Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 07:42 PM EDT

PDB ID	:	6ND5 / pdb_00006nd5
Title	:	Crystal structure of the Thermus thermophilus 70S ribosome in complex with chloramphenicol and bound to mRNA and A-, P-, and E-site tRNAs at 2.60A resolution
Authors	:	Svetlov, M.S.; Plessa, E.; Chen, C.-W.; Bougas, A.; Krokidis, M.G.; Dinos, G.P.; Polikanov, Y.S.
Deposited on	:	2018-12-13
Resolution	:	2.60 Å(reported)

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

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

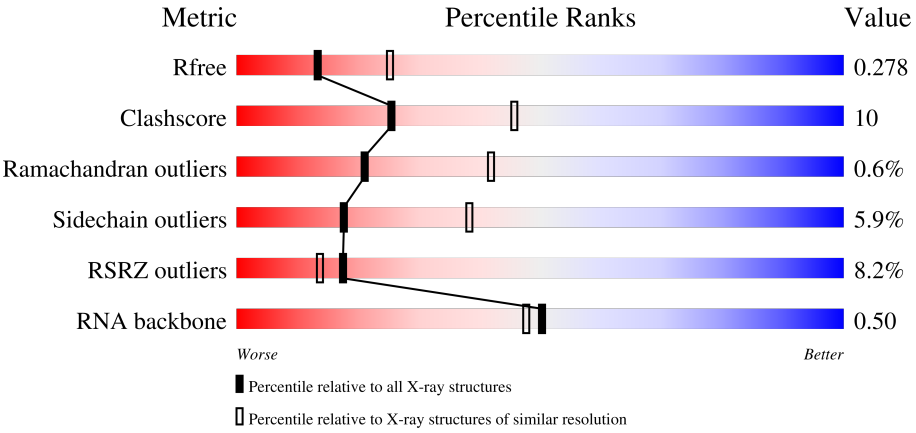
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 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.



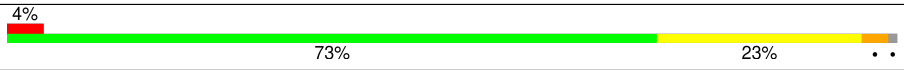
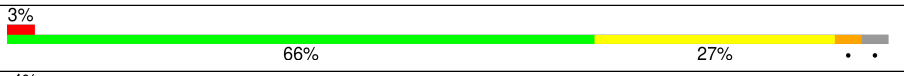
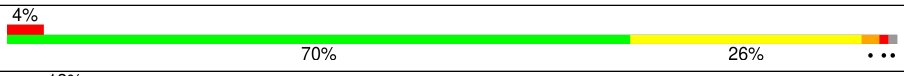
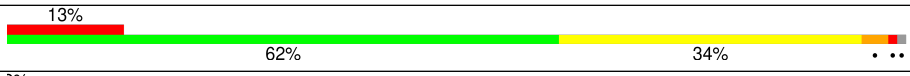
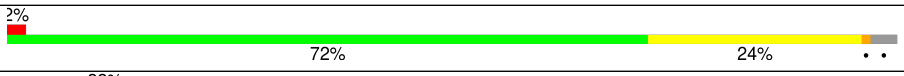
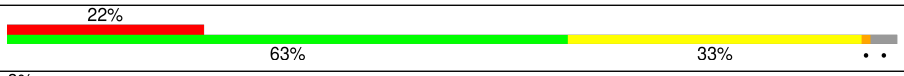
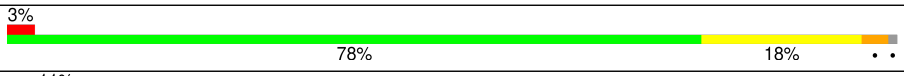
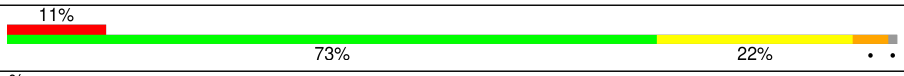
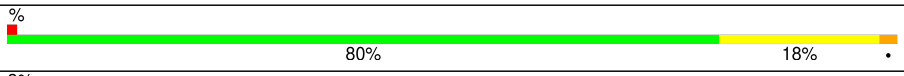
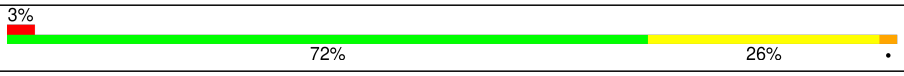
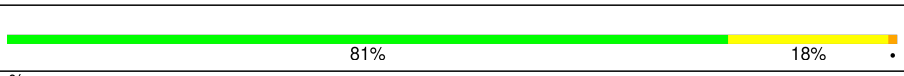
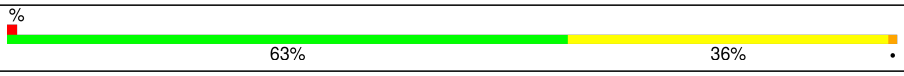
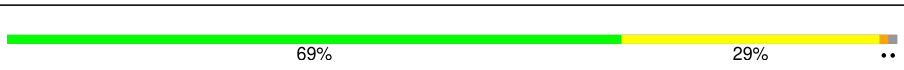
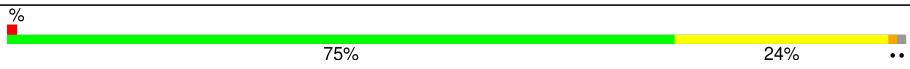
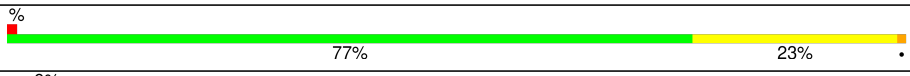
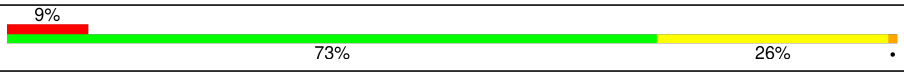
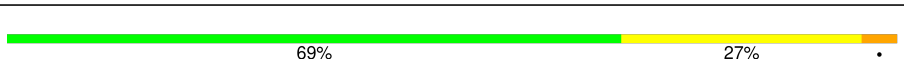
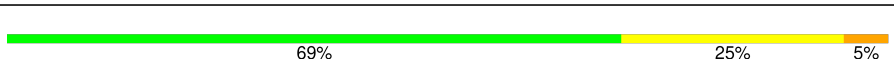
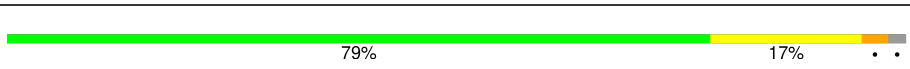
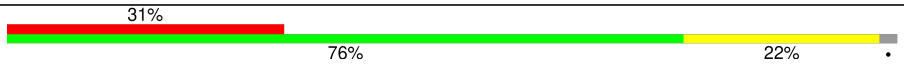
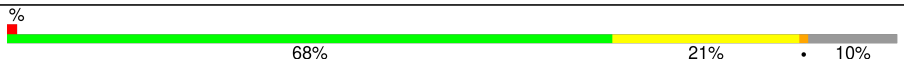
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)
RNA backbone	3983	1014 (2.84-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1A	2915	3% 61% 31% 7%
1	2A	2915	3% 54% 35% 7%
2	1B	121	71% 24%
2	2B	121	7% 44% 44% 12%

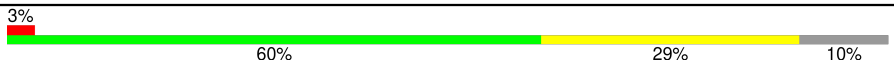
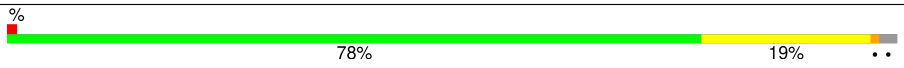
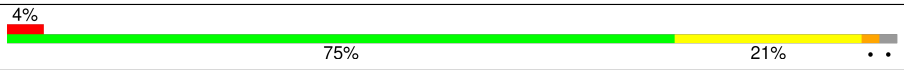
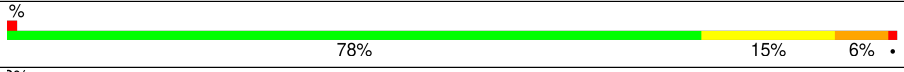
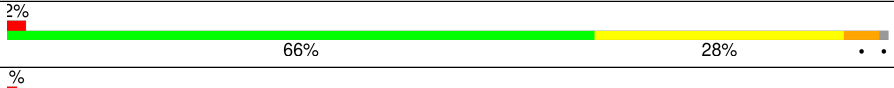
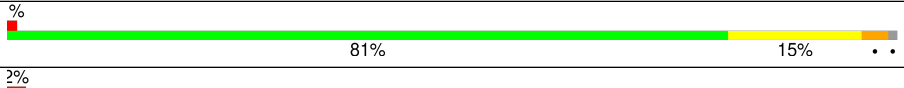
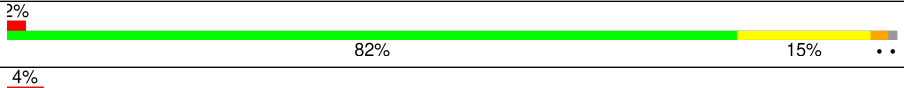
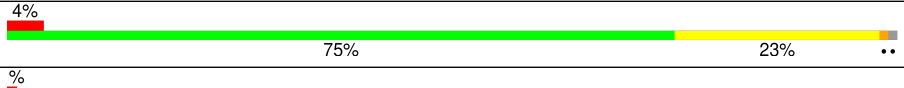
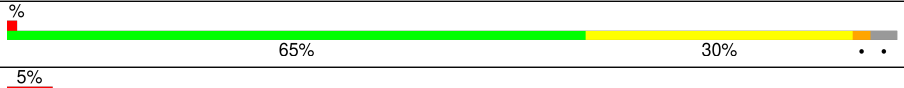
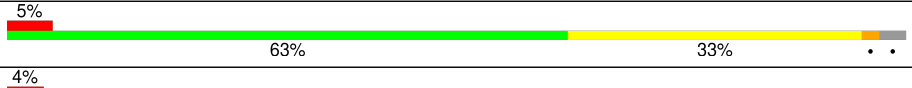
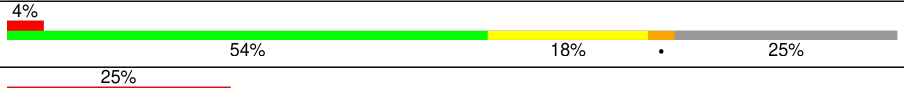
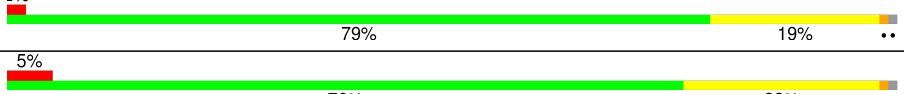
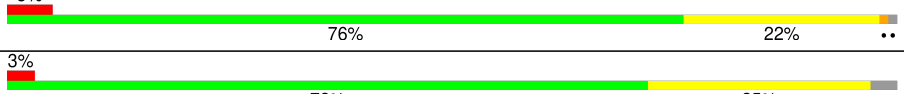
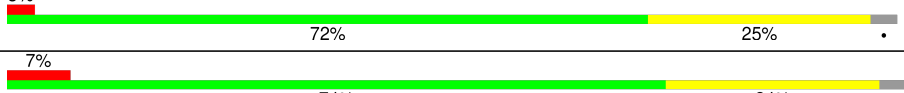
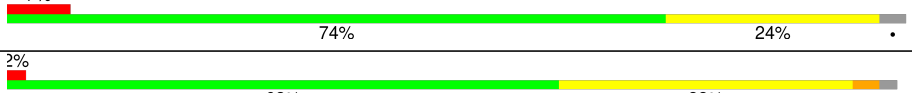
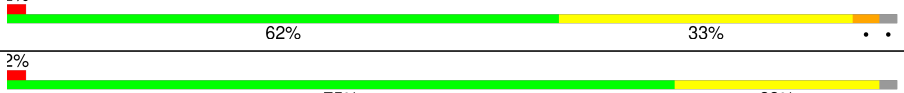
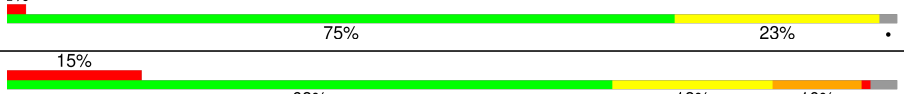
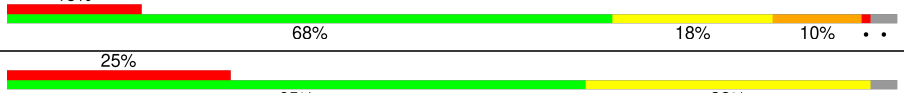
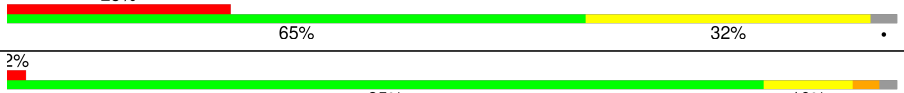
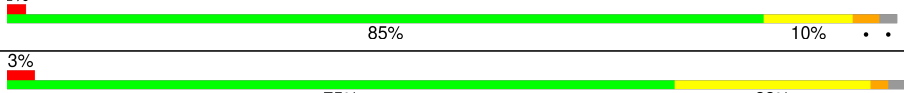
Continued on next page...

Continued from previous page...

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

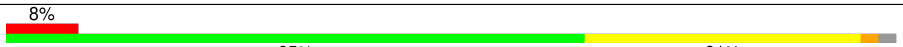
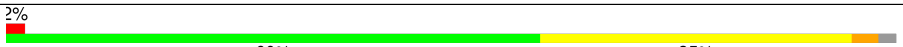
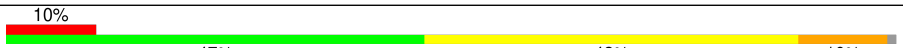
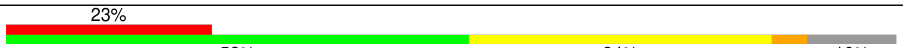
Continued on next page...

Continued from previous page...

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

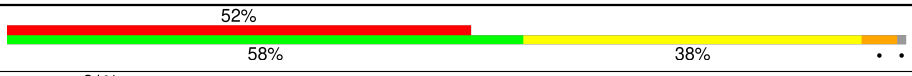
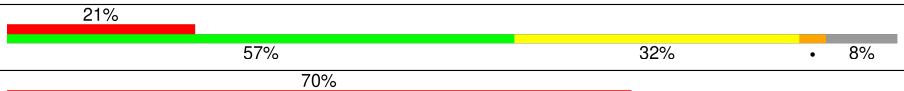
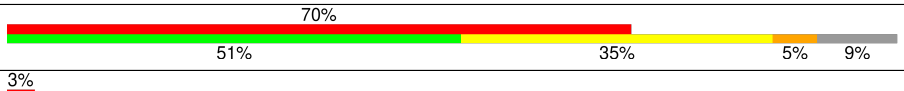
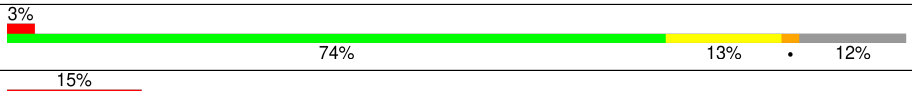
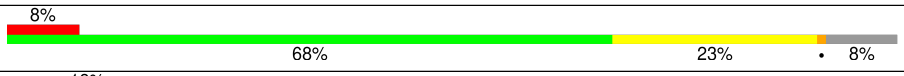
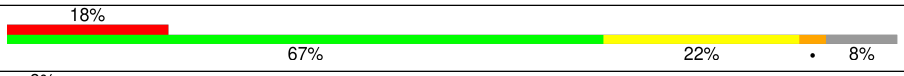
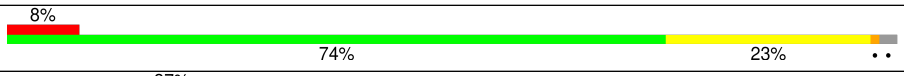
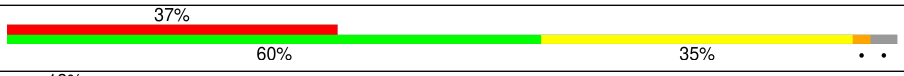
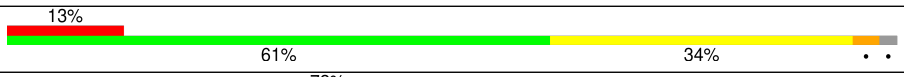
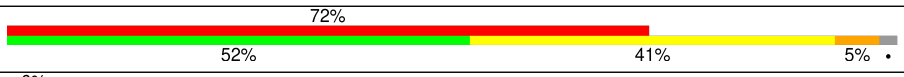
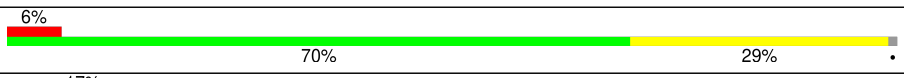
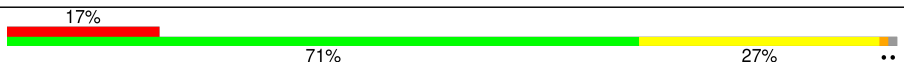
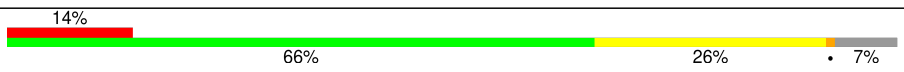
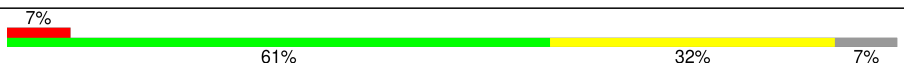
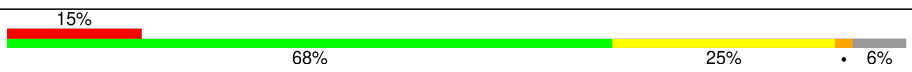
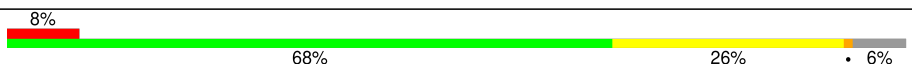
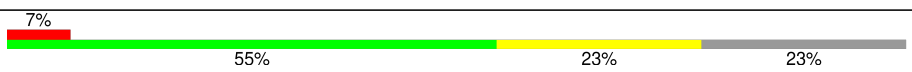
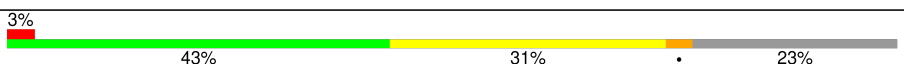
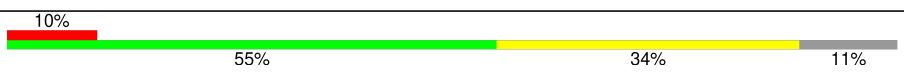
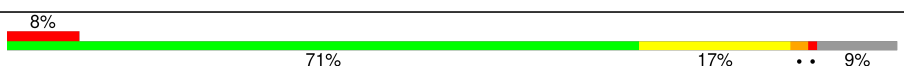
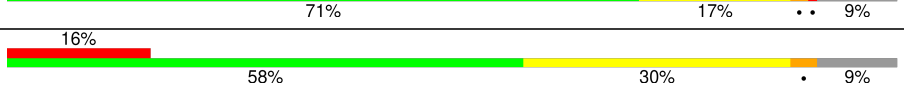
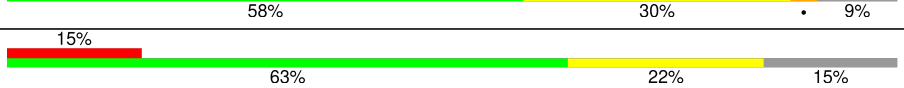
Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	1v	24	4% 38% 12% 46%
53	2v	24	33% 29% 12% 12% 46%
54	1w	76	20% 36% 34% 26%
54	1y	76	4% 42% 37% 16%
54	2w	76	30% 25% 46% 24% 5%
54	2y	76	13% 39% 37% 18%
55	1x	77	4% 64% 27% 8%
55	2x	77	3% 44% 44% 10%

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
60	SF4	1d	302	-	-	X	-
60	SF4	2d	302	-	-	X	-

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 300833 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	2O	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	1S	110	Total	C	N	O	0	0	0
			873	550	174	149			
14	2S	110	Total	C	N	O	0	0	0
			870	549	173	148			

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

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

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	1U	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			
16	2U	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			

- Molecule 17 is a protein called 50S ribosomal protein L21.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 53 is a RNA chain called mRNA.

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

- Molecule 54 is a RNA chain called A-site and E-site tRNAs.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1w	74	Total	C	N	O	P	S	0	0	0
			1592	713	285	518	74	2			
54	1y	74	Total	C	N	O	P	S	0	0	0
			1585	707	285	518	74	1			
54	2w	72	Total	C	N	O	P	S	0	0	0
			1544	690	278	502	72	2			
54	2y	73	Total	C	N	O	P	S	0	0	0
			1565	698	283	510	73	1			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
55	1x	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			
55	2x	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1A	1101	Total	Mg	0	0
			1101	1101		
56	1B	39	Total	Mg	0	0
			39	39		
56	1D	13	Total	Mg	0	0
			13	13		
56	1E	15	Total	Mg	0	0
			15	15		
56	1F	10	Total	Mg	0	0
			10	10		
56	1G	4	Total	Mg	0	0
			4	4		
56	1I	1	Total	Mg	0	0
			1	1		
56	1N	6	Total	Mg	0	0
			6	6		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	1O	5	Total Mg 5 5	0	0
56	1P	9	Total Mg 9 9	0	0
56	1Q	8	Total Mg 8 8	0	0
56	1R	3	Total Mg 3 3	0	0
56	1S	3	Total Mg 3 3	0	0
56	1T	4	Total Mg 4 4	0	0
56	1U	12	Total Mg 12 12	0	0
56	1V	7	Total Mg 7 7	0	0
56	1W	5	Total Mg 5 5	0	0
56	1X	5	Total Mg 5 5	0	0
56	1Y	3	Total Mg 3 3	0	0
56	1Z	3	Total Mg 3 3	0	0
56	10	6	Total Mg 6 6	0	0
56	11	5	Total Mg 5 5	0	0
56	12	2	Total Mg 2 2	0	0
56	13	3	Total Mg 3 3	0	0
56	14	1	Total Mg 1 1	0	0
56	15	5	Total Mg 5 5	0	0
56	16	3	Total Mg 3 3	0	0
56	17	8	Total Mg 8 8	0	0
56	18	7	Total Mg 7 7	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	19	1	Total Mg 1 1	0	0
56	1a	233	Total Mg 233 233	0	0
56	1b	2	Total Mg 2 2	0	0
56	1d	1	Total Mg 1 1	0	0
56	1e	2	Total Mg 2 2	0	0
56	1f	2	Total Mg 2 2	0	0
56	1h	1	Total Mg 1 1	0	0
56	1l	2	Total Mg 2 2	0	0
56	1m	2	Total Mg 2 2	0	0
56	1n	1	Total Mg 1 1	0	0
56	1s	1	Total Mg 1 1	0	0
56	1t	1	Total Mg 1 1	0	0
56	1v	1	Total Mg 1 1	0	0
56	1w	12	Total Mg 12 12	0	0
56	1x	18	Total Mg 18 18	0	0
56	2A	887	Total Mg 887 887	0	0
56	2B	20	Total Mg 20 20	0	0
56	2D	10	Total Mg 10 10	0	0
56	2E	4	Total Mg 4 4	0	0
56	2F	6	Total Mg 6 6	0	0
56	2G	1	Total Mg 1 1	0	0

Continued on next page...

Continued from previous page...

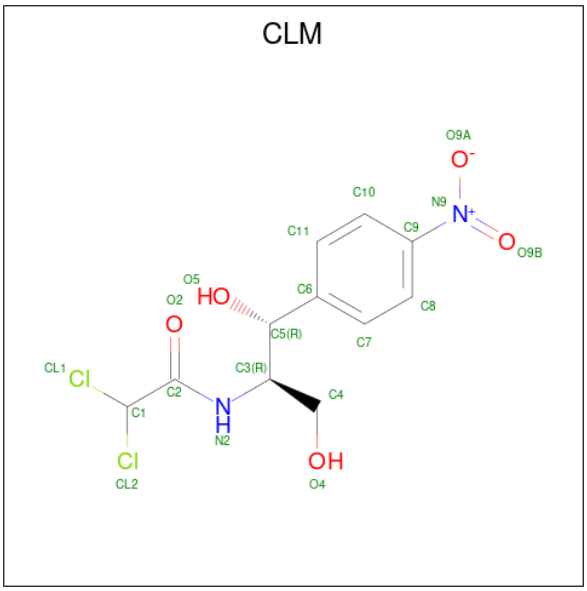
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	2N	1	Total Mg 1 1	0	0
56	2O	1	Total Mg 1 1	0	0
56	2P	4	Total Mg 4 4	0	0
56	2Q	4	Total Mg 4 4	0	0
56	2R	2	Total Mg 2 2	0	0
56	2T	4	Total Mg 4 4	0	0
56	2U	3	Total Mg 3 3	0	0
56	2V	3	Total Mg 3 3	0	0
56	2W	3	Total Mg 3 3	0	0
56	2X	1	Total Mg 1 1	0	0
56	2Z	1	Total Mg 1 1	0	0
56	20	3	Total Mg 3 3	0	0
56	21	1	Total Mg 1 1	0	0
56	23	3	Total Mg 3 3	0	0
56	25	5	Total Mg 5 5	0	0
56	27	2	Total Mg 2 2	0	0
56	28	3	Total Mg 3 3	0	0
56	2a	241	Total Mg 241 241	0	0
56	2d	1	Total Mg 1 1	0	0
56	2e	1	Total Mg 1 1	0	0
56	2f	2	Total Mg 2 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	2g	1	Total Mg 1 1	0	0
56	2i	1	Total Mg 1 1	0	0
56	2j	1	Total Mg 1 1	0	0
56	2k	1	Total Mg 1 1	0	0
56	2l	4	Total Mg 4 4	0	0
56	2m	1	Total Mg 1 1	0	0
56	2q	2	Total Mg 2 2	0	0
56	2r	1	Total Mg 1 1	0	0
56	2t	1	Total Mg 1 1	0	0
56	2v	1	Total Mg 1 1	0	0
56	2w	4	Total Mg 4 4	0	0
56	2x	5	Total Mg 5 5	0	0
56	2y	6	Total Mg 6 6	0	0

- Molecule 57 is CHLORAMPHENICOL (CCD ID: CLM) (formula: $C_{11}H_{12}Cl_2N_2O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
57	1A	1	Total	C	Cl	N	O	0	0
			20	11	2	2	5		
57	2A	1	Total	C	Cl	N	O	0	0
			20	11	2	2	5		

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

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

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

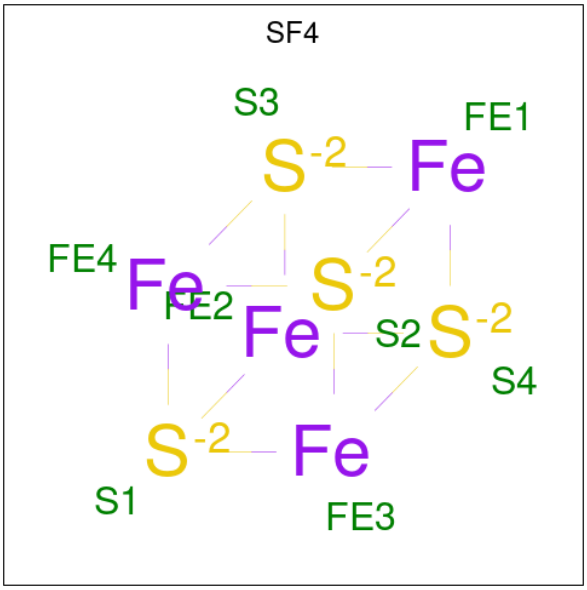
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1Y	1	Total	Zn	0	0
			1	1		
59	14	1	Total	Zn	0	0
			1	1		
59	15	1	Total	Zn	0	0
			1	1		
59	16	1	Total	Zn	0	0
			1	1		
59	19	1	Total	Zn	0	0
			1	1		

Continued on next page...

Continued from previous page...

