	144	LEU
34	2c	181	ASN
48	2q	67	LYS
50	1s	27	GLU
11	2P	45	LEU
40	2i	11	LYS
41	2j	29	ARG
44	2m	6	GLY
6	1G	50	ALA
12	1Q	15	GLY
33	2b	74	LYS
33	2b	78	GLN
41	2j	78	ASN
35	1d	170	VAL
36	1e	69	VAL
40	1i	41	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	1j	77	PRO
48	1q	33	GLY
51	1t	47	GLY
21	2Z	146	ILE
33	2b	125	PRO
51	2t	47	GLY
6	2G	42	GLY
36	2e	11	ILE
11	1P	122	PRO
26	14	56	VAL
35	1d	124	GLY
42	2k	105	VAL
33	1b	229	VAL
39	1h	73	ASP
40	1i	24	GLY
20	2Y	55	TYR
36	2e	96	PRO
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%)	206 (96%)	9 (4%)	26 40
3	2D	215/218 (99%)	203 (94%)	12 (6%)	19 29
4	1E	164/166 (99%)	153 (93%)	11 (7%)	15 21
4	2E	164/166 (99%)	155 (94%)	9 (6%)	19 29
5	1F	160/166 (96%)	143 (89%)	17 (11%)	6 7
5	2F	159/166 (96%)	144 (91%)	15 (9%)	8 10
6	1G	143/156 (92%)	128 (90%)	15 (10%)	6 8
6	2G	143/156 (92%)	131 (92%)	12 (8%)	10 14
7	1H	144/148 (97%)	132 (92%)	12 (8%)	10 14
7	2H	144/148 (97%)	128 (89%)	16 (11%)	6 6

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	1I	113/124 (91%)	96 (85%)	17 (15%)	3 2
8	2I	105/124 (85%)	96 (91%)	9 (9%)	10 13
9	1N	118/119 (99%)	109 (92%)	9 (8%)	12 17
9	2N	118/119 (99%)	110 (93%)	8 (7%)	14 20
10	1O	100/100 (100%)	99 (99%)	1 (1%)	68 80
10	2O	100/100 (100%)	93 (93%)	7 (7%)	14 19
11	1P	115/116 (99%)	108 (94%)	7 (6%)	17 25
11	2P	115/116 (99%)	106 (92%)	9 (8%)	11 16
12	1Q	111/111 (100%)	108 (97%)	3 (3%)	39 58
12	2Q	111/111 (100%)	106 (96%)	5 (4%)	24 38
13	1R	101/101 (100%)	96 (95%)	5 (5%)	22 33
13	2R	101/101 (100%)	97 (96%)	4 (4%)	28 42
14	1S	86/88 (98%)	81 (94%)	5 (6%)	18 27
14	2S	85/88 (97%)	80 (94%)	5 (6%)	18 27
15	1T	115/127 (91%)	109 (95%)	6 (5%)	21 32
15	2T	113/127 (89%)	104 (92%)	9 (8%)	11 15
16	1U	93/94 (99%)	89 (96%)	4 (4%)	26 39
16	2U	93/94 (99%)	88 (95%)	5 (5%)	20 30
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%)	86 (96%)	4 (4%)	25 38
18	2W	90/92 (98%)	87 (97%)	3 (3%)	33 50
19	1X	77/78 (99%)	73 (95%)	4 (5%)	21 32
19	2X	77/78 (99%)	75 (97%)	2 (3%)	40 59
20	1Y	85/91 (93%)	73 (86%)	12 (14%)	3 3
20	2Y	85/91 (93%)	75 (88%)	10 (12%)	5 5
21	1Z	135/179 (75%)	124 (92%)	11 (8%)	11 15
21	2Z	137/179 (76%)	116 (85%)	21 (15%)	3 2
22	10	65/67 (97%)	63 (97%)	2 (3%)	35 53
22	20	65/67 (97%)	63 (97%)	2 (3%)	35 53
23	11	80/83 (96%)	78 (98%)	2 (2%)	42 60

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
23	21	80/83 (96%)	74 (92%)	6 (8%)	12 17
24	12	65/67 (97%)	64 (98%)	1 (2%)	57 74
24	22	65/67 (97%)	63 (97%)	2 (3%)	35 53
25	13	51/52 (98%)	45 (88%)	6 (12%)	5 5
25	23	50/52 (96%)	44 (88%)	6 (12%)	5 5
26	14	59/63 (94%)	51 (86%)	8 (14%)	3 3
26	24	53/63 (84%)	45 (85%)	8 (15%)	3 2
27	15	50/52 (96%)	48 (96%)	2 (4%)	28 42
27	25	50/52 (96%)	48 (96%)	2 (4%)	28 42
28	16	51/52 (98%)	45 (88%)	6 (12%)	5 5
28	26	50/52 (96%)	47 (94%)	3 (6%)	17 26
29	17	41/42 (98%)	37 (90%)	4 (10%)	7 9
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%)	51 (94%)	3 (6%)	19 29
31	19	34/34 (100%)	34 (100%)	0	100 100
31	29	34/34 (100%)	33 (97%)	1 (3%)	37 55
33	1b	192/220 (87%)	170 (88%)	22 (12%)	5 6
33	2b	187/220 (85%)	148 (79%)	39 (21%)	1 1
34	1c	142/188 (76%)	127 (89%)	15 (11%)	6 7
34	2c	140/188 (74%)	125 (89%)	15 (11%)	6 7
35	1d	169/181 (93%)	159 (94%)	10 (6%)	18 27
35	2d	173/181 (96%)	151 (87%)	22 (13%)	4 4
36	1e	113/123 (92%)	106 (94%)	7 (6%)	16 24
36	2e	114/123 (93%)	106 (93%)	8 (7%)	14 19
37	1f	84/90 (93%)	75 (89%)	9 (11%)	6 7
37	2f	85/90 (94%)	81 (95%)	4 (5%)	23 36
38	1g	119/127 (94%)	105 (88%)	14 (12%)	5 5
38	2g	120/127 (94%)	107 (89%)	13 (11%)	6 7
39	1h	114/119 (96%)	107 (94%)	7 (6%)	17 25
39	2h	114/119 (96%)	105 (92%)	9 (8%)	11 16

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
40	1i	90/99 (91%)	77 (86%)	13 (14%)	3 2
40	2i	89/99 (90%)	79 (89%)	10 (11%)	6 6
41	1j	66/92 (72%)	57 (86%)	9 (14%)	3 3
41	2j	69/92 (75%)	57 (83%)	12 (17%)	2 1
42	1k	82/99 (83%)	77 (94%)	5 (6%)	17 25
42	2k	83/99 (84%)	77 (93%)	6 (7%)	13 18
43	1l	96/108 (89%)	88 (92%)	8 (8%)	10 14
43	2l	96/108 (89%)	92 (96%)	4 (4%)	26 40
44	1m	93/101 (92%)	83 (89%)	10 (11%)	6 7
44	2m	92/101 (91%)	81 (88%)	11 (12%)	5 5
45	1n	49/50 (98%)	43 (88%)	6 (12%)	5 4
45	2n	49/50 (98%)	44 (90%)	5 (10%)	7 8
46	1o	78/80 (98%)	76 (97%)	2 (3%)	40 59
46	2o	78/80 (98%)	73 (94%)	5 (6%)	16 23
47	1p	69/74 (93%)	64 (93%)	5 (7%)	13 18
47	2p	68/74 (92%)	64 (94%)	4 (6%)	18 27
48	1q	94/97 (97%)	88 (94%)	6 (6%)	16 23
48	2q	94/97 (97%)	89 (95%)	5 (5%)	20 31
49	1r	59/77 (77%)	55 (93%)	4 (7%)	14 20
49	2r	59/77 (77%)	56 (95%)	3 (5%)	21 33
50	1s	69/80 (86%)	63 (91%)	6 (9%)	9 13
50	2s	67/80 (84%)	61 (91%)	6 (9%)	9 11
51	1t	70/82 (85%)	67 (96%)	3 (4%)	26 39
51	2t	70/82 (85%)	70 (100%)	0	100 100
52	1u	18/22 (82%)	18 (100%)	0	100 100
52	2u	18/22 (82%)	18 (100%)	0	100 100
All	All	9303/10064 (92%)	8569 (92%)	734 (8%)	11 16

All (734) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	3	VAL
3	1D	38	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	1D	61	LEU
3	1D	111	LEU
3	1D	142	VAL
3	1D	165	ILE
3	1D	229	VAL
3	1D	242	ARG
3	1D	259	THR
4	1E	2	LYS
4	1E	45	THR
4	1E	47	VAL
4	1E	49	LEU
4	1E	78	LEU
4	1E	81	ILE
4	1E	116	VAL
4	1E	181	LEU
4	1E	184	VAL
4	1E	188	VAL
4	1E	195	LEU
5	1F	24	LEU
5	1F	33	LEU
5	1F	53	THR
5	1F	57	VAL
5	1F	60	SER
5	1F	70	THR
5	1F	72	ARG
5	1F	74	ARG
5	1F	106	ARG
5	1F	132	VAL
5	1F	140	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	5	VAL
6	1G	7	LEU
6	1G	31	VAL
6	1G	43	LEU
6	1G	47	LYS
6	1G	60	LEU
6	1G	64	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	1G	82	LEU
6	1G	86	MET
6	1G	104	GLU
6	1G	139	LEU
6	1G	148	MET
6	1G	150	ASP
6	1G	159	VAL
6	1G	181	ARG
7	1H	6	ARG
7	1H	13	LYS
7	1H	15	VAL
7	1H	42	ARG
7	1H	45	VAL
7	1H	57	ASP
7	1H	77	LYS
7	1H	87	LEU
7	1H	98	LEU
7	1H	114	VAL
7	1H	122	THR
7	1H	124	GLU
8	1I	3	VAL
8	1I	12	LEU
8	1I	15	VAL
8	1I	38	LEU
8	1I	41	GLU
8	1I	47	LEU
8	1I	48	GLU
8	1I	77	LEU
8	1I	78	THR
8	1I	85	GLU
8	1I	86	THR
8	1I	92	VAL
8	1I	101	LEU
8	1I	108	THR
8	1I	123	LEU
8	1I	129	THR
8	1I	140	LEU
9	1N	1	MET
9	1N	9	VAL
9	1N	10	GLU
9	1N	14	VAL
9	1N	28	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	1N	48	MET
9	1N	62	VAL
9	1N	68	GLU
9	1N	138	LEU
10	1O	20	MET
11	1P	2	LYS
11	1P	45	LEU
11	1P	75	ILE
11	1P	98	GLU
11	1P	125	VAL
11	1P	133	SER
11	1P	149	GLU
12	1Q	1	MET
12	1Q	75	THR
12	1Q	109	VAL
13	1R	36	THR
13	1R	67	LEU
13	1R	111	LEU
13	1R	114	VAL
13	1R	117	VAL
14	1S	14	VAL
14	1S	46	VAL
14	1S	69	VAL
14	1S	73	LEU
14	1S	85	VAL
15	1T	23	ARG
15	1T	28	VAL
15	1T	34	VAL
15	1T	49	VAL
15	1T	85	LYS
15	1T	96	ARG
16	1U	8	VAL
16	1U	74	LEU
16	1U	84	LYS
16	1U	95	LEU
17	1V	79	VAL
17	1V	100	ARG
18	1W	4	LYS
18	1W	11	ARG
18	1W	17	VAL
18	1W	92	ARG
19	1X	38	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	1X	66	LEU
19	1X	72	LYS
19	1X	81	VAL
20	1Y	1	MET
20	1Y	7	VAL
20	1Y	9	LYS
20	1Y	21	LYS
20	1Y	26	LYS
20	1Y	43	ASN
20	1Y	44	ILE
20	1Y	50	ARG
20	1Y	64	GLU
20	1Y	72	VAL
20	1Y	91	GLU
20	1Y	99	CYS
21	1Z	1	MET
21	1Z	33	LEU
21	1Z	42	VAL
21	1Z	72	ARG
21	1Z	124	ILE
21	1Z	126	VAL
21	1Z	132	ASN
21	1Z	154	ASP
21	1Z	155	LEU
21	1Z	170	THR
21	1Z	171	ILE
22	10	10	THR
22	10	82	ARG
23	11	46	LEU
23	11	56	GLN
24	12	43	GLN
25	13	23	LEU
25	13	32	GLN
25	13	34	GLU
25	13	54	VAL
25	13	58	VAL
25	13	60	GLU
26	14	21	VAL
26	14	22	ILE
26	14	33	VAL
26	14	49	PHE
26	14	53	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	14	56	VAL
26	14	66	SER
26	14	69	LYS
27	15	6	VAL
27	15	40	LYS
28	16	5	VAL
28	16	6	ARG
28	16	14	THR
28	16	19	ARG
28	16	35	GLU
28	16	51	GLU
29	17	24	THR
29	17	29	LYS
29	17	43	THR
29	17	46	VAL
30	18	14	VAL
30	18	39	LYS
33	1b	8	LYS
33	1b	12	GLU
33	1b	15	VAL
33	1b	19	HIS
33	1b	21	ARG
33	1b	35	GLU
33	1b	39	ILE
33	1b	48	MET
33	1b	54	THR
33	1b	78	GLN
33	1b	80	ILE
33	1b	93	VAL
33	1b	145	LEU
33	1b	153	ARG
33	1b	164	VAL
33	1b	170	GLU
33	1b	185	ILE
33	1b	208	ILE
33	1b	215	LEU
33	1b	217	ARG
33	1b	229	VAL
33	1b	230	VAL
34	1c	3	ASN
34	1c	5	ILE
34	1c	33	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	1c	46	GLU
34	1c	49	SER
34	1c	66	VAL
34	1c	70	VAL
34	1c	89	GLU
34	1c	132	ARG
34	1c	165	THR
34	1c	172	ARG
34	1c	195	VAL
34	1c	198	VAL
34	1c	206	GLU
34	1c	207	VAL
35	1d	19	LEU
35	1d	21	LEU
35	1d	56	VAL
35	1d	59	ARG
35	1d	76	ARG
35	1d	88	VAL
35	1d	112	VAL
35	1d	135	LEU
35	1d	182	LYS
35	1d	194	LEU
36	1e	10	MET
36	1e	13	ILE
36	1e	41	VAL
36	1e	79	GLU
36	1e	98	THR
36	1e	126	ARG
36	1e	149	GLU
37	1f	10	LEU
37	1f	19	LEU
37	1f	36	ARG
37	1f	37	VAL
37	1f	45	LEU
37	1f	57	GLN
37	1f	72	VAL
37	1f	75	LEU
37	1f	92	LYS
38	1g	9	VAL
38	1g	16	LEU
38	1g	32	ARG
38	1g	59	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	1g	61	VAL
38	1g	72	ARG
38	1g	77	SER
38	1g	80	VAL
38	1g	90	GLU
38	1g	97	GLN
38	1g	104	LEU
38	1g	113	GLU
38	1g	114	ARG
38	1g	155	ARG
39	1h	24	THR
39	1h	32	LYS
39	1h	38	ILE
39	1h	51	VAL
39	1h	52	ASP
39	1h	127	LEU
39	1h	133	LEU
40	1i	14	VAL
40	1i	23	ASN
40	1i	26	VAL
40	1i	27	THR
40	1i	41	VAL
40	1i	48	GLU
40	1i	60	ASP
40	1i	63	ILE
40	1i	64	THR
40	1i	92	TYR
40	1i	104	ARG
40	1i	127	LYS
40	1i	128	ARG
41	1j	38	ILE
41	1j	44	VAL
41	1j	46	ARG
41	1j	51	ARG
41	1j	72	VAL
41	1j	81	THR
41	1j	92	THR
41	1j	95	GLU
41	1j	98	ILE
42	1k	14	VAL
42	1k	48	ILE
42	1k	87	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
42	1k	95	ILE
42	1k	114	VAL
43	1l	36	VAL
43	1l	57	LYS
43	1l	62	SER
43	1l	78	GLN
43	1l	83	VAL
43	1l	97	ARG
43	1l	100	ILE
43	1l	118	SER
44	1m	3	ARG
44	1m	4	ILE
44	1m	11	ARG
44	1m	32	GLU
44	1m	43	THR
44	1m	52	GLU
44	1m	60	VAL
44	1m	106	ASN
44	1m	109	THR
44	1m	122	LYS
45	1n	3	ARG
45	1n	6	LEU
45	1n	15	LYS
45	1n	18	VAL
45	1n	25	VAL
45	1n	53	LEU
46	1o	84	LYS
46	1o	88	ARG
47	1p	5	ARG
47	1p	20	VAL
47	1p	60	LEU
47	1p	61	SER
47	1p	67	THR
48	1q	7	THR
48	1q	10	VAL
48	1q	11	VAL
48	1q	19	VAL
48	1q	60	ILE
48	1q	98	LEU
49	1r	37	VAL
49	1r	47	THR
49	1r	84	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	1r	85	LEU
50	1s	12	ASP
50	1s	15	LEU
50	1s	33	THR
50	1s	41	VAL
50	1s	48	THR
50	1s	56	GLN
51	1t	10	LEU
51	1t	24	LEU
51	1t	100	ILE
3	2D	3	VAL
3	2D	37	LEU
3	2D	39	LYS
3	2D	61	LEU
3	2D	71	ASP
3	2D	99	ASP
3	2D	142	VAL
3	2D	147	LEU
3	2D	181	GLU
3	2D	229	VAL
3	2D	242	ARG
3	2D	259	THR
4	2E	21	VAL
4	2E	55	ASN
4	2E	77	ILE
4	2E	78	LEU
4	2E	91	VAL
4	2E	116	VAL
4	2E	181	LEU
4	2E	184	VAL
4	2E	195	LEU
5	2F	9	ILE
5	2F	17	ARG
5	2F	19	GLU
5	2F	33	LEU
5	2F	74	ARG
5	2F	112	MET
5	2F	124	LEU
5	2F	149	ASP
5	2F	154	VAL
5	2F	158	THR
5	2F	162	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	2F	165	ARG
5	2F	175	THR
5	2F	196	LEU
5	2F	201	VAL
6	2G	18	GLU
6	2G	43	LEU
6	2G	45	GLU
6	2G	53	LEU
6	2G	62	LEU
6	2G	77	ILE
6	2G	116	ASP
6	2G	126	ASP
6	2G	140	ILE
6	2G	149	VAL
6	2G	162	THR
6	2G	165	THR
7	2H	7	LEU
7	2H	23	ARG
7	2H	26	VAL
7	2H	44	VAL
7	2H	45	VAL
7	2H	58	GLU
7	2H	63	SER
7	2H	85	LYS
7	2H	92	ILE
7	2H	95	ARG
7	2H	114	VAL
7	2H	124	GLU
7	2H	134	SER
7	2H	136	ILE
7	2H	139	GLN
7	2H	153	LYS
8	2I	20	ASP
8	2I	38	LEU
8	2I	58	LEU
8	2I	92	VAL
8	2I	101	LEU
8	2I	102	SER
8	2I	104	GLN
8	2I	117	GLU
8	2I	127	VAL
9	2N	1	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	2N	5	VAL
9	2N	48	MET
9	2N	61	ARG
9	2N	62	VAL
9	2N	68	GLU
9	2N	83	LYS
9	2N	138	LEU
10	2O	28	SER
10	2O	42	SER
10	2O	69	ILE
10	2O	77	ILE
10	2O	92	GLU
10	2O	108	GLU
10	2O	116	SER
11	2P	1	MET
11	2P	4	SER
11	2P	45	LEU
11	2P	77	ARG
11	2P	98	GLU
11	2P	135	LEU
11	2P	147	LEU
11	2P	148	LEU
11	2P	149	GLU
12	2Q	7	MET
12	2Q	38	GLU
12	2Q	96	VAL
12	2Q	106	VAL
12	2Q	109	VAL
13	2R	36	THR
13	2R	67	LEU
13	2R	111	LEU
13	2R	114	VAL
14	2S	58	LEU
14	2S	63	THR
14	2S	64	GLU
14	2S	75	GLU
14	2S	110	LEU
15	2T	9	LEU
15	2T	19	LEU
15	2T	40	THR
15	2T	63	VAL
15	2T	72	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	2T	96	ARG
15	2T	107	ASP
15	2T	115	ARG
15	2T	121	ILE
16	2U	8	VAL
16	2U	31	SER
16	2U	74	LEU
16	2U	84	LYS
16	2U	95	LEU
17	2V	33	VAL
17	2V	35	LEU
17	2V	53	GLU
17	2V	61	VAL
17	2V	79	VAL
17	2V	98	GLU
18	2W	11	ARG
18	2W	17	VAL
18	2W	21	VAL
19	2X	38	GLU
19	2X	82	GLN
20	2Y	1	MET
20	2Y	7	VAL
20	2Y	9	LYS
20	2Y	11	ASP
20	2Y	21	LYS
20	2Y	39	VAL
20	2Y	72	VAL
20	2Y	75	ILE
20	2Y	90	LEU
20	2Y	99	CYS
21	2Z	6	LYS
21	2Z	30	ASN
21	2Z	33	LEU
21	2Z	42	VAL
21	2Z	60	GLU
21	2Z	71	VAL
21	2Z	74	VAL
21	2Z	91	LEU
21	2Z	94	GLU
21	2Z	96	VAL
21	2Z	100	VAL
21	2Z	131	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	2Z	136	PHE
21	2Z	137	ILE
21	2Z	146	ILE
21	2Z	150	LEU
21	2Z	151	HIS
21	2Z	155	LEU
21	2Z	170	THR
21	2Z	171	ILE
21	2Z	174	VAL
22	20	9	SER
22	20	80	HIS
23	21	40	ARG
23	21	46	LEU
23	21	69	LYS
23	21	78	LYS
23	21	80	LEU
23	21	85	LEU
24	22	4	SER
24	22	34	GLU
25	23	6	VAL
25	23	29	ARG
25	23	30	ARG
25	23	31	LEU
25	23	54	VAL
25	23	59	VAL
26	24	10	VAL
26	24	26	SER
26	24	49	PHE
26	24	56	VAL
26	24	59	PHE
26	24	61	ARG
26	24	62	ARG
26	24	67	TYR
27	25	6	VAL
27	25	40	LYS
28	26	6	ARG
28	26	9	LEU
28	26	19	ARG
29	27	1	MET
29	27	23	ARG
29	27	24	THR
29	27	43	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
29	27	46	VAL
30	28	14	VAL
30	28	19	SER
30	28	39	LYS
31	29	26	ILE
33	2b	7	VAL
33	2b	8	LYS
33	2b	9	GLU
33	2b	11	LEU
33	2b	15	VAL
33	2b	16	HIS
33	2b	37	ASN
33	2b	39	ILE
33	2b	41	ILE
33	2b	48	MET
33	2b	58	ILE
33	2b	67	THR
33	2b	71	VAL
33	2b	76	GLN
33	2b	79	ASP
33	2b	80	ILE
33	2b	83	MET
33	2b	90	MET
33	2b	94	ASN
33	2b	101	MET
33	2b	107	THR
33	2b	111	ARG
33	2b	112	VAL
33	2b	118	LEU
33	2b	126	GLU
33	2b	127	ILE
33	2b	138	LEU
33	2b	142	LEU
33	2b	143	GLU
33	2b	144	ARG
33	2b	150	SER
33	2b	162	ILE
33	2b	164	VAL
33	2b	168	THR
33	2b	185	ILE
33	2b	189	ASP
33	2b	208	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	2b	217	ARG
33	2b	223	ILE
34	2c	14	ILE
34	2c	15	THR
34	2c	30	ARG
34	2c	47	LEU
34	2c	55	VAL
34	2c	57	ILE
34	2c	85	ARG
34	2c	91	LEU
34	2c	101	LEU
34	2c	104	GLN
34	2c	138	VAL
34	2c	152	ILE
34	2c	190	ARG
34	2c	195	VAL
34	2c	202	ILE
35	2d	5	ILE
35	2d	8	VAL
35	2d	19	LEU
35	2d	28	SER
35	2d	47	ARG
35	2d	58	LEU
35	2d	59	ARG
35	2d	83	SER
35	2d	85	LYS
35	2d	94	LEU
35	2d	127	THR
35	2d	135	LEU
35	2d	155	LEU
35	2d	162	LEU
35	2d	166	LYS
35	2d	169	LYS
35	2d	178	VAL
35	2d	181	MET
35	2d	188	LEU
35	2d	194	LEU
35	2d	196	LEU
35	2d	201	GLN
36	2e	13	ILE
36	2e	24	ARG
36	2e	41	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	2e	51	VAL
36	2e	72	GLN
36	2e	147	ASP
36	2e	148	VAL
36	2e	151	LEU
37	2f	21	LEU
37	2f	70	ASP
37	2f	81	ILE
37	2f	95	GLU
38	2g	4	ARG
38	2g	9	VAL
38	2g	13	GLN
38	2g	24	THR
38	2g	33	ASP
38	2g	53	LYS
38	2g	75	VAL
38	2g	86	GLN
38	2g	97	GLN
38	2g	98	SER
38	2g	110	GLN
38	2g	113	GLU
38	2g	115	ARG
39	2h	26	VAL
39	2h	29	SER
39	2h	51	VAL
39	2h	52	ASP
39	2h	56	LYS
39	2h	86	ILE
39	2h	95	VAL
39	2h	97	VAL
39	2h	119	LEU
40	2i	14	VAL
40	2i	29	ASN
40	2i	63	ILE
40	2i	64	THR
40	2i	65	VAL
40	2i	75	ASP
40	2i	87	GLN
40	2i	99	LEU
40	2i	102	LEU
40	2i	128	ARG
41	2j	9	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	2j	30	SER
41	2j	33	GLN
41	2j	38	ILE
41	2j	66	ARG
41	2j	67	THR
41	2j	72	VAL
41	2j	74	ILE
41	2j	81	THR
41	2j	89	ASP
41	2j	92	THR
41	2j	100	THR
42	2k	14	VAL
42	2k	28	THR
42	2k	53	SER
42	2k	77	MET
42	2k	84	VAL
42	2k	114	VAL
43	2l	33	ARG
43	2l	78	GLN
43	2l	83	VAL
43	2l	97	ARG
44	2m	3	ARG
44	2m	32	GLU
44	2m	45	VAL
44	2m	47	ASP
44	2m	48	LEU
44	2m	53	VAL
44	2m	67	GLU
44	2m	70	LEU
44	2m	90	LEU
44	2m	98	VAL
44	2m	121	LYS
45	2n	3	ARG
45	2n	15	LYS
45	2n	18	VAL
45	2n	25	VAL
45	2n	33	VAL
46	2o	14	GLU
46	2o	24	SER
46	2o	64	ARG
46	2o	87	ILE
46	2o	88	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
47	2p	2	VAL
47	2p	11	SER
47	2p	21	VAL
47	2p	60	LEU
48	2q	36	ILE
48	2q	63	ARG
48	2q	76	LEU
48	2q	96	GLU
48	2q	99	SER
49	2r	26	LEU
49	2r	84	LYS
49	2r	86	VAL
50	2s	12	ASP
50	2s	21	GLU
50	2s	28	LYS
50	2s	30	LEU
50	2s	37	ARG
50	2s	41	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (133) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	166	GLN
4	1E	48	GLN
4	1E	143	ASN
4	1E	180	ASN
5	1F	8	GLN
5	1F	69	HIS
5	1F	203	GLN
6	1G	132	ASN
7	1H	74	ASN
8	1I	74	ASN
9	1N	131	GLN
12	1Q	12	GLN
12	1Q	57	HIS
13	1R	31	HIS
13	1R	71	GLN
14	1S	68	GLN
14	1S	95	HIS
15	1T	38	ASN
15	1T	58	ASN
16	1U	81	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	1U	94	ASN
19	1X	31	HIS
19	1X	82	GLN
20	1Y	43	ASN
21	1Z	34	ASN
21	1Z	73	GLN
22	10	50	ASN
23	11	56	GLN
25	13	32	GLN
33	1b	140	HIS
34	1c	6	HIS
34	1c	104	GLN
34	1c	162	GLN
34	1c	170	GLN
34	1c	181	ASN
36	1e	78	HIS
37	1f	7	ASN
37	1f	13	ASN
37	1f	100	ASN
38	1g	13	GLN
38	1g	28	ASN
40	1i	31	GLN
40	1i	34	ASN
40	1i	117	HIS
40	1i	124	GLN
41	1j	56	HIS
41	1j	62	HIS
42	1k	99	GLN
42	1k	116	HIS
43	1l	99	HIS
44	1m	92	HIS
46	1o	9	GLN
46	1o	62	GLN
47	1p	14	ASN
48	1q	26	GLN
48	1q	94	ASN
50	1s	14	HIS
50	1s	23	ASN
50	1s	47	HIS
50	1s	83	HIS
51	1t	90	GLN
3	2D	87	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	2E	48	GLN
4	2E	143	ASN
5	2F	31	HIS
5	2F	69	HIS
5	2F	75	HIS
5	2F	133	ASN
6	2G	41	GLN
7	2H	74	ASN
8	2I	104	GLN
9	2N	131	GLN
10	2O	5	GLN
12	2Q	123	HIS
13	2R	13	HIS
13	2R	61	HIS
13	2R	71	GLN
14	2S	38	GLN
15	2T	43	GLN
15	2T	58	ASN
16	2U	81	HIS
16	2U	94	ASN
18	2W	60	ASN
19	2X	82	GLN
20	2Y	6	HIS
20	2Y	43	ASN
21	2Z	32	HIS
21	2Z	55	HIS
21	2Z	65	GLN
21	2Z	73	GLN
22	20	3	HIS
23	21	56	GLN
25	23	32	GLN
26	24	46	GLN
28	26	20	ASN
28	26	49	HIS
33	2b	40	HIS
33	2b	76	GLN
33	2b	113	HIS
33	2b	135	GLN
33	2b	204	ASN
34	2c	6	HIS
34	2c	123	GLN
35	2d	77	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	2d	116	GLN
35	2d	119	GLN
35	2d	123	HIS
36	2e	78	HIS
36	2e	141	GLN
37	2f	57	GLN
37	2f	100	ASN
38	2g	13	GLN
38	2g	28	ASN
38	2g	56	GLN
38	2g	122	HIS
38	2g	148	ASN
40	2i	3	GLN
40	2i	58	HIS
40	2i	89	ASN
41	2j	33	GLN
42	2k	22	HIS
42	2k	62	GLN
42	2k	78	GLN
42	2k	104	GLN
43	2l	99	HIS
48	2q	93	GLN
50	2s	47	HIS
50	2s	56	GLN
50	2s	69	HIS
50	2s	83	HIS
51	2t	9	ASN
51	2t	16	HIS
51	2t	75	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	416 (14%)	31 (1%)
1	2A	2791/2915 (95%)	458 (16%)	25 (0%)
2	1B	119/121 (98%)	7 (5%)	0
2	2B	118/121 (97%)	20 (16%)	0
32	1a	1497/1521 (98%)	223 (14%)	0
32	2a	1501/1521 (98%)	255 (16%)	0
53	1v	12/24 (50%)	2 (16%)	0
53	2v	12/24 (50%)	3 (25%)	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
54	1w	71/76 (93%)	22 (30%)	0
54	2w	68/76 (89%)	24 (35%)	0
55	1x	75/77 (97%)	5 (6%)	0
55	2x	75/77 (97%)	8 (10%)	0
56	1y	72/76 (94%)	28 (38%)	0
56	2y	70/76 (92%)	30 (42%)	0
All	All	9345/9620 (97%)	1501 (16%)	56 (0%)

All (1501) 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	55	G
1	1A	71	A
1	1A	74	A
1	1A	75	G
1	1A	84	A
1	1A	95	G
1	1A	118	A
1	1A	119	A
1	1A	120	U
1	1A	196	A
1	1A	197	A
1	1A	205	G
1	1A	214	G
1	1A	215	G
1	1A	216	A
1	1A	222	A
1	1A	228	A
1	1A	229	A
1	1A	233	A
1	1A	248	G
1	1A	269	U
1	1A	271(C)	C
1	1A	271(K)	U
1	1A	271(L)	U
1	1A	271(M)	G
1	1A	271(N)	U
1	1A	271(O)	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	271(P)	C
1	1A	271(S)	G
1	1A	272(B)	G
1	1A	272(I)	U
1	1A	275	G
1	1A	279	C
1	1A	311	A
1	1A	327	G
1	1A	329	G
1	1A	330	A
1	1A	342	G
1	1A	352	G
1	1A	363	G
1	1A	363(B)	G
1	1A	370	G
1	1A	372	G
1	1A	386	G
1	1A	396	G
1	1A	405	U
1	1A	411	G
1	1A	428	A
1	1A	443	A
1	1A	444	C
1	1A	448	U
1	1A	455	C
1	1A	456	C
1	1A	481	G
1	1A	494	G
1	1A	504	U
1	1A	505	A
1	1A	508	G
1	1A	509	C
1	1A	514	A
1	1A	530	G
1	1A	531	C
1	1A	532	A
1	1A	533	G
1	1A	545	G
1	1A	549	G
1	1A	563	G
1	1A	573	G
1	1A	575	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	586	A
1	1A	603	A
1	1A	604	G
1	1A	607	U
1	1A	615	G
1	1A	627	A
1	1A	637	A
1	1A	645	C
1	1A	646	A
1	1A	652(E)	G
1	1A	652(F)	G
1	1A	652(T)	C
1	1A	668	G
1	1A	686	G
1	1A	717	G
1	1A	730	C
1	1A	740	U
1	1A	762	U
1	1A	764	A
1	1A	765	G
1	1A	775	G
1	1A	776	G
1	1A	782	A
1	1A	784	A
1	1A	785	G
1	1A	790	C
1	1A	792	G
1	1A	805	G
1	1A	812	C
1	1A	819	A
1	1A	827	U
1	1A	828	U
1	1A	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	885	C
1	1A	886	C
1	1A	887	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	888	C
1	1A	889	C
1	1A	890	A
1	1A	893	C
1	1A	896	A
1	1A	897	C
1	1A	899	A
1	1A	907	U
1	1A	910	A
1	1A	932	G
1	1A	945	A
1	1A	946	G
1	1A	953	A
1	1A	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	1022	G
1	1A	1026	U
1	1A	1027	A
1	1A	1033	U
1	1A	1041	C
1	1A	1046	A
1	1A	1047	G
1	1A	1054	A
1	1A	1055	G
1	1A	1058	G
1	1A	1059	G
1	1A	1063	G
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	1081	U
1	1A	1082	U
1	1A	1085	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1087	G
1	1A	1088	A
1	1A	1089	G
1	1A	1090	U
1	1A	1091	G
1	1A	1093	G
1	1A	1094	U
1	1A	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	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	1244	G
1	1A	1253	A
1	1A	1256	G
1	1A	1271	G
1	1A	1272	A
1	1A	1273	U
1	1A	1300	U
1	1A	1301	A
1	1A	1303	G
1	1A	1313	U
1	1A	1321	A
1	1A	1345	C
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1386	C
1	1A	1395	A
1	1A	1396	U
1	1A	1416	G
1	1A	1417	C
1	1A	1420	U
1	1A	1421	G
1	1A	1428	C
1	1A	1445	A
1	1A	1450	G
1	1A	1455	G
1	1A	1459	G
1	1A	1467	C
1	1A	1482	G
1	1A	1493	C
1	1A	1494	A
1	1A	1496	A
1	1A	1509	C
1	1A	1509(A)	A
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	1610	A
1	1A	1616	A
1	1A	1647	G
1	1A	1648	C
1	1A	1664	A
1	1A	1674	G
1	1A	1696	G
1	1A	1700	A
1	1A	1701	A
1	1A	1703	G
1	1A	1722	A
1	1A	1739	U
1	1A	1745	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1756	G
1	1A	1763	G
1	1A	1764	G
1	1A	1773	A
1	1A	1780	A
1	1A	1782	C
1	1A	1791	A
1	1A	1800	C
1	1A	1801	G
1	1A	1812	A
1	1A	1816	G
1	1A	1817	G
1	1A	1829	A
1	1A	1839	G
1	1A	1847	A
1	1A	1848	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	2032	G
1	1A	2033	A
1	1A	2043	C
1	1A	2055	C
1	1A	2056	G
1	1A	2060	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2061	G
1	1A	2062	A
1	1A	2069	G
1	1A	2101	G
1	1A	2102	U
1	1A	2107	C
1	1A	2108	C
1	1A	2113	U
1	1A	2116	G
1	1A	2121	G
1	1A	2127	G
1	1A	2131	G
1	1A	2132	U
1	1A	2133	G
1	1A	2134	A
1	1A	2135	A
1	1A	2136	C
1	1A	2142	C
1	1A	2143	C
1	1A	2144	U
1	1A	2145	C
1	1A	2146	C
1	1A	2147	G
1	1A	2148	G
1	1A	2150	U
1	1A	2151	G
1	1A	2155	G
1	1A	2156	G
1	1A	2157	G
1	1A	2158	A
1	1A	2159	G
1	1A	2161	C
1	1A	2163	C
1	1A	2165	G
1	1A	2166	G
1	1A	2167	U
1	1A	2168	G
1	1A	2171	A
1	1A	2172	U
1	1A	2173	A
1	1A	2174	C
1	1A	2181	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2182	G
1	1A	2184	G
1	1A	2189	U
1	1A	2192	G
1	1A	2198	A
1	1A	2206	G
1	1A	2207	G
1	1A	2225	A
1	1A	2238	G
1	1A	2239	G
1	1A	2268	A
1	1A	2269	A
1	1A	2283	C
1	1A	2287	A
1	1A	2289	G
1	1A	2305	A
1	1A	2308	G
1	1A	2312	U
1	1A	2320	A
1	1A	2325	G
1	1A	2334	G
1	1A	2336	A
1	1A	2347	C
1	1A	2350	C
1	1A	2354	G
1	1A	2361	A
1	1A	2372	G
1	1A	2383	G
1	1A	2385	C
1	1A	2406	U
1	1A	2410	G
1	1A	2422	A
1	1A	2424	C
1	1A	2425	A
1	1A	2429	G
1	1A	2430	A
1	1A	2435	A
1	1A	2439	A
1	1A	2440	C
1	1A	2441	C
1	1A	2447	G
1	1A	2448	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2468	G
1	1A	2476	A
1	1A	2477	C
1	1A	2491	U
1	1A	2502	G
1	1A	2505	G
1	1A	2518	A
1	1A	2529	G
1	1A	2549	G
1	1A	2554	U
1	1A	2566	A
1	1A	2567	G
1	1A	2573	C
1	1A	2585	U
1	1A	2602	A
1	1A	2611	U
1	1A	2612	C
1	1A	2629	A
1	1A	2630	G
1	1A	2654	A
1	1A	2663	G
1	1A	2689	U
1	1A	2690	C
1	1A	2691	C
1	1A	2702	U
1	1A	2712(A)	A
1	1A	2713	A
1	1A	2714	G
1	1A	2726	U
1	1A	2733	A
1	1A	2764	A
1	1A	2765	A
1	1A	2778	A
1	1A	2790	A
1	1A	2791	C
1	1A	2794	C
1	1A	2802	G
1	1A	2803	C
1	1A	2805	G
1	1A	2818	G
1	1A	2820	A
1	1A	2821	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2835	A
1	1A	2836	U
1	1A	2872	G
1	1A	2880	C
1	1A	2892	A
1	1A	2894	G
1	1A	2895	U
2	1B	2	C
2	1B	13	A
2	1B	56	G
2	1B	67	G
2	1B	73	A
2	1B	84	C
2	1B	110	G
32	1a	7	G
32	1a	9	G
32	1a	32	A
32	1a	39	G
32	1a	48	C
32	1a	50	A
32	1a	51	A
32	1a	54	C
32	1a	61	G
32	1a	77	G
32	1a	79	G
32	1a	91	C
32	1a	98	G
32	1a	115	G
32	1a	116	A
32	1a	121	C
32	1a	131	C
32	1a	163	C
32	1a	164	U
32	1a	174	C
32	1a	182	U
32	1a	189(A)	C
32	1a	189(F)	U
32	1a	189(G)	G
32	1a	195	A
32	1a	201	C
32	1a	203	U
32	1a	204	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	243	A
32	1a	247	G
32	1a	251	G
32	1a	262	A
32	1a	266	G
32	1a	267	C
32	1a	289	G
32	1a	306	G
32	1a	321	A
32	1a	328	C
32	1a	332	G
32	1a	342	C
32	1a	348	G
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	367	U
32	1a	372	C
32	1a	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	424	G
32	1a	429	U
32	1a	439	A
32	1a	442	C
32	1a	443	C
32	1a	446	G
32	1a	452	A
32	1a	461	A
32	1a	470	C
32	1a	485	G
32	1a	495	A
32	1a	496	A
32	1a	498	U
32	1a	509	A
32	1a	510	A
32	1a	511	C
32	1a	518	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	521	G
32	1a	524	G
32	1a	527	G7M
32	1a	531	U
32	1a	532	A
32	1a	547	A
32	1a	559	A
32	1a	561	U
32	1a	568	G
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	577	G
32	1a	587	G
32	1a	630	G
32	1a	653	A
32	1a	657	G
32	1a	665	A
32	1a	666	G
32	1a	671	G
32	1a	672	U
32	1a	687	A
32	1a	688	G
32	1a	695	A
32	1a	703	G
32	1a	723	U
32	1a	731	G
32	1a	749	C
32	1a	755	G
32	1a	760	G
32	1a	777	A
32	1a	793	U
32	1a	794	A
32	1a	815	A
32	1a	817	C
32	1a	821	G
32	1a	827	U
32	1a	828	A
32	1a	836	G
32	1a	840	C
32	1a	841	U
32	1a	851	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	859	A
32	1a	873	A
32	1a	902	G
32	1a	914	A
32	1a	926	G
32	1a	927	G
32	1a	934	C
32	1a	942	G
32	1a	960	U
32	1a	961	U
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	992	U
32	1a	993	G
32	1a	996	A
32	1a	999	C
32	1a	1000	U
32	1a	1001(A)	G
32	1a	1002	G
32	1a	1003	G
32	1a	1005	A
32	1a	1006	C
32	1a	1020	U
32	1a	1022	G
32	1a	1023	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C
32	1a	1028	C
32	1a	1029	C
32	1a	1030	C
32	1a	1030(A)	G
32	1a	1030(C)	G
32	1a	1031	G
32	1a	1039	C
32	1a	1043	C
32	1a	1044	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	1046	A
32	1a	1066	C
32	1a	1068	G
32	1a	1081	G
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1123	A
32	1a	1124	G
32	1a	1134	G
32	1a	1137	C
32	1a	1138	G
32	1a	1139	G
32	1a	1144	G
32	1a	1146	A
32	1a	1152	A
32	1a	1157	A
32	1a	1159	U
32	1a	1184	G
32	1a	1196	U
32	1a	1197	G
32	1a	1201	A
32	1a	1202	G
32	1a	1212	U
32	1a	1213	A
32	1a	1227	A
32	1a	1236	A
32	1a	1238	A
32	1a	1240	U
32	1a	1241	G
32	1a	1253	G
32	1a	1256	A
32	1a	1257	U
32	1a	1262	C
32	1a	1270	C
32	1a	1275	A
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A
32	1a	1300	G
32	1a	1302	U
32	1a	1305	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	1320	C
32	1a	1338	G
32	1a	1340	A
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1364	U
32	1a	1370	G
32	1a	1394	A
32	1a	1406	U
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1446	U
32	1a	1447	A
32	1a	1452	C
32	1a	1456	G
32	1a	1469	G
32	1a	1487	G
32	1a	1492	A
32	1a	1503	A
32	1a	1504	G
32	1a	1506	U
32	1a	1517	G
32	1a	1529	G
32	1a	1530	G
53	1v	13	A
53	1v	24	A
54	1w	2	C
54	1w	6	G
54	1w	11	C
54	1w	12	U
54	1w	15	G
54	1w	19	G
54	1w	20	U
54	1w	21	A
54	1w	23	A
54	1w	24	G
54	1w	34	G
54	1w	45	U
54	1w	46	G7M

