Full wwPDB X-ray Structure Validation Report (i)

Mar 28, 2026 – 02:37 PM UTC

PDB ID	:	8VTU / pdb_00008vtu
Title	:	Crystal structure of the wild-type Thermus thermophilus 70S ribosome in complex with macrolone MCX-66, mRNA, aminoacylated A-site Phe-tRNAphe, aminoacylated P-site fMet-tRNAmet, and deacylated E-site tRNAphe at 2.40A resolution
Authors	:	Aleksandrova, E.V.; Ma, C.-X.; Klepacki, D.; Alizadeh, F.; Vazquez-Laslop, N.; Liang, J.-H.; Polikanov, Y.S.; Mankin, A.S.
Deposited on	:	2024-01-27
Resolution	:	2.40 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

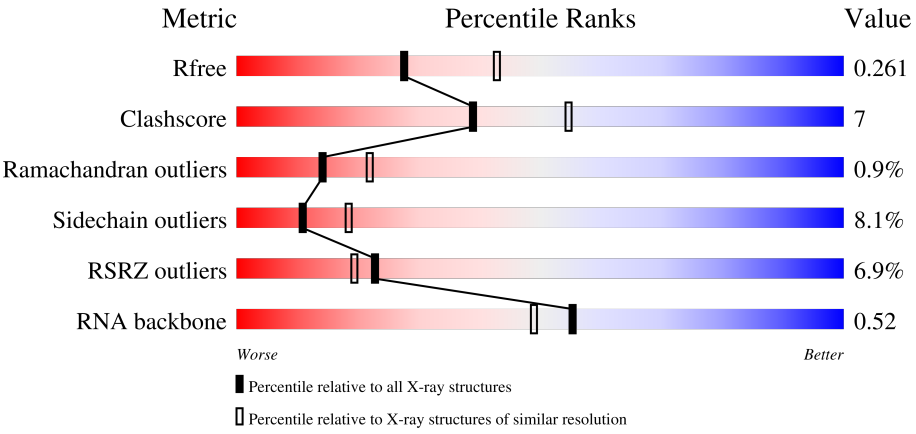
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)
RNA backbone	3983	1155 (2.70-2.10)

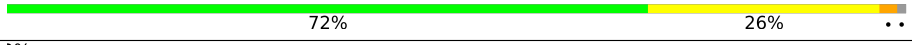
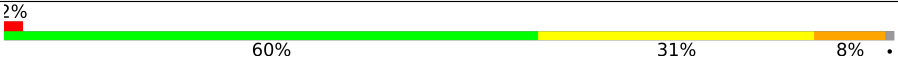
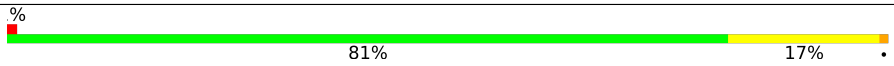
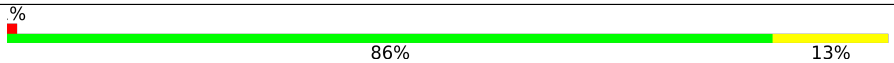
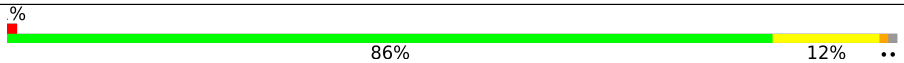
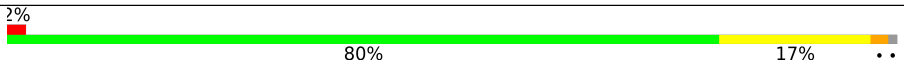
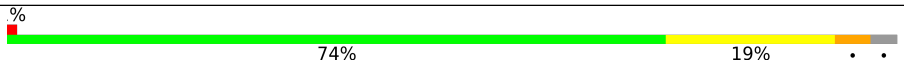
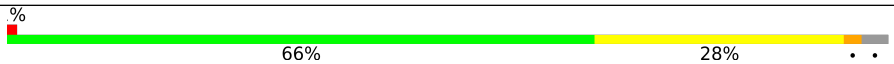
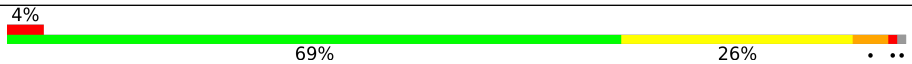
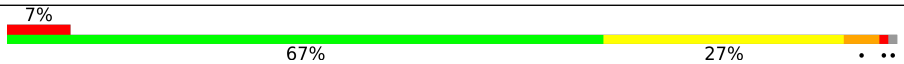
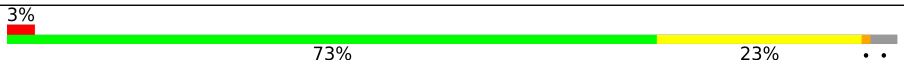
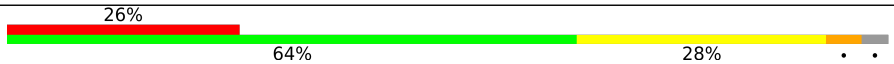
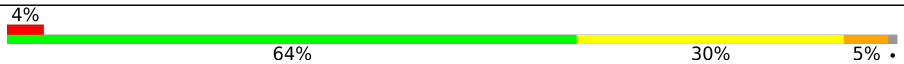
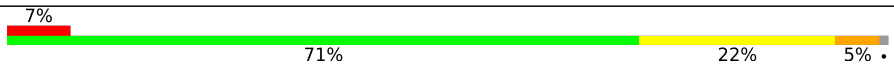
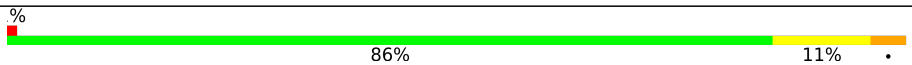
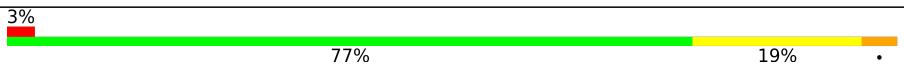
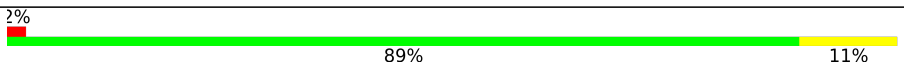
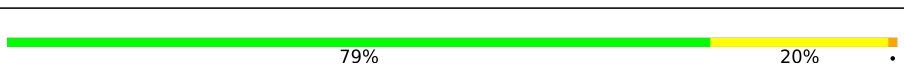
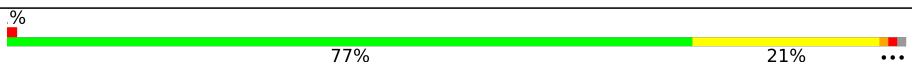
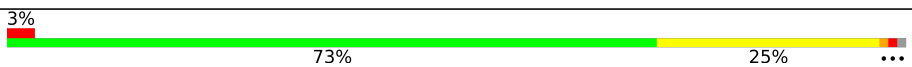
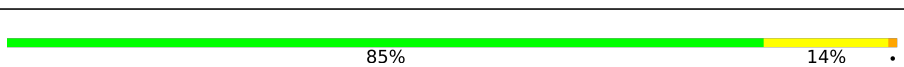
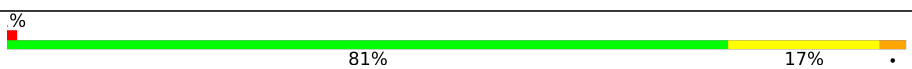
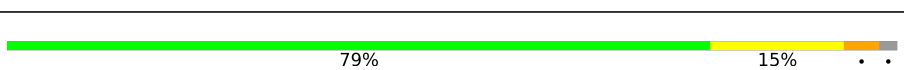
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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% 70% 23% 5% ·
1	2A	2915	5% 64% 26% 6% ·

Continued on next page...

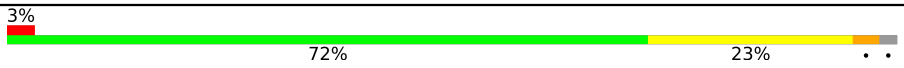
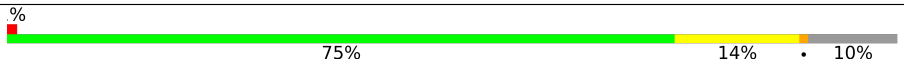
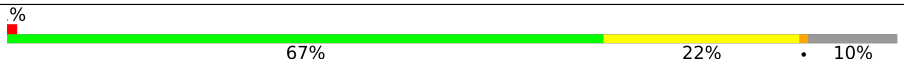
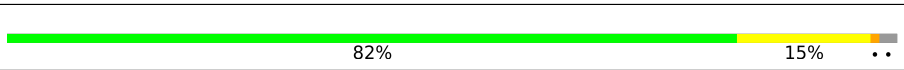
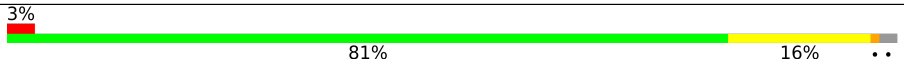
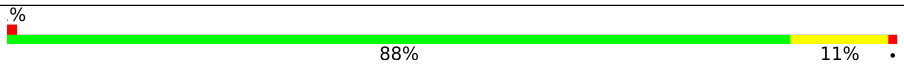
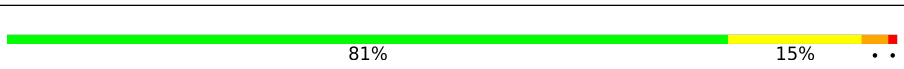
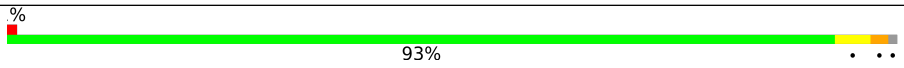
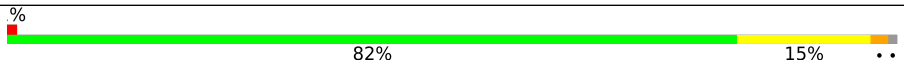
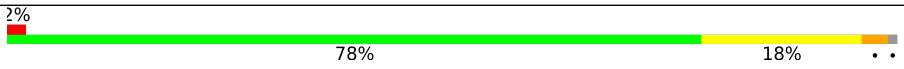
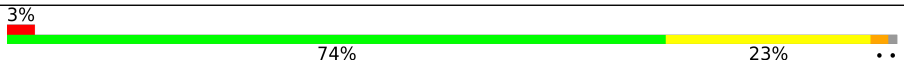
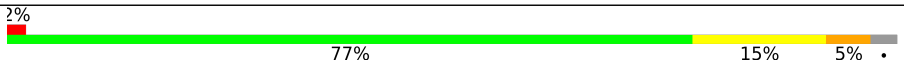
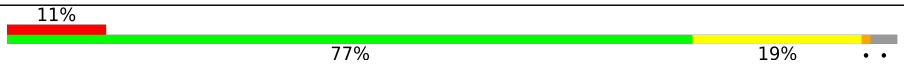
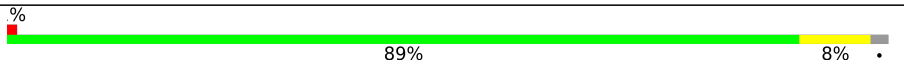
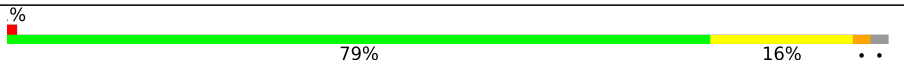
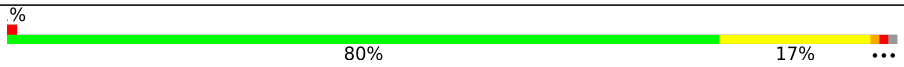
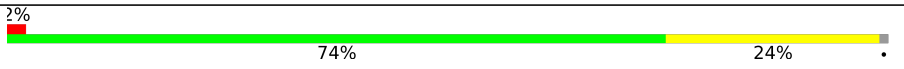
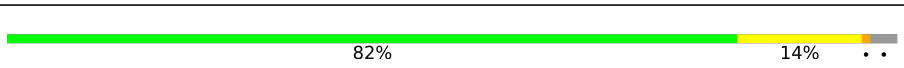
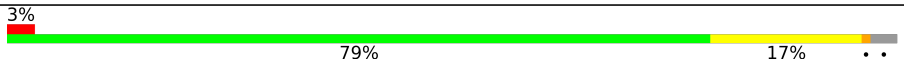
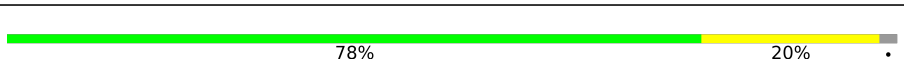
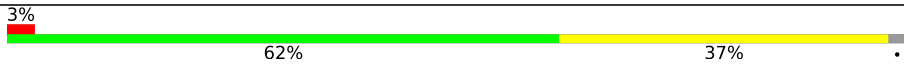
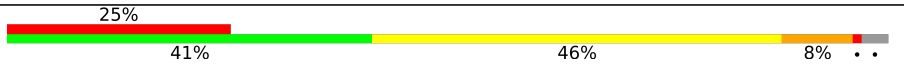
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

Continued from previous page...

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

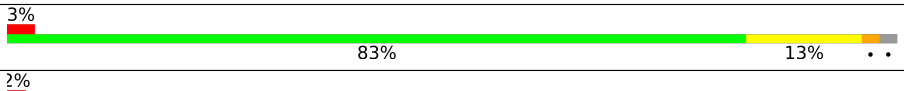
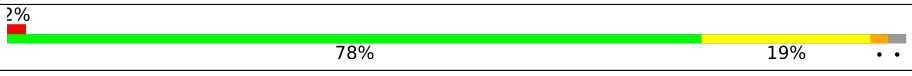
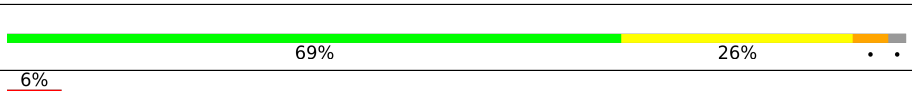
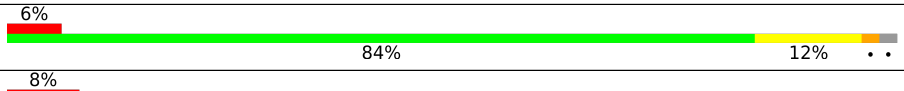
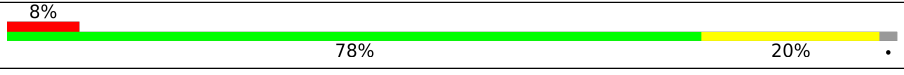
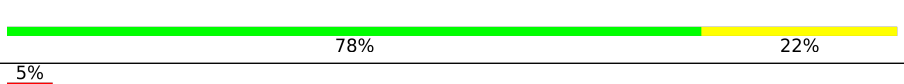
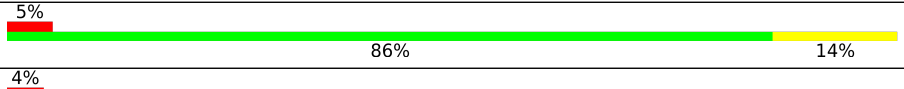
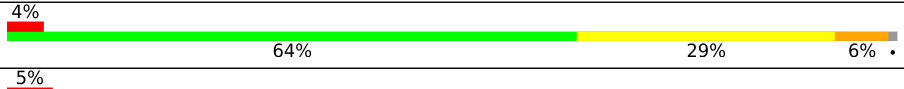
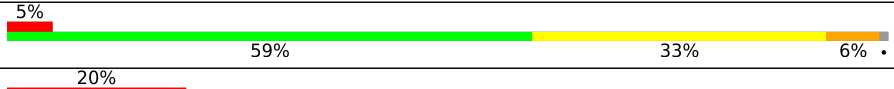
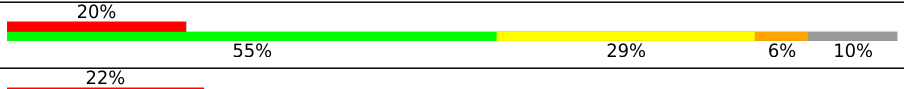
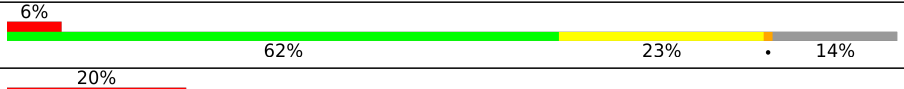
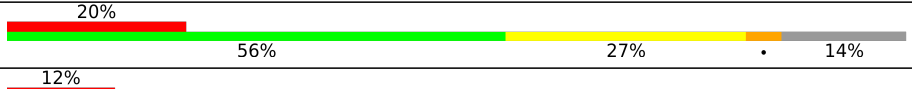
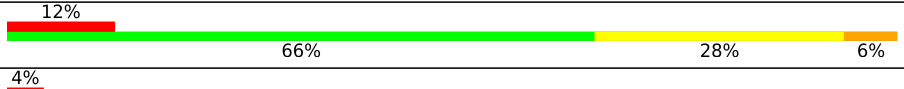
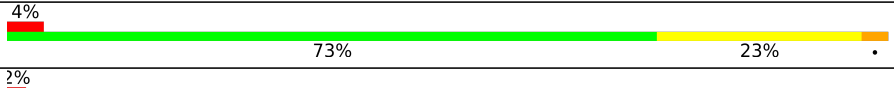
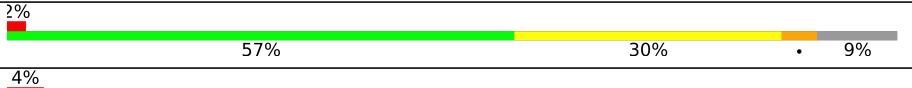
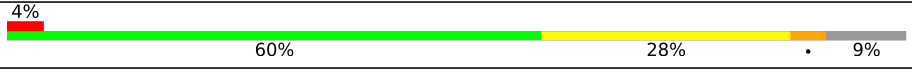
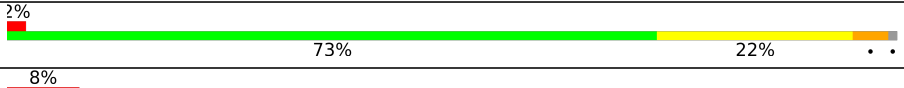
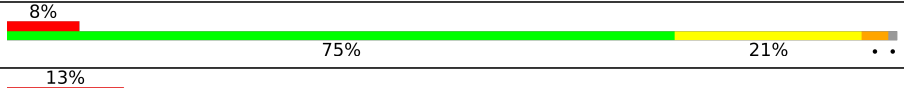
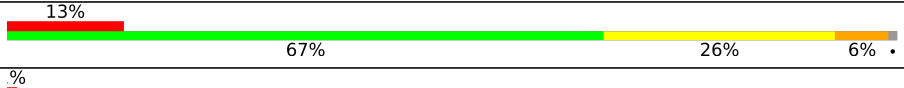
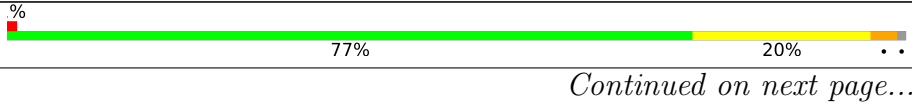
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
14	2S	112	
15	1T	146	
15	2T	146	
16	1U	118	
16	2U	118	
17	1V	101	
17	2V	101	
18	1W	113	
18	2W	113	
19	1X	96	
19	2X	96	
20	1Y	110	
20	2Y	110	
21	1Z	206	
21	2Z	206	
22	10	85	
22	20	85	
23	11	98	
23	21	98	
24	12	72	
24	22	72	
25	13	60	
25	23	60	
26	14	71	
26	24	71	

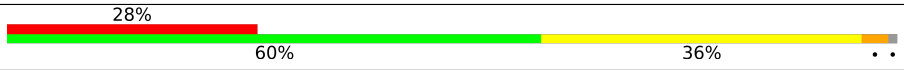
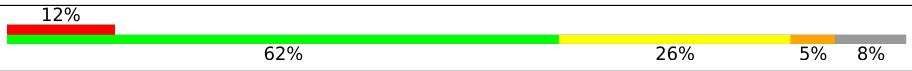
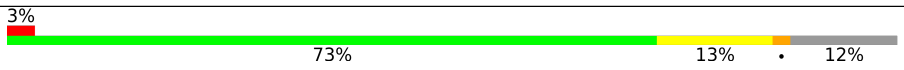
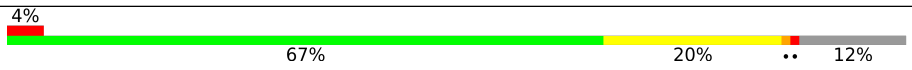
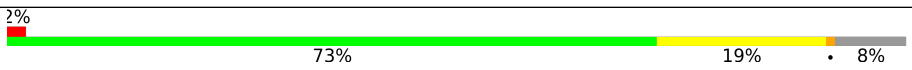
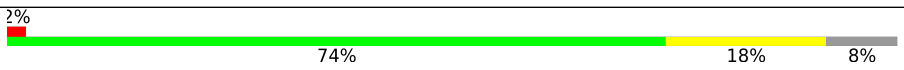
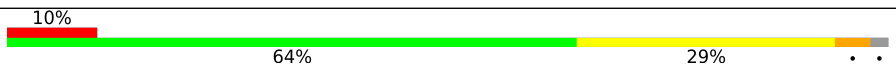
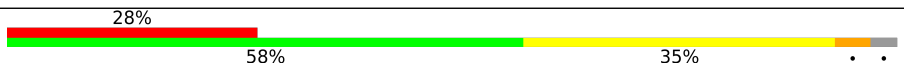
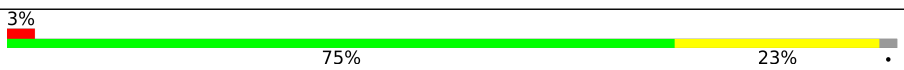
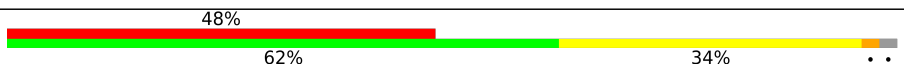
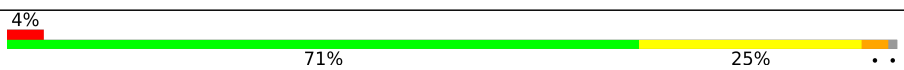
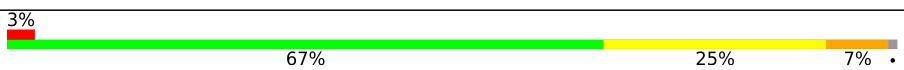
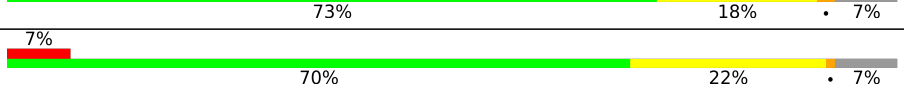
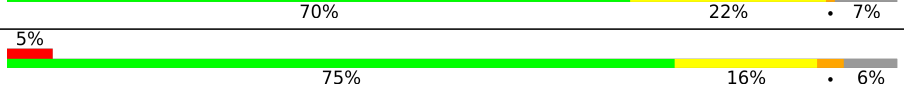
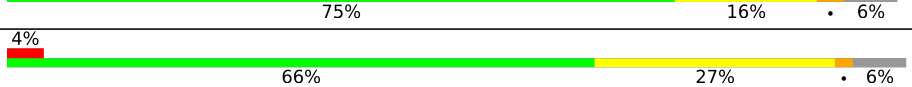
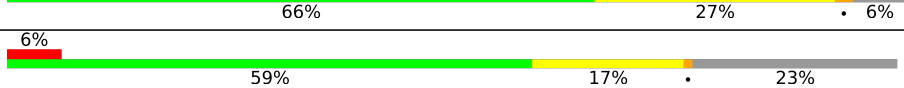
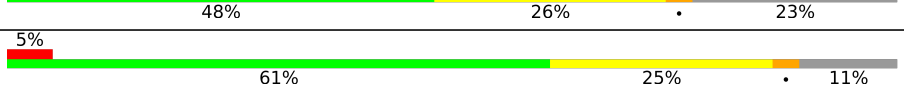
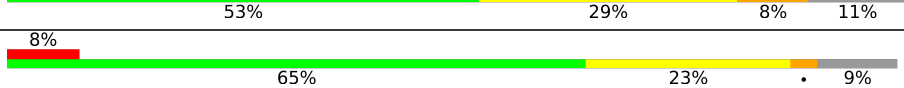
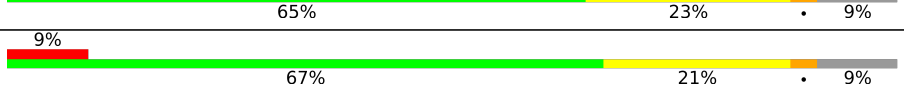
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
27	15	60	
27	25	60	
28	16	54	
28	26	54	
29	17	49	
29	27	49	
30	18	65	
30	28	65	
31	19	37	
31	29	37	
32	1a	1521	
32	2a	1521	
33	1b	256	
33	2b	256	
34	1c	239	
34	2c	239	
35	1d	209	
35	2d	209	
36	1e	162	
36	2e	162	
37	1f	101	
37	2f	101	
38	1g	156	
38	2g	156	
39	1h	138	

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
52	1u	27	7% 67% 15% 15%
52	2u	27	41% 56% 22% 7% 15%
53	1v	24	12% 42% 8% 46%
53	2v	24	12% 38% 12% 46%
54	1w	76	9% 39% 47% 9%
54	2w	76	11% 37% 46% 11% 5%
55	1x	77	4% 81% 14% 5%
55	2x	77	% 74% 22%
56	1y	76	61% 28% 38% 28%
56	2y	76	61% 26% 47% 21%

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	10	107	-	-	-	X
57	MG	1U	211	-	-	-	X
57	MG	2A	3306	-	-	-	X
57	MG	2v	102	-	-	-	X

2 Entry composition

There are 64 unique types of molecules in this entry. The entry contains 300455 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	1F	203	Total	C	N	O	S	0	0	1
			1584	1009	298	275	2			
5	2F	203	Total	C	N	O	S	0	0	1
			1580	1007	297	274	2			

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	2O	122	Total 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 Aminoacylated Phe-tRNAphe.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1w	74	Total	C	N	O	P	S	0	0	0
			1592	713	286	517	74	2			
54	2w	72	Total	C	N	O	P	S	0	0	0
			1544	690	279	501	72	2			

- Molecule 55 is a RNA chain called Aminoacylated fMet-tRNAmet.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
55	1x	77	Total	C	N	O	P	S	0	0	0
			1646	734	298	536	77	1			
55	2x	77	Total	C	N	O	P	S	0	0	0
			1646	734	298	536	77	1			

- Molecule 56 is a RNA chain called 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	1117	Total	Mg	0	0
			1117	1117		
57	1B	37	Total	Mg	0	0
			37	37		
57	1D	15	Total	Mg	0	0
			15	15		
57	1E	15	Total	Mg	0	0
			15	15		
57	1F	12	Total	Mg	0	0
			12	12		

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	16	1	Total Mg 1 1	0	0
57	17	5	Total Mg 5 5	0	0
57	18	5	Total Mg 5 5	0	0
57	19	1	Total Mg 1 1	0	0
57	1a	222	Total Mg 222 222	0	0
57	1b	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	1h	1	Total Mg 1 1	0	0
57	1j	1	Total Mg 1 1	0	0
57	1k	1	Total Mg 1 1	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	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	842	Total Mg 842 842	0	0
57	2B	18	Total Mg 18 18	0	0
57	2D	9	Total Mg 9 9	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	2E	8	Total Mg 8 8	0	0
57	2F	8	Total Mg 8 8	0	0
57	2G	1	Total Mg 1 1	0	0
57	2N	1	Total Mg 1 1	0	0
57	2O	2	Total Mg 2 2	0	0
57	2P	1	Total Mg 1 1	0	0
57	2Q	3	Total Mg 3 3	0	0
57	2R	3	Total Mg 3 3	0	0
57	2T	4	Total Mg 4 4	0	0
57	2U	2	Total Mg 2 2	0	0
57	2V	2	Total Mg 2 2	0	0
57	2W	1	Total Mg 1 1	0	0
57	2X	2	Total Mg 2 2	0	0
57	2Y	1	Total Mg 1 1	0	0
57	2Z	1	Total Mg 1 1	0	0
57	20	1	Total Mg 1 1	0	0
57	21	3	Total Mg 3 3	0	0
57	23	2	Total Mg 2 2	0	0
57	25	4	Total Mg 4 4	0	0
57	27	2	Total Mg 2 2	0	0
57	28	2	Total Mg 2 2	0	0

Continued on next page...

Continued from previous page...

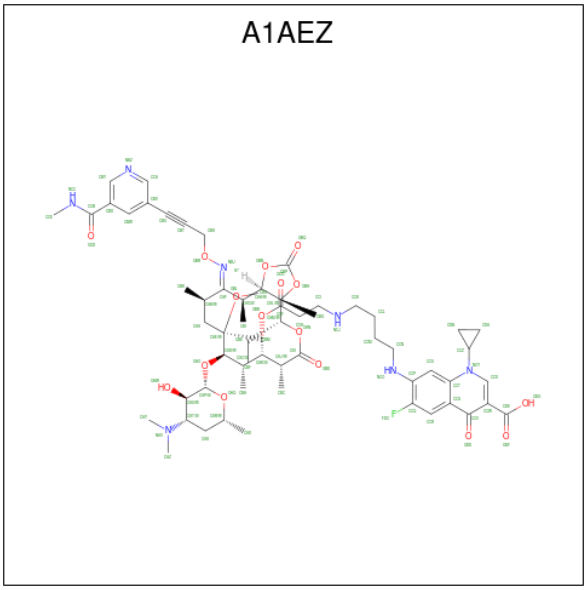
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	2a	231	Total Mg 231 231	0	0
57	2d	1	Total Mg 1 1	0	0
57	2e	1	Total Mg 1 1	0	0
57	2f	2	Total Mg 2 2	0	0
57	2g	1	Total Mg 1 1	0	0
57	2j	1	Total Mg 1 1	0	0
57	2l	4	Total Mg 4 4	0	0
57	2m	1	Total Mg 1 1	0	0
57	2q	2	Total Mg 2 2	0	0
57	2r	1	Total Mg 1 1	0	0
57	2t	1	Total Mg 1 1	0	0
57	2v	2	Total Mg 2 2	0	0
57	2w	7	Total Mg 7 7	0	0
57	2x	7	Total Mg 7 7	0	0
57	2y	2	Total Mg 2 2	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 1-cyclopropyl-7-[(4-{[3-({(3aR,4R,7R,8S,9S,10R,11R,13R,14E,15S,15aR)-10-{[(2S,3R,4S,6R)-4-(dimethylamino)-3-hydroxy-6-methyloxan-2-yl]oxy}-4-ethyl-11-methoxy-3a,7,9,11,13,15-hexamethyl-14-[({3-[5-(methylcarbamoyl)pyridin-3-yl]prop-2-yn-1-yl}oxy)imino]-2,6-dioxododecahydro-2H,4H-[1,3]dioxolo[4,5-c]oxacyclotetradecin-8-yl}ox

y)-3-oxopropyl]amino}butyl)amino]-6-fluoro-4-oxo-1,4-dihydroquinoline-3-carboxylic acid (non-preferred name) (CCD ID: A1AEZ) (formula: $C_{61}H_{84}FN_7O_{16}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
59	1A	1	Total	C	F	N	O	0	0
			85	61	1	7	16		
59	2A	1	Total	C	F	N	O	0	0
			85	61	1	7	16		

- Molecule 60 is ZINC ION (CCD ID: ZN) (formula: Zn).

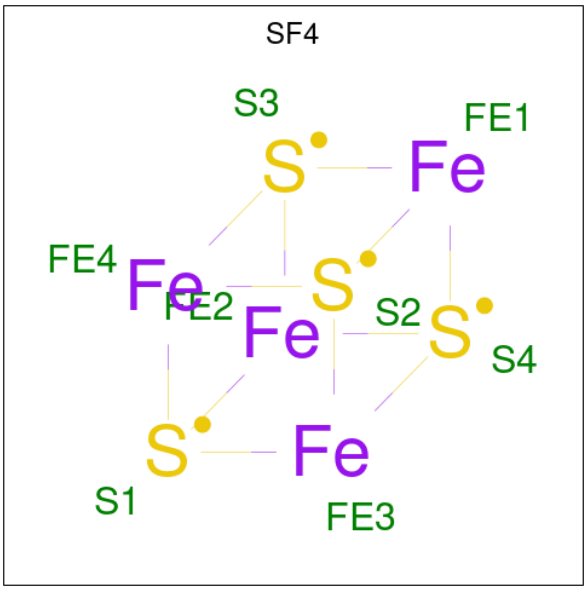
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1Y	1	Total	Zn	0	0
			1	1		
60	14	1	Total	Zn	0	0
			1	1		
60	15	1	Total	Zn	0	0
			1	1		
60	16	1	Total	Zn	0	0
			1	1		
60	19	1	Total	Zn	0	0
			1	1		
60	1n	1	Total	Zn	0	0
			1	1		
60	2Y	1	Total	Zn	0	0
			1	1		
60	24	1	Total	Zn	0	0
			1	1		

Continued on next page...

Continued from previous page...

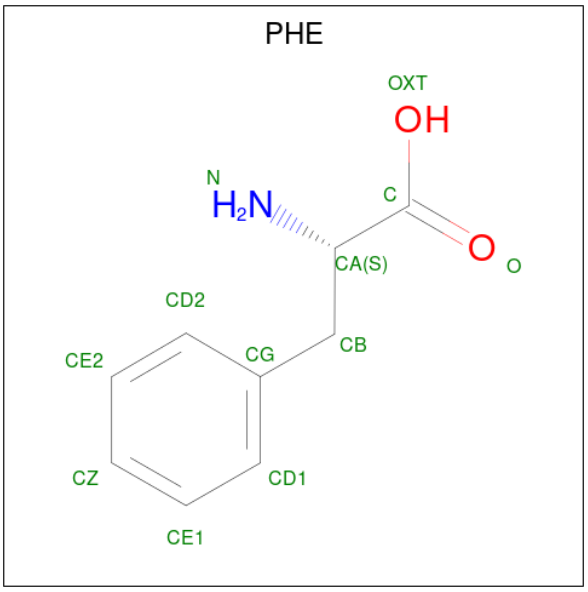
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	25	1	Total Zn 1 1	0	0
60	26	1	Total Zn 1 1	0	0
60	29	1	Total Zn 1 1	0	0
60	2n	1	Total Zn 1 1	0	0

- Molecule 61 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



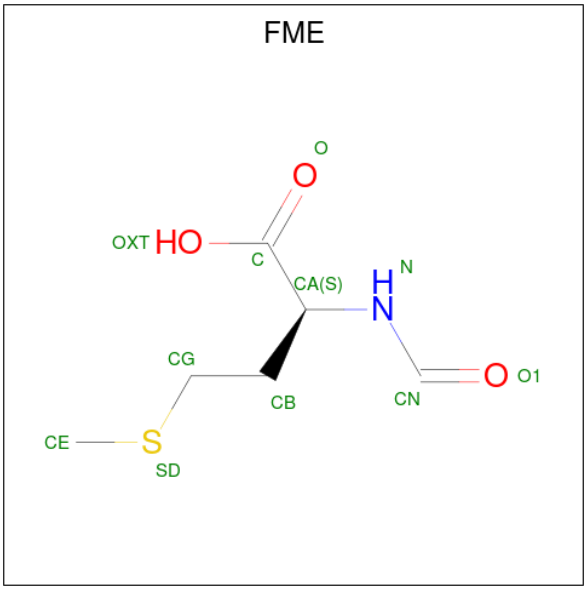
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1d	1	Total Fe S 8 4 4	0	0
61	2d	1	Total Fe S 8 4 4	0	0

- Molecule 62 is PHENYLALANINE (CCD ID: PHE) (formula: $C_9H_{11}NO_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
62	1w	1	Total C N O 11 9 1 1	0	0
62	2w	1	Total C N O 11 9 1 1	0	0

- Molecule 63 is N-FORMYLMETHIONINE (CCD ID: FME) (formula: $C_6H_{11}NO_3S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
63	1x	1	Total C N O S 10 6 1 2 1	0	0
63	2x	1	Total C N O S 10 6 1 2 1	0	0

- Molecule 64 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
64	1A	2052	Total O 2052 2052	0	0
64	1B	64	Total O 64 64	0	0
64	1D	31	Total O 31 31	0	0
64	1E	27	Total O 27 27	0	0
64	1F	19	Total O 19 19	0	0
64	1G	3	Total O 3 3	0	0
64	1H	2	Total O 2 2	0	0
64	1N	5	Total O 5 5	0	0
64	1O	6	Total O 6 6	0	0
64	1P	22	Total O 22 22	0	0
64	1Q	9	Total O 9 9	0	0
64	1R	9	Total O 9 9	0	0
64	1S	4	Total O 4 4	0	0
64	1T	8	Total O 8 8	0	0
64	1U	13	Total O 13 13	0	0
64	1V	8	Total O 8 8	0	0
64	1W	8	Total O 8 8	0	0
64	1X	4	Total O 4 4	0	0
64	1Y	2	Total O 2 2	0	0
64	1Z	1	Total O 1 1	0	0
64	10	12	Total O 12 12	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
64	11	9	Total O 9 9	0	0
64	12	3	Total O 3 3	0	0
64	13	4	Total O 4 4	0	0
64	14	1	Total O 1 1	0	0
64	15	6	Total O 6 6	0	0
64	16	2	Total O 2 2	0	0
64	17	9	Total O 9 9	0	0
64	18	10	Total O 10 10	0	0
64	1a	418	Total O 418 418	0	0
64	1b	1	Total O 1 1	0	0
64	1d	3	Total O 3 3	0	0
64	1e	1	Total O 1 1	0	0
64	1f	2	Total O 2 2	0	0
64	1g	1	Total O 1 1	0	0
64	1i	2	Total O 2 2	0	0
64	1j	2	Total O 2 2	0	0
64	1k	1	Total O 1 1	0	0
64	1l	5	Total O 5 5	0	0
64	1m	2	Total O 2 2	0	0
64	1p	1	Total O 1 1	0	0
64	1q	2	Total O 2 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
64	1r	1	Total O 1 1	0	0
64	1v	4	Total O 4 4	0	0
64	1w	15	Total O 15 15	0	0
64	1x	16	Total O 16 16	0	0
64	1y	1	Total O 1 1	0	0
64	2A	1183	Total O 1183 1183	0	0
64	2B	18	Total O 18 18	0	0
64	2D	22	Total O 22 22	0	0
64	2E	12	Total O 12 12	0	0
64	2F	12	Total O 12 12	0	0
64	2N	2	Total O 2 2	0	0
64	2O	2	Total O 2 2	0	0
64	2P	10	Total O 10 10	0	0
64	2Q	1	Total O 1 1	0	0
64	2R	4	Total O 4 4	0	0
64	2T	6	Total O 6 6	0	0
64	2U	2	Total O 2 2	0	0
64	2W	1	Total O 1 1	0	0
64	2X	2	Total O 2 2	0	0
64	2Y	2	Total O 2 2	0	0
64	20	2	Total O 2 2	0	0

Continued on next page...

Continued from previous page...

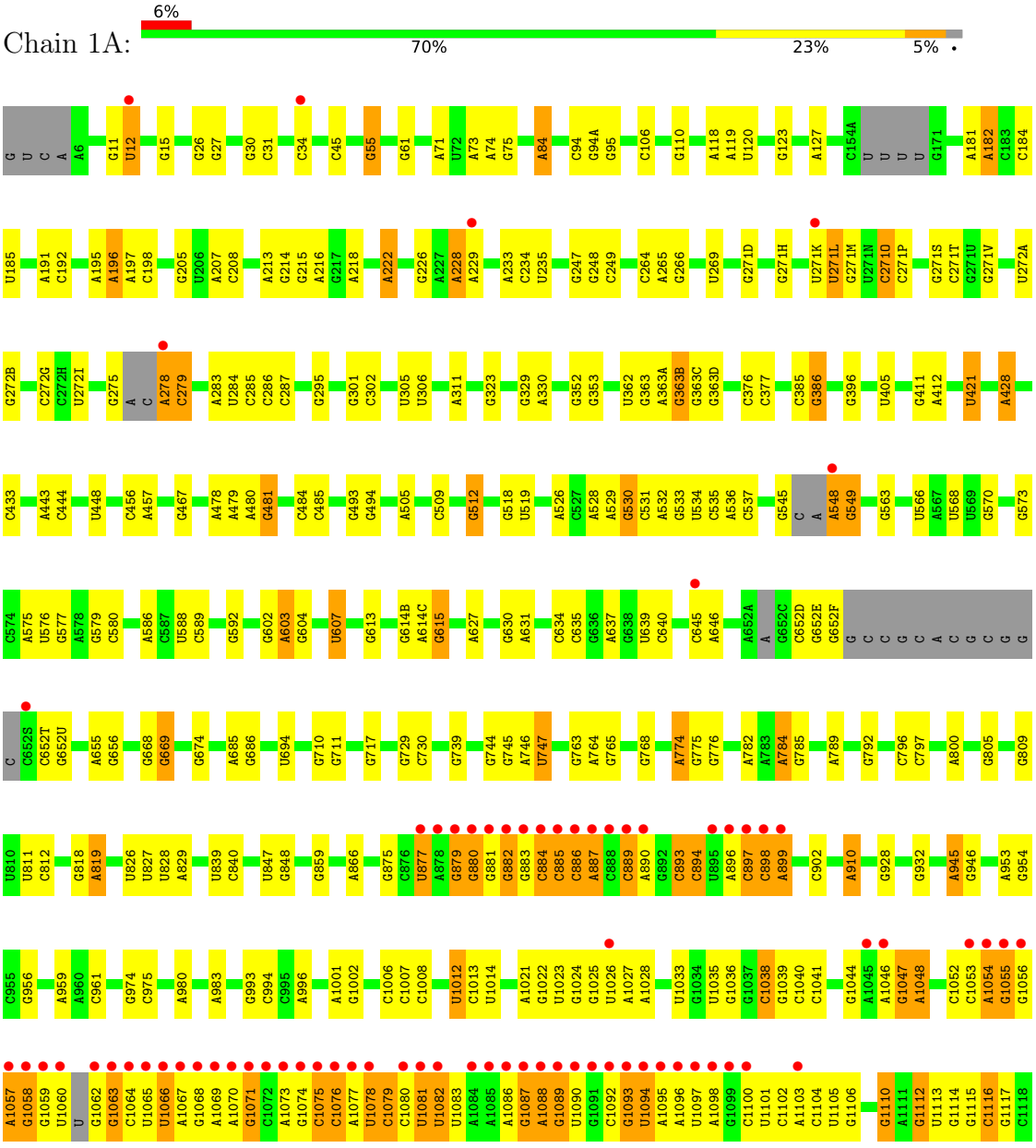
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
64	21	7	Total O 7 7	0	0
64	23	2	Total O 2 2	0	0
64	25	1	Total O 1 1	0	0
64	26	1	Total O 1 1	0	0
64	27	4	Total O 4 4	0	0
64	28	3	Total O 3 3	0	0
64	29	1	Total O 1 1	0	0
64	2a	265	Total O 265 265	0	0
64	2c	2	Total O 2 2	0	0
64	2d	3	Total O 3 3	0	0
64	2e	1	Total O 1 1	0	0
64	2g	1	Total O 1 1	0	0
64	2j	2	Total O 2 2	0	0
64	2l	6	Total O 6 6	0	0
64	2n	1	Total O 1 1	0	0
64	2p	1	Total O 1 1	0	0
64	2r	1	Total O 1 1	0	0
64	2t	5	Total O 5 5	0	0
64	2w	2	Total O 2 2	0	0
64	2x	7	Total O 7 7	0	0
64	2y	3	Total O 3 3	0	0

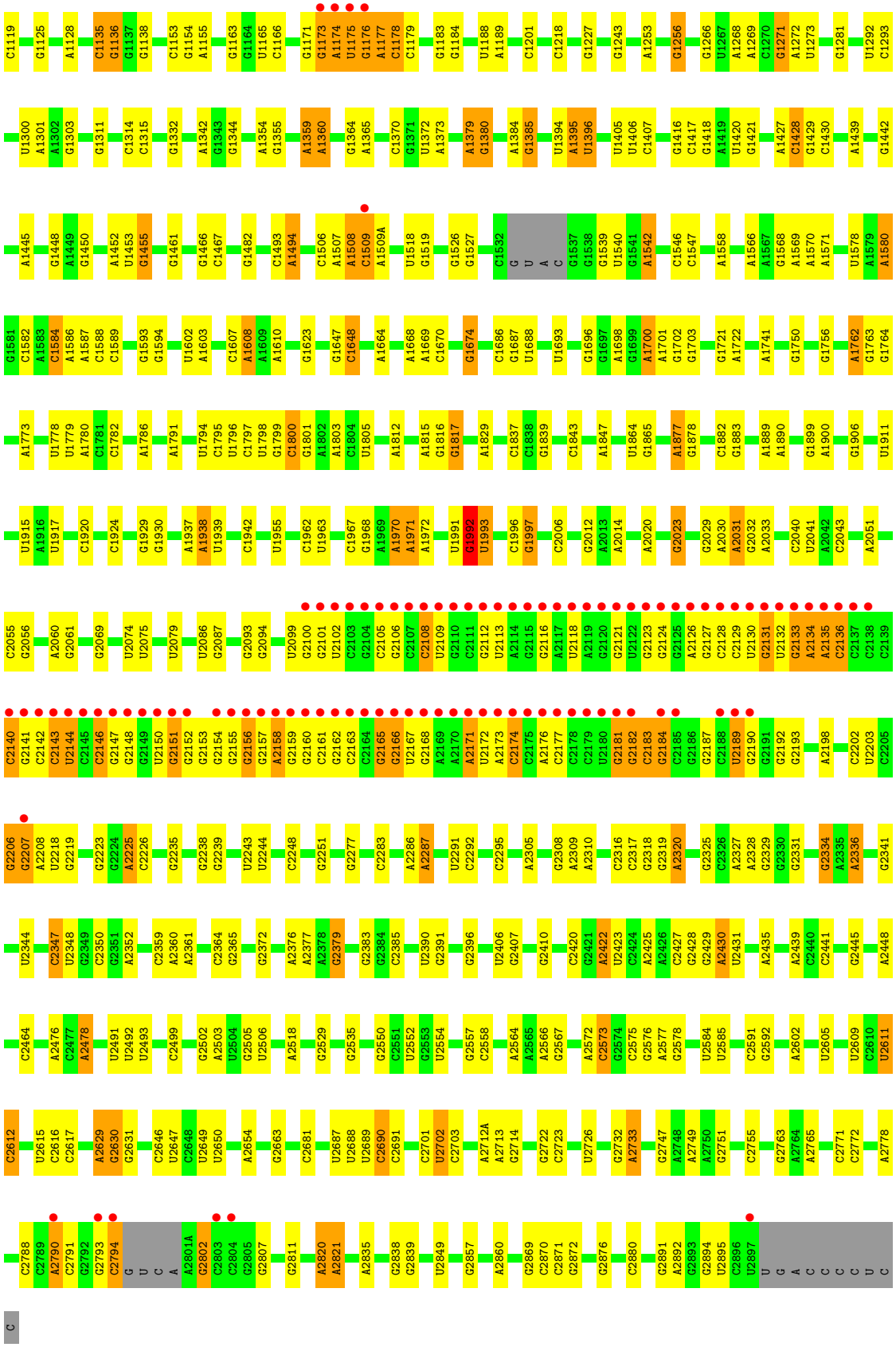
3 Residue-property plots (i)

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

- Molecule 1: 23S Ribosomal RNA

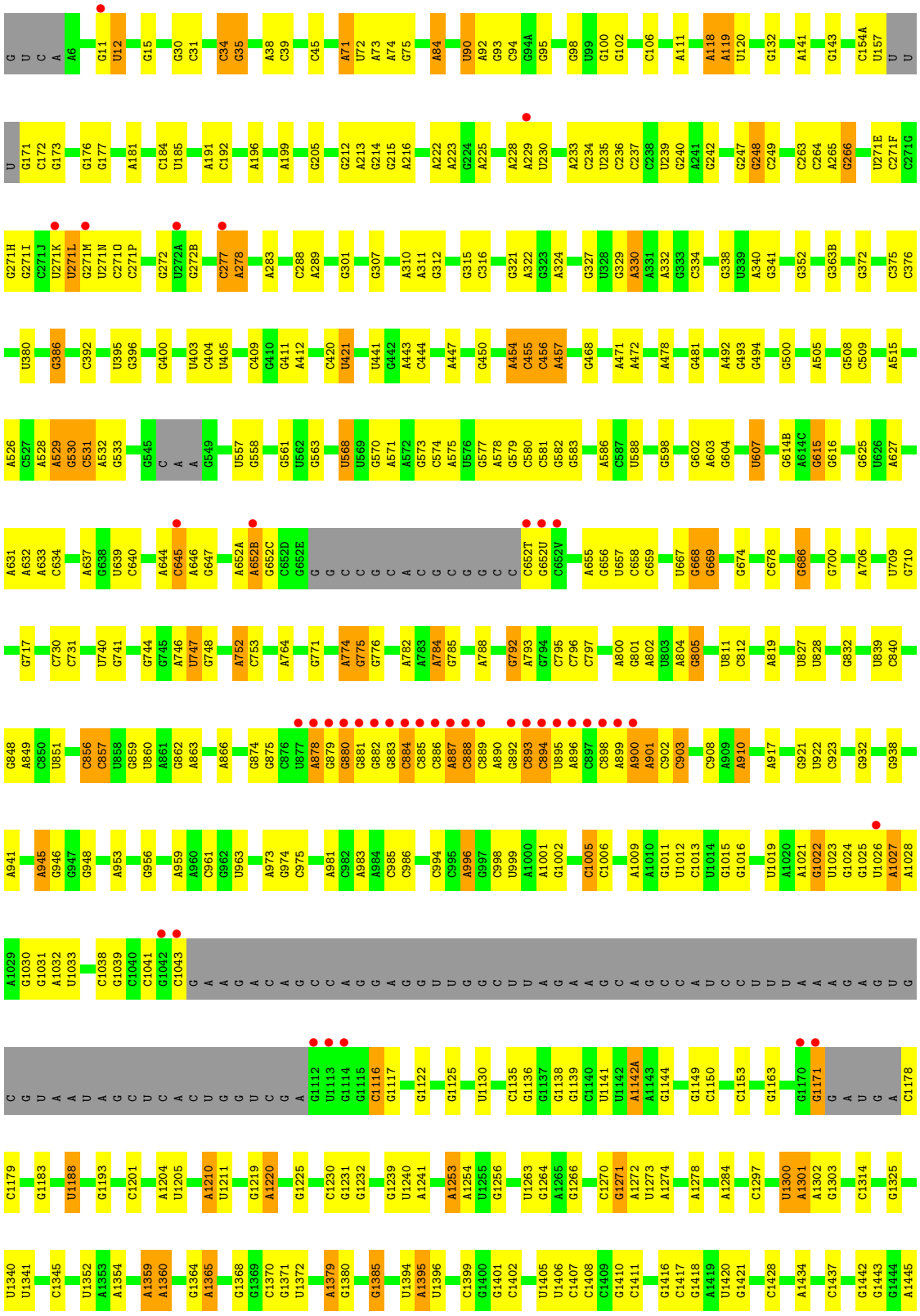
Chain 1A:

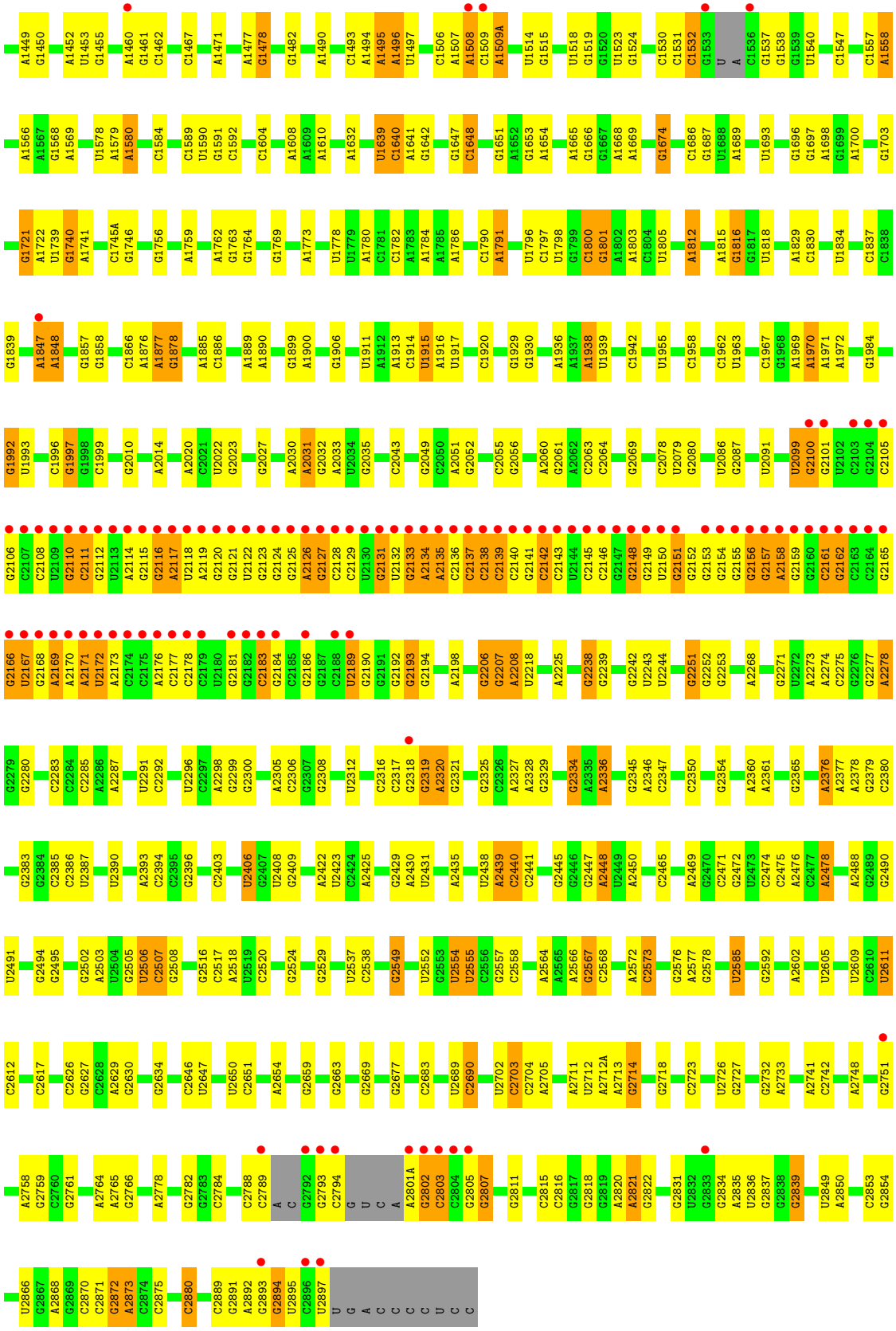




• Molecule 1: 23S Ribosomal RNA

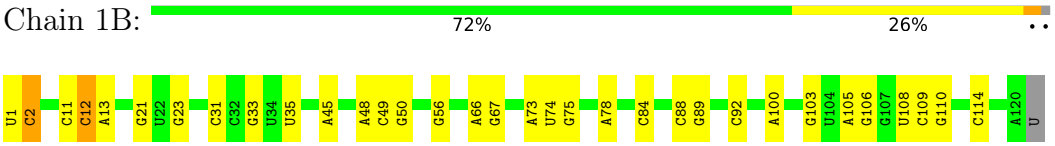
Chain 2A:





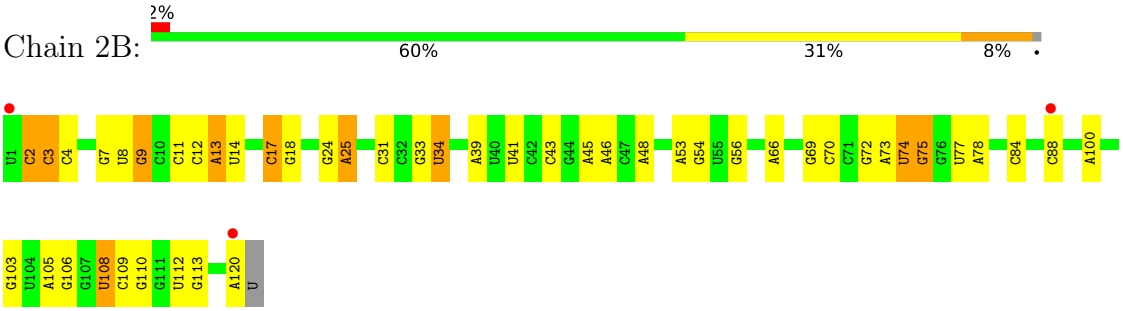
• Molecule 2: 5S Ribosomal RNA

Chain 1B:



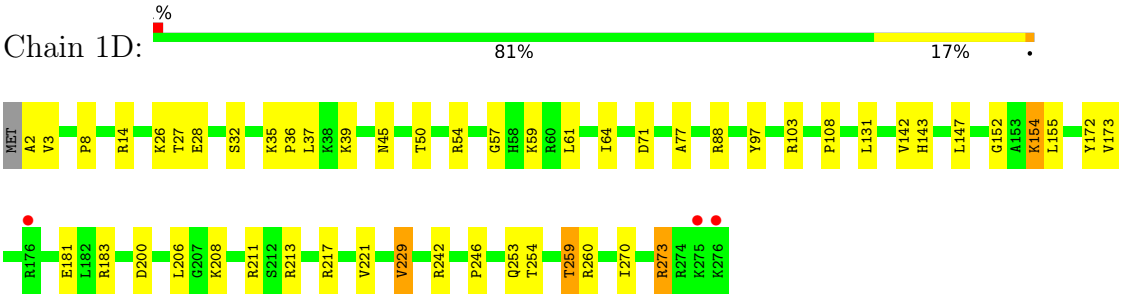
• Molecule 2: 5S Ribosomal RNA

Chain 2B:



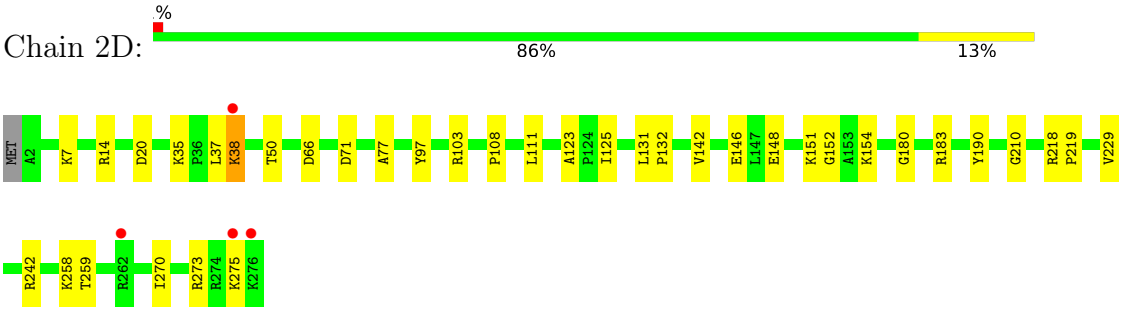
• Molecule 3: 50S ribosomal protein L2

Chain 1D:



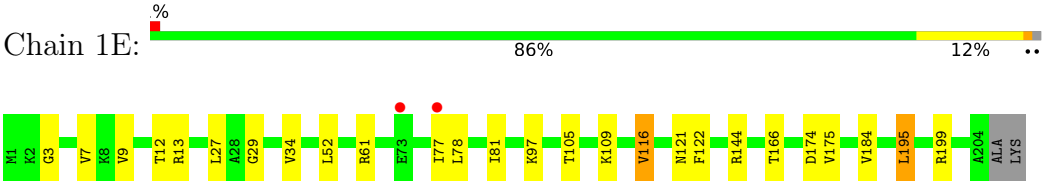
• Molecule 3: 50S ribosomal protein L2

Chain 2D:



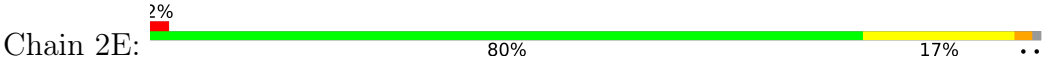
• Molecule 4: 50S ribosomal protein L3

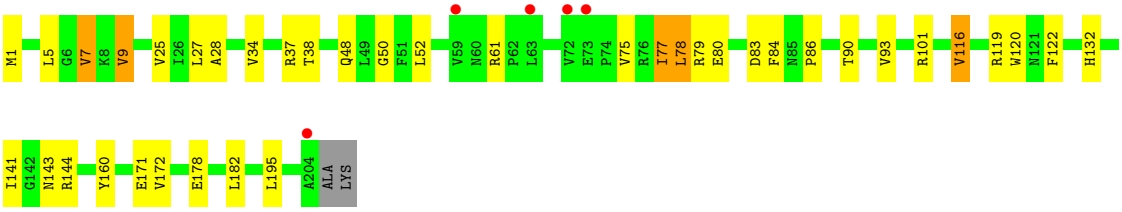
Chain 1E:



• Molecule 4: 50S ribosomal protein L3

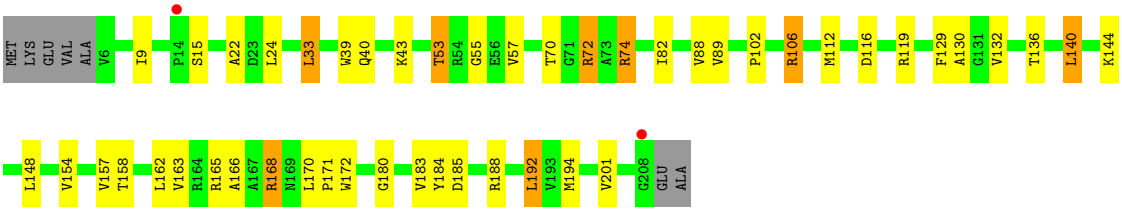
Chain 2E:





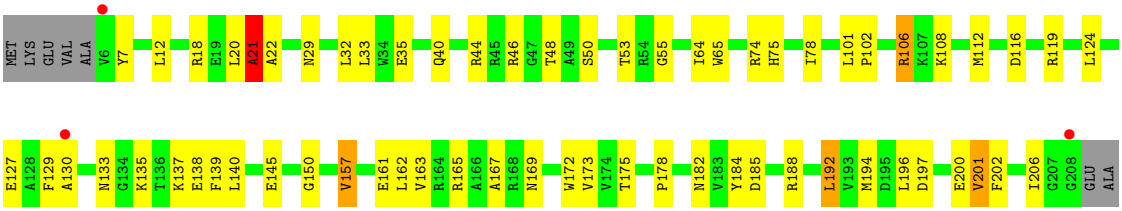
• Molecule 5: 50S ribosomal protein L4

Chain 1F:



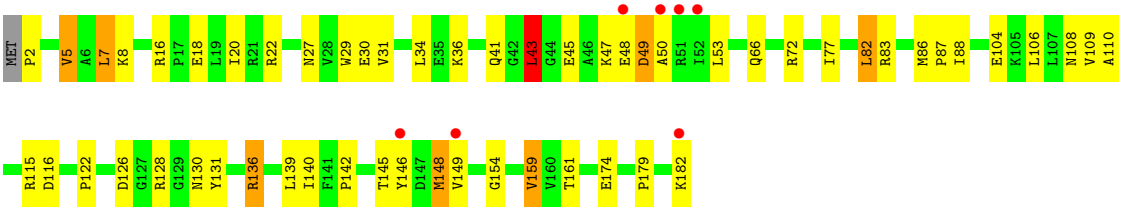
• Molecule 5: 50S ribosomal protein L4

Chain 2F:



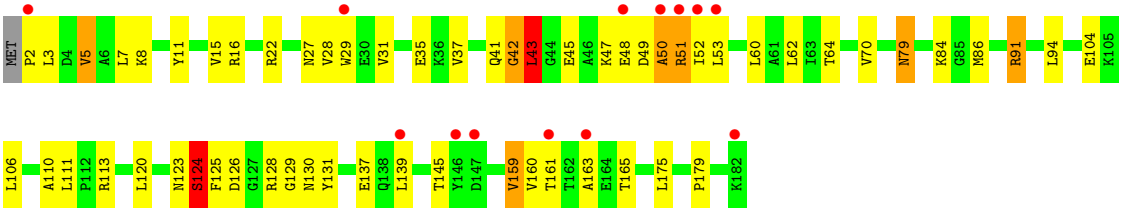
• Molecule 6: 50S ribosomal protein L5

Chain 1G:



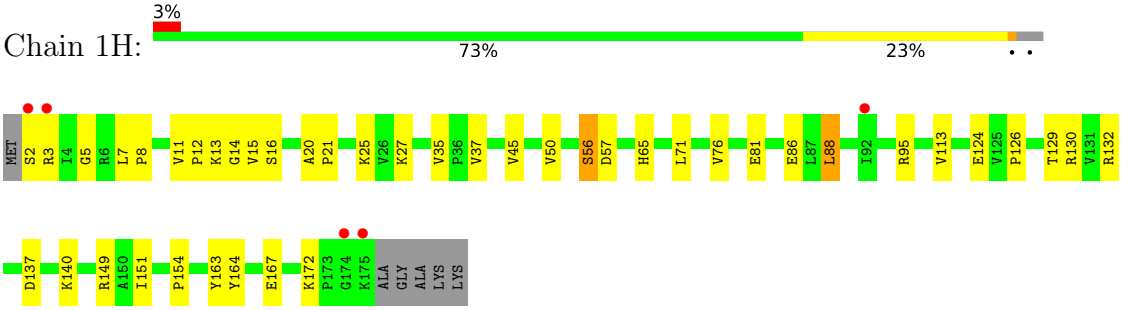
• Molecule 6: 50S ribosomal protein L5

Chain 2G:



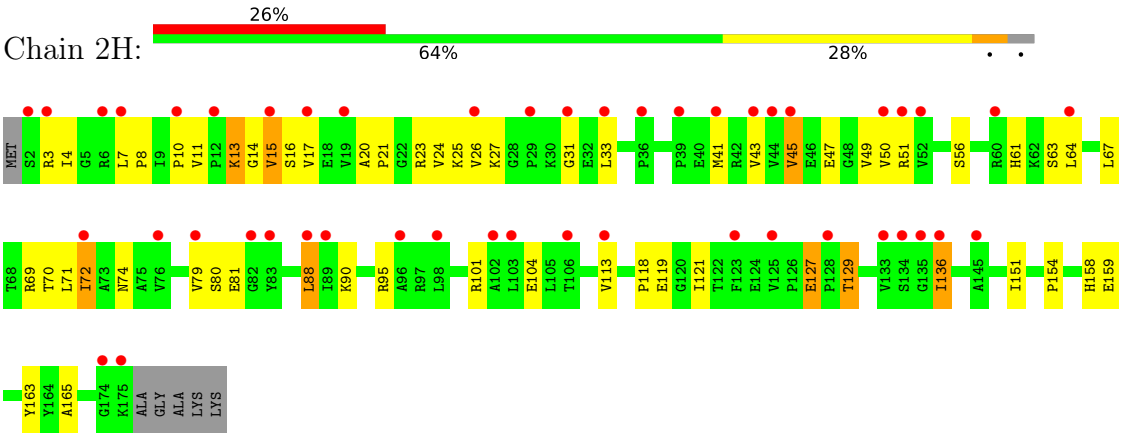
• Molecule 7: 50S ribosomal protein L6

Chain 1H:



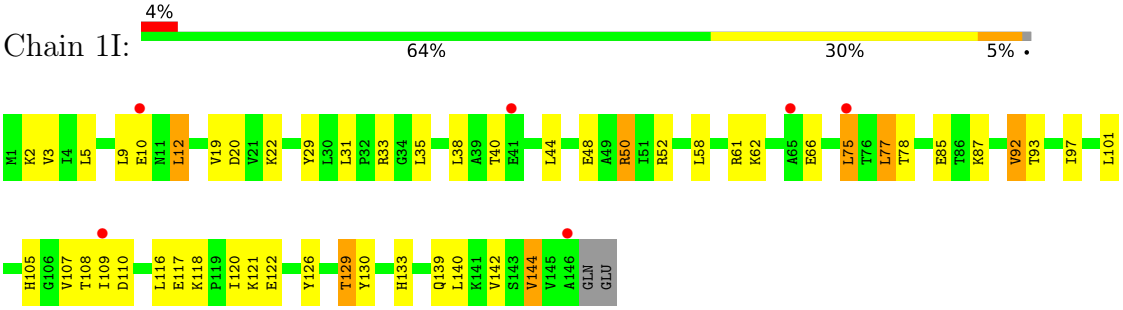
• Molecule 7: 50S ribosomal protein L6

Chain 2H:



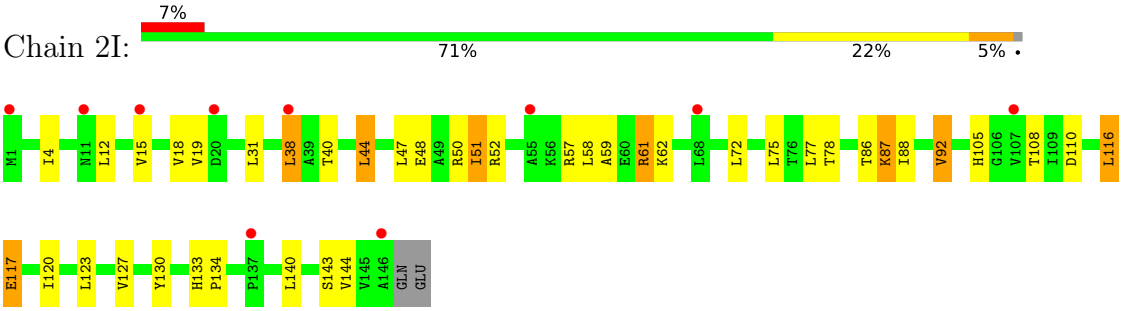
• Molecule 8: 50S ribosomal protein L9

Chain 1I:



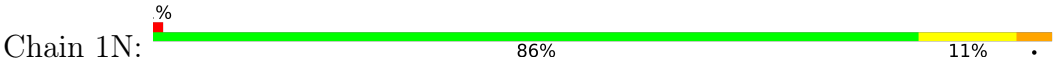
• Molecule 8: 50S ribosomal protein L9

Chain 2I:

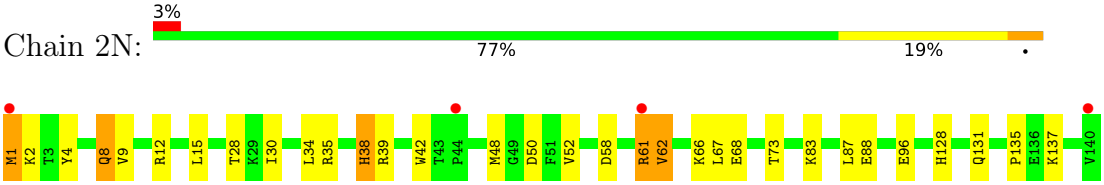


• Molecule 9: 50S ribosomal protein L13

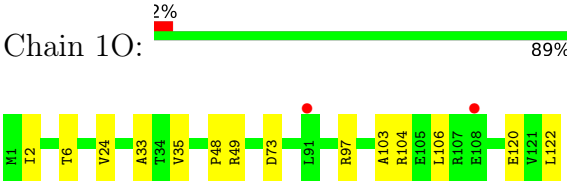
Chain 1N:



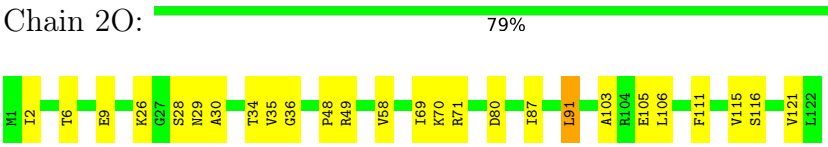
• Molecule 9: 50S ribosomal protein L13



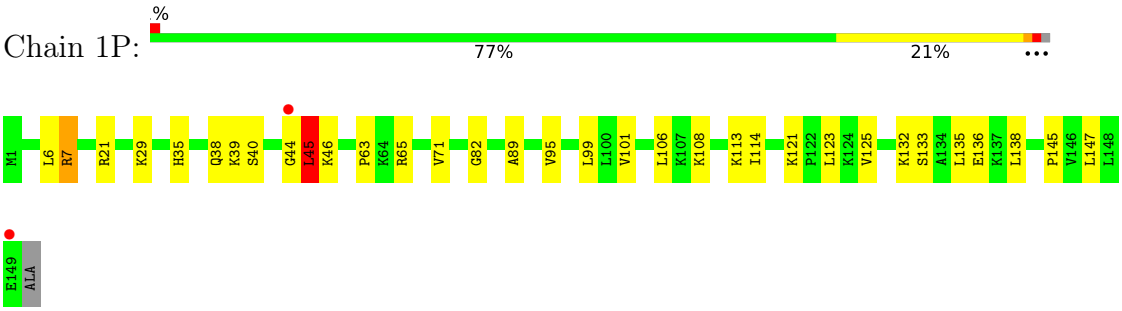
• Molecule 10: 50S ribosomal protein L14



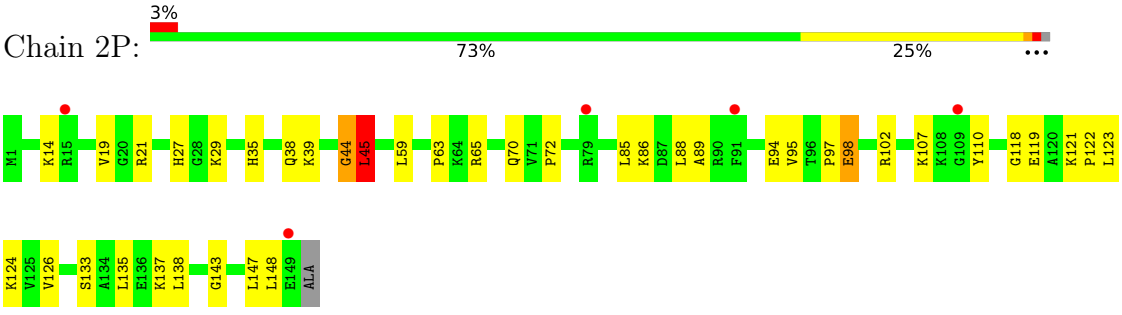
• Molecule 10: 50S ribosomal protein L14



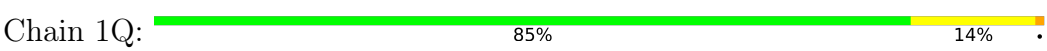
• Molecule 11: 50S ribosomal protein L15

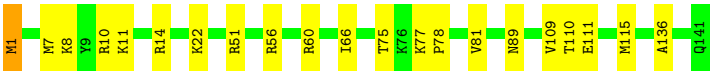


• Molecule 11: 50S ribosomal protein L15



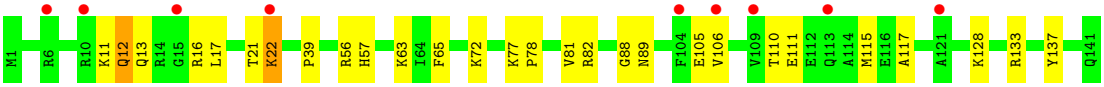
• Molecule 12: 50S ribosomal protein L16





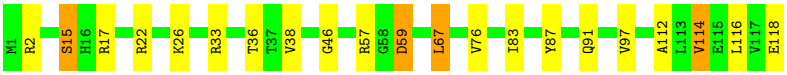
• Molecule 12: 50S ribosomal protein L16

Chain 2Q:



• Molecule 13: 50S ribosomal protein L17

Chain 1R:

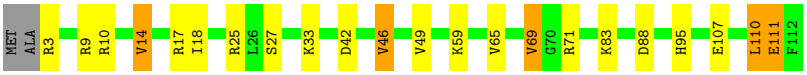


• Molecule 13: 50S ribosomal protein L17

Chain 2R:

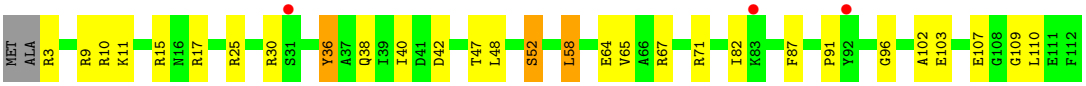
• Molecule 14: 50S ribosomal protein L18

Chain 1S:



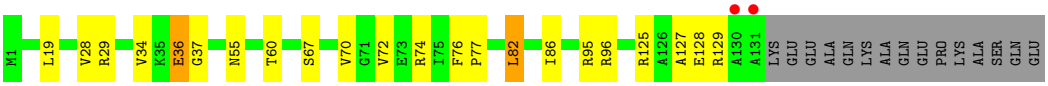
• Molecule 14: 50S ribosomal protein L18

Chain 2S:



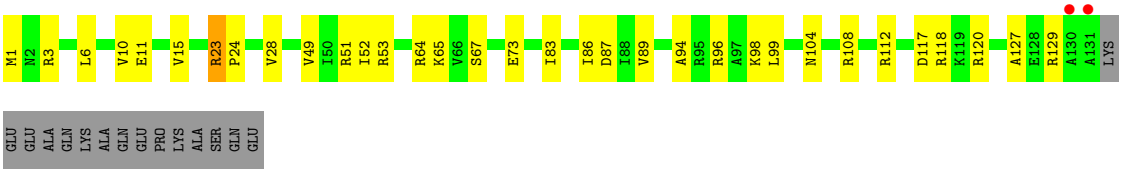
• Molecule 15: 50S ribosomal protein L19

Chain 1T:

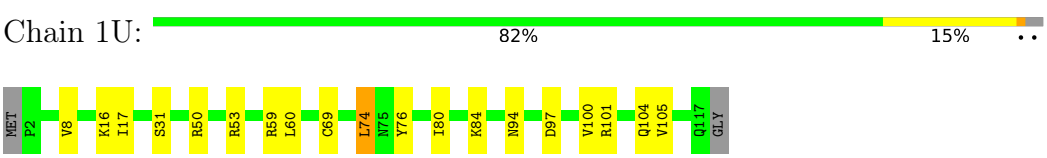


• Molecule 15: 50S ribosomal protein L19

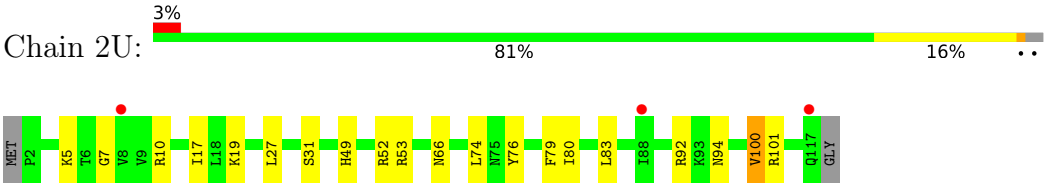
Chain 2T:



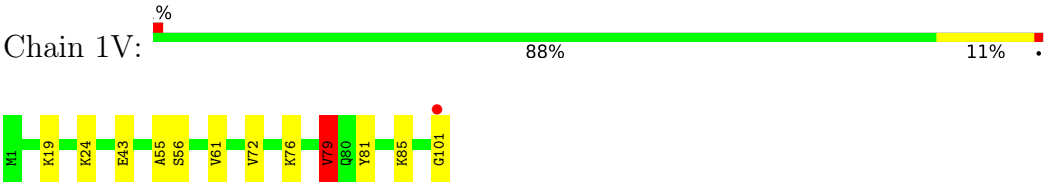
• Molecule 16: 50S ribosomal protein L20



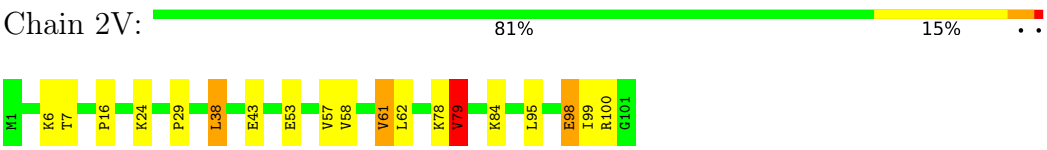
• Molecule 16: 50S ribosomal protein L20



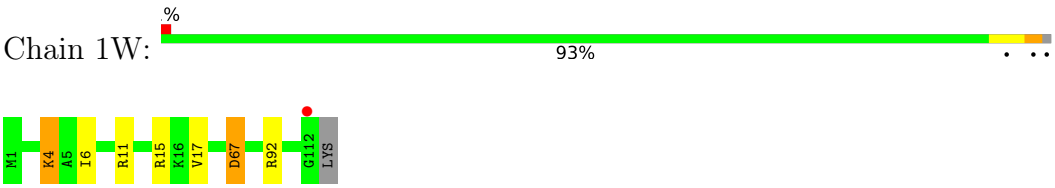
• Molecule 17: 50S ribosomal protein L21



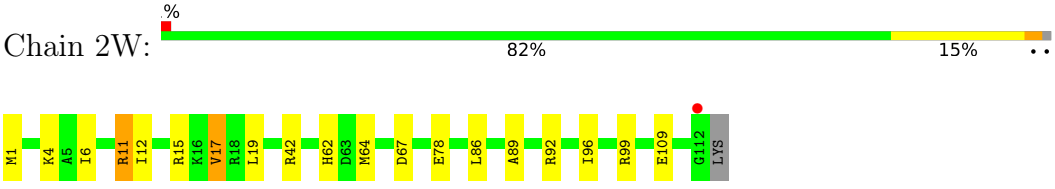
• Molecule 17: 50S ribosomal protein L21



• Molecule 18: 50S ribosomal protein L22

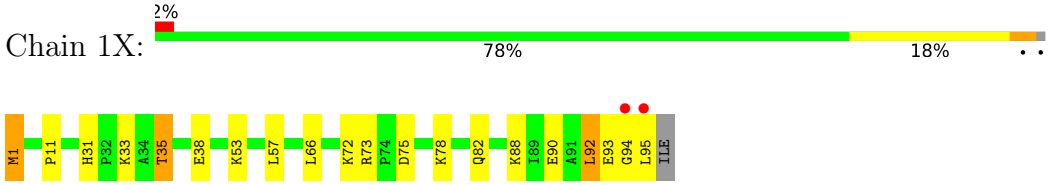


• Molecule 18: 50S ribosomal protein L22



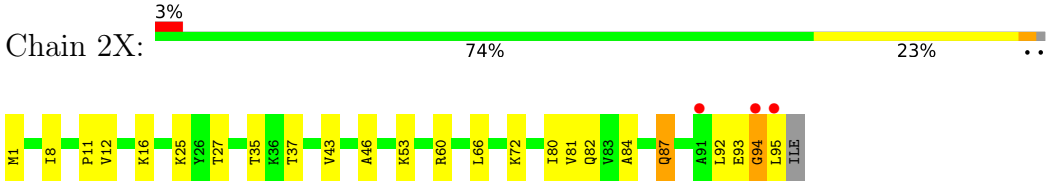
• Molecule 19: 50S ribosomal protein L23

Chain 1X:



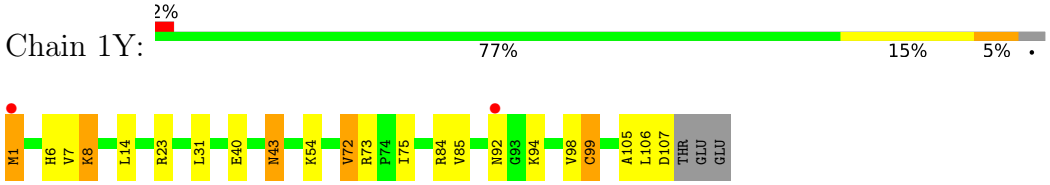
• Molecule 19: 50S ribosomal protein L23

Chain 2X:



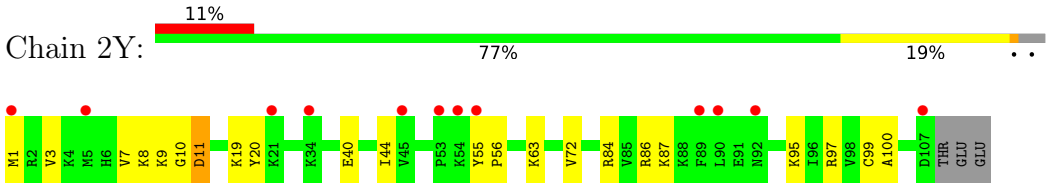
• Molecule 20: 50S ribosomal protein L24

Chain 1Y:



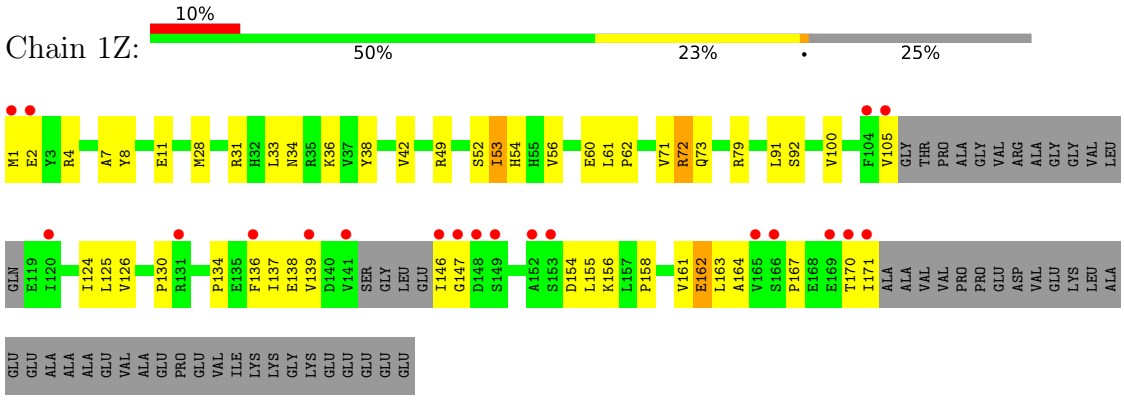
• Molecule 20: 50S ribosomal protein L24

Chain 2Y:



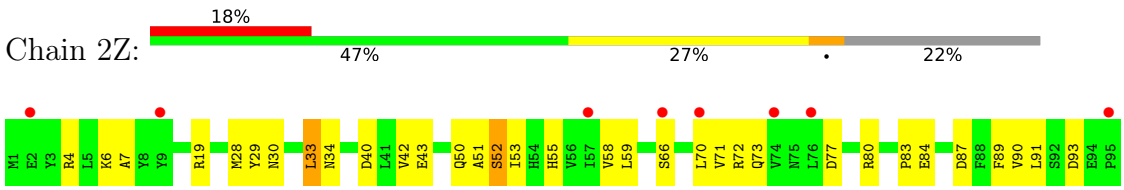
• Molecule 21: 50S ribosomal protein L25

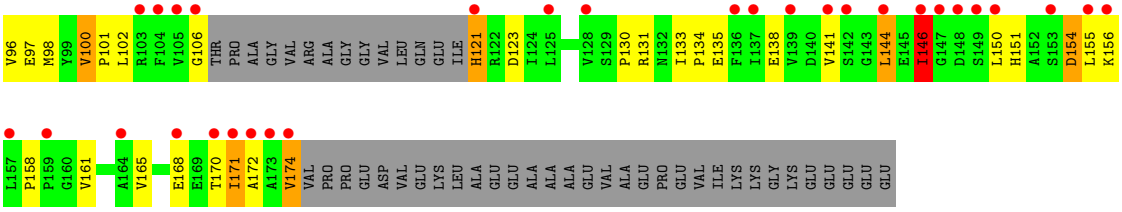
Chain 1Z:



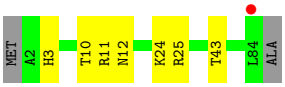
• Molecule 21: 50S ribosomal protein L25

Chain 2Z:

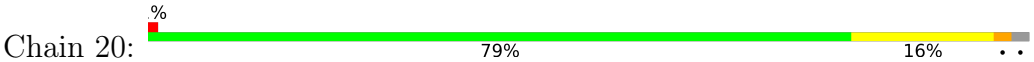




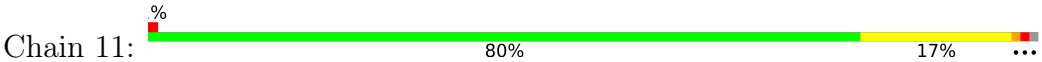
• Molecule 22: 50S ribosomal protein L27

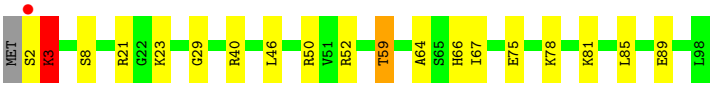


• Molecule 22: 50S ribosomal protein L27

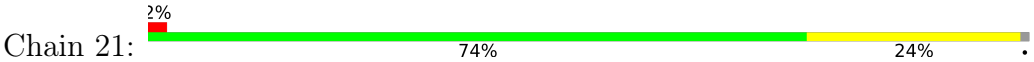


• Molecule 23: 50S ribosomal protein L28

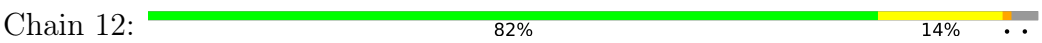


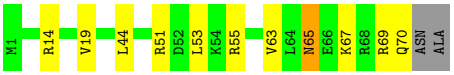


• Molecule 23: 50S ribosomal protein L28

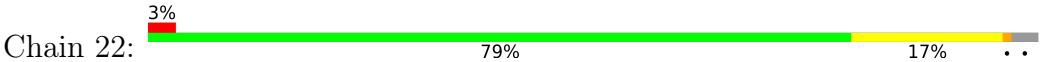


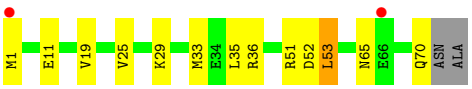
• Molecule 24: 50S ribosomal protein L29





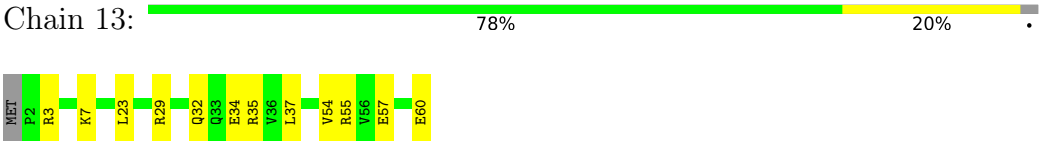
• Molecule 24: 50S ribosomal protein L29





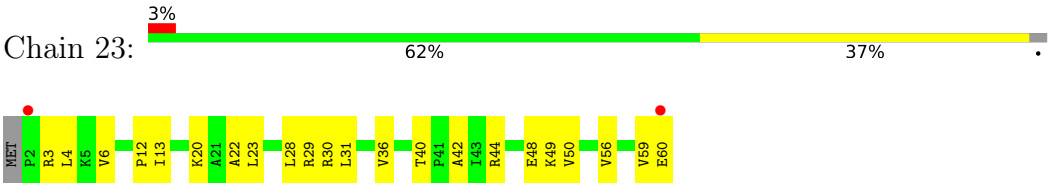
• Molecule 25: 50S ribosomal protein L30

Chain 13:



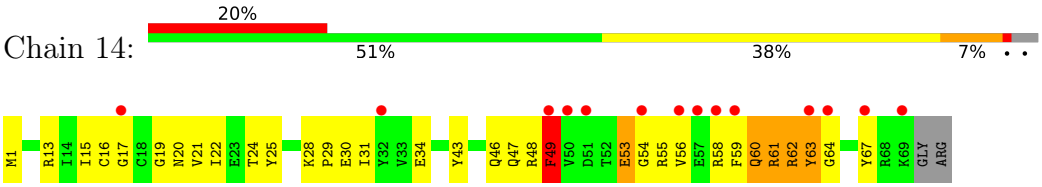
• Molecule 25: 50S ribosomal protein L30

Chain 23:



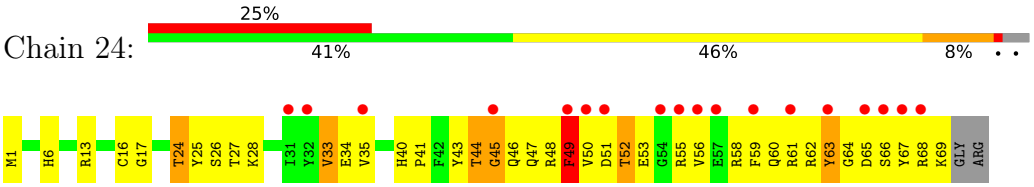
• Molecule 26: 50S ribosomal protein L31

Chain 14:



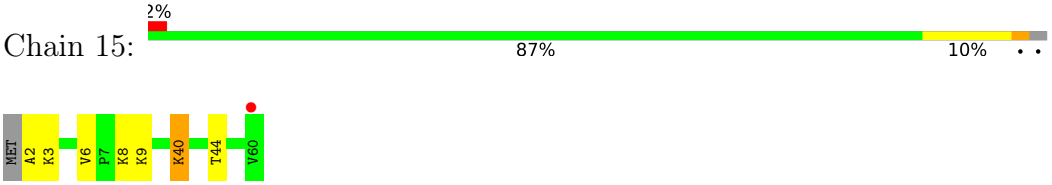
• Molecule 26: 50S ribosomal protein L31

Chain 24:



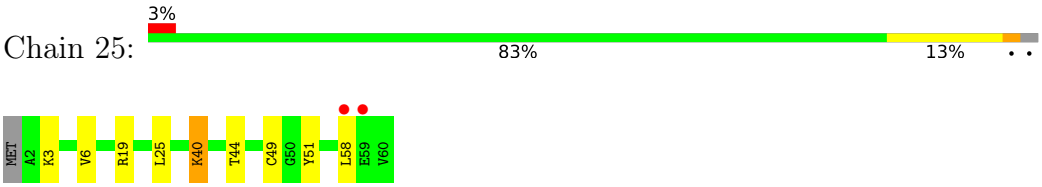
• Molecule 27: 50S ribosomal protein L32

Chain 15:



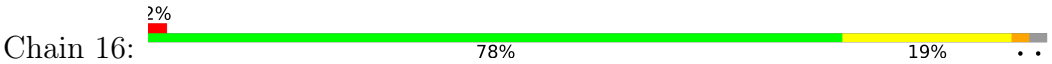
• Molecule 27: 50S ribosomal protein L32

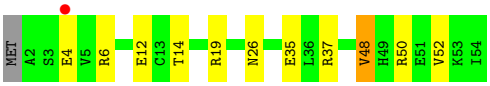
Chain 25:



• Molecule 28: 50S ribosomal protein L33

Chain 16:



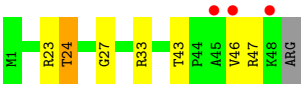


• Molecule 28: 50S ribosomal protein L33

Chain 26:

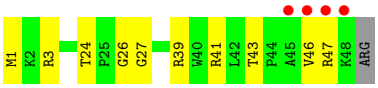
• Molecule 29: 50S ribosomal protein L34

Chain 17:



• Molecule 29: 50S ribosomal protein L34

Chain 27:

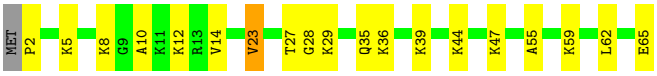


• Molecule 30: 50S ribosomal protein L35

Chain 18:

• Molecule 30: 50S ribosomal protein L35

Chain 28:

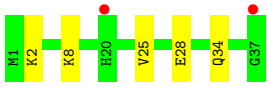


• Molecule 31: 50S ribosomal protein L36

Chain 19:

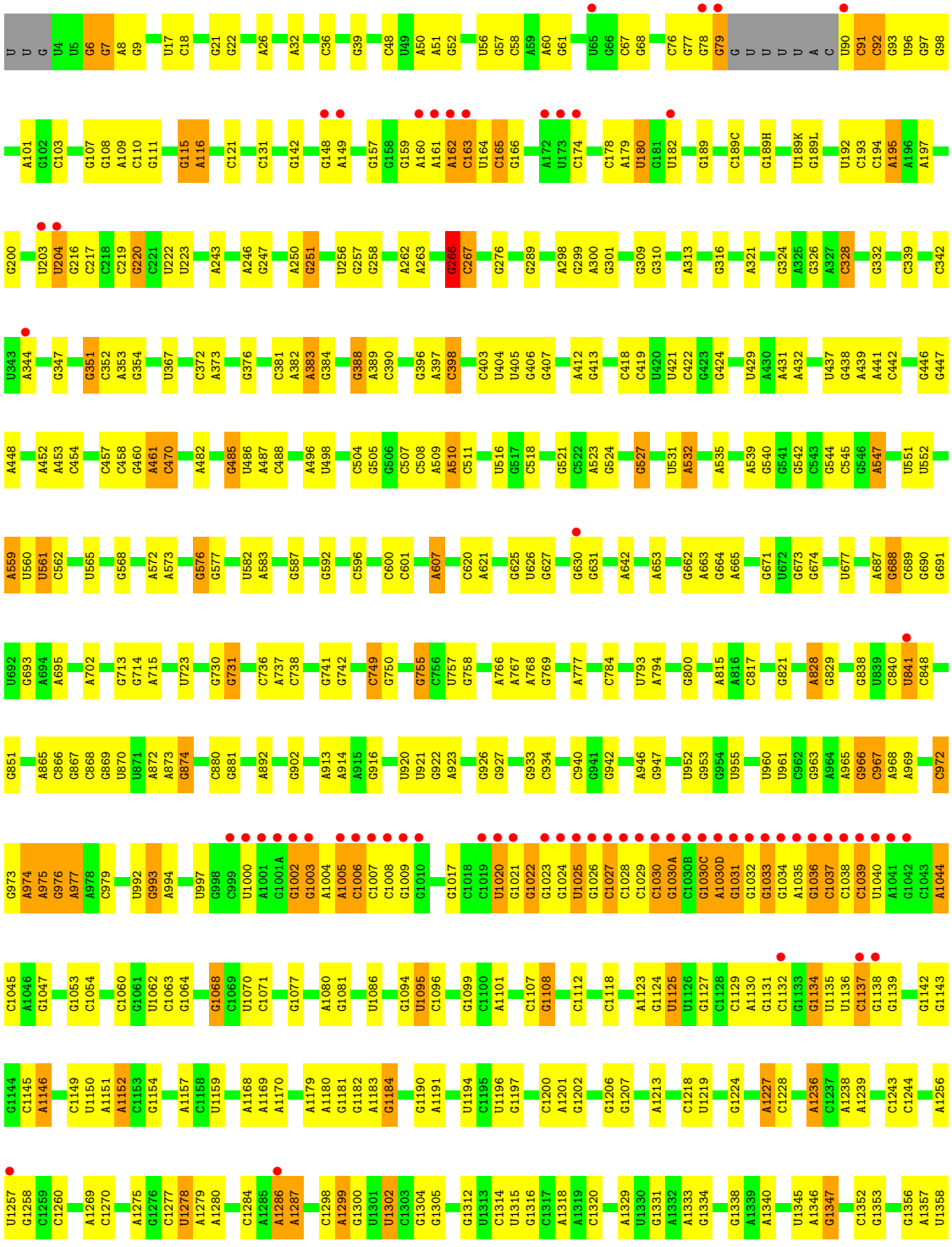
• Molecule 31: 50S ribosomal protein L36

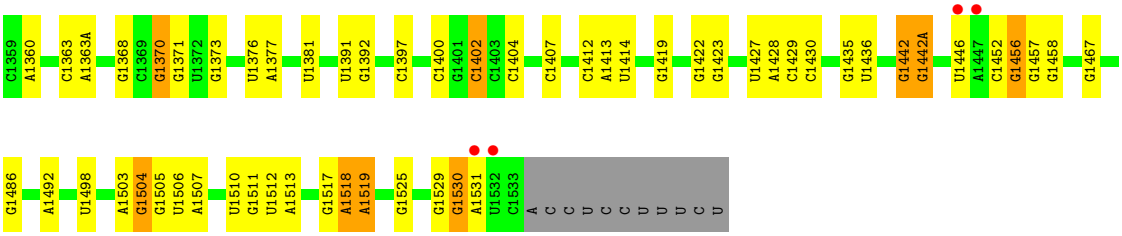
Chain 29:



• Molecule 32: 16S Ribosomal RNA

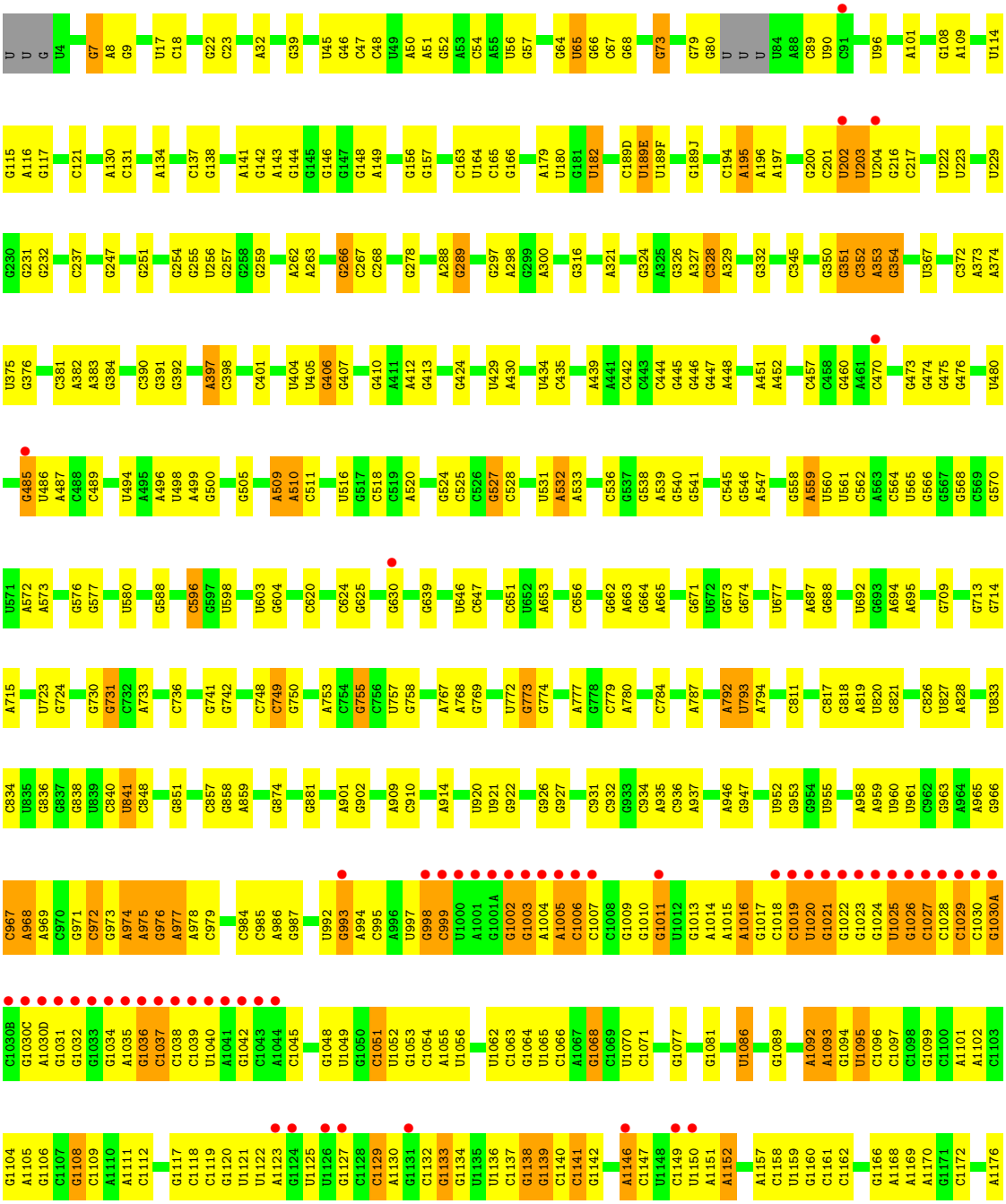
Chain 1a:

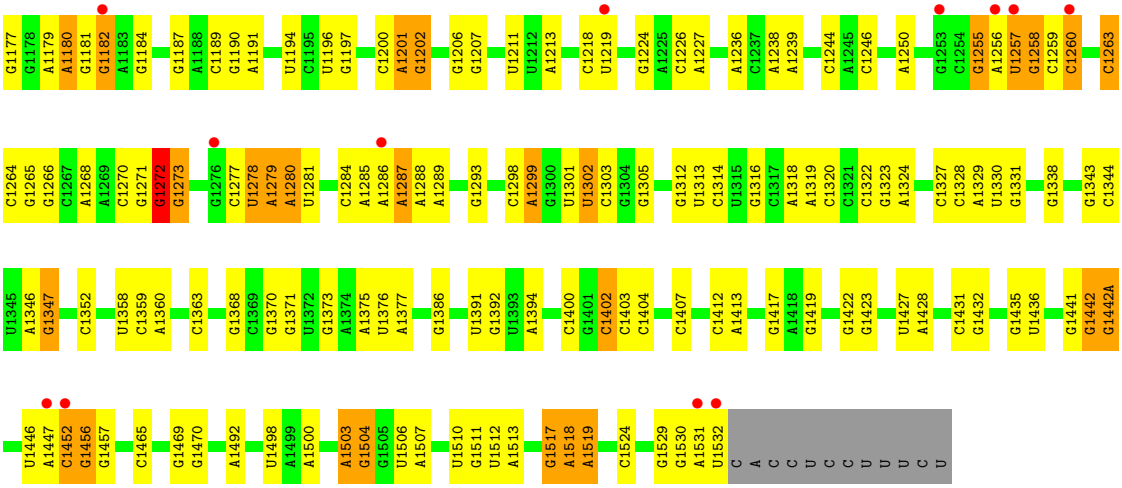




• Molecule 32: 16S Ribosomal RNA

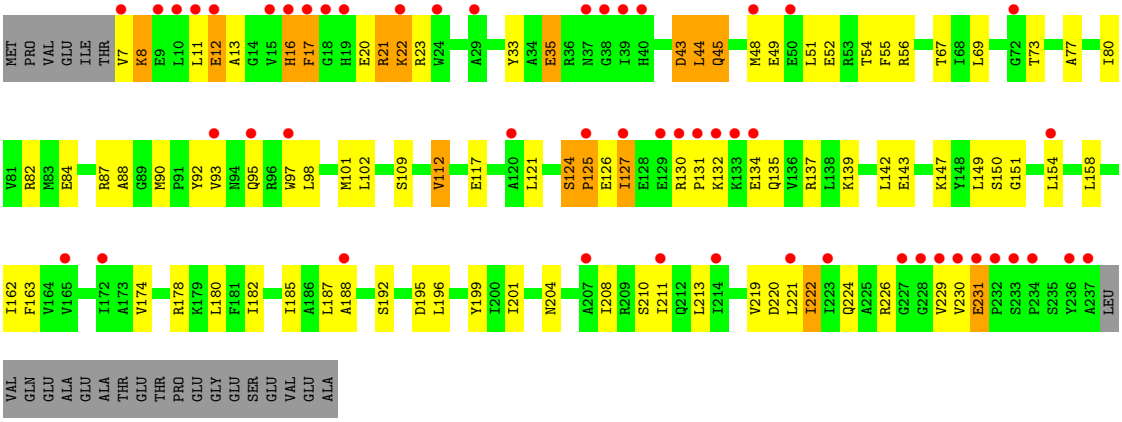
Chain 2a:





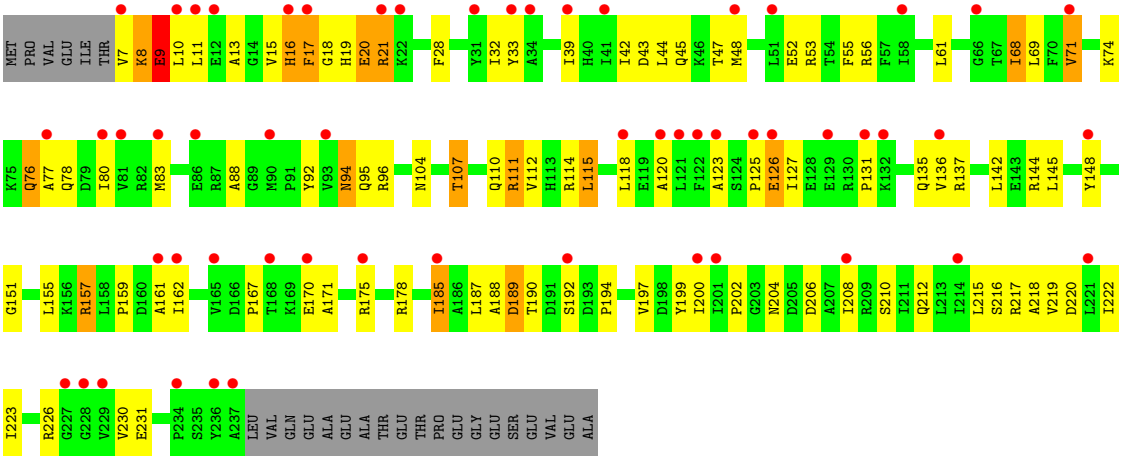
• Molecule 33: 30S ribosomal protein S2

Chain 1b:



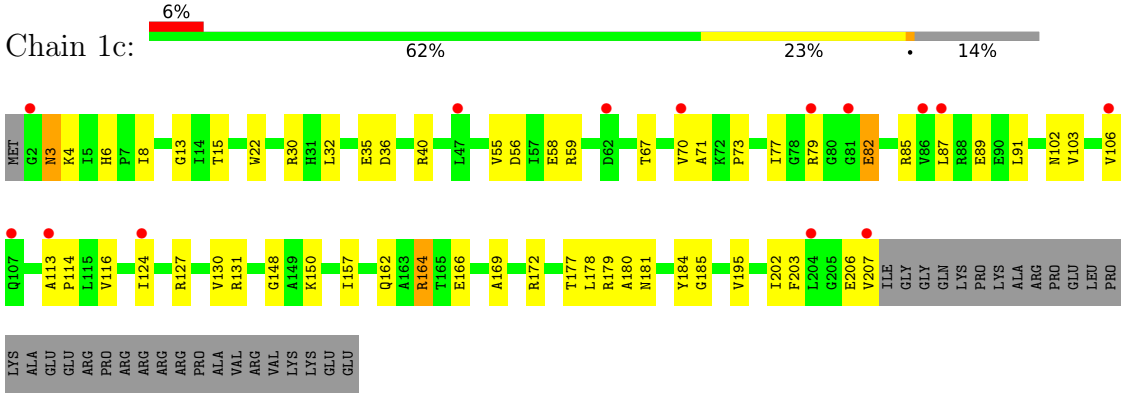
• Molecule 33: 30S ribosomal protein S2

Chain 2b:



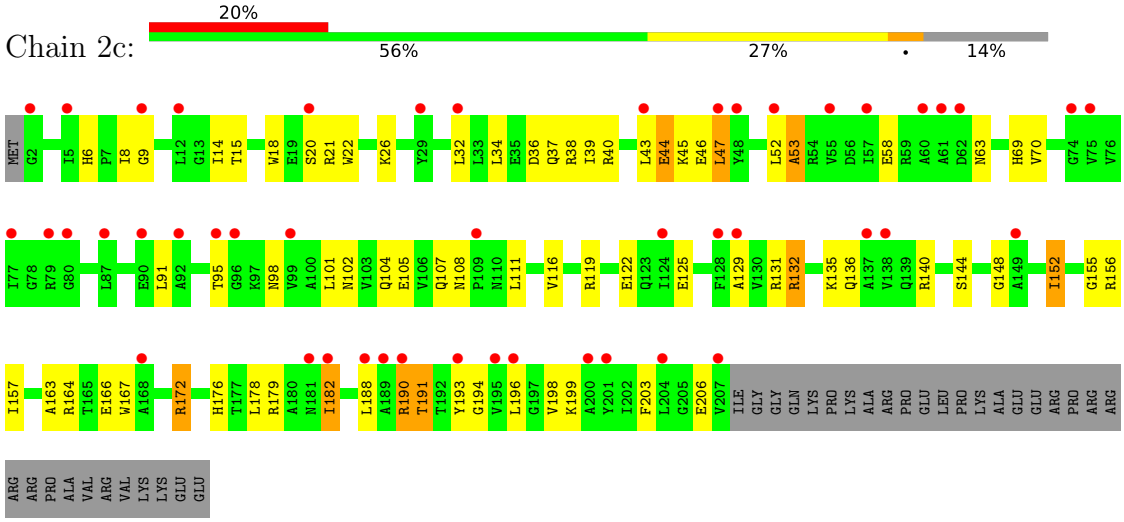
• Molecule 34: 30S ribosomal protein S3

Chain 1c:



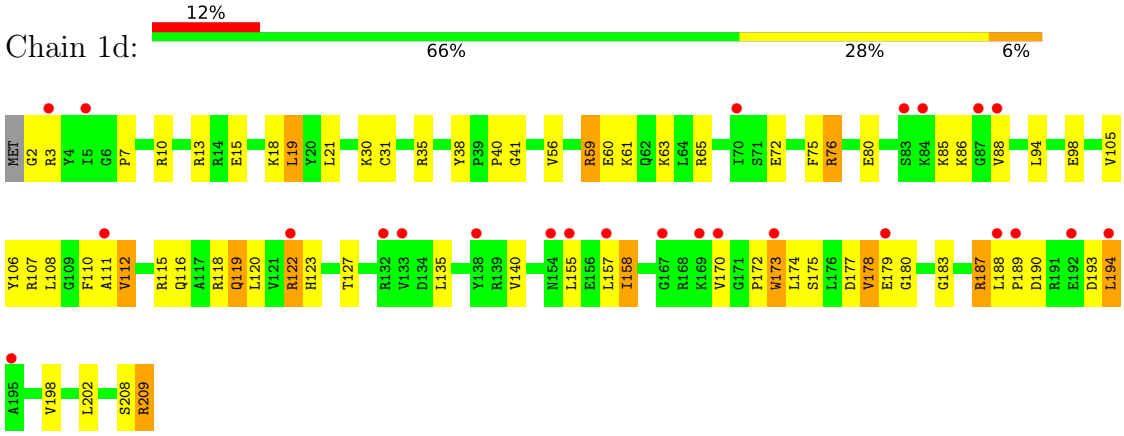
• Molecule 34: 30S ribosomal protein S3

Chain 2c:



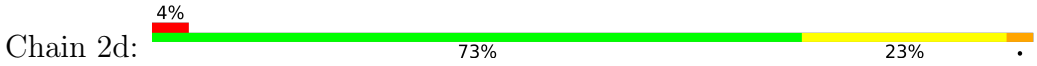
• Molecule 35: 30S ribosomal protein S4

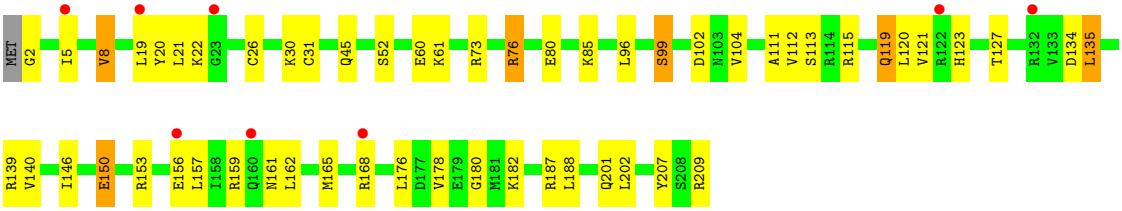
Chain 1d:



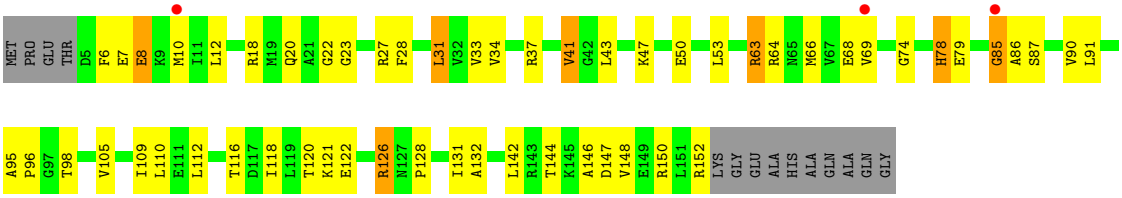
• Molecule 35: 30S ribosomal protein S4

Chain 2d:

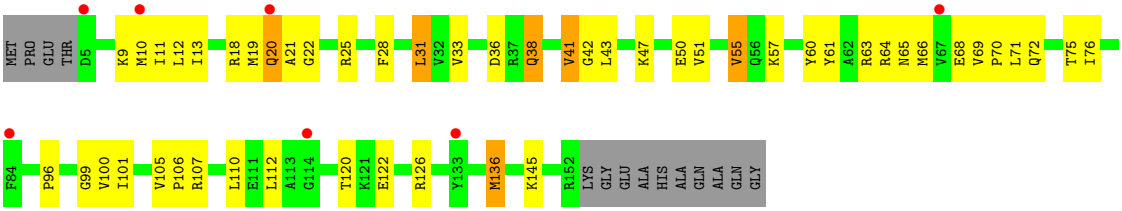




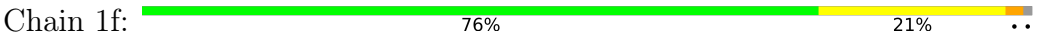
• Molecule 36: 30S ribosomal protein S5

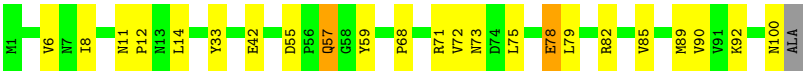


• Molecule 36: 30S ribosomal protein S5

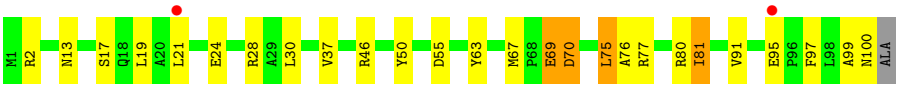


• Molecule 37: 30S ribosomal protein S6

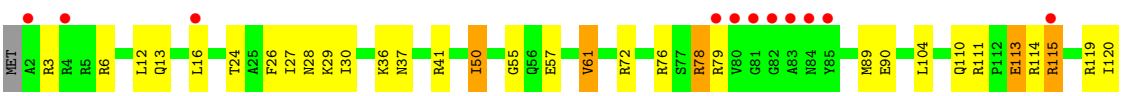




• Molecule 37: 30S ribosomal protein S6

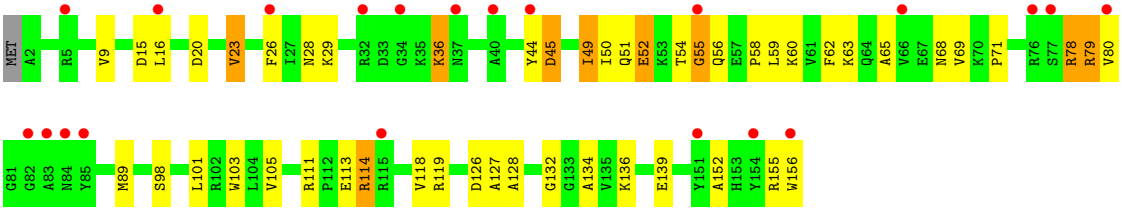


• Molecule 38: 30S ribosomal protein S7



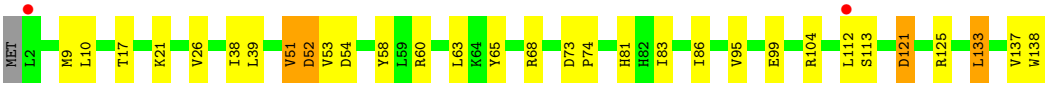
• Molecule 38: 30S ribosomal protein S7

Chain 2g:



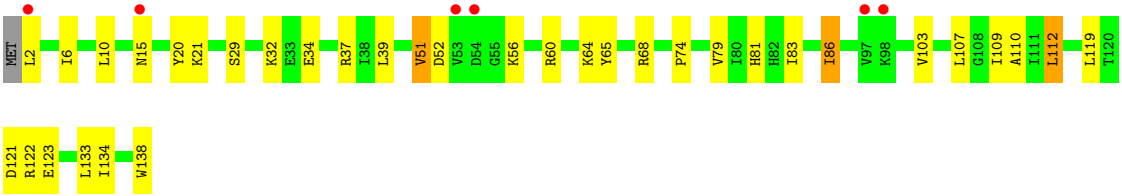
• Molecule 39: 30S ribosomal protein S8

Chain 1h:



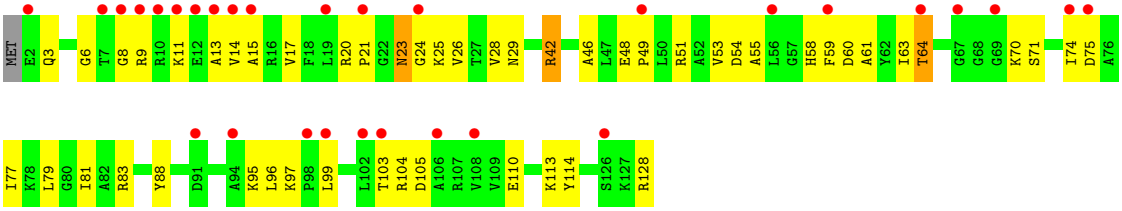
• Molecule 39: 30S ribosomal protein S8

Chain 2h:



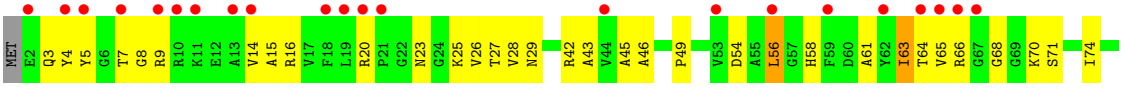
• Molecule 40: 30S ribosomal protein S9

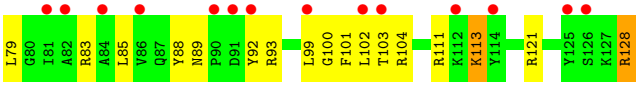
Chain 1i:



• Molecule 40: 30S ribosomal protein S9

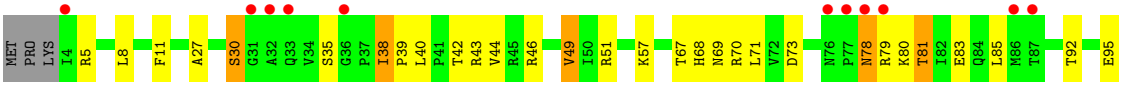
Chain 2i:

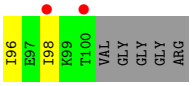




• Molecule 41: 30S ribosomal protein S10

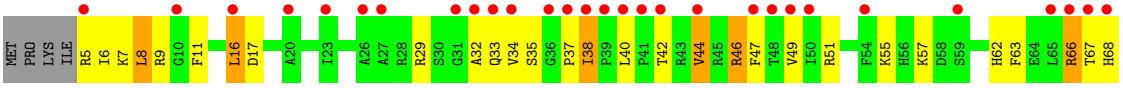
Chain 1j:

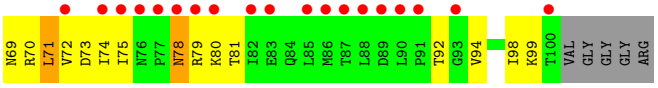




• Molecule 41: 30S ribosomal protein S10

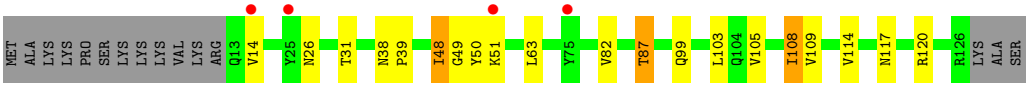
Chain 2j:





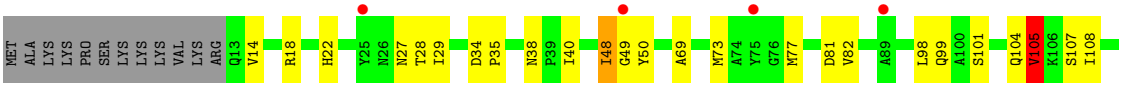
• Molecule 42: 30S ribosomal protein S11

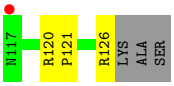
Chain 1k:



• Molecule 42: 30S ribosomal protein S11

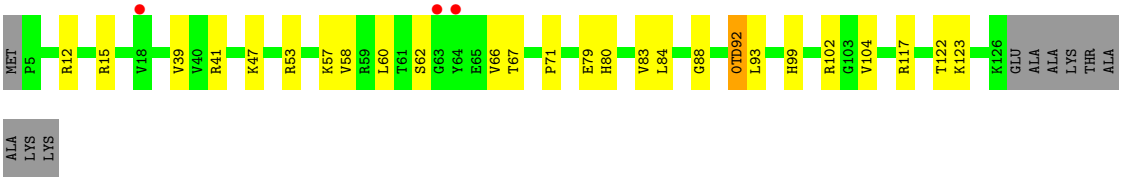
Chain 2k:



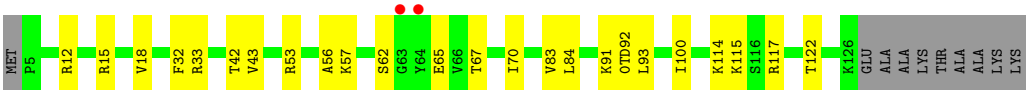


• Molecule 43: 30S ribosomal protein S12

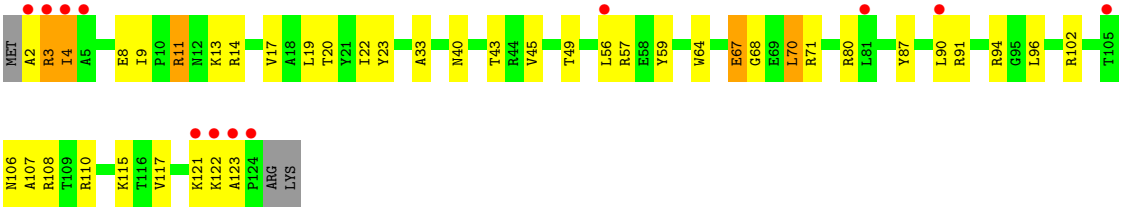
Chain 1l:



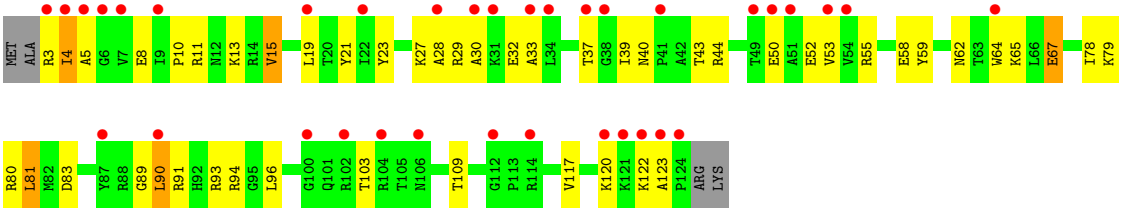
• Molecule 43: 30S ribosomal protein S12



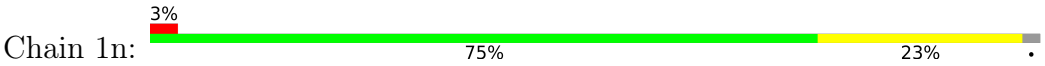
• Molecule 44: 30S ribosomal protein S13



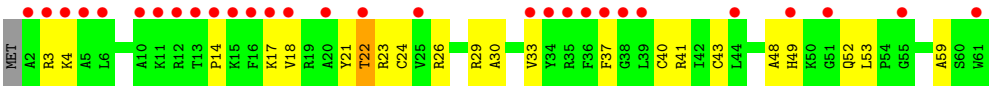
• Molecule 44: 30S ribosomal protein S13



• Molecule 45: 30S ribosomal protein S14 type Z

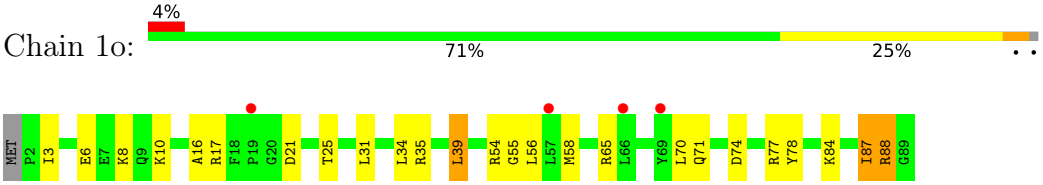


• Molecule 45: 30S ribosomal protein S14 type Z



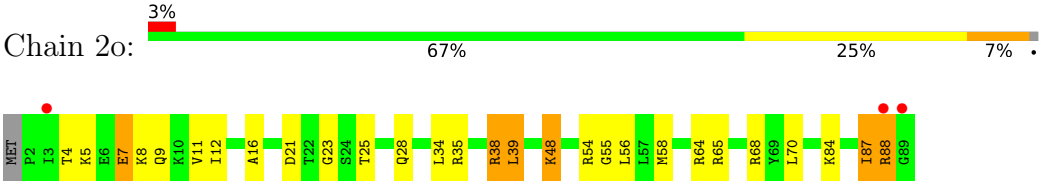
• Molecule 46: 30S ribosomal protein S15

Chain 1o:



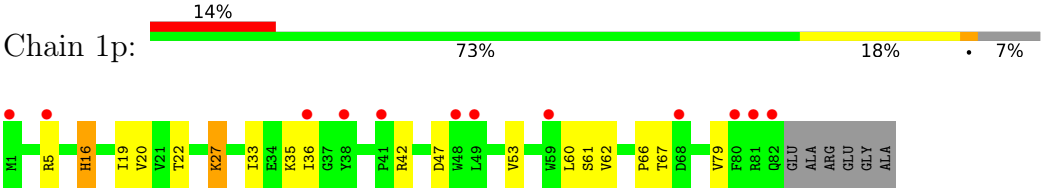
• Molecule 46: 30S ribosomal protein S15

Chain 2o:



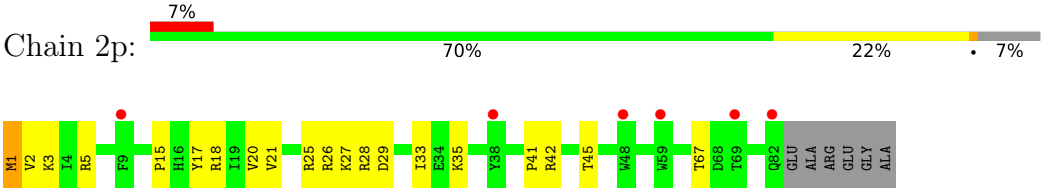
• Molecule 47: 30S ribosomal protein S16

Chain 1p:



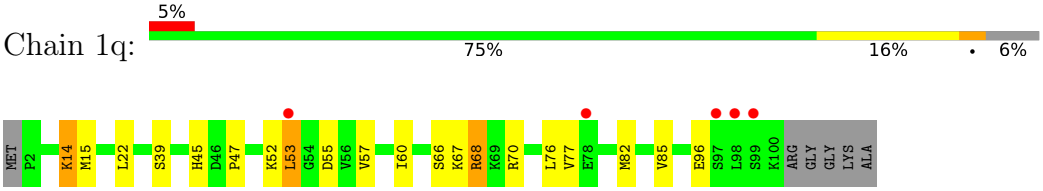
• Molecule 47: 30S ribosomal protein S16

Chain 2p:



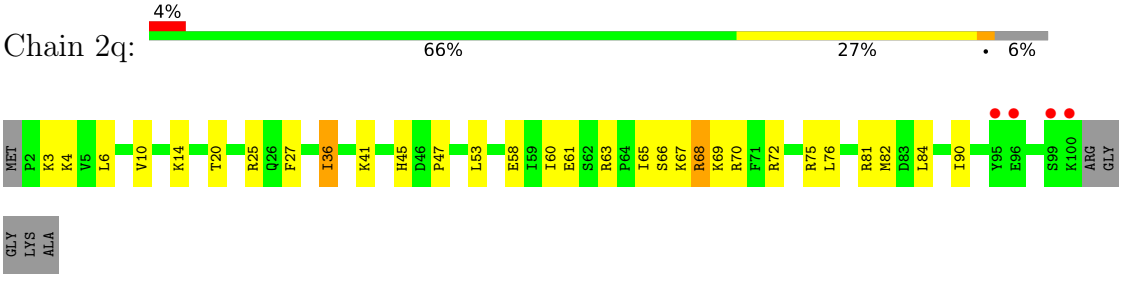
• Molecule 48: 30S ribosomal protein S17

Chain 1q:



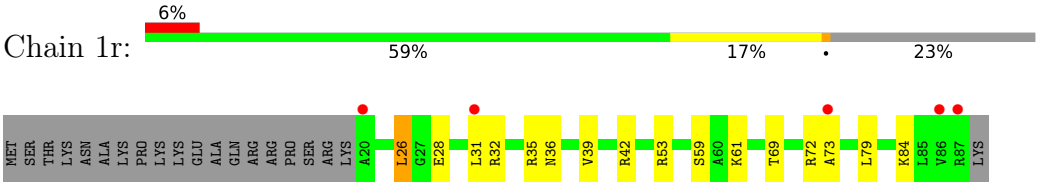
• Molecule 48: 30S ribosomal protein S17

Chain 2q:



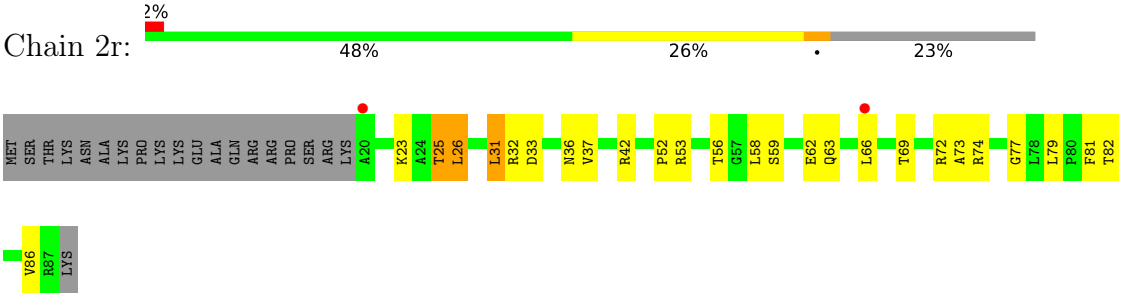
• Molecule 49: 30S ribosomal protein S18

Chain 1r:



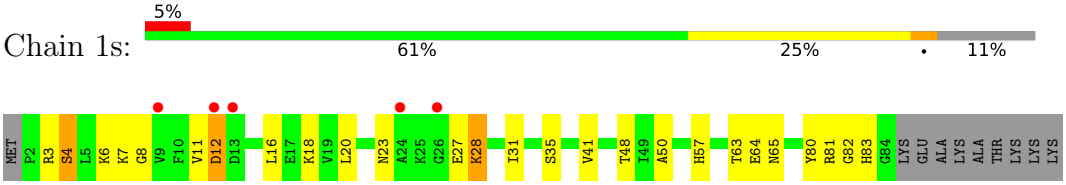
• Molecule 49: 30S ribosomal protein S18

Chain 2r:



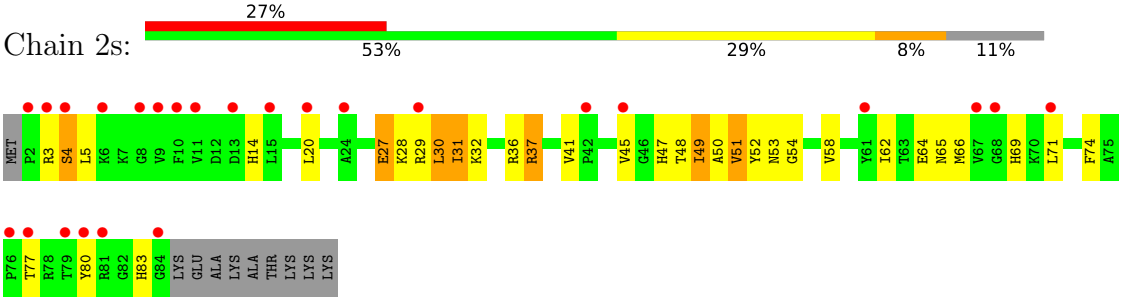
• Molecule 50: 30S ribosomal protein S19

Chain 1s:



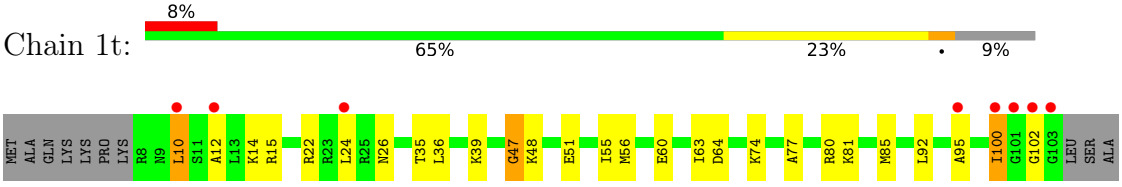
• Molecule 50: 30S ribosomal protein S19

Chain 2s:



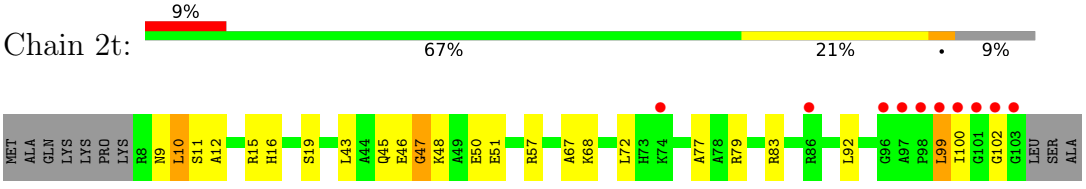
• Molecule 51: 30S ribosomal protein S20

Chain 1t:



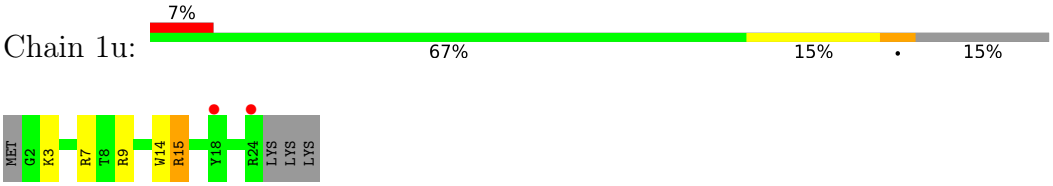
• Molecule 51: 30S ribosomal protein S20

Chain 2t:



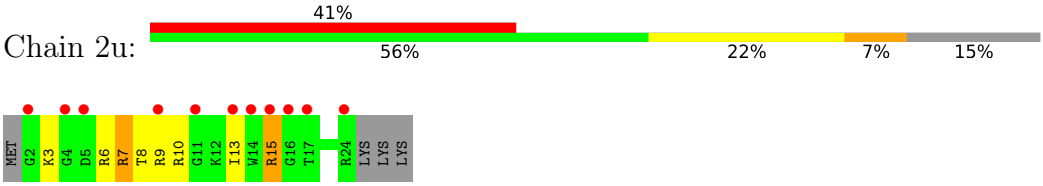
• Molecule 52: 30S ribosomal protein Thx

Chain 1u:



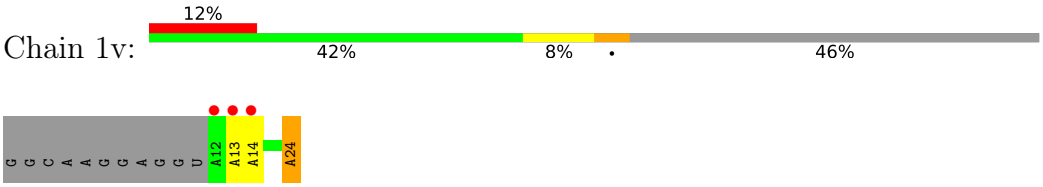
• Molecule 52: 30S ribosomal protein Thx

Chain 2u:



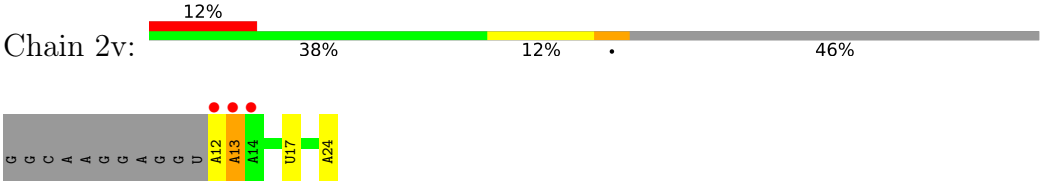
• Molecule 53: MF-mRNA

Chain 1v:



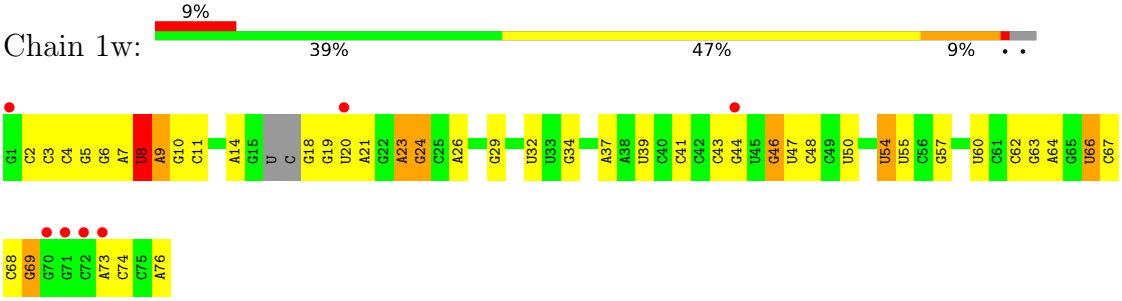
• Molecule 53: MF-mRNA

Chain 2v:



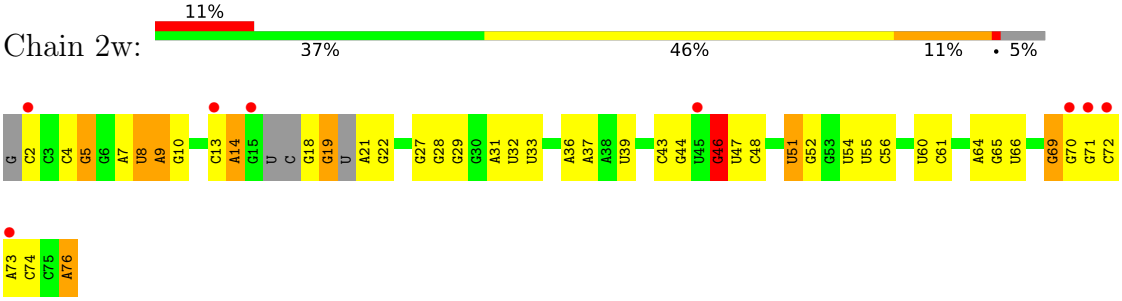
• Molecule 54: Aminoacylated Phe-tRNAphe

Chain 1w:



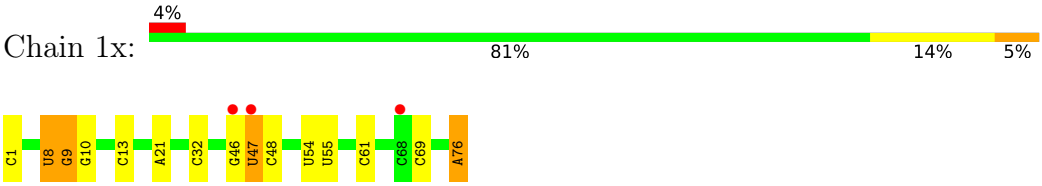
• Molecule 54: Aminoacylated Phe-tRNAphe

Chain 2w:



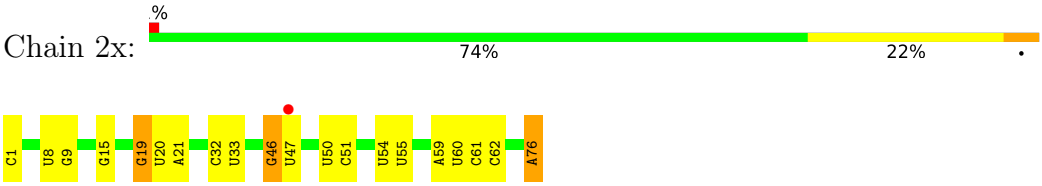
• Molecule 55: Aminoacylated fMet-tRNAmet

Chain 1x:



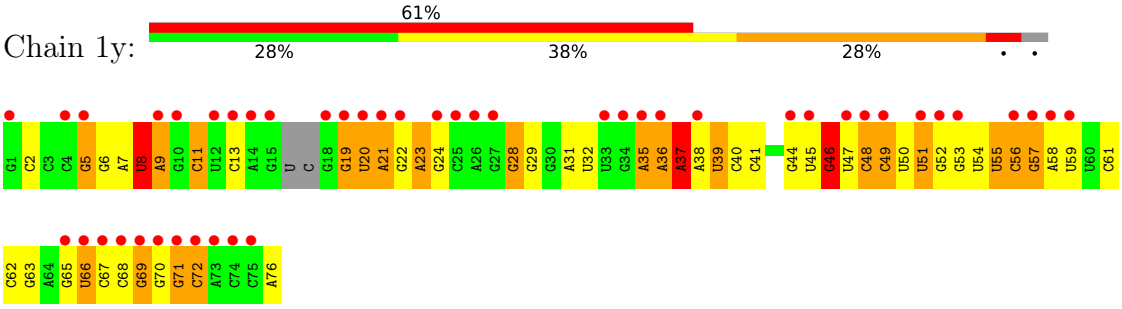
• Molecule 55: Aminoacylated fMet-tRNAmet

Chain 2x:



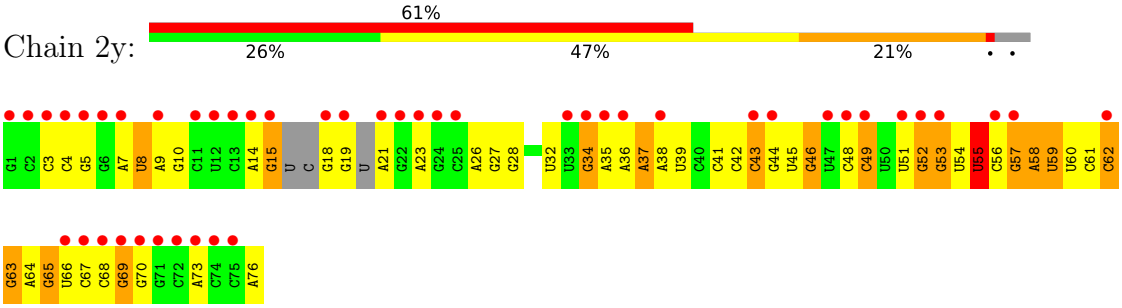
• Molecule 56: Deacylated tRNAphe

Chain 1y:



• Molecule 56: Deacylated tRNAphe

Chain 2y:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	209.98Å 450.78Å 623.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	107.27 – 2.40 107.27 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.9 (107.27-2.40) 98.8 (107.27-2.40)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.15 (at 2.40Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.221 , 0.260 0.223 , 0.261	Depositor DCC
R_{free} test set	112480 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	47.1	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 45.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	300455	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

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

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 2MA, FME, A1AEZ, 4OC, M2G, K, 2MG, ZN, 4SU, OMG, G7M, 5MU, 5MC, SF4, OMU, UR3, MA6, 8AN, 0TD, PSU, MG, MIA, OMC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	1A	0.27	0/69011	0.47	2/107720 (0.0%)
1	2A	0.21	0/67295	0.40	1/105042 (0.0%)
2	1B	0.21	0/2882	0.39	0/4494
2	2B	0.19	0/2879	0.38	0/4487
3	1D	0.26	0/2186	0.51	0/2944
3	2D	0.23	0/2186	0.46	0/2944
4	1E	0.25	0/1592	0.49	0/2149
4	2E	0.20	0/1592	0.43	0/2149
5	1F	0.25	0/1619	0.51	0/2193
5	2F	0.19	0/1615	0.46	2/2188 (0.1%)
6	1G	0.22	0/1448	0.53	2/1957 (0.1%)
6	2G	0.19	0/1453	0.42	0/1963
7	1H	0.21	0/1356	0.40	0/1834
7	2H	0.20	0/1356	0.39	0/1834
8	1I	0.18	0/1112	0.41	0/1514
8	2I	0.18	0/1079	0.44	0/1475
9	1N	0.25	0/1144	0.46	0/1543
9	2N	0.18	0/1144	0.39	0/1543
10	1O	0.24	0/943	0.43	0/1269
10	2O	0.19	0/943	0.39	0/1269
11	1P	0.24	0/1152	0.55	0/1533
11	2P	0.21	0/1152	0.48	0/1533
12	1Q	0.26	0/1143	0.46	0/1527
12	2Q	0.19	0/1143	0.40	0/1527
13	1R	0.27	0/982	0.49	0/1312
13	2R	0.19	0/982	0.42	0/1312
14	1S	0.22	0/883	0.47	0/1176
14	2S	0.20	0/880	0.43	0/1172
15	1T	0.24	0/1105	0.47	0/1477
15	2T	0.20	0/1097	0.41	0/1468
16	1U	0.28	0/977	0.47	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
16	2U	0.19	0/977	0.40	0/1301
17	1V	0.25	0/782	0.49	0/1049
17	2V	0.19	0/782	0.42	0/1049
18	1W	0.26	0/897	0.45	0/1205
18	2W	0.21	0/897	0.40	0/1205
19	1X	0.27	0/764	0.55	0/1025
19	2X	0.21	0/764	0.49	2/1025 (0.2%)
20	1Y	0.22	0/819	0.50	0/1095
20	2Y	0.20	0/819	0.43	0/1095
21	1Z	0.24	0/1267	0.47	0/1717
21	2Z	0.21	0/1299	0.43	0/1763
22	10	0.25	0/662	0.50	0/881
22	20	0.20	0/662	0.45	0/881
23	11	0.23	0/762	0.41	0/1014
23	21	0.22	0/762	0.41	0/1014
24	12	0.24	0/590	0.44	0/781
24	22	0.19	0/590	0.39	0/781
25	13	0.26	0/474	0.47	0/635
25	23	0.18	0/469	0.41	0/630
26	14	0.26	0/565	0.60	1/761 (0.1%)
26	24	0.24	0/545	0.56	0/737
27	15	0.26	0/469	0.50	0/635
27	25	0.19	0/469	0.42	0/635
28	16	0.26	0/460	0.46	0/613
28	26	0.21	0/456	0.44	0/608
29	17	0.29	0/426	0.54	0/561
29	27	0.24	0/426	0.50	0/561
30	18	0.26	0/525	0.47	0/691
30	28	0.20	0/525	0.38	0/691
31	19	0.26	0/310	0.51	0/407
31	29	0.18	0/310	0.41	0/407
32	1a	0.20	0/35795	0.39	2/55864 (0.0%)
32	2a	0.19	0/35886	0.37	3/56005 (0.0%)
33	1b	0.20	0/1881	0.49	0/2542
33	2b	0.21	0/1860	0.48	0/2518
34	1c	0.20	0/1572	0.40	0/2126
34	2c	0.20	0/1566	0.41	0/2119
35	1d	0.19	0/1685	0.44	0/2262
35	2d	0.20	0/1704	0.42	0/2284
36	1e	0.21	0/1145	0.49	1/1543 (0.1%)
36	2e	0.20	0/1149	0.44	0/1548
37	1f	0.17	0/823	0.39	0/1115
37	2f	0.19	0/829	0.39	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	1g	0.19	0/1250	0.42	0/1679
38	2g	0.20	0/1254	0.44	0/1683
39	1h	0.19	0/1108	0.42	0/1494
39	2h	0.17	0/1108	0.41	0/1494
40	1i	0.20	0/1002	0.49	0/1346
40	2i	0.21	0/997	0.46	0/1343
41	1j	0.21	0/722	0.43	0/982
41	2j	0.21	0/727	0.48	0/988
42	1k	0.18	0/844	0.41	0/1145
42	2k	0.17	0/848	0.37	0/1149
43	1l	0.23	0/937	0.42	0/1260
43	2l	0.18	0/937	0.39	0/1260
44	1m	0.20	0/969	0.49	0/1302
44	2m	0.20	0/961	0.47	0/1291
45	1n	0.19	0/501	0.41	0/664
45	2n	0.20	0/501	0.42	0/664
46	1o	0.19	0/739	0.38	0/985
46	2o	0.18	0/739	0.37	0/985
47	1p	0.19	0/697	0.43	0/939
47	2p	0.18	0/693	0.45	0/935
48	1q	0.20	0/836	0.45	0/1117
48	2q	0.19	0/836	0.46	0/1117
49	1r	0.20	0/560	0.38	0/746
49	2r	0.18	0/560	0.40	0/746
50	1s	0.19	0/667	0.49	0/900
50	2s	0.27	0/661	0.57	2/893 (0.2%)
51	1t	0.19	0/730	0.45	0/965
51	2t	0.22	0/729	0.50	0/965
52	1u	0.18	0/203	0.43	0/266
52	2u	0.19	0/203	0.45	0/266
53	1v	0.22	0/310	0.33	0/480
53	2v	0.22	0/310	0.35	0/480
54	1w	0.28	1/1581 (0.1%)	0.43	0/2458
54	2w	0.29	2/1531 (0.1%)	0.39	0/2379
55	1x	0.27	0/1723	0.41	0/2684
55	2x	0.25	1/1723 (0.1%)	0.39	0/2684
56	1y	0.33	2/1606 (0.1%)	0.40	0/2497
56	2y	0.33	2/1583 (0.1%)	0.40	0/2459
All	All	0.23	8/316636 (0.0%)	0.43	18/474041 (0.0%)

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
11	1P	0	1
11	2P	0	1
All	All	0	2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	2y	46	G7M	O3'-P	5.73	1.61	1.56
56	2y	8	4SU	O3'-P	5.52	1.61	1.56
56	1y	46	G7M	O3'-P	5.49	1.61	1.56
54	2w	46	G7M	O3'-P	5.34	1.61	1.56
54	1w	46	G7M	O3'-P	5.25	1.61	1.56
56	1y	8	4SU	O3'-P	5.18	1.61	1.56
54	2w	8	4SU	O3'-P	5.08	1.61	1.56
55	2x	8	4SU	O3'-P	5.06	1.61	1.56

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1992	G	C2'-C3'-O3'	6.76	119.64	109.50
6	1G	49	ASP	CA-C-O	-6.59	111.09	120.51
1	2A	1992	G	C2'-C3'-O3'	6.39	119.08	109.50
26	14	60	GLN	N-CA-C	-6.07	106.23	113.21
32	2a	1272	G	N1-C2-N2	-5.89	98.52	116.20
32	2a	1263	C	N1-C2-O2	5.73	136.09	118.90
6	1G	49	ASP	O-C-N	5.65	130.11	122.59
36	1e	23	GLY	N-CA-C	5.61	118.00	110.43
32	1a	266	G	C2'-C3'-O3'	5.51	117.76	109.50
32	2a	1272	G	N3-C2-N2	5.37	136.02	119.90
19	2X	94	GLY	CA-C-N	5.24	131.12	121.70
19	2X	94	GLY	C-N-CA	5.24	131.12	121.70
1	1A	512	G	O4'-C1'-N9	5.20	116.00	108.20
50	2s	27	GLU	CA-C-N	5.13	130.93	121.70
50	2s	27	GLU	C-N-CA	5.13	130.93	121.70
32	1a	266	G	P-O3'-C3'	5.12	127.88	120.20
5	2F	21	ALA	CA-C-N	5.01	130.73	121.70
5	2F	21	ALA	C-N-CA	5.01	130.73	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

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

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	61852	0	31196	466	0
1	2A	60322	0	30428	523	0
2	1B	2577	0	1305	20	0
2	2B	2575	0	1303	31	0
3	1D	2136	0	2218	35	0
3	2D	2136	0	2218	29	0
4	1E	1559	0	1618	14	0
4	2E	1559	0	1618	26	0
5	1F	1584	0	1625	29	0
5	2F	1580	0	1619	43	0
6	1G	1423	0	1436	33	0
6	2G	1428	0	1438	36	0
7	1H	1330	0	1407	22	0
7	2H	1330	0	1407	28	0
8	1I	1097	0	1140	30	0
8	2I	1064	0	1082	25	0
9	1N	1117	0	1184	11	0
9	2N	1117	0	1184	20	0
10	1O	933	0	996	11	0
10	2O	933	0	996	15	0
11	1P	1135	0	1212	22	0
11	2P	1135	0	1212	23	0
12	1Q	1122	0	1179	12	0
12	2Q	1122	0	1179	18	0
13	1R	968	0	1033	13	0
13	2R	968	0	1033	15	0
14	1S	873	0	927	19	0
14	2S	870	0	923	24	0
15	1T	1091	0	1151	13	0
15	2T	1083	0	1136	20	0
16	1U	959	0	1019	11	0
16	2U	959	0	1019	13	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	1V	771	0	830	7	0
17	2V	771	0	829	11	0
18	1W	886	0	940	3	0
18	2W	886	0	940	11	0
19	1X	750	0	814	12	0
19	2X	750	0	814	17	0
20	1Y	806	0	881	12	0
20	2Y	806	0	881	11	0
21	1Z	1240	0	1240	31	0
21	2Z	1271	0	1273	47	0
22	10	653	0	674	9	0
22	20	653	0	674	12	0
23	11	755	0	826	13	0
23	21	755	0	826	18	0
24	12	588	0	643	5	0
24	22	588	0	643	6	0
25	13	469	0	518	8	0
25	23	464	0	514	12	0
26	14	552	0	533	30	0
26	24	532	0	503	28	0
27	15	455	0	465	5	0
27	25	455	0	465	5	0
28	16	453	0	473	6	0
28	26	449	0	469	8	0
29	17	418	0	467	4	0
29	27	418	0	467	7	0
30	18	517	0	582	12	0
30	28	517	0	582	14	0
31	19	307	0	335	5	0
31	29	307	0	335	3	0
32	1a	32246	0	16295	312	0
32	2a	32327	0	16338	368	0
33	1b	1846	0	1867	55	0
33	2b	1825	0	1828	69	0
34	1c	1548	0	1535	34	0
34	2c	1542	0	1517	53	0
35	1d	1655	0	1672	52	0
35	2d	1674	0	1714	34	0
36	1e	1129	0	1185	31	0
36	2e	1133	0	1191	32	0
37	1f	810	0	804	11	0
37	2f	816	0	808	19	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	1g	1231	0	1238	23	0
38	2g	1235	0	1249	31	0
39	1h	1088	0	1126	17	0
39	2h	1088	0	1126	20	0
40	1i	983	0	986	29	0
40	2i	978	0	966	34	0
41	1j	709	0	650	23	0
41	2j	714	0	672	33	0
42	1k	829	0	825	11	0
42	2k	833	0	836	15	0
43	1l	932	0	981	14	0
43	2l	932	0	981	11	0
44	1m	958	0	1002	26	0
44	2m	950	0	988	31	0
45	1n	492	0	529	10	0
45	2n	492	0	529	20	0
46	1o	728	0	760	14	0
46	2o	728	0	760	19	0
47	1p	681	0	697	9	0
47	2p	677	0	686	15	0
48	1q	823	0	891	11	0
48	2q	823	0	891	17	0
49	1r	555	0	618	7	0
49	2r	555	0	618	21	0
50	1s	652	0	662	17	0
50	2s	646	0	644	29	0
51	1t	728	0	798	19	0
51	2t	727	0	796	19	0
52	1u	199	0	208	4	0
52	2u	199	0	208	6	0
53	1v	277	0	140	1	0
53	2v	277	0	140	2	0
54	1w	1592	0	817	19	0
54	2w	1544	0	786	18	0
55	1x	1646	0	838	9	0
55	2x	1646	0	838	11	0
56	1y	1585	0	803	32	0
56	2y	1565	0	794	40	0
57	10	9	0	0	0	0
57	11	5	0	0	0	0
57	12	2	0	0	0	0
57	13	4	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	14	1	0	0	0	0
57	15	7	0	0	0	0
57	16	1	0	0	0	0
57	17	5	0	0	0	0
57	18	5	0	0	0	0
57	19	1	0	0	0	0
57	1A	1117	0	0	0	0
57	1B	37	0	0	0	0
57	1D	15	0	0	0	0
57	1E	15	0	0	0	0
57	1F	12	0	0	0	0
57	1G	5	0	0	0	0
57	1I	1	0	0	0	0
57	1N	4	0	0	0	0
57	1O	6	0	0	0	0
57	1P	6	0	0	0	0
57	1Q	6	0	0	0	0
57	1R	6	0	0	0	0
57	1S	3	0	0	0	0
57	1T	2	0	0	0	0
57	1U	11	0	0	0	0
57	1V	7	0	0	0	0
57	1W	4	0	0	0	0
57	1X	6	0	0	0	0
57	1Y	2	0	0	0	0
57	1Z	4	0	0	0	0
57	1a	222	0	0	0	0
57	1b	1	0	0	0	0
57	1e	2	0	0	0	0
57	1f	2	0	0	0	0
57	1h	1	0	0	0	0
57	1j	1	0	0	0	0
57	1k	1	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	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	1	0	0	0	0
57	21	3	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	23	2	0	0	0	0
57	25	4	0	0	0	0
57	27	2	0	0	0	0
57	28	2	0	0	0	0
57	2A	842	0	0	0	0
57	2B	18	0	0	0	0
57	2D	9	0	0	0	0
57	2E	8	0	0	0	0
57	2F	8	0	0	0	0
57	2G	1	0	0	0	0
57	2N	1	0	0	0	0
57	2O	2	0	0	0	0
57	2P	1	0	0	0	0
57	2Q	3	0	0	0	0
57	2R	3	0	0	0	0
57	2T	4	0	0	0	0
57	2U	2	0	0	0	0
57	2V	2	0	0	0	0
57	2W	1	0	0	0	0
57	2X	2	0	0	0	0
57	2Y	1	0	0	0	0
57	2Z	1	0	0	0	0
57	2a	231	0	0	0	0
57	2d	1	0	0	0	0
57	2e	1	0	0	0	0
57	2f	2	0	0	0	0
57	2g	1	0	0	0	0
57	2j	1	0	0	0	0
57	2l	4	0	0	0	0
57	2m	1	0	0	0	0
57	2q	2	0	0	0	0
57	2r	1	0	0	0	0
57	2t	1	0	0	0	0
57	2v	2	0	0	0	0
57	2w	7	0	0	0	0
57	2x	7	0	0	0	0
57	2y	2	0	0	0	0
58	1A	1	0	0	0	0
58	2A	1	0	0	0	0
59	1A	85	0	0	2	0
59	2A	85	0	0	1	0
60	14	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	15	1	0	0	0	0
60	16	1	0	0	0	0
60	19	1	0	0	0	0
60	1Y	1	0	0	0	0
60	1n	1	0	0	0	0
60	24	1	0	0	0	0
60	25	1	0	0	0	0
60	26	1	0	0	0	0
60	29	1	0	0	0	0
60	2Y	1	0	0	0	0
60	2n	1	0	0	0	0
61	1d	8	0	0	0	0
61	2d	8	0	0	0	0
62	1w	11	0	8	0	0
62	2w	11	0	8	1	0
63	1x	10	0	10	0	0
63	2x	10	0	10	0	0
64	10	12	0	0	2	0
64	11	9	0	0	0	0
64	12	3	0	0	0	0
64	13	4	0	0	0	0
64	14	1	0	0	0	0
64	15	6	0	0	0	0
64	16	2	0	0	0	0
64	17	9	0	0	1	0
64	18	10	0	0	1	0
64	1A	2052	0	0	67	0
64	1B	64	0	0	2	0
64	1D	31	0	0	0	0
64	1E	27	0	0	2	0
64	1F	19	0	0	1	0
64	1G	3	0	0	1	0
64	1H	2	0	0	0	0
64	1N	5	0	0	0	0
64	1O	6	0	0	0	0
64	1P	22	0	0	0	0
64	1Q	9	0	0	0	0
64	1R	9	0	0	1	0
64	1S	4	0	0	1	0
64	1T	8	0	0	0	0
64	1U	13	0	0	0	0
64	1V	8	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
64	1W	8	0	0	0	0
64	1X	4	0	0	0	0
64	1Y	2	0	0	0	0
64	1Z	1	0	0	0	0
64	1a	418	0	0	25	0
64	1b	1	0	0	0	0
64	1d	3	0	0	0	0
64	1e	1	0	0	0	0
64	1f	2	0	0	0	0
64	1g	1	0	0	0	0
64	1i	2	0	0	0	0
64	1j	2	0	0	0	0
64	1k	1	0	0	0	0
64	1l	5	0	0	0	0
64	1m	2	0	0	0	0
64	1p	1	0	0	0	0
64	1q	2	0	0	0	0
64	1r	1	0	0	0	0
64	1v	4	0	0	0	0
64	1w	15	0	0	0	0
64	1x	16	0	0	1	0
64	1y	1	0	0	0	0
64	20	2	0	0	0	0
64	21	7	0	0	0	0
64	23	2	0	0	1	0
64	25	1	0	0	0	0
64	26	1	0	0	0	0
64	27	4	0	0	0	0
64	28	3	0	0	0	0
64	29	1	0	0	0	0
64	2A	1183	0	0	66	0
64	2B	18	0	0	1	0
64	2D	22	0	0	0	0
64	2E	12	0	0	0	0
64	2F	12	0	0	0	0
64	2N	2	0	0	0	0
64	2O	2	0	0	0	0
64	2P	10	0	0	0	0
64	2Q	1	0	0	0	0
64	2R	4	0	0	0	0
64	2T	6	0	0	0	0
64	2U	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
64	2W	1	0	0	0	0
64	2X	2	0	0	0	0
64	2Y	2	0	0	0	0
64	2a	265	0	0	16	0
64	2c	2	0	0	0	0
64	2d	3	0	0	0	0
64	2e	1	0	0	0	0
64	2g	1	0	0	0	0
64	2j	2	0	0	1	0
64	2l	6	0	0	0	0
64	2n	1	0	0	1	0
64	2p	1	0	0	0	0
64	2r	1	0	0	1	0
64	2t	5	0	0	0	0
64	2w	2	0	0	0	0
64	2x	7	0	0	0	0
64	2y	3	0	0	0	0
All	All	300455	0	196744	3290	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 (3290) 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)
59:1A:4118:A1AEZ:NBJ	59:1A:4118:A1AEZ:OBR	1.56	1.34
1:1A:1082:U:H3	1:1A:1086:A:N6	1.35	1.25
1:1A:1082:U:O4	1:1A:1086:A:N1	1.96	0.99
1:2A:2298:A:H62	1:2A:2318:G:H8	1.14	0.95
1:1A:1054:A:H61	1:1A:1105:U:H3	1.15	0.92
1:1A:1798:U:H5'	3:1D:259:THR:HG22	1.49	0.91
1:1A:1062:G:H1	1:1A:1077:A:H61	1.18	0.91
33:1b:185:ILE:HG22	33:1b:199:TYR:HB2	1.53	0.90
10:2O:48:PRO:HB3	32:2a:1422:G:H5"	1.53	0.89
29:17:24:THR:HG22	29:17:27:GLY:H	1.36	0.89
1:1A:2427:C:OP1	64:1A:4203:HOH:O	1.92	0.87
17:1V:55:ALA:HA	17:1V:101:GLY:HA2	1.56	0.87
1:1A:2099:U:H3	1:1A:2190:G:H1	1.21	0.86
32:2a:975:A:H4'	32:2a:976:G:H5"	1.57	0.85
34:1c:6:HIS:HD2	34:1c:8:ILE:H	1.25	0.84
1:1A:2100:G:H1	1:1A:2189:U:H3	0.85	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:24:53:GLU:HG2	26:24:55:ARG:H	1.42	0.84
1:2A:2319:G:H22	14:2S:3:ARG:HH11	1.26	0.84
56:1y:2:C:H42	56:1y:71:G:H1	1.26	0.84
2:2B:7:G:H21	14:2S:38:GLN:HE22	1.22	0.83
1:1A:993:G:OP1	16:1U:50:ARG:NH2	2.13	0.82
1:1A:1664:A:OP1	64:1A:4204:HOH:O	1.97	0.82
1:1A:2124:G:H1	1:1A:2174:C:H42	1.25	0.82
1:2A:1204:A:H2	1:2A:1241:A:H62	1.27	0.81
1:1A:11:G:H2'	1:1A:12:U:H5"	1.61	0.81
1:1A:847:U:OP2	64:1A:4205:HOH:O	1.98	0.81
35:1d:112:VAL:HG23	35:1d:116:GLN:HE22	1.45	0.81
1:2A:994:C:OP1	16:2U:53:ARG:NH2	2.14	0.81
32:1a:547:A:OP1	64:1a:4803:HOH:O	1.99	0.80
32:2a:1086:U:H3	32:2a:1099:G:H22	1.25	0.80
1:1A:2136:C:N3	1:1A:2155:G:C2	2.50	0.80
1:2A:2131:G:H22	1:2A:2158:A:H62	1.30	0.80
1:2A:2206:G:H3'	1:2A:2207:G:C8	2.17	0.79
1:1A:1057:A:H61	1:1A:1081:U:H3	1.29	0.79
22:10:10:THR:HG22	22:10:12:ASN:H	1.47	0.79
21:2Z:154:ASP:N	21:2Z:154:ASP:OD1	2.15	0.79
32:2a:1106:G:H5"	34:2c:172:ARG:HG2	1.63	0.79
40:2i:3:GLN:HE21	40:2i:20:ARG:HE	1.31	0.79
1:1A:1023:U:OP2	64:1A:4207:HOH:O	2.01	0.78
1:2A:963:U:OP2	64:2A:3902:HOH:O	2.00	0.78
1:2A:2136:C:N4	1:2A:2155:G:H1	1.80	0.78
1:2A:1019:U:H3	1:2A:1142(A):A:H62	1.32	0.78
33:2b:69:LEU:HB3	33:2b:162:ILE:HG22	1.65	0.78
1:2A:1647:G:OP1	64:2A:3903:HOH:O	2.00	0.78
1:2A:2379:G:O2'	14:2S:17:ARG:NH1	2.13	0.78
32:2a:1272:G:N2	32:2a:1273:G:N7	2.32	0.78
32:1a:1314:C:OP2	50:1s:4:SER:OG	2.01	0.78
38:2g:113:GLU:HG2	38:2g:119:ARG:HG2	1.66	0.78
1:1A:1036:G:O6	64:1A:4206:HOH:O	2.00	0.78
32:2a:1314:C:OP2	50:2s:4:SER:OG	2.00	0.77
1:1A:2102:U:H3	1:1A:2187:G:H1	1.31	0.77
34:2c:43:LEU:HD21	34:2c:91:LEU:HD21	1.66	0.77
32:1a:975:A:H4'	32:1a:976:G:H5"	1.66	0.77
10:2O:35:VAL:HG11	10:2O:103:ALA:HB3	1.67	0.77
1:2A:1604:C:OP2	64:2A:3906:HOH:O	2.03	0.77
1:1A:1603:A:OP1	64:1A:4208:HOH:O	2.02	0.77
1:2A:2138:C:H42	1:2A:2153:G:H1	1.29	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2550:G:OP1	64:1A:4209:HOH:O	2.02	0.76
1:2A:678:C:OP1	64:2A:3904:HOH:O	2.02	0.76
44:2m:13:LYS:HA	44:2m:44:ARG:HH11	1.49	0.76
1:1A:1993:U:OP2	64:1A:4210:HOH:O	2.02	0.76
1:1A:2183:C:H2'	1:1A:2184:G:H8	1.49	0.76
21:2Z:171:ILE:HD12	21:2Z:172:ALA:H	1.49	0.76
1:1A:631:A:OP1	11:1P:65:ARG:NH1	2.19	0.76
29:17:23:ARG:NH1	64:17:201:HOH:O	2.16	0.76
32:2a:953:G:H5'	32:2a:965:A:H61	1.49	0.76
32:2a:1286:A:C8	32:2a:1287:A:H4'	2.20	0.76
1:1A:1395:A:OP1	64:1A:4208:HOH:O	2.03	0.76
1:1A:826:U:OP1	64:1A:4203:HOH:O	2.02	0.76
1:2A:1830:C:OP2	64:2A:3905:HOH:O	2.02	0.76
36:2e:20:GLN:NE2	36:2e:21:ALA:O	2.19	0.76
5:2F:21:ALA:HB3	5:2F:22:ALA:HA	1.66	0.76
11:2P:118:GLY:O	11:2P:137:LYS:NZ	2.19	0.76
32:2a:117:G:OP2	64:2a:1901:HOH:O	2.03	0.76
32:2a:278:G:OP2	48:2q:41:LYS:NZ	2.20	0.76
1:1A:763:G:OP1	64:1A:4215:HOH:O	2.05	0.75
32:1a:664:G:H22	32:1a:741:G:H1	1.32	0.75
21:2Z:146:ILE:HG12	21:2Z:174:VAL:HG13	1.68	0.75
32:1a:1027:C:C2	32:1a:1034:G:N2	2.48	0.75
56:2y:18:G:N2	56:2y:55:PSU:N3	2.35	0.75
1:1A:1060:U:H3	1:1A:1088:A:H8	1.34	0.75
1:1A:2849:U:OP2	15:1T:95:ARG:NH1	2.20	0.75
32:2a:157:G:H1	32:2a:164:U:H3	1.33	0.75
49:2r:32:ARG:HA	49:2r:69:THR:HG21	1.68	0.75
1:1A:1082:U:N3	1:1A:1086:A:N6	2.11	0.75
33:1b:33:TYR:HB2	33:1b:43:ASP:HB2	1.66	0.75
1:1A:2575:C:OP2	64:1A:4211:HOH:O	2.03	0.74
4:2E:119:ARG:HD2	4:2E:160:TYR:HB2	1.69	0.74
33:1b:195:ASP:O	39:1h:68:ARG:NH2	2.19	0.74
35:2d:157:LEU:O	35:2d:161:ASN:ND2	2.20	0.74
1:2A:2448:A:OP1	64:2A:3907:HOH:O	2.04	0.74
1:1A:192:C:OP1	64:1A:4214:HOH:O	2.04	0.74
1:1A:1054:A:N6	1:1A:1105:U:H3	1.84	0.74
10:1O:35:VAL:HG11	10:1O:103:ALA:HB3	1.68	0.74
1:1A:1647:G:OP1	64:1A:4213:HOH:O	2.04	0.74
1:2A:2365:G:N7	30:28:39:LYS:NZ	2.35	0.74
44:2m:23:TYR:HB3	44:2m:67:GLU:HA	1.69	0.74
2:2B:75:G:H22	21:2Z:73:GLN:HE21	1.34	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:979:C:N4	64:2a:1913:HOH:O	2.21	0.74
35:2d:8:VAL:HG22	35:2d:21:LEU:HD13	1.68	0.74
1:1A:1332:G:OP1	64:1A:4212:HOH:O	2.04	0.73
28:16:12:GLU:OE1	28:16:19:ARG:NH1	2.21	0.73
59:1A:4118:A1AEZ:NBJ	59:1A:4118:A1AEZ:CBS	2.50	0.73
1:2A:132:G:O6	64:2A:3908:HOH:O	2.06	0.73
32:2a:1286:A:H8	32:2a:1287:A:H4'	1.52	0.73
1:2A:1812:A:OP2	64:2A:3909:HOH:O	2.06	0.73
6:2G:113:ARG:NH2	6:2G:139:LEU:O	2.21	0.73
32:1a:1086:U:H3	32:1a:1099:G:H22	1.35	0.73
1:2A:2099:U:H3	1:2A:2190:G:H1	1.36	0.73
13:2R:97:VAL:HG22	13:2R:114:VAL:HG13	1.70	0.73
1:2A:1271:G:OP2	64:2A:3903:HOH:O	2.06	0.73
56:2y:8:4SU:H5"	56:2y:49:C:H5'	1.70	0.73
41:1j:38:ILE:HG13	41:1j:71:LEU:HB3	1.70	0.73
25:23:13:ILE:O	64:23:201:HOH:O	2.07	0.73
34:2c:125:GLU:HB2	34:2c:190:ARG:HH21	1.53	0.73
1:2A:1253:A:OP1	64:2A:3911:HOH:O	2.07	0.72
1:1A:1669:A:OP2	64:1A:4209:HOH:O	2.07	0.72
4:1E:105:THR:OG1	4:1E:199:ARG:NH2	2.22	0.72
1:1A:1315:C:OP2	64:1A:4212:HOH:O	2.07	0.72
1:1A:1058:G:N2	1:1A:1081:U:O2	2.21	0.72
7:2H:11:VAL:HG13	7:2H:15:VAL:HG23	1.71	0.72
32:2a:266:G:H5"	32:2a:268:C:H41	1.54	0.72
33:2b:189:ASP:OD1	33:2b:189:ASP:N	2.23	0.72
34:2c:182:ILE:HG22	34:2c:203:PHE:HA	1.71	0.72
37:2f:97:PHE:HD2	49:2r:31:LEU:HD11	1.54	0.72
1:2A:2592:G:OP1	64:2A:3910:HOH:O	2.06	0.72
1:1A:110:G:N7	64:1A:4251:HOH:O	2.23	0.72
32:2a:588:G:OP2	64:2a:1902:HOH:O	2.06	0.72
40:2i:16:ARG:HB2	40:2i:64:THR:HG22	1.70	0.72
44:2m:58:GLU:O	44:2m:62:ASN:ND2	2.22	0.72
44:2m:80:ARG:HH22	50:2s:69:HIS:HE1	1.38	0.72
33:1b:12:GLU:HB2	33:1b:213:LEU:HD21	1.72	0.72
1:2A:1024:G:OP2	64:2A:3912:HOH:O	2.07	0.72
41:1j:81:THR:HG22	41:1j:85:LEU:HG	1.72	0.71
5:1F:116:ASP:OD1	5:1F:119:ARG:NH2	2.23	0.71
51:1t:60:GLU:HG3	51:1t:81:LYS:HD2	1.71	0.71
1:2A:880:G:H2'	1:2A:881:G:H8	1.56	0.71
32:2a:671:G:H5'	37:2f:77:ARG:HH22	1.55	0.71
32:2a:1181:G:O2'	32:2a:1182:G:N7	2.24	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1316:G:H22	32:2a:1319:A:H5"	1.55	0.71
56:2y:14:A:H61	56:2y:21:A:H2	1.39	0.71
35:1d:15:GLU:OE2	35:1d:59:ARG:NH1	2.24	0.71
1:2A:1689:A:H62	1:2A:1698:A:H2	1.36	0.71
1:2A:2849:U:O4	15:2T:23:ARG:NH2	2.23	0.71
32:2a:664:G:H22	32:2a:741:G:H1	1.37	0.71
1:2A:2131:G:H22	1:2A:2158:A:N6	1.87	0.71
32:1a:953:G:H5'	32:1a:965:A:H61	1.52	0.71
26:24:24:THR:OG1	26:24:25:TYR:N	2.23	0.71
32:1a:1224:G:OP1	64:1a:4805:HOH:O	2.08	0.71
1:2A:248:G:OP1	64:2A:3913:HOH:O	2.09	0.71
32:2a:353:A:OP1	64:2a:1904:HOH:O	2.09	0.71
1:1A:2749:A:OP1	7:1H:3:ARG:NH1	2.23	0.70
32:1a:116:A:OP1	64:1a:4804:HOH:O	2.08	0.70
1:1A:1266:G:O5'	18:1W:15:ARG:NH2	2.24	0.70
1:2A:973:A:OP2	64:2A:3915:HOH:O	2.09	0.70
1:2A:1031:G:H5"	31:29:8:LYS:HE3	1.73	0.70
26:24:46:GLN:HE21	26:24:48:ARG:HD3	1.56	0.70
25:23:59:VAL:HG12	25:23:60:GLU:H	1.55	0.70
33:2b:16:HIS:HB2	33:2b:204:ASN:HB3	1.73	0.70
1:2A:1693:U:O2'	3:2D:14:ARG:NH2	2.23	0.70
1:2A:2079:U:OP1	23:21:21:ARG:NH2	2.23	0.70
1:1A:1693:U:O2'	3:1D:14:ARG:NH2	2.25	0.70
1:2A:1648:C:OP1	64:2A:3903:HOH:O	2.08	0.70
1:2A:948:G:OP1	64:2A:3902:HOH:O	2.09	0.70
21:2Z:106:GLY:HA3	21:2Z:141:VAL:HB	1.73	0.70
32:2a:1010:G:H2'	32:2a:1011:G:H8	1.55	0.70
1:1A:1024:G:OP2	64:1A:4207:HOH:O	2.08	0.70
1:1A:2131:G:N2	1:1A:2158:A:N1	2.40	0.70
32:2a:289:G:OP2	64:2a:1901:HOH:O	2.09	0.70
56:2y:26:A:N1	56:2y:44:G:C6	2.59	0.70
1:1A:1890:A:OP2	64:1A:4218:HOH:O	2.10	0.69
32:1a:1033:G:H3'	32:1a:1034:G:H8	1.57	0.69
32:2a:922:G:H4'	36:2e:20:GLN:HA	1.73	0.69
36:2e:33:VAL:HG13	36:2e:112:LEU:HD22	1.72	0.69
1:1A:668:G:N7	64:1A:4256:HOH:O	2.25	0.69
1:2A:526:A:OP1	64:2A:3916:HOH:O	2.10	0.69
2:1B:23:G:O6	64:1B:301:HOH:O	2.06	0.69
1:2A:1394:U:OP1	64:2A:3917:HOH:O	2.10	0.69
1:2A:2379:G:HO2'	14:2S:17:ARG:HH12	1.40	0.69
1:1A:2136:C:N4	1:1A:2155:G:C6	2.60	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1602:U:O4	64:1A:4217:HOH:O	2.08	0.69
17:2V:43:GLU:OE1	17:2V:43:GLU:N	2.26	0.69
1:1A:467:G:OP1	29:17:33:ARG:NH1	2.26	0.69
1:1A:2499:C:OP1	64:1A:4221:HOH:O	2.11	0.69
1:2A:752:A:H3'	29:27:1:MET:HE1	1.74	0.69
12:1Q:60:ARG:NH2	54:1w:54:5MU:OP2	2.25	0.69
32:2a:1108:G:O6	64:2a:1903:HOH:O	2.08	0.69
36:2e:122:GLU:O	36:2e:126:ARG:NH1	2.26	0.69
1:1A:2206:G:H3'	1:1A:2207:G:C8	2.28	0.69
41:1j:8:LEU:HD22	41:1j:96:ILE:HG22	1.75	0.69
21:2Z:93:ASP:HA	21:2Z:131:ARG:HH12	1.58	0.69
1:2A:1030:G:OP2	12:2Q:128:LYS:NZ	2.25	0.69
1:2A:1264:G:OP1	27:25:19:ARG:NH2	2.20	0.69
32:2a:1002:G:H1	32:2a:1038:C:H42	1.40	0.69
38:2g:78:ARG:HH21	38:2g:79:ARG:HE	1.40	0.69
54:2w:4:C:H42	54:2w:69:G:H1	1.41	0.69
1:1A:271(V):G:O6	64:1A:4216:HOH:O	2.08	0.68
32:1a:1002:G:H3'	32:1a:1003:G:H4'	1.75	0.68
56:1y:5:G:O2'	56:1y:69:G:N2	2.26	0.68
1:2A:568:U:H5'	1:2A:945:A:N1	2.08	0.68
1:2A:2677:G:N3	64:2A:3966:HOH:O	2.26	0.68
1:1A:1970:A:OP1	64:1A:4219:HOH:O	2.10	0.68
1:2A:1800:C:OP2	3:2D:183:ARG:NH2	2.27	0.68
1:2A:1023:U:OP2	64:2A:3912:HOH:O	2.11	0.68
1:1A:2079:U:OP1	23:11:21:ARG:NH2	2.22	0.68
2:1B:103:G:H21	21:1Z:73:GLN:HE22	1.41	0.68
32:1a:1505:G:OP2	64:1a:4806:HOH:O	2.10	0.68
1:1A:1271:G:OP2	64:1A:4213:HOH:O	2.09	0.68
38:2g:68:ASN:HD22	38:2g:128:ALA:HA	1.57	0.68
50:2s:49:ILE:HG22	50:2s:62:ILE:HD11	1.74	0.68
15:2T:65:LYS:HE3	15:2T:67:SER:HB2	1.76	0.68
32:2a:460:G:O6	64:2a:1905:HOH:O	2.10	0.68
32:2a:1129:C:H2'	32:2a:1139:G:N7	2.09	0.68
46:2o:7:GLU:OE1	46:2o:38:ARG:NH2	2.26	0.68
13:1R:97:VAL:HG22	13:1R:114:VAL:HG13	1.74	0.68
26:14:55:ARG:N	26:14:56:VAL:HA	2.09	0.68
38:1g:115:ARG:H	38:1g:115:ARG:HD2	1.58	0.68
12:2Q:11:LYS:NZ	12:2Q:88:GLY:O	2.24	0.68
32:2a:656:C:O2'	46:2o:28:GLN:OE1	2.07	0.68
1:2A:1021:A:H62	1:2A:1141:U:H3	1.41	0.68
1:2A:2110:G:OP1	1:2A:2118:U:N3	2.25	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:1N:46:VAL:HG23	9:1N:48:MET:HG2	1.76	0.68
33:1b:224:GLN:HG2	33:1b:229:VAL:HG22	1.74	0.68
51:1t:10:LEU:HB3	51:1t:12:ALA:H	1.56	0.68
1:2A:570:G:O6	64:2A:3907:HOH:O	2.08	0.68
1:2A:2154:G:N7	1:2A:2156:G:N2	2.42	0.68
32:2a:1271:G:N2	32:2a:1272:G:N7	2.42	0.68
1:1A:2629:A:O2'	1:1A:2630:G:OP2	2.12	0.67
1:1A:2428:G:OP1	64:1A:4203:HOH:O	2.13	0.67
25:13:55:ARG:HH22	25:13:57:GLU:HB2	1.59	0.67
1:2A:400:G:N7	64:2A:3970:HOH:O	2.27	0.67
47:2p:21:VAL:HG23	47:2p:33:ILE:HB	1.77	0.67
48:2q:66:SER:O	48:2q:70:ARG:NH1	2.27	0.67
32:2a:297:G:N2	32:2a:300:A:OP2	2.27	0.67
32:1a:1467:G:O6	64:1a:4807:HOH:O	2.11	0.67
5:2F:53:THR:HG23	5:2F:55:GLY:H	1.58	0.67
8:2I:59:ALA:HA	8:2I:62:LYS:HG2	1.75	0.67
47:2p:1:MET:HE3	47:2p:3:LYS:HD3	1.76	0.67
40:1i:53:VAL:O	40:1i:55:ALA:N	2.25	0.67
59:2A:3843:A1AEZ:ODD	64:2A:3919:HOH:O	2.12	0.67
7:2H:80:SER:OG	7:2H:81:GLU:OE2	2.13	0.67
43:2l:53:ARG:HG3	43:2l:93:LEU:HD21	1.77	0.67
33:1b:93:VAL:HG11	33:1b:97:TRP:HD1	1.59	0.67
1:1A:2235:G:N7	64:1A:4272:HOH:O	2.28	0.66
1:2A:1006:C:OP1	64:2A:3921:HOH:O	2.12	0.66
46:2o:87:ILE:HG22	46:2o:88:ARG:H	1.59	0.66
1:2A:2524:G:N7	64:2A:3976:HOH:O	2.28	0.66
32:2a:1004:A:N6	32:2a:1037:C:H1'	2.10	0.66
1:2A:106:C:H1'	20:2Y:1:MET:HE2	1.75	0.66
1:1A:2316:C:O2'	6:1G:128:ARG:NH2	2.29	0.66
51:1t:22:ARG:O	51:1t:26:ASN:ND2	2.28	0.66
56:1y:2:C:N4	56:1y:71:G:H1	1.93	0.66
1:2A:2133:G:O2'	1:2A:2157:G:N2	2.28	0.66
40:2i:128:ARG:NH2	55:2x:33:U:OP2	2.28	0.66
10:1O:48:PRO:HB3	32:1a:1422:G:H5"	1.78	0.66
32:1a:324:G:N7	64:1a:4837:HOH:O	2.29	0.66
32:1a:505:G:N7	64:1a:4836:HOH:O	2.29	0.66
1:2A:141:A:H8	1:2A:1408:C:HO2'	1.40	0.66
12:2Q:111:GLU:OE2	12:2Q:133:ARG:NH2	2.27	0.66
15:2T:117:ASP:OD2	15:2T:120:ARG:NE	2.27	0.66
32:1a:702:A:OP2	64:1a:4808:HOH:O	2.12	0.66
43:1l:57:LYS:HG2	43:1l:67:THR:HG22	1.78	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2G:161:THR:HG22	6:2G:163:ALA:H	1.59	0.66
32:2a:999:C:H42	32:2a:1042:G:H1	1.41	0.66
34:2c:36:ASP:HA	34:2c:39:ILE:HD12	1.78	0.66
32:1a:892:A:OP2	64:1a:4809:HOH:O	2.14	0.66
1:2A:1225:G:H4'	17:2V:84:LYS:HG2	1.78	0.66
1:2A:2091:U:O4	64:2A:3920:HOH:O	2.12	0.66
3:2D:148:GLU:HB2	3:2D:151:LYS:HD2	1.78	0.66
56:2y:18:G:N2	56:2y:55:PSU:HN3	1.93	0.66
40:1i:46:ALA:HB2	40:1i:74:ILE:HG23	1.76	0.66
1:2A:143:G:H4'	19:2X:35:THR:HG21	1.77	0.66
1:1A:1607:C:O2	64:1A:4220:HOH:O	2.11	0.66
6:1G:77:ILE:HD12	6:1G:82:LEU:HD12	1.78	0.66
1:2A:1254:A:OP2	64:2A:3923:HOH:O	2.14	0.66
1:2A:1452:A:OP2	64:2A:3924:HOH:O	2.15	0.65
1:2A:2268:A:OP1	64:2A:3922:HOH:O	2.14	0.65
1:2A:2277:G:OP2	22:20:10:THR:HG21	1.96	0.65
23:11:2:SER:HB3	23:11:46:LEU:HD12	1.79	0.65
5:2F:184:TYR:CE2	5:2F:188:ARG:HD2	2.32	0.65
21:1Z:105:VAL:N	21:1Z:139:VAL:O	2.28	0.65
34:1c:71:ALA:HA	34:1c:106:VAL:HG21	1.79	0.65
25:23:40:THR:HG22	25:23:42:ALA:H	1.61	0.65
41:2j:49:VAL:HG23	45:2n:41:ARG:HB2	1.78	0.65
32:1a:559:A:OP1	36:1e:126:ARG:NH2	2.30	0.65
32:2a:1119:C:H2'	32:2a:1120:G:C8	2.32	0.65
43:2l:32:PHE:HB3	43:2l:84:LEU:HD11	1.79	0.65
1:1A:744:G:OP1	64:1A:4224:HOH:O	2.15	0.65
1:1A:2124:G:H1	1:1A:2174:C:N4	1.93	0.65
5:1F:157:VAL:HB	5:1F:194:MET:HG2	1.78	0.65
8:1I:92:VAL:HG13	8:1I:120:ILE:HB	1.77	0.65
42:1k:48:ILE:O	42:1k:50:TYR:N	2.29	0.65
32:2a:1025:U:H3	32:2a:1036:G:H1	1.43	0.65
1:1A:1670:C:OP1	64:1A:4222:HOH:O	2.14	0.65
1:1A:2341:G:N7	64:1A:4279:HOH:O	2.29	0.65
1:2A:1354:A:H5"	3:2D:38:LYS:HD3	1.78	0.65
1:1A:84:A:H5"	20:1Y:8:LYS:HE3	1.79	0.65
1:2A:1721:G:H8	1:2A:1741:A:H62	1.44	0.65
32:1a:1125:U:H4'	41:1j:5:ARG:HH22	1.61	0.65
39:1h:121:ASP:OD1	39:1h:121:ASP:N	2.30	0.65
1:2A:2156:G:H2'	1:2A:2157:G:C2	2.31	0.65
1:2A:2327:A:H2'	1:2A:2328:A:C8	2.31	0.65
1:2A:2788:C:OP1	4:2E:61:ARG:NH2	2.30	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:2X:60:ARG:HH22	29:27:47:ARG:HH12	1.45	0.65
32:2a:1029:C:C4	32:2a:1032:G:N1	2.65	0.65
1:1A:1038:C:H42	1:1A:1117:G:H1	1.45	0.64
1:1A:1105:U:H2'	1:1A:1106:G:C8	2.32	0.64
1:1A:2130:U:H2'	1:1A:2158:A:H61	1.62	0.64
8:1I:75:LEU:HD22	8:1I:105:HIS:CD2	2.32	0.64
1:1A:1105:U:H2'	1:1A:1106:G:H8	1.61	0.64
3:2D:180:GLY:HA3	3:2D:275:LYS:HG2	1.79	0.64
1:1A:2218:U:O4'	23:11:52:ARG:NH2	2.30	0.64
26:14:16:CYS:SG	26:14:17:GLY:N	2.70	0.64
32:1a:1136:U:H5"	32:1a:1137:C:C4	2.32	0.64
46:1o:25:THR:HG21	46:1o:70:LEU:HB2	1.80	0.64
13:2R:67:LEU:HD13	13:2R:76:VAL:HG21	1.79	0.64
51:2t:99:LEU:HD12	51:2t:100:ILE:HG23	1.79	0.64
1:1A:2344:U:OP1	28:16:37:ARG:NH1	2.31	0.64
32:1a:545:C:OP1	35:1d:61:LYS:NZ	2.31	0.64
56:1y:19:G:N2	56:1y:56:C:N3	2.44	0.64
62:2w:108:PHE:N	55:2x:76:8AN:HO2'	1.94	0.64
1:1A:1014:U:OP2	64:1A:4223:HOH:O	2.14	0.64
25:13:3:ARG:NE	25:13:60:GLU:OE2	2.26	0.64
32:1a:1004:A:H5'	32:1a:1024:G:H1	1.63	0.64
34:1c:8:ILE:HD13	34:1c:184:TYR:HB3	1.79	0.64
51:1t:56:MET:HE3	51:1t:85:MET:HE2	1.79	0.64
1:2A:1163:G:OP1	17:2V:24:LYS:NZ	2.28	0.64
1:2A:2646:C:OP2	1:2A:2732:G:O2'	2.14	0.64
32:2a:1272:G:N2	32:2a:1273:G:C5	2.65	0.64
41:2j:40:LEU:HB2	41:2j:69:ASN:HB3	1.80	0.64
40:1i:20:ARG:O	40:1i:60:ASP:N	2.21	0.64
1:2A:2138:C:N4	1:2A:2153:G:H1	1.95	0.64
1:1A:1053:C:H42	1:1A:1106:G:H1	1.43	0.64
34:1c:15:THR:HG21	34:1c:181:ASN:HA	1.80	0.64
1:2A:2839:G:H5'	13:2R:46:GLY:HA2	1.79	0.64
1:1A:1314:C:OP1	64:1A:4212:HOH:O	2.15	0.64
32:1a:159:G:N2	32:1a:162:A:OP2	2.30	0.64
32:1a:800:G:O6	64:1a:4810:HOH:O	2.14	0.64
34:1c:162:GLN:NE2	53:1v:24:A:O2'	2.31	0.64
8:2I:86:THR:HG23	8:2I:87:LYS:HD2	1.80	0.64
32:2a:1189:C:OP1	41:2j:51:ARG:NH2	2.31	0.64
39:1h:86:ILE:HD12	39:1h:133:LEU:HD22	1.80	0.63
6:1G:131:TYR:HB3	6:1G:159:VAL:HG13	1.79	0.63
21:1Z:163:LEU:HD23	21:1Z:167:PRO:HG3	1.80	0.63