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

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



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

- Molecule 61 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	3	Total O 3 3	0	0
61	1A	1	Total O 1 1	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	2	Total O 2 2	0	0
61	1A	4	Total O 4 4	0	0
61	1A	1	Total O 1 1	0	0
61	1A	4	Total O 4 4	0	0
61	1A	3	Total O 3 3	0	0
61	1A	4	Total O 4 4	0	0
61	1A	2	Total O 2 2	0	0
61	1A	2	Total O 2 2	0	0
61	1A	2	Total O 2 2	0	0
61	1A	2	Total O 2 2	0	0
61	1A	5	Total O 5 5	0	0
61	1A	4	Total O 4 4	0	0
61	1A	6	Total O 6 6	0	0
61	1A	1	Total O 1 1	0	0
61	1A	2	Total O 2 2	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	5	Total O 5 5	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	1	Total O 1 1	0	0
61	1A	2	Total O 2 2	0	0
61	1A	2	Total O 2 2	0	0
61	1A	5	Total O 5 5	0	0
61	1A	4	Total O 4 4	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	2	Total O 2 2	0	0
61	1A	4	Total O 4 4	0	0
61	1A	2	Total O 2 2	0	0
61	1A	2	Total O 2 2	0	0
61	1A	2	Total O 2 2	0	0
61	1A	4	Total O 4 4	0	0
61	1A	2	Total O 2 2	0	0
61	1A	4	Total O 4 4	0	0
61	1A	1	Total O 1 1	0	0
61	1A	2	Total O 2 2	0	0
61	1A	2	Total O 2 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	1	Total O 1 1	0	0
61	1A	5	Total O 5 5	0	0
61	1A	1	Total O 1 1	0	0
61	1A	4	Total O 4 4	0	0
61	1A	1	Total O 1 1	0	0
61	1A	3	Total O 3 3	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	2	Total O 2 2	0	0
61	1A	1	Total O 1 1	0	0
61	1A	4	Total O 4 4	0	0
61	1A	3	Total O 3 3	0	0
61	1A	4	Total O 4 4	0	0
61	1A	2	Total O 2 2	0	0
61	1A	1	Total O 1 1	0	0
61	1A	2	Total O 2 2	0	0
61	1A	4	Total O 4 4	0	0
61	1A	4	Total O 4 4	0	0
61	1A	5	Total O 5 5	0	0
61	1A	3	Total O 3 3	0	0
61	1A	4	Total O 4 4	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	5	Total O 5 5	0	0
61	1A	4	Total O 4 4	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	4	Total O 4 4	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	4	Total O 4 4	0	0
61	1A	4	Total O 4 4	0	0
61	1A	5	Total O 5 5	0	0
61	1A	4	Total O 4 4	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	2	Total O 2 2	0	0
61	1A	2	Total O 2 2	0	0
61	1A	4	Total O 4 4	0	0
61	1A	1	Total O 1 1	0	0
61	1A	5	Total O 5 5	0	0
61	1A	1	Total O 1 1	0	0
61	1A	4	Total O 4 4	0	0
61	1A	1	Total O 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	5	Total O 5 5	0	0
61	1A	4	Total O 4 4	0	0
61	1A	4	Total O 4 4	0	0
61	1A	4	Total O 4 4	0	0
61	1A	4	Total O 4 4	0	0
61	1A	3	Total O 3 3	0	0
61	1A	3	Total O 3 3	0	0
61	1A	4	Total O 4 4	0	0
61	1A	4	Total O 4 4	0	0
61	1A	4	Total O 4 4	0	0
61	1A	3	Total O 3 3	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	3	Total O 3 3	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	3	Total O 3 3	0	0
61	1A	3	Total O 3 3	0	0
61	1A	1	Total O 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	2	Total O 2 2	0	0
61	1A	1	Total O 1 1	0	0
61	1A	2	Total O 2 2	0	0
61	1A	1	Total O 1 1	0	0
61	1A	4	Total O 4 4	0	0
61	1A	1	Total O 1 1	0	0
61	1A	2	Total O 2 2	0	0
61	1A	2	Total O 2 2	0	0
61	1A	2	Total O 2 2	0	0
61	1A	3	Total O 3 3	0	0
61	1A	1	Total O 1 1	0	0
61	1A	3	Total O 3 3	0	0
61	1A	2	Total O 2 2	0	0
61	1A	6	Total O 6 6	0	0
61	1A	3	Total O 3 3	0	0
61	1A	2	Total O 2 2	0	0
61	1A	1	Total O 1 1	0	0
61	1A	2	Total O 2 2	0	0
61	1A	5	Total O 5 5	0	0
61	1A	2	Total O 2 2	0	0
61	1A	3	Total O 3 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	2	Total O 2 2	0	0
61	1A	6	Total O 6 6	0	0
61	1A	6	Total O 6 6	0	0
61	1A	4	Total O 4 4	0	0
61	1A	3	Total O 3 3	0	0
61	1A	3	Total O 3 3	0	0
61	1A	4	Total O 4 4	0	0
61	1A	3	Total O 3 3	0	0
61	1A	4	Total O 4 4	0	0
61	1A	2	Total O 2 2	0	0
61	1A	2	Total O 2 2	0	0
61	1A	6	Total O 6 6	0	0
61	1A	3	Total O 3 3	0	0
61	1A	4	Total O 4 4	0	0
61	1A	1	Total O 1 1	0	0
61	1A	5	Total O 5 5	0	0
61	1A	2	Total O 2 2	0	0
61	1A	2	Total O 2 2	0	0
61	1A	4	Total O 4 4	0	0
61	1A	2	Total O 2 2	0	0
61	1A	1	Total O 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	5	Total O 5 5	0	0
61	1A	4	Total O 4 4	0	0
61	1A	5	Total O 5 5	0	0
61	1A	6	Total O 6 6	0	0
61	1A	6	Total O 6 6	0	0
61	1A	5	Total O 5 5	0	0
61	1A	2	Total O 2 2	0	0
61	1A	2	Total O 2 2	0	0
61	1A	3	Total O 3 3	0	0
61	1A	4	Total O 4 4	0	0
61	1A	3	Total O 3 3	0	0
61	1A	6	Total O 6 6	0	0
61	1A	4	Total O 4 4	0	0
61	1A	3	Total O 3 3	0	0
61	1A	5	Total O 5 5	0	0
61	1A	3	Total O 3 3	0	0
61	1A	4	Total O 4 4	0	0
61	1A	4	Total O 4 4	0	0
61	1A	4	Total O 4 4	0	0
61	1A	3	Total O 3 3	0	0
61	1A	5	Total O 5 5	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	3	Total O 3 3	0	0
61	1A	4	Total O 4 4	0	0
61	1A	4	Total O 4 4	0	0
61	1A	3	Total O 3 3	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	4	Total O 4 4	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	4	Total O 4 4	0	0
61	1A	3	Total O 3 3	0	0
61	1A	3	Total O 3 3	0	0
61	1A	1	Total O 1 1	0	0
61	1A	5	Total O 5 5	0	0
61	1A	4	Total O 4 4	0	0
61	1A	1	Total O 1 1	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	2	Total O 2 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	2	Total O 2 2	0	0
61	1A	2	Total O 2 2	0	0
61	1A	2	Total O 2 2	0	0
61	1A	6	Total O 6 6	0	0
61	1A	4	Total O 4 4	0	0
61	1A	3	Total O 3 3	0	0
61	1A	4	Total O 4 4	0	0
61	1A	4	Total O 4 4	0	0
61	1A	3	Total O 3 3	0	0
61	1A	5	Total O 5 5	0	0
61	1A	2	Total O 2 2	0	0
61	1A	2	Total O 2 2	0	0
61	1A	1	Total O 1 1	0	0
61	1A	5	Total O 5 5	0	0
61	1A	6	Total O 6 6	0	0
61	1A	2	Total O 2 2	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	3	Total O 3 3	0	0
61	1A	1	Total O 1 1	0	0
61	1A	5	Total O 5 5	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	1	Total O 1 1	0	0
61	1A	3	Total O 3 3	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	2	Total O 2 2	0	0
61	1A	2	Total O 2 2	0	0
61	1A	1	Total O 1 1	0	0
61	1A	2	Total O 2 2	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	2	Total O 2 2	0	0
61	1A	1	Total O 1 1	0	0
61	1A	2	Total O 2 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	2	Total O 2 2	0	0
61	1A	4	Total O 4 4	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	3	Total O 3 3	0	0
61	1A	4	Total O 4 4	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	3	Total O 3 3	0	0
61	1A	6	Total O 6 6	0	0
61	1A	2	Total O 2 2	0	0
61	1A	3	Total O 3 3	0	0
61	1A	3	Total O 3 3	0	0
61	1A	2	Total O 2 2	0	0
61	1A	2	Total O 2 2	0	0
61	1A	2	Total O 2 2	0	0
61	1A	5	Total O 5 5	0	0
61	1A	1	Total O 1 1	0	0
61	1A	2	Total O 2 2	0	0
61	1A	3	Total O 3 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	3	Total O 3 3	0	0
61	1A	2	Total O 2 2	0	0
61	1A	1	Total O 1 1	0	0
61	1A	2	Total O 2 2	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	2	Total O 2 2	0	0
61	1A	6	Total O 6 6	0	0
61	1A	1	Total O 1 1	0	0
61	1A	2	Total O 2 2	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	2	Total O 2 2	0	0
61	1A	4	Total O 4 4	0	0
61	1A	1	Total O 1 1	0	0
61	1A	2	Total O 2 2	0	0
61	1A	5	Total O 5 5	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	2	Total O 2 2	0	0
61	1A	2	Total O 2 2	0	0
61	1A	6	Total O 6 6	0	0
61	1A	1	Total O 1 1	0	0
61	1A	3	Total O 3 3	0	0
61	1A	5	Total O 5 5	0	0
61	1A	6	Total O 6 6	0	0
61	1A	3	Total O 3 3	0	0
61	1A	1	Total O 1 1	0	0
61	1A	3	Total O 3 3	0	0
61	1A	5	Total O 5 5	0	0
61	1A	4	Total O 4 4	0	0
61	1A	4	Total O 4 4	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	2	Total O 2 2	0	0
61	1A	2	Total O 2 2	0	0
61	1A	1	Total O 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	1	Total O 1 1	0	0
61	1A	3	Total O 3 3	0	0
61	1A	1	Total O 1 1	0	0
61	1A	5	Total O 5 5	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	2	Total O 2 2	0	0
61	1A	2	Total O 2 2	0	0
61	1A	3	Total O 3 3	0	0
61	1A	6	Total O 6 6	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	6	Total O 6 6	0	0
61	1A	6	Total O 6 6	0	0
61	1A	3	Total O 3 3	0	0
61	1A	2	Total O 2 2	0	0
61	1A	1	Total O 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	4	Total O 4 4	0	0
61	1A	6	Total O 6 6	0	0
61	1A	6	Total O 6 6	0	0
61	1A	6	Total O 6 6	0	0
61	1A	4	Total O 4 4	0	0
61	1A	6	Total O 6 6	0	0
61	1A	6	Total O 6 6	0	0
61	1A	6	Total O 6 6	0	0
61	1A	4	Total O 4 4	0	0
61	1A	3	Total O 3 3	0	0
61	1A	5	Total O 5 5	0	0
61	1A	4	Total O 4 4	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	6	Total O 6 6	0	0
61	1A	3	Total O 3 3	0	0
61	1A	4	Total O 4 4	0	0
61	1A	6	Total O 6 6	0	0
61	1A	6	Total O 6 6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	6	Total O 6 6	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	6	Total O 6 6	0	0
61	1A	6	Total O 6 6	0	0
61	1A	6	Total O 6 6	0	0
61	1A	3	Total O 3 3	0	0
61	1A	3	Total O 3 3	0	0
61	1A	5	Total O 5 5	0	0
61	1A	4	Total O 4 4	0	0
61	1A	6	Total O 6 6	0	0
61	1A	6	Total O 6 6	0	0
61	1A	6	Total O 6 6	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	3	Total O 3 3	0	0
61	1A	6	Total O 6 6	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	5	Total O 5 5	0	0
61	1A	4	Total O 4 4	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	6	Total O 6 6	0	0
61	1A	4	Total O 4 4	0	0
61	1A	6	Total O 6 6	0	0
61	1A	3	Total O 3 3	0	0
61	1A	2	Total O 2 2	0	0
61	1A	4	Total O 4 4	0	0
61	1A	2	Total O 2 2	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	6	Total O 6 6	0	0
61	1A	6	Total O 6 6	0	0
61	1A	4	Total O 4 4	0	0
61	1A	5	Total O 5 5	0	0
61	1A	6	Total O 6 6	0	0
61	1A	6	Total O 6 6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	6	Total O 6 6	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	6	Total O 6 6	0	0
61	1A	6	Total O 6 6	0	0
61	1A	5	Total O 5 5	0	0
61	1A	4	Total O 4 4	0	0
61	1A	5	Total O 5 5	0	0
61	1A	4	Total O 4 4	0	0
61	1A	4	Total O 4 4	0	0
61	1A	4	Total O 4 4	0	0
61	1A	6	Total O 6 6	0	0
61	1A	6	Total O 6 6	0	0
61	1A	6	Total O 6 6	0	0
61	1A	6	Total O 6 6	0	0
61	1A	6	Total O 6 6	0	0
61	1A	6	Total O 6 6	0	0
61	1A	4	Total O 4 4	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	6	Total O 6 6	0	0
61	1A	4	Total O 4 4	0	0
61	1A	3	Total O 3 3	0	0
61	1A	2	Total O 2 2	0	0
61	1A	2	Total O 2 2	0	0
61	1A	3	Total O 3 3	0	0
61	1A	6	Total O 6 6	0	0
61	1A	6	Total O 6 6	0	0
61	1A	6	Total O 6 6	0	0
61	1A	6	Total O 6 6	0	0
61	1A	6	Total O 6 6	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	4	Total O 4 4	0	0
61	1A	4	Total O 4 4	0	0
61	1A	5	Total O 5 5	0	0
61	1A	6	Total O 6 6	0	0
61	1A	5	Total O 5 5	0	0
61	1A	4	Total O 4 4	0	0
61	1A	5	Total O 5 5	0	0
61	1A	6	Total O 6 6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	4	Total O 4 4	0	0
61	1A	6	Total O 6 6	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	6	Total O 6 6	0	0
61	1A	4	Total O 4 4	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	6	Total O 6 6	0	0
61	1A	6	Total O 6 6	0	0
61	1A	6	Total O 6 6	0	0
61	1A	5	Total O 5 5	0	0
61	1A	6	Total O 6 6	0	0
61	1A	4	Total O 4 4	0	0
61	1A	4	Total O 4 4	0	0
61	1A	4	Total O 4 4	0	0
61	1A	6	Total O 6 6	0	0
61	1A	5	Total O 5 5	0	0
61	1A	6	Total O 6 6	0	0
61	1A	6	Total O 6 6	0	0
61	1A	6	Total O 6 6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	6	Total O 6 6	0	0
61	1A	5	Total O 5 5	0	0
61	1A	6	Total O 6 6	0	0
61	1A	6	Total O 6 6	0	0
61	1A	5	Total O 5 5	0	0
61	1A	4	Total O 4 4	0	0
61	1A	6	Total O 6 6	0	0
61	1A	4	Total O 4 4	0	0
61	1A	2	Total O 2 2	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	1	Total O 1 1	0	0
61	1A	3	Total O 3 3	0	0
61	1A	4	Total O 4 4	0	0
61	1A	4	Total O 4 4	0	0
61	1A	6	Total O 6 6	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	6	Total O 6 6	0	0
61	1A	5	Total O 5 5	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	3	Total O 3 3	0	0
61	1A	4	Total O 4 4	0	0
61	1A	5	Total O 5 5	0	0
61	1A	5	Total O 5 5	0	0
61	1A	4	Total O 4 4	0	0
61	1A	3	Total O 3 3	0	0
61	1A	1	Total O 1 1	0	0
61	1A	1	Total O 1 1	0	0
61	1A	4	Total O 4 4	0	0
61	1A	3	Total O 3 3	0	0
61	1A	6	Total O 6 6	0	0
61	1A	5	Total O 5 5	0	0
61	1A	6	Total O 6 6	0	0
61	1A	6	Total O 6 6	0	0
61	1A	6	Total O 6 6	0	0
61	1A	1	Total O 1 1	0	0
61	1A	5	Total O 5 5	0	0
61	1A	6	Total O 6 6	0	0
61	1A	1	Total O 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1A	1	Total O 1 1	0	0
61	1A	6	Total O 6 6	0	0
61	1A	2	Total O 2 2	0	0
61	1A	1	Total O 1 1	0	0
61	1A	6	Total O 6 6	0	0
61	1A	2	Total O 2 2	0	0
61	1A	2	Total O 2 2	0	0
61	1A	6	Total O 6 6	0	0
61	1A	2	Total O 2 2	0	0
61	1A	1	Total O 1 1	0	0
61	1A	6	Total O 6 6	0	0
61	1A	500	Total O 500 500	0	0
61	1B	3	Total O 3 3	0	0
61	1B	1	Total O 1 1	0	0
61	1B	5	Total O 5 5	0	0
61	1B	4	Total O 4 4	0	0
61	1B	3	Total O 3 3	0	0
61	1B	1	Total O 1 1	0	0
61	1B	1	Total O 1 1	0	0
61	1B	1	Total O 1 1	0	0
61	1B	1	Total O 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1B	1	Total O 1 1	0	0
61	1B	2	Total O 2 2	0	0
61	1B	2	Total O 2 2	0	0
61	1B	1	Total O 1 1	0	0
61	1B	2	Total O 2 2	0	0
61	1B	1	Total O 1 1	0	0
61	1B	6	Total O 6 6	0	0
61	1B	1	Total O 1 1	0	0
61	1B	2	Total O 2 2	0	0
61	1B	1	Total O 1 1	0	0
61	1B	1	Total O 1 1	0	0
61	1B	3	Total O 3 3	0	0
61	1B	2	Total O 2 2	0	0
61	1B	1	Total O 1 1	0	0
61	1B	2	Total O 2 2	0	0
61	1B	1	Total O 1 1	0	0
61	1B	3	Total O 3 3	0	0
61	1B	5	Total O 5 5	0	0
61	1B	16	Total O 16 16	0	0
61	1D	5	Total O 5 5	0	0
61	1D	2	Total O 2 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1D	1	Total O 1 1	0	0
61	1D	1	Total O 1 1	0	0
61	1D	15	Total O 15 15	0	0
61	1E	2	Total O 2 2	0	0
61	1E	2	Total O 2 2	0	0
61	1E	2	Total O 2 2	0	0
61	1E	2	Total O 2 2	0	0
61	1E	6	Total O 6 6	0	0
61	1E	13	Total O 13 13	0	0
61	1F	1	Total O 1 1	0	0
61	1F	8	Total O 8 8	0	0
61	1G	2	Total O 2 2	0	0
61	1G	3	Total O 3 3	0	0
61	1H	1	Total O 1 1	0	0
61	1I	2	Total O 2 2	0	0
61	1N	4	Total O 4 4	0	0
61	1O	2	Total O 2 2	0	0
61	1O	1	Total O 1 1	0	0
61	1O	4	Total O 4 4	0	0
61	1P	5	Total O 5 5	0	0
61	1P	2	Total O 2 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1P	2	Total O 2 2	0	0
61	1P	1	Total O 1 1	0	0
61	1P	6	Total O 6 6	0	0
61	1P	5	Total O 5 5	0	0
61	1Q	6	Total O 6 6	0	0
61	1Q	1	Total O 1 1	0	0
61	1Q	4	Total O 4 4	0	0
61	1R	1	Total O 1 1	0	0
61	1R	7	Total O 7 7	0	0
61	1S	2	Total O 2 2	0	0
61	1S	2	Total O 2 2	0	0
61	1T	1	Total O 1 1	0	0
61	1T	1	Total O 1 1	0	0
61	1T	4	Total O 4 4	0	0
61	1U	9	Total O 9 9	0	0
61	1V	1	Total O 1 1	0	0
61	1V	6	Total O 6 6	0	0
61	1W	9	Total O 9 9	0	0
61	1X	4	Total O 4 4	0	0
61	1X	3	Total O 3 3	0	0
61	1Y	3	Total O 3 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1Z	1	Total O 1 1	0	0
61	10	3	Total O 3 3	0	0
61	10	2	Total O 2 2	0	0
61	10	7	Total O 7 7	0	0
61	11	1	Total O 1 1	0	0
61	11	1	Total O 1 1	0	0
61	11	8	Total O 8 8	0	0
61	12	4	Total O 4 4	0	0
61	13	1	Total O 1 1	0	0
61	13	3	Total O 3 3	0	0
61	14	2	Total O 2 2	0	0
61	15	2	Total O 2 2	0	0
61	15	5	Total O 5 5	0	0
61	16	1	Total O 1 1	0	0
61	17	2	Total O 2 2	0	0
61	17	5	Total O 5 5	0	0
61	18	5	Total O 5 5	0	0
61	18	2	Total O 2 2	0	0
61	18	1	Total O 1 1	0	0
61	18	2	Total O 2 2	0	0
61	18	6	Total O 6 6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	18	3	Total O 3 3	0	0
61	1a	2	Total O 2 2	0	0
61	1a	3	Total O 3 3	0	0
61	1a	4	Total O 4 4	0	0
61	1a	1	Total O 1 1	0	0
61	1a	2	Total O 2 2	0	0
61	1a	2	Total O 2 2	0	0
61	1a	1	Total O 1 1	0	0
61	1a	5	Total O 5 5	0	0
61	1a	4	Total O 4 4	0	0
61	1a	4	Total O 4 4	0	0
61	1a	5	Total O 5 5	0	0
61	1a	4	Total O 4 4	0	0
61	1a	4	Total O 4 4	0	0
61	1a	1	Total O 1 1	0	0
61	1a	2	Total O 2 2	0	0
61	1a	1	Total O 1 1	0	0
61	1a	3	Total O 3 3	0	0
61	1a	2	Total O 2 2	0	0
61	1a	3	Total O 3 3	0	0
61	1a	5	Total O 5 5	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1a	6	Total O 6 6	0	0
61	1a	3	Total O 3 3	0	0
61	1a	5	Total O 5 5	0	0
61	1a	5	Total O 5 5	0	0
61	1a	3	Total O 3 3	0	0
61	1a	1	Total O 1 1	0	0
61	1a	5	Total O 5 5	0	0
61	1a	2	Total O 2 2	0	0
61	1a	4	Total O 4 4	0	0
61	1a	1	Total O 1 1	0	0
61	1a	1	Total O 1 1	0	0
61	1a	6	Total O 6 6	0	0
61	1a	5	Total O 5 5	0	0
61	1a	4	Total O 4 4	0	0
61	1a	1	Total O 1 1	0	0
61	1a	4	Total O 4 4	0	0
61	1a	2	Total O 2 2	0	0
61	1a	1	Total O 1 1	0	0
61	1a	1	Total O 1 1	0	0
61	1a	1	Total O 1 1	0	0
61	1a	6	Total O 6 6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1a	3	Total O 3 3	0	0
61	1a	1	Total O 1 1	0	0
61	1a	6	Total O 6 6	0	0
61	1a	3	Total O 3 3	0	0
61	1a	1	Total O 1 1	0	0
61	1a	3	Total O 3 3	0	0
61	1a	1	Total O 1 1	0	0
61	1a	4	Total O 4 4	0	0
61	1a	4	Total O 4 4	0	0
61	1a	6	Total O 6 6	0	0
61	1a	5	Total O 5 5	0	0
61	1a	5	Total O 5 5	0	0
61	1a	5	Total O 5 5	0	0
61	1a	5	Total O 5 5	0	0
61	1a	6	Total O 6 6	0	0
61	1a	4	Total O 4 4	0	0
61	1a	4	Total O 4 4	0	0
61	1a	6	Total O 6 6	0	0
61	1a	4	Total O 4 4	0	0
61	1a	4	Total O 4 4	0	0
61	1a	2	Total O 2 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1a	4	Total O 4 4	0	0
61	1a	6	Total O 6 6	0	0
61	1a	4	Total O 4 4	0	0
61	1a	6	Total O 6 6	0	0
61	1a	6	Total O 6 6	0	0
61	1a	6	Total O 6 6	0	0
61	1a	6	Total O 6 6	0	0
61	1a	6	Total O 6 6	0	0
61	1a	5	Total O 5 5	0	0
61	1a	4	Total O 4 4	0	0
61	1a	6	Total O 6 6	0	0
61	1a	6	Total O 6 6	0	0
61	1a	6	Total O 6 6	0	0
61	1a	6	Total O 6 6	0	0
61	1a	6	Total O 6 6	0	0
61	1a	6	Total O 6 6	0	0
61	1a	2	Total O 2 2	0	0
61	1a	4	Total O 4 4	0	0
61	1a	5	Total O 5 5	0	0
61	1a	6	Total O 6 6	0	0
61	1a	6	Total O 6 6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1a	4	Total O 4 4	0	0
61	1a	6	Total O 6 6	0	0
61	1a	5	Total O 5 5	0	0
61	1a	6	Total O 6 6	0	0
61	1a	2	Total O 2 2	0	0
61	1a	1	Total O 1 1	0	0
61	1a	1	Total O 1 1	0	0
61	1a	1	Total O 1 1	0	0
61	1a	2	Total O 2 2	0	0
61	1a	1	Total O 1 1	0	0
61	1a	1	Total O 1 1	0	0
61	1a	2	Total O 2 2	0	0
61	1a	1	Total O 1 1	0	0
61	1a	78	Total O 78 78	0	0
61	1b	1	Total O 1 1	0	0
61	1d	1	Total O 1 1	0	0
61	1f	1	Total O 1 1	0	0
61	1l	6	Total O 6 6	0	0
61	1l	1	Total O 1 1	0	0
61	1q	4	Total O 4 4	0	0
61	1w	6	Total O 6 6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	1w	1	Total O 1 1	0	0
61	1w	9	Total O 9 9	0	0
61	1x	3	Total O 3 3	0	0
61	1x	2	Total O 2 2	0	0
61	1x	1	Total O 1 1	0	0
61	1x	2	Total O 2 2	0	0
61	1x	1	Total O 1 1	0	0
61	1x	1	Total O 1 1	0	0
61	1x	5	Total O 5 5	0	0
61	1y	1	Total O 1 1	0	0
61	2A	6	Total O 6 6	0	0
61	2A	5	Total O 5 5	0	0
61	2A	6	Total O 6 6	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	5	Total O 5 5	0	0
61	2A	4	Total O 4 4	0	0
61	2A	3	Total O 3 3	0	0
61	2A	1	Total O 1 1	0	0
61	2A	3	Total O 3 3	0	0
61	2A	1	Total O 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2A	1	Total O 1 1	0	0
61	2A	5	Total O 5 5	0	0
61	2A	3	Total O 3 3	0	0
61	2A	6	Total O 6 6	0	0
61	2A	1	Total O 1 1	0	0
61	2A	5	Total O 5 5	0	0
61	2A	3	Total O 3 3	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	2	Total O 2 2	0	0
61	2A	5	Total O 5 5	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	4	Total O 4 4	0	0
61	2A	5	Total O 5 5	0	0
61	2A	2	Total O 2 2	0	0
61	2A	5	Total O 5 5	0	0
61	2A	5	Total O 5 5	0	0
61	2A	5	Total O 5 5	0	0
61	2A	2	Total O 2 2	0	0
61	2A	1	Total O 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	2	Total O 2 2	0	0
61	2A	2	Total O 2 2	0	0
61	2A	2	Total O 2 2	0	0
61	2A	2	Total O 2 2	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	3	Total O 3 3	0	0
61	2A	5	Total O 5 5	0	0
61	2A	4	Total O 4 4	0	0
61	2A	5	Total O 5 5	0	0
61	2A	5	Total O 5 5	0	0
61	2A	3	Total O 3 3	0	0
61	2A	1	Total O 1 1	0	0
61	2A	4	Total O 4 4	0	0
61	2A	5	Total O 5 5	0	0
61	2A	5	Total O 5 5	0	0
61	2A	3	Total O 3 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2A	4	Total O 4 4	0	0
61	2A	4	Total O 4 4	0	0
61	2A	3	Total O 3 3	0	0
61	2A	1	Total O 1 1	0	0
61	2A	4	Total O 4 4	0	0
61	2A	4	Total O 4 4	0	0
61	2A	3	Total O 3 3	0	0
61	2A	5	Total O 5 5	0	0
61	2A	5	Total O 5 5	0	0
61	2A	3	Total O 3 3	0	0
61	2A	2	Total O 2 2	0	0
61	2A	3	Total O 3 3	0	0
61	2A	4	Total O 4 4	0	0
61	2A	5	Total O 5 5	0	0
61	2A	4	Total O 4 4	0	0
61	2A	4	Total O 4 4	0	0
61	2A	5	Total O 5 5	0	0
61	2A	2	Total O 2 2	0	0
61	2A	1	Total O 1 1	0	0
61	2A	4	Total O 4 4	0	0
61	2A	2	Total O 2 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2A	4	Total O 4 4	0	0
61	2A	3	Total O 3 3	0	0
61	2A	5	Total O 5 5	0	0
61	2A	3	Total O 3 3	0	0
61	2A	2	Total O 2 2	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	2	Total O 2 2	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	2	Total O 2 2	0	0
61	2A	2	Total O 2 2	0	0
61	2A	6	Total O 6 6	0	0
61	2A	1	Total O 1 1	0	0
61	2A	5	Total O 5 5	0	0
61	2A	1	Total O 1 1	0	0
61	2A	4	Total O 4 4	0	0
61	2A	2	Total O 2 2	0	0
61	2A	6	Total O 6 6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2A	6	Total O 6 6	0	0
61	2A	2	Total O 2 2	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	2	Total O 2 2	0	0
61	2A	2	Total O 2 2	0	0
61	2A	4	Total O 4 4	0	0
61	2A	2	Total O 2 2	0	0
61	2A	2	Total O 2 2	0	0
61	2A	1	Total O 1 1	0	0
61	2A	2	Total O 2 2	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	6	Total O 6 6	0	0
61	2A	5	Total O 5 5	0	0
61	2A	4	Total O 4 4	0	0
61	2A	3	Total O 3 3	0	0
61	2A	2	Total O 2 2	0	0
61	2A	4	Total O 4 4	0	0
61	2A	4	Total O 4 4	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2A	4	Total O 4 4	0	0
61	2A	4	Total O 4 4	0	0
61	2A	3	Total O 3 3	0	0
61	2A	5	Total O 5 5	0	0
61	2A	2	Total O 2 2	0	0
61	2A	1	Total O 1 1	0	0
61	2A	3	Total O 3 3	0	0
61	2A	1	Total O 1 1	0	0
61	2A	5	Total O 5 5	0	0
61	2A	5	Total O 5 5	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	3	Total O 3 3	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	3	Total O 3 3	0	0
61	2A	4	Total O 4 4	0	0
61	2A	3	Total O 3 3	0	0
61	2A	2	Total O 2 2	0	0
61	2A	5	Total O 5 5	0	0
61	2A	1	Total O 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2A	1	Total O 1 1	0	0
61	2A	4	Total O 4 4	0	0
61	2A	4	Total O 4 4	0	0
61	2A	1	Total O 1 1	0	0
61	2A	2	Total O 2 2	0	0
61	2A	2	Total O 2 2	0	0
61	2A	4	Total O 4 4	0	0
61	2A	1	Total O 1 1	0	0
61	2A	2	Total O 2 2	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	5	Total O 5 5	0	0
61	2A	2	Total O 2 2	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	2	Total O 2 2	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	3	Total O 3 3	0	0
61	2A	3	Total O 3 3	0	0
61	2A	2	Total O 2 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2A	1	Total O 1 1	0	0
61	2A	2	Total O 2 2	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	2	Total O 2 2	0	0
61	2A	3	Total O 3 3	0	0
61	2A	1	Total O 1 1	0	0
61	2A	2	Total O 2 2	0	0
61	2A	2	Total O 2 2	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	3	Total O 3 3	0	0
61	2A	1	Total O 1 1	0	0
61	2A	2	Total O 2 2	0	0
61	2A	2	Total O 2 2	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	2	Total O 2 2	0	0
61	2A	4	Total O 4 4	0	0
61	2A	3	Total O 3 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2A	2	Total O 2 2	0	0
61	2A	2	Total O 2 2	0	0
61	2A	2	Total O 2 2	0	0
61	2A	1	Total O 1 1	0	0
61	2A	5	Total O 5 5	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	4	Total O 4 4	0	0
61	2A	2	Total O 2 2	0	0
61	2A	2	Total O 2 2	0	0
61	2A	1	Total O 1 1	0	0
61	2A	2	Total O 2 2	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	2	Total O 2 2	0	0
61	2A	2	Total O 2 2	0	0
61	2A	1	Total O 1 1	0	0
61	2A	4	Total O 4 4	0	0
61	2A	4	Total O 4 4	0	0
61	2A	2	Total O 2 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2A	2	Total O 2 2	0	0
61	2A	3	Total O 3 3	0	0
61	2A	3	Total O 3 3	0	0
61	2A	1	Total O 1 1	0	0
61	2A	2	Total O 2 2	0	0
61	2A	2	Total O 2 2	0	0
61	2A	6	Total O 6 6	0	0
61	2A	3	Total O 3 3	0	0
61	2A	4	Total O 4 4	0	0
61	2A	2	Total O 2 2	0	0
61	2A	1	Total O 1 1	0	0
61	2A	4	Total O 4 4	0	0
61	2A	3	Total O 3 3	0	0
61	2A	3	Total O 3 3	0	0
61	2A	6	Total O 6 6	0	0
61	2A	2	Total O 2 2	0	0
61	2A	4	Total O 4 4	0	0
61	2A	2	Total O 2 2	0	0
61	2A	2	Total O 2 2	0	0
61	2A	1	Total O 1 1	0	0
61	2A	2	Total O 2 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2A	2	Total O 2 2	0	0
61	2A	6	Total O 6 6	0	0
61	2A	4	Total O 4 4	0	0
61	2A	1	Total O 1 1	0	0
61	2A	5	Total O 5 5	0	0
61	2A	4	Total O 4 4	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	2	Total O 2 2	0	0
61	2A	2	Total O 2 2	0	0
61	2A	6	Total O 6 6	0	0
61	2A	2	Total O 2 2	0	0
61	2A	1	Total O 1 1	0	0
61	2A	3	Total O 3 3	0	0
61	2A	1	Total O 1 1	0	0
61	2A	2	Total O 2 2	0	0
61	2A	2	Total O 2 2	0	0
61	2A	2	Total O 2 2	0	0
61	2A	3	Total O 3 3	0	0
61	2A	4	Total O 4 4	0	0
61	2A	4	Total O 4 4	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2A	1	Total O 1 1	0	0
61	2A	2	Total O 2 2	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	6	Total O 6 6	0	0
61	2A	1	Total O 1 1	0	0
61	2A	3	Total O 3 3	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	2	Total O 2 2	0	0
61	2A	2	Total O 2 2	0	0
61	2A	1	Total O 1 1	0	0
61	2A	2	Total O 2 2	0	0
61	2A	2	Total O 2 2	0	0
61	2A	3	Total O 3 3	0	0
61	2A	3	Total O 3 3	0	0
61	2A	1	Total O 1 1	0	0
61	2A	4	Total O 4 4	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	2	Total O 2 2	0	0
61	2A	4	Total O 4 4	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	3	Total O 3 3	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	2	Total O 2 2	0	0
61	2A	2	Total O 2 2	0	0
61	2A	5	Total O 5 5	0	0
61	2A	4	Total O 4 4	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	3	Total O 3 3	0	0
61	2A	2	Total O 2 2	0	0
61	2A	1	Total O 1 1	0	0
61	2A	5	Total O 5 5	0	0
61	2A	1	Total O 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2A	2	Total O 2 2	0	0
61	2A	5	Total O 5 5	0	0
61	2A	6	Total O 6 6	0	0
61	2A	3	Total O 3 3	0	0
61	2A	6	Total O 6 6	0	0
61	2A	6	Total O 6 6	0	0
61	2A	5	Total O 5 5	0	0
61	2A	3	Total O 3 3	0	0
61	2A	6	Total O 6 6	0	0
61	2A	6	Total O 6 6	0	0
61	2A	3	Total O 3 3	0	0
61	2A	4	Total O 4 4	0	0
61	2A	3	Total O 3 3	0	0
61	2A	1	Total O 1 1	0	0
61	2A	6	Total O 6 6	0	0
61	2A	6	Total O 6 6	0	0
61	2A	6	Total O 6 6	0	0
61	2A	5	Total O 5 5	0	0
61	2A	4	Total O 4 4	0	0
61	2A	5	Total O 5 5	0	0
61	2A	6	Total O 6 6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2A	4	Total O 4 4	0	0
61	2A	6	Total O 6 6	0	0
61	2A	5	Total O 5 5	0	0
61	2A	3	Total O 3 3	0	0
61	2A	3	Total O 3 3	0	0
61	2A	5	Total O 5 5	0	0
61	2A	5	Total O 5 5	0	0
61	2A	4	Total O 4 4	0	0
61	2A	5	Total O 5 5	0	0
61	2A	2	Total O 2 2	0	0
61	2A	3	Total O 3 3	0	0
61	2A	4	Total O 4 4	0	0
61	2A	5	Total O 5 5	0	0
61	2A	6	Total O 6 6	0	0
61	2A	4	Total O 4 4	0	0
61	2A	4	Total O 4 4	0	0
61	2A	3	Total O 3 3	0	0
61	2A	3	Total O 3 3	0	0
61	2A	5	Total O 5 5	0	0
61	2A	6	Total O 6 6	0	0
61	2A	6	Total O 6 6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2A	6	Total O 6 6	0	0
61	2A	4	Total O 4 4	0	0
61	2A	6	Total O 6 6	0	0
61	2A	4	Total O 4 4	0	0
61	2A	6	Total O 6 6	0	0
61	2A	5	Total O 5 5	0	0
61	2A	4	Total O 4 4	0	0
61	2A	4	Total O 4 4	0	0
61	2A	4	Total O 4 4	0	0
61	2A	6	Total O 6 6	0	0
61	2A	5	Total O 5 5	0	0
61	2A	5	Total O 5 5	0	0
61	2A	5	Total O 5 5	0	0
61	2A	4	Total O 4 4	0	0
61	2A	5	Total O 5 5	0	0
61	2A	5	Total O 5 5	0	0
61	2A	4	Total O 4 4	0	0
61	2A	6	Total O 6 6	0	0
61	2A	3	Total O 3 3	0	0
61	2A	4	Total O 4 4	0	0
61	2A	6	Total O 6 6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2A	5	Total O 5 5	0	0
61	2A	5	Total O 5 5	0	0
61	2A	6	Total O 6 6	0	0
61	2A	6	Total O 6 6	0	0
61	2A	6	Total O 6 6	0	0
61	2A	4	Total O 4 4	0	0
61	2A	6	Total O 6 6	0	0
61	2A	5	Total O 5 5	0	0
61	2A	4	Total O 4 4	0	0
61	2A	5	Total O 5 5	0	0
61	2A	5	Total O 5 5	0	0
61	2A	5	Total O 5 5	0	0
61	2A	4	Total O 4 4	0	0
61	2A	6	Total O 6 6	0	0
61	2A	6	Total O 6 6	0	0
61	2A	6	Total O 6 6	0	0
61	2A	6	Total O 6 6	0	0
61	2A	5	Total O 5 5	0	0
61	2A	5	Total O 5 5	0	0
61	2A	5	Total O 5 5	0	0
61	2A	6	Total O 6 6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2A	5	Total O 5 5	0	0
61	2A	3	Total O 3 3	0	0
61	2A	6	Total O 6 6	0	0
61	2A	6	Total O 6 6	0	0
61	2A	4	Total O 4 4	0	0
61	2A	4	Total O 4 4	0	0
61	2A	1	Total O 1 1	0	0
61	2A	4	Total O 4 4	0	0
61	2A	2	Total O 2 2	0	0
61	2A	3	Total O 3 3	0	0
61	2A	2	Total O 2 2	0	0
61	2A	2	Total O 2 2	0	0
61	2A	2	Total O 2 2	0	0
61	2A	2	Total O 2 2	0	0
61	2A	1	Total O 1 1	0	0
61	2A	1	Total O 1 1	0	0
61	2A	2	Total O 2 2	0	0
61	2A	1	Total O 1 1	0	0
61	2A	2	Total O 2 2	0	0
61	2A	2	Total O 2 2	0	0
61	2A	2	Total O 2 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2A	6	Total O 6 6	0	0
61	2A	222	Total O 222 222	0	0
61	2B	2	Total O 2 2	0	0
61	2B	3	Total O 3 3	0	0
61	2B	3	Total O 3 3	0	0
61	2B	1	Total O 1 1	0	0
61	2B	2	Total O 2 2	0	0
61	2B	1	Total O 1 1	0	0
61	2B	1	Total O 1 1	0	0
61	2B	12	Total O 12 12	0	0
61	2D	5	Total O 5 5	0	0
61	2D	3	Total O 3 3	0	0
61	2D	2	Total O 2 2	0	0
61	2D	7	Total O 7 7	0	0
61	2E	3	Total O 3 3	0	0
61	2F	6	Total O 6 6	0	0
61	2I	3	Total O 3 3	0	0
61	2N	1	Total O 1 1	0	0
61	2O	1	Total O 1 1	0	0
61	2P	5	Total O 5 5	0	0
61	2P	2	Total O 2 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2P	4	Total O 4 4	0	0
61	2Q	1	Total O 1 1	0	0
61	2Q	1	Total O 1 1	0	0
61	2R	1	Total O 1 1	0	0
61	2R	2	Total O 2 2	0	0
61	2T	2	Total O 2 2	0	0
61	2T	3	Total O 3 3	0	0
61	2U	2	Total O 2 2	0	0
61	2W	3	Total O 3 3	0	0
61	2Z	1	Total O 1 1	0	0
61	20	6	Total O 6 6	0	0
61	20	2	Total O 2 2	0	0
61	20	2	Total O 2 2	0	0
61	21	6	Total O 6 6	0	0
61	22	1	Total O 1 1	0	0
61	25	4	Total O 4 4	0	0
61	27	1	Total O 1 1	0	0
61	27	1	Total O 1 1	0	0
61	28	4	Total O 4 4	0	0
61	28	1	Total O 1 1	0	0
61	28	1	Total O 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	29	1	Total O 1 1	0	0
61	2a	6	Total O 6 6	0	0
61	2a	6	Total O 6 6	0	0
61	2a	5	Total O 5 5	0	0
61	2a	5	Total O 5 5	0	0
61	2a	4	Total O 4 4	0	0
61	2a	6	Total O 6 6	0	0
61	2a	6	Total O 6 6	0	0
61	2a	6	Total O 6 6	0	0
61	2a	5	Total O 5 5	0	0
61	2a	5	Total O 5 5	0	0
61	2a	3	Total O 3 3	0	0
61	2a	5	Total O 5 5	0	0
61	2a	4	Total O 4 4	0	0
61	2a	6	Total O 6 6	0	0
61	2a	3	Total O 3 3	0	0
61	2a	5	Total O 5 5	0	0
61	2a	6	Total O 6 6	0	0
61	2a	4	Total O 4 4	0	0
61	2a	4	Total O 4 4	0	0
61	2a	2	Total O 2 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2a	6	Total O 6 6	0	0
61	2a	5	Total O 5 5	0	0
61	2a	3	Total O 3 3	0	0
61	2a	6	Total O 6 6	0	0
61	2a	3	Total O 3 3	0	0
61	2a	6	Total O 6 6	0	0
61	2a	5	Total O 5 5	0	0
61	2a	4	Total O 4 4	0	0
61	2a	3	Total O 3 3	0	0
61	2a	5	Total O 5 5	0	0
61	2a	6	Total O 6 6	0	0
61	2a	6	Total O 6 6	0	0
61	2a	5	Total O 5 5	0	0
61	2a	5	Total O 5 5	0	0
61	2a	2	Total O 2 2	0	0
61	2a	4	Total O 4 4	0	0
61	2a	6	Total O 6 6	0	0
61	2a	6	Total O 6 6	0	0
61	2a	5	Total O 5 5	0	0
61	2a	5	Total O 5 5	0	0
61	2a	4	Total O 4 4	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2a	5	Total O 5 5	0	0
61	2a	6	Total O 6 6	0	0
61	2a	5	Total O 5 5	0	0
61	2a	6	Total O 6 6	0	0
61	2a	3	Total O 3 3	0	0
61	2a	6	Total O 6 6	0	0
61	2a	1	Total O 1 1	0	0
61	2a	2	Total O 2 2	0	0
61	2a	3	Total O 3 3	0	0
61	2a	2	Total O 2 2	0	0
61	2a	5	Total O 5 5	0	0
61	2a	4	Total O 4 4	0	0
61	2a	2	Total O 2 2	0	0
61	2a	2	Total O 2 2	0	0
61	2a	1	Total O 1 1	0	0
61	2a	2	Total O 2 2	0	0
61	2a	1	Total O 1 1	0	0
61	2a	5	Total O 5 5	0	0
61	2a	1	Total O 1 1	0	0
61	2a	4	Total O 4 4	0	0
61	2a	1	Total O 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2a	2	Total O 2 2	0	0
61	2a	1	Total O 1 1	0	0
61	2a	2	Total O 2 2	0	0
61	2a	2	Total O 2 2	0	0
61	2a	1	Total O 1 1	0	0
61	2a	2	Total O 2 2	0	0
61	2a	1	Total O 1 1	0	0
61	2a	1	Total O 1 1	0	0
61	2a	3	Total O 3 3	0	0
61	2a	3	Total O 3 3	0	0
61	2a	1	Total O 1 1	0	0
61	2a	1	Total O 1 1	0	0
61	2a	3	Total O 3 3	0	0
61	2a	2	Total O 2 2	0	0
61	2a	3	Total O 3 3	0	0
61	2a	4	Total O 4 4	0	0
61	2a	1	Total O 1 1	0	0
61	2a	1	Total O 1 1	0	0
61	2a	4	Total O 4 4	0	0
61	2a	4	Total O 4 4	0	0
61	2a	2	Total O 2 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2a	2	Total O 2 2	0	0
61	2a	2	Total O 2 2	0	0
61	2a	1	Total O 1 1	0	0
61	2a	1	Total O 1 1	0	0
61	2a	1	Total O 1 1	0	0
61	2a	1	Total O 1 1	0	0
61	2a	1	Total O 1 1	0	0
61	2a	1	Total O 1 1	0	0
61	2a	1	Total O 1 1	0	0
61	2a	1	Total O 1 1	0	0
61	2a	1	Total O 1 1	0	0
61	2a	1	Total O 1 1	0	0
61	2a	1	Total O 1 1	0	0
61	2a	1	Total O 1 1	0	0
61	2a	2	Total O 2 2	0	0
61	2a	2	Total O 2 2	0	0
61	2a	2	Total O 2 2	0	0
61	2a	2	Total O 2 2	0	0
61	2a	1	Total O 1 1	0	0
61	2a	2	Total O 2 2	0	0
61	2a	1	Total O 1 1	0	0
61	2a	2	Total O 2 2	0	0