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	1w	47	U
54	1w	48	C
54	1w	50	U
54	1w	66	U
54	1w	68	C
54	1w	69	G
54	1w	70	G
54	1w	73	A
54	1w	74	C
55	1x	9	G
55	1x	19	G
55	1x	21	A
55	1x	47	U
55	1x	61	C
56	1y	5	G
56	1y	7	A
56	1y	8	4SU
56	1y	9	A
56	1y	14	A
56	1y	19	G
56	1y	20	U
56	1y	21	A
56	1y	22	G
56	1y	35	A
56	1y	36	A
56	1y	39	PSU
56	1y	43	C
56	1y	44	G
56	1y	45	U
56	1y	46	G7M
56	1y	47	U
56	1y	48	C
56	1y	49	C
56	1y	53	G
56	1y	56	C
56	1y	57	G
56	1y	58	A
56	1y	59	U
56	1y	69	G
56	1y	70	G
56	1y	71	G
56	1y	76	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	12	U
1	2A	15	G
1	2A	34	C
1	2A	35	G
1	2A	45	C
1	2A	64	A
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	83	G
1	2A	84	A
1	2A	92	A
1	2A	95	G
1	2A	100	G
1	2A	102	G
1	2A	118	A
1	2A	119	A
1	2A	120	U
1	2A	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	197	A
1	2A	199	A
1	2A	205	G
1	2A	215	G
1	2A	216	A
1	2A	221	A
1	2A	222	A
1	2A	228	A
1	2A	229	A
1	2A	230	U
1	2A	233	A
1	2A	248	G
1	2A	250	G
1	2A	266	G
1	2A	267	C
1	2A	271(J)	C
1	2A	271(K)	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	271(O)	C
1	2A	271(P)	C
1	2A	272	G
1	2A	272(B)	G
1	2A	274	G
1	2A	277	C
1	2A	278	A
1	2A	283	A
1	2A	311	A
1	2A	324	A
1	2A	327	G
1	2A	329	G
1	2A	330	A
1	2A	342	G
1	2A	352	G
1	2A	357	A
1	2A	363	G
1	2A	363(B)	G
1	2A	386	G
1	2A	396	G
1	2A	405	U
1	2A	411	G
1	2A	412	A
1	2A	421	U
1	2A	443	A
1	2A	444	C
1	2A	455	C
1	2A	456	C
1	2A	457	A
1	2A	481	G
1	2A	501	A
1	2A	505	A
1	2A	508	G
1	2A	509	C
1	2A	528	A
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	556	G
1	2A	563	G
1	2A	568	U
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	606	U
1	2A	607	U
1	2A	615	G
1	2A	616	G
1	2A	627	A
1	2A	637	A
1	2A	645	C
1	2A	646	A
1	2A	648	G
1	2A	651	G
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	669	G
1	2A	686	G
1	2A	717	G
1	2A	730	C
1	2A	752	A
1	2A	753	C
1	2A	771	G
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	790	C
1	2A	792	G
1	2A	805	G
1	2A	812	C
1	2A	819	A
1	2A	827	U
1	2A	828	U
1	2A	859	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	866	A
1	2A	874	G
1	2A	875	G
1	2A	879	G
1	2A	880	G
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	892	G
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	959	A
1	2A	961	C
1	2A	974	G
1	2A	975	C
1	2A	980	A
1	2A	983	A
1	2A	996	A
1	2A	1005	C
1	2A	1012	U
1	2A	1013	C
1	2A	1020	A
1	2A	1021	A
1	2A	1022	G
1	2A	1025	G
1	2A	1026	U
1	2A	1027	A
1	2A	1033	U
1	2A	1038	C
1	2A	1039	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1041	C
1	2A	1043	C
1	2A	1114	G
1	2A	1117	G
1	2A	1128	A
1	2A	1129	A
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1139	G
1	2A	1155	A
1	2A	1171	G
1	2A	1188	U
1	2A	1195	G
1	2A	1211	U
1	2A	1220	A
1	2A	1230	C
1	2A	1236	G
1	2A	1244	G
1	2A	1247	A
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1273	U
1	2A	1286	A
1	2A	1300	U
1	2A	1301	A
1	2A	1314	C
1	2A	1321	A
1	2A	1352	U
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1368	G
1	2A	1370	C
1	2A	1384	A
1	2A	1385	G
1	2A	1386	C
1	2A	1416	G
1	2A	1417	C
1	2A	1421	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1428	C
1	2A	1437	C
1	2A	1445	A
1	2A	1449	A
1	2A	1450	G
1	2A	1455	G
1	2A	1460	A
1	2A	1461	G
1	2A	1465	G
1	2A	1467	C
1	2A	1471	A
1	2A	1472	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	1505	C
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1531	C
1	2A	1532	C
1	2A	1533	G
1	2A	1542	A
1	2A	1547	C
1	2A	1554	A
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	1587	A
1	2A	1595	G
1	2A	1608	A
1	2A	1609	A
1	2A	1640	C
1	2A	1648	C
1	2A	1653	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1654	A
1	2A	1664	A
1	2A	1674	G
1	2A	1696	G
1	2A	1700	A
1	2A	1721	G
1	2A	1722	A
1	2A	1739	U
1	2A	1740	G
1	2A	1741	A
1	2A	1746	G
1	2A	1756	G
1	2A	1758	G
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A
1	2A	1780	A
1	2A	1782	C
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1816	G
1	2A	1829	A
1	2A	1847	A
1	2A	1848	A
1	2A	1877	A
1	2A	1878	G
1	2A	1889	A
1	2A	1900	A
1	2A	1906	G
1	2A	1929	G
1	2A	1930	G
1	2A	1936	A
1	2A	1938	A
1	2A	1940	U
1	2A	1955	U
1	2A	1963	U
1	2A	1965	C
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1972	A
1	2A	1984	G
1	2A	1993	U
1	2A	1996	C
1	2A	1997	G
1	2A	2020	A
1	2A	2023	G
1	2A	2031	A
1	2A	2032	G
1	2A	2033	A
1	2A	2043	C
1	2A	2049	G
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2062	A
1	2A	2069	G
1	2A	2099	U
1	2A	2101	G
1	2A	2110	G
1	2A	2111	C
1	2A	2116	G
1	2A	2117	A
1	2A	2120	G
1	2A	2122	U
1	2A	2125	G
1	2A	2126	A
1	2A	2127	G
1	2A	2128	C
1	2A	2129	C
1	2A	2130	U
1	2A	2131	G
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2135	A
1	2A	2136	C
1	2A	2137	C
1	2A	2138	C
1	2A	2139	C
1	2A	2141	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2142	C
1	2A	2145	C
1	2A	2146	C
1	2A	2148	G
1	2A	2149	G
1	2A	2150	U
1	2A	2151	G
1	2A	2156	G
1	2A	2157	G
1	2A	2158	A
1	2A	2161	C
1	2A	2166	G
1	2A	2167	U
1	2A	2168	G
1	2A	2169	A
1	2A	2172	U
1	2A	2173	A
1	2A	2174	C
1	2A	2178	C
1	2A	2180	U
1	2A	2185	C
1	2A	2189	U
1	2A	2192	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2218	U
1	2A	2225	A
1	2A	2239	G
1	2A	2268	A
1	2A	2275	C
1	2A	2278	A
1	2A	2280	G
1	2A	2283	C
1	2A	2287	A
1	2A	2305	A
1	2A	2308	G
1	2A	2319	G
1	2A	2320	A
1	2A	2325	G
1	2A	2334	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2336	A
1	2A	2347	C
1	2A	2350	C
1	2A	2354	G
1	2A	2383	G
1	2A	2385	C
1	2A	2406	U
1	2A	2425	A
1	2A	2429	G
1	2A	2430	A
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2448	A
1	2A	2465	C
1	2A	2468	G
1	2A	2469	A
1	2A	2476	A
1	2A	2480	C
1	2A	2487	G
1	2A	2491	U
1	2A	2494	G
1	2A	2502	G
1	2A	2505	G
1	2A	2506	U
1	2A	2507	C
1	2A	2518	A
1	2A	2525	G
1	2A	2529	G
1	2A	2530	A
1	2A	2554	U
1	2A	2564	A
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2578	G
1	2A	2582	G
1	2A	2585	U
1	2A	2602	A
1	2A	2609	U
1	2A	2611	U
1	2A	2612	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2630	G
1	2A	2634	G
1	2A	2646	C
1	2A	2654	A
1	2A	2656	U
1	2A	2667	C
1	2A	2689	U
1	2A	2690	C
1	2A	2702	U
1	2A	2703	C
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2726	U
1	2A	2733	A
1	2A	2748	A
1	2A	2751	G
1	2A	2752	C
1	2A	2764	A
1	2A	2765	A
1	2A	2766	G
1	2A	2778	A
1	2A	2789	C
1	2A	2793	G
1	2A	2802	G
1	2A	2803	C
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2825	C
1	2A	2833	G
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	4	C
2	2B	9	G
2	2B	13	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2B	19	G
2	2B	20	C
2	2B	23	G
2	2B	40	U
2	2B	42	C
2	2B	51	G
2	2B	53	A
2	2B	56	G
2	2B	73	A
2	2B	74	U
2	2B	75	G
2	2B	88	C
2	2B	105	A
2	2B	107	G
2	2B	110	G
2	2B	120	A
32	2a	9	G
32	2a	22	G
32	2a	32	A
32	2a	33	A
32	2a	39	G
32	2a	45	U
32	2a	47	C
32	2a	48	C
32	2a	50	A
32	2a	51	A
32	2a	66	G
32	2a	73	G
32	2a	88	A
32	2a	89	C
32	2a	101	A
32	2a	116	A
32	2a	121	C
32	2a	131	C
32	2a	163	C
32	2a	182	U
32	2a	189	G
32	2a	189(B)	C
32	2a	195	A
32	2a	197	A
32	2a	201	C
32	2a	202	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	203	U
32	2a	204	U
32	2a	216	G
32	2a	220	G
32	2a	231	G
32	2a	247	G
32	2a	251	G
32	2a	258	G
32	2a	266	G
32	2a	267	C
32	2a	289	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	355	C
32	2a	367	U
32	2a	372	C
32	2a	373	A
32	2a	384	G
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	412	A
32	2a	413	G
32	2a	421	U
32	2a	424	G
32	2a	429	U
32	2a	439	A
32	2a	442	C
32	2a	452	A
32	2a	461	A
32	2a	470	C
32	2a	485	G
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	509	A
32	2a	510	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	511	C
32	2a	518	C
32	2a	519	C
32	2a	528	C
32	2a	531	U
32	2a	532	A
32	2a	533	A
32	2a	536	C
32	2a	547	A
32	2a	559	A
32	2a	561	U
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	607	A
32	2a	630	G
32	2a	631	G
32	2a	650	G
32	2a	653	A
32	2a	665	A
32	2a	687	A
32	2a	688	G
32	2a	695	A
32	2a	703	G
32	2a	721	G
32	2a	723	U
32	2a	731	G
32	2a	749	C
32	2a	755	G
32	2a	773	G
32	2a	774	G
32	2a	777	A
32	2a	793	U
32	2a	794	A
32	2a	816	A
32	2a	817	C
32	2a	821	G
32	2a	827	U
32	2a	828	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	840	C
32	2a	841	U
32	2a	851	G
32	2a	859	A
32	2a	873	A
32	2a	874	G
32	2a	884	U
32	2a	902	G
32	2a	914	A
32	2a	926	G
32	2a	927	G
32	2a	934	C
32	2a	935	A
32	2a	936	C
32	2a	958	A
32	2a	960	U
32	2a	961	U
32	2a	963	G
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	972	C
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	978	A
32	2a	990	C
32	2a	991	U
32	2a	992	U
32	2a	993	G
32	2a	996	A
32	2a	997	U
32	2a	999	C
32	2a	1002	G
32	2a	1005	A
32	2a	1006	C
32	2a	1009	G
32	2a	1011	G
32	2a	1020	U
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	1032	G
32	2a	1035	A
32	2a	1037	C
32	2a	1039	C
32	2a	1040	U
32	2a	1044	A
32	2a	1046	A
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	1077	G
32	2a	1081	G
32	2a	1092	A
32	2a	1093	A
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A
32	2a	1108	G
32	2a	1117	G
32	2a	1121	U
32	2a	1125	U
32	2a	1129	C
32	2a	1133	G
32	2a	1135	U
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1140	C
32	2a	1146	A
32	2a	1152	A
32	2a	1155	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1157	A
32	2a	1159	U
32	2a	1160	G
32	2a	1172	C
32	2a	1182	G
32	2a	1184	G
32	2a	1196	U
32	2a	1197	G
32	2a	1201	A
32	2a	1202	G
32	2a	1210	C
32	2a	1213	A
32	2a	1227	A
32	2a	1238	A
32	2a	1240	U
32	2a	1241	G
32	2a	1256	A
32	2a	1257	U
32	2a	1258	G
32	2a	1260	C
32	2a	1270	C
32	2a	1272	G
32	2a	1273	G
32	2a	1279	A
32	2a	1280	A
32	2a	1287	A
32	2a	1299	A
32	2a	1300	G
32	2a	1302	U
32	2a	1303	C
32	2a	1305	G
32	2a	1306	A
32	2a	1320	C
32	2a	1323	G
32	2a	1338	G
32	2a	1340	A
32	2a	1346	A
32	2a	1347	G
32	2a	1353	G
32	2a	1363	C
32	2a	1363(A)	A
32	2a	1368	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1381	U
32	2a	1394	A
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1442(B)	A
32	2a	1447	A
32	2a	1452	C
32	2a	1456	G
32	2a	1492	A
32	2a	1497	G
32	2a	1503	A
32	2a	1504	G
32	2a	1506	U
32	2a	1517	G
32	2a	1529	G
32	2a	1530	G
32	2a	1531	A
32	2a	1532	U
53	2v	13	A
53	2v	14	A
53	2v	24	A
54	2w	3	C
54	2w	4	C
54	2w	5	G
54	2w	11	C
54	2w	12	U
54	2w	13	C
54	2w	14	A
54	2w	19	G
54	2w	22	G
54	2w	46	G7M
54	2w	48	C
54	2w	50	U
54	2w	51	U
54	2w	61	C
54	2w	62	C
54	2w	63	G
54	2w	65	G
54	2w	66	U
54	2w	67	C
54	2w	69	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	2w	70	G
54	2w	72	C
54	2w	73	A
54	2w	74	C
55	2x	9	G
55	2x	10	G
55	2x	21	A
55	2x	47	U
55	2x	48	C
55	2x	52	G
55	2x	53	G
55	2x	61	C
56	2y	7	A
56	2y	12	U
56	2y	14	A
56	2y	15	G
56	2y	19	G
56	2y	25	C
56	2y	26	A
56	2y	27	G
56	2y	36	A
56	2y	43	C
56	2y	45	U
56	2y	48	C
56	2y	49	C
56	2y	50	U
56	2y	51	U
56	2y	52	G
56	2y	53	G
56	2y	54	5MU
56	2y	55	PSU
56	2y	56	C
56	2y	58	A
56	2y	59	U
56	2y	60	U
56	2y	61	C
56	2y	63	G
56	2y	67	C
56	2y	68	C
56	2y	69	G
56	2y	70	G
56	2y	73	A

All (56) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	195	A
1	1A	196	A
1	1A	266	G
1	1A	278	A
1	1A	548	A
1	1A	685	A
1	1A	746	A
1	1A	764	A
1	1A	774	A
1	1A	827	U
1	1A	895	U
1	1A	974	G
1	1A	1067	A
1	1A	1174	A
1	1A	1175	U
1	1A	1176	G
1	1A	1379	A
1	1A	1420	U
1	1A	1442	G
1	1A	1508	A
1	1A	1608	A
1	1A	1762	A
1	1A	1992	G
1	1A	2134	A
1	1A	2181	G
1	1A	2183	C
1	1A	2406	U
1	1A	2439	A
1	1A	2611	U
1	1A	2629	A
1	1A	2689	U
1	2A	195	A
1	2A	196	A
1	2A	228	A
1	2A	229	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	827	U
1	2A	893	C
1	2A	900	A
1	2A	1026	U
1	2A	1210	A
1	2A	1420	U
1	2A	1442	G
1	2A	1530	C
1	2A	1608	A
1	2A	1653	G
1	2A	1992	G
1	2A	2119	A
1	2A	2126	A
1	2A	2689	U

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

88 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	4OC	1a	1402	32	20,23,24	0.79	0	25,32,35	0.86	1 (4%)
1	PSU	2A	1911	1	18,21,22	1.39	3 (16%)	21,30,33	2.23	3 (14%)
55	5MC	1x	32	55	19,22,23	1.67	3 (15%)	26,32,35	1.21	3 (11%)
43	0TD	2l	92	43	8,9,10	4.46	1 (12%)	6,11,13	4.99	3 (50%)
54	PSU	2w	55	54	18,21,22	1.41	2 (11%)	21,30,33	1.94	3 (14%)
56	5MU	2y	54	56	19,22,23	1.41	4 (21%)	27,32,35	2.21	6 (22%)
56	PSU	1y	39	56	18,21,22	1.43	2 (11%)	21,30,33	1.78	3 (14%)
55	31H	1x	76	57,55	31,34,35	1.17	3 (9%)	35,47,50	2.17	14 (40%)
56	MIA	1y	37	56	21,24,32	1.64	3 (14%)	30,35,47	2.00	7 (23%)
32	UR3	1a	1498	32	19,22,23	0.93	1 (5%)	26,32,35	1.78	3 (11%)
32	5MC	2a	967	32	19,22,23	1.65	3 (15%)	26,32,35	1.12	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
54	5MU	1w	54	54	19,22,23	1.50	5 (26%)	27,32,35	1.72	5 (18%)
1	2MU	1A	2552	1	19,22,24	1.20	2 (10%)	25,31,36	2.00	6 (24%)
1	OMC	1A	1920	1	19,22,23	0.77	0	25,31,34	0.98	1 (4%)
55	5MU	2x	54	55	19,22,23	1.44	6 (31%)	27,32,35	1.92	7 (25%)
1	5MU	2A	1915	1	19,22,23	1.43	6 (31%)	27,32,35	2.34	7 (25%)
55	31H	2x	76	57,55	31,34,35	1.23	3 (9%)	35,47,50	2.15	12 (34%)
43	0TD	1l	92	43	8,9,10	4.52	1 (12%)	6,11,13	6.01	2 (33%)
56	G7M	1y	46	56	23,26,27	1.55	4 (17%)	34,39,42	1.78	4 (11%)
1	5MC	2A	1962	1,57	19,22,23	1.52	3 (15%)	26,32,35	1.17	2 (7%)
1	5MU	2A	1939	1,57	19,22,23	1.44	6 (31%)	27,32,35	2.19	6 (22%)
54	PSU	2w	32	54	18,21,22	1.34	2 (11%)	21,30,33	1.89	3 (14%)
54	PSU	1w	39	54	18,21,22	1.43	3 (16%)	21,30,33	1.56	3 (14%)
56	PSU	2y	55	56	18,21,22	1.37	3 (16%)	21,30,33	2.01	5 (23%)
1	PSU	1A	2605	1,57	18,21,22	1.42	2 (11%)	21,30,33	2.25	3 (14%)
56	5MU	1y	54	56	19,22,23	1.42	4 (21%)	27,32,35	2.09	6 (22%)
1	8AH	1A	2503	1,57	22,26,27	1.47	5 (22%)	29,39,42	2.16	7 (24%)
54	F3N	2w	76	54,1	33,36,37	1.49	4 (12%)	41,51,54	1.73	9 (21%)
54	PSU	2w	39	54	18,21,22	1.38	2 (11%)	21,30,33	1.91	3 (14%)
32	5MC	2a	1407	32,57	19,22,23	1.61	3 (15%)	26,32,35	1.22	3 (11%)
1	5MC	1A	1942	1,57	19,22,23	1.60	3 (15%)	26,32,35	1.21	3 (11%)
1	OMC	2A	1920	1	19,22,23	0.80	1 (5%)	25,31,34	1.02	1 (4%)
56	PSU	2y	32	56	18,21,22	1.35	2 (11%)	21,30,33	2.05	3 (14%)
32	2MG	1a	1207	32,57	23,26,27	1.24	2 (8%)	33,38,41	2.22	8 (24%)
55	4SU	1x	8	55	18,21,22	2.37	6 (33%)	25,30,33	1.92	7 (28%)
32	MA6	2a	1519	32	23,26,27	0.48	0	33,38,41	2.10	9 (27%)
54	MIA	1w	37	54	28,31,32	2.30	7 (25%)	38,44,47	2.94	14 (36%)
54	PSU	1w	55	54	18,21,22	1.36	2 (11%)	21,30,33	2.06	3 (14%)
32	5MC	2a	1404	32	19,22,23	1.58	3 (15%)	26,32,35	1.13	3 (11%)
1	5MU	1A	1939	1,57	19,22,23	1.47	6 (31%)	27,32,35	2.16	6 (22%)
54	MIA	2w	37	54	24,27,32	2.14	5 (20%)	32,39,47	2.51	11 (34%)
32	5MC	1a	967	32	19,22,23	1.73	3 (15%)	26,32,35	1.15	2 (7%)
32	G7M	2a	527	32	23,26,27	1.49	4 (17%)	34,39,42	1.67	5 (14%)
32	5MC	1a	1400	32	19,22,23	1.64	3 (15%)	26,32,35	1.08	2 (7%)
32	G7M	1a	527	32	23,26,27	1.48	3 (13%)	34,39,42	1.70	5 (14%)
56	4SU	2y	8	56	18,21,22	1.82	5 (27%)	25,30,33	1.80	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
54	5MU	2w	54	54	19,22,23	1.35	4 (21%)	27,32,35	1.81	7 (25%)
56	PSU	1y	32	56	18,21,22	1.37	2 (11%)	21,30,33	1.99	3 (14%)
1	PSU	1A	1917	1	18,21,22	1.33	2 (11%)	21,30,33	2.15	4 (19%)
55	4SU	2x	8	55	18,21,22	2.07	6 (33%)	25,30,33	1.25	4 (16%)
56	PSU	2y	39	56	18,21,22	1.40	2 (11%)	21,30,33	1.74	4 (19%)
54	F3N	1w	76	54,1	33,36,37	1.49	4 (12%)	41,51,54	1.85	9 (21%)
1	PSU	2A	2605	1	18,21,22	1.24	2 (11%)	21,30,33	2.07	3 (14%)
56	G7M	2y	46	56	23,26,27	1.59	3 (13%)	34,39,42	1.79	4 (11%)
1	OMG	2A	2251	1,55	23,26,27	1.19	3 (13%)	32,38,41	2.04	6 (18%)
32	MA6	2a	1518	32	23,26,27	0.43	0	33,38,41	1.98	9 (27%)
55	5MC	2x	32	55	19,22,23	1.57	3 (15%)	26,32,35	1.24	4 (15%)
1	8AH	2A	2503	1,57	22,26,27	1.66	5 (22%)	29,39,42	2.24	5 (17%)
1	PSU	1A	1911	1	18,21,22	1.42	2 (11%)	21,30,33	1.98	3 (14%)
54	G7M	1w	46	54	23,26,27	1.57	4 (17%)	34,39,42	1.65	4 (11%)
55	5MU	1x	54	57,55	19,22,23	1.45	5 (26%)	27,32,35	1.92	7 (25%)
32	5MC	1a	1404	32	19,22,23	1.65	3 (15%)	26,32,35	1.16	2 (7%)
54	PSU	1w	32	54,57	18,21,22	1.33	2 (11%)	21,30,33	1.99	4 (19%)
32	4OC	2a	1402	32	20,23,24	0.79	0	25,32,35	1.00	1 (4%)
54	G7M	2w	46	54	23,26,27	1.52	4 (17%)	34,39,42	1.61	4 (11%)
32	MA6	1a	1519	32	23,26,27	0.47	0	33,38,41	2.14	9 (27%)
55	PSU	2x	55	55	18,21,22	1.33	2 (11%)	21,30,33	1.92	4 (19%)
54	4SU	2w	8	54	18,21,22	1.83	5 (27%)	25,30,33	2.43	5 (20%)
56	PSU	1y	55	56	18,21,22	1.37	2 (11%)	21,30,33	2.05	3 (14%)
1	5MC	1A	1962	1,57	19,22,23	1.90	3 (15%)	26,32,35	1.24	4 (15%)
32	2MG	2a	1207	32	23,26,27	1.27	3 (13%)	33,38,41	2.23	8 (24%)
56	4SU	1y	8	56	18,21,22	1.78	5 (27%)	25,30,33	1.71	4 (16%)
1	5MC	2A	1942	1	19,22,23	1.65	3 (15%)	26,32,35	1.12	3 (11%)
54	4SU	1w	8	54	18,21,22	1.88	5 (27%)	25,30,33	2.14	5 (20%)
1	OMG	1A	2251	1,55,57	23,26,27	1.22	3 (13%)	32,38,41	2.02	6 (18%)
32	MA6	1a	1518	32	23,26,27	0.44	0	33,38,41	1.95	10 (30%)
32	UR3	2a	1498	32	19,22,23	1.07	2 (10%)	26,32,35	1.72	3 (11%)
32	5MC	2a	1400	32	19,22,23	1.60	3 (15%)	26,32,35	1.16	2 (7%)
32	M2G	2a	966	32	24,27,28	1.30	3 (12%)	33,40,43	1.88	6 (18%)
1	2MU	2A	2552	1,57	19,22,24	1.20	2 (10%)	25,31,36	1.84	6 (24%)
32	M2G	1a	966	32	24,27,28	1.31	3 (12%)	33,40,43	1.84	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
55	PSU	1x	55	57,55	18,21,22	1.30	2 (11%)	21,30,33	1.99	4 (19%)
56	MIA	2y	37	56	21,24,32	1.59	4 (19%)	30,35,47	2.00	7 (23%)
32	PSU	2a	516	32	18,21,22	1.30	2 (11%)	21,30,33	2.05	4 (19%)
32	PSU	1a	516	32	18,21,22	1.36	2 (11%)	21,30,33	1.95	5 (23%)
32	5MC	1a	1407	32	19,22,23	1.65	2 (10%)	26,32,35	1.11	2 (7%)
1	5MU	1A	1915	1	19,22,23	1.38	4 (21%)	27,32,35	2.18	7 (25%)
1	PSU	2A	1917	1	18,21,22	1.35	2 (11%)	21,30,33	1.95	4 (19%)

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	4OC	1a	1402	32	-	1/9/29/30	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	5/7/12/14	-
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
56	5MU	2y	54	56	-	2/7/25/26	0/2/2/2
56	PSU	1y	39	56	-	0/7/25/26	0/2/2/2
55	31H	1x	76	57,55	-	4/22/40/41	0/3/3/3
56	MIA	1y	37	56	-	0/7/25/34	0/3/3/3
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
1	2MU	1A	2552	1	-	0/9/27/28	0/2/2/2
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
55	31H	2x	76	57,55	-	4/22/40/41	0/3/3/3
43	0TD	1l	92	43	-	4/7/12/14	-
56	G7M	1y	46	56	-	3/7/25/26	0/3/3/3
1	5MC	2A	1962	1,57	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	1,57	-	0/7/25/26	0/2/2/2
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
56	PSU	2y	55	56	-	5/7/25/26	0/2/2/2
1	PSU	1A	2605	1,57	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	5MU	1y	54	56	-	1/7/25/26	0/2/2/2
1	8AH	1A	2503	1,57	-	1/7/25/26	0/3/3/3
54	F3N	2w	76	54,1	-	0/19/37/38	0/4/4/4
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
32	5MC	2a	1407	32,57	-	0/7/25/26	0/2/2/2
1	5MC	1A	1942	1,57	-	0/7/25/26	0/2/2/2
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
56	PSU	2y	32	56	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32,57	-	1/9/27/28	0/3/3/3
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	3/11/29/30	0/3/3/3
54	MIA	1w	37	54	-	3/15/33/34	0/3/3/3
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	1,57	-	0/7/25/26	0/2/2/2
54	MIA	2w	37	54	-	2/11/29/34	0/3/3/3
32	5MC	1a	967	32	-	1/7/25/26	0/2/2/2
32	G7M	2a	527	32	-	3/7/25/26	0/3/3/3
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
32	G7M	1a	527	32	-	3/7/25/26	0/3/3/3
56	4SU	2y	8	56	-	0/7/25/26	0/2/2/2
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
56	PSU	1y	32	56	-	0/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
55	4SU	2x	8	55	-	0/7/25/26	0/2/2/2
56	PSU	2y	39	56	-	0/7/25/26	0/2/2/2
54	F3N	1w	76	54,1	-	0/19/37/38	0/4/4/4
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
56	G7M	2y	46	56	-	2/7/25/26	0/3/3/3
1	OMG	2A	2251	1,55	-	0/9/27/28	0/3/3/3
32	MA6	2a	1518	32	-	0/11/29/30	0/3/3/3
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
1	8AH	2A	2503	1,57	-	0/7/25/26	0/3/3/3
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
54	G7M	1w	46	54	-	1/7/25/26	0/3/3/3
55	5MU	1x	54	57,55	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
54	PSU	1w	32	54,57	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32	-	1/9/29/30	0/2/2/2
54	G7M	2w	46	54	-	1/7/25/26	0/3/3/3
32	MA6	1a	1519	32	-	3/11/29/30	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
56	PSU	1y	55	56	-	2/7/25/26	0/2/2/2
1	5MC	1A	1962	1,57	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	1/9/27/28	0/3/3/3
56	4SU	1y	8	56	-	3/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	1,55,57	-	0/9/27/28	0/3/3/3
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
1	2MU	2A	2552	1,57	-	0/9/27/28	0/2/2/2
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
55	PSU	1x	55	57,55	-	0/7/25/26	0/2/2/2
56	MIA	2y	37	56	-	2/7/25/34	0/3/3/3
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
1	5MU	1A	1915	1	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2

All (262) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.29	1.69	1.82
43	1l	92	0TD	CB-SB	-12.24	1.69	1.82
1	1A	1962	5MC	C5-C4	7.33	1.49	1.44
54	1w	37	MIA	C2-S10	-7.16	1.69	1.75
54	2w	37	MIA	C2-S10	-6.92	1.70	1.75
54	1w	37	MIA	C13-C14	6.71	1.52	1.32
32	1a	967	5MC	C5-C4	6.46	1.49	1.44
55	1x	8	4SU	C4-N3	-6.21	1.31	1.37
1	2A	1942	5MC	C5-C4	5.99	1.48	1.44
32	1a	1400	5MC	C5-C4	5.98	1.48	1.44
55	1x	32	5MC	C5-C4	5.95	1.48	1.44
32	2a	967	5MC	C5-C4	5.93	1.48	1.44
32	1a	1407	5MC	C5-C4	5.89	1.48	1.44
32	1a	1404	5MC	C5-C4	5.84	1.48	1.44
32	2a	1400	5MC	C5-C4	5.78	1.48	1.44
1	1A	1942	5MC	C5-C4	5.73	1.48	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2a	1407	5MC	C5-C4	5.72	1.48	1.44
55	2x	32	5MC	C5-C4	5.51	1.48	1.44
32	2a	1404	5MC	C5-C4	5.50	1.48	1.44
1	2A	1962	5MC	C5-C4	5.39	1.48	1.44
54	2w	37	MIA	C5-C4	5.30	1.48	1.39
56	1y	37	MIA	C5-C4	5.17	1.48	1.39
54	1w	8	4SU	C4-S4	-5.16	1.59	1.68
54	2w	8	4SU	C4-S4	-5.10	1.59	1.68
55	2x	8	4SU	C4-N3	-5.06	1.32	1.37
54	1w	76	F3N	CB-CG	-5.02	1.39	1.51
56	2y	37	MIA	C5-C4	5.01	1.48	1.39
54	1w	46	G7M	C5-N7	-4.99	1.33	1.39
54	2w	76	F3N	CB-CG	-4.87	1.39	1.51
56	2y	8	4SU	C4-S4	-4.77	1.60	1.68
32	1a	527	G7M	C5-N7	-4.73	1.33	1.39
56	2y	46	G7M	C5-N7	-4.73	1.33	1.39
54	1w	37	MIA	C5-C4	4.56	1.47	1.39
54	2w	46	G7M	C5-N7	-4.55	1.33	1.39
56	1y	46	G7M	C5-N7	-4.53	1.34	1.39
32	2a	527	G7M	C5-N7	-4.53	1.34	1.39
55	1x	8	4SU	C4-S4	-4.45	1.60	1.68
56	1y	8	4SU	C4-S4	-4.40	1.60	1.68
1	2A	2503	8AH	C5-C4	4.39	1.46	1.39
55	1x	8	4SU	C2-N3	-4.34	1.30	1.38
55	2x	8	4SU	C4-S4	-4.23	1.61	1.68
56	1y	39	PSU	C6-C5	4.19	1.39	1.35
1	1A	1911	PSU	C6-C5	4.11	1.39	1.35
56	2y	39	PSU	C6-C5	4.00	1.39	1.35
54	2w	55	PSU	C6-C5	3.97	1.39	1.35
56	1y	55	PSU	C6-C5	3.96	1.39	1.35
55	2x	76	31H	C5-N7	-3.94	1.31	1.39
56	1y	32	PSU	C6-C5	3.92	1.39	1.35
54	2w	76	F3N	C5-N7	-3.91	1.31	1.39
54	2w	39	PSU	C6-C5	3.87	1.39	1.35
56	2y	32	PSU	C6-C5	3.87	1.39	1.35
54	1w	55	PSU	C6-C5	3.84	1.39	1.35
1	1A	2605	PSU	C6-C5	3.69	1.39	1.35
55	1x	76	31H	C5-N7	-3.67	1.32	1.39
54	1w	32	PSU	C6-C5	3.65	1.39	1.35
1	2A	2503	8AH	C8-N7	3.61	1.36	1.31
56	1y	46	G7M	C5-C4	3.57	1.47	1.38
1	1A	2503	8AH	C4-N9	-3.56	1.33	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	2y	46	G7M	C5-C4	3.56	1.47	1.38
54	1w	76	F3N	C5-N7	-3.54	1.32	1.39
1	2A	1917	PSU	C6-C5	3.51	1.39	1.35
54	2w	32	PSU	C6-C5	3.50	1.39	1.35
1	2A	1911	PSU	C6-C5	3.50	1.39	1.35
32	1a	516	PSU	C6-C5	3.49	1.39	1.35
1	1A	2503	8AH	C5-C4	3.47	1.45	1.39
55	2x	55	PSU	C6-C5	3.45	1.39	1.35
32	2a	516	PSU	C6-C5	3.43	1.39	1.35
54	2w	8	4SU	C4-N3	-3.38	1.34	1.37
54	1w	39	PSU	C6-C5	3.35	1.39	1.35
54	1w	46	G7M	C5-C4	3.34	1.46	1.38
56	1y	8	4SU	C4-N3	-3.33	1.34	1.37
55	1x	8	4SU	C5-C4	-3.33	1.38	1.42
54	2w	46	G7M	C5-C4	3.33	1.46	1.38
32	2a	1207	2MG	C5-C4	3.32	1.47	1.38
56	2y	55	PSU	C6-C5	3.30	1.38	1.35
55	2x	8	4SU	C2-N3	-3.27	1.32	1.38
56	2y	8	4SU	C4-N3	-3.26	1.34	1.37
54	2w	76	F3N	C5-C4	-3.26	1.33	1.39
32	2a	966	M2G	C2-N2	3.25	1.41	1.35
55	1x	55	PSU	C6-C5	3.19	1.38	1.35
32	2a	966	M2G	C5-C4	3.18	1.47	1.38
32	1a	1207	2MG	C5-C4	3.18	1.47	1.38
32	2a	527	G7M	C5-C4	3.15	1.46	1.38
54	1w	76	F3N	C5-C4	-3.14	1.33	1.39
32	2a	1404	5MC	C6-C5	3.13	1.39	1.34
54	1w	54	5MU	C6-C5	3.11	1.39	1.34
55	1x	76	31H	C5-C4	-3.10	1.33	1.39
1	2A	2503	8AH	C4-N9	-3.10	1.34	1.38
55	2x	8	4SU	C5-C4	-3.09	1.38	1.42
32	1a	966	M2G	C5-C4	3.08	1.47	1.38
1	2A	2251	OMG	C5-C4	3.08	1.47	1.38
56	1y	37	MIA	C5-C6	3.07	1.49	1.41
1	1A	1939	5MU	C6-C5	3.07	1.39	1.34
54	1w	8	4SU	C4-N3	-3.07	1.34	1.37
32	1a	966	M2G	C2-N2	3.05	1.40	1.35
1	1A	1939	5MU	C4-N3	-3.01	1.33	1.38
32	1a	1407	5MC	C6-C5	2.98	1.39	1.34
32	1a	527	G7M	C5-C4	2.98	1.45	1.38
55	2x	76	31H	C5-C4	-2.97	1.33	1.39
55	1x	54	5MU	C6-C5	2.97	1.39	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1942	5MC	C6-C5	2.96	1.39	1.34
55	1x	32	5MC	C6-C5	2.94	1.39	1.34
54	1w	8	4SU	C5-C4	-2.94	1.39	1.42
55	2x	54	5MU	C6-C5	2.94	1.39	1.34
1	1A	2251	OMG	C5-C4	2.94	1.46	1.38
56	1y	54	5MU	C6-C5	2.92	1.39	1.34
56	2y	54	5MU	C6-C5	2.92	1.39	1.34
54	1w	54	5MU	C4-N3	-2.91	1.33	1.38
1	1A	1917	PSU	C6-C5	2.90	1.38	1.35
32	2a	1407	5MC	C6-C5	2.89	1.39	1.34
56	2y	37	MIA	C5-C6	2.89	1.49	1.41
54	2w	37	MIA	C5-C6	2.88	1.48	1.41
32	1a	967	5MC	C6-C5	2.86	1.39	1.34
32	1a	1400	5MC	C6-C5	2.86	1.39	1.34
32	1a	1404	5MC	C6-C5	2.84	1.39	1.34
1	1A	1917	PSU	C4-N3	-2.81	1.33	1.38
1	2A	2605	PSU	C6-C5	2.76	1.38	1.35
1	2A	1939	5MU	C4-N3	-2.76	1.33	1.38
54	1w	39	PSU	C4-N3	-2.76	1.33	1.38
1	1A	1915	5MU	C6-C5	2.75	1.39	1.34
1	2A	1939	5MU	C6-C5	2.75	1.39	1.34
56	2y	54	5MU	C2-N1	2.75	1.42	1.38
1	1A	2251	OMG	C6-N1	-2.74	1.33	1.38
56	2y	55	PSU	C4-N3	-2.71	1.33	1.38
55	1x	54	5MU	C4-C5	2.70	1.49	1.44
54	1w	37	MIA	C5-C6	2.69	1.48	1.41
32	2a	967	5MC	C6-C5	2.68	1.39	1.34
1	2A	2503	8AH	C5-C6	2.67	1.48	1.41
56	2y	8	4SU	C5-C4	-2.67	1.39	1.42
1	2A	1915	5MU	C6-C5	2.66	1.38	1.34
55	2x	54	5MU	C4-N3	-2.66	1.33	1.38
1	2A	2251	OMG	C6-N1	-2.65	1.33	1.38
56	1y	54	5MU	C4-C5	2.65	1.49	1.44
55	2x	32	5MC	C6-C5	2.65	1.38	1.34
1	2A	2552	2MU	C4-N3	-2.65	1.34	1.38
1	1A	1915	5MU	C2-N1	2.65	1.42	1.38
54	2w	8	4SU	C5-C4	-2.65	1.39	1.42
1	2A	1915	5MU	C4-N3	-2.63	1.33	1.38
1	1A	1962	5MC	C6-C5	2.62	1.38	1.34
55	1x	76	31H	C5-C6	-2.61	1.33	1.41
54	2w	54	5MU	C4-N3	-2.60	1.34	1.38
54	2w	54	5MU	C6-C5	2.60	1.38	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1x	54	5MU	C4-N3	-2.60	1.34	1.38
55	2x	76	31H	C5-C6	-2.60	1.33	1.41
56	2y	39	PSU	C4-N3	-2.59	1.34	1.38
54	1w	76	F3N	C5-C6	-2.59	1.33	1.41
55	2x	54	5MU	C4-C5	2.59	1.49	1.44
32	1a	516	PSU	C4-N3	-2.59	1.34	1.38
1	1A	2605	PSU	C4-N3	-2.57	1.34	1.38
56	1y	54	5MU	C2-N1	2.57	1.42	1.38
1	1A	2503	8AH	C8-N7	2.56	1.35	1.31
1	2A	1942	5MC	C6-C5	2.55	1.38	1.34
1	1A	1915	5MU	C4-N3	-2.54	1.34	1.38
32	1a	1207	2MG	C6-N1	-2.54	1.34	1.38
32	2a	1400	5MC	C6-C5	2.54	1.38	1.34
1	2A	2503	8AH	C5-N7	-2.52	1.34	1.39
56	1y	39	PSU	C4-N3	-2.51	1.34	1.38
32	2a	1498	UR3	C2-N1	2.51	1.42	1.38
1	2A	1917	PSU	C4-N3	-2.51	1.34	1.38
54	2w	55	PSU	C4-N3	-2.50	1.34	1.38
1	2A	1915	5MU	C4-C5	2.50	1.48	1.44
1	2A	1915	5MU	C2-N1	2.50	1.42	1.38
32	2a	1207	2MG	C6-N1	-2.50	1.34	1.38
1	1A	1911	PSU	C4-N3	-2.49	1.34	1.38
54	2w	76	F3N	C5-C6	-2.47	1.34	1.41
1	2A	1962	5MC	C6-N1	-2.46	1.33	1.38
1	1A	2503	8AH	C5-N7	-2.46	1.35	1.39
1	2A	1911	PSU	C4-N3	-2.45	1.34	1.38
1	2A	1939	5MU	C6-N1	-2.45	1.33	1.38
56	1y	37	MIA	C8-N7	2.45	1.36	1.31
54	1w	32	PSU	C4-N3	-2.45	1.34	1.38
55	1x	55	PSU	C4-N3	-2.44	1.34	1.38
54	2w	39	PSU	C4-N3	-2.44	1.34	1.38
32	2a	527	G7M	C6-N1	-2.43	1.34	1.38
56	1y	8	4SU	C5-C4	-2.42	1.39	1.42
1	2A	1942	5MC	C6-N1	-2.41	1.33	1.38
32	2a	967	5MC	C6-N1	-2.41	1.33	1.38
56	1y	55	PSU	C4-N3	-2.41	1.34	1.38
55	2x	55	PSU	C4-N3	-2.41	1.34	1.38
56	2y	37	MIA	C8-N7	2.40	1.36	1.31
54	1w	54	5MU	C2-N1	2.40	1.42	1.38
32	1a	1404	5MC	C6-N1	-2.40	1.33	1.38
54	1w	8	4SU	C2-N1	2.38	1.42	1.38
54	1w	55	PSU	C4-N3	-2.37	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2552	2MU	C4-N3	-2.37	1.34	1.38
54	1w	54	5MU	C4-C5	2.37	1.48	1.44
56	1y	32	PSU	C4-N3	-2.37	1.34	1.38
56	1y	54	5MU	C4-N3	-2.36	1.34	1.38
55	2x	32	5MC	C6-N1	-2.34	1.34	1.38
1	2A	1962	5MC	C6-C5	2.34	1.38	1.34
54	2w	32	PSU	C4-N3	-2.33	1.34	1.38
56	2y	54	5MU	C4-C5	2.33	1.48	1.44
56	1y	8	4SU	C2-N1	2.33	1.42	1.38
1	1A	1939	5MU	C4-C5	2.32	1.48	1.44
54	2w	37	MIA	C5-N7	-2.32	1.34	1.39
1	1A	1939	5MU	C6-N1	-2.32	1.34	1.38
56	2y	46	G7M	C6-N1	-2.32	1.34	1.38
32	2a	516	PSU	C4-N3	-2.31	1.34	1.38
1	2A	1939	5MU	C2-N1	2.30	1.42	1.38
55	1x	8	4SU	O2-C2	2.30	1.27	1.23
56	2y	8	4SU	C2-N3	-2.29	1.34	1.38
1	2A	2605	PSU	C4-N3	-2.29	1.34	1.38
54	1w	46	G7M	C6-N1	-2.28	1.34	1.38
55	1x	32	5MC	C6-N1	-2.28	1.34	1.38
56	2y	54	5MU	C4-N3	-2.28	1.34	1.38
54	1w	37	MIA	C5-N7	-2.27	1.34	1.39
1	1A	2503	8AH	C5-C6	2.27	1.47	1.41
1	2A	1915	5MU	C6-N1	-2.27	1.34	1.38
32	1a	527	G7M	C6-N1	-2.27	1.34	1.38
54	1w	39	PSU	C2-N3	-2.26	1.33	1.37
1	2A	1939	5MU	C2-N3	-2.25	1.34	1.38
32	2a	1400	5MC	C6-N1	-2.25	1.34	1.38
54	1w	54	5MU	C2-N3	-2.25	1.34	1.38
54	2w	54	5MU	C4-C5	2.25	1.48	1.44
1	1A	1939	5MU	C2-N3	-2.24	1.34	1.38
55	2x	8	4SU	O2-C2	2.22	1.27	1.23
32	1a	966	M2G	C6-N1	-2.21	1.34	1.38
55	2x	54	5MU	C2-N3	-2.21	1.34	1.38
32	2a	1407	5MC	C6-N1	-2.20	1.34	1.38
32	2a	1404	5MC	C6-N1	-2.19	1.34	1.38
1	1A	1962	5MC	C6-N1	-2.19	1.34	1.38
54	1w	37	MIA	C8-N7	2.18	1.35	1.31
1	1A	1915	5MU	C4-C5	2.17	1.48	1.44
54	2w	8	4SU	C2-N3	-2.15	1.34	1.38
1	1A	2251	OMG	C5-N7	-2.15	1.34	1.39
56	1y	46	G7M	C6-N1	-2.15	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	2552	2MU	C2-N1	2.15	1.41	1.38
54	2w	37	MIA	C2-N3	2.14	1.37	1.34
56	2y	8	4SU	C2-N1	2.14	1.41	1.38
1	2A	1915	5MU	C2-N3	-2.14	1.34	1.38
1	1A	1942	5MC	C6-N1	-2.13	1.34	1.38
32	1a	1400	5MC	C6-N1	-2.12	1.34	1.38
56	2y	32	PSU	C4-N3	-2.12	1.34	1.38
55	1x	54	5MU	C2-N1	2.12	1.41	1.38
56	1y	8	4SU	C2-N3	-2.11	1.34	1.38
55	2x	8	4SU	C6-C5	2.10	1.40	1.35
32	2a	1498	UR3	C6-C5	2.10	1.39	1.35
32	2a	1207	2MG	C2-N3	2.10	1.36	1.32
56	1y	46	G7M	C5-C6	2.10	1.49	1.43
32	2a	527	G7M	C5-C6	2.10	1.49	1.43
32	2a	966	M2G	C6-N1	-2.10	1.34	1.38
54	2w	46	G7M	C6-N1	-2.10	1.34	1.38
54	2w	46	G7M	C4-N9	-2.09	1.32	1.38
56	2y	55	PSU	C2-N3	-2.09	1.34	1.37
1	2A	1939	5MU	C4-C5	2.07	1.48	1.44
55	1x	54	5MU	C6-N1	-2.05	1.34	1.38
1	2A	2552	2MU	C5-C4	2.04	1.48	1.43
32	1a	1498	UR3	C6-C5	2.04	1.39	1.35
54	2w	8	4SU	C2-N1	2.04	1.41	1.38
56	2y	37	MIA	C5-N7	-2.04	1.35	1.39
55	2x	54	5MU	C6-N1	-2.03	1.34	1.38
54	2w	54	5MU	C2-N3	-2.03	1.34	1.38
32	1a	967	5MC	C6-N1	-2.03	1.34	1.38
54	1w	8	4SU	O2-C2	2.02	1.26	1.23
55	1x	8	4SU	C6-C5	2.02	1.39	1.35
55	2x	54	5MU	C2-N1	2.01	1.41	1.38
1	2A	1920	OMC	C6-C5	2.01	1.39	1.35
1	1A	1939	5MU	C2-N1	2.01	1.41	1.38
54	1w	37	MIA	C4-N9	-2.01	1.33	1.37
1	2A	2251	OMG	C5-N7	-2.00	1.35	1.39
1	2A	1911	PSU	C2-N1	-2.00	1.34	1.36
54	1w	46	G7M	C4-N9	-2.00	1.33	1.38