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	2.17	0.63
1:2A:1300:U:H4'	1:2A:1301:A:H5"	1.80	0.63
1:2A:1970:A:OP1	64:2A:3925:HOH:O	2.15	0.63
14:2S:48:LEU:HD23	14:2S:82:ILE:HD11	1.80	0.63
32:2a:1375:A:H4'	38:2g:29:LYS:HE3	1.80	0.63
56:2y:18:G:H22	56:2y:55:PSU:HN3	1.46	0.63
32:1a:933:G:O6	38:1g:3:ARG:NH2	2.32	0.63
11:2P:63:PRO:HD3	30:28:27:THR:HG22	1.80	0.63
32:1a:691:G:OP2	42:1k:26:ASN:ND2	2.27	0.63
37:1f:89:MET:HE1	49:1r:72:ARG:HB3	1.80	0.63
55:1x:76:8AN:O2P	64:1x:201:HOH:O	2.15	0.63
8:2I:40:THR:O	8:2I:44:LEU:HB2	1.98	0.63
32:2a:7:G:O2'	36:2e:120:THR:O	2.16	0.63
32:2a:1166:G:N2	32:2a:1170:A:OP2	2.29	0.63
32:2a:1099:G:OP2	33:2b:144:ARG:NH2	2.32	0.63
33:1b:16:HIS:HB2	33:1b:204:ASN:HB3	1.79	0.63
32:2a:410:G:OP1	35:2d:30:LYS:NZ	2.22	0.63
43:1l:88:GLY:O	43:1l:99:HIS:HD2	1.82	0.63
8:2I:12:LEU:HD22	8:2I:19:VAL:HG21	1.80	0.63
26:24:44:THR:O	26:24:46:GLN:N	2.31	0.63
32:2a:662:G:O2'	32:2a:836:G:OP1	2.17	0.63
1:1A:1648:C:OP1	64:1A:4213:HOH:O	2.15	0.63
37:1f:42:GLU:OE2	37:1f:59:TYR:OH	2.13	0.62
21:2Z:4:ARG:NH2	21:2Z:66:SER:OG	2.31	0.62
35:2d:119:GLN:HG2	35:2d:123:HIS:CD2	2.33	0.62
56:1y:51:U:H3	56:1y:63:G:H1	1.47	0.62
1:2A:2136:C:H42	1:2A:2155:G:H1	1.46	0.62
14:2S:71:ARG:NH1	14:2S:107:GLU:OE1	2.33	0.62
32:2a:976:G:H5'	32:2a:1358:U:O2'	1.99	0.62
44:2m:33:ALA:HA	44:2m:59:TYR:HE2	1.64	0.62
1:1A:1047:G:H2'	1:1A:1110:G:H22	1.63	0.62
1:1A:1466:G:O2'	1:1A:1546:C:O2'	2.17	0.62
42:1k:82:VAL:HB	42:1k:108:ILE:HD13	1.81	0.62
44:1m:87:TYR:HA	44:1m:90:LEU:HD12	1.80	0.62
31:29:25:VAL:HB	31:29:34:GLN:HB2	1.80	0.62
32:2a:196:A:OP1	51:2t:68:LYS:NZ	2.25	0.62
32:1a:1030(D):A:H2'	32:1a:1031:G:H4'	1.80	0.62
1:2A:568:U:O4	64:2A:3915:HOH:O	2.13	0.62
1:2A:1193:G:OP1	11:2P:14:LYS:NZ	2.20	0.62
1:2A:1266:G:O5'	18:2W:15:ARG:NH2	2.33	0.62
19:2X:53:LYS:HB3	19:2X:82:GLN:HB3	1.80	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:2t:9:ASN:O	51:2t:10:LEU:HB2	1.98	0.62
5:1F:185:ASP:HA	5:1F:188:ARG:HD3	1.82	0.62
21:1Z:92:SER:O	21:1Z:130:PRO:HG2	1.99	0.62
1:2A:2134:A:H62	1:2A:2157:G:H4'	1.63	0.62
26:14:55:ARG:H	26:14:56:VAL:HA	1.65	0.62
33:1b:93:VAL:HG11	33:1b:97:TRP:CD1	2.34	0.62
32:2a:1020:U:H2'	32:2a:1021:G:C8	2.35	0.62
54:2w:27:G:H1	54:2w:43:C:H42	1.45	0.62
21:2Z:52:SER:OG	21:2Z:53:ILE:N	2.32	0.62
3:1D:147:LEU:HD13	3:1D:155:LEU:HD11	1.81	0.62
32:1a:200:G:H1	32:1a:217:C:H42	1.48	0.62
32:2a:596:C:OP2	64:2a:1907:HOH:O	2.16	0.62
34:2c:191:THR:OG1	34:2c:194:GLY:O	2.17	0.62
33:1b:20:GLU:HG2	33:1b:23:ARG:HH11	1.65	0.62
46:1o:16:ALA:HB1	46:1o:21:ASP:HB3	1.81	0.62
56:1y:8:4SU:H4'	56:1y:48:C:H4'	1.80	0.62
51:2t:57:ARG:HH12	51:2t:100:ILE:HD12	1.64	0.62
1:2A:2136:C:N4	1:2A:2155:G:N1	2.48	0.61
54:2w:2:C:H42	54:2w:71:G:H1	1.48	0.61
1:1A:2334:G:H5'	14:1S:9:ARG:HG2	1.82	0.61
1:1A:2690:C:OP1	13:1R:17:ARG:NH2	2.33	0.61
44:2m:90:LEU:HD23	44:2m:93:ARG:HE	1.65	0.61
50:2s:64:GLU:OE2	50:2s:65:ASN:ND2	2.34	0.61
46:1o:55:GLY:HA2	46:1o:58:MET:HE3	1.81	0.61
1:2A:2298:A:N6	1:2A:2318:G:H8	1.92	0.61
1:2A:2345:G:H4'	1:2A:2346:A:H5"	1.81	0.61
3:2D:108:PRO:HG2	3:2D:111:LEU:HB2	1.82	0.61
33:2b:114:ARG:HG3	33:2b:118:LEU:HD13	1.82	0.61
41:2j:6:ILE:HG12	41:2j:98:ILE:HD12	1.82	0.61
1:1A:2612:C:OP2	27:15:2:ALA:N	2.33	0.61
46:1o:87:ILE:HG22	46:1o:88:ARG:H	1.66	0.61
1:2A:2049:G:N7	64:2A:3997:HOH:O	2.31	0.61
32:2a:407:G:H5"	35:2d:115:ARG:HB3	1.80	0.61
1:2A:307:G:H21	1:2A:330:A:H62	1.46	0.61
33:2b:104:ASN:OD1	33:2b:107:THR:OG1	2.19	0.61
35:1d:187:ARG:NH2	35:1d:190:ASP:OD1	2.34	0.61
1:2A:271(L):U:H5'	8:2I:50:ARG:HH22	1.64	0.61
8:2I:92:VAL:HG13	8:2I:120:ILE:HB	1.83	0.61
1:2A:1537:G:H2'	1:2A:1538:G:H8	1.66	0.61
1:1A:956:G:H5"	12:1Q:77:LYS:HD2	1.83	0.61
1:2A:848:G:H2'	1:2A:849:A:C8	2.35	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:2I:4:ILE:HG12	8:2I:18:VAL:HG22	1.83	0.61
13:2R:51:LEU:HD22	13:2R:66:VAL:HG13	1.83	0.61
40:1i:21:PRO:HA	40:1i:59:PHE:HA	1.83	0.61
1:2A:271(L):U:OP1	8:2I:50:ARG:NH1	2.34	0.61
1:2A:2690:C:OP1	13:2R:17:ARG:NH2	2.34	0.61
32:2a:1030(A):G:N1	32:2a:1030(D):A:OP2	2.33	0.61
1:1A:1057:A:N6	1:1A:1081:U:H3	1.97	0.60
5:1F:89:VAL:O	64:1F:401:HOH:O	2.16	0.60
33:1b:48:MET:HA	33:1b:51:LEU:HD12	1.83	0.60
33:1b:88:ALA:HB2	33:1b:219:VAL:HG13	1.83	0.60
1:2A:1801:G:OP2	3:2D:154:LYS:NZ	2.33	0.60
1:1A:2646:C:OP2	1:1A:2732:G:O2'	2.19	0.60
32:1a:1305:G:N2	32:1a:1331:G:H1'	2.15	0.60
6:2G:124:SER:O	6:2G:124:SER:OG	2.15	0.60
7:2H:56:SER:HB3	7:2H:61:HIS:ND1	2.15	0.60
34:2c:37:GLN:NE2	45:2n:52:GLN:OE1	2.33	0.60
50:2s:28:LYS:HB3	50:2s:29:ARG:HA	1.83	0.60
1:1A:1055:G:H1	1:1A:1104:C:H42	1.50	0.60
1:1A:1452:A:OP2	64:1A:4226:HOH:O	2.16	0.60
31:19:25:VAL:HB	31:19:34:GLN:HB2	1.83	0.60
18:2W:12:ILE:HD13	18:2W:17:VAL:HG13	1.82	0.60
1:2A:2285:C:OP2	28:26:6:ARG:NH1	2.34	0.60
32:2a:1352:C:OP1	52:2u:3:LYS:NZ	2.22	0.60
33:2b:74:LYS:O	33:2b:78:GLN:HG2	2.01	0.60
41:2j:47:PHE:N	41:2j:63:PHE:O	2.30	0.60
8:2I:38:LEU:H	8:2I:38:LEU:HD12	1.66	0.60
1:1A:2788:C:OP1	4:1E:61:ARG:NH2	2.34	0.60
7:1H:7:LEU:HD12	7:1H:8:PRO:HD2	1.84	0.60
6:2G:5:VAL:HG13	6:2G:8:LYS:HE2	1.83	0.60
32:2a:953:G:H5'	32:2a:965:A:N6	2.17	0.60
51:2t:50:GLU:HB2	51:2t:99:LEU:HD11	1.84	0.60
54:2w:51:U:H2'	54:2w:52:G:C8	2.36	0.60
56:2y:15:G:N2	56:2y:48:C:H42	2.00	0.60
1:1A:2023:G:H5'	1:1A:2617:C:H4'	1.84	0.60
8:1I:40:THR:O	8:1I:44:LEU:HB2	2.00	0.60
5:2F:167:ALA:HB1	5:2F:173:VAL:HG11	1.82	0.60
40:2i:46:ALA:HB2	40:2i:74:ILE:HG23	1.83	0.60
44:2m:40:ASN:HD22	44:2m:43:THR:HG23	1.67	0.60
21:2Z:70:LEU:HD12	21:2Z:71:VAL:H	1.66	0.60
32:2a:254:G:OP1	48:2q:66:SER:OG	2.18	0.60
1:1A:1074:G:C2	1:1A:1075:C:H1'	2.37	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2125:G:H1'	1:2A:2173:A:N6	2.17	0.60
21:2Z:53:ILE:HG22	21:2Z:71:VAL:HG23	1.84	0.60
32:2a:559:A:OP1	36:2e:126:ARG:NH2	2.35	0.60
32:2a:1263:C:N3	32:2a:1272:G:O6	2.35	0.60
42:2k:48:ILE:O	42:2k:50:TYR:N	2.30	0.60
32:1a:507:C:OP2	64:1a:4812:HOH:O	2.16	0.60
35:1d:112:VAL:H	35:1d:116:GLN:NE2	2.00	0.60
1:2A:900:A:O2'	1:2A:901:A:OP1	2.20	0.60
1:2A:1495:A:H2'	1:2A:1496:A:C8	2.37	0.60
1:2A:2576:G:OP1	64:2A:3926:HOH:O	2.16	0.60
6:2G:64:THR:HB	6:2G:94:LEU:HD21	1.83	0.60
14:1S:25:ARG:NH1	14:1S:42:ASP:OD1	2.34	0.59
33:1b:21:ARG:O	33:1b:23:ARG:N	2.35	0.59
35:1d:119:GLN:HG2	35:1d:123:HIS:CD2	2.37	0.59
1:2A:1022:G:H22	1:2A:1142(A):A:H2	1.47	0.59
19:2X:46:ALA:HB1	24:22:33:MET:HE1	1.83	0.59
32:2a:1244:C:H42	32:2a:1293:G:H1	1.50	0.59
52:2u:6:ARG:HB3	52:2u:15:ARG:HD2	1.84	0.59
1:1A:1183:G:O2'	25:13:29:ARG:NH1	2.35	0.59
1:1A:2182:G:H2'	1:1A:2183:C:C6	2.36	0.59
1:2A:921:G:O6	64:2A:3914:HOH:O	2.09	0.59
1:1A:1174:A:H4'	1:1A:1175:U:OP1	2.03	0.59
1:1A:2226:C:OP2	64:1A:4228:HOH:O	2.16	0.59
3:1D:35:LYS:HE2	3:1D:64:ILE:HG12	1.85	0.59
14:1S:59:LYS:O	64:1S:301:HOH:O	2.17	0.59
1:2A:2611:U:C4	27:25:3:LYS:HG2	2.37	0.59
10:2O:49:ARG:NH1	32:2a:1422:G:O3'	2.35	0.59
5:1F:140:LEU:HD21	5:1F:170:LEU:HD21	1.84	0.59
46:2o:25:THR:HG21	46:2o:70:LEU:HB2	1.84	0.59
8:1I:129:THR:HG23	8:1I:139:GLN:HE22	1.66	0.59
14:1S:14:VAL:O	14:1S:18:ILE:HG12	2.03	0.59
1:2A:792:G:O6	64:2A:3918:HOH:O	2.10	0.59
39:2h:21:LYS:O	39:2h:65:TYR:OH	2.17	0.59
32:1a:78:G:O6	32:1a:92:C:N4	2.35	0.59
1:2A:2758:A:C2	1:2A:2759:G:H1'	2.36	0.59
12:2Q:78:PRO:HD3	55:2x:1:C:N3	2.18	0.59
32:2a:1027:C:H2'	32:2a:1034:G:H22	1.67	0.59
45:2n:3:ARG:HE	45:2n:3:ARG:HA	1.67	0.59
44:2m:39:ILE:HD13	44:2m:52:GLU:HB3	1.84	0.59
56:2y:58:A:O2'	56:2y:60:U:OP2	2.20	0.59
2:2B:13:A:N1	2:2B:69:G:O2'	2.31	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:21:23:LYS:HB3	23:21:29:GLY:HA3	1.85	0.59
32:2a:1068:G:N2	32:2a:1191:A:N3	2.47	0.59
46:2o:54:ARG:HG2	46:2o:58:MET:HE2	1.84	0.59
50:2s:53:ASN:OD1	50:2s:54:GLY:N	2.36	0.59
1:1A:1971:A:OP1	64:1A:4219:HOH:O	2.17	0.59
1:1A:2183:C:H2'	1:1A:2184:G:C8	2.34	0.59
34:1c:131:ARG:HH11	34:1c:166:GLU:HG3	1.68	0.59
50:1s:20:LEU:HD23	50:1s:23:ASN:HD22	1.68	0.59
32:2a:562:C:H1'	43:2l:15:ARG:HB3	1.85	0.59
32:2a:1194:U:H4'	36:2e:22:GLY:HA2	1.84	0.59
39:2h:10:LEU:HD22	39:2h:83:ILE:HD11	1.85	0.59
1:1A:881:G:H3'	1:1A:882:G:H8	1.68	0.59
1:1A:1025:G:O2'	64:1A:4207:HOH:O	2.03	0.59
1:1A:1702:G:N7	64:1A:4296:HOH:O	2.32	0.59
9:1N:62:VAL:HG22	9:1N:66:LYS:HD2	1.85	0.59
32:1a:405:U:OP2	35:1d:3:ARG:NH1	2.36	0.59
1:2A:631:A:OP1	11:2P:65:ARG:NH1	2.35	0.59
32:2a:662:G:H2'	32:2a:663:A:C8	2.38	0.59
41:2j:62:HIS:HB3	45:2n:59:ALA:HB3	1.84	0.59
1:1A:2165:G:H1	1:1A:2171:A:H2'	1.68	0.58
1:2A:2151:G:H2'	1:2A:2152:G:H8	1.68	0.58
16:2U:49:HIS:HA	16:2U:52:ARG:HB2	1.83	0.58
33:2b:118:LEU:HB3	33:2b:142:LEU:HD13	1.84	0.58
19:1X:88:LYS:NZ	19:1X:90:GLU:OE1	2.25	0.58
32:1a:693:G:OP2	64:1a:4811:HOH:O	2.16	0.58
33:1b:163:PHE:HD1	33:1b:185:ILE:HG13	1.67	0.58
44:1m:122:LYS:HG3	44:1m:123:ALA:H	1.68	0.58
1:2A:893:C:H5'	1:2A:894:C:C5	2.37	0.58
1:2A:2183:C:H2'	1:2A:2184:G:H8	1.68	0.58
14:2S:58:LEU:HD13	14:2S:65:VAL:HB	1.84	0.58
32:2a:972:C:O2'	41:2j:55:LYS:O	2.21	0.58
32:2a:1271:G:C2	32:2a:1272:G:N7	2.71	0.58
54:2w:14:A:H61	54:2w:21:A:H2	1.52	0.58
1:1A:784:A:N6	3:1D:229:VAL:HG11	2.18	0.58
26:14:46:GLN:O	26:14:48:ARG:N	2.35	0.58
32:1a:1302:U:C5	44:1m:17:VAL:HG21	2.38	0.58
1:2A:2875:C:OP1	15:2T:3:ARG:NH2	2.36	0.58
1:1A:1062:G:O5'	1:1A:1070:A:O2'	2.19	0.58
1:1A:1494:A:OP1	64:1A:4225:HOH:O	2.16	0.58
6:1G:142:PRO:HB2	26:14:31:ILE:HG21	1.84	0.58
46:1o:39:LEU:HD13	46:1o:56:LEU:HB2	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2S:67:ARG:NH1	14:2S:107:GLU:OE2	2.36	0.58
8:1I:75:LEU:HD22	8:1I:105:HIS:HD2	1.68	0.58
32:1a:1129:C:O2	32:1a:1130:A:N6	2.32	0.58
36:1e:8:GLU:OE2	36:1e:63:ARG:NH2	2.37	0.58
32:2a:56:U:H2'	32:2a:57:G:C8	2.38	0.58
38:2g:65:ALA:HB1	38:2g:127:ALA:HB3	1.85	0.58
32:1a:742:G:OP2	46:1o:35:ARG:NH2	2.35	0.58
1:2A:2805:G:H2'	1:2A:2807:G:C8	2.39	0.58
27:25:40:LYS:NZ	27:25:44:THR:O	2.37	0.58
32:2a:200:G:H1	32:2a:217:C:H42	1.52	0.58
32:2a:1427:U:H2'	32:2a:1428:A:C8	2.38	0.58
37:2f:67:MET:HE1	37:2f:75:LEU:HD22	1.86	0.58
1:1A:301:G:OP2	20:1Y:84:ARG:NH2	2.37	0.58
5:1F:165:ARG:HA	5:1F:168:ARG:HD2	1.86	0.58
32:1a:148:G:H2'	32:1a:149:A:H8	1.68	0.58
32:1a:404:U:OP1	35:1d:118:ARG:NH1	2.37	0.58
41:1j:27:ALA:HA	41:1j:81:THR:HG21	1.85	0.58
32:2a:1053:G:H4'	32:2a:1054:C:H3'	1.86	0.58
32:1a:1125:U:H4'	41:1j:5:ARG:NH2	2.19	0.58
21:2Z:138:GLU:H	21:2Z:156:LYS:HE2	1.69	0.58
32:2a:165:C:H2'	32:2a:166:G:C8	2.38	0.58
45:2n:48:ALA:HB2	45:2n:53:LEU:HD12	1.85	0.58
1:1A:1025:G:C4	1:1A:1135:C:H1'	2.39	0.58
26:14:54:GLY:N	26:14:55:ARG:HA	2.18	0.58
32:1a:403:C:O2'	35:1d:122:ARG:NH2	2.34	0.58
32:1a:544:G:OP1	35:1d:59:ARG:NH2	2.28	0.58
44:1m:3:ARG:HG2	44:1m:8:GLU:HA	1.86	0.58
1:2A:998:C:N4	64:2A:4037:HOH:O	2.37	0.58
1:2A:1604:C:OP1	64:2A:3917:HOH:O	2.17	0.58
15:2T:108:ARG:HD3	15:2T:112:ARG:HH12	1.69	0.58
32:2a:1224:G:OP1	64:2a:1909:HOH:O	2.17	0.58
3:1D:8:PRO:HB3	3:1D:14:ARG:HG2	1.86	0.58
7:1H:11:VAL:HG13	7:1H:15:VAL:HG23	1.85	0.58
39:1h:51:VAL:HG12	39:1h:52:ASP:H	1.69	0.58
1:2A:880:G:H22	1:2A:898:C:H1'	1.67	0.58
1:2A:1009:A:OP2	64:2A:3928:HOH:O	2.17	0.58
19:2X:35:THR:HG22	19:2X:37:THR:H	1.69	0.58
32:2a:1102:A:O3'	33:2b:96:ARG:NH2	2.37	0.58
32:2a:1347:G:N2	32:2a:1373:G:H2'	2.19	0.58
36:2e:60:TYR:OH	36:2e:64:ARG:NH1	2.37	0.58
1:1A:1379:A:H4'	1:1A:1380:G:OP2	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:1P:38:GLN:O	11:1P:39:LYS:HB3	2.02	0.57
1:2A:249:C:O2	30:28:12:LYS:NZ	2.35	0.57
13:2R:57:ARG:NE	13:2R:59:ASP:OD1	2.31	0.57
24:22:35:LEU:HD12	24:22:53:LEU:HD12	1.85	0.57
26:24:48:ARG:HG3	26:24:52:THR:HG23	1.86	0.57
42:2k:82:VAL:HB	42:2k:108:ILE:HD13	1.85	0.57
1:1A:428:A:OP1	64:1A:4230:HOH:O	2.17	0.57
35:1d:173:TRP:CD1	35:1d:173:TRP:H	2.21	0.57
1:2A:1798:U:H5'	3:2D:259:THR:HG22	1.84	0.57
1:2A:2207:G:H3'	1:2A:2208:A:H5"	1.87	0.57
8:2I:57:ARG:HA	8:2I:61:ARG:HH21	1.69	0.57
12:2Q:57:HIS:HD2	12:2Q:117:ALA:HB2	1.69	0.57
1:1A:2577:A:OP2	27:15:3:LYS:NZ	2.36	0.57
3:1D:108:PRO:HB3	3:1D:143:HIS:CE1	2.40	0.57
32:1a:36:C:OP1	43:1l:123:LYS:NZ	2.36	0.57
37:1f:100:ASN:HB2	49:1r:28:GLU:HA	1.86	0.57
50:2s:30:LEU:HD11	50:2s:50:ALA:HB2	1.87	0.57
15:1T:127:ALA:C	15:1T:129:ARG:H	2.12	0.57
32:1a:92:C:H2'	32:1a:93:G:C8	2.40	0.57
44:1m:11:ARG:HA	44:1m:45:VAL:HB	1.87	0.57
47:1p:47:ASP:OD1	47:1p:47:ASP:N	2.38	0.57
14:2S:11:LYS:HE3	14:2S:15:ARG:HH12	1.69	0.57
26:24:46:GLN:NE2	26:24:48:ARG:HD3	2.18	0.57
34:2c:58:GLU:HB3	41:2j:92:THR:HG21	1.86	0.57
13:1R:67:LEU:HD13	13:1R:76:VAL:HG21	1.86	0.57
4:2E:50:GLY:HA3	4:2E:75:VAL:HG21	1.85	0.57
5:2F:12:LEU:HD12	5:2F:124:LEU:HD21	1.86	0.57
7:2H:88:LEU:HD11	7:2H:165:ALA:HA	1.86	0.57
32:2a:1055:A:N7	32:2a:1200:C:N4	2.52	0.57
32:2a:1280:A:H5'	41:2j:40:LEU:HD22	1.86	0.57
35:2d:140:VAL:HG11	35:2d:146:ILE:HD11	1.86	0.57
32:2a:1029:C:N3	32:2a:1032:G:N2	2.51	0.57
33:2b:21:ARG:HA	33:2b:39:ILE:HA	1.87	0.57
1:1A:630:G:OP2	30:18:15:LYS:NZ	2.25	0.57
1:1A:1800:C:OP1	3:1D:260:ARG:NH2	2.38	0.57
16:1U:104:GLN:HE21	16:1U:105:VAL:HG23	1.69	0.57
32:1a:1183:A:O2'	32:1a:1184:G:OP1	2.23	0.57
32:1a:1530:G:H2'	32:1a:1531:A:C8	2.39	0.57
36:1e:78:HIS:CD2	39:1h:104:ARG:HD2	2.40	0.57
36:1e:110:LEU:HD13	36:1e:118:ILE:HG21	1.87	0.57
36:2e:100:VAL:O	36:2e:107:ARG:NH1	2.33	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1039:G:H1	1:1A:1116:C:H42	1.52	0.57
6:1G:27:ASN:HB3	6:1G:30:GLU:HG3	1.85	0.57
32:1a:222:U:H2'	32:1a:223:U:C6	2.39	0.57
1:2A:1015:G:H2'	1:2A:1016:G:H8	1.70	0.57
21:2Z:33:LEU:HD21	21:2Z:90:VAL:HG21	1.86	0.57
32:2a:17:U:H2'	32:2a:18:C:C6	2.40	0.57
32:2a:973:G:H3'	32:2a:974:A:H5"	1.87	0.57
34:2c:101:LEU:HD22	34:2c:102:ASN:H	1.69	0.57
1:1A:1803:A:O2'	3:1D:259:THR:HG21	2.04	0.57
11:1P:121:LYS:HB3	11:1P:123:LEU:HD13	1.87	0.57
32:1a:78:G:N1	32:1a:91:C:N4	2.53	0.57
32:1a:157:G:H1	32:1a:164:U:H3	1.53	0.57
32:1a:316:G:OP2	32:1a:351:G:O2'	2.23	0.57
1:2A:271(L):U:H5'	8:2I:50:ARG:NH2	2.20	0.57
1:2A:639:U:H2'	1:2A:640:C:C6	2.40	0.57
5:2F:137:LYS:HA	5:2F:140:LEU:HD12	1.87	0.57
9:2N:67:LEU:HB3	9:2N:88:GLU:HG3	1.87	0.57
20:2Y:86:ARG:HE	20:2Y:100:ALA:HA	1.70	0.57
37:2f:2:ARG:NE	37:2f:69:GLU:HG2	2.20	0.57
1:1A:1418:G:OP2	64:1A:4229:HOH:O	2.17	0.57
1:1A:1779:U:OP2	64:1A:4227:HOH:O	2.16	0.57
2:1B:105:A:OP1	21:1Z:72:ARG:NH1	2.34	0.57
3:1D:2:ALA:N	3:1D:200:ASP:OD2	2.37	0.57
21:1Z:136:PHE:O	21:1Z:137:ILE:HG13	2.05	0.57
32:1a:78:G:N2	32:1a:91:C:N3	2.52	0.57
32:1a:1356:G:H2'	32:1a:1357:A:C8	2.40	0.57
1:2A:2136:C:N3	1:2A:2155:G:N2	2.46	0.57
1:2A:2317:C:H2'	1:2A:2318:G:H5'	1.87	0.57
26:24:58:ARG:HH21	50:2s:69:HIS:CE1	2.23	0.57
32:2a:142:G:H2'	32:2a:143:A:C8	2.39	0.57
1:1A:893:C:H2'	1:1A:894:C:C6	2.40	0.56
1:1A:1688:U:O2	1:1A:1700:A:H5'	2.05	0.56
32:1a:1435:G:H2'	32:1a:1436:U:C6	2.40	0.56
11:2P:39:LYS:HB2	11:2P:45:LEU:HD22	1.86	0.56
7:1H:25:LYS:HE2	7:1H:27:LYS:HE3	1.86	0.56
11:1P:39:LYS:HB2	11:1P:45:LEU:HD13	1.87	0.56
32:2a:1190:G:H5'	34:2c:176:HIS:CE1	2.40	0.56
33:2b:16:HIS:O	33:2b:18:GLY:N	2.39	0.56
40:2i:23:ASN:ND2	40:2i:25:LYS:HE3	2.20	0.56
41:2j:9:ARG:NH2	41:2j:69:ASN:HD21	2.02	0.56
1:1A:278:A:O2'	1:1A:279:C:OP1	2.17	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1178:C:H2'	1:1A:1179:C:H6	1.68	0.56
12:1Q:89:ASN:HB2	55:1x:1:C:C4	2.40	0.56
32:1a:1510:U:H2'	32:1a:1511:G:C8	2.40	0.56
46:1o:54:ARG:HG2	46:1o:58:MET:HE2	1.87	0.56
1:2A:271(E):U:H2'	1:2A:271(F):C:C6	2.40	0.56
1:2A:1341:U:OP2	1:2A:1394:U:O2'	2.20	0.56
1:2A:1651:G:OP1	13:2R:40:LYS:NZ	2.37	0.56
15:2T:127:ALA:C	15:2T:129:ARG:H	2.13	0.56
19:2X:94:GLY:H	19:2X:95:LEU:HB2	1.70	0.56
23:21:83:GLU:N	23:21:83:GLU:OE2	2.38	0.56
32:2a:1018:C:H2'	32:2a:1019:C:O4'	2.06	0.56
33:2b:188:ALA:HB1	33:2b:192:SER:HB2	1.86	0.56
56:2y:65:G:H2'	56:2y:66:U:C6	2.40	0.56
1:1A:887:A:H1'	1:1A:889:C:OP2	2.06	0.56
32:1a:677:U:H3	32:1a:713:G:H22	1.53	0.56
41:1j:78:ASN:O	41:1j:80:LYS:N	2.37	0.56
1:2A:804:A:OP1	64:2A:3929:HOH:O	2.18	0.56
1:2A:1639:U:H2'	1:2A:1640:C:H5"	1.88	0.56
12:2Q:17:LEU:HB3	12:2Q:39:PRO:HB2	1.88	0.56
33:1b:112:VAL:HG12	33:1b:149:LEU:HD13	1.87	0.56
2:2B:56:G:H5'	6:2G:27:ASN:ND2	2.20	0.56
41:2j:78:ASN:O	41:2j:80:LYS:N	2.38	0.56
46:2o:11:VAL:HG21	46:2o:34:LEU:HD22	1.88	0.56
56:2y:9:A:H4'	56:2y:46:G7M:H5'	1.88	0.56
21:1Z:52:SER:C	21:1Z:54:HIS:H	2.13	0.56
45:2n:26:ARG:HD3	45:2n:43:CYS:HB3	1.88	0.56
1:1A:2128:C:N3	1:1A:2160:G:N2	2.52	0.56
10:1O:73:ASP:HB2	15:1T:82:LEU:HD13	1.86	0.56
32:1a:662:G:H2'	32:1a:663:A:C8	2.40	0.56
32:1a:1531:A:H8	32:1a:1531:A:O5'	1.89	0.56
1:2A:706:A:OP1	3:2D:7:LYS:NZ	2.39	0.56
32:2a:67:C:H2'	32:2a:68:G:C8	2.40	0.56
32:2a:1376:U:OP1	38:2g:98:SER:OG	2.24	0.56
1:1A:2319:G:H22	14:1S:3:ARG:HE	1.54	0.56
32:1a:946:A:H2'	32:1a:947:G:C8	2.40	0.56
33:1b:95:GLN:NE2	33:1b:147:LYS:O	2.39	0.56
1:2A:796:C:H2'	1:2A:797:C:C6	2.40	0.56
32:2a:446:G:O6	64:2a:1906:HOH:O	2.16	0.56
32:2a:973:G:OP1	41:2j:57:LYS:NZ	2.39	0.56
32:2a:1004:A:C6	32:2a:1037:C:H1'	2.41	0.56
1:1A:739:G:OP1	64:1A:4231:HOH:O	2.18	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1799:G:O2'	3:1D:181:GLU:OE2	2.18	0.56
3:1D:183:ARG:HG3	3:1D:270:ILE:HD13	1.88	0.56
23:11:50:ARG:HG2	23:11:59:THR:HG23	1.88	0.56
32:1a:78:G:C6	32:1a:91:C:N4	2.74	0.56
41:1j:49:VAL:HG22	45:1n:41:ARG:HB2	1.87	0.56
1:2A:878:A:H61	1:2A:899:A:H1'	1.71	0.56
1:2A:2108:C:H42	1:2A:2181:G:H1	1.53	0.56
26:24:68:ARG:HE	26:24:69:LYS:H	1.52	0.56
32:2a:1118:C:H1'	32:2a:1179:A:C4	2.41	0.56
36:2e:10:MET:HE2	36:2e:55:VAL:HG21	1.87	0.56
1:1A:2763:G:OP2	64:1A:4234:HOH:O	2.18	0.56
10:1O:24:VAL:HG13	10:1O:33:ALA:HB2	1.87	0.56
32:1a:560:U:O2'	32:1a:561:U:OP2	2.19	0.56
32:1a:600:C:H2'	32:1a:601:C:C6	2.40	0.56
33:1b:174:VAL:O	33:1b:178:ARG:HG2	2.06	0.56
35:1d:178:VAL:C	35:1d:180:GLY:H	2.14	0.56
32:2a:45:U:H2'	32:2a:46:G:C8	2.41	0.56
32:2a:1010:G:H2'	32:2a:1011:G:C8	2.38	0.56
32:2a:1435:G:H2'	32:2a:1436:U:C6	2.41	0.56
32:2a:1442:G:H2'	32:2a:1442:G:N3	2.20	0.56
4:1E:3:GLY:HA3	4:1E:81:ILE:HD12	1.87	0.55
1:2A:1188:U:H4'	17:2V:79:VAL:HG22	1.88	0.55
2:2B:54:G:OP2	64:2B:301:HOH:O	2.18	0.55
9:2N:128:HIS:O	9:2N:131:GLN:NE2	2.38	0.55
30:28:62:LEU:HB3	30:28:65:GLU:HG2	1.88	0.55
32:2a:165:C:H2'	32:2a:166:G:H8	1.69	0.55
32:2a:539:A:OP2	43:2l:115:LYS:NZ	2.30	0.55
32:2a:620:C:C2	35:2d:135:LEU:HG	2.41	0.55
32:2a:1029:C:N4	32:2a:1032:G:N1	2.54	0.55
34:2c:157:ILE:HD12	34:2c:164:ARG:HB3	1.87	0.55
39:2h:34:GLU:OE1	39:2h:37:ARG:NH1	2.37	0.55
41:2j:44:VAL:HG13	41:2j:66:ARG:HB3	1.88	0.55
51:2t:43:LEU:O	51:2t:47:GLY:N	2.33	0.55
1:1A:1007:C:OP2	64:1A:4233:HOH:O	2.18	0.55
1:1A:2790:A:H3'	1:1A:2790:A:N3	2.21	0.55
21:1Z:11:GLU:O	21:1Z:36:LYS:NZ	2.39	0.55
32:1a:1032:G:H2'	32:1a:1033:G:O4'	2.06	0.55
34:1c:114:PRO:HA	34:1c:185:GLY:HA3	1.87	0.55
1:2A:2064:C:OP2	64:2A:3930:HOH:O	2.18	0.55
1:2A:2659:G:OP1	7:2H:158:HIS:NE2	2.37	0.55
7:2H:70:THR:O	7:2H:74:ASN:ND2	2.39	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1255:G:H5"	34:2c:26:LYS:HE2	1.88	0.55
33:2b:217:ARG:HA	33:2b:220:ASP:HB2	1.87	0.55
1:1A:1786:A:H1'	1:1A:1938:A:N6	2.21	0.55
8:1I:38:LEU:HD23	8:1I:38:LEU:H	1.70	0.55
26:14:15:ILE:HG13	26:14:21:VAL:HG22	1.87	0.55
1:2A:2110:G:H3'	1:2A:2111:C:H5'	1.86	0.55
34:2c:6:HIS:HD2	34:2c:8:ILE:H	1.54	0.55
47:2p:15:PRO:HD2	47:2p:42:ARG:HD2	1.87	0.55
1:1A:877:U:H3	1:1A:899:A:H2	1.52	0.55
1:1A:2870:C:H2'	1:1A:2871:C:O4'	2.06	0.55
7:1H:86:GLU:OE2	7:1H:130:ARG:NH1	2.39	0.55
32:1a:532:A:N6	32:1a:1206:G:O2'	2.39	0.55
36:1e:105:VAL:HG21	36:1e:128:PRO:HB3	1.89	0.55
1:2A:2116:G:N7	1:2A:2166:G:N2	2.51	0.55
1:2A:2136:C:HO2'	1:2A:2137:C:H6	1.53	0.55
2:2B:14:U:OP2	2:2B:70:C:O2'	2.24	0.55
15:2T:24:PRO:HA	15:2T:49:VAL:HG12	1.88	0.55
32:2a:64:G:H4'	32:2a:65:U:H3'	1.87	0.55
32:1a:1518:MA6:H93	32:1a:1519:MA6:H92	1.89	0.55
43:1l:117:ARG:HB3	43:1l:122:THR:HB	1.88	0.55
50:1s:12:ASP:OD2	50:1s:35:SER:OG	2.19	0.55
1:2A:1395:A:OP1	64:2A:3906:HOH:O	2.18	0.55
1:2A:1803:A:O2'	3:2D:259:THR:HG21	2.06	0.55
8:2I:116:LEU:HD11	8:2I:120:ILE:HG13	1.88	0.55
33:2b:144:ARG:NH2	33:2b:148:TYR:OH	2.39	0.55
34:2c:148:GLY:HA3	34:2c:172:ARG:O	2.06	0.55
38:2g:113:GLU:HG3	38:2g:118:VAL:HG12	1.88	0.55
1:1A:1048:A:N1	1:1A:1112:G:O2'	2.34	0.55
1:1A:1077:A:H2'	1:1A:1078:U:H4'	1.87	0.55
32:1a:1391:U:H2'	32:1a:1392:G:C8	2.42	0.55
1:2A:1183:G:H5"	25:23:30:ARG:NH2	2.21	0.55
1:2A:2334:G:H5'	14:2S:9:ARG:HG2	1.88	0.55
11:2P:126:VAL:HG12	11:2P:148:LEU:HD22	1.87	0.55
32:2a:1002:G:H1	32:2a:1038:C:N4	2.04	0.55
32:2a:1301:U:O2'	32:2a:1302:U:H5'	2.06	0.55
33:2b:223:ILE:HA	33:2b:226:ARG:HD3	1.89	0.55
42:2k:73:MET:HA	42:2k:77:MET:H	1.71	0.55
44:2m:3:ARG:NH1	44:2m:8:GLU:OE2	2.39	0.55
1:2A:674:G:H1'	5:2F:74:ARG:HD3	1.87	0.55
1:2A:744:G:OP1	4:2E:132:HIS:ND1	2.36	0.55
8:2I:75:LEU:HD22	8:2I:105:HIS:HD2	1.71	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:24:16:CYS:HA	26:24:33:VAL:HG12	1.89	0.55
32:2a:7:G:H5'	32:2a:298:A:O4'	2.06	0.55
32:2a:406:G:H4'	35:2d:5:ILE:HD11	1.89	0.55
11:1P:63:PRO:HD3	30:18:27:THR:HG22	1.88	0.55
39:1h:51:VAL:HG21	39:1h:60:ARG:HB2	1.89	0.55
56:1y:36:A:H2'	56:1y:37:MIA:O4'	2.07	0.55
3:2D:66:ASP:OD2	3:2D:103:ARG:NH1	2.39	0.55
4:2E:28:ALA:HB3	4:2E:93:VAL:HG12	1.89	0.55
14:2S:38:GLN:NE2	14:2S:47:THR:OG1	2.30	0.55
20:2Y:19:LYS:HD2	20:2Y:20:TYR:CE2	2.42	0.55
32:2a:1318:A:H1'	50:2s:37:ARG:HH21	1.71	0.55
32:1a:509:A:O2'	32:1a:510:A:OP1	2.18	0.55
44:1m:3:ARG:HD2	44:1m:9:ILE:HG12	1.89	0.55
1:1A:1188:U:H4'	17:1V:79:VAL:HG22	1.89	0.55
32:1a:1239:A:H62	32:1a:1299:A:N6	2.05	0.55
34:1c:3:ASN:OD1	34:1c:3:ASN:N	2.40	0.55
1:2A:247:G:H4'	1:2A:386:G:C5	2.42	0.55
12:2Q:111:GLU:O	12:2Q:115:MET:HG2	2.07	0.55
32:2a:148:G:H2'	32:2a:149:A:H8	1.71	0.55
32:2a:624:C:H2'	32:2a:625:G:H8	1.70	0.55
32:2a:673:G:H2'	32:2a:674:G:C8	2.41	0.55
33:2b:88:ALA:HB2	33:2b:219:VAL:HG13	1.89	0.55
34:2c:46:GLU:OE2	34:2c:46:GLU:N	2.37	0.55
44:2m:122:LYS:HG3	44:2m:123:ALA:H	1.72	0.55
1:1A:994:C:OP1	16:1U:53:ARG:NH2	2.40	0.54
1:1A:2422:A:O4'	56:1y:76:A:N6	2.40	0.54
35:1d:108:LEU:HD13	35:1d:183:GLY:HA3	1.89	0.54
1:2A:700:G:O2'	1:2A:1632:A:N3	2.33	0.54
44:2m:37:THR:HB	44:2m:55:ARG:HD2	1.89	0.54
56:2y:8:4SU:O4'	56:2y:48:C:O2'	2.23	0.54
1:1A:1385:G:O2'	1:1A:1396:U:O2	2.24	0.54
1:1A:2108:C:H2'	1:1A:2109:U:H6	1.72	0.54
6:1G:83:ARG:O	6:1G:86:MET:HG3	2.06	0.54
21:1Z:52:SER:O	21:1Z:54:HIS:N	2.40	0.54
38:1g:78:ARG:HG2	38:1g:156:TRP:HZ3	1.72	0.54
5:2F:101:LEU:O	5:2F:106:ARG:NH1	2.41	0.54
32:2a:148:G:H2'	32:2a:149:A:C8	2.41	0.54
32:2a:651:C:N4	32:2a:753:A:OP2	2.41	0.54
32:2a:1305:G:N2	32:2a:1331:G:H1'	2.22	0.54
1:1A:1439:A:OP1	64:1A:4236:HOH:O	2.19	0.54
32:1a:757:U:H2'	32:1a:758:G:O4'	2.06	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1036:G:H5”	32:1a:1037:C:C5	2.42	0.54
1:2A:887:A:H4’	1:2A:888:C:C5	2.43	0.54
1:2A:1365:A:O2’	23:21:11:ARG:NH1	2.39	0.54
1:2A:1507:A:O2’	1:2A:1508:A:O5’	2.24	0.54
1:2A:1778:U:OP1	64:2A:3931:HOH:O	2.18	0.54
6:2G:47:LYS:HG3	6:2G:48:GLU:H	1.72	0.54
32:2a:1402:4OC:HM22	32:2a:1403:C:H5’	1.90	0.54
46:2o:5:LYS:O	46:2o:9:GLN:HG2	2.07	0.54
1:1A:2733:A:OP1	64:1A:4235:HOH:O	2.18	0.54
4:1E:121:ASN:ND2	64:1E:402:HOH:O	2.39	0.54
7:1H:16:SER:HB2	7:1H:27:LYS:HB2	1.88	0.54
24:12:14:ARG:O	24:12:67:LYS:NZ	2.38	0.54
48:1q:53:LEU:HD23	48:1q:82:MET:HE1	1.90	0.54
56:1y:37:MIA:H2’	56:1y:38:A:C8	2.42	0.54
4:2E:7:VAL:HG11	15:2T:1:MET:HE1	1.89	0.54
37:2f:70:ASP:OD1	37:2f:70:ASP:N	2.32	0.54
1:1A:1506:C:H2’	1:1A:1507:A:H8	1.72	0.54
1:1A:2295:C:OP1	14:1S:10:ARG:NH1	2.40	0.54
30:18:62:LEU:HB3	30:18:65:GLU:HG2	1.89	0.54
1:2A:2748:A:H5’	7:2H:4:ILE:HD12	1.90	0.54
32:2a:1089:G:H1	32:2a:1096:C:H42	1.55	0.54
40:2i:9:ARG:HG2	40:2i:14:VAL:HG12	1.89	0.54
46:2o:16:ALA:HB1	46:2o:21:ASP:HB3	1.90	0.54
1:1A:784:A:C6	3:1D:229:VAL:HG11	2.41	0.54
1:1A:1817:G:OP1	3:1D:88:ARG:NH2	2.41	0.54
33:1b:163:PHE:CD1	33:1b:185:ILE:HG13	2.42	0.54
44:1m:67:GLU:HG3	44:1m:71:ARG:NH2	2.23	0.54
1:2A:884:C:H3’	1:2A:885:C:C6	2.43	0.54
1:2A:1116:C:H2’	1:2A:1117:G:C8	2.43	0.54
33:2b:111:ARG:HH11	33:2b:111:ARG:HA	1.72	0.54
3:1D:26:LYS:HE2	3:1D:28:GLU:O	2.07	0.54
55:1x:47:U:H5’	55:1x:48:C:H5’	1.90	0.54
1:2A:1668:A:O2’	1:2A:1674:G:N7	2.34	0.54
37:2f:91:VAL:HG11	49:2r:72:ARG:NH1	2.23	0.54
47:1p:22:THR:HA	47:1p:33:ILE:HD12	1.89	0.54
52:1u:3:LYS:HB3	52:1u:14:TRP:CD1	2.42	0.54
1:2A:307:G:N1	1:2A:310:A:OP2	2.41	0.54
1:2A:1507:A:O2’	1:2A:1508:A:O4’	2.26	0.54
5:2F:7:TYR:O	5:2F:22:ALA:N	2.40	0.54
33:2b:76:GLN:HB2	33:2b:208:ILE:HG12	1.89	0.54
43:1l:84:LEU:HB3	43:1l:104:VAL:HG21	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2507:C:H5”	1:2A:2573:C:N4	2.22	0.54
20:2Y:87:LYS:HB3	20:2Y:95:LYS:HD2	1.89	0.54
21:2Z:77:ASP:OD2	21:2Z:80:ARG:NH1	2.41	0.54
1:2A:468:G:N7	29:27:39:ARG:NH2	2.55	0.54
1:2A:793:A:O2’	64:2A:3932:HOH:O	2.18	0.54
6:2G:129:GLY:O	6:2G:161:THR:HB	2.08	0.54
11:2P:121:LYS:O	11:2P:123:LEU:N	2.41	0.54
32:2a:955:U:O2’	50:2s:83:HIS:HD2	1.90	0.54
36:2e:106:PRO:O	36:2e:110:LEU:HG	2.08	0.54
7:1H:164:TYR:HB2	7:1H:167:GLU:HB2	1.90	0.53
32:1a:1456:G:N2	51:1t:51:GLU:OE2	2.38	0.53
35:1d:111:ALA:HB2	35:1d:120:LEU:HD12	1.91	0.53
1:2A:1278:A:OP1	13:2R:36:THR:HG23	2.07	0.53
1:2A:1518:U:H2’	1:2A:1519:G:O4’	2.08	0.53
6:2G:49:ASP:C	6:2G:51:ARG:H	2.15	0.53
30:28:28:GLY:O	30:28:36:LYS:NZ	2.38	0.53
33:2b:159:PRO:HB2	33:2b:161:ALA:O	2.08	0.53
48:2q:4:LYS:HE3	48:2q:6:LEU:HD21	1.89	0.53
1:1A:674:G:O2’	5:1F:74:ARG:HD3	2.08	0.53
6:1G:7:LEU:HB2	6:1G:104:GLU:HB2	1.90	0.53
24:12:51:ARG:O	24:12:55:ARG:HG2	2.08	0.53
26:14:20:ASN:OD1	26:14:21:VAL:N	2.41	0.53
35:1d:173:TRP:CD2	35:1d:189:PRO:HG3	2.44	0.53
49:2r:53:ARG:HH21	49:2r:59:SER:HA	1.73	0.53
1:1A:1047:G:H2’	1:1A:1110:G:N2	2.23	0.53
1:1A:2243:U:H2’	1:1A:2244:U:C6	2.43	0.53
7:1H:20:ALA:HB1	7:1H:21:PRO:HD2	1.89	0.53
25:13:7:LYS:HE3	25:13:32:GLN:HE21	1.74	0.53
32:1a:625:G:H4’	47:1p:16:HIS:CG	2.43	0.53
2:2B:105:A:H5’	2:2B:106:G:OP2	2.08	0.53
32:2a:1368:G:OP1	40:2i:111:ARG:NH2	2.41	0.53
38:2g:89:MET:SD	38:2g:155:ARG:HB2	2.48	0.53
41:2j:5:ARG:HA	41:2j:73:ASP:OD1	2.08	0.53
6:1G:72:ARG:NH1	6:1G:87:PRO:HG3	2.24	0.53
23:11:75:GLU:OE1	23:11:78:LYS:NZ	2.28	0.53
32:1a:148:G:H2’	32:1a:149:A:C8	2.44	0.53
34:1c:157:ILE:HD12	34:1c:164:ARG:HB3	1.89	0.53
1:2A:668:G:H5’	1:2A:669:G:OP2	2.07	0.53
1:2A:832:G:OP1	64:2A:3934:HOH:O	2.18	0.53
1:2A:2022:U:O2’	1:2A:2617:C:H5’	2.09	0.53
1:2A:2296:U:OP2	14:2S:9:ARG:NH2	2.40	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:8:A:H5'	36:2e:101:ILE:HG22	1.90	0.53
33:2b:16:HIS:HB3	33:2b:210:SER:HB2	1.89	0.53
38:2g:29:LYS:HB3	38:2g:105:VAL:HG21	1.90	0.53
1:1A:2140:C:H2'	1:1A:2141:G:H8	1.72	0.53
2:1B:48:A:H4'	14:1S:95:HIS:HD2	1.73	0.53
32:1a:1278:U:H5"	32:1a:1279:A:O4'	2.07	0.53
1:2A:602:G:O2'	1:2A:655:A:N6	2.42	0.53
1:2A:1340:U:OP1	19:2X:16:LYS:NZ	2.34	0.53
32:2a:141:A:H1'	32:2a:182:U:O2	2.09	0.53
32:2a:401:C:P	35:2d:73:ARG:HH21	2.30	0.53
32:2a:1026:G:O6	32:2a:1036:G:N2	2.41	0.53
32:2a:1257:U:O4	45:2n:17:LYS:NZ	2.41	0.53
1:1A:305:U:H2'	1:1A:306:U:C6	2.44	0.53
1:1A:363(A):A:H2'	1:1A:363(B):G:C8	2.44	0.53
1:1A:2611:U:C4	27:15:3:LYS:HG2	2.43	0.53
3:1D:39:LYS:NZ	3:1D:57:GLY:O	2.41	0.53
32:1a:1457:G:H5"	51:1t:35:THR:HG21	1.91	0.53
1:2A:2135:A:N1	1:2A:2156:G:O2'	2.38	0.53
21:2Z:55:HIS:HE1	21:2Z:135:GLU:HB2	1.74	0.53
32:2a:921:U:O2	36:2e:19:MET:HB2	2.09	0.53
32:2a:1518:MA6:H93	32:2a:1519:MA6:H92	1.91	0.53
1:1A:528:A:O2'	1:1A:529:A:H5'	2.08	0.53
32:1a:56:U:H2'	32:1a:57:G:C8	2.43	0.53
33:1b:22:LYS:HE2	33:1b:35:GLU:OE2	2.09	0.53
34:1c:87:LEU:O	34:1c:91:LEU:N	2.33	0.53
38:1g:113:GLU:HG2	38:1g:119:ARG:HG2	1.90	0.53
1:2A:2131:G:OP2	1:2A:2131:G:N2	2.40	0.53
7:2H:25:LYS:HE2	7:2H:27:LYS:HE3	1.89	0.53
14:2S:11:LYS:HE3	14:2S:15:ARG:NH1	2.22	0.53
20:2Y:8:LYS:HD3	20:2Y:97:ARG:NH1	2.23	0.53
34:2c:34:LEU:O	34:2c:38:ARG:HG3	2.08	0.53
1:1A:1065:U:H5"	1:1A:1066:U:OP2	2.09	0.53
1:1A:1864:U:OP1	1:1A:2410:G:O2'	2.25	0.53
1:1A:2128:C:N4	1:1A:2160:G:N1	2.56	0.53
32:1a:1021:G:O2'	32:1a:1022:G:O5'	2.26	0.53
36:1e:12:LEU:HB3	36:1e:31:LEU:HB2	1.90	0.53
40:1i:26:VAL:HG13	40:1i:61:ALA:HB3	1.91	0.53
48:1q:67:LYS:HA	48:1q:70:ARG:HH12	1.74	0.53
1:2A:307:G:OP2	64:2A:3935:HOH:O	2.19	0.53
1:2A:1996:C:H4'	1:2A:1997:G:OP1	2.08	0.53
1:2A:2801(A):A:H5'	1:2A:2802:G:H8	1.73	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:2H:20:ALA:HB1	7:2H:21:PRO:HD2	1.91	0.53
30:28:29:LYS:HD2	30:28:44:LYS:HB3	1.90	0.53
1:1A:1069:A:H1'	1:1A:1096:A:H4'	1.90	0.53
11:1P:63:PRO:HG2	30:18:25:MET:HB2	1.90	0.53
32:1a:952:U:H2'	32:1a:953:G:H8	1.73	0.53
56:1y:6:G:C6	56:1y:7:A:C6	2.97	0.53
1:2A:2063:C:OP1	64:2A:3930:HOH:O	2.19	0.53
8:2I:123:LEU:HD23	8:2I:144:VAL:HG12	1.90	0.53
19:2X:8:ILE:O	24:22:36:ARG:NH2	2.42	0.53
26:24:64:GLY:C	26:24:66:SER:H	2.17	0.53
41:2j:33:GLN:HG2	41:2j:34:VAL:H	1.73	0.53
1:1A:1178:C:H2'	1:1A:1179:C:C6	2.43	0.53
40:1i:79:LEU:HG	40:1i:83:ARG:HD2	1.91	0.53
1:2A:403:U:H4'	1:2A:404:C:H5'	1.89	0.53
1:2A:800:A:H8	1:2A:800:A:OP1	1.92	0.53
11:2P:38:GLN:O	11:2P:39:LYS:HB3	2.08	0.53
32:2a:1179:A:H2'	32:2a:1180:A:O4'	2.08	0.53
32:2a:1239:A:H62	32:2a:1299:A:N6	2.07	0.53
34:2c:157:ILE:HD13	34:2c:166:GLU:HG3	1.91	0.53
1:1A:484:C:H2'	1:1A:485:C:C6	2.44	0.52
1:1A:615:G:OP1	5:1F:40:GLN:NE2	2.31	0.52
1:2A:223:A:O2'	1:2A:420:C:O2	2.26	0.52
1:2A:2784:C:H1'	4:2E:37:ARG:HH12	1.73	0.52
8:2I:72:LEU:HD23	8:2I:75:LEU:HD21	1.89	0.52
10:2O:80:ASP:OD1	15:2T:64:ARG:NH2	2.42	0.52
22:20:11:ARG:O	22:20:14:ARG:NH2	2.41	0.52
32:2a:1005:A:H3'	32:2a:1006:C:C6	2.44	0.52
32:2a:1330:U:H4'	44:2m:23:TYR:CE1	2.44	0.52
35:2d:111:ALA:HB2	35:2d:120:LEU:HD12	1.90	0.52
40:2i:49:PRO:HG3	40:2i:101:PHE:HD1	1.74	0.52
44:2m:4:ILE:HG23	44:2m:5:ALA:H	1.73	0.52
48:2q:10:VAL:HA	48:2q:20:THR:O	2.09	0.52
1:1A:1071:G:H1'	1:1A:1089:G:H2'	1.90	0.52
32:1a:1381:U:H1'	38:1g:79:ARG:HG2	1.90	0.52
39:1h:10:LEU:HD22	39:1h:83:ILE:HD11	1.91	0.52
44:1m:2:ALA:N	44:1m:8:GLU:OE1	2.43	0.52
56:1y:19:G:N1	56:1y:56:C:N4	2.56	0.52
1:2A:1877:A:H5'	1:2A:1878:G:OP2	2.10	0.52
21:2Z:102:LEU:HD13	21:2Z:123:ASP:HA	1.90	0.52
32:2a:742:G:OP2	46:2o:35:ARG:NH2	2.35	0.52
32:2a:1062:U:H2'	32:2a:1063:C:C6	2.44	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:2b:55:PHE:HE1	33:2b:218:ALA:HA	1.74	0.52
33:2b:126:GLU:H	33:2b:126:GLU:CD	2.17	0.52
6:1G:47:LYS:HG3	6:1G:48:GLU:H	1.73	0.52
9:1N:96:GLU:H	9:1N:96:GLU:CD	2.15	0.52
32:1a:738:C:OP2	37:1f:92:LYS:NZ	2.42	0.52
44:1m:33:ALA:HA	44:1m:59:TYR:CE2	2.44	0.52
1:2A:922:U:H2'	1:2A:923:C:C6	2.45	0.52
1:2A:1816:G:O6	3:2D:35:LYS:NZ	2.31	0.52
26:24:46:GLN:C	26:24:48:ARG:H	2.17	0.52
32:2a:328:C:H4'	32:2a:329:A:H5'	1.92	0.52
32:2a:974:A:H8	32:2a:974:A:OP1	1.93	0.52
32:2a:1119:C:H2'	32:2a:1120:G:H8	1.73	0.52
1:1A:2277:G:OP2	22:10:10:THR:HG21	2.09	0.52
20:1Y:14:LEU:HB2	20:1Y:75:ILE:HD11	1.91	0.52
32:1a:509:A:O3'	64:1a:4814:HOH:O	2.19	0.52
42:1k:99:GLN:HG3	42:1k:105:VAL:HG21	1.90	0.52
1:2A:839:U:H2'	1:2A:840:C:C6	2.44	0.52
1:1A:1359:A:H2	1:1A:1372:U:O4	1.92	0.52
11:1P:138:LEU:HD23	11:1P:145:PRO:HB3	1.92	0.52
28:16:19:ARG:NH1	28:16:52:VAL:HG21	2.25	0.52
35:1d:172:PRO:C	35:1d:174:LEU:H	2.17	0.52
36:1e:33:VAL:HG22	36:1e:112:LEU:HD12	1.91	0.52
43:1l:39:VAL:HG11	43:1l:41:ARG:HH11	1.75	0.52
50:1s:31:ILE:O	50:1s:50:ALA:N	2.41	0.52
7:2H:3:ARG:NH1	7:2H:4:ILE:H	2.06	0.52
13:2R:28:LEU:HD23	13:2R:48:VAL:HG21	1.91	0.52
32:2a:448:A:P	32:2a:485:G:H22	2.31	0.52
47:2p:28:ARG:HG2	47:2p:29:ASP:OD1	2.10	0.52
50:2s:31:ILE:O	50:2s:50:ALA:N	2.37	0.52
1:1A:2155:G:H2'	1:1A:2155:G:N3	2.23	0.52
32:1a:189:G:H1	32:1a:189(K):U:H3	1.57	0.52
56:1y:20:U:H1'	56:1y:21:A:H4'	1.92	0.52
1:2A:340:A:H2'	1:2A:341:G:O4'	2.09	0.52
1:2A:2162:G:H4'	1:2A:2172:U:H2'	1.91	0.52
32:2a:995:C:O2	45:2n:4:LYS:NZ	2.36	0.52
32:2a:1133:G:H1	32:2a:1141:C:H42	1.57	0.52
32:2a:1179:A:H4'	40:2i:103:THR:HA	1.90	0.52
33:2b:197:VAL:HB	33:2b:200:ILE:HG13	1.92	0.52
1:1A:800:A:H8	1:1A:800:A:OP1	1.93	0.52
32:1a:1269:A:H2	32:1a:1312:G:N3	2.08	0.52
33:1b:162:ILE:O	33:1b:185:ILE:HG12	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:1g:78:ARG:HD3	38:1g:79:ARG:HG3	1.91	0.52
1:2A:884:C:H3'	1:2A:885:C:H6	1.74	0.52
1:2A:1796:U:H2'	1:2A:1797:C:C6	2.45	0.52
1:2A:2151:G:H2'	1:2A:2152:G:C8	2.45	0.52
26:24:40:HIS:HB3	26:24:43:TYR:HB2	1.91	0.52
32:2a:532:A:N6	32:2a:1206:G:O2'	2.42	0.52
32:2a:1003:G:H2'	32:2a:1004:A:O4'	2.09	0.52
32:2a:1456:G:N1	51:2t:51:GLU:OE2	2.41	0.52
54:2w:51:U:H2'	54:2w:52:G:H8	1.74	0.52
25:13:35:ARG:HE	25:13:37:LEU:HD21	1.74	0.52
44:1m:17:VAL:O	44:1m:20:THR:OG1	2.21	0.52
1:2A:2134:A:H1'	1:2A:2158:A:C5	2.45	0.52
6:2G:126:ASP:OD2	6:2G:130:ASN:ND2	2.40	0.52
32:2a:952:U:H2'	32:2a:953:G:H8	1.73	0.52
36:2e:20:GLN:HG2	36:2e:25:ARG:HG3	1.92	0.52
1:1A:603:A:O4'	1:1A:655:A:N6	2.43	0.52
1:1A:1762:A:H2'	64:1A:6035:HOH:O	2.10	0.52
40:1i:42:ARG:NH2	40:1i:75:ASP:OD1	2.43	0.52
44:1m:87:TYR:O	44:1m:91:ARG:HG2	2.10	0.52
20:2Y:44:ILE:HA	20:2Y:63:LYS:O	2.10	0.52
32:2a:54:C:N4	32:2a:353:A:OP2	2.42	0.52
32:2a:263:A:OP1	51:2t:79:ARG:NH1	2.42	0.52
38:2g:54:THR:O	38:2g:56:GLN:N	2.43	0.52
38:2g:60:LYS:HA	38:2g:63:LYS:HD2	1.91	0.52
21:1Z:125:LEU:HG	21:1Z:164:ALA:HB3	1.91	0.52
32:1a:204:U:H4'	32:1a:216:G:H5"	1.91	0.52
34:1c:150:LYS:HG3	34:1c:169:ALA:HB2	1.91	0.52
54:1w:18:G:HO2'	54:1w:57:G:H22	1.57	0.52
1:2A:307:G:H21	1:2A:330:A:N6	2.08	0.52
1:2A:1537:G:H2'	1:2A:1538:G:C8	2.45	0.52
11:2P:98:GLU:OE1	11:2P:102:ARG:NH1	2.43	0.52
32:2a:1226:C:OP2	44:2m:91:ARG:NH1	2.38	0.52
4:1E:77:ILE:HD13	4:1E:195:LEU:HD22	1.92	0.51
19:1X:31:HIS:CD2	19:1X:33:LYS:H	2.28	0.51
26:14:59:PHE:C	26:14:61:ARG:H	2.17	0.51
35:1d:112:VAL:HG23	35:1d:116:GLN:NE2	2.21	0.51
36:1e:85:GLY:C	36:1e:87:SER:H	2.18	0.51
40:1i:70:LYS:O	40:1i:74:ILE:HG13	2.11	0.51
42:1k:87:THR:O	42:1k:87:THR:OG1	2.28	0.51
54:1w:4:C:H2'	54:1w:5:G:C8	2.45	0.51
1:2A:242:G:C8	30:28:5:LYS:HG2	2.45	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:395:U:O2'	64:2A:3936:HOH:O	2.19	0.51
8:2I:48:GLU:HG3	8:2I:52:ARG:HH11	1.75	0.51
12:2Q:63:LYS:HG2	12:2Q:65:PHE:CE2	2.45	0.51
32:2a:1202:G:O4'	45:2n:29:ARG:NH1	2.42	0.51
1:1A:2319:G:N1	14:1S:3:ARG:HA	2.25	0.51
9:1N:115:ARG:HA	9:1N:118:LYS:HE3	1.92	0.51
32:1a:1077:G:N2	32:1a:1080:A:OP2	2.41	0.51
32:1a:1376:U:H2'	32:1a:1377:A:C8	2.46	0.51
33:1b:69:LEU:HB3	33:1b:162:ILE:HG22	1.93	0.51
48:1q:22:LEU:HD11	48:1q:39:SER:HB2	1.91	0.51
3:2D:123:ALA:HB3	3:2D:131:LEU:HG	1.91	0.51
41:2j:5:ARG:N	41:2j:99:LYS:O	2.43	0.51
22:10:24:LYS:O	22:10:25:ARG:NH1	2.37	0.51
33:1b:97:TRP:HZ2	33:1b:102:LEU:HD13	1.75	0.51
38:1g:50:ILE:HG13	38:1g:61:VAL:HG11	1.91	0.51
40:1i:23:ASN:OD1	40:1i:23:ASN:N	2.35	0.51
1:2A:2319:G:N2	14:2S:3:ARG:HD2	2.25	0.51
1:2A:2683:C:OP1	15:2T:53:ARG:NH2	2.39	0.51
7:2H:31:GLY:HA3	7:2H:136:ILE:HD13	1.93	0.51
18:2W:19:LEU:HB3	27:25:25:LEU:HG	1.93	0.51
32:2a:946:A:H2'	32:2a:947:G:C8	2.45	0.51
34:2c:20:SER:HB3	34:2c:22:TRP:HE1	1.74	0.51
35:2d:165:MET:HE2	35:2d:168:ARG:NE	2.25	0.51
54:2w:43:C:H2'	54:2w:44:G:C8	2.46	0.51
1:1A:1991:U:H2'	1:1A:1992:G:H5"	1.93	0.51
6:1G:5:VAL:HG22	6:1G:8:LYS:H	1.75	0.51
32:1a:642:A:N3	39:1h:113:SER:OG	2.40	0.51
32:1a:1009:G:O6	32:1a:1020:U:O2	2.28	0.51
54:1w:29:G:H1	54:1w:41:C:H42	1.58	0.51
1:2A:30:G:H2'	1:2A:31:C:C6	2.45	0.51
1:2A:1005:C:H2'	1:2A:1006:C:C6	2.45	0.51
1:2A:2506:U:O2'	54:2w:76:8AN:H4'	2.10	0.51
32:2a:1095:U:H5"	32:2a:1109:C:O2	2.11	0.51
32:2a:1323:G:H2'	32:2a:1324:A:C8	2.45	0.51
38:2g:111:ARG:NH2	38:2g:126:ASP:OD2	2.44	0.51
56:2y:9:A:O2'	56:2y:10:G:N7	2.43	0.51
1:1A:839:U:H2'	1:1A:840:C:C6	2.46	0.51
1:1A:1076:C:O2'	1:1A:1077:A:N7	2.37	0.51
39:1h:17:THR:HG22	39:1h:63:LEU:HD13	1.92	0.51
40:1i:110:GLU:OE2	40:1i:113:LYS:NZ	2.44	0.51
46:1o:8:LYS:HE3	46:1o:31:LEU:HD22	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:1s:50:ALA:HB1	50:1s:57:HIS:HB3	1.92	0.51
8:2I:78:THR:HA	8:2I:143:SER:HB3	1.91	0.51
32:2a:237:C:H5"	48:2q:25:ARG:CZ	2.41	0.51
32:2a:646:U:H2'	32:2a:647:C:C6	2.46	0.51
33:2b:185:ILE:HG22	33:2b:199:TYR:HB2	1.91	0.51
54:2w:18:G:H4'	54:2w:60:U:C5	2.45	0.51
32:1a:79:G:C6	32:1a:90:U:O2	2.63	0.51
32:1a:421:U:O4	34:1c:127:ARG:NH2	2.40	0.51
32:1a:976:G:H5'	32:1a:1358:U:O2'	2.10	0.51
49:1r:26:LEU:HD21	49:1r:39:VAL:HG13	1.92	0.51
1:2A:1568:G:N7	64:2A:4002:HOH:O	2.33	0.51
1:2A:2782:G:OP2	64:2A:3937:HOH:O	2.19	0.51
2:2B:31:C:H4'	6:2G:29:TRP:CH2	2.46	0.51
19:2X:35:THR:HG22	19:2X:37:THR:N	2.25	0.51
32:2a:494:U:OP2	64:2a:1911:HOH:O	2.19	0.51
34:2c:164:ARG:NH2	34:2c:166:GLU:OE1	2.42	0.51
1:1A:530:G:N1	1:1A:2023:G:OP1	2.31	0.51
2:1B:103:G:N2	21:1Z:73:GLN:HE22	2.08	0.51
12:1Q:10:ARG:HH11	12:1Q:11:LYS:HE2	1.76	0.51
17:1V:72:VAL:HB	17:1V:85:LYS:HB3	1.92	0.51
32:1a:504:C:OP1	64:1a:4818:HOH:O	2.19	0.51
32:1a:741:G:H2'	32:1a:742:G:O4'	2.11	0.51
39:1h:21:LYS:O	39:1h:65:TYR:OH	2.26	0.51
43:1l:71:PRO:O	43:1l:102:ARG:NH1	2.40	0.51
1:2A:111:A:O3'	24:22:65:ASN:ND2	2.44	0.51
1:2A:2447:G:N2	1:2A:2450:A:OP2	2.44	0.51
1:2A:2646:C:H2'	1:2A:2647:U:O4'	2.11	0.51
15:2T:108:ARG:NH2	32:2a:1465:C:OP2	2.43	0.51
18:2W:86:LEU:HD22	18:2W:96:ILE:HD11	1.92	0.51
32:2a:179:A:H2'	32:2a:180:U:C6	2.46	0.51
32:2a:316:G:OP2	32:2a:351:G:O2'	2.28	0.51
32:2a:677:U:H3	32:2a:713:G:H22	1.57	0.51
32:2a:769:G:H4'	32:2a:1513:A:H4'	1.93	0.51
1:1A:1243:G:O2'	11:1P:7:ARG:NH2	2.44	0.51
1:1A:2327:A:H2'	1:1A:2328:A:C8	2.46	0.51
17:1V:76:LYS:HB2	17:1V:81:TYR:HB3	1.92	0.51
27:15:40:LYS:NZ	27:15:44:THR:O	2.39	0.51
32:1a:1030:C:N4	32:1a:1030(A):G:N3	2.58	0.51
48:1q:67:LYS:O	48:1q:68:ARG:HB2	2.11	0.51
1:2A:1220:A:OP2	16:2U:19:LYS:NZ	2.41	0.51
3:2D:258:LYS:HE2	3:2D:273:ARG:NH1	2.26	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2Z:7:ALA:HB2	21:2Z:59:LEU:HD22	1.92	0.51
21:2Z:19:ARG:NH1	21:2Z:84:GLU:O	2.44	0.51
56:2y:14:A:O2'	56:2y:15:G:OP1	2.20	0.51
1:1A:668:G:H5'	1:1A:669:G:OP2	2.11	0.51
5:1F:53:THR:CG2	5:1F:55:GLY:H	2.24	0.51
32:1a:975:A:H5'	32:1a:975:A:H8	1.75	0.51
1:2A:531:C:OP1	1:2A:561:G:N1	2.41	0.51
1:2A:775:G:O3'	64:2A:3933:HOH:O	2.18	0.51
3:2D:20:ASP:OD1	3:2D:20:ASP:N	2.40	0.51
5:2F:192:LEU:HD13	5:2F:194:MET:HE2	1.92	0.51
18:2W:1:MET:HE3	18:2W:62:HIS:HB3	1.93	0.51
32:2a:1111:A:H2'	32:2a:1112:C:H6	1.76	0.51
34:2c:32:LEU:O	34:2c:36:ASP:HB2	2.10	0.51
34:2c:39:ILE:O	34:2c:43:LEU:HG	2.11	0.51
38:2g:26:PHE:CD2	38:2g:62:PHE:HE1	2.29	0.51
1:1A:2573:C:OP1	64:1A:4211:HOH:O	2.19	0.51
11:1P:101:VAL:HG21	11:1P:108:LYS:HG2	1.93	0.51
19:1X:94:GLY:H	19:1X:95:LEU:HB2	1.75	0.51
39:1h:81:HIS:N	39:1h:138:TRP:O	2.41	0.51
1:2A:1557:C:OP2	1:2A:1558:A:O2'	2.14	0.51
14:2S:25:ARG:NH1	14:2S:42:ASP:OD2	2.43	0.51
38:2g:16:LEU:HD21	40:2i:45:ALA:HB2	1.93	0.51
43:2l:70:ILE:HG12	43:2l:100:ILE:HD12	1.93	0.51
50:2s:28:LYS:HB3	50:2s:29:ARG:CA	2.41	0.51
1:1A:579:G:H2'	1:1A:580:C:C6	2.46	0.50
1:1A:745:G:O6	64:1A:4232:HOH:O	2.18	0.50
1:1A:2147:G:H3'	1:1A:2147:G:N3	2.26	0.50
1:1A:2611:U:H5'	1:1A:2611:U:H6	1.75	0.50
4:1E:7:VAL:HG12	4:1E:27:LEU:HB3	1.93	0.50
32:1a:276:G:O3'	48:1q:68:ARG:NH1	2.43	0.50
48:1q:57:VAL:HG12	48:1q:76:LEU:HA	1.93	0.50
1:2A:492:A:H2'	1:2A:493:G:O4'	2.11	0.50
1:2A:2136:C:O2'	1:2A:2137:C:H6	1.93	0.50
5:2F:129:PHE:CD2	5:2F:163:VAL:HG21	2.46	0.50
10:2O:49:ARG:HH12	32:2a:1423:G:P	2.33	0.50
15:2T:51:ARG:HG3	15:2T:98:LYS:HD2	1.93	0.50
15:2T:83:ILE:HD13	15:2T:86:ILE:HD11	1.92	0.50
21:2Z:121:HIS:N	21:2Z:171:ILE:O	2.43	0.50
32:2a:109:A:C6	32:2a:326:G:C6	2.99	0.50
32:2a:134:A:H61	47:2p:25:ARG:NH1	2.09	0.50
32:2a:984:C:H2'	32:2a:985:C:C6	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:999:C:N4	32:2a:1042:G:H1	2.08	0.50
32:2a:1417:G:O6	64:2a:1908:HOH:O	2.16	0.50
42:2k:22:HIS:HB3	42:2k:29:ILE:HB	1.93	0.50
43:2l:57:LYS:HG2	43:2l:67:THR:HG22	1.91	0.50
1:1A:1053:C:N4	1:1A:1106:G:H1	2.08	0.50
23:11:85:LEU:HD23	23:11:89:GLU:HB3	1.93	0.50
26:14:58:ARG:HD3	44:1m:80:ARG:HH12	1.77	0.50
36:1e:144:THR:H	36:1e:147:ASP:HB2	1.77	0.50
1:2A:994:C:O2'	1:2A:996:A:OP1	2.22	0.50
1:2A:2320:A:N3	1:2A:2320:A:H2'	2.25	0.50
1:2A:2870:C:H2'	1:2A:2871:C:O4'	2.12	0.50
21:2Z:130:PRO:HA	21:2Z:133:ILE:HG13	1.93	0.50
1:1A:1075:C:H2'	1:1A:1076:C:H5'	1.93	0.50
1:1A:1588:C:H2'	1:1A:1589:C:H6	1.76	0.50
1:1A:2464:C:H1'	64:1A:4469:HOH:O	2.12	0.50
1:1A:2794:C:H42	1:1A:2802:G:H22	1.59	0.50
26:14:58:ARG:O	26:14:61:ARG:N	2.44	0.50
43:1l:53:ARG:HG3	43:1l:93:LEU:HD21	1.93	0.50
1:2A:1665:A:H2'	1:2A:1666:G:O4'	2.11	0.50
32:2a:255:G:OP1	48:2q:69:LYS:NZ	2.43	0.50
32:2a:1446:U:H2'	32:2a:1452:C:C5	2.46	0.50
50:2s:36:ARG:HG2	50:2s:51:VAL:HG12	1.93	0.50
1:1A:1996:C:H4'	1:1A:1997:G:OP1	2.12	0.50
19:1X:11:PRO:HB3	19:1X:92:LEU:HD11	1.92	0.50
32:1a:110:C:H2'	32:1a:111:G:O4'	2.12	0.50
32:1a:559:A:P	36:1e:126:ARG:HH22	2.34	0.50
32:1a:1107:C:OP1	34:1c:172:ARG:HG3	2.12	0.50
33:1b:82:ARG:HD2	33:1b:92:TYR:OH	2.12	0.50
9:2N:4:TYR:CD2	16:2U:100:VAL:HG11	2.46	0.50
23:21:85:LEU:HD23	23:21:89:GLU:HB3	1.94	0.50
47:2p:5:ARG:HH21	47:2p:28:ARG:HA	1.77	0.50
1:1A:323:G:C8	5:1F:171:PRO:HG3	2.47	0.50
32:1a:955:U:O2'	50:1s:83:HIS:HD2	1.95	0.50
32:1a:993:G:H1	32:1a:1045:C:H42	1.59	0.50
33:1b:109:SER:O	33:1b:112:VAL:HG22	2.11	0.50
33:1b:134:GLU:HA	33:1b:137:ARG:HE	1.76	0.50
34:1c:35:GLU:CD	34:1c:59:ARG:HH22	2.20	0.50
40:1i:25:LYS:N	40:1i:60:ASP:OD1	2.45	0.50
1:2A:1786:A:H1'	1:2A:1938:A:N6	2.26	0.50
1:2A:2727:G:O2'	10:2O:70:LYS:NZ	2.39	0.50
28:26:9:LEU:HD13	28:26:51:GLU:HG3	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:2b:155:LEU:HD21	33:2b:159:PRO:HD3	1.93	0.50
1:1A:796:C:H2'	1:1A:797:C:C6	2.46	0.50
6:1G:72:ARG:HH12	6:1G:87:PRO:HG3	1.75	0.50
11:1P:89:ALA:HA	11:1P:121:LYS:HD3	1.94	0.50
32:1a:1305:G:H22	32:1a:1331:G:H1'	1.77	0.50
32:1a:1352:C:OP1	52:1u:3:LYS:NZ	2.34	0.50
49:1r:32:ARG:HA	49:1r:69:THR:HG21	1.94	0.50
50:1s:11:VAL:HG11	50:1s:16:LEU:HB2	1.92	0.50
1:2A:441:U:O2	5:2F:46:ARG:NH2	2.35	0.50
64:2A:4689:HOH:O	11:2P:44:GLY:HA2	2.10	0.50
32:2a:1289:A:OP1	52:2u:10:ARG:NH2	2.45	0.50
34:2c:129:ALA:HB3	34:2c:132:ARG:HB3	1.94	0.50
37:2f:95:GLU:O	49:2r:32:ARG:NH1	2.45	0.50
46:2o:39:LEU:HB3	46:2o:56:LEU:HD13	1.93	0.50
2:1B:103:G:H21	21:1Z:73:GLN:NE2	2.09	0.50
30:18:23:VAL:HG11	30:18:47:LYS:HD3	1.94	0.50
32:1a:920:U:H2'	32:1a:921:U:C6	2.47	0.50
44:1m:19:LEU:HD11	44:1m:56:LEU:HD21	1.93	0.50
1:2A:667:U:O2	30:28:2:PRO:HD2	2.12	0.50
1:2A:1580:A:H8	1:2A:1580:A:OP2	1.95	0.50
28:26:6:ARG:NH1	28:26:26:ASN:HB2	2.27	0.50
32:2a:259:G:OP2	51:2t:83:ARG:NH1	2.44	0.50
32:2a:1068:G:H8	32:2a:1068:G:OP2	1.94	0.50
32:2a:1123:A:H4'	41:2j:37:PRO:HD2	1.94	0.50
32:2a:1239:A:H62	32:2a:1299:A:H62	1.59	0.50
35:2d:121:VAL:O	35:2d:134:ASP:HA	2.12	0.50
1:1A:1062:G:H1'	1:1A:1088:A:C8	2.47	0.50
35:1d:30:LYS:HA	35:1d:35:ARG:NH1	2.26	0.50
40:1i:42:ARG:NH1	40:1i:71:SER:OG	2.45	0.50
1:2A:2183:C:H2'	1:2A:2184:G:C8	2.45	0.50
6:2G:79:ASN:N	6:2G:79:ASN:OD1	2.45	0.50
17:2V:62:LEU:HD11	17:2V:95:LEU:HB2	1.94	0.50
26:24:45:GLY:C	26:24:47:GLN:H	2.20	0.50
32:2a:381:C:H2'	32:2a:382:A:O4'	2.12	0.50
32:2a:664:G:N2	32:2a:741:G:H1	2.08	0.50
34:2c:155:GLY:O	34:2c:157:ILE:N	2.45	0.50
44:2m:79:LYS:HG2	44:2m:83:ASP:OD2	2.12	0.50
1:1A:1062:G:H2'	1:1A:1063:G:C8	2.46	0.50
1:1A:1968:G:OP1	64:1A:4238:HOH:O	2.20	0.50
1:1A:2131:G:H5'	1:1A:2133:G:C8	2.47	0.50
10:1O:122:LEU:HD13	15:1T:72:VAL:HG11	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:407:G:OP1	35:1d:115:ARG:NH2	2.45	0.50
33:1b:84:GLU:HB3	33:1b:219:VAL:HG21	1.94	0.50
33:1b:102:LEU:HB3	33:1b:180:LEU:HD12	1.94	0.50
46:1o:71:GLN:HG3	46:1o:78:TYR:CD2	2.47	0.50
54:1w:43:C:H2'	54:1w:44:G:C8	2.47	0.50
1:2A:2360:A:H2'	1:2A:2361:A:O4'	2.12	0.50
11:2P:97:PRO:HD3	11:2P:126:VAL:O	2.12	0.50
32:2a:1105:A:H2'	32:2a:1106:G:H8	1.77	0.50
32:2a:1376:U:H2'	32:2a:1377:A:C8	2.47	0.50
56:2y:61:C:H2'	56:2y:62:C:C6	2.47	0.50
1:1A:588:U:H2'	1:1A:589:C:C6	2.47	0.49
1:1A:639:U:H2'	1:1A:640:C:C6	2.47	0.49
1:1A:884:C:N3	1:1A:885:C:O2'	2.43	0.49
32:1a:17:U:H2'	32:1a:18:C:C6	2.47	0.49
32:1a:67:C:H2'	32:1a:68:G:C8	2.47	0.49
32:1a:178:C:H2'	32:1a:179:A:H8	1.75	0.49
32:1a:486:U:H2'	32:1a:487:A:H8	1.75	0.49
32:1a:972:C:OP2	41:1j:57:LYS:NZ	2.27	0.49
32:1a:1414:U:O4	64:1a:4816:HOH:O	2.19	0.49
36:1e:43:LEU:HD21	36:1e:132:ALA:HB1	1.94	0.49
55:1x:8:4SU:O5'	55:1x:8:4SU:H6	2.12	0.49
1:2A:1364:G:P	23:21:3:LYS:HG3	2.52	0.49
1:2A:1514:U:H2'	1:2A:1515:G:C8	2.47	0.49
1:2A:2238:G:OP2	64:2A:3939:HOH:O	2.20	0.49
9:2N:38:HIS:CE1	9:2N:39:ARG:HG3	2.47	0.49
20:2Y:11:ASP:OD1	20:2Y:11:ASP:N	2.45	0.49
32:2a:750:G:N3	46:2o:23:GLY:HA3	2.27	0.49
39:2h:20:TYR:HA	39:2h:65:TYR:CZ	2.47	0.49
40:2i:3:GLN:HE21	40:2i:20:ARG:NE	2.06	0.49
17:1V:55:ALA:CA	17:1V:101:GLY:HA2	2.35	0.49
38:1g:76:ARG:HD3	38:1g:156:TRP:HZ2	1.76	0.49
1:2A:981:A:OP1	64:2A:3938:HOH:O	2.20	0.49
4:2E:101:ARG:CZ	4:2E:171:GLU:HB2	2.42	0.49
5:2F:133:ASN:N	5:2F:138:GLU:OE1	2.34	0.49
56:2y:62:C:H2'	56:2y:63:G:C8	2.46	0.49
1:1A:1113:U:H2'	1:1A:1114:G:C8	2.47	0.49
1:1A:1165:U:H2'	1:1A:1166:C:C6	2.47	0.49
1:1A:1166:C:O2'	64:1A:4239:HOH:O	2.20	0.49
64:1A:5543:HOH:O	11:1P:44:GLY:HA2	2.11	0.49
9:1N:4:TYR:CD2	16:1U:100:VAL:HG11	2.48	0.49
46:1o:74:ASP:HB3	46:1o:77:ARG:HB2	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:332:A:O2'	1:2A:334:C:OP2	2.27	0.49
1:2A:2495:G:H5"	12:2Q:82:ARG:HG2	1.94	0.49
6:2G:7:LEU:HD22	6:2G:104:GLU:HA	1.94	0.49
26:24:41:PRO:HG3	26:24:49:PHE:CE1	2.46	0.49
26:24:48:ARG:NH1	26:24:51:ASP:O	2.45	0.49
32:2a:692:U:O2'	32:2a:694:A:N7	2.39	0.49
32:2a:1010:G:N2	32:2a:1020:U:O2'	2.45	0.49
32:2a:1299:A:H2'	32:2a:1299:A:N3	2.27	0.49
32:2a:1312:G:H5'	50:2s:5:LEU:HD11	1.94	0.49
11:1P:39:LYS:HB2	11:1P:45:LEU:HD22	1.94	0.49
56:1y:7:A:O2'	56:1y:49:C:O5'	2.29	0.49
1:2A:774:A:H2'	1:2A:774:A:N3	2.28	0.49
1:2A:2651:C:H42	1:2A:2669:G:H1	1.60	0.49
21:2Z:70:LEU:HD12	21:2Z:71:VAL:N	2.28	0.49
41:2j:74:ILE:HG22	64:2j:301:HOH:O	2.12	0.49
1:1A:2564:A:C2	1:1A:2647:U:H4'	2.47	0.49
31:19:2:LYS:HE2	31:19:31:LYS:O	2.12	0.49
32:1a:8:A:N7	35:1d:208:SER:OG	2.44	0.49
35:1d:107:ARG:HH21	35:1d:194:LEU:HD21	1.77	0.49
39:1h:121:ASP:HB2	39:1h:125:ARG:NH2	2.27	0.49
1:2A:2100:G:H1	1:2A:2189:U:H3	1.59	0.49
19:2X:43:VAL:HG21	19:2X:81:VAL:HG11	1.94	0.49
32:2a:434:U:H2'	32:2a:435:C:C6	2.47	0.49
32:2a:1026:G:H5'	32:2a:1027:C:O5'	2.12	0.49
33:2b:107:THR:O	33:2b:110:GLN:HB3	2.12	0.49
33:2b:118:LEU:HD23	33:2b:142:LEU:HB2	1.93	0.49
51:2t:16:HIS:O	51:2t:19:SER:OG	2.25	0.49
56:2y:51:U:H3	56:2y:63:G:H1	1.60	0.49
1:1A:484:C:H2'	1:1A:485:C:H6	1.78	0.49
1:1A:1038:C:N4	1:1A:1117:G:H1	2.09	0.49
1:1A:2108:C:H2'	1:1A:2109:U:C6	2.47	0.49
1:1A:2591:C:H2'	1:1A:2592:G:C8	2.48	0.49
5:1F:9:ILE:HD13	5:1F:22:ALA:HB3	1.94	0.49
19:1X:35:THR:HG22	19:1X:38:GLU:H	1.77	0.49
32:1a:446:G:H1	32:1a:488:C:H42	1.61	0.49
32:1a:736:C:H2'	32:1a:737:A:C8	2.48	0.49
56:1y:66:U:H2'	56:1y:67:C:C6	2.47	0.49
1:2A:277:C:H4'	1:2A:278:A:OP2	2.12	0.49
1:2A:625:G:O6	11:2P:107:LYS:NZ	2.31	0.49
1:2A:731:C:H5"	64:2A:4039:HOH:O	2.11	0.49
1:2A:2319:G:H22	14:2S:3:ARG:HD2	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2F:53:THR:HG23	5:2F:55:GLY:N	2.26	0.49
9:2N:12:ARG:NH2	9:2N:50:ASP:OD2	2.42	0.49
32:2a:1151:A:O2'	32:2a:1152:A:H8	1.95	0.49
36:2e:63:ARG:C	36:2e:66:MET:HE1	2.37	0.49
56:2y:66:U:H2'	56:2y:67:C:O4'	2.12	0.49
1:1A:1394:U:H2'	1:1A:1395:A:O4'	2.13	0.49
12:1Q:89:ASN:HB2	55:1x:1:C:N3	2.28	0.49
33:1b:131:PRO:O	33:1b:135:GLN:N	2.44	0.49
49:1r:73:ALA:HB3	49:1r:79:LEU:HD12	1.94	0.49
51:1t:47:GLY:N	51:1t:48:LYS:HB2	2.27	0.49
1:2A:1847:A:H3'	1:2A:1848:A:H5'	1.94	0.49
5:2F:157:VAL:HB	5:2F:194:MET:HG2	1.93	0.49
12:2Q:78:PRO:HG2	12:2Q:81:VAL:HG11	1.94	0.49
21:2Z:51:ALA:O	21:2Z:52:SER:HB3	2.13	0.49
32:2a:1051:C:H2'	32:2a:1052:U:C6	2.47	0.49
34:2c:14:ILE:HG21	34:2c:178:LEU:HB3	1.93	0.49
40:2i:5:TYR:OH	40:2i:16:ARG:HG2	2.12	0.49
49:2r:32:ARG:NE	64:2r:201:HOH:O	2.44	0.49
32:1a:68:G:H1	32:1a:101:A:H61	1.61	0.49
32:1a:165:C:H2'	32:1a:166:G:H8	1.78	0.49
32:1a:328:C:OP1	64:1a:4813:HOH:O	2.18	0.49
34:1c:116:VAL:HG21	34:1c:202:ILE:HD11	1.93	0.49
1:2A:234:C:H2'	1:2A:235:U:C6	2.47	0.49
5:2F:116:ASP:OD1	5:2F:119:ARG:NH2	2.46	0.49
32:2a:404:U:H2'	32:2a:405:U:C6	2.47	0.49
1:1A:886:C:H3'	1:1A:887:A:H5"	1.95	0.49
1:1A:1173:G:H22	1:1A:1177:A:P	2.35	0.49
1:1A:1607:C:H4'	1:1A:1608:A:O5'	2.12	0.49
1:1A:2223:G:OP1	3:1D:172:TYR:OH	2.25	0.49
5:1F:53:THR:HG22	5:1F:55:GLY:H	1.77	0.49
19:1X:92:LEU:O	19:1X:94:GLY:N	2.46	0.49
34:1c:6:HIS:CD2	34:1c:8:ILE:H	2.17	0.49
38:1g:28:ASN:HD21	38:1g:36:LYS:NZ	2.11	0.49
1:2A:236:C:H2'	1:2A:237:C:C6	2.47	0.49
1:2A:443:A:H1'	1:2A:1201:C:O4'	2.13	0.49
21:2Z:146:ILE:HG23	21:2Z:174:VAL:C	2.38	0.49
32:2a:1218:C:H2'	32:2a:1219:U:C6	2.47	0.49
33:2b:77:ALA:HA	33:2b:80:ILE:HG22	1.93	0.49
40:2i:28:VAL:HG12	40:2i:63:ILE:HB	1.95	0.49
1:1A:2140:C:H2'	1:1A:2141:G:C8	2.48	0.49
26:14:56:VAL:HB	26:14:60:GLN:HG3	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1d:10:ARG:HB2	35:1d:40:PRO:HG3	1.94	0.49
35:1d:187:ARG:NH1	35:1d:188:LEU:O	2.46	0.49
37:1f:33:TYR:OH	37:1f:78:GLU:HG3	2.13	0.49
54:1w:66:U:H5'	54:1w:67:C:OP2	2.13	0.49
1:2A:1219:G:H1	1:2A:1230:C:H42	1.61	0.49
1:2A:2299:G:H2'	1:2A:2300:G:H8	1.78	0.49
1:2A:2805:G:H2'	1:2A:2807:G:H8	1.77	0.49
32:2a:596:C:OP2	64:2a:1910:HOH:O	2.19	0.49
32:2a:952:U:H2'	32:2a:953:G:C8	2.48	0.49
33:2b:78:GLN:O	33:2b:94:ASN:ND2	2.46	0.49
1:1A:1805:U:O2	3:1D:50:THR:HB	2.12	0.48
1:1A:2156:G:OP2	1:1A:2156:G:H8	1.96	0.48
15:1T:74:ARG:HG2	15:1T:76:PHE:CZ	2.48	0.48
32:1a:195:A:H1'	32:1a:222:U:O2'	2.12	0.48
32:1a:458:C:H2'	32:1a:460:G:O4'	2.12	0.48
32:1a:963:G:H5'	64:1a:4894:HOH:O	2.13	0.48
50:1s:80:TYR:CZ	50:1s:82:GLY:HA2	2.48	0.48
1:2A:652(T):C:H2'	1:2A:652(U):G:C8	2.48	0.48
1:2A:2815:C:H2'	1:2A:2816:C:C6	2.48	0.48
10:2O:36:GLY:HA2	10:2O:106:LEU:HD23	1.95	0.48
19:2X:11:PRO:HB3	19:2X:92:LEU:HD11	1.94	0.48
21:2Z:93:ASP:HA	21:2Z:131:ARG:NH1	2.25	0.48
29:27:24:THR:HG22	29:27:27:GLY:H	1.77	0.48
32:2a:709:G:O6	64:2a:1912:HOH:O	2.20	0.48
56:2y:62:C:H2'	56:2y:63:G:H8	1.78	0.48
1:1A:1119:C:N4	64:1A:4206:HOH:O	2.42	0.48
1:1A:2134:A:O2'	1:1A:2135:A:OP1	2.25	0.48
8:1I:126:TYR:HB2	8:1I:142:VAL:HG23	1.95	0.48
33:1b:87:ARG:NH2	33:1b:220:ASP:OD1	2.37	0.48
41:1j:30:SER:O	41:1j:30:SER:OG	2.31	0.48
1:2A:900:A:HO2'	1:2A:901:A:P	2.36	0.48
1:2A:1514:U:H2'	1:2A:1515:G:H8	1.78	0.48
1:2A:2537:U:H2'	1:2A:2538:C:C6	2.47	0.48
28:26:40:CYS:O	28:26:44:ARG:N	2.45	0.48
32:2a:730:G:C5	32:2a:731:G:H1'	2.48	0.48
32:2a:838:G:H1	32:2a:848:C:H42	1.60	0.48
35:2d:20:TYR:HD1	35:2d:26:CYS:HB3	1.78	0.48
37:2f:46:ARG:HH22	49:2r:37:VAL:HG11	1.78	0.48
40:2i:3:GLN:NE2	40:2i:20:ARG:HE	2.06	0.48
1:1A:1588:C:H2'	1:1A:1589:C:C6	2.49	0.48
26:14:60:GLN:C	26:14:62:ARG:H	2.21	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:438:G:H4'	35:1d:123:HIS:ND1	2.28	0.48
35:1d:60:GLU:HG3	35:1d:202:LEU:HD12	1.95	0.48
39:1h:95:VAL:HB	39:1h:99:GLU:HB2	1.95	0.48
47:1p:19:ILE:HG22	47:1p:36:ILE:HG13	1.95	0.48
48:1q:76:LEU:HD23	48:1q:77:VAL:N	2.28	0.48
1:2A:795:C:H2'	1:2A:796:C:C6	2.48	0.48
32:2a:1263:C:C4	32:2a:1272:G:O6	2.65	0.48
38:2g:15:ASP:OD2	38:2g:44:TYR:OH	2.31	0.48
48:2q:67:LYS:O	48:2q:68:ARG:HB2	2.12	0.48
51:2t:10:LEU:HG	51:2t:12:ALA:H	1.78	0.48
1:1A:694:U:OP1	3:1D:59:LYS:NZ	2.46	0.48
1:1A:2291:U:H2'	1:1A:2292:C:C6	2.49	0.48
32:1a:838:G:H1	32:1a:848:C:H42	1.60	0.48
32:1a:977:A:O2'	32:1a:979:C:OP2	2.30	0.48
2:2B:8:U:O3'	14:2S:25:ARG:NH2	2.46	0.48
9:2N:15:LEU:HB2	9:2N:135:PRO:HB2	1.93	0.48
11:2P:85:LEU:HD23	11:2P:88:LEU:HD12	1.95	0.48
21:2Z:30:ASN:HA	21:2Z:89:PHE:HE1	1.78	0.48
29:27:24:THR:HG22	29:27:26:GLY:N	2.27	0.48
32:2a:975:A:H5'	32:2a:975:A:H8	1.78	0.48
36:2e:145:LYS:HG2	39:2h:107:LEU:HD22	1.95	0.48
39:2h:6:ILE:O	39:2h:10:LEU:HG	2.13	0.48
56:2y:34:G:H2'	56:2y:35:A:C8	2.48	0.48
1:1A:443:A:H1'	1:1A:1201:C:O4'	2.12	0.48
1:1A:518:G:H2'	1:1A:519:U:C6	2.48	0.48
1:1A:1092:C:H2'	1:1A:1093:G:H5'	1.95	0.48
1:1A:1184:G:H5'	25:13:29:ARG:NH1	2.29	0.48
32:1a:200:G:H1	32:1a:217:C:N4	2.10	0.48
32:1a:1145:C:H4'	32:1a:1146:A:H5'	1.95	0.48
33:1b:84:GLU:OE1	33:1b:87:ARG:NH1	2.46	0.48
1:2A:236:C:H2'	1:2A:237:C:H6	1.78	0.48
7:2H:113:VAL:HG11	7:2H:151:ILE:HD13	1.96	0.48
11:2P:19:VAL:HG12	11:2P:27:HIS:HB3	1.96	0.48
17:2V:6:LYS:HB2	17:2V:38:LEU:HD11	1.96	0.48
36:2e:71:LEU:C	36:2e:72:GLN:HE21	2.22	0.48
1:1A:286:C:H2'	1:1A:287:C:H6	1.78	0.48
1:1A:295:G:H4'	20:1Y:1:MET:HE3	1.95	0.48
1:1A:1064:C:H2'	1:1A:1065:U:H5'	1.96	0.48
1:1A:1584:C:O2'	1:1A:1586:A:H5'	2.13	0.48
1:1A:2747:G:O6	1:1A:2755:C:H5"	2.14	0.48
32:1a:757:U:O4	64:1a:4817:HOH:O	2.19	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1095:U:OP2	64:1a:4815:HOH:O	2.20	0.48
32:1a:1318:A:H5"	50:1s:3:ARG:HH12	1.78	0.48
54:1w:63:G:H2'	54:1w:64:A:C8	2.48	0.48
1:2A:301:G:OP2	20:2Y:84:ARG:NH2	2.47	0.48
1:2A:880:G:N2	1:2A:898:C:H1'	2.29	0.48
1:2A:1889:A:H2'	1:2A:1890:A:C8	2.48	0.48
1:2A:2291:U:H2'	1:2A:2292:C:C6	2.49	0.48
32:2a:955:U:OP1	44:2m:120:LYS:NZ	2.37	0.48
32:2a:1146:A:H2'	32:2a:1147:C:O4'	2.13	0.48
35:2d:22:LYS:O	35:2d:113:SER:HB2	2.14	0.48
55:2x:50:U:H2'	55:2x:51:C:C6	2.49	0.48
1:1A:2328:A:H2'	1:1A:2329:G:C8	2.49	0.48
14:1S:27:SER:HA	14:1S:88:ASP:HB3	1.96	0.48
32:1a:116:A:H61	32:1a:313:A:H1'	1.79	0.48
33:1b:230:VAL:HG12	33:1b:231:GLU:H	1.78	0.48
35:1d:30:LYS:HA	35:1d:35:ARG:HH11	1.78	0.48
1:2A:375:C:H2'	1:2A:376:C:C6	2.49	0.48
1:2A:1866:C:H2'	1:2A:1876:A:O4'	2.14	0.48
1:2A:2171:A:N3	1:2A:2172:U:N3	2.62	0.48
1:2A:2712:U:OP1	1:2A:2714:G:H4'	2.14	0.48
12:2Q:89:ASN:HB2	55:2x:1:C:C4	2.49	0.48
21:2Z:29:TYR:HB3	21:2Z:34:ASN:HD22	1.77	0.48
1:1A:1080:C:H5'	1:1A:1081:U:OP2	2.13	0.48
56:1y:5:G:C2	56:1y:69:G:C5	3.02	0.48
1:2A:2136:C:O2'	1:2A:2137:C:O5'	2.31	0.48
21:2Z:40:ASP:OD2	21:2Z:43:GLU:N	2.41	0.48
23:21:2:SER:HB3	23:21:46:LEU:HD12	1.96	0.48
32:2a:1056:U:H5'	34:2c:163:ALA:HB2	1.96	0.48
34:2c:104:GLN:HG3	34:2c:105:GLU:N	2.28	0.48
36:2e:41:VAL:O	36:2e:66:MET:HA	2.13	0.48
37:2f:91:VAL:HG11	49:2r:72:ARG:HH12	1.78	0.48
40:2i:26:VAL:HG22	40:2i:61:ALA:HB3	1.94	0.48
56:2y:9:A:H5'	56:2y:46:G7M:N3	2.27	0.48
1:1A:2153:G:H2'	1:1A:2154:G:C8	2.49	0.48
1:1A:2420:C:OP1	30:18:34:TRP:HB3	2.13	0.48
1:1A:2811:G:N2	1:1A:2891:G:H1'	2.28	0.48
1:1A:2839:G:H5'	13:1R:46:GLY:HA2	1.95	0.48
8:1I:92:VAL:HG11	8:1I:144:VAL:HG11	1.95	0.48
9:1N:75:TYR:CE2	9:1N:77:GLY:HA2	2.49	0.48
10:1O:120:GLU:OE1	15:1T:67:SER:OG	2.30	0.48
32:1a:841:U:C4	32:1a:848:C:H1'	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2115:G:O2'	1:2A:2117:A:N7	2.40	0.48
1:2A:2801(A):A:H5'	1:2A:2802:G:C8	2.48	0.48
32:2a:108:G:C6	51:2t:15:ARG:HG2	2.48	0.48
49:2r:58:LEU:HD22	49:2r:62:GLU:HB3	1.96	0.48
7:1H:3:ARG:CZ	7:1H:5:GLY:H	2.27	0.48
15:1T:19:LEU:HD22	15:1T:86:ILE:HG13	1.95	0.48
32:1a:881:G:P	43:1l:12:ARG:HH22	2.37	0.48
56:1y:19:G:C6	56:1y:56:C:N4	2.81	0.48
1:2A:598:G:N2	5:2F:35:GLU:OE2	2.42	0.48
1:2A:981:A:N1	1:2A:2027:G:O2'	2.43	0.48
1:2A:1495:A:H2'	1:2A:1496:A:H8	1.77	0.48
8:2I:47:LEU:O	8:2I:51:ILE:HB	2.14	0.48
9:2N:35:ARG:O	9:2N:42:TRP:NE1	2.45	0.48
10:2O:2:ILE:HD12	10:2O:6:THR:HG21	1.95	0.48
32:2a:538:G:H5"	43:2l:114:LYS:HB2	1.96	0.48
32:2a:1206:G:O2'	34:2c:193:TYR:HA	2.13	0.48
39:2h:86:ILE:HD13	39:2h:133:LEU:HD22	1.96	0.48
40:2i:100:GLY:O	40:2i:103:THR:HG22	2.13	0.48
1:1A:1311:G:H2'	29:17:47:ARG:HH22	1.79	0.47
1:1A:1796:U:H2'	1:1A:1797:C:C6	2.48	0.47
1:1A:2105:C:H2'	1:1A:2106:G:C8	2.49	0.47
10:1O:2:ILE:HD12	10:1O:6:THR:HG21	1.96	0.47
19:1X:72:LYS:HE2	19:1X:73:ARG:O	2.14	0.47
32:1a:376:G:H5"	47:1p:5:ARG:HG2	1.95	0.47
32:1a:600:C:H2'	32:1a:601:C:H6	1.79	0.47
32:1a:673:G:H2'	32:1a:674:G:C8	2.48	0.47
32:1a:767:A:H2'	32:1a:768:A:O4'	2.14	0.47
34:1c:172:ARG:NH2	34:1c:206:GLU:OE2	2.47	0.47
50:1s:63:THR:OG1	50:1s:65:ASN:OD1	2.31	0.47
1:2A:900:A:H2'	1:2A:901:A:H8	1.79	0.47
5:2F:137:LYS:HE2	5:2F:137:LYS:HB3	1.62	0.47
5:2F:172:TRP:H	5:2F:172:TRP:CD1	2.32	0.47
17:2V:16:PRO:HD3	17:2V:99:ILE:HD11	1.96	0.47
39:2h:119:LEU:HB3	39:2h:123:GLU:HB2	1.95	0.47
1:1A:55:G:O2'	1:1A:127:A:N1	2.42	0.47
1:1A:747:U:O2	1:1A:2014:A:H1'	2.14	0.47
1:1A:2161:C:O2'	1:1A:2162:G:H5"	2.14	0.47
1:1A:2206:G:OP2	1:1A:2206:G:H4'	2.13	0.47
13:1R:57:ARG:HG2	13:1R:59:ASP:OD1	2.14	0.47
21:1Z:1:MET:HA	21:1Z:2:GLU:HA	1.68	0.47
21:1Z:53:ILE:HG22	21:1Z:71:VAL:HG12	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:96:U:H2'	32:1a:97:G:C8	2.49	0.47
32:1a:974:A:H8	32:1a:974:A:OP1	1.96	0.47
32:1a:1025:U:C2	32:1a:1036:G:O6	2.68	0.47
32:1a:1442:G:H2'	32:1a:1442:G:N3	2.28	0.47
50:1s:27:GLU:HB2	50:1s:28:LYS:HA	1.95	0.47
1:2A:2849:U:H4'	1:2A:2868:A:C2	2.49	0.47
2:2B:9:G:H1	2:2B:112:U:H3	1.62	0.47
2:2B:66:A:N6	2:2B:108:U:H3'	2.29	0.47
9:2N:96:GLU:CD	9:2N:96:GLU:H	2.22	0.47
28:26:34:LEU:HB2	28:26:51:GLU:HB2	1.95	0.47
32:2a:936:C:H2'	32:2a:937:A:O4'	2.14	0.47
32:2a:1134:G:H1	32:2a:1140:C:H42	1.62	0.47
38:2g:20:ASP:HB3	38:2g:23:VAL:HB	1.96	0.47
1:1A:2379:G:O2'	14:1S:17:ARG:NH2	2.47	0.47
26:14:46:GLN:HB2	26:14:48:ARG:NE	2.28	0.47
30:18:23:VAL:HG13	30:18:47:LYS:HB3	1.96	0.47
32:1a:542:G:H5'	35:1d:41:GLY:HA3	1.96	0.47
32:1a:867:G:O2'	32:1a:873:A:N1	2.42	0.47
33:1b:77:ALA:HB2	33:1b:211:ILE:HD13	1.95	0.47
5:2F:20:LEU:HG	5:2F:21:ALA:H	1.79	0.47
13:2R:33:ARG:NH2	13:2R:115:GLU:OE1	2.38	0.47
32:2a:137:C:H2'	32:2a:138:G:H8	1.79	0.47
32:2a:920:U:H2'	32:2a:921:U:C6	2.49	0.47
3:1D:77:ALA:HB2	3:1D:97:TYR:CD1	2.49	0.47
6:1G:66:GLN:HG3	26:14:1:MET:HE1	1.97	0.47
8:1I:109:ILE:HD12	8:1I:130:TYR:CE2	2.50	0.47
32:1a:486:U:H2'	32:1a:487:A:C8	2.49	0.47
32:1a:1039:C:H2'	32:1a:1040:U:C6	2.49	0.47
32:1a:1169:A:H2'	32:1a:1170:A:C8	2.49	0.47
33:1b:222:ILE:O	33:1b:226:ARG:HG2	2.14	0.47
46:1o:6:GLU:O	46:1o:10:LYS:HG3	2.14	0.47
54:1w:68:C:H2'	54:1w:69:G:C8	2.49	0.47
1:2A:141:A:H8	1:2A:1408:C:O2'	1.96	0.47
1:2A:171:G:H2'	1:2A:172:C:C6	2.50	0.47
1:2A:900:A:H2'	1:2A:901:A:C8	2.50	0.47
13:2R:56:LYS:NZ	13:2R:90:ARG:O	2.46	0.47
1:1A:302:C:P	20:1Y:73:ARG:HH22	2.37	0.47
1:1A:1266:G:O2'	1:1A:2012:G:O6	2.30	0.47
1:1A:1580:A:OP2	1:1A:1580:A:H8	1.98	0.47
1:1A:2572:A:C8	4:1E:144:ARG:HD3	2.49	0.47
1:1A:2849:U:P	15:1T:95:ARG:HH12	2.36	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1S:71:ARG:NH1	14:1S:107:GLU:OE1	2.43	0.47
32:1a:1194:U:H4'	36:1e:22:GLY:HA2	1.95	0.47
32:1a:1347:G:O2'	32:1a:1373:G:O6	2.28	0.47
1:2A:784:A:C6	3:2D:229:VAL:HG11	2.49	0.47
1:2A:881:G:C2	1:2A:882:G:H1'	2.49	0.47
2:2B:77:U:OP1	21:2Z:19:ARG:NH2	2.47	0.47
4:2E:116:VAL:HG13	4:2E:122:PHE:HB2	1.96	0.47
5:2F:32:LEU:HD22	5:2F:112:MET:HE3	1.95	0.47
14:2S:10:ARG:NE	14:2S:91:PRO:O	2.47	0.47
32:2a:1002:G:N3	32:2a:1003:G:H1'	2.29	0.47
33:2b:178:ARG:HH12	39:2h:68:ARG:HH22	1.62	0.47
33:2b:185:ILE:HG22	33:2b:199:TYR:CD2	2.49	0.47
41:2j:38:ILE:HD11	41:2j:71:LEU:HD23	1.97	0.47
54:2w:4:C:N4	54:2w:69:G:H1	2.09	0.47
1:1A:284:U:H2'	1:1A:285:C:C6	2.48	0.47
1:1A:2123:G:H2'	1:1A:2124:G:H8	1.80	0.47
21:1Z:126:VAL:HG11	21:1Z:161:VAL:HB	1.96	0.47
23:11:64:ALA:HA	23:11:67:ILE:HG13	1.95	0.47
32:1a:262:A:C6	32:1a:263:A:C6	3.02	0.47
32:1a:1260:C:O5'	32:1a:1284:C:H4'	2.15	0.47
33:1b:187:LEU:HD12	33:1b:201:ILE:O	2.15	0.47
34:1c:13:GLY:HA3	45:1n:57:ARG:NH1	2.30	0.47
3:2D:132:PRO:HD3	3:2D:190:TYR:CZ	2.50	0.47
6:2G:41:GLN:HB3	6:2G:43:LEU:HD22	1.97	0.47
32:2a:736:C:OP1	49:2r:72:ARG:NH2	2.48	0.47
32:2a:1318:A:H1'	50:2s:37:ARG:HE	1.80	0.47
32:2a:1327:C:H2'	32:2a:1328:C:C6	2.49	0.47
32:2a:1359:C:OP1	45:2n:22:THR:OG1	2.31	0.47
34:2c:108:ASN:HB3	34:2c:111:LEU:HD12	1.97	0.47
42:2k:27:ASN:OD1	42:2k:28:THR:N	2.43	0.47
1:1A:286:C:H2'	1:1A:287:C:C6	2.50	0.47
1:1A:774:A:N3	1:1A:774:A:H2'	2.28	0.47
1:1A:1092:C:C2'	1:1A:1093:G:H5'	2.44	0.47
1:1A:1102:C:H2'	1:1A:1103:A:H8	1.78	0.47
20:1Y:92:ASN:ND2	20:1Y:94:LYS:HG3	2.29	0.47
21:1Z:158:PRO:O	21:1Z:161:VAL:HG22	2.15	0.47
32:1a:381:C:H2'	32:1a:382:A:O4'	2.15	0.47
32:1a:1027:C:C4	32:1a:1034:G:N1	2.79	0.47
35:1d:65:ARG:NH1	35:1d:72:GLU:HB2	2.29	0.47
56:1y:35:A:OP2	56:1y:35:A:H8	1.97	0.47
1:2A:652(B):A:H61	1:2A:655:A:H1'	1.78	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:882:G:H22	1:2A:894:C:H42	1.63	0.47
1:2A:1647:G:H3'	1:2A:1647:G:OP2	2.14	0.47
1:2A:2836:U:H2'	1:2A:2837:G:C8	2.49	0.47
1:2A:2880:C:O3'	13:2R:90:ARG:NH1	2.48	0.47
5:2F:21:ALA:CB	5:2F:22:ALA:HA	2.41	0.47
9:2N:58:ASP:OD1	9:2N:58:ASP:N	2.46	0.47
17:2V:24:LYS:HB3	17:2V:24:LYS:HE2	1.68	0.47
21:2Z:156:LYS:HE3	21:2Z:158:PRO:HD3	1.96	0.47
23:21:67:ILE:N	23:21:68:PRO:HD2	2.30	0.47
32:2a:509:A:O2'	32:2a:510:A:OP1	2.27	0.47
32:2a:1030(A):G:N2	32:2a:1030(C):G:H3'	2.30	0.47
32:2a:1264:C:C4	32:2a:1272:G:O6	2.68	0.47
41:2j:7:LYS:HB2	41:2j:71:LEU:HD12	1.97	0.47
56:2y:14:A:N6	56:2y:21:A:H2	2.10	0.47
22:10:11:ARG:HG2	64:10:206:HOH:O	2.14	0.47
31:19:17:ILE:HD13	31:19:26:ILE:HD13	1.97	0.47
32:1a:299:G:O5'	32:1a:299:G:H8	1.97	0.47
32:1a:1007:C:H2'	32:1a:1008:C:C6	2.49	0.47
32:1a:1152:A:OP1	41:1j:68:HIS:ND1	2.48	0.47
35:1d:178:VAL:HG12	35:1d:179:GLU:H	1.80	0.47
56:1y:31:A:H61	56:1y:39:PSU:HN3	1.63	0.47
1:2A:747:U:O2	1:2A:2014:A:H1'	2.15	0.47
15:2T:6:LEU:O	15:2T:10:VAL:HG23	2.14	0.47
32:2a:772:U:H2'	32:2a:773:G:O4'	2.15	0.47
32:2a:1302:U:OP2	44:2m:21:TYR:OH	2.17	0.47
32:2a:1456:G:H1	51:2t:51:GLU:CD	2.23	0.47
33:2b:167:PRO:HD3	33:2b:187:LEU:O	2.14	0.47
34:2c:6:HIS:ND1	45:2n:49:HIS:HB3	2.30	0.47
43:2l:117:ARG:HB3	43:2l:122:THR:O	2.15	0.47
44:2m:91:ARG:HH11	44:2m:96:LEU:HD13	1.80	0.47
1:1A:602:G:O2'	1:1A:655:A:N6	2.48	0.47
1:1A:729:G:C6	3:1D:208:LYS:HB2	2.49	0.47
21:1Z:100:VAL:HG11	21:1Z:134:PRO:HG2	1.97	0.47
36:1e:74:GLY:HA3	36:1e:116:THR:HG22	1.97	0.47
1:2A:784:A:N6	3:2D:229:VAL:HG11	2.29	0.47
1:2A:1178:C:H2'	1:2A:1179:C:C6	2.49	0.47
5:2F:65:TRP:CZ2	5:2F:75:HIS:HD2	2.33	0.47
12:2Q:65:PHE:HB2	12:2Q:105:GLU:HB2	1.96	0.47
32:2a:447:G:O6	32:2a:485:G:O2'	2.28	0.47
32:2a:757:U:H2'	32:2a:758:G:O4'	2.15	0.47
32:2a:1117:G:N2	32:2a:1180:A:O2'	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1226:C:H4'	50:2s:80:TYR:CZ	2.50	0.47
1:1A:1065:U:H3'	1:1A:1066:U:C6	2.49	0.47
3:1D:71:ASP:HB2	3:1D:103:ARG:HH12	1.80	0.47
13:1R:118:GLU:H	13:1R:118:GLU:CD	2.23	0.47
14:1S:65:VAL:O	14:1S:69:VAL:HG12	2.15	0.47
32:1a:507:C:OP2	32:1a:508:C:O2'	2.24	0.47
32:1a:731:G:H5'	32:1a:766:A:H4'	1.96	0.47
38:1g:26:PHE:O	38:1g:30:ILE:HG13	2.14	0.47
1:2A:614(B):G:H2'	5:2F:44:ARG:HH11	1.80	0.47
1:2A:908:C:OP1	12:2Q:22:LYS:HG2	2.15	0.47
1:2A:2155:G:C5	1:2A:2156:G:H1'	2.50	0.47
20:2Y:9:LYS:HA	20:2Y:10:GLY:HA2	1.61	0.47
28:26:11:LEU:HB2	28:26:21:TYR:HB2	1.97	0.47
32:2a:779:C:H2'	32:2a:780:A:O4'	2.15	0.47
33:2b:8:LYS:HD2	33:2b:9:GLU:H	1.80	0.47
51:2t:47:GLY:HA2	51:2t:48:LYS:C	2.40	0.47
1:1A:247:G:H4'	1:1A:386:G:C5	2.49	0.46
1:1A:1095:A:C8	1:1A:1096:A:C8	3.04	0.46
1:1A:1173:G:OP2	1:1A:1173:G:H2'	2.15	0.46
8:1I:107:VAL:HG12	8:1I:109:ILE:HG12	1.98	0.46
32:1a:108:G:C6	51:1t:15:ARG:HD2	2.50	0.46
32:1a:1298:C:C4	38:1g:114:ARG:HD3	2.50	0.46
1:2A:2336:A:H61	22:20:43:THR:CG2	2.28	0.46
7:2H:45:VAL:HG13	7:2H:50:VAL:HG22	1.97	0.46
9:2N:4:TYR:HB2	16:2U:101:ARG:NH1	2.30	0.46
32:2a:1053:G:N7	32:2a:1200:C:H5"	2.30	0.46
32:2a:1176:A:H2'	32:2a:1177:G:C8	2.50	0.46
32:2a:1518:MA6:H93	32:2a:1519:MA6:C9	2.46	0.46
34:2c:131:ARG:HH21	34:2c:135:LYS:HE3	1.80	0.46
38:2g:45:ASP:O	38:2g:49:ILE:HD12	2.15	0.46
42:2k:98:LEU:O	42:2k:101:SER:OG	2.21	0.46
42:2k:99:GLN:HG2	42:2k:105:VAL:HG21	1.97	0.46
1:1A:668:G:OP2	64:1A:4240:HOH:O	2.20	0.46
1:1A:2126:A:N1	1:1A:2162:G:O2'	2.43	0.46
8:1I:62:LYS:O	8:1I:66:GLU:HG2	2.16	0.46
32:1a:404:U:P	35:1d:118:ARG:HH12	2.38	0.46
32:1a:766:A:OP2	64:1a:4820:HOH:O	2.20	0.46
32:1a:1025:U:O2	32:1a:1036:G:C6	2.68	0.46
32:1a:1429:C:H2'	32:1a:1430:C:C6	2.51	0.46
39:1h:9:MET:HG3	39:1h:26:VAL:HG21	1.97	0.46
41:1j:39:PRO:HA	41:1j:70:ARG:HD3	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:887:A:H4'	1:2A:888:C:H5	1.79	0.46
1:2A:1443:G:N7	64:2A:4030:HOH:O	2.36	0.46
1:2A:1641:A:H2'	1:2A:1642:G:O4'	2.16	0.46
1:2A:2142:C:H2'	1:2A:2143:C:C6	2.51	0.46
1:2A:2291:U:OP1	1:2A:2380:C:O2'	2.30	0.46
1:2A:2802:G:H2'	1:2A:2803:C:O4'	2.16	0.46
2:2B:75:G:H22	21:2Z:73:GLN:NE2	2.10	0.46
21:2Z:55:HIS:CE1	21:2Z:135:GLU:HB2	2.50	0.46
30:28:23:VAL:HG11	30:28:47:LYS:HD3	1.98	0.46
32:2a:959:A:HO2'	32:2a:984:C:HO2'	1.60	0.46
32:2a:1510:U:H2'	32:2a:1511:G:C8	2.49	0.46
33:2b:215:LEU:HD23	33:2b:215:LEU:HA	1.81	0.46
35:2d:104:VAL:HG21	35:2d:140:VAL:HG21	1.96	0.46
7:1H:149:ARG:NH1	7:1H:167:GLU:OE2	2.41	0.46
16:1U:76:TYR:CZ	16:1U:80:ILE:HG13	2.50	0.46
26:14:24:THR:OG1	26:14:25:TYR:N	2.48	0.46
28:16:6:ARG:NH1	28:16:26:ASN:HB2	2.30	0.46
32:1a:769:G:H4'	32:1a:1513:A:H4'	1.98	0.46
32:1a:1442:G:O2'	32:1a:1442(A):G:H5'	2.15	0.46
36:1e:78:HIS:HE1	36:1e:142:LEU:HA	1.79	0.46
36:1e:148:VAL:O	36:1e:152:ARG:HG3	2.15	0.46
38:1g:13:GLN:O	38:1g:24:THR:HG21	2.15	0.46
51:1t:64:ASP:CG	51:1t:81:LYS:HZ3	2.24	0.46
1:2A:910:A:N1	1:2A:2277:G:H1'	2.31	0.46
2:2B:103:G:H21	21:2Z:73:GLN:HE22	1.64	0.46
5:2F:185:ASP:OD1	5:2F:188:ARG:NH1	2.46	0.46
32:2a:1149:C:H2'	32:2a:1150:U:C6	2.51	0.46
43:2l:56:ALA:HB2	43:2l:70:ILE:HD11	1.98	0.46
45:2n:23:ARG:NH1	45:2n:30:ALA:HB2	2.30	0.46
1:1A:1035:U:H2'	1:1A:1036:G:C8	2.51	0.46
1:1A:1041:C:H42	1:1A:1114:G:H1	1.62	0.46
1:1A:1153:C:H2'	1:1A:1154:G:O4'	2.15	0.46
1:1A:2123:G:H2'	1:1A:2124:G:C8	2.50	0.46
8:1I:3:VAL:HG12	8:1I:38:LEU:HA	1.96	0.46
32:1a:103:C:OP2	51:1t:14:LYS:NZ	2.48	0.46
32:1a:1060:C:H5"	41:1j:51:ARG:HG2	1.98	0.46
32:1a:1136:U:H5"	32:1a:1137:C:N4	2.30	0.46
35:1d:172:PRO:O	35:1d:174:LEU:N	2.47	0.46
40:1i:24:GLY:HA2	40:1i:59:PHE:O	2.15	0.46
40:1i:48:GLU:HA	40:1i:51:ARG:HD3	1.97	0.46
55:1x:8:4SU:O2	55:1x:21:A:H2	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:657:U:H2'	1:2A:658:C:C6	2.50	0.46
6:2G:35:GLU:HB3	6:2G:160:VAL:HG12	1.97	0.46
6:2G:106:LEU:O	6:2G:110:ALA:HB3	2.15	0.46
32:2a:598:U:O4	64:2a:1910:HOH:O	2.18	0.46
32:2a:1056:U:C5'	34:2c:163:ALA:HB2	2.46	0.46
40:2i:58:HIS:H	40:2i:58:HIS:CD2	2.33	0.46
44:2m:50:GLU:O	44:2m:53:VAL:HG22	2.15	0.46
1:1A:271(L):U:P	8:1I:50:ARG:HH12	2.37	0.46
1:1A:271(O):C:H2'	1:1A:271(P):C:C6	2.51	0.46
32:1a:447:G:H2'	32:1a:485:G:N2	2.31	0.46
32:1a:509:A:HO2'	32:1a:510:A:P	2.35	0.46
34:1c:124:ILE:HG22	34:1c:130:VAL:HG22	1.98	0.46
35:1d:105:VAL:HG13	35:1d:110:PHE:HB2	1.97	0.46
39:1h:53:VAL:HB	39:1h:58:TYR:CD2	2.51	0.46
1:2A:324:A:N6	1:2A:338:G:O2'	2.47	0.46
1:2A:392:C:H5"	1:2A:409:C:H5"	1.98	0.46
1:2A:893:C:H2'	1:2A:894:C:C4	2.50	0.46
1:2A:1579:A:H2'	1:2A:1580:A:C8	2.49	0.46
1:2A:1589:C:H2'	1:2A:1590:U:C6	2.51	0.46
1:2A:2169:A:H2'	1:2A:2170:A:C8	2.50	0.46
32:2a:352:C:O2'	32:2a:354:G:OP1	2.31	0.46
32:2a:376:G:H5"	47:2p:5:ARG:HB2	1.97	0.46
32:2a:445:G:H1	32:2a:489:C:H42	1.63	0.46
32:2a:792:A:H4'	32:2a:793:U:H5"	1.97	0.46
32:2a:1329:A:OP2	52:2u:7:ARG:NH1	2.40	0.46
38:2g:51:GLN:O	38:2g:55:GLY:HA2	2.15	0.46
45:2n:3:ARG:HE	45:2n:3:ARG:CA	2.28	0.46
51:2t:50:GLU:O	51:2t:100:ILE:HD11	2.15	0.46
1:1A:1429:G:H2'	1:1A:1430:C:C6	2.50	0.46
1:1A:1721:G:H1'	1:1A:1741:A:H61	1.80	0.46
2:1B:108:U:H2'	2:1B:109:C:H5"	1.97	0.46
26:14:59:PHE:CD2	50:1s:64:GLU:HB3	2.50	0.46
28:16:14:THR:HG21	28:16:48:VAL:HG13	1.97	0.46
32:1a:952:U:H2'	32:1a:953:G:C8	2.51	0.46
32:1a:1218:C:H2'	32:1a:1219:U:C6	2.51	0.46
33:1b:13:ALA:HB2	33:1b:44:LEU:HD13	1.98	0.46
36:1e:95:ALA:HB1	36:1e:96:PRO:HD2	1.98	0.46
48:1q:45:HIS:NE2	48:1q:47:PRO:HG3	2.29	0.46
4:2E:9:VAL:HG22	4:2E:25:VAL:HB	1.98	0.46
32:2a:229:U:H5"	47:2p:33:ILE:HD13	1.97	0.46
32:2a:1139:G:N2	32:2a:1142:G:O6	2.39	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:2g:50:ILE:HD11	38:2g:58:PRO:HA	1.96	0.46
40:2i:4:TYR:CE1	40:2i:88:TYR:HA	2.51	0.46
41:2j:9:ARG:HH22	41:2j:69:ASN:HD21	1.63	0.46
48:2q:3:LYS:HD3	48:2q:61:GLU:O	2.16	0.46
48:2q:45:HIS:NE2	48:2q:47:PRO:HG3	2.30	0.46
49:2r:73:ALA:HB3	49:2r:79:LEU:HD12	1.97	0.46
1:1A:2286:A:H4'	1:1A:2287:A:O4'	2.15	0.46
32:1a:625:G:H4'	47:1p:16:HIS:CD2	2.51	0.46
32:1a:1030(A):G:O2'	32:1a:1031:G:N2	2.49	0.46
32:1a:1239:A:C4	32:1a:1298:C:N4	2.84	0.46
35:1d:65:ARG:HG3	35:1d:75:PHE:CD1	2.51	0.46
54:1w:9:A:H8	54:1w:11:C:H41	1.63	0.46
1:2A:805:G:OP1	64:2A:3929:HOH:O	2.20	0.46
1:2A:1006:C:OP2	64:2A:3940:HOH:O	2.20	0.46
1:2A:1405:U:H2'	1:2A:1406:U:C6	2.51	0.46
3:2D:77:ALA:HA	3:2D:97:TYR:HA	1.97	0.46
3:2D:125:ILE:HB	37:2f:81:ILE:HD11	1.97	0.46
5:2F:127:GLU:HG2	5:2F:196:LEU:HD12	1.98	0.46
7:2H:118:PRO:HD2	7:2H:121:ILE:HB	1.98	0.46
17:2V:29:PRO:HA	17:2V:61:VAL:HG22	1.97	0.46
1:1A:362:U:H6	1:1A:362:U:H2'	1.57	0.46
1:1A:1058:G:H1	1:1A:1080:C:H42	1.63	0.46
1:1A:1587:A:H2'	1:1A:1588:C:C6	2.51	0.46
1:1A:2478:A:H5'	31:19:31:LYS:HE2	1.98	0.46
11:1P:135:LEU:HD23	11:1P:135:LEU:HA	1.77	0.46
13:1R:38:VAL:HG22	13:1R:112:ALA:HB2	1.97	0.46
19:1X:57:LEU:HD11	19:1X:78:LYS:HE2	1.96	0.46
32:1a:109:A:H2'	32:1a:326:G:N2	2.31	0.46
32:1a:1360:A:OP2	45:1n:35:ARG:NH2	2.49	0.46
33:1b:125:PRO:O	33:1b:127:ILE:N	2.49	0.46
37:1f:8:ILE:HD11	37:1f:79:LEU:HD13	1.98	0.46
38:1g:89:MET:SD	38:1g:155:ARG:HB2	2.56	0.46
1:2A:272:G:O2'	1:2A:421:U:OP2	2.22	0.46
1:2A:529:A:H2	64:2A:4517:HOH:O	1.99	0.46
1:2A:2134:A:H2'	1:2A:2134:A:N3	2.31	0.46
5:2F:64:ILE:HG21	5:2F:78:ILE:HG23	1.98	0.46
8:2I:133:HIS:ND1	8:2I:134:PRO:O	2.49	0.46
12:2Q:57:HIS:CD2	12:2Q:117:ALA:HB2	2.50	0.46
15:2T:64:ARG:HB2	15:2T:73:GLU:HG2	1.98	0.46
15:2T:94:ALA:HB1	15:2T:99:LEU:HD21	1.97	0.46
32:2a:486:U:H2'	32:2a:487:A:C8	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:520:A:N1	32:2a:536:C:H1'	2.31	0.46
32:2a:1095:U:H2'	32:2a:1096:C:C6	2.50	0.46
37:2f:24:GLU:O	37:2f:28:ARG:N	2.47	0.46
41:2j:44:VAL:HA	41:2j:66:ARG:HA	1.98	0.46
1:1A:526:A:OP1	64:1A:4241:HOH:O	2.21	0.46
1:1A:1176:G:H1'	1:1A:1177:A:C5'	2.46	0.46
1:1A:1359:A:C2	1:1A:1372:U:O4	2.68	0.46
7:1H:12:PRO:O	7:1H:15:VAL:HG22	2.16	0.46
10:1O:49:ARG:HH12	32:1a:1423:G:P	2.39	0.46
32:1a:79:G:O6	32:1a:90:U:C2	2.69	0.46
32:1a:1006:C:H2'	32:1a:1007:C:C6	2.50	0.46
33:1b:16:HIS:HB3	33:1b:210:SER:HB2	1.98	0.46
33:1b:158:LEU:HD22	33:1b:182:ILE:HD11	1.98	0.46
54:1w:18:G:H4'	54:1w:60:U:C5	2.50	0.46
1:2A:271(H):G:H2'	1:2A:271(I):G:C8	2.51	0.46
1:2A:656:G:H2'	1:2A:657:U:O4'	2.15	0.46
1:2A:1401:G:H2'	1:2A:1402:C:O4'	2.16	0.46
1:2A:2010:G:H5"	18:2W:42:ARG:HB2	1.97	0.46
4:2E:172:VAL:HG13	4:2E:182:LEU:HD11	1.98	0.46
21:2Z:151:HIS:HD2	21:2Z:168:GLU:C	2.23	0.46
32:2a:324:G:N1	32:2a:327:A:OP2	2.49	0.46
32:2a:560:U:H5'	32:2a:566:G:N2	2.30	0.46
32:2a:841:U:C5	32:2a:848:C:H1'	2.51	0.46
32:2a:1288:A:N1	32:2a:1371:G:H1'	2.31	0.46
32:2a:1427:U:H2'	32:2a:1428:A:H8	1.79	0.46
33:2b:45:GLN:HE21	33:2b:45:GLN:HB3	1.61	0.46
56:2y:42:C:H2'	56:2y:43:C:C6	2.51	0.46
56:2y:68:C:C4	56:2y:69:G:C8	3.04	0.46
1:1A:528:A:OP2	9:1N:114:ARG:NH1	2.49	0.46
1:1A:1076:C:H4'	1:1A:1077:A:OP1	2.15	0.46
1:1A:1113:U:H2'	1:1A:1114:G:H8	1.81	0.46
1:1A:1899:G:N3	1:1A:1899:G:H2'	2.31	0.46
5:1F:192:LEU:HD13	5:1F:194:MET:HE2	1.98	0.46
12:1Q:1:MET:HE2	12:1Q:1:MET:HB2	1.69	0.46
28:16:35:GLU:OE2	28:16:50:ARG:NH1	2.47	0.46
32:1a:576:G:O6	32:1a:880:C:O2'	2.30	0.46
32:1a:1004:A:H5"	32:1a:1025:U:C5	2.50	0.46
41:1j:81:THR:C	41:1j:83:GLU:N	2.74	0.46
44:1m:108:ARG:HD3	44:1m:108:ARG:HA	1.69	0.46
1:2A:811:U:H2'	11:2P:21:ARG:HA	1.98	0.46
1:2A:1028:A:N6	1:2A:1125:G:H2'	2.31	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1899:G:H2'	1:2A:1899:G:N3	2.31	0.46
5:2F:197:ASP:O	5:2F:200:GLU:HB3	2.15	0.46
10:2O:34:THR:OG1	10:2O:35:VAL:N	2.50	0.46
17:2V:58:VAL:HB	17:2V:98:GLU:HG3	1.98	0.46
32:2a:909:A:H2'	32:2a:910:C:O4'	2.16	0.46
32:2a:986:A:H2'	32:2a:987:G:O4'	2.16	0.46
32:2a:1376:U:H2'	32:2a:1377:A:H8	1.80	0.46
33:2b:18:GLY:HA2	33:2b:42:ILE:HG13	1.97	0.46
37:2f:100:ASN:HD21	49:2r:23:LYS:HE3	1.81	0.46
56:2y:52:G:H5'	56:2y:53:G:OP2	2.16	0.46
1:1A:634:C:H2'	1:1A:635:C:C6	2.51	0.45
1:1A:899:A:H2'	1:1A:899:A:N3	2.31	0.45
1:1A:1453:U:O2'	1:1A:1455:G:N7	2.45	0.45
3:1D:152:GLY:O	3:1D:154:LYS:HD3	2.15	0.45
4:1E:116:VAL:HG13	4:1E:122:PHE:HB2	1.98	0.45
5:1F:129:PHE:CD2	5:1F:163:VAL:HG21	2.51	0.45
7:1H:88:LEU:HD23	7:1H:130:ARG:HG3	1.98	0.45
11:1P:132:LYS:O	11:1P:136:GLU:HG3	2.16	0.45
32:1a:382:A:H2'	32:1a:383:A:C8	2.51	0.45
32:1a:523:A:H61	43:1l:92:0TD:CG	2.29	0.45
55:1x:9:G:O2'	55:1x:10:G:N7	2.47	0.45
56:1y:9:A:H4'	56:1y:46:G7M:OP2	2.15	0.45
1:2A:1532:C:H42	1:2A:1537:G:H1	1.65	0.45
1:2A:2572:A:C8	4:2E:144:ARG:HD3	2.51	0.45
1:2A:2811:G:N2	1:2A:2891:G:H1'	2.31	0.45
6:2G:43:LEU:HA	6:2G:43:LEU:HD13	1.72	0.45
11:2P:138:LEU:HG	11:2P:143:GLY:HA3	1.98	0.45
32:2a:397:A:H3'	32:2a:397:A:N3	2.31	0.45
32:2a:748:C:H4'	32:2a:749:C:O5'	2.16	0.45
32:2a:978:A:O2'	32:2a:1322:C:N3	2.46	0.45
32:2a:1318:A:H5"	50:2s:3:ARG:NH2	2.31	0.45
34:2c:179:ARG:NH1	34:2c:206:GLU:HB2	2.31	0.45
55:2x:61:C:H2'	55:2x:62:C:H6	1.80	0.45
1:1A:271(D):G:H1	1:1A:271(T):C:H42	1.65	0.45
1:1A:1843:C:H5'	3:1D:253:GLN:OE1	2.15	0.45
1:1A:2136:C:C2	1:1A:2155:G:N2	2.83	0.45
1:1A:2163:C:OP1	1:1A:2165:G:N2	2.49	0.45
5:1F:144:LYS:HB3	5:1F:144:LYS:HE3	1.75	0.45
32:1a:1037:C:H2'	32:1a:1038:C:H6	1.81	0.45
32:1a:1068:G:H8	32:1a:1068:G:OP2	1.99	0.45
34:1c:73:PRO:HB3	34:1c:103:VAL:HG11	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:1p:60:LEU:HD11	47:1p:66:PRO:HD3	1.97	0.45
1:2A:1274:A:N3	1:2A:1297:C:H1'	2.31	0.45
1:2A:1508:A:H4'	1:2A:1509(A):A:C5	2.51	0.45
4:2E:119:ARG:HG2	4:2E:120:TRP:NE1	2.31	0.45
21:2Z:77:ASP:CG	21:2Z:80:ARG:HH11	2.24	0.45
54:2w:19:G:H1	54:2w:56:C:H42	1.64	0.45
1:1A:1359:A:H2'	1:1A:1360:A:H5'	1.97	0.45
1:1A:2181:G:HO2'	1:1A:2182:G:P	2.39	0.45
23:11:23:LYS:HB3	23:11:29:GLY:HA3	1.99	0.45
32:1a:828:A:H2'	32:1a:829:G:O4'	2.16	0.45
32:1a:1002:G:H3'	32:1a:1003:G:C4'	2.44	0.45
38:1g:72:ARG:HD3	38:1g:142:GLU:OE2	2.16	0.45
44:1m:3:ARG:HG3	44:1m:4:ILE:H	1.80	0.45
54:1w:23:A:H3'	54:1w:24:G:H8	1.81	0.45
1:2A:184:C:H2'	1:2A:185:U:C6	2.52	0.45
9:2N:8:GLN:HE21	9:2N:8:GLN:HB2	1.62	0.45
28:26:32:ASN:OD1	28:26:32:ASN:N	2.48	0.45
29:27:24:THR:HG22	29:27:26:GLY:H	1.80	0.45
32:2a:405:U:O4	35:2d:2:GLY:N	2.50	0.45
32:2a:1006:C:H2'	32:2a:1007:C:C6	2.51	0.45
32:2a:1442:G:O2'	32:2a:1442(A):G:H5'	2.17	0.45
35:2d:60:GLU:HG3	35:2d:202:LEU:HD12	1.99	0.45
54:2w:27:G:H1	54:2w:43:C:N4	2.12	0.45
56:2y:15:G:H22	56:2y:48:C:N4	2.14	0.45
1:1A:222:A:H3'	1:1A:421:U:H5'	1.98	0.45
1:1A:2331:G:O2'	22:10:43:THR:HG22	2.16	0.45
21:1Z:7:ALA:O	21:1Z:62:PRO:HD3	2.15	0.45
21:1Z:52:SER:C	21:1Z:54:HIS:N	2.75	0.45
56:1y:71:G:H2'	56:1y:72:C:H6	1.81	0.45
1:2A:1015:G:H2'	1:2A:1016:G:C8	2.49	0.45
1:2A:1171:G:H8	1:2A:1171:G:O5'	2.00	0.45
1:2A:2242:G:OP1	64:2A:3944:HOH:O	2.21	0.45
1:2A:2577:A:H5"	1:2A:2578:G:H5'	1.98	0.45
2:2B:75:G:N2	21:2Z:87:ASP:OD1	2.50	0.45
12:2Q:12:GLN:NE2	12:2Q:72:LYS:HG3	2.31	0.45
32:2a:524:G:H2'	32:2a:525:C:C6	2.51	0.45
32:2a:1278:U:H5'	32:2a:1279:A:OP1	2.17	0.45
32:2a:1305:G:O2'	32:2a:1331:G:N2	2.48	0.45
41:2j:47:PHE:CZ	45:2n:37:PHE:HE2	2.34	0.45
44:2m:78:ILE:HA	44:2m:81:LEU:HD12	1.98	0.45
45:2n:21:TYR:HB3	64:2n:601:HOH:O	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1028:A:N6	1:1A:1125:G:H2'	2.31	0.45
1:1A:1066:U:H2'	1:1A:1068:G:OP2	2.17	0.45
1:1A:2051:A:H5'	1:1A:2578:G:O4'	2.16	0.45
12:1Q:78:PRO:HD3	55:1x:1:C:N3	2.32	0.45
15:1T:127:ALA:O	15:1T:129:ARG:N	2.48	0.45
31:19:2:LYS:HD3	31:19:4:ARG:NH2	2.31	0.45
32:1a:310:G:OP2	47:1p:27:LYS:HE2	2.17	0.45
32:1a:966:M2G:HM13	32:1a:967:5MC:H1'	1.99	0.45
32:1a:1458:G:OP1	51:1t:35:THR:OG1	2.33	0.45
44:1m:11:ARG:C	44:1m:13:LYS:H	2.23	0.45
54:1w:9:A:O2'	54:1w:10:G:N7	2.50	0.45
1:2A:2080:G:OP1	23:21:35:THR:HG21	2.16	0.45
1:2A:2273:A:H2'	1:2A:2274:A:C8	2.51	0.45
6:2G:50:ALA:O	6:2G:52:ILE:N	2.40	0.45
19:2X:1:MET:N	24:22:29:LYS:HE3	2.31	0.45
32:2a:1004:A:H5"	32:2a:1024:G:H22	1.82	0.45
32:2a:1005:A:H5"	32:2a:1006:C:C5	2.51	0.45
32:2a:1412:C:H2'	32:2a:1413:A:C8	2.51	0.45
35:2d:180:GLY:O	35:2d:182:LYS:HG3	2.16	0.45
1:1A:954:G:OP1	12:1Q:14:ARG:O	2.35	0.45
6:1G:41:GLN:HG2	6:1G:154:GLY:O	2.16	0.45
21:1Z:146:ILE:HA	21:1Z:147:GLY:HA2	1.70	0.45
32:1a:1035:A:C4	32:1a:1036:G:N2	2.84	0.45
36:1e:85:GLY:O	36:1e:87:SER:N	2.49	0.45
1:2A:38:A:H2'	1:2A:39:C:C6	2.52	0.45
1:2A:1385:G:O2'	1:2A:1396:U:O2	2.32	0.45
1:2A:2316:C:O2'	6:2G:128:ARG:NH2	2.49	0.45
1:2A:2431:U:OP2	64:2A:3942:HOH:O	2.20	0.45
4:2E:48:GLN:HE21	4:2E:78:LEU:HG	1.82	0.45
4:2E:48:GLN:HA	4:2E:80:GLU:HA	1.98	0.45
15:2T:118:ARG:HG2	32:2a:1442(A):G:C8	2.51	0.45
32:2a:23:C:H5	32:2a:561:U:O4	1.98	0.45
32:2a:316:G:H4'	64:2a:2028:HOH:O	2.16	0.45
32:2a:1049:U:C6	32:2a:1201:A:H5'	2.52	0.45
33:2b:71:VAL:HG12	33:2b:170:GLU:HG2	1.97	0.45
34:2c:152:ILE:HG13	34:2c:152:ILE:O	2.15	0.45
35:2d:162:LEU:HD23	35:2d:162:LEU:HA	1.74	0.45
37:2f:30:LEU:HD23	37:2f:75:LEU:HD11	1.98	0.45
47:2p:26:ARG:HG3	47:2p:27:LYS:O	2.17	0.45
1:1A:548:A:H1'	1:1A:549:G:OP1	2.16	0.45
1:1A:1001:A:H2'	1:1A:1002:G:O4'	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1815:A:P	3:1D:54:ARG:HH22	2.39	0.45
1:1A:2029:G:H2'	1:1A:2031:A:OP1	2.16	0.45
3:1D:273:ARG:HE	3:1D:273:ARG:HB3	1.58	0.45
32:1a:7:G:H5'	32:1a:298:A:O4'	2.17	0.45
33:1b:16:HIS:HB2	33:1b:204:ASN:CB	2.46	0.45
1:2A:1834:U:H4'	1:2A:1969:A:C6	2.52	0.45
1:2A:1837:C:OP1	32:2a:784:C:H4'	2.17	0.45
1:2A:2516:G:C6	1:2A:2517:C:C4	3.04	0.45
1:2A:2557:G:H2'	1:2A:2558:C:C6	2.52	0.45
4:2E:77:ILE:HG21	4:2E:195:LEU:HD22	1.98	0.45
13:2R:2:ARG:HG2	13:2R:5:LYS:HB2	1.98	0.45
25:23:12:PRO:HB2	25:23:20:LYS:HG2	1.98	0.45
26:24:26:SER:OG	26:24:28:LYS:O	2.35	0.45
32:2a:841:U:H6	32:2a:841:U:P	2.40	0.45
33:2b:33:TYR:HB2	33:2b:43:ASP:HA	1.98	0.45
33:2b:92:TYR:CE2	33:2b:151:GLY:HA3	2.51	0.45
37:2f:50:TYR:CE2	49:2r:77:GLY:HA2	2.51	0.45
1:1A:226:G:N2	1:1A:228:A:H62	2.15	0.45
21:1Z:72:ARG:HD3	21:1Z:72:ARG:HA	1.63	0.45
32:1a:189(K):U:H2'	32:1a:189(L):G:C8	2.52	0.45
32:1a:404:U:H2'	32:1a:405:U:C6	2.51	0.45
32:1a:1227:A:OP1	50:1s:80:TYR:OH	2.24	0.45
32:1a:1345:U:H2'	64:1a:4997:HOH:O	2.17	0.45
33:1b:139:LYS:O	33:1b:143:GLU:HG3	2.17	0.45
35:1d:194:LEU:HA	35:1d:194:LEU:HD13	1.69	0.45
37:1f:68:PRO:HG2	37:1f:71:ARG:HD2	1.98	0.45
38:1g:37:ASN:O	38:1g:41:ARG:HD3	2.16	0.45
41:1j:11:PHE:HE1	41:1j:67:THR:HG22	1.82	0.45
1:2A:93:G:H2'	1:2A:94:C:C6	2.52	0.45
1:2A:856:C:H2'	1:2A:857:C:C6	2.52	0.45
1:2A:1523:U:H2'	1:2A:1524:G:C8	2.52	0.45
1:2A:1740:G:H2'	1:2A:1740:G:N3	2.32	0.45
1:2A:2139:C:H2'	1:2A:2140:C:C6	2.52	0.45
6:2G:11:TYR:CZ	6:2G:16:ARG:HD3	2.51	0.45
7:2H:26:VAL:HG12	7:2H:79:VAL:HG21	1.99	0.45
23:21:7:ILE:HG23	23:21:98:LEU:HD11	1.98	0.45
32:2a:8:A:N6	35:2d:209:ARG:HB2	2.32	0.45
32:2a:565:U:OP2	32:2a:566:G:O2'	2.31	0.45
32:2a:1280:A:O2'	32:2a:1281:U:H5'	2.16	0.45
34:2c:119:ARG:HE	34:2c:140:ARG:NH2	2.13	0.45
36:2e:75:THR:OG1	36:2e:76:ILE:N	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:2g:68:ASN:ND2	38:2g:128:ALA:HA	2.28	0.45
47:2p:17:TYR:HE2	47:2p:41:PRO:HG3	1.82	0.45
48:2q:81:ARG:NH2	48:2q:84:LEU:HD21	2.32	0.45
1:1A:249:C:O2	30:18:12:LYS:NZ	2.43	0.45
1:1A:2143:C:H2'	1:1A:2144:U:O4'	2.17	0.45
1:1A:2646:C:H2'	1:1A:2647:U:O4'	2.17	0.45
4:1E:29:GLY:HA3	64:1E:405:HOH:O	2.16	0.45
5:1F:39:TRP:CZ2	5:1F:43:LYS:HE2	2.52	0.45
5:1F:184:TYR:O	5:1F:188:ARG:HG3	2.17	0.45
32:1a:690:G:C6	32:1a:691:G:C6	3.05	0.45
64:1a:4979:HOH:O	45:1n:3:ARG:HG2	2.16	0.45
38:1g:90:GLU:CD	38:1g:90:GLU:H	2.25	0.45
1:2A:330:A:H2	1:2A:1210:A:O2'	2.00	0.45
1:2A:748:G:C8	18:2W:89:ALA:HB1	2.52	0.45
1:2A:1759:A:H1'	1:2A:2711:A:C2	2.51	0.45
1:2A:1769:G:O2'	1:2A:1958:C:OP1	2.32	0.45
1:2A:1778:U:H2'	1:2A:1784:A:N6	2.31	0.45
1:2A:2131:G:N2	1:2A:2158:A:H62	2.05	0.45
7:2H:154:PRO:HB3	7:2H:163:TYR:CE1	2.52	0.45
25:23:23:LEU:HG	25:23:50:VAL:HG11	1.99	0.45
26:24:60:GLN:O	26:24:62:ARG:NH1	2.49	0.45
30:28:55:ALA:O	30:28:59:LYS:HG3	2.17	0.45
32:2a:1119:C:OP2	40:2i:9:ARG:NH2	2.50	0.45
32:2a:1149:C:O2'	32:2a:1280:A:N1	2.49	0.45
32:2a:1320:C:N3	50:2s:36:ARG:NH2	2.65	0.45
33:2b:219:VAL:HA	33:2b:222:ILE:HG12	1.99	0.45
1:1A:614(C):A:C4	5:1F:180:GLY:HA2	2.52	0.45
1:1A:1406:U:H2'	1:1A:1407:C:C6	2.52	0.45
5:1F:170:LEU:HD13	5:1F:172:TRP:CZ2	2.51	0.45
32:1a:262:A:H2'	32:1a:263:A:C8	2.53	0.45
32:1a:1031:G:H2'	32:1a:1032:G:C8	2.52	0.45
54:1w:26:A:H61	54:1w:44:G:H1	1.65	0.45
56:1y:28:G:H2'	56:1y:29:G:C8	2.51	0.45
1:2A:271(O):C:H2'	1:2A:271(P):C:C6	2.52	0.45
1:2A:646:A:H2'	1:2A:647:G:O4'	2.17	0.45
1:2A:1399:C:OP1	19:2X:25:LYS:NZ	2.49	0.45
1:2A:1418:G:H2'	1:2A:1579:A:H62	1.82	0.45
6:2G:111:LEU:HD21	6:2G:120:LEU:HD21	1.98	0.45
18:2W:64:MET:HE2	18:2W:109:GLU:HG3	1.99	0.45
33:2b:16:HIS:C	33:2b:18:GLY:H	2.25	0.45
56:2y:5:G:H1	56:2y:68:C:H42	1.63	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1B:78:A:C2	2:1B:100:A:C4	3.05	0.44
32:1a:250:A:H4'	32:1a:251:G:O5'	2.15	0.44
33:1b:45:GLN:O	33:1b:49:GLU:HG3	2.16	0.44
34:1c:56:ASP:HB2	34:1c:67:THR:HB	1.98	0.44
35:1d:85:LYS:HG3	35:1d:86:LYS:H	1.83	0.44
40:1i:11:LYS:C	40:1i:13:ALA:H	2.25	0.44
44:1m:40:ASN:HB3	44:1m:43:THR:HG23	1.97	0.44
44:1m:70:LEU:HD23	44:1m:70:LEU:HA	1.83	0.44
1:2A:35:G:H1'	1:2A:454:A:C4	2.52	0.44
1:2A:801:G:O6	5:2F:53:THR:OG1	2.35	0.44
1:2A:894:C:O2'	1:2A:895:U:H5"	2.16	0.44
1:2A:1434:A:H61	1:2A:1558:A:H62	1.65	0.44
1:2A:2507:C:H5"	1:2A:2573:C:C4	2.52	0.44
2:2B:39:A:O2'	2:2B:46:A:N1	2.48	0.44
11:2P:89:ALA:HA	11:2P:121:LYS:HD3	1.99	0.44
16:2U:5:LYS:HG3	16:2U:7:GLY:N	2.33	0.44
21:2Z:138:GLU:N	21:2Z:156:LYS:HE2	2.31	0.44
33:2b:16:HIS:CG	33:2b:17:PHE:N	2.86	0.44
38:2g:78:ARG:HG3	38:2g:156:TRP:CZ3	2.52	0.44
48:2q:45:HIS:HB2	48:2q:65:ILE:HD13	1.98	0.44
53:2v:12:A:N3	53:2v:12:A:H2'	2.32	0.44
55:2x:15:G:H2'	55:2x:59:A:N1	2.32	0.44
56:2y:68:C:H3'	56:2y:69:G:H5"	1.99	0.44
1:1A:1062:G:C8	1:1A:1088:A:H2'	2.53	0.44
1:1A:2181:G:O2'	1:1A:2182:G:OP1	2.30	0.44
1:1A:2649:U:H2'	1:1A:2650:U:C6	2.52	0.44
32:1a:976:G:OP1	45:1n:32:SER:N	2.49	0.44
32:1a:1062:U:H2'	32:1a:1063:C:C6	2.52	0.44
33:1b:16:HIS:CG	33:1b:17:PHE:H	2.34	0.44
38:1g:78:ARG:HG2	38:1g:156:TRP:CZ3	2.52	0.44
1:2A:322:A:OP2	5:2F:169:ASN:HB2	2.17	0.44
1:2A:764:A:H5"	3:2D:210:GLY:HA3	1.98	0.44
1:2A:1379:A:H4'	1:2A:1380:G:OP2	2.16	0.44
1:2A:1915:5MU:H2'	1:2A:1916:A:O4'	2.17	0.44
1:2A:2166:G:H3'	1:2A:2167:U:H5"	1.99	0.44
1:2A:2278:A:OP2	22:20:12:ASN:ND2	2.50	0.44
5:2F:40:GLN:NE2	5:2F:182:ASN:HB2	2.32	0.44
5:2F:150:GLY:HA2	5:2F:172:TRP:CD2	2.52	0.44
32:2a:1391:U:H2'	32:2a:1392:G:C8	2.52	0.44
1:1A:73:A:OP1	64:1A:4243:HOH:O	2.21	0.44
1:1A:185:U:H4'	1:1A:218:A:H4'	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1865:G:N2	1:1A:1877:A:OP2	2.49	0.44
5:1F:184:TYR:CE2	5:1F:188:ARG:HD2	2.53	0.44
6:1G:18:GLU:HG3	6:1G:22:ARG:HD2	1.98	0.44
6:1G:115:ARG:HG2	6:1G:136:ARG:HH22	1.82	0.44
32:1a:1095:U:H2'	32:1a:1096:C:C6	2.52	0.44
32:1a:1412:C:H2'	32:1a:1413:A:C8	2.53	0.44
35:1d:13:ARG:HB3	35:1d:38:TYR:O	2.17	0.44
35:1d:173:TRP:CE3	35:1d:174:LEU:HG	2.52	0.44
1:2A:579:G:H2'	1:2A:580:C:C6	2.52	0.44
1:2A:1477:A:H2'	1:2A:1478:G:O4'	2.17	0.44
1:2A:2105:C:H2'	1:2A:2106:G:C8	2.52	0.44
1:2A:2156:G:H4'	1:2A:2157:G:OP1	2.17	0.44
1:2A:2271:G:OP1	22:20:18:ALA:HB1	2.17	0.44
10:2O:26:LYS:O	10:2O:30:ALA:HB2	2.17	0.44
32:2a:546:G:OP1	35:2d:73:ARG:HG2	2.17	0.44
33:2b:131:PRO:O	33:2b:135:GLN:HG3	2.17	0.44
34:2c:40:ARG:O	34:2c:44:GLU:HB2	2.17	0.44
48:2q:3:LYS:HD2	48:2q:60:ILE:HD11	1.99	0.44
50:2s:66:MET:HB2	50:2s:74:PHE:CZ	2.52	0.44
56:2y:67:C:H2'	56:2y:68:C:C6	2.52	0.44
1:1A:184:C:H2'	1:1A:185:U:C6	2.52	0.44
1:1A:363(C):G:H2'	1:1A:363(D):G:C8	2.52	0.44
1:1A:493:G:H2'	1:1A:494:G:O4'	2.17	0.44
1:1A:2430:A:N3	1:1A:2430:A:H2'	2.32	0.44
1:1A:2492:U:H2'	1:1A:2493:U:C6	2.53	0.44
26:14:62:ARG:C	26:14:63:TYR:CG	2.95	0.44
32:1a:1003:G:C4	32:1a:1004:A:H2	2.35	0.44
33:1b:52:GLU:OE2	33:1b:56:ARG:NH2	2.51	0.44
35:1d:76:ARG:NE	35:1d:80:GLU:OE2	2.39	0.44
1:2A:234:C:H2'	1:2A:235:U:H6	1.82	0.44
1:2A:1032:A:H2	1:2A:1122:G:H22	1.65	0.44
1:2A:2161:C:H2'	1:2A:2162:G:O4'	2.17	0.44
1:2A:2872:G:O2'	1:2A:2873:A:H5'	2.18	0.44
2:2B:11:C:OP2	22:20:72:ARG:NH2	2.44	0.44
9:2N:62:VAL:HG13	9:2N:66:LYS:HB2	1.99	0.44
21:2Z:72:ARG:NH2	21:2Z:97:GLU:O	2.50	0.44
21:2Z:138:GLU:HB2	21:2Z:156:LYS:HD3	1.98	0.44
26:24:46:GLN:O	26:24:48:ARG:N	2.37	0.44
54:2w:33:U:N3	54:2w:36:A:OP2	2.41	0.44
1:1A:1012:U:C5	9:1N:28:THR:HG21	2.52	0.44
1:1A:1364:G:P	23:11:3:LYS:HG3	2.57	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2176:A:H2'	1:1A:2177:C:C6	2.53	0.44
1:1A:2506:U:C2	1:1A:2585:U:O4	2.71	0.44
15:1T:127:ALA:C	15:1T:129:ARG:N	2.73	0.44
30:18:42:ARG:HD2	64:18:203:HOH:O	2.16	0.44
32:1a:396:G:O2'	32:1a:398:C:OP1	2.18	0.44
32:1a:922:G:C6	32:1a:923:A:C6	3.06	0.44
33:1b:124:SER:HA	33:1b:125:PRO:HA	1.71	0.44
36:1e:90:VAL:O	36:1e:120:THR:HA	2.18	0.44
36:1e:122:GLU:O	36:1e:126:ARG:NH1	2.50	0.44
42:1k:48:ILE:HD12	42:1k:63:LEU:HB2	2.00	0.44
1:2A:557:U:H2'	1:2A:558:G:C8	2.53	0.44
1:2A:1591:G:H2'	1:2A:1592:C:C6	2.53	0.44
1:2A:2206:G:H5"	1:2A:2207:G:C5	2.52	0.44
1:2A:2386:C:H2'	1:2A:2387:U:C6	2.52	0.44
2:2B:72:G:O2'	2:2B:105:A:N6	2.50	0.44
5:2F:29:ASN:O	5:2F:33:LEU:HD23	2.17	0.44
7:2H:41:MET:HE3	7:2H:64:LEU:HB2	1.98	0.44
14:2S:87:PHE:CE1	14:2S:102:ALA:HB2	2.52	0.44
32:2a:406:G:H5'	35:2d:5:ILE:HG12	1.98	0.44
32:2a:473:G:H2'	32:2a:474:G:H8	1.83	0.44
32:2a:1004:A:H61	32:2a:1037:C:H1'	1.80	0.44
32:2a:1118:C:H1'	32:2a:1179:A:C5	2.52	0.44
32:2a:1343:G:H2'	32:2a:1344:C:C6	2.53	0.44
41:2j:8:LEU:HG	41:2j:70:ARG:HB2	2.00	0.44
46:2o:39:LEU:HD13	46:2o:56:LEU:HB2	1.98	0.44
56:2y:8:4SU:H2'	56:2y:46:G7M:N2	2.33	0.44
1:1A:613:G:N2	1:1A:614(C):A:O2'	2.51	0.44
1:1A:652(T):C:H2'	1:1A:652(U):G:C8	2.53	0.44
1:1A:1075:C:O2	1:1A:1076:C:H2'	2.18	0.44
1:1A:1094:U:H2'	1:1A:1095:A:C8	2.53	0.44
1:1A:2074:U:H2'	1:1A:2075:U:C6	2.52	0.44
1:1A:2155:G:H5'	1:1A:2156:G:OP2	2.17	0.44
11:1P:101:VAL:HA	11:1P:106:LEU:O	2.18	0.44
32:1a:523:A:N1	43:1l:92:0TD:H6	2.33	0.44
32:1a:1033:G:H3'	32:1a:1034:G:C8	2.46	0.44
35:1d:94:LEU:O	35:1d:98:GLU:HG2	2.17	0.44
38:1g:111:ARG:NE	38:1g:113:GLU:OE2	2.43	0.44
1:2A:856:C:O4'	22:20:27:GLU:HB3	2.18	0.44
1:2A:902:C:H2'	1:2A:903:C:C6	2.53	0.44
1:2A:1011:G:OP2	16:2U:66:ASN:ND2	2.50	0.44
1:2A:1406:U:H2'	1:2A:1407:C:C6	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2133:G:HO2'	1:2A:2157:G:N2	2.15	0.44
14:2S:36:TYR:CD1	14:2S:52:SER:HB3	2.53	0.44
25:23:4:LEU:O	25:23:36:VAL:HA	2.18	0.44
26:24:33:VAL:HG13	26:24:35:VAL:H	1.82	0.44
32:2a:1002:G:C2	32:2a:1003:G:H1'	2.52	0.44
34:2c:152:ILE:HG22	34:2c:167:TRP:HB2	1.99	0.44
35:2d:201:GLN:NE2	36:2e:99:GLY:HA2	2.33	0.44
37:2f:99:ALA:HB1	49:2r:23:LYS:NZ	2.32	0.44
42:2k:18:ARG:NH2	42:2k:35:PRO:O	2.51	0.44
44:2m:15:VAL:O	44:2m:19:LEU:HG	2.18	0.44
1:1A:234:C:H2'	1:1A:235:U:H6	1.83	0.44
1:1A:568:U:H5'	1:1A:945:A:N6	2.33	0.44
1:1A:1815:A:OP2	3:1D:54:ARG:NH2	2.49	0.44
1:1A:1837:C:OP1	32:1a:784:C:H4'	2.18	0.44
1:1A:2086:U:H2'	1:1A:2087:G:C8	2.53	0.44
1:1A:2319:G:H22	14:1S:3:ARG:NE	2.13	0.44
1:1A:2687:U:H2'	1:1A:2688:U:O4'	2.17	0.44
1:1A:2820:A:O2'	1:1A:2821:A:OP1	2.29	0.44
6:1G:16:ARG:O	6:1G:20:ILE:HG13	2.17	0.44
26:14:63:TYR:HA	26:14:64:GLY:HA2	1.79	0.44
32:1a:161:A:H2'	32:1a:162:A:C8	2.53	0.44
32:1a:453:A:C5	32:1a:454:C:C4	3.05	0.44
33:1b:17:PHE:HB3	33:1b:44:LEU:HD21	2.00	0.44
1:2A:1001:A:H2'	1:2A:1002:G:O4'	2.18	0.44
1:2A:1153:C:OP1	16:2U:92:ARG:NH2	2.46	0.44
4:2E:48:GLN:NE2	4:2E:78:LEU:HG	2.32	0.44
6:2G:37:VAL:O	6:2G:94:LEU:N	2.48	0.44
8:2I:48:GLU:HG3	8:2I:52:ARG:NH1	2.33	0.44
18:2W:4:LYS:HD3	18:2W:6:ILE:HD11	2.00	0.44
22:20:37:LEU:HG	22:20:60:PHE:HA	1.99	0.44
32:2a:826:C:O2	39:2h:15:ASN:ND2	2.51	0.44
33:2b:15:VAL:O	33:2b:17:PHE:N	2.48	0.44
33:2b:111:ARG:HA	33:2b:111:ARG:HD3	1.81	0.44
40:2i:70:LYS:O	40:2i:74:ILE:HG13	2.17	0.44
40:2i:99:LEU:HB3	40:2i:101:PHE:CE2	2.53	0.44
1:1A:234:C:H2'	1:1A:235:U:C6	2.53	0.44
1:1A:512:G:OP2	64:1A:4245:HOH:O	2.21	0.44
1:1A:884:C:C4	1:1A:885:C:H1'	2.53	0.44
4:1E:12:THR:OG1	4:1E:13:ARG:N	2.51	0.44
6:1G:179:PRO:HG3	26:14:43:TYR:OH	2.18	0.44
15:1T:60:THR:HG22	15:1T:77:PRO:HA	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:755:G:OP2	46:1o:65:ARG:HD2	2.17	0.44
40:1i:28:VAL:HG22	40:1i:63:ILE:HB	1.99	0.44
47:1p:53:VAL:HG13	47:1p:79:VAL:HG22	2.00	0.44
1:2A:1270:C:H5"	1:2A:1271:G:O5'	2.18	0.44
1:2A:2086:U:H2'	1:2A:2087:G:C8	2.53	0.44
1:2A:2390:U:P	30:28:35:GLN:HE22	2.41	0.44
1:2A:2650:U:H2'	1:2A:2651:C:C6	2.53	0.44
2:2B:78:A:C2	2:2B:100:A:C4	3.06	0.44
2:2B:103:G:H21	21:2Z:73:GLN:NE2	2.16	0.44
10:2O:71:ARG:NE	10:2O:105:GLU:OE2	2.50	0.44
21:2Z:171:ILE:H	21:2Z:171:ILE:HG13	1.54	0.44
25:23:22:ALA:HB2	25:23:49:LYS:HD3	2.00	0.44
32:2a:1016:A:H2'	32:2a:1017:G:O4'	2.17	0.44
33:2b:185:ILE:O	33:2b:185:ILE:HG12	2.17	0.44
36:2e:105:VAL:HB	36:2e:106:PRO:HD3	2.00	0.44
46:2o:4:THR:N	46:2o:7:GLU:OE2	2.39	0.44
1:1A:182:A:H2	1:1A:433:C:O2	2.01	0.44
1:1A:264:C:O2'	1:1A:265:A:H2'	2.18	0.44
1:1A:819:A:C4	1:1A:1189:A:C2	3.06	0.44
1:1A:1593:G:H2'	1:1A:1594:G:C8	2.53	0.44
3:1D:71:ASP:CB	3:1D:103:ARG:HH12	2.31	0.44
6:1G:43:LEU:HD23	6:1G:53:LEU:HD23	2.00	0.44
6:1G:126:ASP:HB2	6:1G:130:ASN:O	2.18	0.44
9:1N:15:LEU:HB2	9:1N:135:PRO:HB2	1.99	0.44
32:1a:1054:C:C5	54:1w:34:G:H1'	2.53	0.44
32:1a:1333:A:H2'	32:1a:1334:G:O4'	2.18	0.44
33:1b:55:PHE:O	33:1b:221:LEU:HD21	2.18	0.44
48:1q:14:LYS:N	48:1q:14:LYS:HD2	2.32	0.44
1:2A:84:A:H5"	20:2Y:8:LYS:HE3	2.00	0.44
1:2A:571:A:O2'	17:2V:78:LYS:HE2	2.18	0.44
1:2A:1263:U:C4	1:2A:1264:G:C6	3.06	0.44
1:2A:2408:U:H2'	1:2A:2409:G:C8	2.53	0.44
2:2B:3:C:H2'	2:2B:4:C:C6	2.53	0.44
6:2G:131:TYR:HB3	6:2G:159:VAL:HG13	1.99	0.44
8:2I:31:LEU:HD21	8:2I:38:LEU:HG	1.98	0.44
25:23:44:ARG:O	25:23:48:GLU:HG3	2.17	0.44
26:24:16:CYS:SG	26:24:17:GLY:N	2.91	0.44
32:2a:1431:C:H2'	32:2a:1432:G:O4'	2.17	0.44
32:2a:1504:G:OP1	32:2a:1507:A:H4'	2.17	0.44
46:2o:55:GLY:HA2	46:2o:58:MET:HE3	2.00	0.44
50:2s:49:ILE:H	50:2s:62:ILE:HD11	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:2w:10:G:H8	54:2w:10:G:OP1	2.01	0.44
1:1A:196:A:H2'	1:1A:196:A:N3	2.33	0.43
1:1A:1568:G:H5"	3:1D:61:LEU:HG	2.00	0.43
1:1A:1623:G:N7	64:1A:4314:HOH:O	2.36	0.43
6:1G:179:PRO:HG3	26:14:43:TYR:CZ	2.53	0.43
16:1U:76:TYR:CE2	16:1U:80:ILE:HG13	2.53	0.43
32:1a:21:G:H2'	32:1a:22:G:C8	2.53	0.43
32:1a:1142:G:H2'	32:1a:1143:G:O4'	2.18	0.43
38:1g:26:PHE:CE2	38:1g:30:ILE:HD11	2.53	0.43
42:1k:38:ASN:HA	42:1k:39:PRO:HD3	1.91	0.43
1:2A:1116:C:H2'	1:2A:1117:G:H8	1.81	0.43
10:2O:115:VAL:HG13	10:2O:121:VAL:HG21	2.00	0.43
16:2U:27:LEU:HB3	16:2U:31:SER:HB3	2.00	0.43
32:2a:444:C:H2'	32:2a:445:G:H8	1.83	0.43
32:2a:540:G:H2'	32:2a:541:G:O4'	2.18	0.43
32:2a:714:G:H2'	32:2a:715:A:C8	2.52	0.43
32:2a:1132:C:H3'	32:2a:1133:G:H8	1.83	0.43
33:2b:157:ARG:HE	33:2b:157:ARG:HB3	1.68	0.43
33:2b:219:VAL:O	33:2b:223:ILE:HG13	2.18	0.43
41:2j:32:ALA:HA	41:2j:33:GLN:HA	1.77	0.43
52:2u:9:ARG:O	52:2u:13:ILE:HG13	2.17	0.43
56:2y:15:G:H22	56:2y:48:C:H42	1.66	0.43
56:2y:36:A:H2'	56:2y:37:MIA:O4'	2.18	0.43
1:1A:534:U:H2'	1:1A:535:C:C6	2.53	0.43
1:1A:1087:G:H2'	1:1A:1089:G:C8	2.53	0.43
8:1I:109:ILE:HD13	8:1I:109:ILE:HA	1.83	0.43
16:1U:97:ASP:OD1	16:1U:101:ARG:HD2	2.18	0.43
32:1a:562:C:H1'	43:1l:15:ARG:HB3	1.99	0.43
33:1b:97:TRP:CZ2	33:1b:102:LEU:HD13	2.51	0.43
48:1q:66:SER:O	48:1q:70:ARG:NH1	2.51	0.43
1:2A:11:G:C2'	1:2A:12:U:H5'	2.48	0.43
1:2A:652(A):A:H3'	1:2A:652(B):A:H5"	2.00	0.43
1:2A:985:C:H2'	1:2A:986:C:H6	1.84	0.43
1:2A:1885:A:H2'	1:2A:1886:C:O4'	2.17	0.43
1:2A:2135:A:C8	1:2A:2136:C:H5	2.36	0.43
4:2E:178:GLU:H	4:2E:178:GLU:CD	2.22	0.43
5:2F:108:LYS:HB2	5:2F:108:LYS:HE2	1.84	0.43
32:2a:767:A:H2'	32:2a:768:A:O4'	2.18	0.43
32:2a:1138:G:O2'	32:2a:1140:C:H5'	2.18	0.43
34:2c:63:ASN:HB3	34:2c:98:ASN:HD22	1.83	0.43
35:2d:156:GLU:CD	35:2d:159:ARG:HH21	2.26	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:2h:81:HIS:ND1	39:2h:138:TRP:OXT	2.41	0.43
40:2i:9:ARG:O	40:2i:104:ARG:HG3	2.18	0.43
42:2k:34:ASP:HB3	42:2k:40:ILE:HD11	2.00	0.43
1:1A:385:C:O2	11:1P:71:VAL:HG21	2.19	0.43
1:1A:548:A:N6	17:1V:19:LYS:H	2.16	0.43
1:1A:1364:G:OP2	23:11:3:LYS:HG3	2.17	0.43
1:1A:1427:A:H4'	1:1A:1428:C:O4'	2.18	0.43
1:1A:1924:C:H4'	55:1x:13:C:O2'	2.18	0.43
1:1A:2701:C:H2'	1:1A:2702:U:H2'	2.00	0.43
5:1F:33:LEU:HB3	11:1P:6:LEU:HD21	1.99	0.43
14:1S:83:LYS:HB3	14:1S:111:GLU:HG3	2.00	0.43
22:10:3:HIS:HB3	64:10:210:HOH:O	2.18	0.43
26:14:13:ARG:HB3	26:14:30:GLU:HG2	1.99	0.43
32:1a:510:A:P	64:1a:4814:HOH:O	2.76	0.43
32:1a:714:G:H2'	32:1a:715:A:C8	2.53	0.43
32:1a:1315:U:H2'	32:1a:1316:G:O4'	2.17	0.43
34:1c:22:TRP:CZ2	45:1n:54:PRO:HG2	2.53	0.43
51:1t:39:LYS:HG2	51:1t:55:ILE:HG21	2.00	0.43
1:2A:171:G:P	1:2A:171:G:H8	2.42	0.43
1:2A:890:A:H2'	1:2A:892:G:C8	2.54	0.43
1:2A:1790:C:H5"	1:2A:1791:A:OP1	2.18	0.43
1:2A:2626:C:H2'	1:2A:2627:G:O4'	2.19	0.43
6:2G:15:VAL:HG13	6:2G:175:LEU:HB2	2.00	0.43
6:2G:179:PRO:HG3	26:24:43:TYR:OH	2.18	0.43
32:2a:232:G:H1'	32:2a:262:A:N1	2.33	0.43
1:1A:566:U:H5"	11:1P:29:LYS:HE3	2.00	0.43
1:1A:1227:G:OP2	16:1U:16:LYS:NZ	2.43	0.43
1:1A:1372:U:H2'	1:1A:1373:A:O4'	2.19	0.43
1:1A:1518:U:H2'	1:1A:1519:G:O4'	2.18	0.43
1:1A:1526:G:C6	1:1A:1527:G:C2	3.05	0.43
1:1A:1582:C:O2'	1:1A:1586:A:N3	2.49	0.43
1:1A:1812:A:O2'	3:1D:45:ASN:N	2.46	0.43
6:1G:34:LEU:HD23	6:1G:161:THR:HG22	2.01	0.43
8:1I:2:LYS:HA	8:1I:19:VAL:O	2.17	0.43
16:1U:104:GLN:NE2	16:1U:105:VAL:HG23	2.34	0.43
32:1a:115:G:H4'	32:1a:116:A:O5'	2.17	0.43
32:1a:542:G:OP1	35:1d:10:ARG:NH2	2.43	0.43
32:1a:1027:C:N1	32:1a:1034:G:N2	2.64	0.43
32:1a:1191:A:H5"	34:1c:4:LYS:HE3	2.00	0.43
32:1a:1402:4OC:O5'	32:1a:1402:4OC:H6	2.19	0.43
33:1b:151:GLY:HA2	33:1b:154:LEU:HD13	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:1j:30:SER:OG	41:1j:81:THR:OG1	2.22	0.43
41:1j:40:LEU:HB2	41:1j:69:ASN:HB2	2.00	0.43
1:2A:631:A:H2'	1:2A:632:A:O4'	2.17	0.43
1:2A:2306:C:N4	6:2G:42:GLY:O	2.46	0.43
2:2B:48:A:OP1	14:2S:30:ARG:NH2	2.52	0.43
16:2U:79:PHE:CZ	16:2U:83:LEU:HD11	2.53	0.43
33:2b:115:LEU:HG	33:2b:145:LEU:HB3	2.00	0.43
35:2d:19:LEU:O	35:2d:21:LEU:N	2.50	0.43
38:2g:132:GLY:O	38:2g:136:LYS:HG2	2.18	0.43
44:2m:28:ALA:C	44:2m:30:ALA:H	2.25	0.43
44:2m:89:GLY:O	44:2m:93:ARG:HG2	2.18	0.43
48:2q:53:LEU:HD23	48:2q:82:MET:HE1	2.00	0.43
55:2x:61:C:H2'	55:2x:62:C:C6	2.54	0.43
1:1A:910:A:N1	1:1A:2277:G:H1'	2.33	0.43
5:1F:136:THR:HA	5:1F:166:ALA:O	2.18	0.43
10:1O:48:PRO:CB	32:1a:1422:G:H5"	2.48	0.43
25:13:55:ARG:NH2	25:13:57:GLU:HB2	2.29	0.43
32:1a:26:A:O2'	35:1d:209:ARG:NH2	2.48	0.43
32:1a:243:A:C2	32:1a:246:A:C8	3.07	0.43
32:1a:1149:C:H2'	32:1a:1150:U:C6	2.53	0.43
36:1e:10:MET:H	36:1e:10:MET:HG2	1.58	0.43
37:1f:82:ARG:HB2	37:1f:85:VAL:HG23	2.01	0.43
50:1s:3:ARG:NE	50:1s:8:GLY:O	2.44	0.43
9:2N:38:HIS:NE2	9:2N:50:ASP:OD2	2.48	0.43
11:2P:94:GLU:OE2	11:2P:124:LYS:NZ	2.44	0.43
23:21:89:GLU:O	23:21:93:GLU:HG2	2.18	0.43
25:23:6:VAL:HG12	25:23:28:LEU:HD11	1.99	0.43
32:2a:266:G:N3	32:2a:266:G:H2'	2.32	0.43
32:2a:382:A:H2'	32:2a:383:A:C8	2.54	0.43
32:2a:838:G:H1	32:2a:848:C:N4	2.15	0.43
32:2a:947:G:O3'	44:2m:109:THR:OG1	2.34	0.43
32:2a:1394:A:N1	32:2a:1500:A:O2'	2.50	0.43
32:2a:1512:U:H2'	32:2a:1513:A:C8	2.53	0.43
32:2a:1524:C:OP1	42:2k:120:ARG:NH1	2.45	0.43
35:2d:61:LYS:HD2	35:2d:207:TYR:OH	2.18	0.43
1:1A:1056:G:H5"	1:1A:1057:A:C4'	2.48	0.43
2:1B:92:C:H5"	21:1Z:79:ARG:NH1	2.33	0.43
4:1E:174:ASP:OD1	4:1E:175:VAL:N	2.51	0.43
6:1G:106:LEU:HA	6:1G:110:ALA:HB3	2.01	0.43
11:1P:82:GLY:HA2	11:1P:113:LYS:O	2.18	0.43
26:14:49:PHE:HD1	26:14:49:PHE:HA	1.74	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:18:26:LYS:HG2	30:18:46:ARG:O	2.18	0.43
32:1a:256:U:H2'	32:1a:257:G:O4'	2.18	0.43
32:1a:405:U:O4	35:1d:2:GLY:N	2.51	0.43
32:1a:973:G:H3'	32:1a:974:A:H5"	2.01	0.43
34:1c:177:THR:HG22	34:1c:180:ALA:H	1.84	0.43
35:1d:158:ILE:H	35:1d:158:ILE:HG13	1.48	0.43
36:1e:18:ARG:HH11	36:1e:27:ARG:HH12	1.66	0.43
39:1h:83:ILE:HG13	39:1h:137:VAL:HG22	2.00	0.43
44:1m:4:ILE:HD12	44:1m:57:ARG:HA	1.99	0.43
52:1u:14:TRP:HE3	52:1u:15:ARG:HG2	1.82	0.43
54:1w:66:U:C4	54:1w:67:C:N4	2.87	0.43
1:2A:72:U:OP1	64:2A:3943:HOH:O	2.20	0.43
1:2A:709:U:H2'	1:2A:710:G:C8	2.54	0.43
1:2A:2336:A:H61	22:20:43:THR:HG22	1.84	0.43
1:2A:2758:A:C4	7:2H:67:LEU:HD21	2.54	0.43
1:2A:2815:C:H2'	1:2A:2816:C:H6	1.83	0.43
22:20:6:GLY:O	22:20:7:LEU:HD23	2.19	0.43
23:21:81:LYS:HE2	23:21:81:LYS:HB3	1.65	0.43
33:2b:212:GLN:OE1	33:2b:216:SER:HB3	2.19	0.43
36:2e:42:GLY:HA2	36:2e:65:ASN:O	2.17	0.43
36:2e:68:GLU:OE2	36:2e:70:PRO:HG3	2.18	0.43
41:2j:6:ILE:HG12	41:2j:98:ILE:HG23	2.00	0.43
44:2m:80:ARG:HH22	50:2s:69:HIS:CE1	2.26	0.43
1:1A:26:G:C6	1:1A:27:G:N1	2.87	0.43
1:1A:1082:U:C4	1:1A:1086:A:N1	2.83	0.43
1:1A:2151:G:H2'	1:1A:2152:G:C8	2.54	0.43
7:1H:56:SER:OG	7:1H:57:ASP:N	2.50	0.43
8:1I:121:LYS:HE3	8:1I:121:LYS:HB3	1.86	0.43
32:1a:309:G:O2'	32:1a:607:A:N1	2.48	0.43
32:1a:1329:A:N7	52:1u:7:ARG:NH2	2.67	0.43
34:1c:203:PHE:HZ	34:1c:206:GLU:HG3	1.84	0.43
40:1i:77:ILE:O	40:1i:81:ILE:HG22	2.18	0.43
43:1l:79:GLU:HG2	43:1l:80:HIS:CD2	2.54	0.43
1:2A:1359:A:H2'	1:2A:1360:A:H5'	2.00	0.43
1:2A:2166:G:O6	1:2A:2171:A:N6	2.52	0.43
1:2A:2252:G:H2'	1:2A:2253:G:O4'	2.19	0.43
1:2A:2564:A:C2	1:2A:2647:U:H4'	2.54	0.43
5:2F:178:PRO:HB2	5:2F:201:VAL:HG21	2.01	0.43
19:2X:84:ALA:HB3	19:2X:87:GLN:NE2	2.33	0.43
21:2Z:53:ILE:HA	21:2Z:71:VAL:HG23	2.00	0.43
32:2a:580:U:H5"	46:2o:58:MET:HG2	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:993:G:N3	32:2a:993:G:H2'	2.33	0.43
32:2a:1260:C:O5'	32:2a:1284:C:H4'	2.18	0.43
33:2b:19:HIS:CE1	33:2b:206:ASP:HB2	2.53	0.43
1:1A:479:A:N3	1:1A:481:G:H5"	2.34	0.43
1:1A:1698:A:C8	1:1A:1700:A:O4'	2.71	0.43
20:1Y:6:HIS:HE1	20:1Y:72:VAL:O	2.01	0.43
32:1a:6:G:H1	36:1e:98:THR:HG21	1.84	0.43
34:1c:36:ASP:O	34:1c:40:ARG:HG3	2.18	0.43
1:2A:315:G:H2'	1:2A:316:C:C6	2.54	0.43
1:2A:644:A:H4'	1:2A:645:C:C5	2.54	0.43
1:2A:1359:A:C2	1:2A:1372:U:O4	2.71	0.43
1:2A:2516:G:O6	1:2A:2517:C:N4	2.52	0.43
7:2H:127:GLU:C	7:2H:129:THR:H	2.27	0.43
8:2I:140:LEU:HD12	8:2I:140:LEU:HA	1.81	0.43
14:2S:38:GLN:HG2	14:2S:40:ILE:HD11	2.01	0.43
32:2a:1010:G:N2	32:2a:1020:U:HO2'	2.17	0.43
32:2a:1161:C:H2'	32:2a:1162:C:C6	2.54	0.43
36:2e:31:LEU:HD23	36:2e:31:LEU:HA	1.79	0.43
38:2g:16:LEU:HD12	40:2i:42:ARG:HA	2.01	0.43
1:1A:1778:U:OP1	64:1A:4242:HOH:O	2.21	0.43
7:1H:35:VAL:O	7:1H:37:VAL:HG23	2.19	0.43
8:1I:12:LEU:HD23	8:1I:12:LEU:HA	1.81	0.43
10:1O:104:ARG:NE	15:1T:36:GLU:OE2	2.36	0.43
21:1Z:4:ARG:NE	21:1Z:60:GLU:OE2	2.38	0.43
32:1a:582:U:H2'	32:1a:583:A:C8	2.54	0.43
32:1a:1414:U:H3	32:1a:1486:G:H1	1.66	0.43
32:1a:1504:G:OP1	32:1a:1507:A:H4'	2.19	0.43
32:1a:1525:G:P	42:1k:120:ARG:HH22	2.41	0.43
36:1e:31:LEU:HD23	36:1e:31:LEU:HA	1.76	0.43
38:1g:78:ARG:HD3	38:1g:79:ARG:H	1.83	0.43
1:2A:471:A:H2'	1:2A:472:A:O4'	2.19	0.43
1:2A:1818:U:O2'	3:2D:154:LYS:O	2.35	0.43
1:2A:2438:U:O2'	1:2A:2440:C:OP1	2.32	0.43
1:2A:2472:G:H2'	1:2A:2475:C:H42	1.84	0.43
3:2D:218:ARG:HB3	3:2D:219:PRO:HD2	2.01	0.43
10:2O:29:ASN:OD1	10:2O:29:ASN:N	2.52	0.43
23:21:64:ALA:HA	23:21:67:ILE:HG13	2.01	0.43
32:2a:986:A:H1'	50:2s:54:GLY:O	2.19	0.43
32:2a:1064:G:OP1	32:2a:1386:G:H4'	2.19	0.43
33:2b:10:LEU:HD12	33:2b:10:LEU:HA	1.83	0.43
33:2b:185:ILE:HG22	33:2b:199:TYR:HD2	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:2f:69:GLU:CD	37:2f:69:GLU:H	2.27	0.43
41:2j:42:THR:HG23	41:2j:68:HIS:HA	2.01	0.43
41:2j:46:ARG:HB2	41:2j:46:ARG:HH11	1.84	0.43
48:2q:27:PHE:CE1	48:2q:36:ILE:HD11	2.53	0.43
49:2r:52:PRO:O	49:2r:56:THR:HG23	2.19	0.43
1:1A:2206:G:H5"	1:1A:2207:G:C5	2.54	0.43
1:1A:2615:U:H2'	1:1A:2616:C:H6	1.84	0.43
2:1B:114:C:H4'	14:1S:46:VAL:HG22	2.01	0.43
5:1F:148:LEU:HD22	5:1F:154:VAL:HG21	2.01	0.43
14:1S:10:ARG:O	14:1S:14:VAL:HG13	2.18	0.43
21:1Z:28:MET:O	21:1Z:34:ASN:HA	2.19	0.43
32:1a:868:C:H2'	32:1a:869:G:O4'	2.19	0.43
32:1a:1134:G:N3	32:1a:1134:G:H2'	2.34	0.43
33:1b:132:LYS:HA	33:1b:135:GLN:HB3	2.00	0.43
36:1e:33:VAL:HG21	36:1e:109:ILE:HA	1.99	0.43
56:1y:55:PSU:C4	56:1y:57:G:H5'	2.54	0.43
1:2A:34:C:N4	1:2A:454:A:O2'	2.52	0.43
1:2A:632:A:H2'	1:2A:633:A:C8	2.54	0.43
1:2A:764:A:H5"	3:2D:210:GLY:CA	2.48	0.43
1:2A:851:U:H5'	25:23:49:LYS:HD2	2.01	0.43
1:2A:1371:G:H2'	1:2A:1372:U:H5	1.83	0.43
1:2A:2328:A:H2'	1:2A:2329:G:C8	2.54	0.43
32:2a:1244:C:N4	32:2a:1293:G:H1	2.15	0.43
33:2b:47:THR:HA	33:2b:202:PRO:HG2	2.01	0.43
34:2c:131:ARG:NH2	36:2e:50:GLU:HG3	2.34	0.43
35:2d:150:GLU:CD	35:2d:150:GLU:H	2.27	0.43
55:2x:21:A:N6	55:2x:46:G:H2'	2.33	0.43
1:1A:768:G:O2'	1:1A:1379:A:N1	2.47	0.42
1:1A:1176:G:H4'	1:1A:1177:A:OP1	2.18	0.42
1:1A:1508:A:O2'	1:1A:1509:C:H5"	2.19	0.42
1:1A:2319:G:H1	14:1S:3:ARG:HA	1.83	0.42
12:1Q:136:ALA:HB1	21:1Z:52:SER:HB2	1.99	0.42
18:1W:67:ASP:OD1	18:1W:67:ASP:N	2.48	0.42
20:1Y:99:CYS:HB2	20:1Y:106:LEU:HD21	2.01	0.42
32:1a:219:C:H2'	32:1a:220:G:O4'	2.19	0.42
32:1a:389:A:C6	32:1a:390:C:H1'	2.54	0.42
32:1a:688:G:H2'	32:1a:689:C:H6	1.83	0.42
36:1e:7:GLU:OE2	36:1e:37:ARG:NH2	2.52	0.42
51:1t:77:ALA:O	51:1t:81:LYS:HG3	2.19	0.42
1:2A:530:G:O4'	1:2A:530:G:N3	2.51	0.42
1:2A:1231:G:H2'	1:2A:1232:G:C8	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2B:17:C:H2'	2:2B:18:G:O4'	2.19	0.42
6:2G:179:PRO:HG3	26:24:43:TYR:CZ	2.54	0.42
7:2H:90:LYS:HD2	7:2H:159:GLU:CD	2.44	0.42
16:2U:76:TYR:CZ	16:2U:80:ILE:HG13	2.54	0.42
32:2a:157:G:N2	32:2a:164:U:O2	2.41	0.42
32:2a:1024:G:H2'	32:2a:1025:U:H5"	2.00	0.42
32:2a:1168:A:C6	32:2a:1169:A:C6	3.06	0.42
32:2a:1190:G:H5'	34:2c:176:HIS:HE1	1.82	0.42
32:2a:1312:G:H5'	50:2s:5:LEU:CD1	2.49	0.42
33:2b:178:ARG:HH22	39:2h:68:ARG:HH12	1.67	0.42
34:2c:52:LEU:HD12	34:2c:53:ALA:H	1.82	0.42
35:2d:99:SER:HB3	35:2d:139:ARG:HG3	2.01	0.42
44:2m:3:ARG:HH22	44:2m:11:ARG:HG3	1.84	0.42
52:2u:6:ARG:C	52:2u:8:THR:H	2.27	0.42
1:1A:226:G:H21	1:1A:228:A:H62	1.67	0.42
1:1A:576:U:H2'	1:1A:577:G:C8	2.54	0.42
1:1A:879:G:N2	1:1A:880:G:N3	2.67	0.42
1:1A:1021:A:H3'	1:1A:1021:A:N3	2.34	0.42
1:1A:2317:C:H2'	1:1A:2318:G:O4'	2.19	0.42
21:1Z:163:LEU:HD12	21:1Z:163:LEU:HA	1.87	0.42
32:1a:1039:C:H2'	32:1a:1040:U:H6	1.84	0.42
34:1c:148:GLY:HA3	34:1c:172:ARG:H	1.84	0.42
44:1m:23:TYR:HB3	44:1m:67:GLU:HA	2.01	0.42
1:2A:580:C:H2'	1:2A:581:C:H6	1.84	0.42
1:2A:2127:G:N2	1:2A:2161:C:N3	2.67	0.42
5:2F:139:PHE:CG	5:2F:167:ALA:HB2	2.54	0.42
6:2G:41:GLN:O	6:2G:43:LEU:N	2.51	0.42
7:2H:33:LEU:HD21	7:2H:136:ILE:HB	2.01	0.42
21:2Z:100:VAL:HG21	21:2Z:134:PRO:HG2	2.01	0.42
26:24:1:MET:HE2	26:24:6:HIS:CE1	2.54	0.42
26:24:50:VAL:HG21	44:2m:65:LYS:HA	2.01	0.42
32:2a:73:G:H1	32:2a:96:U:H3	1.67	0.42
32:2a:390:C:O3'	47:2p:28:ARG:NH2	2.53	0.42
32:2a:741:G:H2'	32:2a:742:G:O4'	2.18	0.42
32:2a:818:G:O2'	32:2a:819:A:H5'	2.19	0.42
32:2a:1133:G:H2'	32:2a:1134:G:O4'	2.18	0.42
34:2c:6:HIS:HB3	45:2n:49:HIS:CD2	2.54	0.42
34:2c:20:SER:HB3	34:2c:22:TRP:NE1	2.33	0.42
36:2e:36:ASP:O	36:2e:38:GLN:N	2.46	0.42
36:2e:36:ASP:C	36:2e:38:GLN:H	2.27	0.42
41:2j:16:LEU:HD22	41:2j:94:VAL:HG13	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:2s:36:ARG:HD2	50:2s:52:TYR:O	2.19	0.42
56:2y:63:G:H2'	56:2y:64:A:C8	2.53	0.42
1:1A:829:A:N7	1:1A:2248:C:H5'	2.34	0.42
1:1A:898:C:N4	1:1A:899:A:H62	2.17	0.42
1:1A:2390:U:O2'	1:1A:2391:G:H5'	2.18	0.42
64:1A:4619:HOH:O	13:1R:15:SER:HB3	2.19	0.42
13:1R:22:ARG:O	13:1R:26:LYS:HG3	2.19	0.42
27:15:8:LYS:O	27:15:9:LYS:HD2	2.20	0.42
33:1b:16:HIS:CG	33:1b:17:PHE:N	2.88	0.42
34:1c:13:GLY:HA3	45:1n:57:ARG:HH12	1.82	0.42
36:1e:28:PHE:O	36:1e:47:LYS:HA	2.19	0.42
36:1e:41:VAL:O	36:1e:66:MET:HA	2.19	0.42
54:1w:18:G:H4'	54:1w:60:U:C6	2.54	0.42
1:2A:582:G:H2'	1:2A:583:G:C8	2.54	0.42
1:2A:645:C:H5"	1:2A:646:A:OP2	2.18	0.42
1:2A:1669:A:O2'	1:2A:2549:G:OP1	2.28	0.42
1:2A:2052:G:H4'	4:2E:143:ASN:O	2.19	0.42
2:2B:56:G:H5'	6:2G:27:ASN:HD21	1.82	0.42
4:2E:1:MET:HB3	4:2E:83:ASP:O	2.19	0.42
9:2N:1:MET:HE1	16:2U:94:ASN:ND2	2.34	0.42
15:2T:127:ALA:C	15:2T:129:ARG:N	2.77	0.42
32:2a:200:G:H1	32:2a:217:C:N4	2.16	0.42
32:2a:1121:U:H2'	32:2a:1122:U:C6	2.54	0.42
39:2h:51:VAL:HG11	39:2h:60:ARG:HH11	1.84	0.42
48:2q:45:HIS:HB3	48:2q:72:ARG:HG2	2.00	0.42
1:1A:272(G):C:H42	1:1A:363(C):G:H1	1.67	0.42
1:1A:655:A:H2'	1:1A:656:G:O4'	2.19	0.42
1:1A:875:G:H1	1:1A:902:C:H42	1.67	0.42
1:1A:1686:C:H2'	1:1A:1687:G:O4'	2.20	0.42
1:1A:2309:A:N6	1:1A:2310:A:N1	2.67	0.42
6:1G:7:LEU:N	6:1G:104:GLU:OE1	2.52	0.42
20:1Y:43:ASN:HD22	20:1Y:43:ASN:HA	1.51	0.42
25:13:7:LYS:HE3	25:13:32:GLN:NE2	2.32	0.42
32:1a:7:G:H21	36:1e:121:LYS:HG2	1.82	0.42
32:1a:192:U:H2'	32:1a:193:C:H6	1.83	0.42
32:1a:1181:G:O2'	32:1a:1182:G:N7	2.50	0.42
33:1b:8:LYS:HE2	33:1b:8:LYS:HB2	1.91	0.42
40:1i:55:ALA:HA	40:1i:58:HIS:HD2	1.84	0.42
41:1j:5:ARG:NH2	41:1j:73:ASP:OD2	2.32	0.42
48:1q:55:ASP:O	48:1q:57:VAL:HG13	2.19	0.42
56:1y:5:G:N1	56:1y:6:G:C5	2.87	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:1y:40:C:H2'	56:1y:41:C:C6	2.55	0.42
1:2A:84:A:N1	1:2A:98:G:O2'	2.49	0.42
1:2A:171:G:H2'	1:2A:172:C:H6	1.84	0.42
1:2A:1325:G:OP1	1:2A:1647:G:O2'	2.27	0.42
1:2A:1686:C:H2'	1:2A:1687:G:O4'	2.18	0.42
1:2A:2377:A:H2'	1:2A:2378:A:C8	2.54	0.42
2:2B:2:C:H2'	2:2B:3:C:C6	2.54	0.42
18:2W:11:ARG:NH1	18:2W:99:ARG:O	2.50	0.42
32:2a:1122:U:C4	32:2a:1123:A:N7	2.87	0.42
32:2a:1187:G:H5'	40:2i:113:LYS:NZ	2.33	0.42
32:2a:1517:G:N7	32:2a:1518:MA6:H103	2.35	0.42
34:2c:47:LEU:HB2	34:2c:52:LEU:HD22	2.01	0.42
41:2j:17:ASP:OD1	41:2j:70:ARG:NE	2.48	0.42
49:2r:74:ARG:HB3	49:2r:81:PHE:CE1	2.55	0.42
1:1A:586:A:N1	1:1A:809:G:O2'	2.46	0.42
1:1A:1075:C:C2'	1:1A:1076:C:H5'	2.48	0.42
3:1D:246:PRO:O	3:1D:254:THR:HG22	2.19	0.42
7:1H:3:ARG:NH2	7:1H:65:HIS:HB3	2.34	0.42
20:1Y:98:VAL:HG12	20:1Y:105:ALA:HA	2.01	0.42
33:1b:98:LEU:HD12	33:1b:101:MET:HE3	2.02	0.42
37:1f:11:ASN:HB3	37:1f:14:LEU:HD11	2.02	0.42
43:1l:60:LEU:HD11	43:1l:66:VAL:HG22	2.02	0.42
1:2A:515:A:H1'	1:2A:581:C:H1'	2.02	0.42
1:2A:557:U:H2'	1:2A:558:G:H8	1.85	0.42
1:2A:570:G:H2'	1:2A:2030:A:C5	2.54	0.42
1:2A:607:U:OP1	5:2F:102:PRO:HA	2.19	0.42
1:2A:2142:C:N4	1:2A:2148:G:O6	2.52	0.42
1:2A:2705:A:OP2	64:2A:3948:HOH:O	2.22	0.42
1:2A:2784:C:H1'	4:2E:37:ARG:NH1	2.34	0.42
6:2G:120:LEU:N	6:2G:179:PRO:O	2.33	0.42
9:2N:62:VAL:CG1	9:2N:66:LYS:HB2	2.49	0.42
15:2T:24:PRO:HD3	15:2T:52:ILE:HD12	2.02	0.42
23:21:26:ARG:HG3	23:21:27:GLU:HG3	2.01	0.42
32:2a:130:A:H1'	32:2a:263:A:O2'	2.18	0.42
32:2a:1266:G:N2	32:2a:1268:A:H3'	2.35	0.42
33:2b:78:GLN:HE22	33:2b:95:GLN:HE22	1.66	0.42
34:2c:18:TRP:HE3	34:2c:18:TRP:H	1.66	0.42
36:2e:31:LEU:HD22	36:2e:43:LEU:HD11	2.00	0.42
42:2k:34:ASP:OD2	42:2k:38:ASN:HB2	2.20	0.42
45:2n:24:CYS:HB2	45:2n:40:CYS:HB3	2.00	0.42
49:2r:33:ASP:OD2	49:2r:36:ASN:HB2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:2w:4:C:H2'	54:2w:5:G:O4'	2.19	0.42
1:1A:11:G:C2'	1:1A:12:U:H5"	2.41	0.42
1:1A:191:A:H2'	1:1A:192:C:C6	2.53	0.42
1:1A:897:C:N3	1:1A:898:C:N4	2.67	0.42
1:1A:1078:U:H5'	1:1A:1079:C:OP1	2.20	0.42
1:1A:2006:C:OP2	64:1A:4244:HOH:O	2.21	0.42
3:1D:206:LEU:HD22	3:1D:211:ARG:HG2	2.02	0.42
20:1Y:14:LEU:HD12	20:1Y:23:ARG:O	2.20	0.42
32:1a:79:G:H1	32:1a:90:U:H1'	1.84	0.42
32:1a:418:C:H2'	32:1a:419:C:C6	2.54	0.42
32:1a:544:G:P	35:1d:59:ARG:HH22	2.42	0.42
32:1a:1118:C:H1'	32:1a:1179:A:C4	2.55	0.42
32:1a:1286:A:H2'	32:1a:1287:A:H4'	2.01	0.42
35:1d:173:TRP:NE1	35:1d:193:ASP:HB3	2.34	0.42
40:1i:6:GLY:O	40:1i:17:VAL:HG12	2.19	0.42
1:2A:450:G:OP1	64:2A:3946:HOH:O	2.21	0.42
1:2A:910:A:C5	12:2Q:13:GLN:HG3	2.54	0.42
1:2A:956:G:H5"	12:2Q:77:LYS:HD2	2.01	0.42
1:2A:1410:G:H2'	1:2A:1411:C:C6	2.54	0.42
1:2A:2567:G:H2'	1:2A:2568:C:C6	2.54	0.42
1:2A:2850:A:OP2	1:2A:2866:U:H5	2.01	0.42
1:2A:2889:C:H2'	1:2A:2891:G:O4'	2.20	0.42
2:2B:34:U:OP1	6:2G:2:PRO:HG3	2.19	0.42
6:2G:16:ARG:NE	6:2G:31:VAL:HG11	2.35	0.42
7:2H:17:VAL:HG11	7:2H:50:VAL:HG21	2.01	0.42
22:20:33:ALA:N	22:20:64:ASP:OD1	2.37	0.42
32:2a:79:G:H1	32:2a:90:U:H3	1.68	0.42
32:2a:1265:G:C4	32:2a:1271:G:N2	2.87	0.42
36:2e:57:LYS:HG2	36:2e:61:TYR:CE2	2.55	0.42
39:2h:29:SER:OG	39:2h:32:LYS:HG3	2.19	0.42
44:2m:90:LEU:O	44:2m:94:ARG:HB2	2.19	0.42
46:2o:48:LYS:HD3	46:2o:48:LYS:HA	1.70	0.42
47:2p:15:PRO:HD2	47:2p:42:ARG:CD	2.49	0.42
51:2t:67:ALA:HA	51:2t:72:LEU:O	2.19	0.42
56:2y:14:A:H3'	56:2y:15:G:C8	2.54	0.42
1:1A:1292:U:H2'	1:1A:1293:C:C6	2.55	0.42
1:1A:2109:U:C2	1:1A:2181:G:C2	3.08	0.42
1:1A:2128:C:N4	1:1A:2160:G:H1	2.17	0.42
2:1B:1:U:H2'	2:1B:2:C:C6	2.54	0.42
3:1D:35:LYS:HB2	3:1D:36:PRO:HD2	2.01	0.42
8:1I:77:LEU:HD23	8:1I:77:LEU:HA	1.82	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1Z:138:GLU:H	21:1Z:156:LYS:HD3	1.84	0.42
26:14:17:GLY:C	26:14:19:GLY:H	2.28	0.42
32:1a:160:A:H1'	32:1a:344:A:C5	2.55	0.42
32:1a:487:A:H2'	32:1a:488:C:O4'	2.19	0.42
32:1a:1044:A:C5	32:1a:1045:C:H1'	2.54	0.42
34:1c:6:HIS:CD2	34:1c:8:ILE:HB	2.55	0.42
37:1f:6:VAL:HG22	37:1f:90:VAL:HG22	2.01	0.42
51:1t:47:GLY:HA2	51:1t:48:LYS:C	2.45	0.42
56:1y:71:G:H2'	56:1y:72:C:C6	2.54	0.42
1:2A:1364:G:OP2	23:21:3:LYS:HG3	2.20	0.42
1:2A:1805:U:O2	3:2D:50:THR:HB	2.19	0.42
1:2A:2507:C:H2'	1:2A:2508:G:O4'	2.20	0.42
8:2I:110:ASP:N	8:2I:130:TYR:OH	2.35	0.42
13:2R:12:ARG:O	13:2R:17:ARG:NH1	2.53	0.42
21:2Z:100:VAL:HA	21:2Z:101:PRO:HD3	1.93	0.42
28:26:38:LYS:HB3	28:26:38:LYS:HE3	1.72	0.42
32:2a:811:C:O2'	32:2a:901:A:N1	2.49	0.42
32:2a:1004:A:N3	32:2a:1038:C:C2	2.88	0.42
32:2a:1201:A:H4'	32:2a:1202:G:O5'	2.20	0.42
32:2a:1272:G:C2	32:2a:1273:G:C8	3.08	0.42
34:2c:69:HIS:HA	34:2c:104:GLN:HB3	2.00	0.42
56:2y:8:4SU:S4	56:2y:14:A:N7	2.93	0.42
1:1A:1750:G:O2'	1:1A:2860:A:N1	2.46	0.42
1:1A:1794:U:H2'	1:1A:1795:C:C6	2.55	0.42
1:1A:2112:G:H1'	56:1y:19:G:O2'	2.19	0.42
1:1A:2202:C:H2'	1:1A:2203:U:O4'	2.19	0.42
1:1A:2320:A:H2'	1:1A:2320:A:N3	2.35	0.42
2:1B:21:G:N7	64:1B:305:HOH:O	2.37	0.42
2:1B:106:G:H5'	21:1Z:31:ARG:HG2	2.02	0.42
7:1H:11:VAL:HG21	7:1H:50:VAL:HG23	2.02	0.42
11:1P:121:LYS:HE2	11:1P:123:LEU:HD11	2.01	0.42
23:11:8:SER:HB3	23:11:66:HIS:CD2	2.54	0.42
32:1a:582:U:H2'	32:1a:583:A:H8	1.84	0.42
35:1d:19:LEU:O	35:1d:21:LEU:HG	2.19	0.42
35:1d:63:LYS:HD2	35:1d:198:VAL:HG22	2.02	0.42
42:1k:103:LEU:HD23	42:1k:103:LEU:HA	1.90	0.42
1:2A:192:C:O2'	1:2A:802:A:N3	2.48	0.42
1:2A:1693:U:H1'	3:2D:14:ARG:HH21	1.85	0.42
1:2A:2123:G:H2'	1:2A:2124:G:C8	2.55	0.42
1:2A:2406:U:H6	1:2A:2406:U:H2'	1.67	0.42
1:2A:2439:A:N6	55:2x:76:8AN:O1P	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2741:A:H2'	1:2A:2742:C:O4'	2.20	0.42
2:2B:43:C:H5"	26:24:1:MET:HG2	2.01	0.42
6:2G:3:LEU:O	6:2G:8:LYS:NZ	2.35	0.42
7:2H:13:LYS:HA	7:2H:14:GLY:HA2	1.55	0.42
9:2N:30:ILE:HG23	9:2N:52:VAL:HG11	2.01	0.42
12:2Q:137:TYR:CE1	21:2Z:83:PRO:HG3	2.55	0.42
21:2Z:150:LEU:O	21:2Z:171:ILE:HG13	2.19	0.42
32:2a:288:A:H2'	32:2a:289:G:H4'	2.02	0.42
32:2a:1264:C:H42	32:2a:1271:G:H1	1.66	0.42
32:2a:1327:C:H2'	32:2a:1328:C:H6	1.85	0.42
48:2q:58:GLU:OE2	48:2q:75:ARG:NH2	2.53	0.42
1:1A:198:C:H5'	1:1A:2244:U:OP1	2.19	0.42
1:1A:1163:G:OP1	17:1V:24:LYS:NZ	2.52	0.42
1:1A:2336:A:H61	22:10:43:THR:HG22	1.85	0.42
5:1F:33:LEU:HD13	5:1F:112:MET:HE2	2.02	0.42
8:1I:48:GLU:HB3	8:1I:52:ARG:NH1	2.35	0.42
12:1Q:78:PRO:HG2	12:1Q:81:VAL:HG11	2.01	0.42
12:1Q:111:GLU:O	12:1Q:115:MET:HG2	2.20	0.42
32:1a:60:A:N1	32:1a:107:G:O2'	2.47	0.42
32:1a:437:U:H5"	35:1d:155:LEU:HD11	2.00	0.42
32:1a:730:G:C5	32:1a:731:G:H1'	2.55	0.42
32:1a:1151:A:O4'	41:1j:39:PRO:HB2	2.20	0.42
32:1a:1239:A:H62	32:1a:1299:A:H62	1.66	0.42
32:1a:1318:A:OP1	50:1s:7:LYS:NZ	2.40	0.42
35:1d:107:ARG:NH2	35:1d:194:LEU:HD21	2.34	0.42
36:1e:146:ALA:O	36:1e:150:ARG:HG3	2.20	0.42
40:1i:49:PRO:HG2	40:1i:81:ILE:HG23	2.01	0.42
46:1o:3:ILE:HG21	46:1o:34:LEU:HD21	2.02	0.42
1:2A:1453:U:H3'	64:2A:3953:HOH:O	2.20	0.42
1:2A:2137:C:N4	1:2A:2155:G:O6	2.53	0.42
4:2E:84:PHE:CZ	4:2E:86:PRO:HB3	2.54	0.42
7:2H:8:PRO:O	7:2H:10:PRO:HD3	2.20	0.42
32:2a:407:G:OP1	35:2d:115:ARG:NH2	2.53	0.42
32:2a:545:C:OP1	35:2d:61:LYS:NZ	2.52	0.42
32:2a:570:G:H1'	32:2a:820:U:C4	2.55	0.42
32:2a:755:G:OP2	46:2o:65:ARG:HD2	2.20	0.42
32:2a:1013:G:O2'	32:2a:1015:A:N7	2.49	0.42
32:2a:1469:G:H2'	32:2a:1470:G:C8	2.55	0.42
33:2b:167:PRO:HG2	33:2b:192:SER:HB3	2.02	0.42
37:2f:76:ALA:HB1	37:2f:80:ARG:NH2	2.35	0.42
38:2g:28:ASN:HD21	38:2g:36:LYS:NZ	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:2i:71:SER:HA	40:2i:74:ILE:HD12	2.02	0.42
50:2s:27:GLU:HB2	50:2s:28:LYS:HA	2.01	0.42
1:1A:376:C:H2'	1:1A:377:C:C6	2.55	0.42
1:1A:1268:A:H2'	1:1A:1269:A:O4'	2.20	0.42
1:1A:1466:G:H2'	1:1A:1547:C:N4	2.35	0.42
1:1A:1668:A:O2'	1:1A:1674:G:N7	2.39	0.42
1:1A:2376:A:H2'	1:1A:2377:A:O4'	2.20	0.42
5:1F:72:ARG:HE	5:1F:72:ARG:HB3	1.57	0.42
14:1S:110:LEU:HD12	14:1S:110:LEU:HA	1.78	0.42
32:1a:78:G:O2'	32:1a:79:G:O5'	2.38	0.42
32:1a:535:A:H5"	64:1a:4844:HOH:O	2.19	0.42
32:1a:551:U:H2'	32:1a:552:U:C6	2.55	0.42
32:1a:872:A:C8	32:1a:874:G:C8	3.08	0.42
32:1a:1168:A:H2'	32:1a:1169:A:C8	2.55	0.42
34:1c:30:ARG:HB3	45:1n:36:PHE:O	2.20	0.42
35:1d:106:TYR:HD2	35:1d:107:ARG:HD3	1.83	0.42
45:1n:48:ALA:HB2	45:1n:53:LEU:HD12	2.01	0.42
54:1w:8:4SU:O5'	54:1w:8:4SU:H6	2.19	0.42
56:1y:52:G:H2'	56:1y:53:G:O4'	2.20	0.42
1:2A:118:A:C8	1:2A:119:A:C8	3.08	0.42
1:2A:2030:A:H4'	1:2A:2031:A:C8	2.55	0.42
1:2A:2138:C:H2'	1:2A:2139:C:O4'	2.20	0.42
3:2D:146:GLU:HG2	3:2D:152:GLY:C	2.45	0.42
6:2G:123:ASN:O	6:2G:125:PHE:N	2.44	0.42
23:21:98:LEU:HD23	23:21:98:LEU:HA	1.85	0.42
32:2a:109:A:H2'	32:2a:326:G:N2	2.34	0.42
32:2a:473:G:H2'	32:2a:474:G:C8	2.55	0.42
32:2a:1004:A:N6	32:2a:1037:C:O2	2.45	0.42
32:2a:1441:G:H8	32:2a:1441:G:O5'	2.03	0.42
44:2m:33:ALA:HA	44:2m:59:TYR:CE2	2.50	0.42
49:2r:26:LEU:HD11	49:2r:42:ARG:HD3	2.02	0.42
49:2r:53:ARG:HG2	49:2r:63:GLN:HE21	1.84	0.42
1:1A:1065:U:H1'	1:1A:1074:G:C2	2.54	0.41
1:1A:1506:C:H2'	1:1A:1507:A:C8	2.53	0.41
13:1R:2:ARG:HD2	64:1R:307:HOH:O	2.19	0.41
30:18:26:LYS:HD2	30:18:48:PHE:CD2	2.55	0.41
32:1a:1004:A:H5"	32:1a:1025:U:H5	1.85	0.41
32:1a:1030(A):G:H2'	32:1a:1030(C):G:OP2	2.20	0.41
32:1a:1064:G:O2'	32:1a:1190:G:N2	2.53	0.41
32:1a:1179:A:H2'	32:1a:1180:A:O4'	2.20	0.41
36:1e:6:PHE:HB3	36:1e:34:VAL:HG22	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:1f:12:PRO:HG3	37:1f:57:GLN:O	2.19	0.41
40:1i:9:ARG:HG2	40:1i:14:VAL:HG12	2.01	0.41
44:1m:102:ARG:HE	44:1m:102:ARG:HB2	1.67	0.41
44:1m:122:LYS:HG3	44:1m:123:ALA:N	2.33	0.41
1:2A:176:G:O2'	1:2A:177:G:H5'	2.20	0.41
1:2A:263:C:H2'	1:2A:264:C:O4'	2.20	0.41
1:2A:577:G:C6	1:2A:578:A:C6	3.08	0.41
1:2A:860:U:H1'	1:2A:2268:A:H5'	2.01	0.41
1:2A:1803:A:H4'	3:2D:259:THR:HG23	2.02	0.41
1:2A:2125:G:H2'	1:2A:2126:A:C8	2.55	0.41
1:2A:2577:A:OP1	64:2A:3926:HOH:O	2.22	0.41
1:2A:2821:A:H2'	1:2A:2822:G:C8	2.55	0.41
7:2H:7:LEU:HD23	7:2H:69:ARG:NH2	2.35	0.41
8:2I:88:ILE:HD11	8:2I:144:VAL:HG11	2.02	0.41
21:2Z:144:LEU:HD11	21:2Z:150:LEU:HD22	2.01	0.41
22:20:23:VAL:HG22	22:20:38:VAL:HG22	2.02	0.41
24:22:1:MET:N	24:22:52:ASP:OD1	2.52	0.41
32:2a:881:G:P	43:2l:12:ARG:HH22	2.43	0.41
32:2a:1070:U:H2'	32:2a:1071:C:C6	2.55	0.41
32:2a:1250:A:H4'	40:2i:68:GLY:N	2.34	0.41
32:2a:1313:U:OP1	50:2s:5:LEU:HB2	2.20	0.41
33:2b:171:ALA:O	33:2b:175:ARG:N	2.41	0.41
36:2e:69:VAL:HG12	36:2e:71:LEU:HD21	2.01	0.41
38:2g:69:VAL:HG13	38:2g:134:ALA:O	2.20	0.41
39:2h:121:ASP:N	39:2h:121:ASP:OD1	2.53	0.41
40:2i:93:ARG:HD3	40:2i:93:ARG:HA	1.89	0.41
49:2r:53:ARG:HA	49:2r:56:THR:OG1	2.20	0.41
1:1A:106:C:H1'	20:1Y:1:MET:HE2	2.02	0.41
1:1A:710:G:H2'	1:1A:711:G:C8	2.54	0.41
1:1A:710:G:H2'	1:1A:711:G:H8	1.85	0.41
1:1A:811:U:H2'	11:1P:21:ARG:HA	2.02	0.41
1:1A:1052:C:H2'	1:1A:1053:C:H6	1.85	0.41
1:1A:2857:G:N2	1:1A:2860:A:OP2	2.41	0.41
16:1U:69:CYS:HB3	16:1U:74:LEU:HD13	2.01	0.41
19:1X:92:LEU:HD12	19:1X:92:LEU:HA	1.88	0.41
26:14:28:LYS:HA	26:14:29:PRO:HD3	1.94	0.41
32:1a:1228:C:OP1	44:1m:115:LYS:NZ	2.46	0.41
32:1a:1427:U:H2'	32:1a:1428:A:C8	2.55	0.41
34:1c:79:ARG:O	34:1c:82:GLU:HB2	2.20	0.41
56:1y:6:G:O2'	56:1y:7:A:H5'	2.21	0.41
1:2A:478:A:N1	1:2A:500:G:H4'	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2393:A:H5"	11:2P:63:PRO:HB3	2.01	0.41
2:2B:74:U:H3'	2:2B:75:G:H5"	2.01	0.41
11:2P:107:LYS:O	11:2P:110:TYR:HB2	2.20	0.41
13:2R:9:LYS:O	13:2R:17:ARG:HD3	2.20	0.41
26:24:62:ARG:HB2	26:24:63:TYR:CE2	2.55	0.41
32:2a:114:U:O2'	32:2a:115:G:H5'	2.20	0.41
32:2a:1014:A:H4'	50:2s:14:HIS:CE1	2.55	0.41
34:2c:45:LYS:HE2	34:2c:45:LYS:HB3	1.72	0.41
40:2i:7:THR:HB	40:2i:83:ARG:NH1	2.34	0.41
40:2i:85:LEU:HB3	40:2i:92:TYR:CD2	2.55	0.41
51:2t:92:LEU:HD23	51:2t:92:LEU:HA	1.91	0.41
54:2w:2:C:N4	54:2w:71:G:H1	2.14	0.41
1:1A:1173:G:O2'	1:1A:1174:A:O4'	2.32	0.41
1:1A:2135:A:H2'	1:1A:2135:A:N3	2.35	0.41
1:1A:2144:U:H3'	1:1A:2146:C:N4	2.35	0.41
1:1A:2352:A:N6	1:1A:2365:G:O2'	2.52	0.41
2:1B:11:C:H3'	2:1B:12:C:C6	2.56	0.41
2:1B:31:C:H4'	6:1G:29:TRP:CH2	2.56	0.41
3:1D:213:ARG:HD2	3:1D:217:ARG:O	2.21	0.41
7:1H:86:GLU:CD	7:1H:132:ARG:HH21	2.27	0.41
7:1H:137:ASP:HB3	7:1H:140:LYS:HB3	2.02	0.41
8:1I:61:ARG:HD3	8:1I:61:ARG:HA	1.96	0.41
19:1X:1:MET:HE2	19:1X:1:MET:HB2	1.77	0.41
32:1a:940:C:OP1	38:1g:29:LYS:NZ	2.53	0.41
33:1b:134:GLU:HA	33:1b:137:ARG:NE	2.35	0.41
35:1d:65:ARG:HH11	35:1d:72:GLU:HB2	1.84	0.41
56:1y:22:G:H3'	56:1y:23:A:H8	1.86	0.41
1:2A:740:U:H2'	1:2A:741:G:C8	2.56	0.41
1:2A:1301:A:O2'	1:2A:1302:A:H3'	2.20	0.41
1:2A:1359:A:H2	1:2A:1372:U:O4	2.04	0.41
1:2A:1639:U:C2'	1:2A:1640:C:H5"	2.51	0.41
1:2A:1857:G:C6	1:2A:1858:G:C6	3.08	0.41
1:2A:2126:A:N3	1:2A:2127:G:H1'	2.35	0.41
1:2A:2554:U:H2'	1:2A:2555:U:C6	2.55	0.41
4:2E:5:LEU:HD21	4:2E:79:ARG:HB2	2.02	0.41
5:2F:185:ASP:HA	5:2F:188:ARG:HD3	2.02	0.41
5:2F:202:PHE:O	5:2F:206:ILE:HG12	2.20	0.41
32:2a:202:U:H3'	32:2a:203:U:C6	2.56	0.41
32:2a:222:U:H2'	32:2a:223:U:C6	2.55	0.41
32:2a:1503:A:H2	53:2v:13:A:N7	2.18	0.41
34:2c:152:ILE:HD11	34:2c:199:LYS:NZ	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:2i:9:ARG:H	40:2i:79:LEU:HD23	1.85	0.41
40:2i:42:ARG:HB3	40:2i:42:ARG:NH2	2.36	0.41
40:2i:85:LEU:HB3	40:2i:92:TYR:HD2	1.86	0.41
46:2o:64:ARG:HD3	46:2o:68:ARG:NH2	2.35	0.41
50:2s:51:VAL:O	50:2s:58:VAL:N	2.53	0.41
56:2y:3:C:H2'	56:2y:4:C:C6	2.55	0.41
56:2y:59:U:H2'	56:2y:60:U:H5'	2.01	0.41
1:1A:271(L):U:OP1	8:1I:50:ARG:NH1	2.36	0.41
1:1A:570:G:H2'	1:1A:2030:A:N7	2.36	0.41
1:1A:1093:G:H3'	1:1A:1094:U:H5"	2.02	0.41
1:1A:1256:G:H1'	5:1F:82:ILE:HD11	2.03	0.41
7:1H:13:LYS:HA	7:1H:14:GLY:HA2	1.53	0.41
8:1I:29:TYR:O	8:1I:33:ARG:HG3	2.20	0.41
32:1a:266:G:O2'	32:1a:267:C:OP2	2.26	0.41
32:1a:300:A:H1'	32:1a:565:U:O2	2.21	0.41
32:1a:1030:C:H42	32:1a:1031:G:H1	1.67	0.41
32:1a:1370:G:C2	32:1a:1371:G:C8	3.08	0.41
33:1b:158:LEU:HD23	33:1b:158:LEU:HA	1.95	0.41
41:1j:78:ASN:C	41:1j:80:LYS:H	2.28	0.41
1:2A:455:C:N3	1:2A:472:A:H2'	2.36	0.41
1:2A:2121:G:H1	1:2A:2177:C:H42	1.68	0.41
1:2A:2135:A:H2'	1:2A:2136:C:C5	2.56	0.41
1:2A:2155:G:N7	1:2A:2156:G:H1'	2.36	0.41
1:2A:2319:G:N2	14:2S:3:ARG:HA	2.35	0.41
7:2H:11:VAL:HG21	7:2H:17:VAL:HG21	2.02	0.41
32:2a:976:G:C8	32:2a:1358:U:C2	3.09	0.41
33:2b:13:ALA:C	33:2b:15:VAL:H	2.28	0.41
35:2d:102:ASP:OD1	35:2d:102:ASP:N	2.53	0.41
38:2g:60:LYS:HA	38:2g:63:LYS:CD	2.51	0.41
39:2h:2:LEU:HD12	39:2h:2:LEU:HA	1.91	0.41
47:2p:18:ARG:HD3	47:2p:35:LYS:HD2	2.02	0.41
54:2w:9:A:H5'	54:2w:46:G7M:H1'	2.02	0.41
1:1A:94:C:H2'	1:1A:94(A):G:O4'	2.21	0.41
6:1G:122:PRO:HG3	6:1G:182:LYS:H	1.84	0.41
19:1X:72:LYS:HE3	19:1X:75:ASP:OD1	2.19	0.41
24:12:44:LEU:HD12	24:12:44:LEU:HA	1.96	0.41
32:1a:448:A:C4	32:1a:487:A:C2	3.09	0.41
32:1a:620:C:H2'	32:1a:621:A:O4'	2.19	0.41
32:1a:994:A:N1	32:1a:1047:G:H4'	2.35	0.41
33:1b:188:ALA:HB1	33:1b:192:SER:OG	2.20	0.41
44:1m:20:THR:C	44:1m:22:ILE:H	2.27	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:1y:11:C:H42	56:1y:24:G:H1	1.68	0.41
1:2A:265:A:H1'	1:2A:266:G:O4'	2.20	0.41
1:2A:615:G:OP1	5:2F:40:GLN:NE2	2.46	0.41
1:2A:686:G:N2	1:2A:788:A:H61	2.19	0.41
1:2A:1999:C:H4'	1:2A:2723:C:O2	2.20	0.41
1:2A:2193:G:H2'	1:2A:2194:G:C8	2.56	0.41
1:2A:2478:A:OP2	31:29:2:LYS:NZ	2.32	0.41
5:2F:46:ARG:HB3	5:2F:48:THR:HG23	2.03	0.41
9:2N:73:THR:HA	9:2N:83:LYS:O	2.21	0.41
18:2W:92:ARG:HG3	18:2W:92:ARG:HH21	1.86	0.41
23:21:73:LEU:HD23	23:21:73:LEU:HA	1.82	0.41
32:2a:499:A:H4'	32:2a:500:G:OP1	2.20	0.41
32:2a:1092:A:H2'	32:2a:1093:A:C8	2.55	0.41
33:2b:8:LYS:O	33:2b:9:GLU:HB2	2.20	0.41
33:2b:120:ALA:O	33:2b:125:PRO:HD2	2.20	0.41
54:2w:28:G:H2'	54:2w:29:G:O4'	2.21	0.41
1:1A:123:G:OP2	64:1A:4247:HOH:O	2.22	0.41
1:1A:478:A:C6	1:1A:480:A:C6	3.08	0.41
1:1A:536:A:H2'	1:1A:537:C:C6	2.55	0.41
1:1A:818:G:H5'	1:1A:839:U:OP1	2.20	0.41
1:1A:880:G:H2'	1:1A:881:G:C8	2.54	0.41
1:1A:2093:G:C6	1:1A:2225:A:C8	3.08	0.41
1:1A:2094:G:OP1	8:1I:22:LYS:HD2	2.20	0.41
1:1A:2364:C:H2'	1:1A:2365:G:O4'	2.21	0.41
1:1A:2869:G:H2'	1:1A:2870:C:O4'	2.21	0.41
5:1F:106:ARG:H	5:1F:106:ARG:HG2	1.72	0.41
6:1G:108:ASN:HB3	26:14:22:ILE:HD13	2.01	0.41
8:1I:117:GLU:HG3	8:1I:118:LYS:H	1.85	0.41
26:14:59:PHE:HD2	50:1s:64:GLU:HB3	1.86	0.41
42:1k:48:ILE:O	42:1k:48:ILE:HG12	2.20	0.41
56:1y:67:C:H2'	56:1y:68:C:O4'	2.21	0.41
1:2A:658:C:H2'	1:2A:659:C:C6	2.56	0.41
1:2A:862:G:H2'	1:2A:863:A:O4'	2.21	0.41
1:2A:921:G:H2'	1:2A:922:U:C6	2.55	0.41
1:2A:1239:G:H2'	1:2A:1240:U:O4'	2.20	0.41
1:2A:1341:U:O2	19:2X:80:ILE:HD12	2.21	0.41
1:2A:1506:C:H2'	1:2A:1507:A:H5'	2.03	0.41
1:2A:2317:C:C2'	1:2A:2318:G:H5'	2.48	0.41
1:2A:2853:C:H2'	1:2A:2854:G:C8	2.55	0.41
4:2E:9:VAL:HG13	4:2E:25:VAL:O	2.20	0.41
7:2H:80:SER:OG	7:2H:81:GLU:N	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:2X:92:LEU:O	19:2X:94:GLY:N	2.54	0.41
21:2Z:50:GLN:OE1	21:2Z:50:GLN:N	2.52	0.41
29:27:1:MET:HE3	29:27:3:ARG:NH2	2.35	0.41
32:2a:833:U:H2'	32:2a:834:C:C6	2.55	0.41
32:2a:1104:G:H4'	33:2b:111:ARG:NH2	2.35	0.41
35:2d:150:GLU:HA	35:2d:153:ARG:HG3	2.01	0.41
36:2e:43:LEU:HB2	36:2e:136:MET:SD	2.60	0.41
39:2h:112:LEU:HA	39:2h:134:ILE:HG12	2.02	0.41
44:2m:10:PRO:HG2	44:2m:21:TYR:CE1	2.56	0.41
55:2x:19:G:H5"	55:2x:60:U:O4	2.21	0.41
1:1A:278:A:H2'	1:1A:279:C:C6	2.55	0.41
1:1A:1448:G:H4'	1:1A:1542:A:OP1	2.21	0.41
2:1B:66:A:H61	2:1B:109:C:H5'	1.85	0.41
4:1E:77:ILE:HD12	4:1E:195:LEU:HD13	2.01	0.41
6:1G:146:TYR:O	6:1G:149:VAL:HG12	2.21	0.41
13:1R:87:TYR:OH	13:1R:116:LEU:HB3	2.20	0.41
24:12:63:VAL:O	24:12:67:LYS:HG3	2.20	0.41
26:14:53:GLU:HB2	26:14:55:ARG:C	2.45	0.41
32:1a:58:C:O2'	32:1a:388:G:N7	2.44	0.41
32:1a:625:G:H2'	32:1a:626:U:C6	2.56	0.41
32:1a:626:U:C2	32:1a:627:G:C8	3.09	0.41
33:1b:178:ARG:HH22	39:1h:74:PRO:HB3	1.86	0.41
54:1w:4:C:H2'	54:1w:5:G:H8	1.83	0.41
1:2A:1798:U:H5'	3:2D:259:THR:CG2	2.50	0.41
1:2A:2831:G:OP1	1:2A:2834:G:H4'	2.21	0.41
1:2A:2893:G:H5"	1:2A:2894:G:O4'	2.21	0.41
2:2B:24:G:H4'	2:2B:25:A:C8	2.55	0.41
7:2H:24:VAL:HG21	7:2H:72:ILE:HD13	2.03	0.41
25:23:3:ARG:NH2	25:23:36:VAL:HG11	2.36	0.41
27:25:49:CYS:SG	27:25:51:TYR:HB2	2.61	0.41
32:2a:194:C:H2'	32:2a:195:A:H5"	2.03	0.41
32:2a:603:U:H2'	32:2a:604:G:H8	1.85	0.41
32:2a:998:G:OP2	32:2a:998:G:H8	2.03	0.41
32:2a:1029:C:N4	32:2a:1032:G:C6	2.89	0.41
33:2b:20:GLU:HB2	33:2b:190:THR:OG1	2.20	0.41
33:2b:178:ARG:NH2	39:2h:74:PRO:HB3	2.35	0.41
42:2k:81:ASP:OD1	42:2k:107:SER:OG	2.29	0.41
44:2m:29:ARG:HD3	44:2m:64:TRP:CE2	2.55	0.41
1:1A:1342:A:O2'	1:1A:1344:G:OP2	2.34	0.41
1:1A:1354:A:H2'	1:1A:1355:G:O4'	2.21	0.41
1:1A:1364:G:N7	23:11:3:LYS:HD2	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1G:34:LEU:HD23	6:1G:34:LEU:HA	1.87	0.41
6:1G:116:ASP:OD2	44:1m:68:GLY:HA3	2.21	0.41
12:1Q:51:ARG:HD3	12:1Q:66:ILE:HD11	2.02	0.41
15:1T:127:ALA:O	15:1T:128:GLU:HB3	2.19	0.41
19:1X:53:LYS:HB3	19:1X:82:GLN:HB3	2.03	0.41
30:18:54:GLU:O	30:18:58:ILE:HG13	2.20	0.41
32:1a:162:A:N7	32:1a:163:C:H1'	2.36	0.41
32:1a:461:A:O2'	32:1a:470:C:H5'	2.20	0.41
32:1a:1108:G:O6	64:1a:4815:HOH:O	2.19	0.41
32:1a:1243:C:H2'	32:1a:1244:C:C6	2.55	0.41
34:1c:113:ALA:HB2	34:1c:202:ILE:HG13	2.02	0.41
41:1j:96:ILE:HD12	41:1j:98:ILE:HD11	2.03	0.41
44:1m:96:LEU:C	44:1m:110:ARG:HG2	2.46	0.41
1:2A:239:U:H2'	1:2A:240:G:O4'	2.21	0.41
1:2A:583:G:OP2	16:2U:10:ARG:HD2	2.20	0.41
1:2A:2035:G:OP1	64:2A:3947:HOH:O	2.21	0.41
5:2F:20:LEU:HD12	5:2F:20:LEU:HA	1.77	0.41
21:2Z:28:MET:HE3	21:2Z:28:MET:HB2	1.89	0.41
30:28:8:LYS:HB3	30:28:12:LYS:HE3	2.01	0.41
32:2a:1285:A:H5'	32:2a:1286:A:C2	2.55	0.41
33:2b:28:PHE:CD1	33:2b:194:PRO:HG3	2.55	0.41
33:2b:52:GLU:O	33:2b:56:ARG:NH1	2.54	0.41
34:2c:188:LEU:HD12	34:2c:188:LEU:HA	1.89	0.41
38:2g:71:PRO:HG3	38:2g:103:TRP:CH2	2.56	0.41
39:2h:103:VAL:HG21	39:2h:110:ALA:HB2	2.02	0.41
51:2t:10:LEU:HD12	51:2t:11:SER:H	1.84	0.41
1:1A:207:A:H2'	1:1A:208:C:O4'	2.20	0.41
1:1A:1056:G:H5"	1:1A:1057:A:H4'	2.02	0.41
1:1A:1570:A:H2'	1:1A:1571:A:C8	2.56	0.41
1:1A:2124:G:N2	1:1A:2174:C:N3	2.59	0.41
1:1A:2319:G:C2	14:1S:3:ARG:HA	2.56	0.41
1:1A:2347:C:H2'	1:1A:2348:U:C6	2.56	0.41
1:1A:2681:C:OP2	4:1E:109:LYS:NZ	2.44	0.41
1:1A:2722:G:H2'	1:1A:2723:C:C6	2.56	0.41
1:1A:2838:G:C6	1:1A:2839:G:C5	3.08	0.41
18:1W:4:LYS:HD3	18:1W:6:ILE:HD11	2.02	0.41
21:1Z:8:TYR:HB2	21:1Z:38:TYR:CE2	2.55	0.41
21:1Z:126:VAL:HG13	21:1Z:162:GLU:H	1.85	0.41
32:1a:108:G:O6	51:1t:15:ARG:HD2	2.21	0.41
32:1a:193:C:H2'	32:1a:194:C:C6	2.56	0.41
32:1a:299:G:C6	32:1a:300:A:C6	3.08	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:539:A:H2'	32:1a:540:G:C8	2.56	0.41
32:1a:1004:A:H5'	32:1a:1024:G:N1	2.34	0.41
32:1a:1112:C:H1'	34:1c:179:ARG:HH11	1.85	0.41
32:1a:1511:G:H2'	32:1a:1512:U:O4'	2.20	0.41
35:1d:7:PRO:HB2	35:1d:10:ARG:HD2	2.02	0.41
36:1e:50:GLU:HB2	36:1e:53:LEU:HD13	2.03	0.41
40:1i:29:ASN:OD1	40:1i:64:THR:HA	2.20	0.41
40:1i:95:LYS:O	40:1i:99:LEU:HD13	2.21	0.41
41:1j:11:PHE:CE1	41:1j:67:THR:HG22	2.56	0.41
45:1n:6:LEU:HB3	45:1n:23:ARG:NH2	2.35	0.41
46:1o:17:ARG:HG3	46:1o:17:ARG:HH11	1.85	0.41
51:1t:92:LEU:HD23	51:1t:92:LEU:HA	1.88	0.41
1:2A:90:U:H1'	1:2A:92:A:C8	2.56	0.41
1:2A:288:C:H2'	1:2A:289:A:C8	2.55	0.41
1:2A:1149:G:H2'	1:2A:1150:C:C6	2.56	0.41
1:2A:1697:G:OP2	1:2A:1698:A:O2'	2.32	0.41
1:2A:1815:A:H8	1:2A:1815:A:OP1	2.03	0.41
1:2A:2051:A:H4'	4:2E:141:ILE:HG12	2.02	0.41
1:2A:2078:C:C4	1:2A:2079:U:C4	3.09	0.41
1:2A:2243:U:H2'	1:2A:2244:U:C6	2.55	0.41
1:2A:2704:C:H2'	1:2A:2705:A:O4'	2.21	0.41
10:2O:111:PHE:O	10:2O:115:VAL:HG23	2.20	0.41
19:2X:12:VAL:HG21	19:2X:27:THR:HG22	2.03	0.41
32:2a:451:A:N6	32:2a:480:U:H2'	2.36	0.41
32:2a:857:C:H2'	32:2a:858:G:O4'	2.21	0.41
32:2a:967:5MC:H2'	32:2a:968:A:C8	2.55	0.41
32:2a:977:A:H2'	32:2a:978:A:H5"	2.03	0.41
32:2a:1027:C:C2'	32:2a:1034:G:H22	2.32	0.41
32:2a:1048:G:OP1	45:2n:3:ARG:HB3	2.21	0.41
32:2a:1313:U:P	50:2s:5:LEU:HD12	2.61	0.41
34:2c:101:LEU:HD22	34:2c:102:ASN:N	2.35	0.41
35:2d:76:ARG:O	35:2d:80:GLU:HG2	2.20	0.41
35:2d:176:LEU:HD12	35:2d:182:LYS:O	2.21	0.41
37:2f:76:ALA:HB1	37:2f:80:ARG:HH22	1.85	0.41
39:2h:64:LYS:HD2	39:2h:79:VAL:HG21	2.03	0.41
40:2i:8:GLY:O	40:2i:15:ALA:N	2.46	0.41
41:2j:35:SER:HB3	41:2j:73:ASP:H	1.85	0.41
41:2j:49:VAL:HG21	45:2n:41:ARG:O	2.21	0.41
43:2l:33:ARG:HD2	43:2l:33:ARG:HA	1.87	0.41
1:1A:607:U:OP1	5:1F:102:PRO:HA	2.21	0.41
1:1A:1405:U:H2'	1:1A:1406:U:C6	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1882:C:H2'	1:1A:1883:G:O4'	2.21	0.41
1:1A:2445:G:OP1	5:1F:74:ARG:NH2	2.49	0.41
1:1A:2557:G:H2'	1:1A:2558:C:C6	2.55	0.41
1:1A:2584:U:H2'	1:1A:2585:U:C6	2.56	0.41
1:1A:2771:C:H2'	1:1A:2772:C:C6	2.55	0.41
2:1B:48:A:H2'	2:1B:49:C:C6	2.56	0.41
2:1B:74:U:H2'	2:1B:75:G:O4'	2.21	0.41
4:1E:105:THR:OG1	4:1E:166:THR:OG1	2.28	0.41
8:1I:33:ARG:C	8:1I:35:LEU:H	2.29	0.41
8:1I:93:THR:O	8:1I:97:ILE:HG13	2.21	0.41
13:1R:33:ARG:HA	13:1R:114:VAL:O	2.20	0.41
32:1a:1005:A:H1'	32:1a:1036:G:O6	2.21	0.41
32:1a:1070:U:H2'	32:1a:1071:C:C6	2.56	0.41
32:1a:1131:G:OP1	40:1i:20:ARG:NH2	2.54	0.41
32:1a:1277:C:O2'	32:1a:1279:A:H1'	2.21	0.41
40:1i:8:GLY:O	40:1i:15:ALA:N	2.54	0.41
41:1j:38:ILE:HD11	41:1j:71:LEU:HD23	2.02	0.41
49:1r:53:ARG:HH21	49:1r:59:SER:HA	1.86	0.41
1:2A:456:C:O2'	1:2A:457:A:OP2	2.34	0.41
1:2A:1523:U:H2'	1:2A:1524:G:H8	1.85	0.41
1:2A:2127:G:N1	1:2A:2161:C:N4	2.68	0.41
9:2N:61:ARG:HD3	9:2N:61:ARG:HA	1.93	0.41
23:21:52:ARG:HE	23:21:52:ARG:HB2	1.68	0.41
32:2a:374:A:C6	32:2a:375:U:C4	3.09	0.41
33:2b:61:LEU:HD11	33:2b:68:ILE:HG13	2.03	0.41
34:2c:136:GLN:O	34:2c:140:ARG:HG3	2.21	0.41
40:2i:43:ALA:HA	40:2i:74:ILE:HD13	2.02	0.41
42:2k:48:ILE:H	42:2k:48:ILE:HG12	1.67	0.41
1:1A:848:G:O6	1:1A:928:G:H2'	2.22	0.40
1:1A:1006:C:C2	1:1A:1138:G:N2	2.89	0.40
7:1H:113:VAL:HG11	7:1H:151:ILE:HG21	2.03	0.40
32:1a:179:A:H2'	32:1a:180:U:H6	1.86	0.40
32:1a:865:A:H2'	32:1a:866:C:C6	2.56	0.40
32:1a:1236:A:H4'	32:1a:1304:G:H4'	2.02	0.40
34:1c:40:ARG:HG2	34:1c:55:VAL:HG11	2.03	0.40
38:1g:78:ARG:NH1	38:1g:154:TYR:O	2.54	0.40
51:1t:36:LEU:HA	51:1t:39:LYS:HB3	2.01	0.40
56:1y:21:A:N6	56:1y:46:G7M:O2'	2.55	0.40
1:2A:191:A:H2'	1:2A:192:C:C6	2.55	0.40
1:2A:212:G:H2'	1:2A:213:A:O4'	2.21	0.40
1:2A:321:G:OP1	5:2F:135:LYS:NZ	2.52	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2100:G:H2'	1:2A:2101:G:C8	2.56	0.40
1:2A:2376:A:H2'	1:2A:2377:A:O4'	2.22	0.40
2:2B:11:C:H3'	2:2B:12:C:C6	2.56	0.40
6:2G:49:ASP:C	6:2G:51:ARG:N	2.77	0.40
8:2I:75:LEU:HD13	8:2I:105:HIS:CD2	2.55	0.40
10:2O:87:ILE:HD12	10:2O:91:LEU:HA	2.03	0.40
32:2a:137:C:H2'	32:2a:138:G:C8	2.56	0.40
32:2a:256:U:H2'	32:2a:257:G:C8	2.56	0.40
32:2a:1360:A:H8	32:2a:1360:A:OP1	2.04	0.40
33:2b:28:PHE:O	33:2b:32:ILE:HG13	2.21	0.40
33:2b:44:LEU:HA	33:2b:47:THR:OG1	2.20	0.40
37:2f:13:ASN:ND2	37:2f:55:ASP:OD2	2.49	0.40
38:2g:60:LYS:O	38:2g:63:LYS:HG2	2.21	0.40
38:2g:101:LEU:O	38:2g:105:VAL:HG23	2.20	0.40
1:1A:218:A:C2	1:1A:235:U:H4'	2.55	0.40
1:1A:980:A:C4	1:1A:1136:G:O4'	2.74	0.40
1:1A:1055:G:H1	1:1A:1104:C:N4	2.15	0.40
1:1A:1803:A:H4'	3:1D:259:THR:HG23	2.03	0.40
1:1A:2165:G:H2'	1:1A:2166:G:C5	2.56	0.40
1:1A:2359:C:H2'	1:1A:2360:A:O4'	2.20	0.40
1:1A:2576:G:H1'	64:1A:5518:HOH:O	2.21	0.40
1:1A:2820:A:OP2	13:1R:2:ARG:NH2	2.54	0.40
2:1B:33:G:H5'	6:1G:2:PRO:HD3	2.03	0.40
9:1N:1:MET:HE1	16:1U:94:ASN:ND2	2.36	0.40
10:1O:97:ARG:NH1	32:1a:339:C:OP2	2.52	0.40
32:1a:626:U:H2'	32:1a:627:G:C8	2.57	0.40
32:1a:975:A:H5'	32:1a:975:A:C8	2.55	0.40
32:1a:1036:G:H5"	32:1a:1037:C:H5	1.86	0.40
40:1i:55:ALA:HA	40:1i:58:HIS:CD2	2.56	0.40
51:1t:63:ILE:HD13	51:1t:80:ARG:HB3	2.03	0.40
6:2G:91:ARG:CZ	6:2G:91:ARG:HB3	2.51	0.40
9:2N:67:LEU:HA	9:2N:87:LEU:HD23	2.02	0.40
11:2P:59:LEU:HD11	30:28:10:ALA:HA	2.03	0.40
15:2T:11:GLU:O	15:2T:15:VAL:HG23	2.21	0.40
32:2a:792:A:H4'	32:2a:793:U:C5'	2.51	0.40
34:2c:9:GLY:HA3	45:2n:49:HIS:HD2	1.85	0.40
34:2c:122:GLU:HA	34:2c:125:GLU:HG2	2.02	0.40
49:2r:25:THR:O	49:2r:26:LEU:HD12	2.21	0.40
51:2t:72:LEU:HD23	51:2t:77:ALA:HB2	2.04	0.40
1:1A:2040:C:H2'	1:1A:2041:U:O4'	2.22	0.40
1:1A:2751:G:C5	7:1H:2:SER:N	2.88	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1G:45:GLU:OE2	64:1G:301:HOH:O	2.21	0.40
7:1H:154:PRO:HB3	7:1H:163:TYR:CE1	2.56	0.40
8:1I:31:LEU:HD21	8:1I:38:LEU:HD22	2.04	0.40
8:1I:58:LEU:O	8:1I:61:ARG:N	2.55	0.40
8:1I:101:LEU:HG	8:1I:107:VAL:HB	2.04	0.40
22:10:10:THR:HG22	22:10:12:ASN:N	2.25	0.40
24:12:65:ASN:HD22	24:12:69:ARG:NH1	2.18	0.40
32:1a:431:A:H2'	32:1a:432:A:O4'	2.22	0.40
40:1i:25:LYS:HB2	40:1i:60:ASP:OD2	2.22	0.40
49:1r:26:LEU:HD11	49:1r:42:ARG:HD3	2.03	0.40
50:1s:27:GLU:HG3	50:1s:28:LYS:HE3	2.02	0.40
51:1t:74:LYS:HE2	51:1t:74:LYS:HB3	1.84	0.40
1:2A:580:C:H2'	1:2A:581:C:C6	2.56	0.40
1:2A:1022:G:N2	1:2A:1023:U:O4	2.52	0.40
1:2A:1478:G:O2'	1:2A:1558:A:N1	2.51	0.40
1:2A:2251:OMG:HM23	1:2A:2251:OMG:H1'	1.93	0.40
2:2B:14:U:H1'	2:2B:108:U:O2'	2.21	0.40
32:2a:189(D):C:H2'	32:2a:189(E):U:O4'	2.21	0.40
32:2a:624:C:H2'	32:2a:625:G:C8	2.52	0.40
32:2a:1298:C:H2'	38:2g:114:ARG:NH2	2.35	0.40
38:2g:152:ALA:O	38:2g:155:ARG:HD3	2.20	0.40
42:2k:121:PRO:HG2	42:2k:126:ARG:HG2	2.03	0.40
56:2y:55:PSU:N1	56:2y:57:G:H5'	2.36	0.40
1:1A:30:G:H2'	1:1A:31:C:C6	2.56	0.40
1:1A:271(H):G:H4'	23:11:81:LYS:HG2	2.02	0.40
1:1A:2630:G:H2'	1:1A:2631:G:C8	2.56	0.40
2:1B:88:C:H2'	2:1B:89:G:O4'	2.21	0.40
6:1G:82:LEU:HD21	6:1G:88:ILE:HG21	2.03	0.40
8:1I:116:LEU:HD11	8:1I:120:ILE:HG13	2.03	0.40
9:1N:138:LEU:HD23	9:1N:138:LEU:HA	1.84	0.40
11:1P:46:LYS:HE3	11:1P:46:LYS:HB3	1.86	0.40
26:14:34:GLU:H	26:14:34:GLU:CD	2.30	0.40
32:1a:749:C:H2'	32:1a:750:G:H8	1.87	0.40
32:1a:1070:U:H2'	32:1a:1071:C:H6	1.86	0.40
40:1i:3:GLN:HG2	40:1i:20:ARG:HE	1.86	0.40
42:1k:51:LYS:HE2	42:1k:51:LYS:HA	2.04	0.40
54:1w:63:G:H2'	54:1w:64:A:H8	1.86	0.40
1:2A:71:A:H5"	1:2A:73:A:C8	2.57	0.40
1:2A:184:C:H2'	1:2A:185:U:H6	1.86	0.40
1:2A:2114:A:N6	1:2A:2115:G:H21	2.19	0.40
1:2A:2394:C:N3	56:2y:76:A:O2'	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2807:G:N2	1:2A:2893:G:O6	2.53	0.40
4:2E:7:VAL:HG13	4:2E:27:LEU:HB3	2.03	0.40
9:2N:30:ILE:O	9:2N:34:LEU:HG	2.20	0.40
11:2P:121:LYS:HB3	11:2P:123:LEU:HD13	2.04	0.40
32:2a:391:G:C6	32:2a:392:G:C5	3.09	0.40
42:2k:69:ALA:O	42:2k:73:MET:HG3	2.21	0.40
46:2o:8:LYS:HG2	46:2o:12:ILE:HD11	2.02	0.40
1:1A:213:A:H2'	1:1A:214:G:O4'	2.21	0.40
1:1A:886:C:N3	1:1A:887:A:C8	2.90	0.40
1:1A:1116:C:H5'	1:1A:1117:G:OP2	2.21	0.40
6:1G:148:MET:H	6:1G:148:MET:HG3	1.55	0.40
21:1Z:91:LEU:HD22	21:1Z:130:PRO:HG3	2.04	0.40
22:10:43:THR:HG23	22:10:43:THR:O	2.22	0.40
26:14:53:GLU:HB2	26:14:55:ARG:O	2.22	0.40
32:1a:1136:U:H5"	32:1a:1137:C:N3	2.36	0.40
32:1a:1368:G:OP1	40:1i:114:TYR:N	2.54	0.40
38:1g:111:ARG:HD2	38:1g:123:GLU:HB2	2.03	0.40
1:2A:1006:C:C2	1:2A:1138:G:N2	2.90	0.40
1:2A:1027:A:C2	1:2A:2488:A:H5'	2.57	0.40
1:2A:1462:C:H4'	1:2A:2703:C:H5'	2.04	0.40
1:2A:2379:G:HO2'	14:2S:17:ARG:NH1	2.08	0.40
1:2A:2406:U:C2	11:2P:72:PRO:HG2	2.57	0.40
1:2A:2506:U:C2	1:2A:2585:U:O4	2.74	0.40
20:2Y:55:TYR:N	20:2Y:56:PRO:HD3	2.37	0.40
26:24:40:HIS:O	26:24:44:THR:OG1	2.34	0.40
26:24:46:GLN:C	26:24:48:ARG:N	2.80	0.40
30:28:23:VAL:CG1	30:28:47:LYS:HD3	2.52	0.40
32:2a:1258:G:H2'	32:2a:1259:C:C6	2.56	0.40
34:2c:111:LEU:HD11	34:2c:144:SER:O	2.22	0.40
36:2e:28:PHE:O	36:2e:47:LYS:HA	2.21	0.40
41:2j:11:PHE:HE1	41:2j:67:THR:HG22	1.86	0.40
47:2p:1:MET:HE2	47:2p:1:MET:N	2.36	0.40
47:2p:28:ARG:HG2	47:2p:28:ARG:HH11	1.86	0.40
56:2y:15:G:N1	56:2y:48:C:N3	2.67	0.40
56:2y:18:G:N1	56:2y:55:PSU:C4	2.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	1D	273/276 (99%)	258 (94%)	15 (6%)	0	100 100
3	2D	273/276 (99%)	261 (96%)	12 (4%)	0	100 100
4	1E	202/206 (98%)	192 (95%)	9 (4%)	1 (0%)	24 37
4	2E	202/206 (98%)	188 (93%)	13 (6%)	1 (0%)	24 37
5	1F	201/210 (96%)	194 (96%)	5 (2%)	2 (1%)	12 20
5	2F	201/210 (96%)	192 (96%)	6 (3%)	3 (2%)	8 12
6	1G	179/182 (98%)	170 (95%)	6 (3%)	3 (2%)	7 10
6	2G	179/182 (98%)	157 (88%)	16 (9%)	6 (3%)	3 2
7	1H	172/180 (96%)	162 (94%)	9 (5%)	1 (1%)	21 32
7	2H	172/180 (96%)	154 (90%)	17 (10%)	1 (1%)	21 32
8	1I	144/148 (97%)	121 (84%)	23 (16%)	0	100 100
8	2I	144/148 (97%)	118 (82%)	25 (17%)	1 (1%)	18 28
9	1N	138/140 (99%)	132 (96%)	6 (4%)	0	100 100
9	2N	138/140 (99%)	128 (93%)	9 (6%)	1 (1%)	18 28
10	1O	120/122 (98%)	114 (95%)	6 (5%)	0	100 100
10	2O	120/122 (98%)	112 (93%)	8 (7%)	0	100 100
11	1P	147/150 (98%)	131 (89%)	15 (10%)	1 (1%)	18 28
11	2P	147/150 (98%)	133 (90%)	10 (7%)	4 (3%)	4 4
12	1Q	139/141 (99%)	134 (96%)	5 (4%)	0	100 100
12	2Q	139/141 (99%)	127 (91%)	11 (8%)	1 (1%)	18 28
13	1R	116/118 (98%)	112 (97%)	4 (3%)	0	100 100
13	2R	116/118 (98%)	112 (97%)	4 (3%)	0	100 100
14	1S	108/112 (96%)	105 (97%)	3 (3%)	0	100 100
14	2S	108/112 (96%)	103 (95%)	3 (3%)	2 (2%)	6 8
15	1T	129/146 (88%)	124 (96%)	3 (2%)	2 (2%)	7 11