Continued on next page...

Continued from previous page...

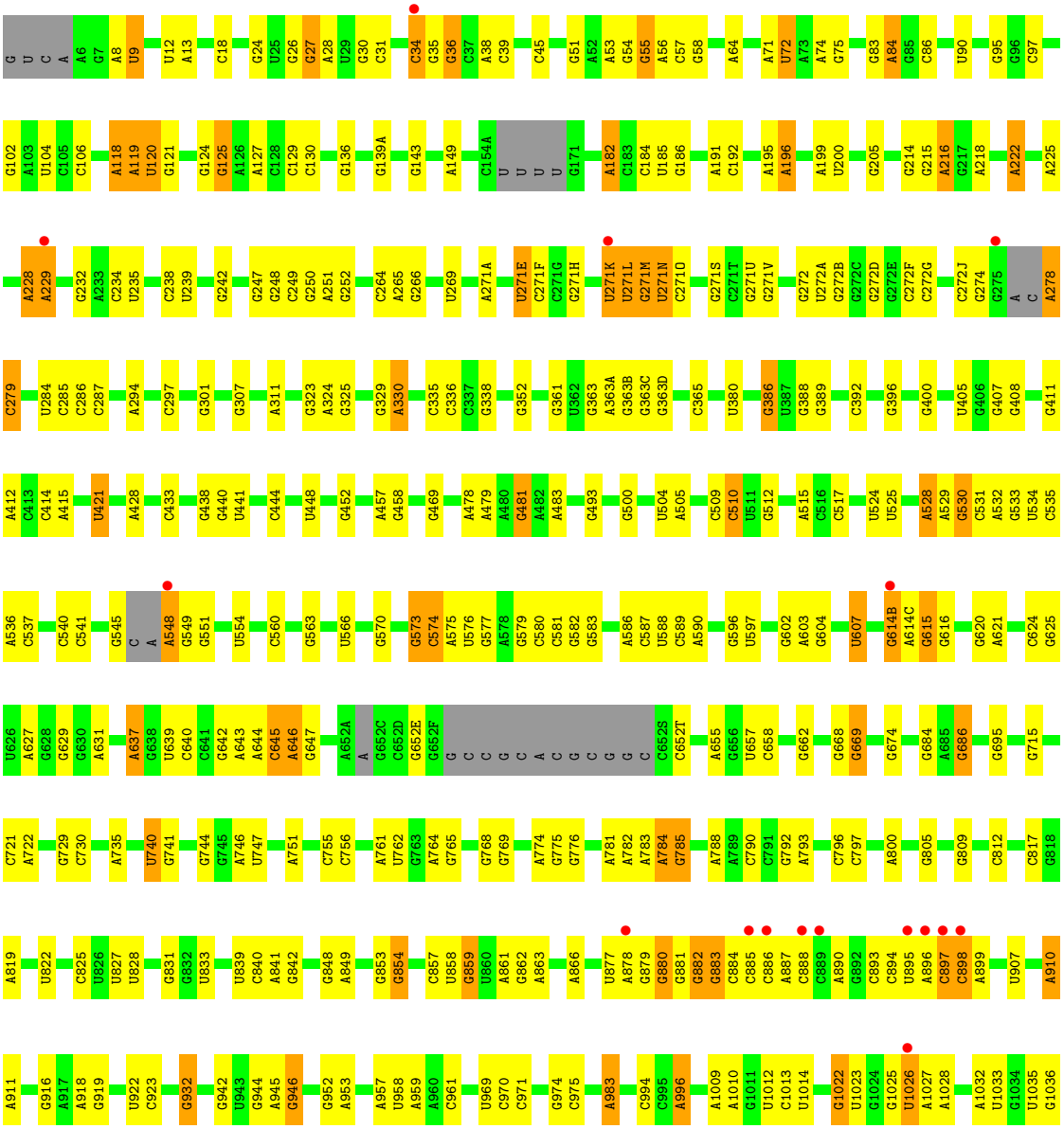
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	2a	2	Total O 2 2	0	0
61	2a	2	Total O 2 2	0	0
61	2a	40	Total O 40 40	0	0
61	2d	1	Total O 1 1	0	0
61	2g	1	Total O 1 1	0	0
61	2i	1	Total O 1 1	0	0
61	2j	2	Total O 2 2	0	0
61	2j	1	Total O 1 1	0	0
61	2l	1	Total O 1 1	0	0
61	2l	1	Total O 1 1	0	0
61	2p	1	Total O 1 1	0	0
61	2r	1	Total O 1 1	0	0
61	2t	2	Total O 2 2	0	0
61	2x	2	Total O 2 2	0	0
61	2x	2	Total O 2 2	0	0
61	2x	3	Total O 3 3	0	0
61	2y	6	Total O 6 6	0	0
61	2y	1	Total O 1 1	0	0
61	2y	6	Total O 6 6	0	0

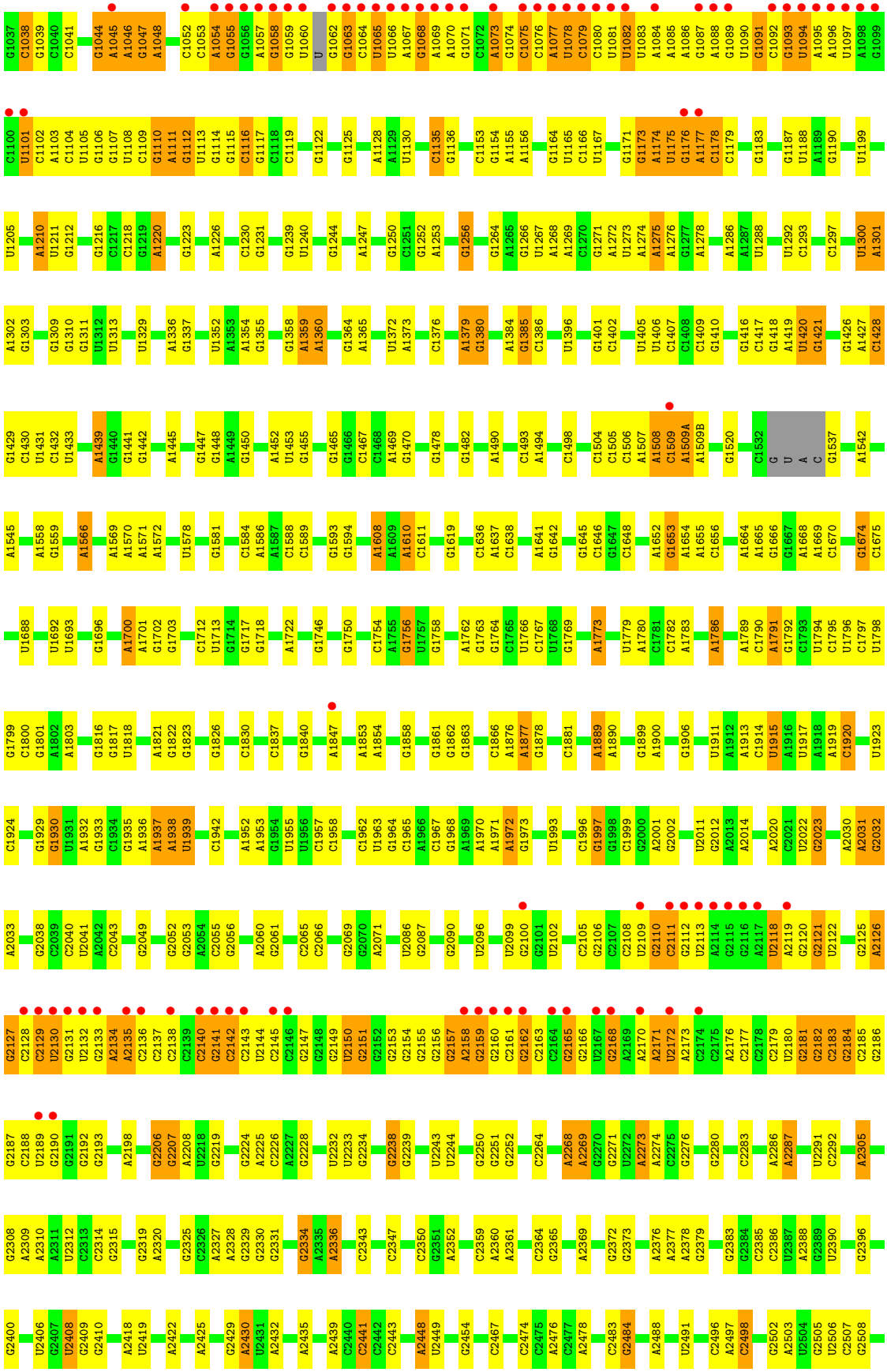
3 Residue-property plots (i)

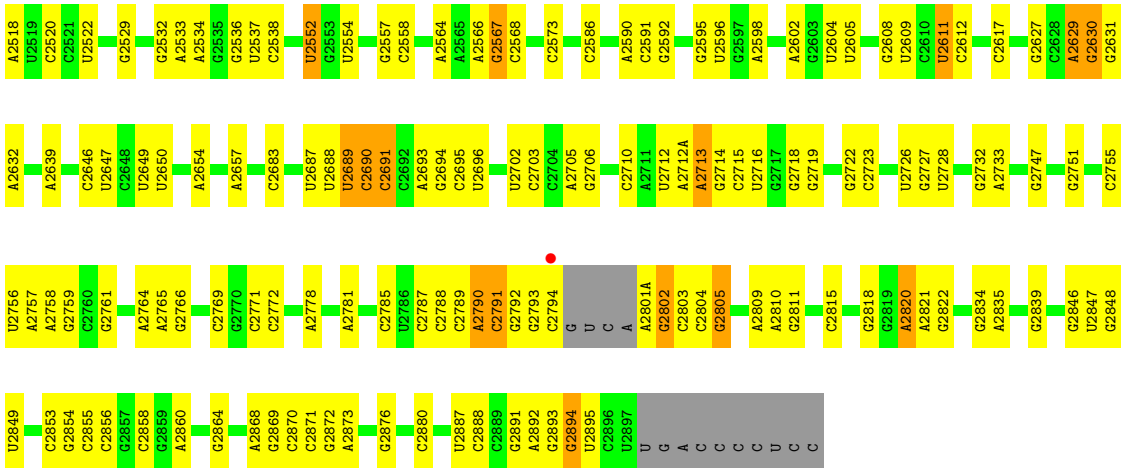
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

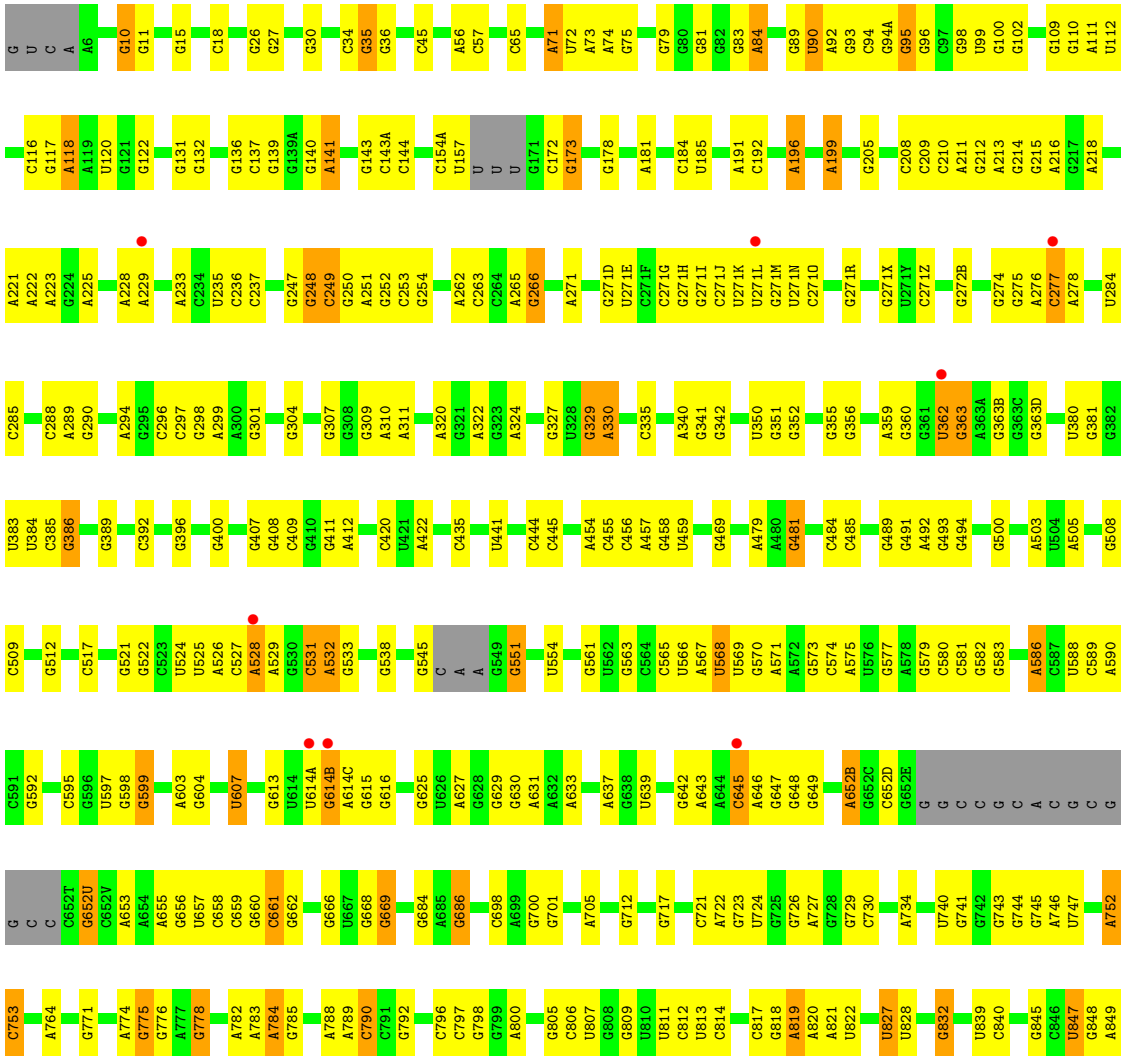


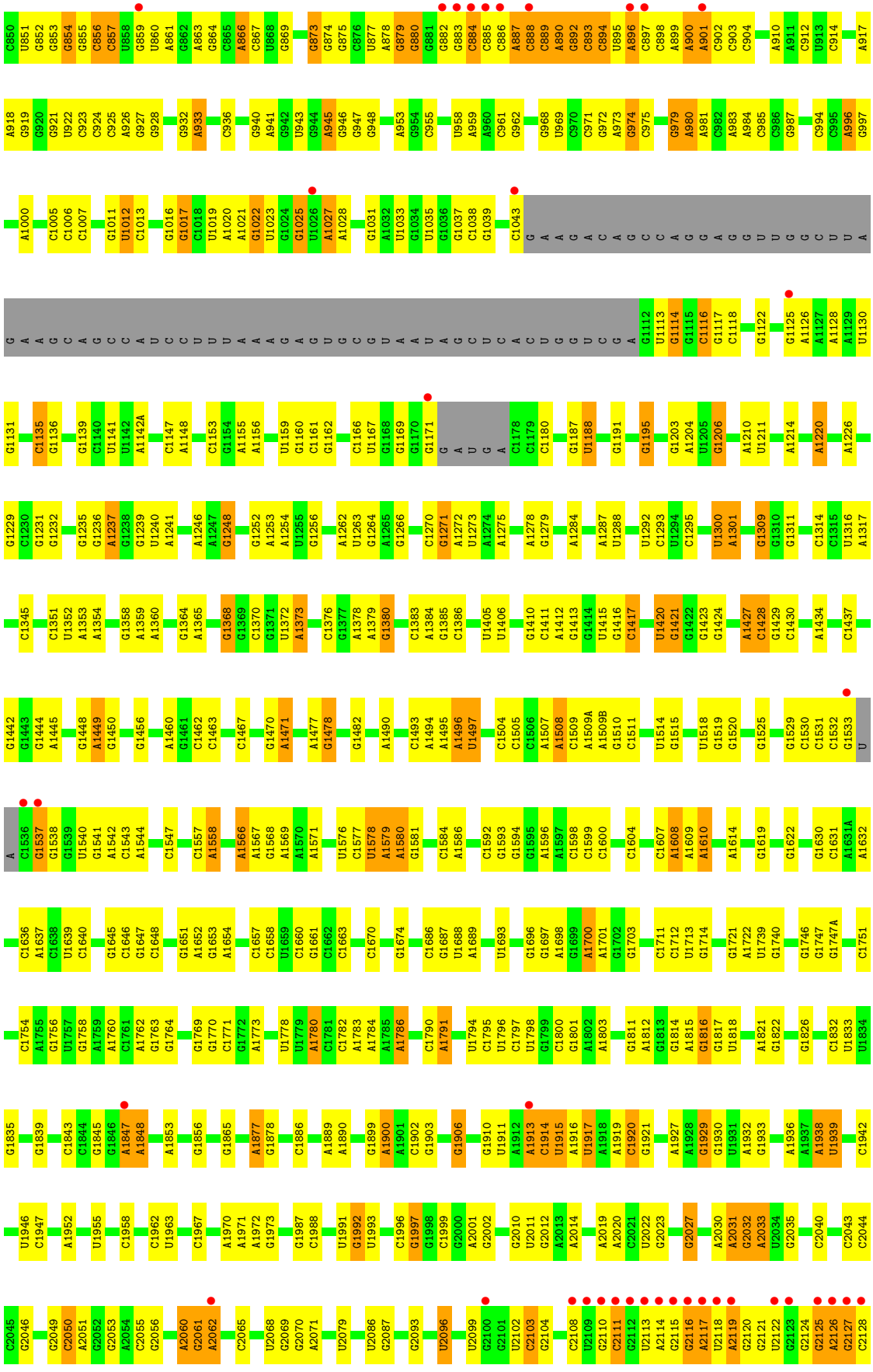

G1037 C1038 G1039 C1040 C1041 G1044 A1045 A1046 G1047 A1048 C1052 C1053 A1054 G1055 G1056 A1057 G1058 G1059 U1060 U G1062 G1063 C1064 U1065 U1066 A1067 G1068 A1069 A1070 G1071 C1072 A1073 G1074 C1075 C1076 A1077 U1078 C1079 C1080 U1081 U1082 U1083 A1084 A1085 A1086 G1087 A1088 G1089 U1090 G1091 C1092 G1093 U1094 A1095 A1096 U1097 A1098 G1099
C1100 U1101 C1102 A1103 C1104 U1105 G1106 G1107 U1108 C1109 G1110 A1111 G1112 U1113 G1114 G1115 C1116 G1117 C1118 C1119 G1122 G1125 A1128 A1129 U1130 C1135 G1136 C1153 G1154 A1155 A1156 G1164 U1165 C1166 U1167 G1171 G1173 A1174 U1175 G1176 A1177 C1178 C1179 G1183 G1187 U1188 A1189 G1190 U1199
U1205 A1210 U1211 G1212 G1216 C1217 C1218 G1219 A1220 G1223 A1226 C1230 G1231 G1239 U1240 G1244 A1247 G1250 C1251 G1252 A1253 G1256 G1264 A1265 C1266 U1267 A1268 A1269 C1270 G1271 A1272 U1273 A1274 A1275 A1276 G1277 A1278 A1286 A1287 U1288 U1292 C1293 C1297 U1300 A1301
A1302 G1303 G1309 G1310 G1311 U1312 U1313 U1329 A1336 G1337 U1352 A1353 A1354 G1355 G1358 A1359 A1360 G1364 A1365 U1372 A1373 C1376 A1379 G1380 A1384 G1385 C1386 U1396 G1401 C1402 U1405 U1406 C1407 C1408 C1409 G1410 G1416 C1417 G1418 A1419 U1420 G1421 G1426 A1427 C1428
G1429 C1430 U1431 C1432 U1433 A1439 G1440 G1441 G1442 A1445 G1447 G1448 A1449 G1450 A1452 U1453 G1455 G1465 G1466 C1467 C1468 A1469 G1470 G1478 G1482 A1490 C1493 A1494 C1498 C1504 C1505 C1506 A1507 A1508 C1509 A1509A A1509B G1520 C1532 G U A C G1537 A1542
A1545 A1558 G1559 A1566 A1569 A1570 A1571 A1572 U1578 G1581 C1584 A1586 A1587 C1588 C1589 G1593 G1594 A1608 A1609 A1610 C1611 G1619 C1636 A1637 C1638 A1641 G1642 G1645 C1646 G1647 C1648 A1652 G1653 A1654 A1655 C1656 A1664 A1665 G1666 G1667 A1668 A1669 C1670 G1674 C1675
U1688 U1692 U1693 G1696 A1700 A1701 G1702 G1703 C1712 U1713 G1714 G1717 G1718 A1722 G1746 G1750 C1754 A1755 G1756 U1757 G1758 A1762 G1763 G1764 C1765 U1766 C1767 U1768 G1769 A1773 U1779 A1780 C1781 C1782 A1783 A1786 A1789 C1790 A1791 G1792 C1793 U1794 C1795 U1796 C1797 U1798
G1799 C1800 G1801 A1802 A1803 G1816 G1817 U1818 A1821 G1822 G1823 G1826 C1830 C1837 G1840 A1847 A1853 A1854 G1858 G1861 G1862 G1863 C1866 A1876 A1877 G1878 C1881 A1889 A1890 G1899 A1900 G1906 U1911 A1912 A1913 C1914 U1915 A1916 U1917 A1918 A1919 C1920 U1923
C1924 G1929 G1930 U1931 A1932 G1933 C1934 G1935 A1936 A1937 A1938 U1939 C1942 A1952 A1953 G1954 U1955 U1956 C1957 C1958 C1962 U1963 G1964 C1965 A1966 A1969 A1970 A1971 A1972 G1973 U1993 C1996 G1997 G1998 C1999 G2000 A2001 G2002 U2011 G2012 A2013 A2014 A2020 C2021 U2022 G2023 A2030 A2031 G2032
A2033 G2038 C2039 C2040 U2041 A2042 C2043 G2049 G2052 G2053 A2054 C2055 G2056 A2060 G2061 C2065 C2066 G2069 G2070 A2071 U2086 G2087 G2090 U2096 U2099 G2100 G2101 U2102 C2105 G2106 C2107 C2108 U2109 G2110 C2111 G2112 U2113 A2114 G2115 G2116 A2117 U2118 A2119 G2120 G2121 U2122 G2125 A2126
G2127 C2128 C2129 U2130 G2131 U2132 G2133 A2134 A2135 C2136 C2137 C2138 C2139 C2140 G2141 C2142 C2143 U2144 C2145 C2146 C2147 G2148 G2149 U2150 G2151 G2152 G2153 G2154 G2155 G2156 G2157 A2158 G2159 G2160 C2161 G2162 C2163 C2164 G2165 G2166 U2167 G2168 A2169 A2170 A2171 U2172 A2173 C2174 C2175 A2176 C2177 C2178 C2179 U2180 G2181 G2182 C2183 G2184 C2185 C2186
G2187 C2188 U2189 G2190 G2191 G2192 G2193 A2198 G2206 G2207 A2208 U2218 G2219 G2224 A2225 C2226 A2227 G2228 U2232 U2233 G2234 G2238 G2239 U2243 U2244 G2250 G2251 G2252 C2264 A2268 A2269 G2270 G2271 U2272 A2273 A2274 C2275 G2276 G2280 C2283 A2286 A2287 U2291 C2292 A2305
G2308 A2309 A2310 A2311 U2312 C2313 C2314 G2315 G2319 A2320 G2326 C2326 A2327 A2328 G2329 G2330 G2331 G2334 A2335 A2336 C2343 C2347 C2350 G2351 A2352 C2359 A2360 A2361 C2364 G2365 A2369 G2372 G2373 A2376 A2377 A2378 G2379 G2383 G2384 C2385 C2386 U2387 A2388 G2389 U2390 G2396
G2400 U2406 G2407 U2408 G2409 G2410 A2418 U2419 A2422 A2425 G2429 A2430 U2431 A2432 A2435 A2439 C2440 C2441 C2442 C2443 A2448 U2449 G2454 C2467 C2474 C2475 A2476 C2477 A2478 C2483 G2484 A2488 U2491 C2496 A2497 C2498 G2502 A2503 U2504 G2505 U2506 C2507 G2508