All (432) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	1l	92	0TD	CSB-SB-CB	-14.25	76.74	102.36
43	2l	92	0TD	CSB-SB-CB	-11.44	81.80	102.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	1w	37	MIA	C12-C13-C14	-10.07	108.93	127.01
54	2w	37	MIA	C5-C4-N3	-8.70	118.01	127.18
1	2A	2503	8AH	C5-C4-N3	-8.65	118.07	127.18
54	1w	37	MIA	C5-C4-N3	-7.66	119.11	127.18
1	1A	2503	8AH	C5-C4-N3	-7.59	119.19	127.18
54	2w	8	4SU	C4-N3-C2	-7.44	120.18	127.31
54	2w	37	MIA	N3-C4-N9	7.33	136.29	126.99
32	2a	1207	2MG	C2-N3-C4	7.26	121.08	112.00
32	1a	1498	UR3	C4-N3-C2	-7.09	118.88	124.58
32	2a	1498	UR3	C4-N3-C2	-6.85	119.07	124.58
1	2A	1911	PSU	N1-C2-N3	6.83	122.38	115.17
32	1a	1207	2MG	C2-N3-C4	6.80	120.50	112.00
1	1A	1917	PSU	N1-C2-N3	6.73	122.27	115.17
1	1A	2605	PSU	N1-C2-N3	6.65	122.19	115.17
54	2w	8	4SU	C5-C4-N3	6.41	120.71	114.75
56	2y	55	PSU	N1-C2-N3	6.39	121.91	115.17
32	2a	1207	2MG	C5-C4-N3	-6.35	118.28	128.39
1	2A	2251	OMG	C5-C4-N3	-6.32	118.33	128.39
56	2y	32	PSU	N1-C2-N3	6.32	121.84	115.17
1	1A	1911	PSU	N1-C2-N3	6.31	121.82	115.17
1	2A	2605	PSU	N1-C2-N3	6.22	121.72	115.17
56	1y	55	PSU	N1-C2-N3	6.21	121.72	115.17
54	1w	37	MIA	N3-C4-N9	6.21	134.87	126.99
56	1y	32	PSU	N1-C2-N3	6.16	121.67	115.17
54	1w	8	4SU	C5-C4-N3	6.16	120.48	114.75
1	1A	2251	OMG	C5-C4-N3	-6.09	118.70	128.39
54	1w	32	PSU	N1-C2-N3	6.06	121.56	115.17
54	1w	55	PSU	N1-C2-N3	6.04	121.54	115.17
54	2w	55	PSU	N1-C2-N3	5.99	121.49	115.17
1	2A	1917	PSU	N1-C2-N3	5.98	121.47	115.17
32	2a	516	PSU	N1-C2-N3	5.95	121.44	115.17
55	1x	55	PSU	N1-C2-N3	5.91	121.40	115.17
54	2w	39	PSU	N1-C2-N3	5.89	121.38	115.17
54	2w	32	PSU	N1-C2-N3	5.88	121.37	115.17
54	1w	76	F3N	N1-C2-N3	-5.85	119.72	128.58
32	1a	516	PSU	N1-C2-N3	5.84	121.33	115.17
56	1y	37	MIA	C5-C4-N3	-5.84	118.68	126.72
56	2y	46	G7M	N9-C4-N3	5.82	137.59	125.95
55	2x	76	31H	N1-C2-N3	-5.82	119.77	128.58
55	2x	55	PSU	N1-C2-N3	5.81	121.29	115.17
56	2y	37	MIA	C5-C4-N3	-5.81	118.72	126.72
55	1x	76	31H	N1-C2-N3	-5.79	119.81	128.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	2w	76	F3N	N1-C2-N3	-5.78	119.83	128.58
32	2a	966	M2G	C5-C4-N3	-5.77	119.20	128.39
32	1a	1207	2MG	C5-C4-N3	-5.74	119.26	128.39
1	2A	1915	5MU	C4-N3-C2	-5.73	119.83	127.34
56	1y	46	G7M	N9-C4-N3	5.72	137.40	125.95
32	1a	966	M2G	C5-C4-N3	-5.69	119.34	128.39
1	2A	1915	5MU	C5-C4-N3	5.60	120.19	115.32
56	1y	46	G7M	C5-C4-N3	-5.55	117.66	128.15
54	1w	8	4SU	C4-N3-C2	-5.54	122.01	127.31
56	2y	46	G7M	C5-C4-N3	-5.44	117.86	128.15
1	2A	1939	5MU	C4-N3-C2	-5.39	120.28	127.34
54	1w	76	F3N	C5-C4-N3	-5.37	119.32	126.72
56	2y	39	PSU	N1-C2-N3	5.36	120.82	115.17
56	1y	39	PSU	N1-C2-N3	5.35	120.81	115.17
1	1A	1939	5MU	C4-N3-C2	-5.34	120.34	127.34
56	1y	54	5MU	N3-C2-N1	5.32	121.81	114.89
56	2y	54	5MU	C4-N3-C2	-5.28	120.42	127.34
54	1w	46	G7M	N9-C4-N3	5.27	136.50	125.95
32	2a	527	G7M	N9-C4-N3	5.26	136.46	125.95
32	2a	527	G7M	C5-C4-N3	-5.22	118.29	128.15
1	1A	1915	5MU	N3-C2-N1	5.21	121.68	114.89
1	1A	1915	5MU	C4-N3-C2	-5.15	120.59	127.34
55	1x	76	31H	C5-C4-N3	-5.15	119.63	126.72
55	2x	76	31H	C5-C4-N3	-5.13	119.65	126.72
1	2A	1939	5MU	N3-C2-N1	5.13	121.56	114.89
56	2y	54	5MU	O4-C4-C5	-5.13	119.05	124.92
1	2A	2251	OMG	N9-C4-N3	5.12	136.19	125.95
1	2A	1911	PSU	O2-C2-N1	-5.07	117.56	122.79
1	1A	1939	5MU	N3-C2-N1	5.07	121.49	114.89
56	2y	8	4SU	C5-C4-N3	5.06	119.46	114.75
1	2A	1915	5MU	N3-C2-N1	5.05	121.46	114.89
56	2y	54	5MU	N3-C2-N1	5.05	121.46	114.89
32	1a	527	G7M	N9-C4-N3	5.04	136.04	125.95
54	2w	46	G7M	N9-C4-N3	5.00	135.95	125.95
32	1a	1519	MA6	N1-C2-N3	-5.00	121.02	128.58
1	2A	2251	OMG	C2-N3-C4	4.98	120.88	112.30
56	1y	54	5MU	C4-N3-C2	-4.98	120.81	127.34
32	1a	527	G7M	C5-C4-N3	-4.96	118.78	128.15
1	1A	2251	OMG	C2-N3-C4	4.95	120.82	112.30
1	1A	2552	2MU	N3-C2-N1	4.89	121.26	114.89
54	1w	39	PSU	N1-C2-N3	4.88	120.31	115.17
54	1w	46	G7M	C5-C4-N3	-4.87	118.95	128.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	2552	2MU	C4-N3-C2	-4.86	120.58	126.61
54	2w	76	F3N	C5-C4-N3	-4.86	120.03	126.72
56	1y	46	G7M	C2-N3-C4	4.84	120.64	112.30
55	1x	54	5MU	N3-C2-N1	4.83	121.18	114.89
32	1a	527	G7M	C2-N3-C4	4.82	120.61	112.30
1	2A	1939	5MU	C5-C4-N3	4.81	119.51	115.32
1	2A	2503	8AH	C6-C5-N7	4.80	136.48	131.72
1	1A	1939	5MU	C5-C4-N3	4.79	119.49	115.32
56	2y	54	5MU	C5-C4-N3	4.79	119.48	115.32
55	2x	54	5MU	N3-C2-N1	4.78	121.11	114.89
1	2A	2552	2MU	N3-C2-N1	4.76	121.09	114.89
56	1y	8	4SU	C4-N3-C2	-4.76	122.75	127.31
56	2y	46	G7M	C2-N3-C4	4.76	120.49	112.30
32	2a	1519	MA6	N1-C2-N3	-4.76	121.38	128.58
1	1A	2503	8AH	C6-C5-N7	4.75	136.43	131.72
1	1A	2251	OMG	N9-C4-N3	4.75	135.45	125.95
56	2y	37	MIA	N3-C4-N9	4.73	135.21	127.17
32	2a	1518	MA6	N1-C2-N3	-4.72	121.43	128.58
54	2w	46	G7M	C5-C4-N3	-4.66	119.34	128.15
56	1y	37	MIA	N3-C4-N9	4.65	135.07	127.17
32	2a	1519	MA6	C5-C4-N3	-4.64	120.33	126.72
54	1w	8	4SU	C5-C4-S4	-4.62	119.02	124.31
32	2a	527	G7M	C2-N3-C4	4.62	120.26	112.30
1	1A	2605	PSU	O2-C2-N1	-4.61	118.04	122.79
55	1x	54	5MU	C4-N3-C2	-4.60	121.31	127.34
1	2A	1939	5MU	O4-C4-C5	-4.58	119.67	124.92
1	2A	2503	8AH	C4-C5-N7	-4.56	106.24	110.91
32	2a	966	M2G	C2-N3-C4	4.55	120.93	112.51
1	1A	2605	PSU	C4-N3-C2	-4.55	120.11	126.37
32	1a	1519	MA6	C5-C4-N3	-4.54	120.46	126.72
55	2x	54	5MU	C4-N3-C2	-4.50	121.44	127.34
56	1y	8	4SU	C5-C4-N3	4.50	118.94	114.75
55	1x	8	4SU	S4-C4-N3	-4.48	115.51	120.20
1	1A	1915	5MU	C5-C4-N3	4.47	119.21	115.32
1	1A	1939	5MU	C5-C6-N1	-4.47	118.46	123.31
56	2y	8	4SU	C4-N3-C2	-4.46	123.04	127.31
54	1w	54	5MU	N3-C2-N1	4.45	120.68	114.89
1	2A	2552	2MU	C4-N3-C2	-4.45	121.09	126.61
1	2A	1915	5MU	O4-C4-C5	-4.43	119.84	124.92
55	1x	8	4SU	C6-C5-C4	-4.42	116.12	119.95
54	2w	8	4SU	N3-C2-N1	4.42	120.64	114.89
32	2a	516	PSU	C4-N3-C2	-4.41	120.30	126.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	1a	966	M2G	N9-C4-N3	4.40	134.74	125.95
54	2w	46	G7M	C2-N3-C4	4.35	119.79	112.30
32	2a	966	M2G	N9-C4-N3	4.34	134.63	125.95
1	1A	1915	5MU	O4-C4-C5	-4.33	119.96	124.92
1	1A	1917	PSU	C4-N3-C2	-4.33	120.41	126.37
1	2A	2605	PSU	C4-N3-C2	-4.33	120.41	126.37
32	1a	966	M2G	C2-N3-C4	4.33	120.51	112.51
32	2a	1518	MA6	C5-C4-N3	-4.31	120.78	126.72
54	1w	32	PSU	C4-N3-C2	-4.30	120.44	126.37
54	1w	55	PSU	C4-N3-C2	-4.28	120.48	126.37
55	1x	55	PSU	C4-N3-C2	-4.26	120.51	126.37
54	2w	54	5MU	N3-C2-N1	4.25	120.42	114.89
54	1w	46	G7M	C2-N3-C4	4.24	119.59	112.30
56	2y	32	PSU	O2-C2-N1	-4.23	118.43	122.79
32	1a	516	PSU	C4-N3-C2	-4.19	120.60	126.37
32	1a	1518	MA6	N1-C2-N3	-4.17	122.27	128.58
54	1w	37	MIA	C15-C14-C13	-4.16	110.17	122.66
32	1a	1519	MA6	C5-N7-C8	4.15	109.98	103.45
32	2a	1207	2MG	N9-C4-N3	4.15	134.24	125.95
55	2x	55	PSU	C4-N3-C2	-4.13	120.69	126.37
54	2w	8	4SU	C5-C4-S4	-4.10	119.62	124.31
56	1y	55	PSU	C4-N3-C2	-4.10	120.72	126.37
56	2y	55	PSU	C4-N3-C2	-4.08	120.76	126.37
1	2A	1917	PSU	C4-N3-C2	-4.08	120.76	126.37
1	2A	1911	PSU	C4-N3-C2	-4.07	120.76	126.37
32	1a	1518	MA6	C5-C4-N3	-4.07	121.11	126.72
1	1A	1917	PSU	O2-C2-N1	-4.06	118.60	122.79
32	1a	1519	MA6	C4-C5-N7	-4.04	105.96	110.58
56	1y	54	5MU	C5-C4-N3	4.04	118.83	115.32
32	2a	1518	MA6	C2-N1-C6	4.04	121.69	111.83
32	2a	1519	MA6	C4-C5-N7	-4.03	105.97	110.58
54	2w	54	5MU	C4-N3-C2	-4.03	122.06	127.34
32	2a	1519	MA6	C5-N7-C8	4.03	109.78	103.45
55	1x	8	4SU	O2-C2-N1	4.00	128.01	122.80
32	1a	1207	2MG	C6-C5-N7	3.99	137.55	130.29
56	1y	32	PSU	C4-N3-C2	-3.95	120.93	126.37
56	1y	54	5MU	O4-C4-C5	-3.94	120.41	124.92
1	1A	1911	PSU	C4-N3-C2	-3.94	120.95	126.37
54	1w	37	MIA	C11-S10-C2	-3.93	99.30	102.25
32	1a	1518	MA6	C2-N1-C6	3.92	121.40	111.83
54	2w	39	PSU	C4-N3-C2	-3.91	120.99	126.37
1	1A	1939	5MU	O4-C4-C5	-3.90	120.46	124.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	1w	37	MIA	C6-C5-N7	3.90	136.68	132.43
32	2a	1519	MA6	C2-N1-C6	3.89	121.34	111.83
54	1w	37	MIA	C16-C14-C13	-3.89	110.98	122.66
32	1a	1519	MA6	C2-N1-C6	3.87	121.29	111.83
1	1A	2503	8AH	C4-C5-N7	-3.86	106.96	110.91
1	1A	1942	5MC	C5-C6-N1	-3.86	119.12	123.31
55	2x	54	5MU	C5-C4-N3	3.85	118.67	115.32
54	2w	32	PSU	C4-N3-C2	-3.85	121.07	126.37
56	2y	32	PSU	C4-N3-C2	-3.84	121.08	126.37
54	1w	54	5MU	C4-N3-C2	-3.83	122.32	127.34
54	2w	54	5MU	C5-C4-N3	3.79	118.61	115.32
32	1a	1518	MA6	C5-N7-C8	3.77	109.38	103.45
32	1a	1519	MA6	N9-C8-N7	-3.77	108.59	113.94
32	1a	967	5MC	C5-C6-N1	-3.76	119.23	123.31
54	2w	55	PSU	C4-N3-C2	-3.76	121.19	126.37
32	2a	516	PSU	O2-C2-N1	-3.75	118.92	122.79
55	1x	54	5MU	C5-C4-N3	3.73	118.56	115.32
1	2A	2605	PSU	O2-C2-N1	-3.72	118.95	122.79
56	1y	55	PSU	O2-C2-N1	-3.70	118.97	122.79
32	1a	1207	2MG	N9-C4-N3	3.69	133.33	125.95
1	2A	1939	5MU	C5-C6-N1	-3.69	119.31	123.31
56	1y	37	MIA	C2-N3-C4	3.66	120.78	111.83
55	2x	76	31H	O4'-C1'-N9	3.66	115.11	108.09
32	1a	1404	5MC	C5-C6-N1	-3.65	119.35	123.31
32	2a	1518	MA6	C5-N7-C8	3.63	109.16	103.45
1	1A	2552	2MU	C2'-C1'-N1	-3.63	107.36	114.24
56	1y	32	PSU	O2-C2-N1	-3.62	119.06	122.79
54	1w	54	5MU	C5-C4-N3	3.61	118.46	115.32
32	2a	967	5MC	C5-C6-N1	-3.60	119.40	123.31
1	2A	1915	5MU	C5-C6-N1	-3.60	119.40	123.31
55	1x	32	5MC	C5-C6-N1	-3.59	119.41	123.31
1	2A	1962	5MC	C5-C6-N1	-3.58	119.43	123.31
32	1a	1519	MA6	C2-N3-C4	3.57	120.56	111.83
56	2y	37	MIA	C2-N3-C4	3.57	120.56	111.83
55	1x	55	PSU	O2-C2-N1	-3.56	119.11	122.79
32	2a	1518	MA6	C4-C5-N7	-3.54	106.53	110.58
54	2w	54	5MU	O4-C4-C5	-3.54	120.87	124.92
54	1w	76	F3N	C2-N3-C4	3.54	120.47	111.83
55	1x	54	5MU	C5-C6-N1	-3.52	119.49	123.31
32	2a	1207	2MG	C6-C5-N7	3.52	136.70	130.29
32	2a	1519	MA6	N9-C8-N7	-3.52	108.94	113.94
32	1a	1518	MA6	N9-C8-N7	-3.52	108.94	113.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	1w	55	PSU	O2-C2-N1	-3.51	119.16	122.79
55	2x	76	31H	N9-C8-N7	-3.51	108.96	113.94
56	1y	37	MIA	C4-C5-N7	-3.50	106.58	110.58
32	2a	1400	5MC	C5-C6-N1	-3.50	119.51	123.31
32	2a	1407	5MC	C5-C6-N1	-3.50	119.51	123.31
54	1w	76	F3N	N9-C8-N7	-3.49	108.98	113.94
32	2a	1519	MA6	C2-N3-C4	3.47	120.31	111.83
54	1w	37	MIA	C4-C5-N7	-3.47	106.61	110.58
32	1a	1518	MA6	C4-C5-N7	-3.47	106.62	110.58
55	2x	76	31H	C2-N3-C4	3.46	120.28	111.83
55	1x	76	31H	N9-C8-N7	-3.45	109.04	113.94
55	1x	76	31H	C4'-O4'-C1'	-3.44	101.87	109.47
54	2w	76	F3N	N9-C8-N7	-3.43	109.07	113.94
32	2a	966	M2G	C6-C5-N7	3.43	136.53	130.29
55	1x	76	31H	C2-N3-C4	3.42	120.19	111.83
55	2x	54	5MU	C5-C6-N1	-3.42	119.60	123.31
56	1y	39	PSU	C4-N3-C2	-3.42	121.66	126.37
56	2y	37	MIA	C4-C5-N7	-3.40	106.69	110.58
1	2A	1917	PSU	O2-C2-N1	-3.38	119.30	122.79
32	1a	1407	5MC	C5-C6-N1	-3.38	119.64	123.31
1	2A	1942	5MC	C5-C6-N1	-3.36	119.66	123.31
54	2w	76	F3N	C2-N3-C4	3.36	120.04	111.83
1	1A	2552	2MU	O4-C4-C5	-3.35	119.38	125.16
56	1y	37	MIA	N3-C2-N1	-3.33	123.54	128.58
56	1y	8	4SU	N3-C2-N1	3.30	119.18	114.89
56	2y	54	5MU	C5-C6-N1	-3.29	119.74	123.31
55	2x	54	5MU	O4-C4-C5	-3.28	121.17	124.92
56	2y	39	PSU	C4-N3-C2	-3.28	121.85	126.37
32	1a	1498	UR3	C5-C4-N3	3.27	119.35	115.04
32	2a	1518	MA6	C2-N3-C4	3.27	119.81	111.83
1	2A	2552	2MU	C5-C4-N3	3.24	119.34	114.80
55	2x	32	5MC	C5-C6-N1	-3.23	119.80	123.31
54	1w	37	MIA	C2-N3-C4	3.23	120.75	112.29
54	1w	54	5MU	O4-C4-C5	-3.22	121.23	124.92
32	1a	1207	2MG	C4-C5-N7	-3.21	105.58	110.67
32	2a	1518	MA6	N9-C8-N7	-3.21	109.39	113.94
32	1a	966	M2G	C6-C5-N7	3.20	136.12	130.29
43	2l	92	0TD	OD2-CG-CB	3.19	120.04	113.15
32	2a	1498	UR3	C5-C4-N3	3.18	119.23	115.04
56	2y	37	MIA	N3-C2-N1	-3.18	123.78	128.58
54	2w	55	PSU	O2-C2-N1	-3.16	119.53	122.79
54	2w	37	MIA	C4-C5-N7	-3.16	106.97	110.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	1a	1400	5MC	C5-C6-N1	-3.15	119.89	123.31
54	1w	37	MIA	C4-N9-C8	3.15	109.05	105.74
54	1w	54	5MU	C5-C6-N1	-3.15	119.89	123.31
54	2w	32	PSU	O2-C2-N1	-3.15	119.54	122.79
32	1a	1404	5MC	C5-C4-N3	-3.15	118.53	121.75
55	1x	32	5MC	C5-C4-N3	-3.13	118.54	121.75
32	2a	1404	5MC	C5-C6-N1	-3.12	119.93	123.31
1	1A	2552	2MU	C5-C4-N3	3.12	119.16	114.80
55	2x	76	31H	C5-N7-C8	3.10	108.32	103.45
1	1A	2251	OMG	C6-C5-N7	3.10	135.93	130.29
1	1A	2552	2MU	O2-C2-N1	-3.10	118.76	122.80
56	2y	8	4SU	C5-C4-S4	-3.08	120.79	124.31
55	1x	54	5MU	O4-C4-C5	-3.08	121.40	124.92
55	2x	8	4SU	C6-C5-C4	-3.07	117.29	119.95
54	2w	37	MIA	C2-N3-C4	3.06	120.30	112.29
32	2a	1207	2MG	C4-C5-N7	-3.05	105.84	110.67
32	1a	1207	2MG	N1-C2-N2	3.03	119.65	116.56
1	1A	1962	5MC	C5-C6-N1	-3.02	120.03	123.31
32	2a	1404	5MC	C5-C4-N3	-3.02	118.66	121.75
1	1A	1911	PSU	O2-C2-N1	-3.00	119.70	122.79
55	1x	76	31H	C5-N7-C8	2.99	108.14	103.45
1	1A	2503	8AH	C2-N1-C6	2.96	122.66	118.10
55	1x	8	4SU	C4-N3-C2	2.96	130.16	127.31
54	2w	76	F3N	C5-N7-C8	2.96	108.10	103.45
54	1w	76	F3N	C5-N7-C8	2.95	108.09	103.45
1	1A	2503	8AH	N6-C6-N1	2.95	121.00	117.03
54	1w	76	F3N	C5-C4-N9	2.94	109.01	105.81
56	2y	8	4SU	N3-C2-N1	2.93	118.70	114.89
56	2y	55	PSU	O2-C2-N1	-2.92	119.77	122.79
32	2a	1407	5MC	C5-C4-N3	-2.91	118.77	121.75
1	1A	1915	5MU	C5-C6-N1	-2.90	120.16	123.31
32	1a	1518	MA6	C2-N3-C4	2.90	118.92	111.83
55	2x	76	31H	C4'-O4'-C1'	-2.89	103.08	109.47
32	1a	1207	2MG	N2-C2-N3	-2.88	116.84	120.51
1	1A	1942	5MC	C5-C4-N3	-2.88	118.80	121.75
54	2w	39	PSU	O2-C2-N1	-2.85	119.85	122.79
1	2A	2251	OMG	C6-C5-N7	2.83	135.44	130.29
1	2A	2552	2MU	O4-C4-C5	-2.83	120.28	125.16
32	1a	967	5MC	C5-C4-N3	-2.81	118.87	121.75
54	1w	32	PSU	O2-C2-N1	-2.81	119.89	122.79
54	1w	8	4SU	N3-C2-N1	2.80	118.53	114.89
32	2a	1519	MA6	N3-C4-N9	2.79	131.92	127.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	1x	76	31H	C5-C4-N9	2.78	108.84	105.81
32	1a	1519	MA6	N3-C4-N9	2.78	131.90	127.17
43	1l	92	0TD	OD2-CG-CB	2.77	119.14	113.15
55	2x	32	5MC	C5-C4-N3	-2.77	118.92	121.75
54	2w	37	MIA	C12-N6-C6	-2.76	120.29	122.85
56	1y	54	5MU	C5-C6-N1	-2.75	120.33	123.31
1	2A	1920	OMC	O2-C2-N3	-2.74	118.00	122.33
56	1y	8	4SU	C5-C4-S4	-2.74	121.17	124.31
32	1a	1518	MA6	N3-C4-N9	2.73	131.82	127.17
55	2x	55	PSU	O2-C2-N1	-2.73	119.97	122.79
32	1a	516	PSU	O2-C2-N1	-2.73	119.97	122.79
55	1x	8	4SU	C5-C4-N3	2.72	117.28	114.75
32	1a	1518	MA6	C4-C5-C6	2.72	118.72	115.91
54	2w	54	5MU	C5-C6-N1	-2.69	120.40	123.31
32	2a	1518	MA6	N3-C4-N9	2.67	131.71	127.17
54	1w	37	MIA	C5-N7-C8	2.66	107.63	103.45
1	1A	1962	5MC	CM5-C5-C6	-2.66	119.25	122.85
55	2x	76	31H	C5-C4-N9	2.66	108.71	105.81
56	2y	37	MIA	C4-N9-C8	2.65	108.52	105.74
54	1w	76	F3N	N3-C4-N9	2.65	131.67	127.17
55	1x	76	31H	CA-N-CN	-2.65	118.75	122.82
32	1a	1498	UR3	C3U-N3-C4	2.64	121.53	117.87
54	1w	39	PSU	C4-N3-C2	-2.64	122.73	126.37
1	2A	1915	5MU	C5M-C5-C4	2.63	121.59	118.78
55	2x	76	31H	N3-C4-N9	2.63	131.64	127.17
32	1a	527	G7M	O6-C6-C5	-2.62	122.17	128.01
54	2w	76	F3N	C5-C4-N9	2.61	108.66	105.81
54	1w	76	F3N	C6-C5-C4	2.61	120.74	117.18
32	2a	1407	5MC	O2-C2-N3	-2.60	118.22	122.33
1	2A	1962	5MC	C5-C4-N3	-2.59	119.10	121.75
1	2A	2552	2MU	C2'-C1'-N1	-2.59	109.33	114.24
1	1A	2251	OMG	C4-C5-N7	-2.58	106.58	110.67
1	1A	1915	5MU	O2-C2-N1	-2.58	119.44	122.80
56	1y	54	5MU	O2-C2-N1	-2.57	119.45	122.80
32	2a	966	M2G	C4-C5-N7	-2.57	106.60	110.67
55	1x	76	31H	O2'-C2'-C3'	2.56	117.44	111.16
55	1x	76	31H	N3-C4-N9	2.56	131.52	127.17
56	2y	37	MIA	C5-N7-C8	2.55	107.46	103.45
55	1x	76	31H	O4'-C1'-N9	2.55	112.98	108.09
1	1A	1920	OMC	O2-C2-N3	-2.54	118.32	122.33
55	1x	8	4SU	C5-C4-S4	2.54	127.20	124.31
54	1w	37	MIA	C2-N1-C6	2.54	122.36	117.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	1y	37	MIA	C5-N7-C8	2.53	107.43	103.45
32	1a	1400	5MC	C5-C4-N3	-2.53	119.16	121.75
32	2a	967	5MC	C5-C4-N3	-2.53	119.16	121.75
32	2a	1519	MA6	C4-C5-C6	2.52	118.51	115.91
1	1A	1962	5MC	C5-C4-N3	-2.52	119.17	121.75
54	1w	8	4SU	C1'-N1-C2	2.52	122.11	117.59
32	1a	1407	5MC	C5-C4-N3	-2.51	119.18	121.75
55	1x	54	5MU	O2-C2-N1	-2.50	119.54	122.80
56	1y	39	PSU	C6-C5-C4	-2.50	116.48	118.17
43	2l	92	0TD	OD1-CG-CB	-2.50	117.21	122.44
32	2a	1518	MA6	C4-C5-C6	2.49	118.48	115.91
1	2A	1942	5MC	C5-C4-N3	-2.49	119.20	121.75
54	2w	54	5MU	O2-C2-N1	-2.48	119.57	122.80
54	2w	46	G7M	O6-C6-C5	-2.48	122.48	128.01
32	1a	966	M2G	O6-C6-C5	-2.46	120.05	126.53
54	1w	46	G7M	O6-C6-C5	-2.45	122.54	128.01
56	1y	37	MIA	C4-N9-C8	2.45	108.31	105.74
1	2A	2503	8AH	N6-C6-N1	2.44	120.33	117.03
54	2w	76	F3N	N3-C4-N9	2.44	131.32	127.17
32	2a	1402	4OC	C6-C5-C4	2.44	119.94	117.00
56	1y	46	G7M	O6-C6-C5	-2.43	122.59	128.01
1	2A	1939	5MU	O2-C2-N1	-2.41	119.66	122.80
1	1A	1939	5MU	O2-C2-N1	-2.41	119.66	122.80
1	2A	2503	8AH	C2-N1-C6	2.40	121.79	118.10
54	2w	37	MIA	C2-N1-C6	2.40	122.09	117.54
55	1x	76	31H	C6-C5-C4	2.37	120.42	117.18
55	1x	32	5MC	O2-C2-N3	-2.36	118.60	122.33
55	1x	76	31H	OCN-CN-N	-2.35	119.23	125.32
56	2y	46	G7M	O6-C6-C5	-2.35	122.76	128.01
32	1a	966	M2G	C4-C5-N7	-2.35	106.94	110.67
55	2x	8	4SU	C5-C4-N3	2.35	116.93	114.75
32	2a	1400	5MC	C5-C4-N3	-2.34	119.35	121.75
55	2x	54	5MU	O2-C2-N1	-2.34	119.75	122.80
1	2A	1915	5MU	O2-C2-N1	-2.33	119.77	122.80
54	1w	76	F3N	C4-C5-N7	-2.32	107.92	110.58
54	1w	37	MIA	N3-C2-N1	-2.32	122.76	127.00
32	1a	516	PSU	C5-C6-N1	-2.32	118.92	122.14
1	2A	2251	OMG	C4-C5-N7	-2.31	107.01	110.67
54	2w	37	MIA	C5-N7-C8	2.31	107.08	103.45
55	1x	55	PSU	C5-C6-N1	-2.31	118.94	122.14
55	1x	76	31H	C4-C5-N7	-2.30	107.95	110.58
1	2A	2251	OMG	O6-C6-C5	-2.30	120.45	126.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	1w	37	MIA	N9-C8-N7	-2.28	110.70	113.94
54	2w	54	5MU	C5M-C5-C4	2.28	121.22	118.78
54	2w	37	MIA	C4-N9-C8	2.28	108.13	105.74
55	2x	76	31H	C4-C5-N7	-2.27	107.98	110.58
32	1a	527	G7M	C5-C6-N1	2.27	116.53	111.84
32	2a	527	G7M	C5-C6-N1	2.27	116.52	111.84
32	2a	966	M2G	O6-C6-C5	-2.26	120.56	126.53
32	2a	1207	2MG	N1-C2-N2	2.26	118.86	116.56
1	2A	2552	2MU	O2-C2-N1	-2.23	119.89	122.80
55	2x	55	PSU	C5-C6-N1	-2.23	119.04	122.14
54	2w	37	MIA	C1'-N9-C8	-2.23	122.16	127.09
1	1A	2251	OMG	O6-C6-C5	-2.22	120.67	126.53
54	2w	37	MIA	C4-C5-C6	2.21	118.62	116.78
55	2x	76	31H	C6-C5-C4	2.21	120.19	117.18
1	1A	1942	5MC	O2-C2-N3	-2.21	118.85	122.33
32	2a	1498	UR3	C3U-N3-C4	2.20	120.92	117.87
32	2a	1207	2MG	N2-C2-N3	-2.19	117.72	120.51
54	2w	76	F3N	C6-C5-C4	2.16	120.13	117.18
55	1x	8	4SU	O2-C2-N3	-2.16	117.51	121.49
55	2x	8	4SU	C1'-N1-C2	2.15	121.46	117.59
54	2w	37	MIA	C11-S10-C2	-2.15	100.64	102.25
32	1a	1518	MA6	C4-N9-C8	2.14	107.99	105.74
55	2x	8	4SU	O2-C2-N1	2.14	125.58	122.80
1	2A	1917	PSU	C5-C6-N1	-2.13	119.18	122.14
54	1w	32	PSU	C5-C6-N1	-2.12	119.20	122.14
1	1A	2503	8AH	C2'-C1'-N9	-2.11	112.39	115.44
56	2y	55	PSU	O4'-C1'-C2'	2.11	108.06	105.15
56	2y	55	PSU	C5-C6-N1	-2.10	119.22	122.14
32	1a	1207	2MG	C8-N7-C5	2.10	108.00	104.26
32	1a	1402	4OC	C6-C5-C4	2.10	119.53	117.00
1	1A	1962	5MC	C1'-N1-C6	-2.10	117.70	121.15
55	2x	54	5MU	C5M-C5-C4	2.10	121.02	118.78
1	1A	1915	5MU	C5M-C5-C4	2.09	121.02	118.78
54	2w	8	4SU	O2-C2-N1	-2.09	120.07	122.80
55	2x	76	31H	O2'-C2'-C3'	2.07	116.23	111.16
32	2a	527	G7M	O6-C6-C5	-2.07	123.40	128.01
1	1A	2503	8AH	N1-C2-N3	-2.07	122.12	125.77
32	1a	1519	MA6	C4-C5-C6	2.06	118.04	115.91
56	2y	54	5MU	C1'-N1-C2	2.05	121.27	117.59
32	2a	1404	5MC	O2-C2-N3	-2.04	119.12	122.33
1	1A	1917	PSU	C5-C6-N1	-2.04	119.31	122.14
32	2a	516	PSU	C5-C6-N1	-2.03	119.32	122.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	2y	39	PSU	C6-C5-C4	-2.03	116.80	118.17
32	2a	1207	2MG	C2-N1-C6	-2.02	122.10	124.55
55	2x	32	5MC	C1'-N1-C6	-2.02	117.82	121.15
55	2x	32	5MC	O2-C2-N3	-2.01	119.16	122.33
1	2A	1942	5MC	CM5-C5-C6	-2.01	120.13	122.85
55	1x	54	5MU	C5M-C5-C4	2.01	120.92	118.78
54	2w	76	F3N	C4-C5-N7	-2.01	108.29	110.58
54	1w	39	PSU	O2-C2-N1	-2.00	120.72	122.79
56	2y	39	PSU	O2-C2-N1	-2.00	120.72	122.79
32	1a	516	PSU	O4'-C1'-C2'	2.00	107.92	105.15

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	1207	2MG	N3-C2-N2-CM2
43	1l	92	0TD	O-C-CA-CB
43	1l	92	0TD	CA-CB-SB-CSB
43	1l	92	0TD	CG-CB-SB-CSB
54	1w	37	MIA	N6-C12-C13-C14
54	1w	37	MIA	C12-C13-C14-C15
54	1w	37	MIA	C12-C13-C14-C16
55	1x	76	31H	C3'-C4'-C5'-O5'
55	1x	76	31H	O4'-C4'-C5'-O5'
56	1y	46	G7M	C4'-C5'-O5'-P
32	2a	1207	2MG	N3-C2-N2-CM2
43	2l	92	0TD	O-C-CA-CB
43	2l	92	0TD	CG-CB-SB-CSB
43	2l	92	0TD	SB-CB-CG-OD2
43	2l	92	0TD	SB-CB-CG-OD1
54	2w	37	MIA	C5-C6-N6-C12
54	2w	37	MIA	N1-C6-N6-C12
55	2x	76	31H	C3'-C4'-C5'-O5'
55	2x	76	31H	O4'-C4'-C5'-O5'
56	2y	54	5MU	O4'-C4'-C5'-O5'
56	2y	55	PSU	C2'-C1'-C5-C4
56	2y	55	PSU	C2'-C1'-C5-C6
56	2y	55	PSU	C3'-C4'-C5'-O5'
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1519	MA6	O4'-C4'-C5'-O5'
56	2y	54	5MU	C3'-C4'-C5'-O5'
56	2y	55	PSU	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
55	2x	76	31H	CB-CG-SD-CE
32	1a	527	G7M	C3'-C4'-C5'-O5'
56	1y	46	G7M	C3'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
56	1y	8	4SU	C3'-C4'-C5'-O5'
56	1y	8	4SU	O4'-C4'-C5'-O5'
55	1x	76	31H	CB-CG-SD-CE
56	2y	46	G7M	O4'-C1'-N9-C4
32	2a	527	G7M	C3'-C4'-C5'-O5'
56	2y	37	MIA	C3'-C4'-C5'-O5'
54	2w	46	G7M	C4'-C5'-O5'-P
54	1w	46	G7M	C4'-C5'-O5'-P
43	1l	92	0TD	SB-CB-CG-OD1
55	1x	76	31H	C4'-C5'-O5'-P
32	1a	1402	4OC	O4'-C4'-C5'-O5'
55	2x	76	31H	C4'-C5'-O5'-P
56	1y	55	PSU	O4'-C1'-C5-C4
56	2y	55	PSU	O4'-C1'-C5-C4
32	1a	527	G7M	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C4'-C5'-O5'-P
56	2y	46	G7M	O4'-C1'-N9-C8
32	1a	1519	MA6	C4'-C5'-O5'-P
32	2a	527	G7M	C4'-C5'-O5'-P
56	1y	54	5MU	O4'-C4'-C5'-O5'
56	1y	8	4SU	C4'-C5'-O5'-P
1	1A	2503	8AH	C4'-C5'-O5'-P
56	1y	46	G7M	O4'-C4'-C5'-O5'
43	2l	92	0TD	CA-CB-SB-CSB
32	1a	527	G7M	C4'-C5'-O5'-P
56	1y	55	PSU	O4'-C1'-C5-C6
32	1a	967	5MC	O4'-C4'-C5'-O5'
32	2a	1402	4OC	O4'-C4'-C5'-O5'
32	2a	527	G7M	O4'-C4'-C5'-O5'
1	1A	1920	OMC	C2'-C1'-N1-C2
56	2y	37	MIA	O4'-C4'-C5'-O5'

There are no ring outliers.

38 monomers are involved in 54 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	1a	1402	4OC	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
43	2l	92	0TD	1	0
56	2y	54	5MU	1	0
56	1y	39	PSU	1	0
32	2a	967	5MC	1	0
1	1A	2552	2MU	1	0
55	2x	54	5MU	2	0
1	2A	1915	5MU	1	0
55	2x	76	31H	2	0
1	2A	1939	5MU	1	0
54	1w	39	PSU	1	0
56	2y	55	PSU	6	0
54	2w	76	F3N	3	0
54	2w	39	PSU	1	0
55	1x	8	4SU	1	0
32	2a	1519	MA6	1	0
54	1w	37	MIA	2	0
1	1A	1939	5MU	1	0
54	2w	37	MIA	1	0
56	2y	8	4SU	1	0
1	1A	1917	PSU	1	0
55	2x	8	4SU	1	0
54	1w	76	F3N	1	0
56	2y	46	G7M	2	0
1	2A	2251	OMG	1	0
32	2a	1518	MA6	2	0
54	2w	46	G7M	1	0
32	1a	1519	MA6	1	0
54	2w	8	4SU	1	0
56	1y	55	PSU	2	0
56	1y	8	4SU	2	0
54	1w	8	4SU	2	0
32	1a	1518	MA6	2	0
1	2A	2552	2MU	2	0
32	1a	966	M2G	2	0
56	2y	37	MIA	2	0
32	1a	516	PSU	1	0
1	2A	1917	PSU	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2472 ligands modelled in this entry, 2470 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	2d	501	35	0,12,12	-	-	-		
60	SF4	1d	302	35	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	SF4	2d	501	35	-	-	0/6/5/5
60	SF4	1d	302	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.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.35	189 (6%) 24 24	22, 39, 97, 108	0
1	2A	2789/2915 (95%)	0.15	156 (5%) 30 29	38, 59, 96, 109	0
2	1B	120/121 (99%)	-0.23	0 100 100	34, 53, 65, 87	0
2	2B	120/121 (99%)	0.46	3 (2%) 58 59	62, 73, 84, 97	0
3	1D	275/276 (99%)	0.02	3 (1%) 78 79	24, 39, 53, 84	0
3	2D	275/276 (99%)	0.23	3 (1%) 78 79	34, 50, 62, 78	0
4	1E	204/206 (99%)	-0.08	1 (0%) 87 89	21, 41, 60, 73	0
4	2E	204/206 (99%)	0.83	5 (2%) 58 59	41, 64, 76, 83	0
5	1F	202/210 (96%)	0.08	4 (1%) 65 65	21, 44, 68, 82	0
5	2F	202/210 (96%)	0.58	6 (2%) 52 54	38, 64, 78, 85	0
6	1G	181/182 (99%)	0.59	9 (4%) 34 33	46, 58, 72, 86	0
6	2G	181/182 (99%)	1.14	19 (10%) 11 11	63, 74, 82, 88	0
7	1H	174/180 (96%)	0.39	4 (2%) 61 62	39, 54, 67, 72	0
7	2H	174/180 (96%)	2.03	88 (50%) 0 0	73, 86, 92, 97	0
8	1I	146/148 (98%)	0.97	9 (6%) 26 26	51, 73, 80, 84	0
8	2I	146/148 (98%)	1.23	22 (15%) 5 5	52, 73, 84, 91	0
9	1N	140/140 (100%)	-0.07	1 (0%) 84 86	26, 38, 59, 75	0
9	2N	140/140 (100%)	1.10	9 (6%) 25 24	51, 69, 80, 84	0
10	1O	122/122 (100%)	0.02	1 (0%) 82 84	30, 42, 59, 62	0
10	2O	122/122 (100%)	0.81	1 (0%) 82 84	50, 63, 73, 78	0
11	1P	149/150 (99%)	0.30	4 (2%) 56 57	24, 52, 69, 77	0
11	2P	149/150 (99%)	0.72	5 (3%) 48 49	42, 64, 79, 88	0
12	1Q	141/141 (100%)	0.08	1 (0%) 84 86	26, 42, 57, 71	0
12	2Q	141/141 (100%)	1.15	15 (10%) 11 11	46, 68, 78, 84	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%)	-0.18	0 100 100	28, 37, 51, 57	0
13	2R	118/118 (100%)	0.64	2 (1%) 69 69	48, 58, 66, 76	0
14	1S	110/112 (98%)	0.26	1 (0%) 81 83	40, 53, 64, 69	0
14	2S	110/112 (98%)	0.86	4 (3%) 46 47	59, 70, 78, 84	0
15	1T	131/146 (89%)	0.37	5 (3%) 44 45	37, 46, 72, 84	0
15	2T	131/146 (89%)	1.02	12 (9%) 14 14	56, 66, 81, 84	0
16	1U	116/118 (98%)	-0.30	1 (0%) 81 83	22, 31, 44, 62	0
16	2U	116/118 (98%)	0.88	7 (6%) 27 27	45, 66, 76, 81	0
17	1V	101/101 (100%)	-0.22	0 100 100	24, 38, 55, 65	0
17	2V	101/101 (100%)	0.98	6 (5%) 28 27	47, 72, 79, 84	0
18	1W	112/113 (99%)	-0.21	1 (0%) 81 83	25, 33, 56, 80	0
18	2W	112/113 (99%)	0.42	3 (2%) 56 57	43, 52, 67, 90	0
19	1X	95/96 (98%)	0.07	3 (3%) 50 51	30, 42, 65, 75	0
19	2X	95/96 (98%)	0.70	7 (7%) 20 19	49, 58, 76, 82	0
20	1Y	107/110 (97%)	0.50	3 (2%) 55 56	39, 52, 69, 82	0
20	2Y	107/110 (97%)	1.47	23 (21%) 2 2	58, 70, 84, 89	0
21	1Z	154/206 (74%)	0.95	17 (11%) 10 10	41, 66, 84, 89	0
21	2Z	160/206 (77%)	1.69	44 (27%) 1 1	72, 82, 90, 92	0
22	10	83/85 (97%)	-0.03	1 (1%) 76 77	27, 40, 52, 63	0
22	20	83/85 (97%)	0.84	6 (7%) 21 20	45, 62, 70, 77	0
23	11	97/98 (98%)	0.51	3 (3%) 51 52	31, 50, 71, 76	0
23	21	97/98 (98%)	0.67	4 (4%) 41 42	42, 56, 75, 84	0
24	12	70/72 (97%)	0.44	2 (2%) 53 55	38, 50, 61, 76	0
24	22	70/72 (97%)	0.90	4 (5%) 29 29	56, 68, 76, 86	0
25	13	59/60 (98%)	0.00	2 (3%) 48 49	27, 37, 63, 82	0
25	23	59/60 (98%)	0.76	3 (5%) 33 33	53, 67, 78, 85	0
26	14	69/71 (97%)	1.19	14 (20%) 3 2	59, 75, 87, 90	0
26	24	69/71 (97%)	1.45	14 (20%) 3 2	71, 84, 91, 93	0
27	15	59/60 (98%)	-0.14	0 100 100	22, 34, 49, 57	0
27	25	59/60 (98%)	0.49	1 (1%) 69 69	41, 57, 69, 78	0
28	16	53/54 (98%)	0.20	1 (1%) 66 66	36, 45, 57, 61	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	26	53/54 (98%)	0.59	1 (1%) 66 66	47, 59, 67, 77	0
29	17	48/49 (97%)	0.06	4 (8%) 17 17	26, 31, 56, 66	0
29	27	48/49 (97%)	0.52	5 (10%) 11 11	38, 42, 67, 71	0
30	18	64/65 (98%)	-0.09	0 100 100	29, 37, 44, 56	0
30	28	64/65 (98%)	0.46	0 100 100	46, 56, 61, 68	0
31	19	37/37 (100%)	-0.06	0 100 100	32, 40, 61, 62	0
31	29	37/37 (100%)	1.39	7 (18%) 3 2	64, 73, 84, 88	0
32	1a	1488/1521 (97%)	0.31	58 (3%) 43 44	35, 67, 94, 109	0
32	2a	1491/1521 (98%)	0.54	78 (5%) 33 32	45, 72, 94, 108	0
33	1b	231/256 (90%)	1.51	62 (26%) 1 1	62, 78, 87, 93	0
33	2b	231/256 (90%)	1.74	81 (35%) 1 0	69, 83, 89, 93	0
34	1c	206/239 (86%)	1.15	22 (10%) 11 10	63, 73, 83, 90	0
34	2c	206/239 (86%)	1.72	69 (33%) 1 0	70, 79, 86, 90	0
35	1d	208/209 (99%)	1.12	20 (9%) 13 13	57, 69, 78, 89	0
35	2d	208/209 (99%)	0.89	11 (5%) 32 31	56, 66, 75, 85	0
36	1e	148/162 (91%)	0.85	7 (4%) 36 36	48, 64, 75, 81	0
36	2e	148/162 (91%)	1.02	6 (4%) 41 42	54, 71, 80, 87	0
37	1f	100/101 (99%)	0.85	5 (5%) 34 33	55, 68, 76, 80	0
37	2f	100/101 (99%)	0.65	2 (2%) 65 65	55, 66, 74, 81	0
38	1g	155/156 (99%)	1.02	19 (12%) 8 7	61, 71, 85, 91	0
38	2g	155/156 (99%)	1.25	23 (14%) 5 5	68, 75, 85, 96	0
39	1h	137/138 (99%)	0.74	2 (1%) 72 73	55, 65, 72, 76	0
39	2h	137/138 (99%)	0.93	7 (5%) 33 33	64, 72, 78, 81	0
40	1i	127/128 (99%)	1.60	30 (23%) 2 1	51, 78, 85, 88	0
40	2i	127/128 (99%)	1.98	61 (48%) 0 0	68, 83, 88, 91	0
41	1j	97/105 (92%)	1.85	43 (44%) 0 0	57, 78, 87, 93	0
41	2j	96/105 (91%)	2.38	59 (61%) 0 0	72, 83, 89, 96	0
42	1k	114/129 (88%)	0.86	9 (7%) 18 18	44, 64, 76, 80	0
42	2k	114/129 (88%)	1.05	13 (11%) 10 9	54, 71, 80, 84	0
43	1l	121/132 (91%)	0.38	3 (2%) 58 59	48, 54, 65, 71	0
43	2l	121/132 (91%)	0.87	7 (5%) 29 28	58, 65, 73, 77	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%)	1.13	17 (13%) 6 5	54, 70, 77, 86	0
44	2m	122/126 (96%)	1.51	27 (22%) 2 2	67, 78, 84, 90	0
45	1n	60/61 (98%)	1.13	6 (10%) 12 12	61, 69, 77, 78	0
45	2n	60/61 (98%)	2.23	30 (50%) 0 0	72, 79, 87, 89	0
46	1o	88/89 (98%)	0.85	7 (7%) 18 18	45, 65, 73, 77	0
46	2o	88/89 (98%)	0.86	4 (4%) 38 38	54, 66, 78, 86	0
47	1p	82/88 (93%)	1.43	19 (23%) 2 1	59, 71, 79, 84	0
47	2p	82/88 (93%)	1.02	9 (10%) 10 10	58, 68, 77, 79	0
48	1q	99/105 (94%)	1.03	5 (5%) 33 33	53, 66, 74, 76	0
48	2q	99/105 (94%)	1.02	6 (6%) 27 26	58, 70, 79, 80	0
49	1r	68/88 (77%)	0.61	4 (5%) 28 27	56, 64, 77, 79	0
49	2r	68/88 (77%)	0.75	2 (2%) 53 55	58, 67, 76, 79	0
50	1s	83/93 (89%)	1.09	11 (13%) 7 6	62, 73, 81, 86	0
50	2s	83/93 (89%)	1.76	29 (34%) 1 0	72, 82, 88, 90	0
51	1t	96/106 (90%)	1.14	14 (14%) 6 5	61, 71, 80, 85	0
51	2t	96/106 (90%)	1.33	15 (15%) 5 4	60, 72, 82, 85	0
52	1u	23/27 (85%)	1.69	7 (30%) 1 0	62, 66, 72, 78	0
52	2u	23/27 (85%)	1.84	9 (39%) 1 0	67, 75, 81, 84	0
53	1v	13/24 (54%)	0.81	3 (23%) 2 1	48, 55, 91, 97	0
53	2v	13/24 (54%)	1.10	3 (23%) 2 1	60, 70, 96, 103	0
54	1w	66/76 (86%)	1.34	15 (22%) 2 2	31, 86, 98, 102	0
54	2w	64/76 (84%)	1.48	17 (26%) 1 1	50, 95, 100, 104	0
55	1x	72/77 (93%)	0.24	2 (2%) 55 56	28, 60, 79, 90	0
55	2x	72/77 (93%)	0.36	1 (1%) 73 74	45, 72, 84, 100	0
56	1y	67/76 (88%)	1.96	31 (46%) 0 0	58, 99, 103, 105	0
56	2y	66/76 (86%)	2.24	41 (62%) 0 0	69, 101, 104, 107	0
All	All	20871/21748 (95%)	0.52	1800 (8%) 16 15	21, 64, 89, 109	0