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
15	2T	129/146 (88%)	119 (92%)	10 (8%)	0	100 100
16	1U	114/118 (97%)	114 (100%)	0	0	100 100
16	2U	114/118 (97%)	114 (100%)	0	0	100 100
17	1V	99/101 (98%)	93 (94%)	4 (4%)	2 (2%)	6 7
17	2V	99/101 (98%)	91 (92%)	6 (6%)	2 (2%)	6 7
18	1W	110/113 (97%)	109 (99%)	1 (1%)	0	100 100
18	2W	110/113 (97%)	108 (98%)	2 (2%)	0	100 100
19	1X	93/96 (97%)	89 (96%)	3 (3%)	1 (1%)	11 18
19	2X	93/96 (97%)	87 (94%)	5 (5%)	1 (1%)	11 18
20	1Y	105/110 (96%)	99 (94%)	5 (5%)	1 (1%)	12 20
20	2Y	105/110 (96%)	100 (95%)	5 (5%)	0	100 100
21	1Z	148/206 (72%)	133 (90%)	14 (10%)	1 (1%)	18 28
21	2Z	156/206 (76%)	134 (86%)	18 (12%)	4 (3%)	4 4
22	10	81/85 (95%)	79 (98%)	2 (2%)	0	100 100
22	20	81/85 (95%)	77 (95%)	4 (5%)	0	100 100
23	11	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	11 18
23	21	95/98 (97%)	92 (97%)	3 (3%)	0	100 100
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100 100
24	22	68/72 (94%)	68 (100%)	0	0	100 100
25	13	57/60 (95%)	56 (98%)	1 (2%)	0	100 100
25	23	57/60 (95%)	53 (93%)	4 (7%)	0	100 100
26	14	67/71 (94%)	53 (79%)	10 (15%)	4 (6%)	1 0
26	24	67/71 (94%)	52 (78%)	11 (16%)	4 (6%)	1 0
27	15	57/60 (95%)	56 (98%)	1 (2%)	0	100 100
27	25	57/60 (95%)	56 (98%)	1 (2%)	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%)	61 (98%)	1 (2%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
31	19	35/37 (95%)	35 (100%)	0	0	100 100
31	29	35/37 (95%)	35 (100%)	0	0	100 100
33	1b	229/256 (90%)	195 (85%)	27 (12%)	7 (3%)	3 3
33	2b	229/256 (90%)	191 (83%)	31 (14%)	7 (3%)	3 3
34	1c	204/239 (85%)	191 (94%)	13 (6%)	0	100 100
34	2c	204/239 (85%)	182 (89%)	18 (9%)	4 (2%)	6 7
35	1d	206/209 (99%)	196 (95%)	9 (4%)	1 (0%)	24 37
35	2d	206/209 (99%)	195 (95%)	11 (5%)	0	100 100
36	1e	146/162 (90%)	128 (88%)	15 (10%)	3 (2%)	5 7
36	2e	146/162 (90%)	134 (92%)	11 (8%)	1 (1%)	18 28
37	1f	98/101 (97%)	93 (95%)	5 (5%)	0	100 100
37	2f	98/101 (97%)	95 (97%)	3 (3%)	0	100 100
38	1g	153/156 (98%)	140 (92%)	11 (7%)	2 (1%)	9 14
38	2g	153/156 (98%)	136 (89%)	14 (9%)	3 (2%)	6 7
39	1h	135/138 (98%)	129 (96%)	5 (4%)	1 (1%)	18 28
39	2h	135/138 (98%)	127 (94%)	8 (6%)	0	100 100
40	1i	125/128 (98%)	112 (90%)	12 (10%)	1 (1%)	16 25
40	2i	125/128 (98%)	109 (87%)	14 (11%)	2 (2%)	7 11
41	1j	95/105 (90%)	83 (87%)	10 (10%)	2 (2%)	5 7
41	2j	94/105 (90%)	82 (87%)	9 (10%)	3 (3%)	3 3
42	1k	112/129 (87%)	103 (92%)	8 (7%)	1 (1%)	14 22
42	2k	112/129 (87%)	105 (94%)	5 (4%)	2 (2%)	6 9
43	1l	119/132 (90%)	112 (94%)	7 (6%)	0	100 100
43	2l	119/132 (90%)	111 (93%)	7 (6%)	1 (1%)	16 25
44	1m	121/126 (96%)	106 (88%)	13 (11%)	2 (2%)	7 10
44	2m	120/126 (95%)	107 (89%)	12 (10%)	1 (1%)	16 25
45	1n	58/61 (95%)	56 (97%)	2 (3%)	0	100 100
45	2n	58/61 (95%)	53 (91%)	4 (7%)	1 (2%)	7 10
46	1o	86/89 (97%)	81 (94%)	5 (6%)	0	100 100
46	2o	86/89 (97%)	82 (95%)	4 (5%)	0	100 100
47	1p	80/88 (91%)	74 (92%)	6 (8%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
47	2p	80/88 (91%)	75 (94%)	5 (6%)	0	100 100
48	1q	97/105 (92%)	91 (94%)	5 (5%)	1 (1%)	12 20
48	2q	97/105 (92%)	91 (94%)	5 (5%)	1 (1%)	12 20
49	1r	66/88 (75%)	60 (91%)	6 (9%)	0	100 100
49	2r	66/88 (75%)	62 (94%)	4 (6%)	0	100 100
50	1s	81/93 (87%)	71 (88%)	9 (11%)	1 (1%)	10 16
50	2s	81/93 (87%)	68 (84%)	13 (16%)	0	100 100
51	1t	94/106 (89%)	84 (89%)	6 (6%)	4 (4%)	2 1
51	2t	94/106 (89%)	85 (90%)	6 (6%)	3 (3%)	3 3
52	1u	21/27 (78%)	19 (90%)	2 (10%)	0	100 100
52	2u	21/27 (78%)	19 (90%)	2 (10%)	0	100 100
All	All	11370/12128 (94%)	10541 (93%)	723 (6%)	106 (1%)	14 22