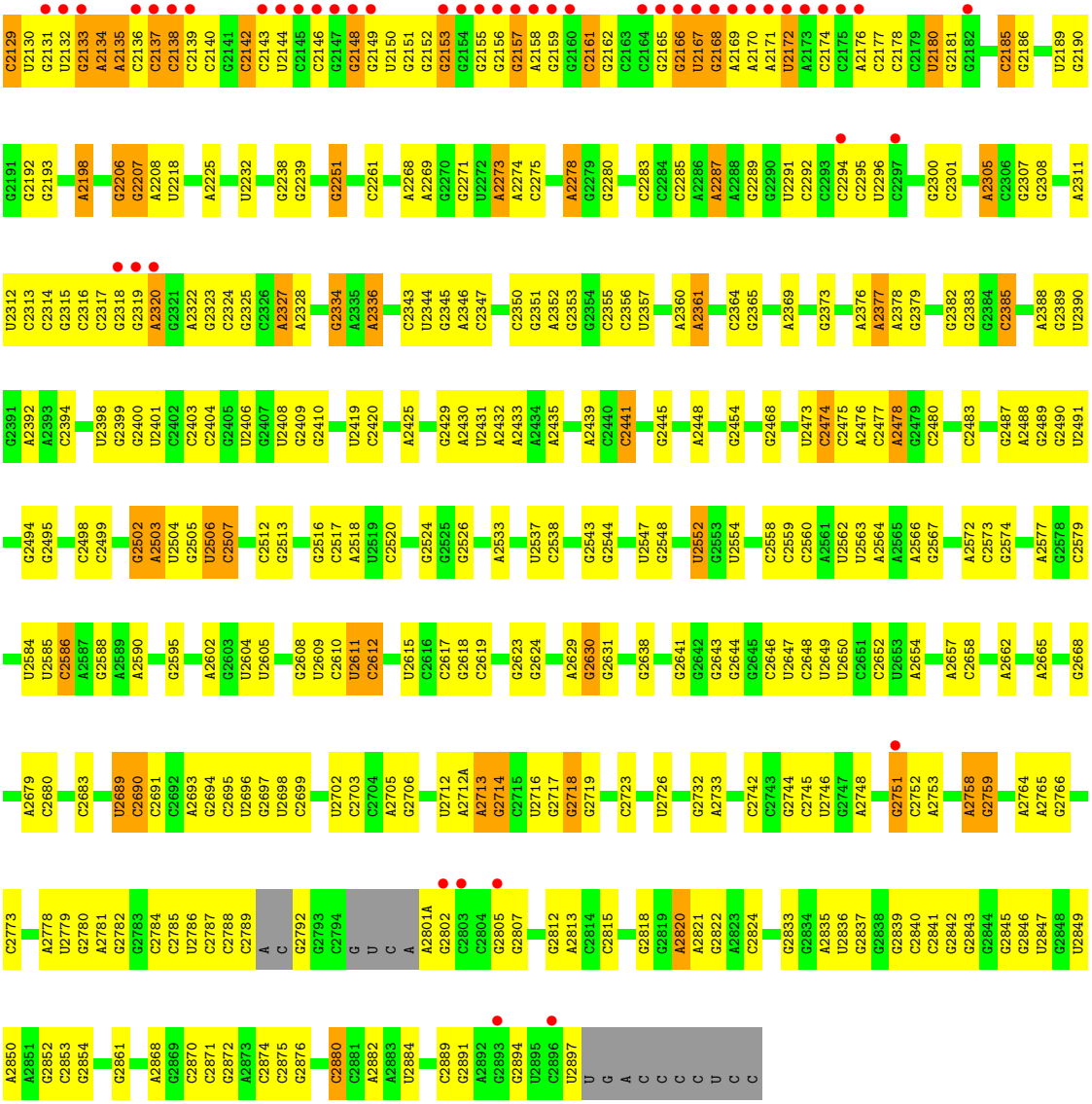


• Molecule 1: 23S Ribosomal RNA

Chain 2A:

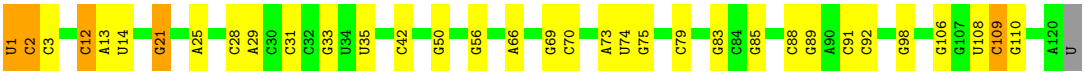



C850 U851 G852 G853 G854 G855 C856 C857 U858 G859 U860 A861 G862 A863 G864 C865 A866 C867 U868 G869 G873 G874 G875 C876 U877 A878 G879 G880 G881 G882 G883 C884 C885 C886 A887 C888 C889 A890 G892 C893 C894 U895 A896 C897 C898 A899 A900 A901 C902 C903 C904 A910 A911 C912 U913 C914 A917
A918 G919 G920 G921 U922 C923 C924 C925 A926 G927 G928 G932 A933 C936 G940 A941 G942 U943 G944 A945 G946 G947 G948 A953 G954 C955 U958 A959 A960 C961 G962 G968 U969 C970 C971 G972 A973 G974 C975 G979 A980 A981 C982 A983 A984 C985 C986 G987 C994 C995 A996 G997
A1000 C1005 C1006 C1007 G1011 U1012 C1013 G1016 G1017 C1018 U1019 A1020 A1021 G1022 U1023 G1024 G1025 U1026 A1027 A1028 G1031 A1032 U1033 G1034 U1035 G1036 G1037 C1038 G1039 C1043 G A A A G A C A G C C A G C C U U U U A A A G U C C U U U U C C G U A A C C U G G U U C G A G C C A G1112 U1113 G1114 G1115 C1116 G1117 C1118 G1122 G1125 A1126 A1127 A1128 A1129 U1130
G1131 C1135 G1136 G1139 C1140 U1141 U1142 A1142A C1147 A1148 C1153 G1154 A1155 A1156 U1159 G1160 C1161 G1162 C1166 U1167 G1168 G1169 G1170 G1171 G A U G A C1178 C1179 C1180 G1187 U1188 G1191 G1195 G1203 A1204 U1205 G1206 A1210 U1211 A1214 A1220 A1226
G1229 C1230 G1231 G1232 G1235 G1236 A1237 G1238 G1239 U1240 A1241 A1246 A1247 G1248 G1252 A1253 A1254 U1255 G1256 A1262 U1263 G1264 A1265 G1266 C1270 G1271 A1272 U1273 A1274 A1275 A1278 G1279 A1284 A1287 U1288 U1292 C1293 U1294 C1295 U1300 A1301 G1309 G1310 G1311 C1314 C1315 U1316 A1317
C1345 C1351 U1352 A1353 A1354 G1358 A1359 A1360 G1364 A1365 G1368 G1369 C1370 G1371 U1372 A1373 C1376 G1377 A1378 A1379 G1380 C1383 A1384 G1385 C1386 U1405 U1406 G1410 C1411 A1412 G1413 G1414 U1415 G1416 C1417 U1420 G1421 G1422 G1423 G1424 A1427 C1428 G1429 C1430 A1434 C1437
G1442 G1443 G1444 A1445 G1448 A1449 G1450 G1456 A1460 G1461 C1462 C1463 C1467 G1470 A1471 A1477 G1478 G1482 A1490 C1493 A1494 A1495 A1496 U1497 C1504 C1505 C1506 A1507 A1508 C1509 A1509A A1509B G1510 C1511 U1514 G1515 U1518 G1519 G1520 G1525 G1529 C1530 C1531 C1532 G1533 U
A C1536 C1537 G1538 G1539 U1540 G1541 A1542 C1543 A1544 C1547 C1557 A1558 A1566 A1567 G1568 A1569 A1570 A1571 U1576 C1577 U1578 A1579 A1580 G1581 C1584 A1586 C1592 G1593 G1594 G1595 A1596 A1597 C1598 C1599 C1600 C1604 C1607 A1608 A1609 A1610 A1614 G1619 G1622 G1630 C1631 A1631A A1632
C1636 A1637 C1638 U1639 C1640 G1645 C1646 G1647 C1648 G1651 A1652 G1653 A1654 C1657 C1658 U1659 C1660 G1661 C1662 C1663 C1670 G1674 C1686 G1687 U1688 A1689 U1693 G1696 G1697 A1698 G1699 A1700 A1701 G1702 G1703 C1711 C1712 U1713 G1714 G1721 A1722 U1739 G1740 G1746 G1747 G1747A C1751
C1754 A1755 G1756 U1757 G1758 A1759 A1760 C1761 A1762 G1763 G1764 G1769 G1770 C1771 G1772 A1773 U1778 U1779 A1780 C1781 C1782 A1783 A1784 A1785 A1786 C1790 A1791 U1794 C1795 U1796 C1797 U1798 G1799 C1800 G1801 A1802 A1803 G1811 A1812 G1813 G1814 A1815 G1816 G1817 U1818 A1821 G1822 G1826 C1832 U1833 U1834
G1835 G1839 C1843 C1844 G1845 G1846 A1847 A1848 A1853 G1856 G1865 A1877 G1878 C1886 A1889 A1890 G1899 A1900 A1901 C1902 C1903 G1906 G1910 U1911 A1912 A1913 C1914 U1915 A1916 U1917 A1918 A1919 C1920 G1921 A1927 A1928 G1929 G1930 U1931 A1932 G1933 A1936 A1937 A1938 U1939 C1942
U1946 C1947 A1952 U1955 C1958 C1962 U1963 C1967 A1970 A1971 A1972 G1973 G1987 C1988 U1991 G1992 U1993 C1996 G1997 G1998 C1999 G2000 A2001 G2002 G2010 U2011 G2012 A2013 A2014 A2019 A2020 C2021 U2022 G2023 G2027 A2030 A2031 G2032 A2033 U2034 G2035 C2040 C2043 C2044
C2045 G2046 G2049 C2050 A2051 G2052 G2053 A2054 C2055 G2056 A2060 G2061 A2062 C2065 U2068 G2069 C2070 A2071 U2079 U2086 C2087 G2093 U2096 U2099 G2100 G2101 U2102 C2103 G2104 C2108 U2109 C2110 C2111 C2112 U2113 A2114 G2115 G2116 A2117 U2118 A2119 G2120 G2121 U2122 G2123 G2124 G2125 A2126 G2127 C2128



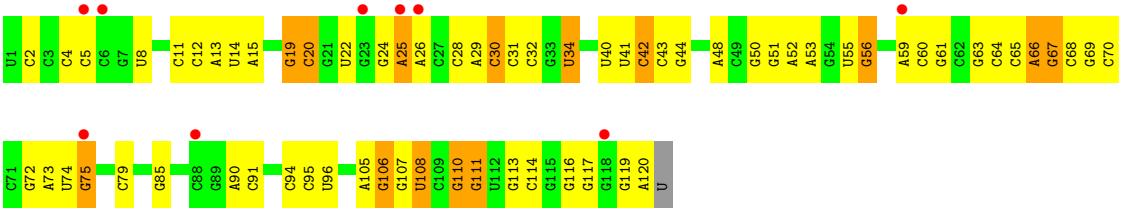
• Molecule 2: 5S Ribosomal RNA

Chain 1B:



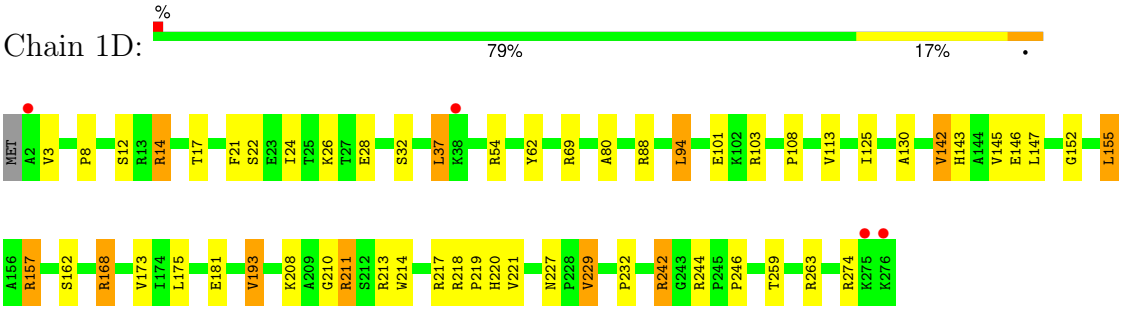
• Molecule 2: 5S Ribosomal RNA

Chain 2B:



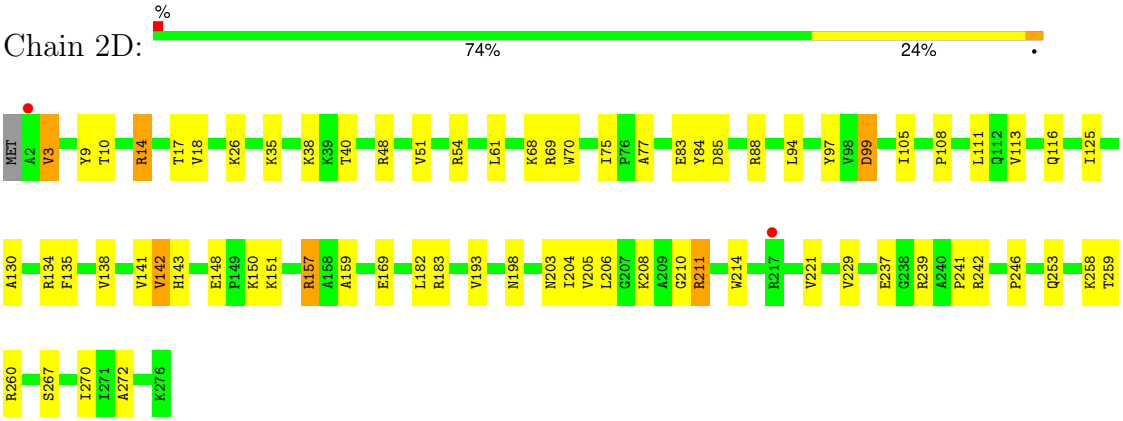
• Molecule 3: 50S ribosomal protein L2

Chain 1D:



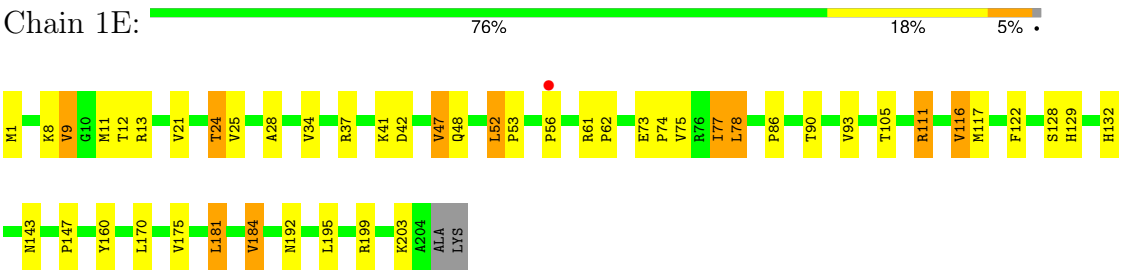
• Molecule 3: 50S ribosomal protein L2

Chain 2D:



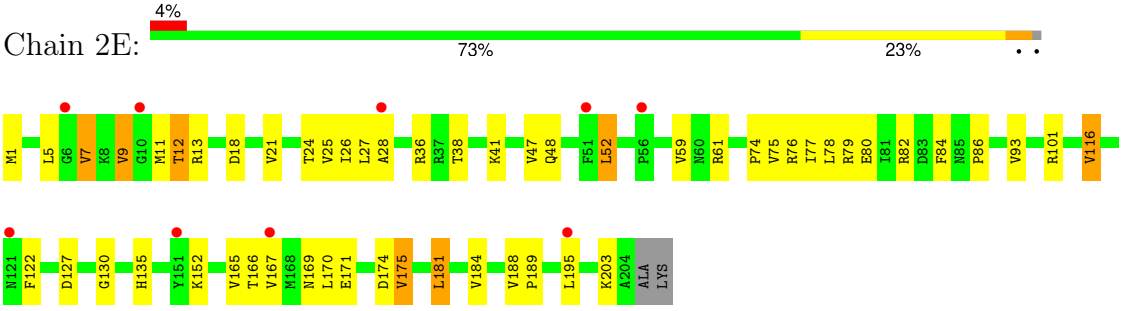
• Molecule 4: 50S ribosomal protein L3

Chain 1E:



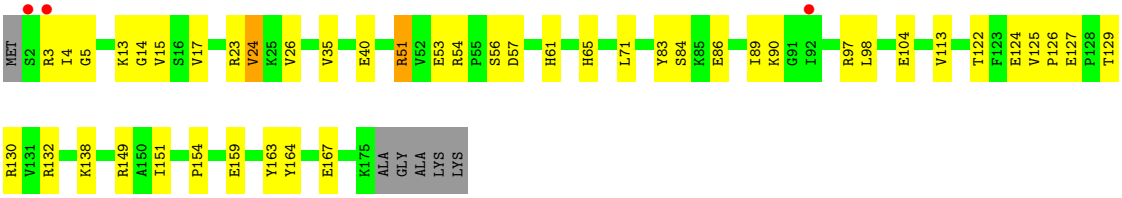
• Molecule 4: 50S ribosomal protein L3

Chain 2E:



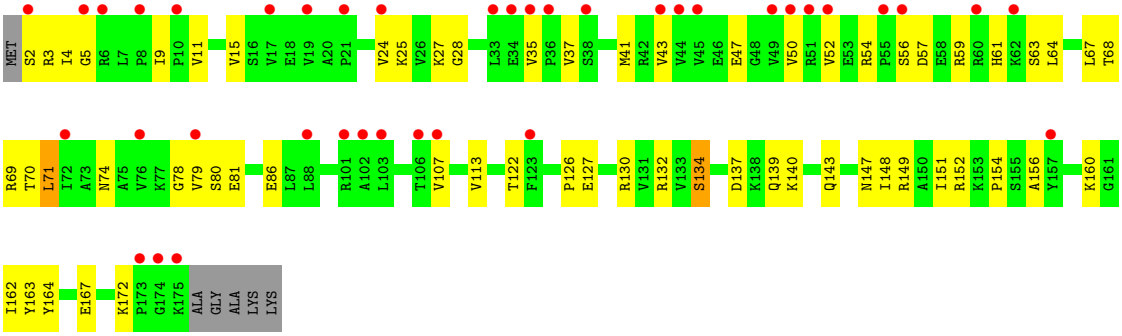
• Molecule 5: 50S ribosomal protein L4

Chain 1F:



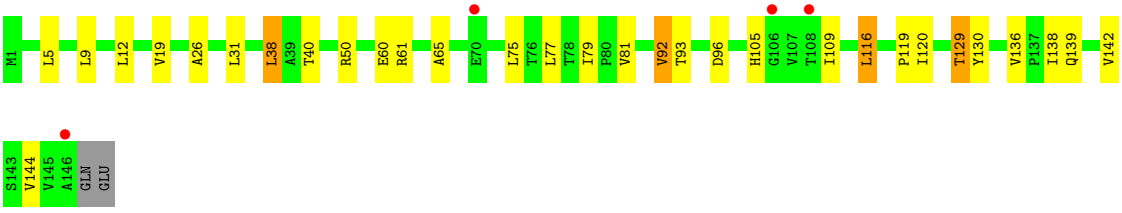
• Molecule 7: 50S ribosomal protein L6

Chain 2H:



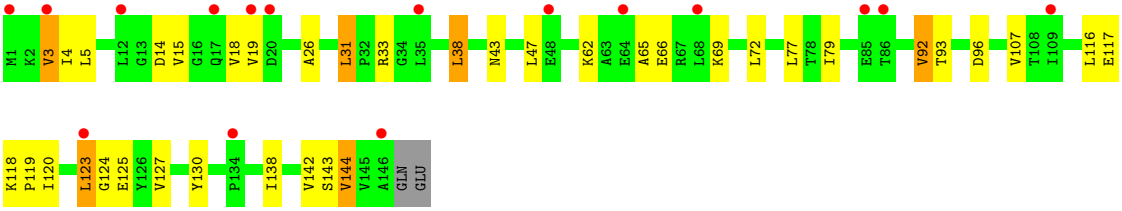
• Molecule 8: 50S ribosomal protein L9

Chain 1I:



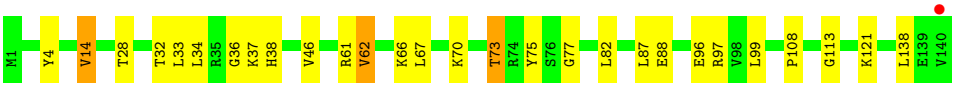
• Molecule 8: 50S ribosomal protein L9

Chain 2I:



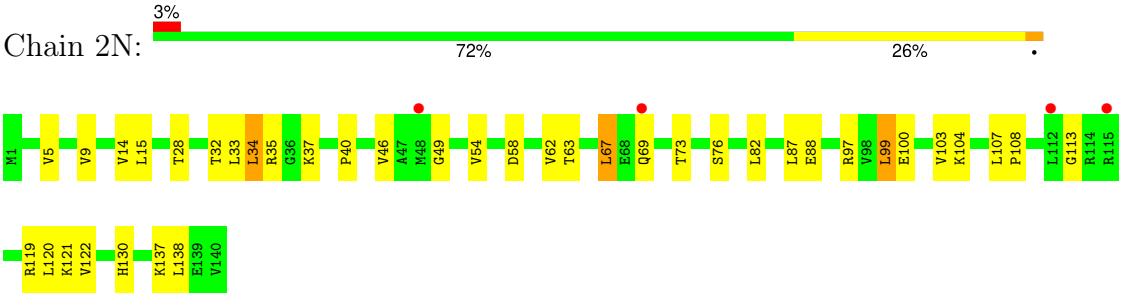
• Molecule 9: 50S ribosomal protein L13

Chain 1N:



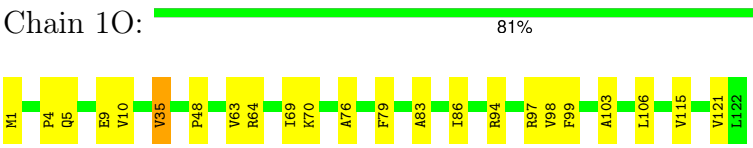
• Molecule 9: 50S ribosomal protein L13

Chain 2N:



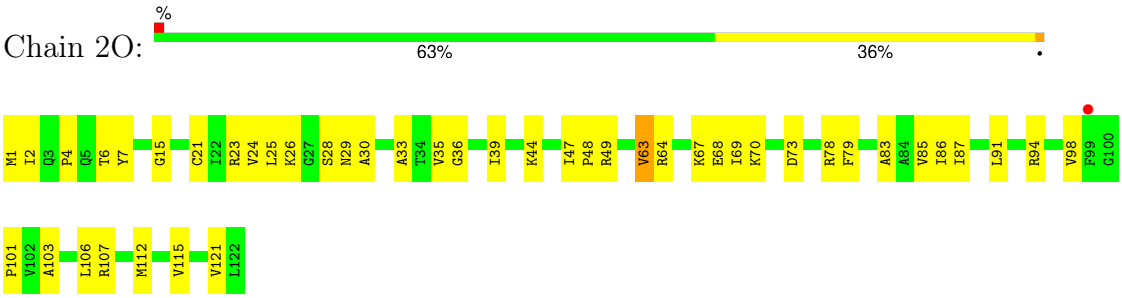
• Molecule 10: 50S ribosomal protein L14

Chain 1O:



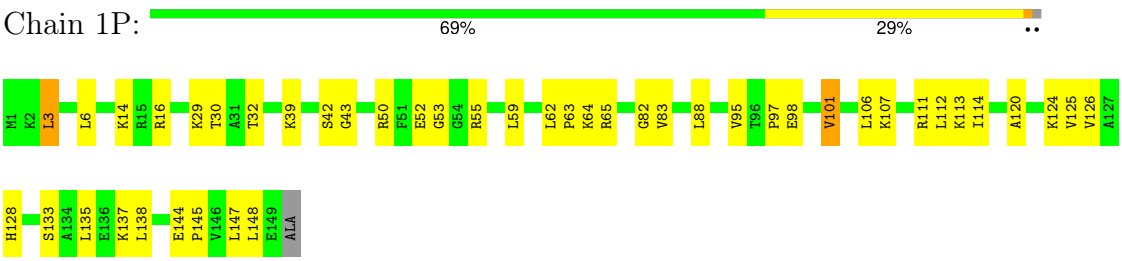
• Molecule 10: 50S ribosomal protein L14

Chain 2O:



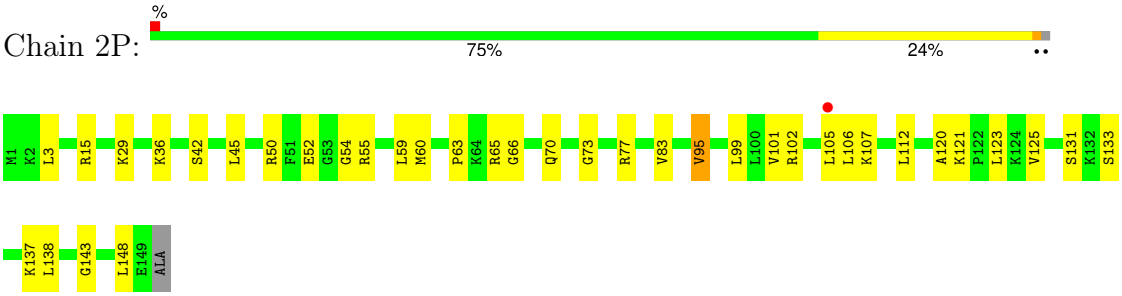
• Molecule 11: 50S ribosomal protein L15

Chain 1P:



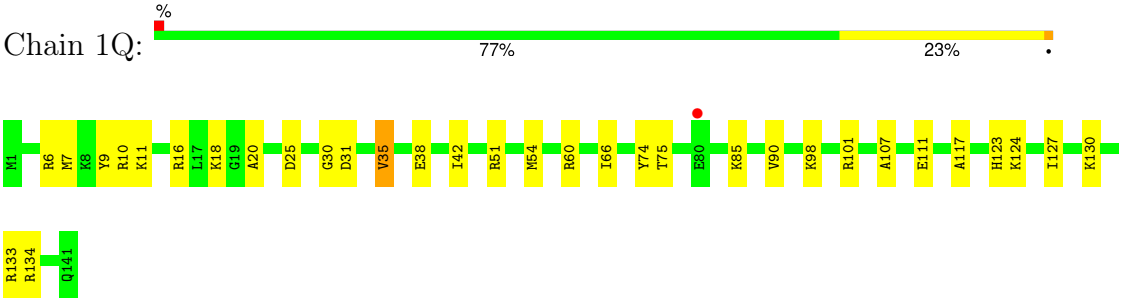
• Molecule 11: 50S ribosomal protein L15

Chain 2P:



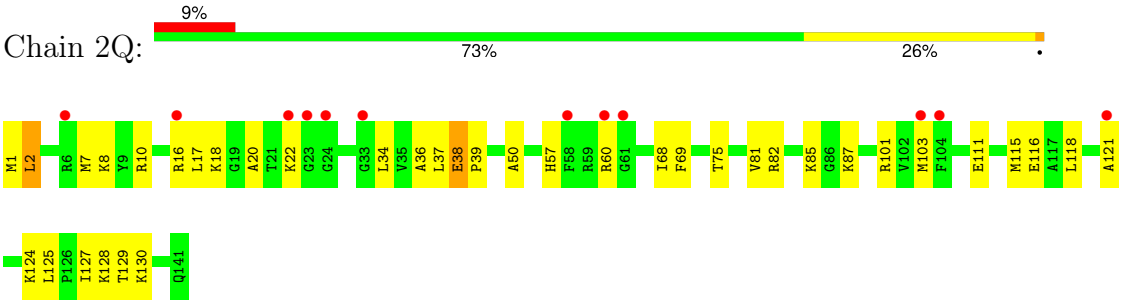
• Molecule 12: 50S ribosomal protein L16

Chain 1Q:



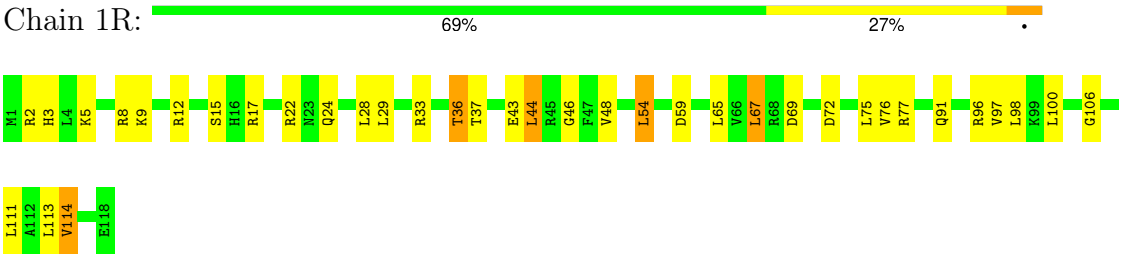
• Molecule 12: 50S ribosomal protein L16

Chain 2Q:



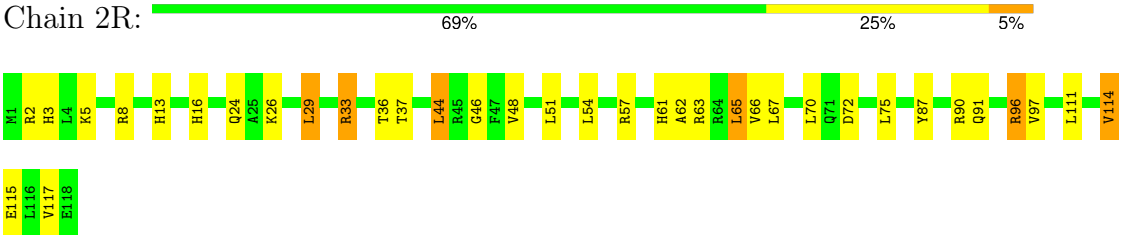
• Molecule 13: 50S ribosomal protein L17

Chain 1R:



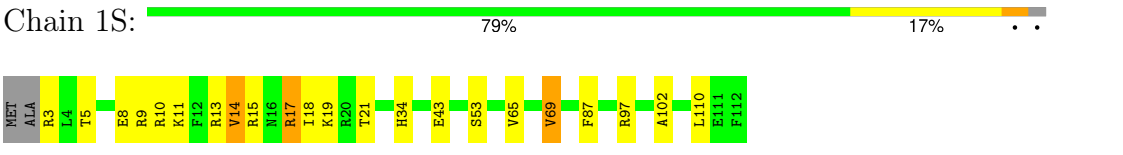
• Molecule 13: 50S ribosomal protein L17

Chain 2R:



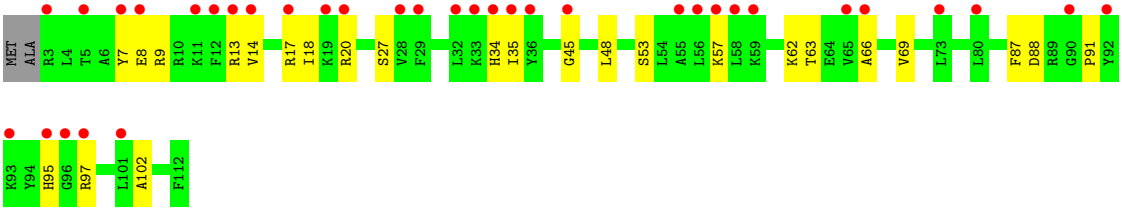
• Molecule 14: 50S ribosomal protein L18

Chain 1S:



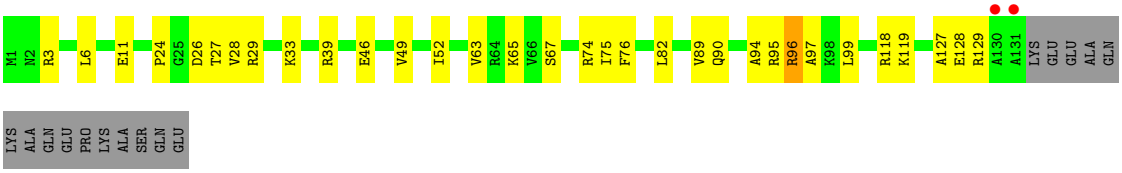
• Molecule 14: 50S ribosomal protein L18