All (1800) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	2A	652(V)	C	10.3
1	2A	652(U)	G	10.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	653	A	9.4
1	2A	654	A	7.5
1	1A	653	A	7.3
44	1m	123	ALA	7.2
44	2m	123	ALA	7.1
45	2n	2	ALA	6.9
21	1Z	141	VAL	6.9
1	2A	2802	G	6.8
1	1A	652(U)	G	6.8
35	1d	167	GLY	6.7
44	2m	124	PRO	6.6
38	1g	80	VAL	6.6
23	11	2	SER	6.6
23	21	2	SER	6.5
21	2Z	172	ALA	6.4
1	2A	652(T)	C	6.4
1	1A	654	A	6.3
38	2g	80	VAL	6.2
1	1A	652(C)	G	6.1
1	2A	883	G	6.1
1	1A	652(V)	C	6.1
44	1m	2	ALA	6.1
41	2j	32	ALA	6.1
45	1n	2	ALA	6.1
1	1A	1094	U	6.0
38	2g	85	TYR	6.0
33	2b	121	LEU	5.8
1	2A	652(C)	G	5.8
44	2m	102	ARG	5.7
33	1b	237	ALA	5.7
1	1A	1095	A	5.6
1	1A	1096	A	5.6
34	2c	2	GLY	5.6
21	1Z	146	ILE	5.6
41	2j	37	PRO	5.6
54	1w	73	A	5.4
1	2A	2111	C	5.3
1	2A	2803	C	5.3
1	1A	652(T)	C	5.2
1	1A	2114	A	5.2
51	1t	103	GLY	5.1
40	1i	64	THR	5.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	2110	G	5.1
7	2H	128	PRO	5.0
1	1A	2115	G	4.9
1	2A	2147	G	4.9
51	2t	103	GLY	4.9
1	1A	884	C	4.9
26	14	56	VAL	4.9
21	2Z	146	ILE	4.8
1	1A	652(S)	C	4.8
1	1A	2145	C	4.8
1	2A	2145	C	4.8
20	2Y	1	MET	4.8
1	1A	885	C	4.8
26	24	56	VAL	4.8
38	1g	84	ASN	4.8
15	1T	130	ALA	4.7
54	2w	71	G	4.7
44	1m	124	PRO	4.7
1	2A	882	G	4.7
50	2s	13	ASP	4.7
1	1A	1068	G	4.7
32	2a	1033	G	4.7
21	2Z	171	ILE	4.7
41	2j	74	ILE	4.7
3	1D	276	LYS	4.7
21	2Z	141	VAL	4.6
1	1A	2111	C	4.6
1	1A	2119	A	4.6
32	2a	1286	A	4.6
20	2Y	107	ASP	4.6
50	1s	13	ASP	4.6
1	1A	1064	C	4.5
33	2b	225	ALA	4.5
44	2m	122	LYS	4.5
38	2g	154	TYR	4.5
1	2A	2112	G	4.5
1	2A	2896	C	4.5
1	1A	1057	A	4.5
1	1A	2117	A	4.5
1	2A	652(D)	C	4.5
7	1H	2	SER	4.5
38	2g	81	GLY	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
42	2k	14	VAL	4.5
41	2j	36	GLY	4.4
32	1a	1035	A	4.4
33	2b	236	TYR	4.4
6	2G	50	ALA	4.4
46	2o	89	GLY	4.4
9	2N	9	VAL	4.4
38	2g	84	ASN	4.4
1	1A	1058	G	4.4
32	1a	1036	G	4.4
1	2A	652(B)	A	4.4
32	2a	1032	G	4.3
40	2i	11	LYS	4.3
1	2A	884	C	4.3
40	2i	14	VAL	4.3
1	1A	2112	G	4.3
32	2a	1030(A)	G	4.3
7	2H	19	VAL	4.3
41	2j	14	LYS	4.3
42	2k	25	TYR	4.3
12	2Q	10	ARG	4.3
43	2l	18	VAL	4.3
1	1A	888	C	4.3
1	1A	2790	A	4.3
34	2c	190	ARG	4.3
1	1A	1087	G	4.2
32	2a	1001(A)	G	4.2
33	2b	7	VAL	4.2
41	2j	90	LEU	4.2
40	1i	15	ALA	4.2
1	2A	2893	G	4.2
51	2t	28	ALA	4.2
33	1b	22	LYS	4.2
1	1A	1081	U	4.2
1	1A	1082	U	4.2
33	1b	19	HIS	4.2
44	2m	121	LYS	4.2
7	2H	26	VAL	4.2
1	2A	2805	G	4.2
26	24	63	TYR	4.1
38	2g	82	GLY	4.1
1	2A	896	A	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
6	2G	52	ILE	4.1
1	1A	2113	U	4.1
29	27	48	LYS	4.1
1	2A	2125	G	4.1
51	1t	69	GLY	4.1
1	1A	2803	C	4.1
1	1A	882	G	4.1
5	1F	207	GLY	4.1
41	2j	10	GLY	4.1
41	2j	31	GLY	4.1
7	2H	45	VAL	4.1
21	1Z	105	VAL	4.1
21	2Z	174	VAL	4.1
41	2j	65	LEU	4.1
1	2A	1536	C	4.1
38	2g	83	ALA	4.1
41	2j	77	PRO	4.1
1	1A	879	G	4.1
7	2H	33	LEU	4.1
21	2Z	166	SER	4.0
38	1g	81	GLY	4.0
29	17	48	LYS	4.0
44	1m	122	LYS	4.0
1	1A	2166	G	4.0
1	1A	1069	A	4.0
1	2A	2135	A	4.0
6	1G	50	ALA	4.0
32	2a	1030	C	4.0
1	2A	2144	U	4.0
32	1a	1025	U	4.0
48	1q	98	LEU	4.0
45	2n	33	VAL	4.0
21	2Z	159	PRO	4.0
1	1A	2170	A	4.0
33	2b	38	GLY	4.0
33	2b	165	VAL	4.0
25	23	2	PRO	4.0
1	1A	2116	G	4.0
1	1A	1509	C	4.0
1	1A	2109	U	4.0
7	2H	7	LEU	4.0
7	2H	21	PRO	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
41	2j	47	PHE	3.9
41	1j	32	ALA	3.9
1	1A	2802	G	3.9
32	1a	1003	G	3.9
1	1A	2135	A	3.9
32	2a	1030(B)	C	3.9
40	1i	59	PHE	3.9
20	1Y	1	MET	3.9
33	2b	201	ILE	3.9
1	1A	2793	G	3.9
32	1a	1034	G	3.9
1	2A	2113	U	3.9
1	2A	1509	C	3.9
33	1b	232	PRO	3.9
45	2n	39	LEU	3.9
1	1A	1098	A	3.9
55	2x	47	U	3.9
32	1a	1027	C	3.9
32	2a	1018	C	3.9
54	2w	72	C	3.9
15	2T	131	ALA	3.9
41	2j	26	ALA	3.9
23	11	93	GLU	3.9
47	2p	82	GLN	3.9
1	1A	878	A	3.9
1	1A	1066	U	3.8
56	2y	7	A	3.9
15	2T	130	ALA	3.8
26	14	63	TYR	3.8
21	2Z	105	VAL	3.8
15	1T	131	ALA	3.8
21	2Z	104	PHE	3.8
33	2b	34	ALA	3.8
40	2i	36	TYR	3.8
1	2A	1533	G	3.8
1	2A	2110	G	3.8
38	1g	82	GLY	3.8
7	2H	136	ILE	3.8
40	2i	126	SER	3.8
41	2j	34	VAL	3.8
8	1I	146	ALA	3.8
46	2o	88	ARG	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
45	2n	34	TYR	3.8
41	1j	10	GLY	3.8
1	1A	2136	C	3.8
1	1A	652(E)	G	3.8
32	1a	1033	G	3.8
45	2n	3	ARG	3.8
26	14	54	GLY	3.8
36	2e	114	GLY	3.8
6	2G	53	LEU	3.8
21	2Z	150	LEU	3.8
1	2A	2804	C	3.8
32	1a	630	G	3.8
54	1w	1	G	3.8
33	1b	17	PHE	3.7
1	2A	2126	A	3.7
26	24	31	ILE	3.7
34	1c	39	ILE	3.7
56	1y	36	A	3.7
33	1b	10	LEU	3.7
1	2A	2138	C	3.7
1	1A	2165	G	3.7
1	2A	2148	G	3.7
54	1w	71	G	3.7
21	2Z	164	ALA	3.7
33	2b	237	ALA	3.7
38	1g	83	ALA	3.7
24	22	70	GLN	3.7
1	2A	2134	A	3.7
6	1G	51	ARG	3.7
41	1j	66	ARG	3.7
7	2H	2	SER	3.7
1	1A	880	G	3.7
1	1A	1063	G	3.7
8	2I	63	ALA	3.7
15	2T	128	GLU	3.7
33	2b	17	PHE	3.7
19	1X	95	LEU	3.7
1	1A	2130	U	3.7
1	2A	1026	U	3.7
36	1e	10	MET	3.7
32	2a	1005	A	3.7
53	1v	12	A	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
54	2w	73	A	3.7
40	1i	14	VAL	3.7
1	1A	897	C	3.7
1	2A	2174	C	3.7
45	2n	7	ILE	3.7
1	2A	1509(A)	A	3.6
32	1a	1531	A	3.6
6	2G	48	GLU	3.6
1	1A	2143	C	3.6
1	2A	2137	C	3.6
12	2Q	104	PHE	3.6
8	2I	68	LEU	3.6
1	1A	2160	G	3.6
1	2A	11	G	3.6
54	1w	70	G	3.6
32	1a	1030(D)	A	3.6
34	2c	207	VAL	3.6
44	1m	121	LYS	3.6
1	2A	2136	C	3.6
1	1A	2159	G	3.6
32	2a	1002	G	3.6
32	2a	1034	G	3.6
56	2y	34	G	3.6
7	2H	52	VAL	3.6
1	1A	896	A	3.6
54	2w	2	C	3.6
26	14	51	ASP	3.6
33	1b	236	TYR	3.6
33	2b	86	GLU	3.6
1	1A	655	A	3.6
47	1p	82	GLN	3.6
35	2d	155	LEU	3.6
40	1i	8	GLY	3.6
41	2j	93	GLY	3.6
26	24	65	ASP	3.6
1	1A	1065	U	3.5
32	1a	1024	G	3.5
5	2F	207	GLY	3.5
33	2b	221	LEU	3.5
50	2s	84	GLY	3.5
32	2a	1035	A	3.5
7	2H	126	PRO	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	2129	C	3.5
1	2A	885	C	3.5
7	2H	17	VAL	3.5
21	2Z	144	LEU	3.5
41	2j	40	LEU	3.5
35	2d	23	GLY	3.5
7	2H	12	PRO	3.5
20	2Y	44	ILE	3.5
53	2v	12	A	3.5
1	1A	652(D)	C	3.5
32	1a	1028	C	3.5
33	1b	15	VAL	3.5
45	2n	13	THR	3.5
1	2A	271(K)	U	3.5
33	1b	11	LEU	3.5
40	1i	47	LEU	3.5
40	1i	13	ALA	3.5
40	2i	39	GLY	3.5
40	2i	46	ALA	3.5
1	1A	1059	G	3.5
1	1A	2121	G	3.5
32	1a	1030(A)	G	3.5
7	2H	15	VAL	3.5
50	1s	9	VAL	3.5
1	2A	2143	C	3.5
1	1A	899	A	3.4
52	1u	9	ARG	3.4
52	1u	24	ARG	3.4
32	1a	79	G	3.4
32	2a	1003	G	3.4
45	2n	25	VAL	3.4
34	2c	188	LEU	3.4
51	1t	10	LEU	3.4
1	1A	2167	U	3.4
1	2A	888	C	3.4
49	1r	20	ALA	3.4
54	1w	72	C	3.4
21	1Z	52	SER	3.4
7	2H	123	PHE	3.4
1	1A	652(F)	G	3.4
7	2H	24	VAL	3.4
7	2H	50	VAL	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
50	2s	16	LEU	3.4
40	2i	63	ILE	3.4
1	1A	271(K)	U	3.4
1	2A	2146	C	3.4
34	2c	62	ASP	3.4
1	1A	887	A	3.4
51	2t	10	LEU	3.4
32	2a	1031	G	3.4
33	2b	192	SER	3.4
1	2A	2109	U	3.4
32	2a	470	C	3.4
20	2Y	45	VAL	3.4
40	2i	19	LEU	3.4
41	2j	92	THR	3.4
50	2s	9	VAL	3.4
35	1d	87	GLY	3.4
33	2b	39	ILE	3.4
11	1P	149	GLU	3.4
33	2b	134	GLU	3.4
42	2k	75	TYR	3.3
54	2w	70	G	3.3
1	1A	2172	U	3.3
54	2w	3	C	3.3
44	1m	27	LYS	3.3
33	2b	187	LEU	3.3
40	2i	56	LEU	3.3
50	2s	15	LEU	3.3
51	2t	98	PRO	3.3
1	1A	1088	A	3.3
35	1d	5	ILE	3.3
13	2R	14	SER	3.3
33	2b	163	PHE	3.3
56	2y	19	G	3.3
24	12	70	GLN	3.3
1	1A	889	C	3.3
1	2A	897	C	3.3
1	2A	2794	C	3.3
7	2H	64	LEU	3.3
33	1b	61	LEU	3.3
21	2Z	170	THR	3.3
51	1t	8	ARG	3.3
33	1b	9	GLU	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	1c	2	GLY	3.3
45	2n	38	GLY	3.3
1	1A	2158	A	3.3
1	2A	2801(A)	A	3.3
41	2j	78	ASN	3.3
1	2A	881	G	3.3
1	2A	2156	G	3.3
1	1A	2108	C	3.3
32	2a	1027	C	3.3
40	2i	9	ARG	3.3
8	2I	48	GLU	3.3
34	2c	95	THR	3.3
51	2t	97	ALA	3.3
53	1v	13	A	3.3
53	2v	13	A	3.3
45	2n	36	PHE	3.3
35	2d	154	ASN	3.3
32	1a	1532	U	3.3
7	2H	10	PRO	3.3
11	2P	15	ARG	3.3
40	2i	44	VAL	3.3
1	1A	2164	C	3.3
1	1A	2896	C	3.3
7	2H	92	ILE	3.3
3	1D	275	LYS	3.3
7	2H	145	ALA	3.3
21	1Z	136	PHE	3.2
32	1a	1447	A	3.2
33	1b	70	PHE	3.2
51	2t	9	ASN	3.2
1	1A	2897	U	3.2
51	2t	99	LEU	3.2
20	1Y	91	GLU	3.2
52	2u	16	GLY	3.2
41	1j	98	ILE	3.2
1	1A	886	C	3.2
1	1A	2141	G	3.2
56	2y	15	G	3.2
1	1A	1073	A	3.2
1	1A	1086	A	3.2
1	1A	1509(A)	A	3.2
33	2b	19	HIS	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
54	1w	20	U	3.2
20	2Y	49	VAL	3.2
29	27	45	ALA	3.2
1	2A	2128	C	3.2
32	1a	1030	C	3.2
1	1A	1176	G	3.2
1	2A	2154	G	3.2
56	2y	18	G	3.2
1	1A	1508	A	3.2
40	2i	96	LEU	3.2
56	2y	36	A	3.2
5	2F	6	VAL	3.2
29	27	46	VAL	3.2
50	1s	8	GLY	3.2
21	2Z	173	ALA	3.2
1	1A	1075	C	3.2
32	2a	1029	C	3.2
32	2a	1149	C	3.2
33	2b	70	PHE	3.2
1	2A	2149	G	3.2
32	1a	1026	G	3.2
33	2b	22	LYS	3.2
40	1i	56	LEU	3.2
1	1A	1070	A	3.2
56	1y	35	A	3.2
7	2H	125	VAL	3.2
21	2Z	106	GLY	3.2
34	2c	138	VAL	3.2
41	1j	4	ILE	3.2
14	1S	3	ARG	3.1
22	20	11	ARG	3.1
29	27	47	ARG	3.1
41	2j	63	PHE	3.1
6	2G	54	GLU	3.1
50	2s	12	ASP	3.1
31	29	20	HIS	3.1
41	2j	91	PRO	3.1
44	2m	106	ASN	3.1
1	1A	2151	G	3.1
1	2A	2751	G	3.1
32	1a	1023	G	3.1
32	1a	1032	G	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
38	1g	154	TYR	3.1
56	2y	14	A	3.1
33	1b	201	ILE	3.1
40	2i	106	ALA	3.1
40	2i	18	PHE	3.1
6	2G	49	ASP	3.1
38	1g	156	TRP	3.1
40	1i	19	LEU	3.1
1	2A	2140	C	3.1
21	2Z	160	GLY	3.1
1	2A	2793	G	3.1
7	2H	44	VAL	3.1
39	2h	90	GLY	3.1
40	1i	67	GLY	3.1
1	2A	2117	A	3.1
19	2X	68	ARG	3.1
40	2i	94	ALA	3.1
33	2b	11	LEU	3.1
48	2q	99	SER	3.1
44	2m	6	GLY	3.1
15	2T	28	VAL	3.1
21	2Z	139	VAL	3.1
52	2u	6	ARG	3.1
7	2H	94	TYR	3.1
22	20	43	THR	3.1
33	2b	148	TYR	3.1
40	2i	125	TYR	3.1
1	1A	2131	G	3.1
1	2A	2158	A	3.1
32	1a	1286	A	3.1
32	2a	1001	A	3.1
33	2b	132	LYS	3.1
33	2b	188	ALA	3.1
56	1y	1	G	3.1
56	1y	19	G	3.1
56	2y	35	A	3.1
40	1i	18	PHE	3.1
49	2r	66	LEU	3.1
50	2s	36	ARG	3.1
1	1A	898	C	3.1
1	1A	2794	C	3.1
1	2A	2179	C	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
35	2d	5	ILE	3.1
26	14	69	LYS	3.0
12	1Q	32	TYR	3.0
40	2i	114	TYR	3.0
1	1A	2171	A	3.0
1	2A	887	A	3.0
32	2a	1004	A	3.0
32	2a	1257	U	3.0
41	1j	77	PRO	3.0
7	2H	82	GLY	3.0
33	1b	222	ILE	3.0
41	1j	74	ILE	3.0
41	2j	87	THR	3.0
50	2s	79	THR	3.0
1	1A	2128	C	3.0
1	2A	2139	C	3.0
5	2F	21	ALA	3.0
33	1b	13	ALA	3.0
48	2q	95	TYR	3.0
33	2b	140	HIS	3.0
1	1A	1077	A	3.0
1	1A	2169	A	3.0
1	2A	2170	A	3.0
32	1a	204	U	3.0
32	2a	1030(D)	A	3.0
40	2i	21	PRO	3.0
40	2i	102	LEU	3.0
45	2n	6	LEU	3.0
1	1A	881	G	3.0
1	1A	2120	G	3.0
1	2A	271(M)	G	3.0
29	17	47	ARG	3.0
40	2i	66	ARG	3.0
56	2y	6	G	3.0
26	24	66	SER	3.0
3	2D	276	LYS	3.0
44	2m	12	ASN	3.0
35	2d	87	GLY	3.0
12	2Q	121	ALA	3.0
20	2Y	91	GLU	3.0
34	2c	92	ALA	3.0
1	1A	2137	C	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	2804	C	3.0
1	2A	2175	C	3.0
34	2c	47	LEU	3.0
40	2i	79	LEU	3.0
1	1A	895	U	3.0
32	2a	1148	U	3.0
33	2b	175	ARG	3.0
54	2w	45	U	3.0
56	1y	12	U	3.0
41	2j	59	SER	3.0
42	2k	51	LYS	3.0
1	2A	2141	G	3.0
44	2m	100	GLY	3.0
41	1j	33	GLN	3.0
43	1l	18	VAL	3.0
51	1t	100	ILE	3.0
21	1Z	1	MET	3.0
38	1g	85	TYR	3.0
1	1A	2174	C	3.0
3	2D	275	LYS	3.0
12	2Q	65	PHE	3.0
21	2Z	136	PHE	3.0
32	2a	1040	U	3.0
32	2a	1532	U	3.0
56	1y	20	U	3.0
56	2y	58	A	3.0
4	2E	29	GLY	3.0
15	1T	123	GLN	3.0
7	2H	35	VAL	2.9
9	1N	9	VAL	2.9
1	1A	2207	G	2.9
1	2A	2133	G	2.9
32	2a	1021	G	2.9
40	2i	2	GLU	2.9
40	2i	52	ALA	2.9
21	2Z	167	PRO	2.9
24	22	69	ARG	2.9
41	1j	41	PRO	2.9
34	2c	52	LEU	2.9
1	1A	2140	C	2.9
26	24	59	PHE	2.9
33	1b	124	SER	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
40	2i	8	GLY	2.9
42	2k	117	ASN	2.9
7	2H	43	VAL	2.9
40	1i	2	GLU	2.9
27	25	29	THR	2.9
1	2A	652(E)	G	2.9
1	2A	2127	G	2.9
1	2A	2157	G	2.9
1	2A	2894	G	2.9
26	14	55	ARG	2.9
32	1a	1001(A)	G	2.9
38	2g	5	ARG	2.9
41	2j	79	ARG	2.9
50	2s	2	PRO	2.9
39	1h	112	LEU	2.9
26	24	67	TYR	2.9
42	1k	25	TYR	2.9
1	1A	1078	U	2.9
1	2A	886	C	2.9
1	2A	2164	C	2.9
50	2s	4	SER	2.9
56	2y	33	U	2.9
38	2g	37	ASN	2.9
41	2j	76	ASN	2.9
42	1k	117	ASN	2.9
1	1A	2173	A	2.9
1	1A	2801(A)	A	2.9
33	2b	12	GLU	2.9
33	1b	7	VAL	2.9
37	1f	90	VAL	2.9
40	1i	17	VAL	2.9
50	2s	19	VAL	2.9
35	1d	191	ARG	2.9
3	1D	38	LYS	2.9
7	2H	175	LYS	2.9
1	1A	2133	G	2.9
1	2A	880	G	2.9
1	2A	2124	G	2.9
32	2a	1036	G	2.9
34	2c	193	TYR	2.9
50	2s	80	TYR	2.9
34	2c	142	MET	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
35	2d	156	GLU	2.9
40	2i	67	GLY	2.9
32	2a	1038	C	2.9
32	2a	1039	C	2.9
1	2A	2119	A	2.9
1	2A	2892	A	2.9
32	2a	978	A	2.9
32	2a	1251	A	2.9
7	2H	29	PRO	2.9
41	2j	39	PRO	2.9
41	2j	100	THR	2.9
50	2s	63	THR	2.9
52	1u	23	PRO	2.9
8	2I	75	LEU	2.9
33	2b	118	LEU	2.9
1	1A	2123	G	2.9
1	2A	2155	G	2.9
40	2i	101	PHE	2.9
54	1w	69	G	2.9
7	2H	40	GLU	2.9
21	2Z	168	GLU	2.9
7	2H	60	ARG	2.8
21	2Z	149	SER	2.8
34	2c	3	ASN	2.8
41	2j	38	ILE	2.8
1	1A	1060	U	2.8
1	1A	2146	C	2.8
1	2A	898	C	2.8
1	2A	1508	A	2.8
1	2A	2173	A	2.8
1	2A	2629	A	2.8
33	1b	125	PRO	2.8
56	2y	21	A	2.8
33	2b	138	LEU	2.8
50	2s	71	LEU	2.8
6	1G	48	GLU	2.8
33	1b	231	GLU	2.8
36	2e	133	TYR	2.8
7	2H	120	GLY	2.8
45	1n	57	ARG	2.8
51	2t	96	GLY	2.8
52	2u	24	ARG	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	2115	G	2.8
7	2H	4	ILE	2.8
32	2a	630	G	2.8
32	2a	1026	G	2.8
41	2j	56	HIS	2.8
44	2m	92	HIS	2.8
35	1d	170	VAL	2.8
48	2q	23	VAL	2.8
52	2u	23	PRO	2.8
1	1A	2138	C	2.8
8	2I	53	ALA	2.8
21	2Z	51	ALA	2.8
32	1a	1008	C	2.8
40	2i	82	ALA	2.8
1	1A	1067	A	2.8
1	2A	899	A	2.8
1	2A	2114	A	2.8
17	2V	94	LEU	2.8
19	2X	95	LEU	2.8
20	2Y	90	LEU	2.8
32	2a	1248	A	2.8
41	1j	86	MET	2.8
21	1Z	2	GLU	2.8
21	2Z	103	ARG	2.8
38	1g	79	ARG	2.8
47	1p	80	PHE	2.8
34	2c	51	GLY	2.8
40	2i	62	TYR	2.8
43	1l	64	TYR	2.8
1	1A	1093	G	2.8
7	2H	36	PRO	2.8
21	2Z	95	PRO	2.8
26	14	50	VAL	2.8
33	1b	229	VAL	2.8
32	1a	1031	G	2.8
32	2a	1023	G	2.8
55	1x	46	G	2.8
1	1A	1097	U	2.8
1	2A	2897	U	2.8
47	2p	69	THR	2.8
56	2y	59	U	2.8
7	2H	20	ALA	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
11	1P	15	ARG	2.8
45	2n	4	LYS	2.8
33	2b	122	PHE	2.8
35	1d	173	TRP	2.8
47	2p	59	TRP	2.8
8	1I	109	ILE	2.8
33	2b	41	ILE	2.8
38	1g	151	TYR	2.8
50	2s	52	TYR	2.8
20	2Y	53	PRO	2.8
21	2Z	71	VAL	2.8
45	2n	18	VAL	2.8
32	1a	1257	U	2.8
36	1e	48	ALA	2.8
1	1A	2168	G	2.8
1	2A	1537	G	2.8
1	2A	2151	G	2.8
1	2A	2165	G	2.8
32	1a	1002	G	2.8
54	1w	5	G	2.8
44	2m	120	LYS	2.8
1	2A	271(J)	C	2.8
32	2a	1037	C	2.8
56	2y	67	C	2.8
33	2b	166	ASP	2.8
15	1T	37	GLY	2.7
26	14	49	PHE	2.8
33	2b	200	ILE	2.7
34	2c	8	ILE	2.7
34	2c	14	ILE	2.7
38	2g	156	TRP	2.7
20	2Y	55	TYR	2.7
34	1c	184	TYR	2.7
38	2g	151	TYR	2.7
7	2H	49	VAL	2.7
29	17	46	VAL	2.7
33	1b	71	VAL	2.7
21	1Z	170	THR	2.7
40	2i	43	ALA	2.7
1	2A	2167	U	2.7
48	2q	100	LYS	2.7
56	2y	12	U	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
11	2P	79	ARG	2.7
40	1i	66	ARG	2.7
40	2i	12	GLU	2.7
42	1k	13	GLN	2.7
1	1A	883	G	2.7
1	1A	1089	G	2.7
1	2A	2160	G	2.7
32	1a	1030(C)	G	2.7
1	1A	2142	C	2.7
1	2A	878	A	2.7
8	2I	20	ASP	2.7
21	1Z	140	ASP	2.7
32	2a	1531	A	2.7
6	2G	127	GLY	2.7
34	2c	182	ILE	2.7
33	1b	131	PRO	2.7
12	2Q	96	VAL	2.7
21	1Z	149	SER	2.7
31	29	16	VAL	2.7
34	2c	106	VAL	2.7
41	2j	44	VAL	2.7
11	1P	148	LEU	2.7
34	1c	47	LEU	2.7
45	2n	47	LEU	2.7
34	2c	189	ALA	2.7
38	2g	152	ALA	2.7
45	2n	35	ARG	2.7
33	2b	170	GLU	2.7
1	1A	2189	U	2.7
1	2A	9	U	2.7
32	1a	90	U	2.7
32	2a	1150	U	2.7
41	1j	84	GLN	2.7
1	1A	2893	G	2.7
1	2A	2116	G	2.7
18	1W	112	GLY	2.7
32	2a	1024	G	2.7
33	1b	38	GLY	2.7
56	1y	15	G	2.7
1	1A	1053	C	2.7
1	1A	1072	C	2.7
32	1a	1030(B)	C	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	2a	1223	C	2.7
41	1j	38	ILE	2.7
33	2b	234	PRO	2.7
6	2G	76	SER	2.7
8	2I	87	LYS	2.7
33	2b	164	VAL	2.7
34	2c	195	VAL	2.7
36	1e	69	VAL	2.7
39	2h	129	VAL	2.7
20	2Y	5	MET	2.7
22	10	84	LEU	2.7
40	1i	95	LYS	2.7
21	1Z	152	ALA	2.7
38	2g	32	ARG	2.7
41	1j	29	ARG	2.7
49	2r	20	ALA	2.7
1	1A	2144	U	2.7
1	2A	895	U	2.7
1	2A	2150	U	2.7
33	1b	140	HIS	2.7
34	2c	6	HIS	2.7
56	2y	47	U	2.7
12	2Q	30	GLY	2.7
25	13	2	PRO	2.7
33	2b	232	PRO	2.7
35	1d	70	ILE	2.7
1	1A	548	A	2.7
1	1A	2125	G	2.7
1	2A	2123	G	2.7
1	1A	2175	C	2.7
1	2A	229	A	2.7
1	2A	2108	C	2.7
20	1Y	92	ASN	2.7
7	2H	113	VAL	2.7
33	1b	230	VAL	2.7
38	2g	16	LEU	2.7
39	2h	2	LEU	2.7
40	2i	10	ARG	2.7
40	2i	17	VAL	2.7
44	2m	7	VAL	2.7
26	14	67	TYR	2.7
34	2c	29	TYR	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	1b	186	ALA	2.7
33	2b	67	THR	2.7
47	1p	22	THR	2.7
1	2A	2895	U	2.7
7	2H	8	PRO	2.6
7	2H	27	LYS	2.6
20	2Y	23	ARG	2.6
32	1a	1005	A	2.6
1	1A	2139	C	2.6
1	1A	2162	G	2.6
1	2A	879	G	2.6
1	2A	2159	G	2.6
32	2a	1030(C)	G	2.6
32	2a	1249	C	2.6
41	2j	72	VAL	2.6
45	1n	60	SER	2.6
56	2y	1	G	2.6
56	2y	13	C	2.6
56	2y	65	G	2.6
36	2e	20	GLN	2.6
41	1j	26	ALA	2.6
47	2p	48	TRP	2.6
1	1A	2180	U	2.6
23	21	81	LYS	2.6
33	2b	8	LYS	2.6
26	14	59	PHE	2.6
33	2b	125	PRO	2.6
34	1c	128	PHE	2.6
34	2c	7	PRO	2.6
7	2H	23	ARG	2.6
41	1j	46	ARG	2.6
34	2c	87	LEU	2.6
45	2n	44	LEU	2.6
50	2s	20	LEU	2.6
7	2H	11	VAL	2.6
20	2Y	72	VAL	2.6
26	14	57	GLU	2.6
1	1A	652(A)	A	2.6
7	2H	156	ALA	2.6
8	2I	98	ALA	2.6
40	2i	13	ALA	2.6
41	1j	67	THR	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
44	2m	118	ALA	2.6
6	1G	146	TYR	2.6
56	1y	53	G	2.6
56	2y	44	G	2.6
7	2H	100	GLY	2.6
36	1e	85	GLY	2.6
46	1o	89	GLY	2.6
32	2a	1025	U	2.6
32	2a	1219	U	2.6
33	1b	127	ILE	2.6
40	2i	16	ARG	2.6
50	2s	76	PRO	2.6
56	1y	59	U	2.6
9	2N	1	MET	2.6
7	2H	71	LEU	2.6
21	1Z	33	LEU	2.6
25	13	60	GLU	2.6
33	1b	44	LEU	2.6
40	2i	99	LEU	2.6
44	2m	90	LEU	2.6
7	2H	79	VAL	2.6
12	2Q	109	VAL	2.6
35	1d	88	VAL	2.6
21	2Z	152	ALA	2.6
38	2g	2	ALA	2.6
41	2j	18	ALA	2.6
40	2i	4	TYR	2.6
42	1k	75	TYR	2.6
40	2i	97	LYS	2.6
1	1A	545	G	2.6
1	1A	2792	G	2.6
1	2A	10	G	2.6
1	2A	1171	G	2.6
1	2A	2153	G	2.6
54	2w	5	G	2.6
7	1H	3	ARG	2.6
21	1Z	148	ASP	2.6
33	1b	223	ILE	2.6
34	2c	5	ILE	2.6
32	2a	961	U	2.6
56	2y	66	U	2.6
8	1I	68	LEU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
8	2I	64	GLU	2.6
45	2n	53	LEU	2.6
21	2Z	96	VAL	2.6
33	1b	165	VAL	2.6
41	1j	76	ASN	2.6
43	2l	39	VAL	2.6
6	1G	76	SER	2.6
34	2c	71	ALA	2.6
45	2n	5	ALA	2.6
34	2c	4	LYS	2.6
42	2k	55	LYS	2.6
1	1A	1084	A	2.6
1	2A	528	A	2.6
32	1a	1001	A	2.6
53	2v	14	A	2.6
1	1A	1076	C	2.5
1	1A	2107	C	2.5
44	2m	94	ARG	2.5
34	2c	167	TRP	2.5
52	2u	14	TRP	2.5
7	2H	39	PRO	2.5
9	2N	80	GLY	2.5
11	1P	44	GLY	2.5
15	2T	124	ASP	2.5
52	2u	2	GLY	2.5
1	1A	1062	G	2.5
1	2A	2190	G	2.5
21	2Z	133	ILE	2.5
32	1a	346	G	2.5
33	1b	214	ILE	2.5
35	2d	158	ILE	2.5
56	2y	22	G	2.5
1	1A	2132	U	2.5
1	1A	2808	U	2.5
1	2A	2118	U	2.5
35	1d	120	LEU	2.5
56	1y	47	U	2.5
40	2i	53	VAL	2.5
44	1m	15	VAL	2.5
45	2n	56	VAL	2.5
41	1j	68	HIS	2.5
7	2H	16	SER	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	2H	165	ALA	2.5
41	2j	48	THR	2.5
15	2T	112	ARG	2.5
33	1b	21	ARG	2.5
1	1A	1103	A	2.5
42	2k	50	TYR	2.5
54	2w	7	A	2.5
21	1Z	159	PRO	2.5
21	2Z	158	PRO	2.5
33	2b	131	PRO	2.5
32	2a	1006	C	2.5
50	1s	68	GLY	2.5
33	1b	97	TRP	2.5
34	2c	22	TRP	2.5
1	1A	271(M)	G	2.5
1	1A	1071	G	2.5
1	1A	2152	G	2.5
1	1A	2156	G	2.5
1	2A	2318	G	2.5
32	2a	1131	G	2.5
41	2j	88	LEU	2.5
49	1r	78	LEU	2.5
56	2y	57	G	2.5
1	1A	2118	U	2.5
32	2a	1020	U	2.5
34	1c	107	GLN	2.5
7	1H	17	VAL	2.5
9	2N	46	VAL	2.5
33	2b	71	VAL	2.5
42	1k	51	LYS	2.5
33	2b	77	ALA	2.5
33	2b	123	ALA	2.5
7	2H	129	THR	2.5
14	2S	50	SER	2.5
16	2U	59	ARG	2.5
41	1j	45	ARG	2.5
33	2b	48	MET	2.5
4	2E	56	PRO	2.5
33	2b	31	TYR	2.5
40	1i	21	PRO	2.5
46	1o	69	TYR	2.5
1	1A	229	A	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	2H	48	GLY	2.5
21	2Z	169	GLU	2.5
41	2j	61	GLU	2.5
48	2q	96	GLU	2.5
1	1A	154(A)	C	2.5
4	2E	195	LEU	2.5
33	2b	55	PHE	2.5
49	1r	76	LEU	2.5
6	1G	182	LYS	2.5
33	1b	40	HIS	2.5
24	22	65	ASN	2.5
33	2b	136	VAL	2.5
44	2m	98	VAL	2.5
1	2A	1112	G	2.5
1	2A	2792	G	2.5
32	1a	70	G	2.5
54	2w	15	G	2.5
56	2y	5	G	2.5
34	2c	160	ALA	2.5
38	1g	115	ARG	2.5
42	2k	89	ALA	2.5
6	2G	164	GLU	2.5
8	2I	135	GLU	2.5
26	24	32	TYR	2.5
34	2c	201	TYR	2.5
7	2H	9	ILE	2.5
1	2A	6	A	2.5
32	2a	1447	A	2.5
7	2H	67	LEU	2.5
41	2j	85	LEU	2.5
48	1q	100	LYS	2.5
51	2t	74	LYS	2.5
21	1Z	104	PHE	2.5
42	2k	13	GLN	2.5
32	2a	1019	C	2.5
32	2a	1054	C	2.5
54	1w	4	C	2.5
34	2c	55	VAL	2.5
36	1e	67	VAL	2.5
7	2H	6	ARG	2.5
26	24	68	ARG	2.5
32	2a	1125	U	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
41	2j	43	ARG	2.5
45	2n	12	ARG	2.5
47	1p	75	ARG	2.5
33	1b	120	ALA	2.5
1	1A	1056	G	2.5
1	1A	2147	G	2.5
1	1A	2153	G	2.5
1	1A	2154	G	2.5
7	2H	63	SER	2.5
7	2H	134	SER	2.5
54	2w	69	G	2.5
19	2X	94	GLY	2.4
33	1b	12	GLU	2.4
41	1j	97	GLU	2.4
16	2U	76	TYR	2.4
33	2b	222	ILE	2.4
34	2c	48	TYR	2.4
41	2j	89	ASP	2.4
7	2H	88	LEU	2.4
34	2c	43	LEU	2.4
32	2a	977	A	2.4
32	2a	1250	A	2.4
34	1c	28	GLN	2.4
34	1c	10	PHE	2.4
15	2T	115	ARG	2.4
36	2e	27	ARG	2.4
37	1f	46	ARG	2.4
46	2o	72	ARG	2.4
1	1A	34	C	2.4
1	1A	2163	C	2.4
1	2A	2129	C	2.4
40	2i	41	VAL	2.4
56	1y	67	C	2.4
1	1A	2122	U	2.4
7	2H	41	MET	2.4
34	2c	200	ALA	2.4
42	1k	15	ALA	2.4
25	23	40	THR	2.4
40	2i	27	THR	2.4
40	1i	126	SER	2.4
41	2j	30	SER	2.4
1	1A	2127	G	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	2149	G	2.4
1	2A	2166	G	2.4
26	24	54	GLY	2.4
35	2d	151	LYS	2.4
42	2k	124	LYS	2.4
56	1y	6	G	2.4
56	2y	24	G	2.4
34	2c	57	ILE	2.4
39	2h	4	ASP	2.4
41	1j	75	ILE	2.4
45	2n	42	ILE	2.4
33	2b	196	LEU	2.4
38	2g	153	HIS	2.4
34	2c	127	ARG	2.4
40	1i	10	ARG	2.4
1	2A	652(A)	A	2.4
1	2A	2169	A	2.4
56	2y	73	A	2.4
8	1I	107	VAL	2.4
20	2Y	92	ASN	2.4
33	1b	136	VAL	2.4
47	1p	62	VAL	2.4
1	1A	271(J)	C	2.4
1	1A	2185	C	2.4
4	2E	204	ALA	2.4
32	1a	1037	C	2.4
34	2c	146	ALA	2.4
40	1i	94	ALA	2.4
56	2y	4	C	2.4
41	1j	42	THR	2.4
41	2j	42	THR	2.4
6	2G	2	PRO	2.4
7	2H	55	PRO	2.4
7	2H	173	PRO	2.4
33	2b	147	LYS	2.4
34	2c	161	GLU	2.4
35	2d	150	GLU	2.4
38	2g	77	SER	2.4
51	1t	98	PRO	2.4
51	2t	11	SER	2.4
12	2Q	63	LYS	2.4
50	2s	18	LYS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
12	2Q	15	GLY	2.4
33	2b	223	ILE	2.4
40	1i	91	ASP	2.4
41	2j	82	ILE	2.4
44	1m	4	ILE	2.4
1	1A	2181	G	2.4
1	2A	530	G	2.4
6	2G	152	LEU	2.4
22	20	84	LEU	2.4
32	1a	1042	G	2.4
32	2a	1197	G	2.4
38	1g	16	LEU	2.4
41	1j	88	LEU	2.4
56	1y	34	G	2.4
9	2N	61	ARG	2.4
14	2S	3	ARG	2.4
38	2g	155	ARG	2.4
48	1q	91	ARG	2.4
26	14	32	TYR	2.4
38	1g	43	PHE	2.4
5	1F	89	VAL	2.4
9	2N	5	VAL	2.4
44	2m	53	VAL	2.4
1	1A	1177	A	2.4
6	2G	132	ASN	2.4
51	1t	9	ASN	2.4
7	2H	96	ALA	2.4
8	2I	55	ALA	2.4
33	2b	97	TRP	2.4
45	2n	10	ALA	2.4
7	2H	32	GLU	2.4
33	2b	168	THR	2.4
44	1m	43	THR	2.4
1	2A	894	C	2.4
7	2H	168	PRO	2.4
45	2n	8	GLU	2.4
1	2A	2130	U	2.4
32	2a	1129	C	2.4
54	2w	13	C	2.4
56	2y	75	C	2.4
42	2k	86	GLY	2.4
44	2m	112	GLY	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
8	2I	71	ILE	2.4
7	2H	42	ARG	2.4
8	2I	50	ARG	2.4
31	29	18	ARG	2.4
33	2b	10	LEU	2.4
34	2c	21	ARG	2.4
34	2c	30	ARG	2.4
41	2j	73	ASP	2.4
44	1m	3	ARG	2.4
52	2u	22	ARG	2.4
33	1b	55	PHE	2.4
33	1b	105	PHE	2.4
34	2c	23	TYR	2.4
19	2X	1	MET	2.4
41	1j	47	PHE	2.4
12	2Q	102	VAL	2.4
39	2h	93	VAL	2.4
41	1j	72	VAL	2.4
20	2Y	48	ALA	2.4
21	2Z	162	GLU	2.4
32	1a	152	A	2.4
33	1b	188	ALA	2.4
41	1j	27	ALA	2.4
44	2m	42	ALA	2.4
41	2j	83	GLU	2.4
35	1d	189	PRO	2.3
40	2i	64	THR	2.3
47	1p	48	TRP	2.4
41	2j	35	SER	2.3
1	2A	2808	U	2.3
32	1a	223	U	2.3
32	1a	1000	U	2.3
32	1a	1446	U	2.3
33	2b	36	ARG	2.3
34	1c	79	ARG	2.3
40	2i	104	ARG	2.3
44	2m	99	ARG	2.3
51	2t	25	ARG	2.3
8	1I	38	LEU	2.3
33	1b	121	LEU	2.3
33	2b	40	HIS	2.3
34	2c	196	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
37	2f	21	LEU	2.3
7	2H	83	TYR	2.3
50	2s	10	PHE	2.3
7	2H	99	VAL	2.3
34	1c	99	VAL	2.3
34	2c	70	VAL	2.3
40	2i	65	VAL	2.3
40	2i	86	VAL	2.3
40	2i	95	LYS	2.3
43	2l	126	LYS	2.3
1	1A	1047	G	2.3
1	1A	1091	G	2.3
1	2A	2106	G	2.3
56	2y	53	G	2.3
35	1d	179	GLU	2.3
40	2i	45	ALA	2.3
46	1o	19	PRO	2.3
44	1m	105	THR	2.3
1	1A	1054	A	2.3
32	2a	1287	A	2.3
7	2H	155	SER	2.3
8	1I	42	SER	2.3
33	2b	21	ARG	2.3
38	1g	77	SER	2.3
7	1H	174	GLY	2.3
34	2c	205	GLY	2.3
41	1j	28	ARG	2.3
47	1p	71	ARG	2.3
1	1A	2150	U	2.3
2	2B	1	U	2.3
32	2a	84	U	2.3
7	2H	121	ILE	2.3
8	2I	54	GLN	2.3
15	2T	123	GLN	2.3
21	2Z	157	LEU	2.3
42	2k	48	ILE	2.3
51	2t	24	LEU	2.3
13	2R	69	ASP	2.3
32	1a	1029	C	2.3
33	2b	189	ASP	2.3
40	2i	91	ASP	2.3
54	1w	67	C	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
54	2w	67	C	2.3
56	2y	11	C	2.3
33	2b	90	MET	2.3
33	2b	101	MET	2.3
9	2N	51	PHE	2.3
35	1d	84	LYS	2.3
51	1t	14	LYS	2.3
34	1c	207	VAL	2.3
52	1u	18	TYR	2.3
8	1I	117	GLU	2.3
8	2I	10	GLU	2.3
26	24	57	GLU	2.3
10	2O	11	ALA	2.3
34	2c	180	ALA	2.3
41	1j	37	PRO	2.3
44	1m	18	ALA	2.3
51	1t	94	ALA	2.3
51	2t	95	ALA	2.3
1	2A	2120	G	2.3
1	2A	2168	G	2.3
7	2H	3	ARG	2.3
34	2c	79	ARG	2.3
50	1s	29	ARG	2.3
52	2u	15	ARG	2.3
56	1y	65	G	2.3
1	1A	900	A	2.3
1	2A	909	A	2.3
44	1m	6	GLY	2.3
50	1s	26	GLY	2.3
53	1v	15	A	2.3
7	2H	148	ILE	2.3
23	11	82	LEU	2.3
40	1i	85	LEU	2.3
40	2i	74	ILE	2.3
41	1j	40	LEU	2.3
46	1o	31	LEU	2.3
1	2A	1113	U	2.3
6	1G	147	ASP	2.3
1	1A	1100	C	2.3
1	2A	645	C	2.3
11	2P	76	LYS	2.3
32	1a	1137	C	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	2a	1043	C	2.3
56	1y	4	C	2.3
56	2y	56	C	2.3
45	2n	16	PHE	2.3
10	1O	108	GLU	2.3
20	2Y	7	VAL	2.3
41	2j	94	VAL	2.3
33	2b	29	ALA	2.3
34	2c	149	ALA	2.3
42	1k	74	ALA	2.3
50	2s	42	PRO	2.3
7	2H	69	ARG	2.3
8	2I	52	ARG	2.3
45	1n	3	ARG	2.3
40	2i	103	THR	2.3
18	2W	112	GLY	2.3
40	2i	72	GLY	2.3
45	1n	51	GLY	2.3
50	2s	26	GLY	2.3
1	1A	1099	G	2.3
1	1A	2157	G	2.3
1	2A	100	G	2.3
1	2A	2182	G	2.3
32	2a	1221	G	2.3
1	1A	890	A	2.3
2	2B	120	A	2.3
7	2H	72	ILE	2.3
33	2b	185	ILE	2.3
34	1c	124	ILE	2.3
34	2c	18	TRP	2.3
34	2c	178	LEU	2.3
39	2h	112	LEU	2.3
41	1j	8	LEU	2.3
56	1y	18	G	2.3
21	2Z	1	MET	2.3
56	1y	21	A	2.3
44	2m	13	LYS	2.3
50	1s	12	ASP	2.3
51	2t	30	LYS	2.3
1	2A	12	U	2.3
1	2A	1043	C	2.3
1	2A	2107	C	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
8	2I	41	GLU	2.3
32	1a	1038	C	2.3
35	1d	110	PHE	2.3
41	2j	25	GLU	2.3
54	1w	2	C	2.3
7	2H	141	VAL	2.3
8	2I	107	VAL	2.3
37	1f	88	VAL	2.3
41	1j	24	VAL	2.3
18	2W	92	ARG	2.3
38	1g	4	ARG	2.3
34	1c	60	ALA	2.2
39	2h	94	TYR	2.3
50	2s	29	ARG	2.3
31	29	37	GLY	2.2
33	2b	113	HIS	2.2
34	1c	25	GLY	2.2
8	2I	79	ILE	2.2
16	2U	62	ILE	2.2
31	29	15	LYS	2.2
33	1b	39	ILE	2.2
33	1b	215	LEU	2.2
1	1A	1046	A	2.2
32	1a	143	A	2.2
32	2a	1123	A	2.2
1	1A	2148	G	2.2
1	2A	545	G	2.2
1	2A	2319	G	2.2
54	1w	18	G	2.2
54	2w	6	G	2.2
56	2y	69	G	2.2
32	2a	1126	U	2.2
41	1j	83	GLU	2.2
34	2c	128	PHE	2.2
6	2G	51	ARG	2.2
33	1b	30	ARG	2.2
38	2g	76	ARG	2.2
40	2i	107	ARG	2.2
42	1k	54	ARG	2.2
47	1p	25	ARG	2.2
1	1A	2161	C	2.2
1	2A	1530	C	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	2789	C	2.2
54	2w	4	C	2.2
56	2y	49	C	2.2
19	2X	91	ALA	2.2
33	1b	207	ALA	2.2
34	1c	92	ALA	2.2
51	1t	59	ALA	2.2
33	2b	33	TYR	2.2
35	1d	38	TYR	2.2
8	2I	86	THR	2.2
29	27	24	THR	2.2
33	2b	107	THR	2.2
40	2i	73	GLN	2.2
41	1j	87	THR	2.2
17	2V	85	LYS	2.2
34	2c	194	GLY	2.2
35	2d	124	GLY	2.2
38	2g	35	LYS	2.2
41	1j	93	GLY	2.2
43	2l	63	GLY	2.2
50	1s	84	GLY	2.2
50	2s	8	GLY	2.2
40	1i	102	LEU	2.2
41	1j	65	LEU	2.2
12	2Q	127	ILE	2.2
26	14	15	ILE	2.2
41	2j	75	ILE	2.2
50	2s	34	TRP	2.2
1	1A	2126	A	2.2
1	1A	2134	A	2.2
1	1A	2892	A	2.2
32	2a	1151	A	2.2
32	2a	1225	A	2.2
32	2a	1503	A	2.2
34	2c	90	GLU	2.2
1	1A	1055	G	2.2
1	2A	2131	G	2.2
32	1a	1009	G	2.2
32	2a	1224	G	2.2
35	1d	3	ARG	2.2
45	1n	29	ARG	2.2
45	2n	57	ARG	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
47	1p	72	ARG	2.2
51	2t	8	ARG	2.2
16	2U	79	PHE	2.2
40	2i	37	PHE	2.2
41	1j	11	PHE	2.2
33	2b	112	VAL	2.2
40	1i	26	VAL	2.2
43	2l	48	PRO	2.2
22	20	12	ASN	2.2
29	17	45	ALA	2.2
47	1p	24	ALA	2.2
54	1w	3	C	2.2
56	1y	48	C	2.2
5	2F	8	GLN	2.2
20	2Y	54	LYS	2.2
21	2Z	127	LYS	2.2
24	12	15	LYS	2.2
51	1t	74	LYS	2.2
34	2c	191	THR	2.2
44	2m	105	THR	2.2
7	2H	14	GLY	2.2
7	2H	93	GLY	2.2
7	2H	135	GLY	2.2
20	2Y	80	GLY	2.2
34	1c	81	GLY	2.2
40	1i	39	GLY	2.2
12	2Q	47	ILE	2.2
33	2b	211	ILE	2.2
36	1e	13	ILE	2.2
26	24	51	ASP	2.2
40	2i	20	ARG	2.2
44	2m	80	ARG	2.2
45	2n	31	ARG	2.2
1	1A	1085	A	2.2
1	1A	1460	A	2.2
1	1A	2062	A	2.2
1	2A	272(A)	U	2.2
9	2N	126	PRO	2.2
33	1b	122	PHE	2.2
38	1g	26	PHE	2.2
5	1F	6	VAL	2.2
34	2c	64	VAL	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
40	2i	109	VAL	2.2
1	1A	892	G	2.2
20	2Y	81	LYS	2.2
21	2Z	156	LYS	2.2
24	22	8	LYS	2.2
32	1a	78	G	2.2
32	1a	216	G	2.2
32	2a	1010	G	2.2
32	2a	1124	G	2.2
32	2a	1222	G	2.2
33	1b	34	ALA	2.2
36	1e	21	ALA	2.2
40	2i	78	LYS	2.2
56	2y	10	G	2.2
7	2H	61	HIS	2.2
21	2Z	121	HIS	2.2
50	2s	47	HIS	2.2
51	1t	76	ALA	2.2
41	2j	21	GLN	2.2
41	2j	84	GLN	2.2
1	2A	893	C	2.2
3	2D	37	LEU	2.2
34	1c	23	TYR	2.2
34	2c	41	GLY	2.2
34	2c	184	TYR	2.2
37	1f	63	TYR	2.2
41	1j	36	GLY	2.2
56	2y	62	C	2.2
21	1Z	120	ILE	2.2
21	2Z	53	ILE	2.2
7	2H	57	ASP	2.2
33	1b	20	GLU	2.2
33	2b	129	GLU	2.2
5	2F	14	PRO	2.2
34	2c	73	PRO	2.2
1	2A	900	A	2.1
1	2A	2122	U	2.2
33	2b	169	LYS	2.2
37	2f	97	PHE	2.2
6	2G	31	VAL	2.1
26	24	50	VAL	2.1
32	2a	1130	A	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	2c	66	VAL	2.1
47	1p	2	VAL	2.1
55	1x	47	U	2.2
56	1y	33	U	2.2
7	2H	75	ALA	2.1
12	2Q	7	MET	2.1
33	1b	62	ALA	2.1
33	2b	186	ALA	2.1
34	2c	24	ALA	2.1
34	2c	65	ALA	2.1
36	2e	48	ALA	2.1
40	2i	15	ALA	2.1
44	1m	5	ALA	2.1
44	2m	101	GLN	2.1
1	1A	1537	G	2.1
1	1A	2100	G	2.1
1	2A	271(I)	G	2.1
4	2E	186	GLY	2.1
7	2H	174	GLY	2.1
19	1X	94	GLY	2.1
33	1b	72	GLY	2.1
40	2i	57	GLY	2.1
40	2i	69	GLY	2.1
41	1j	90	LEU	2.1
41	2j	71	LEU	2.1
44	1m	24	GLY	2.1
52	1u	19	GLY	2.1
54	1w	19	G	2.1
56	1y	22	G	2.1
56	1y	27	G	2.1
56	2y	52	G	2.1
15	2T	68	TYR	2.1
34	1c	14	ILE	2.1
43	2l	70	ILE	2.1
46	1o	3	ILE	2.1
1	1A	1079	C	2.1
1	1A	2178	C	2.1
32	2a	1028	C	2.1
56	2y	68	C	2.1
20	2Y	2	ARG	2.1
28	16	4	GLU	2.1
33	2b	144	ARG	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
38	2g	78	ARG	2.1
21	2Z	154	ASP	2.1
7	2H	13	LYS	2.1
7	2H	138	LYS	2.1
17	2V	6	LYS	2.1
33	1b	133	LYS	2.1
45	2n	11	LYS	2.1
48	1q	28	PRO	2.1
12	2Q	106	VAL	2.1
21	2Z	165	VAL	2.1
33	1b	81	VAL	2.1
34	1c	70	VAL	2.1
35	1d	133	VAL	2.1
40	1i	86	VAL	2.1
1	2A	2132	U	2.1
1	2A	2062	A	2.1
1	2A	2176	A	2.1
16	1U	117	GLN	2.1
32	1a	162	A	2.1
32	1a	1041	A	2.1
47	2p	76	GLN	2.1
33	2b	88	ALA	2.1
16	2U	44	ASN	2.1
19	2X	67	GLY	2.1
34	1c	87	LEU	2.1
34	2c	111	LEU	2.1
35	1d	176	LEU	2.1
41	1j	85	LEU	2.1
47	1p	6	LEU	2.1
47	2p	45	THR	2.1
16	2U	88	ILE	2.1