All (106) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
21	1Z	53	ILE
23	11	3	LYS
33	1b	22	LYS
33	1b	126	GLU
35	1d	173	TRP
40	1i	54	ASP
44	1m	67	GLU
44	1m	107	ALA
5	2F	130	ALA
33	2b	17	PHE
38	2g	55	GLY
38	2g	80	VAL
41	2j	79	ARG
44	2m	67	GLU
5	1F	15	SER
6	1G	50	ALA
19	1X	93	GLU
26	14	47	GLN
26	14	49	PHE
26	14	62	ARG
33	1b	17	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	1e	85	GLY
41	1j	79	ARG
42	1k	49	GLY
48	1q	68	ARG
50	1s	81	ARG
51	1t	100	ILE
6	2G	84	LYS
17	2V	53	GLU
17	2V	79	VAL
21	2Z	146	ILE
26	24	45	GLY
33	2b	123	ALA
34	2c	107	GLN
34	2c	156	ARG
42	2k	49	GLY
48	2q	68	ARG
4	1E	52	LEU
6	1G	43	LEU
17	1V	43	GLU
17	1V	79	VAL
20	1Y	54	LYS
33	1b	231	GLU
38	1g	6	ARG
51	1t	47	GLY
6	2G	43	LEU
6	2G	50	ALA
11	2P	44	GLY
12	2Q	16	ARG
19	2X	93	GLU
21	2Z	52	SER
21	2Z	144	LEU
26	24	49	PHE
26	24	61	ARG
33	2b	20	GLU
33	2b	21	ARG
33	2b	126	GLU
34	2c	95	THR
38	2g	52	GLU
41	2j	78	ASN
6	1G	49	ASP
15	1T	37	GLY
26	14	61	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	1b	8	LYS
33	1b	124	SER
36	1e	86	ALA
4	2E	52	LEU
5	2F	18	ARG
6	2G	42	GLY
9	2N	2	LYS
11	2P	29	LYS
33	2b	9	GLU
40	2i	56	LEU
43	2l	91	LYS
51	2t	10	LEU
51	2t	47	GLY
7	1H	126	PRO
11	1P	45	LEU
15	1T	55	ASN
41	1j	78	ASN
51	1t	95	ALA
5	2F	21	ALA
7	2H	47	GLU
8	2I	117	GLU
11	2P	45	LEU
34	2c	53	ALA
40	2i	121	ARG
36	1e	69	VAL
6	2G	51	ARG
6	2G	124	SER
26	24	65	ASP
41	2j	75	ILE
42	2k	105	VAL
11	2P	122	PRO
14	2S	96	GLY
51	2t	102	GLY
38	1g	55	GLY
51	1t	102	GLY
21	2Z	165	VAL
33	2b	231	GLU
36	2e	96	PRO
45	2n	14	PRO
39	1h	73	ASP
14	2S	109	GLY
33	1b	125	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	1D	215/218 (99%)	202 (94%)	13 (6%)	17 31
3	2D	215/218 (99%)	209 (97%)	6 (3%)	38 60
4	1E	164/166 (99%)	157 (96%)	7 (4%)	26 44
4	2E	164/166 (99%)	156 (95%)	8 (5%)	22 39
5	1F	160/166 (96%)	143 (89%)	17 (11%)	6 10
5	2F	159/166 (96%)	149 (94%)	10 (6%)	16 29
6	1G	143/156 (92%)	129 (90%)	14 (10%)	7 12
6	2G	143/156 (92%)	126 (88%)	17 (12%)	5 7
7	1H	144/148 (97%)	134 (93%)	10 (7%)	14 24
7	2H	144/148 (97%)	125 (87%)	19 (13%)	4 5
8	1I	113/124 (91%)	94 (83%)	19 (17%)	2 3
8	2I	105/124 (85%)	92 (88%)	13 (12%)	4 6
9	1N	118/119 (99%)	109 (92%)	9 (8%)	12 21
9	2N	118/119 (99%)	108 (92%)	10 (8%)	10 16
10	1O	100/100 (100%)	99 (99%)	1 (1%)	68 84
10	2O	100/100 (100%)	94 (94%)	6 (6%)	17 31
11	1P	115/116 (99%)	106 (92%)	9 (8%)	11 20
11	2P	115/116 (99%)	106 (92%)	9 (8%)	11 20
12	1Q	111/111 (100%)	103 (93%)	8 (7%)	13 23
12	2Q	111/111 (100%)	105 (95%)	6 (5%)	20 35
13	1R	101/101 (100%)	94 (93%)	7 (7%)	14 24
13	2R	101/101 (100%)	97 (96%)	4 (4%)	28 47
14	1S	86/88 (98%)	79 (92%)	7 (8%)	11 18
14	2S	85/88 (97%)	79 (93%)	6 (7%)	13 23
15	1T	115/127 (91%)	107 (93%)	8 (7%)	14 24
15	2T	113/127 (89%)	107 (95%)	6 (5%)	20 36

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
16	1U	93/94 (99%)	86 (92%)	7 (8%)	12 21
16	2U	93/94 (99%)	90 (97%)	3 (3%)	34 56
17	1V	80/82 (98%)	77 (96%)	3 (4%)	29 49
17	2V	80/82 (98%)	73 (91%)	7 (9%)	9 15
18	1W	90/92 (98%)	85 (94%)	5 (6%)	19 33
18	2W	90/92 (98%)	86 (96%)	4 (4%)	25 43
19	1X	77/78 (99%)	73 (95%)	4 (5%)	21 36
19	2X	77/78 (99%)	74 (96%)	3 (4%)	28 48
20	1Y	85/91 (93%)	75 (88%)	10 (12%)	5 7
20	2Y	85/91 (93%)	79 (93%)	6 (7%)	13 23
21	1Z	135/179 (75%)	123 (91%)	12 (9%)	9 15
21	2Z	137/179 (76%)	121 (88%)	16 (12%)	5 7
22	10	65/67 (97%)	65 (100%)	0	100 100
22	20	65/67 (97%)	63 (97%)	2 (3%)	35 57
23	11	80/83 (96%)	77 (96%)	3 (4%)	29 49
23	21	80/83 (96%)	78 (98%)	2 (2%)	42 64
24	12	65/67 (97%)	61 (94%)	4 (6%)	16 29
24	22	65/67 (97%)	59 (91%)	6 (9%)	8 14
25	13	51/52 (98%)	48 (94%)	3 (6%)	18 31
25	23	50/52 (96%)	47 (94%)	3 (6%)	17 31
26	14	59/63 (94%)	55 (93%)	4 (7%)	14 25
26	24	53/63 (84%)	41 (77%)	12 (23%)	1 1
27	15	50/52 (96%)	48 (96%)	2 (4%)	28 47
27	25	50/52 (96%)	47 (94%)	3 (6%)	17 31
28	16	51/52 (98%)	49 (96%)	2 (4%)	28 48
28	26	50/52 (96%)	43 (86%)	7 (14%)	3 4
29	17	41/42 (98%)	38 (93%)	3 (7%)	13 22
29	27	41/42 (98%)	38 (93%)	3 (7%)	13 22
30	18	54/55 (98%)	52 (96%)	2 (4%)	30 51
30	28	54/55 (98%)	52 (96%)	2 (4%)	30 51
31	19	34/34 (100%)	33 (97%)	1 (3%)	37 60

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
31	29	34/34 (100%)	33 (97%)	1 (3%)	37 60
33	1b	192/220 (87%)	168 (88%)	24 (12%)	4 6
33	2b	187/220 (85%)	164 (88%)	23 (12%)	4 6
34	1c	142/188 (76%)	129 (91%)	13 (9%)	8 14
34	2c	140/188 (74%)	126 (90%)	14 (10%)	7 11
35	1d	169/181 (93%)	147 (87%)	22 (13%)	4 5
35	2d	173/181 (96%)	157 (91%)	16 (9%)	8 14
36	1e	113/123 (92%)	101 (89%)	12 (11%)	6 10
36	2e	114/123 (93%)	102 (90%)	12 (10%)	6 10
37	1f	84/90 (93%)	78 (93%)	6 (7%)	13 23
37	2f	85/90 (94%)	76 (89%)	9 (11%)	6 10
38	1g	119/127 (94%)	106 (89%)	13 (11%)	6 9
38	2g	120/127 (94%)	109 (91%)	11 (9%)	8 14
39	1h	114/119 (96%)	106 (93%)	8 (7%)	14 24
39	2h	114/119 (96%)	106 (93%)	8 (7%)	14 24
40	1i	90/99 (91%)	80 (89%)	10 (11%)	6 9
40	2i	89/99 (90%)	78 (88%)	11 (12%)	4 6
41	1j	66/92 (72%)	55 (83%)	11 (17%)	2 3
41	2j	69/92 (75%)	59 (86%)	10 (14%)	3 4
42	1k	82/99 (83%)	74 (90%)	8 (10%)	7 12
42	2k	83/99 (84%)	79 (95%)	4 (5%)	23 40
43	1l	96/108 (89%)	92 (96%)	4 (4%)	26 45
43	2l	96/108 (89%)	90 (94%)	6 (6%)	16 29
44	1m	93/101 (92%)	82 (88%)	11 (12%)	5 7
44	2m	92/101 (91%)	84 (91%)	8 (9%)	9 16
45	1n	49/50 (98%)	46 (94%)	3 (6%)	17 30
45	2n	49/50 (98%)	46 (94%)	3 (6%)	17 30
46	1o	78/80 (98%)	74 (95%)	4 (5%)	21 37
46	2o	78/80 (98%)	71 (91%)	7 (9%)	9 15
47	1p	69/74 (93%)	61 (88%)	8 (12%)	5 8
47	2p	68/74 (92%)	63 (93%)	5 (7%)	13 22

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
48	1q	94/97 (97%)	87 (93%)	7 (7%)	13 22
48	2q	94/97 (97%)	89 (95%)	5 (5%)	20 36
49	1r	59/77 (77%)	53 (90%)	6 (10%)	7 11
49	2r	59/77 (77%)	53 (90%)	6 (10%)	7 11
50	1s	69/80 (86%)	62 (90%)	7 (10%)	7 11
50	2s	67/80 (84%)	53 (79%)	14 (21%)	1 1
51	1t	70/82 (85%)	67 (96%)	3 (4%)	26 44
51	2t	70/82 (85%)	67 (96%)	3 (4%)	26 44
52	1u	18/22 (82%)	16 (89%)	2 (11%)	6 9
52	2u	18/22 (82%)	16 (89%)	2 (11%)	6 9
All	All	9303/10064 (92%)	8550 (92%)	753 (8%)	11 18

All (753) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	3	VAL
3	1D	27	THR
3	1D	32	SER
3	1D	37	LEU
3	1D	131	LEU
3	1D	142	VAL
3	1D	154	LYS
3	1D	173	VAL
3	1D	221	VAL
3	1D	229	VAL
3	1D	242	ARG
3	1D	259	THR
3	1D	273	ARG
4	1E	9	VAL
4	1E	34	VAL
4	1E	78	LEU
4	1E	97	LYS
4	1E	116	VAL
4	1E	184	VAL
4	1E	195	LEU
5	1F	24	LEU
5	1F	33	LEU
5	1F	53	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	1F	57	VAL
5	1F	70	THR
5	1F	72	ARG
5	1F	74	ARG
5	1F	88	VAL
5	1F	106	ARG
5	1F	132	VAL
5	1F	140	LEU
5	1F	158	THR
5	1F	162	LEU
5	1F	168	ARG
5	1F	183	VAL
5	1F	192	LEU
5	1F	201	VAL
6	1G	5	VAL
6	1G	7	LEU
6	1G	31	VAL
6	1G	36	LYS
6	1G	43	LEU
6	1G	82	LEU
6	1G	109	VAL
6	1G	136	ARG
6	1G	139	LEU
6	1G	140	ILE
6	1G	145	THR
6	1G	148	MET
6	1G	159	VAL
6	1G	174	GLU
7	1H	45	VAL
7	1H	56	SER
7	1H	71	LEU
7	1H	76	VAL
7	1H	81	GLU
7	1H	88	LEU
7	1H	95	ARG
7	1H	124	GLU
7	1H	129	THR
7	1H	172	LYS
8	1I	5	LEU
8	1I	9	LEU
8	1I	10	GLU
8	1I	12	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	1I	20	ASP
8	1I	50	ARG
8	1I	75	LEU
8	1I	77	LEU
8	1I	78	THR
8	1I	85	GLU
8	1I	87	LYS
8	1I	92	VAL
8	1I	108	THR
8	1I	110	ASP
8	1I	122	GLU
8	1I	129	THR
8	1I	133	HIS
8	1I	140	LEU
8	1I	144	VAL
9	1N	1	MET
9	1N	9	VAL
9	1N	10	GLU
9	1N	14	VAL
9	1N	28	THR
9	1N	48	MET
9	1N	62	VAL
9	1N	96	GLU
9	1N	136	GLU
10	1O	106	LEU
11	1P	7	ARG
11	1P	40	SER
11	1P	45	LEU
11	1P	95	VAL
11	1P	99	LEU
11	1P	114	ILE
11	1P	125	VAL
11	1P	133	SER
11	1P	147	LEU
12	1Q	1	MET
12	1Q	7	MET
12	1Q	8	LYS
12	1Q	22	LYS
12	1Q	56	ARG
12	1Q	75	THR
12	1Q	109	VAL
12	1Q	110	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	1R	15	SER
13	1R	36	THR
13	1R	59	ASP
13	1R	67	LEU
13	1R	83	ILE
13	1R	91	GLN
13	1R	114	VAL
14	1S	14	VAL
14	1S	33	LYS
14	1S	46	VAL
14	1S	49	VAL
14	1S	69	VAL
14	1S	110	LEU
14	1S	111	GLU
15	1T	28	VAL
15	1T	29	ARG
15	1T	34	VAL
15	1T	36	GLU
15	1T	70	VAL
15	1T	82	LEU
15	1T	96	ARG
15	1T	125	ARG
16	1U	8	VAL
16	1U	17	ILE
16	1U	31	SER
16	1U	59	ARG
16	1U	60	LEU
16	1U	74	LEU
16	1U	84	LYS
17	1V	56	SER
17	1V	61	VAL
17	1V	79	VAL
18	1W	4	LYS
18	1W	11	ARG
18	1W	17	VAL
18	1W	67	ASP
18	1W	92	ARG
19	1X	1	MET
19	1X	35	THR
19	1X	66	LEU
19	1X	92	LEU
20	1Y	1	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	1Y	7	VAL
20	1Y	8	LYS
20	1Y	31	LEU
20	1Y	40	GLU
20	1Y	43	ASN
20	1Y	72	VAL
20	1Y	85	VAL
20	1Y	99	CYS
20	1Y	107	ASP
21	1Z	33	LEU
21	1Z	42	VAL
21	1Z	49	ARG
21	1Z	56	VAL
21	1Z	61	LEU
21	1Z	72	ARG
21	1Z	124	ILE
21	1Z	154	ASP
21	1Z	155	LEU
21	1Z	162	GLU
21	1Z	170	THR
21	1Z	171	ILE
23	11	3	LYS
23	11	40	ARG
23	11	59	THR
24	12	19	VAL
24	12	53	LEU
24	12	65	ASN
24	12	70	GLN
25	13	23	LEU
25	13	34	GLU
25	13	54	VAL
26	14	49	PHE
26	14	53	GLU
26	14	63	TYR
26	14	67	TYR
27	15	6	VAL
27	15	40	LYS
28	16	4	GLU
28	16	48	VAL
29	17	24	THR
29	17	43	THR
29	17	46	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	18	14	VAL
30	18	23	VAL
31	19	28	GLU
33	1b	7	VAL
33	1b	11	LEU
33	1b	12	GLU
33	1b	16	HIS
33	1b	21	ARG
33	1b	35	GLU
33	1b	43	ASP
33	1b	44	LEU
33	1b	45	GLN
33	1b	54	THR
33	1b	67	THR
33	1b	73	THR
33	1b	80	ILE
33	1b	90	MET
33	1b	112	VAL
33	1b	117	GLU
33	1b	121	LEU
33	1b	127	ILE
33	1b	130	ARG
33	1b	142	LEU
33	1b	150	SER
33	1b	196	LEU
33	1b	208	ILE
33	1b	222	ILE
34	1c	3	ASN
34	1c	32	LEU
34	1c	58	GLU
34	1c	70	VAL
34	1c	77	ILE
34	1c	82	GLU
34	1c	85	ARG
34	1c	89	GLU
34	1c	102	ASN
34	1c	164	ARG
34	1c	178	LEU
34	1c	195	VAL
34	1c	207	VAL
35	1d	18	LYS
35	1d	19	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	1d	31	CYS
35	1d	56	VAL
35	1d	59	ARG
35	1d	76	ARG
35	1d	88	VAL
35	1d	112	VAL
35	1d	119	GLN
35	1d	122	ARG
35	1d	127	THR
35	1d	135	LEU
35	1d	140	VAL
35	1d	157	LEU
35	1d	158	ILE
35	1d	170	VAL
35	1d	175	SER
35	1d	177	ASP
35	1d	178	VAL
35	1d	187	ARG
35	1d	194	LEU
35	1d	209	ARG
36	1e	8	GLU
36	1e	20	GLN
36	1e	31	LEU
36	1e	41	VAL
36	1e	63	ARG
36	1e	64	ARG
36	1e	68	GLU
36	1e	78	HIS
36	1e	79	GLU
36	1e	91	LEU
36	1e	126	ARG
36	1e	131	ILE
37	1f	55	ASP
37	1f	57	GLN
37	1f	72	VAL
37	1f	73	ASN
37	1f	75	LEU
37	1f	78	GLU
38	1g	12	LEU
38	1g	16	LEU
38	1g	27	ILE
38	1g	50	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	1g	57	GLU
38	1g	61	VAL
38	1g	78	ARG
38	1g	104	LEU
38	1g	110	GLN
38	1g	113	GLU
38	1g	115	ARG
38	1g	120	ILE
38	1g	131	LYS
39	1h	38	ILE
39	1h	39	LEU
39	1h	51	VAL
39	1h	52	ASP
39	1h	54	ASP
39	1h	112	LEU
39	1h	121	ASP
39	1h	133	LEU
40	1i	23	ASN
40	1i	42	ARG
40	1i	64	THR
40	1i	88	TYR
40	1i	96	LEU
40	1i	97	LYS
40	1i	103	THR
40	1i	104	ARG
40	1i	105	ASP
40	1i	128	ARG
41	1j	30	SER
41	1j	35	SER
41	1j	38	ILE
41	1j	42	THR
41	1j	43	ARG
41	1j	44	VAL
41	1j	46	ARG
41	1j	49	VAL
41	1j	81	THR
41	1j	92	THR
41	1j	95	GLU
42	1k	14	VAL
42	1k	31	THR
42	1k	48	ILE
42	1k	87	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
42	1k	108	ILE
42	1k	109	VAL
42	1k	114	VAL
42	1k	117	ASN
43	1l	47	LYS
43	1l	58	VAL
43	1l	62	SER
43	1l	83	VAL
44	1m	3	ARG
44	1m	4	ILE
44	1m	11	ARG
44	1m	14	ARG
44	1m	49	THR
44	1m	64	TRP
44	1m	70	LEU
44	1m	94	ARG
44	1m	106	ASN
44	1m	117	VAL
44	1m	121	LYS
45	1n	4	LYS
45	1n	18	VAL
45	1n	33	VAL
46	1o	39	LEU
46	1o	84	LYS
46	1o	87	ILE
46	1o	88	ARG
47	1p	16	HIS
47	1p	20	VAL
47	1p	27	LYS
47	1p	35	LYS
47	1p	42	ARG
47	1p	61	SER
47	1p	62	VAL
47	1p	67	THR
48	1q	14	LYS
48	1q	15	MET
48	1q	52	LYS
48	1q	53	LEU
48	1q	60	ILE
48	1q	85	VAL
48	1q	96	GLU
49	1r	26	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
49	1r	31	LEU
49	1r	35	ARG
49	1r	36	ASN
49	1r	61	LYS
49	1r	84	LYS
50	1s	4	SER
50	1s	6	LYS
50	1s	12	ASP
50	1s	18	LYS
50	1s	28	LYS
50	1s	41	VAL
50	1s	48	THR
51	1t	10	LEU
51	1t	24	LEU
51	1t	100	ILE
52	1u	9	ARG
52	1u	15	ARG
3	2D	37	LEU
3	2D	38	LYS
3	2D	71	ASP
3	2D	142	VAL
3	2D	242	ARG
3	2D	270	ILE
4	2E	7	VAL
4	2E	9	VAL
4	2E	34	VAL
4	2E	38	THR
4	2E	77	ILE
4	2E	78	LEU
4	2E	90	THR
4	2E	116	VAL
5	2F	50	SER
5	2F	106	ARG
5	2F	145	GLU
5	2F	157	VAL
5	2F	161	GLU
5	2F	162	LEU
5	2F	165	ARG
5	2F	175	THR
5	2F	192	LEU
5	2F	201	VAL
6	2G	5	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	2G	22	ARG
6	2G	28	VAL
6	2G	43	LEU
6	2G	45	GLU
6	2G	53	LEU
6	2G	60	LEU
6	2G	62	LEU
6	2G	70	VAL
6	2G	79	ASN
6	2G	86	MET
6	2G	91	ARG
6	2G	124	SER
6	2G	137	GLU
6	2G	145	THR
6	2G	159	VAL
6	2G	165	THR
7	2H	13	LYS
7	2H	15	VAL
7	2H	16	SER
7	2H	23	ARG
7	2H	43	VAL
7	2H	45	VAL
7	2H	49	VAL
7	2H	51	ARG
7	2H	63	SER
7	2H	71	LEU
7	2H	72	ILE
7	2H	88	LEU
7	2H	95	ARG
7	2H	101	ARG
7	2H	104	GLU
7	2H	119	GLU
7	2H	127	GLU
7	2H	129	THR
7	2H	136	ILE
8	2I	15	VAL
8	2I	38	LEU
8	2I	44	LEU
8	2I	51	ILE
8	2I	58	LEU
8	2I	61	ARG
8	2I	77	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	2I	87	LYS
8	2I	92	VAL
8	2I	108	THR
8	2I	116	LEU
8	2I	117	GLU
8	2I	127	VAL
9	2N	1	MET
9	2N	8	GLN
9	2N	9	VAL
9	2N	28	THR
9	2N	38	HIS
9	2N	48	MET
9	2N	61	ARG
9	2N	62	VAL
9	2N	68	GLU
9	2N	137	LYS
10	2O	9	GLU
10	2O	28	SER
10	2O	58	VAL
10	2O	69	ILE
10	2O	91	LEU
10	2O	116	SER
11	2P	45	LEU
11	2P	70	GLN
11	2P	86	LYS
11	2P	95	VAL
11	2P	98	GLU
11	2P	119	GLU
11	2P	133	SER
11	2P	135	LEU
11	2P	147	LEU
12	2Q	12	GLN
12	2Q	21	THR
12	2Q	22	LYS
12	2Q	56	ARG
12	2Q	106	VAL
12	2Q	110	THR
13	2R	6	SER
13	2R	36	THR
13	2R	67	LEU
13	2R	114	VAL
14	2S	36	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	2S	52	SER
14	2S	58	LEU
14	2S	64	GLU
14	2S	103	GLU
14	2S	110	LEU
15	2T	23	ARG
15	2T	28	VAL
15	2T	87	ASP
15	2T	89	VAL
15	2T	96	ARG
15	2T	104	ASN
16	2U	17	ILE
16	2U	74	LEU
16	2U	100	VAL
17	2V	7	THR
17	2V	38	LEU
17	2V	57	VAL
17	2V	61	VAL
17	2V	79	VAL
17	2V	98	GLU
17	2V	100	ARG
18	2W	11	ARG
18	2W	17	VAL
18	2W	67	ASP
18	2W	78	GLU
19	2X	66	LEU
19	2X	72	LYS
19	2X	87	GLN
20	2Y	3	VAL
20	2Y	7	VAL
20	2Y	11	ASP
20	2Y	40	GLU
20	2Y	72	VAL
20	2Y	99	CYS
21	2Z	6	LYS
21	2Z	33	LEU
21	2Z	42	VAL
21	2Z	58	VAL
21	2Z	91	LEU
21	2Z	96	VAL
21	2Z	98	MET
21	2Z	100	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	2Z	121	HIS
21	2Z	146	ILE
21	2Z	154	ASP
21	2Z	155	LEU
21	2Z	161	VAL
21	2Z	170	THR
21	2Z	171	ILE
21	2Z	174	VAL
22	20	10	THR
22	20	11	ARG
23	21	40	ARG
23	21	59	THR
24	22	11	GLU
24	22	19	VAL
24	22	25	VAL
24	22	51	ARG
24	22	53	LEU
24	22	70	GLN
25	23	29	ARG
25	23	31	LEU
25	23	56	VAL
26	24	13	ARG
26	24	24	THR
26	24	27	THR
26	24	33	VAL
26	24	34	GLU
26	24	44	THR
26	24	49	PHE
26	24	52	THR
26	24	56	VAL
26	24	59	PHE
26	24	63	TYR
26	24	67	TYR
27	25	6	VAL
27	25	40	LYS
27	25	58	LEU
28	26	5	VAL
28	26	6	ARG
28	26	13	CYS
28	26	19	ARG
28	26	30	THR
28	26	32	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	26	48	VAL
29	27	41	ARG
29	27	43	THR
29	27	46	VAL
30	28	14	VAL
30	28	23	VAL
31	29	28	GLU
33	2b	7	VAL
33	2b	8	LYS
33	2b	9	GLU
33	2b	11	LEU
33	2b	16	HIS
33	2b	48	MET
33	2b	53	ARG
33	2b	68	ILE
33	2b	71	VAL
33	2b	76	GLN
33	2b	83	MET
33	2b	94	ASN
33	2b	107	THR
33	2b	111	ARG
33	2b	112	VAL
33	2b	115	LEU
33	2b	127	ILE
33	2b	136	VAL
33	2b	137	ARG
33	2b	157	ARG
33	2b	185	ILE
33	2b	189	ASP
33	2b	230	VAL
34	2c	15	THR
34	2c	21	ARG
34	2c	44	GLU
34	2c	47	LEU
34	2c	70	VAL
34	2c	116	VAL
34	2c	132	ARG
34	2c	152	ILE
34	2c	172	ARG
34	2c	182	ILE
34	2c	190	ARG
34	2c	191	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	2c	196	LEU
34	2c	198	VAL
35	2d	8	VAL
35	2d	31	CYS
35	2d	45	GLN
35	2d	52	SER
35	2d	76	ARG
35	2d	85	LYS
35	2d	96	LEU
35	2d	99	SER
35	2d	112	VAL
35	2d	119	GLN
35	2d	127	THR
35	2d	135	LEU
35	2d	150	GLU
35	2d	178	VAL
35	2d	187	ARG
35	2d	188	LEU
36	2e	9	LYS
36	2e	11	ILE
36	2e	12	LEU
36	2e	13	ILE
36	2e	18	ARG
36	2e	20	GLN
36	2e	31	LEU
36	2e	38	GLN
36	2e	41	VAL
36	2e	51	VAL
36	2e	55	VAL
36	2e	136	MET
37	2f	17	SER
37	2f	19	LEU
37	2f	21	LEU
37	2f	37	VAL
37	2f	63	TYR
37	2f	69	GLU
37	2f	70	ASP
37	2f	75	LEU
37	2f	81	ILE
38	2g	9	VAL
38	2g	23	VAL
38	2g	36	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	2g	45	ASP
38	2g	49	ILE
38	2g	52	GLU
38	2g	59	LEU
38	2g	78	ARG
38	2g	79	ARG
38	2g	114	ARG
38	2g	139	GLU
39	2h	39	LEU
39	2h	51	VAL
39	2h	52	ASP
39	2h	56	LYS
39	2h	86	ILE
39	2h	109	ILE
39	2h	112	LEU
39	2h	122	ARG
40	2i	27	THR
40	2i	29	ASN
40	2i	54	ASP
40	2i	56	LEU
40	2i	63	ILE
40	2i	65	VAL
40	2i	66	ARG
40	2i	89	ASN
40	2i	102	LEU
40	2i	113	LYS
40	2i	128	ARG
41	2j	8	LEU
41	2j	16	LEU
41	2j	29	ARG
41	2j	38	ILE
41	2j	44	VAL
41	2j	46	ARG
41	2j	66	ARG
41	2j	71	LEU
41	2j	72	VAL
41	2j	81	THR
42	2k	14	VAL
42	2k	48	ILE
42	2k	104	GLN
42	2k	105	VAL
43	2l	18	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
43	2l	42	THR
43	2l	43	VAL
43	2l	62	SER
43	2l	65	GLU
43	2l	83	VAL
44	2m	4	ILE
44	2m	15	VAL
44	2m	27	LYS
44	2m	32	GLU
44	2m	81	LEU
44	2m	90	LEU
44	2m	103	THR
44	2m	117	VAL
45	2n	18	VAL
45	2n	22	THR
45	2n	33	VAL
46	2o	7	GLU
46	2o	38	ARG
46	2o	39	LEU
46	2o	48	LYS
46	2o	84	LYS
46	2o	87	ILE
46	2o	88	ARG
47	2p	1	MET
47	2p	2	VAL
47	2p	20	VAL
47	2p	45	THR
47	2p	67	THR
48	2q	14	LYS
48	2q	36	ILE
48	2q	63	ARG
48	2q	76	LEU
48	2q	90	ILE
49	2r	25	THR
49	2r	26	LEU
49	2r	31	LEU
49	2r	66	LEU
49	2r	82	THR
49	2r	86	VAL
50	2s	4	SER
50	2s	20	LEU
50	2s	30	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	2s	31	ILE
50	2s	32	LYS
50	2s	37	ARG
50	2s	41	VAL
50	2s	45	VAL
50	2s	47	HIS
50	2s	48	THR
50	2s	49	ILE
50	2s	51	VAL
50	2s	71	LEU
50	2s	77	THR
51	2t	45	GLN
51	2t	46	GLU
51	2t	99	LEU
52	2u	7	ARG
52	2u	15	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (147) such sidechains are listed below:

Mol	Chain	Res	Type
4	1E	48	GLN
4	1E	121	ASN
5	1F	8	GLN
5	1F	69	HIS
5	1F	203	GLN
6	1G	26	GLN
8	1I	104	GLN
8	1I	139	GLN
9	1N	8	GLN
12	1Q	12	GLN
12	1Q	57	HIS
13	1R	13	HIS
13	1R	31	HIS
14	1S	95	HIS
15	1T	58	ASN
15	1T	84	GLN
16	1U	94	ASN
16	1U	104	GLN
19	1X	31	HIS
19	1X	82	GLN
20	1Y	6	HIS
20	1Y	43	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	1Z	55	HIS
21	1Z	73	GLN
21	1Z	151	HIS
23	11	19	GLN
24	12	9	GLN
24	12	65	ASN
25	13	32	GLN
33	1b	40	HIS
33	1b	95	GLN
33	1b	135	GLN
34	1c	6	HIS
34	1c	69	HIS
34	1c	102	ASN
34	1c	123	GLN
34	1c	162	GLN
34	1c	181	ASN
35	1d	116	GLN
35	1d	123	HIS
35	1d	201	GLN
36	1e	20	GLN
36	1e	78	HIS
36	1e	141	GLN
37	1f	32	ASN
37	1f	57	GLN
37	1f	73	ASN
37	1f	100	ASN
38	1g	13	GLN
38	1g	28	ASN
38	1g	106	GLN
40	1i	31	GLN
40	1i	34	ASN
40	1i	58	HIS
40	1i	124	GLN
41	1j	56	HIS
42	1k	116	HIS
43	1l	8	ASN
43	1l	99	HIS
44	1m	77	ASN
44	1m	92	HIS
47	1p	16	HIS
47	1p	76	GLN
50	1s	23	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	1s	47	HIS
50	1s	83	HIS
51	1t	16	HIS
51	1t	18	GLN
51	1t	75	ASN
4	2E	48	GLN
5	2F	40	GLN
5	2F	133	ASN
5	2F	203	GLN
6	2G	27	ASN
8	2I	105	HIS
9	2N	8	GLN
9	2N	94	HIS
10	2O	5	GLN
11	2P	70	GLN
12	2Q	12	GLN
13	2R	31	HIS
13	2R	71	GLN
14	2S	38	GLN
14	2S	68	GLN
15	2T	58	ASN
16	2U	94	ASN
19	2X	82	GLN
20	2Y	6	HIS
20	2Y	43	ASN
21	2Z	34	ASN
21	2Z	55	HIS
21	2Z	73	GLN
21	2Z	132	ASN
21	2Z	151	HIS
24	22	43	GLN
25	23	32	GLN
26	24	46	GLN
28	26	20	ASN
30	28	35	GLN
33	2b	37	ASN
33	2b	45	GLN
33	2b	76	GLN
33	2b	94	ASN
33	2b	95	GLN
33	2b	113	HIS
33	2b	135	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	2b	140	HIS
34	2c	6	HIS
34	2c	98	ASN
34	2c	162	GLN
35	2d	77	ASN
35	2d	116	GLN
35	2d	160	GLN
35	2d	199	ASN
36	2e	72	GLN
36	2e	73	ASN
36	2e	130	ASN
36	2e	141	GLN
37	2f	73	ASN
37	2f	100	ASN
38	2g	28	ASN
38	2g	68	ASN
38	2g	86	GLN
38	2g	148	ASN
40	2i	3	GLN
40	2i	38	GLN
40	2i	58	HIS
40	2i	117	HIS
41	2j	13	HIS
41	2j	33	GLN
41	2j	62	HIS
41	2j	69	ASN
42	2k	38	ASN
42	2k	104	GLN
43	2l	99	HIS
44	2m	40	ASN
44	2m	92	HIS
45	2n	49	HIS
46	2o	62	GLN
47	2p	76	GLN
49	2r	63	GLN
50	2s	47	HIS
50	2s	69	HIS
50	2s	83	HIS
51	2t	42	GLN
51	2t	75	ASN
51	2t	90	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	405 (14%)	30 (1%)
1	2A	2791/2915 (95%)	444 (15%)	26 (0%)
2	1B	119/121 (98%)	11 (9%)	0
2	2B	118/121 (97%)	21 (17%)	0
32	1a	1497/1521 (98%)	230 (15%)	0
32	2a	1501/1521 (98%)	253 (16%)	0
53	1v	12/24 (50%)	3 (25%)	0
53	2v	12/24 (50%)	3 (25%)	0
54	1w	71/76 (93%)	21 (29%)	0
54	2w	68/76 (89%)	22 (32%)	0
55	1x	75/77 (97%)	5 (6%)	0
55	2x	75/77 (97%)	5 (6%)	0
56	1y	72/76 (94%)	33 (45%)	0
56	2y	70/76 (92%)	25 (35%)	0
All	All	9345/9620 (97%)	1481 (15%)	56 (0%)

All (1481) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	15	G
1	1A	34	C
1	1A	45	C
1	1A	55	G
1	1A	61	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	181	A
1	1A	182	A
1	1A	196	A
1	1A	197	A
1	1A	205	G
1	1A	215	G
1	1A	216	A
1	1A	222	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	228	A
1	1A	229	A
1	1A	233	A
1	1A	248	G
1	1A	269	U
1	1A	271(K)	U
1	1A	271(L)	U
1	1A	271(M)	G
1	1A	271(O)	C
1	1A	271(S)	G
1	1A	272(A)	U
1	1A	272(B)	G
1	1A	272(I)	U
1	1A	275	G
1	1A	279	C
1	1A	283	A
1	1A	311	A
1	1A	329	G
1	1A	330	A
1	1A	352	G
1	1A	353	G
1	1A	363	G
1	1A	363(B)	G
1	1A	386	G
1	1A	396	G
1	1A	405	U
1	1A	411	G
1	1A	412	A
1	1A	421	U
1	1A	428	A
1	1A	444	C
1	1A	448	U
1	1A	456	C
1	1A	457	A
1	1A	481	G
1	1A	505	A
1	1A	509	C
1	1A	530	G
1	1A	531	C
1	1A	532	A
1	1A	533	G
1	1A	545	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	549	G
1	1A	563	G
1	1A	573	G
1	1A	575	A
1	1A	592	G
1	1A	603	A
1	1A	604	G
1	1A	607	U
1	1A	614(B)	G
1	1A	615	G
1	1A	627	A
1	1A	637	A
1	1A	645	C
1	1A	646	A
1	1A	652(D)	C
1	1A	652(E)	G
1	1A	652(F)	G
1	1A	669	G
1	1A	686	G
1	1A	717	G
1	1A	730	C
1	1A	746	A
1	1A	747	U
1	1A	764	A
1	1A	765	G
1	1A	775	G
1	1A	776	G
1	1A	782	A
1	1A	784	A
1	1A	785	G
1	1A	789	A
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	882	G
1	1A	883	G
1	1A	884	C
1	1A	885	C
1	1A	886	C
1	1A	887	A
1	1A	889	C
1	1A	890	A
1	1A	893	C
1	1A	894	C
1	1A	896	A
1	1A	897	C
1	1A	898	C
1	1A	899	A
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	1008	C
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	1038	C
1	1A	1040	C
1	1A	1044	G
1	1A	1046	A
1	1A	1047	G
1	1A	1048	A
1	1A	1054	A
1	1A	1055	G
1	1A	1057	A
1	1A	1058	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1059	G
1	1A	1063	G
1	1A	1066	U
1	1A	1071	G
1	1A	1073	A
1	1A	1075	C
1	1A	1076	C
1	1A	1078	U
1	1A	1079	C
1	1A	1081	U
1	1A	1082	U
1	1A	1083	U
1	1A	1087	G
1	1A	1088	A
1	1A	1089	G
1	1A	1090	U
1	1A	1093	G
1	1A	1094	U
1	1A	1097	U
1	1A	1098	A
1	1A	1100	C
1	1A	1101	U
1	1A	1110	G
1	1A	1112	G
1	1A	1115	G
1	1A	1116	C
1	1A	1128	A
1	1A	1135	C
1	1A	1136	G
1	1A	1155	A
1	1A	1171	G
1	1A	1173	G
1	1A	1174	A
1	1A	1175	U
1	1A	1176	G
1	1A	1177	A
1	1A	1178	C
1	1A	1218	C
1	1A	1253	A
1	1A	1256	G
1	1A	1271	G
1	1A	1272	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1273	U
1	1A	1281	G
1	1A	1300	U
1	1A	1301	A
1	1A	1303	G
1	1A	1359	A
1	1A	1360	A
1	1A	1365	A
1	1A	1370	C
1	1A	1380	G
1	1A	1384	A
1	1A	1385	G
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	1461	G
1	1A	1467	C
1	1A	1482	G
1	1A	1493	C
1	1A	1494	A
1	1A	1508	A
1	1A	1509	C
1	1A	1509(A)	A
1	1A	1539	G
1	1A	1540	U
1	1A	1542	A
1	1A	1558	A
1	1A	1566	A
1	1A	1569	A
1	1A	1578	U
1	1A	1580	A
1	1A	1584	C
1	1A	1608	A
1	1A	1610	A
1	1A	1648	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1674	G
1	1A	1696	G
1	1A	1700	A
1	1A	1701	A
1	1A	1703	G
1	1A	1722	A
1	1A	1756	G
1	1A	1762	A
1	1A	1763	G
1	1A	1764	G
1	1A	1773	A
1	1A	1780	A
1	1A	1782	C
1	1A	1791	A
1	1A	1800	C
1	1A	1801	G
1	1A	1816	G
1	1A	1817	G
1	1A	1829	A
1	1A	1839	G
1	1A	1847	A
1	1A	1877	A
1	1A	1878	G
1	1A	1889	A
1	1A	1900	A
1	1A	1906	G
1	1A	1929	G
1	1A	1930	G
1	1A	1937	A
1	1A	1938	A
1	1A	1955	U
1	1A	1963	U
1	1A	1967	C
1	1A	1970	A
1	1A	1971	A
1	1A	1972	A
1	1A	1992	G
1	1A	1993	U
1	1A	1997	G
1	1A	2020	A
1	1A	2023	G
1	1A	2031	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2032	G
1	1A	2033	A
1	1A	2043	C
1	1A	2055	C
1	1A	2056	G
1	1A	2060	A
1	1A	2061	G
1	1A	2069	G
1	1A	2101	G
1	1A	2108	C
1	1A	2113	U
1	1A	2116	G
1	1A	2118	U
1	1A	2121	G
1	1A	2127	G
1	1A	2129	C
1	1A	2131	G
1	1A	2132	U
1	1A	2133	G
1	1A	2134	A
1	1A	2135	A
1	1A	2136	C
1	1A	2140	C
1	1A	2142	C
1	1A	2143	C
1	1A	2144	U
1	1A	2146	C
1	1A	2148	G
1	1A	2150	U
1	1A	2151	G
1	1A	2156	G
1	1A	2157	G
1	1A	2158	A
1	1A	2159	G
1	1A	2165	G
1	1A	2166	G
1	1A	2167	U
1	1A	2168	G
1	1A	2171	A
1	1A	2172	U
1	1A	2173	A
1	1A	2174	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2181	G
1	1A	2182	G
1	1A	2184	G
1	1A	2189	U
1	1A	2192	G
1	1A	2193	G
1	1A	2198	A
1	1A	2206	G
1	1A	2207	G
1	1A	2208	A
1	1A	2219	G
1	1A	2225	A
1	1A	2238	G
1	1A	2239	G
1	1A	2283	C
1	1A	2287	A
1	1A	2305	A
1	1A	2308	G
1	1A	2320	A
1	1A	2325	G
1	1A	2334	G
1	1A	2336	A
1	1A	2347	C
1	1A	2350	C
1	1A	2361	A
1	1A	2372	G
1	1A	2379	G
1	1A	2383	G
1	1A	2385	C
1	1A	2396	G
1	1A	2406	U
1	1A	2407	G
1	1A	2422	A
1	1A	2423	U
1	1A	2425	A
1	1A	2429	G
1	1A	2430	A
1	1A	2431	U
1	1A	2435	A
1	1A	2439	A
1	1A	2441	C
1	1A	2448	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2476	A
1	1A	2478	A
1	1A	2491	U
1	1A	2502	G
1	1A	2505	G
1	1A	2518	A
1	1A	2529	G
1	1A	2535	G
1	1A	2554	U
1	1A	2566	A
1	1A	2567	G
1	1A	2573	C
1	1A	2602	A
1	1A	2609	U
1	1A	2611	U
1	1A	2612	C
1	1A	2629	A
1	1A	2630	G
1	1A	2654	A
1	1A	2663	G
1	1A	2689	U
1	1A	2690	C
1	1A	2691	C
1	1A	2702	U
1	1A	2703	C
1	1A	2712(A)	A
1	1A	2713	A
1	1A	2714	G
1	1A	2726	U
1	1A	2733	A
1	1A	2765	A
1	1A	2778	A
1	1A	2790	A
1	1A	2791	C
1	1A	2793	G
1	1A	2794	C
1	1A	2802	G
1	1A	2807	G
1	1A	2820	A
1	1A	2821	A
1	1A	2835	A
1	1A	2872	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2876	G
1	1A	2880	C
1	1A	2892	A
1	1A	2894	G
1	1A	2895	U
2	1B	2	C
2	1B	12	C
2	1B	13	A
2	1B	35	U
2	1B	45	A
2	1B	50	G
2	1B	56	G
2	1B	67	G
2	1B	73	A
2	1B	84	C
2	1B	110	G
32	1a	6	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	52	G
32	1a	61	G
32	1a	76	C
32	1a	77	G
32	1a	79	G
32	1a	91	C
32	1a	92	C
32	1a	98	G
32	1a	115	G
32	1a	116	A
32	1a	121	C
32	1a	131	C
32	1a	142	G
32	1a	162	A
32	1a	163	C
32	1a	165	C
32	1a	174	C
32	1a	180	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	182	U
32	1a	189(C)	C
32	1a	189(H)	G
32	1a	195	A
32	1a	197	A
32	1a	203	U
32	1a	204	U
32	1a	220	G
32	1a	247	G
32	1a	251	G
32	1a	258	G
32	1a	266	G
32	1a	267	C
32	1a	289	G
32	1a	301	G
32	1a	321	A
32	1a	328	C
32	1a	332	G
32	1a	342	C
32	1a	347	G
32	1a	351	G
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	383	A
32	1a	384	G
32	1a	388	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	441	A
32	1a	442	C
32	1a	452	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	457	C
32	1a	461	A
32	1a	470	C
32	1a	482	A
32	1a	485	G
32	1a	496	A
32	1a	498	U
32	1a	510	A
32	1a	511	C
32	1a	518	C
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	592	G
32	1a	596	C
32	1a	607	A
32	1a	630	G
32	1a	631	G
32	1a	653	A
32	1a	665	A
32	1a	671	G
32	1a	687	A
32	1a	688	G
32	1a	695	A
32	1a	723	U
32	1a	731	G
32	1a	749	C
32	1a	755	G
32	1a	777	A
32	1a	793	U
32	1a	794	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	815	A
32	1a	817	C
32	1a	821	G
32	1a	828	A
32	1a	840	C
32	1a	841	U
32	1a	851	G
32	1a	870	U
32	1a	874	G
32	1a	902	G
32	1a	913	A
32	1a	914	A
32	1a	916	G
32	1a	926	G
32	1a	927	G
32	1a	934	C
32	1a	942	G
32	1a	960	U
32	1a	961	U
32	1a	968	A
32	1a	969	A
32	1a	972	C
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	997	U
32	1a	1000	U
32	1a	1002	G
32	1a	1003	G
32	1a	1005	A
32	1a	1006	C
32	1a	1017	G
32	1a	1020	U
32	1a	1022	G
32	1a	1023	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C
32	1a	1028	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	1029	C
32	1a	1030	C
32	1a	1030(A)	G
32	1a	1030(C)	G
32	1a	1030(D)	A
32	1a	1031	G
32	1a	1033	G
32	1a	1036	G
32	1a	1037	C
32	1a	1039	C
32	1a	1044	A
32	1a	1053	G
32	1a	1068	G
32	1a	1081	G
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1108	G
32	1a	1123	A
32	1a	1124	G
32	1a	1125	U
32	1a	1127	G
32	1a	1132	C
32	1a	1134	G
32	1a	1135	U
32	1a	1137	C
32	1a	1138	G
32	1a	1139	G
32	1a	1146	A
32	1a	1152	A
32	1a	1154	G
32	1a	1157	A
32	1a	1159	U
32	1a	1184	G
32	1a	1196	U
32	1a	1197	G
32	1a	1200	C
32	1a	1201	A
32	1a	1202	G
32	1a	1213	A
32	1a	1227	A
32	1a	1236	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	1238	A
32	1a	1256	A
32	1a	1257	U
32	1a	1258	G
32	1a	1270	C
32	1a	1275	A
32	1a	1278	U
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1320	C
32	1a	1338	G
32	1a	1340	A
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1363(A)	A
32	1a	1370	G
32	1a	1397	C
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1446	U
32	1a	1452	C
32	1a	1456	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	14	A
53	1v	24	A
54	1w	2	C
54	1w	3	C
54	1w	6	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	1w	7	A
54	1w	8	4SU
54	1w	9	A
54	1w	14	A
54	1w	19	G
54	1w	20	U
54	1w	21	A
54	1w	23	A
54	1w	24	G
54	1w	46	G7M
54	1w	47	U
54	1w	48	C
54	1w	50	U
54	1w	62	C
54	1w	66	U
54	1w	69	G
54	1w	73	A
54	1w	74	C
55	1x	9	G
55	1x	46	G
55	1x	47	U
55	1x	61	C
55	1x	69	C
56	1y	5	G
56	1y	8	4SU
56	1y	9	A
56	1y	11	C
56	1y	13	C
56	1y	19	G
56	1y	20	U
56	1y	21	A
56	1y	23	A
56	1y	28	G
56	1y	35	A
56	1y	36	A
56	1y	37	MIA
56	1y	44	G
56	1y	45	U
56	1y	46	G7M
56	1y	47	U
56	1y	48	C
56	1y	49	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
56	1y	50	U
56	1y	51	U
56	1y	56	C
56	1y	57	G
56	1y	58	A
56	1y	59	U
56	1y	61	C
56	1y	62	C
56	1y	65	G
56	1y	66	U
56	1y	69	G
56	1y	70	G
56	1y	71	G
56	1y	72	C
1	2A	12	U
1	2A	15	G
1	2A	34	C
1	2A	35	G
1	2A	45	C
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	84	A
1	2A	90	U
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	154(A)	C
1	2A	157	U
1	2A	173	G
1	2A	181	A
1	2A	196	A
1	2A	199	A
1	2A	205	G
1	2A	214	G
1	2A	215	G
1	2A	216	A
1	2A	222	A
1	2A	225	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	228	A
1	2A	229	A
1	2A	230	U
1	2A	233	A
1	2A	248	G
1	2A	266	G
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	272(B)	G
1	2A	277	C
1	2A	278	A
1	2A	283	A
1	2A	311	A
1	2A	312	G
1	2A	327	G
1	2A	329	G
1	2A	330	A
1	2A	352	G
1	2A	363(B)	G
1	2A	372	G
1	2A	380	U
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	444	C
1	2A	447	A
1	2A	454	A
1	2A	455	C
1	2A	456	C
1	2A	457	A
1	2A	481	G
1	2A	494	G
1	2A	505	A
1	2A	508	G
1	2A	509	C
1	2A	528	A
1	2A	529	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	563	G
1	2A	568	U
1	2A	573	G
1	2A	574	C
1	2A	575	A
1	2A	586	A
1	2A	588	U
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	615	G
1	2A	616	G
1	2A	627	A
1	2A	634	C
1	2A	637	A
1	2A	645	C
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	668	G
1	2A	669	G
1	2A	686	G
1	2A	717	G
1	2A	730	C
1	2A	746	A
1	2A	747	U
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	792	G
1	2A	805	G
1	2A	812	C
1	2A	819	A
1	2A	827	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	828	U
1	2A	857	C
1	2A	859	G
1	2A	866	A
1	2A	874	G
1	2A	875	G
1	2A	878	A
1	2A	879	G
1	2A	880	G
1	2A	883	G
1	2A	884	C
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	893	C
1	2A	894	C
1	2A	896	A
1	2A	900	A
1	2A	901	A
1	2A	903	C
1	2A	910	A
1	2A	917	A
1	2A	932	G
1	2A	938	G
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	953	A
1	2A	959	A
1	2A	961	C
1	2A	974	G
1	2A	975	C
1	2A	983	A
1	2A	996	A
1	2A	999	U
1	2A	1005	C
1	2A	1012	U
1	2A	1013	C
1	2A	1022	G
1	2A	1025	G
1	2A	1026	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1027	A
1	2A	1033	U
1	2A	1038	C
1	2A	1039	G
1	2A	1041	C
1	2A	1043	C
1	2A	1116	C
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1139	G
1	2A	1144	G
1	2A	1171	G
1	2A	1188	U
1	2A	1205	U
1	2A	1211	U
1	2A	1220	A
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1273	U
1	2A	1284	A
1	2A	1300	U
1	2A	1301	A
1	2A	1303	G
1	2A	1314	C
1	2A	1345	C
1	2A	1352	U
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1368	G
1	2A	1370	C
1	2A	1379	A
1	2A	1385	G
1	2A	1395	A
1	2A	1416	G
1	2A	1417	C
1	2A	1421	G
1	2A	1428	C
1	2A	1437	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1445	A
1	2A	1449	A
1	2A	1450	G
1	2A	1455	G
1	2A	1460	A
1	2A	1461	G
1	2A	1467	C
1	2A	1471	A
1	2A	1478	G
1	2A	1482	G
1	2A	1490	A
1	2A	1493	C
1	2A	1494	A
1	2A	1495	A
1	2A	1496	A
1	2A	1497	U
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1531	C
1	2A	1532	C
1	2A	1540	U
1	2A	1547	C
1	2A	1558	A
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1580	A
1	2A	1584	C
1	2A	1608	A
1	2A	1610	A
1	2A	1639	U
1	2A	1640	C
1	2A	1648	C
1	2A	1654	A
1	2A	1674	G
1	2A	1696	G
1	2A	1700	A
1	2A	1703	G
1	2A	1721	G
1	2A	1722	A
1	2A	1739	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1740	G
1	2A	1745(A)	C
1	2A	1746	G
1	2A	1756	G
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A
1	2A	1780	A
1	2A	1782	C
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1812	A
1	2A	1816	G
1	2A	1829	A
1	2A	1839	G
1	2A	1847	A
1	2A	1848	A
1	2A	1877	A
1	2A	1878	G
1	2A	1900	A
1	2A	1906	G
1	2A	1913	A
1	2A	1914	C
1	2A	1929	G
1	2A	1930	G
1	2A	1936	A
1	2A	1938	A
1	2A	1955	U
1	2A	1963	U
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1984	G
1	2A	1992	G
1	2A	1993	U
1	2A	1997	G
1	2A	2020	A
1	2A	2023	G
1	2A	2031	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2032	G
1	2A	2033	A
1	2A	2043	C
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2069	G
1	2A	2099	U
1	2A	2100	G
1	2A	2110	G
1	2A	2111	C
1	2A	2112	G
1	2A	2116	G
1	2A	2117	A
1	2A	2120	G
1	2A	2122	U
1	2A	2126	A
1	2A	2127	G
1	2A	2128	C
1	2A	2129	C
1	2A	2131	G
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2135	A
1	2A	2137	C
1	2A	2138	C
1	2A	2139	C
1	2A	2141	G
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	2157	G
1	2A	2158	A
1	2A	2159	G
1	2A	2161	C
1	2A	2162	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2165	G
1	2A	2166	G
1	2A	2167	U
1	2A	2168	G
1	2A	2169	A
1	2A	2171	A
1	2A	2172	U
1	2A	2176	A
1	2A	2178	C
1	2A	2183	C
1	2A	2186	G
1	2A	2189	U
1	2A	2192	G
1	2A	2193	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2218	U
1	2A	2225	A
1	2A	2238	G
1	2A	2239	G
1	2A	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	2312	U
1	2A	2319	G
1	2A	2320	A
1	2A	2321	G
1	2A	2325	G
1	2A	2334	G
1	2A	2336	A
1	2A	2347	C
1	2A	2350	C
1	2A	2354	G
1	2A	2376	A
1	2A	2383	G
1	2A	2385	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2396	G
1	2A	2403	C
1	2A	2406	U
1	2A	2422	A
1	2A	2423	U
1	2A	2425	A
1	2A	2429	G
1	2A	2430	A
1	2A	2435	A
1	2A	2439	A
1	2A	2440	C
1	2A	2441	C
1	2A	2445	G
1	2A	2448	A
1	2A	2465	C
1	2A	2469	A
1	2A	2471	C
1	2A	2474	C
1	2A	2476	A
1	2A	2478	A
1	2A	2490	G
1	2A	2491	U
1	2A	2494	G
1	2A	2502	G
1	2A	2505	G
1	2A	2506	U
1	2A	2507	C
1	2A	2518	A
1	2A	2520	C
1	2A	2529	G
1	2A	2549	G
1	2A	2554	U
1	2A	2555	U
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2585	U
1	2A	2602	A
1	2A	2609	U
1	2A	2611	U
1	2A	2612	C
1	2A	2629	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2630	G
1	2A	2634	G
1	2A	2654	A
1	2A	2663	G
1	2A	2689	U
1	2A	2690	C
1	2A	2702	U
1	2A	2703	C
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2718	G
1	2A	2726	U
1	2A	2733	A
1	2A	2751	G
1	2A	2761	G
1	2A	2764	A
1	2A	2765	A
1	2A	2766	G
1	2A	2778	A
1	2A	2789	C
1	2A	2793	G
1	2A	2794	C
1	2A	2802	G
1	2A	2803	C
1	2A	2807	G
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2835	A
1	2A	2839	G
1	2A	2872	G
1	2A	2873	A
1	2A	2880	C
1	2A	2892	A
1	2A	2894	G
1	2A	2895	U
1	2A	2897	U
2	2B	2	C
2	2B	3	C
2	2B	9	G
2	2B	13	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2B	17	C
2	2B	25	A
2	2B	33	G
2	2B	34	U
2	2B	41	U
2	2B	45	A
2	2B	53	A
2	2B	73	A
2	2B	74	U
2	2B	75	G
2	2B	84	C
2	2B	88	C
2	2B	108	U
2	2B	109	C
2	2B	110	G
2	2B	113	G
2	2B	120	A
32	2a	7	G
32	2a	9	G
32	2a	22	G
32	2a	32	A
32	2a	39	G
32	2a	47	C
32	2a	48	C
32	2a	50	A
32	2a	51	A
32	2a	52	G
32	2a	65	U
32	2a	66	G
32	2a	73	G
32	2a	80	G
32	2a	89	C
32	2a	101	A
32	2a	116	A
32	2a	121	C
32	2a	131	C
32	2a	144	G
32	2a	146	G
32	2a	156	G
32	2a	163	C
32	2a	182	U
32	2a	189(E)	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	189(F)	U
32	2a	189(J)	G
32	2a	195	A
32	2a	197	A
32	2a	201	C
32	2a	202	U
32	2a	203	U
32	2a	204	U
32	2a	216	G
32	2a	231	G
32	2a	247	G
32	2a	251	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	345	C
32	2a	350	G
32	2a	351	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	367	U
32	2a	372	C
32	2a	373	A
32	2a	384	G
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	412	A
32	2a	413	G
32	2a	424	G
32	2a	429	U
32	2a	430	A
32	2a	439	A
32	2a	442	C
32	2a	452	A
32	2a	457	C
32	2a	470	C
32	2a	475	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	476	G
32	2a	485	G
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	509	A
32	2a	510	A
32	2a	511	C
32	2a	518	C
32	2a	527	G7M
32	2a	528	C
32	2a	531	U
32	2a	532	A
32	2a	533	A
32	2a	547	A
32	2a	558	G
32	2a	559	A
32	2a	564	C
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	630	G
32	2a	639	G
32	2a	653	A
32	2a	665	A
32	2a	687	A
32	2a	688	G
32	2a	695	A
32	2a	723	U
32	2a	724	G
32	2a	731	G
32	2a	733	A
32	2a	749	C
32	2a	755	G
32	2a	773	G
32	2a	774	G
32	2a	777	A
32	2a	787	A
32	2a	792	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	793	U
32	2a	794	A
32	2a	817	C
32	2a	821	G
32	2a	827	U
32	2a	828	A
32	2a	840	C
32	2a	841	U
32	2a	851	G
32	2a	859	A
32	2a	874	G
32	2a	902	G
32	2a	914	A
32	2a	926	G
32	2a	927	G
32	2a	931	C
32	2a	932	C
32	2a	934	C
32	2a	935	A
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	992	U
32	2a	993	G
32	2a	994	A
32	2a	997	U
32	2a	998	G
32	2a	999	C
32	2a	1002	G
32	2a	1003	G
32	2a	1005	A
32	2a	1006	C
32	2a	1009	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1011	G
32	2a	1016	A
32	2a	1019	C
32	2a	1020	U
32	2a	1021	G
32	2a	1022	G
32	2a	1023	G
32	2a	1025	U
32	2a	1026	G
32	2a	1027	C
32	2a	1028	C
32	2a	1029	C
32	2a	1030	C
32	2a	1030(A)	G
32	2a	1031	G
32	2a	1035	A
32	2a	1036	G
32	2a	1037	C
32	2a	1039	C
32	2a	1040	U
32	2a	1045	C
32	2a	1051	C
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1077	G
32	2a	1081	G
32	2a	1086	U
32	2a	1092	A
32	2a	1093	A
32	2a	1094	G
32	2a	1095	U
32	2a	1097	C
32	2a	1101	A
32	2a	1108	G
32	2a	1125	U
32	2a	1127	G
32	2a	1129	C
32	2a	1130	A
32	2a	1133	G
32	2a	1136	U
32	2a	1137	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1138	G
32	2a	1139	G
32	2a	1141	C
32	2a	1146	A
32	2a	1152	A
32	2a	1157	A
32	2a	1158	C
32	2a	1159	U
32	2a	1160	G
32	2a	1172	C
32	2a	1180	A
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	1211	U
32	2a	1213	A
32	2a	1227	A
32	2a	1236	A
32	2a	1238	A
32	2a	1246	C
32	2a	1255	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	1277	C
32	2a	1278	U
32	2a	1279	A
32	2a	1280	A
32	2a	1287	A
32	2a	1299	A
32	2a	1302	U
32	2a	1303	C
32	2a	1338	G
32	2a	1346	A
32	2a	1347	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1363	C
32	2a	1370	G
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1447	A
32	2a	1452	C
32	2a	1456	G
32	2a	1457	G
32	2a	1492	A
32	2a	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	17	U
53	2v	24	A
54	2w	5	G
54	2w	7	A
54	2w	8	4SU
54	2w	9	A
54	2w	13	C
54	2w	14	A
54	2w	19	G
54	2w	22	G
54	2w	31	A
54	2w	46	G7M
54	2w	47	U
54	2w	48	C
54	2w	51	U
54	2w	61	C
54	2w	64	A
54	2w	65	G
54	2w	66	U
54	2w	69	G
54	2w	70	G
54	2w	72	C
54	2w	73	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	2w	74	C
55	2x	9	G
55	2x	19	G
55	2x	20	U
55	2x	46	G
55	2x	47	U
56	2y	7	A
56	2y	15	G
56	2y	19	G
56	2y	23	A
56	2y	27	G
56	2y	28	G
56	2y	34	G
56	2y	38	A
56	2y	41	C
56	2y	43	C
56	2y	45	U
56	2y	49	C
56	2y	52	G
56	2y	53	G
56	2y	55	PSU
56	2y	56	C
56	2y	57	G
56	2y	58	A
56	2y	59	U
56	2y	62	C
56	2y	63	G
56	2y	65	G
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	669	G
1	1A	685	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	746	A
1	1A	764	A
1	1A	774	A
1	1A	827	U
1	1A	974	G
1	1A	1047	G
1	1A	1067	A
1	1A	1174	A
1	1A	1176	G
1	1A	1379	A
1	1A	1442	G
1	1A	1508	A
1	1A	1608	A
1	1A	1992	G
1	1A	2134	A
1	1A	2181	G
1	1A	2183	C
1	1A	2406	U
1	1A	2422	A
1	1A	2430	A
1	1A	2439	A
1	1A	2629	A
1	1A	2689	U
1	2A	196	A
1	2A	228	A
1	2A	266	G
1	2A	271(M)	G
1	2A	277	C
1	2A	528	A
1	2A	746	A
1	2A	752	A
1	2A	774	A
1	2A	827	U
1	2A	856	C
1	2A	900	A
1	2A	1142(A)	A
1	2A	1210	A
1	2A	1420	U
1	2A	1442	G
1	2A	1530	C
1	2A	1653	G
1	2A	1913	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1992	G
1	2A	2119	A
1	2A	2126	A
1	2A	2156	G
1	2A	2406	U
1	2A	2439	A
1	2A	2689	U

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

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	G7M	1a	527	57,32	23,26,27	1.55	4 (17%)	34,39,42	1.67	5 (14%)
32	5MC	2a	967	32	19,22,23	1.66	3 (15%)	26,32,35	1.11	2 (7%)
54	4SU	1w	8	54	18,21,22	1.80	4 (22%)	25,30,33	1.96	4 (16%)
32	UR3	2a	1498	32	19,22,23	1.02	2 (10%)	26,32,35	1.73	3 (11%)
1	PSU	2A	2605	1	18,21,22	1.30	2 (11%)	21,30,33	2.04	3 (14%)
1	OMU	2A	2552	1	19,22,23	1.07	1 (5%)	25,31,34	1.90	5 (20%)
54	G7M	2w	46	54	23,26,27	1.49	4 (17%)	34,39,42	1.73	6 (17%)
1	OMG	1A	2251	1,55,57	23,26,27	1.23	3 (13%)	32,38,41	1.99	5 (15%)
56	5MU	1y	54	56	19,22,23	1.49	4 (21%)	27,32,35	1.82	6 (22%)
1	OMU	1A	2552	1,57	19,22,23	1.11	2 (10%)	25,31,34	1.94	5 (20%)
1	5MU	1A	1939	1,57	19,22,23	1.55	6 (31%)	27,32,35	1.98	7 (25%)
1	5MC	2A	1942	1	19,22,23	1.59	3 (15%)	26,32,35	1.08	2 (7%)
54	PSU	2w	32	54	18,21,22	1.39	2 (11%)	21,30,33	1.84	3 (14%)
55	4SU	1x	8	55	18,21,22	2.25	6 (33%)	25,30,33	1.70	7 (28%)
56	MIA	2y	37	56	21,24,32	1.65	3 (14%)	30,35,47	2.02	7 (23%)
32	5MC	2a	1400	32	19,22,23	1.71	3 (15%)	26,32,35	1.20	3 (11%)
54	G7M	1w	46	54	23,26,27	1.55	4 (17%)	34,39,42	1.63	4 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
56	MIA	1y	37	56	21,24,32	1.64	4 (19%)	30,35,47	2.02	7 (23%)
54	5MU	1w	54	54	19,22,23	1.48	5 (26%)	27,32,35	1.88	6 (22%)
56	PSU	1y	32	56	18,21,22	1.36	2 (11%)	21,30,33	1.95	3 (14%)
1	2MA	1A	2503	1,57	22,25,26	1.53	4 (18%)	32,37,40	2.26	6 (18%)
32	UR3	1a	1498	32	19,22,23	0.94	0	26,32,35	1.83	3 (11%)
54	PSU	2w	39	54	18,21,22	1.38	2 (11%)	21,30,33	1.91	3 (14%)
1	5MC	1A	1942	1	19,22,23	1.86	3 (15%)	26,32,35	1.23	3 (11%)
32	4OC	1a	1402	32	20,23,24	0.74	0	25,32,35	1.00	1 (4%)
1	PSU	1A	1917	1	18,21,22	1.32	2 (11%)	21,30,33	2.03	4 (19%)
56	5MU	2y	54	56	19,22,23	1.44	4 (21%)	27,32,35	1.77	5 (18%)
55	5MU	1x	54	57,55	19,22,23	1.43	5 (26%)	27,32,35	1.98	6 (22%)
32	2MG	1a	1207	32	23,26,27	1.24	3 (13%)	33,38,41	2.15	6 (18%)
54	MIA	1w	37	54	28,31,32	2.25	6 (21%)	38,44,47	2.80	13 (34%)
54	8AN	2w	76	62,1,54	21,24,25	1.49	4 (19%)	26,35,38	2.13	9 (34%)
1	PSU	1A	1911	1	18,21,22	1.40	2 (11%)	21,30,33	2.03	5 (23%)
54	PSU	1w	39	54	18,21,22	1.34	2 (11%)	21,30,33	2.08	4 (19%)
55	5MC	1x	32	55	19,22,23	1.70	3 (15%)	26,32,35	1.23	3 (11%)
54	5MU	2w	54	54	19,22,23	1.36	5 (26%)	27,32,35	1.86	7 (25%)
1	PSU	1A	2605	1,57	18,21,22	1.40	3 (16%)	21,30,33	2.06	5 (23%)
1	PSU	2A	1911	1	18,21,22	1.38	2 (11%)	21,30,33	2.12	4 (19%)
43	0TD	1l	92	43	8,9,10	4.68	1 (12%)	6,11,13	1.36	1 (16%)
54	MIA	2w	37	54	24,27,32	2.05	6 (25%)	32,39,47	2.67	12 (37%)
32	5MC	1a	1407	32	19,22,23	1.52	3 (15%)	26,32,35	1.13	3 (11%)
32	2MG	2a	1207	32	23,26,27	1.24	2 (8%)	33,38,41	2.29	7 (21%)
55	PSU	2x	55	55	18,21,22	1.37	2 (11%)	21,30,33	1.93	5 (23%)
32	4OC	2a	1402	32	20,23,24	0.78	0	25,32,35	0.99	1 (4%)
32	M2G	1a	966	32	24,27,28	1.32	3 (12%)	33,40,43	1.89	6 (18%)
56	G7M	1y	46	56	23,26,27	1.53	4 (17%)	34,39,42	1.74	4 (11%)
32	5MC	1a	1404	32	19,22,23	1.70	3 (15%)	26,32,35	1.22	4 (15%)
32	MA6	1a	1519	32	23,26,27	0.43	0	33,38,41	2.04	9 (27%)
1	OMC	1A	1920	1	19,22,23	0.78	0	25,31,34	0.91	1 (4%)
1	OMC	2A	1920	1	19,22,23	0.82	0	25,31,34	0.96	1 (4%)
1	5MC	2A	1962	1	19,22,23	1.69	3 (15%)	26,32,35	1.13	2 (7%)
32	5MC	2a	1407	32	19,22,23	1.66	3 (15%)	26,32,35	1.20	3 (11%)
32	MA6	2a	1519	32	23,26,27	0.44	0	33,38,41	2.15	8 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	5MC	1a	967	32	19,22,23	1.73	3 (15%)	26,32,35	1.19	3 (11%)
32	MA6	1a	1518	32	23,26,27	0.42	0	33,38,41	2.00	9 (27%)
1	5MU	1A	1915	1	19,22,23	1.35	5 (26%)	27,32,35	2.22	8 (29%)
1	OMG	2A	2251	1,55,57	23,26,27	1.22	3 (13%)	32,38,41	1.94	6 (18%)
56	PSU	1y	55	56	18,21,22	1.38	2 (11%)	21,30,33	2.08	4 (19%)
55	8AN	2x	76	57,55,63	21,24,25	1.41	3 (14%)	26,35,38	2.28	10 (38%)
32	G7M	2a	527	57,32	23,26,27	1.48	4 (17%)	34,39,42	1.72	5 (14%)
56	4SU	1y	8	56	18,21,22	1.78	6 (33%)	25,30,33	1.83	5 (20%)
55	4SU	2x	8	57,55	18,21,22	2.10	6 (33%)	25,30,33	1.38	6 (24%)
1	5MC	1A	1962	1,57	19,22,23	1.65	3 (15%)	26,32,35	1.15	3 (11%)
54	PSU	2w	55	54	18,21,22	1.38	2 (11%)	21,30,33	2.03	3 (14%)
55	8AN	1x	76	57,55,63	21,24,25	1.51	4 (19%)	26,35,38	2.61	11 (42%)
54	PSU	1w	32	54	18,21,22	1.39	3 (16%)	21,30,33	1.82	3 (14%)
32	PSU	1a	516	32	18,21,22	1.36	2 (11%)	21,30,33	1.93	5 (23%)
56	G7M	2y	46	56	23,26,27	1.63	5 (21%)	34,39,42	1.98	5 (14%)
56	PSU	2y	39	56	18,21,22	1.44	2 (11%)	21,30,33	1.68	3 (14%)
32	M2G	2a	966	32	24,27,28	1.26	3 (12%)	33,40,43	1.82	5 (15%)
54	4SU	2w	8	54	18,21,22	1.70	3 (16%)	25,30,33	2.50	5 (20%)
55	5MU	2x	54	55	19,22,23	1.42	5 (26%)	27,32,35	2.14	6 (22%)
56	PSU	1y	39	56	18,21,22	1.43	2 (11%)	21,30,33	1.86	4 (19%)
1	5MU	2A	1939	1,57	19,22,23	1.44	6 (31%)	27,32,35	2.28	6 (22%)
56	4SU	2y	8	56	18,21,22	1.72	4 (22%)	25,30,33	2.38	5 (20%)
54	PSU	1w	55	54	18,21,22	1.37	2 (11%)	21,30,33	2.05	3 (14%)
32	MA6	2a	1518	32	23,26,27	0.43	0	33,38,41	2.05	9 (27%)
56	PSU	2y	32	56	18,21,22	1.36	2 (11%)	21,30,33	1.99	3 (14%)
32	5MC	1a	1400	32	19,22,23	1.55	3 (15%)	26,32,35	1.16	3 (11%)
55	5MC	2x	32	55	19,22,23	1.63	3 (15%)	26,32,35	1.27	3 (11%)
1	5MU	2A	1915	1	19,22,23	1.44	4 (21%)	27,32,35	2.11	6 (22%)
43	0TD	2l	92	43	8,9,10	4.59	2 (25%)	6,11,13	2.49	1 (16%)
32	PSU	2a	516	32	18,21,22	1.35	2 (11%)	21,30,33	2.03	3 (14%)
56	PSU	2y	55	56	18,21,22	1.43	3 (16%)	21,30,33	2.01	4 (19%)
1	2MA	2A	2503	1,57	22,25,26	1.51	4 (18%)	32,37,40	2.43	8 (25%)
55	PSU	1x	55	55	18,21,22	1.35	2 (11%)	21,30,33	2.00	4 (19%)
32	5MC	2a	1404	32	19,22,23	1.73	3 (15%)	26,32,35	1.12	2 (7%)
54	8AN	1w	76	62,1,54	21,24,25	1.45	3 (14%)	26,35,38	2.14	9 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	PSU	2A	1917	1	18,21,22	1.35	2 (11%)	21,30,33	2.05	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	G7M	1a	527	57,32	-	3/7/25/26	0/3/3/3
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
1	OMU	2A	2552	1	-	0/9/27/28	0/2/2/2
54	G7M	2w	46	54	-	3/7/25/26	0/3/3/3
1	OMG	1A	2251	1,55,57	-	0/9/27/28	0/3/3/3
56	5MU	1y	54	56	-	0/7/25/26	0/2/2/2
1	OMU	1A	2552	1,57	-	0/9/27/28	0/2/2/2
1	5MU	1A	1939	1,57	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
56	MIA	2y	37	56	-	3/7/25/34	0/3/3/3
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
54	G7M	1w	46	54	-	1/7/25/26	0/3/3/3
56	MIA	1y	37	56	-	2/7/25/34	0/3/3/3
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
56	PSU	1y	32	56	-	0/7/25/26	0/2/2/2
1	2MA	1A	2503	1,57	-	1/7/25/26	0/3/3/3
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	1/9/29/30	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
56	5MU	2y	54	56	-	0/7/25/26	0/2/2/2
55	5MU	1x	54	57,55	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/9/27/28	0/3/3/3
54	MIA	1w	37	54	-	1/15/33/34	0/3/3/3
54	8AN	2w	76	62,1,54	-	0/7/25/26	0/3/3/3
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
1	PSU	1A	2605	1,57	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	2/7/12/14	-
54	MIA	2w	37	54	-	2/11/29/34	0/3/3/3
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	0/9/27/28	0/3/3/3
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32	-	1/9/29/30	0/2/2/2
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
56	G7M	1y	46	56	-	1/7/25/26	0/3/3/3
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	3/11/29/30	0/3/3/3
1	OMC	1A	1920	1	-	1/9/27/28	0/2/2/2
1	OMC	2A	1920	1	-	0/9/27/28	0/2/2/2
1	5MC	2A	1962	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	3/11/29/30	0/3/3/3
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	0/11/29/30	0/3/3/3
1	5MU	1A	1915	1	-	1/7/25/26	0/2/2/2
1	OMG	2A	2251	1,55,57	-	0/9/27/28	0/3/3/3
56	PSU	1y	55	56	-	1/7/25/26	0/2/2/2
55	8AN	2x	76	57,55,63	-	3/7/25/26	0/3/3/3
32	G7M	2a	527	57,32	-	3/7/25/26	0/3/3/3
56	4SU	1y	8	56	-	3/7/25/26	0/2/2/2
55	4SU	2x	8	57,55	-	0/7/25/26	0/2/2/2
1	5MC	1A	1962	1,57	-	0/7/25/26	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
55	8AN	1x	76	57,55,63	-	3/7/25/26	0/3/3/3
54	PSU	1w	32	54	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
56	G7M	2y	46	56	-	2/7/25/26	0/3/3/3
56	PSU	2y	39	56	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
56	PSU	1y	39	56	-	0/7/25/26	0/2/2/2
1	5MU	2A	1939	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	4SU	2y	8	56	-	1/7/25/26	0/2/2/2
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	0/11/29/30	0/3/3/3
56	PSU	2y	32	56	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	2/7/12/14	-
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
56	PSU	2y	55	56	-	2/7/25/26	0/2/2/2
1	2MA	2A	2503	1,57	-	2/7/25/26	0/3/3/3
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
54	8AN	1w	76	62,1,54	-	0/7/25/26	0/3/3/3
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2

All (258) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-12.72	1.69	1.82
43	2l	92	0TD	CB-SB	-12.44	1.69	1.82
1	1A	1942	5MC	C5-C4	7.05	1.49	1.44
54	1w	37	MIA	C13-C14	6.81	1.52	1.32
32	1a	967	5MC	C5-C4	6.47	1.49	1.44
32	2a	1404	5MC	C5-C4	6.34	1.48	1.44
54	2w	37	MIA	C2-S10	-6.28	1.70	1.75
32	2a	1400	5MC	C5-C4	6.17	1.48	1.44
55	1x	32	5MC	C5-C4	6.16	1.48	1.44
1	2A	1962	5MC	C5-C4	6.15	1.48	1.44
32	2a	967	5MC	C5-C4	6.14	1.48	1.44
32	1a	1404	5MC	C5-C4	6.09	1.48	1.44
1	1A	1962	5MC	C5-C4	6.06	1.48	1.44
54	1w	37	MIA	C2-S10	-6.04	1.70	1.75
32	2a	1407	5MC	C5-C4	5.96	1.48	1.44
55	2x	32	5MC	C5-C4	5.77	1.48	1.44
1	2A	1942	5MC	C5-C4	5.73	1.48	1.44
55	1x	8	4SU	C4-N3	-5.62	1.31	1.37
32	1a	1400	5MC	C5-C4	5.39	1.48	1.44
32	1a	1407	5MC	C5-C4	5.37	1.48	1.44
56	2y	37	MIA	C5-C4	5.27	1.48	1.39
56	1y	37	MIA	C5-C4	5.20	1.48	1.39
54	2w	37	MIA	C5-C4	5.07	1.48	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	2x	8	4SU	C4-N3	-5.06	1.32	1.37
54	1w	37	MIA	C5-C4	4.96	1.47	1.39
32	1a	527	G7M	C5-N7	-4.93	1.33	1.39
54	1w	46	G7M	C5-N7	-4.80	1.33	1.39
56	2y	8	4SU	C4-S4	-4.78	1.60	1.68
54	2w	8	4SU	C4-S4	-4.75	1.60	1.68
54	1w	8	4SU	C4-S4	-4.75	1.60	1.68
56	2y	46	G7M	C5-N7	-4.63	1.33	1.39
54	2w	46	G7M	C5-N7	-4.60	1.33	1.39
1	2A	2503	2MA	C5-C4	4.58	1.47	1.39
1	1A	2503	2MA	C5-C4	4.53	1.47	1.39
56	1y	8	4SU	C4-S4	-4.47	1.60	1.68
55	1x	8	4SU	C4-S4	-4.44	1.60	1.68
32	2a	527	G7M	C5-N7	-4.35	1.34	1.39
56	1y	39	PSU	C6-C5	4.26	1.40	1.35
55	2x	8	4SU	C4-S4	-4.26	1.61	1.68
56	1y	46	G7M	C5-N7	-4.25	1.34	1.39
56	2y	39	PSU	C6-C5	4.16	1.39	1.35
56	2y	32	PSU	C6-C5	4.06	1.39	1.35
56	1y	55	PSU	C6-C5	4.04	1.39	1.35
55	2x	76	8AN	C5-N7	-3.94	1.31	1.39
54	2w	55	PSU	C6-C5	3.93	1.39	1.35
55	1x	76	8AN	C5-N7	-3.92	1.31	1.39
56	1y	32	PSU	C6-C5	3.90	1.39	1.35
54	2w	39	PSU	C6-C5	3.88	1.39	1.35
55	1x	8	4SU	C2-N3	-3.88	1.31	1.38
54	2w	76	8AN	C5-N7	-3.87	1.32	1.39
54	1w	55	PSU	C6-C5	3.85	1.39	1.35
54	1w	76	8AN	C5-N7	-3.83	1.32	1.39
32	2a	516	PSU	C6-C5	3.80	1.39	1.35
56	2y	46	G7M	C5-C4	3.78	1.47	1.38
54	2w	32	PSU	C6-C5	3.74	1.39	1.35
1	1A	1911	PSU	C6-C5	3.74	1.39	1.35
1	2A	1917	PSU	C6-C5	3.64	1.39	1.35
1	2A	1911	PSU	C6-C5	3.58	1.39	1.35
55	2x	55	PSU	C6-C5	3.55	1.39	1.35
56	1y	46	G7M	C5-C4	3.55	1.47	1.38
32	1a	516	PSU	C6-C5	3.54	1.39	1.35
55	1x	55	PSU	C6-C5	3.46	1.39	1.35
55	2x	8	4SU	C2-N3	-3.44	1.32	1.38
54	1w	32	PSU	C6-C5	3.43	1.39	1.35
1	1A	1917	PSU	C6-C5	3.43	1.39	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	8	4SU	C4-N3	-3.40	1.34	1.37
56	2y	55	PSU	C6-C5	3.36	1.39	1.35
55	1x	8	4SU	C5-C4	-3.35	1.38	1.42
56	1y	8	4SU	C4-N3	-3.30	1.34	1.37
32	2a	966	M2G	C5-C4	3.29	1.47	1.38
54	1w	39	PSU	C6-C5	3.27	1.38	1.35
54	2w	46	G7M	C5-C4	3.26	1.46	1.38
32	1a	527	G7M	C5-C4	3.25	1.46	1.38
32	2a	1207	2MG	C5-C4	3.24	1.47	1.38
54	1w	46	G7M	C5-C4	3.22	1.46	1.38
1	2A	2251	OMG	C5-C4	3.22	1.47	1.38
55	2x	76	8AN	C5-C4	-3.20	1.33	1.39
54	2w	76	8AN	C5-C4	-3.20	1.33	1.39
1	2A	2605	PSU	C6-C5	3.17	1.38	1.35
32	1a	1207	2MG	C5-C4	3.17	1.47	1.38
54	1w	54	5MU	C6-C5	3.17	1.39	1.34
32	2a	527	G7M	C5-C4	3.14	1.46	1.38
1	1A	2251	OMG	C5-C4	3.12	1.47	1.38
1	1A	2605	PSU	C6-C5	3.11	1.38	1.35
56	2y	54	5MU	C6-C5	3.10	1.39	1.34
54	2w	37	MIA	C5-C6	3.09	1.49	1.41
32	1a	966	M2G	C5-C4	3.08	1.47	1.38
32	1a	966	M2G	C2-N2	3.07	1.40	1.35
55	1x	76	8AN	C5-C4	-3.07	1.33	1.39
1	2A	1939	5MU	C4-N3	-3.07	1.33	1.38
54	1w	76	8AN	C5-C4	-3.03	1.33	1.39
1	2A	1915	5MU	C6-C5	3.02	1.39	1.34
56	2y	37	MIA	C5-C6	3.01	1.49	1.41
56	1y	37	MIA	C5-C6	3.00	1.49	1.41
55	2x	8	4SU	C5-C4	-2.96	1.39	1.42
1	1A	2605	PSU	C4-N3	-2.96	1.33	1.38
55	1x	54	5MU	C6-C5	2.95	1.39	1.34
32	1a	1400	5MC	C6-C5	2.94	1.39	1.34
32	2a	1404	5MC	C6-C5	2.92	1.39	1.34
1	2A	1942	5MC	C6-C5	2.88	1.39	1.34
1	2A	1939	5MU	C6-C5	2.86	1.39	1.34
1	1A	1939	5MU	C4-N3	-2.85	1.33	1.38
55	2x	32	5MC	C6-C5	2.85	1.39	1.34
56	1y	54	5MU	C6-C5	2.85	1.39	1.34
55	2x	54	5MU	C6-C5	2.82	1.39	1.34
1	1A	1939	5MU	C6-C5	2.82	1.39	1.34
32	1a	1407	5MC	C6-C5	2.80	1.39	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	32	PSU	C4-N3	-2.79	1.33	1.38
56	1y	54	5MU	C2-N1	2.79	1.42	1.38
54	2w	8	4SU	C4-N3	-2.78	1.34	1.37
32	2a	1400	5MC	C6-C5	2.78	1.39	1.34
32	2a	1407	5MC	C6-C5	2.76	1.39	1.34
1	1A	1939	5MU	C2-N3	-2.75	1.33	1.38
55	1x	32	5MC	C6-C5	2.75	1.39	1.34
1	2A	2251	OMG	C6-N1	-2.73	1.33	1.38
1	1A	1911	PSU	C4-N3	-2.68	1.33	1.38
1	2A	1915	5MU	C2-N1	2.67	1.42	1.38
55	1x	54	5MU	C4-N3	-2.67	1.33	1.38
1	1A	1942	5MC	C6-C5	2.67	1.39	1.34
1	1A	2503	2MA	C5-C6	2.66	1.48	1.41
32	1a	966	M2G	C6-N1	-2.66	1.33	1.38
32	1a	1404	5MC	C6-C5	2.64	1.38	1.34
32	2a	967	5MC	C6-C5	2.64	1.38	1.34
1	2A	1962	5MC	C6-C5	2.63	1.38	1.34
54	2w	54	5MU	C6-C5	2.63	1.38	1.34
54	1w	37	MIA	C5-C6	2.62	1.48	1.41
56	2y	39	PSU	C4-N3	-2.61	1.34	1.38
1	1A	1915	5MU	C6-C5	2.61	1.38	1.34
1	1A	1962	5MC	C6-C5	2.61	1.38	1.34
54	1w	39	PSU	C4-N3	-2.60	1.34	1.38
56	2y	8	4SU	C4-N3	-2.60	1.34	1.37
1	1A	2503	2MA	C8-N7	2.60	1.36	1.31
54	1w	54	5MU	C4-N3	-2.59	1.34	1.38
1	1A	1939	5MU	C6-N1	-2.58	1.33	1.38
55	2x	55	PSU	C4-N3	-2.58	1.34	1.38
54	1w	37	MIA	C5-N7	-2.57	1.34	1.39
55	2x	54	5MU	C2-N1	2.57	1.42	1.38
56	1y	8	4SU	C2-N1	2.56	1.42	1.38
56	1y	39	PSU	C4-N3	-2.56	1.34	1.38
55	1x	76	8AN	C5-C6	-2.55	1.33	1.41
1	2A	1917	PSU	C4-N3	-2.54	1.34	1.38
1	2A	1911	PSU	C4-N3	-2.54	1.34	1.38
32	1a	1207	2MG	C6-N1	-2.54	1.34	1.38
56	2y	37	MIA	C8-N7	2.54	1.36	1.31
56	1y	54	5MU	C4-C5	2.53	1.48	1.44
1	1A	1939	5MU	C4-C5	2.53	1.48	1.44
56	1y	54	5MU	C4-N3	-2.52	1.34	1.38
1	1A	2503	2MA	C5-N7	-2.52	1.34	1.39
56	2y	55	PSU	C4-N3	-2.52	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	2503	2MA	C5-C6	2.52	1.48	1.41
1	1A	1942	5MC	C6-N1	-2.52	1.33	1.38
54	2w	54	5MU	C4-N3	-2.52	1.34	1.38
1	2A	1915	5MU	C4-C5	2.51	1.48	1.44
54	1w	54	5MU	C4-C5	2.51	1.48	1.44
56	2y	54	5MU	C2-N1	2.50	1.42	1.38
1	1A	1917	PSU	C4-N3	-2.50	1.34	1.38
54	1w	8	4SU	C5-C4	-2.50	1.39	1.42
1	1A	1915	5MU	C4-C5	2.50	1.48	1.44
32	1a	527	G7M	C6-N1	-2.49	1.34	1.38
43	2l	92	0TD	CB-CA	2.49	1.55	1.54
56	2y	8	4SU	C2-N1	2.48	1.42	1.38
55	2x	76	8AN	C5-C6	-2.48	1.34	1.41
56	2y	46	G7M	C6-N1	-2.48	1.34	1.38
54	2w	76	8AN	C5-C6	-2.47	1.34	1.41
32	1a	516	PSU	C4-N3	-2.46	1.34	1.38
32	1a	967	5MC	C6-C5	2.45	1.38	1.34
54	1w	76	8AN	C5-C6	-2.45	1.34	1.41
1	2A	1962	5MC	C6-N1	-2.45	1.33	1.38
54	2w	39	PSU	C4-N3	-2.45	1.34	1.38
54	2w	55	PSU	C4-N3	-2.44	1.34	1.38
32	2a	1400	5MC	C6-N1	-2.44	1.33	1.38
55	1x	55	PSU	C4-N3	-2.44	1.34	1.38
56	2y	54	5MU	C4-C5	2.43	1.48	1.44
32	2a	527	G7M	C6-N1	-2.43	1.34	1.38
1	2A	2503	2MA	C5-N7	-2.43	1.34	1.39
56	1y	32	PSU	C4-N3	-2.42	1.34	1.38
55	2x	54	5MU	C4-C5	2.41	1.48	1.44
1	1A	2251	OMG	C5-N7	-2.41	1.34	1.39
55	1x	8	4SU	O2-C2	2.41	1.27	1.23
55	2x	54	5MU	C4-N3	-2.40	1.34	1.38
54	2w	8	4SU	C5-C4	-2.39	1.39	1.42
54	1w	55	PSU	C4-N3	-2.38	1.34	1.38
1	1A	1915	5MU	C4-N3	-2.38	1.34	1.38
32	2a	966	M2G	C2-N2	2.38	1.39	1.35
32	1a	1404	5MC	C6-N1	-2.36	1.34	1.38
1	2A	1915	5MU	C4-N3	-2.36	1.34	1.38
32	2a	1207	2MG	C6-N1	-2.35	1.34	1.38
55	1x	54	5MU	C4-C5	2.35	1.48	1.44
54	2w	37	MIA	C2-N3	2.33	1.37	1.34
1	1A	2251	OMG	C6-N1	-2.33	1.34	1.38
55	1x	32	5MC	C6-N1	-2.33	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	2503	2MA	C8-N7	2.32	1.36	1.31
54	1w	46	G7M	C6-N1	-2.32	1.34	1.38
1	2A	2605	PSU	C4-N3	-2.32	1.34	1.38
54	2w	32	PSU	C4-N3	-2.32	1.34	1.38
1	2A	1939	5MU	C6-N1	-2.32	1.34	1.38
32	2a	966	M2G	C6-N1	-2.32	1.34	1.38
54	1w	8	4SU	C2-N3	-2.31	1.33	1.38
32	1a	967	5MC	C6-N1	-2.31	1.34	1.38
56	2y	8	4SU	C5-C4	-2.31	1.39	1.42
32	2a	1407	5MC	C6-N1	-2.30	1.34	1.38
54	2w	76	8AN	C2'-C3'	-2.29	1.50	1.53
56	2y	54	5MU	C4-N3	-2.29	1.34	1.38
55	2x	32	5MC	C6-N1	-2.28	1.34	1.38
54	2w	37	MIA	C5-N7	-2.28	1.34	1.39
55	1x	54	5MU	C2-N1	2.28	1.42	1.38
55	2x	8	4SU	O2-C2	2.28	1.27	1.23
1	1A	1915	5MU	C2-N1	2.27	1.42	1.38
56	1y	37	MIA	C8-N7	2.26	1.36	1.31
56	1y	55	PSU	C4-N3	-2.26	1.34	1.38
1	1A	1962	5MC	C6-N1	-2.25	1.34	1.38
1	2A	1939	5MU	C2-N1	2.25	1.42	1.38
54	2w	54	5MU	C4-C5	2.23	1.48	1.44
56	1y	8	4SU	C5-C4	-2.23	1.39	1.42
56	1y	8	4SU	C2-N3	-2.22	1.34	1.38
32	1a	1400	5MC	C6-N1	-2.22	1.34	1.38
32	2a	516	PSU	C4-N3	-2.21	1.34	1.38
1	1A	2552	OMU	C4-N3	-2.20	1.34	1.38
56	1y	46	G7M	C6-N1	-2.19	1.34	1.38
54	1w	54	5MU	C2-N1	2.17	1.41	1.38
1	1A	2552	OMU	C5-C4	-2.17	1.39	1.43
54	1w	54	5MU	C2-N3	-2.16	1.34	1.38
32	2a	1404	5MC	C6-N1	-2.16	1.34	1.38
1	2A	2251	OMG	C5-N7	-2.15	1.34	1.39
54	2w	37	MIA	C8-N7	2.14	1.35	1.31
32	2a	1498	UR3	C2-N1	2.14	1.41	1.38
1	1A	1915	5MU	C6-N1	-2.14	1.34	1.38
54	1w	37	MIA	C8-N7	2.13	1.35	1.31
1	1A	2605	PSU	C2-N3	-2.12	1.34	1.37
1	2A	1939	5MU	C2-N3	-2.12	1.34	1.38
54	1w	32	PSU	C2-N3	-2.12	1.34	1.37
55	2x	54	5MU	C6-N1	-2.12	1.34	1.38
32	2a	967	5MC	C6-N1	-2.10	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	2y	32	PSU	C4-N3	-2.09	1.34	1.38
32	1a	1207	2MG	C2-N3	2.09	1.35	1.32
55	2x	8	4SU	C6-C5	2.08	1.39	1.35
54	2w	54	5MU	C2-N3	-2.08	1.34	1.38
1	1A	1939	5MU	C2-N1	2.08	1.41	1.38
56	1y	8	4SU	C6-C5	2.07	1.39	1.35
1	2A	1942	5MC	C6-N1	-2.07	1.34	1.38
54	2w	54	5MU	C6-N1	-2.07	1.34	1.38
32	2a	527	G7M	C5-C6	2.06	1.48	1.43
56	1y	46	G7M	C5-C6	2.06	1.48	1.43
56	2y	46	G7M	C2-N3	2.06	1.38	1.33
1	2A	1939	5MU	C4-C5	2.06	1.48	1.44
54	2w	46	G7M	C5-C6	2.05	1.48	1.43
56	1y	37	MIA	C5-N7	-2.04	1.35	1.39
56	2y	46	G7M	C5-C6	2.03	1.48	1.43
32	1a	1407	5MC	C6-N1	-2.03	1.34	1.38
55	1x	54	5MU	C6-N1	-2.03	1.34	1.38
54	2w	46	G7M	C4-N9	-2.03	1.32	1.38
32	1a	527	G7M	C4-N9	-2.01	1.32	1.38
1	2A	2552	OMU	C4-N3	-2.01	1.35	1.38
55	1x	8	4SU	C6-C5	2.01	1.39	1.35
54	1w	46	G7M	C4-N9	-2.01	1.32	1.38
55	1x	76	8AN	P-O5'	-2.01	1.57	1.62
56	2y	55	PSU	C2-N3	-2.00	1.34	1.37
32	2a	1498	UR3	C6-C5	2.00	1.39	1.35