Chain 2S:



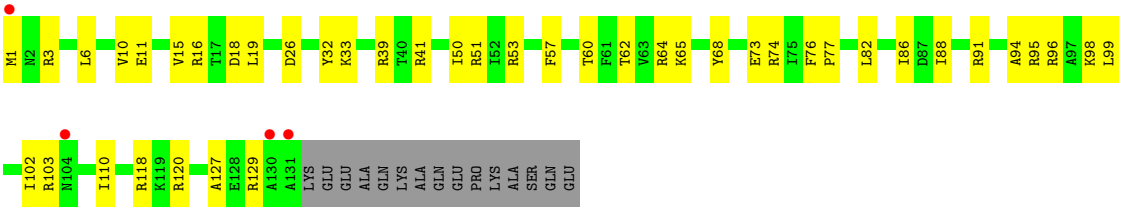
• Molecule 15: 50S ribosomal protein L19

Chain 1T:



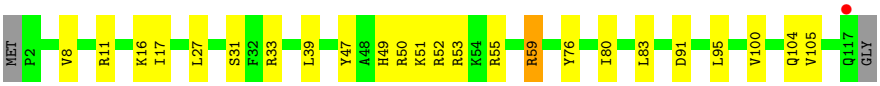
• Molecule 15: 50S ribosomal protein L19

Chain 2T:



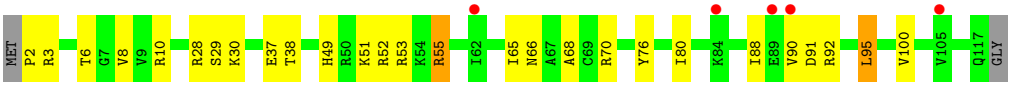
• Molecule 16: 50S ribosomal protein L20

Chain 1U:



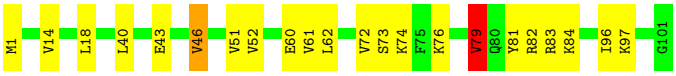
• Molecule 16: 50S ribosomal protein L20

Chain 2U:



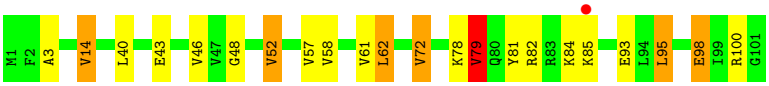
• Molecule 17: 50S ribosomal protein L21

Chain 1V:



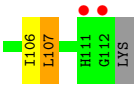
• Molecule 17: 50S ribosomal protein L21

Chain 2V:



• Molecule 18: 50S ribosomal protein L22

Chain 1W:



• Molecule 18: 50S ribosomal protein L22

Chain 2W:

• Molecule 19: 50S ribosomal protein L23

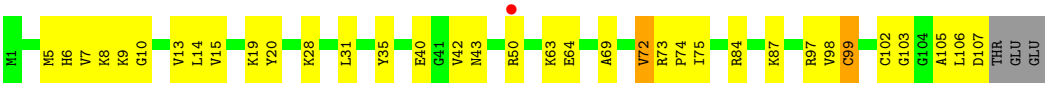
Chain 1X:

• Molecule 19: 50S ribosomal protein L23

Chain 2X:

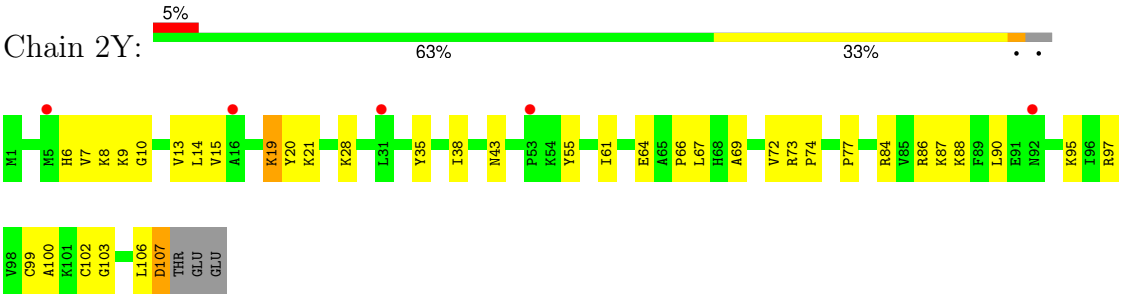
• Molecule 20: 50S ribosomal protein L24

Chain 1Y:



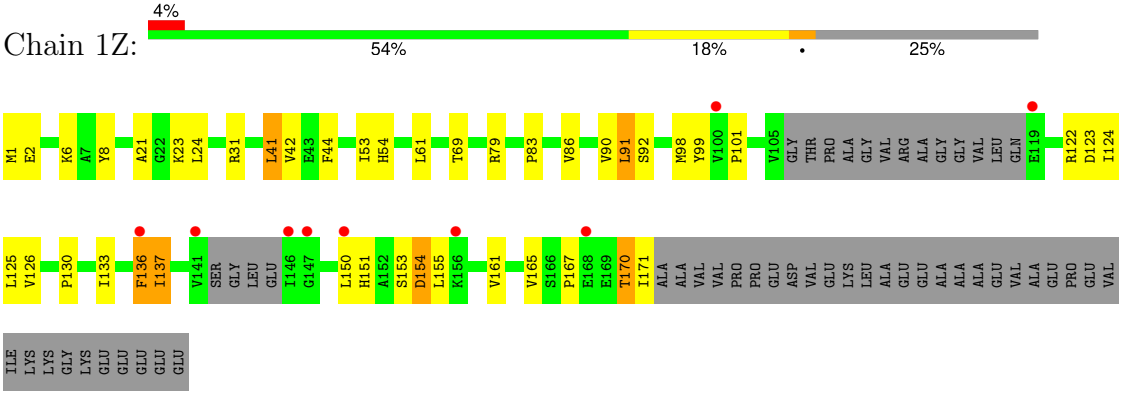
• Molecule 20: 50S ribosomal protein L24

Chain 2Y:



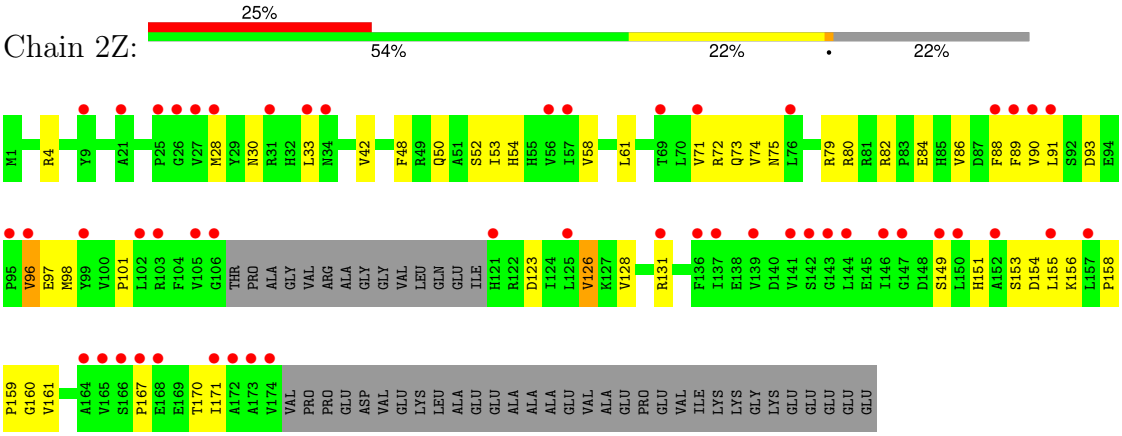
• Molecule 21: 50S ribosomal protein L25

Chain 1Z:



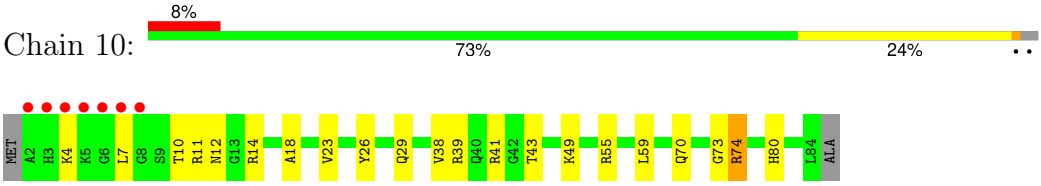
• Molecule 21: 50S ribosomal protein L25

Chain 2Z:



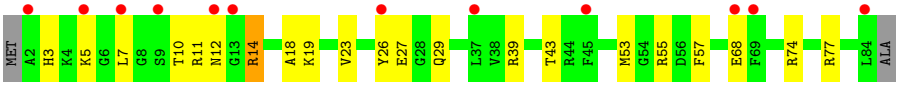
• Molecule 22: 50S ribosomal protein L27

Chain 10:



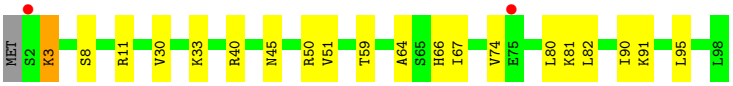
• Molecule 22: 50S ribosomal protein L27

Chain 20:



• Molecule 23: 50S ribosomal protein L28

Chain 11:

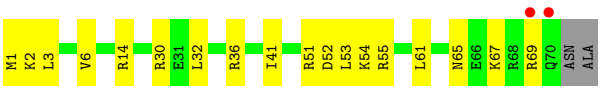


• Molecule 23: 50S ribosomal protein L28

Chain 21:

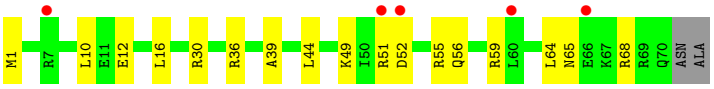
• Molecule 24: 50S ribosomal protein L29

Chain 12:



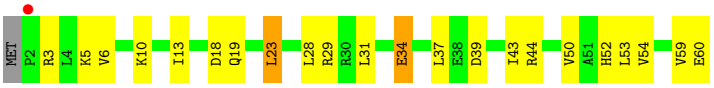
• Molecule 24: 50S ribosomal protein L29

Chain 22:



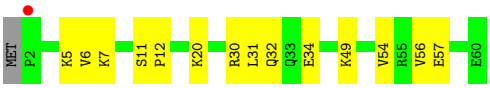
• Molecule 25: 50S ribosomal protein L30

Chain 13:



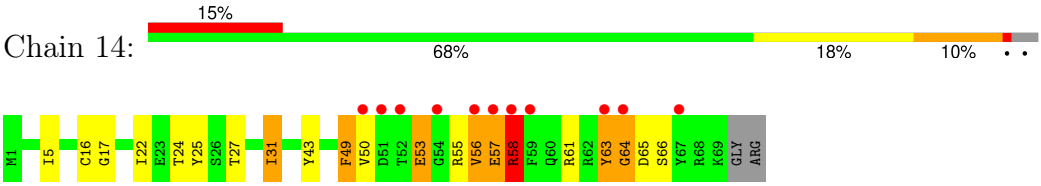
• Molecule 25: 50S ribosomal protein L30

Chain 23:



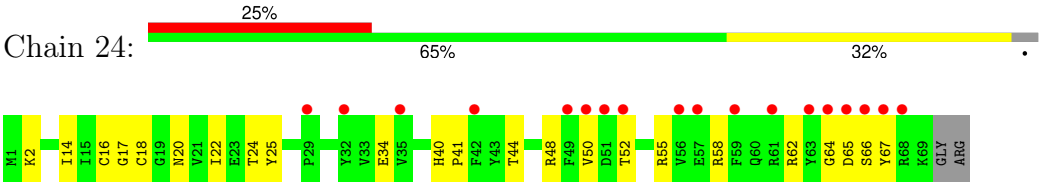
• Molecule 26: 50S ribosomal protein L31

Chain 14:



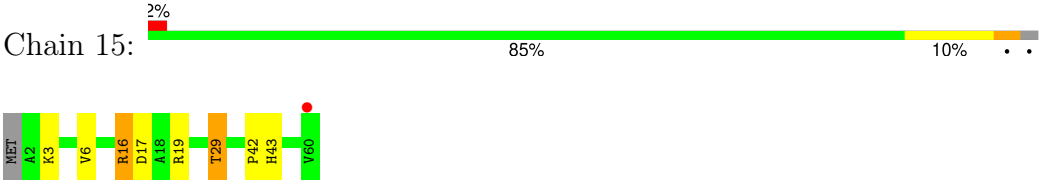
• Molecule 26: 50S ribosomal protein L31

Chain 24:



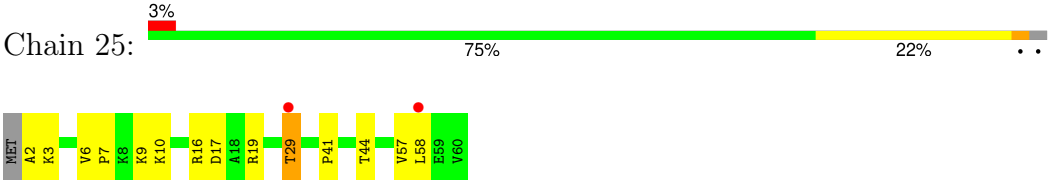
• Molecule 27: 50S ribosomal protein L32

Chain 15:



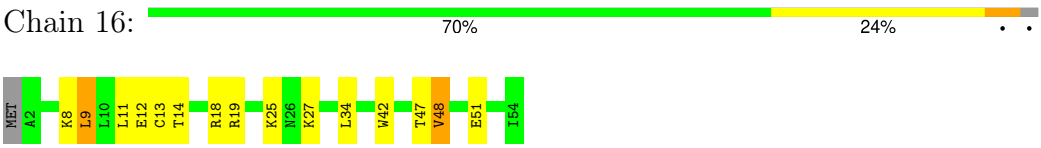
• Molecule 27: 50S ribosomal protein L32

Chain 25:



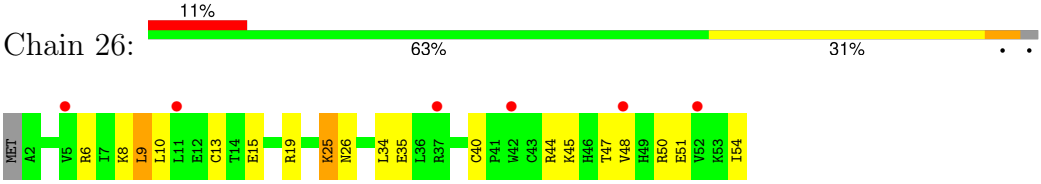
• Molecule 28: 50S ribosomal protein L33

Chain 16:



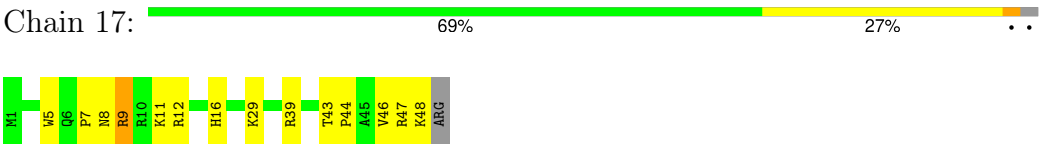
• Molecule 28: 50S ribosomal protein L33

Chain 26:



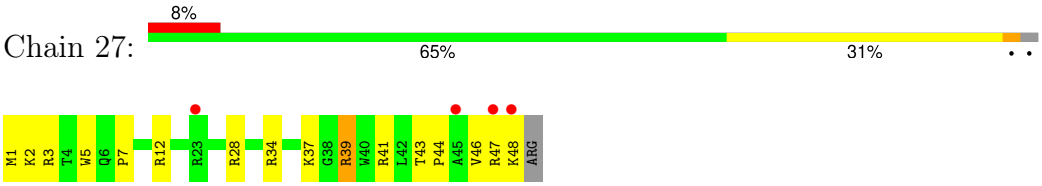
• Molecule 29: 50S ribosomal protein L34

Chain 17:



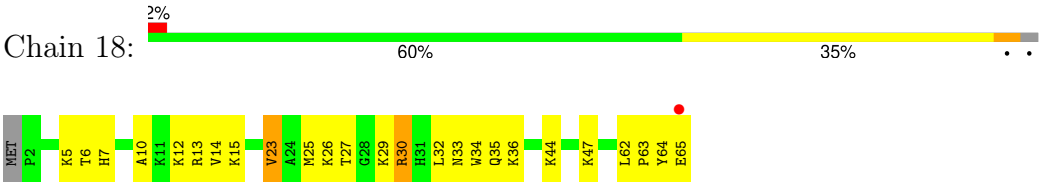
• Molecule 29: 50S ribosomal protein L34

Chain 27:



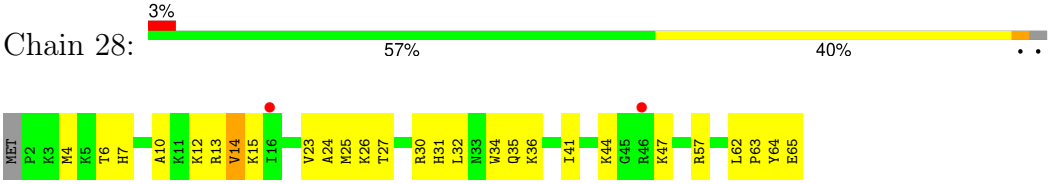
• Molecule 30: 50S ribosomal protein L35

Chain 18:



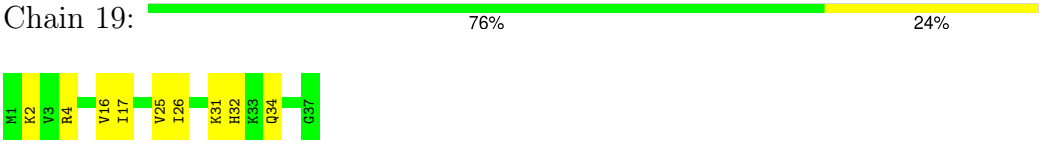
• Molecule 30: 50S ribosomal protein L35

Chain 28:



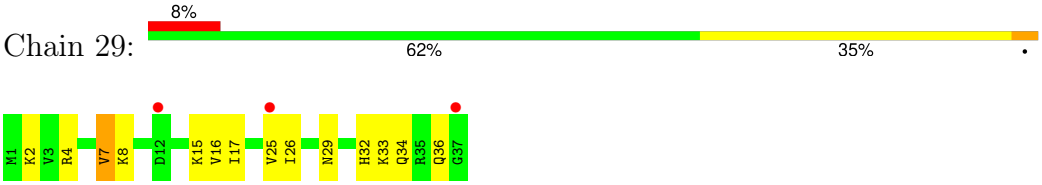
• Molecule 31: 50S ribosomal protein L36

Chain 19:



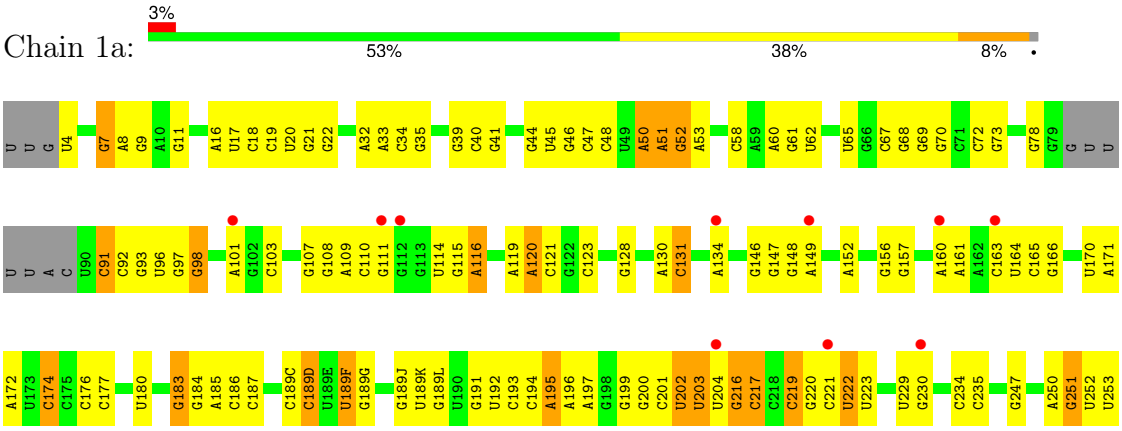
• Molecule 31: 50S ribosomal protein L36

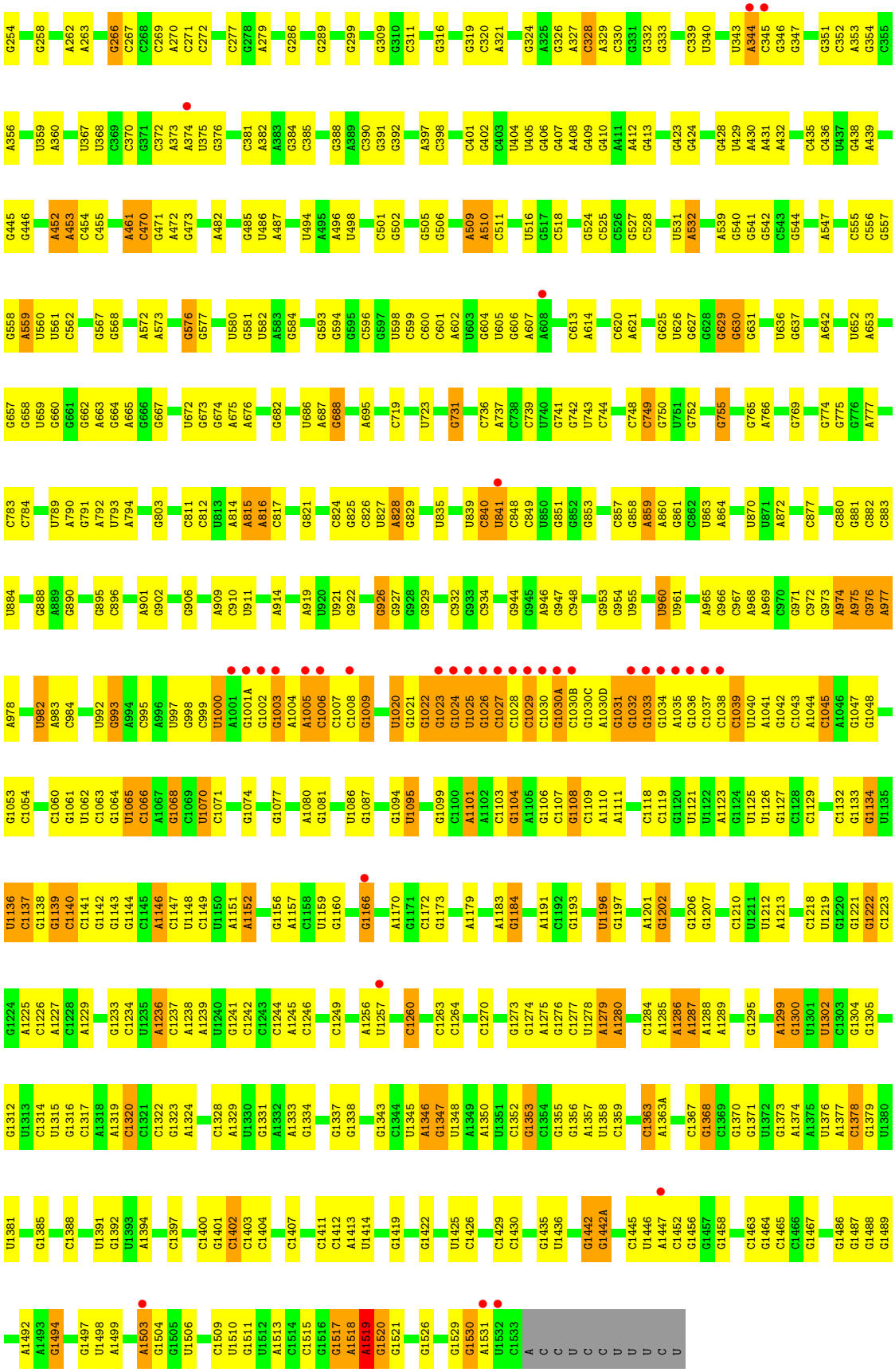
Chain 29:



• Molecule 32: 16S Ribosomal RNA

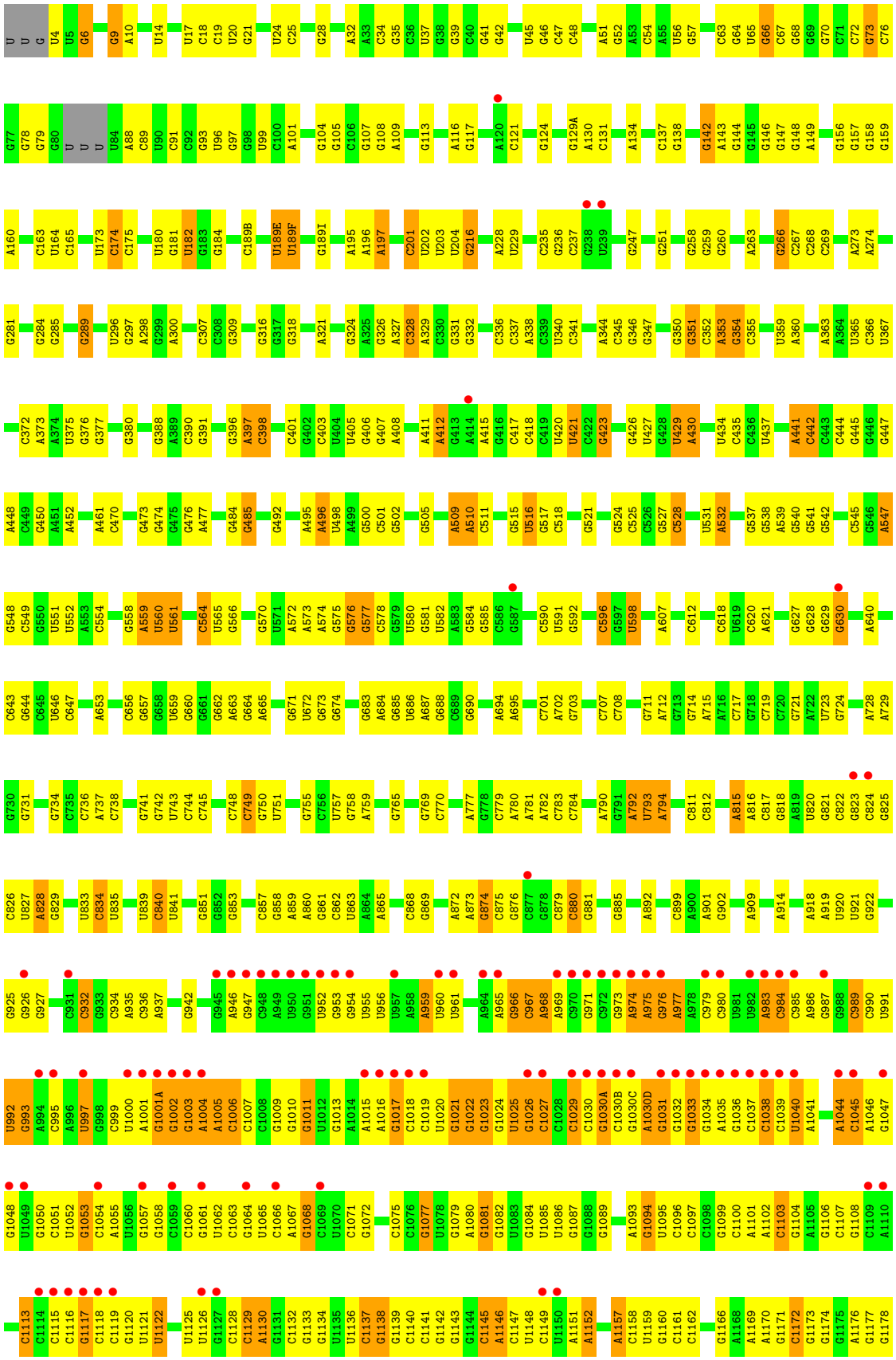
Chain 1a:

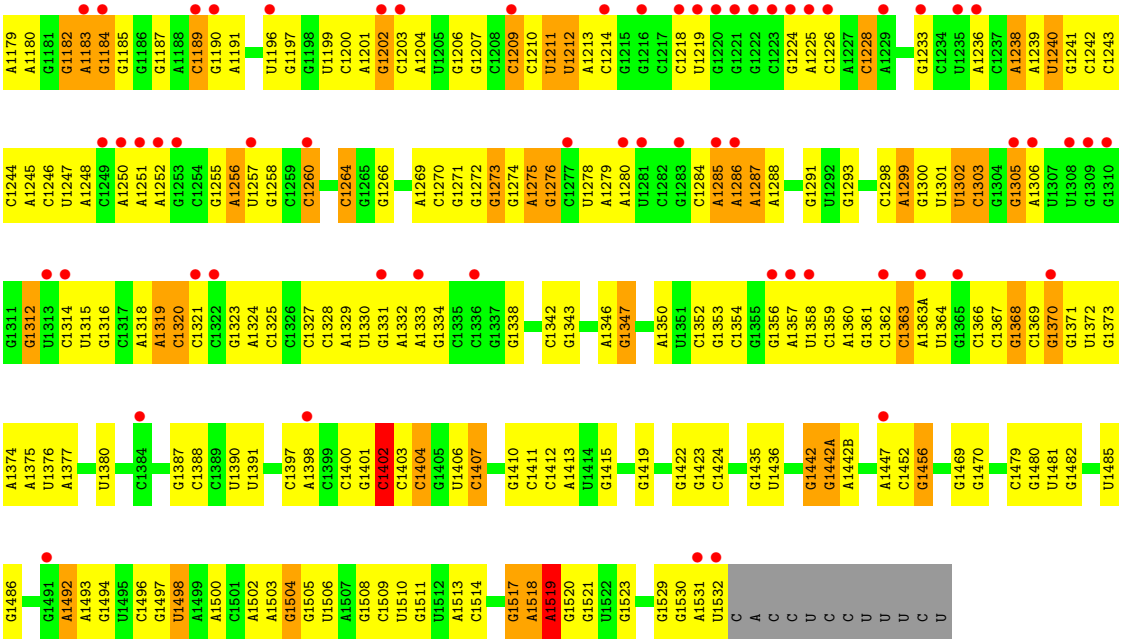




• Molecule 32: 16S Ribosomal RNA

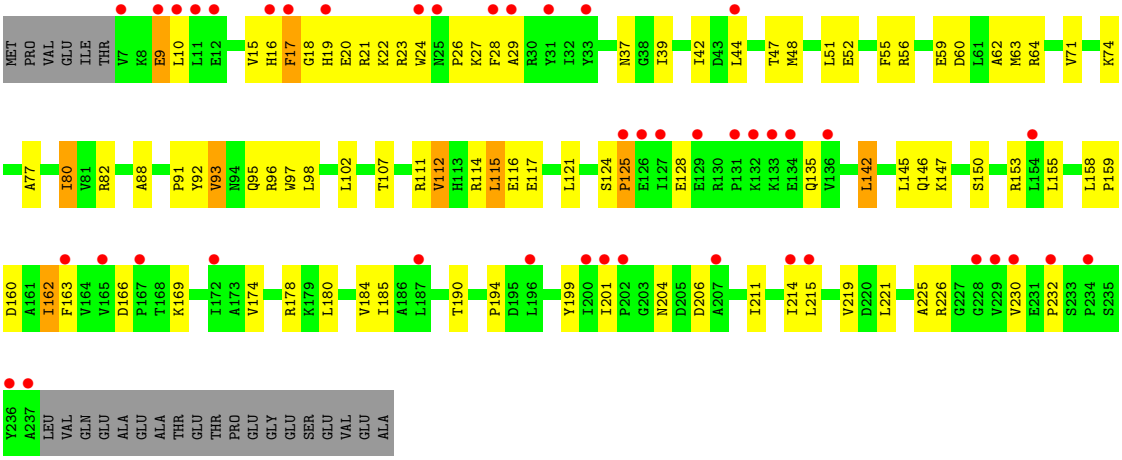
Chain 2a:





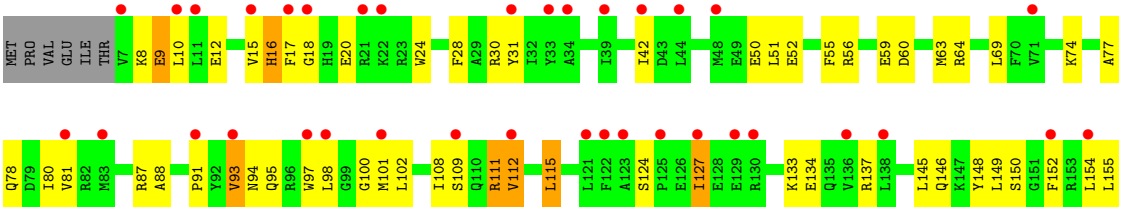
• Molecule 33: 30S ribosomal protein S2

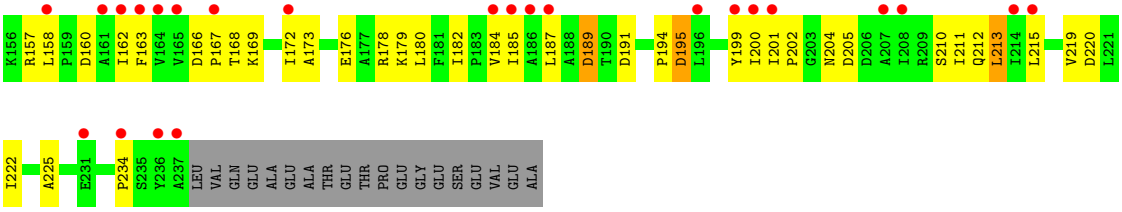
Chain 1b:



• Molecule 33: 30S ribosomal protein S2

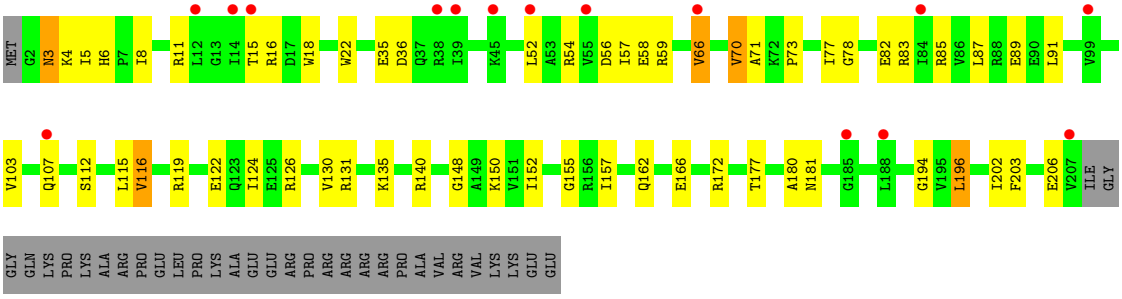
Chain 2b:





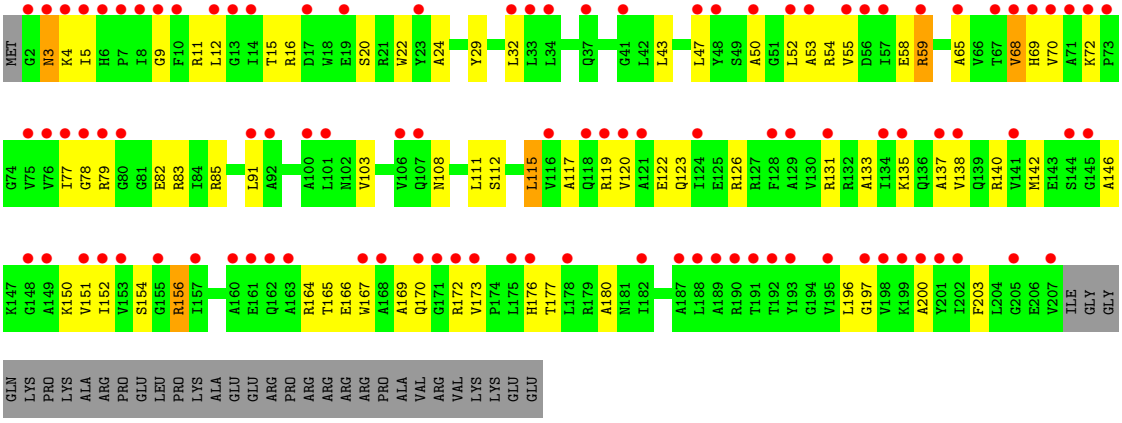
• Molecule 34: 30S ribosomal protein S3

Chain 1c:



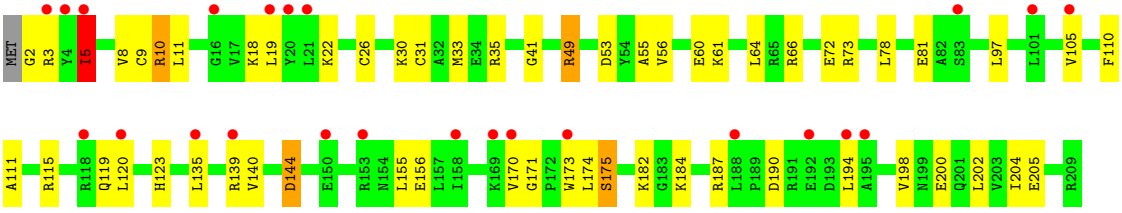
• Molecule 34: 30S ribosomal protein S3

Chain 2c:



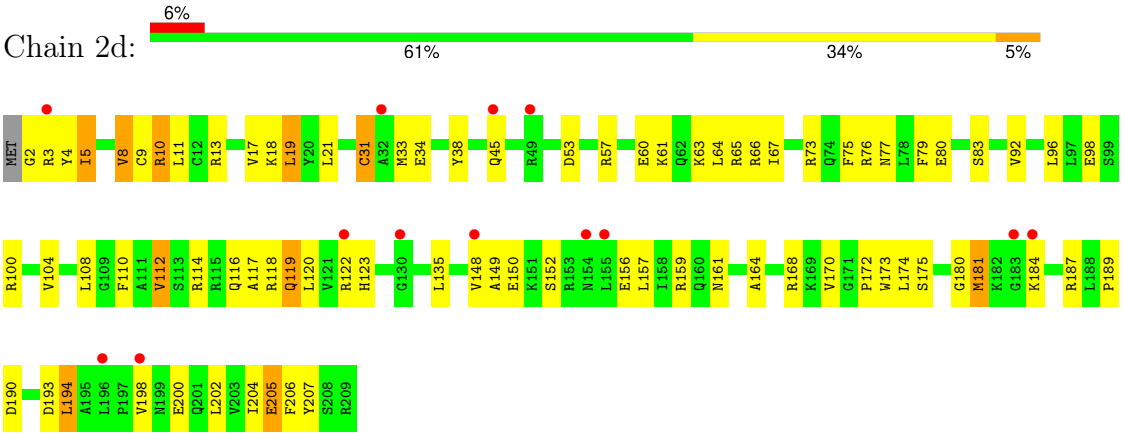
• Molecule 35: 30S ribosomal protein S4

Chain 1d:



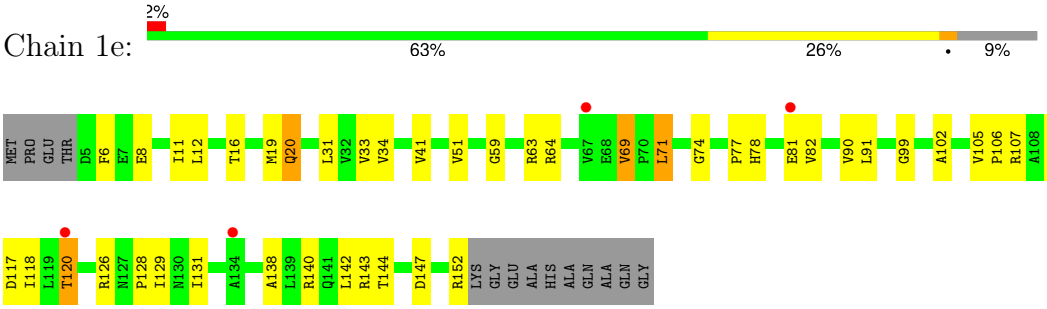
• Molecule 35: 30S ribosomal protein S4

Chain 2d:



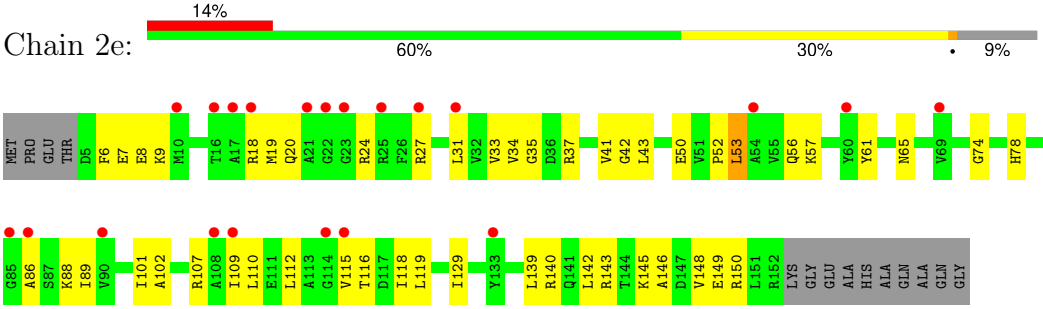
• Molecule 36: 30S ribosomal protein S5

Chain 1e:



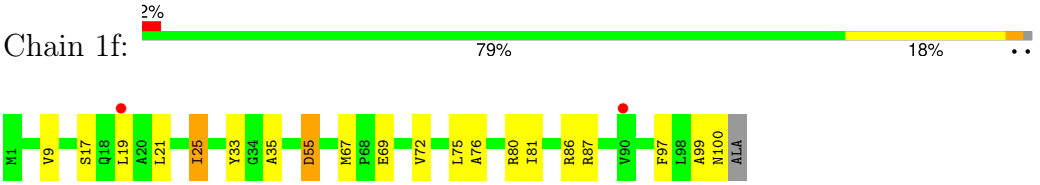
• Molecule 36: 30S ribosomal protein S5

Chain 2e:



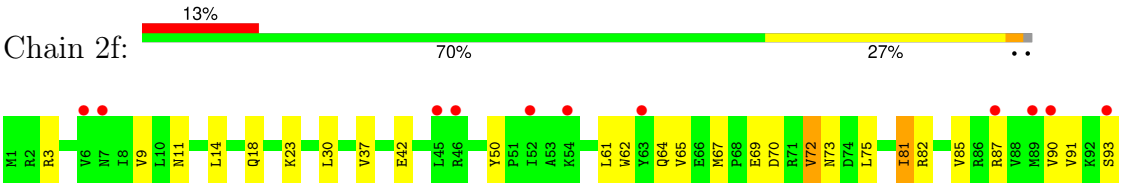
• Molecule 37: 30S ribosomal protein S6

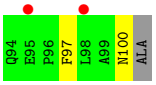
Chain 1f:



• Molecule 37: 30S ribosomal protein S6

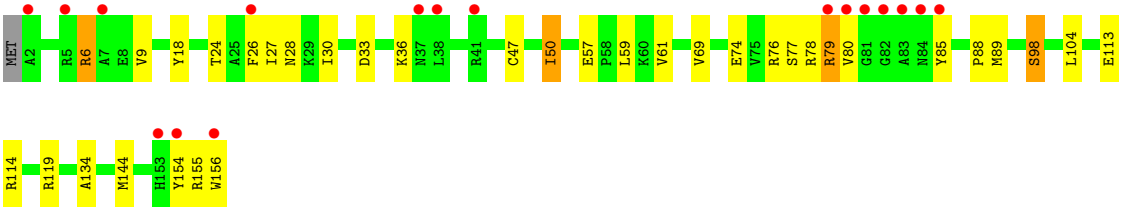
Chain 2f:





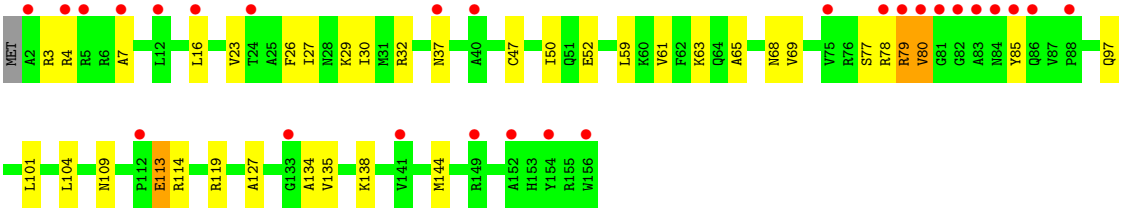
• Molecule 38: 30S ribosomal protein S7

Chain 1g:



• Molecule 38: 30S ribosomal protein S7

Chain 2g:

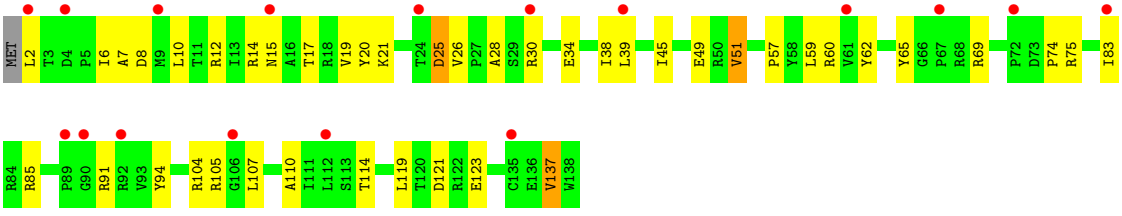


• Molecule 39: 30S ribosomal protein S8

Chain 1h:

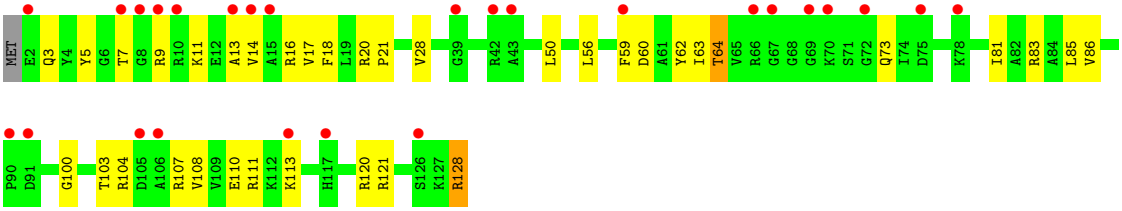
• Molecule 39: 30S ribosomal protein S8

Chain 2h:



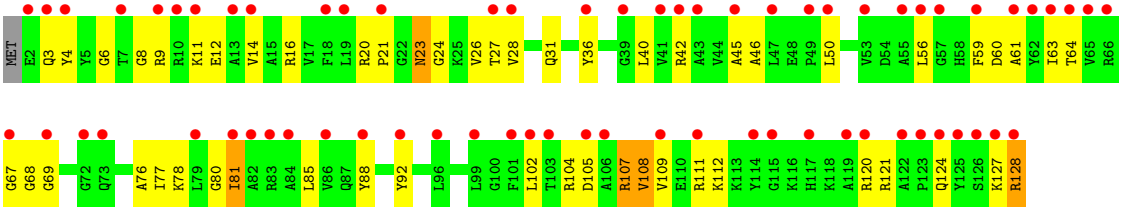
• Molecule 40: 30S ribosomal protein S9

Chain 1i:



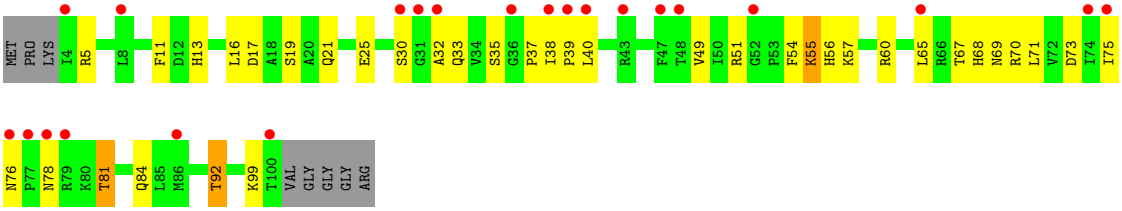
• Molecule 40: 30S ribosomal protein S9

Chain 2i:



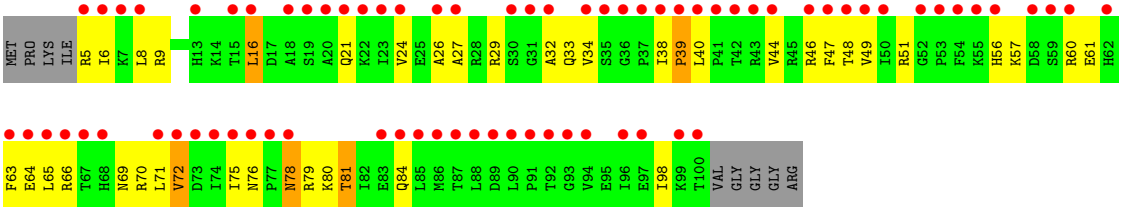
• Molecule 41: 30S ribosomal protein S10

Chain 1j:



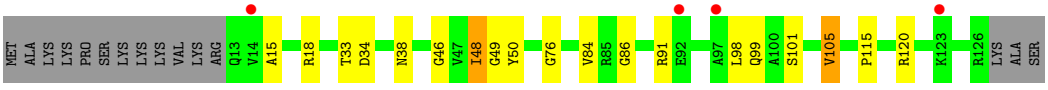
• Molecule 41: 30S ribosomal protein S10

Chain 2j:



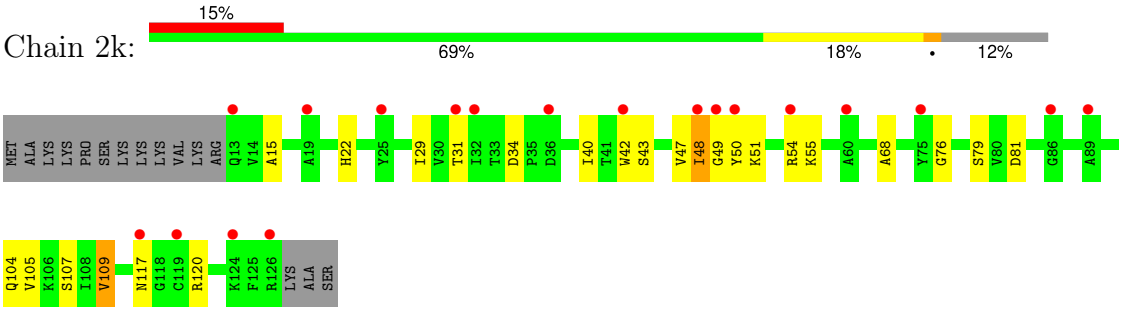
• Molecule 42: 30S ribosomal protein S11

Chain 1k:



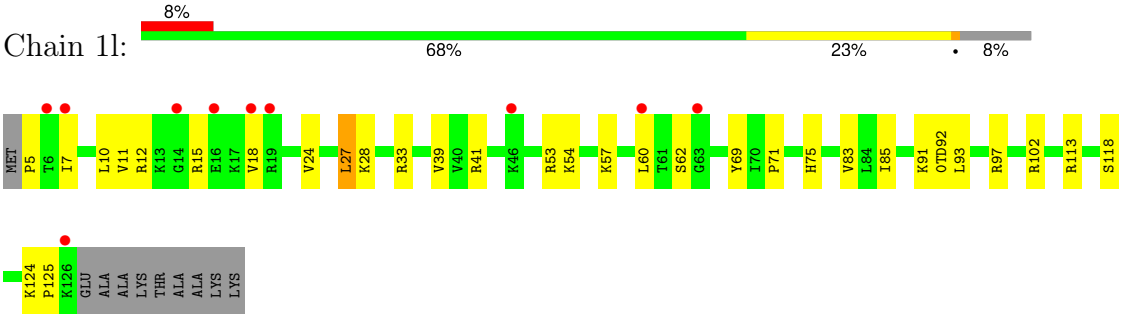
• Molecule 42: 30S ribosomal protein S11

Chain 2k:



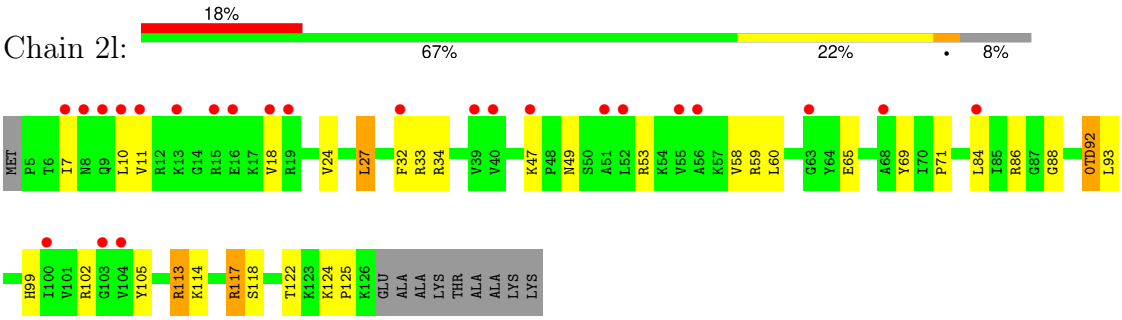
• Molecule 43: 30S ribosomal protein S12

Chain 1l:



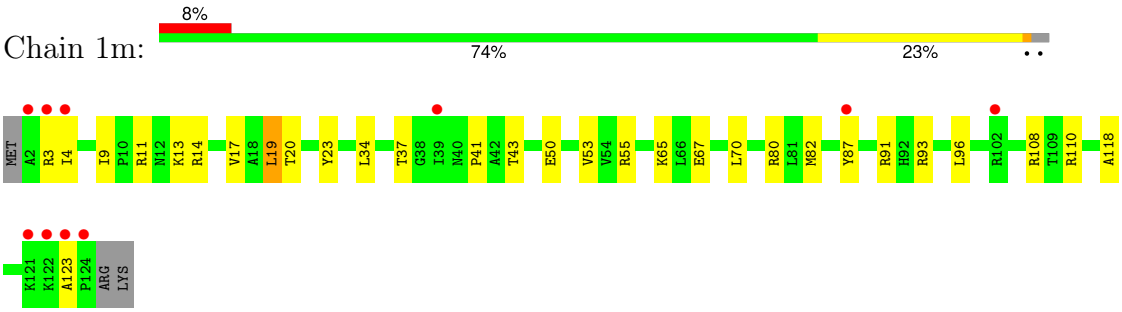
• Molecule 43: 30S ribosomal protein S12

Chain 2l:



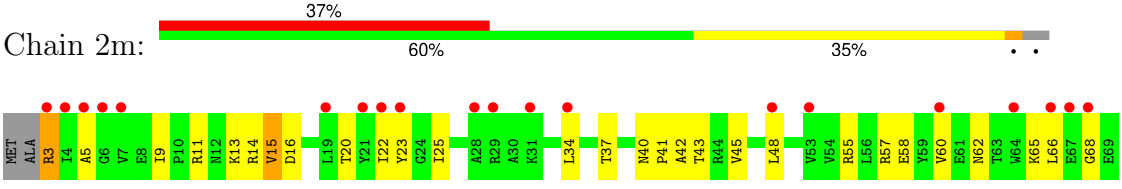
• Molecule 44: 30S ribosomal protein S13

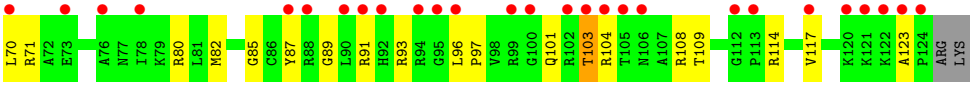
Chain 1m:



• Molecule 44: 30S ribosomal protein S13

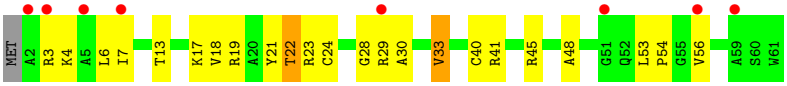
Chain 2m:





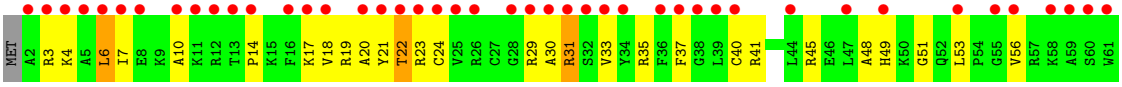
• Molecule 45: 30S ribosomal protein S14 type Z

Chain 1n:



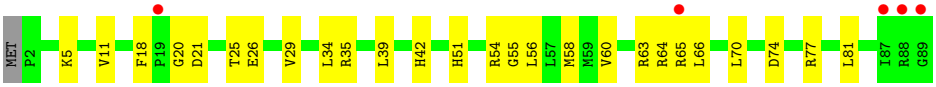
• Molecule 45: 30S ribosomal protein S14 type Z

Chain 2n:



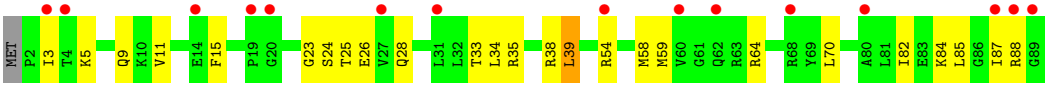
• Molecule 46: 30S ribosomal protein S15

Chain 1o:



• Molecule 46: 30S ribosomal protein S15

Chain 2o:

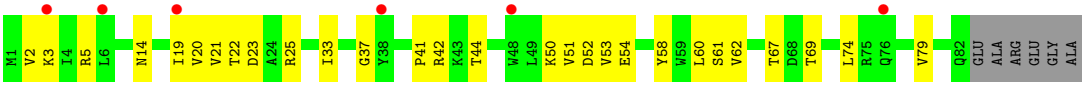


• Molecule 47: 30S ribosomal protein S16

Chain 1p:

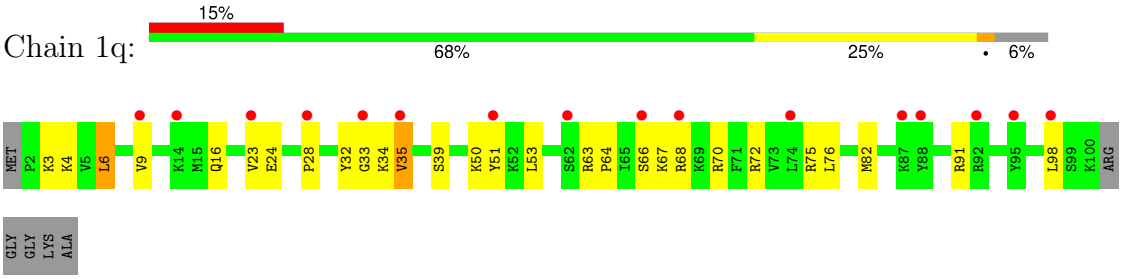
• Molecule 47: 30S ribosomal protein S16

Chain 2p:



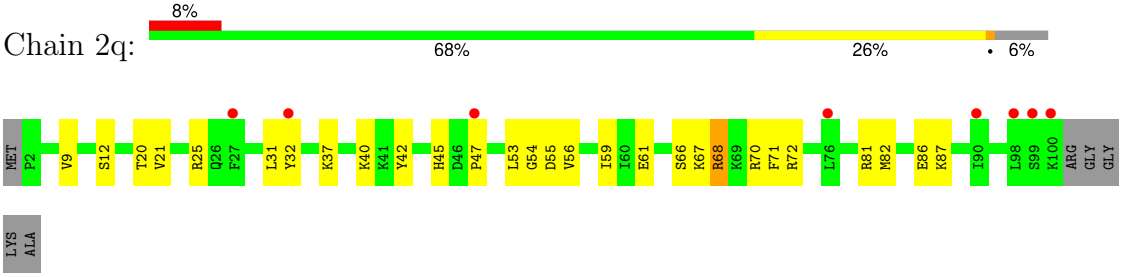
• Molecule 48: 30S ribosomal protein S17

Chain 1q:



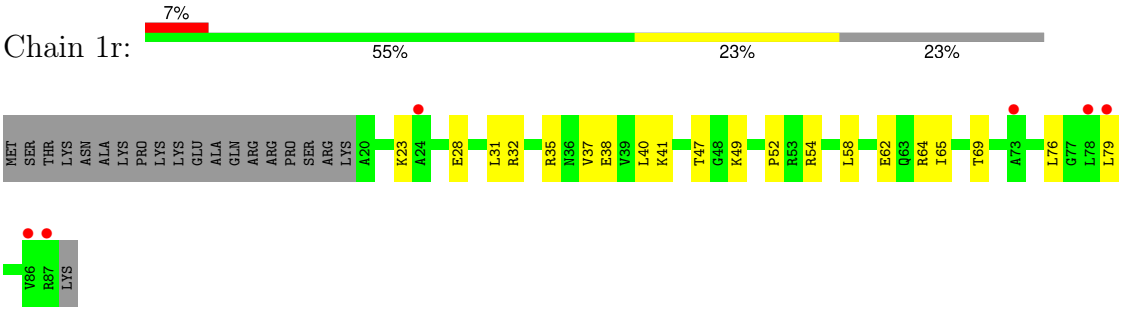
• Molecule 48: 30S ribosomal protein S17

Chain 2q:



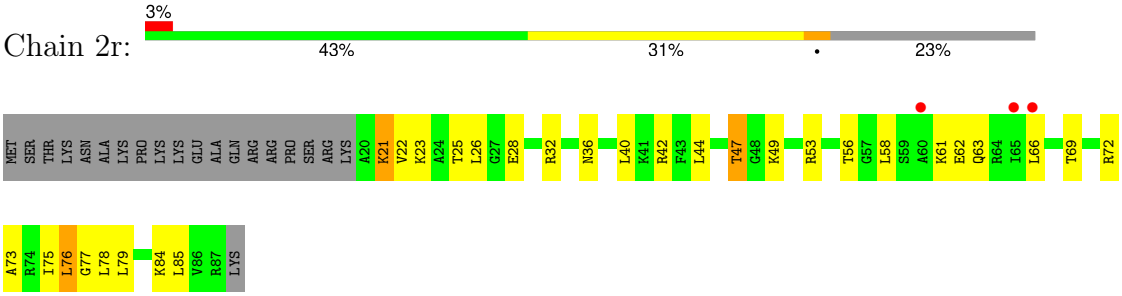
• Molecule 49: 30S ribosomal protein S18

Chain 1r:



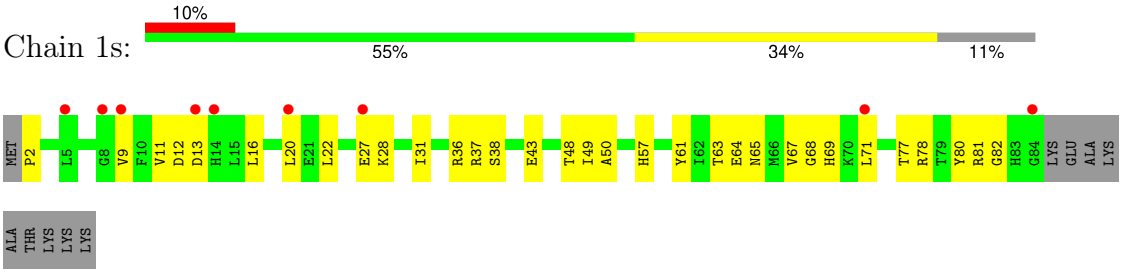
• Molecule 49: 30S ribosomal protein S18

Chain 2r:



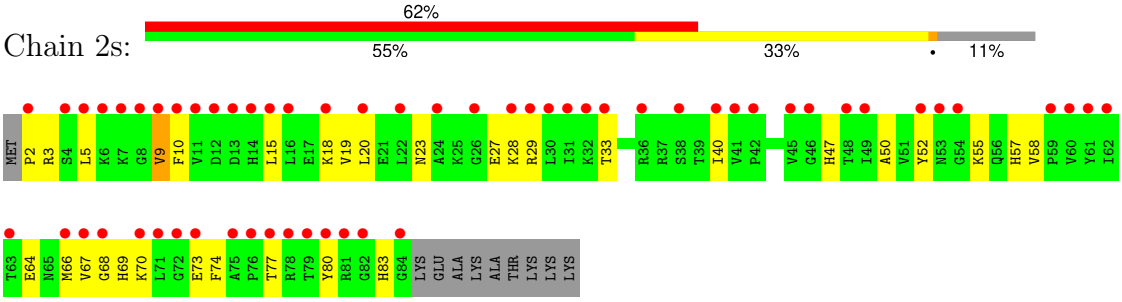
• Molecule 50: 30S ribosomal protein S19

Chain 1s:



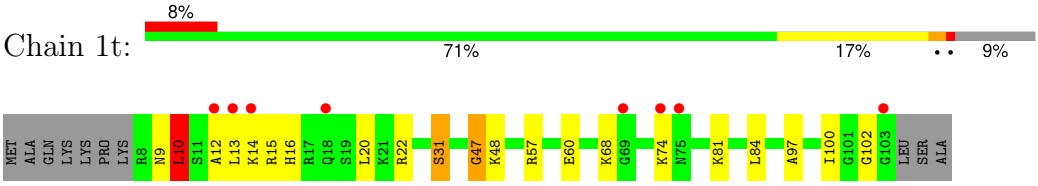
• Molecule 50: 30S ribosomal protein S19

Chain 2s:



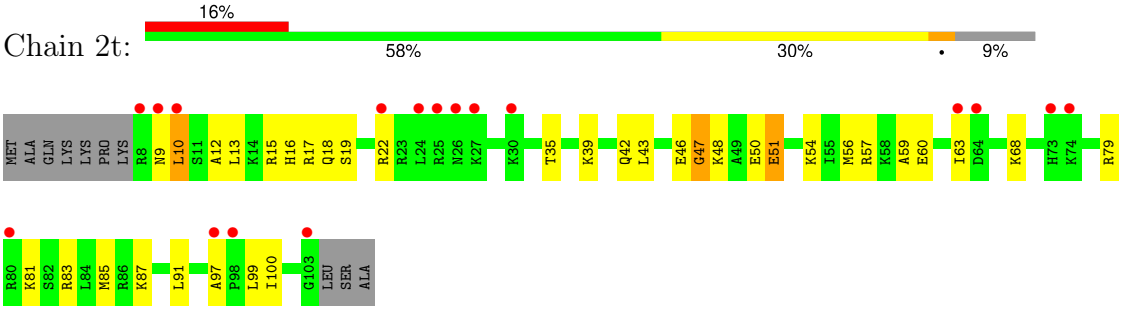
• Molecule 51: 30S ribosomal protein S20

Chain 1t:



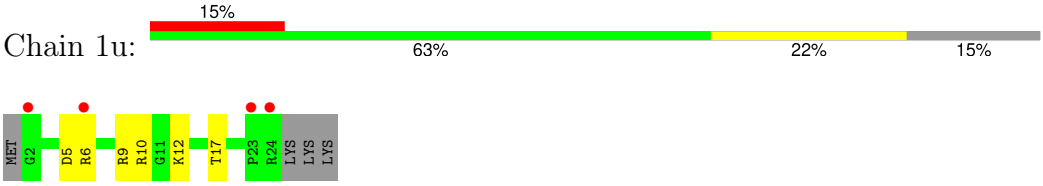
• Molecule 51: 30S ribosomal protein S20

Chain 2t:



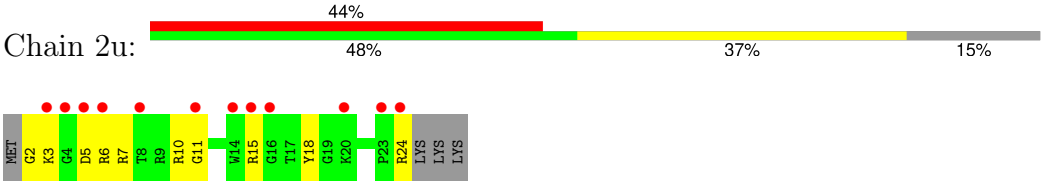
• Molecule 52: 30S ribosomal protein Thx

Chain 1u:



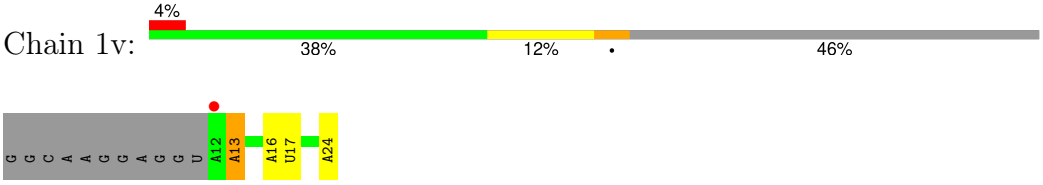
• Molecule 52: 30S ribosomal protein Thx

Chain 2u:



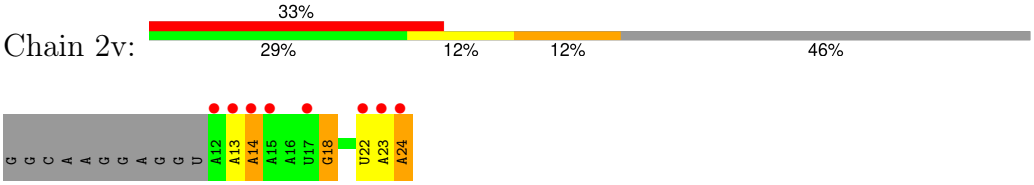
• Molecule 53: mRNA

Chain 1v:



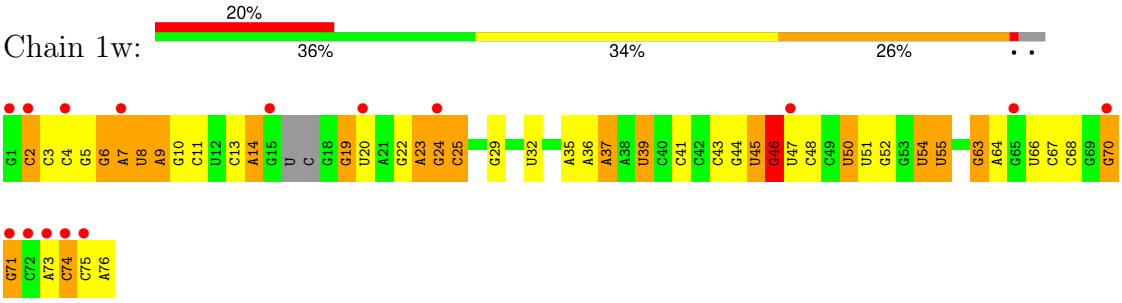
• Molecule 53: mRNA

Chain 2v:



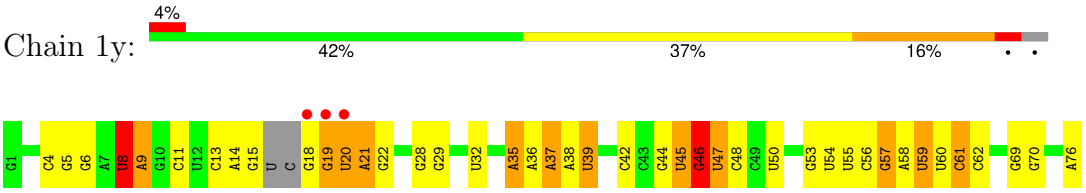
• Molecule 54: A-site and E-site tRNAs

Chain 1w:



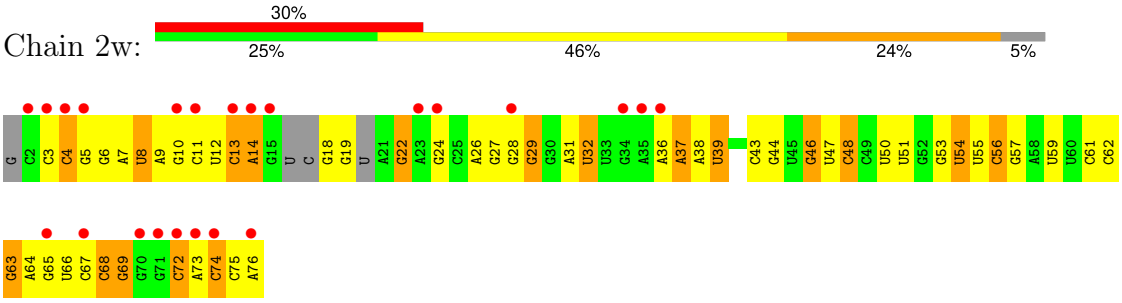
• Molecule 54: A-site and E-site tRNAs

Chain 1y:



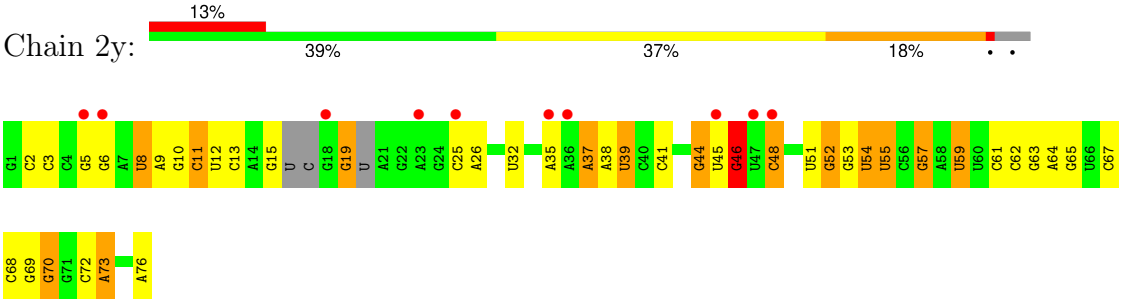
• Molecule 54: A-site and E-site tRNAs

Chain 2w:



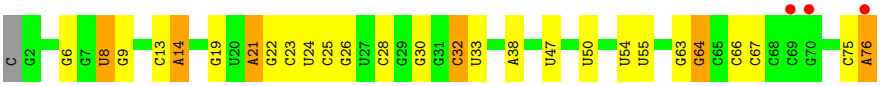
• Molecule 54: A-site and E-site tRNAs

Chain 2y:



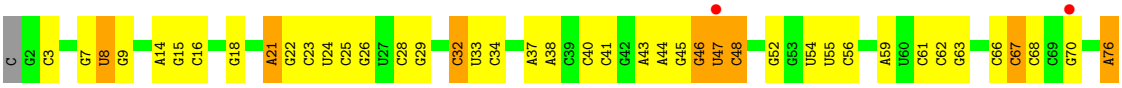
• Molecule 55: P-site tRNA

Chain 1x:



• Molecule 55: P-site tRNA

Chain 2x:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	208.99Å 448.29Å 618.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	127.28 – 2.60 127.28 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.7 (127.28-2.60) 98.7 (127.28-2.60)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.19 (at 2.62Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.229 , 0.276 0.234 , 0.278	Depositor DCC
R_{free} test set	86986 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	52.3	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 50.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	300833	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.59% 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: 5MU, 4OC, K, 0TD, MA6, OMG, MG, MIA, 2MG, SF4, 4SU, M2G, PSU, CLM, UR3, 5MC, 2MA, 7MG, 2MU, ZN

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	0.19	0/69009	0.37	0/107712
1	2A	0.14	0/67293	0.32	0/105034
2	1B	0.14	0/2882	0.31	0/4494
2	2B	0.13	0/2879	0.32	0/4487
3	1D	0.25	0/2186	0.46	0/2944
3	2D	0.17	0/2186	0.41	0/2944
4	1E	0.18	0/1592	0.43	0/2149
4	2E	0.15	0/1592	0.39	0/2149
5	1F	0.17	0/1619	0.42	0/2193
5	2F	0.14	0/1615	0.35	0/2188
6	1G	0.16	0/1448	0.37	0/1957
6	2G	0.13	0/1453	0.39	0/1963
7	1H	0.16	0/1356	0.35	0/1834
7	2H	0.13	0/1356	0.33	0/1834
8	1I	0.13	0/1112	0.33	0/1514
8	2I	0.14	0/1079	0.36	0/1475
9	1N	0.18	0/1144	0.39	0/1543
9	2N	0.13	0/1144	0.36	0/1543
10	1O	0.19	0/943	0.38	0/1269
10	2O	0.15	0/943	0.35	0/1269
11	1P	0.19	0/1152	0.41	0/1533
11	2P	0.15	0/1152	0.39	0/1533
12	1Q	0.18	0/1143	0.38	0/1527
12	2Q	0.14	0/1143	0.37	0/1527
13	1R	0.18	0/982	0.41	0/1312
13	2R	0.14	0/982	0.37	0/1312
14	1S	0.15	0/883	0.41	0/1176
14	2S	0.13	0/880	0.37	0/1172
15	1T	0.17	0/1105	0.39	0/1477
15	2T	0.14	0/1097	0.37	0/1468
16	1U	0.19	0/977	0.38	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	2U	0.14	0/977	0.34	0/1301
17	1V	0.19	0/782	0.39	0/1049
17	2V	0.15	0/782	0.37	0/1049
18	1W	0.19	0/897	0.40	0/1205
18	2W	0.14	0/897	0.34	0/1205
19	1X	0.18	0/764	0.44	0/1025
19	2X	0.13	0/764	0.35	0/1025
20	1Y	0.17	0/819	0.41	0/1095
20	2Y	0.14	0/819	0.38	0/1095
21	1Z	0.16	0/1267	0.39	0/1717
21	2Z	0.15	0/1299	0.39	0/1763
22	10	0.18	0/662	0.43	0/881
22	20	0.15	0/662	0.43	0/881
23	11	0.16	0/762	0.36	0/1014
23	21	0.15	0/762	0.34	0/1014
24	12	0.16	0/590	0.36	0/781
24	22	0.14	0/590	0.31	0/781
25	13	0.18	0/474	0.38	0/635
25	23	0.15	0/469	0.36	0/630
26	14	0.20	0/565	0.53	0/761
26	24	0.19	0/545	0.46	0/737
27	15	0.20	0/469	0.48	0/635
27	25	0.16	0/469	0.38	0/635
28	16	0.18	0/460	0.42	0/613
28	26	0.15	0/456	0.41	0/608
29	17	0.19	0/426	0.42	0/561
29	27	0.17	0/426	0.42	0/561
30	18	0.18	0/525	0.38	0/691
30	28	0.14	0/525	0.32	0/691
31	19	0.18	0/310	0.38	0/407
31	29	0.15	0/310	0.40	0/407
32	1a	0.14	1/35795 (0.0%)	0.32	0/55864
32	2a	0.14	0/35886	0.32	0/56005
33	1b	0.15	0/1881	0.42	0/2542
33	2b	0.17	0/1860	0.42	0/2518
34	1c	0.14	0/1572	0.34	0/2126
34	2c	0.14	0/1566	0.37	0/2119
35	1d	0.15	0/1685	0.37	0/2262
35	2d	0.14	0/1704	0.38	0/2284
36	1e	0.14	0/1145	0.40	0/1543
36	2e	0.15	0/1149	0.43	0/1548
37	1f	0.14	0/823	0.35	0/1115
37	2f	0.14	0/829	0.34	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	1g	0.14	0/1250	0.35	0/1679
38	2g	0.14	0/1254	0.38	0/1683
39	1h	0.13	0/1108	0.34	0/1494
39	2h	0.12	0/1108	0.36	0/1494
40	1i	0.16	0/1002	0.42	0/1346
40	2i	0.15	0/997	0.42	0/1343
41	1j	0.14	0/722	0.41	0/982
41	2j	0.15	0/727	0.43	0/988
42	1k	0.12	0/844	0.32	0/1145
42	2k	0.12	0/848	0.31	0/1149
43	1l	0.14	0/937	0.38	0/1260
43	2l	0.14	0/937	0.37	0/1260
44	1m	0.16	0/969	0.37	0/1302
44	2m	0.16	0/961	0.39	0/1291
45	1n	0.13	0/501	0.36	0/664
45	2n	0.14	0/501	0.35	0/664
46	1o	0.13	0/739	0.33	0/985
46	2o	0.12	0/739	0.33	0/985
47	1p	0.14	0/697	0.39	0/939
47	2p	0.18	0/693	0.43	0/935
48	1q	0.14	0/836	0.34	0/1117
48	2q	0.14	0/836	0.36	0/1117
49	1r	0.13	0/560	0.33	0/746
49	2r	0.12	0/560	0.33	0/746
50	1s	0.17	0/667	0.46	0/900
50	2s	0.20	0/661	0.55	0/893
51	1t	0.14	0/730	0.41	0/965
51	2t	0.16	0/729	0.43	0/965
52	1u	0.15	0/203	0.42	0/266
52	2u	0.17	0/203	0.43	0/266
53	1v	0.16	0/310	0.29	0/480
53	2v	0.19	0/310	0.34	0/480
54	1w	0.21	1/1606 (0.1%)	0.37	0/2497
54	1y	0.20	1/1606 (0.1%)	0.35	0/2497
54	2w	0.21	0/1556	0.35	0/2418
54	2y	0.20	0/1583	0.35	0/2459
55	1x	0.21	0/1725	0.36	0/2689
55	2x	0.19	0/1725	0.31	0/2689
All	All	0.16	3/316686 (0.0%)	0.35	0/474113

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
26	14	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	8	4SU	O3'-P	5.09	1.61	1.56
54	1y	8	4SU	O3'-P	5.07	1.61	1.56
32	1a	1498	UR3	O3'-P	5.03	1.61	1.56

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	14	57	GLU	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	31191	679	0
1	2A	60322	0	30425	778	0
2	1B	2577	0	1305	23	0
2	2B	2575	0	1303	45	0
3	1D	2136	0	2218	45	0
3	2D	2136	0	2218	61	0
4	1E	1559	0	1618	31	0
4	2E	1559	0	1618	38	0
5	1F	1584	0	1625	44	0
5	2F	1580	0	1619	40	0
6	1G	1423	0	1436	34	0
6	2G	1428	0	1438	46	0
7	1H	1330	0	1407	24	0
7	2H	1330	0	1407	41	0
8	1I	1097	0	1140	17	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	2I	1064	0	1082	20	0
9	1N	1117	0	1184	18	0
9	2N	1117	0	1184	26	0
10	1O	933	0	996	18	0
10	2O	933	0	996	31	0
11	1P	1135	0	1212	38	0
11	2P	1135	0	1212	28	0
12	1Q	1122	0	1179	27	0
12	2Q	1122	0	1179	28	0
13	1R	968	0	1033	27	0
13	2R	968	0	1033	26	0
14	1S	873	0	927	18	0
14	2S	870	0	923	18	0
15	1T	1091	0	1151	26	0
15	2T	1083	0	1136	34	0
16	1U	959	0	1019	22	0
16	2U	959	0	1018	20	0
17	1V	771	0	829	10	0
17	2V	771	0	830	15	0
18	1W	886	0	940	24	0
18	2W	886	0	940	11	0
19	1X	750	0	814	9	0
19	2X	750	0	814	16	0
20	1Y	806	0	881	22	0
20	2Y	806	0	881	24	0
21	1Z	1240	0	1240	27	0
21	2Z	1271	0	1273	30	0
22	10	653	0	674	18	0
22	20	653	0	674	20	0
23	11	755	0	826	13	0
23	21	755	0	826	19	0
24	12	588	0	643	12	0
24	22	588	0	643	13	0
25	13	469	0	518	15	0
25	23	464	0	514	9	0
26	14	552	0	533	24	0
26	24	532	0	503	16	0
27	15	455	0	465	6	0
27	25	455	0	465	13	0
28	16	453	0	473	10	0
28	26	449	0	469	13	0
29	17	418	0	467	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	27	418	0	467	14	0
30	18	517	0	582	22	0
30	28	517	0	582	23	0
31	19	307	0	335	5	0
31	29	307	0	335	10	0
32	1a	32246	0	16295	479	0
32	2a	32327	0	16340	586	0
33	1b	1846	0	1867	67	0
33	2b	1825	0	1828	76	0
34	1c	1548	0	1535	39	0
34	2c	1542	0	1517	57	0
35	1d	1655	0	1675	50	0
35	2d	1674	0	1714	61	0
36	1e	1129	0	1184	31	0
36	2e	1133	0	1191	39	0
37	1f	810	0	804	13	0
37	2f	816	0	808	24	0
38	1g	1231	0	1238	21	0
38	2g	1235	0	1249	28	0
39	1h	1088	0	1126	29	0
39	2h	1088	0	1126	33	0
40	1i	983	0	986	24	0
40	2i	978	0	966	44	0
41	1j	709	0	650	24	0
41	2j	714	0	672	31	0
42	1k	829	0	825	10	0
42	2k	833	0	836	16	0
43	1l	932	0	981	19	0
43	2l	932	0	981	25	0
44	1m	958	0	1002	22	0
44	2m	950	0	988	35	0
45	1n	492	0	529	20	0
45	2n	492	0	529	24	0
46	1o	728	0	760	20	0
46	2o	728	0	760	19	0
47	1p	681	0	697	19	0
47	2p	677	0	686	16	0
48	1q	823	0	891	19	0
48	2q	823	0	891	22	0
49	1r	555	0	618	12	0
49	2r	555	0	618	21	0
50	1s	652	0	662	31	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	2s	646	0	644	27	0
51	1t	728	0	798	17	0
51	2t	727	0	796	25	0
52	1u	199	0	208	4	0
52	2u	199	0	208	9	0
53	1v	277	0	140	3	0
53	2v	277	0	140	5	0
54	1w	1592	0	819	42	0
54	1y	1585	0	804	30	0
54	2w	1544	0	788	45	0
54	2y	1565	0	795	26	0
55	1x	1625	0	829	14	0
55	2x	1625	0	829	28	0
56	10	6	0	0	0	0
56	11	5	0	0	0	0
56	12	2	0	0	0	0
56	13	3	0	0	0	0
56	14	1	0	0	0	0
56	15	5	0	0	0	0
56	16	3	0	0	0	0
56	17	8	0	0	0	0
56	18	7	0	0	0	0
56	19	1	0	0	0	0
56	1A	1101	0	0	0	0
56	1B	39	0	0	0	0
56	1D	13	0	0	0	0
56	1E	15	0	0	0	0
56	1F	10	0	0	0	0
56	1G	4	0	0	0	0
56	1I	1	0	0	0	0
56	1N	6	0	0	0	0
56	1O	5	0	0	0	0
56	1P	9	0	0	0	0
56	1Q	8	0	0	0	0
56	1R	3	0	0	0	0
56	1S	3	0	0	0	0
56	1T	4	0	0	0	0
56	1U	12	0	0	0	0
56	1V	7	0	0	0	0
56	1W	5	0	0	0	0
56	1X	5	0	0	0	0
56	1Y	3	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	1Z	3	0	0	0	0
56	1a	233	0	0	0	0
56	1b	2	0	0	0	0
56	1d	1	0	0	0	0
56	1e	2	0	0	0	0
56	1f	2	0	0	0	0
56	1h	1	0	0	0	0
56	1l	2	0	0	0	0
56	1m	2	0	0	0	0
56	1n	1	0	0	0	0
56	1s	1	0	0	0	0
56	1t	1	0	0	0	0
56	1v	1	0	0	0	0
56	1w	12	0	0	0	0
56	1x	18	0	0	0	0
56	20	3	0	0	0	0
56	21	1	0	0	0	0
56	23	3	0	0	0	0
56	25	5	0	0	0	0
56	27	2	0	0	0	0
56	28	3	0	0	0	0
56	2A	887	0	0	0	0
56	2B	20	0	0	0	0
56	2D	10	0	0	0	0
56	2E	4	0	0	0	0
56	2F	6	0	0	0	0
56	2G	1	0	0	0	0
56	2N	1	0	0	0	0
56	2O	1	0	0	0	0
56	2P	4	0	0	0	0
56	2Q	4	0	0	0	0
56	2R	2	0	0	0	0
56	2T	4	0	0	0	0
56	2U	3	0	0	0	0
56	2V	3	0	0	0	0
56	2W	3	0	0	0	0
56	2X	1	0	0	0	0
56	2Z	1	0	0	0	0
56	2a	241	0	0	0	0
56	2d	1	0	0	0	0
56	2e	1	0	0	0	0
56	2f	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	2g	1	0	0	0	0
56	2i	1	0	0	0	0
56	2j	1	0	0	0	0
56	2k	1	0	0	0	0
56	2l	4	0	0	0	0
56	2m	1	0	0	0	0
56	2q	2	0	0	0	0
56	2r	1	0	0	0	0
56	2t	1	0	0	0	0
56	2v	1	0	0	0	0
56	2w	4	0	0	0	0
56	2x	5	0	0	0	0
56	2y	6	0	0	0	0
57	1A	20	0	11	0	0
57	2A	20	0	11	1	0
58	1A	1	0	0	0	0
58	2A	1	0	0	0	0
59	14	1	0	0	0	0
59	15	1	0	0	0	0
59	16	1	0	0	0	0
59	19	1	0	0	0	0
59	1Y	1	0	0	0	0
59	1n	1	0	0	0	0
59	24	1	0	0	0	0
59	25	1	0	0	0	0
59	26	1	0	0	0	0
59	29	1	0	0	0	0
59	2Y	1	0	0	0	0
59	2n	1	0	0	0	0
60	1d	8	0	0	11	0
60	2d	8	0	0	3	0
61	10	12	0	0	1	0
61	11	10	0	0	0	0
61	12	4	0	0	0	0
61	13	4	0	0	0	0
61	14	2	0	0	0	0
61	15	7	0	0	0	0
61	16	1	0	0	1	0
61	17	7	0	0	0	0
61	18	19	0	0	2	0
61	1A	2246	0	0	71	0
61	1B	73	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	1D	24	0	0	1	0
61	1E	27	0	0	0	0
61	1F	9	0	0	0	0
61	1G	5	0	0	0	0
61	1H	1	0	0	0	0
61	1I	2	0	0	0	0
61	1N	4	0	0	0	0
61	1O	7	0	0	0	0
61	1P	21	0	0	0	0
61	1Q	11	0	0	0	0
61	1R	8	0	0	1	0
61	1S	4	0	0	0	0
61	1T	6	0	0	0	0
61	1U	9	0	0	0	0
61	1V	7	0	0	0	0
61	1W	9	0	0	2	0
61	1X	7	0	0	0	0
61	1Y	3	0	0	0	0
61	1Z	1	0	0	0	0
61	1a	430	0	0	26	0
61	1b	1	0	0	0	0
61	1d	1	0	0	0	0
61	1f	1	0	0	0	0
61	1l	7	0	0	0	0
61	1q	4	0	0	0	0
61	1w	16	0	0	0	0
61	1x	15	0	0	0	0
61	1y	1	0	0	0	0
61	20	10	0	0	1	0
61	21	6	0	0	0	0
61	22	1	0	0	0	0
61	25	4	0	0	0	0
61	27	2	0	0	1	0
61	28	6	0	0	0	0
61	29	1	0	0	0	0
61	2A	1405	0	0	57	0
61	2B	25	0	0	1	0
61	2D	17	0	0	0	0
61	2E	3	0	0	0	0
61	2F	6	0	0	0	0
61	2I	3	0	0	0	0
61	2N	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	2O	1	0	0	0	0
61	2P	11	0	0	1	0
61	2Q	2	0	0	0	0
61	2R	3	0	0	0	0
61	2T	5	0	0	0	0
61	2U	2	0	0	0	0
61	2W	3	0	0	0	0
61	2Z	1	0	0	0	0
61	2a	380	0	0	22	0
61	2d	1	0	0	0	0
61	2g	1	0	0	0	0
61	2i	1	0	0	0	0
61	2j	3	0	0	2	0
61	2l	2	0	0	1	0
61	2p	1	0	0	0	0
61	2r	1	0	0	0	0
61	2t	2	0	0	0	0
61	2x	7	0	0	1	0
61	2y	13	0	0	0	0
All	All	300833	0	196713	4469	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 10.