7	2H	157	TYR	2.1
15	2T	125	ARG	2.1
2	2B	119	G	2.1
6	2G	45	GLU	2.1
33	1b	130	ARG	2.1
40	1i	12	GLU	2.1
41	2j	66	ARG	2.1
43	2l	64	TYR	2.1
44	1m	102	ARG	2.1
47	1p	5	ARG	2.1
47	1p	38	TYR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
49	1r	87	ARG	2.1
32	1a	1021	G	2.1
54	1w	15	G	2.1
54	2w	19	G	2.1
1	1A	2177	C	2.1
32	1a	163	C	2.1
32	1a	848	C	2.1
33	1b	192	SER	2.1
33	1b	156	LYS	2.1
33	2b	133	LYS	2.1
41	2j	80	LYS	2.1
44	1m	98	VAL	2.1
44	2m	17	VAL	2.1
50	1s	41	VAL	2.1
51	1t	97	ALA	2.1
34	2c	181	ASN	2.1
56	1y	45	U	2.1
56	1y	66	U	2.1
7	2H	122	THR	2.1
8	2I	108	THR	2.1
20	2Y	93	GLY	2.1
23	21	28	GLY	2.1
23	21	94	LEU	2.1
33	2b	228	GLY	2.1
34	2c	96	GLY	2.1
37	1f	79	LEU	2.1
41	2j	16	LEU	2.1
44	2m	48	LEU	2.1
56	2y	23	A	2.1
39	1h	128	GLY	2.1
40	2i	100	GLY	2.1
51	1t	101	GLY	2.1
5	1F	17	ARG	2.1
15	1T	115	ARG	2.1
20	2Y	73	ARG	2.1
22	20	44	ARG	2.1
35	1d	115	ARG	2.1
36	2e	25	ARG	2.1
35	2d	54	TYR	2.1
44	2m	23	TYR	2.1
47	2p	38	TYR	2.1
7	2H	38	SER	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	1074	G	2.1
1	2A	171	G	2.1
1	2A	2207	G	2.1
56	2y	63	G	2.1
56	1y	68	C	2.1
56	2y	40	C	2.1
19	1X	1	MET	2.1
34	2c	176	HIS	2.1
41	2j	62	HIS	2.1
6	1G	26	GLN	2.1
8	1I	142	VAL	2.1
26	24	49	PHE	2.1
34	1c	106	VAL	2.1
34	2c	76	VAL	2.1
34	2c	198	VAL	2.1
41	1j	34	VAL	2.1
41	2j	11	PHE	2.1
33	2b	207	ALA	2.1
1	1A	1101	U	2.1
1	2A	2172	U	2.1
5	2F	20	LEU	2.1
14	2S	61	ASN	2.1
25	23	53	LEU	2.1
11	2P	28	GLY	2.1
11	2P	44	GLY	2.1
12	2Q	6	ARG	2.1
15	2T	96	ARG	2.1
21	2Z	59	LEU	2.1
33	2b	155	LEU	2.1
34	2c	25	GLY	2.1
38	2g	79	ARG	2.1
43	1l	41	ARG	2.1
47	1p	74	LEU	2.1
17	2V	63	GLY	2.1
50	2s	46	GLY	2.1
52	2u	9	ARG	2.1
1	2A	1847	A	2.1
4	1E	77	ILE	2.1
32	1a	344	A	2.1
32	1a	1503	A	2.1
32	2a	1357	A	2.1
47	2p	33	ILE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
48	2q	90	ILE	2.1
56	1y	58	A	2.1
56	1y	73	A	2.1
56	2y	64	A	2.1
9	2N	104	LYS	2.1
41	1j	7	LYS	2.1
21	2Z	148	ASP	2.1
40	2i	105	ASP	2.1
47	1p	39	TYR	2.1
47	1p	68	ASP	2.1
21	2Z	153	SER	2.1
50	1s	4	SER	2.1
45	2n	54	PRO	2.1
46	1o	2	PRO	2.1
1	1A	894	C	2.1
1	2A	889	C	2.1
21	2Z	151	HIS	2.1
1	2A	2807	G	2.0
32	1a	221	C	2.1
20	2Y	57	GLN	2.0
32	2a	1117	G	2.0
32	2a	1260	C	2.1
50	2s	14	HIS	2.1
56	1y	24	G	2.0
56	1y	71	G	2.0
6	2G	5	VAL	2.0
14	2S	46	VAL	2.0
41	2j	54	PHE	2.0
33	1b	53	ARG	2.0
38	2g	3	ARG	2.0
42	1k	96	ARG	2.0
46	1o	64	ARG	2.0
8	1I	5	LEU	2.0
8	2I	38	LEU	2.0
18	2W	60	ASN	2.0
33	2b	213	LEU	2.0
33	2b	215	LEU	2.0
50	2s	22	LEU	2.0
33	1b	24	TRP	2.0
34	1c	9	GLY	2.0
38	1g	55	GLY	2.0
1	1A	1175	U	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	2180	U	2.0
22	20	49	LYS	2.0
34	2c	152	ILE	2.0
35	1d	169	LYS	2.0
40	1i	7	THR	2.0
41	2j	55	LYS	2.0
45	2n	22	THR	2.0
56	1y	50	U	2.0
41	1j	82	ILE	2.0
1	1A	2629	A	2.0
32	1a	171	A	2.0
32	1a	1151	A	2.0
32	2a	1146	A	2.0
6	2G	146	TYR	2.0
7	2H	84	SER	2.0
33	1b	234	PRO	2.0
41	1j	30	SER	2.0
45	2n	14	PRO	2.0
50	1s	38	SER	2.0
33	2b	16	HIS	2.0
41	2j	33	GLN	2.0
1	1A	2105	C	2.0
1	2A	271(O)	C	2.0
1	2A	2142	C	2.0
6	1G	5	VAL	2.0
21	2Z	48	PHE	2.0
26	14	68	ARG	2.0
32	1a	91	C	2.0
32	2a	1145	C	2.0
33	1b	163	PHE	2.0
38	1g	6	ARG	2.0
40	1i	33	PHE	2.0
40	1i	101	PHE	2.0
41	2j	46	ARG	2.0
46	2o	18	PHE	2.0
47	1p	21	VAL	2.0
47	2p	80	PHE	2.0
50	2s	81	ARG	2.0
52	1u	10	ARG	2.0
52	1u	15	ARG	2.0
56	1y	2	C	2.0
56	1y	72	C	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	271(I)	G	2.0
1	2A	2152	G	2.0
6	2G	133	LEU	2.0
15	2T	127	ALA	2.0
32	2a	1022	G	2.0
17	2V	95	LEU	2.0
33	1b	50	GLU	2.0
33	1b	149	LEU	2.0
35	1d	195	ALA	2.0
47	1p	70	ALA	2.0
6	2G	182	LYS	2.0
7	2H	74	ASN	2.0
20	2Y	47	LYS	2.0
31	29	8	LYS	2.0
33	1b	18	GLY	2.0
33	2b	75	LYS	2.0
17	2V	92	THR	2.0
21	1Z	53	ILE	2.0
28	26	54	ILE	2.0
31	29	26	ILE	2.0
41	2j	50	ILE	2.0
16	2U	25	TRP	2.0
32	2a	1000	U	2.0
1	1A	1045	A	2.0
1	2A	1507	A	2.0
41	2j	86	MET	2.0
42	2k	36	ASP	2.0
54	2w	14	A	2.0
38	1g	89	MET	2.0
7	2H	56	SER	2.0
7	2H	164	TYR	2.0
19	2X	69	TYR	2.0
40	1i	125	TYR	2.0
48	1q	99	SER	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
56	4SU	2y	8	20/21	0.37	0.19	98,102,113,128	0
56	5MU	2y	54	21/22	0.45	0.21	94,100,111,124	0
56	PSU	2y	55	20/21	0.45	0.16	92,99,110,115	0
56	MIA	2y	37	22/30	0.47	0.17	88,94,108,126	0
56	G7M	2y	46	24/25	0.48	0.17	86,101,106,121	0
56	PSU	1y	55	20/21	0.52	0.17	96,101,103,114	0
56	G7M	1y	46	24/25	0.52	0.16	90,98,107,113	0
56	4SU	1y	8	20/21	0.54	0.15	97,101,109,117	0
56	MIA	1y	37	22/30	0.56	0.18	88,95,103,115	0
56	PSU	1y	39	20/21	0.59	0.16	88,94,105,106	0
56	5MU	1y	54	21/22	0.61	0.16	89,98,103,112	0
56	PSU	2y	39	20/21	0.62	0.17	88,94,105,111	0
56	PSU	2y	32	20/21	0.67	0.16	89,96,103,113	0
54	G7M	2w	46	24/25	0.68	0.16	87,94,105,120	0
56	PSU	1y	32	20/21	0.74	0.16	90,96,105,109	0
54	G7M	1w	46	24/25	0.75	0.15	79,86,99,118	0
54	4SU	2w	8	20/21	0.77	0.14	89,94,104,105	0
54	PSU	2w	55	20/21	0.83	0.11	85,89,96,99	0
54	MIA	2w	37	25/30	0.84	0.17	56,74,82,100	0
54	4SU	1w	8	20/21	0.84	0.14	83,88,93,95	0
54	PSU	1w	55	20/21	0.85	0.12	59,73,84,87	0
54	5MU	2w	54	21/22	0.86	0.12	79,84,89,93	0
55	PSU	2x	55	20/21	0.87	0.12	69,75,87,90	0
55	PSU	1x	55	20/21	0.89	0.12	57,63,72,72	0
54	PSU	2w	32	20/21	0.90	0.12	73,78,86,86	0
55	4SU	2x	8	20/21	0.90	0.12	71,78,82,83	0
55	5MU	1x	54	21/22	0.90	0.11	58,63,72,74	0
32	2MG	2a	1207	24/25	0.90	0.11	71,81,83,85	0
54	MIA	1w	37	29/30	0.90	0.17	51,59,73,87	0
55	5MU	2x	54	21/22	0.91	0.12	72,77,80,83	0
43	0TD	2l	92	10/11	0.91	0.11	63,65,68,72	0
32	G7M	2a	527	24/25	0.91	0.14	56,64,71,72	0
54	5MU	1w	54	21/22	0.92	0.09	52,63,66,70	0
32	PSU	2a	516	20/21	0.92	0.10	53,67,71,74	0
43	0TD	1l	92	10/11	0.92	0.12	47,52,55,67	0
32	5MC	2a	1400	21/22	0.93	0.14	61,66,74,74	0
54	PSU	1w	32	20/21	0.93	0.11	56,62,69,71	0
55	4SU	1x	8	20/21	0.93	0.10	55,62,66,67	0
32	5MC	2a	967	21/22	0.93	0.13	59,66,72,75	0
55	5MC	2x	32	21/22	0.93	0.13	63,68,73,78	0
55	5MC	1x	32	21/22	0.93	0.12	51,56,60,64	0
54	PSU	2w	39	20/21	0.93	0.11	68,78,84,85	0
1	5MU	2A	1915	21/22	0.93	0.10	53,61,65,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	M2G	2a	966	25/26	0.94	0.14	53,62,68,73	0
32	2MG	1a	1207	24/25	0.94	0.09	66,70,74,75	0
32	G7M	1a	527	24/25	0.94	0.10	36,49,56,60	0
32	M2G	1a	966	25/26	0.94	0.11	39,49,60,63	0
32	MA6	2a	1518	24/25	0.95	0.11	52,59,64,67	0
32	MA6	2a	1519	24/25	0.95	0.11	48,59,64,66	0
32	5MC	1a	967	21/22	0.95	0.10	45,50,59,62	0
55	31H	1x	76	32/33	0.95	0.09	21,27,33,45	10
32	PSU	1a	516	20/21	0.95	0.07	51,57,62,62	0
32	4OC	2a	1402	22/23	0.95	0.10	53,59,63,66	0
32	UR3	2a	1498	21/22	0.95	0.10	51,56,59,62	0
1	5MU	1A	1915	21/22	0.95	0.09	44,49,57,57	0
55	31H	2x	76	32/33	0.95	0.10	39,47,57,57	0
1	PSU	2A	1917	20/21	0.95	0.08	50,57,63,64	0
1	OMC	2A	1920	21/22	0.95	0.10	51,56,60,62	0
32	5MC	1a	1407	21/22	0.96	0.09	35,44,46,50	0
32	5MC	2a	1404	21/22	0.96	0.09	49,52,56,58	0
1	PSU	2A	1911	20/21	0.96	0.08	49,53,58,64	0
32	5MC	2a	1407	21/22	0.96	0.09	49,56,60,62	0
32	5MC	1a	1400	21/22	0.96	0.10	45,51,56,56	0
1	PSU	1A	1917	20/21	0.96	0.07	47,51,55,55	0
54	PSU	1w	39	20/21	0.96	0.09	47,61,66,69	0
32	4OC	1a	1402	22/23	0.96	0.09	36,43,46,50	0
1	5MC	2A	1942	21/22	0.96	0.08	50,57,63,73	0
1	5MC	2A	1962	21/22	0.96	0.09	43,48,53,61	0
1	OMG	2A	2251	24/25	0.96	0.09	40,45,50,52	0
1	2MU	2A	2552	21/23	0.96	0.09	44,49,52,58	0
1	PSU	2A	2605	20/21	0.96	0.08	36,42,47,51	0
1	5MC	1A	1942	21/22	0.97	0.08	35,41,46,50	0
54	F3N	2w	76	33/34	0.97	0.08	36,43,47,50	0
1	PSU	1A	1911	20/21	0.97	0.07	40,51,54,55	0
32	MA6	1a	1518	24/25	0.97	0.08	34,40,47,47	0
1	8AH	2A	2503	24/25	0.97	0.10	35,40,43,49	0
32	MA6	1a	1519	24/25	0.97	0.08	33,41,45,49	0
1	PSU	1A	2605	20/21	0.97	0.07	23,29,32,35	0
1	5MU	2A	1939	21/22	0.97	0.07	33,41,46,51	0
32	5MC	1a	1404	21/22	0.98	0.06	34,40,45,47	0
1	5MU	1A	1939	21/22	0.98	0.07	25,31,35,42	0
1	8AH	1A	2503	24/25	0.98	0.07	16,25,30,32	0
32	UR3	1a	1498	21/22	0.98	0.07	37,42,45,48	0
1	2MU	1A	2552	21/23	0.98	0.07	24,29,34,35	0
54	F3N	1w	76	33/34	0.98	0.07	19,27,32,33	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	OMC	1A	1920	21/22	0.98	0.07	38,47,50,52	0
1	5MC	1A	1962	21/22	0.98	0.06	28,34,37,41	0
1	OMG	1A	2251	24/25	0.99	0.05	22,26,30,33	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, 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
57	MG	1B	230	1/1	-0.02	0.25	84,84,84,84	0
57	MG	1A	4003	1/1	0.38	0.19	75,75,75,75	0
57	MG	2A	3264	1/1	0.49	0.36	82,82,82,82	0
57	MG	2A	3384	1/1	0.49	0.32	91,91,91,91	0
57	MG	2A	3674	1/1	0.54	0.29	57,57,57,57	0
57	MG	2A	3592	1/1	0.55	0.32	73,73,73,73	0
57	MG	10	106	1/1	0.58	0.28	68,68,68,68	0
57	MG	1A	4041	1/1	0.59	0.33	70,70,70,70	0
57	MG	1x	111	1/1	0.60	0.20	78,78,78,78	0
57	MG	1A	3562	1/1	0.61	0.32	70,70,70,70	0
57	MG	2A	3451	1/1	0.61	0.25	68,68,68,68	0
57	MG	2E	302	1/1	0.63	0.17	67,67,67,67	0
57	MG	2y	105	1/1	0.63	0.28	89,89,89,89	0
57	MG	2A	3491	1/1	0.65	0.17	82,82,82,82	0
57	MG	2A	3772	1/1	0.65	0.30	77,77,77,77	0
57	MG	1O	204	1/1	0.66	0.29	67,67,67,67	0
57	MG	1A	3884	1/1	0.66	0.30	47,47,47,47	0
57	MG	2w	103	1/1	0.66	0.21	93,93,93,93	0
57	MG	1B	237	1/1	0.66	0.17	62,62,62,62	0
57	MG	2A	3791	1/1	0.68	0.19	71,71,71,71	0
57	MG	1A	4035	1/1	0.68	0.17	65,65,65,65	0
57	MG	2A	3235	1/1	0.69	0.21	80,80,80,80	0
57	MG	2A	3639	1/1	0.69	0.19	88,88,88,88	0
57	MG	1A	4101	1/1	0.69	0.21	65,65,65,65	0
57	MG	2A	3316	1/1	0.69	0.39	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	2A	3525	1/1	0.70	0.16	65,65,65,65	0
57	MG	2A	3790	1/1	0.70	0.19	75,75,75,75	0
57	MG	1A	3356	1/1	0.70	0.24	68,68,68,68	0
57	MG	2A	3792	1/1	0.70	0.27	78,78,78,78	0
57	MG	2A	3634	1/1	0.70	0.21	66,66,66,66	0
57	MG	18	105	1/1	0.70	0.27	78,78,78,78	0
57	MG	1A	4022	1/1	0.70	0.24	55,55,55,55	0
57	MG	1a	1629	1/1	0.71	0.18	77,77,77,77	0
57	MG	2A	3387	1/1	0.71	0.33	79,79,79,79	0
57	MG	2A	3062	1/1	0.71	0.20	73,73,73,73	0
57	MG	2A	3097	1/1	0.71	0.28	75,75,75,75	0
57	MG	2A	3749	1/1	0.72	0.20	65,65,65,65	0
57	MG	2A	3502	1/1	0.72	0.13	70,70,70,70	0
57	MG	2A	3161	1/1	0.72	0.12	87,87,87,87	0
57	MG	2A	3031	1/1	0.72	0.29	70,70,70,70	0
57	MG	1A	3641	1/1	0.72	0.21	53,53,53,53	0
57	MG	1A	3983	1/1	0.72	0.18	43,43,43,43	0
57	MG	2A	3500	1/1	0.72	0.25	84,84,84,84	0
57	MG	2y	104	1/1	0.72	0.15	71,71,71,71	0
57	MG	2A	3721	1/1	0.72	0.16	69,69,69,69	0
57	MG	1A	3795	1/1	0.73	0.17	51,51,51,51	0
57	MG	1A	3819	1/1	0.73	0.22	70,70,70,70	0
57	MG	1A	3506	1/1	0.73	0.24	65,65,65,65	0
57	MG	2A	3499	1/1	0.73	0.23	75,75,75,75	0
57	MG	1A	3925	1/1	0.73	0.18	73,73,73,73	0
57	MG	1A	3939	1/1	0.73	0.23	74,74,74,74	0
57	MG	1A	4050	1/1	0.73	0.18	56,56,56,56	0
57	MG	1A	4073	1/1	0.73	0.15	73,73,73,73	0
57	MG	1a	1655	1/1	0.73	0.18	66,66,66,66	0
57	MG	2y	102	1/1	0.73	0.22	87,87,87,87	0
57	MG	1a	1786	1/1	0.73	0.17	71,71,71,71	0
57	MG	2A	3657	1/1	0.73	0.19	68,68,68,68	0
57	MG	2A	3733	1/1	0.74	0.19	57,57,57,57	0
57	MG	1A	3092	1/1	0.74	0.14	79,79,79,79	0
57	MG	2A	3562	1/1	0.74	0.22	56,56,56,56	0
57	MG	2A	3141	1/1	0.74	0.25	74,74,74,74	0
57	MG	2A	3620	1/1	0.74	0.16	77,77,77,77	0
57	MG	2A	3633	1/1	0.74	0.26	74,74,74,74	0
57	MG	1A	3499	1/1	0.74	0.23	51,51,51,51	0
57	MG	2A	3016	1/1	0.74	0.30	67,67,67,67	0
57	MG	15	108	1/1	0.74	0.44	60,60,60,60	0
57	MG	2A	3269	1/1	0.74	0.21	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	1685	1/1	0.74	0.21	61,61,61,61	0
57	MG	1a	1645	1/1	0.75	0.26	78,78,78,78	0
57	MG	2A	3318	1/1	0.75	0.41	72,72,72,72	0
57	MG	1S	201	1/1	0.75	0.35	60,60,60,60	0
57	MG	1A	4070	1/1	0.75	0.17	71,71,71,71	0
57	MG	1a	1785	1/1	0.75	0.19	76,76,76,76	0
57	MG	1A	3479	1/1	0.75	0.23	65,65,65,65	0
57	MG	2A	3494	1/1	0.75	0.19	56,56,56,56	0
57	MG	2A	3644	1/1	0.75	0.14	63,63,63,63	0
57	MG	1b	301	1/1	0.75	0.22	86,86,86,86	0
57	MG	1D	311	1/1	0.75	0.20	65,65,65,65	0
57	MG	1A	3814	1/1	0.75	0.16	41,41,41,41	0
57	MG	1a	1659	1/1	0.76	0.45	80,80,80,80	0
57	MG	1S	203	1/1	0.76	0.15	72,72,72,72	0
57	MG	2A	3673	1/1	0.76	0.19	64,64,64,64	0
57	MG	1a	1725	1/1	0.76	0.15	75,75,75,75	0
57	MG	2A	3686	1/1	0.76	0.34	58,58,58,58	0
57	MG	1A	3072	1/1	0.76	0.30	69,69,69,69	0
57	MG	1A	3757	1/1	0.76	0.12	22,22,22,22	0
57	MG	1a	1818	1/1	0.76	0.19	54,54,54,54	0
57	MG	1A	4042	1/1	0.76	0.28	40,40,40,40	0
57	MG	1q	201	1/1	0.76	0.18	64,64,64,64	0
57	MG	2A	3567	1/1	0.76	0.37	73,73,73,73	0
57	MG	1A	3503	1/1	0.76	0.18	57,57,57,57	0
57	MG	2B	201	1/1	0.76	0.32	75,75,75,75	0
57	MG	2B	203	1/1	0.76	0.14	68,68,68,68	0
57	MG	2A	3617	1/1	0.76	0.25	76,76,76,76	0
57	MG	1A	3908	1/1	0.76	0.14	52,52,52,52	0
57	MG	1A	3909	1/1	0.76	0.12	61,61,61,61	0
57	MG	2A	3403	1/1	0.76	0.35	76,76,76,76	0
57	MG	2A	3404	1/1	0.76	0.22	72,72,72,72	0
57	MG	2y	107	1/1	0.76	0.19	84,84,84,84	0
57	MG	1a	1648	1/1	0.77	0.25	79,79,79,79	0
57	MG	1A	4103	1/1	0.77	0.12	63,63,63,63	0
57	MG	2A	3704	1/1	0.77	0.18	68,68,68,68	0
57	MG	2A	3708	1/1	0.77	0.19	73,73,73,73	0
57	MG	1A	3978	1/1	0.77	0.16	66,66,66,66	0
57	MG	1B	231	1/1	0.77	0.24	67,67,67,67	0
57	MG	2A	3532	1/1	0.77	0.17	52,52,52,52	0
57	MG	1A	3776	1/1	0.77	0.25	84,84,84,84	0
57	MG	1A	3291	1/1	0.77	0.18	64,64,64,64	0
57	MG	1A	3428	1/1	0.77	0.22	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	3533	1/1	0.77	0.20	60,60,60,60	0
57	MG	1A	3824	1/1	0.77	0.22	64,64,64,64	0
57	MG	1A	3293	1/1	0.77	0.33	64,64,64,64	0
57	MG	1A	3485	1/1	0.77	0.17	69,69,69,69	0
57	MG	1A	3673	1/1	0.77	0.13	61,61,61,61	0
57	MG	1A	3734	1/1	0.77	0.16	62,62,62,62	0
57	MG	2A	3649	1/1	0.77	0.15	67,67,67,67	0
57	MG	2A	3041	1/1	0.77	0.36	71,71,71,71	0
57	MG	1A	3352	1/1	0.77	0.30	64,64,64,64	0
57	MG	2A	3564	1/1	0.78	0.14	70,70,70,70	0
57	MG	2A	3271	1/1	0.78	0.21	80,80,80,80	0
57	MG	2A	3669	1/1	0.78	0.17	44,44,44,44	0
57	MG	2A	3580	1/1	0.78	0.24	75,75,75,75	0
57	MG	2A	3106	1/1	0.78	0.28	69,69,69,69	0
57	MG	1A	3669	1/1	0.78	0.24	70,70,70,70	0
57	MG	1A	4010	1/1	0.78	0.12	83,83,83,83	0
57	MG	2Z	301	1/1	0.78	0.14	80,80,80,80	0
57	MG	2A	3057	1/1	0.78	0.21	72,72,72,72	0
57	MG	2A	3709	1/1	0.78	0.17	52,52,52,52	0
57	MG	2A	3238	1/1	0.78	0.17	65,65,65,65	0
57	MG	1A	4018	1/1	0.78	0.23	56,56,56,56	0
57	MG	1A	3945	1/1	0.78	0.12	57,57,57,57	0
57	MG	1a	1604	1/1	0.79	0.20	68,68,68,68	0
57	MG	1A	3711	1/1	0.79	0.26	61,61,61,61	0
57	MG	1a	1632	1/1	0.79	0.35	70,70,70,70	0
57	MG	1A	4008	1/1	0.79	0.15	73,73,73,73	0
57	MG	1A	3721	1/1	0.79	0.16	66,66,66,66	0
57	MG	1a	1650	1/1	0.79	0.25	74,74,74,74	0
57	MG	1A	4014	1/1	0.79	0.14	59,59,59,59	0
57	MG	1A	3895	1/1	0.79	0.22	67,67,67,67	0
57	MG	2A	3518	1/1	0.79	0.20	69,69,69,69	0
57	MG	2A	3144	1/1	0.79	0.36	62,62,62,62	0
57	MG	1A	3729	1/1	0.79	0.25	47,47,47,47	0
57	MG	2A	3762	1/1	0.79	0.14	78,78,78,78	0
57	MG	2A	3221	1/1	0.79	0.28	77,77,77,77	0
57	MG	1E	311	1/1	0.79	0.14	53,53,53,53	0
57	MG	1a	1727	1/1	0.79	0.16	82,82,82,82	0
57	MG	1A	3329	1/1	0.79	0.20	59,59,59,59	0
57	MG	2A	3591	1/1	0.79	0.20	61,61,61,61	0
57	MG	1A	3222	1/1	0.79	0.18	61,61,61,61	0
57	MG	1A	3051	1/1	0.79	0.17	54,54,54,54	0
57	MG	2A	3298	1/1	0.79	0.26	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	2A	3301	1/1	0.79	0.34	55,55,55,55	0
57	MG	2w	105	1/1	0.79	0.21	79,79,79,79	0
57	MG	1A	3198	1/1	0.79	0.19	58,58,58,58	0
57	MG	1A	3447	1/1	0.79	0.15	57,57,57,57	0
57	MG	1v	101	1/1	0.79	0.24	74,74,74,74	0
57	MG	1A	3696	1/1	0.79	0.21	54,54,54,54	0
57	MG	2A	3456	1/1	0.80	0.19	64,64,64,64	0
57	MG	2A	3247	1/1	0.80	0.16	76,76,76,76	0
57	MG	2A	3252	1/1	0.80	0.27	76,76,76,76	0
57	MG	1A	3699	1/1	0.80	0.19	55,55,55,55	0
57	MG	1a	1814	1/1	0.80	0.21	64,64,64,64	0
57	MG	1A	3521	1/1	0.80	0.25	77,77,77,77	0
57	MG	2A	3099	1/1	0.80	0.26	59,59,59,59	0
57	MG	1A	3831	1/1	0.80	0.14	57,57,57,57	0
57	MG	2A	3310	1/1	0.80	0.33	61,61,61,61	0
57	MG	2A	3312	1/1	0.80	0.24	75,75,75,75	0
57	MG	2A	3753	1/1	0.80	0.18	48,48,48,48	0
57	MG	1A	3975	1/1	0.80	0.11	32,32,32,32	0
57	MG	1A	3712	1/1	0.80	0.18	74,74,74,74	0
57	MG	2A	3789	1/1	0.80	0.20	69,69,69,69	0
57	MG	2A	3329	1/1	0.80	0.23	73,73,73,73	0
57	MG	2A	3338	1/1	0.80	0.28	51,51,51,51	0
57	MG	2A	3355	1/1	0.80	0.12	63,63,63,63	0
57	MG	2A	3598	1/1	0.80	0.16	57,57,57,57	0
57	MG	1A	3786	1/1	0.80	0.13	56,56,56,56	0
57	MG	2B	208	1/1	0.80	0.18	66,66,66,66	0
57	MG	2A	3182	1/1	0.80	0.20	69,69,69,69	0
57	MG	1A	3199	1/1	0.80	0.18	70,70,70,70	0
57	MG	1A	3666	1/1	0.80	0.18	63,63,63,63	0
57	MG	2A	3410	1/1	0.80	0.12	73,73,73,73	0
57	MG	2x	103	1/1	0.80	0.14	76,76,76,76	0
57	MG	2x	107	1/1	0.80	0.13	49,49,49,49	0
57	MG	2A	3426	1/1	0.80	0.18	57,57,57,57	0
57	MG	2y	103	1/1	0.80	0.14	80,80,80,80	0
57	MG	2A	3648	1/1	0.80	0.21	68,68,68,68	0
57	MG	2A	3427	1/1	0.80	0.17	63,63,63,63	0
57	MG	1A	4058	1/1	0.80	0.22	61,61,61,61	0
57	MG	1A	3302	1/1	0.81	0.19	50,50,50,50	0
57	MG	2A	3142	1/1	0.81	0.19	64,64,64,64	0
57	MG	1A	3882	1/1	0.81	0.15	64,64,64,64	0
57	MG	2A	3160	1/1	0.81	0.19	68,68,68,68	0
57	MG	1a	1742	1/1	0.81	0.15	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	1782	1/1	0.81	0.28	85,85,85,85	0
57	MG	2A	3188	1/1	0.81	0.16	68,68,68,68	0
57	MG	1A	4061	1/1	0.81	0.12	28,28,28,28	0
57	MG	1A	3281	1/1	0.81	0.34	77,77,77,77	0
57	MG	2A	3715	1/1	0.81	0.14	62,62,62,62	0
57	MG	1A	3693	1/1	0.81	0.15	35,35,35,35	0
57	MG	2A	3731	1/1	0.81	0.20	52,52,52,52	0
57	MG	1A	3331	1/1	0.81	0.21	67,67,67,67	0
57	MG	1a	1623	1/1	0.81	0.14	57,57,57,57	0
57	MG	2A	3514	1/1	0.81	0.17	69,69,69,69	0
57	MG	1A	3560	1/1	0.81	0.12	47,47,47,47	0
57	MG	1A	4104	1/1	0.81	0.22	64,64,64,64	0
57	MG	1a	1634	1/1	0.81	0.28	74,74,74,74	0
57	MG	2A	3538	1/1	0.81	0.26	75,75,75,75	0
57	MG	2A	3546	1/1	0.81	0.18	60,60,60,60	0
57	MG	1A	3350	1/1	0.81	0.38	67,67,67,67	0
57	MG	2A	3023	1/1	0.81	0.28	71,71,71,71	0
57	MG	1A	3160	1/1	0.81	0.32	68,68,68,68	0
57	MG	1A	4024	1/1	0.81	0.31	74,74,74,74	0
57	MG	2B	210	1/1	0.81	0.13	68,68,68,68	0
57	MG	1A	3713	1/1	0.81	0.18	54,54,54,54	0
57	MG	1a	1656	1/1	0.81	0.22	68,68,68,68	0
57	MG	25	103	1/1	0.81	0.15	76,76,76,76	0
57	MG	2w	102	1/1	0.81	0.28	86,86,86,86	0
57	MG	2A	3328	1/1	0.81	0.17	73,73,73,73	0
57	MG	2A	3605	1/1	0.81	0.28	67,67,67,67	0
57	MG	2A	3082	1/1	0.81	0.28	69,69,69,69	0
57	MG	1A	3949	1/1	0.81	0.12	49,49,49,49	0
57	MG	1A	3246	1/1	0.81	0.15	56,56,56,56	0
57	MG	2A	3356	1/1	0.81	0.25	53,53,53,53	0
57	MG	2A	3369	1/1	0.81	0.22	73,73,73,73	0
57	MG	2A	3102	1/1	0.81	0.14	72,72,72,72	0
57	MG	1a	1711	1/1	0.81	0.13	71,71,71,71	0
57	MG	1A	3788	1/1	0.82	0.12	54,54,54,54	0
57	MG	1a	1710	1/1	0.82	0.28	68,68,68,68	0
57	MG	2A	3571	1/1	0.82	0.25	84,84,84,84	0
57	MG	2A	3408	1/1	0.82	0.10	81,81,81,81	0
57	MG	2A	3757	1/1	0.82	0.12	64,64,64,64	0
57	MG	2A	3294	1/1	0.82	0.24	63,63,63,63	0
57	MG	2A	3422	1/1	0.82	0.12	67,67,67,67	0
57	MG	2A	3423	1/1	0.82	0.17	69,69,69,69	0
57	MG	1A	3840	1/1	0.82	0.13	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	3607	1/1	0.82	0.13	66,66,66,66	0
57	MG	1w	104	1/1	0.82	0.17	65,65,65,65	0
57	MG	1a	1722	1/1	0.82	0.18	71,71,71,71	0
57	MG	1A	3653	1/1	0.82	0.18	40,40,40,40	0
57	MG	2B	205	1/1	0.82	0.25	67,67,67,67	0
57	MG	2A	3477	1/1	0.82	0.15	54,54,54,54	0
57	MG	1A	3968	1/1	0.82	0.14	65,65,65,65	0
57	MG	2B	214	1/1	0.82	0.24	69,69,69,69	0
57	MG	2A	3493	1/1	0.82	0.20	77,77,77,77	0
57	MG	1a	1741	1/1	0.82	0.15	65,65,65,65	0
57	MG	2A	3322	1/1	0.82	0.16	70,70,70,70	0
57	MG	1A	3520	1/1	0.82	0.12	71,71,71,71	0
57	MG	2A	3050	1/1	0.82	0.28	73,73,73,73	0
57	MG	1A	3818	1/1	0.82	0.16	62,62,62,62	0
57	MG	2w	106	1/1	0.82	0.37	82,82,82,82	0
57	MG	2A	3352	1/1	0.82	0.24	65,65,65,65	0
57	MG	2x	106	1/1	0.82	0.19	66,66,66,66	0
57	MG	2A	3237	1/1	0.82	0.23	79,79,79,79	0
57	MG	1A	3456	1/1	0.82	0.14	61,61,61,61	0
57	MG	1B	222	1/1	0.82	0.12	61,61,61,61	0
57	MG	1A	3823	1/1	0.82	0.18	67,67,67,67	0
57	MG	2A	3560	1/1	0.82	0.17	44,44,44,44	0
57	MG	1A	3381	1/1	0.82	0.20	65,65,65,65	0
57	MG	1A	3680	1/1	0.83	0.13	65,65,65,65	0
57	MG	1A	4113	1/1	0.83	0.15	56,56,56,56	0
57	MG	1a	1810	1/1	0.83	0.19	69,69,69,69	0
57	MG	1a	1635	1/1	0.83	0.23	62,62,62,62	0
57	MG	2A	3662	1/1	0.83	0.20	71,71,71,71	0
57	MG	1a	1816	1/1	0.83	0.35	67,67,67,67	0
57	MG	2A	3229	1/1	0.83	0.12	76,76,76,76	0
57	MG	1a	1817	1/1	0.83	0.17	66,66,66,66	0
57	MG	1A	3444	1/1	0.83	0.13	69,69,69,69	0
57	MG	2A	3700	1/1	0.83	0.16	62,62,62,62	0
57	MG	1a	1646	1/1	0.83	0.16	66,66,66,66	0
57	MG	2A	3240	1/1	0.83	0.17	66,66,66,66	0
57	MG	1A	3296	1/1	0.83	0.22	58,58,58,58	0
57	MG	1A	3697	1/1	0.83	0.12	59,59,59,59	0
57	MG	1A	3239	1/1	0.83	0.21	59,59,59,59	0
57	MG	1A	3475	1/1	0.83	0.17	65,65,65,65	0
57	MG	1A	3117	1/1	0.83	0.22	59,59,59,59	0
57	MG	2A	3275	1/1	0.83	0.29	71,71,71,71	0
57	MG	2A	3511	1/1	0.83	0.24	74,74,74,74	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	1664	1/1	0.83	0.29	73,73,73,73	0
57	MG	1a	1666	1/1	0.83	0.19	73,73,73,73	0
57	MG	1A	3631	1/1	0.83	0.22	72,72,72,72	0
57	MG	2A	3783	1/1	0.83	0.20	75,75,75,75	0
57	MG	2A	3529	1/1	0.83	0.24	70,70,70,70	0
57	MG	1a	1686	1/1	0.83	0.18	76,76,76,76	0
57	MG	1A	4051	1/1	0.83	0.13	54,54,54,54	0
57	MG	2A	3543	1/1	0.83	0.26	65,65,65,65	0
57	MG	2A	3804	1/1	0.83	0.26	79,79,79,79	0
57	MG	1A	4056	1/1	0.83	0.09	51,51,51,51	0
57	MG	2B	202	1/1	0.83	0.24	67,67,67,67	0
57	MG	1A	3247	1/1	0.83	0.19	74,74,74,74	0
57	MG	2A	3320	1/1	0.83	0.20	70,70,70,70	0
57	MG	2A	3084	1/1	0.83	0.27	57,57,57,57	0
57	MG	1A	3496	1/1	0.83	0.16	87,87,87,87	0
57	MG	1A	3989	1/1	0.83	0.11	68,68,68,68	0
57	MG	2A	3332	1/1	0.83	0.22	72,72,72,72	0
57	MG	2E	307	1/1	0.83	0.17	71,71,71,71	0
57	MG	2A	3581	1/1	0.83	0.16	64,64,64,64	0
57	MG	1A	3387	1/1	0.83	0.20	75,75,75,75	0
57	MG	27	102	1/1	0.83	0.32	67,67,67,67	0
57	MG	1A	3399	1/1	0.83	0.27	64,64,64,64	0
57	MG	2A	3108	1/1	0.83	0.14	58,58,58,58	0
57	MG	2A	3125	1/1	0.83	0.12	65,65,65,65	0
57	MG	2A	3365	1/1	0.83	0.23	62,62,62,62	0
57	MG	2A	3608	1/1	0.83	0.14	62,62,62,62	0
57	MG	2A	3610	1/1	0.83	0.23	49,49,49,49	0
57	MG	2A	3615	1/1	0.83	0.20	63,63,63,63	0
57	MG	1a	1746	1/1	0.83	0.12	78,78,78,78	0
57	MG	1a	1755	1/1	0.83	0.14	70,70,70,70	0
57	MG	2A	3386	1/1	0.83	0.14	68,68,68,68	0
57	MG	1A	3338	1/1	0.83	0.21	62,62,62,62	0
57	MG	2A	3158	1/1	0.83	0.34	79,79,79,79	0
57	MG	2A	3018	1/1	0.84	0.20	66,66,66,66	0
57	MG	1A	3905	1/1	0.84	0.10	40,40,40,40	0
57	MG	2A	3375	1/1	0.84	0.23	72,72,72,72	0
57	MG	1A	3596	1/1	0.84	0.13	57,57,57,57	0
57	MG	1A	3238	1/1	0.84	0.21	66,66,66,66	0
57	MG	1A	3476	1/1	0.84	0.17	61,61,61,61	0
57	MG	2A	3245	1/1	0.84	0.34	72,72,72,72	0
57	MG	2A	3590	1/1	0.84	0.32	78,78,78,78	0
57	MG	1A	3927	1/1	0.84	0.12	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	1A	3408	1/1	0.84	0.23	55,55,55,55	0
57	MG	2A	3076	1/1	0.84	0.18	58,58,58,58	0
57	MG	1a	1787	1/1	0.84	0.11	74,74,74,74	0
57	MG	1a	1795	1/1	0.84	0.19	68,68,68,68	0
57	MG	1a	1807	1/1	0.84	0.15	61,61,61,61	0
57	MG	1a	1809	1/1	0.84	0.16	66,66,66,66	0
57	MG	2A	3297	1/1	0.84	0.37	74,74,74,74	0
57	MG	1A	3367	1/1	0.84	0.17	60,60,60,60	0
57	MG	1A	3514	1/1	0.84	0.25	62,62,62,62	0
57	MG	2A	3480	1/1	0.84	0.19	55,55,55,55	0
57	MG	1B	233	1/1	0.84	0.21	61,61,61,61	0
57	MG	1a	1691	1/1	0.84	0.28	68,68,68,68	0
57	MG	2D	306	1/1	0.84	0.16	62,62,62,62	0
57	MG	1A	4059	1/1	0.84	0.14	55,55,55,55	0
57	MG	1A	3951	1/1	0.84	0.19	55,55,55,55	0
57	MG	2O	201	1/1	0.84	0.13	55,55,55,55	0
57	MG	2A	3143	1/1	0.84	0.22	72,72,72,72	0
57	MG	1l	201	1/1	0.84	0.17	82,82,82,82	0
57	MG	2A	3510	1/1	0.84	0.13	71,71,71,71	0
57	MG	2w	101	1/1	0.84	0.12	75,75,75,75	0
57	MG	2A	3327	1/1	0.84	0.17	73,73,73,73	0
57	MG	2A	3151	1/1	0.84	0.38	67,67,67,67	0
57	MG	2w	104	1/1	0.84	0.11	80,80,80,80	0
57	MG	1D	312	1/1	0.84	0.27	47,47,47,47	0
57	MG	2A	3331	1/1	0.84	0.14	75,75,75,75	0
57	MG	2A	3696	1/1	0.84	0.17	82,82,82,82	0
57	MG	1a	1643	1/1	0.84	0.28	60,60,60,60	0
57	MG	2A	3701	1/1	0.84	0.11	68,68,68,68	0
57	MG	1A	3708	1/1	0.84	0.21	44,44,44,44	0
57	MG	2A	3705	1/1	0.84	0.11	68,68,68,68	0
57	MG	1x	108	1/1	0.84	0.31	72,72,72,72	0
57	MG	1a	1736	1/1	0.84	0.23	76,76,76,76	0
57	MG	1O	203	1/1	0.84	0.12	62,62,62,62	0
57	MG	2A	3398	1/1	0.85	0.17	67,67,67,67	0
57	MG	2A	3400	1/1	0.85	0.17	65,65,65,65	0
57	MG	2A	3653	1/1	0.85	0.20	76,76,76,76	0
57	MG	1A	3027	1/1	0.85	0.14	51,51,51,51	0
57	MG	2A	3661	1/1	0.85	0.17	72,72,72,72	0
57	MG	2A	3181	1/1	0.85	0.25	64,64,64,64	0
57	MG	1A	3853	1/1	0.85	0.16	47,47,47,47	0
57	MG	2A	3184	1/1	0.85	0.14	57,57,57,57	0
57	MG	2A	3187	1/1	0.85	0.13	49,49,49,49	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	3679	1/1	0.85	0.20	71,71,71,71	0
57	MG	1m	3001	1/1	0.85	0.15	61,61,61,61	0
57	MG	2A	3189	1/1	0.85	0.17	67,67,67,67	0
57	MG	2A	3198	1/1	0.85	0.30	73,73,73,73	0
57	MG	1A	4060	1/1	0.85	0.17	43,43,43,43	0
57	MG	2A	3455	1/1	0.85	0.45	72,72,72,72	0
57	MG	2A	3226	1/1	0.85	0.16	69,69,69,69	0
57	MG	1a	1692	1/1	0.85	0.20	63,63,63,63	0
57	MG	2A	3231	1/1	0.85	0.28	73,73,73,73	0
57	MG	2A	3710	1/1	0.85	0.24	85,85,85,85	0
57	MG	1w	101	1/1	0.85	0.37	74,74,74,74	0
57	MG	1a	1694	1/1	0.85	0.24	62,62,62,62	0
57	MG	1w	108	1/1	0.85	0.29	66,66,66,66	0
57	MG	1A	3870	1/1	0.85	0.14	25,25,25,25	0
57	MG	11	105	1/1	0.85	0.20	78,78,78,78	0
57	MG	1a	1718	1/1	0.85	0.17	68,68,68,68	0
57	MG	1A	3703	1/1	0.85	0.15	58,58,58,58	0
57	MG	1A	3284	1/1	0.85	0.31	66,66,66,66	0
57	MG	1A	4007	1/1	0.85	0.13	77,77,77,77	0
57	MG	1A	3889	1/1	0.85	0.16	55,55,55,55	0
57	MG	2A	3523	1/1	0.85	0.11	73,73,73,73	0
57	MG	2A	3272	1/1	0.85	0.13	59,59,59,59	0
57	MG	2A	3274	1/1	0.85	0.25	76,76,76,76	0
57	MG	2A	3042	1/1	0.85	0.18	74,74,74,74	0
57	MG	2A	3794	1/1	0.85	0.19	63,63,63,63	0
57	MG	1A	3002	1/1	0.85	0.16	55,55,55,55	0
57	MG	2A	3054	1/1	0.85	0.18	66,66,66,66	0
57	MG	1A	3794	1/1	0.85	0.22	69,69,69,69	0
57	MG	2A	3547	1/1	0.85	0.20	49,49,49,49	0
57	MG	1a	1743	1/1	0.85	0.12	87,87,87,87	0
57	MG	1B	212	1/1	0.85	0.17	58,58,58,58	0
57	MG	1A	3425	1/1	0.85	0.21	63,63,63,63	0
57	MG	1a	1771	1/1	0.85	0.17	69,69,69,69	0
57	MG	2A	3090	1/1	0.85	0.20	69,69,69,69	0
57	MG	2A	3575	1/1	0.85	0.17	61,61,61,61	0
57	MG	1B	224	1/1	0.85	0.16	59,59,59,59	0
57	MG	2A	3098	1/1	0.85	0.17	82,82,82,82	0
57	MG	1B	227	1/1	0.85	0.20	67,67,67,67	0
57	MG	23	101	1/1	0.85	0.19	70,70,70,70	0
57	MG	1A	3507	1/1	0.85	0.21	47,47,47,47	0
57	MG	1A	3604	1/1	0.85	0.16	16,16,16,16	0
57	MG	1a	1649	1/1	0.85	0.12	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	2A	3604	1/1	0.85	0.23	61,61,61,61	0
57	MG	2A	3110	1/1	0.85	0.15	73,73,73,73	0
57	MG	1A	3101	1/1	0.85	0.31	44,44,44,44	0
57	MG	2A	3138	1/1	0.85	0.18	58,58,58,58	0
57	MG	2A	3139	1/1	0.85	0.31	61,61,61,61	0
57	MG	1a	1654	1/1	0.85	0.20	61,61,61,61	0
57	MG	1A	3295	1/1	0.85	0.12	47,47,47,47	0
57	MG	1a	1813	1/1	0.85	0.14	57,57,57,57	0
57	MG	2A	3625	1/1	0.85	0.19	72,72,72,72	0
57	MG	1A	3735	1/1	0.85	0.14	45,45,45,45	0
57	MG	1A	3825	1/1	0.85	0.14	51,51,51,51	0
57	MG	1A	3830	1/1	0.85	0.09	61,61,61,61	0
57	MG	2y	106	1/1	0.85	0.21	71,71,71,71	0
57	MG	1A	3741	1/1	0.85	0.10	30,30,30,30	0
57	MG	1A	3832	1/1	0.86	0.11	60,60,60,60	0
57	MG	2A	3585	1/1	0.86	0.12	59,59,59,59	0
57	MG	1A	3567	1/1	0.86	0.19	46,46,46,46	0
57	MG	2A	3270	1/1	0.86	0.28	76,76,76,76	0
57	MG	1A	3588	1/1	0.86	0.15	53,53,53,53	0
57	MG	2A	3595	1/1	0.86	0.11	52,52,52,52	0
57	MG	1A	3858	1/1	0.86	0.07	38,38,38,38	0
57	MG	2A	3599	1/1	0.86	0.31	75,75,75,75	0
57	MG	1A	3859	1/1	0.86	0.14	42,42,42,42	0
57	MG	1A	3716	1/1	0.86	0.10	49,49,49,49	0
57	MG	2A	3281	1/1	0.86	0.22	70,70,70,70	0
57	MG	1A	3874	1/1	0.86	0.12	39,39,39,39	0
57	MG	2A	3295	1/1	0.86	0.26	59,59,59,59	0
57	MG	1x	106	1/1	0.86	0.22	58,58,58,58	0
57	MG	1x	107	1/1	0.86	0.24	63,63,63,63	0
57	MG	1A	3877	1/1	0.86	0.10	29,29,29,29	0
57	MG	2A	3305	1/1	0.86	0.40	71,71,71,71	0
57	MG	1x	109	1/1	0.86	0.14	32,32,32,32	0
57	MG	1A	4052	1/1	0.86	0.14	22,22,22,22	0
57	MG	1A	3484	1/1	0.86	0.20	62,62,62,62	0
57	MG	2A	3642	1/1	0.86	0.14	69,69,69,69	0
57	MG	2A	3317	1/1	0.86	0.22	71,71,71,71	0
57	MG	1A	3725	1/1	0.86	0.11	52,52,52,52	0
57	MG	2A	3020	1/1	0.86	0.13	62,62,62,62	0
57	MG	1A	3726	1/1	0.86	0.18	68,68,68,68	0
57	MG	1A	3893	1/1	0.86	0.12	45,45,45,45	0
57	MG	2A	3658	1/1	0.86	0.24	68,68,68,68	0
57	MG	2A	3659	1/1	0.86	0.14	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	3359	1/1	0.86	0.12	70,70,70,70	0
57	MG	1a	1651	1/1	0.86	0.17	60,60,60,60	0
57	MG	2A	3330	1/1	0.86	0.34	60,60,60,60	0
57	MG	2A	3672	1/1	0.86	0.15	43,43,43,43	0
57	MG	1a	1652	1/1	0.86	0.12	69,69,69,69	0
57	MG	1A	3901	1/1	0.86	0.12	23,23,23,23	0
57	MG	1A	4071	1/1	0.86	0.20	56,56,56,56	0
57	MG	2A	3343	1/1	0.86	0.34	59,59,59,59	0
57	MG	1A	3902	1/1	0.86	0.14	46,46,46,46	0
57	MG	2A	3065	1/1	0.86	0.17	54,54,54,54	0
57	MG	1A	4091	1/1	0.86	0.11	68,68,68,68	0
57	MG	2A	3357	1/1	0.86	0.26	59,59,59,59	0
57	MG	1A	3625	1/1	0.86	0.21	55,55,55,55	0
57	MG	1A	3413	1/1	0.86	0.30	66,66,66,66	0
57	MG	2A	3085	1/1	0.86	0.21	64,64,64,64	0
57	MG	2A	3380	1/1	0.86	0.16	75,75,75,75	0
57	MG	2A	3382	1/1	0.86	0.17	65,65,65,65	0
57	MG	2A	3720	1/1	0.86	0.17	69,69,69,69	0
57	MG	1a	1667	1/1	0.86	0.26	64,64,64,64	0
57	MG	2A	3724	1/1	0.86	0.13	56,56,56,56	0
57	MG	1a	1676	1/1	0.86	0.22	61,61,61,61	0
57	MG	1A	3640	1/1	0.86	0.13	50,50,50,50	0
57	MG	1A	4105	1/1	0.86	0.19	68,68,68,68	0
57	MG	1A	4109	1/1	0.86	0.20	52,52,52,52	0
57	MG	1A	3911	1/1	0.86	0.12	29,29,29,29	0
57	MG	1B	203	1/1	0.86	0.21	60,60,60,60	0
57	MG	1A	3417	1/1	0.86	0.15	48,48,48,48	0
57	MG	2A	3778	1/1	0.86	0.12	61,61,61,61	0
57	MG	1B	216	1/1	0.86	0.15	54,54,54,54	0
57	MG	2A	3784	1/1	0.86	0.14	56,56,56,56	0
57	MG	2A	3786	1/1	0.86	0.20	72,72,72,72	0
57	MG	1B	219	1/1	0.86	0.15	57,57,57,57	0
57	MG	1A	3423	1/1	0.86	0.20	45,45,45,45	0
57	MG	1B	223	1/1	0.86	0.17	60,60,60,60	0