All (429) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	2w	37	MIA	C5-C4-N3	-9.25	117.44	127.18
54	1w	37	MIA	C12-C13-C14	-9.04	110.78	127.01
1	2A	2503	2MA	C5-C4-N3	-8.48	118.24	127.18
1	1A	2503	2MA	C5-C4-N3	-8.18	118.56	127.18
54	1w	37	MIA	C5-C4-N3	-8.09	118.66	127.18
54	2w	8	4SU	C4-N3-C2	-7.81	119.83	127.31
54	2w	37	MIA	N3-C4-N9	7.42	136.40	126.99
32	1a	1498	UR3	C4-N3-C2	-7.33	118.68	124.58
56	2y	8	4SU	C4-N3-C2	-7.10	120.51	127.31
32	2a	1207	2MG	C2-N3-C4	7.07	120.84	112.00
1	2A	2503	2MA	N3-C4-N9	6.99	135.86	126.99
32	1a	1207	2MG	C2-N3-C4	6.94	120.69	112.00
32	2a	1498	UR3	C4-N3-C2	-6.74	119.15	124.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	1w	37	MIA	N3-C4-N9	6.69	135.47	126.99
1	2A	1911	PSU	N1-C2-N3	6.59	122.12	115.17
56	2y	46	G7M	N9-C4-N3	6.57	139.08	125.95
56	1y	55	PSU	N1-C2-N3	6.56	122.08	115.17
1	1A	2605	PSU	N1-C2-N3	6.50	122.03	115.17
1	1A	1911	PSU	N1-C2-N3	6.46	121.98	115.17
54	1w	39	PSU	N1-C2-N3	6.43	121.95	115.17
1	2A	1917	PSU	N1-C2-N3	6.37	121.89	115.17
54	2w	55	PSU	N1-C2-N3	6.31	121.83	115.17
54	1w	55	PSU	N1-C2-N3	6.22	121.73	115.17
55	1x	55	PSU	N1-C2-N3	6.21	121.72	115.17
32	1a	966	M2G	C5-C4-N3	-6.21	118.51	128.39
1	1A	2251	OMG	C5-C4-N3	-6.20	118.52	128.39
54	2w	8	4SU	C5-C4-N3	6.19	120.51	114.75
32	2a	516	PSU	N1-C2-N3	6.14	121.65	115.17
56	2y	32	PSU	N1-C2-N3	6.14	121.64	115.17
55	1x	76	8AN	O4'-C1'-N9	6.08	119.76	108.09
1	1A	1917	PSU	N1-C2-N3	6.08	121.58	115.17
56	2y	46	G7M	C5-C4-N3	-6.03	116.76	128.15
32	2a	1207	2MG	C5-C4-N3	-6.03	118.80	128.39
1	2A	2251	OMG	C5-C4-N3	-6.02	118.81	128.39
56	2y	55	PSU	N1-C2-N3	6.00	121.50	115.17
32	2a	966	M2G	C5-C4-N3	-5.96	118.91	128.39
55	2x	55	PSU	N1-C2-N3	5.94	121.44	115.17
56	1y	32	PSU	N1-C2-N3	5.93	121.42	115.17
56	2y	8	4SU	C5-C4-N3	5.91	120.25	114.75
1	2A	2605	PSU	N1-C2-N3	5.90	121.39	115.17
32	1a	1207	2MG	C5-C4-N3	-5.90	119.00	128.39
56	1y	39	PSU	N1-C2-N3	5.89	121.38	115.17
32	1a	516	PSU	N1-C2-N3	5.86	121.35	115.17
54	2w	39	PSU	N1-C2-N3	5.84	121.33	115.17
56	1y	37	MIA	C5-C4-N3	-5.83	118.69	126.72
1	1A	2503	2MA	N3-C4-N9	5.83	134.38	126.99
54	2w	32	PSU	N1-C2-N3	5.80	121.29	115.17
54	2w	76	8AN	N1-C2-N3	-5.80	119.81	128.58
55	1x	76	8AN	N1-C2-N3	-5.78	119.83	128.58
55	2x	76	8AN	N1-C2-N3	-5.77	119.84	128.58
54	1w	76	8AN	N1-C2-N3	-5.72	119.92	128.58
56	1y	46	G7M	N9-C4-N3	5.71	137.38	125.95
54	1w	8	4SU	C4-N3-C2	-5.69	121.86	127.31
56	2y	37	MIA	C5-C4-N3	-5.64	118.95	126.72
54	1w	32	PSU	N1-C2-N3	5.62	121.09	115.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2A	1939	5MU	C4-N3-C2	-5.60	120.00	127.34
1	2A	1939	5MU	N3-C2-N1	5.59	122.17	114.89
43	2l	92	0TD	CSB-SB-CB	-5.43	92.60	102.36
32	2a	527	G7M	N9-C4-N3	5.42	136.80	125.95
56	2y	39	PSU	N1-C2-N3	5.36	120.82	115.17
1	1A	1915	5MU	C4-N3-C2	-5.35	120.32	127.34
32	2a	527	G7M	C5-C4-N3	-5.35	118.04	128.15
32	1a	527	G7M	N9-C4-N3	5.34	136.63	125.95
54	1w	8	4SU	C5-C4-N3	5.33	119.71	114.75
56	1y	46	G7M	C5-C4-N3	-5.32	118.10	128.15
1	1A	1915	5MU	N3-C2-N1	5.26	121.74	114.89
55	1x	76	8AN	C5-C4-N3	-5.17	119.60	126.72
32	2a	1519	MA6	N1-C2-N3	-5.15	120.78	128.58
54	1w	46	G7M	N9-C4-N3	5.15	136.26	125.95
55	2x	54	5MU	C4-N3-C2	-5.13	120.61	127.34
1	1A	2251	OMG	C2-N3-C4	5.12	121.13	112.30
32	1a	527	G7M	C5-C4-N3	-5.09	118.53	128.15
1	2A	1915	5MU	C4-N3-C2	-5.06	120.71	127.34
56	1y	8	4SU	C4-N3-C2	-5.05	122.47	127.31
55	2x	54	5MU	N3-C2-N1	5.04	121.45	114.89
54	2w	46	G7M	C5-C4-N3	-5.04	118.63	128.15
56	2y	46	G7M	C2-N3-C4	5.03	120.96	112.30
55	1x	54	5MU	N3-C2-N1	5.02	121.42	114.89
54	1w	76	8AN	C5-C4-N3	-4.99	119.84	126.72
32	1a	1518	MA6	N1-C2-N3	-4.97	121.05	128.58
1	2A	1915	5MU	N3-C2-N1	4.95	121.33	114.89
54	2w	76	8AN	C5-C4-N3	-4.92	119.94	126.72
55	2x	76	8AN	C5-C4-N3	-4.90	119.97	126.72
32	2a	1518	MA6	C5-C4-N3	-4.88	120.00	126.72
32	1a	1519	MA6	N1-C2-N3	-4.87	121.21	128.58
1	1A	2552	OMU	C4-N3-C2	-4.87	120.57	126.61
56	1y	46	G7M	C2-N3-C4	4.86	120.68	112.30
56	1y	37	MIA	N3-C4-N9	4.85	135.41	127.17
54	1w	46	G7M	C5-C4-N3	-4.83	119.02	128.15
1	2A	1939	5MU	C5-C4-N3	4.81	119.50	115.32
1	2A	2552	OMU	C4-N3-C2	-4.78	120.68	126.61
1	2A	2251	OMG	N9-C4-N3	4.77	135.50	125.95
32	2a	527	G7M	C2-N3-C4	4.77	120.52	112.30
54	1w	54	5MU	N3-C2-N1	4.72	121.03	114.89
55	1x	54	5MU	C4-N3-C2	-4.72	121.16	127.34
1	2A	2251	OMG	C2-N3-C4	4.70	120.39	112.30
56	2y	37	MIA	N3-C4-N9	4.67	135.10	127.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1939	5MU	C4-N3-C2	-4.66	121.22	127.34
56	1y	8	4SU	C5-C4-N3	4.66	119.08	114.75
54	2w	46	G7M	N9-C4-N3	4.65	135.25	125.95
32	2a	1518	MA6	N1-C2-N3	-4.64	121.56	128.58
1	2A	1915	5MU	C5-C4-N3	4.60	119.32	115.32
1	1A	2552	OMU	N3-C2-N1	4.56	120.83	114.89
32	1a	966	M2G	C2-N3-C4	4.55	120.93	112.51
32	1a	966	M2G	N9-C4-N3	4.55	135.04	125.95
1	2A	1915	5MU	O4-C4-C5	-4.53	119.74	124.92
1	1A	1939	5MU	C5-C4-N3	4.50	119.24	115.32
54	2w	8	4SU	C5-C4-S4	-4.50	119.17	124.31
54	2w	46	G7M	C2-N3-C4	4.49	120.04	112.30
54	1w	54	5MU	C4-N3-C2	-4.48	121.46	127.34
56	2y	8	4SU	C5-C4-S4	-4.47	119.19	124.31
55	2x	54	5MU	O4-C4-C5	-4.47	119.80	124.92
32	2a	1519	MA6	C5-C4-N3	-4.47	120.56	126.72
32	1a	1519	MA6	C5-C4-N3	-4.46	120.57	126.72
32	2a	966	M2G	N9-C4-N3	4.43	134.82	125.95
1	1A	1915	5MU	C5-C4-N3	4.41	119.16	115.32
54	2w	8	4SU	N3-C2-N1	4.40	120.62	114.89
1	2A	2605	PSU	C4-N3-C2	-4.38	120.34	126.37
1	1A	1939	5MU	N3-C2-N1	4.37	120.58	114.89
1	2A	2552	OMU	O2-C2-N1	-4.37	117.11	122.80
1	1A	2552	OMU	O2-C2-N1	-4.36	117.12	122.80
32	1a	527	G7M	C2-N3-C4	4.35	119.79	112.30
1	1A	2251	OMG	N9-C4-N3	4.32	134.59	125.95
1	1A	1915	5MU	O4-C4-C5	-4.31	119.99	124.92
54	1w	37	MIA	C15-C14-C13	-4.30	109.76	122.66
1	2A	2552	OMU	N3-C2-N1	4.29	120.47	114.89
54	2w	54	5MU	C4-N3-C2	-4.28	121.73	127.34
1	2A	1911	PSU	O2-C2-N1	-4.28	118.38	122.79
54	1w	46	G7M	C2-N3-C4	4.26	119.64	112.30
1	1A	2605	PSU	C4-N3-C2	-4.24	120.53	126.37
54	2w	54	5MU	N3-C2-N1	4.23	120.40	114.89
1	2A	1939	5MU	O4-C4-C5	-4.23	120.08	124.92
55	2x	54	5MU	C5-C4-N3	4.22	118.99	115.32
1	1A	1917	PSU	C4-N3-C2	-4.20	120.59	126.37
1	1A	1911	PSU	C4-N3-C2	-4.18	120.61	126.37
54	1w	39	PSU	C4-N3-C2	-4.18	120.61	126.37
1	2A	1911	PSU	C4-N3-C2	-4.17	120.63	126.37
32	1a	1207	2MG	N9-C4-N3	4.16	134.27	125.95
1	2A	1917	PSU	C4-N3-C2	-4.14	120.67	126.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	966	M2G	C2-N3-C4	4.14	120.16	112.51
55	1x	55	PSU	C4-N3-C2	-4.13	120.68	126.37
56	2y	8	4SU	N3-C2-N1	4.13	120.27	114.89
32	2a	516	PSU	C4-N3-C2	-4.13	120.68	126.37
32	1a	1518	MA6	C2-N1-C6	4.11	121.86	111.83
56	2y	54	5MU	C5-C4-N3	4.09	118.88	115.32
32	1a	516	PSU	C4-N3-C2	-4.08	120.75	126.37
56	1y	54	5MU	N3-C2-N1	4.07	120.19	114.89
55	2x	55	PSU	C4-N3-C2	-4.07	120.77	126.37
54	1w	55	PSU	O2-C2-N1	-4.06	118.61	122.79
56	1y	54	5MU	C4-N3-C2	-4.04	122.04	127.34
56	1y	55	PSU	C4-N3-C2	-4.04	120.81	126.37
54	2w	55	PSU	C4-N3-C2	-4.03	120.81	126.37
32	2a	1519	MA6	C5-N7-C8	4.03	109.78	103.45
1	1A	1917	PSU	O2-C2-N1	-4.02	118.65	122.79
32	2a	1519	MA6	C4-C5-N7	-4.01	105.99	110.58
1	1A	1939	5MU	C5-C6-N1	-4.01	118.95	123.31
54	1w	54	5MU	C5-C4-N3	3.98	118.78	115.32
54	2w	54	5MU	C5-C4-N3	3.97	118.78	115.32
55	1x	8	4SU	C6-C5-C4	-3.95	116.53	119.95
56	2y	54	5MU	O4-C4-C5	-3.94	120.41	124.92
54	2w	39	PSU	C4-N3-C2	-3.94	120.94	126.37
56	1y	54	5MU	C5-C4-N3	3.93	118.74	115.32
54	1w	55	PSU	C4-N3-C2	-3.93	120.95	126.37
56	1y	32	PSU	C4-N3-C2	-3.91	120.98	126.37
32	2a	1519	MA6	C2-N1-C6	3.90	121.36	111.83
54	1w	39	PSU	O2-C2-N1	-3.90	118.77	122.79
55	1x	54	5MU	C5-C4-N3	3.89	118.70	115.32
32	1a	1519	MA6	C4-C5-N7	-3.86	106.17	110.58
54	2w	54	5MU	O4-C4-C5	-3.86	120.50	124.92
32	2a	1207	2MG	C6-C5-N7	3.86	137.31	130.29
32	1a	1518	MA6	C5-C4-N3	-3.84	121.42	126.72
32	1a	1519	MA6	C2-N1-C6	3.83	121.19	111.83
32	2a	1518	MA6	C2-N1-C6	3.83	121.18	111.83
32	1a	1518	MA6	C5-N7-C8	3.82	109.46	103.45
1	2A	1939	5MU	C5-C6-N1	-3.82	119.16	123.31
56	2y	32	PSU	C4-N3-C2	-3.82	121.11	126.37
55	1x	8	4SU	O2-C2-N1	3.82	127.76	122.80
56	2y	54	5MU	C4-N3-C2	-3.81	122.34	127.34
55	1x	54	5MU	O4-C4-C5	-3.76	120.61	124.92
32	1a	1519	MA6	C5-N7-C8	3.76	109.35	103.45
56	2y	32	PSU	O2-C2-N1	-3.75	118.93	122.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	2a	1207	2MG	N9-C4-N3	3.74	133.43	125.95
56	2y	54	5MU	N3-C2-N1	3.74	119.76	114.89
32	1a	1518	MA6	N9-C8-N7	-3.73	108.64	113.94
1	2A	1917	PSU	O2-C2-N1	-3.73	118.94	122.79
32	2a	1518	MA6	C4-C5-N7	-3.73	106.32	110.58
54	1w	8	4SU	N3-C2-N1	3.72	119.74	114.89
32	2a	1518	MA6	C5-N7-C8	3.70	109.27	103.45
54	1w	32	PSU	C4-N3-C2	-3.70	121.28	126.37
32	1a	1207	2MG	C6-C5-N7	3.68	136.99	130.29
56	2y	55	PSU	O2-C2-N1	-3.67	119.00	122.79
56	1y	8	4SU	N3-C2-N1	3.67	119.67	114.89
54	2w	37	MIA	C12-N6-C6	-3.66	119.45	122.85
56	1y	55	PSU	O2-C2-N1	-3.66	119.02	122.79
56	1y	39	PSU	C4-N3-C2	-3.65	121.34	126.37
56	2y	37	MIA	C2-N3-C4	3.65	120.75	111.83
32	2a	1519	MA6	C2-N3-C4	3.65	120.74	111.83
32	1a	1400	5MC	C5-C6-N1	-3.64	119.36	123.31
56	1y	37	MIA	C2-N3-C4	3.64	120.72	111.83
54	1w	37	MIA	C16-C14-C13	-3.64	111.74	122.66
54	2w	37	MIA	C4-C5-N7	-3.63	106.44	110.58
56	2y	55	PSU	C4-N3-C2	-3.59	121.43	126.37
32	2a	516	PSU	O2-C2-N1	-3.58	119.10	122.79
1	1A	2503	2MA	N6-C6-N1	3.57	121.85	117.03
32	2a	1519	MA6	N9-C8-N7	-3.57	108.87	113.94
55	2x	54	5MU	C5-C6-N1	-3.57	119.44	123.31
1	2A	2605	PSU	O2-C2-N1	-3.57	119.11	122.79
54	2w	55	PSU	O2-C2-N1	-3.55	119.13	122.79
56	2y	37	MIA	N3-C2-N1	-3.54	123.23	128.58
32	1a	967	5MC	C5-C6-N1	-3.53	119.48	123.31
32	2a	1400	5MC	C5-C6-N1	-3.52	119.49	123.31
1	1A	2503	2MA	C4-C5-N7	-3.52	106.56	110.58
32	1a	1519	MA6	C2-N3-C4	3.50	120.39	111.83
54	2w	32	PSU	C4-N3-C2	-3.49	121.57	126.37
55	2x	32	5MC	C5-C6-N1	-3.49	119.53	123.31
32	2a	1518	MA6	C2-N3-C4	3.48	120.34	111.83
1	1A	1942	5MC	C5-C6-N1	-3.47	119.54	123.31
56	1y	54	5MU	O4-C4-C5	-3.47	120.95	124.92
54	1w	54	5MU	C5-C6-N1	-3.47	119.55	123.31
55	1x	76	8AN	N9-C8-N7	-3.46	109.03	113.94
54	1w	76	8AN	C2-N3-C4	3.46	120.28	111.83
32	1a	1404	5MC	C5-C4-N3	-3.45	118.22	121.75
55	1x	76	8AN	C2-N3-C4	3.44	120.24	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	2x	76	8AN	N9-C8-N7	-3.43	109.06	113.94
1	2A	2503	2MA	C4-C5-N7	-3.43	106.66	110.58
54	1w	76	8AN	N9-C8-N7	-3.43	109.07	113.94
32	2a	1404	5MC	C5-C6-N1	-3.43	119.59	123.31
32	2a	1207	2MG	N1-C2-N2	3.43	120.06	116.56
1	2A	1962	5MC	C5-C6-N1	-3.40	119.62	123.31
54	1w	54	5MU	O4-C4-C5	-3.40	121.03	124.92
54	2w	37	MIA	C2-N3-C4	3.39	121.17	112.29
1	2A	2552	OMU	C5-C4-N3	3.38	119.54	114.80
54	2w	76	8AN	N9-C8-N7	-3.38	109.15	113.94
56	2y	37	MIA	C4-C5-N7	-3.37	106.73	110.58
1	2A	1942	5MC	C5-C6-N1	-3.37	119.66	123.31
32	2a	1407	5MC	C5-C6-N1	-3.37	119.66	123.31
55	2x	76	8AN	C2-N3-C4	3.36	120.03	111.83
54	2w	76	8AN	C2-N3-C4	3.36	120.03	111.83
56	1y	37	MIA	N3-C2-N1	-3.35	123.51	128.58
55	1x	54	5MU	C5-C6-N1	-3.34	119.69	123.31
1	1A	2251	OMG	C6-C5-N7	3.34	136.36	130.29
56	2y	55	PSU	C6-C5-C4	-3.33	115.92	118.17
32	1a	1518	MA6	C4-C5-N7	-3.33	106.78	110.58
56	1y	37	MIA	C4-C5-N7	-3.33	106.78	110.58
56	1y	32	PSU	O2-C2-N1	-3.31	119.38	122.79
32	1a	1498	UR3	C5-C4-N3	3.30	119.39	115.04
1	2A	1915	5MU	C5-C6-N1	-3.29	119.74	123.31
1	2A	2503	2MA	N6-C6-N1	3.29	121.46	117.03
54	2w	32	PSU	O2-C2-N1	-3.29	119.40	122.79
32	2a	967	5MC	C5-C6-N1	-3.29	119.74	123.31
55	1x	32	5MC	C5-C4-N3	-3.28	118.39	121.75
32	2a	1207	2MG	C4-C5-N7	-3.27	105.48	110.67
1	1A	2552	OMU	C5-C4-N3	3.26	119.36	114.80
55	1x	32	5MC	C5-C6-N1	-3.26	119.78	123.31
32	2a	1407	5MC	C5-C4-N3	-3.26	118.42	121.75
54	1w	37	MIA	C2-N3-C4	3.25	120.81	112.29
1	1A	2552	OMU	O4-C4-C5	-3.25	119.56	125.16
55	1x	8	4SU	S4-C4-N3	-3.24	116.81	120.20
32	1a	1518	MA6	C2-N3-C4	3.24	119.75	111.83
54	1w	37	MIA	C4-C5-N7	-3.19	106.93	110.58
32	2a	1207	2MG	N2-C2-N3	-3.18	116.46	120.51
1	1A	1915	5MU	O2-C2-N1	-3.17	118.67	122.80
32	1a	1519	MA6	N9-C8-N7	-3.15	109.47	113.94
32	1a	966	M2G	C6-C5-N7	3.15	136.02	130.29
32	1a	1404	5MC	C5-C6-N1	-3.14	119.91	123.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2A	2552	OMU	O4-C4-C5	-3.13	119.77	125.16
32	2a	1518	MA6	N9-C8-N7	-3.13	109.50	113.94
32	2a	966	M2G	C6-C5-N7	3.11	135.94	130.29
55	1x	76	8AN	C4'-O4'-C1'	-3.08	102.67	109.47
55	1x	76	8AN	C5-N7-C8	3.07	108.27	103.45
32	2a	1498	UR3	C5-C4-N3	3.06	119.07	115.04
54	1w	8	4SU	C5-C4-S4	-3.05	120.83	124.31
54	2w	54	5MU	C5-C6-N1	-3.04	120.01	123.31
55	2x	8	4SU	O2-C2-N1	3.03	126.74	122.80
1	2A	2251	OMG	C6-C5-N7	3.02	135.78	130.29
1	2A	2503	2MA	C4-N9-C8	3.01	108.90	105.74
55	1x	55	PSU	O2-C2-N1	-3.00	119.69	122.79
54	1w	76	8AN	C5-N7-C8	3.00	108.17	103.45
1	1A	1942	5MC	C5-C4-N3	-3.00	118.68	121.75
32	2a	1518	MA6	N3-C4-N9	3.00	132.27	127.17
54	2w	76	8AN	C5-N7-C8	2.98	108.14	103.45
55	2x	76	8AN	C5-N7-C8	2.96	108.10	103.45
1	1A	1911	PSU	O2-C2-N1	-2.93	119.77	122.79
1	1A	1962	5MC	C5-C6-N1	-2.93	120.14	123.31
55	2x	76	8AN	C4'-O4'-C1'	-2.93	103.01	109.47
56	1y	54	5MU	C5-C6-N1	-2.92	120.14	123.31
32	1a	1407	5MC	C5-C6-N1	-2.92	120.14	123.31
1	1A	1915	5MU	C5-C6-N1	-2.91	120.15	123.31
54	1w	37	MIA	C6-C5-N7	2.91	135.60	132.43
32	1a	1207	2MG	C4-C5-N7	-2.89	106.09	110.67
56	2y	39	PSU	C4-N3-C2	-2.88	122.40	126.37
32	2a	1518	MA6	C4-C5-C6	2.87	118.88	115.91
56	2y	54	5MU	C5-C6-N1	-2.87	120.20	123.31
54	2w	39	PSU	O2-C2-N1	-2.87	119.83	122.79
1	1A	2251	OMG	C4-C5-N7	-2.83	106.18	110.67
55	2x	32	5MC	C5-C4-N3	-2.82	118.87	121.75
1	1A	2503	2MA	C2-N1-C6	2.81	122.42	118.10
1	1A	2605	PSU	O2-C2-N1	-2.81	119.89	122.79
55	2x	8	4SU	C6-C5-C4	-2.80	117.53	119.95
55	1x	8	4SU	C5-C4-N3	2.79	117.34	114.75
1	2A	1962	5MC	C5-C4-N3	-2.78	118.90	121.75
32	1a	1407	5MC	O2-C2-N3	-2.78	117.95	122.33
54	2w	37	MIA	C5-N7-C8	2.77	107.80	103.45
56	2y	37	MIA	C4-N9-C8	2.76	108.64	105.74
54	1w	37	MIA	C2-N1-C6	2.76	122.78	117.54
1	2A	1942	5MC	C5-C4-N3	-2.76	118.93	121.75
1	1A	1939	5MU	C5M-C5-C4	2.76	121.72	118.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1A	1939	5MU	O4-C4-C5	-2.74	121.78	124.92
1	2A	2503	2MA	C5-N7-C8	2.74	107.76	103.45
1	1A	1962	5MC	C5-C4-N3	-2.72	118.96	121.75
54	2w	76	8AN	C5-C4-N9	2.69	108.75	105.81
32	1a	1400	5MC	C5-C4-N3	-2.68	119.01	121.75
32	1a	1518	MA6	N3-C4-N9	2.68	131.72	127.17
32	2a	1404	5MC	C5-C4-N3	-2.67	119.02	121.75
55	1x	76	8AN	N3-C4-N9	2.66	131.70	127.17
54	2w	8	4SU	O2-C2-N1	-2.66	119.33	122.80
1	2A	2503	2MA	C2-N1-C6	2.65	122.18	118.10
54	1w	76	8AN	N3-C4-N9	2.65	131.68	127.17
55	1x	76	8AN	C5-C4-N9	2.65	108.69	105.81
32	1a	966	M2G	C4-C5-N7	-2.63	106.50	110.67
32	2a	1519	MA6	N3-C4-N9	2.61	131.61	127.17
32	2a	966	M2G	C4-C5-N7	-2.60	106.55	110.67
32	1a	516	PSU	O2-C2-N1	-2.60	120.11	122.79
54	1w	46	G7M	O6-C6-C5	-2.59	122.23	128.01
54	1w	37	MIA	C4-N9-C8	2.59	108.46	105.74
32	1a	1402	4OC	C6-C5-C4	2.59	120.12	117.00
54	2w	46	G7M	O6-C6-C5	-2.59	122.24	128.01
1	2A	1939	5MU	O2-C2-N1	-2.57	119.45	122.80
1	1A	1942	5MC	CM5-C5-C6	-2.57	119.37	122.85
56	1y	37	MIA	C4-N9-C8	2.57	108.43	105.74
1	1A	1915	5MU	C5M-C5-C4	2.56	121.52	118.78
32	2a	1400	5MC	C5-C4-N3	-2.55	119.14	121.75
32	1a	1519	MA6	N3-C4-N9	2.54	131.49	127.17
54	1w	54	5MU	O2-C2-N1	-2.54	119.50	122.80
55	2x	8	4SU	C5-C4-N3	2.53	117.11	114.75
55	2x	76	8AN	C5-C4-N9	2.53	108.56	105.81
55	2x	76	8AN	N3-C4-N9	2.52	131.45	127.17
56	2y	37	MIA	C5-N7-C8	2.52	107.41	103.45
55	1x	8	4SU	C1'-N1-C2	2.52	122.11	117.59
56	1y	37	MIA	C5-N7-C8	2.50	107.38	103.45
56	1y	8	4SU	C1'-N1-C2	2.50	122.08	117.59
56	1y	39	PSU	O2-C2-N3	-2.48	117.46	121.86
55	1x	54	5MU	O2-C2-N1	-2.47	119.58	122.80
54	1w	37	MIA	N3-C2-N1	-2.46	122.51	127.00
55	2x	54	5MU	O2-C2-N1	-2.46	119.59	122.80
54	1w	76	8AN	C5-C4-N9	2.45	108.48	105.81
32	1a	527	G7M	O6-C6-C5	-2.44	122.56	128.01
32	1a	1407	5MC	C5-C4-N3	-2.44	119.25	121.75
54	2w	37	MIA	C6-C5-N7	2.44	135.09	132.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	2w	76	8AN	N3-C4-N9	2.44	131.31	127.17
55	2x	32	5MC	O2-C2-N3	-2.42	118.51	122.33
32	1a	1518	MA6	C4-N9-C8	2.41	108.27	105.74
55	2x	8	4SU	S4-C4-N3	-2.41	117.68	120.20
56	2y	8	4SU	O2-C2-N1	-2.40	119.67	122.80
55	2x	8	4SU	C1'-N1-C2	2.40	121.90	117.59
54	1w	32	PSU	O2-C2-N1	-2.39	120.32	122.79
54	1w	37	MIA	C5-N7-C8	2.39	107.21	103.45
56	1y	8	4SU	C5-C4-S4	-2.39	121.58	124.31
55	2x	55	PSU	O2-C2-N1	-2.38	120.33	122.79
55	1x	55	PSU	C5-C6-N1	-2.38	118.84	122.14
55	2x	76	8AN	O4'-C1'-N9	2.37	112.65	108.09
32	2a	1400	5MC	O2-C2-N3	-2.37	118.59	122.33
1	1A	2503	2MA	C5-N7-C8	2.35	107.15	103.45
55	1x	76	8AN	C6-C5-C4	2.35	120.38	117.18
32	2a	527	G7M	C5-C6-N1	2.34	116.69	111.84
32	2a	967	5MC	C5-C4-N3	-2.34	119.36	121.75
54	2w	37	MIA	C11-S10-C2	-2.33	100.50	102.25
56	1y	46	G7M	O6-C6-C5	-2.31	122.85	128.01
55	1x	8	4SU	C4-N3-C2	2.31	129.53	127.31
32	1a	967	5MC	C5-C4-N3	-2.31	119.39	121.75
32	2a	1407	5MC	O2-C2-N3	-2.30	118.71	122.33
43	1l	92	0TD	OD2-CG-CB	2.29	118.09	113.15
1	2A	2251	OMG	C4-C5-N7	-2.28	107.05	110.67
56	2y	39	PSU	O2-C2-N3	-2.28	117.82	121.86
54	2w	54	5MU	O2-C2-N1	-2.27	119.84	122.80
55	1x	76	8AN	C4-C5-N7	-2.25	108.01	110.58
32	2a	1402	4OC	C6-C5-C4	2.23	119.69	117.00
56	2y	46	G7M	O6-C6-C5	-2.23	123.04	128.01
1	2A	2503	2MA	N9-C8-N7	-2.23	110.78	113.94
54	1w	39	PSU	C5-C6-N1	-2.22	119.06	122.14
32	1a	1400	5MC	O2-C2-N3	-2.22	118.83	122.33
32	2a	527	G7M	O6-C6-C5	-2.20	123.09	128.01
1	2A	2251	OMG	O6-C6-C5	-2.18	120.77	126.53
1	1A	1962	5MC	O2-C2-N3	-2.18	118.89	122.33
32	1a	1498	UR3	C3U-N3-C2	2.18	121.13	117.33
54	2w	76	8AN	C6-C5-C4	2.17	120.14	117.18
32	2a	1498	UR3	C6-N1-C2	-2.17	120.02	121.80
54	2w	46	G7M	N2-C2-N3	-2.16	115.45	119.67
1	2A	1920	OMC	O2-C2-N3	-2.16	118.93	122.33
32	1a	516	PSU	O4'-C1'-C2'	2.16	108.13	105.15
55	2x	76	8AN	C6-C5-C4	2.16	120.12	117.18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	1a	1404	5MC	O2-C2-N3	-2.15	118.94	122.33
54	1w	37	MIA	C11-S10-C2	-2.15	100.64	102.25
54	2w	37	MIA	C4-N9-C8	2.14	107.99	105.74
54	2w	37	MIA	C2-N1-C6	2.14	121.61	117.54
1	1A	2605	PSU	C5-C6-N1	-2.14	119.17	122.14
1	2A	1917	PSU	C5-C6-N1	-2.14	119.17	122.14
1	1A	1911	PSU	C5-C6-N1	-2.13	119.18	122.14
32	1a	527	G7M	C5-C6-N1	2.13	116.25	111.84
56	1y	39	PSU	O4'-C1'-C2'	2.13	108.10	105.15
1	1A	2605	PSU	O2-C2-N3	-2.13	118.08	121.86
55	1x	8	4SU	O2-C2-N3	-2.13	117.56	121.49
54	2w	46	G7M	C5-C6-N1	2.13	116.24	111.84
55	1x	32	5MC	O2-C2-N3	-2.12	118.98	122.33
32	1a	1404	5MC	CM5-C5-C6	-2.10	120.00	122.85
54	2w	76	8AN	C4-C5-N7	-2.10	108.18	110.58
56	1y	55	PSU	O4'-C1'-C2'	2.10	108.06	105.15
1	1A	1915	5MU	C5M-C5-C6	-2.10	120.01	122.85
32	1a	516	PSU	C5-C6-N1	-2.10	119.23	122.14
55	2x	55	PSU	C5-C6-N1	-2.09	119.24	122.14
54	2w	54	5MU	C5M-C5-C4	2.08	121.00	118.78
32	1a	967	5MC	CM5-C5-C6	-2.07	120.05	122.85
1	2A	1915	5MU	O2-C2-N1	-2.07	120.10	122.80
1	1A	1920	OMC	O2-C2-N3	-2.07	119.07	122.33
54	1w	76	8AN	C6-C5-C4	2.07	120.00	117.18
55	2x	8	4SU	O2-C2-N3	-2.05	117.70	121.49
55	2x	55	PSU	O2-C2-N3	-2.04	118.23	121.86
54	2w	37	MIA	C4-C5-C6	2.04	118.47	116.78
1	1A	1911	PSU	O2-C2-N3	-2.03	118.25	121.86
32	1a	1207	2MG	C8-N7-C5	2.03	107.87	104.26
32	1a	1519	MA6	C4-C5-C6	2.02	118.00	115.91
54	1w	76	8AN	C4-C5-N7	-2.02	108.27	110.58
1	1A	1939	5MU	C5M-C5-C6	-2.02	120.11	122.85
1	1A	1917	PSU	C5-C6-N1	-2.01	119.34	122.14
56	1y	54	5MU	C5M-C5-C4	2.01	120.93	118.78
56	2y	46	G7M	C5-C6-N1	2.01	116.00	111.84
1	2A	1911	PSU	C5-C6-N1	-2.01	119.35	122.14
32	1a	966	M2G	O6-C6-C5	-2.01	121.24	126.53
54	2w	37	MIA	C1'-N9-C8	-2.00	122.65	127.09

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	1w	37	MIA	C12-C13-C14-C16
56	1y	46	G7M	C4'-C5'-O5'-P
55	2x	76	8AN	O4'-C4'-C5'-O5'
55	2x	76	8AN	C3'-C4'-C5'-O5'
56	2y	55	PSU	C2'-C1'-C5-C4
55	1x	76	8AN	C3'-C4'-C5'-O5'
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1519	MA6	O4'-C4'-C5'-O5'
54	2w	46	G7M	O4'-C4'-C5'-O5'
55	1x	76	8AN	O4'-C4'-C5'-O5'
56	1y	37	MIA	C3'-C4'-C5'-O5'
32	2a	527	G7M	C3'-C4'-C5'-O5'
54	2w	46	G7M	C3'-C4'-C5'-O5'
32	1a	527	G7M	C3'-C4'-C5'-O5'
56	1y	8	4SU	C3'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
56	2y	37	MIA	C3'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
56	1y	8	4SU	O4'-C4'-C5'-O5'
56	2y	46	G7M	O4'-C1'-N9-C4
54	1w	46	G7M	C4'-C5'-O5'-P
54	2w	46	G7M	C4'-C5'-O5'-P
56	1y	37	MIA	O4'-C4'-C5'-O5'
32	2a	527	G7M	O4'-C4'-C5'-O5'
54	2w	37	MIA	N3-C2-S10-C11
55	2x	76	8AN	C4'-C5'-O5'-P
54	2w	37	MIA	N1-C2-S10-C11
32	1a	527	G7M	O4'-C4'-C5'-O5'
56	2y	37	MIA	O4'-C4'-C5'-O5'
43	1l	92	0TD	CG-CB-SB-CSB
43	2l	92	0TD	CG-CB-SB-CSB
43	1l	92	0TD	SB-CB-CG-OD1
56	2y	46	G7M	O4'-C1'-N9-C8
55	1x	76	8AN	C4'-C5'-O5'-P
56	1y	55	PSU	O4'-C1'-C5-C4
56	2y	55	PSU	O4'-C1'-C5-C4
32	1a	527	G7M	C4'-C5'-O5'-P
32	2a	527	G7M	C4'-C5'-O5'-P
32	2a	1519	MA6	C4'-C5'-O5'-P
32	1a	1402	4OC	O4'-C4'-C5'-O5'
32	2a	1402	4OC	O4'-C4'-C5'-O5'
1	1A	2503	2MA	C4'-C5'-O5'-P
56	2y	8	4SU	C4'-C5'-O5'-P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
43	2l	92	0TD	SB-CB-CG-OD2
1	2A	2503	2MA	O4'-C4'-C5'-O5'
1	1A	1915	5MU	O4'-C4'-C5'-O5'
1	1A	1920	OMC	C2'-C1'-N1-C2
32	1a	1519	MA6	C4'-C5'-O5'-P
1	2A	2503	2MA	C4'-C5'-O5'-P
56	2y	37	MIA	C4'-C5'-O5'-P
56	1y	8	4SU	C2'-C1'-N1-C2

There are no ring outliers.

28 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	2a	967	5MC	1	0
54	1w	8	4SU	1	0
54	2w	46	G7M	1	0
55	1x	8	4SU	2	0
56	2y	37	MIA	1	0
56	1y	37	MIA	2	0
54	1w	54	5MU	1	0
32	1a	1402	4OC	1	0
54	2w	76	8AN	1	0
43	1l	92	0TD	2	0
32	2a	1402	4OC	1	0
32	1a	966	M2G	1	0
56	1y	46	G7M	2	0
32	1a	1519	MA6	1	0
32	2a	1519	MA6	2	0
32	1a	967	5MC	1	0
32	1a	1518	MA6	1	0
1	2A	2251	OMG	1	0
56	1y	55	PSU	1	0
55	2x	76	8AN	2	0
56	1y	8	4SU	1	0
55	1x	76	8AN	1	0
56	2y	46	G7M	3	0
56	1y	39	PSU	1	0
56	2y	8	4SU	4	0
32	2a	1518	MA6	3	0
1	2A	1915	5MU	1	0
56	2y	55	PSU	5	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2777 ligands modelled in this entry, 2769 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
61	SF4	2d	302	35	0,12,12	-	-	-		
63	FME	2x	108	55	8,9,10	0.44	0	8,9,11	1.32	2 (25%)
62	PHE	1w	110	54	10,11,12	1.48	1 (10%)	8,13,15	0.54	0
59	A1AEZ	2A	3843	57	90,91,91	2.39	16 (17%)	126,132,132	2.22	32 (25%)
62	PHE	2w	108	54	10,11,12	1.56	1 (10%)	8,13,15	0.52	0
61	SF4	1d	501	35	0,12,12	-	-	-		
63	FME	1x	115	55	8,9,10	0.50	0	8,9,11	1.50	2 (25%)
59	A1AEZ	1A	4118	57	90,91,91	2.45	18 (20%)	126,132,132	2.05	31 (24%)

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
61	SF4	2d	302	35	-	-	0/6/5/5
63	FME	2x	108	55	-	0/7/9/11	-
62	PHE	1w	110	54	-	0/5/6/8	0/1/1/1
59	A1AEZ	2A	3843	57	-	16/98/132/132	0/7/7/7
62	PHE	2w	108	54	-	2/5/6/8	0/1/1/1
61	SF4	1d	501	35	-	-	0/6/5/5
63	FME	1x	115	55	-	2/7/9/11	-
59	A1AEZ	1A	4118	57	-	18/98/132/132	0/7/7/7

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	2A	3843	A1AEZ	CAG-CAF	-12.87	1.41	1.53
59	1A	4118	A1AEZ	CAG-CAF	-11.84	1.42	1.53
59	2A	3843	A1AEZ	CBU-CBT	8.71	1.30	1.19
59	1A	4118	A1AEZ	OBR-NBJ	8.19	1.56	1.42
59	1A	4118	A1AEZ	CBU-CBT	7.52	1.29	1.19
59	2A	3843	A1AEZ	CAB-CAF	-7.19	1.40	1.52
59	1A	4118	A1AEZ	CAB-CAF	-5.87	1.42	1.52
59	1A	4118	A1AEZ	CCW-CDE	-5.53	1.40	1.48
59	2A	3843	A1AEZ	CAJ-CAI	-5.50	1.39	1.51
59	2A	3843	A1AEZ	CCW-CDE	-5.20	1.40	1.48
59	1A	4118	A1AEZ	CBX-CCB	-5.09	1.39	1.50
59	1A	4118	A1AEZ	CAJ-CAI	-4.89	1.41	1.51
62	2w	108	PHE	CB-CG	-4.71	1.40	1.51
59	2A	3843	A1AEZ	CBX-CCB	-4.63	1.40	1.50
62	1w	110	PHE	CB-CG	-4.49	1.40	1.51
59	1A	4118	A1AEZ	CCS-CCV	-4.41	1.39	1.48
59	2A	3843	A1AEZ	CCS-CCV	-4.31	1.39	1.48
59	1A	4118	A1AEZ	CAF-NBJ	4.23	1.34	1.28
59	2A	3843	A1AEZ	CAF-NBJ	3.57	1.33	1.28
59	2A	3843	A1AEZ	CCX-NCY	3.56	1.40	1.34
59	1A	4118	A1AEZ	CCA-NBZ	3.36	1.41	1.34
59	1A	4118	A1AEZ	CCX-NCY	3.35	1.40	1.34
59	2A	3843	A1AEZ	OBH-CAL	-3.21	1.42	1.47
59	2A	3843	A1AEZ	CBY-NBZ	3.16	1.41	1.34
59	1A	4118	A1AEZ	CAG-CAH	3.08	1.58	1.54
59	2A	3843	A1AEZ	CCZ-NCY	2.98	1.51	1.46
59	2A	3843	A1AEZ	CCA-NBZ	2.94	1.40	1.34
59	1A	4118	A1AEZ	CCT-NCY	-2.91	1.36	1.40
59	1A	4118	A1AEZ	FDC-CCQ	-2.75	1.28	1.35
59	1A	4118	A1AEZ	OBH-CAL	-2.61	1.43	1.47
59	1A	4118	A1AEZ	CCZ-NCY	2.60	1.51	1.46
59	1A	4118	A1AEZ	CBY-NBZ	2.55	1.39	1.34
59	2A	3843	A1AEZ	CCT-NCY	-2.46	1.37	1.40
59	2A	3843	A1AEZ	CAG-CAH	2.45	1.57	1.54
59	1A	4118	A1AEZ	OAN-CAM	-2.22	1.42	1.46
59	2A	3843	A1AEZ	CDB-CCZ	2.07	1.53	1.48

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
59	2A	3843	A1AEZ	CAB-CAF-NBJ	-11.32	117.86	126.21
59	2A	3843	A1AEZ	CCT-NCY-CCZ	9.62	129.90	119.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
59	1A	4118	A1AEZ	CCT-NCY-CCZ	9.59	129.87	119.88
59	1A	4118	A1AEZ	CAB-CAF-NBJ	-9.02	119.56	126.21
59	2A	3843	A1AEZ	CCZ-NCY-CCX	-5.92	111.06	119.74
59	2A	3843	A1AEZ	CCQ-CCP-NCO	-5.87	115.12	119.26
59	1A	4118	A1AEZ	CCZ-NCY-CCX	-5.65	111.45	119.74
59	2A	3843	A1AEZ	CAB-CAF-CAG	4.49	124.14	119.34
59	2A	3843	A1AEZ	CCU-CCT-NCY	4.40	124.29	120.49
59	1A	4118	A1AEZ	CAB-CAF-CAG	4.36	124.00	119.34
59	2A	3843	A1AEZ	CCR-CCQ-CCP	-4.11	119.23	123.43
59	2A	3843	A1AEZ	CAE-CAD-CAC	-4.04	107.37	113.54
59	1A	4118	A1AEZ	OBR-NBJ-CAF	3.77	121.16	111.53
59	2A	3843	A1AEZ	CBE-CAM-CAL	-3.68	110.15	115.23
59	1A	4118	A1AEZ	CDB-CCZ-NCY	3.61	124.58	118.87
59	1A	4118	A1AEZ	CCR-CCQ-CCP	-3.61	119.74	123.43
59	2A	3843	A1AEZ	CAG-CAF-NBJ	3.46	117.97	114.40
59	1A	4118	A1AEZ	CBS-OBR-NBJ	3.38	111.80	108.03
59	2A	3843	A1AEZ	CDB-CCZ-NCY	3.26	124.02	118.87
59	1A	4118	A1AEZ	CCU-CCT-NCY	3.24	123.30	120.49
59	1A	4118	A1AEZ	CDE-CCW-CCV	3.18	126.33	121.61
59	1A	4118	A1AEZ	CBE-CAM-CAL	-3.17	110.86	115.23
59	2A	3843	A1AEZ	CCU-CCP-CCQ	3.12	120.64	117.65
59	1A	4118	A1AEZ	OBH-CAL-CBG	3.05	112.18	106.80
59	1A	4118	A1AEZ	CAE-CAD-CAC	-3.01	108.95	113.54
59	1A	4118	A1AEZ	CBW-CBX-CBY	2.90	120.90	117.92
59	1A	4118	A1AEZ	CCU-CCP-CCQ	2.86	120.40	117.65
59	1A	4118	A1AEZ	OAO-CAD-CAE	2.83	113.02	106.44
63	1x	115	FME	CA-N-CN	-2.82	118.48	122.82
59	2A	3843	A1AEZ	CCS-CCV-CCW	2.81	119.18	115.64
59	2A	3843	A1AEZ	CAX-CAR-CAS	-2.80	109.04	113.27
59	1A	4118	A1AEZ	OBH-CAL-CAM	2.77	111.76	105.63
59	2A	3843	A1AEZ	CCX-CCW-CCV	-2.73	117.93	119.94
59	1A	4118	A1AEZ	CCE-NCC-CCB	-2.64	116.77	121.80
59	2A	3843	A1AEZ	OBH-CAL-CAM	2.63	111.46	105.63
59	1A	4118	A1AEZ	CBX-CBY-NBZ	-2.62	119.60	123.50
59	2A	3843	A1AEZ	CBV-CCA-NBZ	-2.62	119.24	123.37
63	1x	115	FME	O1-CN-N	-2.59	118.63	125.32
59	2A	3843	A1AEZ	CBI-CAG-CAH	2.50	116.35	112.94
59	2A	3843	A1AEZ	CCI-CCH-CCF	-2.44	107.77	113.12
59	1A	4118	A1AEZ	CCI-CCH-CCF	-2.43	107.80	113.12
59	2A	3843	A1AEZ	CBW-CBV-CCA	2.42	120.60	118.28
59	1A	4118	A1AEZ	CBX-CCB-NCC	-2.41	114.00	117.01
59	2A	3843	A1AEZ	CCR-CCS-CCT	2.39	121.57	118.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
63	2x	108	FME	CA-N-CN	-2.38	119.16	122.82
59	2A	3843	A1AEZ	CBS-OBR-NBJ	2.38	110.68	108.03
59	2A	3843	A1AEZ	OBR-NBJ-CAF	2.35	117.55	111.53
59	2A	3843	A1AEZ	CCE-NCC-CCB	-2.33	117.37	121.80
59	2A	3843	A1AEZ	OBH-CAL-CBG	2.32	110.90	106.80
59	1A	4118	A1AEZ	ODG-CDE-ODF	-2.31	118.40	123.90
59	1A	4118	A1AEZ	CCX-CCW-CCV	-2.30	118.25	119.94
59	2A	3843	A1AEZ	CCU-CCT-CCS	-2.29	116.90	120.18
63	2x	108	FME	O1-CN-N	-2.27	119.45	125.32
59	1A	4118	A1AEZ	CCQ-CCP-NCO	-2.22	117.69	119.26
59	2A	3843	A1AEZ	CAH-OBN-CBP	-2.22	105.72	109.45
59	2A	3843	A1AEZ	OAN-CAI-CAJ	2.16	116.14	111.53
59	1A	4118	A1AEZ	CBI-CAG-CAH	2.15	115.88	112.94
59	1A	4118	A1AEZ	OAO-CAD-CAC	-2.14	108.48	111.58
59	2A	3843	A1AEZ	CBX-CBY-NBZ	-2.14	120.32	123.50
59	2A	3843	A1AEZ	OBL-CAE-CAA	2.14	110.21	105.71
59	1A	4118	A1AEZ	CCS-CCV-CCW	2.13	118.33	115.64
59	1A	4118	A1AEZ	CAX-CAR-CAS	-2.09	110.11	113.27
59	2A	3843	A1AEZ	CCR-CCS-CCV	-2.09	116.44	119.94
59	1A	4118	A1AEZ	FDC-CCQ-CCP	2.06	120.15	117.59
59	1A	4118	A1AEZ	CCR-CCS-CCT	2.04	121.17	118.76
59	1A	4118	A1AEZ	CCR-CCS-CCV	-2.04	116.52	119.94
59	2A	3843	A1AEZ	OAO-CAD-CAE	2.03	111.15	106.44

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	1A	4118	A1AEZ	OBR-CBS-CBT-CBU
59	1A	4118	A1AEZ	CBT-CBS-OBR-NBJ
59	1A	4118	A1AEZ	CDB-CCZ-NCY-CCT
59	1A	4118	A1AEZ	CDB-CCZ-NCY-CCX
59	2A	3843	A1AEZ	OBR-CBS-CBT-CBU
59	2A	3843	A1AEZ	CBT-CBS-OBR-NBJ
59	2A	3843	A1AEZ	CDB-CCZ-NCY-CCT
59	2A	3843	A1AEZ	CDB-CCZ-NCY-CCX
62	2w	108	PHE	O-C-CA-CB
59	2A	3843	A1AEZ	NCJ-CCK-CCL-CCM
59	1A	4118	A1AEZ	NCJ-CCK-CCL-CCM
59	2A	3843	A1AEZ	CDA-CCZ-NCY-CCX
59	1A	4118	A1AEZ	CCL-CCK-NCJ-CCI
59	2A	3843	A1AEZ	CCH-CCI-NCJ-CCK

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
59	2A	3843	A1AEZ	CCL-CCM-CCN-NCO
59	2A	3843	A1AEZ	CCV-CCW-CDE-ODF
59	2A	3843	A1AEZ	CCV-CCW-CDE-ODG
59	2A	3843	A1AEZ	CCX-CCW-CDE-ODG
59	2A	3843	A1AEZ	CDA-CCZ-NCY-CCT
59	2A	3843	A1AEZ	CCX-CCW-CDE-ODF
59	1A	4118	A1AEZ	CCF-CCH-CCI-NCJ
59	2A	3843	A1AEZ	CCF-CCH-CCI-NCJ
63	1x	115	FME	N-CA-CB-CG
59	1A	4118	A1AEZ	NBJ-CAF-CAG-CBI
59	1A	4118	A1AEZ	CCM-CCN-NCO-CCP
59	1A	4118	A1AEZ	CDA-CCZ-NCY-CCX
59	2A	3843	A1AEZ	CCL-CCK-NCJ-CCI
62	2w	108	PHE	C-CA-CB-CG
59	1A	4118	A1AEZ	CCK-CCL-CCM-CCN
59	1A	4118	A1AEZ	CCH-CCI-NCJ-CCK
63	1x	115	FME	CB-CG-SD-CE
59	1A	4118	A1AEZ	CCL-CCM-CCN-NCO
59	1A	4118	A1AEZ	CDA-CCZ-NCY-CCT
59	1A	4118	A1AEZ	CBK-CAB-CAF-NBJ
59	1A	4118	A1AEZ	CCV-CCW-CDE-ODF
59	1A	4118	A1AEZ	CCV-CCW-CDE-ODG
59	1A	4118	A1AEZ	CAU-CAP-OAO-CAD
59	2A	3843	A1AEZ	OAN-CAM-CBE-CBF

There are no ring outliers.

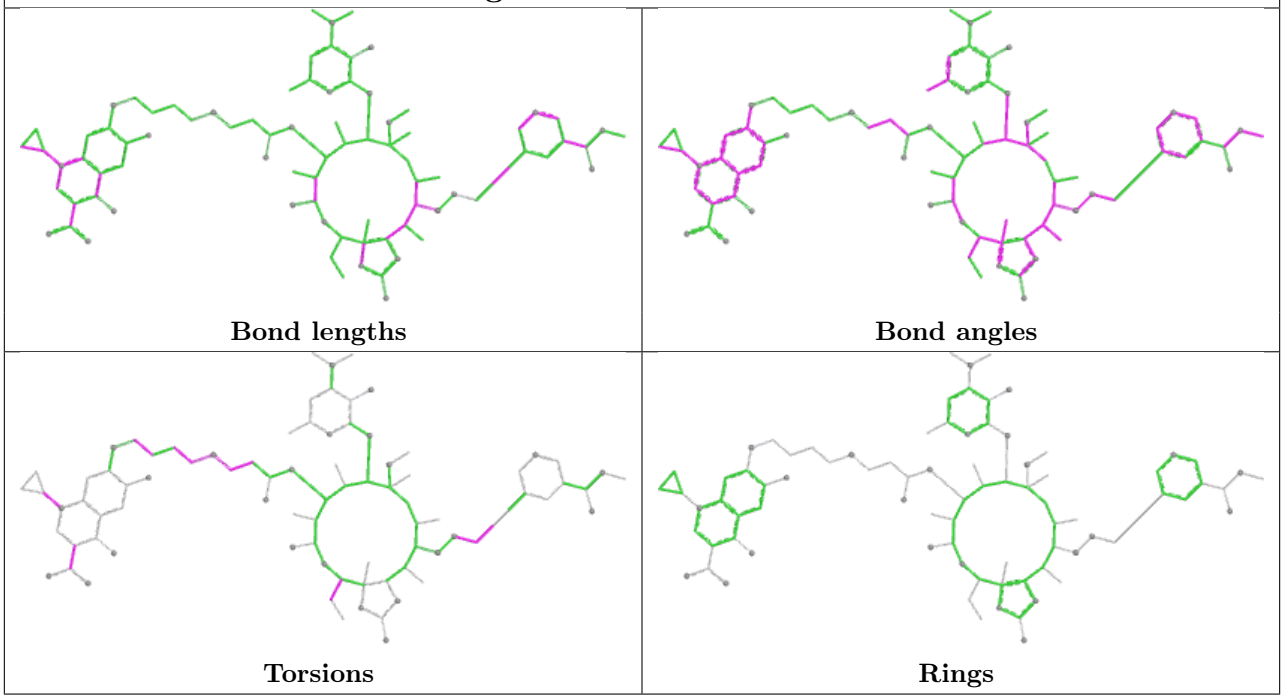
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	2A	3843	A1AEZ	1	0
62	2w	108	PHE	1	0
59	1A	4118	A1AEZ	2	0

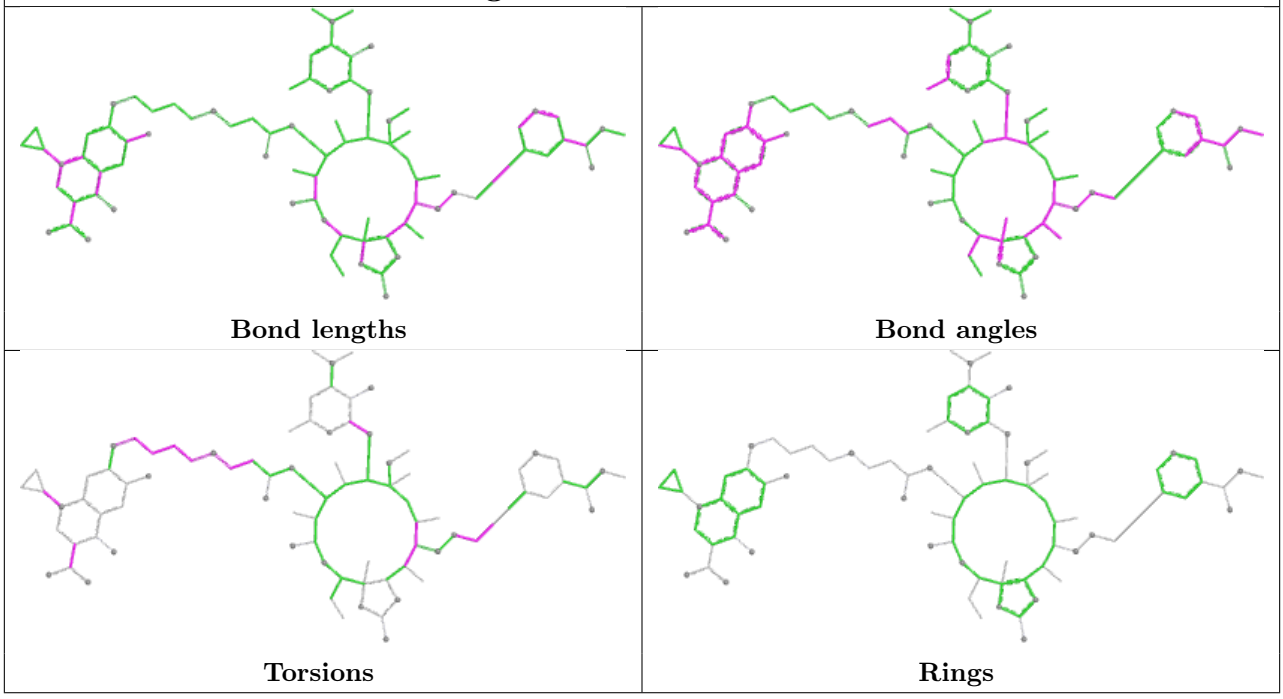
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand A1AEZ 2A 3843



Ligand A1AEZ 1A 4118



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	-0.55	174 (6%) 27 23	16, 32, 83, 94	0
1	2A	2789/2915 (95%)	-0.08	147 (5%) 32 28	29, 50, 81, 93	0
2	1B	120/121 (99%)	-0.42	0 100 100	26, 44, 57, 75	0
2	2B	120/121 (99%)	0.47	3 (2%) 58 54	52, 64, 71, 81	0
3	1D	275/276 (99%)	-0.25	3 (1%) 78 74	17, 33, 46, 68	0
3	2D	275/276 (99%)	0.15	4 (1%) 72 68	27, 43, 54, 72	0
4	1E	204/206 (99%)	-0.21	2 (0%) 79 76	17, 35, 55, 63	0
4	2E	204/206 (99%)	0.37	5 (2%) 58 54	30, 52, 63, 71	0
5	1F	203/210 (96%)	-0.13	2 (0%) 79 76	16, 38, 60, 72	0
5	2F	203/210 (96%)	0.47	3 (1%) 72 68	30, 58, 70, 77	0
6	1G	181/182 (99%)	0.42	7 (3%) 43 39	36, 51, 64, 76	0
6	2G	181/182 (99%)	0.97	13 (7%) 21 18	53, 65, 73, 77	0
7	1H	174/180 (96%)	0.28	5 (2%) 53 50	35, 47, 59, 64	0
7	2H	174/180 (96%)	1.52	47 (27%) 1 1	62, 72, 78, 82	0
8	1I	146/148 (98%)	0.83	6 (4%) 41 37	42, 63, 71, 75	0
8	2I	146/148 (98%)	1.01	10 (6%) 23 20	49, 63, 72, 75	0
9	1N	140/140 (100%)	-0.17	2 (1%) 73 69	22, 35, 53, 61	0
9	2N	140/140 (100%)	0.71	4 (2%) 53 50	41, 56, 68, 74	0
10	1O	122/122 (100%)	-0.12	2 (1%) 70 66	23, 36, 52, 57	0
10	2O	122/122 (100%)	0.36	0 100 100	42, 52, 62, 65	0
11	1P	149/150 (99%)	0.04	2 (1%) 75 71	16, 41, 59, 64	0
11	2P	149/150 (99%)	0.62	5 (3%) 48 44	32, 58, 70, 77	0
12	1Q	141/141 (100%)	-0.17	0 100 100	21, 36, 50, 64	0
12	2Q	141/141 (100%)	0.86	9 (6%) 25 22	40, 56, 66, 69	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%)	-0.39	0 100 100	23, 30, 44, 51	0
13	2R	118/118 (100%)	0.16	1 (0%) 82 80	34, 46, 55, 63	0
14	1S	110/112 (98%)	0.11	0 100 100	31, 43, 55, 59	0
14	2S	110/112 (98%)	0.93	3 (2%) 56 52	52, 61, 68, 74	0
15	1T	131/146 (89%)	0.07	2 (1%) 72 68	29, 40, 60, 69	0
15	2T	131/146 (89%)	0.46	2 (1%) 72 68	43, 54, 66, 70	0
16	1U	116/118 (98%)	-0.46	0 100 100	18, 27, 43, 57	0
16	2U	116/118 (98%)	0.54	3 (2%) 57 53	37, 52, 64, 69	0
17	1V	101/101 (100%)	-0.28	1 (0%) 79 76	18, 34, 50, 58	0
17	2V	101/101 (100%)	0.71	0 100 100	38, 60, 66, 71	0
18	1W	112/113 (99%)	-0.41	1 (0%) 81 78	20, 28, 46, 72	0
18	2W	112/113 (99%)	0.10	1 (0%) 81 78	36, 43, 58, 76	0
19	1X	95/96 (98%)	-0.12	2 (2%) 63 59	23, 34, 59, 73	0
19	2X	95/96 (98%)	0.58	3 (3%) 50 46	39, 51, 66, 76	0
20	1Y	107/110 (97%)	0.22	2 (1%) 66 62	33, 44, 58, 66	0
20	2Y	107/110 (97%)	1.19	12 (11%) 10 7	51, 62, 71, 76	0
21	1Z	154/206 (74%)	0.90	20 (12%) 7 5	34, 56, 72, 78	0
21	2Z	160/206 (77%)	1.48	38 (23%) 2 1	56, 69, 77, 83	0
22	10	83/85 (97%)	-0.13	1 (1%) 76 73	24, 32, 43, 61	0
22	20	83/85 (97%)	0.59	1 (1%) 76 73	38, 52, 60, 74	0
23	11	97/98 (98%)	0.16	1 (1%) 79 76	26, 41, 63, 66	0
23	21	97/98 (98%)	0.43	2 (2%) 63 59	33, 49, 64, 68	0
24	12	70/72 (97%)	0.09	0 100 100	29, 42, 54, 62	0
24	22	70/72 (97%)	0.66	2 (2%) 53 50	49, 60, 68, 72	0
25	13	59/60 (98%)	-0.29	0 100 100	19, 30, 55, 70	0
25	23	59/60 (98%)	0.47	2 (3%) 48 44	47, 55, 65, 74	0
26	14	69/71 (97%)	1.04	14 (20%) 3 2	43, 65, 76, 79	0
26	24	69/71 (97%)	1.50	18 (26%) 1 1	62, 71, 79, 81	0
27	15	59/60 (98%)	-0.39	1 (1%) 69 65	17, 30, 50, 58	0
27	25	59/60 (98%)	0.12	2 (3%) 48 44	30, 46, 60, 72	0
28	16	53/54 (98%)	-0.17	1 (1%) 66 62	28, 38, 49, 55	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%)	0.52	0 100 100	44, 52, 60, 62	0
29	17	48/49 (97%)	-0.27	3 (6%) 26 22	17, 24, 50, 57	0
29	27	48/49 (97%)	0.07	4 (8%) 17 14	27, 36, 61, 65	0
30	18	64/65 (98%)	-0.45	0 100 100	22, 29, 36, 53	0
30	28	64/65 (98%)	0.44	0 100 100	41, 47, 53, 59	0
31	19	37/37 (100%)	-0.19	0 100 100	24, 35, 44, 54	0
31	29	37/37 (100%)	0.96	2 (5%) 31 28	50, 59, 68, 71	0
32	1a	1488/1521 (97%)	0.21	67 (4%) 38 34	31, 57, 80, 94	0
32	2a	1491/1521 (98%)	0.48	70 (4%) 36 32	42, 65, 81, 92	0
33	1b	231/256 (90%)	1.33	51 (22%) 2 2	55, 66, 75, 79	0
33	2b	231/256 (90%)	1.52	56 (24%) 2 1	60, 71, 76, 81	0
34	1c	206/239 (86%)	0.91	14 (6%) 23 20	50, 62, 70, 75	0
34	2c	206/239 (86%)	1.56	47 (22%) 2 1	62, 70, 76, 78	0
35	1d	208/209 (99%)	1.04	25 (12%) 9 6	49, 61, 69, 72	0
35	2d	208/209 (99%)	0.79	8 (3%) 44 40	50, 60, 67, 73	0
36	1e	148/162 (91%)	0.65	3 (2%) 65 60	44, 55, 64, 71	0
36	2e	148/162 (91%)	0.98	7 (4%) 36 32	53, 64, 70, 76	0
37	1f	100/101 (99%)	0.65	0 100 100	47, 58, 66, 69	0
37	2f	100/101 (99%)	0.66	2 (2%) 65 60	49, 58, 66, 72	0
38	1g	155/156 (99%)	0.83	13 (8%) 17 14	53, 62, 73, 77	0
38	2g	155/156 (99%)	1.31	21 (13%) 7 5	61, 68, 76, 82	0
39	1h	137/138 (99%)	0.51	2 (1%) 72 68	47, 57, 62, 68	0
39	2h	137/138 (99%)	0.94	6 (4%) 39 34	56, 64, 69, 72	0
40	1i	127/128 (99%)	1.34	30 (23%) 2 1	48, 66, 73, 74	0
40	2i	127/128 (99%)	1.73	36 (28%) 1 1	60, 71, 76, 79	0
41	1j	97/105 (92%)	1.36	13 (13%) 7 5	51, 66, 76, 77	0
41	2j	96/105 (91%)	2.14	48 (50%) 0 0	63, 72, 78, 80	0
42	1k	114/129 (88%)	0.60	4 (3%) 47 43	37, 58, 67, 69	0
42	2k	114/129 (88%)	0.79	5 (4%) 39 34	46, 63, 71, 73	0
43	1l	121/132 (91%)	0.20	3 (2%) 58 54	37, 46, 56, 65	0
43	2l	121/132 (91%)	0.61	2 (1%) 69 65	50, 56, 63, 70	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	1m	123/126 (97%)	0.86	12 (9%) 13 10	48, 60, 68, 73	0
44	2m	122/126 (96%)	1.72	35 (28%) 1 1	60, 69, 73, 78	0
45	1n	60/61 (98%)	0.92	2 (3%) 49 45	53, 58, 65, 66	0
45	2n	60/61 (98%)	2.06	29 (48%) 0 0	63, 70, 74, 76	0
46	1o	88/89 (98%)	0.62	4 (4%) 38 34	40, 56, 63, 69	0
46	2o	88/89 (98%)	0.70	3 (3%) 48 44	50, 60, 68, 73	0
47	1p	82/88 (93%)	1.38	12 (14%) 6 4	49, 60, 67, 74	0
47	2p	82/88 (93%)	1.03	6 (7%) 21 17	53, 60, 68, 70	0
48	1q	99/105 (94%)	0.84	5 (5%) 33 30	47, 58, 66, 70	0
48	2q	99/105 (94%)	0.72	4 (4%) 42 38	55, 62, 70, 73	0
49	1r	68/88 (77%)	0.61	5 (7%) 20 17	49, 59, 67, 71	0
49	2r	68/88 (77%)	0.63	2 (2%) 53 50	52, 60, 69, 72	0
50	1s	83/93 (89%)	0.92	5 (6%) 27 24	53, 61, 70, 74	0
50	2s	83/93 (89%)	1.65	25 (30%) 1 1	63, 71, 75, 79	0
51	1t	96/106 (90%)	1.01	8 (8%) 17 14	51, 61, 68, 71	0
51	2t	96/106 (90%)	1.07	10 (10%) 11 9	53, 60, 70, 72	0
52	1u	23/27 (85%)	1.17	2 (8%) 16 13	54, 57, 64, 64	0
52	2u	23/27 (85%)	1.94	11 (47%) 0 0	63, 67, 71, 76	0
53	1v	13/24 (54%)	0.82	3 (23%) 2 1	42, 47, 81, 87	0
53	2v	13/24 (54%)	1.21	3 (23%) 2 1	55, 60, 84, 89	0
54	1w	66/76 (86%)	0.86	7 (10%) 11 8	23, 69, 77, 85	0
54	2w	64/76 (84%)	1.09	8 (12%) 8 6	39, 77, 83, 86	0
55	1x	72/77 (93%)	0.12	3 (4%) 40 36	22, 54, 71, 77	0
55	2x	72/77 (93%)	0.33	1 (1%) 73 69	35, 64, 75, 83	0
56	1y	67/76 (88%)	2.30	46 (68%) 0 0	56, 86, 89, 90	0
56	2y	66/76 (86%)	2.28	46 (69%) 0 0	65, 87, 90, 91	0
All	All	20873/21748 (95%)	0.34	1430 (6%) 23 19	16, 55, 76, 94	0