57	MG	1A	3361	1/1	0.86	0.16	58,58,58,58	0
57	MG	1a	1731	1/1	0.86	0.28	57,57,57,57	0
57	MG	2A	3796	1/1	0.86	0.18	70,70,70,70	0
57	MG	1A	3141	1/1	0.86	0.13	49,49,49,49	0
57	MG	1A	3510	1/1	0.86	0.28	64,64,64,64	0
57	MG	2A	3465	1/1	0.86	0.16	59,59,59,59	0
57	MG	2A	3154	1/1	0.86	0.25	68,68,68,68	0
57	MG	1A	3377	1/1	0.86	0.15	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	3519	1/1	0.86	0.18	61,61,61,61	0
57	MG	1A	3325	1/1	0.86	0.15	44,44,44,44	0
57	MG	2A	3171	1/1	0.86	0.22	61,61,61,61	0
57	MG	2D	303	1/1	0.86	0.36	54,54,54,54	0
57	MG	1a	1753	1/1	0.86	0.09	48,48,48,48	0
57	MG	1A	3042	1/1	0.86	0.13	47,47,47,47	0
57	MG	1a	1756	1/1	0.86	0.17	55,55,55,55	0
57	MG	2G	201	1/1	0.86	0.15	66,66,66,66	0
57	MG	1A	3979	1/1	0.86	0.10	52,52,52,52	0
57	MG	1E	306	1/1	0.86	0.16	58,58,58,58	0
57	MG	21	101	1/1	0.86	0.14	68,68,68,68	0
57	MG	1A	3391	1/1	0.86	0.17	58,58,58,58	0
57	MG	25	101	1/1	0.86	0.11	59,59,59,59	0
57	MG	1A	3396	1/1	0.86	0.27	62,62,62,62	0
57	MG	2A	3202	1/1	0.86	0.16	53,53,53,53	0
57	MG	1A	3292	1/1	0.86	0.19	55,55,55,55	0
57	MG	1Q	204	1/1	0.86	0.20	73,73,73,73	0
57	MG	1Q	207	1/1	0.86	0.18	54,54,54,54	0
57	MG	1R	204	1/1	0.86	0.19	53,53,53,53	0
57	MG	2A	3540	1/1	0.86	0.10	77,77,77,77	0
57	MG	1A	3827	1/1	0.86	0.30	68,68,68,68	0
57	MG	1A	3829	1/1	0.86	0.11	69,69,69,69	0
57	MG	1T	203	1/1	0.86	0.19	64,64,64,64	0
57	MG	1V	207	1/1	0.86	0.13	53,53,53,53	0
57	MG	1W	202	1/1	0.86	0.11	58,58,58,58	0
57	MG	1A	3710	1/1	0.86	0.15	59,59,59,59	0
57	MG	2A	3250	1/1	0.86	0.25	74,74,74,74	0
57	MG	1A	3565	1/1	0.86	0.27	68,68,68,68	0
57	MG	2A	3253	1/1	0.86	0.30	64,64,64,64	0
57	MG	2A	3256	1/1	0.86	0.24	68,68,68,68	0
57	MG	2A	3244	1/1	0.87	0.14	72,72,72,72	0
57	MG	1B	214	1/1	0.87	0.28	69,69,69,69	0
57	MG	2A	3413	1/1	0.87	0.35	68,68,68,68	0
57	MG	1A	3752	1/1	0.87	0.10	26,26,26,26	0
57	MG	1A	3162	1/1	0.87	0.23	41,41,41,41	0
57	MG	1a	1764	1/1	0.87	0.14	77,77,77,77	0
57	MG	1A	3762	1/1	0.87	0.12	66,66,66,66	0
57	MG	2A	3440	1/1	0.87	0.14	69,69,69,69	0
57	MG	2A	3079	1/1	0.87	0.27	58,58,58,58	0
57	MG	2A	3081	1/1	0.87	0.16	58,58,58,58	0
57	MG	1A	3467	1/1	0.87	0.17	65,65,65,65	0
57	MG	2A	3461	1/1	0.87	0.17	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	3683	1/1	0.87	0.17	66,66,66,66	0
57	MG	1A	4038	1/1	0.87	0.24	69,69,69,69	0
57	MG	2A	3687	1/1	0.87	0.25	69,69,69,69	0
57	MG	2A	3688	1/1	0.87	0.17	69,69,69,69	0
57	MG	2A	3466	1/1	0.87	0.11	55,55,55,55	0
57	MG	2A	3467	1/1	0.87	0.18	55,55,55,55	0
57	MG	2A	3474	1/1	0.87	0.17	65,65,65,65	0
57	MG	1A	3914	1/1	0.87	0.12	57,57,57,57	0
57	MG	1A	3243	1/1	0.87	0.21	65,65,65,65	0
57	MG	1a	1790	1/1	0.87	0.17	56,56,56,56	0
57	MG	1A	4044	1/1	0.87	0.09	42,42,42,42	0
57	MG	2A	3279	1/1	0.87	0.23	61,61,61,61	0
57	MG	1A	3851	1/1	0.87	0.24	68,68,68,68	0
57	MG	2A	3285	1/1	0.87	0.16	65,65,65,65	0
57	MG	1A	3373	1/1	0.87	0.19	69,69,69,69	0
57	MG	2A	3506	1/1	0.87	0.22	69,69,69,69	0
57	MG	2A	3728	1/1	0.87	0.15	62,62,62,62	0
57	MG	2A	3730	1/1	0.87	0.10	79,79,79,79	0
57	MG	1A	3854	1/1	0.87	0.10	40,40,40,40	0
57	MG	1A	4053	1/1	0.87	0.16	74,74,74,74	0
57	MG	2A	3736	1/1	0.87	0.13	58,58,58,58	0
57	MG	2A	3109	1/1	0.87	0.21	58,58,58,58	0
57	MG	1A	3580	1/1	0.87	0.15	51,51,51,51	0
57	MG	1A	3581	1/1	0.87	0.21	64,64,64,64	0
57	MG	2A	3761	1/1	0.87	0.14	85,85,85,85	0
57	MG	2A	3524	1/1	0.87	0.19	75,75,75,75	0
57	MG	1F	311	1/1	0.87	0.13	64,64,64,64	0
57	MG	2A	3311	1/1	0.87	0.23	69,69,69,69	0
57	MG	2A	3780	1/1	0.87	0.14	63,63,63,63	0
57	MG	2A	3781	1/1	0.87	0.21	75,75,75,75	0
57	MG	1A	3953	1/1	0.87	0.24	53,53,53,53	0
57	MG	1A	3800	1/1	0.87	0.16	64,64,64,64	0
57	MG	1a	1674	1/1	0.87	0.32	64,64,64,64	0
57	MG	2A	3788	1/1	0.87	0.14	65,65,65,65	0
57	MG	1l	202	1/1	0.87	0.12	65,65,65,65	0
57	MG	1A	3970	1/1	0.87	0.11	33,33,33,33	0
57	MG	1Q	206	1/1	0.87	0.10	51,51,51,51	0
57	MG	1A	3811	1/1	0.87	0.10	39,39,39,39	0
57	MG	2A	3561	1/1	0.87	0.14	55,55,55,55	0
57	MG	2A	3795	1/1	0.87	0.22	62,62,62,62	0
57	MG	1A	3174	1/1	0.87	0.18	63,63,63,63	0
57	MG	2A	3799	1/1	0.87	0.18	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3803	1/1	0.87	0.18	59,59,59,59	0
57	MG	1w	102	1/1	0.87	0.11	60,60,60,60	0
57	MG	1R	206	1/1	0.87	0.23	44,44,44,44	0
57	MG	2A	3569	1/1	0.87	0.20	55,55,55,55	0
57	MG	2A	3165	1/1	0.87	0.25	66,66,66,66	0
57	MG	1w	106	1/1	0.87	0.16	82,82,82,82	0
57	MG	2B	207	1/1	0.87	0.22	61,61,61,61	0
57	MG	2A	3577	1/1	0.87	0.16	60,60,60,60	0
57	MG	2A	3334	1/1	0.87	0.23	50,50,50,50	0
57	MG	2B	211	1/1	0.87	0.19	71,71,71,71	0
57	MG	2A	3177	1/1	0.87	0.27	70,70,70,70	0
57	MG	2B	215	1/1	0.87	0.12	73,73,73,73	0
57	MG	2A	3582	1/1	0.87	0.10	59,59,59,59	0
57	MG	1w	107	1/1	0.87	0.27	68,68,68,68	0
57	MG	2A	3587	1/1	0.87	0.19	62,62,62,62	0
57	MG	1A	3817	1/1	0.87	0.18	66,66,66,66	0
57	MG	1w	109	1/1	0.87	0.21	79,79,79,79	0
57	MG	1A	4083	1/1	0.87	0.19	58,58,58,58	0
57	MG	1A	3443	1/1	0.87	0.13	55,55,55,55	0
57	MG	2A	3597	1/1	0.87	0.35	65,65,65,65	0
57	MG	2A	3362	1/1	0.87	0.44	71,71,71,71	0
57	MG	1a	1714	1/1	0.87	0.21	78,78,78,78	0
57	MG	1A	3378	1/1	0.87	0.18	49,49,49,49	0
57	MG	2A	3372	1/1	0.87	0.22	52,52,52,52	0
57	MG	1A	4102	1/1	0.87	0.14	64,64,64,64	0
57	MG	2A	3212	1/1	0.87	0.17	52,52,52,52	0
57	MG	1A	3995	1/1	0.87	0.13	41,41,41,41	0
57	MG	1A	3891	1/1	0.87	0.13	42,42,42,42	0
57	MG	1A	3136	1/1	0.87	0.21	48,48,48,48	0
57	MG	2A	3618	1/1	0.87	0.11	59,59,59,59	0
57	MG	1A	3522	1/1	0.87	0.21	60,60,60,60	0
57	MG	2A	3388	1/1	0.87	0.32	70,70,70,70	0
57	MG	2A	3632	1/1	0.87	0.15	69,69,69,69	0
57	MG	2A	3397	1/1	0.87	0.16	57,57,57,57	0
57	MG	1A	3448	1/1	0.87	0.10	50,50,50,50	0
57	MG	1a	1611	1/1	0.87	0.23	74,74,74,74	0
57	MG	2A	3402	1/1	0.87	0.27	56,56,56,56	0
57	MG	1A	4012	1/1	0.87	0.12	49,49,49,49	0
57	MG	1A	3743	1/1	0.87	0.16	44,44,44,44	0
57	MG	1A	3493	1/1	0.88	0.15	68,68,68,68	0
57	MG	1A	3314	1/1	0.88	0.28	57,57,57,57	0
57	MG	2A	3660	1/1	0.88	0.07	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	1A	3317	1/1	0.88	0.11	54,54,54,54	0
57	MG	2A	3415	1/1	0.88	0.29	66,66,66,66	0
57	MG	2A	3667	1/1	0.88	0.11	69,69,69,69	0
57	MG	1A	4072	1/1	0.88	0.14	49,49,49,49	0
57	MG	1A	3838	1/1	0.88	0.20	52,52,52,52	0
57	MG	2A	3028	1/1	0.88	0.36	62,62,62,62	0
57	MG	1V	206	1/1	0.88	0.18	57,57,57,57	0
57	MG	2A	3676	1/1	0.88	0.18	60,60,60,60	0
57	MG	2A	3428	1/1	0.88	0.13	52,52,52,52	0
57	MG	2A	3438	1/1	0.88	0.10	57,57,57,57	0
57	MG	2A	3033	1/1	0.88	0.22	56,56,56,56	0
57	MG	1A	3080	1/1	0.88	0.21	50,50,50,50	0
57	MG	2A	3453	1/1	0.88	0.15	55,55,55,55	0
57	MG	2A	3691	1/1	0.88	0.12	60,60,60,60	0
57	MG	1A	3736	1/1	0.88	0.11	45,45,45,45	0
57	MG	2A	3699	1/1	0.88	0.13	56,56,56,56	0
57	MG	2A	3044	1/1	0.88	0.28	71,71,71,71	0
57	MG	2A	3459	1/1	0.88	0.13	69,69,69,69	0
57	MG	1W	206	1/1	0.88	0.18	27,27,27,27	0
57	MG	2A	3462	1/1	0.88	0.14	41,41,41,41	0
57	MG	1A	4095	1/1	0.88	0.10	65,65,65,65	0
57	MG	1A	3976	1/1	0.88	0.22	60,60,60,60	0
57	MG	2A	3257	1/1	0.88	0.14	64,64,64,64	0
57	MG	2A	3261	1/1	0.88	0.22	69,69,69,69	0
57	MG	11	106	1/1	0.88	0.14	54,54,54,54	0
57	MG	2A	3267	1/1	0.88	0.17	61,61,61,61	0
57	MG	1a	1748	1/1	0.88	0.13	57,57,57,57	0
57	MG	2A	3067	1/1	0.88	0.22	65,65,65,65	0
57	MG	1A	3244	1/1	0.88	0.14	55,55,55,55	0
57	MG	1A	3436	1/1	0.88	0.26	65,65,65,65	0
57	MG	1a	1602	1/1	0.88	0.19	62,62,62,62	0
57	MG	1A	3085	1/1	0.88	0.16	37,37,37,37	0
57	MG	1A	3332	1/1	0.88	0.12	64,64,64,64	0
57	MG	1A	3867	1/1	0.88	0.10	39,39,39,39	0
57	MG	1a	1625	1/1	0.88	0.27	63,63,63,63	0
57	MG	2A	3096	1/1	0.88	0.11	57,57,57,57	0
57	MG	2A	3517	1/1	0.88	0.15	62,62,62,62	0
57	MG	2A	3763	1/1	0.88	0.10	42,42,42,42	0
57	MG	1A	3335	1/1	0.88	0.29	65,65,65,65	0
57	MG	2A	3296	1/1	0.88	0.19	65,65,65,65	0
57	MG	1A	4006	1/1	0.88	0.11	70,70,70,70	0
57	MG	1a	1633	1/1	0.88	0.30	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	3782	1/1	0.88	0.11	50,50,50,50	0
57	MG	1a	1793	1/1	0.88	0.15	66,66,66,66	0
57	MG	1B	211	1/1	0.88	0.23	50,50,50,50	0
57	MG	2A	3537	1/1	0.88	0.15	54,54,54,54	0
57	MG	2A	3308	1/1	0.88	0.18	65,65,65,65	0
57	MG	1A	3382	1/1	0.88	0.14	50,50,50,50	0
57	MG	1a	1808	1/1	0.88	0.24	67,67,67,67	0
57	MG	1a	1636	1/1	0.88	0.21	69,69,69,69	0
57	MG	2A	3113	1/1	0.88	0.35	73,73,73,73	0
57	MG	1A	3785	1/1	0.88	0.11	44,44,44,44	0
57	MG	2A	3126	1/1	0.88	0.19	47,47,47,47	0
57	MG	1A	3878	1/1	0.88	0.11	30,30,30,30	0
57	MG	1A	3452	1/1	0.88	0.20	55,55,55,55	0
57	MG	1A	3337	1/1	0.88	0.13	59,59,59,59	0
57	MG	1A	3461	1/1	0.88	0.24	61,61,61,61	0
57	MG	1A	3535	1/1	0.88	0.32	56,56,56,56	0
57	MG	1A	3796	1/1	0.88	0.10	44,44,44,44	0
57	MG	1d	301	1/1	0.88	0.34	61,61,61,61	0
57	MG	1A	3554	1/1	0.88	0.35	65,65,65,65	0
57	MG	2A	3155	1/1	0.88	0.27	64,64,64,64	0
57	MG	2A	3336	1/1	0.88	0.28	55,55,55,55	0
57	MG	1A	4037	1/1	0.88	0.08	17,17,17,17	0
57	MG	1A	3068	1/1	0.88	0.16	54,54,54,54	0
57	MG	2A	3347	1/1	0.88	0.32	61,61,61,61	0
57	MG	2A	3349	1/1	0.88	0.19	69,69,69,69	0
57	MG	2B	216	1/1	0.88	0.28	74,74,74,74	0
57	MG	2A	3350	1/1	0.88	0.21	58,58,58,58	0
57	MG	1B	236	1/1	0.88	0.17	71,71,71,71	0
57	MG	2E	301	1/1	0.88	0.15	70,70,70,70	0
57	MG	1A	3813	1/1	0.88	0.17	50,50,50,50	0
57	MG	2A	3166	1/1	0.88	0.23	74,74,74,74	0
57	MG	2A	3167	1/1	0.88	0.17	65,65,65,65	0
57	MG	1A	3253	1/1	0.88	0.14	69,69,69,69	0
57	MG	2W	203	1/1	0.88	0.26	65,65,65,65	0
57	MG	1A	3260	1/1	0.88	0.15	56,56,56,56	0
57	MG	20	101	1/1	0.88	0.18	67,67,67,67	0
57	MG	1w	103	1/1	0.88	0.21	75,75,75,75	0
57	MG	2A	3370	1/1	0.88	0.10	63,63,63,63	0
57	MG	1A	3407	1/1	0.88	0.11	52,52,52,52	0
57	MG	1A	3480	1/1	0.88	0.13	45,45,45,45	0
57	MG	1F	310	1/1	0.88	0.16	38,38,38,38	0
57	MG	1A	3353	1/1	0.88	0.14	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	3719	1/1	0.88	0.12	69,69,69,69	0
57	MG	1A	3720	1/1	0.88	0.08	69,69,69,69	0
57	MG	2A	3200	1/1	0.88	0.23	66,66,66,66	0
57	MG	1A	3929	1/1	0.88	0.11	62,62,62,62	0
57	MG	2A	3390	1/1	0.88	0.09	75,75,75,75	0
57	MG	2x	101	1/1	0.88	0.14	71,71,71,71	0
57	MG	2A	3204	1/1	0.88	0.38	55,55,55,55	0
57	MG	2x	104	1/1	0.88	0.38	73,73,73,73	0
57	MG	2A	3205	1/1	0.88	0.21	58,58,58,58	0
57	MG	1A	3099	1/1	0.88	0.14	68,68,68,68	0
57	MG	2y	101	1/1	0.88	0.09	57,57,57,57	0
57	MG	2A	3645	1/1	0.88	0.12	68,68,68,68	0
57	MG	2A	3401	1/1	0.88	0.13	67,67,67,67	0
57	MG	2A	3218	1/1	0.88	0.24	68,68,68,68	0
57	MG	2A	3651	1/1	0.88	0.25	62,62,62,62	0
57	MG	1A	3488	1/1	0.88	0.42	43,43,43,43	0
57	MG	2A	3222	1/1	0.88	0.10	72,72,72,72	0
57	MG	2A	3239	1/1	0.89	0.27	73,73,73,73	0
57	MG	1A	3783	1/1	0.89	0.08	23,23,23,23	0
57	MG	1A	3058	1/1	0.89	0.18	59,59,59,59	0
57	MG	1A	4026	1/1	0.89	0.07	43,43,43,43	0
57	MG	2A	3668	1/1	0.89	0.20	61,61,61,61	0
57	MG	1A	3542	1/1	0.89	0.11	62,62,62,62	0
57	MG	1A	3433	1/1	0.89	0.26	57,57,57,57	0
57	MG	1A	3888	1/1	0.89	0.14	48,48,48,48	0
57	MG	1A	3789	1/1	0.89	0.08	24,24,24,24	0
57	MG	2A	3434	1/1	0.89	0.31	55,55,55,55	0
57	MG	2A	3061	1/1	0.89	0.12	51,51,51,51	0
57	MG	1A	3176	1/1	0.89	0.07	45,45,45,45	0
57	MG	2A	3258	1/1	0.89	0.17	67,67,67,67	0
57	MG	1Q	205	1/1	0.89	0.29	55,55,55,55	0
57	MG	1A	3438	1/1	0.89	0.09	69,69,69,69	0
57	MG	2A	3071	1/1	0.89	0.23	71,71,71,71	0
57	MG	2A	3457	1/1	0.89	0.14	59,59,59,59	0
57	MG	1A	4045	1/1	0.89	0.13	64,64,64,64	0
57	MG	1A	3564	1/1	0.89	0.26	54,54,54,54	0
57	MG	1A	3701	1/1	0.89	0.24	69,69,69,69	0
57	MG	1A	3801	1/1	0.89	0.12	32,32,32,32	0
57	MG	1A	3393	1/1	0.89	0.13	64,64,64,64	0
57	MG	1A	3566	1/1	0.89	0.19	57,57,57,57	0
57	MG	2A	3087	1/1	0.89	0.15	55,55,55,55	0
57	MG	1A	3186	1/1	0.89	0.37	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	3714	1/1	0.89	0.19	66,66,66,66	0
57	MG	2A	3093	1/1	0.89	0.20	71,71,71,71	0
57	MG	2A	3716	1/1	0.89	0.11	70,70,70,70	0
57	MG	2A	3490	1/1	0.89	0.19	55,55,55,55	0
57	MG	2A	3287	1/1	0.89	0.18	77,77,77,77	0
57	MG	1a	1752	1/1	0.89	0.16	61,61,61,61	0
57	MG	1A	3815	1/1	0.89	0.24	53,53,53,53	0
57	MG	1A	3816	1/1	0.89	0.27	64,64,64,64	0
57	MG	1A	3196	1/1	0.89	0.12	50,50,50,50	0
57	MG	1X	105	1/1	0.89	0.16	51,51,51,51	0
57	MG	2A	3105	1/1	0.89	0.22	65,65,65,65	0
57	MG	2A	3740	1/1	0.89	0.12	56,56,56,56	0
57	MG	2A	3302	1/1	0.89	0.24	55,55,55,55	0
57	MG	2A	3750	1/1	0.89	0.13	63,63,63,63	0
57	MG	10	104	1/1	0.89	0.18	57,57,57,57	0
57	MG	1A	4064	1/1	0.89	0.12	54,54,54,54	0
57	MG	1A	3404	1/1	0.89	0.11	49,49,49,49	0
57	MG	1A	3928	1/1	0.89	0.10	26,26,26,26	0
57	MG	2A	3112	1/1	0.89	0.18	49,49,49,49	0
57	MG	2A	3764	1/1	0.89	0.13	57,57,57,57	0
57	MG	1A	3582	1/1	0.89	0.22	47,47,47,47	0
57	MG	1A	3822	1/1	0.89	0.12	59,59,59,59	0
57	MG	1A	3449	1/1	0.89	0.20	51,51,51,51	0
57	MG	1A	3946	1/1	0.89	0.10	32,32,32,32	0
57	MG	2A	3534	1/1	0.89	0.11	63,63,63,63	0
57	MG	2A	3321	1/1	0.89	0.29	62,62,62,62	0
57	MG	1a	1608	1/1	0.89	0.35	70,70,70,70	0
57	MG	2A	3325	1/1	0.89	0.09	77,77,77,77	0
57	MG	1A	3948	1/1	0.89	0.21	59,59,59,59	0
57	MG	1a	1621	1/1	0.89	0.14	59,59,59,59	0
57	MG	1A	3592	1/1	0.89	0.12	58,58,58,58	0
57	MG	2A	3558	1/1	0.89	0.18	59,59,59,59	0
57	MG	1A	3041	1/1	0.89	0.16	68,68,68,68	0
57	MG	1a	1628	1/1	0.89	0.22	58,58,58,58	0
57	MG	1A	3826	1/1	0.89	0.08	40,40,40,40	0
57	MG	1A	3966	1/1	0.89	0.16	73,73,73,73	0
57	MG	2A	3335	1/1	0.89	0.24	46,46,46,46	0
57	MG	1A	3149	1/1	0.89	0.25	48,48,48,48	0
57	MG	1A	3969	1/1	0.89	0.19	67,67,67,67	0
57	MG	2A	3573	1/1	0.89	0.16	65,65,65,65	0
57	MG	2A	3574	1/1	0.89	0.23	68,68,68,68	0
57	MG	2A	3339	1/1	0.89	0.15	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	2A	3340	1/1	0.89	0.29	58,58,58,58	0
57	MG	1A	3513	1/1	0.89	0.34	54,54,54,54	0
57	MG	1A	4114	1/1	0.89	0.15	61,61,61,61	0
57	MG	2B	209	1/1	0.89	0.10	78,78,78,78	0
57	MG	1A	3102	1/1	0.89	0.30	50,50,50,50	0
57	MG	2A	3583	1/1	0.89	0.11	64,64,64,64	0
57	MG	2B	212	1/1	0.89	0.22	73,73,73,73	0
57	MG	1B	204	1/1	0.89	0.19	62,62,62,62	0
57	MG	1p	101	1/1	0.89	0.17	57,57,57,57	0
57	MG	1B	208	1/1	0.89	0.13	63,63,63,63	0
57	MG	1t	201	1/1	0.89	0.13	55,55,55,55	0
57	MG	1B	209	1/1	0.89	0.17	54,54,54,54	0
57	MG	2A	3359	1/1	0.89	0.14	67,67,67,67	0
57	MG	2A	3360	1/1	0.89	0.28	66,66,66,66	0
57	MG	1A	3634	1/1	0.89	0.08	37,37,37,37	0
57	MG	2A	3363	1/1	0.89	0.21	63,63,63,63	0
57	MG	2A	3364	1/1	0.89	0.23	46,46,46,46	0
57	MG	1A	3349	1/1	0.89	0.23	47,47,47,47	0
57	MG	1A	3473	1/1	0.89	0.08	53,53,53,53	0
57	MG	1A	3650	1/1	0.89	0.11	44,44,44,44	0
57	MG	2A	3195	1/1	0.89	0.33	68,68,68,68	0
57	MG	2A	3374	1/1	0.89	0.15	69,69,69,69	0
57	MG	1A	3847	1/1	0.89	0.11	43,43,43,43	0
57	MG	1A	3990	1/1	0.89	0.12	75,75,75,75	0
57	MG	2A	3619	1/1	0.89	0.10	81,81,81,81	0
57	MG	1A	3651	1/1	0.89	0.11	49,49,49,49	0
57	MG	2A	3624	1/1	0.89	0.09	37,37,37,37	0
57	MG	2A	3383	1/1	0.89	0.34	58,58,58,58	0
57	MG	1a	1658	1/1	0.89	0.38	77,77,77,77	0
57	MG	2A	3385	1/1	0.89	0.40	59,59,59,59	0
57	MG	1A	3418	1/1	0.89	0.18	50,50,50,50	0
57	MG	2A	3636	1/1	0.89	0.15	53,53,53,53	0
57	MG	1a	1661	1/1	0.89	0.20	66,66,66,66	0
57	MG	1A	3748	1/1	0.89	0.11	23,23,23,23	0
57	MG	2x	105	1/1	0.89	0.10	56,56,56,56	0
57	MG	2A	3219	1/1	0.89	0.22	71,71,71,71	0
57	MG	1A	3855	1/1	0.89	0.17	39,39,39,39	0
57	MG	1A	3656	1/1	0.89	0.12	37,37,37,37	0
57	MG	1A	3278	1/1	0.89	0.20	66,66,66,66	0
57	MG	1A	3097	1/1	0.89	0.15	62,62,62,62	0
57	MG	1a	1682	1/1	0.89	0.23	64,64,64,64	0
57	MG	1a	1684	1/1	0.89	0.26	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	3775	1/1	0.89	0.11	23,23,23,23	0
57	MG	1A	3671	1/1	0.89	0.10	43,43,43,43	0
57	MG	1a	1703	1/1	0.90	0.14	67,67,67,67	0
57	MG	1a	1705	1/1	0.90	0.11	57,57,57,57	0
57	MG	1a	1706	1/1	0.90	0.11	53,53,53,53	0
57	MG	1A	3249	1/1	0.90	0.08	43,43,43,43	0
57	MG	1A	3330	1/1	0.90	0.15	60,60,60,60	0
57	MG	1A	3251	1/1	0.90	0.16	49,49,49,49	0
57	MG	2A	3348	1/1	0.90	0.20	64,64,64,64	0
57	MG	1A	3147	1/1	0.90	0.18	45,45,45,45	0
57	MG	1A	3494	1/1	0.90	0.17	59,59,59,59	0
57	MG	2A	3627	1/1	0.90	0.17	60,60,60,60	0
57	MG	2A	3351	1/1	0.90	0.33	62,62,62,62	0
57	MG	1A	3254	1/1	0.90	0.24	65,65,65,65	0
57	MG	2A	3353	1/1	0.90	0.22	54,54,54,54	0
57	MG	2A	3635	1/1	0.90	0.16	64,64,64,64	0
57	MG	1A	3086	1/1	0.90	0.12	42,42,42,42	0
57	MG	2A	3117	1/1	0.90	0.10	58,58,58,58	0
57	MG	2A	3640	1/1	0.90	0.10	42,42,42,42	0
57	MG	1A	3276	1/1	0.90	0.15	56,56,56,56	0
57	MG	1a	1734	1/1	0.90	0.17	66,66,66,66	0
57	MG	1A	3277	1/1	0.90	0.13	43,43,43,43	0
57	MG	1E	308	1/1	0.90	0.20	55,55,55,55	0
57	MG	1A	3684	1/1	0.90	0.11	41,41,41,41	0
57	MG	1A	3688	1/1	0.90	0.11	28,28,28,28	0
57	MG	1A	3155	1/1	0.90	0.16	64,64,64,64	0
57	MG	2A	3656	1/1	0.90	0.16	49,49,49,49	0
57	MG	1N	205	1/1	0.90	0.36	53,53,53,53	0
57	MG	1N	206	1/1	0.90	0.12	45,45,45,45	0
57	MG	2A	3371	1/1	0.90	0.14	59,59,59,59	0
57	MG	2A	3153	1/1	0.90	0.17	53,53,53,53	0
57	MG	1A	3351	1/1	0.90	0.18	60,60,60,60	0
57	MG	1A	4001	1/1	0.90	0.11	54,54,54,54	0
57	MG	2A	3665	1/1	0.90	0.22	61,61,61,61	0
57	MG	1P	204	1/1	0.90	0.06	40,40,40,40	0
57	MG	1P	205	1/1	0.90	0.16	45,45,45,45	0
57	MG	1Q	203	1/1	0.90	0.11	50,50,50,50	0
57	MG	1a	1772	1/1	0.90	0.09	86,86,86,86	0
57	MG	1a	1780	1/1	0.90	0.23	66,66,66,66	0
57	MG	1A	3512	1/1	0.90	0.18	46,46,46,46	0
57	MG	2A	3168	1/1	0.90	0.30	64,64,64,64	0
57	MG	1A	3430	1/1	0.90	0.12	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	3175	1/1	0.90	0.14	68,68,68,68	0
57	MG	2A	3392	1/1	0.90	0.19	65,65,65,65	0
57	MG	2A	3395	1/1	0.90	0.11	65,65,65,65	0
57	MG	1A	3214	1/1	0.90	0.14	45,45,45,45	0
57	MG	1A	3282	1/1	0.90	0.10	45,45,45,45	0
57	MG	1A	3437	1/1	0.90	0.24	44,44,44,44	0
57	MG	1a	1791	1/1	0.90	0.10	62,62,62,62	0
57	MG	1A	3283	1/1	0.90	0.20	40,40,40,40	0
57	MG	1A	3833	1/1	0.90	0.13	68,68,68,68	0
57	MG	1A	3357	1/1	0.90	0.14	58,58,58,58	0
57	MG	1A	3839	1/1	0.90	0.16	61,61,61,61	0
57	MG	2A	3706	1/1	0.90	0.09	54,54,54,54	0
57	MG	2A	3409	1/1	0.90	0.17	55,55,55,55	0
57	MG	1A	3216	1/1	0.90	0.18	57,57,57,57	0
57	MG	1A	3843	1/1	0.90	0.07	29,29,29,29	0
57	MG	1A	3845	1/1	0.90	0.23	33,33,33,33	0
57	MG	2A	3420	1/1	0.90	0.21	60,60,60,60	0
57	MG	1A	3445	1/1	0.90	0.12	55,55,55,55	0
57	MG	1A	3537	1/1	0.90	0.12	54,54,54,54	0
57	MG	2A	3211	1/1	0.90	0.16	67,67,67,67	0
57	MG	2A	3722	1/1	0.90	0.14	69,69,69,69	0
57	MG	2A	3723	1/1	0.90	0.12	80,80,80,80	0
57	MG	1A	3446	1/1	0.90	0.15	55,55,55,55	0
57	MG	2A	3216	1/1	0.90	0.20	56,56,56,56	0
57	MG	1A	3550	1/1	0.90	0.14	48,48,48,48	0
57	MG	11	102	1/1	0.90	0.10	54,54,54,54	0
57	MG	1A	3125	1/1	0.90	0.18	59,59,59,59	0
57	MG	1A	3857	1/1	0.90	0.19	38,38,38,38	0
57	MG	2A	3225	1/1	0.90	0.35	64,64,64,64	0
57	MG	2A	3746	1/1	0.90	0.10	60,60,60,60	0
57	MG	2A	3747	1/1	0.90	0.14	63,63,63,63	0
57	MG	1A	3724	1/1	0.90	0.09	54,54,54,54	0
57	MG	1A	3235	1/1	0.90	0.19	52,52,52,52	0
57	MG	1A	3863	1/1	0.90	0.13	42,42,42,42	0
57	MG	1A	3866	1/1	0.90	0.15	66,66,66,66	0
57	MG	2A	3760	1/1	0.90	0.12	39,39,39,39	0
57	MG	2A	3460	1/1	0.90	0.13	46,46,46,46	0
57	MG	1a	1607	1/1	0.90	0.20	60,60,60,60	0
57	MG	1A	3135	1/1	0.90	0.18	47,47,47,47	0
57	MG	1A	3869	1/1	0.90	0.09	48,48,48,48	0
57	MG	1a	1614	1/1	0.90	0.09	73,73,73,73	0
57	MG	1A	3727	1/1	0.90	0.09	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3374	1/1	0.90	0.27	40,40,40,40	0
57	MG	1A	3163	1/1	0.90	0.21	63,63,63,63	0
57	MG	1A	3457	1/1	0.90	0.10	49,49,49,49	0
57	MG	2A	3484	1/1	0.90	0.18	62,62,62,62	0
57	MG	2A	3487	1/1	0.90	0.14	35,35,35,35	0
57	MG	1A	3460	1/1	0.90	0.15	64,64,64,64	0
57	MG	1A	3241	1/1	0.90	0.08	61,61,61,61	0
57	MG	1x	101	1/1	0.90	0.32	69,69,69,69	0
57	MG	1x	102	1/1	0.90	0.30	73,73,73,73	0
57	MG	2A	3495	1/1	0.90	0.11	43,43,43,43	0
57	MG	1A	3887	1/1	0.90	0.10	46,46,46,46	0
57	MG	1A	3463	1/1	0.90	0.20	46,46,46,46	0
57	MG	1A	4074	1/1	0.90	0.13	62,62,62,62	0
57	MG	2A	3266	1/1	0.90	0.36	49,49,49,49	0
57	MG	1A	4081	1/1	0.90	0.22	53,53,53,53	0
57	MG	1a	1637	1/1	0.90	0.29	63,63,63,63	0
57	MG	2A	3001	1/1	0.90	0.39	68,68,68,68	0
57	MG	2A	3515	1/1	0.90	0.21	56,56,56,56	0
57	MG	1A	3744	1/1	0.90	0.12	59,59,59,59	0
57	MG	1A	3745	1/1	0.90	0.09	24,24,24,24	0
57	MG	2B	204	1/1	0.90	0.23	71,71,71,71	0
57	MG	1A	3466	1/1	0.90	0.11	60,60,60,60	0
57	MG	1A	4096	1/1	0.90	0.13	69,69,69,69	0
57	MG	2A	3278	1/1	0.90	0.18	58,58,58,58	0
57	MG	1A	3018	1/1	0.90	0.17	57,57,57,57	0
57	MG	2A	3280	1/1	0.90	0.15	57,57,57,57	0
57	MG	1A	3471	1/1	0.90	0.16	48,48,48,48	0
57	MG	2A	3283	1/1	0.90	0.19	59,59,59,59	0
57	MG	1A	3595	1/1	0.90	0.10	35,35,35,35	0
57	MG	2A	3040	1/1	0.90	0.11	58,58,58,58	0
57	MG	2A	3541	1/1	0.90	0.12	46,46,46,46	0
57	MG	1A	3766	1/1	0.90	0.10	28,28,28,28	0
57	MG	1A	3769	1/1	0.90	0.09	31,31,31,31	0
57	MG	1A	3770	1/1	0.90	0.08	72,72,72,72	0
57	MG	2A	3553	1/1	0.90	0.24	55,55,55,55	0
57	MG	2E	305	1/1	0.90	0.18	60,60,60,60	0
57	MG	2E	306	1/1	0.90	0.16	56,56,56,56	0
57	MG	2A	3047	1/1	0.90	0.36	68,68,68,68	0
57	MG	2F	302	1/1	0.90	0.26	65,65,65,65	0
57	MG	1A	3910	1/1	0.90	0.12	56,56,56,56	0
57	MG	1A	3312	1/1	0.90	0.24	59,59,59,59	0
57	MG	2U	201	1/1	0.90	0.15	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2W	201	1/1	0.90	0.27	72,72,72,72	0
57	MG	2A	3055	1/1	0.90	0.32	64,64,64,64	0
57	MG	2A	3303	1/1	0.90	0.17	68,68,68,68	0
57	MG	1B	201	1/1	0.90	0.11	54,54,54,54	0
57	MG	2A	3058	1/1	0.90	0.17	61,61,61,61	0
57	MG	1a	1660	1/1	0.90	0.15	58,58,58,58	0
57	MG	1A	3597	1/1	0.90	0.11	36,36,36,36	0
57	MG	1A	3782	1/1	0.90	0.10	32,32,32,32	0
57	MG	2A	3314	1/1	0.90	0.11	77,77,77,77	0
57	MG	2A	3315	1/1	0.90	0.23	67,67,67,67	0
57	MG	2A	3578	1/1	0.90	0.15	65,65,65,65	0
57	MG	1A	3598	1/1	0.90	0.15	62,62,62,62	0
57	MG	2A	3070	1/1	0.90	0.12	59,59,59,59	0
57	MG	1A	3474	1/1	0.90	0.08	52,52,52,52	0
57	MG	1a	1669	1/1	0.90	0.20	47,47,47,47	0
57	MG	1A	3619	1/1	0.90	0.10	30,30,30,30	0
57	MG	2x	102	1/1	0.90	0.28	76,76,76,76	0
57	MG	1A	3937	1/1	0.90	0.15	75,75,75,75	0
57	MG	2A	3589	1/1	0.90	0.11	47,47,47,47	0
57	MG	2A	3323	1/1	0.90	0.12	62,62,62,62	0
57	MG	1a	1681	1/1	0.90	0.29	70,70,70,70	0
57	MG	1A	3621	1/1	0.90	0.15	59,59,59,59	0
57	MG	1A	3060	1/1	0.90	0.13	34,34,34,34	0
57	MG	1A	3315	1/1	0.90	0.12	57,57,57,57	0
57	MG	2A	3089	1/1	0.90	0.18	72,72,72,72	0
57	MG	1B	220	1/1	0.90	0.23	53,53,53,53	0
57	MG	1A	3477	1/1	0.90	0.13	53,53,53,53	0
57	MG	1A	3145	1/1	0.90	0.14	45,45,45,45	0
57	MG	1A	3193	1/1	0.90	0.20	63,63,63,63	0
57	MG	2A	3616	1/1	0.91	0.14	62,62,62,62	0
57	MG	1a	1789	1/1	0.91	0.10	48,48,48,48	0
57	MG	2A	3354	1/1	0.91	0.20	61,61,61,61	0
57	MG	15	104	1/1	0.91	0.22	44,44,44,44	0
57	MG	15	106	1/1	0.91	0.32	46,46,46,46	0
57	MG	2A	3156	1/1	0.91	0.14	52,52,52,52	0
57	MG	1a	1792	1/1	0.91	0.11	66,66,66,66	0
57	MG	2A	3159	1/1	0.91	0.23	71,71,71,71	0
57	MG	1A	3424	1/1	0.91	0.09	67,67,67,67	0
57	MG	1a	1794	1/1	0.91	0.23	64,64,64,64	0
57	MG	1A	4075	1/1	0.91	0.16	60,60,60,60	0
57	MG	1a	1804	1/1	0.91	0.19	56,56,56,56	0
57	MG	2A	3366	1/1	0.91	0.41	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	3368	1/1	0.91	0.33	57,57,57,57	0
57	MG	1A	4076	1/1	0.91	0.17	60,60,60,60	0
57	MG	1A	3704	1/1	0.91	0.13	47,47,47,47	0
57	MG	1A	3318	1/1	0.91	0.11	62,62,62,62	0
57	MG	1A	3237	1/1	0.91	0.13	58,58,58,58	0
57	MG	1A	4093	1/1	0.91	0.07	43,43,43,43	0
57	MG	1A	3573	1/1	0.91	0.12	57,57,57,57	0
57	MG	1a	1618	1/1	0.91	0.11	54,54,54,54	0
57	MG	2A	3381	1/1	0.91	0.19	56,56,56,56	0
57	MG	2A	3655	1/1	0.91	0.11	54,54,54,54	0
57	MG	1A	3938	1/1	0.91	0.08	50,50,50,50	0
57	MG	1A	4099	1/1	0.91	0.10	64,64,64,64	0
57	MG	1a	1820	1/1	0.91	0.11	45,45,45,45	0
57	MG	1a	1624	1/1	0.91	0.17	60,60,60,60	0
57	MG	2A	3192	1/1	0.91	0.14	57,57,57,57	0
57	MG	2A	3193	1/1	0.91	0.13	56,56,56,56	0
57	MG	1A	3429	1/1	0.91	0.33	47,47,47,47	0
57	MG	1e	202	1/1	0.91	0.25	64,64,64,64	0
57	MG	2A	3199	1/1	0.91	0.10	52,52,52,52	0
57	MG	2A	3393	1/1	0.91	0.11	44,44,44,44	0
57	MG	1A	3328	1/1	0.91	0.24	40,40,40,40	0
57	MG	1A	3127	1/1	0.91	0.11	66,66,66,66	0
57	MG	1a	1631	1/1	0.91	0.09	51,51,51,51	0
57	MG	1A	3947	1/1	0.91	0.07	45,45,45,45	0
57	MG	1A	3583	1/1	0.91	0.09	36,36,36,36	0
57	MG	1A	3287	1/1	0.91	0.32	62,62,62,62	0
57	MG	2A	3680	1/1	0.91	0.14	66,66,66,66	0
57	MG	2A	3682	1/1	0.91	0.17	60,60,60,60	0
57	MG	1A	3591	1/1	0.91	0.11	39,39,39,39	0
57	MG	1A	3173	1/1	0.91	0.16	54,54,54,54	0
57	MG	1A	3593	1/1	0.91	0.10	30,30,30,30	0
57	MG	2A	3220	1/1	0.91	0.31	62,62,62,62	0
57	MG	2A	3689	1/1	0.91	0.22	73,73,73,73	0
57	MG	1a	1639	1/1	0.91	0.10	56,56,56,56	0
57	MG	2A	3693	1/1	0.91	0.19	64,64,64,64	0
57	MG	1B	202	1/1	0.91	0.16	59,59,59,59	0
57	MG	2A	3224	1/1	0.91	0.24	53,53,53,53	0
57	MG	1A	3256	1/1	0.91	0.15	61,61,61,61	0
57	MG	1A	3441	1/1	0.91	0.11	54,54,54,54	0
57	MG	1A	3257	1/1	0.91	0.12	63,63,63,63	0
57	MG	2A	3425	1/1	0.91	0.11	60,60,60,60	0
57	MG	2A	3230	1/1	0.91	0.21	57,57,57,57	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	3973	1/1	0.91	0.10	21,21,21,21	0
57	MG	1A	3836	1/1	0.91	0.23	41,41,41,41	0
57	MG	2A	3432	1/1	0.91	0.24	57,57,57,57	0
57	MG	1A	3730	1/1	0.91	0.09	28,28,28,28	0
57	MG	2A	3435	1/1	0.91	0.15	51,51,51,51	0
57	MG	1A	3502	1/1	0.91	0.26	38,38,38,38	0
57	MG	1B	215	1/1	0.91	0.13	71,71,71,71	0
57	MG	2A	3447	1/1	0.91	0.09	42,42,42,42	0
57	MG	1A	3599	1/1	0.91	0.13	37,37,37,37	0
57	MG	1A	3113	1/1	0.91	0.17	49,49,49,49	0
57	MG	2A	3454	1/1	0.91	0.12	62,62,62,62	0
57	MG	1a	1657	1/1	0.91	0.33	67,67,67,67	0
57	MG	1A	3737	1/1	0.91	0.07	48,48,48,48	0
57	MG	2A	3248	1/1	0.91	0.09	60,60,60,60	0
57	MG	2A	3732	1/1	0.91	0.09	36,36,36,36	0
57	MG	2A	3458	1/1	0.91	0.19	57,57,57,57	0
57	MG	2A	3005	1/1	0.91	0.38	71,71,71,71	0
57	MG	2A	3737	1/1	0.91	0.23	66,66,66,66	0
57	MG	2A	3007	1/1	0.91	0.14	54,54,54,54	0
57	MG	2A	3010	1/1	0.91	0.10	56,56,56,56	0
57	MG	2A	3011	1/1	0.91	0.14	58,58,58,58	0
57	MG	2A	3463	1/1	0.91	0.17	59,59,59,59	0
57	MG	1A	3505	1/1	0.91	0.20	57,57,57,57	0
57	MG	1A	3993	1/1	0.91	0.08	25,25,25,25	0
57	MG	2A	3756	1/1	0.91	0.09	67,67,67,67	0
57	MG	1A	3211	1/1	0.91	0.10	45,45,45,45	0
57	MG	1a	1663	1/1	0.91	0.24	77,77,77,77	0
57	MG	1B	226	1/1	0.91	0.14	62,62,62,62	0
57	MG	1A	3997	1/1	0.91	0.08	50,50,50,50	0
57	MG	2A	3032	1/1	0.91	0.19	47,47,47,47	0
57	MG	1B	228	1/1	0.91	0.09	54,54,54,54	0
57	MG	2A	3765	1/1	0.91	0.10	66,66,66,66	0
57	MG	2A	3767	1/1	0.91	0.08	51,51,51,51	0
57	MG	2A	3771	1/1	0.91	0.14	57,57,57,57	0
57	MG	2A	3488	1/1	0.91	0.11	49,49,49,49	0
57	MG	2A	3776	1/1	0.91	0.17	63,63,63,63	0
57	MG	2A	3489	1/1	0.91	0.10	39,39,39,39	0
57	MG	2A	3036	1/1	0.91	0.10	56,56,56,56	0
57	MG	1A	3339	1/1	0.91	0.10	54,54,54,54	0
57	MG	2A	3273	1/1	0.91	0.14	59,59,59,59	0
57	MG	1a	1670	1/1	0.91	0.31	49,49,49,49	0
57	MG	1A	3627	1/1	0.91	0.16	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	2A	3785	1/1	0.91	0.20	51,51,51,51	0
57	MG	1a	1675	1/1	0.91	0.17	61,61,61,61	0
57	MG	1A	4005	1/1	0.91	0.11	64,64,64,64	0
57	MG	1a	1677	1/1	0.91	0.23	63,63,63,63	0
57	MG	2A	3052	1/1	0.91	0.17	61,61,61,61	0
57	MG	2A	3508	1/1	0.91	0.12	54,54,54,54	0
57	MG	1B	234	1/1	0.91	0.14	56,56,56,56	0
57	MG	1A	3509	1/1	0.91	0.27	58,58,58,58	0
57	MG	2A	3286	1/1	0.91	0.26	69,69,69,69	0
57	MG	1A	3750	1/1	0.91	0.08	27,27,27,27	0
57	MG	2A	3797	1/1	0.91	0.17	72,72,72,72	0
57	MG	1A	3394	1/1	0.91	0.11	54,54,54,54	0
57	MG	1A	3344	1/1	0.91	0.16	42,42,42,42	0
57	MG	2A	3520	1/1	0.91	0.22	67,67,67,67	0
57	MG	2A	3521	1/1	0.91	0.18	67,67,67,67	0
57	MG	1A	3297	1/1	0.91	0.14	50,50,50,50	0
57	MG	1A	3400	1/1	0.91	0.27	56,56,56,56	0
57	MG	1a	1693	1/1	0.91	0.26	58,58,58,58	0
57	MG	2A	3527	1/1	0.91	0.12	48,48,48,48	0
57	MG	2A	3528	1/1	0.91	0.11	56,56,56,56	0
57	MG	2A	3299	1/1	0.91	0.22	64,64,64,64	0
57	MG	2A	3300	1/1	0.91	0.19	67,67,67,67	0
57	MG	1A	3516	1/1	0.91	0.11	51,51,51,51	0
57	MG	1A	4021	1/1	0.91	0.18	57,57,57,57	0
57	MG	1A	3298	1/1	0.91	0.16	58,58,58,58	0
57	MG	2A	3304	1/1	0.91	0.26	65,65,65,65	0
57	MG	1A	3774	1/1	0.91	0.09	45,45,45,45	0
57	MG	1A	3872	1/1	0.91	0.12	32,32,32,32	0
57	MG	1A	4032	1/1	0.91	0.09	48,48,48,48	0
57	MG	1A	3406	1/1	0.91	0.17	61,61,61,61	0
57	MG	1A	3175	1/1	0.91	0.18	73,73,73,73	0
57	MG	2A	3313	1/1	0.91	0.10	73,73,73,73	0
57	MG	1A	3311	1/1	0.91	0.11	56,56,56,56	0
57	MG	1a	1724	1/1	0.91	0.21	59,59,59,59	0
57	MG	1A	4040	1/1	0.91	0.13	52,52,52,52	0
57	MG	1A	3411	1/1	0.91	0.24	39,39,39,39	0
57	MG	1A	3089	1/1	0.91	0.30	65,65,65,65	0
57	MG	2A	3319	1/1	0.91	0.09	75,75,75,75	0
57	MG	2R	201	1/1	0.91	0.11	64,64,64,64	0
57	MG	1a	1733	1/1	0.91	0.12	57,57,57,57	0
57	MG	2V	201	1/1	0.91	0.12	65,65,65,65	0
57	MG	1A	3679	1/1	0.91	0.10	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	3415	1/1	0.91	0.23	45,45,45,45	0
57	MG	1a	1739	1/1	0.91	0.17	58,58,58,58	0
57	MG	2A	3576	1/1	0.91	0.19	76,76,76,76	0
57	MG	2A	3324	1/1	0.91	0.15	78,78,78,78	0
57	MG	21	102	1/1	0.91	0.52	59,59,59,59	0
57	MG	1A	3541	1/1	0.91	0.21	59,59,59,59	0
57	MG	2A	3326	1/1	0.91	0.12	61,61,61,61	0
57	MG	1A	3685	1/1	0.91	0.13	36,36,36,36	0
57	MG	2A	3107	1/1	0.91	0.36	69,69,69,69	0
57	MG	2a	1602	1/1	0.91	0.33	70,70,70,70	0
57	MG	1A	3892	1/1	0.91	0.21	64,64,64,64	0
57	MG	1A	3469	1/1	0.91	0.20	31,31,31,31	0
57	MG	1A	3280	1/1	0.91	0.10	44,44,44,44	0
57	MG	1A	3798	1/1	0.91	0.11	73,73,73,73	0
57	MG	1A	3472	1/1	0.91	0.22	39,39,39,39	0
57	MG	1A	3118	1/1	0.91	0.14	37,37,37,37	0
57	MG	1A	3907	1/1	0.91	0.12	51,51,51,51	0
57	MG	1A	3802	1/1	0.91	0.18	59,59,59,59	0
57	MG	2A	3135	1/1	0.91	0.26	64,64,64,64	0
57	MG	2A	3136	1/1	0.91	0.20	45,45,45,45	0
57	MG	1Z	302	1/1	0.91	0.21	54,54,54,54	0
57	MG	2A	3601	1/1	0.91	0.14	43,43,43,43	0
57	MG	2A	3603	1/1	0.91	0.11	65,65,65,65	0
57	MG	1A	4066	1/1	0.91	0.20	56,56,56,56	0
57	MG	1A	3809	1/1	0.91	0.11	43,43,43,43	0
57	MG	10	107	1/1	0.91	0.12	59,59,59,59	0
57	MG	1A	3698	1/1	0.91	0.11	64,64,64,64	0
57	MG	1A	3422	1/1	0.91	0.12	56,56,56,56	0
57	MG	2A	3611	1/1	0.91	0.11	66,66,66,66	0
57	MG	1A	3006	1/1	0.91	0.09	38,38,38,38	0
57	MG	2A	3176	1/1	0.92	0.17	67,67,67,67	0
57	MG	1A	3123	1/1	0.92	0.30	41,41,41,41	0
57	MG	2A	3376	1/1	0.92	0.14	60,60,60,60	0
57	MG	1A	3915	1/1	0.92	0.07	43,43,43,43	0
57	MG	1a	1811	1/1	0.92	0.15	53,53,53,53	0
57	MG	1A	3922	1/1	0.92	0.15	55,55,55,55	0
57	MG	1A	3530	1/1	0.92	0.45	50,50,50,50	0
57	MG	1A	4087	1/1	0.92	0.11	58,58,58,58	0
57	MG	1A	3691	1/1	0.92	0.14	58,58,58,58	0
57	MG	2A	3190	1/1	0.92	0.29	57,57,57,57	0
57	MG	1A	3806	1/1	0.92	0.07	25,25,25,25	0
57	MG	1A	3228	1/1	0.92	0.14	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	3695	1/1	0.92	0.12	42,42,42,42	0
57	MG	2A	3391	1/1	0.92	0.18	48,48,48,48	0
57	MG	1A	4098	1/1	0.92	0.09	43,43,43,43	0
57	MG	1A	3091	1/1	0.92	0.21	56,56,56,56	0
57	MG	2A	3394	1/1	0.92	0.18	58,58,58,58	0
57	MG	1A	4100	1/1	0.92	0.10	53,53,53,53	0
57	MG	2A	3396	1/1	0.92	0.11	39,39,39,39	0
57	MG	1a	1630	1/1	0.92	0.15	56,56,56,56	0
57	MG	1A	3384	1/1	0.92	0.14	51,51,51,51	0
57	MG	1A	3940	1/1	0.92	0.13	64,64,64,64	0
57	MG	2A	3663	1/1	0.92	0.17	54,54,54,54	0
57	MG	2A	3207	1/1	0.92	0.11	61,61,61,61	0
57	MG	1A	3385	1/1	0.92	0.28	49,49,49,49	0
57	MG	1A	3321	1/1	0.92	0.12	58,58,58,58	0
57	MG	2A	3213	1/1	0.92	0.09	59,59,59,59	0
57	MG	2A	3671	1/1	0.92	0.12	65,65,65,65	0
57	MG	1A	3458	1/1	0.92	0.32	53,53,53,53	0
57	MG	1A	4106	1/1	0.92	0.16	53,53,53,53	0
57	MG	1A	4107	1/1	0.92	0.11	47,47,47,47	0
57	MG	1A	3388	1/1	0.92	0.13	59,59,59,59	0
57	MG	1A	3559	1/1	0.92	0.20	40,40,40,40	0
57	MG	2A	3418	1/1	0.92	0.24	60,60,60,60	0
57	MG	2A	3681	1/1	0.92	0.14	57,57,57,57	0
57	MG	1A	3390	1/1	0.92	0.17	49,49,49,49	0
57	MG	1A	3172	1/1	0.92	0.13	39,39,39,39	0
57	MG	1a	1647	1/1	0.92	0.17	59,59,59,59	0
57	MG	1A	3955	1/1	0.92	0.14	49,49,49,49	0
57	MG	1A	3961	1/1	0.92	0.12	42,42,42,42	0
57	MG	1A	3963	1/1	0.92	0.09	64,64,64,64	0
57	MG	2A	3690	1/1	0.92	0.14	71,71,71,71	0
57	MG	1A	3965	1/1	0.92	0.09	69,69,69,69	0
57	MG	1A	3465	1/1	0.92	0.16	50,50,50,50	0
57	MG	2A	3694	1/1	0.92	0.13	68,68,68,68	0
57	MG	1a	1653	1/1	0.92	0.15	61,61,61,61	0
57	MG	1A	3070	1/1	0.92	0.18	35,35,35,35	0
57	MG	2A	3437	1/1	0.92	0.12	57,57,57,57	0
57	MG	1A	3130	1/1	0.92	0.14	46,46,46,46	0
57	MG	1x	113	1/1	0.92	0.14	66,66,66,66	0
57	MG	2A	3442	1/1	0.92	0.16	65,65,65,65	0
57	MG	1B	213	1/1	0.92	0.26	61,61,61,61	0
57	MG	2A	3449	1/1	0.92	0.12	43,43,43,43	0
57	MG	2A	3002	1/1	0.92	0.28	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	2A	3246	1/1	0.92	0.09	72,72,72,72	0
57	MG	1A	3004	1/1	0.92	0.10	34,34,34,34	0
57	MG	2A	3006	1/1	0.92	0.25	59,59,59,59	0
57	MG	1A	3036	1/1	0.92	0.07	51,51,51,51	0
57	MG	2A	3008	1/1	0.92	0.08	59,59,59,59	0
57	MG	1A	3575	1/1	0.92	0.14	41,41,41,41	0
57	MG	1A	3286	1/1	0.92	0.35	60,60,60,60	0
57	MG	1A	3403	1/1	0.92	0.16	46,46,46,46	0
57	MG	1A	3081	1/1	0.92	0.08	41,41,41,41	0
57	MG	2A	3259	1/1	0.92	0.20	58,58,58,58	0
57	MG	1A	3289	1/1	0.92	0.11	52,52,52,52	0
57	MG	1a	1665	1/1	0.92	0.22	64,64,64,64	0
57	MG	1A	3984	1/1	0.92	0.08	15,15,15,15	0
57	MG	1A	3985	1/1	0.92	0.30	43,43,43,43	0
57	MG	1A	3587	1/1	0.92	0.12	49,49,49,49	0
57	MG	1A	3189	1/1	0.92	0.09	39,39,39,39	0
57	MG	2A	3478	1/1	0.92	0.15	55,55,55,55	0
57	MG	1a	1671	1/1	0.92	0.26	54,54,54,54	0
57	MG	2A	3482	1/1	0.92	0.11	56,56,56,56	0
57	MG	1A	3047	1/1	0.92	0.06	31,31,31,31	0
57	MG	1A	3731	1/1	0.92	0.08	24,24,24,24	0
57	MG	1A	3410	1/1	0.92	0.14	47,47,47,47	0
57	MG	1A	3340	1/1	0.92	0.10	51,51,51,51	0
57	MG	2A	3046	1/1	0.92	0.31	63,63,63,63	0
57	MG	1B	235	1/1	0.92	0.12	60,60,60,60	0
57	MG	1A	4002	1/1	0.92	0.10	54,54,54,54	0
57	MG	1A	3849	1/1	0.92	0.12	53,53,53,53	0
57	MG	2A	3053	1/1	0.92	0.15	58,58,58,58	0
57	MG	2A	3284	1/1	0.92	0.11	58,58,58,58	0
57	MG	1A	3341	1/1	0.92	0.08	55,55,55,55	0
57	MG	1A	3342	1/1	0.92	0.23	54,54,54,54	0
57	MG	2A	3769	1/1	0.92	0.15	42,42,42,42	0
57	MG	1A	3248	1/1	0.92	0.19	32,32,32,32	0
57	MG	2A	3289	1/1	0.92	0.10	64,64,64,64	0
57	MG	1A	3490	1/1	0.92	0.16	53,53,53,53	0
57	MG	1E	309	1/1	0.92	0.10	29,29,29,29	0
57	MG	1A	3856	1/1	0.92	0.09	38,38,38,38	0
57	MG	2A	3063	1/1	0.92	0.30	67,67,67,67	0
57	MG	1a	1696	1/1	0.92	0.19	58,58,58,58	0
57	MG	1a	1699	1/1	0.92	0.23	59,59,59,59	0
57	MG	1a	1700	1/1	0.92	0.15	62,62,62,62	0
57	MG	1A	3294	1/1	0.92	0.31	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	3074	1/1	0.92	0.12	53,53,53,53	0
57	MG	1A	3146	1/1	0.92	0.26	37,37,37,37	0
57	MG	1N	202	1/1	0.92	0.19	52,52,52,52	0
57	MG	1N	204	1/1	0.92	0.17	40,40,40,40	0
57	MG	2A	3306	1/1	0.92	0.20	55,55,55,55	0
57	MG	1A	3112	1/1	0.92	0.12	42,42,42,42	0
57	MG	2A	3793	1/1	0.92	0.10	64,64,64,64	0
57	MG	2A	3531	1/1	0.92	0.09	42,42,42,42	0
57	MG	1A	3749	1/1	0.92	0.10	47,47,47,47	0
57	MG	1O	201	1/1	0.92	0.25	51,51,51,51	0
57	MG	2A	3536	1/1	0.92	0.14	55,55,55,55	0
57	MG	1O	202	1/1	0.92	0.13	61,61,61,61	0
57	MG	1A	3148	1/1	0.92	0.17	40,40,40,40	0
57	MG	1A	3201	1/1	0.92	0.14	50,50,50,50	0
57	MG	2A	3091	1/1	0.92	0.10	63,63,63,63	0
57	MG	1A	4025	1/1	0.92	0.07	58,58,58,58	0
57	MG	2A	3094	1/1	0.92	0.11	76,76,76,76	0
57	MG	1a	1730	1/1	0.92	0.12	61,61,61,61	0
57	MG	1A	3754	1/1	0.92	0.10	39,39,39,39	0
57	MG	1Q	202	1/1	0.92	0.14	34,34,34,34	0
57	MG	1A	4028	1/1	0.92	0.12	32,32,32,32	0
57	MG	1A	3301	1/1	0.92	0.22	36,36,36,36	0
57	MG	1A	3504	1/1	0.92	0.27	55,55,55,55	0
57	MG	1A	3062	1/1	0.92	0.24	54,54,54,54	0
57	MG	2A	3566	1/1	0.92	0.12	60,60,60,60	0
57	MG	2B	213	1/1	0.92	0.20	60,60,60,60	0
57	MG	1A	3767	1/1	0.92	0.11	54,54,54,54	0
57	MG	2A	3568	1/1	0.92	0.21	50,50,50,50	0
57	MG	1A	3304	1/1	0.92	0.11	51,51,51,51	0
57	MG	1R	205	1/1	0.92	0.11	34,34,34,34	0
57	MG	1a	1747	1/1	0.92	0.12	66,66,66,66	0
57	MG	1A	3360	1/1	0.92	0.13	53,53,53,53	0
57	MG	1A	3772	1/1	0.92	0.07	42,42,42,42	0
57	MG	2E	304	1/1	0.92	0.12	40,40,40,40	0
57	MG	1A	3435	1/1	0.92	0.09	60,60,60,60	0
57	MG	2A	3119	1/1	0.92	0.12	61,61,61,61	0
57	MG	2A	3122	1/1	0.92	0.10	73,73,73,73	0
57	MG	1A	3306	1/1	0.92	0.14	46,46,46,46	0
57	MG	1A	3511	1/1	0.92	0.07	24,24,24,24	0
57	MG	2A	3129	1/1	0.92	0.23	59,59,59,59	0
57	MG	2Q	201	1/1	0.92	0.09	64,64,64,64	0
57	MG	2Q	202	1/1	0.92	0.12	57,57,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3780	1/1	0.92	0.08	22,22,22,22	0
57	MG	1A	3362	1/1	0.92	0.23	71,71,71,71	0
57	MG	2U	202	1/1	0.92	0.20	62,62,62,62	0
57	MG	2A	3586	1/1	0.92	0.13	63,63,63,63	0
57	MG	1A	3365	1/1	0.92	0.18	25,25,25,25	0
57	MG	2A	3344	1/1	0.92	0.26	53,53,53,53	0
57	MG	1a	1777	1/1	0.92	0.13	58,58,58,58	0
57	MG	2A	3140	1/1	0.92	0.28	60,60,60,60	0
57	MG	20	102	1/1	0.92	0.17	72,72,72,72	0
57	MG	1A	3310	1/1	0.92	0.12	42,42,42,42	0
57	MG	1A	4057	1/1	0.92	0.11	47,47,47,47	0
57	MG	1Z	303	1/1	0.92	0.23	59,59,59,59	0
57	MG	1A	3898	1/1	0.92	0.22	37,37,37,37	0
57	MG	1A	3372	1/1	0.92	0.30	68,68,68,68	0
57	MG	1a	1788	1/1	0.92	0.13	68,68,68,68	0
57	MG	28	101	1/1	0.92	0.31	64,64,64,64	0
57	MG	1A	3787	1/1	0.92	0.09	47,47,47,47	0
57	MG	1A	3903	1/1	0.92	0.11	40,40,40,40	0
57	MG	1A	3517	1/1	0.92	0.25	58,58,58,58	0
57	MG	1A	3677	1/1	0.92	0.15	30,30,30,30	0
57	MG	1A	3678	1/1	0.92	0.10	28,28,28,28	0
57	MG	2A	3609	1/1	0.92	0.10	54,54,54,54	0
57	MG	1A	3087	1/1	0.92	0.09	45,45,45,45	0
57	MG	1A	3050	1/1	0.92	0.08	24,24,24,24	0
57	MG	2A	3613	1/1	0.92	0.10	60,60,60,60	0
57	MG	1a	1798	1/1	0.92	0.10	63,63,63,63	0
57	MG	1a	1802	1/1	0.92	0.12	75,75,75,75	0
57	MG	1A	3261	1/1	0.92	0.18	49,49,49,49	0
57	MG	1a	1806	1/1	0.92	0.15	65,65,65,65	0
57	MG	2A	3169	1/1	0.92	0.19	54,54,54,54	0
57	MG	1a	1601	1/1	0.92	0.11	59,59,59,59	0
57	MG	2A	3621	1/1	0.92	0.17	65,65,65,65	0
57	MG	2A	3172	1/1	0.92	0.12	59,59,59,59	0
57	MG	1A	3913	1/1	0.92	0.10	44,44,44,44	0
57	MG	2A	3626	1/1	0.92	0.22	56,56,56,56	0
57	MG	2A	3373	1/1	0.92	0.12	71,71,71,71	0
57	MG	2A	3631	1/1	0.92	0.12	49,49,49,49	0
57	MG	1a	1776	1/1	0.93	0.09	50,50,50,50	0
57	MG	2A	3358	1/1	0.93	0.25	48,48,48,48	0
57	MG	1A	3778	1/1	0.93	0.17	50,50,50,50	0
57	MG	1A	3316	1/1	0.93	0.18	50,50,50,50	0
57	MG	1a	1781	1/1	0.93	0.12	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	1Y	201	1/1	0.93	0.25	69,69,69,69	0
57	MG	1a	1783	1/1	0.93	0.30	70,70,70,70	0
57	MG	2A	3149	1/1	0.93	0.14	61,61,61,61	0
57	MG	1Y	202	1/1	0.93	0.32	53,53,53,53	0
57	MG	1A	3518	1/1	0.93	0.12	60,60,60,60	0
57	MG	1A	3459	1/1	0.93	0.09	60,60,60,60	0
57	MG	1A	3658	1/1	0.93	0.13	51,51,51,51	0
57	MG	1A	3131	1/1	0.93	0.16	45,45,45,45	0
57	MG	2A	3638	1/1	0.93	0.10	49,49,49,49	0
57	MG	1A	3048	1/1	0.93	0.07	43,43,43,43	0
57	MG	1A	3259	1/1	0.93	0.23	54,54,54,54	0
57	MG	1A	3526	1/1	0.93	0.15	41,41,41,41	0
57	MG	1A	3790	1/1	0.93	0.09	25,25,25,25	0
57	MG	2A	3164	1/1	0.93	0.13	50,50,50,50	0
57	MG	1A	3912	1/1	0.93	0.10	50,50,50,50	0
57	MG	1A	3676	1/1	0.93	0.17	35,35,35,35	0
57	MG	1A	3322	1/1	0.93	0.22	60,60,60,60	0
57	MG	16	102	1/1	0.93	0.20	51,51,51,51	0
57	MG	1A	3324	1/1	0.93	0.18	45,45,45,45	0
57	MG	2A	3170	1/1	0.93	0.15	44,44,44,44	0
57	MG	1a	1805	1/1	0.93	0.15	59,59,59,59	0
57	MG	1A	3918	1/1	0.93	0.10	78,78,78,78	0
57	MG	2A	3173	1/1	0.93	0.14	61,61,61,61	0
57	MG	1A	3920	1/1	0.93	0.07	39,39,39,39	0
57	MG	1A	3409	1/1	0.93	0.10	41,41,41,41	0
57	MG	1a	1606	1/1	0.93	0.08	67,67,67,67	0
57	MG	2A	3178	1/1	0.93	0.16	59,59,59,59	0
57	MG	1A	4088	1/1	0.93	0.17	45,45,45,45	0
57	MG	2A	3666	1/1	0.93	0.19	75,75,75,75	0
57	MG	1A	3161	1/1	0.93	0.18	43,43,43,43	0
57	MG	1a	1812	1/1	0.93	0.17	73,73,73,73	0
57	MG	2A	3185	1/1	0.93	0.11	55,55,55,55	0
57	MG	2A	3186	1/1	0.93	0.07	57,57,57,57	0
57	MG	1A	3096	1/1	0.93	0.10	55,55,55,55	0
57	MG	1A	3265	1/1	0.93	0.10	51,51,51,51	0
57	MG	1A	3804	1/1	0.93	0.08	55,55,55,55	0
57	MG	1a	1619	1/1	0.93	0.07	56,56,56,56	0
57	MG	1a	1620	1/1	0.93	0.08	61,61,61,61	0
57	MG	2A	3407	1/1	0.93	0.09	54,54,54,54	0
57	MG	1a	1819	1/1	0.93	0.09	76,76,76,76	0
57	MG	2A	3194	1/1	0.93	0.12	65,65,65,65	0
57	MG	1A	3930	1/1	0.93	0.11	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3197	1/1	0.93	0.09	56,56,56,56	0
57	MG	1A	3934	1/1	0.93	0.07	72,72,72,72	0
57	MG	2A	3416	1/1	0.93	0.09	53,53,53,53	0
57	MG	1A	3936	1/1	0.93	0.11	66,66,66,66	0
57	MG	1A	3546	1/1	0.93	0.17	41,41,41,41	0
57	MG	1f	202	1/1	0.93	0.07	70,70,70,70	0
57	MG	2A	3692	1/1	0.93	0.12	55,55,55,55	0
57	MG	2A	3203	1/1	0.93	0.09	52,52,52,52	0
57	MG	1a	1626	1/1	0.93	0.22	51,51,51,51	0
57	MG	1A	3808	1/1	0.93	0.08	29,29,29,29	0
57	MG	1A	3369	1/1	0.93	0.50	44,44,44,44	0
57	MG	1A	3552	1/1	0.93	0.08	49,49,49,49	0
57	MG	1A	3371	1/1	0.93	0.08	54,54,54,54	0
57	MG	1A	3556	1/1	0.93	0.15	49,49,49,49	0
57	MG	1A	3103	1/1	0.93	0.12	42,42,42,42	0
57	MG	2A	3217	1/1	0.93	0.10	58,58,58,58	0
57	MG	1A	3124	1/1	0.93	0.32	37,37,37,37	0
57	MG	1A	4110	1/1	0.93	0.10	36,36,36,36	0
57	MG	1A	3299	1/1	0.93	0.24	70,70,70,70	0
57	MG	2A	3712	1/1	0.93	0.12	66,66,66,66	0
57	MG	2A	3713	1/1	0.93	0.11	53,53,53,53	0
57	MG	2A	3445	1/1	0.93	0.10	47,47,47,47	0
57	MG	1A	3375	1/1	0.93	0.08	38,38,38,38	0
57	MG	1A	3376	1/1	0.93	0.17	37,37,37,37	0
57	MG	2A	3718	1/1	0.93	0.14	57,57,57,57	0
57	MG	2A	3719	1/1	0.93	0.08	65,65,65,65	0
57	MG	1a	1641	1/1	0.93	0.26	53,53,53,53	0
57	MG	2A	3452	1/1	0.93	0.09	40,40,40,40	0
57	MG	1A	3482	1/1	0.93	0.23	49,49,49,49	0
57	MG	1A	3960	1/1	0.93	0.19	76,76,76,76	0
57	MG	1A	3426	1/1	0.93	0.08	50,50,50,50	0
57	MG	1A	3962	1/1	0.93	0.14	74,74,74,74	0
57	MG	2A	3729	1/1	0.93	0.14	62,62,62,62	0
57	MG	1x	104	1/1	0.93	0.20	67,67,67,67	0
57	MG	2A	3233	1/1	0.93	0.14	64,64,64,64	0
57	MG	1A	3569	1/1	0.93	0.29	48,48,48,48	0
57	MG	2A	3236	1/1	0.93	0.16	61,61,61,61	0
57	MG	1B	210	1/1	0.93	0.10	48,48,48,48	0
57	MG	1A	3105	1/1	0.93	0.34	44,44,44,44	0
57	MG	1A	3486	1/1	0.93	0.22	37,37,37,37	0
57	MG	2A	3743	1/1	0.93	0.09	64,64,64,64	0
57	MG	1x	110	1/1	0.93	0.18	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	3242	1/1	0.93	0.26	56,56,56,56	0
57	MG	2A	3748	1/1	0.93	0.09	69,69,69,69	0
57	MG	1A	3487	1/1	0.93	0.20	42,42,42,42	0
57	MG	1x	112	1/1	0.93	0.25	67,67,67,67	0
57	MG	2A	3752	1/1	0.93	0.07	56,56,56,56	0
57	MG	1A	3336	1/1	0.93	0.09	49,49,49,49	0
57	MG	1A	3379	1/1	0.93	0.11	55,55,55,55	0
57	MG	1A	3491	1/1	0.93	0.20	36,36,36,36	0
57	MG	2A	3481	1/1	0.93	0.14	57,57,57,57	0
57	MG	1A	3584	1/1	0.93	0.06	41,41,41,41	0
57	MG	1A	3722	1/1	0.93	0.09	49,49,49,49	0
57	MG	1A	3977	1/1	0.93	0.14	49,49,49,49	0
57	MG	2A	3254	1/1	0.93	0.14	66,66,66,66	0
57	MG	1A	3835	1/1	0.93	0.18	68,68,68,68	0
57	MG	1A	3492	1/1	0.93	0.11	56,56,56,56	0
57	MG	1B	225	1/1	0.93	0.16	57,57,57,57	0
57	MG	1A	3980	1/1	0.93	0.16	43,43,43,43	0
57	MG	2A	3017	1/1	0.93	0.26	54,54,54,54	0
57	MG	1A	3090	1/1	0.93	0.11	65,65,65,65	0
57	MG	2A	3498	1/1	0.93	0.14	52,52,52,52	0
57	MG	2A	3019	1/1	0.93	0.07	44,44,44,44	0
57	MG	1A	3303	1/1	0.93	0.24	40,40,40,40	0
57	MG	1B	229	1/1	0.93	0.11	43,43,43,43	0
57	MG	2A	3026	1/1	0.93	0.22	56,56,56,56	0
57	MG	1A	3383	1/1	0.93	0.16	56,56,56,56	0
57	MG	1A	3497	1/1	0.93	0.11	61,61,61,61	0
57	MG	1A	3129	1/1	0.93	0.09	37,37,37,37	0
57	MG	1A	3846	1/1	0.93	0.07	53,53,53,53	0
57	MG	1a	1672	1/1	0.93	0.25	49,49,49,49	0
57	MG	1a	1673	1/1	0.93	0.32	60,60,60,60	0
57	MG	1A	3305	1/1	0.93	0.22	60,60,60,60	0
57	MG	2A	3519	1/1	0.93	0.10	43,43,43,43	0
57	MG	1A	3732	1/1	0.93	0.17	56,56,56,56	0
57	MG	1A	3015	1/1	0.93	0.30	51,51,51,51	0
57	MG	2A	3045	1/1	0.93	0.18	48,48,48,48	0
57	MG	1D	303	1/1	0.93	0.13	40,40,40,40	0
57	MG	1a	1678	1/1	0.93	0.14	56,56,56,56	0
57	MG	1A	3309	1/1	0.93	0.15	48,48,48,48	0
57	MG	2A	3051	1/1	0.93	0.05	51,51,51,51	0
57	MG	1A	3220	1/1	0.93	0.18	54,54,54,54	0
57	MG	1A	3348	1/1	0.93	0.12	51,51,51,51	0
57	MG	1A	3612	1/1	0.93	0.15	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3618	1/1	0.93	0.08	21,21,21,21	0
57	MG	2A	3535	1/1	0.93	0.20	46,46,46,46	0
57	MG	2A	3056	1/1	0.93	0.15	66,66,66,66	0
57	MG	2B	206	1/1	0.93	0.10	71,71,71,71	0
57	MG	1E	310	1/1	0.93	0.12	33,33,33,33	0
57	MG	1A	3180	1/1	0.93	0.17	33,33,33,33	0
57	MG	2A	3060	1/1	0.93	0.16	51,51,51,51	0
57	MG	1F	302	1/1	0.93	0.17	35,35,35,35	0
57	MG	1F	304	1/1	0.93	0.13	42,42,42,42	0
57	MG	1F	308	1/1	0.93	0.09	59,59,59,59	0
57	MG	1A	3620	1/1	0.93	0.10	22,22,22,22	0
57	MG	2A	3550	1/1	0.93	0.12	61,61,61,61	0
57	MG	1A	3861	1/1	0.93	0.23	39,39,39,39	0
57	MG	2A	3554	1/1	0.93	0.17	54,54,54,54	0
57	MG	2D	302	1/1	0.93	0.33	72,72,72,72	0
57	MG	2A	3069	1/1	0.93	0.08	57,57,57,57	0
57	MG	1G	202	1/1	0.93	0.15	64,64,64,64	0
57	MG	1H	201	1/1	0.93	0.17	54,54,54,54	0
57	MG	1A	4013	1/1	0.93	0.06	45,45,45,45	0
57	MG	1A	3746	1/1	0.93	0.15	52,52,52,52	0
57	MG	1A	4015	1/1	0.93	0.10	51,51,51,51	0
57	MG	1A	3508	1/1	0.93	0.19	44,44,44,44	0
57	MG	1a	1717	1/1	0.93	0.09	61,61,61,61	0
57	MG	2F	301	1/1	0.93	0.15	60,60,60,60	0
57	MG	2A	3083	1/1	0.93	0.14	63,63,63,63	0
57	MG	2F	303	1/1	0.93	0.10	45,45,45,45	0
57	MG	2A	3570	1/1	0.93	0.10	59,59,59,59	0
57	MG	1A	3224	1/1	0.93	0.25	48,48,48,48	0
57	MG	1A	3395	1/1	0.93	0.12	63,63,63,63	0
57	MG	1A	3628	1/1	0.93	0.11	23,23,23,23	0
57	MG	1A	3753	1/1	0.93	0.13	32,32,32,32	0
57	MG	2T	201	1/1	0.93	0.10	62,62,62,62	0
57	MG	2T	202	1/1	0.93	0.13	52,52,52,52	0
57	MG	2T	203	1/1	0.93	0.11	72,72,72,72	0
57	MG	1A	3873	1/1	0.93	0.12	31,31,31,31	0
57	MG	1A	3630	1/1	0.93	0.10	66,66,66,66	0
57	MG	1Q	201	1/1	0.93	0.21	41,41,41,41	0
57	MG	1a	1732	1/1	0.93	0.08	54,54,54,54	0
57	MG	1A	4031	1/1	0.93	0.08	49,49,49,49	0
57	MG	2X	101	1/1	0.93	0.18	61,61,61,61	0
57	MG	1A	3182	1/1	0.93	0.09	47,47,47,47	0
57	MG	1A	3633	1/1	0.93	0.08	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	2A	3584	1/1	0.93	0.08	37,37,37,37	0
57	MG	1a	1738	1/1	0.93	0.09	63,63,63,63	0
57	MG	2A	3101	1/1	0.93	0.17	48,48,48,48	0
57	MG	21	103	1/1	0.93	0.13	54,54,54,54	0
57	MG	1A	3879	1/1	0.93	0.08	26,26,26,26	0
57	MG	1A	3880	1/1	0.93	0.07	25,25,25,25	0
57	MG	1A	3397	1/1	0.93	0.22	48,48,48,48	0
57	MG	2A	3333	1/1	0.93	0.14	45,45,45,45	0
57	MG	1A	3637	1/1	0.93	0.07	59,59,59,59	0
57	MG	2A	3593	1/1	0.93	0.12	78,78,78,78	0
57	MG	2A	3594	1/1	0.93	0.23	49,49,49,49	0
57	MG	1a	1744	1/1	0.93	0.08	64,64,64,64	0
57	MG	1A	3768	1/1	0.93	0.14	57,57,57,57	0
57	MG	1A	3455	1/1	0.93	0.12	41,41,41,41	0
57	MG	1A	3398	1/1	0.93	0.11	55,55,55,55	0
57	MG	1a	1750	1/1	0.93	0.15	78,78,78,78	0
57	MG	2A	3115	1/1	0.93	0.24	67,67,67,67	0
57	MG	1a	1751	1/1	0.93	0.09	71,71,71,71	0
57	MG	2A	3346	1/1	0.93	0.31	63,63,63,63	0
57	MG	2A	3606	1/1	0.93	0.16	64,64,64,64	0
57	MG	2A	3118	1/1	0.93	0.29	68,68,68,68	0
57	MG	1S	202	1/1	0.93	0.15	52,52,52,52	0
57	MG	1A	3643	1/1	0.93	0.12	46,46,46,46	0
57	MG	2A	3124	1/1	0.93	0.13	52,52,52,52	0
57	MG	1A	3645	1/1	0.93	0.14	40,40,40,40	0
57	MG	1A	3649	1/1	0.93	0.07	27,27,27,27	0
57	MG	1A	3255	1/1	0.93	0.14	57,57,57,57	0
57	MG	1a	1769	1/1	0.93	0.09	81,81,81,81	0
57	MG	1W	201	1/1	0.93	0.19	51,51,51,51	0
57	MG	1A	3896	1/1	0.93	0.09	42,42,42,42	0
57	MG	1A	3215	1/1	0.94	0.14	56,56,56,56	0
57	MG	2A	3630	1/1	0.94	0.09	34,34,34,34	0
57	MG	1A	3820	1/1	0.94	0.31	45,45,45,45	0
57	MG	1A	3821	1/1	0.94	0.06	38,38,38,38	0
57	MG	2A	3162	1/1	0.94	0.11	65,65,65,65	0
57	MG	1A	3106	1/1	0.94	0.28	33,33,33,33	0
57	MG	1A	3950	1/1	0.94	0.05	33,33,33,33	0
57	MG	1A	3023	1/1	0.94	0.10	39,39,39,39	0
57	MG	1A	3017	1/1	0.94	0.09	33,33,33,33	0
57	MG	1A	4112	1/1	0.94	0.14	55,55,55,55	0
57	MG	1A	3954	1/1	0.94	0.13	51,51,51,51	0
57	MG	2A	3641	1/1	0.94	0.17	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	3715	1/1	0.94	0.10	49,49,49,49	0
57	MG	1A	3223	1/1	0.94	0.13	50,50,50,50	0
57	MG	1A	3307	1/1	0.94	0.20	63,63,63,63	0
57	MG	1A	3354	1/1	0.94	0.24	37,37,37,37	0
57	MG	1A	3600	1/1	0.94	0.10	46,46,46,46	0
57	MG	1B	205	1/1	0.94	0.29	62,62,62,62	0
57	MG	1B	207	1/1	0.94	0.15	51,51,51,51	0
57	MG	2A	3654	1/1	0.94	0.10	62,62,62,62	0
57	MG	1A	3601	1/1	0.94	0.10	45,45,45,45	0
57	MG	2A	3179	1/1	0.94	0.08	67,67,67,67	0
57	MG	1A	3308	1/1	0.94	0.20	47,47,47,47	0
57	MG	1A	3607	1/1	0.94	0.20	60,60,60,60	0
57	MG	2A	3183	1/1	0.94	0.26	54,54,54,54	0
57	MG	1A	3834	1/1	0.94	0.11	51,51,51,51	0
57	MG	1A	3608	1/1	0.94	0.10	31,31,31,31	0
57	MG	1a	1640	1/1	0.94	0.13	54,54,54,54	0
57	MG	1A	3462	1/1	0.94	0.18	50,50,50,50	0
57	MG	2A	3399	1/1	0.94	0.10	56,56,56,56	0
57	MG	1A	3114	1/1	0.94	0.28	51,51,51,51	0
57	MG	1A	3464	1/1	0.94	0.12	56,56,56,56	0
57	MG	1A	3225	1/1	0.94	0.14	52,52,52,52	0
57	MG	2A	3191	1/1	0.94	0.30	66,66,66,66	0
57	MG	1A	3266	1/1	0.94	0.16	42,42,42,42	0
57	MG	1A	3844	1/1	0.94	0.14	63,63,63,63	0
57	MG	1B	221	1/1	0.94	0.10	46,46,46,46	0
57	MG	1w	105	1/1	0.94	0.14	63,63,63,63	0
57	MG	2A	3675	1/1	0.94	0.10	58,58,58,58	0
57	MG	1A	3622	1/1	0.94	0.09	34,34,34,34	0
57	MG	2A	3677	1/1	0.94	0.18	66,66,66,66	0
57	MG	1A	3624	1/1	0.94	0.10	61,61,61,61	0
57	MG	1A	3268	1/1	0.94	0.09	40,40,40,40	0
57	MG	1A	3626	1/1	0.94	0.12	40,40,40,40	0
57	MG	2A	3417	1/1	0.94	0.09	57,57,57,57	0
57	MG	1A	3739	1/1	0.94	0.11	41,41,41,41	0
57	MG	2A	3684	1/1	0.94	0.08	46,46,46,46	0
57	MG	2A	3685	1/1	0.94	0.16	45,45,45,45	0
57	MG	1A	3468	1/1	0.94	0.23	48,48,48,48	0
57	MG	1x	103	1/1	0.94	0.11	55,55,55,55	0
57	MG	1A	3991	1/1	0.94	0.14	50,50,50,50	0
57	MG	1A	3742	1/1	0.94	0.10	52,52,52,52	0
57	MG	2A	3208	1/1	0.94	0.13	66,66,66,66	0
57	MG	2A	3210	1/1	0.94	0.08	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	3994	1/1	0.94	0.05	32,32,32,32	0
57	MG	2A	3430	1/1	0.94	0.19	71,71,71,71	0
57	MG	1A	3177	1/1	0.94	0.07	49,49,49,49	0
57	MG	2A	3695	1/1	0.94	0.11	49,49,49,49	0
57	MG	1B	232	1/1	0.94	0.09	72,72,72,72	0
57	MG	2A	3697	1/1	0.94	0.18	74,74,74,74	0
57	MG	2A	3698	1/1	0.94	0.07	60,60,60,60	0
57	MG	1A	3528	1/1	0.94	0.13	40,40,40,40	0
57	MG	1A	3529	1/1	0.94	0.18	38,38,38,38	0
57	MG	1A	3470	1/1	0.94	0.20	30,30,30,30	0
57	MG	2A	3702	1/1	0.94	0.10	46,46,46,46	0
57	MG	2A	3703	1/1	0.94	0.10	58,58,58,58	0
57	MG	1A	3531	1/1	0.94	0.13	46,46,46,46	0
57	MG	1x	114	1/1	0.94	0.14	54,54,54,54	0
57	MG	2A	3444	1/1	0.94	0.12	64,64,64,64	0
57	MG	1A	3860	1/1	0.94	0.14	37,37,37,37	0
57	MG	1D	302	1/1	0.94	0.13	49,49,49,49	0
57	MG	2A	3004	1/1	0.94	0.29	67,67,67,67	0
57	MG	2A	3450	1/1	0.94	0.13	62,62,62,62	0
57	MG	1a	1668	1/1	0.94	0.07	70,70,70,70	0
57	MG	1A	3232	1/1	0.94	0.24	37,37,37,37	0
57	MG	2A	3227	1/1	0.94	0.09	60,60,60,60	0
57	MG	1D	307	1/1	0.94	0.29	45,45,45,45	0
57	MG	1A	3534	1/1	0.94	0.22	60,60,60,60	0
57	MG	1A	3751	1/1	0.94	0.09	37,37,37,37	0
57	MG	1A	4009	1/1	0.94	0.10	61,61,61,61	0
57	MG	2A	3012	1/1	0.94	0.09	55,55,55,55	0
57	MG	2A	3014	1/1	0.94	0.07	46,46,46,46	0
57	MG	1A	3233	1/1	0.94	0.27	42,42,42,42	0
57	MG	1A	4011	1/1	0.94	0.08	59,59,59,59	0
57	MG	1A	3868	1/1	0.94	0.06	30,30,30,30	0
57	MG	1A	3279	1/1	0.94	0.10	49,49,49,49	0
57	MG	2A	3464	1/1	0.94	0.10	39,39,39,39	0
57	MG	1E	312	1/1	0.94	0.23	48,48,48,48	0
57	MG	2A	3022	1/1	0.94	0.24	47,47,47,47	0
57	MG	1a	1679	1/1	0.94	0.10	58,58,58,58	0
57	MG	2A	3735	1/1	0.94	0.07	38,38,38,38	0
57	MG	2A	3024	1/1	0.94	0.10	60,60,60,60	0
57	MG	2A	3475	1/1	0.94	0.13	48,48,48,48	0
57	MG	2A	3025	1/1	0.94	0.13	54,54,54,54	0
57	MG	1E	314	1/1	0.94	0.05	36,36,36,36	0
57	MG	1A	3054	1/1	0.94	0.26	49,49,49,49	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	3251	1/1	0.94	0.22	54,54,54,54	0
57	MG	2A	3029	1/1	0.94	0.09	68,68,68,68	0
57	MG	2A	3483	1/1	0.94	0.10	38,38,38,38	0
57	MG	1A	3648	1/1	0.94	0.07	23,23,23,23	0
57	MG	1F	305	1/1	0.94	0.13	43,43,43,43	0
57	MG	2A	3255	1/1	0.94	0.27	62,62,62,62	0
57	MG	1A	3760	1/1	0.94	0.07	26,26,26,26	0
57	MG	1a	1687	1/1	0.94	0.17	55,55,55,55	0
57	MG	1a	1690	1/1	0.94	0.27	58,58,58,58	0
57	MG	1A	3421	1/1	0.94	0.24	40,40,40,40	0
57	MG	1A	3764	1/1	0.94	0.08	33,33,33,33	0
57	MG	1F	312	1/1	0.94	0.19	56,56,56,56	0
57	MG	1A	3543	1/1	0.94	0.17	38,38,38,38	0
57	MG	1G	203	1/1	0.94	0.10	65,65,65,65	0
57	MG	2A	3766	1/1	0.94	0.06	49,49,49,49	0
57	MG	1a	1697	1/1	0.94	0.14	59,59,59,59	0
57	MG	2A	3501	1/1	0.94	0.11	38,38,38,38	0
57	MG	2A	3770	1/1	0.94	0.17	62,62,62,62	0
57	MG	1a	1698	1/1	0.94	0.08	46,46,46,46	0
57	MG	1A	3236	1/1	0.94	0.14	48,48,48,48	0
57	MG	2A	3774	1/1	0.94	0.11	58,58,58,58	0
57	MG	2A	3775	1/1	0.94	0.09	65,65,65,65	0
57	MG	1A	3075	1/1	0.94	0.25	44,44,44,44	0
57	MG	2A	3509	1/1	0.94	0.20	65,65,65,65	0
57	MG	1a	1701	1/1	0.94	0.20	58,58,58,58	0
57	MG	1A	3654	1/1	0.94	0.06	30,30,30,30	0
57	MG	1A	3551	1/1	0.94	0.29	42,42,42,42	0
57	MG	2A	3276	1/1	0.94	0.08	52,52,52,52	0
57	MG	2A	3516	1/1	0.94	0.30	62,62,62,62	0
57	MG	2A	3277	1/1	0.94	0.26	69,69,69,69	0
57	MG	1A	3657	1/1	0.94	0.08	30,30,30,30	0
57	MG	2A	3787	1/1	0.94	0.16	60,60,60,60	0
57	MG	1A	4033	1/1	0.94	0.07	50,50,50,50	0
57	MG	1A	3076	1/1	0.94	0.20	53,53,53,53	0
57	MG	1a	1712	1/1	0.94	0.16	55,55,55,55	0
57	MG	1A	3056	1/1	0.94	0.07	50,50,50,50	0
57	MG	1a	1716	1/1	0.94	0.06	37,37,37,37	0
57	MG	1A	3667	1/1	0.94	0.10	51,51,51,51	0
57	MG	1A	3192	1/1	0.94	0.22	39,39,39,39	0
57	MG	1A	3242	1/1	0.94	0.19	59,59,59,59	0
57	MG	2A	3288	1/1	0.94	0.13	78,78,78,78	0
57	MG	2A	3068	1/1	0.94	0.16	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	3293	1/1	0.94	0.12	63,63,63,63	0
57	MG	2A	3801	1/1	0.94	0.10	56,56,56,56	0
57	MG	2A	3802	1/1	0.94	0.08	59,59,59,59	0
57	MG	1a	1723	1/1	0.94	0.08	53,53,53,53	0
57	MG	1A	3043	1/1	0.94	0.27	31,31,31,31	0
57	MG	2A	3805	1/1	0.94	0.14	58,58,58,58	0
57	MG	1A	4043	1/1	0.94	0.05	25,25,25,25	0
57	MG	1A	3561	1/1	0.94	0.16	35,35,35,35	0
57	MG	1a	1729	1/1	0.94	0.07	50,50,50,50	0
57	MG	2A	3077	1/1	0.94	0.19	52,52,52,52	0
57	MG	2A	3078	1/1	0.94	0.21	57,57,57,57	0
57	MG	1A	3897	1/1	0.94	0.21	40,40,40,40	0
57	MG	2A	3545	1/1	0.94	0.07	42,42,42,42	0
57	MG	1A	4047	1/1	0.94	0.07	43,43,43,43	0
57	MG	1A	3784	1/1	0.94	0.09	42,42,42,42	0
57	MG	2A	3548	1/1	0.94	0.20	68,68,68,68	0
57	MG	1A	3290	1/1	0.94	0.20	48,48,48,48	0
57	MG	1R	201	1/1	0.94	0.16	45,45,45,45	0
57	MG	1a	1735	1/1	0.94	0.12	68,68,68,68	0
57	MG	2A	3557	1/1	0.94	0.11	46,46,46,46	0
57	MG	1A	3084	1/1	0.94	0.21	44,44,44,44	0
57	MG	2A	3559	1/1	0.94	0.11	72,72,72,72	0
57	MG	2D	301	1/1	0.94	0.12	57,57,57,57	0
57	MG	1A	3030	1/1	0.94	0.10	33,33,33,33	0
57	MG	1A	3016	1/1	0.94	0.14	51,51,51,51	0
57	MG	1A	3906	1/1	0.94	0.11	65,65,65,65	0
57	MG	1A	3682	1/1	0.94	0.13	51,51,51,51	0
57	MG	1A	3200	1/1	0.94	0.09	42,42,42,42	0
57	MG	1A	3568	1/1	0.94	0.13	64,64,64,64	0
57	MG	1U	204	1/1	0.94	0.33	46,46,46,46	0
57	MG	1A	3686	1/1	0.94	0.05	24,24,24,24	0
57	MG	1A	3065	1/1	0.94	0.12	57,57,57,57	0
57	MG	1A	3570	1/1	0.94	0.17	50,50,50,50	0
57	MG	1A	3799	1/1	0.94	0.08	56,56,56,56	0
57	MG	1W	205	1/1	0.94	0.17	42,42,42,42	0
57	MG	1A	3692	1/1	0.94	0.07	33,33,33,33	0
57	MG	1X	104	1/1	0.94	0.20	45,45,45,45	0
57	MG	2P	201	1/1	0.94	0.11	57,57,57,57	0
57	MG	1A	3386	1/1	0.94	0.10	55,55,55,55	0
57	MG	1a	1757	1/1	0.94	0.09	53,53,53,53	0
57	MG	2A	3579	1/1	0.94	0.19	68,68,68,68	0
57	MG	1A	3442	1/1	0.94	0.24	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	3803	1/1	0.94	0.20	26,26,26,26	0
57	MG	1Z	301	1/1	0.94	0.09	61,61,61,61	0
57	MG	2A	3114	1/1	0.94	0.21	61,61,61,61	0
57	MG	1A	3250	1/1	0.94	0.08	44,44,44,44	0
57	MG	2U	203	1/1	0.94	0.15	68,68,68,68	0
57	MG	1a	1773	1/1	0.94	0.07	71,71,71,71	0
57	MG	1a	1775	1/1	0.94	0.07	70,70,70,70	0
57	MG	1A	3805	1/1	0.94	0.08	48,48,48,48	0
57	MG	2A	3120	1/1	0.94	0.10	54,54,54,54	0
57	MG	1A	4077	1/1	0.94	0.14	57,57,57,57	0
57	MG	1A	3204	1/1	0.94	0.18	52,52,52,52	0
57	MG	2A	3337	1/1	0.94	0.26	45,45,45,45	0
57	MG	1A	4082	1/1	0.94	0.14	49,49,49,49	0
57	MG	1A	3252	1/1	0.94	0.12	66,66,66,66	0
57	MG	2A	3127	1/1	0.94	0.27	68,68,68,68	0
57	MG	11	104	1/1	0.94	0.08	48,48,48,48	0
57	MG	2A	3130	1/1	0.94	0.09	49,49,49,49	0
57	MG	2A	3131	1/1	0.94	0.13	44,44,44,44	0
57	MG	2A	3600	1/1	0.94	0.08	71,71,71,71	0
57	MG	2A	3134	1/1	0.94	0.16	59,59,59,59	0
57	MG	1A	3165	1/1	0.94	0.08	48,48,48,48	0
57	MG	1A	3700	1/1	0.94	0.07	48,48,48,48	0
57	MG	12	101	1/1	0.94	0.17	51,51,51,51	0
57	MG	13	103	1/1	0.94	0.07	51,51,51,51	0
57	MG	1A	3812	1/1	0.94	0.07	42,42,42,42	0
57	MG	1A	3343	1/1	0.94	0.11	50,50,50,50	0
57	MG	1A	4094	1/1	0.94	0.10	63,63,63,63	0
57	MG	1A	3133	1/1	0.94	0.25	35,35,35,35	0
57	MG	1A	3347	1/1	0.94	0.12	48,48,48,48	0
57	MG	2A	3612	1/1	0.94	0.08	30,30,30,30	0
57	MG	2A	3145	1/1	0.94	0.10	40,40,40,40	0
57	MG	2A	3146	1/1	0.94	0.22	58,58,58,58	0
57	MG	2A	3147	1/1	0.94	0.14	69,69,69,69	0
57	MG	1A	4097	1/1	0.94	0.07	55,55,55,55	0
57	MG	1A	3706	1/1	0.94	0.22	48,48,48,48	0
57	MG	1a	1796	1/1	0.94	0.10	66,66,66,66	0
57	MG	1A	3707	1/1	0.94	0.09	55,55,55,55	0
57	MG	1A	3943	1/1	0.94	0.09	50,50,50,50	0
57	MG	1A	3944	1/1	0.94	0.07	44,44,44,44	0
57	MG	2A	3367	1/1	0.94	0.39	65,65,65,65	0
57	MG	1A	3451	1/1	0.94	0.13	48,48,48,48	0
57	MG	2A	3103	1/1	0.95	0.17	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3933	1/1	0.95	0.08	45,45,45,45	0
57	MG	1A	3756	1/1	0.95	0.07	32,32,32,32	0
57	MG	2A	3282	1/1	0.95	0.09	54,54,54,54	0
57	MG	1A	3935	1/1	0.95	0.07	61,61,61,61	0
57	MG	2A	3678	1/1	0.95	0.06	61,61,61,61	0
57	MG	2A	3470	1/1	0.95	0.15	39,39,39,39	0
57	MG	1a	1803	1/1	0.95	0.13	62,62,62,62	0
57	MG	1A	3432	1/1	0.95	0.10	39,39,39,39	0
57	MG	1a	1642	1/1	0.95	0.12	58,58,58,58	0
57	MG	1A	4046	1/1	0.95	0.08	44,44,44,44	0
57	MG	1A	3758	1/1	0.95	0.06	56,56,56,56	0
57	MG	1A	3589	1/1	0.95	0.07	42,42,42,42	0
57	MG	2A	3290	1/1	0.95	0.21	65,65,65,65	0
57	MG	1A	3219	1/1	0.95	0.19	37,37,37,37	0
57	MG	2A	3116	1/1	0.95	0.08	56,56,56,56	0
57	MG	1F	301	1/1	0.95	0.16	30,30,30,30	0
57	MG	1A	3137	1/1	0.95	0.12	38,38,38,38	0
57	MG	1A	3942	1/1	0.95	0.08	56,56,56,56	0
57	MG	1A	4054	1/1	0.95	0.08	46,46,46,46	0
57	MG	1A	3681	1/1	0.95	0.10	29,29,29,29	0
57	MG	1a	1815	1/1	0.95	0.09	74,74,74,74	0
57	MG	1F	309	1/1	0.95	0.08	51,51,51,51	0
57	MG	1A	3008	1/1	0.95	0.05	23,23,23,23	0
57	MG	2A	3497	1/1	0.95	0.07	49,49,49,49	0
57	MG	1A	3848	1/1	0.95	0.05	42,42,42,42	0
57	MG	2A	3128	1/1	0.95	0.24	47,47,47,47	0
57	MG	1A	3683	1/1	0.95	0.08	33,33,33,33	0
57	MG	1F	313	1/1	0.95	0.10	57,57,57,57	0
57	MG	1A	3594	1/1	0.95	0.11	36,36,36,36	0
57	MG	2A	3504	1/1	0.95	0.24	64,64,64,64	0
57	MG	2A	3133	1/1	0.95	0.19	70,70,70,70	0
57	MG	2A	3507	1/1	0.95	0.08	47,47,47,47	0
57	MG	1A	3523	1/1	0.95	0.20	42,42,42,42	0
57	MG	1e	201	1/1	0.95	0.11	69,69,69,69	0
57	MG	1G	205	1/1	0.95	0.15	57,57,57,57	0
57	MG	1f	201	1/1	0.95	0.19	52,52,52,52	0
57	MG	1A	3525	1/1	0.95	0.10	55,55,55,55	0
57	MG	1a	1662	1/1	0.95	0.10	48,48,48,48	0
57	MG	1N	201	1/1	0.95	0.15	40,40,40,40	0
57	MG	1A	3179	1/1	0.95	0.18	50,50,50,50	0
57	MG	1n	101	1/1	0.95	0.09	50,50,50,50	0
57	MG	2A	3717	1/1	0.95	0.09	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	4067	1/1	0.95	0.14	52,52,52,52	0
57	MG	1A	3689	1/1	0.95	0.05	31,31,31,31	0
57	MG	1A	3952	1/1	0.95	0.06	50,50,50,50	0
57	MG	2A	3522	1/1	0.95	0.08	66,66,66,66	0
57	MG	1A	3478	1/1	0.95	0.16	40,40,40,40	0
57	MG	2A	3148	1/1	0.95	0.08	61,61,61,61	0
57	MG	1A	3028	1/1	0.95	0.08	60,60,60,60	0
57	MG	2A	3526	1/1	0.95	0.14	63,63,63,63	0
57	MG	1A	3115	1/1	0.95	0.19	27,27,27,27	0
57	MG	1A	3956	1/1	0.95	0.16	69,69,69,69	0
57	MG	1A	3183	1/1	0.95	0.25	39,39,39,39	0
57	MG	1A	3532	1/1	0.95	0.17	41,41,41,41	0
57	MG	1A	4079	1/1	0.95	0.06	29,29,29,29	0
57	MG	2A	3533	1/1	0.95	0.12	51,51,51,51	0
57	MG	1A	4080	1/1	0.95	0.07	46,46,46,46	0
57	MG	1A	3862	1/1	0.95	0.25	35,35,35,35	0
57	MG	1A	3327	1/1	0.95	0.27	46,46,46,46	0
57	MG	1A	3865	1/1	0.95	0.17	36,36,36,36	0
57	MG	1A	4086	1/1	0.95	0.11	61,61,61,61	0
57	MG	1A	3010	1/1	0.95	0.07	49,49,49,49	0