All (1430) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	2m	123	ALA	12.0
45	1n	2	ALA	7.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
44	2m	122	LYS	7.4
44	2m	124	PRO	7.2
1	1A	2174	C	6.5
1	1A	2115	G	6.5
1	1A	1096	A	6.4
1	1A	2111	C	6.2
1	2A	883	G	6.1
1	1A	2112	G	6.0
1	2A	2111	C	5.9
1	1A	2110	G	5.8
21	1Z	141	VAL	5.8
1	1A	2114	A	5.8
1	2A	2145	C	5.7
1	1A	2113	U	5.7
44	1m	123	ALA	5.6
1	2A	2146	C	5.5
45	2n	2	ALA	5.5
21	1Z	146	ILE	5.4
1	1A	2145	C	5.4
1	1A	2175	C	5.3
15	1T	131	ALA	5.3
1	2A	884	C	5.3
38	2g	83	ALA	5.2
1	1A	1094	U	5.2
23	11	2	SER	5.2
1	1A	898	C	5.1
33	2b	237	ALA	5.1
1	2A	2112	G	5.1
32	2a	1036	G	5.1
1	2A	2113	U	5.0
34	2c	2	GLY	5.0
1	1A	2109	U	5.0
44	2m	102	ARG	5.0
41	2j	32	ALA	4.9
1	1A	1057	A	4.9
1	1A	885	C	4.9
1	2A	2147	G	4.9
1	2A	2134	A	4.9
33	2b	236	TYR	4.9
1	2A	885	C	4.9
32	2a	1033	G	4.9
33	1b	232	PRO	4.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	2a	1032	G	4.8
1	2A	2115	G	4.8
1	2A	2159	G	4.8
1	2A	2138	C	4.8
1	1A	2130	U	4.8
1	1A	1064	C	4.8
7	1H	2	SER	4.8
1	1A	2119	A	4.7
1	2A	882	G	4.7
1	1A	1081	U	4.7
3	1D	276	LYS	4.7
47	2p	82	GLN	4.7
26	14	56	VAL	4.7
1	2A	2126	A	4.7
1	2A	2120	G	4.7
32	2a	1034	G	4.7
56	1y	75	C	4.7
1	2A	2117	A	4.7
1	1A	2129	C	4.6
32	2a	1030(B)	C	4.6
32	1a	1035	A	4.6
1	2A	2125	G	4.6
1	1A	1095	A	4.6
54	2w	73	A	4.6
1	2A	2139	C	4.5
32	2a	1027	C	4.5
1	2A	896	A	4.5
1	1A	2108	C	4.5
1	1A	2143	C	4.5
38	2g	80	VAL	4.5
33	1b	11	LEU	4.5
1	1A	2159	G	4.5
38	2g	82	GLY	4.5
1	1A	1065	U	4.5
1	1A	1097	U	4.5
19	1X	94	GLY	4.5
1	2A	2110	G	4.5
1	2A	2154	G	4.5
1	2A	2135	A	4.5
21	2Z	146	ILE	4.4
21	2Z	174	VAL	4.4
1	1A	1078	U	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	2130	U	4.4
1	1A	2160	G	4.4
1	2A	2155	G	4.4
1	2A	2128	C	4.4
41	2j	75	ILE	4.4
1	1A	2120	G	4.4
1	2A	2160	G	4.4
53	2v	12	A	4.3
51	2t	103	GLY	4.3
47	1p	82	GLN	4.3
1	2A	2174	C	4.3
1	2A	2123	G	4.3
32	1a	1034	G	4.3
32	2a	1026	G	4.3
23	21	2	SER	4.3
51	1t	103	GLY	4.3
1	1A	884	C	4.3
1	1A	1070	A	4.3
1	1A	2170	A	4.3
53	1v	13	A	4.3
1	1A	1087	G	4.2
32	2a	1031	G	4.2
38	2g	156	TRP	4.2
38	1g	80	VAL	4.2
20	2Y	1	MET	4.2
32	1a	1025	U	4.2
21	1Z	1	MET	4.2
6	2G	182	LYS	4.2
33	2b	121	LEU	4.2
1	1A	1068	G	4.2
1	1A	1098	A	4.1
21	1Z	120	ILE	4.1
1	1A	2136	C	4.1
1	2A	2170	A	4.1
32	2a	1002	G	4.1
1	1A	897	C	4.1
32	2a	1030	C	4.1
53	1v	12	A	4.1
1	2A	2149	G	4.1
32	1a	1030(A)	G	4.1
20	2Y	54	LYS	4.1
1	1A	2161	C	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	898	C	4.1
32	1a	1027	C	4.1
33	1b	237	ALA	4.1
42	2k	25	TYR	4.1
32	2a	1030(A)	G	4.1
21	1Z	105	VAL	4.1
1	1A	2117	A	4.1
32	1a	1038	C	4.0
50	2s	2	PRO	4.0
1	2A	2148	G	4.0
50	1s	9	VAL	4.0
1	1A	1073	A	4.0
1	2A	2119	A	4.0
1	2A	2136	C	4.0
1	2A	2137	C	4.0
21	1Z	170	THR	4.0
40	2i	102	LEU	4.0
1	2A	2127	G	4.0
44	1m	122	LYS	4.0
33	1b	127	ILE	4.0
8	2I	146	ALA	4.0
1	1A	2147	G	4.0
1	2A	2166	G	4.0
1	2A	2168	G	4.0
1	1A	896	A	4.0
1	1A	2135	A	4.0
1	1A	1066	U	4.0
1	1A	2146	C	4.0
32	1a	1257	U	4.0
38	2g	84	ASN	3.9
1	1A	2165	G	3.9
1	1A	2168	G	3.9
32	1a	1003	G	3.9
1	2A	2169	A	3.9
1	2A	1536	C	3.9
50	2s	45	VAL	3.9
45	2n	55	GLY	3.9
32	2a	1035	A	3.9
53	2v	13	A	3.9
15	2T	131	ALA	3.9
46	2o	89	GLY	3.9
32	2a	1001	A	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	2165	G	3.9
1	1A	1058	G	3.8
1	1A	1063	G	3.8
1	2A	2104	G	3.8
1	1A	1072	C	3.8
32	2a	1038	C	3.8
22	20	84	LEU	3.8
41	2j	65	LEU	3.8
33	1b	229	VAL	3.8
1	2A	2143	C	3.8
41	2j	41	PRO	3.8
1	1A	2189	U	3.8
1	2A	2167	U	3.8
1	1A	1069	A	3.8
21	2Z	172	ALA	3.8
38	1g	85	TYR	3.8
50	2s	68	GLY	3.8
1	1A	2138	C	3.8
1	1A	2166	G	3.8
38	2g	16	LEU	3.8
1	2A	2802	G	3.8
32	2a	1021	G	3.8
1	2A	2144	U	3.7
1	1A	2169	A	3.7
1	1A	2171	A	3.7
1	2A	2114	A	3.7
1	1A	2121	G	3.7
32	2a	1024	G	3.7
41	2j	44	VAL	3.7
33	1b	9	GLU	3.7
40	2i	67	GLY	3.7
45	2n	34	TYR	3.7
1	1A	888	C	3.7
1	1A	1099	G	3.7
1	1A	2141	G	3.7
33	1b	10	LEU	3.7
1	1A	1088	A	3.7
32	2a	1004	A	3.7
40	2i	126	SER	3.7
41	2j	34	VAL	3.7
1	2A	2116	G	3.7
32	1a	1036	G	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
56	1y	19	G	3.7
44	2m	121	LYS	3.7
1	2A	2109	U	3.7
12	2Q	6	ARG	3.7
43	2l	64	TYR	3.7
1	1A	899	A	3.6
34	2c	189	ALA	3.6
21	1Z	136	PHE	3.6
34	1c	2	GLY	3.6
1	1A	2116	G	3.6
32	1a	1026	G	3.6
32	1a	1031	G	3.6
56	1y	15	G	3.6
26	24	63	TYR	3.6
1	2A	878	A	3.6
32	2a	1005	A	3.6
1	2A	888	C	3.6
1	2A	2129	C	3.6
1	2A	2179	C	3.6
26	24	49	PHE	3.6
54	1w	20	U	3.6
1	1A	882	G	3.6
1	1A	1071	G	3.6
1	1A	2133	G	3.6
1	1A	2181	G	3.6
54	1w	73	A	3.6
50	2s	84	GLY	3.6
51	2t	98	PRO	3.6
1	2A	2133	G	3.6
34	1c	207	VAL	3.6
38	2g	77	SER	3.6
32	2a	1030(D)	A	3.6
41	2j	76	ASN	3.6
1	1A	2178	C	3.5
1	2A	2108	C	3.5
32	1a	1029	C	3.5
3	2D	275	LYS	3.5
32	1a	1000	U	3.5
33	2b	165	VAL	3.5
45	2n	33	VAL	3.5
38	2g	32	ARG	3.5
21	2Z	159	PRO	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	2b	17	PHE	3.5
1	2A	2803	C	3.5
21	2Z	141	VAL	3.5
43	2l	63	GLY	3.5
44	2m	33	ALA	3.5
1	2A	2173	A	3.5
56	1y	1	G	3.5
32	2a	1000	U	3.5
7	2H	2	SER	3.5
1	1A	1089	G	3.5
1	2A	2157	G	3.5
38	1g	84	ASN	3.5
34	2c	190	ARG	3.5
21	2Z	105	VAL	3.5
41	1j	100	THR	3.5
1	1A	886	C	3.5
32	2a	1028	C	3.5
1	1A	2167	U	3.5
1	1A	2172	U	3.5
32	1a	1532	U	3.5
45	2n	6	LEU	3.5
19	2X	94	GLY	3.5
33	1b	227	GLY	3.5
41	2j	74	ILE	3.5
44	1m	121	LYS	3.5
1	1A	1059	G	3.4
1	2A	2124	G	3.4
26	24	56	VAL	3.4
29	27	46	VAL	3.4
1	1A	2118	U	3.4
1	1A	2128	C	3.4
1	2A	2804	C	3.4
32	1a	204	U	3.4
32	2a	1257	U	3.4
38	2g	85	TYR	3.4
33	1b	230	VAL	3.4
52	2u	2	GLY	3.4
1	1A	2107	C	3.4
1	2A	2175	C	3.4
45	2n	3	ARG	3.4
1	1A	2173	A	3.4
34	2c	195	VAL	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
41	2j	88	LEU	3.4
1	1A	1091	G	3.4
41	1j	32	ALA	3.4
56	2y	19	G	3.4
32	2a	1532	U	3.4
1	1A	2137	C	3.4
1	2A	2164	C	3.4
35	1d	173	TRP	3.4
35	1d	167	GLY	3.4
38	1g	81	GLY	3.4
41	2j	10	GLY	3.4
21	2Z	149	SER	3.4
32	1a	1028	C	3.3
33	1b	15	VAL	3.3
41	2j	91	PRO	3.3
1	1A	887	A	3.3
1	2A	2158	A	3.3
32	1a	1531	A	3.3
15	1T	130	ALA	3.3
38	2g	154	TYR	3.3
1	2A	2150	U	3.3
1	2A	2172	U	3.3
1	2A	2189	U	3.3
56	2y	33	U	3.3
1	1A	1176	G	3.3
1	1A	2125	G	3.3
19	2X	95	LEU	3.3
35	1d	194	LEU	3.3
41	2j	40	LEU	3.3
35	1d	192	GLU	3.3
8	1I	146	ALA	3.3
6	1G	182	LYS	3.3
26	24	59	PHE	3.3
33	1b	132	LYS	3.3
40	2i	11	LYS	3.3
1	2A	2118	U	3.3
1	1A	879	G	3.3
1	2A	2156	G	3.3
1	2A	2893	G	3.3
32	1a	1033	G	3.3
32	2a	1003	G	3.3
1	1A	2164	C	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	1a	1030	C	3.3
41	1j	77	PRO	3.3
56	2y	13	C	3.3
26	14	64	GLY	3.3
35	2d	156	GLU	3.3
1	1A	2790	A	3.3
3	2D	276	LYS	3.3
33	1b	236	TYR	3.3
41	2j	78	ASN	3.3
1	1A	2150	U	3.3
7	2H	6	ARG	3.3
32	1a	630	G	3.3
56	2y	1	G	3.3
1	2A	894	C	3.3
32	1a	1008	C	3.3
36	1e	85	GLY	3.3
38	1g	82	GLY	3.3
34	2c	182	ILE	3.3
32	2a	1531	A	3.2
26	24	32	TYR	3.2
51	1t	10	LEU	3.2
44	2m	4	ILE	3.2
1	1A	883	G	3.2
1	1A	1076	C	3.2
1	1A	2149	G	3.2
1	2A	2188	C	3.2
12	2Q	104	PHE	3.2
41	2j	59	SER	3.2
52	2u	24	ARG	3.2
33	1b	188	ALA	3.2
54	2w	2	C	3.2
1	1A	1056	G	3.2
32	1a	1032	G	3.2
56	2y	34	G	3.2
26	14	49	PHE	3.2
33	2b	11	LEU	3.2
6	1G	146	TYR	3.2
48	2q	100	LYS	3.2
1	1A	1060	U	3.2
1	1A	2122	U	3.2
33	2b	7	VAL	3.2
34	2c	207	VAL	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
44	2m	6	GLY	3.2
1	2A	897	C	3.2
32	1a	163	C	3.2
1	1A	2207	G	3.2
1	2A	881	G	3.2
56	2y	57	G	3.2
3	2D	38	LYS	3.2
40	2i	19	LEU	3.2
1	1A	1103	A	3.2
53	2v	14	A	3.2
56	1y	35	A	3.2
34	2c	75	VAL	3.2
1	1A	2180	U	3.2
1	2A	2122	U	3.2
40	1i	15	ALA	3.1
11	2P	15	ARG	3.1
1	1A	2105	C	3.1
1	2A	2105	C	3.1
33	2b	86	GLU	3.1
40	2i	91	ASP	3.1
41	2j	77	PRO	3.1
45	2n	14	PRO	3.1
56	2y	2	C	3.1
7	2H	33	LEU	3.1
1	1A	2148	G	3.1
56	2y	18	G	3.1
41	1j	31	GLY	3.1
34	2c	77	ILE	3.1
19	2X	91	ALA	3.1
29	27	47	ARG	3.1
33	2b	123	ALA	3.1
50	2s	13	ASP	3.1
1	1A	1075	C	3.1
32	2a	1018	C	3.1
32	2a	1037	C	3.1
1	1A	881	G	3.1
7	2H	15	VAL	3.1
26	14	67	TYR	3.1
56	2y	6	G	3.1
32	1a	160	A	3.1
56	2y	21	A	3.1
1	1A	2144	U	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
21	2Z	173	ALA	3.1
33	2b	77	ALA	3.1
40	2i	82	ALA	3.1
45	2n	39	LEU	3.1
42	2k	117	ASN	3.1
1	1A	2142	C	3.1
31	29	37	GLY	3.1
56	2y	68	C	3.1
40	2i	9	ARG	3.1
32	1a	1023	G	3.1
41	2j	20	ALA	3.1
56	1y	57	G	3.1
1	1A	1082	U	3.1
54	2w	45	U	3.1
33	1b	97	TRP	3.1
33	1b	165	VAL	3.1
32	2a	1029	C	3.1
41	1j	4	ILE	3.1
56	1y	74	C	3.1
33	2b	33	TYR	3.0
25	23	60	GLU	3.0
32	2a	1020	U	3.0
1	2A	2805	G	3.0
54	2w	71	G	3.0
56	2y	15	G	3.0
26	14	58	ARG	3.0
34	2c	79	ARG	3.0
38	1g	4	ARG	3.0
7	2H	44	VAL	3.0
7	2H	136	ILE	3.0
45	2n	22	THR	3.0
32	2a	1006	C	3.0
34	2c	48	TYR	3.0
43	1l	64	TYR	3.0
1	2A	2176	A	3.0
44	1m	124	PRO	3.0
56	1y	20	U	3.0
21	2Z	104	PHE	3.0
26	24	65	ASP	3.0
1	1A	1062	G	3.0
1	1A	2793	G	3.0
1	2A	892	G	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	2100	G	3.0
1	2A	2131	G	3.0
32	2a	1030(C)	G	3.0
54	1w	70	G	3.0
21	2Z	142	SER	3.0
44	2m	106	ASN	3.0
5	2F	208	GLY	3.0
33	1b	18	GLY	3.0
45	2n	38	GLY	3.0
8	2I	107	VAL	3.0
35	1d	88	VAL	3.0
33	1b	19	HIS	3.0
32	2a	1039	C	3.0
32	1a	1447	A	3.0
32	2a	1040	U	3.0
1	1A	1093	G	3.0
1	1A	2131	G	3.0
32	1a	1001(A)	G	3.0
56	2y	22	G	3.0
33	2b	80	ILE	3.0
34	2c	55	VAL	3.0
6	1G	50	ALA	3.0
44	1m	2	ALA	3.0
51	1t	24	LEU	3.0
29	27	48	LYS	3.0
45	2n	11	LYS	3.0
1	1A	271(K)	U	3.0
1	2A	652(B)	A	3.0
12	2Q	15	GLY	3.0
26	24	54	GLY	3.0
35	1d	87	GLY	3.0
41	1j	33	GLN	3.0
7	2H	52	VAL	2.9
50	2s	9	VAL	2.9
1	1A	2106	G	2.9
1	2A	11	G	2.9
32	1a	1024	G	2.9
56	2y	5	G	2.9
40	2i	103	THR	2.9
4	2E	204	ALA	2.9
12	2Q	22	LYS	2.9
1	1A	2794	C	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	886	C	2.9
21	2Z	136	PHE	2.9
56	1y	49	C	2.9
1	1A	2132	U	2.9
1	2A	2132	U	2.9
55	2x	47	U	2.9
56	2y	36	A	2.9
33	1b	134	GLU	2.9
40	2i	14	VAL	2.9
45	2n	18	VAL	2.9
33	1b	40	HIS	2.9
1	1A	2127	G	2.9
35	1d	169	LYS	2.9
20	2Y	90	LEU	2.9
26	14	59	PHE	2.9
56	2y	56	C	2.9
32	1a	344	A	2.9
32	1a	1001	A	2.9
33	2b	136	VAL	2.9
34	2c	43	LEU	2.9
1	2A	2792	G	2.9
32	2a	1023	G	2.9
21	1Z	148	ASP	2.9
21	2Z	106	GLY	2.9
24	22	66	GLU	2.9
27	25	59	GLU	2.9
40	1i	2	GLU	2.9
44	2m	38	GLY	2.9
41	2j	82	ILE	2.9
32	2a	1286	A	2.9
33	1b	133	LYS	2.9
56	2y	35	A	2.9
40	2i	7	THR	2.9
7	2H	96	ALA	2.9
51	2t	97	ALA	2.9
8	2I	68	LEU	2.9
21	2Z	157	LEU	2.9
34	2c	47	LEU	2.9
50	2s	71	LEU	2.9
1	2A	1533	G	2.9
1	2A	2121	G	2.9
21	1Z	104	PHE	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
26	14	63	TYR	2.9
32	2a	1001(A)	G	2.9
48	1q	99	SER	2.8
52	2u	9	ARG	2.8
45	2n	25	VAL	2.8
1	1A	1077	A	2.8
41	2j	27	ALA	2.8
19	1X	95	LEU	2.8
26	24	51	ASP	2.8
47	1p	68	ASP	2.8
21	2Z	168	GLU	2.8
33	1b	17	PHE	2.8
33	2b	122	PHE	2.8
40	2i	18	PHE	2.8
7	2H	174	GLY	2.8
41	2j	31	GLY	2.8
1	2A	652(U)	G	2.8
8	1I	109	ILE	2.8
32	1a	1030(C)	G	2.8
56	1y	24	G	2.8
1	1A	1100	C	2.8
1	2A	889	C	2.8
38	1g	83	ALA	2.8
56	1y	13	C	2.8
1	1A	878	A	2.8
1	1A	2158	A	2.8
49	2r	66	LEU	2.8
56	1y	21	A	2.8
33	1b	231	GLU	2.8
38	2g	26	PHE	2.8
11	2P	109	GLY	2.8
34	1c	81	GLY	2.8
34	2c	201	TYR	2.8
42	1k	25	TYR	2.8
1	1A	2100	G	2.8
1	2A	2153	G	2.8
54	1w	71	G	2.8
56	1y	18	G	2.8
1	2A	1026	U	2.8
21	2Z	150	LEU	2.8
1	2A	652(T)	C	2.8
56	1y	67	C	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	1086	A	2.8
1	2A	2171	A	2.8
41	2j	86	MET	2.8
56	1y	36	A	2.8
56	1y	73	A	2.8
21	2Z	148	ASP	2.8
18	1W	112	GLY	2.8
33	2b	200	ILE	2.8
47	1p	38	TYR	2.8
21	1Z	153	SER	2.8
41	1j	78	ASN	2.8
7	2H	43	VAL	2.8
1	2A	895	U	2.8
21	2Z	125	LEU	2.8
33	1b	120	ALA	2.8
34	2c	60	ALA	2.8
34	2c	61	ALA	2.8
44	1m	5	ALA	2.8
1	2A	1042	G	2.8
1	2A	2793	G	2.8
45	2n	4	LYS	2.8
1	1A	2179	C	2.8
32	1a	1030(D)	A	2.8
33	2b	41	ILE	2.7
33	2b	185	ILE	2.7
44	2m	64	TRP	2.7
21	1Z	149	SER	2.7
41	2j	37	PRO	2.7
41	2j	49	VAL	2.7
41	2j	90	LEU	2.7
42	2k	89	ALA	2.7
50	2s	24	ALA	2.7
1	1A	2151	G	2.7
1	1A	2162	G	2.7
56	2y	71	G	2.7
1	1A	1046	A	2.7
1	1A	1174	A	2.7
32	2a	999	C	2.7
32	2a	1447	A	2.7
45	2n	37	PHE	2.7
21	2Z	171	ILE	2.7
34	2c	5	ILE	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
49	1r	31	LEU	2.7
9	2N	61	ARG	2.7
41	2j	66	ARG	2.7
1	1A	880	G	2.7
1	1A	2182	G	2.7
1	2A	879	G	2.7
1	1A	1054	A	2.7
1	1A	1092	C	2.7
32	1a	1005	A	2.7
7	2H	89	ILE	2.7
32	1a	1037	C	2.7
32	1a	1286	A	2.7
32	2a	1041	A	2.7
41	2j	47	PHE	2.7
46	2o	3	ILE	2.7
56	1y	48	C	2.7
7	2H	39	PRO	2.7
46	1o	19	PRO	2.7
21	1Z	139	VAL	2.7
44	2m	120	LYS	2.7
41	1j	86	MET	2.7
21	2Z	103	ARG	2.7
41	2j	100	THR	2.7
40	2i	2	GLU	2.7
1	2A	1113	U	2.7
41	2j	68	HIS	2.7
56	1y	59	U	2.7
4	1E	77	ILE	2.7
33	2b	201	ILE	2.7
35	1d	5	ILE	2.7
1	1A	2190	G	2.7
1	2A	2106	G	2.7
1	2A	2141	G	2.7
32	2a	630	G	2.7
32	2a	1124	G	2.7
56	2y	69	G	2.7
1	1A	2188	C	2.7
1	2A	2107	C	2.7
1	2A	2142	C	2.7
32	2a	1019	C	2.7
41	1j	76	ASN	2.7
56	2y	25	C	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	2H	79	VAL	2.7
21	2Z	144	LEU	2.7
33	2b	48	MET	2.7
38	2g	5	ARG	2.7
40	1i	19	LEU	2.7
41	2j	79	ARG	2.7
44	2m	53	VAL	2.7
48	1q	98	LEU	2.7
33	1b	129	GLU	2.7
1	1A	12	U	2.7
1	1A	2102	U	2.7
32	1a	1040	U	2.7
51	2t	102	GLY	2.6
33	1b	125	PRO	2.6
33	1b	234	PRO	2.6
1	2A	1847	A	2.6
44	2m	34	LEU	2.6
49	1r	86	VAL	2.6
56	1y	58	A	2.6
1	1A	2140	C	2.6
1	2A	1112	G	2.6
1	2A	2318	G	2.6
32	1a	1030(B)	C	2.6
32	2a	1149	C	2.6
54	2w	72	C	2.6
26	14	57	GLU	2.6
21	2Z	9	TYR	2.6
36	2e	20	GLN	2.6
40	2i	64	THR	2.6
45	2n	13	THR	2.6
1	1A	1175	U	2.6
14	2S	83	LYS	2.6
6	2G	52	ILE	2.6
33	2b	214	ILE	2.6
47	1p	80	PHE	2.6
6	1G	51	ARG	2.6
47	1p	1	MET	2.6
40	2i	99	LEU	2.6
42	1k	14	VAL	2.6
29	27	45	ALA	2.6
41	1j	87	THR	2.6
44	2m	49	THR	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
44	2m	51	ALA	2.6
1	1A	1173	G	2.6
1	2A	880	G	2.6
26	14	32	TYR	2.6
40	2i	5	TYR	2.6
56	1y	27	G	2.6
45	2n	17	LYS	2.6
33	2b	66	GLY	2.6
38	2g	34	GLY	2.6
32	2a	1025	U	2.6
32	2a	1150	U	2.6
33	1b	39	ILE	2.6
40	2i	20	ARG	2.6
40	2i	66	ARG	2.6
56	1y	45	U	2.6
56	1y	47	U	2.6
7	2H	123	PHE	2.6
33	1b	37	ASN	2.6
35	1d	179	GLU	2.6
41	2j	85	LEU	2.6
7	2H	19	VAL	2.6
33	1b	95	GLN	2.6
6	2G	163	ALA	2.6
1	1A	1067	A	2.6
1	1A	652(S)	C	2.6
1	1A	1509	C	2.6
1	2A	2178	C	2.6
32	2a	1260	C	2.6
46	1o	69	TYR	2.6
33	1b	22	LYS	2.6
33	2b	22	LYS	2.6
1	2A	1170	G	2.6
18	2W	112	GLY	2.6
36	2e	114	GLY	2.6
44	1m	4	ILE	2.6
2	2B	1	U	2.6
55	1x	47	U	2.6
41	2j	83	GLU	2.6
34	1c	107	GLN	2.6
35	1d	170	VAL	2.6
40	1i	13	ALA	2.6
48	2q	99	SER	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
29	17	48	LYS	2.6
2	2B	120	A	2.6
56	2y	14	A	2.6
20	2Y	55	TYR	2.6
33	2b	31	TYR	2.6
1	1A	2185	C	2.5
1	1A	2803	C	2.5
1	2A	2140	C	2.5
20	2Y	107	ASP	2.5
26	14	54	GLY	2.5
41	2j	36	GLY	2.5
1	1A	2155	G	2.5
1	1A	2156	G	2.5
1	1A	2157	G	2.5
1	2A	1171	G	2.5
1	2A	2182	G	2.5
32	2a	1022	G	2.5
56	2y	24	G	2.5
6	1G	48	GLU	2.5
39	1h	2	LEU	2.5
56	2y	12	U	2.5
6	1G	149	VAL	2.5
41	2j	80	LYS	2.5
6	2G	161	THR	2.5
1	2A	2794	C	2.5
5	1F	208	GLY	2.5
33	2b	234	PRO	2.5
44	2m	100	GLY	2.5
56	2y	67	C	2.5
41	2j	38	ILE	2.5
51	2t	100	ILE	2.5
32	1a	78	G	2.5
32	2a	485	G	2.5
51	2t	99	LEU	2.5
1	1A	1026	U	2.5
32	1a	1020	U	2.5
40	2i	44	VAL	2.5
15	2T	130	ALA	2.5
41	2j	26	ALA	2.5
21	1Z	166	SER	2.5
40	1i	10	ARG	2.5
36	1e	10	MET	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	2H	12	PRO	2.5
40	2i	21	PRO	2.5
40	1i	67	GLY	2.5
41	2j	93	GLY	2.5
41	1j	98	ILE	2.5
6	2G	139	LEU	2.5
33	1b	221	LEU	2.5
34	2c	12	LEU	2.5
34	2c	87	LEU	2.5
51	2t	74	LYS	2.5
33	2b	93	VAL	2.5
34	1c	70	VAL	2.5
36	2e	67	VAL	2.5
1	1A	2101	G	2.5
1	2A	2181	G	2.5
32	1a	1002	G	2.5
56	1y	34	G	2.5
7	2H	145	ALA	2.5
21	2Z	164	ALA	2.5
26	24	55	ARG	2.5
29	17	45	ALA	2.5
34	2c	149	ALA	2.5
38	2g	40	ALA	2.5
40	2i	13	ALA	2.5
44	2m	114	ARG	2.5
41	2j	42	THR	2.5
33	1b	48	MET	2.5
33	2b	125	PRO	2.5
21	2Z	2	GLU	2.5
51	2t	101	GLY	2.5
50	1s	12	ASP	2.5
51	1t	100	ILE	2.5
1	1A	2176	A	2.5
56	2y	23	A	2.5
33	2b	221	LEU	2.5
40	1i	102	LEU	2.5
1	2A	2163	C	2.5
32	2a	1007	C	2.5
56	2y	49	C	2.5
7	2H	125	VAL	2.5
26	14	50	VAL	2.5
39	2h	53	VAL	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	1b	130	ARG	2.5
38	2g	115	ARG	2.5
50	2s	3	ARG	2.5
44	2m	5	ALA	2.5
45	2n	5	ALA	2.5
1	2A	271(M)	G	2.5
7	2H	134	SER	2.5
32	1a	1042	G	2.5
33	2b	83	MET	2.5
36	2e	10	MET	2.5
56	2y	70	G	2.5
7	2H	10	PRO	2.4
9	2N	44	PRO	2.4
34	2c	109	PRO	2.4
4	2E	73	GLU	2.4
6	2G	48	GLU	2.4
34	2c	124	ILE	2.4
40	2i	125	TYR	2.4
50	2s	80	TYR	2.4
16	2U	117	GLN	2.4
7	2H	51	ARG	2.4
41	2j	5	ARG	2.4
51	2t	86	ARG	2.4
1	1A	2177	C	2.4
16	2U	8	VAL	2.4
32	1a	999	C	2.4
32	1a	1039	C	2.4
34	2c	99	VAL	2.4
40	1i	14	VAL	2.4
56	2y	75	C	2.4
1	1A	895	U	2.4
33	2b	120	ALA	2.4
41	2j	48	THR	2.4
44	2m	37	THR	2.4
8	1I	41	GLU	2.4
1	1A	2123	G	2.4
1	1A	2152	G	2.4
1	2A	2151	G	2.4
21	2Z	156	LYS	2.4
32	1a	1009	G	2.4
34	2c	80	GLY	2.4
40	1i	8	GLY	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
35	1d	70	ILE	2.4
35	2d	5	ILE	2.4
50	1s	13	ASP	2.4
26	24	67	TYR	2.4
34	1c	47	LEU	2.4
34	2c	32	LEU	2.4
38	2g	44	TYR	2.4
42	1k	75	TYR	2.4
42	2k	75	TYR	2.4
21	1Z	131	ARG	2.4
34	2c	128	PHE	2.4
35	2d	132	ARG	2.4
40	2i	10	ARG	2.4
1	2A	887	A	2.4
56	2y	7	A	2.4
56	2y	73	A	2.4
33	2b	81	VAL	2.4
38	1g	156	TRP	2.4
41	2j	72	VAL	2.4
52	2u	14	TRP	2.4
1	2A	277	C	2.4
1	2A	1509	C	2.4
32	2a	1043	C	2.4
34	2c	137	ALA	2.4
35	1d	111	ALA	2.4
40	1i	94	ALA	2.4
1	2A	272(A)	U	2.4
33	2b	168	THR	2.4
7	2H	36	PRO	2.4
33	1b	131	PRO	2.4
33	1b	233	SER	2.4
33	2b	131	PRO	2.4
33	2b	170	GLU	2.4
40	1i	126	SER	2.4
7	1H	174	GLY	2.4
17	1V	101	GLY	2.4
1	1A	2104	G	2.4
10	1O	91	LEU	2.4
32	1a	1021	G	2.4
56	2y	53	G	2.4
7	2H	83	TYR	2.4
40	2i	114	TYR	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	2H	113	VAL	2.4
21	1Z	165	VAL	2.4
29	17	46	VAL	2.4
33	2b	71	VAL	2.4
39	2h	97	VAL	2.4
34	2c	181	ASN	2.4
53	1v	14	A	2.4
56	1y	38	A	2.4
44	2m	28	ALA	2.4
21	2Z	170	THR	2.4
44	2m	41	PRO	2.4
48	2q	96	GLU	2.4
1	2A	2161	C	2.4
14	2S	31	SER	2.4
32	1a	1006	C	2.4
32	2a	1126	U	2.4
56	2y	4	C	2.4
21	2Z	147	GLY	2.4
43	1l	63	GLY	2.4
51	2t	96	GLY	2.4
7	2H	72	ILE	2.4
34	2c	52	LEU	2.4
34	2c	62	ASP	2.4
33	1b	16	HIS	2.4
35	2d	168	ARG	2.4
47	1p	81	ARG	2.4
32	2a	1182	G	2.4
34	2c	193	TYR	2.4
20	2Y	5	MET	2.4
56	1y	5	G	2.4
56	1y	53	G	2.4
56	1y	65	G	2.4
40	2i	65	VAL	2.4
1	1A	1045	A	2.4
1	2A	899	A	2.4
21	1Z	169	GLU	2.4
32	1a	162	A	2.4
34	1c	113	ALA	2.4
51	1t	12	ALA	2.4
33	2b	12	GLU	2.4
7	2H	29	PRO	2.3
21	2Z	95	PRO	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
47	1p	41	PRO	2.3
56	2y	66	U	2.3
2	2B	88	C	2.3
7	2H	82	GLY	2.3
7	2H	135	GLY	2.3
11	1P	44	GLY	2.3
41	1j	36	GLY	2.3
34	1c	124	ILE	2.3
52	1u	24	ARG	2.3
6	2G	53	LEU	2.3
27	25	58	LEU	2.3
33	2b	16	HIS	2.3
34	1c	204	LEU	2.3
34	2c	196	LEU	2.3
34	2c	29	TYR	2.3
36	2e	84	PHE	2.3
40	2i	62	TYR	2.3
7	2H	50	VAL	2.3
12	2Q	109	VAL	2.3
26	24	50	VAL	2.3
34	1c	86	VAL	2.3
40	1i	11	LYS	2.3
43	1l	18	VAL	2.3
44	2m	31	LYS	2.3
50	2s	11	VAL	2.3
1	2A	2162	G	2.3
20	1Y	92	ASN	2.3
39	2h	15	ASN	2.3
54	2w	70	G	2.3
12	2Q	121	ALA	2.3
26	24	57	GLU	2.3
33	1b	12	GLU	2.3
49	1r	20	ALA	2.3
40	1i	21	PRO	2.3
1	1A	229	A	2.3
1	1A	548	A	2.3
32	2a	1146	A	2.3
56	2y	9	A	2.3
26	24	45	GLY	2.3
33	2b	21	ARG	2.3
33	2b	227	GLY	2.3
35	1d	3	ARG	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
38	1g	115	ARG	2.3
50	1s	26	GLY	2.3
1	2A	2897	U	2.3
56	1y	33	U	2.3
7	2H	103	LEU	2.3
21	2Z	121	HIS	2.3
33	2b	10	LEU	2.3
35	1d	188	LEU	2.3
35	2d	19	LEU	2.3
41	2j	50	ILE	2.3
1	1A	889	C	2.3
1	2A	645	C	2.3
1	2A	2177	C	2.3
56	1y	4	C	2.3
11	2P	91	PHE	2.3
45	2n	15	LYS	2.3
6	2G	146	TYR	2.3
7	2H	17	VAL	2.3
34	2c	138	VAL	2.3
35	1d	138	TYR	2.3
6	2G	50	ALA	2.3
7	2H	128	PRO	2.3
34	2c	129	ALA	2.3
35	1d	195	ALA	2.3
45	2n	20	ALA	2.3
7	2H	106	THR	2.3
40	1i	64	THR	2.3
40	1i	103	THR	2.3
50	2s	29	ARG	2.3
56	1y	44	G	2.3
1	1A	890	A	2.3
1	1A	2134	A	2.3
32	2a	1123	A	2.3
47	2p	48	TRP	2.3
50	2s	8	GLY	2.3
34	2c	188	LEU	2.3
39	1h	112	LEU	2.3
40	2i	81	ILE	2.3
47	1p	49	LEU	2.3
32	1a	90	U	2.3
34	1c	62	ASP	2.3
1	1A	34	C	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	1080	C	2.3
1	2A	893	C	2.3
32	1a	1019	C	2.3
32	1a	1137	C	2.3
56	1y	72	C	2.3
7	2H	133	VAL	2.3
33	2b	148	TYR	2.3
40	1i	108	VAL	2.3
40	2i	92	TYR	2.3
44	2m	54	VAL	2.3
44	2m	87	TYR	2.3
25	23	2	PRO	2.3
40	1i	106	ALA	2.3
40	2i	84	ALA	2.3
45	2n	12	ARG	2.3
47	2p	69	THR	2.3
33	2b	228	GLY	2.3
21	2Z	57	ILE	2.3
32	2a	993	G	2.3
32	2a	1131	G	2.3
33	1b	24	TRP	2.3
33	2b	39	ILE	2.3
35	1d	157	LEU	2.3
40	1i	56	LEU	2.3
44	2m	19	LEU	2.3
54	2w	15	G	2.3
56	1y	10	G	2.3
8	2I	1	MET	2.3
20	1Y	1	MET	2.3
32	1a	161	A	2.3
32	1a	172	A	2.3
32	2a	1044	A	2.3
33	2b	90	MET	2.3
7	1H	175	LYS	2.3
39	2h	98	LYS	2.3
42	1k	51	LYS	2.3
1	1A	1090	U	2.3
56	1y	25	C	2.3
40	2i	86	VAL	2.3
38	1g	79	ARG	2.3
41	1j	79	ARG	2.3
44	2m	104	ARG	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	1b	29	ALA	2.2
33	2b	34	ALA	2.2
34	2c	9	GLY	2.2
34	2c	74	GLY	2.2
7	2H	88	LEU	2.2
26	24	66	SER	2.2
33	2b	118	LEU	2.2
33	2b	132	LYS	2.2
39	2h	2	LEU	2.2
44	2m	22	ILE	2.2
46	1o	57	LEU	2.2
50	2s	20	LEU	2.2
1	2A	229	A	2.2
32	1a	149	A	2.2
1	1A	2154	G	2.2
1	2A	2101	G	2.2
1	2A	2751	G	2.2
32	2a	1042	G	2.2
56	1y	22	G	2.2
56	1y	52	G	2.2
56	2y	44	G	2.2
56	2y	52	G	2.2
1	2A	271(K)	U	2.2
56	2y	47	U	2.2
33	1b	50	GLU	2.2
34	2c	90	GLU	2.2
40	1i	12	GLU	2.2
7	2H	60	ARG	2.2
1	1A	1053	C	2.2
1	1A	2103	C	2.2
1	1A	2804	C	2.2
1	2A	2103	C	2.2
1	2A	2183	C	2.2
1	2A	2789	C	2.2
4	2E	59	VAL	2.2
5	1F	14	PRO	2.2
8	2I	15	VAL	2.2
33	2b	175	ARG	2.2
45	2n	35	ARG	2.2
50	2s	42	PRO	2.2
5	2F	130	ALA	2.2
38	2g	37	ASN	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
45	1n	5	ALA	2.2
51	1t	95	ALA	2.2
36	2e	133	TYR	2.2
35	1d	84	LYS	2.2
35	2d	23	GLY	2.2
51	1t	101	GLY	2.2
8	2I	38	LEU	2.2
34	2c	204	LEU	2.2
21	1Z	171	ILE	2.2
33	1b	211	ILE	2.2
33	1b	214	ILE	2.2
35	1d	83	SER	2.2
8	2I	20	ASP	2.2
36	2e	5	ASP	2.2
6	2G	29	TRP	2.2
11	1P	149	GLU	2.2
33	2b	129	GLU	2.2
32	1a	65	U	2.2
46	2o	88	ARG	2.2
56	1y	69	G	2.2
56	1y	70	G	2.2
4	2E	72	VAL	2.2
6	2G	2	PRO	2.2
20	2Y	45	VAL	2.2
35	1d	189	PRO	2.2
40	2i	53	VAL	2.2
1	2A	2896	C	2.2
33	2b	161	ALA	2.2
34	2c	200	ALA	2.2
54	2w	13	C	2.2
56	1y	56	C	2.2
56	2y	48	C	2.2
56	2y	62	C	2.2
14	2S	92	TYR	2.2
38	1g	154	TYR	2.2
52	2u	17	THR	2.2
7	2H	64	LEU	2.2
21	1Z	147	GLY	2.2
33	1b	228	GLY	2.2
40	1i	24	GLY	2.2
50	2s	15	LEU	2.2
51	1t	102	GLY	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
52	2u	16	GLY	2.2
33	1b	172	ILE	2.2
21	2Z	153	SER	2.2
40	1i	91	ASP	2.2
44	2m	50	GLU	2.2
44	1m	3	ARG	2.2
47	1p	48	TRP	2.2
56	1y	9	A	2.2
56	1y	26	A	2.2
9	1N	9	VAL	2.2
33	1b	93	VAL	2.2
1	1A	2124	G	2.2
1	2A	2833	G	2.2
7	2H	175	LYS	2.2
8	2I	55	ALA	2.2
26	14	69	LYS	2.2
32	1a	79	G	2.2
31	29	20	HIS	2.2
34	2c	168	ALA	2.2
41	2j	33	GLN	2.2
1	2A	1043	C	2.2
7	2H	7	LEU	2.2
32	1a	1007	C	2.2
32	1a	1132	C	2.2
41	2j	87	THR	2.2
44	1m	105	THR	2.2
33	1b	38	GLY	2.2
46	1o	66	LEU	2.2
54	1w	72	C	2.2
47	1p	36	ILE	2.2
48	1q	97	SER	2.2
4	1E	73	GLU	2.2
7	2H	3	ARG	2.2
11	2P	79	ARG	2.2
34	1c	79	ARG	2.2
50	2s	81	ARG	2.2
20	2Y	53	PRO	2.2
40	1i	49	PRO	2.2
41	2j	39	PRO	2.2
47	1p	59	TRP	2.2
47	2p	59	TRP	2.2
20	2Y	89	PHE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	1a	1446	U	2.2
32	2a	1219	U	2.2
40	2i	59	PHE	2.2
50	2s	67	VAL	2.1
56	1y	12	U	2.2
56	1y	14	A	2.1
20	2Y	92	ASN	2.1
1	2A	2184	G	2.1
22	10	84	LEU	2.1
32	1a	1138	G	2.1
32	2a	1011	G	2.1
37	2f	21	LEU	2.1
38	2g	55	GLY	2.1
44	1m	56	LEU	2.1
45	2n	44	LEU	2.1
48	1q	53	LEU	2.1
55	1x	46	G	2.1
7	1H	92	ILE	2.1
52	2u	13	ILE	2.1
1	1A	645	C	2.1
56	1y	68	C	2.1
6	2G	51	ARG	2.1
28	16	4	GLU	2.1
35	1d	122	ARG	2.1
40	1i	59	PHE	2.1
47	2p	9	PHE	2.1
12	2Q	106	VAL	2.1
26	24	35	VAL	2.1
33	1b	7	VAL	2.1
35	1d	133	VAL	2.1
24	22	1	MET	2.1
1	2A	1508	A	2.1
7	2H	102	ALA	2.1
32	1a	1041	A	2.1
38	1g	2	ALA	2.1
45	2n	10	ALA	2.1
7	2H	98	LEU	2.1
26	14	17	GLY	2.1
33	1b	154	LEU	2.1
40	2i	56	LEU	2.1
41	2j	16	LEU	2.1
42	2k	49	GLY	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
44	2m	112	GLY	2.1
33	1b	223	ILE	2.1
33	2b	162	ILE	2.1
1	1A	1055	G	2.1
1	1A	1074	G	2.1
10	1O	108	GLU	2.1
11	2P	149	GLU	2.1
12	2Q	10	ARG	2.1
21	1Z	2	GLU	2.1
40	1i	9	ARG	2.1
52	1u	18	TYR	2.1
52	2u	15	ARG	2.1
32	1a	148	G	2.1
56	1y	71	G	2.1
56	2y	11	C	2.1
23	21	81	LYS	2.1
8	2I	137	PRO	2.1
7	2H	41	MET	2.1
7	2H	26	VAL	2.1
27	15	60	VAL	2.1
36	1e	69	VAL	2.1
1	1A	877	U	2.1
1	1A	2897	U	2.1
8	1I	65	ALA	2.1
45	2n	61	TRP	2.1
50	1s	24	ALA	2.1
8	2I	11	ASN	2.1
1	1A	1084	A	2.1
1	2A	1460	A	2.1
21	2Z	70	LEU	2.1
21	2Z	76	LEU	2.1
44	1m	90	LEU	2.1
56	2y	38	A	2.1
34	2c	95	THR	2.1
40	1i	7	THR	2.1
40	1i	69	GLY	2.1
41	2j	67	THR	2.1
33	2b	58	ILE	2.1
33	2b	208	ILE	2.1
34	2c	57	ILE	2.1
41	2j	23	ILE	2.1
38	2g	151	TYR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
48	2q	95	TYR	2.1
6	2G	147	ASP	2.1
20	2Y	21	LYS	2.1
20	2Y	34	LYS	2.1
33	2b	192	SER	2.1
41	2j	89	ASP	2.1
1	1A	2184	G	2.1
1	2A	1114	G	2.1
1	2A	2186	G	2.1
32	1a	1010	G	2.1
32	2a	1452	C	2.1
40	2i	90	PRO	2.1
21	2Z	74	VAL	2.1
21	2Z	128	VAL	2.1
41	2j	54	PHE	2.1
45	2n	36	PHE	2.1
50	2s	10	PHE	2.1
21	1Z	152	ALA	2.1
33	1b	207	ALA	2.1
3	1D	176	ARG	2.1
7	1H	3	ARG	2.1
32	1a	173	U	2.1
33	2b	51	LEU	2.1
35	1d	132	ARG	2.1
40	1i	99	LEU	2.1
44	2m	90	LEU	2.1
56	1y	51	U	2.1
8	1I	10	GLU	2.1
37	2f	95	GLU	2.1
50	2s	77	THR	2.1
1	1A	278	A	2.1
32	2a	1256	A	2.1
13	2R	69	ASP	2.1
26	14	51	ASP	2.1
52	2u	5	ASP	2.1
34	2c	20	SER	2.1
50	2s	4	SER	2.1
40	1i	98	PRO	2.1
1	1A	2163	C	2.1
32	1a	174	C	2.1
32	2a	91	C	2.1
32	2a	470	C	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
45	2n	49	HIS	2.1
32	2a	1276	G	2.0
55	1x	68	C	2.1
56	2y	72	C	2.1
12	2Q	113	GLN	2.0
35	2d	160	GLN	2.0
9	1N	140	VAL	2.0
9	2N	140	VAL	2.0
21	2Z	139	VAL	2.0
33	2b	229	VAL	2.0
38	2g	66	VAL	2.0
45	2n	16	PHE	2.0
3	2D	262	ARG	2.0
26	24	61	ARG	2.0
35	2d	122	ARG	2.0
44	2m	3	ARG	2.0
47	1p	5	ARG	2.0
49	1r	87	ARG	2.0
8	1I	75	LEU	2.0
34	1c	87	LEU	2.0
7	2H	31	GLY	2.0
33	2b	126	GLU	2.0
45	2n	51	GLY	2.0
52	2u	4	GLY	2.0
52	2u	11	GLY	2.0
1	2A	877	U	2.0
32	1a	203	U	2.0
32	1a	841	U	2.0
32	2a	202	U	2.0
40	2i	112	LYS	2.0
50	2s	6	LYS	2.0
56	1y	66	U	2.0
56	2y	51	U	2.0
26	24	31	ILE	2.0
1	1A	1085	A	2.0
1	2A	900	A	2.0
1	2A	2801(A)	A	2.0
40	1i	75	ASP	2.0
40	2i	4	TYR	2.0
47	2p	38	TYR	2.0
50	2s	61	TYR	2.0
9	2N	1	MET	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	652(V)	C	2.0
5	2F	6	VAL	2.0
7	2H	45	VAL	2.0
7	2H	76	VAL	2.0
26	24	68	ARG	2.0
34	1c	106	VAL	2.0
38	2g	76	ARG	2.0
44	2m	7	VAL	2.0
56	2y	3	C	2.0
56	2y	43	C	2.0
56	2y	74	C	2.0
32	2a	998	G	2.0
32	2a	1127	G	2.0
32	2a	1253	G	2.0
34	2c	92	ALA	2.0
44	1m	81	LEU	2.0
44	2m	30	ALA	2.0
49	1r	73	ALA	2.0
49	2r	20	ALA	2.0
54	1w	1	G	2.0
54	1w	44	G	2.0
4	2E	63	LEU	2.0
21	2Z	155	LEU	2.0
35	1d	155	LEU	2.0
38	1g	16	LEU	2.0
3	1D	275	LYS	2.0
48	1q	78	GLU	2.0
33	1b	72	GLY	2.0
34	2c	96	GLY	2.0
35	1d	154	ASN	2.0
6	1G	52	ILE	2.0
16	2U	88	ILE	2.0
21	2Z	137	ILE	2.0
40	1i	74	ILE	2.0
44	2m	9	ILE	2.0
50	2s	79	THR	2.0
32	1a	182	U	2.0
32	2a	204	U	2.0
1	1A	2126	A	2.0
39	2h	54	ASP	2.0
50	2s	76	PRO	2.0
21	2Z	66	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	PSU	1y	55	20/21	0.41	0.19	84,88,95,104	0
56	MIA	2y	37	22/30	0.43	0.18	78,86,97,113	0
56	G7M	2y	46	24/25	0.45	0.18	78,86,88,102	0
56	5MU	1y	54	21/22	0.47	0.18	79,85,91,102	0
56	G7M	1y	46	24/25	0.50	0.20	78,84,88,98	0
56	4SU	2y	8	20/21	0.51	0.19	83,92,98,108	0
56	MIA	1y	37	22/30	0.52	0.19	79,83,92,104	0
56	PSU	2y	55	20/21	0.52	0.16	78,83,93,106	0
56	PSU	2y	39	20/21	0.53	0.18	78,83,94,102	0
56	5MU	2y	54	21/22	0.55	0.18	72,81,94,108	0
56	4SU	1y	8	20/21	0.62	0.16	80,87,95,105	0
56	PSU	2y	32	20/21	0.68	0.15	74,80,88,108	0
56	PSU	1y	39	20/21	0.68	0.17	75,83,89,91	0
56	PSU	1y	32	20/21	0.69	0.16	76,83,91,102	0
54	G7M	2w	46	24/25	0.70	0.16	73,80,92,107	0
54	G7M	1w	46	24/25	0.70	0.17	62,70,91,106	0
54	PSU	2w	55	20/21	0.84	0.12	67,71,77,81	0
54	MIA	2w	37	25/30	0.87	0.14	55,63,68,93	0
54	4SU	2w	8	20/21	0.87	0.13	72,77,85,92	0
55	4SU	2x	8	20/21	0.89	0.14	62,68,71,75	0
32	2MG	2a	1207	24/25	0.89	0.12	61,70,73,77	0
55	PSU	2x	55	20/21	0.90	0.10	62,65,71,74	0
54	4SU	1w	8	20/21	0.90	0.13	63,67,72,75	0
54	5MU	2w	54	21/22	0.90	0.11	57,62,68,70	0
55	5MU	2x	54	21/22	0.90	0.12	63,67,71,72	0
55	5MU	1x	54	21/22	0.91	0.11	54,60,68,73	0
32	G7M	2a	527	24/25	0.91	0.13	51,57,62,63	0
55	PSU	1x	55	20/21	0.91	0.10	47,57,71,71	0
43	0TD	2l	92	10/11	0.91	0.12	55,57,63,70	0
55	5MC	2x	32	21/22	0.91	0.14	58,63,65,67	0
54	MIA	1w	37	29/30	0.91	0.14	32,46,60,87	0
43	0TD	1l	92	10/11	0.91	0.11	43,47,50,67	0
54	PSU	1w	55	20/21	0.92	0.10	48,57,66,67	0
1	5MU	2A	1915	21/22	0.92	0.11	50,56,59,59	0
54	PSU	2w	32	20/21	0.92	0.10	59,67,76,76	0
32	5MC	2a	1400	21/22	0.93	0.13	56,59,65,69	0
32	5MC	2a	1404	21/22	0.93	0.11	44,50,53,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	PSU	1w	32	20/21	0.93	0.10	46,53,59,60	0
32	M2G	2a	966	25/26	0.93	0.13	51,59,70,72	0
32	2MG	1a	1207	24/25	0.93	0.10	49,56,61,63	0
32	4OC	2a	1402	22/23	0.94	0.11	49,54,56,59	0
1	PSU	2A	1917	20/21	0.94	0.09	47,54,59,62	0
32	5MC	2a	967	21/22	0.94	0.12	52,59,66,68	0
32	PSU	2a	516	20/21	0.94	0.10	54,61,66,67	0
55	4SU	1x	8	20/21	0.94	0.10	50,56,62,63	0
32	M2G	1a	966	25/26	0.95	0.10	39,45,50,54	0
54	PSU	2w	39	20/21	0.95	0.09	59,67,72,72	0
1	PSU	2A	1911	20/21	0.95	0.08	48,50,54,56	0
55	5MC	1x	32	21/22	0.95	0.10	43,48,54,59	0
1	5MU	1A	1915	21/22	0.96	0.09	40,46,50,52	0
32	5MC	1a	967	21/22	0.96	0.10	42,47,53,55	0
54	PSU	1w	39	20/21	0.96	0.08	47,53,59,65	0
32	5MC	2a	1407	21/22	0.96	0.09	36,46,56,56	0
32	UR3	2a	1498	21/22	0.96	0.10	44,49,52,53	0
55	8AN	2x	76	22/23	0.96	0.09	32,37,42,50	0
1	5MC	2A	1942	21/22	0.96	0.08	42,49,54,56	0
1	5MC	2A	1962	21/22	0.96	0.08	30,42,48,55	0
1	5MC	1A	1942	21/22	0.96	0.08	26,32,35,45	0
32	5MC	1a	1407	21/22	0.96	0.09	30,37,40,42	0
32	MA6	1a	1519	24/25	0.96	0.09	32,36,41,50	0
32	PSU	1a	516	20/21	0.96	0.08	43,49,54,55	0
32	G7M	1a	527	24/25	0.96	0.08	37,43,48,50	0
32	4OC	1a	1402	22/23	0.97	0.08	35,40,44,47	0
55	8AN	1x	76	22/23	0.97	0.07	16,21,28,34	0
54	8AN	2w	76	22/23	0.97	0.07	28,34,37,38	0
32	5MC	1a	1404	21/22	0.97	0.08	29,36,40,42	0
1	OMC	2A	1920	21/22	0.97	0.08	43,51,54,59	0
1	5MU	2A	1939	21/22	0.97	0.08	30,35,39,40	0
1	OMC	1A	1920	21/22	0.97	0.07	31,40,43,45	0
32	MA6	2a	1518	24/25	0.97	0.09	39,50,55,56	0
32	MA6	2a	1519	24/25	0.97	0.09	41,50,54,57	0
54	5MU	1w	54	21/22	0.97	0.07	37,49,52,55	0
1	OMU	2A	2552	21/22	0.97	0.08	31,37,44,50	0
1	PSU	1A	1911	20/21	0.97	0.07	32,40,45,47	0
1	5MC	1A	1962	21/22	0.97	0.07	25,30,34,36	0
1	PSU	1A	1917	20/21	0.97	0.08	34,43,46,50	0
32	5MC	1a	1400	21/22	0.97	0.08	37,43,47,51	0
1	PSU	1A	2605	20/21	0.98	0.06	17,23,26,27	0
32	UR3	1a	1498	21/22	0.98	0.07	31,36,39,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	5MU	1A	1939	21/22	0.98	0.06	17,22,26,30	0
1	OMG	2A	2251	24/25	0.98	0.06	31,34,37,39	0
1	2MA	2A	2503	23/24	0.98	0.07	25,33,38,38	0
54	8AN	1w	76	22/23	0.98	0.07	14,20,23,24	0
1	PSU	2A	2605	20/21	0.98	0.06	28,32,36,36	0
1	2MA	1A	2503	23/24	0.98	0.06	13,17,20,23	0
1	OMU	1A	2552	21/22	0.99	0.05	20,23,27,27	0
1	OMG	1A	2251	24/25	0.99	0.06	16,23,25,26	0
32	MA6	1a	1518	24/25	0.99	0.06	30,35,40,41	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	10	107	1/1	0.47	0.41	70,70,70,70	0
57	MG	1U	211	1/1	0.49	0.64	69,69,69,69	0
57	MG	1a	1778	1/1	0.49	0.22	77,77,77,77	0
57	MG	2a	1772	1/1	0.57	0.39	77,77,77,77	0
57	MG	1A	4048	1/1	0.58	0.27	73,73,73,73	0
57	MG	1A	3990	1/1	0.59	0.26	50,50,50,50	0
57	MG	1A	3968	1/1	0.59	0.15	73,73,73,73	0
57	MG	1B	229	1/1	0.60	0.21	66,66,66,66	0
57	MG	2A	3734	1/1	0.61	0.20	54,54,54,54	0
57	MG	1w	108	1/1	0.64	0.29	71,71,71,71	0
57	MG	2A	3718	1/1	0.65	0.18	65,65,65,65	0
57	MG	1A	4055	1/1	0.65	0.24	61,61,61,61	0
57	MG	1A	3574	1/1	0.65	0.13	27,27,27,27	0
57	MG	2v	102	1/1	0.65	0.42	79,79,79,79	0
57	MG	1A	3992	1/1	0.66	0.19	52,52,52,52	0
57	MG	2B	213	1/1	0.66	0.35	72,72,72,72	0
57	MG	2A	3285	1/1	0.66	0.34	68,68,68,68	0
57	MG	1A	4119	1/1	0.66	0.15	43,43,43,43	0
57	MG	2A	3723	1/1	0.67	0.21	82,82,82,82	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3961	1/1	0.67	0.21	46,46,46,46	0
57	MG	1A	3476	1/1	0.67	0.38	69,69,69,69	0
57	MG	2A	3562	1/1	0.67	0.26	66,66,66,66	0
57	MG	1B	230	1/1	0.67	0.21	77,77,77,77	0
57	MG	1A	3850	1/1	0.68	0.23	41,41,41,41	0
57	MG	2A	3593	1/1	0.68	0.26	68,68,68,68	0
57	MG	2A	3656	1/1	0.68	0.18	67,67,67,67	0
57	MG	2A	3683	1/1	0.69	0.18	39,39,39,39	0
57	MG	1A	3889	1/1	0.69	0.14	29,29,29,29	0
57	MG	2A	3805	1/1	0.69	0.21	65,65,65,65	0
57	MG	2A	3689	1/1	0.70	0.17	48,48,48,48	0
57	MG	2A	3616	1/1	0.70	0.25	64,64,64,64	0
57	MG	2A	3737	1/1	0.70	0.20	52,52,52,52	0
57	MG	2A	3777	1/1	0.70	0.24	66,66,66,66	0
57	MG	1A	3764	1/1	0.71	0.16	56,56,56,56	0
57	MG	1A	3491	1/1	0.71	0.18	72,72,72,72	0
57	MG	2A	3182	1/1	0.71	0.17	69,69,69,69	0
57	MG	2A	3280	1/1	0.71	0.34	68,68,68,68	0
57	MG	1A	3754	1/1	0.72	0.24	80,80,80,80	0
57	MG	2a	1605	1/1	0.72	0.26	65,65,65,65	0
57	MG	1a	1822	1/1	0.72	0.20	64,64,64,64	0
57	MG	2A	3518	1/1	0.72	0.15	56,56,56,56	0
57	MG	1A	3669	1/1	0.73	0.16	27,27,27,27	0
57	MG	1a	1814	1/1	0.73	0.27	69,69,69,69	0
57	MG	1E	312	1/1	0.74	0.19	65,65,65,65	0
57	MG	1A	4030	1/1	0.74	0.13	44,44,44,44	0
57	MG	1A	3500	1/1	0.74	0.16	58,58,58,58	0
57	MG	2a	1756	1/1	0.74	0.21	68,68,68,68	0
57	MG	2A	3551	1/1	0.74	0.15	40,40,40,40	0
57	MG	2a	1796	1/1	0.74	0.30	66,66,66,66	0
57	MG	1E	310	1/1	0.74	0.10	25,25,25,25	0
57	MG	1A	3824	1/1	0.75	0.18	56,56,56,56	0
57	MG	2a	1626	1/1	0.75	0.34	74,74,74,74	0
57	MG	1a	1725	1/1	0.75	0.23	56,56,56,56	0
57	MG	1A	3392	1/1	0.75	0.30	63,63,63,63	0
57	MG	2A	3838	1/1	0.75	0.16	64,64,64,64	0
57	MG	2A	3572	1/1	0.75	0.22	43,43,43,43	0
57	MG	2A	3579	1/1	0.76	0.16	45,45,45,45	0
57	MG	2a	1641	1/1	0.76	0.28	63,63,63,63	0
57	MG	1A	3672	1/1	0.76	0.18	45,45,45,45	0
57	MG	2A	3306	1/1	0.76	0.41	69,69,69,69	0
57	MG	2A	3565	1/1	0.76	0.21	53,53,53,53	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	3082	1/1	0.76	0.20	72,72,72,72	0
57	MG	1A	4102	1/1	0.77	0.26	59,59,59,59	0
57	MG	1A	3917	1/1	0.77	0.22	67,67,67,67	0
57	MG	1B	215	1/1	0.77	0.15	54,54,54,54	0
57	MG	2A	3299	1/1	0.77	0.18	57,57,57,57	0
57	MG	2A	3729	1/1	0.77	0.14	61,61,61,61	0
57	MG	1A	3996	1/1	0.77	0.30	55,55,55,55	0
57	MG	1x	111	1/1	0.77	0.27	62,62,62,62	0
57	MG	2A	3622	1/1	0.77	0.28	72,72,72,72	0
57	MG	1A	4001	1/1	0.77	0.17	47,47,47,47	0
57	MG	1a	1741	1/1	0.78	0.13	74,74,74,74	0
57	MG	2A	3316	1/1	0.78	0.20	60,60,60,60	0
57	MG	1A	3847	1/1	0.78	0.15	27,27,27,27	0
57	MG	1a	1790	1/1	0.78	0.14	62,62,62,62	0
57	MG	1A	3547	1/1	0.78	0.29	60,60,60,60	0
57	MG	2A	3743	1/1	0.78	0.11	66,66,66,66	0
57	MG	2A	3744	1/1	0.78	0.22	50,50,50,50	0
57	MG	2A	3762	1/1	0.78	0.14	41,41,41,41	0
57	MG	2A	3563	1/1	0.78	0.23	56,56,56,56	0
57	MG	1A	3879	1/1	0.78	0.12	21,21,21,21	0
57	MG	2A	3811	1/1	0.78	0.21	62,62,62,62	0
57	MG	1A	3734	1/1	0.78	0.08	15,15,15,15	0
57	MG	1B	231	1/1	0.78	0.13	65,65,65,65	0
57	MG	1A	4007	1/1	0.78	0.13	34,34,34,34	0
57	MG	2A	3602	1/1	0.78	0.18	65,65,65,65	0
57	MG	2A	3167	1/1	0.78	0.14	47,47,47,47	0
57	MG	2a	1705	1/1	0.78	0.22	67,67,67,67	0
57	MG	1A	3573	1/1	0.78	0.14	51,51,51,51	0
57	MG	2a	1765	1/1	0.78	0.31	63,63,63,63	0
57	MG	1A	3384	1/1	0.78	0.18	56,56,56,56	0
57	MG	1A	3967	1/1	0.78	0.10	57,57,57,57	0
57	MG	1A	3505	1/1	0.78	0.22	58,58,58,58	0
57	MG	2A	3614	1/1	0.79	0.18	62,62,62,62	0
57	MG	1A	3701	1/1	0.79	0.11	63,63,63,63	0
57	MG	2a	1610	1/1	0.79	0.31	68,68,68,68	0
57	MG	2A	3158	1/1	0.79	0.11	73,73,73,73	0
57	MG	2a	1633	1/1	0.79	0.26	62,62,62,62	0
57	MG	1A	3554	1/1	0.79	0.20	61,61,61,61	0
57	MG	2a	1689	1/1	0.79	0.29	68,68,68,68	0
57	MG	1A	3584	1/1	0.79	0.16	60,60,60,60	0
57	MG	2A	3309	1/1	0.79	0.19	69,69,69,69	0
57	MG	2A	3783	1/1	0.79	0.17	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	1770	1/1	0.79	0.18	63,63,63,63	0
57	MG	2A	3311	1/1	0.79	0.23	67,67,67,67	0
57	MG	2A	3199	1/1	0.79	0.36	70,70,70,70	0
57	MG	2f	202	1/1	0.79	0.17	71,71,71,71	0
57	MG	2A	3266	1/1	0.79	0.29	71,71,71,71	0
57	MG	2A	3519	1/1	0.80	0.25	66,66,66,66	0
57	MG	2A	3541	1/1	0.80	0.27	55,55,55,55	0
57	MG	1O	206	1/1	0.80	0.28	61,61,61,61	0
57	MG	2A	3552	1/1	0.80	0.14	45,45,45,45	0
57	MG	1A	3419	1/1	0.80	0.27	68,68,68,68	0
57	MG	1A	3378	1/1	0.80	0.39	71,71,71,71	0
57	MG	1a	1710	1/1	0.80	0.22	67,67,67,67	0
57	MG	1A	3832	1/1	0.80	0.12	45,45,45,45	0
57	MG	2A	3822	1/1	0.80	0.17	59,59,59,59	0
57	MG	1A	3981	1/1	0.80	0.16	59,59,59,59	0
57	MG	1A	3697	1/1	0.80	0.18	58,58,58,58	0
57	MG	2D	304	1/1	0.80	0.30	74,74,74,74	0
57	MG	1a	1779	1/1	0.80	0.26	60,60,60,60	0
57	MG	2A	3291	1/1	0.80	0.18	67,67,67,67	0
57	MG	1A	3504	1/1	0.80	0.26	61,61,61,61	0
57	MG	1A	3731	1/1	0.80	0.14	38,38,38,38	0
57	MG	2A	3627	1/1	0.80	0.20	43,43,43,43	0
57	MG	1a	1815	1/1	0.80	0.31	77,77,77,77	0
57	MG	2A	3668	1/1	0.80	0.18	59,59,59,59	0
57	MG	2A	3681	1/1	0.80	0.21	68,68,68,68	0
57	MG	1A	3629	1/1	0.80	0.13	32,32,32,32	0
57	MG	1A	3654	1/1	0.80	0.13	22,22,22,22	0
57	MG	2A	3388	1/1	0.80	0.19	61,61,61,61	0
57	MG	2a	1780	1/1	0.80	0.29	59,59,59,59	0
57	MG	2a	1785	1/1	0.80	0.27	64,64,64,64	0
57	MG	2A	3471	1/1	0.80	0.17	58,58,58,58	0
57	MG	2a	1814	1/1	0.80	0.29	62,62,62,62	0
57	MG	2A	3513	1/1	0.80	0.21	50,50,50,50	0
57	MG	2j	201	1/1	0.80	0.16	65,65,65,65	0
57	MG	1A	3940	1/1	0.80	0.14	66,66,66,66	0
57	MG	1x	112	1/1	0.81	0.16	61,61,61,61	0
57	MG	2A	3056	1/1	0.81	0.17	65,65,65,65	0
57	MG	2A	3749	1/1	0.81	0.17	56,56,56,56	0
57	MG	2A	3536	1/1	0.81	0.23	64,64,64,64	0
57	MG	1A	4095	1/1	0.81	0.12	56,56,56,56	0
57	MG	1a	1643	1/1	0.81	0.23	62,62,62,62	0
57	MG	1a	1659	1/1	0.81	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	1a	1702	1/1	0.81	0.21	54,54,54,54	0
57	MG	2A	3192	1/1	0.81	0.16	60,60,60,60	0
57	MG	1A	3796	1/1	0.81	0.20	64,64,64,64	0
57	MG	2A	3844	1/1	0.81	0.27	67,67,67,67	0
57	MG	2A	3242	1/1	0.81	0.17	56,56,56,56	0
57	MG	2A	3264	1/1	0.81	0.24	58,58,58,58	0
57	MG	2U	202	1/1	0.81	0.12	60,60,60,60	0
57	MG	2a	1601	1/1	0.81	0.16	71,71,71,71	0
57	MG	2a	1604	1/1	0.81	0.27	71,71,71,71	0
57	MG	2A	3580	1/1	0.81	0.15	46,46,46,46	0
57	MG	1A	3802	1/1	0.81	0.18	61,61,61,61	0
57	MG	2a	1611	1/1	0.81	0.19	62,62,62,62	0
57	MG	2A	3600	1/1	0.81	0.12	59,59,59,59	0
57	MG	2A	3268	1/1	0.81	0.17	68,68,68,68	0
57	MG	1A	3818	1/1	0.81	0.14	59,59,59,59	0
57	MG	1B	222	1/1	0.81	0.21	57,57,57,57	0
57	MG	1A	3400	1/1	0.81	0.25	61,61,61,61	0
57	MG	1A	3957	1/1	0.81	0.12	59,59,59,59	0
57	MG	1A	3602	1/1	0.81	0.12	39,39,39,39	0
57	MG	1A	3677	1/1	0.81	0.25	55,55,55,55	0
57	MG	1a	1819	1/1	0.81	0.17	53,53,53,53	0
57	MG	1A	3782	1/1	0.81	0.11	47,47,47,47	0
57	MG	1v	101	1/1	0.81	0.36	74,74,74,74	0
57	MG	1A	3969	1/1	0.81	0.16	50,50,50,50	0
57	MG	2A	3481	1/1	0.81	0.11	34,34,34,34	0
57	MG	2A	3493	1/1	0.81	0.14	70,70,70,70	0
57	MG	1A	4076	1/1	0.81	0.12	56,56,56,56	0
57	MG	2A	3517	1/1	0.81	0.16	45,45,45,45	0
57	MG	2A	3750	1/1	0.82	0.13	40,40,40,40	0
57	MG	1a	1807	1/1	0.82	0.23	65,65,65,65	0
57	MG	2A	3227	1/1	0.82	0.15	54,54,54,54	0
57	MG	2A	3234	1/1	0.82	0.35	63,63,63,63	0
57	MG	2A	3801	1/1	0.82	0.17	52,52,52,52	0
57	MG	2A	3554	1/1	0.82	0.18	46,46,46,46	0
57	MG	1A	4002	1/1	0.82	0.10	33,33,33,33	0
57	MG	1A	3653	1/1	0.82	0.14	27,27,27,27	0
57	MG	1A	4024	1/1	0.82	0.15	58,58,58,58	0
57	MG	1a	1680	1/1	0.82	0.17	66,66,66,66	0
57	MG	1A	3613	1/1	0.82	0.14	55,55,55,55	0
57	MG	1a	1706	1/1	0.82	0.22	70,70,70,70	0
57	MG	1A	4043	1/1	0.82	0.19	38,38,38,38	0
57	MG	2Z	301	1/1	0.82	0.12	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	3296	1/1	0.82	0.22	56,56,56,56	0
57	MG	1A	3441	1/1	0.82	0.22	68,68,68,68	0
57	MG	2A	3033	1/1	0.82	0.18	61,61,61,61	0
57	MG	2A	3615	1/1	0.82	0.19	60,60,60,60	0
57	MG	2A	3039	1/1	0.82	0.20	67,67,67,67	0
57	MG	2a	1612	1/1	0.82	0.24	67,67,67,67	0
57	MG	2a	1617	1/1	0.82	0.15	57,57,57,57	0
57	MG	1a	1727	1/1	0.82	0.20	56,56,56,56	0
57	MG	2A	3313	1/1	0.82	0.30	74,74,74,74	0
57	MG	2A	3059	1/1	0.82	0.31	64,64,64,64	0
57	MG	2a	1688	1/1	0.82	0.27	64,64,64,64	0
57	MG	2A	3667	1/1	0.82	0.12	45,45,45,45	0
57	MG	2A	3351	1/1	0.82	0.26	52,52,52,52	0
57	MG	2a	1721	1/1	0.82	0.20	68,68,68,68	0
57	MG	2a	1754	1/1	0.82	0.15	69,69,69,69	0
57	MG	1A	3711	1/1	0.82	0.16	55,55,55,55	0
57	MG	2A	3399	1/1	0.82	0.14	64,64,64,64	0
57	MG	2A	3462	1/1	0.82	0.20	63,63,63,63	0
57	MG	2A	3089	1/1	0.82	0.21	69,69,69,69	0
57	MG	2A	3151	1/1	0.82	0.21	59,59,59,59	0
57	MG	2a	1784	1/1	0.82	0.21	72,72,72,72	0
57	MG	1A	3795	1/1	0.82	0.18	50,50,50,50	0
57	MG	2a	1787	1/1	0.82	0.26	64,64,64,64	0
57	MG	2a	1792	1/1	0.82	0.25	62,62,62,62	0
57	MG	1A	3644	1/1	0.82	0.09	28,28,28,28	0
57	MG	1A	3871	1/1	0.82	0.14	50,50,50,50	0
57	MG	2A	3191	1/1	0.82	0.23	63,63,63,63	0
57	MG	1a	1806	1/1	0.82	0.22	62,62,62,62	0
57	MG	2A	3198	1/1	0.82	0.13	69,69,69,69	0
57	MG	2y	102	1/1	0.82	0.21	77,77,77,77	0
57	MG	1A	4050	1/1	0.83	0.16	52,52,52,52	0
57	MG	1A	3766	1/1	0.83	0.16	54,54,54,54	0
57	MG	1a	1766	1/1	0.83	0.17	60,60,60,60	0
57	MG	2A	3695	1/1	0.83	0.17	59,59,59,59	0
57	MG	2A	3221	1/1	0.83	0.23	62,62,62,62	0
57	MG	2A	3332	1/1	0.83	0.17	55,55,55,55	0
57	MG	2A	3728	1/1	0.83	0.13	44,44,44,44	0
57	MG	1A	3993	1/1	0.83	0.13	55,55,55,55	0
57	MG	2a	1630	1/1	0.83	0.21	67,67,67,67	0
57	MG	2a	1631	1/1	0.83	0.33	65,65,65,65	0
57	MG	2A	3385	1/1	0.83	0.26	56,56,56,56	0
57	MG	1A	3953	1/1	0.83	0.11	34,34,34,34	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3375	1/1	0.83	0.20	55,55,55,55	0
57	MG	2A	3401	1/1	0.83	0.15	65,65,65,65	0
57	MG	2a	1701	1/1	0.83	0.27	65,65,65,65	0
57	MG	2A	3746	1/1	0.83	0.14	41,41,41,41	0
57	MG	2A	3583	1/1	0.83	0.14	60,60,60,60	0
57	MG	2A	3412	1/1	0.83	0.23	64,64,64,64	0
57	MG	2A	3458	1/1	0.83	0.17	57,57,57,57	0
57	MG	1A	3025	1/1	0.83	0.19	51,51,51,51	0
57	MG	1A	3752	1/1	0.83	0.08	40,40,40,40	0
57	MG	1A	3327	1/1	0.83	0.20	59,59,59,59	0
57	MG	1A	3763	1/1	0.83	0.10	41,41,41,41	0
57	MG	2A	3618	1/1	0.83	0.18	64,64,64,64	0
57	MG	1A	3649	1/1	0.83	0.18	64,64,64,64	0
57	MG	1A	3924	1/1	0.83	0.10	30,30,30,30	0
57	MG	2A	3842	1/1	0.83	0.15	61,61,61,61	0
57	MG	2A	3632	1/1	0.83	0.18	56,56,56,56	0
57	MG	2a	1811	1/1	0.83	0.13	65,65,65,65	0
57	MG	2B	209	1/1	0.83	0.26	73,73,73,73	0
57	MG	2A	3653	1/1	0.83	0.17	59,59,59,59	0
57	MG	1E	309	1/1	0.83	0.14	59,59,59,59	0
57	MG	2A	3189	1/1	0.83	0.30	63,63,63,63	0
57	MG	1w	107	1/1	0.83	0.17	66,66,66,66	0
57	MG	1A	3809	1/1	0.84	0.15	47,47,47,47	0
57	MG	1a	1604	1/1	0.84	0.23	55,55,55,55	0
57	MG	1a	1639	1/1	0.84	0.26	64,64,64,64	0
57	MG	2T	204	1/1	0.84	0.14	69,69,69,69	0
57	MG	2A	3195	1/1	0.84	0.18	65,65,65,65	0
57	MG	2A	3428	1/1	0.84	0.28	66,66,66,66	0
57	MG	1a	1816	1/1	0.84	0.24	62,62,62,62	0
57	MG	2A	3652	1/1	0.84	0.14	52,52,52,52	0
57	MG	1A	3911	1/1	0.84	0.10	51,51,51,51	0
57	MG	1A	3817	1/1	0.84	0.15	57,57,57,57	0
57	MG	1h	201	1/1	0.84	0.12	63,63,63,63	0
57	MG	1A	3923	1/1	0.84	0.09	45,45,45,45	0
57	MG	2A	3674	1/1	0.84	0.17	51,51,51,51	0
57	MG	2a	1619	1/1	0.84	0.32	62,62,62,62	0
57	MG	2A	3496	1/1	0.84	0.18	41,41,41,41	0
57	MG	1a	1688	1/1	0.84	0.27	58,58,58,58	0
57	MG	2A	3248	1/1	0.84	0.25	70,70,70,70	0
57	MG	1A	3676	1/1	0.84	0.12	53,53,53,53	0
57	MG	2A	3700	1/1	0.84	0.19	47,47,47,47	0
57	MG	2a	1683	1/1	0.84	0.33	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	3624	1/1	0.84	0.09	23,23,23,23	0
57	MG	2A	3521	1/1	0.84	0.12	62,62,62,62	0
57	MG	1A	3949	1/1	0.84	0.13	34,34,34,34	0
57	MG	2A	3540	1/1	0.84	0.17	64,64,64,64	0
57	MG	2A	3731	1/1	0.84	0.16	58,58,58,58	0
57	MG	2a	1725	1/1	0.84	0.18	64,64,64,64	0
57	MG	2a	1727	1/1	0.84	0.15	65,65,65,65	0
57	MG	1A	3438	1/1	0.84	0.14	60,60,60,60	0
57	MG	1A	3956	1/1	0.84	0.12	60,60,60,60	0
57	MG	1D	313	1/1	0.84	0.21	41,41,41,41	0
57	MG	1a	1751	1/1	0.84	0.14	47,47,47,47	0
57	MG	1A	3514	1/1	0.84	0.14	61,61,61,61	0
57	MG	2A	3088	1/1	0.84	0.18	62,62,62,62	0
57	MG	1A	3761	1/1	0.84	0.10	17,17,17,17	0
57	MG	1A	3855	1/1	0.84	0.11	29,29,29,29	0
57	MG	1A	3799	1/1	0.84	0.10	35,35,35,35	0
57	MG	2A	3162	1/1	0.84	0.21	67,67,67,67	0
57	MG	2A	3331	1/1	0.84	0.28	59,59,59,59	0
57	MG	2a	1808	1/1	0.84	0.20	60,60,60,60	0
57	MG	2A	3589	1/1	0.84	0.21	55,55,55,55	0
57	MG	2A	3590	1/1	0.84	0.26	68,68,68,68	0
57	MG	1a	1794	1/1	0.84	0.18	59,59,59,59	0
57	MG	2A	3168	1/1	0.84	0.29	62,62,62,62	0
57	MG	2m	201	1/1	0.84	0.26	68,68,68,68	0
57	MG	2A	3354	1/1	0.84	0.12	68,68,68,68	0
57	MG	1A	3304	1/1	0.84	0.17	57,57,57,57	0
57	MG	2A	3794	1/1	0.85	0.22	64,64,64,64	0
57	MG	2A	3799	1/1	0.85	0.14	74,74,74,74	0
57	MG	2A	3270	1/1	0.85	0.23	62,62,62,62	0
57	MG	2A	3025	1/1	0.85	0.15	56,56,56,56	0
57	MG	2A	3809	1/1	0.85	0.13	51,51,51,51	0
57	MG	1A	3565	1/1	0.85	0.15	57,57,57,57	0
57	MG	1A	3791	1/1	0.85	0.17	50,50,50,50	0
57	MG	2A	3825	1/1	0.85	0.16	56,56,56,56	0
57	MG	2A	3292	1/1	0.85	0.25	68,68,68,68	0
57	MG	2A	3839	1/1	0.85	0.13	53,53,53,53	0
57	MG	1a	1711	1/1	0.85	0.18	59,59,59,59	0
57	MG	1a	1712	1/1	0.85	0.20	60,60,60,60	0
57	MG	2B	203	1/1	0.85	0.16	54,54,54,54	0
57	MG	1A	3831	1/1	0.85	0.17	48,48,48,48	0
57	MG	2A	3584	1/1	0.85	0.22	50,50,50,50	0
57	MG	2A	3083	1/1	0.85	0.17	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	2Q	203	1/1	0.85	0.37	67,67,67,67	0
57	MG	1A	3683	1/1	0.85	0.12	46,46,46,46	0
57	MG	1a	1739	1/1	0.85	0.11	59,59,59,59	0
57	MG	2A	3092	1/1	0.85	0.20	59,59,59,59	0
57	MG	2A	3324	1/1	0.85	0.18	63,63,63,63	0
57	MG	2A	3117	1/1	0.85	0.14	55,55,55,55	0
57	MG	1A	3936	1/1	0.85	0.12	65,65,65,65	0
57	MG	2A	3335	1/1	0.85	0.24	54,54,54,54	0
57	MG	2A	3617	1/1	0.85	0.27	68,68,68,68	0
57	MG	1A	3840	1/1	0.85	0.13	35,35,35,35	0
57	MG	1A	3426	1/1	0.85	0.11	54,54,54,54	0
57	MG	2A	3624	1/1	0.85	0.18	56,56,56,56	0
57	MG	2a	1624	1/1	0.85	0.15	80,80,80,80	0
57	MG	2A	3358	1/1	0.85	0.12	57,57,57,57	0
57	MG	2A	3370	1/1	0.85	0.25	57,57,57,57	0
57	MG	2A	3376	1/1	0.85	0.27	58,58,58,58	0
57	MG	2A	3164	1/1	0.85	0.12	58,58,58,58	0
57	MG	2A	3387	1/1	0.85	0.22	53,53,53,53	0
57	MG	1A	3432	1/1	0.85	0.22	59,59,59,59	0
57	MG	1A	4021	1/1	0.85	0.16	33,33,33,33	0
57	MG	1A	3703	1/1	0.85	0.13	48,48,48,48	0
57	MG	2a	1697	1/1	0.85	0.20	64,64,64,64	0
57	MG	2A	3188	1/1	0.85	0.52	70,70,70,70	0
57	MG	2A	3414	1/1	0.85	0.21	54,54,54,54	0
57	MG	2a	1706	1/1	0.85	0.11	68,68,68,68	0
57	MG	1A	3858	1/1	0.85	0.11	21,21,21,21	0
57	MG	2A	3190	1/1	0.85	0.22	53,53,53,53	0
57	MG	1A	4038	1/1	0.85	0.13	51,51,51,51	0
57	MG	1A	4039	1/1	0.85	0.15	38,38,38,38	0
57	MG	2A	3476	1/1	0.85	0.17	57,57,57,57	0
57	MG	1A	3960	1/1	0.85	0.12	47,47,47,47	0
57	MG	2a	1766	1/1	0.85	0.25	64,64,64,64	0
57	MG	1A	4046	1/1	0.85	0.22	52,52,52,52	0
57	MG	2a	1771	1/1	0.85	0.15	57,57,57,57	0
57	MG	1a	1605	1/1	0.85	0.22	62,62,62,62	0
57	MG	2a	1773	1/1	0.85	0.20	64,64,64,64	0
57	MG	1A	3386	1/1	0.85	0.20	59,59,59,59	0
57	MG	1A	3810	1/1	0.85	0.12	52,52,52,52	0
57	MG	2A	3228	1/1	0.85	0.24	58,58,58,58	0
57	MG	2A	3233	1/1	0.85	0.23	66,66,66,66	0
57	MG	1A	3886	1/1	0.85	0.11	42,42,42,42	0
57	MG	1a	1661	1/1	0.85	0.33	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	1802	1/1	0.85	0.23	56,56,56,56	0
57	MG	1a	1666	1/1	0.85	0.21	73,73,73,73	0
57	MG	2A	3756	1/1	0.85	0.13	65,65,65,65	0
57	MG	2A	3761	1/1	0.85	0.15	53,53,53,53	0
57	MG	2a	1819	1/1	0.85	0.28	67,67,67,67	0
57	MG	1A	3227	1/1	0.85	0.12	56,56,56,56	0
57	MG	2A	3776	1/1	0.85	0.16	47,47,47,47	0
57	MG	2l	202	1/1	0.85	0.18	59,59,59,59	0
57	MG	1A	4091	1/1	0.85	0.20	65,65,65,65	0
57	MG	2A	3779	1/1	0.85	0.12	56,56,56,56	0
57	MG	1A	3973	1/1	0.85	0.12	31,31,31,31	0
57	MG	2A	3218	1/1	0.86	0.33	49,49,49,49	0
57	MG	2A	3077	1/1	0.86	0.18	55,55,55,55	0
57	MG	2a	1616	1/1	0.86	0.12	65,65,65,65	0
57	MG	1a	1799	1/1	0.86	0.11	57,57,57,57	0
57	MG	1D	302	1/1	0.86	0.18	60,60,60,60	0
57	MG	2a	1621	1/1	0.86	0.18	58,58,58,58	0
57	MG	2a	1622	1/1	0.86	0.14	54,54,54,54	0
57	MG	2a	1623	1/1	0.86	0.18	59,59,59,59	0
57	MG	1A	3092	1/1	0.86	0.15	59,59,59,59	0
57	MG	1A	3154	1/1	0.86	0.19	57,57,57,57	0
57	MG	1A	3443	1/1	0.86	0.15	52,52,52,52	0
57	MG	2A	3093	1/1	0.86	0.23	66,66,66,66	0
57	MG	2a	1632	1/1	0.86	0.22	67,67,67,67	0
57	MG	2A	3393	1/1	0.86	0.32	68,68,68,68	0
57	MG	2a	1640	1/1	0.86	0.34	63,63,63,63	0
57	MG	2A	3398	1/1	0.86	0.20	58,58,58,58	0
57	MG	2a	1646	1/1	0.86	0.17	65,65,65,65	0
57	MG	2a	1682	1/1	0.86	0.45	67,67,67,67	0
57	MG	2A	3260	1/1	0.86	0.23	62,62,62,62	0
57	MG	1A	3185	1/1	0.86	0.16	46,46,46,46	0
57	MG	2A	3404	1/1	0.86	0.14	63,63,63,63	0
57	MG	2A	3766	1/1	0.86	0.14	39,39,39,39	0
57	MG	2A	3770	1/1	0.86	0.10	65,65,65,65	0
57	MG	1G	205	1/1	0.86	0.17	57,57,57,57	0
57	MG	2A	3610	1/1	0.86	0.17	48,48,48,48	0
57	MG	1A	3719	1/1	0.86	0.16	60,60,60,60	0
57	MG	1A	4014	1/1	0.86	0.12	46,46,46,46	0
57	MG	2A	3440	1/1	0.86	0.18	50,50,50,50	0
57	MG	2a	1728	1/1	0.86	0.16	63,63,63,63	0
57	MG	2a	1733	1/1	0.86	0.18	56,56,56,56	0
57	MG	1l	201	1/1	0.86	0.12	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	1A	3725	1/1	0.86	0.12	21,21,21,21	0
57	MG	1A	3188	1/1	0.86	0.16	60,60,60,60	0
57	MG	2A	3808	1/1	0.86	0.20	62,62,62,62	0
57	MG	2A	3475	1/1	0.86	0.12	43,43,43,43	0
57	MG	2A	3174	1/1	0.86	0.19	54,54,54,54	0
57	MG	2A	3480	1/1	0.86	0.23	59,59,59,59	0
57	MG	2A	3293	1/1	0.86	0.22	60,60,60,60	0
57	MG	1A	4029	1/1	0.86	0.17	53,53,53,53	0
57	MG	1x	101	1/1	0.86	0.29	60,60,60,60	0
57	MG	2A	3661	1/1	0.86	0.12	46,46,46,46	0
57	MG	1A	3379	1/1	0.86	0.11	47,47,47,47	0
57	MG	2a	1789	1/1	0.86	0.27	69,69,69,69	0
57	MG	2a	1790	1/1	0.86	0.18	55,55,55,55	0
57	MG	1A	3047	1/1	0.86	0.15	48,48,48,48	0
57	MG	1a	1647	1/1	0.86	0.21	62,62,62,62	0
57	MG	2a	1801	1/1	0.86	0.22	59,59,59,59	0
57	MG	2B	211	1/1	0.86	0.23	61,61,61,61	0
57	MG	2a	1806	1/1	0.86	0.23	63,63,63,63	0
57	MG	2A	3679	1/1	0.86	0.12	63,63,63,63	0
57	MG	2A	3680	1/1	0.86	0.14	57,57,57,57	0
57	MG	1A	3686	1/1	0.86	0.14	59,59,59,59	0
57	MG	2A	3682	1/1	0.86	0.22	61,61,61,61	0
57	MG	1a	1789	1/1	0.86	0.17	66,66,66,66	0
57	MG	2A	3321	1/1	0.86	0.26	65,65,65,65	0
57	MG	1A	3689	1/1	0.86	0.21	64,64,64,64	0
57	MG	2l	204	1/1	0.86	0.14	59,59,59,59	0
57	MG	1A	4044	1/1	0.86	0.19	44,44,44,44	0
57	MG	2v	101	1/1	0.86	0.17	57,57,57,57	0
57	MG	2A	3201	1/1	0.86	0.29	66,66,66,66	0
57	MG	2x	104	1/1	0.86	0.22	60,60,60,60	0
57	MG	2A	3209	1/1	0.86	0.31	60,60,60,60	0
57	MG	1A	3786	1/1	0.87	0.10	23,23,23,23	0
57	MG	2A	3713	1/1	0.87	0.11	55,55,55,55	0
57	MG	2A	3537	1/1	0.87	0.21	59,59,59,59	0
57	MG	2A	3538	1/1	0.87	0.10	34,34,34,34	0
57	MG	1b	301	1/1	0.87	0.12	61,61,61,61	0
57	MG	1a	1670	1/1	0.87	0.19	64,64,64,64	0
57	MG	1A	3713	1/1	0.87	0.11	34,34,34,34	0
57	MG	2a	1629	1/1	0.87	0.27	56,56,56,56	0
57	MG	2A	3732	1/1	0.87	0.14	72,72,72,72	0
57	MG	1A	3263	1/1	0.87	0.14	53,53,53,53	0
57	MG	2A	3334	1/1	0.87	0.23	71,71,71,71	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3558	1/1	0.87	0.19	54,54,54,54	0
57	MG	2a	1634	1/1	0.87	0.26	60,60,60,60	0
57	MG	1A	3607	1/1	0.87	0.20	61,61,61,61	0
57	MG	1B	232	1/1	0.87	0.15	61,61,61,61	0
57	MG	1A	3026	1/1	0.87	0.19	73,73,73,73	0
57	MG	2a	1666	1/1	0.87	0.26	59,59,59,59	0
57	MG	1x	108	1/1	0.87	0.32	66,66,66,66	0
57	MG	2A	3367	1/1	0.87	0.21	54,54,54,54	0
57	MG	2a	1687	1/1	0.87	0.17	64,64,64,64	0
57	MG	1A	3880	1/1	0.87	0.12	39,39,39,39	0
57	MG	1A	3733	1/1	0.87	0.09	29,29,29,29	0
57	MG	2A	3210	1/1	0.87	0.15	61,61,61,61	0
57	MG	2A	3006	1/1	0.87	0.14	50,50,50,50	0
57	MG	1A	3408	1/1	0.87	0.10	61,61,61,61	0
57	MG	1A	3907	1/1	0.87	0.09	56,56,56,56	0
57	MG	2a	1708	1/1	0.87	0.22	67,67,67,67	0
57	MG	1A	3454	1/1	0.87	0.15	48,48,48,48	0
57	MG	2A	3230	1/1	0.87	0.13	61,61,61,61	0
57	MG	1A	3630	1/1	0.87	0.07	27,27,27,27	0
57	MG	2A	3057	1/1	0.87	0.20	58,58,58,58	0
57	MG	2a	1729	1/1	0.87	0.11	62,62,62,62	0
57	MG	2A	3409	1/1	0.87	0.21	64,64,64,64	0
57	MG	1U	202	1/1	0.87	0.25	45,45,45,45	0
57	MG	1A	3633	1/1	0.87	0.09	35,35,35,35	0
57	MG	2A	3417	1/1	0.87	0.28	69,69,69,69	0
57	MG	1Z	304	1/1	0.87	0.11	53,53,53,53	0
57	MG	1A	3307	1/1	0.87	0.13	50,50,50,50	0
57	MG	2A	3446	1/1	0.87	0.11	53,53,53,53	0
57	MG	1a	1785	1/1	0.87	0.13	54,54,54,54	0
57	MG	2A	3633	1/1	0.87	0.15	53,53,53,53	0
57	MG	2A	3634	1/1	0.87	0.31	63,63,63,63	0
57	MG	2A	3640	1/1	0.87	0.09	27,27,27,27	0
57	MG	1A	3312	1/1	0.87	0.15	57,57,57,57	0
57	MG	1A	3430	1/1	0.87	0.17	52,52,52,52	0
57	MG	1a	1606	1/1	0.87	0.11	56,56,56,56	0
57	MG	2A	3096	1/1	0.87	0.24	64,64,64,64	0
57	MG	2B	217	1/1	0.87	0.12	69,69,69,69	0
57	MG	2A	3097	1/1	0.87	0.21	63,63,63,63	0
57	MG	2Q	202	1/1	0.87	0.16	55,55,55,55	0
57	MG	1a	1797	1/1	0.87	0.19	57,57,57,57	0
57	MG	2A	3670	1/1	0.87	0.16	52,52,52,52	0
57	MG	2A	3673	1/1	0.87	0.16	53,53,53,53	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	1611	1/1	0.87	0.26	59,59,59,59	0
57	MG	21	101	1/1	0.87	0.18	62,62,62,62	0
57	MG	1A	4003	1/1	0.87	0.17	42,42,42,42	0
57	MG	2a	1820	1/1	0.87	0.16	70,70,70,70	0
57	MG	2a	1825	1/1	0.87	0.17	69,69,69,69	0
57	MG	2a	1602	1/1	0.87	0.28	59,59,59,59	0
57	MG	2a	1603	1/1	0.87	0.22	61,61,61,61	0
57	MG	1A	4104	1/1	0.87	0.12	75,75,75,75	0
57	MG	1A	3780	1/1	0.87	0.23	57,57,57,57	0
57	MG	2a	1606	1/1	0.87	0.29	64,64,64,64	0
57	MG	2t	201	1/1	0.87	0.15	52,52,52,52	0
57	MG	1a	1650	1/1	0.87	0.28	63,63,63,63	0
57	MG	1B	202	1/1	0.87	0.28	56,56,56,56	0
57	MG	1A	3151	1/1	0.87	0.24	53,53,53,53	0
57	MG	2A	3523	1/1	0.87	0.14	47,47,47,47	0
57	MG	1A	3808	1/1	0.88	0.09	55,55,55,55	0
57	MG	1A	4066	1/1	0.88	0.16	53,53,53,53	0
57	MG	2A	3836	1/1	0.88	0.10	54,54,54,54	0
57	MG	2A	3245	1/1	0.88	0.11	56,56,56,56	0
57	MG	1A	4073	1/1	0.88	0.14	49,49,49,49	0
57	MG	1a	1619	1/1	0.88	0.12	58,58,58,58	0
57	MG	1a	1631	1/1	0.88	0.23	60,60,60,60	0
57	MG	1a	1633	1/1	0.88	0.17	56,56,56,56	0
57	MG	2A	3267	1/1	0.88	0.10	67,67,67,67	0
57	MG	1A	3909	1/1	0.88	0.08	48,48,48,48	0
57	MG	1A	4089	1/1	0.88	0.11	51,51,51,51	0
57	MG	2A	3273	1/1	0.88	0.20	55,55,55,55	0
57	MG	2A	3276	1/1	0.88	0.28	54,54,54,54	0
57	MG	2A	3278	1/1	0.88	0.20	55,55,55,55	0
57	MG	1x	103	1/1	0.88	0.13	58,58,58,58	0
57	MG	1A	3453	1/1	0.88	0.24	59,59,59,59	0
57	MG	1A	3735	1/1	0.88	0.10	52,52,52,52	0
57	MG	2X	101	1/1	0.88	0.18	56,56,56,56	0
57	MG	2A	3582	1/1	0.88	0.15	42,42,42,42	0
57	MG	1a	1656	1/1	0.88	0.27	53,53,53,53	0
57	MG	1A	3999	1/1	0.88	0.08	45,45,45,45	0
57	MG	2A	3011	1/1	0.88	0.22	66,66,66,66	0
57	MG	2A	3298	1/1	0.88	0.34	71,71,71,71	0
57	MG	2A	3592	1/1	0.88	0.13	54,54,54,54	0
57	MG	2A	3017	1/1	0.88	0.21	64,64,64,64	0
57	MG	2A	3305	1/1	0.88	0.14	73,73,73,73	0
57	MG	2a	1607	1/1	0.88	0.31	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	4000	1/1	0.88	0.11	43,43,43,43	0
57	MG	2A	3604	1/1	0.88	0.11	47,47,47,47	0
57	MG	1a	1662	1/1	0.88	0.17	61,61,61,61	0
57	MG	1A	4112	1/1	0.88	0.16	64,64,64,64	0
57	MG	1a	1668	1/1	0.88	0.34	68,68,68,68	0
57	MG	2A	3315	1/1	0.88	0.10	73,73,73,73	0
57	MG	1A	4113	1/1	0.88	0.18	45,45,45,45	0
57	MG	1a	1679	1/1	0.88	0.12	53,53,53,53	0
57	MG	2A	3065	1/1	0.88	0.13	49,49,49,49	0
57	MG	2A	3326	1/1	0.88	0.26	64,64,64,64	0
57	MG	2A	3329	1/1	0.88	0.25	62,62,62,62	0
57	MG	1A	3423	1/1	0.88	0.17	51,51,51,51	0
57	MG	1a	1683	1/1	0.88	0.17	60,60,60,60	0
57	MG	1A	3365	1/1	0.88	0.23	35,35,35,35	0
57	MG	1a	1693	1/1	0.88	0.29	58,58,58,58	0
57	MG	2A	3649	1/1	0.88	0.19	60,60,60,60	0
57	MG	2A	3650	1/1	0.88	0.15	51,51,51,51	0
57	MG	1B	213	1/1	0.88	0.26	65,65,65,65	0
57	MG	2A	3352	1/1	0.88	0.21	66,66,66,66	0
57	MG	1A	3927	1/1	0.88	0.16	43,43,43,43	0
57	MG	2a	1660	1/1	0.88	0.39	65,65,65,65	0
57	MG	2A	3659	1/1	0.88	0.13	60,60,60,60	0
57	MG	2A	3355	1/1	0.88	0.11	63,63,63,63	0
57	MG	2A	3662	1/1	0.88	0.10	57,57,57,57	0
57	MG	2a	1684	1/1	0.88	0.20	53,53,53,53	0
57	MG	1A	4004	1/1	0.88	0.10	54,54,54,54	0
57	MG	1A	3389	1/1	0.88	0.15	51,51,51,51	0
57	MG	1A	4008	1/1	0.88	0.10	21,21,21,21	0
57	MG	2A	3373	1/1	0.88	0.22	54,54,54,54	0
57	MG	2A	3375	1/1	0.88	0.35	54,54,54,54	0
57	MG	1a	1721	1/1	0.88	0.19	65,65,65,65	0
57	MG	2A	3382	1/1	0.88	0.26	54,54,54,54	0
57	MG	1A	3051	1/1	0.88	0.10	49,49,49,49	0
57	MG	2a	1712	1/1	0.88	0.22	72,72,72,72	0
57	MG	2A	3155	1/1	0.88	0.24	57,57,57,57	0
57	MG	2a	1722	1/1	0.88	0.36	64,64,64,64	0
57	MG	1A	3248	1/1	0.88	0.10	51,51,51,51	0
57	MG	1a	1729	1/1	0.88	0.20	62,62,62,62	0
57	MG	2A	3395	1/1	0.88	0.19	48,48,48,48	0
57	MG	2A	3696	1/1	0.88	0.23	70,70,70,70	0
57	MG	2a	1732	1/1	0.88	0.09	72,72,72,72	0
57	MG	1a	1735	1/1	0.88	0.17	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	1738	1/1	0.88	0.16	69,69,69,69	0
57	MG	1B	237	1/1	0.88	0.09	39,39,39,39	0
57	MG	2A	3721	1/1	0.88	0.14	58,58,58,58	0
57	MG	2A	3722	1/1	0.88	0.17	41,41,41,41	0
57	MG	1A	4023	1/1	0.88	0.10	36,36,36,36	0
57	MG	2A	3179	1/1	0.88	0.19	62,62,62,62	0
57	MG	2A	3181	1/1	0.88	0.38	64,64,64,64	0
57	MG	2A	3730	1/1	0.88	0.14	61,61,61,61	0
57	MG	2a	1779	1/1	0.88	0.16	63,63,63,63	0
57	MG	1A	3709	1/1	0.88	0.26	54,54,54,54	0
57	MG	2A	3415	1/1	0.88	0.22	63,63,63,63	0
57	MG	1E	306	1/1	0.88	0.20	53,53,53,53	0
57	MG	1A	3146	1/1	0.88	0.12	58,58,58,58	0
57	MG	2a	1788	1/1	0.88	0.31	54,54,54,54	0
57	MG	2A	3741	1/1	0.88	0.12	58,58,58,58	0
57	MG	2A	3429	1/1	0.88	0.28	58,58,58,58	0
57	MG	1A	3665	1/1	0.88	0.10	28,28,28,28	0
57	MG	1A	3716	1/1	0.88	0.16	47,47,47,47	0
57	MG	2a	1800	1/1	0.88	0.20	71,71,71,71	0
57	MG	2A	3448	1/1	0.88	0.12	34,34,34,34	0
57	MG	1G	204	1/1	0.88	0.10	65,65,65,65	0
57	MG	2A	3193	1/1	0.88	0.14	61,61,61,61	0
57	MG	1A	3718	1/1	0.88	0.10	28,28,28,28	0
57	MG	2a	1810	1/1	0.88	0.23	57,57,57,57	0
57	MG	1A	4040	1/1	0.88	0.09	24,24,24,24	0
57	MG	1A	3282	1/1	0.88	0.10	58,58,58,58	0
57	MG	1A	3445	1/1	0.88	0.19	59,59,59,59	0
57	MG	1a	1805	1/1	0.88	0.12	58,58,58,58	0
57	MG	1Z	302	1/1	0.88	0.08	57,57,57,57	0
57	MG	1A	3626	1/1	0.88	0.12	55,55,55,55	0
57	MG	2A	3503	1/1	0.88	0.11	59,59,59,59	0
57	MG	2A	3791	1/1	0.88	0.13	66,66,66,66	0
57	MG	2A	3508	1/1	0.88	0.09	34,34,34,34	0
57	MG	2A	3509	1/1	0.88	0.25	56,56,56,56	0
57	MG	1A	3800	1/1	0.88	0.10	39,39,39,39	0
57	MG	17	105	1/1	0.88	0.23	38,38,38,38	0
57	MG	18	105	1/1	0.88	0.14	63,63,63,63	0
57	MG	2w	103	1/1	0.88	0.10	65,65,65,65	0
57	MG	2w	106	1/1	0.88	0.15	65,65,65,65	0
57	MG	2w	107	1/1	0.88	0.33	70,70,70,70	0
57	MG	1a	1817	1/1	0.88	0.22	62,62,62,62	0
57	MG	1A	3627	1/1	0.88	0.09	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
57	MG	1A	3813	1/1	0.89	0.11	55,55,55,55	0
57	MG	1A	4015	1/1	0.89	0.15	59,59,59,59	0
57	MG	1A	3931	1/1	0.89	0.17	50,50,50,50	0
57	MG	25	101	1/1	0.89	0.19	57,57,57,57	0
57	MG	2A	3383	1/1	0.89	0.24	55,55,55,55	0
57	MG	1A	3182	1/1	0.89	0.11	51,51,51,51	0
57	MG	2A	3208	1/1	0.89	0.34	58,58,58,58	0
57	MG	1A	3938	1/1	0.89	0.15	65,65,65,65	0
57	MG	2A	3390	1/1	0.89	0.29	58,58,58,58	0
57	MG	2A	3636	1/1	0.89	0.14	68,68,68,68	0
57	MG	1A	3329	1/1	0.89	0.12	49,49,49,49	0
57	MG	2A	3641	1/1	0.89	0.16	60,60,60,60	0
57	MG	2A	3643	1/1	0.89	0.30	67,67,67,67	0
57	MG	1A	3946	1/1	0.89	0.13	59,59,59,59	0
57	MG	1A	3589	1/1	0.89	0.14	46,46,46,46	0
57	MG	1x	109	1/1	0.89	0.26	61,61,61,61	0
57	MG	1A	3452	1/1	0.89	0.13	49,49,49,49	0
57	MG	1A	3333	1/1	0.89	0.16	46,46,46,46	0
57	MG	2A	3407	1/1	0.89	0.10	57,57,57,57	0
57	MG	2A	3232	1/1	0.89	0.27	59,59,59,59	0
57	MG	2A	3411	1/1	0.89	0.17	64,64,64,64	0
57	MG	2A	3666	1/1	0.89	0.16	53,53,53,53	0
57	MG	1a	1707	1/1	0.89	0.21	48,48,48,48	0
57	MG	1A	3405	1/1	0.89	0.28	49,49,49,49	0
57	MG	1E	314	1/1	0.89	0.14	55,55,55,55	0
57	MG	1A	3406	1/1	0.89	0.24	51,51,51,51	0
57	MG	2A	3425	1/1	0.89	0.23	59,59,59,59	0
57	MG	2A	3427	1/1	0.89	0.12	59,59,59,59	0
57	MG	1A	3342	1/1	0.89	0.22	47,47,47,47	0
57	MG	2A	3255	1/1	0.89	0.15	62,62,62,62	0
57	MG	2A	3256	1/1	0.89	0.20	58,58,58,58	0
57	MG	2a	1654	1/1	0.89	0.24	64,64,64,64	0
57	MG	1A	3851	1/1	0.89	0.08	20,20,20,20	0
57	MG	2a	1661	1/1	0.89	0.21	57,57,57,57	0
57	MG	1A	3773	1/1	0.89	0.13	37,37,37,37	0
57	MG	2a	1677	1/1	0.89	0.21	60,60,60,60	0
57	MG	1A	3038	1/1	0.89	0.26	55,55,55,55	0
57	MG	1A	3082	1/1	0.89	0.17	52,52,52,52	0
57	MG	1a	1737	1/1	0.89	0.10	61,61,61,61	0
57	MG	2A	3474	1/1	0.89	0.23	58,58,58,58	0
57	MG	1A	4069	1/1	0.89	0.09	43,43,43,43	0
57	MG	2A	3271	1/1	0.89	0.27	63,63,63,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3203	1/1	0.89	0.18	45,45,45,45	0
57	MG	2a	1698	1/1	0.89	0.25	64,64,64,64	0
57	MG	2a	1699	1/1	0.89	0.12	67,67,67,67	0
57	MG	14	101	1/1	0.89	0.27	68,68,68,68	0
57	MG	2A	3277	1/1	0.89	0.20	68,68,68,68	0
57	MG	15	107	1/1	0.89	0.09	53,53,53,53	0
57	MG	1A	3989	1/1	0.89	0.11	58,58,58,58	0
57	MG	2a	1710	1/1	0.89	0.37	68,68,68,68	0
57	MG	2A	3282	1/1	0.89	0.12	47,47,47,47	0
57	MG	2a	1716	1/1	0.89	0.19	71,71,71,71	0
57	MG	1A	4080	1/1	0.89	0.09	33,33,33,33	0
57	MG	2A	3288	1/1	0.89	0.17	55,55,55,55	0
57	MG	2a	1724	1/1	0.89	0.27	66,66,66,66	0
57	MG	1A	4083	1/1	0.89	0.11	48,48,48,48	0
57	MG	2A	3094	1/1	0.89	0.23	53,53,53,53	0
57	MG	1A	4086	1/1	0.89	0.16	57,57,57,57	0
57	MG	1a	1786	1/1	0.89	0.12	47,47,47,47	0
57	MG	2A	3106	1/1	0.89	0.20	52,52,52,52	0
57	MG	1a	1787	1/1	0.89	0.18	56,56,56,56	0
57	MG	2a	1741	1/1	0.89	0.17	69,69,69,69	0
57	MG	2A	3135	1/1	0.89	0.34	61,61,61,61	0
57	MG	1A	3211	1/1	0.89	0.25	59,59,59,59	0
57	MG	2A	3154	1/1	0.89	0.33	70,70,70,70	0
57	MG	1A	3884	1/1	0.89	0.08	67,67,67,67	0
57	MG	2A	3542	1/1	0.89	0.16	51,51,51,51	0
57	MG	2A	3544	1/1	0.89	0.19	55,55,55,55	0
57	MG	2A	3772	1/1	0.89	0.13	62,62,62,62	0
57	MG	1A	3526	1/1	0.89	0.15	52,52,52,52	0
57	MG	1a	1796	1/1	0.89	0.11	56,56,56,56	0
57	MG	1a	1628	1/1	0.89	0.25	60,60,60,60	0
57	MG	2A	3557	1/1	0.89	0.19	59,59,59,59	0
57	MG	1A	4098	1/1	0.89	0.13	40,40,40,40	0
57	MG	1a	1802	1/1	0.89	0.11	63,63,63,63	0
57	MG	2A	3796	1/1	0.89	0.21	69,69,69,69	0
57	MG	2A	3797	1/1	0.89	0.15	54,54,54,54	0
57	MG	2A	3325	1/1	0.89	0.17	52,52,52,52	0
57	MG	2A	3171	1/1	0.89	0.23	52,52,52,52	0
57	MG	2A	3568	1/1	0.89	0.08	36,36,36,36	0
57	MG	2A	3172	1/1	0.89	0.12	42,42,42,42	0
57	MG	2A	3574	1/1	0.89	0.09	34,34,34,34	0
57	MG	1A	3157	1/1	0.89	0.15	52,52,52,52	0
57	MG	2a	1804	1/1	0.89	0.20	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	3552	1/1	0.89	0.12	35,35,35,35	0
57	MG	2A	3180	1/1	0.89	0.14	60,60,60,60	0
57	MG	1A	3317	1/1	0.89	0.15	56,56,56,56	0
57	MG	2A	3338	1/1	0.89	0.31	61,61,61,61	0
57	MG	2A	3586	1/1	0.89	0.27	63,63,63,63	0
57	MG	2a	1815	1/1	0.89	0.24	62,62,62,62	0
57	MG	2a	1818	1/1	0.89	0.12	61,61,61,61	0
57	MG	2A	3840	1/1	0.89	0.10	59,59,59,59	0
57	MG	2A	3343	1/1	0.89	0.16	64,64,64,64	0
57	MG	2a	1824	1/1	0.89	0.25	65,65,65,65	0
57	MG	1a	1646	1/1	0.89	0.31	59,59,59,59	0
57	MG	2B	201	1/1	0.89	0.17	66,66,66,66	0
57	MG	2A	3185	1/1	0.89	0.14	55,55,55,55	0
57	MG	1A	3729	1/1	0.89	0.10	25,25,25,25	0
57	MG	2A	3599	1/1	0.89	0.15	58,58,58,58	0
57	MG	1A	3916	1/1	0.89	0.10	46,46,46,46	0
57	MG	2A	3357	1/1	0.89	0.15	54,54,54,54	0
57	MG	1A	3730	1/1	0.89	0.13	27,27,27,27	0
57	MG	2E	305	1/1	0.89	0.10	34,34,34,34	0
57	MG	2F	307	1/1	0.89	0.29	48,48,48,48	0
57	MG	2A	3364	1/1	0.89	0.23	43,43,43,43	0
57	MG	1A	3922	1/1	0.89	0.08	28,28,28,28	0
57	MG	1A	3440	1/1	0.89	0.21	59,59,59,59	0
57	MG	1A	3388	1/1	0.89	0.20	54,54,54,54	0
57	MG	2A	3133	1/1	0.90	0.32	67,67,67,67	0
57	MG	2A	3328	1/1	0.90	0.31	64,64,64,64	0
57	MG	2D	309	1/1	0.90	0.10	46,46,46,46	0
57	MG	1A	3205	1/1	0.90	0.11	44,44,44,44	0
57	MG	1A	3908	1/1	0.90	0.10	46,46,46,46	0
57	MG	2F	308	1/1	0.90	0.17	55,55,55,55	0
57	MG	2P	201	1/1	0.90	0.17	56,56,56,56	0
57	MG	1O	201	1/1	0.90	0.10	52,52,52,52	0
57	MG	2A	3333	1/1	0.90	0.30	62,62,62,62	0
57	MG	2R	201	1/1	0.90	0.10	57,57,57,57	0
57	MG	2T	202	1/1	0.90	0.16	63,63,63,63	0
57	MG	1a	1750	1/1	0.90	0.11	57,57,57,57	0
57	MG	1O	202	1/1	0.90	0.27	49,49,49,49	0
57	MG	1a	1759	1/1	0.90	0.14	73,73,73,73	0
57	MG	1A	3660	1/1	0.90	0.09	31,31,31,31	0
57	MG	2A	3345	1/1	0.90	0.13	66,66,66,66	0
57	MG	2A	3347	1/1	0.90	0.29	61,61,61,61	0
57	MG	25	103	1/1	0.90	0.17	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	28	102	1/1	0.90	0.22	48,48,48,48	0
57	MG	1T	202	1/1	0.90	0.20	48,48,48,48	0
57	MG	1A	3559	1/1	0.90	0.26	56,56,56,56	0
57	MG	1A	3913	1/1	0.90	0.08	55,55,55,55	0
57	MG	1A	3667	1/1	0.90	0.14	44,44,44,44	0
57	MG	1A	3561	1/1	0.90	0.20	43,43,43,43	0
57	MG	10	102	1/1	0.90	0.21	39,39,39,39	0
57	MG	1A	3670	1/1	0.90	0.10	39,39,39,39	0
57	MG	2A	3626	1/1	0.90	0.10	41,41,41,41	0
57	MG	2A	3366	1/1	0.90	0.20	37,37,37,37	0
57	MG	2A	3630	1/1	0.90	0.12	63,63,63,63	0
57	MG	1A	3562	1/1	0.90	0.18	59,59,59,59	0
57	MG	2A	3368	1/1	0.90	0.22	47,47,47,47	0
57	MG	1A	3166	1/1	0.90	0.16	43,43,43,43	0
57	MG	2A	3371	1/1	0.90	0.15	58,58,58,58	0
57	MG	2A	3639	1/1	0.90	0.15	65,65,65,65	0
57	MG	1A	3569	1/1	0.90	0.10	49,49,49,49	0
57	MG	2A	3374	1/1	0.90	0.19	58,58,58,58	0
57	MG	2A	3642	1/1	0.90	0.11	51,51,51,51	0
57	MG	1a	1798	1/1	0.90	0.10	62,62,62,62	0
57	MG	1A	3325	1/1	0.90	0.11	55,55,55,55	0
57	MG	1A	4053	1/1	0.90	0.09	48,48,48,48	0
57	MG	1A	3180	1/1	0.90	0.09	34,34,34,34	0
57	MG	1A	4057	1/1	0.90	0.14	59,59,59,59	0
57	MG	1A	3015	1/1	0.90	0.19	46,46,46,46	0
57	MG	1a	1809	1/1	0.90	0.23	56,56,56,56	0
57	MG	2A	3389	1/1	0.90	0.30	59,59,59,59	0
57	MG	2a	1642	1/1	0.90	0.27	65,65,65,65	0
57	MG	2A	3197	1/1	0.90	0.18	53,53,53,53	0
57	MG	2a	1651	1/1	0.90	0.17	63,63,63,63	0
57	MG	1a	1614	1/1	0.90	0.28	55,55,55,55	0
57	MG	1A	3939	1/1	0.90	0.11	42,42,42,42	0
57	MG	1A	3690	1/1	0.90	0.15	47,47,47,47	0
57	MG	2A	3207	1/1	0.90	0.19	60,60,60,60	0
57	MG	2a	1673	1/1	0.90	0.20	64,64,64,64	0
57	MG	2A	3672	1/1	0.90	0.19	62,62,62,62	0
57	MG	1A	3696	1/1	0.90	0.10	63,63,63,63	0
57	MG	1A	3803	1/1	0.90	0.16	44,44,44,44	0
57	MG	1a	1638	1/1	0.90	0.18	53,53,53,53	0
57	MG	2a	1685	1/1	0.90	0.20	62,62,62,62	0
57	MG	2A	3212	1/1	0.90	0.20	67,67,67,67	0
57	MG	1A	3807	1/1	0.90	0.12	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	1f	201	1/1	0.90	0.16	42,42,42,42	0
57	MG	2a	1690	1/1	0.90	0.13	64,64,64,64	0
57	MG	2a	1693	1/1	0.90	0.13	54,54,54,54	0
57	MG	1A	3090	1/1	0.90	0.18	63,63,63,63	0
57	MG	2A	3685	1/1	0.90	0.10	52,52,52,52	0
57	MG	2A	3688	1/1	0.90	0.34	42,42,42,42	0
57	MG	1A	3458	1/1	0.90	0.17	57,57,57,57	0
57	MG	2A	3691	1/1	0.90	0.15	63,63,63,63	0
57	MG	1A	3604	1/1	0.90	0.08	20,20,20,20	0
57	MG	1A	3811	1/1	0.90	0.10	51,51,51,51	0
57	MG	1a	1655	1/1	0.90	0.25	58,58,58,58	0
57	MG	1A	3606	1/1	0.90	0.14	49,49,49,49	0
57	MG	2A	3235	1/1	0.90	0.15	59,59,59,59	0
57	MG	1A	3468	1/1	0.90	0.08	40,40,40,40	0
57	MG	1x	107	1/1	0.90	0.23	63,63,63,63	0
57	MG	2a	1723	1/1	0.90	0.17	59,59,59,59	0
57	MG	1A	3270	1/1	0.90	0.20	59,59,59,59	0
57	MG	2A	3725	1/1	0.90	0.20	50,50,50,50	0
57	MG	2A	3450	1/1	0.90	0.15	64,64,64,64	0
57	MG	2A	3454	1/1	0.90	0.21	51,51,51,51	0
57	MG	2A	3250	1/1	0.90	0.20	65,65,65,65	0
57	MG	2A	3253	1/1	0.90	0.15	60,60,60,60	0
57	MG	2A	3254	1/1	0.90	0.16	56,56,56,56	0
57	MG	1A	3819	1/1	0.90	0.08	18,18,18,18	0
57	MG	2a	1748	1/1	0.90	0.10	63,63,63,63	0
57	MG	1A	3976	1/1	0.90	0.08	38,38,38,38	0
57	MG	1A	3353	1/1	0.90	0.29	62,62,62,62	0
57	MG	2a	1764	1/1	0.90	0.17	49,49,49,49	0
57	MG	2A	3263	1/1	0.90	0.17	55,55,55,55	0
57	MG	1A	3493	1/1	0.90	0.12	64,64,64,64	0
57	MG	2A	3483	1/1	0.90	0.11	42,42,42,42	0
57	MG	1a	1671	1/1	0.90	0.28	66,66,66,66	0
57	MG	1A	3002	1/1	0.90	0.17	53,53,53,53	0
57	MG	2A	3499	1/1	0.90	0.16	46,46,46,46	0
57	MG	2a	1778	1/1	0.90	0.10	60,60,60,60	0
57	MG	2A	3018	1/1	0.90	0.11	41,41,41,41	0
57	MG	2A	3023	1/1	0.90	0.21	54,54,54,54	0
57	MG	2A	3763	1/1	0.90	0.10	51,51,51,51	0
57	MG	1A	3721	1/1	0.90	0.12	40,40,40,40	0
57	MG	1A	3722	1/1	0.90	0.09	14,14,14,14	0
57	MG	2A	3036	1/1	0.90	0.29	57,57,57,57	0
57	MG	1a	1684	1/1	0.90	0.31	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	3040	1/1	0.90	0.14	46,46,46,46	0
57	MG	2A	3048	1/1	0.90	0.20	60,60,60,60	0
57	MG	2A	3782	1/1	0.90	0.08	54,54,54,54	0
57	MG	2a	1798	1/1	0.90	0.28	61,61,61,61	0
57	MG	2a	1799	1/1	0.90	0.13	63,63,63,63	0
57	MG	2A	3055	1/1	0.90	0.21	70,70,70,70	0
57	MG	2A	3786	1/1	0.90	0.12	55,55,55,55	0
57	MG	2A	3530	1/1	0.90	0.26	54,54,54,54	0
57	MG	2a	1803	1/1	0.90	0.14	69,69,69,69	0
57	MG	2A	3284	1/1	0.90	0.14	58,58,58,58	0
57	MG	1B	226	1/1	0.90	0.11	41,41,41,41	0
57	MG	1A	3723	1/1	0.90	0.09	38,38,38,38	0
57	MG	1a	1697	1/1	0.90	0.09	56,56,56,56	0
57	MG	1A	3283	1/1	0.90	0.19	49,49,49,49	0
57	MG	1A	3289	1/1	0.90	0.15	53,53,53,53	0
57	MG	2A	3080	1/1	0.90	0.15	58,58,58,58	0
57	MG	1A	3194	1/1	0.90	0.14	49,49,49,49	0
57	MG	1A	3122	1/1	0.90	0.12	33,33,33,33	0
57	MG	2A	3820	1/1	0.90	0.10	60,60,60,60	0
57	MG	2A	3303	1/1	0.90	0.17	58,58,58,58	0
57	MG	2A	3823	1/1	0.90	0.17	57,57,57,57	0
57	MG	1A	3873	1/1	0.90	0.17	57,57,57,57	0
57	MG	1A	3645	1/1	0.90	0.24	59,59,59,59	0
57	MG	1a	1719	1/1	0.90	0.19	55,55,55,55	0
57	MG	1A	3647	1/1	0.90	0.09	39,39,39,39	0
57	MG	1A	3439	1/1	0.90	0.25	66,66,66,66	0
57	MG	1A	3652	1/1	0.90	0.13	33,33,33,33	0
57	MG	1A	3311	1/1	0.90	0.17	41,41,41,41	0
57	MG	2A	3318	1/1	0.90	0.14	64,64,64,64	0
57	MG	1A	3906	1/1	0.90	0.09	24,24,24,24	0
57	MG	1F	311	1/1	0.90	0.12	56,56,56,56	0
57	MG	2B	210	1/1	0.90	0.27	66,66,66,66	0
57	MG	2A	3581	1/1	0.90	0.10	43,43,43,43	0
57	MG	2A	3128	1/1	0.90	0.18	59,59,59,59	0
57	MG	2A	3827	1/1	0.91	0.10	63,63,63,63	0
57	MG	13	104	1/1	0.91	0.09	45,45,45,45	0
57	MG	1A	4017	1/1	0.91	0.13	63,63,63,63	0
57	MG	2A	3529	1/1	0.91	0.12	51,51,51,51	0
57	MG	1A	4019	1/1	0.91	0.08	52,52,52,52	0
57	MG	2A	3261	1/1	0.91	0.21	54,54,54,54	0
57	MG	16	101	1/1	0.91	0.09	54,54,54,54	0
57	MG	1A	3496	1/1	0.91	0.22	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	2A	3539	1/1	0.91	0.14	59,59,59,59	0
57	MG	1A	3765	1/1	0.91	0.09	48,48,48,48	0
57	MG	1A	3883	1/1	0.91	0.09	29,29,29,29	0
57	MG	1A	3429	1/1	0.91	0.26	38,38,38,38	0
57	MG	2A	3269	1/1	0.91	0.18	58,58,58,58	0
57	MG	2A	3547	1/1	0.91	0.10	51,51,51,51	0
57	MG	2A	3549	1/1	0.91	0.17	57,57,57,57	0
57	MG	1A	3501	1/1	0.91	0.24	44,44,44,44	0
57	MG	1A	3777	1/1	0.91	0.14	56,56,56,56	0
57	MG	1A	3900	1/1	0.91	0.10	42,42,42,42	0
57	MG	2A	3556	1/1	0.91	0.11	42,42,42,42	0
57	MG	1A	3905	1/1	0.91	0.10	24,24,24,24	0
57	MG	1a	1621	1/1	0.91	0.08	40,40,40,40	0
57	MG	1x	113	1/1	0.91	0.12	55,55,55,55	0
57	MG	2A	3002	1/1	0.91	0.17	49,49,49,49	0
57	MG	2A	3281	1/1	0.91	0.13	58,58,58,58	0
57	MG	1a	1625	1/1	0.91	0.21	60,60,60,60	0
57	MG	1A	3302	1/1	0.91	0.16	47,47,47,47	0
57	MG	1A	3237	1/1	0.91	0.11	44,44,44,44	0
57	MG	1A	3693	1/1	0.91	0.08	42,42,42,42	0
57	MG	1A	3239	1/1	0.91	0.20	66,66,66,66	0
57	MG	1A	3794	1/1	0.91	0.26	58,58,58,58	0
57	MG	1A	4051	1/1	0.91	0.10	47,47,47,47	0
57	MG	25	104	1/1	0.91	0.20	66,66,66,66	0
57	MG	27	101	1/1	0.91	0.13	53,53,53,53	0
57	MG	2A	3035	1/1	0.91	0.25	63,63,63,63	0
57	MG	1A	3515	1/1	0.91	0.13	56,56,56,56	0
57	MG	2A	3037	1/1	0.91	0.15	58,58,58,58	0
57	MG	1A	3914	1/1	0.91	0.13	50,50,50,50	0
57	MG	1A	3241	1/1	0.91	0.10	43,43,43,43	0
57	MG	1a	1653	1/1	0.91	0.11	60,60,60,60	0
57	MG	2A	3051	1/1	0.91	0.20	62,62,62,62	0
57	MG	2A	3310	1/1	0.91	0.21	63,63,63,63	0
57	MG	1A	3797	1/1	0.91	0.09	54,54,54,54	0
57	MG	1A	3918	1/1	0.91	0.12	52,52,52,52	0
57	MG	1a	1657	1/1	0.91	0.28	54,54,54,54	0
57	MG	2a	1613	1/1	0.91	0.17	55,55,55,55	0
57	MG	2A	3607	1/1	0.91	0.12	55,55,55,55	0
57	MG	1A	3921	1/1	0.91	0.06	39,39,39,39	0
57	MG	2A	3060	1/1	0.91	0.08	40,40,40,40	0
57	MG	1A	3527	1/1	0.91	0.27	49,49,49,49	0
57	MG	1A	4079	1/1	0.91	0.22	53,53,53,53	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	3632	1/1	0.91	0.12	31,31,31,31	0
57	MG	1a	1667	1/1	0.91	0.19	66,66,66,66	0
57	MG	1A	3801	1/1	0.91	0.12	60,60,60,60	0
57	MG	2A	3087	1/1	0.91	0.12	38,38,38,38	0
57	MG	1A	3058	1/1	0.91	0.10	43,43,43,43	0
57	MG	1A	3712	1/1	0.91	0.14	42,42,42,42	0
57	MG	1A	3805	1/1	0.91	0.17	51,51,51,51	0
57	MG	1A	3637	1/1	0.91	0.05	18,18,18,18	0
57	MG	1a	1681	1/1	0.91	0.10	58,58,58,58	0
57	MG	2a	1637	1/1	0.91	0.17	53,53,53,53	0
57	MG	2a	1638	1/1	0.91	0.18	52,52,52,52	0
57	MG	1A	3715	1/1	0.91	0.09	35,35,35,35	0
57	MG	2A	3341	1/1	0.91	0.29	50,50,50,50	0
57	MG	2A	3637	1/1	0.91	0.16	56,56,56,56	0
57	MG	1A	3642	1/1	0.91	0.14	46,46,46,46	0
57	MG	2a	1647	1/1	0.91	0.18	64,64,64,64	0
57	MG	2a	1649	1/1	0.91	0.18	54,54,54,54	0
57	MG	1A	3005	1/1	0.91	0.12	43,43,43,43	0
57	MG	2A	3346	1/1	0.91	0.23	67,67,67,67	0
57	MG	2A	3110	1/1	0.91	0.24	58,58,58,58	0
57	MG	2A	3348	1/1	0.91	0.12	54,54,54,54	0
57	MG	2A	3116	1/1	0.91	0.20	53,53,53,53	0
57	MG	1A	4111	1/1	0.91	0.17	42,42,42,42	0
57	MG	2a	1675	1/1	0.91	0.31	56,56,56,56	0
57	MG	2A	3651	1/1	0.91	0.14	48,48,48,48	0
57	MG	2A	3353	1/1	0.91	0.12	55,55,55,55	0
57	MG	2A	3125	1/1	0.91	0.20	48,48,48,48	0
57	MG	2A	3655	1/1	0.91	0.10	48,48,48,48	0
57	MG	1A	3083	1/1	0.91	0.12	51,51,51,51	0
57	MG	2A	3130	1/1	0.91	0.17	54,54,54,54	0
57	MG	1A	3951	1/1	0.91	0.10	22,22,22,22	0
57	MG	2A	3361	1/1	0.91	0.21	61,61,61,61	0
57	MG	2A	3362	1/1	0.91	0.11	56,56,56,56	0
57	MG	2a	1691	1/1	0.91	0.10	58,58,58,58	0
57	MG	1A	4116	1/1	0.91	0.10	48,48,48,48	0
57	MG	1A	3812	1/1	0.91	0.15	50,50,50,50	0
57	MG	1A	3281	1/1	0.91	0.12	54,54,54,54	0
57	MG	1B	212	1/1	0.91	0.30	59,59,59,59	0
57	MG	1A	3126	1/1	0.91	0.12	50,50,50,50	0
57	MG	1A	3223	1/1	0.91	0.20	51,51,51,51	0
57	MG	2A	3675	1/1	0.91	0.08	60,60,60,60	0
57	MG	2A	3676	1/1	0.91	0.15	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	1B	221	1/1	0.91	0.11	52,52,52,52	0
57	MG	1A	3284	1/1	0.91	0.27	55,55,55,55	0
57	MG	2a	1713	1/1	0.91	0.31	53,53,53,53	0
57	MG	1B	224	1/1	0.91	0.12	53,53,53,53	0
57	MG	2a	1718	1/1	0.91	0.36	57,57,57,57	0
57	MG	1A	3566	1/1	0.91	0.16	43,43,43,43	0
57	MG	1B	227	1/1	0.91	0.08	37,37,37,37	0
57	MG	1A	3828	1/1	0.91	0.08	40,40,40,40	0
57	MG	2A	3178	1/1	0.91	0.10	64,64,64,64	0
57	MG	1A	3659	1/1	0.91	0.09	38,38,38,38	0
57	MG	1A	3970	1/1	0.91	0.06	27,27,27,27	0
57	MG	1A	3350	1/1	0.91	0.12	64,64,64,64	0
57	MG	1a	1742	1/1	0.91	0.13	53,53,53,53	0
57	MG	2A	3392	1/1	0.91	0.13	47,47,47,47	0
57	MG	1a	1746	1/1	0.91	0.10	64,64,64,64	0
57	MG	2a	1736	1/1	0.91	0.11	56,56,56,56	0
57	MG	2A	3394	1/1	0.91	0.13	47,47,47,47	0
57	MG	2A	3187	1/1	0.91	0.18	59,59,59,59	0
57	MG	2a	1749	1/1	0.91	0.12	64,64,64,64	0
57	MG	1B	234	1/1	0.91	0.13	66,66,66,66	0
57	MG	1A	3975	1/1	0.91	0.08	43,43,43,43	0
57	MG	1A	3412	1/1	0.91	0.14	44,44,44,44	0
57	MG	1a	1765	1/1	0.91	0.12	67,67,67,67	0
57	MG	1A	3979	1/1	0.91	0.12	43,43,43,43	0
57	MG	1a	1768	1/1	0.91	0.09	72,72,72,72	0
57	MG	1a	1776	1/1	0.91	0.31	48,48,48,48	0
57	MG	1A	3842	1/1	0.91	0.16	30,30,30,30	0
57	MG	1A	3982	1/1	0.91	0.08	55,55,55,55	0
57	MG	2A	3735	1/1	0.91	0.11	63,63,63,63	0
57	MG	1A	3986	1/1	0.91	0.09	57,57,57,57	0
57	MG	2A	3740	1/1	0.91	0.07	44,44,44,44	0
57	MG	1A	3844	1/1	0.91	0.08	27,27,27,27	0
57	MG	2A	3204	1/1	0.91	0.15	44,44,44,44	0
57	MG	2A	3205	1/1	0.91	0.12	47,47,47,47	0
57	MG	2A	3745	1/1	0.91	0.08	34,34,34,34	0
57	MG	1A	3845	1/1	0.91	0.06	35,35,35,35	0
57	MG	1A	3846	1/1	0.91	0.10	38,38,38,38	0
57	MG	2a	1791	1/1	0.91	0.26	56,56,56,56	0
57	MG	2A	3430	1/1	0.91	0.14	58,58,58,58	0
57	MG	1A	3158	1/1	0.91	0.10	38,38,38,38	0
57	MG	2A	3759	1/1	0.91	0.08	55,55,55,55	0
57	MG	2A	3760	1/1	0.91	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	1A	3488	1/1	0.91	0.10	42,42,42,42	0
57	MG	1A	3743	1/1	0.91	0.11	25,25,25,25	0
57	MG	2A	3214	1/1	0.91	0.14	53,53,53,53	0
57	MG	1A	3364	1/1	0.91	0.10	66,66,66,66	0
57	MG	2A	3457	1/1	0.91	0.14	60,60,60,60	0
57	MG	2A	3220	1/1	0.91	0.14	49,49,49,49	0
57	MG	2A	3773	1/1	0.91	0.09	25,25,25,25	0
57	MG	2a	1809	1/1	0.91	0.23	68,68,68,68	0
57	MG	1O	205	1/1	0.91	0.11	45,45,45,45	0
57	MG	2A	3224	1/1	0.91	0.15	43,43,43,43	0
57	MG	1A	3856	1/1	0.91	0.12	20,20,20,20	0
57	MG	1Q	204	1/1	0.91	0.14	64,64,64,64	0
57	MG	1R	205	1/1	0.91	0.12	43,43,43,43	0
57	MG	1S	202	1/1	0.91	0.11	49,49,49,49	0
57	MG	1A	3596	1/1	0.91	0.10	21,21,21,21	0
57	MG	2a	1821	1/1	0.91	0.17	58,58,58,58	0
57	MG	2a	1822	1/1	0.91	0.12	61,61,61,61	0
57	MG	2a	1823	1/1	0.91	0.14	48,48,48,48	0
57	MG	1A	3864	1/1	0.91	0.09	42,42,42,42	0
57	MG	1A	3868	1/1	0.91	0.12	42,42,42,42	0
57	MG	2a	1826	1/1	0.91	0.09	62,62,62,62	0
57	MG	2A	3239	1/1	0.91	0.15	60,60,60,60	0
57	MG	2A	3498	1/1	0.91	0.08	34,34,34,34	0
57	MG	1V	204	1/1	0.91	0.19	49,49,49,49	0
57	MG	1A	3870	1/1	0.91	0.17	52,52,52,52	0
57	MG	2A	3247	1/1	0.91	0.11	57,57,57,57	0
57	MG	1A	3675	1/1	0.91	0.20	53,53,53,53	0
57	MG	2A	3511	1/1	0.91	0.09	38,38,38,38	0
57	MG	1A	3295	1/1	0.91	0.13	44,44,44,44	0
57	MG	2w	101	1/1	0.91	0.19	61,61,61,61	0
57	MG	2A	3251	1/1	0.91	0.13	50,50,50,50	0
57	MG	10	103	1/1	0.91	0.11	42,42,42,42	0
57	MG	2A	3824	1/1	0.91	0.17	59,59,59,59	0
57	MG	2x	101	1/1	0.91	0.20	59,59,59,59	0
57	MG	1A	3876	1/1	0.91	0.15	27,27,27,27	0
57	MG	2A	3826	1/1	0.91	0.14	67,67,67,67	0
57	MG	1A	3772	1/1	0.92	0.13	49,49,49,49	0
57	MG	1A	3656	1/1	0.92	0.08	52,52,52,52	0
57	MG	1A	3776	1/1	0.92	0.10	59,59,59,59	0
57	MG	2A	3512	1/1	0.92	0.13	64,64,64,64	0
57	MG	1x	106	1/1	0.92	0.20	62,62,62,62	0
57	MG	1A	3529	1/1	0.92	0.12	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	2A	3833	1/1	0.92	0.08	49,49,49,49	0
57	MG	1A	3778	1/1	0.92	0.15	58,58,58,58	0
57	MG	2A	3837	1/1	0.92	0.20	56,56,56,56	0
57	MG	1A	4049	1/1	0.92	0.23	67,67,67,67	0
57	MG	1A	3546	1/1	0.92	0.13	44,44,44,44	0
57	MG	2A	3522	1/1	0.92	0.26	58,58,58,58	0
57	MG	1A	3912	1/1	0.92	0.09	67,67,67,67	0
57	MG	2A	3524	1/1	0.92	0.14	53,53,53,53	0
57	MG	1A	3663	1/1	0.92	0.24	53,53,53,53	0
57	MG	2A	3001	1/1	0.92	0.12	54,54,54,54	0
57	MG	2B	205	1/1	0.92	0.12	61,61,61,61	0
57	MG	1A	3276	1/1	0.92	0.32	50,50,50,50	0
57	MG	1A	4056	1/1	0.92	0.10	45,45,45,45	0
57	MG	1a	1634	1/1	0.92	0.20	60,60,60,60	0
57	MG	1a	1635	1/1	0.92	0.26	56,56,56,56	0
57	MG	2B	215	1/1	0.92	0.13	63,63,63,63	0
57	MG	2A	3272	1/1	0.92	0.23	56,56,56,56	0