57	MG	1A	3967	1/1	0.95	0.14	71,71,71,71	0
57	MG	2A	3542	1/1	0.95	0.06	39,39,39,39	0
57	MG	1x	105	1/1	0.95	0.21	53,53,53,53	0
57	MG	2A	3544	1/1	0.95	0.16	52,52,52,52	0
57	MG	1A	3609	1/1	0.95	0.09	44,44,44,44	0
57	MG	2A	3755	1/1	0.95	0.11	83,83,83,83	0
57	MG	1A	3611	1/1	0.95	0.09	46,46,46,46	0
57	MG	1A	3031	1/1	0.95	0.17	26,26,26,26	0
57	MG	2A	3758	1/1	0.95	0.10	58,58,58,58	0
57	MG	1A	3971	1/1	0.95	0.06	39,39,39,39	0
57	MG	2A	3549	1/1	0.95	0.11	40,40,40,40	0
57	MG	2A	3345	1/1	0.95	0.40	65,65,65,65	0
57	MG	2A	3551	1/1	0.95	0.11	63,63,63,63	0
57	MG	1A	3613	1/1	0.95	0.07	48,48,48,48	0
57	MG	1A	3121	1/1	0.95	0.07	44,44,44,44	0
57	MG	2A	3555	1/1	0.95	0.10	44,44,44,44	0
57	MG	1A	3405	1/1	0.95	0.14	50,50,50,50	0
57	MG	1A	3489	1/1	0.95	0.30	38,38,38,38	0
57	MG	1V	203	1/1	0.95	0.14	30,30,30,30	0
57	MG	1A	3055	1/1	0.95	0.09	53,53,53,53	0
57	MG	1A	3194	1/1	0.95	0.08	25,25,25,25	0
57	MG	2A	3773	1/1	0.95	0.08	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	3450	1/1	0.95	0.07	42,42,42,42	0
57	MG	2A	3563	1/1	0.95	0.09	36,36,36,36	0
57	MG	2A	3180	1/1	0.95	0.24	56,56,56,56	0
57	MG	2A	3565	1/1	0.95	0.09	62,62,62,62	0
57	MG	1A	3982	1/1	0.95	0.11	47,47,47,47	0
57	MG	1W	204	1/1	0.95	0.15	38,38,38,38	0
57	MG	1A	3333	1/1	0.95	0.09	35,35,35,35	0
57	MG	1a	1702	1/1	0.95	0.19	61,61,61,61	0
57	MG	1A	3881	1/1	0.95	0.08	19,19,19,19	0
57	MG	1a	1704	1/1	0.95	0.06	51,51,51,51	0
57	MG	2A	3572	1/1	0.95	0.26	56,56,56,56	0
57	MG	2A	3361	1/1	0.95	0.10	44,44,44,44	0
57	MG	1X	101	1/1	0.95	0.25	41,41,41,41	0
57	MG	1A	3014	1/1	0.95	0.20	44,44,44,44	0
57	MG	1A	3986	1/1	0.95	0.09	24,24,24,24	0
57	MG	1X	106	1/1	0.95	0.08	42,42,42,42	0
57	MG	1X	107	1/1	0.95	0.08	65,65,65,65	0
57	MG	1A	3495	1/1	0.95	0.06	68,68,68,68	0
57	MG	1a	1715	1/1	0.95	0.18	44,44,44,44	0
57	MG	1A	3555	1/1	0.95	0.07	40,40,40,40	0
57	MG	1A	3454	1/1	0.95	0.17	40,40,40,40	0
57	MG	1A	3557	1/1	0.95	0.23	47,47,47,47	0
57	MG	1a	1721	1/1	0.95	0.12	59,59,59,59	0
57	MG	1A	3272	1/1	0.95	0.25	35,35,35,35	0
57	MG	10	101	1/1	0.95	0.10	47,47,47,47	0
57	MG	1A	3273	1/1	0.95	0.10	44,44,44,44	0
57	MG	2A	3588	1/1	0.95	0.11	59,59,59,59	0
57	MG	2A	3030	1/1	0.95	0.12	50,50,50,50	0
57	MG	1A	3996	1/1	0.95	0.06	29,29,29,29	0
57	MG	1a	1726	1/1	0.95	0.15	60,60,60,60	0
57	MG	2A	3206	1/1	0.95	0.10	59,59,59,59	0
57	MG	1A	3412	1/1	0.95	0.10	42,42,42,42	0
57	MG	2A	3034	1/1	0.95	0.13	53,53,53,53	0
57	MG	11	101	1/1	0.95	0.25	42,42,42,42	0
57	MG	2A	3596	1/1	0.95	0.09	64,64,64,64	0
57	MG	2A	3039	1/1	0.95	0.10	53,53,53,53	0
57	MG	1A	3998	1/1	0.95	0.06	40,40,40,40	0
57	MG	11	103	1/1	0.95	0.07	45,45,45,45	0
57	MG	1A	3810	1/1	0.95	0.08	44,44,44,44	0
57	MG	1A	3639	1/1	0.95	0.11	48,48,48,48	0
57	MG	2A	3602	1/1	0.95	0.19	57,57,57,57	0
57	MG	1A	3019	1/1	0.95	0.08	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	4004	1/1	0.95	0.09	76,76,76,76	0
57	MG	13	102	1/1	0.95	0.16	39,39,39,39	0
57	MG	2A	3049	1/1	0.95	0.20	50,50,50,50	0
57	MG	1A	3563	1/1	0.95	0.19	45,45,45,45	0
57	MG	14	101	1/1	0.95	0.09	74,74,74,74	0
57	MG	2D	304	1/1	0.95	0.12	35,35,35,35	0
57	MG	2D	305	1/1	0.95	0.26	42,42,42,42	0
57	MG	1a	1740	1/1	0.95	0.10	56,56,56,56	0
57	MG	1A	3642	1/1	0.95	0.08	46,46,46,46	0
57	MG	15	105	1/1	0.95	0.13	40,40,40,40	0
57	MG	2E	303	1/1	0.95	0.12	52,52,52,52	0
57	MG	2A	3228	1/1	0.95	0.19	56,56,56,56	0
57	MG	1A	3414	1/1	0.95	0.10	62,62,62,62	0
57	MG	2A	3614	1/1	0.95	0.09	58,58,58,58	0
57	MG	1A	3003	1/1	0.95	0.06	25,25,25,25	0
57	MG	16	101	1/1	0.95	0.09	56,56,56,56	0
57	MG	2A	3232	1/1	0.95	0.17	52,52,52,52	0
57	MG	1A	3904	1/1	0.95	0.14	55,55,55,55	0
57	MG	2A	3234	1/1	0.95	0.13	72,72,72,72	0
57	MG	17	103	1/1	0.95	0.16	37,37,37,37	0
57	MG	18	101	1/1	0.95	0.16	59,59,59,59	0
57	MG	2A	3622	1/1	0.95	0.11	66,66,66,66	0
57	MG	2A	3623	1/1	0.95	0.13	62,62,62,62	0
57	MG	2Q	204	1/1	0.95	0.16	59,59,59,59	0
57	MG	1A	3025	1/1	0.95	0.32	59,59,59,59	0
57	MG	1A	3045	1/1	0.95	0.09	46,46,46,46	0
57	MG	2A	3064	1/1	0.95	0.30	62,62,62,62	0
57	MG	1B	217	1/1	0.95	0.07	54,54,54,54	0
57	MG	2A	3241	1/1	0.95	0.15	50,50,50,50	0
57	MG	2A	3421	1/1	0.95	0.07	62,62,62,62	0
57	MG	2A	3066	1/1	0.95	0.11	42,42,42,42	0
57	MG	1A	3170	1/1	0.95	0.06	22,22,22,22	0
57	MG	1a	1605	1/1	0.95	0.11	60,60,60,60	0
57	MG	2W	202	1/1	0.95	0.12	54,54,54,54	0
57	MG	1A	3205	1/1	0.95	0.21	57,57,57,57	0
57	MG	1A	3088	1/1	0.95	0.24	57,57,57,57	0
57	MG	1A	3346	1/1	0.95	0.11	57,57,57,57	0
57	MG	2A	3072	1/1	0.95	0.12	47,47,47,47	0
57	MG	2A	3431	1/1	0.95	0.13	47,47,47,47	0
57	MG	1A	3655	1/1	0.95	0.06	23,23,23,23	0
57	MG	1a	1613	1/1	0.95	0.15	63,63,63,63	0
57	MG	1A	4019	1/1	0.95	0.14	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	1616	1/1	0.95	0.09	67,67,67,67	0
57	MG	2A	3647	1/1	0.95	0.18	54,54,54,54	0
57	MG	1A	3110	1/1	0.95	0.14	39,39,39,39	0
57	MG	27	101	1/1	0.95	0.09	52,52,52,52	0
57	MG	1A	3576	1/1	0.95	0.11	35,35,35,35	0
57	MG	2A	3650	1/1	0.95	0.28	61,61,61,61	0
57	MG	2a	1601	1/1	0.95	0.09	55,55,55,55	0
57	MG	2A	3441	1/1	0.95	0.12	46,46,46,46	0
57	MG	2A	3652	1/1	0.95	0.09	70,70,70,70	0
57	MG	1a	1778	1/1	0.95	0.07	67,67,67,67	0
57	MG	1A	4023	1/1	0.95	0.06	34,34,34,34	0
57	MG	1A	3579	1/1	0.95	0.15	48,48,48,48	0
57	MG	2A	3260	1/1	0.95	0.11	65,65,65,65	0
57	MG	1A	3661	1/1	0.95	0.06	27,27,27,27	0
57	MG	2A	3086	1/1	0.95	0.18	44,44,44,44	0
57	MG	1A	3917	1/1	0.95	0.07	44,44,44,44	0
57	MG	1A	4027	1/1	0.95	0.09	50,50,50,50	0
57	MG	1A	3662	1/1	0.95	0.14	22,22,22,22	0
57	MG	1A	3111	1/1	0.95	0.16	41,41,41,41	0
57	MG	1A	3427	1/1	0.95	0.11	60,60,60,60	0
57	MG	2A	3664	1/1	0.95	0.09	62,62,62,62	0
57	MG	1A	3923	1/1	0.95	0.11	46,46,46,46	0
57	MG	1A	3515	1/1	0.95	0.22	60,60,60,60	0
57	MG	1A	4036	1/1	0.95	0.07	49,49,49,49	0
57	MG	1A	3313	1/1	0.95	0.17	49,49,49,49	0
57	MG	1A	3285	1/1	0.95	0.06	31,31,31,31	0
57	MG	1A	3674	1/1	0.95	0.06	30,30,30,30	0
57	MG	1A	3026	1/1	0.95	0.17	42,42,42,42	0
58	K	2A	3377	1/1	0.95	0.07	65,65,65,65	0
57	MG	1A	3021	1/1	0.96	0.09	51,51,51,51	0
57	MG	1A	3007	1/1	0.96	0.06	25,25,25,25	0
57	MG	1A	3664	1/1	0.96	0.06	28,28,28,28	0
57	MG	1A	3931	1/1	0.96	0.05	51,51,51,51	0
57	MG	1A	3665	1/1	0.96	0.06	32,32,32,32	0
57	MG	1A	3221	1/1	0.96	0.27	47,47,47,47	0
57	MG	15	107	1/1	0.96	0.06	49,49,49,49	0
57	MG	2A	3711	1/1	0.96	0.07	59,59,59,59	0
57	MG	1A	3270	1/1	0.96	0.14	31,31,31,31	0
57	MG	1A	3035	1/1	0.96	0.09	40,40,40,40	0
57	MG	1A	3074	1/1	0.96	0.05	30,30,30,30	0
57	MG	2A	3539	1/1	0.96	0.12	54,54,54,54	0
57	MG	17	101	1/1	0.96	0.12	35,35,35,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	17	102	1/1	0.96	0.21	38,38,38,38	0
57	MG	1A	3841	1/1	0.96	0.11	21,21,21,21	0
57	MG	17	104	1/1	0.96	0.08	57,57,57,57	0
57	MG	1A	3274	1/1	0.96	0.17	51,51,51,51	0
57	MG	18	102	1/1	0.96	0.15	47,47,47,47	0
57	MG	18	103	1/1	0.96	0.17	44,44,44,44	0
57	MG	2A	3196	1/1	0.96	0.31	65,65,65,65	0
57	MG	1A	3044	1/1	0.96	0.13	35,35,35,35	0
57	MG	2A	3725	1/1	0.96	0.06	59,59,59,59	0
57	MG	2A	3727	1/1	0.96	0.08	56,56,56,56	0
57	MG	2A	3043	1/1	0.96	0.06	56,56,56,56	0
57	MG	19	101	1/1	0.96	0.19	42,42,42,42	0
57	MG	1A	3941	1/1	0.96	0.06	39,39,39,39	0
57	MG	2A	3552	1/1	0.96	0.09	40,40,40,40	0
57	MG	2A	3201	1/1	0.96	0.11	67,67,67,67	0
57	MG	1A	3061	1/1	0.96	0.08	53,53,53,53	0
57	MG	1a	1603	1/1	0.96	0.09	62,62,62,62	0
57	MG	1D	305	1/1	0.96	0.06	39,39,39,39	0
57	MG	1D	306	1/1	0.96	0.16	41,41,41,41	0
57	MG	2A	3738	1/1	0.96	0.10	46,46,46,46	0
57	MG	2A	3739	1/1	0.96	0.10	55,55,55,55	0
57	MG	1A	3139	1/1	0.96	0.10	49,49,49,49	0
57	MG	1D	309	1/1	0.96	0.17	46,46,46,46	0
57	MG	1A	4048	1/1	0.96	0.10	14,14,14,14	0
57	MG	2A	3209	1/1	0.96	0.10	59,59,59,59	0
57	MG	1a	1609	1/1	0.96	0.08	61,61,61,61	0
57	MG	1A	3759	1/1	0.96	0.10	19,19,19,19	0
57	MG	1E	302	1/1	0.96	0.13	40,40,40,40	0
57	MG	2A	3751	1/1	0.96	0.08	41,41,41,41	0
57	MG	1E	305	1/1	0.96	0.14	38,38,38,38	0
57	MG	1a	1615	1/1	0.96	0.15	53,53,53,53	0
57	MG	2A	3059	1/1	0.96	0.13	56,56,56,56	0
57	MG	1a	1761	1/1	0.96	0.10	66,66,66,66	0
57	MG	1A	3416	1/1	0.96	0.18	44,44,44,44	0
57	MG	1A	3524	1/1	0.96	0.22	34,34,34,34	0
57	MG	1A	3850	1/1	0.96	0.06	48,48,48,48	0
57	MG	1A	3763	1/1	0.96	0.05	40,40,40,40	0
57	MG	1A	3852	1/1	0.96	0.08	25,25,25,25	0
57	MG	1A	3319	1/1	0.96	0.38	47,47,47,47	0
57	MG	1E	313	1/1	0.96	0.09	48,48,48,48	0
57	MG	1A	3765	1/1	0.96	0.05	23,23,23,23	0
57	MG	1A	3320	1/1	0.96	0.08	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	1627	1/1	0.96	0.08	46,46,46,46	0
57	MG	1A	3419	1/1	0.96	0.21	43,43,43,43	0
57	MG	1F	303	1/1	0.96	0.17	40,40,40,40	0
57	MG	2A	3073	1/1	0.96	0.32	49,49,49,49	0
57	MG	1A	3140	1/1	0.96	0.07	58,58,58,58	0
57	MG	1a	1784	1/1	0.96	0.20	57,57,57,57	0
57	MG	1A	4063	1/1	0.96	0.14	40,40,40,40	0
57	MG	1F	306	1/1	0.96	0.13	33,33,33,33	0
57	MG	1A	3077	1/1	0.96	0.10	30,30,30,30	0
57	MG	2A	3777	1/1	0.96	0.08	58,58,58,58	0
57	MG	2A	3080	1/1	0.96	0.11	59,59,59,59	0
57	MG	2A	3779	1/1	0.96	0.08	59,59,59,59	0
57	MG	1A	3234	1/1	0.96	0.08	47,47,47,47	0
57	MG	1A	3959	1/1	0.96	0.06	47,47,47,47	0
57	MG	1A	3771	1/1	0.96	0.06	49,49,49,49	0
57	MG	2A	3406	1/1	0.96	0.18	52,52,52,52	0
57	MG	1A	3602	1/1	0.96	0.06	26,26,26,26	0
57	MG	1A	3687	1/1	0.96	0.11	45,45,45,45	0
57	MG	1A	3184	1/1	0.96	0.28	30,30,30,30	0
57	MG	1A	3864	1/1	0.96	0.11	30,30,30,30	0
57	MG	2A	3411	1/1	0.96	0.24	54,54,54,54	0
57	MG	1G	204	1/1	0.96	0.10	50,50,50,50	0
57	MG	1A	3606	1/1	0.96	0.07	32,32,32,32	0
57	MG	2A	3249	1/1	0.96	0.27	75,75,75,75	0
57	MG	1a	1797	1/1	0.96	0.16	57,57,57,57	0
57	MG	2A	3092	1/1	0.96	0.09	60,60,60,60	0
57	MG	1a	1644	1/1	0.96	0.10	47,47,47,47	0
57	MG	1A	3142	1/1	0.96	0.26	36,36,36,36	0
57	MG	1A	3187	1/1	0.96	0.10	43,43,43,43	0
57	MG	1A	3188	1/1	0.96	0.18	34,34,34,34	0
57	MG	1A	3610	1/1	0.96	0.10	29,29,29,29	0
57	MG	1A	3079	1/1	0.96	0.17	36,36,36,36	0
57	MG	2A	3100	1/1	0.96	0.18	57,57,57,57	0
57	MG	1A	3380	1/1	0.96	0.08	54,54,54,54	0
57	MG	1A	3974	1/1	0.96	0.11	30,30,30,30	0
57	MG	1A	4084	1/1	0.96	0.07	47,47,47,47	0
57	MG	2A	3262	1/1	0.96	0.09	62,62,62,62	0
57	MG	2A	3263	1/1	0.96	0.21	70,70,70,70	0
57	MG	2A	3104	1/1	0.96	0.18	42,42,42,42	0
57	MG	2A	3265	1/1	0.96	0.20	56,56,56,56	0
57	MG	1A	3483	1/1	0.96	0.23	56,56,56,56	0
57	MG	2A	3439	1/1	0.96	0.08	49,49,49,49	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	3098	1/1	0.96	0.17	53,53,53,53	0
57	MG	2A	3268	1/1	0.96	0.06	58,58,58,58	0
57	MG	1P	202	1/1	0.96	0.14	31,31,31,31	0
57	MG	1A	3119	1/1	0.96	0.27	43,43,43,43	0
57	MG	1A	4090	1/1	0.96	0.07	28,28,28,28	0
57	MG	2A	3446	1/1	0.96	0.09	53,53,53,53	0
57	MG	1A	3548	1/1	0.96	0.22	29,29,29,29	0
57	MG	1A	3120	1/1	0.96	0.11	44,44,44,44	0
57	MG	1A	3434	1/1	0.96	0.07	44,44,44,44	0
57	MG	1A	3705	1/1	0.96	0.12	58,58,58,58	0
57	MG	1A	3334	1/1	0.96	0.09	60,60,60,60	0
57	MG	1A	3797	1/1	0.96	0.09	53,53,53,53	0
57	MG	1A	3885	1/1	0.96	0.10	46,46,46,46	0
57	MG	1A	3886	1/1	0.96	0.10	32,32,32,32	0
57	MG	1R	202	1/1	0.96	0.15	35,35,35,35	0
57	MG	1A	3553	1/1	0.96	0.15	38,38,38,38	0
57	MG	1A	3053	1/1	0.96	0.12	29,29,29,29	0
57	MG	1A	3197	1/1	0.96	0.07	47,47,47,47	0
57	MG	1A	3153	1/1	0.96	0.36	37,37,37,37	0
57	MG	1A	3629	1/1	0.96	0.08	17,17,17,17	0
57	MG	1A	3122	1/1	0.96	0.22	33,33,33,33	0
57	MG	1A	3714	1/1	0.96	0.09	50,50,50,50	0
57	MG	1U	202	1/1	0.96	0.29	36,36,36,36	0
57	MG	1A	3558	1/1	0.96	0.17	41,41,41,41	0
57	MG	1U	206	1/1	0.96	0.26	32,32,32,32	0
57	MG	2A	3291	1/1	0.96	0.22	65,65,65,65	0
57	MG	2F	306	1/1	0.96	0.23	53,53,53,53	0
57	MG	2A	3469	1/1	0.96	0.07	47,47,47,47	0
57	MG	2A	3132	1/1	0.96	0.11	49,49,49,49	0
57	MG	2A	3471	1/1	0.96	0.07	34,34,34,34	0
57	MG	2A	3473	1/1	0.96	0.09	48,48,48,48	0
57	MG	1A	4108	1/1	0.96	0.07	59,59,59,59	0
57	MG	1V	204	1/1	0.96	0.20	50,50,50,50	0
57	MG	1V	205	1/1	0.96	0.12	34,34,34,34	0
57	MG	2R	202	1/1	0.96	0.19	52,52,52,52	0
57	MG	1a	1680	1/1	0.96	0.19	59,59,59,59	0
57	MG	1A	3632	1/1	0.96	0.10	26,26,26,26	0
57	MG	1A	3999	1/1	0.96	0.09	46,46,46,46	0
57	MG	1A	3389	1/1	0.96	0.06	47,47,47,47	0
57	MG	1A	3159	1/1	0.96	0.20	34,34,34,34	0
57	MG	1A	3100	1/1	0.96	0.07	41,41,41,41	0
57	MG	2A	3485	1/1	0.96	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	3392	1/1	0.96	0.15	48,48,48,48	0
57	MG	1a	1688	1/1	0.96	0.15	49,49,49,49	0
57	MG	1a	1689	1/1	0.96	0.30	57,57,57,57	0
57	MG	1A	3203	1/1	0.96	0.08	45,45,45,45	0
57	MG	2A	3307	1/1	0.96	0.06	58,58,58,58	0
57	MG	1A	3063	1/1	0.96	0.25	56,56,56,56	0
57	MG	2A	3670	1/1	0.96	0.07	52,52,52,52	0
57	MG	1X	102	1/1	0.96	0.12	40,40,40,40	0
57	MG	1A	3064	1/1	0.96	0.08	38,38,38,38	0
57	MG	2A	3496	1/1	0.96	0.10	44,44,44,44	0
57	MG	2A	3150	1/1	0.96	0.23	46,46,46,46	0
57	MG	1A	3207	1/1	0.96	0.10	41,41,41,41	0
57	MG	25	102	1/1	0.96	0.11	53,53,53,53	0
57	MG	1a	1695	1/1	0.96	0.23	51,51,51,51	0
57	MG	1A	3728	1/1	0.96	0.11	21,21,21,21	0
57	MG	1A	3644	1/1	0.96	0.09	46,46,46,46	0
57	MG	1A	3210	1/1	0.96	0.25	46,46,46,46	0
57	MG	28	102	1/1	0.96	0.11	62,62,62,62	0
57	MG	2A	3503	1/1	0.96	0.27	58,58,58,58	0
57	MG	1A	3646	1/1	0.96	0.05	30,30,30,30	0
57	MG	2A	3505	1/1	0.96	0.09	48,48,48,48	0
57	MG	1A	3126	1/1	0.96	0.14	45,45,45,45	0
57	MG	1A	3213	1/1	0.96	0.09	30,30,30,30	0
57	MG	1A	3453	1/1	0.96	0.09	48,48,48,48	0
57	MG	1A	3258	1/1	0.96	0.17	35,35,35,35	0
57	MG	2A	3163	1/1	0.96	0.11	35,35,35,35	0
57	MG	1A	3916	1/1	0.96	0.04	16,16,16,16	0
57	MG	1A	3574	1/1	0.96	0.45	43,43,43,43	0
57	MG	1A	3402	1/1	0.96	0.18	40,40,40,40	0
57	MG	1A	3740	1/1	0.96	0.05	16,16,16,16	0
57	MG	1A	3921	1/1	0.96	0.08	37,37,37,37	0
57	MG	1A	3029	1/1	0.96	0.39	37,37,37,37	0
57	MG	1a	1713	1/1	0.96	0.09	49,49,49,49	0
57	MG	1A	3577	1/1	0.96	0.33	62,62,62,62	0
57	MG	1A	3128	1/1	0.96	0.28	48,48,48,48	0
57	MG	2A	3015	1/1	0.96	0.07	41,41,41,41	0
57	MG	2A	3174	1/1	0.96	0.07	51,51,51,51	0
57	MG	1A	3066	1/1	0.96	0.10	32,32,32,32	0
57	MG	1A	4029	1/1	0.96	0.07	27,27,27,27	0
57	MG	12	102	1/1	0.96	0.08	50,50,50,50	0
58	K	1A	3536	1/1	0.96	0.07	42,42,42,42	0
57	MG	1a	1720	1/1	0.96	0.06	47,47,47,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	ZN	14	102	1/1	0.96	0.09	113,113,113,113	0
59	ZN	24	501	1/1	0.96	0.12	127,127,127,127	0
57	MG	2A	3726	1/1	0.97	0.06	54,54,54,54	0
57	MG	2A	3243	1/1	0.97	0.07	49,49,49,49	0
57	MG	1A	3094	1/1	0.97	0.07	38,38,38,38	0
57	MG	1U	205	1/1	0.97	0.23	40,40,40,40	0
57	MG	1A	3368	1/1	0.97	0.36	44,44,44,44	0
57	MG	1V	202	1/1	0.97	0.30	34,34,34,34	0
57	MG	1A	3132	1/1	0.97	0.13	47,47,47,47	0
57	MG	1A	3370	1/1	0.97	0.10	58,58,58,58	0
57	MG	1A	3738	1/1	0.97	0.05	49,49,49,49	0
57	MG	1A	3001	1/1	0.97	0.10	38,38,38,38	0
57	MG	1A	3585	1/1	0.97	0.21	32,32,32,32	0
57	MG	2A	3405	1/1	0.97	0.10	42,42,42,42	0
57	MG	1A	3586	1/1	0.97	0.07	47,47,47,47	0
57	MG	1A	3022	1/1	0.97	0.04	18,18,18,18	0
57	MG	1A	3046	1/1	0.97	0.10	34,34,34,34	0
57	MG	2A	3744	1/1	0.97	0.06	46,46,46,46	0
57	MG	2A	3745	1/1	0.97	0.05	59,59,59,59	0
57	MG	1A	3663	1/1	0.97	0.06	28,28,28,28	0
57	MG	2A	3111	1/1	0.97	0.10	40,40,40,40	0
57	MG	1A	3323	1/1	0.97	0.22	38,38,38,38	0
57	MG	2A	3412	1/1	0.97	0.09	48,48,48,48	0
57	MG	1A	3590	1/1	0.97	0.07	27,27,27,27	0
57	MG	2A	3414	1/1	0.97	0.07	50,50,50,50	0
57	MG	1A	3083	1/1	0.97	0.19	31,31,31,31	0
57	MG	1X	103	1/1	0.97	0.08	44,44,44,44	0
57	MG	1A	3167	1/1	0.97	0.27	34,34,34,34	0
57	MG	1A	3668	1/1	0.97	0.05	27,27,27,27	0
57	MG	1a	1683	1/1	0.97	0.12	41,41,41,41	0
57	MG	1B	218	1/1	0.97	0.11	46,46,46,46	0
57	MG	1A	3527	1/1	0.97	0.09	37,37,37,37	0
57	MG	2A	3121	1/1	0.97	0.09	47,47,47,47	0
57	MG	2A	3424	1/1	0.97	0.09	41,41,41,41	0
57	MG	1A	3168	1/1	0.97	0.23	43,43,43,43	0
57	MG	2A	3123	1/1	0.97	0.10	52,52,52,52	0
57	MG	1A	3040	1/1	0.97	0.27	33,33,33,33	0
57	MG	1A	3005	1/1	0.97	0.14	39,39,39,39	0
57	MG	1A	3755	1/1	0.97	0.06	31,31,31,31	0
57	MG	1A	4030	1/1	0.97	0.07	40,40,40,40	0
57	MG	1A	3932	1/1	0.97	0.05	49,49,49,49	0
57	MG	2A	3433	1/1	0.97	0.14	25,25,25,25	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	10	103	1/1	0.97	0.15	47,47,47,47	0
57	MG	1A	3675	1/1	0.97	0.10	32,32,32,32	0
57	MG	2A	3436	1/1	0.97	0.08	47,47,47,47	0
57	MG	10	105	1/1	0.97	0.05	34,34,34,34	0
57	MG	1A	3842	1/1	0.97	0.15	26,26,26,26	0
57	MG	1A	4034	1/1	0.97	0.06	29,29,29,29	0
57	MG	1A	3059	1/1	0.97	0.20	47,47,47,47	0
57	MG	1A	3245	1/1	0.97	0.18	29,29,29,29	0
57	MG	1A	3206	1/1	0.97	0.13	42,42,42,42	0
57	MG	2A	3443	1/1	0.97	0.05	35,35,35,35	0
57	MG	1A	3431	1/1	0.97	0.07	51,51,51,51	0
57	MG	1A	4039	1/1	0.97	0.15	69,69,69,69	0
57	MG	1A	3761	1/1	0.97	0.06	41,41,41,41	0
57	MG	1A	3073	1/1	0.97	0.04	28,28,28,28	0
57	MG	2A	3448	1/1	0.97	0.06	47,47,47,47	0
57	MG	1A	3143	1/1	0.97	0.13	30,30,30,30	0
57	MG	1A	3603	1/1	0.97	0.04	34,34,34,34	0
57	MG	1B	238	1/1	0.97	0.06	37,37,37,37	0
57	MG	1A	3538	1/1	0.97	0.08	33,33,33,33	0
57	MG	15	102	1/1	0.97	0.17	32,32,32,32	0
57	MG	2A	3292	1/1	0.97	0.11	62,62,62,62	0
57	MG	1A	3539	1/1	0.97	0.07	23,23,23,23	0
57	MG	1A	3049	1/1	0.97	0.08	40,40,40,40	0
57	MG	2A	3003	1/1	0.97	0.11	49,49,49,49	0
57	MG	1A	3011	1/1	0.97	0.05	36,36,36,36	0
57	MG	1A	3107	1/1	0.97	0.34	34,34,34,34	0
57	MG	2A	3152	1/1	0.97	0.12	55,55,55,55	0
57	MG	2A	3800	1/1	0.97	0.06	65,65,65,65	0
57	MG	1A	3545	1/1	0.97	0.12	46,46,46,46	0
57	MG	1A	3020	1/1	0.97	0.06	30,30,30,30	0
57	MG	1A	3181	1/1	0.97	0.34	39,39,39,39	0
57	MG	2A	3628	1/1	0.97	0.09	55,55,55,55	0
57	MG	2A	3009	1/1	0.97	0.06	39,39,39,39	0
57	MG	2A	3157	1/1	0.97	0.11	53,53,53,53	0
57	MG	1E	301	1/1	0.97	0.28	31,31,31,31	0
57	MG	1A	3773	1/1	0.97	0.04	38,38,38,38	0
57	MG	2A	3468	1/1	0.97	0.07	45,45,45,45	0
57	MG	1E	303	1/1	0.97	0.07	36,36,36,36	0
57	MG	2A	3013	1/1	0.97	0.09	55,55,55,55	0
57	MG	1E	304	1/1	0.97	0.12	32,32,32,32	0
57	MG	17	105	1/1	0.97	0.13	46,46,46,46	0
57	MG	17	106	1/1	0.97	0.07	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	3549	1/1	0.97	0.07	44,44,44,44	0
57	MG	1A	3615	1/1	0.97	0.07	51,51,51,51	0
57	MG	1E	307	1/1	0.97	0.16	32,32,32,32	0
57	MG	2A	3479	1/1	0.97	0.09	37,37,37,37	0
57	MG	18	104	1/1	0.97	0.12	43,43,43,43	0
57	MG	1A	3694	1/1	0.97	0.06	41,41,41,41	0
57	MG	1A	3777	1/1	0.97	0.06	52,52,52,52	0
57	MG	1A	3617	1/1	0.97	0.05	39,39,39,39	0
57	MG	1A	3957	1/1	0.97	0.06	62,62,62,62	0
57	MG	1A	3958	1/1	0.97	0.07	59,59,59,59	0
57	MG	1A	3779	1/1	0.97	0.07	39,39,39,39	0
57	MG	1a	1737	1/1	0.97	0.06	60,60,60,60	0
57	MG	1A	3439	1/1	0.97	0.14	37,37,37,37	0
57	MG	1A	3440	1/1	0.97	0.07	50,50,50,50	0
57	MG	1A	3217	1/1	0.97	0.07	30,30,30,30	0
57	MG	2A	3492	1/1	0.97	0.08	40,40,40,40	0
57	MG	1A	4068	1/1	0.97	0.05	44,44,44,44	0
57	MG	1A	3218	1/1	0.97	0.11	29,29,29,29	0
57	MG	1a	1610	1/1	0.97	0.16	45,45,45,45	0
57	MG	2A	3037	1/1	0.97	0.06	44,44,44,44	0
57	MG	1A	3964	1/1	0.97	0.04	37,37,37,37	0
57	MG	1A	3052	1/1	0.97	0.09	26,26,26,26	0
57	MG	1F	307	1/1	0.97	0.12	31,31,31,31	0
57	MG	2F	304	1/1	0.97	0.12	55,55,55,55	0
57	MG	2F	305	1/1	0.97	0.27	50,50,50,50	0
57	MG	1A	3871	1/1	0.97	0.07	24,24,24,24	0
57	MG	1A	3300	1/1	0.97	0.15	35,35,35,35	0
57	MG	1a	1617	1/1	0.97	0.11	50,50,50,50	0
57	MG	1A	3151	1/1	0.97	0.08	36,36,36,36	0
57	MG	1A	3345	1/1	0.97	0.13	41,41,41,41	0
57	MG	1A	3875	1/1	0.97	0.10	50,50,50,50	0
57	MG	2Q	203	1/1	0.97	0.37	58,58,58,58	0
57	MG	2A	3048	1/1	0.97	0.19	39,39,39,39	0
57	MG	1A	3876	1/1	0.97	0.04	50,50,50,50	0
57	MG	2A	3342	1/1	0.97	0.09	48,48,48,48	0
57	MG	1G	201	1/1	0.97	0.11	39,39,39,39	0
57	MG	1a	1758	1/1	0.97	0.07	77,77,77,77	0
57	MG	1A	3972	1/1	0.97	0.09	38,38,38,38	0
57	MG	2A	3513	1/1	0.97	0.04	51,51,51,51	0
57	MG	1a	1762	1/1	0.97	0.07	62,62,62,62	0
57	MG	1A	3152	1/1	0.97	0.10	46,46,46,46	0
57	MG	1a	1767	1/1	0.97	0.10	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	1A	3498	1/1	0.97	0.07	45,45,45,45	0
57	MG	1A	3791	1/1	0.97	0.05	46,46,46,46	0
57	MG	1A	3185	1/1	0.97	0.24	36,36,36,36	0
57	MG	1A	3500	1/1	0.97	0.28	38,38,38,38	0
57	MG	2X	102	1/1	0.97	0.09	50,50,50,50	0
57	MG	1A	3078	1/1	0.97	0.09	40,40,40,40	0
57	MG	1A	3883	1/1	0.97	0.04	37,37,37,37	0
57	MG	1A	4089	1/1	0.97	0.04	17,17,17,17	0
57	MG	1A	3093	1/1	0.97	0.12	40,40,40,40	0
57	MG	1A	3262	1/1	0.97	0.20	36,36,36,36	0
57	MG	1A	4092	1/1	0.97	0.17	32,32,32,32	0
57	MG	1A	3263	1/1	0.97	0.06	48,48,48,48	0
57	MG	1A	3635	1/1	0.97	0.04	25,25,25,25	0
57	MG	1a	1638	1/1	0.97	0.08	48,48,48,48	0
57	MG	2A	3530	1/1	0.97	0.10	61,61,61,61	0
57	MG	1P	201	1/1	0.97	0.32	29,29,29,29	0
57	MG	2A	3214	1/1	0.97	0.07	63,63,63,63	0
57	MG	2A	3215	1/1	0.97	0.07	52,52,52,52	0
57	MG	1A	3636	1/1	0.97	0.04	28,28,28,28	0
57	MG	1A	3264	1/1	0.97	0.23	44,44,44,44	0
57	MG	1A	3988	1/1	0.97	0.05	60,60,60,60	0
57	MG	1A	3717	1/1	0.97	0.07	28,28,28,28	0
57	MG	1A	3638	1/1	0.97	0.06	44,44,44,44	0
57	MG	1A	3156	1/1	0.97	0.23	31,31,31,31	0
57	MG	1A	3992	1/1	0.97	0.07	33,33,33,33	0
57	MG	1A	3226	1/1	0.97	0.20	30,30,30,30	0
57	MG	2A	3707	1/1	0.97	0.10	56,56,56,56	0
57	MG	1A	3157	1/1	0.97	0.18	33,33,33,33	0
57	MG	1A	3269	1/1	0.97	0.32	41,41,41,41	0
57	MG	1A	3572	1/1	0.97	0.23	54,54,54,54	0
57	MG	1A	3900	1/1	0.97	0.03	33,33,33,33	0
57	MG	1A	3229	1/1	0.97	0.16	33,33,33,33	0
57	MG	1a	1801	1/1	0.97	0.19	47,47,47,47	0
57	MG	1A	3230	1/1	0.97	0.05	41,41,41,41	0
57	MG	1A	3231	1/1	0.97	0.34	35,35,35,35	0
57	MG	1A	3647	1/1	0.97	0.05	27,27,27,27	0
57	MG	1A	4111	1/1	0.97	0.13	49,49,49,49	0
57	MG	1A	3158	1/1	0.97	0.17	29,29,29,29	0
57	MG	1T	201	1/1	0.97	0.14	50,50,50,50	0
57	MG	1T	202	1/1	0.97	0.15	59,59,59,59	0
57	MG	1A	3364	1/1	0.97	0.17	28,28,28,28	0
57	MG	1U	201	1/1	0.97	0.12	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	2A	3095	1/1	0.97	0.13	37,37,37,37	0
57	MG	1A	3275	1/1	0.97	0.08	34,34,34,34	0
59	ZN	2Y	501	1/1	0.97	0.05	105,105,105,105	0
57	MG	1U	203	1/1	0.97	0.11	37,37,37,37	0
59	ZN	2n	501	1/1	0.97	0.06	96,96,96,96	0
57	MG	1A	3578	1/1	0.98	0.06	49,49,49,49	0
57	MG	1A	4017	1/1	0.98	0.07	50,50,50,50	0
57	MG	1A	3038	1/1	0.98	0.07	25,25,25,25	0
57	MG	2A	3309	1/1	0.98	0.11	53,53,53,53	0
57	MG	1A	3108	1/1	0.98	0.06	39,39,39,39	0
57	MG	1A	4020	1/1	0.98	0.04	58,58,58,58	0
57	MG	1A	3138	1/1	0.98	0.06	23,23,23,23	0
57	MG	10	102	1/1	0.98	0.10	50,50,50,50	0
57	MG	1A	3267	1/1	0.98	0.24	30,30,30,30	0
57	MG	2A	3429	1/1	0.98	0.18	46,46,46,46	0
57	MG	1A	3208	1/1	0.98	0.09	49,49,49,49	0
57	MG	1A	3209	1/1	0.98	0.27	41,41,41,41	0
57	MG	1a	1749	1/1	0.98	0.05	59,59,59,59	0
57	MG	1A	3109	1/1	0.98	0.20	34,34,34,34	0
57	MG	1A	3271	1/1	0.98	0.25	38,38,38,38	0
57	MG	1A	3540	1/1	0.98	0.10	33,33,33,33	0
57	MG	1A	3240	1/1	0.98	0.08	40,40,40,40	0
57	MG	2A	3798	1/1	0.98	0.08	73,73,73,73	0
57	MG	1a	1754	1/1	0.98	0.05	64,64,64,64	0
57	MG	1A	3032	1/1	0.98	0.08	31,31,31,31	0
57	MG	2A	3556	1/1	0.98	0.06	48,48,48,48	0
57	MG	1A	3212	1/1	0.98	0.06	42,42,42,42	0
57	MG	1A	3544	1/1	0.98	0.24	40,40,40,40	0
57	MG	1A	3067	1/1	0.98	0.09	30,30,30,30	0
57	MG	1A	3890	1/1	0.98	0.07	38,38,38,38	0
57	MG	1A	3501	1/1	0.98	0.26	40,40,40,40	0
57	MG	1a	1763	1/1	0.98	0.07	43,43,43,43	0
57	MG	1A	3702	1/1	0.98	0.04	18,18,18,18	0
57	MG	2A	3223	1/1	0.98	0.05	65,65,65,65	0
57	MG	1a	1765	1/1	0.98	0.04	62,62,62,62	0
57	MG	1A	3547	1/1	0.98	0.19	27,27,27,27	0
57	MG	1a	1768	1/1	0.98	0.07	59,59,59,59	0
57	MG	1A	3420	1/1	0.98	0.24	32,32,32,32	0
57	MG	1a	1770	1/1	0.98	0.05	76,76,76,76	0
57	MG	1A	3033	1/1	0.98	0.18	32,32,32,32	0
57	MG	15	103	1/1	0.98	0.41	32,32,32,32	0
57	MG	1A	3069	1/1	0.98	0.09	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	3144	1/1	0.98	0.07	30,30,30,30	0
57	MG	2A	3341	1/1	0.98	0.05	40,40,40,40	0
57	MG	1A	3164	1/1	0.98	0.06	17,17,17,17	0
57	MG	2A	3021	1/1	0.98	0.11	32,32,32,32	0
57	MG	1A	3012	1/1	0.98	0.12	27,27,27,27	0
57	MG	1N	203	1/1	0.98	0.04	37,37,37,37	0
57	MG	1B	206	1/1	0.98	0.05	54,54,54,54	0
57	MG	1A	3652	1/1	0.98	0.09	38,38,38,38	0
57	MG	1A	3190	1/1	0.98	0.14	29,29,29,29	0
57	MG	2A	3027	1/1	0.98	0.14	40,40,40,40	0
57	MG	1A	3837	1/1	0.98	0.09	21,21,21,21	0
57	MG	1A	3191	1/1	0.98	0.09	36,36,36,36	0
57	MG	1A	3166	1/1	0.98	0.14	32,32,32,32	0
57	MG	2A	3137	1/1	0.98	0.05	41,41,41,41	0
57	MG	1A	3009	1/1	0.98	0.06	36,36,36,36	0
57	MG	1A	3605	1/1	0.98	0.09	39,39,39,39	0
57	MG	1A	3116	1/1	0.98	0.19	33,33,33,33	0
57	MG	2A	3472	1/1	0.98	0.07	34,34,34,34	0
57	MG	1P	203	1/1	0.98	0.29	33,33,33,33	0
57	MG	2A	3035	1/1	0.98	0.09	33,33,33,33	0
57	MG	1A	3718	1/1	0.98	0.03	24,24,24,24	0
57	MG	2A	3476	1/1	0.98	0.11	33,33,33,33	0
57	MG	1A	3659	1/1	0.98	0.05	27,27,27,27	0
57	MG	1A	3660	1/1	0.98	0.08	27,27,27,27	0
57	MG	1A	4055	1/1	0.98	0.06	38,38,38,38	0
57	MG	1A	3781	1/1	0.98	0.06	26,26,26,26	0
57	MG	1A	3195	1/1	0.98	0.09	36,36,36,36	0
57	MG	1A	3082	1/1	0.98	0.18	36,36,36,36	0
57	MG	1A	3723	1/1	0.98	0.09	55,55,55,55	0
57	MG	1A	3355	1/1	0.98	0.04	41,41,41,41	0
57	MG	1a	1799	1/1	0.98	0.05	65,65,65,65	0
57	MG	1a	1800	1/1	0.98	0.07	32,32,32,32	0
57	MG	1A	3288	1/1	0.98	0.11	40,40,40,40	0
57	MG	1A	4062	1/1	0.98	0.07	37,37,37,37	0
57	MG	1A	3919	1/1	0.98	0.07	30,30,30,30	0
57	MG	1A	3104	1/1	0.98	0.04	25,25,25,25	0
57	MG	1A	4065	1/1	0.98	0.11	44,44,44,44	0
57	MG	1A	3358	1/1	0.98	0.29	27,27,27,27	0
57	MG	1a	1612	1/1	0.98	0.07	26,26,26,26	0
57	MG	2A	3378	1/1	0.98	0.13	53,53,53,53	0
57	MG	2A	3379	1/1	0.98	0.11	25,25,25,25	0
57	MG	2A	3734	1/1	0.98	0.11	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	1A	3227	1/1	0.98	0.07	28,28,28,28	0
57	MG	1A	3614	1/1	0.98	0.09	28,28,28,28	0
57	MG	1A	4069	1/1	0.98	0.14	47,47,47,47	0
57	MG	1A	3924	1/1	0.98	0.04	54,54,54,54	0
57	MG	1A	3150	1/1	0.98	0.07	36,36,36,36	0
57	MG	1A	3792	1/1	0.98	0.04	27,27,27,27	0
57	MG	2A	3741	1/1	0.98	0.09	47,47,47,47	0
57	MG	1a	1707	1/1	0.98	0.03	32,32,32,32	0
57	MG	1a	1708	1/1	0.98	0.08	34,34,34,34	0
57	MG	23	102	1/1	0.98	0.06	59,59,59,59	0
57	MG	1a	1709	1/1	0.98	0.07	36,36,36,36	0
57	MG	2A	3389	1/1	0.98	0.04	37,37,37,37	0
57	MG	1A	3793	1/1	0.98	0.29	24,24,24,24	0
57	MG	1A	3670	1/1	0.98	0.08	22,22,22,22	0
57	MG	1A	3616	1/1	0.98	0.04	28,28,28,28	0
57	MG	1a	1622	1/1	0.98	0.06	53,53,53,53	0
57	MG	1D	301	1/1	0.98	0.14	35,35,35,35	0
57	MG	2A	3629	1/1	0.98	0.04	40,40,40,40	0
57	MG	1A	4000	1/1	0.98	0.05	36,36,36,36	0
57	MG	1V	201	1/1	0.98	0.19	40,40,40,40	0
57	MG	1A	3733	1/1	0.98	0.07	58,58,58,58	0
57	MG	1D	304	1/1	0.98	0.04	21,21,21,21	0
57	MG	1a	1719	1/1	0.98	0.06	58,58,58,58	0
57	MG	2A	3759	1/1	0.98	0.13	63,63,63,63	0
57	MG	1A	3037	1/1	0.98	0.14	37,37,37,37	0
57	MG	2A	3075	1/1	0.98	0.23	40,40,40,40	0
57	MG	2A	3637	1/1	0.98	0.05	56,56,56,56	0
57	MG	1A	3326	1/1	0.98	0.17	40,40,40,40	0
57	MG	1A	3481	1/1	0.98	0.18	24,24,24,24	0
57	MG	1D	308	1/1	0.98	0.17	44,44,44,44	0
57	MG	1A	3401	1/1	0.98	0.17	39,39,39,39	0
57	MG	1D	310	1/1	0.98	0.23	27,27,27,27	0
57	MG	2A	3768	1/1	0.98	0.06	45,45,45,45	0
57	MG	1W	203	1/1	0.98	0.23	43,43,43,43	0
57	MG	1A	3571	1/1	0.98	0.07	30,30,30,30	0
57	MG	1A	3363	1/1	0.98	0.31	44,44,44,44	0
57	MG	1A	4085	1/1	0.98	0.05	61,61,61,61	0
57	MG	1A	3623	1/1	0.98	0.04	24,24,24,24	0
57	MG	1A	3134	1/1	0.98	0.27	41,41,41,41	0
57	MG	1A	3057	1/1	0.98	0.06	38,38,38,38	0
57	MG	2A	3088	1/1	0.98	0.06	47,47,47,47	0
57	MG	1A	3366	1/1	0.98	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	3807	1/1	0.98	0.15	33,33,33,33	0
57	MG	1A	3154	1/1	0.98	0.06	42,42,42,42	0
59	ZN	29	501	1/1	0.98	0.04	84,84,84,84	0
57	MG	1A	3178	1/1	0.98	0.10	41,41,41,41	0
60	SF4	2d	501	8/8	0.98	0.04	61,68,76,83	0
57	MG	1A	4078	1/1	0.99	0.06	34,34,34,34	0
57	MG	1a	1728	1/1	0.99	0.04	55,55,55,55	0
57	MG	1A	4016	1/1	0.99	0.02	23,23,23,23	0
57	MG	2A	3754	1/1	0.99	0.06	33,33,33,33	0
57	MG	15	101	1/1	0.99	0.21	44,44,44,44	0
57	MG	1A	3894	1/1	0.99	0.07	43,43,43,43	0
57	MG	1a	1759	1/1	0.99	0.07	70,70,70,70	0
57	MG	1a	1760	1/1	0.99	0.04	57,57,57,57	0
57	MG	2A	3643	1/1	0.99	0.04	38,38,38,38	0
57	MG	1A	3034	1/1	0.99	0.27	29,29,29,29	0
57	MG	1A	3747	1/1	0.99	0.05	44,44,44,44	0
57	MG	2A	3646	1/1	0.99	0.04	39,39,39,39	0
57	MG	1A	3981	1/1	0.99	0.03	28,28,28,28	0
57	MG	1A	3095	1/1	0.99	0.12	19,19,19,19	0
57	MG	1A	3024	1/1	0.99	0.16	29,29,29,29	0
57	MG	1a	1766	1/1	0.99	0.03	48,48,48,48	0
57	MG	2A	3038	1/1	0.99	0.15	31,31,31,31	0
57	MG	1A	3899	1/1	0.99	0.02	24,24,24,24	0
57	MG	1A	3828	1/1	0.99	0.11	33,33,33,33	0
57	MG	1A	3690	1/1	0.99	0.04	15,15,15,15	0
57	MG	1A	3987	1/1	0.99	0.04	40,40,40,40	0
57	MG	1R	203	1/1	0.99	0.28	39,39,39,39	0
57	MG	1A	3169	1/1	0.99	0.04	31,31,31,31	0
57	MG	2A	3512	1/1	0.99	0.04	43,43,43,43	0
57	MG	1A	3202	1/1	0.99	0.13	33,33,33,33	0
57	MG	1a	1774	1/1	0.99	0.05	61,61,61,61	0
57	MG	1A	4049	1/1	0.99	0.06	28,28,28,28	0
57	MG	1a	1745	1/1	0.99	0.04	67,67,67,67	0
57	MG	1A	3672	1/1	0.99	0.08	32,32,32,32	0
57	MG	1A	3071	1/1	0.99	0.10	15,15,15,15	0
57	MG	1a	1779	1/1	0.99	0.04	62,62,62,62	0
57	MG	1A	3171	1/1	0.99	0.04	35,35,35,35	0
57	MG	1A	3039	1/1	0.99	0.15	31,31,31,31	0
59	ZN	1Y	203	1/1	0.99	0.03	72,72,72,72	0
57	MG	2A	3486	1/1	0.99	0.05	45,45,45,45	0
59	ZN	15	109	1/1	0.99	0.03	43,43,43,43	0
59	ZN	16	103	1/1	0.99	0.03	42,42,42,42	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	ZN	19	102	1/1	0.99	0.04	46,46,46,46	0
59	ZN	1n	102	1/1	0.99	0.03	68,68,68,68	0
57	MG	1A	3013	1/1	0.99	0.07	29,29,29,29	0
57	MG	2A	3419	1/1	0.99	0.06	64,64,64,64	0
59	ZN	25	104	1/1	0.99	0.05	60,60,60,60	0
57	MG	1A	3709	1/1	0.99	0.06	23,23,23,23	0
57	MG	13	101	1/1	0.99	0.05	32,32,32,32	0
60	SF4	1d	302	8/8	0.99	0.04	58,66,72,72	0
57	MG	1A	3926	1/1	0.99	0.04	51,51,51,51	0
57	MG	2A	3742	1/1	1.00	0.06	37,37,37,37	0
59	ZN	26	501	1/1	1.00	0.03	60,60,60,60	0

6.5 Other polymers (i)

There are no such residues in this entry.