57	MG	1A	3280	1/1	0.92	0.34	53,53,53,53	0
57	MG	1A	4058	1/1	0.92	0.11	43,43,43,43	0
57	MG	1A	3370	1/1	0.92	0.12	58,58,58,58	0
57	MG	2F	305	1/1	0.92	0.11	47,47,47,47	0
57	MG	2A	3027	1/1	0.92	0.15	49,49,49,49	0
57	MG	1A	3308	1/1	0.92	0.10	54,54,54,54	0
57	MG	2G	201	1/1	0.92	0.14	58,58,58,58	0
57	MG	2N	201	1/1	0.92	0.14	64,64,64,64	0
57	MG	1A	4072	1/1	0.92	0.12	34,34,34,34	0
57	MG	1A	3560	1/1	0.92	0.18	58,58,58,58	0
57	MG	2A	3283	1/1	0.92	0.17	53,53,53,53	0
57	MG	1A	3674	1/1	0.92	0.10	51,51,51,51	0
57	MG	2A	3038	1/1	0.92	0.10	48,48,48,48	0
57	MG	2A	3286	1/1	0.92	0.19	64,64,64,64	0
57	MG	2A	3559	1/1	0.92	0.17	56,56,56,56	0
57	MG	2V	202	1/1	0.92	0.13	52,52,52,52	0
57	MG	1A	3376	1/1	0.92	0.18	43,43,43,43	0
57	MG	2A	3289	1/1	0.92	0.22	65,65,65,65	0
57	MG	20	101	1/1	0.92	0.21	57,57,57,57	0
57	MG	1A	3085	1/1	0.92	0.11	51,51,51,51	0
57	MG	2A	3566	1/1	0.92	0.15	42,42,42,42	0
57	MG	25	102	1/1	0.92	0.14	46,46,46,46	0
57	MG	2A	3046	1/1	0.92	0.22	66,66,66,66	0
57	MG	1A	3119	1/1	0.92	0.17	47,47,47,47	0
57	MG	2A	3295	1/1	0.92	0.10	53,53,53,53	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	4084	1/1	0.92	0.11	45,45,45,45	0
57	MG	1A	3928	1/1	0.92	0.09	23,23,23,23	0
57	MG	1A	3929	1/1	0.92	0.10	44,44,44,44	0
57	MG	2A	3302	1/1	0.92	0.11	57,57,57,57	0
57	MG	1A	3380	1/1	0.92	0.09	45,45,45,45	0
57	MG	1A	3934	1/1	0.92	0.17	55,55,55,55	0
57	MG	2A	3585	1/1	0.92	0.10	58,58,58,58	0
57	MG	1A	4097	1/1	0.92	0.15	57,57,57,57	0
57	MG	1A	3444	1/1	0.92	0.12	45,45,45,45	0
57	MG	2A	3066	1/1	0.92	0.17	68,68,68,68	0
57	MG	1A	3937	1/1	0.92	0.07	62,62,62,62	0
57	MG	1a	1672	1/1	0.92	0.28	57,57,57,57	0
57	MG	1a	1675	1/1	0.92	0.18	62,62,62,62	0
57	MG	1A	3313	1/1	0.92	0.22	60,60,60,60	0
57	MG	2A	3086	1/1	0.92	0.12	42,42,42,42	0
57	MG	1A	4108	1/1	0.92	0.09	53,53,53,53	0
57	MG	2A	3605	1/1	0.92	0.12	52,52,52,52	0
57	MG	2A	3606	1/1	0.92	0.10	45,45,45,45	0
57	MG	1A	3385	1/1	0.92	0.07	44,44,44,44	0
57	MG	2A	3609	1/1	0.92	0.11	47,47,47,47	0
57	MG	1A	3575	1/1	0.92	0.10	48,48,48,48	0
57	MG	1A	3945	1/1	0.92	0.12	57,57,57,57	0
57	MG	1a	1687	1/1	0.92	0.14	47,47,47,47	0
57	MG	1A	3578	1/1	0.92	0.10	43,43,43,43	0
57	MG	1a	1690	1/1	0.92	0.29	57,57,57,57	0
57	MG	1A	3246	1/1	0.92	0.15	37,37,37,37	0
57	MG	2a	1636	1/1	0.92	0.15	56,56,56,56	0
57	MG	1a	1695	1/1	0.92	0.14	49,49,49,49	0
57	MG	2A	3107	1/1	0.92	0.18	62,62,62,62	0
57	MG	2a	1639	1/1	0.92	0.20	63,63,63,63	0
57	MG	2A	3625	1/1	0.92	0.10	47,47,47,47	0
57	MG	1A	3588	1/1	0.92	0.11	49,49,49,49	0
57	MG	2A	3336	1/1	0.92	0.17	48,48,48,48	0
57	MG	2A	3111	1/1	0.92	0.22	63,63,63,63	0
57	MG	2A	3340	1/1	0.92	0.18	58,58,58,58	0
57	MG	1A	3322	1/1	0.92	0.15	66,66,66,66	0
57	MG	1A	3954	1/1	0.92	0.20	47,47,47,47	0
57	MG	2A	3344	1/1	0.92	0.12	65,65,65,65	0
57	MG	2A	3120	1/1	0.92	0.13	61,61,61,61	0
57	MG	1A	3705	1/1	0.92	0.10	19,19,19,19	0
57	MG	1A	3456	1/1	0.92	0.11	44,44,44,44	0
57	MG	2a	1671	1/1	0.92	0.21	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	1672	1/1	0.92	0.26	57,57,57,57	0
57	MG	1A	3710	1/1	0.92	0.08	57,57,57,57	0
57	MG	2A	3132	1/1	0.92	0.26	53,53,53,53	0
57	MG	2a	1676	1/1	0.92	0.08	66,66,66,66	0
57	MG	1A	3597	1/1	0.92	0.10	54,54,54,54	0
57	MG	2A	3647	1/1	0.92	0.13	30,30,30,30	0
57	MG	1a	1715	1/1	0.92	0.07	46,46,46,46	0
57	MG	2A	3138	1/1	0.92	0.17	45,45,45,45	0
57	MG	2A	3141	1/1	0.92	0.16	59,59,59,59	0
57	MG	2A	3149	1/1	0.92	0.15	63,63,63,63	0
57	MG	1A	3225	1/1	0.92	0.15	50,50,50,50	0
57	MG	1a	1720	1/1	0.92	0.08	54,54,54,54	0
57	MG	1A	3827	1/1	0.92	0.12	53,53,53,53	0
57	MG	2A	3657	1/1	0.92	0.12	43,43,43,43	0
57	MG	2a	1692	1/1	0.92	0.12	58,58,58,58	0
57	MG	1a	1724	1/1	0.92	0.10	50,50,50,50	0
57	MG	2a	1696	1/1	0.92	0.20	57,57,57,57	0
57	MG	2A	3365	1/1	0.92	0.20	46,46,46,46	0
57	MG	1A	3464	1/1	0.92	0.23	54,54,54,54	0
57	MG	1A	3714	1/1	0.92	0.10	52,52,52,52	0
57	MG	2a	1700	1/1	0.92	0.33	62,62,62,62	0
57	MG	1A	3286	1/1	0.92	0.36	64,64,64,64	0
57	MG	2A	3369	1/1	0.92	0.15	35,35,35,35	0
57	MG	1a	1732	1/1	0.92	0.14	63,63,63,63	0
57	MG	1A	3472	1/1	0.92	0.11	61,61,61,61	0
57	MG	1B	233	1/1	0.92	0.10	45,45,45,45	0
57	MG	1A	3474	1/1	0.92	0.10	48,48,48,48	0
57	MG	1A	3619	1/1	0.92	0.13	50,50,50,50	0
57	MG	1A	3720	1/1	0.92	0.11	44,44,44,44	0
57	MG	2a	1717	1/1	0.92	0.19	49,49,49,49	0
57	MG	2A	3380	1/1	0.92	0.26	53,53,53,53	0
57	MG	2a	1719	1/1	0.92	0.22	62,62,62,62	0
57	MG	1A	3622	1/1	0.92	0.07	25,25,25,25	0
57	MG	1A	3121	1/1	0.92	0.14	63,63,63,63	0
57	MG	2A	3384	1/1	0.92	0.12	65,65,65,65	0
57	MG	1a	1747	1/1	0.92	0.10	40,40,40,40	0
57	MG	2A	3183	1/1	0.92	0.14	59,59,59,59	0
57	MG	1A	3625	1/1	0.92	0.06	18,18,18,18	0
57	MG	1A	3481	1/1	0.92	0.16	56,56,56,56	0
57	MG	1a	1752	1/1	0.92	0.13	50,50,50,50	0
57	MG	2A	3693	1/1	0.92	0.08	48,48,48,48	0
57	MG	1A	3728	1/1	0.92	0.08	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	3292	1/1	0.92	0.10	57,57,57,57	0
57	MG	1E	315	1/1	0.92	0.09	34,34,34,34	0
57	MG	2a	1747	1/1	0.92	0.11	65,65,65,65	0
57	MG	2A	3704	1/1	0.92	0.12	57,57,57,57	0
57	MG	1A	3857	1/1	0.92	0.08	30,30,30,30	0
57	MG	2a	1753	1/1	0.92	0.18	62,62,62,62	0
57	MG	2A	3716	1/1	0.92	0.09	56,56,56,56	0
57	MG	2A	3397	1/1	0.92	0.24	36,36,36,36	0
57	MG	2a	1762	1/1	0.92	0.18	46,46,46,46	0
57	MG	2A	3719	1/1	0.92	0.07	35,35,35,35	0
57	MG	1A	3336	1/1	0.92	0.14	50,50,50,50	0
57	MG	1A	3861	1/1	0.92	0.13	29,29,29,29	0
57	MG	2a	1767	1/1	0.92	0.12	57,57,57,57	0
57	MG	1N	201	1/1	0.92	0.15	39,39,39,39	0
57	MG	2A	3724	1/1	0.92	0.12	44,44,44,44	0
57	MG	1A	3862	1/1	0.92	0.09	48,48,48,48	0
57	MG	1A	3340	1/1	0.92	0.11	47,47,47,47	0
57	MG	2a	1775	1/1	0.92	0.23	55,55,55,55	0
57	MG	2a	1776	1/1	0.92	0.26	55,55,55,55	0
57	MG	2A	3200	1/1	0.92	0.12	64,64,64,64	0
57	MG	1O	203	1/1	0.92	0.15	52,52,52,52	0
57	MG	2A	3202	1/1	0.92	0.19	58,58,58,58	0
57	MG	1A	3269	1/1	0.92	0.21	48,48,48,48	0
57	MG	1A	3417	1/1	0.92	0.11	53,53,53,53	0
57	MG	1A	3346	1/1	0.92	0.12	40,40,40,40	0
57	MG	2A	3736	1/1	0.92	0.09	73,73,73,73	0
57	MG	2A	3421	1/1	0.92	0.20	56,56,56,56	0
57	MG	2A	3738	1/1	0.92	0.10	55,55,55,55	0
57	MG	2A	3422	1/1	0.92	0.10	58,58,58,58	0
57	MG	1A	3420	1/1	0.92	0.14	56,56,56,56	0
57	MG	2A	3426	1/1	0.92	0.09	41,41,41,41	0
57	MG	1A	4009	1/1	0.92	0.06	30,30,30,30	0
57	MG	1A	4010	1/1	0.92	0.07	41,41,41,41	0
57	MG	1A	3421	1/1	0.92	0.14	40,40,40,40	0
57	MG	1A	3512	1/1	0.92	0.12	58,58,58,58	0
57	MG	2A	3435	1/1	0.92	0.09	43,43,43,43	0
57	MG	2A	3751	1/1	0.92	0.12	42,42,42,42	0
57	MG	2A	3437	1/1	0.92	0.19	54,54,54,54	0
57	MG	1A	4016	1/1	0.92	0.06	11,11,11,11	0
57	MG	1V	207	1/1	0.92	0.09	46,46,46,46	0
57	MG	1A	3756	1/1	0.92	0.11	46,46,46,46	0
57	MG	2A	3449	1/1	0.92	0.20	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	4018	1/1	0.92	0.13	53,53,53,53	0
57	MG	2A	3451	1/1	0.92	0.12	35,35,35,35	0
57	MG	2A	3452	1/1	0.92	0.13	40,40,40,40	0
57	MG	1A	3300	1/1	0.92	0.07	36,36,36,36	0
57	MG	1A	3425	1/1	0.92	0.11	54,54,54,54	0
57	MG	1A	3518	1/1	0.92	0.14	51,51,51,51	0
57	MG	2A	3231	1/1	0.92	0.12	57,57,57,57	0
57	MG	2A	3467	1/1	0.92	0.10	34,34,34,34	0
57	MG	2A	3469	1/1	0.92	0.07	33,33,33,33	0
57	MG	11	105	1/1	0.92	0.10	47,47,47,47	0
57	MG	1A	3887	1/1	0.92	0.09	48,48,48,48	0
57	MG	2A	3789	1/1	0.92	0.11	60,60,60,60	0
57	MG	2a	1828	1/1	0.92	0.15	63,63,63,63	0
57	MG	2e	201	1/1	0.92	0.07	56,56,56,56	0
57	MG	1A	3888	1/1	0.92	0.08	52,52,52,52	0
57	MG	15	105	1/1	0.92	0.16	30,30,30,30	0
57	MG	2A	3795	1/1	0.92	0.10	49,49,49,49	0
57	MG	2A	3236	1/1	0.92	0.11	67,67,67,67	0
57	MG	2A	3237	1/1	0.92	0.11	66,66,66,66	0
57	MG	1A	3206	1/1	0.92	0.15	59,59,59,59	0
57	MG	1f	202	1/1	0.92	0.09	65,65,65,65	0
57	MG	1A	4034	1/1	0.92	0.09	49,49,49,49	0
57	MG	2A	3806	1/1	0.92	0.14	65,65,65,65	0
57	MG	2w	102	1/1	0.92	0.11	74,74,74,74	0
57	MG	1A	3893	1/1	0.92	0.07	35,35,35,35	0
57	MG	18	104	1/1	0.92	0.12	45,45,45,45	0
57	MG	2A	3500	1/1	0.92	0.13	59,59,59,59	0
57	MG	2A	3815	1/1	0.92	0.09	63,63,63,63	0
57	MG	2A	3816	1/1	0.92	0.09	61,61,61,61	0
57	MG	1A	3427	1/1	0.92	0.12	44,44,44,44	0
57	MG	2A	3812	1/1	0.93	0.16	58,58,58,58	0
57	MG	1A	3471	1/1	0.93	0.08	51,51,51,51	0
57	MG	1A	3285	1/1	0.93	0.16	50,50,50,50	0
57	MG	2A	3818	1/1	0.93	0.12	72,72,72,72	0
57	MG	1A	3473	1/1	0.93	0.09	45,45,45,45	0
57	MG	2A	3506	1/1	0.93	0.13	28,28,28,28	0
57	MG	2A	3507	1/1	0.93	0.10	38,38,38,38	0
57	MG	1A	3698	1/1	0.93	0.08	47,47,47,47	0
57	MG	1A	3331	1/1	0.93	0.09	48,48,48,48	0
57	MG	1A	3133	1/1	0.93	0.08	49,49,49,49	0
57	MG	1A	4085	1/1	0.93	0.10	48,48,48,48	0
57	MG	2A	3829	1/1	0.93	0.07	53,53,53,53	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	3832	1/1	0.93	0.09	57,57,57,57	0
57	MG	1A	3601	1/1	0.93	0.13	48,48,48,48	0
57	MG	1A	3944	1/1	0.93	0.08	55,55,55,55	0
57	MG	1A	3409	1/1	0.93	0.10	39,39,39,39	0
57	MG	1A	3816	1/1	0.93	0.17	42,42,42,42	0
57	MG	2A	3013	1/1	0.93	0.18	52,52,52,52	0
57	MG	1A	4096	1/1	0.93	0.12	58,58,58,58	0
57	MG	1A	3603	1/1	0.93	0.10	45,45,45,45	0
57	MG	2A	3020	1/1	0.93	0.13	40,40,40,40	0
57	MG	1A	3950	1/1	0.93	0.13	34,34,34,34	0
57	MG	1A	4099	1/1	0.93	0.08	44,44,44,44	0
57	MG	2B	204	1/1	0.93	0.17	49,49,49,49	0
57	MG	1A	3483	1/1	0.93	0.24	34,34,34,34	0
57	MG	2B	206	1/1	0.93	0.10	50,50,50,50	0
57	MG	2B	208	1/1	0.93	0.09	71,71,71,71	0
57	MG	2A	3031	1/1	0.93	0.14	49,49,49,49	0
57	MG	2A	3274	1/1	0.93	0.21	64,64,64,64	0
57	MG	1A	3134	1/1	0.93	0.10	33,33,33,33	0
57	MG	2B	212	1/1	0.93	0.09	64,64,64,64	0
57	MG	1A	3822	1/1	0.93	0.11	47,47,47,47	0
57	MG	2B	214	1/1	0.93	0.19	54,54,54,54	0
57	MG	1A	3955	1/1	0.93	0.09	40,40,40,40	0
57	MG	1A	3490	1/1	0.93	0.10	46,46,46,46	0
57	MG	2B	218	1/1	0.93	0.26	67,67,67,67	0
57	MG	1A	3610	1/1	0.93	0.08	26,26,26,26	0
57	MG	1A	3242	1/1	0.93	0.10	53,53,53,53	0
57	MG	2E	302	1/1	0.93	0.07	51,51,51,51	0
57	MG	1A	4117	1/1	0.93	0.25	50,50,50,50	0
57	MG	2E	306	1/1	0.93	0.15	57,57,57,57	0
57	MG	2A	3550	1/1	0.93	0.08	26,26,26,26	0
57	MG	2A	3041	1/1	0.93	0.26	51,51,51,51	0
57	MG	2A	3045	1/1	0.93	0.08	50,50,50,50	0
57	MG	2A	3553	1/1	0.93	0.12	49,49,49,49	0
57	MG	1A	3204	1/1	0.93	0.10	36,36,36,36	0
57	MG	2A	3555	1/1	0.93	0.11	42,42,42,42	0
57	MG	1a	1674	1/1	0.93	0.22	44,44,44,44	0
57	MG	1A	3343	1/1	0.93	0.08	44,44,44,44	0
57	MG	2A	3052	1/1	0.93	0.14	49,49,49,49	0
57	MG	2T	201	1/1	0.93	0.07	52,52,52,52	0
57	MG	1a	1676	1/1	0.93	0.18	49,49,49,49	0
57	MG	2A	3560	1/1	0.93	0.09	33,33,33,33	0
57	MG	1a	1677	1/1	0.93	0.21	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	1B	207	1/1	0.93	0.12	50,50,50,50	0
57	MG	2W	201	1/1	0.93	0.09	50,50,50,50	0
57	MG	1A	3833	1/1	0.93	0.10	27,27,27,27	0
57	MG	1A	3345	1/1	0.93	0.07	35,35,35,35	0
57	MG	1A	3298	1/1	0.93	0.33	53,53,53,53	0
57	MG	2A	3570	1/1	0.93	0.16	54,54,54,54	0
57	MG	21	102	1/1	0.93	0.18	49,49,49,49	0
57	MG	21	103	1/1	0.93	0.11	49,49,49,49	0
57	MG	2A	3300	1/1	0.93	0.10	63,63,63,63	0
57	MG	1B	216	1/1	0.93	0.07	60,60,60,60	0
57	MG	2A	3067	1/1	0.93	0.10	41,41,41,41	0
57	MG	2A	3072	1/1	0.93	0.10	44,44,44,44	0
57	MG	2A	3074	1/1	0.93	0.19	56,56,56,56	0
57	MG	2A	3308	1/1	0.93	0.10	54,54,54,54	0
57	MG	2A	3075	1/1	0.93	0.12	48,48,48,48	0
57	MG	1A	3502	1/1	0.93	0.20	44,44,44,44	0
57	MG	1A	3503	1/1	0.93	0.25	46,46,46,46	0
57	MG	2A	3312	1/1	0.93	0.21	64,64,64,64	0
57	MG	1B	223	1/1	0.93	0.11	41,41,41,41	0
57	MG	1A	3349	1/1	0.93	0.15	35,35,35,35	0
57	MG	2A	3591	1/1	0.93	0.24	51,51,51,51	0
57	MG	2a	1608	1/1	0.93	0.32	66,66,66,66	0
57	MG	2a	1609	1/1	0.93	0.21	62,62,62,62	0
57	MG	1B	225	1/1	0.93	0.07	43,43,43,43	0
57	MG	1A	3171	1/1	0.93	0.10	42,42,42,42	0
57	MG	1a	1698	1/1	0.93	0.08	55,55,55,55	0
57	MG	2A	3322	1/1	0.93	0.16	50,50,50,50	0
57	MG	2a	1614	1/1	0.93	0.14	60,60,60,60	0
57	MG	2a	1615	1/1	0.93	0.13	69,69,69,69	0
57	MG	2A	3323	1/1	0.93	0.14	58,58,58,58	0
57	MG	1a	1700	1/1	0.93	0.18	38,38,38,38	0
57	MG	1A	3848	1/1	0.93	0.06	24,24,24,24	0
57	MG	1a	1703	1/1	0.93	0.08	44,44,44,44	0
57	MG	1a	1704	1/1	0.93	0.14	51,51,51,51	0
57	MG	1a	1705	1/1	0.93	0.12	51,51,51,51	0
57	MG	1A	3727	1/1	0.93	0.05	22,22,22,22	0
57	MG	2A	3611	1/1	0.93	0.12	60,60,60,60	0
57	MG	2A	3613	1/1	0.93	0.11	41,41,41,41	0
57	MG	2A	3098	1/1	0.93	0.12	45,45,45,45	0
57	MG	2A	3101	1/1	0.93	0.08	63,63,63,63	0
57	MG	2A	3104	1/1	0.93	0.14	49,49,49,49	0
57	MG	1A	3301	1/1	0.93	0.11	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	3175	1/1	0.93	0.09	41,41,41,41	0
57	MG	2A	3621	1/1	0.93	0.17	44,44,44,44	0
57	MG	1A	3264	1/1	0.93	0.07	37,37,37,37	0
57	MG	1A	3431	1/1	0.93	0.16	58,58,58,58	0
57	MG	2A	3115	1/1	0.93	0.08	58,58,58,58	0
57	MG	1A	3643	1/1	0.93	0.11	46,46,46,46	0
57	MG	1a	1716	1/1	0.93	0.24	61,61,61,61	0
57	MG	1A	3859	1/1	0.93	0.16	63,63,63,63	0
57	MG	2a	1645	1/1	0.93	0.07	63,63,63,63	0
57	MG	1A	3998	1/1	0.93	0.06	31,31,31,31	0
57	MG	1A	3522	1/1	0.93	0.30	41,41,41,41	0
57	MG	1A	3523	1/1	0.93	0.13	41,41,41,41	0
57	MG	1A	3736	1/1	0.93	0.08	15,15,15,15	0
57	MG	2a	1653	1/1	0.93	0.36	65,65,65,65	0
57	MG	1a	1726	1/1	0.93	0.10	52,52,52,52	0
57	MG	2A	3134	1/1	0.93	0.20	58,58,58,58	0
57	MG	1A	3865	1/1	0.93	0.09	50,50,50,50	0
57	MG	1A	3741	1/1	0.93	0.07	27,27,27,27	0
57	MG	2a	1669	1/1	0.93	0.14	58,58,58,58	0
57	MG	2a	1670	1/1	0.93	0.17	54,54,54,54	0
57	MG	1E	313	1/1	0.93	0.12	36,36,36,36	0
57	MG	2A	3144	1/1	0.93	0.12	46,46,46,46	0
57	MG	2A	3644	1/1	0.93	0.11	49,49,49,49	0
57	MG	1A	3369	1/1	0.93	0.08	40,40,40,40	0
57	MG	1A	4005	1/1	0.93	0.08	39,39,39,39	0
57	MG	1A	3433	1/1	0.93	0.12	33,33,33,33	0
57	MG	2a	1679	1/1	0.93	0.35	58,58,58,58	0
57	MG	1A	3305	1/1	0.93	0.18	51,51,51,51	0
57	MG	2A	3156	1/1	0.93	0.12	41,41,41,41	0
57	MG	1A	3755	1/1	0.93	0.15	53,53,53,53	0
57	MG	1A	3014	1/1	0.93	0.10	37,37,37,37	0
57	MG	1A	3760	1/1	0.93	0.16	29,29,29,29	0
57	MG	1A	3095	1/1	0.93	0.24	46,46,46,46	0
57	MG	1A	3762	1/1	0.93	0.09	37,37,37,37	0
57	MG	2A	3170	1/1	0.93	0.10	45,45,45,45	0
57	MG	1A	3655	1/1	0.93	0.10	26,26,26,26	0
57	MG	1A	3551	1/1	0.93	0.21	35,35,35,35	0
57	MG	1A	3657	1/1	0.93	0.13	28,28,28,28	0
57	MG	2a	1694	1/1	0.93	0.18	57,57,57,57	0
57	MG	2a	1695	1/1	0.93	0.22	52,52,52,52	0
57	MG	2A	3378	1/1	0.93	0.31	58,58,58,58	0
57	MG	2A	3669	1/1	0.93	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	3175	1/1	0.93	0.10	46,46,46,46	0
57	MG	2A	3176	1/1	0.93	0.14	52,52,52,52	0
57	MG	1R	201	1/1	0.93	0.09	43,43,43,43	0
57	MG	1A	3658	1/1	0.93	0.13	39,39,39,39	0
57	MG	2a	1703	1/1	0.93	0.30	57,57,57,57	0
57	MG	2a	1704	1/1	0.93	0.18	62,62,62,62	0
57	MG	1R	206	1/1	0.93	0.15	41,41,41,41	0
57	MG	1a	1771	1/1	0.93	0.08	51,51,51,51	0
57	MG	2A	3677	1/1	0.93	0.09	57,57,57,57	0
57	MG	1a	1775	1/1	0.93	0.20	47,47,47,47	0
57	MG	1A	3310	1/1	0.93	0.18	44,44,44,44	0
57	MG	1A	3895	1/1	0.93	0.07	38,38,38,38	0
57	MG	2A	3186	1/1	0.93	0.15	56,56,56,56	0
57	MG	1A	4028	1/1	0.93	0.11	27,27,27,27	0
57	MG	2A	3684	1/1	0.93	0.10	53,53,53,53	0
57	MG	1a	1780	1/1	0.93	0.16	58,58,58,58	0
57	MG	2a	1720	1/1	0.93	0.28	67,67,67,67	0
57	MG	2A	3686	1/1	0.93	0.10	36,36,36,36	0
57	MG	1U	203	1/1	0.93	0.12	47,47,47,47	0
57	MG	1A	3224	1/1	0.93	0.09	47,47,47,47	0
57	MG	2A	3690	1/1	0.93	0.14	60,60,60,60	0
57	MG	1A	3904	1/1	0.93	0.07	45,45,45,45	0
57	MG	2a	1726	1/1	0.93	0.15	66,66,66,66	0
57	MG	1A	3661	1/1	0.93	0.08	22,22,22,22	0
57	MG	2A	3694	1/1	0.93	0.20	57,57,57,57	0
57	MG	1W	202	1/1	0.93	0.08	44,44,44,44	0
57	MG	1A	3556	1/1	0.93	0.19	43,43,43,43	0
57	MG	2A	3697	1/1	0.93	0.10	48,48,48,48	0
57	MG	2A	3699	1/1	0.93	0.12	39,39,39,39	0
57	MG	2a	1738	1/1	0.93	0.12	63,63,63,63	0
57	MG	2a	1739	1/1	0.93	0.09	82,82,82,82	0
57	MG	2A	3406	1/1	0.93	0.23	55,55,55,55	0
57	MG	2a	1744	1/1	0.93	0.06	46,46,46,46	0
57	MG	2A	3702	1/1	0.93	0.17	58,58,58,58	0
57	MG	1A	3277	1/1	0.93	0.19	46,46,46,46	0
57	MG	1A	3779	1/1	0.93	0.07	25,25,25,25	0
57	MG	2a	1751	1/1	0.93	0.10	42,42,42,42	0
57	MG	2A	3715	1/1	0.93	0.08	32,32,32,32	0
57	MG	1A	3382	1/1	0.93	0.27	56,56,56,56	0
57	MG	1A	3450	1/1	0.93	0.15	35,35,35,35	0
57	MG	2A	3413	1/1	0.93	0.24	47,47,47,47	0
57	MG	2a	1763	1/1	0.93	0.07	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	1801	1/1	0.93	0.13	57,57,57,57	0
57	MG	1A	3113	1/1	0.93	0.18	41,41,41,41	0
57	MG	1a	1804	1/1	0.93	0.13	54,54,54,54	0
57	MG	2A	3418	1/1	0.93	0.18	51,51,51,51	0
57	MG	2a	1768	1/1	0.93	0.27	67,67,67,67	0
57	MG	2A	3419	1/1	0.93	0.23	64,64,64,64	0
57	MG	2A	3420	1/1	0.93	0.07	36,36,36,36	0
57	MG	1A	4047	1/1	0.93	0.10	42,42,42,42	0
57	MG	2A	3206	1/1	0.93	0.09	49,49,49,49	0
57	MG	2A	3424	1/1	0.93	0.07	50,50,50,50	0
57	MG	1A	3187	1/1	0.93	0.10	46,46,46,46	0
57	MG	2A	3733	1/1	0.93	0.09	68,68,68,68	0
57	MG	1A	3793	1/1	0.93	0.15	36,36,36,36	0
57	MG	1a	1808	1/1	0.93	0.28	56,56,56,56	0
57	MG	1A	3229	1/1	0.93	0.14	59,59,59,59	0
57	MG	1A	3323	1/1	0.93	0.13	39,39,39,39	0
57	MG	2a	1786	1/1	0.93	0.13	67,67,67,67	0
57	MG	1A	4052	1/1	0.93	0.09	55,55,55,55	0
57	MG	2A	3431	1/1	0.93	0.12	35,35,35,35	0
57	MG	2A	3215	1/1	0.93	0.12	43,43,43,43	0
57	MG	2A	3742	1/1	0.93	0.09	48,48,48,48	0
57	MG	2A	3436	1/1	0.93	0.10	50,50,50,50	0
57	MG	2A	3216	1/1	0.93	0.20	51,51,51,51	0
57	MG	18	101	1/1	0.93	0.29	45,45,45,45	0
57	MG	2A	3442	1/1	0.93	0.19	53,53,53,53	0
57	MG	2A	3748	1/1	0.93	0.10	32,32,32,32	0
57	MG	2A	3445	1/1	0.93	0.13	60,60,60,60	0
57	MG	1A	3570	1/1	0.93	0.10	26,26,26,26	0
57	MG	1A	4054	1/1	0.93	0.13	51,51,51,51	0
57	MG	2A	3752	1/1	0.93	0.14	45,45,45,45	0
57	MG	2A	3222	1/1	0.93	0.08	63,63,63,63	0
57	MG	1a	1821	1/1	0.93	0.15	62,62,62,62	0
57	MG	1A	3233	1/1	0.93	0.14	61,61,61,61	0
57	MG	1A	3463	1/1	0.93	0.09	44,44,44,44	0
57	MG	2A	3229	1/1	0.93	0.20	48,48,48,48	0
57	MG	1A	3326	1/1	0.93	0.12	39,39,39,39	0
57	MG	1A	3688	1/1	0.93	0.10	45,45,45,45	0
57	MG	2A	3768	1/1	0.93	0.23	67,67,67,67	0
57	MG	2a	1816	1/1	0.93	0.11	65,65,65,65	0
57	MG	2A	3769	1/1	0.93	0.11	54,54,54,54	0
57	MG	2A	3459	1/1	0.93	0.12	46,46,46,46	0
57	MG	1A	4061	1/1	0.93	0.05	26,26,26,26	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3463	1/1	0.93	0.07	42,42,42,42	0
57	MG	2A	3774	1/1	0.93	0.09	70,70,70,70	0
57	MG	2A	3464	1/1	0.93	0.10	53,53,53,53	0
57	MG	2A	3466	1/1	0.93	0.09	49,49,49,49	0
57	MG	1a	1615	1/1	0.93	0.10	54,54,54,54	0
57	MG	1t	201	1/1	0.93	0.12	51,51,51,51	0
57	MG	1A	3114	1/1	0.93	0.16	50,50,50,50	0
57	MG	2a	1830	1/1	0.93	0.12	55,55,55,55	0
57	MG	2A	3472	1/1	0.93	0.07	25,25,25,25	0
57	MG	2A	3787	1/1	0.93	0.08	59,59,59,59	0
57	MG	2A	3473	1/1	0.93	0.12	66,66,66,66	0
57	MG	1w	102	1/1	0.93	0.11	75,75,75,75	0
57	MG	2A	3792	1/1	0.93	0.19	60,60,60,60	0
57	MG	1a	1620	1/1	0.93	0.10	49,49,49,49	0
57	MG	2A	3238	1/1	0.93	0.18	52,52,52,52	0
57	MG	1A	3581	1/1	0.93	0.15	14,14,14,14	0
57	MG	1w	109	1/1	0.93	0.09	67,67,67,67	0
57	MG	2A	3798	1/1	0.93	0.21	46,46,46,46	0
57	MG	2A	3243	1/1	0.93	0.12	50,50,50,50	0
57	MG	2A	3485	1/1	0.93	0.08	43,43,43,43	0
57	MG	2A	3486	1/1	0.93	0.11	45,45,45,45	0
57	MG	2A	3488	1/1	0.93	0.09	34,34,34,34	0
57	MG	2A	3244	1/1	0.93	0.12	59,59,59,59	0
57	MG	2x	103	1/1	0.93	0.13	62,62,62,62	0
57	MG	1a	1623	1/1	0.93	0.24	54,54,54,54	0
57	MG	2x	107	1/1	0.93	0.12	38,38,38,38	0
57	MG	1A	3804	1/1	0.93	0.05	29,29,29,29	0
57	MG	1A	3268	1/1	0.94	0.07	34,34,34,34	0
57	MG	1A	3852	1/1	0.94	0.12	50,50,50,50	0
57	MG	2U	201	1/1	0.94	0.21	43,43,43,43	0
57	MG	1B	201	1/1	0.94	0.18	51,51,51,51	0
57	MG	1A	3854	1/1	0.94	0.13	26,26,26,26	0
57	MG	2A	3203	1/1	0.94	0.13	41,41,41,41	0
57	MG	1x	104	1/1	0.94	0.19	58,58,58,58	0
57	MG	1A	3373	1/1	0.94	0.09	46,46,46,46	0
57	MG	2A	3635	1/1	0.94	0.09	53,53,53,53	0
57	MG	1a	1658	1/1	0.94	0.29	60,60,60,60	0
57	MG	1B	209	1/1	0.94	0.10	43,43,43,43	0
57	MG	1a	1660	1/1	0.94	0.24	54,54,54,54	0
57	MG	1A	3064	1/1	0.94	0.12	51,51,51,51	0
57	MG	1A	3745	1/1	0.94	0.08	42,42,42,42	0
57	MG	2A	3211	1/1	0.94	0.27	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	1665	1/1	0.94	0.13	41,41,41,41	0
57	MG	1A	3074	1/1	0.94	0.22	40,40,40,40	0
57	MG	27	102	1/1	0.94	0.12	53,53,53,53	0
57	MG	2A	3645	1/1	0.94	0.10	52,52,52,52	0
57	MG	2A	3400	1/1	0.94	0.25	50,50,50,50	0
57	MG	1A	3753	1/1	0.94	0.04	14,14,14,14	0
57	MG	2A	3003	1/1	0.94	0.16	55,55,55,55	0
57	MG	1B	219	1/1	0.94	0.21	41,41,41,41	0
57	MG	1A	3377	1/1	0.94	0.12	42,42,42,42	0
57	MG	2A	3012	1/1	0.94	0.18	45,45,45,45	0
57	MG	1A	3534	1/1	0.94	0.23	53,53,53,53	0
57	MG	1A	3544	1/1	0.94	0.12	65,65,65,65	0
57	MG	2A	3225	1/1	0.94	0.17	56,56,56,56	0
57	MG	1A	3759	1/1	0.94	0.05	15,15,15,15	0
57	MG	2A	3019	1/1	0.94	0.12	50,50,50,50	0
57	MG	1A	3866	1/1	0.94	0.13	49,49,49,49	0
57	MG	1A	3271	1/1	0.94	0.12	49,49,49,49	0
57	MG	1A	3080	1/1	0.94	0.09	39,39,39,39	0
57	MG	1A	3212	1/1	0.94	0.11	47,47,47,47	0
57	MG	2A	3030	1/1	0.94	0.09	56,56,56,56	0
57	MG	1A	3320	1/1	0.94	0.09	59,59,59,59	0
57	MG	2A	3671	1/1	0.94	0.11	35,35,35,35	0
57	MG	2a	1620	1/1	0.94	0.16	61,61,61,61	0
57	MG	1A	3553	1/1	0.94	0.07	32,32,32,32	0
57	MG	1A	3878	1/1	0.94	0.06	33,33,33,33	0
57	MG	1A	3222	1/1	0.94	0.09	37,37,37,37	0
57	MG	1A	3167	1/1	0.94	0.11	59,59,59,59	0
57	MG	1A	3881	1/1	0.94	0.10	33,33,33,33	0
57	MG	2a	1627	1/1	0.94	0.25	47,47,47,47	0
57	MG	2A	3240	1/1	0.94	0.13	44,44,44,44	0
57	MG	1A	3558	1/1	0.94	0.24	51,51,51,51	0
57	MG	1D	303	1/1	0.94	0.16	48,48,48,48	0
57	MG	2A	3433	1/1	0.94	0.18	39,39,39,39	0
57	MG	2A	3434	1/1	0.94	0.15	42,42,42,42	0
57	MG	1D	312	1/1	0.94	0.09	49,49,49,49	0
57	MG	2A	3042	1/1	0.94	0.16	45,45,45,45	0
57	MG	1A	3169	1/1	0.94	0.11	40,40,40,40	0
57	MG	2A	3438	1/1	0.94	0.18	46,46,46,46	0
57	MG	2A	3687	1/1	0.94	0.16	53,53,53,53	0
57	MG	1D	314	1/1	0.94	0.23	34,34,34,34	0
57	MG	1A	3387	1/1	0.94	0.14	48,48,48,48	0
57	MG	1A	3023	1/1	0.94	0.13	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	2a	1644	1/1	0.94	0.19	63,63,63,63	0
57	MG	2A	3252	1/1	0.94	0.13	58,58,58,58	0
57	MG	2A	3692	1/1	0.94	0.13	54,54,54,54	0
57	MG	2A	3447	1/1	0.94	0.09	45,45,45,45	0
57	MG	2a	1648	1/1	0.94	0.11	68,68,68,68	0
57	MG	1A	3024	1/1	0.94	0.17	34,34,34,34	0
57	MG	2A	3053	1/1	0.94	0.15	50,50,50,50	0
57	MG	2A	3054	1/1	0.94	0.10	42,42,42,42	0
57	MG	1A	3459	1/1	0.94	0.17	50,50,50,50	0
57	MG	2a	1655	1/1	0.94	0.16	47,47,47,47	0
57	MG	2a	1658	1/1	0.94	0.26	56,56,56,56	0
57	MG	2A	3257	1/1	0.94	0.08	47,47,47,47	0
57	MG	2A	3258	1/1	0.94	0.13	51,51,51,51	0
57	MG	2a	1662	1/1	0.94	0.21	58,58,58,58	0
57	MG	2a	1663	1/1	0.94	0.09	55,55,55,55	0
57	MG	2A	3701	1/1	0.94	0.14	53,53,53,53	0
57	MG	2a	1667	1/1	0.94	0.23	52,52,52,52	0
57	MG	2a	1668	1/1	0.94	0.22	52,52,52,52	0
57	MG	2A	3259	1/1	0.94	0.21	64,64,64,64	0
57	MG	1A	3890	1/1	0.94	0.09	37,37,37,37	0
57	MG	2A	3712	1/1	0.94	0.08	47,47,47,47	0
57	MG	1A	3328	1/1	0.94	0.12	51,51,51,51	0
57	MG	2A	3714	1/1	0.94	0.08	59,59,59,59	0
57	MG	2A	3460	1/1	0.94	0.08	54,54,54,54	0
57	MG	2A	3262	1/1	0.94	0.12	57,57,57,57	0
57	MG	2A	3058	1/1	0.94	0.21	51,51,51,51	0
57	MG	1A	4020	1/1	0.94	0.14	54,54,54,54	0
57	MG	2a	1680	1/1	0.94	0.19	54,54,54,54	0
57	MG	2a	1681	1/1	0.94	0.18	64,64,64,64	0
57	MG	1F	308	1/1	0.94	0.08	38,38,38,38	0
57	MG	1F	310	1/1	0.94	0.15	28,28,28,28	0
57	MG	1A	3396	1/1	0.94	0.08	42,42,42,42	0
57	MG	2A	3470	1/1	0.94	0.14	57,57,57,57	0
57	MG	1G	202	1/1	0.94	0.12	51,51,51,51	0
57	MG	1A	3465	1/1	0.94	0.21	46,46,46,46	0
57	MG	1A	3787	1/1	0.94	0.07	31,31,31,31	0
57	MG	1I	201	1/1	0.94	0.07	55,55,55,55	0
57	MG	1A	3399	1/1	0.94	0.08	45,45,45,45	0
57	MG	1A	3470	1/1	0.94	0.11	54,54,54,54	0
57	MG	2A	3081	1/1	0.94	0.13	56,56,56,56	0
57	MG	1A	3001	1/1	0.94	0.15	38,38,38,38	0
57	MG	2A	3482	1/1	0.94	0.06	43,43,43,43	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	4031	1/1	0.94	0.09	15,15,15,15	0
57	MG	1O	204	1/1	0.94	0.20	63,63,63,63	0
57	MG	1A	3402	1/1	0.94	0.11	45,45,45,45	0
57	MG	1a	1730	1/1	0.94	0.15	56,56,56,56	0
57	MG	2A	3489	1/1	0.94	0.13	47,47,47,47	0
57	MG	1A	4035	1/1	0.94	0.08	47,47,47,47	0
57	MG	2A	3494	1/1	0.94	0.13	35,35,35,35	0
57	MG	1A	4037	1/1	0.94	0.12	45,45,45,45	0
57	MG	1A	3132	1/1	0.94	0.10	41,41,41,41	0
57	MG	1A	3692	1/1	0.94	0.10	52,52,52,52	0
57	MG	2a	1707	1/1	0.94	0.16	50,50,50,50	0
57	MG	2A	3287	1/1	0.94	0.26	48,48,48,48	0
57	MG	1A	3287	1/1	0.94	0.05	32,32,32,32	0
57	MG	2a	1711	1/1	0.94	0.19	52,52,52,52	0
57	MG	1S	201	1/1	0.94	0.16	40,40,40,40	0
57	MG	1A	3587	1/1	0.94	0.12	35,35,35,35	0
57	MG	2a	1715	1/1	0.94	0.25	61,61,61,61	0
57	MG	1S	203	1/1	0.94	0.06	53,53,53,53	0
57	MG	1A	3086	1/1	0.94	0.18	36,36,36,36	0
57	MG	2A	3510	1/1	0.94	0.18	54,54,54,54	0
57	MG	1A	3915	1/1	0.94	0.06	46,46,46,46	0
57	MG	1A	3477	1/1	0.94	0.15	20,20,20,20	0
57	MG	2A	3109	1/1	0.94	0.08	42,42,42,42	0
57	MG	2A	3515	1/1	0.94	0.10	36,36,36,36	0
57	MG	2A	3764	1/1	0.94	0.07	37,37,37,37	0
57	MG	1U	205	1/1	0.94	0.14	51,51,51,51	0
57	MG	1a	1753	1/1	0.94	0.10	58,58,58,58	0
57	MG	2A	3301	1/1	0.94	0.25	52,52,52,52	0
57	MG	2A	3520	1/1	0.94	0.07	30,30,30,30	0
57	MG	2A	3112	1/1	0.94	0.29	61,61,61,61	0
57	MG	2A	3113	1/1	0.94	0.21	47,47,47,47	0
57	MG	1A	3480	1/1	0.94	0.10	55,55,55,55	0
57	MG	1A	3019	1/1	0.94	0.10	46,46,46,46	0
57	MG	2a	1734	1/1	0.94	0.09	70,70,70,70	0
57	MG	2A	3307	1/1	0.94	0.14	56,56,56,56	0
57	MG	1A	3411	1/1	0.94	0.14	52,52,52,52	0
57	MG	2A	3535	1/1	0.94	0.09	53,53,53,53	0
57	MG	2A	3119	1/1	0.94	0.12	43,43,43,43	0
57	MG	1A	3706	1/1	0.94	0.08	29,29,29,29	0
57	MG	1A	3708	1/1	0.94	0.05	11,11,11,11	0
57	MG	2A	3788	1/1	0.94	0.10	45,45,45,45	0
57	MG	2A	3126	1/1	0.94	0.22	40,40,40,40	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3790	1/1	0.94	0.14	55,55,55,55	0
57	MG	1a	1772	1/1	0.94	0.08	49,49,49,49	0
57	MG	1Z	303	1/1	0.94	0.17	44,44,44,44	0
57	MG	2A	3793	1/1	0.94	0.09	61,61,61,61	0
57	MG	2a	1758	1/1	0.94	0.12	59,59,59,59	0
57	MG	2a	1759	1/1	0.94	0.17	53,53,53,53	0
57	MG	1A	3484	1/1	0.94	0.24	34,34,34,34	0
57	MG	1A	3341	1/1	0.94	0.14	46,46,46,46	0
57	MG	2A	3545	1/1	0.94	0.15	56,56,56,56	0
57	MG	2A	3546	1/1	0.94	0.12	40,40,40,40	0
57	MG	2A	3320	1/1	0.94	0.25	53,53,53,53	0
57	MG	2A	3548	1/1	0.94	0.12	60,60,60,60	0
57	MG	2A	3800	1/1	0.94	0.13	46,46,46,46	0
57	MG	2a	1769	1/1	0.94	0.23	50,50,50,50	0
57	MG	1A	3489	1/1	0.94	0.11	57,57,57,57	0
57	MG	2A	3802	1/1	0.94	0.12	59,59,59,59	0
57	MG	2A	3803	1/1	0.94	0.07	57,57,57,57	0
57	MG	2A	3804	1/1	0.94	0.08	65,65,65,65	0
57	MG	10	105	1/1	0.94	0.17	51,51,51,51	0
57	MG	1A	3144	1/1	0.94	0.06	33,33,33,33	0
57	MG	2a	1777	1/1	0.94	0.17	58,58,58,58	0
57	MG	2A	3807	1/1	0.94	0.14	50,50,50,50	0
57	MG	1A	3296	1/1	0.94	0.16	48,48,48,48	0
57	MG	2A	3142	1/1	0.94	0.12	54,54,54,54	0
57	MG	2a	1782	1/1	0.94	0.20	55,55,55,55	0
57	MG	2a	1783	1/1	0.94	0.18	63,63,63,63	0
57	MG	1A	3492	1/1	0.94	0.17	67,67,67,67	0
57	MG	2A	3148	1/1	0.94	0.10	54,54,54,54	0
57	MG	1A	3935	1/1	0.94	0.07	58,58,58,58	0
57	MG	1A	4065	1/1	0.94	0.09	17,17,17,17	0
57	MG	1A	3193	1/1	0.94	0.09	37,37,37,37	0
57	MG	1A	3618	1/1	0.94	0.09	36,36,36,36	0
57	MG	2A	3821	1/1	0.94	0.11	54,54,54,54	0
57	MG	1A	3494	1/1	0.94	0.08	45,45,45,45	0
57	MG	1A	3299	1/1	0.94	0.17	49,49,49,49	0
57	MG	2A	3159	1/1	0.94	0.08	54,54,54,54	0
57	MG	2a	1797	1/1	0.94	0.11	57,57,57,57	0
57	MG	2A	3160	1/1	0.94	0.18	64,64,64,64	0
57	MG	1A	3422	1/1	0.94	0.14	52,52,52,52	0
57	MG	2A	3567	1/1	0.94	0.10	48,48,48,48	0
57	MG	1A	3245	1/1	0.94	0.25	50,50,50,50	0
57	MG	2A	3342	1/1	0.94	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	3165	1/1	0.94	0.09	58,58,58,58	0
57	MG	1a	1602	1/1	0.94	0.23	54,54,54,54	0
57	MG	2a	1805	1/1	0.94	0.16	61,61,61,61	0
57	MG	1A	3424	1/1	0.94	0.13	43,43,43,43	0
57	MG	1A	3829	1/1	0.94	0.15	56,56,56,56	0
57	MG	1A	3948	1/1	0.94	0.10	22,22,22,22	0
57	MG	1A	3059	1/1	0.94	0.30	53,53,53,53	0
57	MG	2A	3350	1/1	0.94	0.13	58,58,58,58	0
57	MG	1A	3198	1/1	0.94	0.12	31,31,31,31	0
57	MG	1A	3358	1/1	0.94	0.08	49,49,49,49	0
57	MG	1A	3834	1/1	0.94	0.17	27,27,27,27	0
57	MG	2a	1817	1/1	0.94	0.14	58,58,58,58	0
57	MG	2A	3587	1/1	0.94	0.22	39,39,39,39	0
57	MG	2A	3588	1/1	0.94	0.12	41,41,41,41	0
57	MG	1A	3836	1/1	0.94	0.13	29,29,29,29	0
57	MG	1A	3428	1/1	0.94	0.17	54,54,54,54	0
57	MG	1A	3513	1/1	0.94	0.06	51,51,51,51	0
57	MG	1a	1818	1/1	0.94	0.17	53,53,53,53	0
57	MG	2A	3359	1/1	0.94	0.13	43,43,43,43	0
57	MG	2A	3596	1/1	0.94	0.11	55,55,55,55	0
57	MG	2A	3360	1/1	0.94	0.09	63,63,63,63	0
57	MG	1A	3843	1/1	0.94	0.10	56,56,56,56	0
57	MG	2A	3601	1/1	0.94	0.17	53,53,53,53	0
57	MG	1A	3958	1/1	0.94	0.14	47,47,47,47	0
57	MG	2A	3184	1/1	0.94	0.27	52,52,52,52	0
57	MG	1A	3251	1/1	0.94	0.11	41,41,41,41	0
57	MG	1A	4103	1/1	0.94	0.10	50,50,50,50	0
57	MG	2l	203	1/1	0.94	0.09	58,58,58,58	0
57	MG	2E	301	1/1	0.94	0.17	59,59,59,59	0
57	MG	1A	3638	1/1	0.94	0.12	24,24,24,24	0
57	MG	2q	201	1/1	0.94	0.09	67,67,67,67	0
57	MG	2q	202	1/1	0.94	0.07	69,69,69,69	0
57	MG	2r	101	1/1	0.94	0.09	64,64,64,64	0
57	MG	1A	4107	1/1	0.94	0.13	53,53,53,53	0
57	MG	1A	3962	1/1	0.94	0.07	11,11,11,11	0
57	MG	1A	3732	1/1	0.94	0.10	23,23,23,23	0
57	MG	1A	3060	1/1	0.94	0.23	43,43,43,43	0
57	MG	1a	1645	1/1	0.94	0.20	52,52,52,52	0
57	MG	1A	3096	1/1	0.94	0.12	28,28,28,28	0
57	MG	2A	3194	1/1	0.94	0.10	50,50,50,50	0
57	MG	1w	105	1/1	0.94	0.14	72,72,72,72	0
57	MG	1w	106	1/1	0.94	0.10	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	3379	1/1	0.94	0.14	49,49,49,49	0
57	MG	1A	3521	1/1	0.94	0.13	33,33,33,33	0
57	MG	2x	105	1/1	0.94	0.13	58,58,58,58	0
57	MG	2R	203	1/1	0.94	0.12	48,48,48,48	0
57	MG	2y	101	1/1	0.94	0.15	70,70,70,70	0
57	MG	2A	3381	1/1	0.94	0.15	61,61,61,61	0
58	K	2A	3402	1/1	0.94	0.07	49,49,49,49	0
59	A1AEZ	2A	3843	85/85	0.94	0.11	30,40,54,61	0
60	ZN	24	501	1/1	0.94	0.11	104,104,104,104	0
57	MG	2A	3543	1/1	0.95	0.17	57,57,57,57	0
57	MG	1x	105	1/1	0.95	0.16	50,50,50,50	0
57	MG	1A	3901	1/1	0.95	0.08	33,33,33,33	0
57	MG	1A	3902	1/1	0.95	0.05	56,56,56,56	0
57	MG	17	104	1/1	0.95	0.16	47,47,47,47	0
57	MG	1A	3903	1/1	0.95	0.12	46,46,46,46	0
57	MG	1x	110	1/1	0.95	0.11	23,23,23,23	0
57	MG	1A	3163	1/1	0.95	0.11	20,20,20,20	0
57	MG	2D	308	1/1	0.95	0.15	56,56,56,56	0
57	MG	1A	3662	1/1	0.95	0.06	16,16,16,16	0
57	MG	2A	3275	1/1	0.95	0.09	57,57,57,57	0
57	MG	1A	3339	1/1	0.95	0.14	46,46,46,46	0
57	MG	1x	114	1/1	0.95	0.17	54,54,54,54	0
57	MG	1a	1601	1/1	0.95	0.14	52,52,52,52	0
57	MG	2E	307	1/1	0.95	0.13	47,47,47,47	0
57	MG	2E	308	1/1	0.95	0.12	35,35,35,35	0
57	MG	2F	303	1/1	0.95	0.08	56,56,56,56	0
57	MG	2F	304	1/1	0.95	0.08	43,43,43,43	0
57	MG	2A	3279	1/1	0.95	0.30	52,52,52,52	0
57	MG	1A	3401	1/1	0.95	0.10	47,47,47,47	0
57	MG	1a	1603	1/1	0.95	0.07	38,38,38,38	0
57	MG	1A	3199	1/1	0.95	0.11	45,45,45,45	0
57	MG	2A	3007	1/1	0.95	0.08	38,38,38,38	0
57	MG	2O	201	1/1	0.95	0.20	68,68,68,68	0
57	MG	1A	3200	1/1	0.95	0.09	39,39,39,39	0
57	MG	1A	3165	1/1	0.95	0.09	37,37,37,37	0
57	MG	1a	1607	1/1	0.95	0.07	45,45,45,45	0
57	MG	1a	1610	1/1	0.95	0.26	47,47,47,47	0
57	MG	2R	202	1/1	0.95	0.24	50,50,50,50	0
57	MG	1A	3788	1/1	0.95	0.09	35,35,35,35	0
57	MG	1a	1612	1/1	0.95	0.09	53,53,53,53	0
57	MG	2A	3290	1/1	0.95	0.12	57,57,57,57	0
57	MG	1a	1613	1/1	0.95	0.06	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	4059	1/1	0.95	0.07	44,44,44,44	0
57	MG	2A	3575	1/1	0.95	0.09	37,37,37,37	0
57	MG	2A	3576	1/1	0.95	0.10	41,41,41,41	0
57	MG	2A	3577	1/1	0.95	0.13	47,47,47,47	0
57	MG	2A	3578	1/1	0.95	0.12	55,55,55,55	0
57	MG	2A	3024	1/1	0.95	0.19	44,44,44,44	0
57	MG	1A	3789	1/1	0.95	0.07	31,31,31,31	0
57	MG	2A	3026	1/1	0.95	0.12	37,37,37,37	0
57	MG	1A	4064	1/1	0.95	0.07	25,25,25,25	0
57	MG	1A	3790	1/1	0.95	0.06	34,34,34,34	0
57	MG	1A	3671	1/1	0.95	0.07	27,27,27,27	0
57	MG	1a	1622	1/1	0.95	0.21	54,54,54,54	0
57	MG	1A	4067	1/1	0.95	0.06	17,17,17,17	0
57	MG	1a	1624	1/1	0.95	0.11	49,49,49,49	0
57	MG	1A	3792	1/1	0.95	0.09	36,36,36,36	0
57	MG	1a	1626	1/1	0.95	0.17	58,58,58,58	0
57	MG	1A	4071	1/1	0.95	0.07	28,28,28,28	0
57	MG	1a	1629	1/1	0.95	0.21	67,67,67,67	0
57	MG	1A	3407	1/1	0.95	0.08	55,55,55,55	0
57	MG	1a	1632	1/1	0.95	0.28	58,58,58,58	0
57	MG	1A	3673	1/1	0.95	0.11	50,50,50,50	0
57	MG	2A	3598	1/1	0.95	0.11	46,46,46,46	0
57	MG	1A	3919	1/1	0.95	0.07	39,39,39,39	0
57	MG	2A	3047	1/1	0.95	0.08	47,47,47,47	0
57	MG	1A	3920	1/1	0.95	0.11	47,47,47,47	0
57	MG	1a	1637	1/1	0.95	0.12	50,50,50,50	0
57	MG	2A	3603	1/1	0.95	0.06	28,28,28,28	0
57	MG	2A	3317	1/1	0.95	0.14	61,61,61,61	0
57	MG	1A	3567	1/1	0.95	0.09	20,20,20,20	0
57	MG	2A	3319	1/1	0.95	0.13	54,54,54,54	0
57	MG	1A	4081	1/1	0.95	0.09	16,16,16,16	0
57	MG	1a	1640	1/1	0.95	0.07	45,45,45,45	0
57	MG	1A	3568	1/1	0.95	0.08	31,31,31,31	0
57	MG	1A	3297	1/1	0.95	0.14	42,42,42,42	0
57	MG	2a	1618	1/1	0.95	0.14	58,58,58,58	0
57	MG	1A	3247	1/1	0.95	0.09	41,41,41,41	0
57	MG	1A	3681	1/1	0.95	0.08	42,42,42,42	0
57	MG	1A	4087	1/1	0.95	0.08	50,50,50,50	0
57	MG	2A	3327	1/1	0.95	0.12	57,57,57,57	0
57	MG	1a	1651	1/1	0.95	0.20	60,60,60,60	0
57	MG	2A	3064	1/1	0.95	0.08	43,43,43,43	0
57	MG	2a	1625	1/1	0.95	0.09	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	3330	1/1	0.95	0.37	49,49,49,49	0
57	MG	1A	3682	1/1	0.95	0.17	41,41,41,41	0
57	MG	1a	1654	1/1	0.95	0.13	51,51,51,51	0
57	MG	1A	3572	1/1	0.95	0.10	30,30,30,30	0
57	MG	2A	3068	1/1	0.95	0.21	38,38,38,38	0
57	MG	2A	3069	1/1	0.95	0.06	46,46,46,46	0
57	MG	2A	3628	1/1	0.95	0.08	63,63,63,63	0
57	MG	1A	4092	1/1	0.95	0.07	37,37,37,37	0
57	MG	2a	1635	1/1	0.95	0.11	56,56,56,56	0
57	MG	1A	3930	1/1	0.95	0.11	52,52,52,52	0
57	MG	1A	3684	1/1	0.95	0.13	39,39,39,39	0
57	MG	1A	3933	1/1	0.95	0.15	58,58,58,58	0
57	MG	1A	3475	1/1	0.95	0.11	37,37,37,37	0
57	MG	1A	3687	1/1	0.95	0.07	42,42,42,42	0
57	MG	1A	4100	1/1	0.95	0.14	49,49,49,49	0
57	MG	1A	3806	1/1	0.95	0.10	24,24,24,24	0
57	MG	2a	1643	1/1	0.95	0.09	61,61,61,61	0
57	MG	1A	3130	1/1	0.95	0.14	40,40,40,40	0
57	MG	1A	3250	1/1	0.95	0.06	37,37,37,37	0
57	MG	1A	3576	1/1	0.95	0.07	32,32,32,32	0
57	MG	1A	3413	1/1	0.95	0.16	39,39,39,39	0
57	MG	2A	3091	1/1	0.95	0.08	43,43,43,43	0
57	MG	1A	4110	1/1	0.95	0.17	36,36,36,36	0
57	MG	1A	3943	1/1	0.95	0.06	55,55,55,55	0
57	MG	1A	3579	1/1	0.95	0.07	22,22,22,22	0
57	MG	1A	3414	1/1	0.95	0.08	42,42,42,42	0
57	MG	2A	3356	1/1	0.95	0.15	58,58,58,58	0
57	MG	2a	1656	1/1	0.95	0.16	48,48,48,48	0
57	MG	2a	1657	1/1	0.95	0.16	41,41,41,41	0
57	MG	1A	3110	1/1	0.95	0.13	47,47,47,47	0
57	MG	1A	3947	1/1	0.95	0.15	46,46,46,46	0
57	MG	1A	3815	1/1	0.95	0.09	16,16,16,16	0
57	MG	2A	3102	1/1	0.95	0.14	48,48,48,48	0
57	MG	2A	3103	1/1	0.95	0.14	34,34,34,34	0
57	MG	2a	1664	1/1	0.95	0.10	54,54,54,54	0
57	MG	2a	1665	1/1	0.95	0.10	47,47,47,47	0
57	MG	1A	3586	1/1	0.95	0.10	25,25,25,25	0
57	MG	2A	3363	1/1	0.95	0.13	38,38,38,38	0
57	MG	2A	3105	1/1	0.95	0.10	46,46,46,46	0
57	MG	2A	3665	1/1	0.95	0.16	58,58,58,58	0
57	MG	1A	3699	1/1	0.95	0.07	47,47,47,47	0
57	MG	1a	1682	1/1	0.95	0.21	52,52,52,52	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3108	1/1	0.95	0.08	26,26,26,26	0
57	MG	1B	206	1/1	0.95	0.10	41,41,41,41	0
57	MG	1A	3700	1/1	0.95	0.07	36,36,36,36	0
57	MG	1a	1686	1/1	0.95	0.13	44,44,44,44	0
57	MG	1B	208	1/1	0.95	0.18	60,60,60,60	0
57	MG	2A	3372	1/1	0.95	0.36	56,56,56,56	0
57	MG	1A	3952	1/1	0.95	0.10	26,26,26,26	0
57	MG	1B	210	1/1	0.95	0.11	49,49,49,49	0
57	MG	1a	1692	1/1	0.95	0.17	52,52,52,52	0
57	MG	1A	3351	1/1	0.95	0.08	36,36,36,36	0
57	MG	2A	3118	1/1	0.95	0.12	41,41,41,41	0
57	MG	1a	1694	1/1	0.95	0.10	57,57,57,57	0
57	MG	2a	1686	1/1	0.95	0.10	55,55,55,55	0
57	MG	1A	3820	1/1	0.95	0.11	22,22,22,22	0
57	MG	2A	3121	1/1	0.95	0.06	60,60,60,60	0
57	MG	1A	3821	1/1	0.95	0.05	25,25,25,25	0
57	MG	1A	3702	1/1	0.95	0.06	46,46,46,46	0
57	MG	1A	3486	1/1	0.95	0.15	44,44,44,44	0
57	MG	2A	3129	1/1	0.95	0.16	37,37,37,37	0
57	MG	1A	3010	1/1	0.95	0.14	37,37,37,37	0
57	MG	1A	3594	1/1	0.95	0.09	23,23,23,23	0
57	MG	1A	3303	1/1	0.95	0.20	47,47,47,47	0
57	MG	1A	3830	1/1	0.95	0.06	17,17,17,17	0
57	MG	2A	3391	1/1	0.95	0.21	45,45,45,45	0
57	MG	1A	3964	1/1	0.95	0.10	20,20,20,20	0
57	MG	2A	3136	1/1	0.95	0.18	37,37,37,37	0
57	MG	1A	3362	1/1	0.95	0.09	53,53,53,53	0
57	MG	2A	3139	1/1	0.95	0.13	41,41,41,41	0
57	MG	2a	1702	1/1	0.95	0.14	44,44,44,44	0
57	MG	1A	3600	1/1	0.95	0.09	52,52,52,52	0
57	MG	1B	228	1/1	0.95	0.05	32,32,32,32	0
57	MG	1A	3363	1/1	0.95	0.22	49,49,49,49	0
57	MG	1a	1713	1/1	0.95	0.06	53,53,53,53	0
57	MG	1A	3091	1/1	0.95	0.07	39,39,39,39	0
57	MG	1A	3972	1/1	0.95	0.04	20,20,20,20	0
57	MG	2A	3405	1/1	0.95	0.13	53,53,53,53	0
57	MG	2A	3705	1/1	0.95	0.10	43,43,43,43	0
57	MG	2A	3706	1/1	0.95	0.18	66,66,66,66	0
57	MG	2A	3708	1/1	0.95	0.07	61,61,61,61	0
57	MG	1a	1718	1/1	0.95	0.07	42,42,42,42	0
57	MG	1A	3265	1/1	0.95	0.15	52,52,52,52	0
57	MG	2A	3408	1/1	0.95	0.24	41,41,41,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3266	1/1	0.95	0.10	47,47,47,47	0
57	MG	1A	3141	1/1	0.95	0.10	37,37,37,37	0
57	MG	1B	235	1/1	0.95	0.19	65,65,65,65	0
57	MG	1B	236	1/1	0.95	0.07	35,35,35,35	0
57	MG	1A	3977	1/1	0.95	0.08	41,41,41,41	0
57	MG	1A	3372	1/1	0.95	0.07	44,44,44,44	0
57	MG	1a	1728	1/1	0.95	0.07	55,55,55,55	0
57	MG	1A	3179	1/1	0.95	0.13	29,29,29,29	0
57	MG	1D	304	1/1	0.95	0.10	32,32,32,32	0
57	MG	2A	3726	1/1	0.95	0.11	34,34,34,34	0
57	MG	2A	3727	1/1	0.95	0.10	37,37,37,37	0
57	MG	1A	3611	1/1	0.95	0.09	30,30,30,30	0
57	MG	1a	1733	1/1	0.95	0.14	43,43,43,43	0
57	MG	1A	3984	1/1	0.95	0.07	48,48,48,48	0
57	MG	1a	1736	1/1	0.95	0.07	60,60,60,60	0
57	MG	1A	3985	1/1	0.95	0.07	55,55,55,55	0
57	MG	1A	3142	1/1	0.95	0.06	32,32,32,32	0
57	MG	1A	3616	1/1	0.95	0.09	34,34,34,34	0
57	MG	1A	3118	1/1	0.95	0.17	34,34,34,34	0
57	MG	2a	1742	1/1	0.95	0.08	69,69,69,69	0
57	MG	1A	3849	1/1	0.95	0.09	30,30,30,30	0
57	MG	1a	1743	1/1	0.95	0.06	52,52,52,52	0
57	MG	1a	1744	1/1	0.95	0.06	46,46,46,46	0
57	MG	1A	3272	1/1	0.95	0.09	51,51,51,51	0
57	MG	1A	3620	1/1	0.95	0.12	46,46,46,46	0
57	MG	1A	3726	1/1	0.95	0.07	31,31,31,31	0
57	MG	1A	3853	1/1	0.95	0.06	39,39,39,39	0
57	MG	2a	1755	1/1	0.95	0.10	68,68,68,68	0
57	MG	1F	309	1/1	0.95	0.10	50,50,50,50	0
57	MG	2a	1757	1/1	0.95	0.06	60,60,60,60	0
57	MG	1A	3042	1/1	0.95	0.11	33,33,33,33	0
57	MG	1A	3623	1/1	0.95	0.06	21,21,21,21	0
57	MG	2a	1760	1/1	0.95	0.13	54,54,54,54	0
57	MG	2a	1761	1/1	0.95	0.26	60,60,60,60	0
57	MG	1A	3506	1/1	0.95	0.32	52,52,52,52	0
57	MG	2A	3444	1/1	0.95	0.08	36,36,36,36	0
57	MG	1G	203	1/1	0.95	0.07	55,55,55,55	0
57	MG	1A	3508	1/1	0.95	0.16	44,44,44,44	0
57	MG	1A	3510	1/1	0.95	0.23	54,54,54,54	0
57	MG	2A	3753	1/1	0.95	0.07	39,39,39,39	0
57	MG	1A	3434	1/1	0.95	0.19	33,33,33,33	0
57	MG	1a	1774	1/1	0.95	0.06	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3436	1/1	0.95	0.07	48,48,48,48	0
57	MG	1N	204	1/1	0.95	0.13	43,43,43,43	0
57	MG	1a	1777	1/1	0.95	0.20	59,59,59,59	0
57	MG	1A	3437	1/1	0.95	0.09	44,44,44,44	0
57	MG	2a	1774	1/1	0.95	0.15	61,61,61,61	0
57	MG	1A	3863	1/1	0.95	0.10	25,25,25,25	0
57	MG	1A	3120	1/1	0.95	0.08	38,38,38,38	0
57	MG	1a	1781	1/1	0.95	0.16	58,58,58,58	0
57	MG	1a	1782	1/1	0.95	0.07	45,45,45,45	0
57	MG	2A	3461	1/1	0.95	0.08	39,39,39,39	0
57	MG	1a	1784	1/1	0.95	0.21	61,61,61,61	0
57	MG	2a	1781	1/1	0.95	0.20	58,58,58,58	0
57	MG	1A	4012	1/1	0.95	0.10	43,43,43,43	0
57	MG	1A	4013	1/1	0.95	0.08	24,24,24,24	0
57	MG	1A	3321	1/1	0.95	0.11	47,47,47,47	0
57	MG	1a	1788	1/1	0.95	0.12	45,45,45,45	0
57	MG	2A	3778	1/1	0.95	0.07	33,33,33,33	0
57	MG	1P	205	1/1	0.95	0.05	33,33,33,33	0
57	MG	2A	3781	1/1	0.95	0.09	39,39,39,39	0
57	MG	1A	3044	1/1	0.95	0.08	31,31,31,31	0
57	MG	1a	1791	1/1	0.95	0.11	59,59,59,59	0
57	MG	2A	3784	1/1	0.95	0.10	39,39,39,39	0
57	MG	1a	1792	1/1	0.95	0.08	45,45,45,45	0
57	MG	2a	1794	1/1	0.95	0.08	58,58,58,58	0
57	MG	1Q	205	1/1	0.95	0.11	53,53,53,53	0
57	MG	1a	1795	1/1	0.95	0.07	43,43,43,43	0
57	MG	1A	3230	1/1	0.95	0.17	43,43,43,43	0
57	MG	1A	3869	1/1	0.95	0.24	22,22,22,22	0
57	MG	2A	3477	1/1	0.95	0.16	56,56,56,56	0
57	MG	2A	3479	1/1	0.95	0.08	41,41,41,41	0
57	MG	1A	3442	1/1	0.95	0.11	55,55,55,55	0
57	MG	1A	3232	1/1	0.95	0.07	54,54,54,54	0
57	MG	1a	1800	1/1	0.95	0.07	70,70,70,70	0
57	MG	1A	3089	1/1	0.95	0.10	46,46,46,46	0
57	MG	2A	3484	1/1	0.95	0.06	37,37,37,37	0
57	MG	1A	3234	1/1	0.95	0.12	27,27,27,27	0
57	MG	1A	3533	1/1	0.95	0.07	46,46,46,46	0
57	MG	1A	3447	1/1	0.95	0.11	49,49,49,49	0
57	MG	1A	3758	1/1	0.95	0.06	15,15,15,15	0
57	MG	2a	1812	1/1	0.95	0.21	48,48,48,48	0
57	MG	2a	1813	1/1	0.95	0.17	55,55,55,55	0
57	MG	1U	204	1/1	0.95	0.20	32,32,32,32	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	3650	1/1	0.95	0.06	25,25,25,25	0
57	MG	2A	3495	1/1	0.95	0.11	34,34,34,34	0
57	MG	1U	207	1/1	0.95	0.14	30,30,30,30	0
57	MG	1a	1811	1/1	0.95	0.06	44,44,44,44	0
57	MG	1A	3651	1/1	0.95	0.07	25,25,25,25	0
57	MG	1A	3540	1/1	0.95	0.08	24,24,24,24	0
57	MG	2A	3502	1/1	0.95	0.07	35,35,35,35	0
57	MG	1V	206	1/1	0.95	0.11	51,51,51,51	0
57	MG	1A	3106	1/1	0.95	0.20	36,36,36,36	0
57	MG	2A	3814	1/1	0.95	0.19	53,53,53,53	0
57	MG	1W	201	1/1	0.95	0.23	47,47,47,47	0
57	MG	1A	3238	1/1	0.95	0.09	56,56,56,56	0
57	MG	1X	102	1/1	0.95	0.12	40,40,40,40	0
57	MG	1Z	301	1/1	0.95	0.07	50,50,50,50	0
57	MG	1A	4036	1/1	0.95	0.09	30,30,30,30	0
57	MG	1e	202	1/1	0.95	0.11	50,50,50,50	0
57	MG	2g	201	1/1	0.95	0.13	66,66,66,66	0
57	MG	2A	3246	1/1	0.95	0.25	53,53,53,53	0
57	MG	2A	3514	1/1	0.95	0.09	35,35,35,35	0
57	MG	1A	3391	1/1	0.95	0.08	45,45,45,45	0
57	MG	1A	3197	1/1	0.95	0.10	45,45,45,45	0
57	MG	2A	3249	1/1	0.95	0.12	51,51,51,51	0
57	MG	2A	3828	1/1	0.95	0.07	62,62,62,62	0
57	MG	1A	3395	1/1	0.95	0.18	40,40,40,40	0
57	MG	2A	3830	1/1	0.95	0.10	38,38,38,38	0
57	MG	1k	201	1/1	0.95	0.12	44,44,44,44	0
57	MG	1A	3288	1/1	0.95	0.16	47,47,47,47	0
57	MG	1n	101	1/1	0.95	0.08	39,39,39,39	0
57	MG	1A	4042	1/1	0.95	0.12	40,40,40,40	0
57	MG	1A	3398	1/1	0.95	0.11	60,60,60,60	0
57	MG	10	108	1/1	0.95	0.17	62,62,62,62	0
57	MG	2w	104	1/1	0.95	0.09	48,48,48,48	0
57	MG	1w	104	1/1	0.95	0.10	59,59,59,59	0
57	MG	2A	3533	1/1	0.95	0.10	54,54,54,54	0
57	MG	2A	3534	1/1	0.95	0.10	52,52,52,52	0
57	MG	10	109	1/1	0.95	0.07	39,39,39,39	0
57	MG	2B	202	1/1	0.95	0.15	64,64,64,64	0
57	MG	11	103	1/1	0.95	0.07	31,31,31,31	0
57	MG	1A	3898	1/1	0.95	0.04	34,34,34,34	0
57	MG	12	102	1/1	0.95	0.09	42,42,42,42	0
57	MG	1A	4045	1/1	0.95	0.14	46,46,46,46	0
57	MG	1A	3899	1/1	0.95	0.11	33,33,33,33	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
59	A1AEZ	1A	4118	85/85	0.95	0.09	10,28,38,42	0
57	MG	15	103	1/1	0.95	0.17	33,33,33,33	0
57	MG	1A	3462	1/1	0.95	0.07	44,44,44,44	0
62	PHE	2w	108	11/12	0.95	0.11	31,35,38,42	0
63	FME	1x	115	10/11	0.95	0.15	17,19,23,28	10
57	MG	1A	3680	1/1	0.96	0.07	28,28,28,28	0
57	MG	1a	1669	1/1	0.96	0.05	48,48,48,48	0
57	MG	1A	3314	1/1	0.96	0.10	40,40,40,40	0
57	MG	1A	4022	1/1	0.96	0.06	16,16,16,16	0
57	MG	1A	3189	1/1	0.96	0.09	43,43,43,43	0
57	MG	1a	1673	1/1	0.96	0.06	55,55,55,55	0
57	MG	1A	3590	1/1	0.96	0.05	18,18,18,18	0
57	MG	1A	3592	1/1	0.96	0.07	28,28,28,28	0
57	MG	1A	3593	1/1	0.96	0.06	35,35,35,35	0
57	MG	1A	3275	1/1	0.96	0.04	19,19,19,19	0
57	MG	2A	3022	1/1	0.96	0.22	45,45,45,45	0
57	MG	1A	3045	1/1	0.96	0.14	30,30,30,30	0
57	MG	1A	3381	1/1	0.96	0.11	37,37,37,37	0
57	MG	1A	3599	1/1	0.96	0.07	17,17,17,17	0
57	MG	1A	3691	1/1	0.96	0.16	57,57,57,57	0
57	MG	1A	3039	1/1	0.96	0.06	31,31,31,31	0
57	MG	2A	3029	1/1	0.96	0.07	25,25,25,25	0
57	MG	1A	3383	1/1	0.96	0.15	37,37,37,37	0
57	MG	2A	3456	1/1	0.96	0.08	39,39,39,39	0
57	MG	1A	3694	1/1	0.96	0.05	24,24,24,24	0
57	MG	1A	3279	1/1	0.96	0.16	47,47,47,47	0
57	MG	2A	3034	1/1	0.96	0.08	44,44,44,44	0
57	MG	2A	3698	1/1	0.96	0.08	30,30,30,30	0
57	MG	1A	3324	1/1	0.96	0.08	49,49,49,49	0
57	MG	1a	1689	1/1	0.96	0.15	37,37,37,37	0
57	MG	1N	202	1/1	0.96	0.09	43,43,43,43	0
57	MG	1a	1691	1/1	0.96	0.22	63,63,63,63	0
57	MG	1A	3511	1/1	0.96	0.06	38,38,38,38	0
57	MG	1A	3195	1/1	0.96	0.15	39,39,39,39	0
57	MG	1A	3104	1/1	0.96	0.11	35,35,35,35	0
57	MG	1A	3609	1/1	0.96	0.06	28,28,28,28	0
57	MG	2A	3710	1/1	0.96	0.05	49,49,49,49	0
57	MG	2A	3711	1/1	0.96	0.08	50,50,50,50	0
57	MG	2A	3044	1/1	0.96	0.20	58,58,58,58	0
57	MG	1a	1696	1/1	0.96	0.09	46,46,46,46	0
57	MG	1A	3105	1/1	0.96	0.07	34,34,34,34	0
57	MG	1A	3127	1/1	0.96	0.11	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	2a	1650	1/1	0.96	0.18	37,37,37,37	0
57	MG	1a	1699	1/1	0.96	0.07	30,30,30,30	0
57	MG	2a	1652	1/1	0.96	0.07	58,58,58,58	0
57	MG	2A	3049	1/1	0.96	0.08	43,43,43,43	0
57	MG	2A	3050	1/1	0.96	0.18	59,59,59,59	0
57	MG	1A	3240	1/1	0.96	0.10	44,44,44,44	0
57	MG	2A	3478	1/1	0.96	0.10	41,41,41,41	0
57	MG	1a	1701	1/1	0.96	0.08	38,38,38,38	0
57	MG	1A	3614	1/1	0.96	0.09	56,56,56,56	0
57	MG	1A	3925	1/1	0.96	0.04	43,43,43,43	0
57	MG	1A	3615	1/1	0.96	0.07	32,32,32,32	0
57	MG	1Q	206	1/1	0.96	0.09	35,35,35,35	0
57	MG	1A	3814	1/1	0.96	0.10	35,35,35,35	0
57	MG	1R	203	1/1	0.96	0.28	44,44,44,44	0
57	MG	1a	1709	1/1	0.96	0.09	40,40,40,40	0
57	MG	2A	3487	1/1	0.96	0.08	38,38,38,38	0
57	MG	1R	204	1/1	0.96	0.07	25,25,25,25	0
57	MG	2A	3062	1/1	0.96	0.09	48,48,48,48	0
57	MG	2A	3063	1/1	0.96	0.17	44,44,44,44	0
57	MG	1A	3448	1/1	0.96	0.09	36,36,36,36	0
57	MG	1A	3330	1/1	0.96	0.12	51,51,51,51	0
57	MG	1A	3034	1/1	0.96	0.09	34,34,34,34	0
57	MG	1A	3932	1/1	0.96	0.12	45,45,45,45	0
57	MG	2a	1674	1/1	0.96	0.14	48,48,48,48	0
57	MG	1A	3107	1/1	0.96	0.17	39,39,39,39	0
57	MG	1T	201	1/1	0.96	0.11	50,50,50,50	0
57	MG	2A	3501	1/1	0.96	0.09	52,52,52,52	0
57	MG	2a	1678	1/1	0.96	0.20	38,38,38,38	0
57	MG	2A	3071	1/1	0.96	0.10	39,39,39,39	0
57	MG	1A	3621	1/1	0.96	0.07	22,22,22,22	0
57	MG	2A	3505	1/1	0.96	0.09	37,37,37,37	0
57	MG	2A	3073	1/1	0.96	0.09	44,44,44,44	0
57	MG	1A	3334	1/1	0.96	0.11	54,54,54,54	0
57	MG	1A	4062	1/1	0.96	0.08	30,30,30,30	0
57	MG	1A	3243	1/1	0.96	0.11	28,28,28,28	0
57	MG	2A	3079	1/1	0.96	0.08	41,41,41,41	0
57	MG	1A	3530	1/1	0.96	0.09	29,29,29,29	0
57	MG	1U	206	1/1	0.96	0.15	40,40,40,40	0
57	MG	2A	3754	1/1	0.96	0.08	34,34,34,34	0
57	MG	1A	3457	1/1	0.96	0.12	46,46,46,46	0
57	MG	2A	3758	1/1	0.96	0.09	47,47,47,47	0
57	MG	1A	3825	1/1	0.96	0.08	43,43,43,43	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3085	1/1	0.96	0.15	48,48,48,48	0
57	MG	2A	3297	1/1	0.96	0.06	39,39,39,39	0
57	MG	1A	3244	1/1	0.96	0.12	39,39,39,39	0
57	MG	1A	3941	1/1	0.96	0.06	53,53,53,53	0
57	MG	1A	3535	1/1	0.96	0.11	38,38,38,38	0
57	MG	2A	3765	1/1	0.96	0.08	53,53,53,53	0
57	MG	1A	3538	1/1	0.96	0.32	36,36,36,36	0
57	MG	2A	3090	1/1	0.96	0.17	48,48,48,48	0
57	MG	1a	1734	1/1	0.96	0.10	50,50,50,50	0
57	MG	1A	3539	1/1	0.96	0.08	42,42,42,42	0
57	MG	2A	3527	1/1	0.96	0.13	53,53,53,53	0
57	MG	1W	204	1/1	0.96	0.10	37,37,37,37	0
57	MG	1A	4077	1/1	0.96	0.05	51,51,51,51	0
57	MG	1X	105	1/1	0.96	0.12	37,37,37,37	0
57	MG	1X	106	1/1	0.96	0.06	34,34,34,34	0
57	MG	1Y	201	1/1	0.96	0.11	46,46,46,46	0
57	MG	2A	3099	1/1	0.96	0.17	45,45,45,45	0
57	MG	2A	3780	1/1	0.96	0.08	34,34,34,34	0
57	MG	2A	3100	1/1	0.96	0.09	35,35,35,35	0
57	MG	1A	3072	1/1	0.96	0.06	37,37,37,37	0
57	MG	2a	1714	1/1	0.96	0.23	51,51,51,51	0
57	MG	2A	3314	1/1	0.96	0.18	54,54,54,54	0
57	MG	1A	3542	1/1	0.96	0.10	35,35,35,35	0
57	MG	2A	3785	1/1	0.96	0.10	42,42,42,42	0
57	MG	1A	3634	1/1	0.96	0.09	42,42,42,42	0
57	MG	1a	1745	1/1	0.96	0.06	55,55,55,55	0
57	MG	1A	4082	1/1	0.96	0.07	35,35,35,35	0
57	MG	1A	3635	1/1	0.96	0.08	19,19,19,19	0
57	MG	1A	3835	1/1	0.96	0.06	41,41,41,41	0
57	MG	1A	3461	1/1	0.96	0.16	39,39,39,39	0
57	MG	10	106	1/1	0.96	0.08	40,40,40,40	0
57	MG	1A	3837	1/1	0.96	0.12	26,26,26,26	0
57	MG	1a	1757	1/1	0.96	0.06	59,59,59,59	0
57	MG	1A	3111	1/1	0.96	0.05	33,33,33,33	0
57	MG	1a	1764	1/1	0.96	0.06	71,71,71,71	0
57	MG	2A	3114	1/1	0.96	0.07	45,45,45,45	0
57	MG	2a	1730	1/1	0.96	0.08	65,65,65,65	0
57	MG	1A	3841	1/1	0.96	0.08	25,25,25,25	0
57	MG	1A	3293	1/1	0.96	0.13	35,35,35,35	0
57	MG	1a	1767	1/1	0.96	0.06	61,61,61,61	0
57	MG	11	104	1/1	0.96	0.06	54,54,54,54	0
57	MG	1A	3172	1/1	0.96	0.14	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	4094	1/1	0.96	0.13	52,52,52,52	0
57	MG	2a	1740	1/1	0.96	0.08	59,59,59,59	0
57	MG	13	102	1/1	0.96	0.11	37,37,37,37	0
57	MG	13	103	1/1	0.96	0.08	37,37,37,37	0
57	MG	2a	1743	1/1	0.96	0.08	48,48,48,48	0
57	MG	1A	3344	1/1	0.96	0.12	27,27,27,27	0
57	MG	2a	1745	1/1	0.96	0.20	53,53,53,53	0
57	MG	1A	3466	1/1	0.96	0.08	28,28,28,28	0
57	MG	1A	3959	1/1	0.96	0.05	43,43,43,43	0
57	MG	1A	3210	1/1	0.96	0.16	47,47,47,47	0
57	MG	2a	1750	1/1	0.96	0.06	76,76,76,76	0
57	MG	2A	3131	1/1	0.96	0.14	39,39,39,39	0
57	MG	2a	1752	1/1	0.96	0.14	60,60,60,60	0
57	MG	1A	3138	1/1	0.96	0.18	32,32,32,32	0
57	MG	1A	3178	1/1	0.96	0.19	28,28,28,28	0
57	MG	17	101	1/1	0.96	0.06	31,31,31,31	0
57	MG	17	103	1/1	0.96	0.09	33,33,33,33	0
57	MG	1A	3252	1/1	0.96	0.07	38,38,38,38	0
57	MG	2A	3819	1/1	0.96	0.08	70,70,70,70	0
57	MG	1A	3253	1/1	0.96	0.07	34,34,34,34	0
57	MG	2A	3349	1/1	0.96	0.15	43,43,43,43	0
57	MG	1A	3744	1/1	0.96	0.07	42,42,42,42	0
57	MG	2A	3140	1/1	0.96	0.21	50,50,50,50	0
57	MG	1A	4106	1/1	0.96	0.18	30,30,30,30	0
57	MG	1A	3257	1/1	0.96	0.12	30,30,30,30	0
57	MG	19	101	1/1	0.96	0.16	45,45,45,45	0
57	MG	1A	3746	1/1	0.96	0.08	22,22,22,22	0
57	MG	1A	4109	1/1	0.96	0.20	30,30,30,30	0
57	MG	1A	3971	1/1	0.96	0.07	20,20,20,20	0
57	MG	1A	3748	1/1	0.96	0.07	42,42,42,42	0
57	MG	1A	3750	1/1	0.96	0.05	36,36,36,36	0
57	MG	1A	3415	1/1	0.96	0.13	32,32,32,32	0
57	MG	1A	4115	1/1	0.96	0.10	45,45,45,45	0
57	MG	1a	1608	1/1	0.96	0.21	59,59,59,59	0
57	MG	1A	3563	1/1	0.96	0.16	42,42,42,42	0
57	MG	1A	3564	1/1	0.96	0.27	36,36,36,36	0
57	MG	2A	3163	1/1	0.96	0.21	52,52,52,52	0
57	MG	2A	3594	1/1	0.96	0.09	44,44,44,44	0
57	MG	2A	3595	1/1	0.96	0.13	54,54,54,54	0
57	MG	1A	3978	1/1	0.96	0.05	28,28,28,28	0
57	MG	1A	3416	1/1	0.96	0.25	34,34,34,34	0
57	MG	1A	3258	1/1	0.96	0.24	29,29,29,29	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1B	205	1/1	0.96	0.06	45,45,45,45	0
57	MG	1a	1616	1/1	0.96	0.11	48,48,48,48	0
57	MG	1a	1617	1/1	0.96	0.10	42,42,42,42	0
57	MG	2B	207	1/1	0.96	0.18	50,50,50,50	0
57	MG	1A	3478	1/1	0.96	0.06	45,45,45,45	0
57	MG	2A	3173	1/1	0.96	0.09	32,32,32,32	0
57	MG	1a	1810	1/1	0.96	0.20	56,56,56,56	0
57	MG	1A	3360	1/1	0.96	0.25	32,32,32,32	0
57	MG	1a	1812	1/1	0.96	0.07	71,71,71,71	0
57	MG	2A	3377	1/1	0.96	0.33	59,59,59,59	0
57	MG	1A	3361	1/1	0.96	0.16	55,55,55,55	0
57	MG	2a	1793	1/1	0.96	0.19	53,53,53,53	0
57	MG	1A	3261	1/1	0.96	0.10	42,42,42,42	0
57	MG	2a	1795	1/1	0.96	0.06	53,53,53,53	0
57	MG	2B	216	1/1	0.96	0.10	53,53,53,53	0
57	MG	1A	3988	1/1	0.96	0.12	70,70,70,70	0
57	MG	1A	3214	1/1	0.96	0.10	51,51,51,51	0
57	MG	2D	302	1/1	0.96	0.15	50,50,50,50	0
57	MG	2D	303	1/1	0.96	0.17	46,46,46,46	0
57	MG	1A	3664	1/1	0.96	0.07	27,27,27,27	0
57	MG	1B	214	1/1	0.96	0.07	55,55,55,55	0
57	MG	1a	1820	1/1	0.96	0.15	54,54,54,54	0
57	MG	1A	3991	1/1	0.96	0.05	35,35,35,35	0
57	MG	2A	3619	1/1	0.96	0.11	36,36,36,36	0
57	MG	2E	303	1/1	0.96	0.12	49,49,49,49	0
57	MG	2a	1807	1/1	0.96	0.17	51,51,51,51	0
57	MG	1A	3221	1/1	0.96	0.14	43,43,43,43	0
57	MG	1B	217	1/1	0.96	0.10	45,45,45,45	0
57	MG	2A	3623	1/1	0.96	0.12	53,53,53,53	0
57	MG	1e	201	1/1	0.96	0.14	63,63,63,63	0
57	MG	2F	302	1/1	0.96	0.13	49,49,49,49	0
57	MG	1A	3306	1/1	0.96	0.09	39,39,39,39	0
57	MG	1B	220	1/1	0.96	0.06	34,34,34,34	0
57	MG	1A	3995	1/1	0.96	0.06	45,45,45,45	0
57	MG	1A	3139	1/1	0.96	0.16	30,30,30,30	0
57	MG	1a	1636	1/1	0.96	0.17	48,48,48,48	0
57	MG	2A	3631	1/1	0.96	0.05	57,57,57,57	0
57	MG	1A	3769	1/1	0.96	0.06	41,41,41,41	0
57	MG	2A	3396	1/1	0.96	0.07	59,59,59,59	0
57	MG	2O	202	1/1	0.96	0.15	54,54,54,54	0
57	MG	1l	202	1/1	0.96	0.05	53,53,53,53	0
57	MG	2Q	201	1/1	0.96	0.10	44,44,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3196	1/1	0.96	0.06	54,54,54,54	0
57	MG	1A	3875	1/1	0.96	0.11	32,32,32,32	0
57	MG	1A	3112	1/1	0.96	0.28	39,39,39,39	0
57	MG	2A	3638	1/1	0.96	0.05	50,50,50,50	0
57	MG	2a	1829	1/1	0.96	0.10	46,46,46,46	0
57	MG	1A	3371	1/1	0.96	0.07	44,44,44,44	0
57	MG	2a	1831	1/1	0.96	0.06	78,78,78,78	0
57	MG	1w	101	1/1	0.96	0.12	38,38,38,38	0
57	MG	1A	3774	1/1	0.96	0.05	32,32,32,32	0
57	MG	1A	3775	1/1	0.96	0.08	35,35,35,35	0
57	MG	1A	3055	1/1	0.96	0.09	41,41,41,41	0
57	MG	2l	201	1/1	0.96	0.07	61,61,61,61	0
57	MG	1A	3076	1/1	0.96	0.14	19,19,19,19	0
57	MG	1a	1649	1/1	0.96	0.09	47,47,47,47	0
57	MG	2A	3410	1/1	0.96	0.13	44,44,44,44	0
57	MG	2A	3648	1/1	0.96	0.07	33,33,33,33	0
57	MG	1A	4006	1/1	0.96	0.10	25,25,25,25	0
57	MG	1A	3079	1/1	0.96	0.12	29,29,29,29	0
57	MG	1a	1652	1/1	0.96	0.08	48,48,48,48	0
57	MG	1A	3885	1/1	0.96	0.14	39,39,39,39	0
57	MG	1A	3585	1/1	0.96	0.06	28,28,28,28	0
57	MG	23	102	1/1	0.96	0.08	45,45,45,45	0
57	MG	1A	3495	1/1	0.96	0.09	47,47,47,47	0
57	MG	1A	3781	1/1	0.96	0.22	22,22,22,22	0
57	MG	1A	3016	1/1	0.96	0.08	41,41,41,41	0
57	MG	2A	3658	1/1	0.96	0.12	38,38,38,38	0
57	MG	2w	105	1/1	0.96	0.09	55,55,55,55	0
57	MG	1A	3783	1/1	0.96	0.10	32,32,32,32	0
57	MG	1A	3892	1/1	0.96	0.07	29,29,29,29	0
57	MG	28	101	1/1	0.96	0.13	45,45,45,45	0
57	MG	2x	102	1/1	0.96	0.18	58,58,58,58	0
57	MG	1A	3784	1/1	0.96	0.05	19,19,19,19	0
57	MG	2A	3664	1/1	0.96	0.09	50,50,50,50	0
57	MG	2A	3423	1/1	0.96	0.09	32,32,32,32	0
57	MG	1D	310	1/1	0.96	0.06	39,39,39,39	0
57	MG	1A	3785	1/1	0.96	0.05	24,24,24,24	0
57	MG	1a	1664	1/1	0.96	0.23	51,51,51,51	0
57	MG	2A	3223	1/1	0.96	0.10	48,48,48,48	0
57	MG	1A	3678	1/1	0.96	0.05	14,14,14,14	0
57	MG	1A	3679	1/1	0.96	0.17	51,51,51,51	0
57	MG	2A	3226	1/1	0.96	0.17	47,47,47,47	0
57	MG	1D	315	1/1	0.96	0.17	30,30,30,30	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3432	1/1	0.96	0.09	46,46,46,46	0
63	FME	2x	108	10/11	0.96	0.10	36,41,46,49	0
57	MG	1A	3087	1/1	0.97	0.08	33,33,33,33	0
57	MG	2A	3455	1/1	0.97	0.12	36,36,36,36	0
57	MG	1N	203	1/1	0.97	0.05	28,28,28,28	0
57	MG	2A	3241	1/1	0.97	0.06	58,58,58,58	0
57	MG	1A	3390	1/1	0.97	0.05	45,45,45,45	0
57	MG	2A	3032	1/1	0.97	0.07	24,24,24,24	0
57	MG	1A	3910	1/1	0.97	0.06	45,45,45,45	0
57	MG	1A	3030	1/1	0.97	0.12	25,25,25,25	0
57	MG	2a	1628	1/1	0.97	0.23	45,45,45,45	0
57	MG	1A	3467	1/1	0.97	0.15	25,25,25,25	0
57	MG	1A	3267	1/1	0.97	0.22	31,31,31,31	0
57	MG	1A	3469	1/1	0.97	0.10	30,30,30,30	0
57	MG	1A	3394	1/1	0.97	0.08	31,31,31,31	0
57	MG	1P	203	1/1	0.97	0.12	27,27,27,27	0
57	MG	2A	3468	1/1	0.97	0.05	41,41,41,41	0
57	MG	2A	3707	1/1	0.97	0.10	37,37,37,37	0
57	MG	1A	3032	1/1	0.97	0.19	23,23,23,23	0
57	MG	2A	3709	1/1	0.97	0.10	43,43,43,43	0
57	MG	1Q	201	1/1	0.97	0.12	35,35,35,35	0
57	MG	1A	3008	1/1	0.97	0.04	22,22,22,22	0
57	MG	2A	3043	1/1	0.97	0.07	19,19,19,19	0
57	MG	1A	3397	1/1	0.97	0.08	40,40,40,40	0
57	MG	1A	3218	1/1	0.97	0.07	26,26,26,26	0
57	MG	1A	3220	1/1	0.97	0.18	37,37,37,37	0
57	MG	1R	202	1/1	0.97	0.14	39,39,39,39	0
57	MG	1A	3798	1/1	0.97	0.08	37,37,37,37	0
57	MG	1A	3577	1/1	0.97	0.10	38,38,38,38	0
57	MG	2A	3720	1/1	0.97	0.11	46,46,46,46	0
57	MG	1A	3168	1/1	0.97	0.06	28,28,28,28	0
57	MG	1A	3274	1/1	0.97	0.08	26,26,26,26	0
57	MG	1a	1708	1/1	0.97	0.05	35,35,35,35	0
57	MG	1A	3073	1/1	0.97	0.17	35,35,35,35	0
57	MG	2A	3265	1/1	0.97	0.17	52,52,52,52	0
57	MG	1A	3926	1/1	0.97	0.08	48,48,48,48	0
57	MG	1A	3403	1/1	0.97	0.13	34,34,34,34	0
57	MG	1A	4060	1/1	0.97	0.08	18,18,18,18	0
57	MG	1A	3123	1/1	0.97	0.05	35,35,35,35	0
57	MG	1a	1714	1/1	0.97	0.09	46,46,46,46	0
57	MG	1A	3093	1/1	0.97	0.07	24,24,24,24	0
57	MG	2A	3491	1/1	0.97	0.09	33,33,33,33	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	2A	3492	1/1	0.97	0.11	49,49,49,49	0
57	MG	1A	4063	1/1	0.97	0.06	16,16,16,16	0
57	MG	2A	3061	1/1	0.97	0.08	29,29,29,29	0
57	MG	1a	1717	1/1	0.97	0.16	37,37,37,37	0
57	MG	1A	3173	1/1	0.97	0.09	29,29,29,29	0
57	MG	1A	3485	1/1	0.97	0.20	34,34,34,34	0
57	MG	2A	3739	1/1	0.97	0.04	48,48,48,48	0
57	MG	1A	3337	1/1	0.97	0.08	34,34,34,34	0
57	MG	1A	3695	1/1	0.97	0.05	21,21,21,21	0
57	MG	1U	209	1/1	0.97	0.14	33,33,33,33	0
57	MG	1A	3338	1/1	0.97	0.11	40,40,40,40	0
57	MG	1A	3410	1/1	0.97	0.10	32,32,32,32	0
57	MG	2A	3070	1/1	0.97	0.10	26,26,26,26	0
57	MG	1V	205	1/1	0.97	0.07	29,29,29,29	0
57	MG	2A	3747	1/1	0.97	0.09	40,40,40,40	0
57	MG	1A	3226	1/1	0.97	0.14	38,38,38,38	0
57	MG	1A	3049	1/1	0.97	0.09	42,42,42,42	0
57	MG	1A	3228	1/1	0.97	0.07	50,50,50,50	0
57	MG	1A	3176	1/1	0.97	0.22	33,33,33,33	0
57	MG	2A	3076	1/1	0.97	0.06	40,40,40,40	0
57	MG	1A	4078	1/1	0.97	0.04	50,50,50,50	0
57	MG	2A	3078	1/1	0.97	0.09	51,51,51,51	0
57	MG	2A	3755	1/1	0.97	0.07	37,37,37,37	0
57	MG	1A	3177	1/1	0.97	0.17	25,25,25,25	0
57	MG	1A	3231	1/1	0.97	0.10	24,24,24,24	0
57	MG	2A	3516	1/1	0.97	0.12	27,27,27,27	0
57	MG	1A	3704	1/1	0.97	0.04	50,50,50,50	0
57	MG	2A	3294	1/1	0.97	0.15	59,59,59,59	0
57	MG	1A	3075	1/1	0.97	0.10	34,34,34,34	0
57	MG	1A	3498	1/1	0.97	0.17	32,32,32,32	0
57	MG	1A	3707	1/1	0.97	0.09	18,18,18,18	0
57	MG	1a	1740	1/1	0.97	0.05	68,68,68,68	0
57	MG	1A	3499	1/1	0.97	0.13	37,37,37,37	0
57	MG	1A	3098	1/1	0.97	0.19	35,35,35,35	0
57	MG	2A	3525	1/1	0.97	0.10	55,55,55,55	0
57	MG	10	101	1/1	0.97	0.14	36,36,36,36	0
57	MG	2A	3771	1/1	0.97	0.06	60,60,60,60	0
57	MG	1A	3347	1/1	0.97	0.06	39,39,39,39	0
57	MG	1A	4088	1/1	0.97	0.06	64,64,64,64	0
57	MG	2A	3304	1/1	0.97	0.05	37,37,37,37	0
57	MG	2A	3775	1/1	0.97	0.06	50,50,50,50	0
57	MG	10	104	1/1	0.97	0.11	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	3826	1/1	0.97	0.11	51,51,51,51	0
57	MG	1a	1748	1/1	0.97	0.06	57,57,57,57	0
57	MG	2A	3095	1/1	0.97	0.07	31,31,31,31	0
57	MG	1A	3103	1/1	0.97	0.14	27,27,27,27	0
57	MG	1A	3236	1/1	0.97	0.05	31,31,31,31	0
57	MG	1A	4093	1/1	0.97	0.04	57,57,57,57	0
57	MG	1A	3290	1/1	0.97	0.20	34,34,34,34	0
57	MG	1a	1756	1/1	0.97	0.06	54,54,54,54	0
57	MG	11	101	1/1	0.97	0.19	32,32,32,32	0
57	MG	1a	1758	1/1	0.97	0.09	42,42,42,42	0
57	MG	1A	3352	1/1	0.97	0.06	45,45,45,45	0
57	MG	1a	1763	1/1	0.97	0.07	54,54,54,54	0
57	MG	1A	3612	1/1	0.97	0.03	26,26,26,26	0
57	MG	1A	3291	1/1	0.97	0.17	27,27,27,27	0
57	MG	12	101	1/1	0.97	0.05	41,41,41,41	0
57	MG	1A	3717	1/1	0.97	0.04	14,14,14,14	0
57	MG	1A	3507	1/1	0.97	0.09	24,24,24,24	0
57	MG	1A	3354	1/1	0.97	0.14	38,38,38,38	0
57	MG	1A	4101	1/1	0.97	0.32	29,29,29,29	0
57	MG	1a	1773	1/1	0.97	0.05	49,49,49,49	0
57	MG	1A	3509	1/1	0.97	0.07	46,46,46,46	0
57	MG	15	101	1/1	0.97	0.15	25,25,25,25	0
57	MG	15	102	1/1	0.97	0.16	35,35,35,35	0
57	MG	1A	3617	1/1	0.97	0.06	38,38,38,38	0
57	MG	1A	3355	1/1	0.97	0.19	28,28,28,28	0
57	MG	1A	4105	1/1	0.97	0.04	60,60,60,60	0
57	MG	2A	3561	1/1	0.97	0.06	33,33,33,33	0
57	MG	1A	3963	1/1	0.97	0.20	21,21,21,21	0
57	MG	1A	3357	1/1	0.97	0.07	31,31,31,31	0
57	MG	1A	3965	1/1	0.97	0.04	27,27,27,27	0
57	MG	2a	1735	1/1	0.97	0.07	60,60,60,60	0
57	MG	2A	3122	1/1	0.97	0.09	42,42,42,42	0
57	MG	2A	3124	1/1	0.97	0.05	33,33,33,33	0
57	MG	1A	3050	1/1	0.97	0.05	43,43,43,43	0
57	MG	2A	3569	1/1	0.97	0.08	51,51,51,51	0
57	MG	2A	3339	1/1	0.97	0.10	47,47,47,47	0
57	MG	2A	3813	1/1	0.97	0.07	48,48,48,48	0
57	MG	1A	3359	1/1	0.97	0.24	38,38,38,38	0
57	MG	2A	3127	1/1	0.97	0.12	32,32,32,32	0
57	MG	1A	3183	1/1	0.97	0.09	16,16,16,16	0
57	MG	2A	3817	1/1	0.97	0.07	51,51,51,51	0
57	MG	18	103	1/1	0.97	0.10	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	3294	1/1	0.97	0.21	35,35,35,35	0
57	MG	1A	3516	1/1	0.97	0.09	33,33,33,33	0
57	MG	1A	4114	1/1	0.97	0.09	28,28,28,28	0
57	MG	1A	3517	1/1	0.97	0.13	26,26,26,26	0
57	MG	1A	3137	1/1	0.97	0.18	37,37,37,37	0
57	MG	1a	1793	1/1	0.97	0.11	55,55,55,55	0
57	MG	1A	3974	1/1	0.97	0.08	28,28,28,28	0
57	MG	2A	3137	1/1	0.97	0.05	35,35,35,35	0
57	MG	1A	3186	1/1	0.97	0.09	32,32,32,32	0
57	MG	1A	3628	1/1	0.97	0.09	33,33,33,33	0
57	MG	1A	3435	1/1	0.97	0.07	41,41,41,41	0
57	MG	1B	203	1/1	0.97	0.10	46,46,46,46	0
57	MG	2A	3831	1/1	0.97	0.07	61,61,61,61	0
57	MG	1B	204	1/1	0.97	0.21	48,48,48,48	0
57	MG	1a	1609	1/1	0.97	0.05	42,42,42,42	0
57	MG	2A	3834	1/1	0.97	0.12	48,48,48,48	0
57	MG	2A	3146	1/1	0.97	0.10	45,45,45,45	0
57	MG	1A	3077	1/1	0.97	0.13	27,27,27,27	0
57	MG	1A	3631	1/1	0.97	0.06	19,19,19,19	0
57	MG	1a	1803	1/1	0.97	0.07	54,54,54,54	0
57	MG	2A	3153	1/1	0.97	0.05	33,33,33,33	0
57	MG	1A	3980	1/1	0.97	0.06	47,47,47,47	0
57	MG	2A	3597	1/1	0.97	0.08	48,48,48,48	0
57	MG	1A	3737	1/1	0.97	0.06	23,23,23,23	0
57	MG	1A	3739	1/1	0.97	0.05	51,51,51,51	0
57	MG	2A	3157	1/1	0.97	0.08	37,37,37,37	0
57	MG	1A	3983	1/1	0.97	0.09	48,48,48,48	0
57	MG	1B	211	1/1	0.97	0.11	44,44,44,44	0
57	MG	1A	3740	1/1	0.97	0.07	34,34,34,34	0
57	MG	2A	3161	1/1	0.97	0.10	53,53,53,53	0
57	MG	1A	3011	1/1	0.97	0.04	25,25,25,25	0
57	MG	1A	3742	1/1	0.97	0.03	16,16,16,16	0
57	MG	1A	3987	1/1	0.97	0.05	35,35,35,35	0
57	MG	2A	3608	1/1	0.97	0.07	36,36,36,36	0
57	MG	1a	1813	1/1	0.97	0.05	37,37,37,37	0
57	MG	1A	3366	1/1	0.97	0.04	23,23,23,23	0
57	MG	1A	3368	1/1	0.97	0.11	40,40,40,40	0
57	MG	2A	3169	1/1	0.97	0.23	51,51,51,51	0
57	MG	1B	218	1/1	0.97	0.06	41,41,41,41	0
57	MG	1A	3140	1/1	0.97	0.07	31,31,31,31	0
57	MG	1A	3636	1/1	0.97	0.06	22,22,22,22	0
57	MG	1A	3747	1/1	0.97	0.04	53,53,53,53	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	3531	1/1	0.97	0.08	18,18,18,18	0
57	MG	1a	1630	1/1	0.97	0.10	39,39,39,39	0
57	MG	2D	305	1/1	0.97	0.05	31,31,31,31	0
57	MG	2D	307	1/1	0.97	0.21	48,48,48,48	0
57	MG	2A	3620	1/1	0.97	0.13	46,46,46,46	0
57	MG	1A	3749	1/1	0.97	0.05	32,32,32,32	0
57	MG	2A	3177	1/1	0.97	0.06	48,48,48,48	0
57	MG	2A	3386	1/1	0.97	0.07	34,34,34,34	0
57	MG	1A	3867	1/1	0.97	0.07	39,39,39,39	0
57	MG	2E	304	1/1	0.97	0.09	36,36,36,36	0
57	MG	1A	3190	1/1	0.97	0.09	36,36,36,36	0
57	MG	1A	3640	1/1	0.97	0.07	21,21,21,21	0
57	MG	1A	3641	1/1	0.97	0.04	24,24,24,24	0
57	MG	1A	3009	1/1	0.97	0.08	26,26,26,26	0
57	MG	2F	301	1/1	0.97	0.07	39,39,39,39	0
57	MG	2A	3629	1/1	0.97	0.05	25,25,25,25	0
57	MG	1A	3872	1/1	0.97	0.06	30,30,30,30	0
57	MG	1j	201	1/1	0.97	0.09	63,63,63,63	0
57	MG	1A	3108	1/1	0.97	0.14	23,23,23,23	0
57	MG	1A	3056	1/1	0.97	0.10	39,39,39,39	0
57	MG	1A	3057	1/1	0.97	0.06	30,30,30,30	0
57	MG	1A	3646	1/1	0.97	0.06	15,15,15,15	0
57	MG	1A	3446	1/1	0.97	0.15	48,48,48,48	0
57	MG	1A	3541	1/1	0.97	0.12	31,31,31,31	0
57	MG	1A	3084	1/1	0.97	0.06	49,49,49,49	0
57	MG	1a	1648	1/1	0.97	0.06	49,49,49,49	0
57	MG	1w	103	1/1	0.97	0.07	53,53,53,53	0
57	MG	1A	3882	1/1	0.97	0.19	51,51,51,51	0
57	MG	1D	301	1/1	0.97	0.11	25,25,25,25	0
57	MG	1A	3543	1/1	0.97	0.07	31,31,31,31	0
57	MG	1A	3152	1/1	0.97	0.07	37,37,37,37	0
57	MG	1A	3449	1/1	0.97	0.14	46,46,46,46	0
57	MG	1D	306	1/1	0.97	0.06	30,30,30,30	0
57	MG	1D	309	1/1	0.97	0.08	39,39,39,39	0
57	MG	2T	203	1/1	0.97	0.17	49,49,49,49	0
57	MG	1x	102	1/1	0.97	0.26	58,58,58,58	0
57	MG	2a	1827	1/1	0.97	0.04	73,73,73,73	0
57	MG	1A	3153	1/1	0.97	0.12	29,29,29,29	0
57	MG	1D	311	1/1	0.97	0.17	24,24,24,24	0
57	MG	2V	201	1/1	0.97	0.20	45,45,45,45	0
57	MG	1A	3768	1/1	0.97	0.06	16,16,16,16	0
57	MG	2d	301	1/1	0.97	0.12	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	3548	1/1	0.97	0.09	40,40,40,40	0
57	MG	1A	3771	1/1	0.97	0.22	20,20,20,20	0
57	MG	2X	102	1/1	0.97	0.11	47,47,47,47	0
57	MG	2Y	201	1/1	0.97	0.13	48,48,48,48	0
57	MG	1A	3549	1/1	0.97	0.09	39,39,39,39	0
57	MG	1E	302	1/1	0.97	0.12	36,36,36,36	0
57	MG	1a	1663	1/1	0.97	0.12	49,49,49,49	0
57	MG	1E	305	1/1	0.97	0.12	26,26,26,26	0
57	MG	1A	3550	1/1	0.97	0.12	36,36,36,36	0
57	MG	1A	3201	1/1	0.97	0.06	37,37,37,37	0
57	MG	1A	3040	1/1	0.97	0.07	27,27,27,27	0
57	MG	1E	311	1/1	0.97	0.10	20,20,20,20	0
57	MG	1A	3896	1/1	0.97	0.04	54,54,54,54	0
57	MG	2A	3217	1/1	0.97	0.25	41,41,41,41	0
57	MG	1A	3021	1/1	0.97	0.07	36,36,36,36	0
57	MG	2A	3219	1/1	0.97	0.26	32,32,32,32	0
57	MG	2A	3005	1/1	0.97	0.12	45,45,45,45	0
57	MG	1A	4026	1/1	0.97	0.06	39,39,39,39	0
57	MG	1A	4027	1/1	0.97	0.10	11,11,11,11	0
57	MG	2A	3008	1/1	0.97	0.07	38,38,38,38	0
57	MG	1F	303	1/1	0.97	0.11	31,31,31,31	0
57	MG	1F	304	1/1	0.97	0.06	29,29,29,29	0
57	MG	1A	3455	1/1	0.97	0.13	42,42,42,42	0
57	MG	2A	3014	1/1	0.97	0.08	55,55,55,55	0
57	MG	2A	3015	1/1	0.97	0.10	24,24,24,24	0
57	MG	1A	3259	1/1	0.97	0.21	34,34,34,34	0
57	MG	2A	3443	1/1	0.97	0.08	56,56,56,56	0
57	MG	1A	3557	1/1	0.97	0.19	32,32,32,32	0
57	MG	1a	1678	1/1	0.97	0.05	50,50,50,50	0
57	MG	1A	3260	1/1	0.97	0.16	39,39,39,39	0
57	MG	1A	4032	1/1	0.97	0.07	43,43,43,43	0
57	MG	1A	3117	1/1	0.97	0.13	37,37,37,37	0
57	MG	1A	3316	1/1	0.97	0.15	29,29,29,29	0
60	ZN	2Y	202	1/1	0.97	0.05	87,87,87,87	0
57	MG	1A	3262	1/1	0.97	0.13	31,31,31,31	0
60	ZN	29	501	1/1	0.97	0.05	70,70,70,70	0
60	ZN	2n	501	1/1	0.97	0.05	83,83,83,83	0
62	PHE	1w	110	11/12	0.97	0.09	14,19,25,25	0
57	MG	1A	3162	1/1	0.97	0.08	23,23,23,23	0
57	MG	1A	3208	1/1	0.97	0.08	24,24,24,24	0
57	MG	2A	3453	1/1	0.97	0.08	13,13,13,13	0
57	MG	1D	305	1/1	0.98	0.09	17,17,17,17	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	0.98	0.17	25,25,25,25	0
57	MG	1A	3757	1/1	0.98	0.05	39,39,39,39	0
57	MG	2A	3841	1/1	0.98	0.06	58,58,58,58	0
57	MG	2A	3021	1/1	0.98	0.09	33,33,33,33	0
57	MG	1D	307	1/1	0.98	0.04	29,29,29,29	0
57	MG	1a	1731	1/1	0.98	0.05	43,43,43,43	0
57	MG	1A	3497	1/1	0.98	0.12	37,37,37,37	0
57	MG	1A	3668	1/1	0.98	0.09	29,29,29,29	0
57	MG	2A	3497	1/1	0.98	0.06	36,36,36,36	0
57	MG	18	102	1/1	0.98	0.11	31,31,31,31	0
57	MG	1A	3580	1/1	0.98	0.04	29,29,29,29	0
57	MG	2A	3337	1/1	0.98	0.06	35,35,35,35	0
57	MG	2A	3028	1/1	0.98	0.07	38,38,38,38	0
57	MG	1A	3128	1/1	0.98	0.28	27,27,27,27	0
57	MG	1A	3583	1/1	0.98	0.05	26,26,26,26	0
57	MG	2A	3678	1/1	0.98	0.08	38,38,38,38	0
57	MG	2A	3504	1/1	0.98	0.08	33,33,33,33	0
57	MG	1A	3129	1/1	0.98	0.10	36,36,36,36	0
57	MG	1A	3235	1/1	0.98	0.06	26,26,26,26	0
57	MG	1E	301	1/1	0.98	0.12	25,25,25,25	0
57	MG	1A	3069	1/1	0.98	0.22	43,43,43,43	0
57	MG	1E	303	1/1	0.98	0.07	29,29,29,29	0
57	MG	1A	3181	1/1	0.98	0.09	28,28,28,28	0
57	MG	2D	301	1/1	0.98	0.09	34,34,34,34	0
57	MG	1A	3860	1/1	0.98	0.06	35,35,35,35	0
57	MG	1E	307	1/1	0.98	0.04	35,35,35,35	0
57	MG	1E	308	1/1	0.98	0.05	38,38,38,38	0
57	MG	1A	3767	1/1	0.98	0.04	16,16,16,16	0
57	MG	2D	306	1/1	0.98	0.27	40,40,40,40	0
57	MG	1A	3131	1/1	0.98	0.09	27,27,27,27	0
57	MG	1A	3070	1/1	0.98	0.09	33,33,33,33	0
57	MG	1A	3770	1/1	0.98	0.05	16,16,16,16	0
57	MG	1A	3184	1/1	0.98	0.06	26,26,26,26	0
57	MG	1A	3966	1/1	0.98	0.04	49,49,49,49	0
57	MG	1a	1754	1/1	0.98	0.04	46,46,46,46	0
57	MG	1a	1755	1/1	0.98	0.05	48,48,48,48	0
57	MG	2a	1731	1/1	0.98	0.06	53,53,53,53	0
57	MG	1A	3071	1/1	0.98	0.10	24,24,24,24	0
57	MG	1F	301	1/1	0.98	0.10	32,32,32,32	0
57	MG	1F	302	1/1	0.98	0.09	23,23,23,23	0
57	MG	1a	1618	1/1	0.98	0.05	37,37,37,37	0
57	MG	2A	3526	1/1	0.98	0.07	36,36,36,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1a	1762	1/1	0.98	0.06	56,56,56,56	0
57	MG	2A	3528	1/1	0.98	0.08	59,59,59,59	0
57	MG	1A	4074	1/1	0.98	0.05	29,29,29,29	0
57	MG	1A	4075	1/1	0.98	0.19	29,29,29,29	0
57	MG	1A	3367	1/1	0.98	0.16	32,32,32,32	0
57	MG	1A	3097	1/1	0.98	0.04	24,24,24,24	0
57	MG	1A	3595	1/1	0.98	0.03	23,23,23,23	0
57	MG	2A	3213	1/1	0.98	0.07	45,45,45,45	0
57	MG	2a	1746	1/1	0.98	0.05	53,53,53,53	0
57	MG	1A	3135	1/1	0.98	0.15	25,25,25,25	0
57	MG	1a	1769	1/1	0.98	0.05	61,61,61,61	0
57	MG	1a	1770	1/1	0.98	0.04	63,63,63,63	0
57	MG	1F	312	1/1	0.98	0.09	45,45,45,45	0
57	MG	1A	3020	1/1	0.98	0.06	24,24,24,24	0
57	MG	1A	3598	1/1	0.98	0.06	22,22,22,22	0
57	MG	2A	3717	1/1	0.98	0.09	60,60,60,60	0
57	MG	1A	3099	1/1	0.98	0.21	31,31,31,31	0
57	MG	1A	3100	1/1	0.98	0.19	22,22,22,22	0
57	MG	1A	3191	1/1	0.98	0.14	25,25,25,25	0
57	MG	1A	3877	1/1	0.98	0.08	23,23,23,23	0
57	MG	1A	3192	1/1	0.98	0.04	32,32,32,32	0
57	MG	1A	3249	1/1	0.98	0.12	22,22,22,22	0
57	MG	1A	3309	1/1	0.98	0.04	36,36,36,36	0
57	MG	1A	3605	1/1	0.98	0.06	11,11,11,11	0
57	MG	1A	4090	1/1	0.98	0.05	33,33,33,33	0
57	MG	1A	3101	1/1	0.98	0.04	33,33,33,33	0
57	MG	1A	3033	1/1	0.98	0.05	40,40,40,40	0
57	MG	1A	3608	1/1	0.98	0.09	18,18,18,18	0
57	MG	1a	1641	1/1	0.98	0.11	35,35,35,35	0
57	MG	1a	1642	1/1	0.98	0.10	41,41,41,41	0
57	MG	1A	3520	1/1	0.98	0.13	26,26,26,26	0
57	MG	1a	1644	1/1	0.98	0.04	41,41,41,41	0
57	MG	1P	201	1/1	0.98	0.20	26,26,26,26	0
57	MG	1A	3006	1/1	0.98	0.05	32,32,32,32	0
57	MG	1A	3196	1/1	0.98	0.16	36,36,36,36	0
57	MG	1P	206	1/1	0.98	0.07	35,35,35,35	0
57	MG	1A	3255	1/1	0.98	0.07	25,25,25,25	0
57	MG	2A	3564	1/1	0.98	0.04	38,38,38,38	0
57	MG	1Q	202	1/1	0.98	0.07	20,20,20,20	0
57	MG	1A	3524	1/1	0.98	0.14	35,35,35,35	0
57	MG	1A	3525	1/1	0.98	0.11	27,27,27,27	0
57	MG	1A	3891	1/1	0.98	0.10	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	1A	3256	1/1	0.98	0.23	33,33,33,33	0
57	MG	1A	3143	1/1	0.98	0.07	30,30,30,30	0
57	MG	2A	3571	1/1	0.98	0.08	27,27,27,27	0
57	MG	2A	3403	1/1	0.98	0.09	17,17,17,17	0
57	MG	2A	3573	1/1	0.98	0.12	39,39,39,39	0
57	MG	1A	3319	1/1	0.98	0.10	34,34,34,34	0
57	MG	1A	3007	1/1	0.98	0.10	23,23,23,23	0
57	MG	1A	3052	1/1	0.98	0.10	33,33,33,33	0
57	MG	1A	3148	1/1	0.98	0.12	26,26,26,26	0
57	MG	1A	3053	1/1	0.98	0.14	40,40,40,40	0
57	MG	1A	3078	1/1	0.98	0.13	36,36,36,36	0
57	MG	1A	3536	1/1	0.98	0.10	32,32,32,32	0
57	MG	1A	3004	1/1	0.98	0.06	37,37,37,37	0
57	MG	2A	3757	1/1	0.98	0.04	48,48,48,48	0
57	MG	1A	3460	1/1	0.98	0.20	40,40,40,40	0
57	MG	1A	3017	1/1	0.98	0.11	26,26,26,26	0
57	MG	1A	3393	1/1	0.98	0.16	33,33,33,33	0
57	MG	1A	3156	1/1	0.98	0.19	32,32,32,32	0
57	MG	2A	3416	1/1	0.98	0.04	23,23,23,23	0
57	MG	1A	3081	1/1	0.98	0.22	42,42,42,42	0
57	MG	1A	3209	1/1	0.98	0.10	28,28,28,28	0
57	MG	1A	3545	1/1	0.98	0.03	27,27,27,27	0
57	MG	1U	208	1/1	0.98	0.22	34,34,34,34	0
57	MG	1A	4011	1/1	0.98	0.04	31,31,31,31	0
57	MG	1U	210	1/1	0.98	0.14	29,29,29,29	0
57	MG	1A	3041	1/1	0.98	0.16	28,28,28,28	0
57	MG	1V	201	1/1	0.98	0.16	27,27,27,27	0
57	MG	1V	202	1/1	0.98	0.17	28,28,28,28	0
57	MG	1A	3159	1/1	0.98	0.07	31,31,31,31	0
57	MG	1A	3332	1/1	0.98	0.16	30,30,30,30	0
57	MG	1A	3161	1/1	0.98	0.14	29,29,29,29	0
57	MG	1A	3213	1/1	0.98	0.18	42,42,42,42	0
57	MG	1A	3335	1/1	0.98	0.18	34,34,34,34	0
57	MG	1A	3018	1/1	0.98	0.28	46,46,46,46	0
57	MG	1A	3639	1/1	0.98	0.06	18,18,18,18	0
57	MG	1A	3273	1/1	0.98	0.09	32,32,32,32	0
57	MG	1a	1685	1/1	0.98	0.13	37,37,37,37	0
57	MG	1X	103	1/1	0.98	0.09	41,41,41,41	0
57	MG	1m	3001	1/1	0.98	0.08	51,51,51,51	0
57	MG	1X	104	1/1	0.98	0.10	32,32,32,32	0
57	MG	1A	3215	1/1	0.98	0.28	33,33,33,33	0
57	MG	2A	3439	1/1	0.98	0.04	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	3216	1/1	0.98	0.08	25,25,25,25	0
57	MG	2A	3441	1/1	0.98	0.07	58,58,58,58	0
57	MG	1A	3823	1/1	0.98	0.23	32,32,32,32	0
57	MG	1Y	202	1/1	0.98	0.20	41,41,41,41	0
57	MG	1A	3217	1/1	0.98	0.12	23,23,23,23	0
57	MG	1A	4025	1/1	0.98	0.04	38,38,38,38	0
57	MG	1A	3115	1/1	0.98	0.13	28,28,28,28	0
57	MG	1A	3278	1/1	0.98	0.03	26,26,26,26	0
57	MG	1A	3479	1/1	0.98	0.23	42,42,42,42	0
57	MG	1A	3116	1/1	0.98	0.19	27,27,27,27	0
57	MG	1A	3648	1/1	0.98	0.05	23,23,23,23	0
57	MG	1A	3028	1/1	0.98	0.18	30,30,30,30	0
57	MG	2f	201	1/1	0.98	0.14	42,42,42,42	0
57	MG	1A	3482	1/1	0.98	0.14	29,29,29,29	0
57	MG	1A	3012	1/1	0.98	0.07	21,21,21,21	0
57	MG	1A	3061	1/1	0.98	0.14	33,33,33,33	0
57	MG	1A	3062	1/1	0.98	0.14	46,46,46,46	0
57	MG	1A	3170	1/1	0.98	0.12	38,38,38,38	0
57	MG	2A	3143	1/1	0.98	0.12	44,44,44,44	0
57	MG	2a	1659	1/1	0.98	0.08	42,42,42,42	0
57	MG	1A	3487	1/1	0.98	0.11	25,25,25,25	0
57	MG	2A	3145	1/1	0.98	0.08	31,31,31,31	0
57	MG	11	102	1/1	0.98	0.04	29,29,29,29	0
57	MG	2A	3147	1/1	0.98	0.06	56,56,56,56	0
57	MG	1A	3088	1/1	0.98	0.10	17,17,17,17	0
57	MG	2A	3810	1/1	0.98	0.09	33,33,33,33	0
57	MG	1A	3838	1/1	0.98	0.21	27,27,27,27	0
57	MG	2A	3150	1/1	0.98	0.19	39,39,39,39	0
57	MG	2A	3465	1/1	0.98	0.06	32,32,32,32	0
57	MG	1A	4041	1/1	0.98	0.06	31,31,31,31	0
57	MG	2A	3152	1/1	0.98	0.14	44,44,44,44	0
57	MG	1A	3839	1/1	0.98	0.20	32,32,32,32	0
57	MG	1A	3418	1/1	0.98	0.11	35,35,35,35	0
57	MG	13	101	1/1	0.98	0.06	28,28,28,28	0
57	MG	1A	3571	1/1	0.98	0.04	29,29,29,29	0
57	MG	1A	3046	1/1	0.98	0.03	10,10,10,10	0
57	MG	1A	3942	1/1	0.98	0.03	34,34,34,34	0
57	MG	2A	3004	1/1	0.98	0.07	31,31,31,31	0
57	MG	1A	3066	1/1	0.98	0.16	27,27,27,27	0
57	MG	2x	106	1/1	0.98	0.04	29,29,29,29	0
57	MG	1A	3751	1/1	0.98	0.04	34,34,34,34	0
57	MG	1A	3174	1/1	0.98	0.13	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	3125	1/1	0.98	0.06	32,32,32,32	0
57	MG	2A	3010	1/1	0.98	0.06	45,45,45,45	0
57	MG	15	104	1/1	0.98	0.22	32,32,32,32	0
57	MG	2A	3166	1/1	0.98	0.09	30,30,30,30	0
60	ZN	14	102	1/1	0.98	0.07	79,79,79,79	0
57	MG	2A	3654	1/1	0.98	0.04	48,48,48,48	0
57	MG	1A	3067	1/1	0.98	0.05	11,11,11,11	0
60	ZN	25	105	1/1	0.98	0.04	67,67,67,67	0
57	MG	1a	1723	1/1	0.98	0.03	35,35,35,35	0
57	MG	15	106	1/1	0.98	0.13	43,43,43,43	0
61	SF4	2d	302	8/8	0.98	0.05	55,62,70,73	0
57	MG	1A	3356	1/1	0.98	0.24	36,36,36,36	0
57	MG	2A	3835	1/1	0.98	0.05	65,65,65,65	0
57	MG	2A	3016	1/1	0.98	0.10	39,39,39,39	0
57	MG	1A	3068	1/1	0.98	0.03	24,24,24,24	0
57	MG	2a	1709	1/1	0.99	0.18	38,38,38,38	0
57	MG	1A	3003	1/1	0.99	0.11	23,23,23,23	0
57	MG	1A	3532	1/1	0.99	0.13	29,29,29,29	0
57	MG	1A	3063	1/1	0.99	0.05	22,22,22,22	0
57	MG	1A	3027	1/1	0.99	0.12	25,25,25,25	0
57	MG	1P	204	1/1	0.99	0.11	25,25,25,25	0
57	MG	1A	3164	1/1	0.99	0.03	29,29,29,29	0
57	MG	1A	3065	1/1	0.99	0.09	11,11,11,11	0
57	MG	1A	3537	1/1	0.99	0.13	25,25,25,25	0
57	MG	1A	3043	1/1	0.99	0.03	29,29,29,29	0
57	MG	1Q	203	1/1	0.99	0.03	35,35,35,35	0
57	MG	2A	3123	1/1	0.99	0.07	39,39,39,39	0
57	MG	1D	308	1/1	0.99	0.07	33,33,33,33	0
57	MG	1A	3219	1/1	0.99	0.15	27,27,27,27	0
57	MG	1A	3124	1/1	0.99	0.03	37,37,37,37	0
57	MG	1A	3874	1/1	0.99	0.04	32,32,32,32	0
57	MG	1A	3054	1/1	0.99	0.05	16,16,16,16	0
57	MG	2A	3490	1/1	0.99	0.09	27,27,27,27	0
57	MG	2F	306	1/1	0.99	0.17	41,41,41,41	0
57	MG	1A	3109	1/1	0.99	0.12	30,30,30,30	0
57	MG	1A	3404	1/1	0.99	0.03	35,35,35,35	0
57	MG	1A	3582	1/1	0.99	0.04	30,30,30,30	0
57	MG	1A	4068	1/1	0.99	0.03	22,22,22,22	0
57	MG	2A	3646	1/1	0.99	0.03	28,28,28,28	0
57	MG	1A	3145	1/1	0.99	0.19	27,27,27,27	0
57	MG	1A	4070	1/1	0.99	0.05	11,11,11,11	0
57	MG	1a	1783	1/1	0.99	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	1E	304	1/1	0.99	0.08	25,25,25,25	0
57	MG	2a	1737	1/1	0.99	0.03	57,57,57,57	0
57	MG	1A	3094	1/1	0.99	0.07	33,33,33,33	0
57	MG	1A	3374	1/1	0.99	0.07	42,42,42,42	0
57	MG	1U	201	1/1	0.99	0.06	24,24,24,24	0
57	MG	1A	3666	1/1	0.99	0.06	10,10,10,10	0
57	MG	1A	3147	1/1	0.99	0.06	27,27,27,27	0
57	MG	1A	3254	1/1	0.99	0.08	22,22,22,22	0
57	MG	1a	1722	1/1	0.99	0.08	55,55,55,55	0
57	MG	1A	3013	1/1	0.99	0.03	19,19,19,19	0
57	MG	1A	3149	1/1	0.99	0.07	24,24,24,24	0
57	MG	2A	3660	1/1	0.99	0.04	32,32,32,32	0
57	MG	1A	3315	1/1	0.99	0.21	25,25,25,25	0
57	MG	1A	3591	1/1	0.99	0.05	39,39,39,39	0
57	MG	2A	3663	1/1	0.99	0.08	38,38,38,38	0
57	MG	1A	3150	1/1	0.99	0.17	26,26,26,26	0
57	MG	1A	3036	1/1	0.99	0.16	28,28,28,28	0
57	MG	1A	3318	1/1	0.99	0.20	33,33,33,33	0
57	MG	2A	3009	1/1	0.99	0.02	34,34,34,34	0
57	MG	1A	3555	1/1	0.99	0.10	30,30,30,30	0
57	MG	1A	4033	1/1	0.99	0.14	36,36,36,36	0
57	MG	1V	203	1/1	0.99	0.12	24,24,24,24	0
57	MG	1A	3202	1/1	0.99	0.07	37,37,37,37	0
57	MG	23	101	1/1	0.99	0.04	45,45,45,45	0
57	MG	2A	3084	1/1	0.99	0.13	36,36,36,36	0
57	MG	1F	305	1/1	0.99	0.04	34,34,34,34	0
57	MG	1F	306	1/1	0.99	0.06	22,22,22,22	0
57	MG	1F	307	1/1	0.99	0.11	28,28,28,28	0
57	MG	1A	3894	1/1	0.99	0.04	8,8,8,8	0
57	MG	1A	3037	1/1	0.99	0.19	26,26,26,26	0
57	MG	1W	203	1/1	0.99	0.13	35,35,35,35	0
57	MG	1A	3519	1/1	0.99	0.13	29,29,29,29	0
57	MG	1X	101	1/1	0.99	0.16	29,29,29,29	0
57	MG	1A	3897	1/1	0.99	0.09	34,34,34,34	0
57	MG	1A	3451	1/1	0.99	0.10	28,28,28,28	0
57	MG	1G	201	1/1	0.99	0.10	36,36,36,36	0
57	MG	1A	3029	1/1	0.99	0.07	30,30,30,30	0
57	MG	2A	3531	1/1	0.99	0.08	32,32,32,32	0
57	MG	2A	3532	1/1	0.99	0.06	34,34,34,34	0
57	MG	2A	3767	1/1	0.99	0.06	32,32,32,32	0
57	MG	1A	3724	1/1	0.99	0.07	32,32,32,32	0
57	MG	1A	3048	1/1	0.99	0.07	17,17,17,17	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	0.99	0.04	22,22,22,22	0
57	MG	1a	1749	1/1	0.99	0.04	65,65,65,65	0
58	K	1A	3528	1/1	0.99	0.04	36,36,36,36	0
57	MG	2A	3612	1/1	0.99	0.10	29,29,29,29	0
57	MG	1A	3155	1/1	0.99	0.09	12,12,12,12	0
57	MG	1A	3207	1/1	0.99	0.09	26,26,26,26	0
60	ZN	1Y	203	1/1	0.99	0.02	55,55,55,55	0
57	MG	1A	3997	1/1	0.99	0.05	43,43,43,43	0
60	ZN	15	108	1/1	0.99	0.02	42,42,42,42	0
60	ZN	1n	102	1/1	0.99	0.04	56,56,56,56	0
57	MG	1A	3685	1/1	0.99	0.07	19,19,19,19	0
57	MG	1A	3022	1/1	0.99	0.06	11,11,11,11	0
57	MG	1A	3031	1/1	0.99	0.23	29,29,29,29	0
57	MG	1A	3102	1/1	0.99	0.11	25,25,25,25	0
57	MG	1a	1627	1/1	0.99	0.14	26,26,26,26	0
61	SF4	1d	501	8/8	0.99	0.05	56,57,62,66	0
57	MG	1A	3136	1/1	0.99	0.07	26,26,26,26	0
57	MG	1A	3160	1/1	0.99	0.28	30,30,30,30	0
57	MG	1a	1760	1/1	0.99	0.06	56,56,56,56	0
57	MG	2A	3703	1/1	0.99	0.05	57,57,57,57	0
57	MG	1a	1761	1/1	0.99	0.03	44,44,44,44	0
60	ZN	19	102	1/1	1.00	0.03	34,34,34,34	0
57	MG	1A	3738	1/1	1.00	0.04	30,30,30,30	0
57	MG	1A	3035	1/1	1.00	0.12	17,17,17,17	0
57	MG	1A	3348	1/1	1.00	0.06	16,16,16,16	0
57	MG	1P	202	1/1	1.00	0.17	27,27,27,27	0
60	ZN	26	501	1/1	1.00	0.03	53,53,53,53	0
60	ZN	16	102	1/1	1.00	0.04	39,39,39,39	0

6.5 Other polymers (i)

There are no such residues in this entry.