All (4469) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2138:C:N4	1:2A:2153:G:H1	1.53	1.07
35:1d:22:LYS:HB2	35:1d:26:CYS:SG	1.95	1.05
54:1w:7:A:N6	54:1w:66:U:H3	1.54	1.05
1:2A:2129:C:N4	1:2A:2159:G:H1	1.55	1.03
1:1A:1058:G:H1	1:1A:1080:C:N4	1.56	1.01
32:2a:1002:G:H1	32:2a:1038:C:N4	1.56	1.01
54:2y:52:G:H1	54:2y:62:C:H42	1.05	1.00
54:2w:50:U:H3	54:2w:64:A:N6	1.59	1.00
54:2w:50:U:H3	54:2w:64:A:H61	1.01	0.98
32:1a:998:G:H1	32:1a:1043:C:H42	1.06	0.97
32:2a:1132:C:H42	32:2a:1142:G:H1	1.11	0.97
1:1A:1082:U:O4	1:1A:1086:A:N1	1.96	0.97
1:1A:2100:G:H1	1:1A:2189:U:H3	1.11	0.96
32:2a:1000:U:H3	32:2a:1041:A:H61	1.09	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2136:C:N4	1:1A:2155:G:H1	1.64	0.95
32:2a:1089:G:H1	32:2a:1096:C:H42	1.02	0.94
1:1A:2136:C:H42	1:1A:2155:G:H1	0.97	0.94
1:1A:1059:G:H1	1:1A:1079:C:N4	1.65	0.92
32:2a:1264:C:H42	32:2a:1271:G:H1	0.98	0.92
32:2a:997:U:H3	32:2a:1044:A:H61	0.97	0.92
1:2A:2136:C:N4	1:2A:2155:G:H1	1.68	0.92
1:2A:2121:G:H1	1:2A:2177:C:H42	0.99	0.92
1:2A:2099:U:H3	1:2A:2190:G:H1	1.18	0.91
32:2a:1011:G:H1	32:2a:1018:C:N4	1.68	0.91
1:1A:1082:U:H3	1:1A:1086:A:N6	1.68	0.91
32:1a:664:G:H22	32:1a:741:G:H1	1.18	0.91
1:1A:1059:G:H1	1:1A:1079:C:H42	0.92	0.91
1:1A:1082:U:H3	1:1A:1086:A:H61	0.92	0.91
55:2x:3:C:H42	55:2x:70:G:H1	0.94	0.91
55:2x:3:C:N4	55:2x:70:G:H1	1.68	0.91
32:2a:1089:G:H1	32:2a:1096:C:N4	1.70	0.90
32:2a:1133:G:H1	32:2a:1141:C:H42	0.98	0.90
54:1y:28:G:H1	54:1y:42:C:H42	1.19	0.90
32:2a:997:U:H3	32:2a:1044:A:N6	1.69	0.90
32:2a:1011:G:H1	32:2a:1018:C:H42	1.18	0.90
32:1a:1004:A:N6	32:1a:1037:C:N3	2.19	0.89
1:2A:2096:U:H3	1:2A:2193:G:H1	1.20	0.89
1:1A:1055:G:H1	1:1A:1104:C:H42	1.21	0.89
54:1w:6:G:H1	54:1w:67:C:H42	1.18	0.89
35:1d:31:CYS:SG	60:1d:302:SF4:FE4	1.64	0.88
1:2A:2127:G:C2	1:2A:2161:C:N3	2.41	0.88
32:2a:1025:U:H3	32:2a:1036:G:H1	1.13	0.88
32:2a:1264:C:N4	32:2a:1271:G:H1	1.72	0.87
35:1d:26:CYS:SG	60:1d:302:SF4:FE2	1.66	0.87
1:2A:2121:G:H1	1:2A:2177:C:N4	1.73	0.87
32:2a:1000:U:H3	32:2a:1041:A:N6	1.72	0.87
32:2a:1133:G:H1	32:2a:1141:C:N4	1.71	0.86
35:1d:9:CYS:SG	60:1d:302:SF4:FE1	1.65	0.86
1:1A:2136:C:N3	1:1A:2155:G:N2	2.23	0.85
1:1A:1054:A:H61	1:1A:1105:U:H3	1.25	0.85
1:2A:2127:G:N1	1:2A:2161:C:C4	2.45	0.85
32:2a:559:A:H4'	32:2a:560:U:H3'	1.57	0.85
1:2A:2127:G:N2	1:2A:2161:C:C2	2.44	0.85
35:1d:9:CYS:HG	60:1d:302:SF4:FE1	0.54	0.85
1:2A:2127:G:C6	1:2A:2161:C:N4	2.45	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2129:C:H42	1:2A:2159:G:H1	0.89	0.84
10:2O:35:VAL:HG11	10:2O:103:ALA:HB3	1.60	0.84
32:1a:998:G:H1	32:1a:1043:C:N4	1.76	0.84
54:2y:15:G:H22	54:2y:48:C:H42	1.26	0.84
22:10:10:THR:HG22	22:10:12:ASN:H	1.43	0.83
1:1A:1058:G:N2	1:1A:1080:C:N3	2.24	0.83
1:1A:1054:A:N6	1:1A:1105:U:H3	1.76	0.83
11:1P:52:GLU:OE1	11:1P:55:ARG:NH1	2.11	0.83
54:2w:4:C:H42	54:2w:69:G:H1	1.26	0.83
54:2y:52:G:H1	54:2y:62:C:N4	1.75	0.83
11:1P:126:VAL:HG12	11:1P:148:LEU:HD23	1.60	0.83
1:2A:2127:G:C2	1:2A:2161:C:C4	2.67	0.83
1:1A:2690:C:OP1	13:1R:17:ARG:NH2	2.10	0.83
32:2a:1002:G:N2	32:2a:1038:C:N3	2.27	0.83
1:2A:2138:C:N3	1:2A:2153:G:N2	2.26	0.82
1:1A:1065:U:O2	1:1A:1073:A:N6	2.12	0.82
1:2A:878:A:H61	1:2A:899:A:H1'	1.43	0.82
32:2a:1316:G:H22	32:2a:1319:A:H5"	1.44	0.82
32:1a:1402:4OC:HM22	32:1a:1403:C:H5'	1.62	0.82
1:2A:1566:A:OP1	3:2D:211:ARG:NH1	2.13	0.81
1:1A:1818:U:OP2	3:1D:157:ARG:NH1	2.13	0.81
1:2A:1607:C:N4	1:2A:1622:G:OP2	2.14	0.81
32:2a:1273:G:H3'	32:2a:1274:G:H8	1.44	0.81
54:2w:7:A:H5'	54:2w:8:4SU:H5	1.62	0.81
32:2a:266:G:H5"	32:2a:268:C:H41	1.43	0.81
32:2a:1055:A:N7	32:2a:1200:C:N4	2.27	0.81
1:1A:2135:A:H5'	1:1A:2160:G:H4'	1.62	0.81
1:1A:1058:G:H1	1:1A:1080:C:H42	0.82	0.80
1:2A:2167:U:H2'	1:2A:2168:G:H21	1.42	0.80
2:1B:33:G:H5'	6:1G:2:PRO:HD3	1.64	0.80
32:1a:1027:C:C2	32:1a:1034:G:N2	2.50	0.80
33:2b:185:ILE:HG22	33:2b:199:TYR:HB2	1.61	0.80
50:1s:27:GLU:HB2	50:1s:28:LYS:HA	1.62	0.80
1:2A:2129:C:N3	1:2A:2159:G:N2	2.29	0.80
32:2a:975:A:H4'	32:2a:976:G:H5"	1.62	0.80
32:1a:1008:C:N3	32:1a:1021:G:O6	2.15	0.80
1:1A:2099:U:H3	1:1A:2190:G:H1	1.27	0.79
1:2A:652(D):C:H42	1:2A:652(U):G:H1	1.28	0.79
1:1A:882:G:H1	1:1A:894:C:H42	1.26	0.79
3:2D:69:ARG:HE	3:2D:130:ALA:HB2	1.47	0.79
31:29:25:VAL:HB	31:29:34:GLN:HB2	1.64	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:1b:185:ILE:HG22	33:1b:199:TYR:HB2	1.65	0.79
33:2b:8:LYS:HG3	33:2b:9:GLU:HG3	1.65	0.79
41:2j:49:VAL:HG23	45:2n:41:ARG:HB2	1.63	0.79
1:1A:880:G:H2'	1:1A:881:G:H8	1.48	0.78
32:1a:189(F):U:H3	48:1q:72:ARG:HH22	1.30	0.78
6:2G:38:VAL:HG22	6:2G:93:THR:HG23	1.65	0.78
1:1A:1817:G:OP1	3:1D:88:ARG:NH2	2.16	0.78
26:14:58:ARG:HB3	50:1s:67:VAL:HB	1.63	0.78
35:1d:31:CYS:HG	60:1d:302:SF4:FE4	0.52	0.78
32:2a:1047:G:H5"	45:2n:4:LYS:HD3	1.65	0.78
36:1e:105:VAL:HG21	36:1e:128:PRO:HB3	1.66	0.78
35:2d:53:ASP:HB3	35:2d:57:ARG:HH12	1.49	0.78
32:2a:953:G:H5'	32:2a:965:A:H61	1.47	0.77
54:1w:22:G:N7	54:1w:46:7MG:N2	2.30	0.77
1:2A:2206:G:H3'	1:2A:2207:G:C8	2.19	0.77
4:2E:47:VAL:HG11	4:2E:86:PRO:HD2	1.67	0.77
10:1O:48:PRO:HB3	32:1a:1422:G:H5"	1.66	0.77
1:2A:1689:A:H62	1:2A:1698:A:H2	1.31	0.77
1:2A:2595:G:N7	61:2A:6286:HOH:O	2.17	0.77
32:2a:1086:U:H3	32:2a:1099:G:H22	1.30	0.77
32:2a:1350:A:N6	61:2a:3301:HOH:O	2.16	0.77
33:2b:16:HIS:HB2	33:2b:204:ASN:HB3	1.66	0.77
54:2y:26:A:N6	54:2y:44:G:N1	2.33	0.77
44:2m:80:ARG:HH12	50:2s:69:HIS:HE1	1.29	0.76
33:2b:16:HIS:HB3	33:2b:210:SER:HB2	1.64	0.76
32:2a:1264:C:N3	32:2a:1271:G:N2	2.32	0.76
32:2a:1129:C:O2'	32:2a:1130:A:N7	2.19	0.76
34:2c:78:GLY:HA3	34:2c:83:ARG:H	1.51	0.76
1:2A:888:C:OP1	44:2m:93:ARG:NH1	2.18	0.76
8:2I:124:GLY:H	8:2I:144:VAL:HG23	1.50	0.76
54:1w:6:G:H1	54:1w:67:C:N4	1.84	0.76
4:2E:28:ALA:HB3	4:2E:93:VAL:HG12	1.68	0.76
32:1a:559:A:H4'	32:1a:560:U:H3'	1.68	0.75
32:2a:782:A:OP1	32:2a:1521:G:N2	2.19	0.75
1:1A:2163:C:OP1	1:1A:2165:G:N2	2.19	0.75
32:1a:1133:G:H1	32:1a:1141:C:H42	1.34	0.75
1:2A:994:C:OP1	16:2U:53:ARG:NH2	2.19	0.75
1:2A:1818:U:OP2	3:2D:157:ARG:NH1	2.20	0.75
32:2a:664:G:H22	32:2a:741:G:H1	1.33	0.75
1:1A:1039:G:H1	1:1A:1116:C:H42	1.33	0.75
32:2a:993:G:O6	32:2a:1045:C:N4	2.18	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1002:G:H1	32:2a:1038:C:H42	0.81	0.74
32:1a:682:G:N7	61:1a:2309:HOH:O	2.19	0.74
32:2a:673:G:H2'	32:2a:674:G:C8	2.23	0.74
32:2a:1030:C:H42	32:2a:1031:G:H1	1.32	0.74
54:1y:28:G:H1	54:1y:42:C:N4	1.85	0.74
1:2A:143:G:H4'	19:2X:35:THR:HG21	1.70	0.74
1:2A:775:G:O3'	61:2A:4892:HOH:O	2.06	0.74
11:2P:52:GLU:OE1	11:2P:55:ARG:NH1	2.21	0.74
33:2b:77:ALA:HB2	33:2b:211:ILE:HD13	1.70	0.74
54:2y:15:G:N2	54:2y:48:C:H42	1.86	0.74
1:2A:2127:G:C2	1:2A:2161:C:C2	2.75	0.74
32:2a:1132:C:N4	32:2a:1142:G:H1	1.84	0.74
44:2m:40:ASN:HB3	44:2m:43:THR:HG23	1.69	0.74
1:1A:2129:C:H42	1:1A:2159:G:H1	1.36	0.74
35:1d:26:CYS:HG	60:1d:302:SF4:FE2	0.49	0.74
32:2a:324:G:OP1	51:2t:22:ARG:NH1	2.20	0.74
42:2k:22:HIS:HB3	42:2k:29:ILE:HB	1.68	0.74
32:1a:976:G:N2	32:1a:1363:C:OP2	2.17	0.73
1:1A:510:C:OP1	61:1A:6777:HOH:O	2.05	0.73
1:1A:2759:G:N7	61:1A:4924:HOH:O	2.20	0.73
32:2a:1007:C:N3	32:2a:1022:G:O6	2.20	0.73
1:2A:2875:C:OP1	15:2T:3:ARG:NH1	2.22	0.73
1:1A:400:G:N7	61:1A:6131:HOH:O	2.20	0.73
32:2a:1118:C:OP1	40:2i:104:ARG:NH1	2.22	0.73
1:1A:272(J):C:H2'	1:1A:274:G:H8	1.52	0.73
4:2E:36:ARG:HG2	4:2E:47:VAL:HG12	1.71	0.73
32:2a:1030(A):G:N2	32:2a:1030(D):A:OP2	2.21	0.73
24:12:65:ASN:OD1	24:12:69:ARG:NH1	2.21	0.73
38:1g:78:ARG:NH1	38:1g:154:TYR:O	2.21	0.73
7:2H:41:MET:HE2	7:2H:64:LEU:HB2	1.70	0.73
32:2a:1113:C:H42	32:2a:1187:G:H1	1.36	0.73
61:1a:2406:HOH:O	52:1u:5:ASP:OD2	2.05	0.73
32:2a:1316:G:H5"	45:2n:17:LYS:HE3	1.70	0.73
32:1a:148:G:H2'	32:1a:149:A:H8	1.52	0.73
1:2A:1153:C:OP1	16:2U:92:ARG:NH2	2.21	0.73
54:1y:8:4SU:O2'	54:1y:21:A:N1	2.20	0.73
1:2A:1011:G:OP2	16:2U:66:ASN:ND2	2.21	0.73
25:23:5:LYS:NZ	25:23:34:GLU:OE2	2.21	0.72
32:2a:363:A:OP2	43:2l:34:ARG:NH1	2.22	0.72
11:1P:50:ARG:HD3	30:18:7:HIS:CD2	2.23	0.72
41:2j:6:ILE:HG12	41:2j:98:ILE:HG13	1.72	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:2w:51:U:H3	54:2w:63:G:H1	1.37	0.72
1:1A:1105:U:H2'	1:1A:1106:G:H8	1.55	0.72
1:2A:89:G:H3'	1:2A:90:U:H5"	1.71	0.72
32:2a:829:G:N7	61:2a:3539:HOH:O	2.22	0.72
20:2Y:77:PRO:HD2	20:2Y:106:LEU:HD22	1.70	0.72
30:28:32:LEU:O	30:28:36:LYS:NZ	2.21	0.72
38:2g:113:GLU:HG2	38:2g:119:ARG:HG2	1.69	0.72
32:1a:1086:U:H3	32:1a:1099:G:H22	1.36	0.72
4:1E:77:ILE:HG21	4:1E:195:LEU:HD11	1.72	0.72
1:1A:279:C:H42	1:1A:361:G:H1	1.36	0.71
54:1w:29:G:H1	54:1w:41:C:H42	1.38	0.71
32:2a:737:A:H1'	37:2f:73:ASN:HD21	1.55	0.71
1:2A:698:C:O2'	1:2A:734:A:N6	2.23	0.71
39:1h:14:ARG:NH1	39:1h:83:ILE:O	2.23	0.71
43:1l:71:PRO:O	43:1l:102:ARG:NH1	2.22	0.71
43:2l:117:ARG:HG2	43:2l:122:THR:HB	1.72	0.71
1:1A:1783:A:N7	61:1A:6221:HOH:O	2.24	0.71
32:1a:1006:C:H42	32:1a:1023:G:H1	1.36	0.71
32:2a:1010:G:N2	32:2a:1020:U:HO2'	1.89	0.71
44:2m:91:ARG:NE	44:2m:97:PRO:O	2.22	0.71
54:2w:26:A:N1	54:2w:44:G:O6	2.22	0.71
32:2a:297:G:N2	32:2a:300:A:OP2	2.23	0.71
10:1O:63:VAL:HG12	10:1O:106:LEU:HD11	1.72	0.71
11:1P:59:LEU:HD11	30:18:10:ALA:HB2	1.73	0.71
12:1Q:10:ARG:HH11	12:1Q:11:LYS:HE2	1.56	0.71
32:2a:953:G:N7	44:2m:104:ARG:NH2	2.38	0.71
32:1a:324:G:OP1	51:1t:22:ARG:NH1	2.24	0.71
32:2a:1011:G:N2	32:2a:1018:C:N3	2.37	0.71
54:1w:7:A:H61	54:1w:66:U:H3	0.77	0.71
17:2V:40:LEU:HB2	17:2V:46:VAL:HG22	1.72	0.71
1:1A:1059:G:N2	1:1A:1079:C:N3	2.37	0.70
32:1a:324:G:N7	61:1a:1902:HOH:O	2.22	0.70
1:2A:307:G:N1	1:2A:310:A:OP2	2.24	0.70
1:2A:309:G:N3	1:2A:329:G:O2'	2.24	0.70
1:2A:1780:A:N7	61:2A:4441:HOH:O	2.24	0.70
40:2i:23:ASN:N	40:2i:23:ASN:OD1	2.24	0.70
1:1A:2153:G:H2'	1:1A:2154:G:H8	1.56	0.70
1:2A:2121:G:N2	1:2A:2177:C:N3	2.33	0.70
1:2A:2502:G:N7	61:2A:5288:HOH:O	2.23	0.70
1:2A:2683:C:O2	10:2O:70:LYS:NZ	2.20	0.70
61:2a:3487:HOH:O	52:2u:2:GLY:N	2.24	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:2b:69:LEU:HB3	33:2b:162:ILE:HG22	1.72	0.70
1:1A:1023:U:OP2	61:1A:5955:HOH:O	2.09	0.70
1:2A:897:C:H1'	54:2w:56:C:H5	1.56	0.70
1:2A:2138:C:H42	1:2A:2153:G:H1	0.77	0.70
22:20:10:THR:HG22	22:20:12:ASN:H	1.57	0.70
9:1N:67:LEU:HA	9:1N:87:LEU:HD22	1.74	0.70
36:2e:31:LEU:HD11	36:2e:129:ILE:HA	1.73	0.70
54:2y:46:7MG:O2'	54:2y:48:C:OP2	2.09	0.70
1:1A:2722:G:OP2	61:1A:4900:HOH:O	2.10	0.70
1:1A:1506:C:H2'	1:1A:1507:A:H8	1.55	0.70
33:2b:134:GLU:HA	33:2b:137:ARG:HE	1.57	0.70
32:1a:975:A:H4'	32:1a:976:G:H5"	1.73	0.70
32:1a:1009:G:O6	32:1a:1020:U:O2	2.08	0.70
1:1A:2789:C:O2	1:1A:2894:G:N2	2.17	0.70
1:2A:500:G:N1	1:2A:503:A:OP2	2.25	0.70
6:2G:79:ASN:N	6:2G:79:ASN:OD1	2.25	0.70
3:1D:125:ILE:HB	37:1f:81:ILE:HD11	1.74	0.70
1:2A:947:G:OP2	61:2A:5952:HOH:O	2.10	0.70
32:2a:501:C:H2'	32:2a:502:G:H8	1.56	0.70
34:2c:20:SER:HB3	34:2c:22:TRP:HE1	1.57	0.70
1:1A:2810:A:N6	1:1A:2891:G:O2'	2.23	0.69
34:1c:6:HIS:HD2	34:1c:8:ILE:H	1.40	0.69
32:2a:662:G:H2'	32:2a:663:A:C8	2.27	0.69
1:1A:2507:C:O2'	54:1w:74:C:N4	2.25	0.69
30:18:6:THR:HG22	30:18:63:PRO:HD2	1.72	0.69
1:2A:630:G:OP2	30:28:15:LYS:NZ	2.24	0.69
32:2a:1010:G:N2	32:2a:1020:U:O2'	2.25	0.69
32:2a:1020:U:H2'	32:2a:1021:G:C8	2.28	0.69
42:2k:54:ARG:NH1	54:2y:39:PSU:O2'	2.25	0.69
1:2A:1204:A:H2	1:2A:1241:A:H62	1.40	0.69
12:1Q:111:GLU:OE2	12:1Q:133:ARG:NH2	2.24	0.69
1:2A:854:G:H2'	1:2A:855:G:H8	1.57	0.69
9:2N:34:LEU:HD21	9:2N:120:LEU:HB2	1.73	0.69
14:2S:27:SER:HA	14:2S:88:ASP:HB3	1.75	0.69
32:2a:1203:C:H2'	32:2a:1204:A:H8	1.57	0.69
54:1w:6:G:N2	54:1w:67:C:N3	2.39	0.69
1:2A:962:G:OP1	61:2A:4963:HOH:O	2.11	0.69
32:2a:380:G:N7	61:2a:3596:HOH:O	2.24	0.69
32:2a:1040:U:H2'	32:2a:1041:A:H8	1.57	0.69
33:2b:87:ARG:NH2	33:2b:220:ASP:OD1	2.23	0.69
17:2V:46:VAL:HG23	17:2V:52:VAL:HG11	1.73	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:26:10:LEU:HD13	28:26:19:ARG:HD3	1.75	0.69
32:2a:25:C:H5'	32:2a:524:G:H1'	1.73	0.69
1:1A:1311:G:H2'	29:17:47:ARG:HH22	1.57	0.69
28:26:34:LEU:H	28:26:51:GLU:HG2	1.58	0.69
36:2e:74:GLY:HA3	36:2e:116:THR:HG22	1.75	0.69
1:1A:1055:G:H1	1:1A:1104:C:N4	1.89	0.69
40:1i:128:ARG:NH2	55:1x:33:U:OP2	2.26	0.69
1:2A:84:A:N1	1:2A:98:G:O2'	2.24	0.69
6:2G:64:THR:HB	6:2G:94:LEU:HD21	1.74	0.68
55:2x:3:C:N3	55:2x:70:G:N2	2.38	0.68
41:1j:49:VAL:HG23	45:1n:41:ARG:HB2	1.75	0.68
6:2G:18:GLU:OE1	6:2G:21:ARG:NH1	2.26	0.68
32:2a:542:G:OP1	35:2d:10:ARG:NH2	2.25	0.68
32:2a:976:G:H5'	32:2a:1358:U:O2'	1.93	0.68
1:1A:1053:C:H42	1:1A:1106:G:H1	1.40	0.68
33:2b:212:GLN:NE2	33:2b:234:PRO:O	2.25	0.68
1:1A:2683:C:O2	10:1O:70:LYS:NZ	2.20	0.68
1:2A:2805:G:H2'	1:2A:2807:G:C8	2.29	0.68
35:2d:98:GLU:HG3	35:2d:194:LEU:HD11	1.74	0.68
1:1A:1009:A:OP2	9:1N:37:LYS:NZ	2.27	0.68
46:2o:25:THR:HG21	46:2o:70:LEU:HB2	1.74	0.68
34:1c:131:ARG:NH1	34:1c:166:GLU:OE2	2.26	0.68
35:1d:18:LYS:NZ	35:1d:31:CYS:SG	2.66	0.68
1:2A:2136:C:N3	1:2A:2155:G:N2	2.36	0.68
1:2A:2431:U:OP1	61:2A:4426:HOH:O	2.12	0.68
34:2c:11:ARG:HB3	34:2c:15:THR:HB	1.74	0.68
47:2p:14:ASN:OD1	47:2p:42:ARG:NH2	2.27	0.68
12:1Q:10:ARG:HH12	12:1Q:90:VAL:H	1.40	0.68
1:2A:586:A:N1	1:2A:809:G:O2'	2.25	0.68
1:2A:987:G:O2'	1:2A:1000:A:N3	2.24	0.68
32:2a:1209:C:O2'	32:2a:1214:C:N4	2.25	0.68
41:2j:5:ARG:N	61:2j:303:HOH:O	2.27	0.68
1:2A:2355:C:H1'	22:20:39:ARG:HH21	1.57	0.68
9:2N:40:PRO:HB3	16:2U:68:ALA:HB2	1.76	0.68
23:21:59:THR:O	23:21:91:LYS:NZ	2.27	0.68
32:2a:1133:G:N2	32:2a:1141:C:N3	2.42	0.68
43:2l:86:ARG:NH1	61:2l:301:HOH:O	2.26	0.68
1:1A:272(G):C:H42	1:1A:363(C):G:H1	1.40	0.68
40:1i:50:LEU:HD13	40:1i:56:LEU:HA	1.76	0.68
1:1A:9:U:H3	1:1A:2629:A:H2	1.40	0.68
32:1a:1133:G:H1	32:1a:1141:C:N4	1.91	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1773:A:OP2	61:1A:5760:HOH:O	2.12	0.67
1:2A:81:G:N7	61:2A:4126:HOH:O	2.27	0.67
1:2A:2126:A:N6	1:2A:2162:G:O2'	2.26	0.67
1:1A:1026:U:OP1	61:1A:5955:HOH:O	2.11	0.67
40:1i:16:ARG:HB2	40:1i:64:THR:HB	1.76	0.67
1:2A:857:C:OP2	22:20:77:ARG:NH2	2.28	0.67
19:2X:8:ILE:O	24:22:36:ARG:NH2	2.27	0.67
26:24:64:GLY:O	26:24:66:SER:N	2.26	0.67
55:2x:7:G:H5"	55:2x:8:4SU:H5	1.75	0.67
1:1A:2121:G:H1	1:1A:2177:C:H42	1.42	0.67
7:2H:113:VAL:HG11	7:2H:151:ILE:HG21	1.76	0.67
15:2T:41:ARG:NH2	32:2a:346:G:OP1	2.27	0.67
23:21:50:ARG:HG2	23:21:59:THR:HG22	1.76	0.67
5:1F:101:LEU:O	5:1F:106:ARG:NH1	2.27	0.67
10:1O:97:ARG:NH1	32:1a:339:C:OP2	2.27	0.67
32:1a:946:A:H2'	32:1a:947:G:C8	2.28	0.67
1:2A:2136:C:N4	1:2A:2155:G:N1	2.41	0.67
32:2a:429:U:OP1	35:2d:13:ARG:NH1	2.27	0.67
32:2a:1312:G:H1	32:2a:1325:C:H42	1.43	0.67
54:2y:15:G:H22	54:2y:48:C:N4	1.93	0.67
1:1A:1077:A:H2'	1:1A:1078:U:H4'	1.75	0.67
1:1A:2022:U:OP1	61:1A:7049:HOH:O	2.12	0.67
32:1a:1166:G:N2	32:1a:1170:A:OP2	2.28	0.67
1:2A:882:G:H2'	1:2A:883:G:C8	2.29	0.67
1:2A:922:U:O2'	22:20:29:GLN:NE2	2.26	0.67
32:2a:974:A:OP2	45:2n:29:ARG:NH2	2.28	0.67
35:2d:8:VAL:HG22	35:2d:21:LEU:HD13	1.76	0.67
5:1F:158:THR:O	5:1F:164:ARG:NH1	2.28	0.67
18:1W:25:ARG:NH2	18:1W:74:ALA:O	2.27	0.67
23:21:50:ARG:NH1	23:21:57:GLU:OE2	2.28	0.67
44:2m:3:ARG:NH2	44:2m:9:ILE:O	2.27	0.67
34:1c:150:LYS:HE3	34:1c:152:ILE:HD11	1.77	0.67
36:1e:8:GLU:HG2	36:1e:34:VAL:HG23	1.76	0.67
6:2G:105:LYS:NZ	26:24:25:TYR:O	2.28	0.67
32:2a:107:G:N7	51:2t:15:ARG:NH2	2.43	0.67
8:1I:92:VAL:HG13	8:1I:120:ILE:HB	1.77	0.66
32:1a:299:G:O6	61:1a:2088:HOH:O	2.09	0.66
34:1c:82:GLU:OE2	34:1c:85:ARG:NH1	2.28	0.66
35:1d:205:GLU:OE2	36:1e:107:ARG:NH1	2.28	0.66
8:1I:77:LEU:HB3	8:1I:142:VAL:HG12	1.75	0.66
25:13:5:LYS:NZ	25:13:34:GLU:OE2	2.28	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:184:G:H2'	32:1a:185:A:H8	1.60	0.66
61:2A:4822:HOH:O	11:2P:42:SER:O	2.13	0.66
51:2t:56:MET:HE3	51:2t:85:MET:HG2	1.77	0.66
32:1a:954:G:N7	61:1a:2359:HOH:O	2.28	0.66
1:2A:1817:G:OP1	3:2D:88:ARG:NH2	2.28	0.66
1:2A:2296:U:OP2	14:2S:9:ARG:NH2	2.28	0.66
1:1A:2632:A:HO2'	1:1A:2811:G:HO2'	1.39	0.66
32:1a:584:G:H5'	48:1q:91:ARG:HH22	1.61	0.66
41:1j:35:SER:HB3	41:1j:73:ASP:HB2	1.77	0.66
1:2A:1771:C:OP1	61:2A:6272:HOH:O	2.14	0.66
1:2A:2049:G:N7	61:2A:6105:HOH:O	2.26	0.66
1:1A:500:G:N7	61:1A:6883:HOH:O	2.27	0.66
1:1A:530:G:N1	1:1A:2023:G:OP1	2.25	0.66
32:1a:1435:G:H2'	32:1a:1436:U:C6	2.30	0.66
34:1c:3:ASN:OD1	34:1c:3:ASN:N	2.28	0.66
1:2A:271(H):G:H2'	1:2A:271(I):G:H8	1.61	0.66
35:2d:205:GLU:OE2	36:2e:107:ARG:NH1	2.29	0.66
4:1E:105:THR:OG1	4:1E:199:ARG:NH2	2.29	0.66
32:1a:1000:U:O4	32:1a:1041:A:N1	2.28	0.66
1:2A:392:C:H5"	1:2A:409:C:H5"	1.76	0.66
4:2E:18:ASP:OD2	15:2T:33:LYS:NZ	2.28	0.66
7:2H:59:ARG:O	7:2H:63:SER:OG	2.14	0.66
32:2a:289:G:OP2	61:2a:3917:HOH:O	2.13	0.66
55:2x:14:A:N6	55:2x:21:A:C2	2.63	0.66
1:1A:1176:G:H1'	1:1A:1177:A:H5"	1.78	0.66
46:1o:54:ARG:HG2	46:1o:58:MET:HE2	1.77	0.66
11:2P:59:LEU:HD11	30:28:10:ALA:HB2	1.77	0.66
26:24:14:ILE:HB	26:24:22:ILE:HB	1.78	0.66
3:1D:242:ARG:HG3	3:1D:242:ARG:HH11	1.61	0.66
37:1f:9:VAL:HB	37:1f:87:ARG:HB2	1.78	0.66
1:2A:299:A:H5"	20:2Y:86:ARG:HH21	1.60	0.66
32:2a:1119:C:H2'	32:2a:1120:G:C8	2.30	0.66
41:2j:98:ILE:O	61:2j:301:HOH:O	2.13	0.66
1:1A:392:C:OP1	61:1A:6959:HOH:O	2.13	0.65
1:2A:1537:G:H2'	1:2A:1538:G:H8	1.60	0.65
40:2i:105:ASP:HB2	40:2i:107:ARG:HG3	1.77	0.65
43:1l:28:LYS:HD3	43:1l:62:SER:HB2	1.77	0.65
1:2A:2577:A:OP1	61:2A:4831:HOH:O	2.13	0.65
13:2R:97:VAL:HG22	13:2R:114:VAL:HG13	1.78	0.65
32:2a:1027:C:C2	32:2a:1034:G:N2	2.61	0.65
40:2i:31:GLN:HE21	40:2i:36:TYR:HD1	1.44	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:483:A:H5"	20:1Y:50:ARG:HG2	1.78	0.65
32:2a:576:G:OP1	61:2a:3629:HOH:O	2.13	0.65
35:2d:57:ARG:HB3	35:2d:206:PHE:HB2	1.77	0.65
50:2s:50:ALA:HB1	50:2s:57:HIS:HB3	1.77	0.65
1:1A:2053:G:OP1	61:1A:7036:HOH:O	2.14	0.65
10:2O:24:VAL:HG13	10:2O:33:ALA:HB2	1.78	0.65
55:2x:28:C:H2'	55:2x:29:G:H8	1.61	0.65
1:1A:250:G:OP2	30:18:13:ARG:NH2	2.30	0.65
18:1W:1:MET:HE2	18:1W:62:HIS:HB3	1.78	0.65
33:1b:201:ILE:HG21	33:1b:214:ILE:HG21	1.78	0.65
51:2t:9:ASN:O	51:2t:10:LEU:HB2	1.96	0.65
1:1A:1447:G:N7	61:1A:6819:HOH:O	2.29	0.65
1:2A:1514:U:H2'	1:2A:1515:G:H8	1.61	0.65
44:2m:14:ARG:HE	44:2m:42:ALA:HA	1.61	0.65
54:2w:18:G:O2'	54:2w:57:G:N2	2.25	0.65
1:1A:2646:C:OP2	1:1A:2732:G:O2'	2.10	0.65
1:2A:72:U:OP1	61:2A:6029:HOH:O	2.14	0.65
61:2A:6386:HOH:O	4:2E:127:ASP:OD2	2.14	0.65
32:2a:1266:G:N2	32:2a:1269:A:OP2	2.22	0.65
5:1F:157:VAL:HB	5:1F:194:MET:HG2	1.77	0.65
20:1Y:14:LEU:HB2	20:1Y:75:ILE:HD11	1.79	0.65
32:1a:1355:G:N7	61:1a:2283:HOH:O	2.29	0.65
1:2A:1798:U:H5'	3:2D:259:THR:HG22	1.78	0.65
51:2t:57:ARG:HH12	51:2t:100:ILE:HD12	1.62	0.65
1:1A:1173:G:N1	1:1A:1176:G:OP2	2.30	0.65
32:1a:1035:A:H2'	32:1a:1036:G:H21	1.60	0.65
32:1a:1385:G:N7	61:1a:2460:HOH:O	2.30	0.65
1:2A:2815:C:H5'	27:25:29:THR:HG21	1.78	0.65
1:1A:1267:U:OP1	61:1A:6299:HOH:O	2.15	0.65
1:1A:631:A:OP1	11:1P:65:ARG:NE	2.30	0.64
1:1A:1113:U:H2'	1:1A:1114:G:H8	1.62	0.64
23:11:50:ARG:HG2	23:11:59:THR:HG22	1.80	0.64
12:2Q:16:ARG:HG2	12:2Q:18:LYS:HG3	1.78	0.64
43:2l:71:PRO:O	43:2l:102:ARG:NH1	2.26	0.64
1:1A:192:C:OP1	61:1A:4755:HOH:O	2.14	0.64
1:1A:1469:A:OP2	61:1A:6789:HOH:O	2.13	0.64
12:1Q:18:LYS:O	12:1Q:98:LYS:NZ	2.22	0.64
36:1e:74:GLY:HA3	36:1e:116:THR:HG22	1.78	0.64
44:1m:3:ARG:HG3	44:1m:4:ILE:H	1.61	0.64
32:2a:236:G:OP1	48:2q:40:LYS:NZ	2.31	0.64
32:2a:1402:4OC:HM22	32:2a:1403:C:H5'	1.78	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2153:G:H2'	1:1A:2154:G:C8	2.32	0.64
1:2A:2127:G:C6	1:2A:2161:C:C4	2.85	0.64
30:28:6:THR:HG22	30:28:63:PRO:HD2	1.80	0.64
32:2a:1166:G:N2	32:2a:1170:A:OP2	2.30	0.64
1:1A:2422:A:O4'	54:1y:76:A:N6	2.29	0.64
1:1A:2839:G:OP1	61:1A:6632:HOH:O	2.15	0.64
21:1Z:41:LEU:HD11	21:1Z:83:PRO:HG2	1.79	0.64
32:1a:510:A:OP2	35:1d:49:ARG:NH1	2.27	0.64
32:1a:582:U:OP1	46:1o:64:ARG:NH1	2.30	0.64
32:1a:974:A:OP2	45:1n:29:ARG:NH2	2.30	0.64
34:1c:58:GLU:HB3	41:1j:92:THR:HG21	1.78	0.64
35:1d:26:CYS:HB3	60:1d:302:SF4:S1	2.37	0.64
54:1w:9:A:O2'	54:1w:10:G:N7	2.30	0.64
1:2A:2280:G:N7	61:20:206:HOH:O	2.29	0.64
32:2a:640:A:N6	61:2a:3427:HOH:O	2.30	0.64
43:1l:39:VAL:HG11	43:1l:41:ARG:HH11	1.61	0.64
1:2A:1557:C:OP2	1:2A:1558:A:O2'	2.15	0.64
1:2A:2151:G:H2'	1:2A:2152:G:H8	1.63	0.64
10:2O:115:VAL:HG13	10:2O:121:VAL:HG21	1.78	0.64
32:1a:161:A:N1	32:1a:347:G:O2'	2.31	0.64
32:1a:542:G:OP1	35:1d:10:ARG:NH2	2.31	0.64
32:1a:1147:C:O2	40:1i:16:ARG:NH1	2.30	0.64
1:2A:307:G:H21	1:2A:330:A:H62	1.46	0.64
48:2q:66:SER:O	48:2q:70:ARG:NH1	2.31	0.64
1:1A:307:G:N7	61:1A:5169:HOH:O	2.30	0.64
4:1E:47:VAL:HG11	4:1E:86:PRO:HD2	1.78	0.64
7:1H:86:GLU:OE2	7:1H:132:ARG:NH2	2.31	0.64
32:1a:1518:MA6:N6	32:1a:1519:MA6:H103	2.13	0.64
38:1g:113:GLU:HG2	38:1g:119:ARG:HG2	1.79	0.64
8:2I:4:ILE:HG12	8:2I:18:VAL:HG22	1.78	0.64
41:2j:40:LEU:HB2	41:2j:69:ASN:HB2	1.78	0.64
1:2A:1264:G:OP1	27:25:19:ARG:NH2	2.31	0.64
32:2a:922:G:H4'	36:2e:20:GLN:HA	1.80	0.64
34:2c:79:ARG:H	34:2c:82:GLU:HB3	1.63	0.64
32:2a:790:A:N6	32:2a:1498:UR3:OP1	2.31	0.64
54:2y:67:C:H2'	54:2y:68:C:C6	2.32	0.64
5:1F:70:THR:HG23	5:1F:72:ARG:H	1.63	0.64
33:1b:24:TRP:CD1	33:1b:24:TRP:H	2.16	0.64
35:2d:18:LYS:NZ	35:2d:31:CYS:SG	2.71	0.64
41:2j:26:ALA:O	41:2j:84:GLN:NE2	2.31	0.64
1:1A:517:C:OP1	27:15:16:ARG:NH2	2.30	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1007:C:OP1	9:2N:35:ARG:NH1	2.31	0.63
1:2A:1226:A:OP1	17:2V:84:LYS:NZ	2.21	0.63
1:2A:2507:C:O2'	54:2w:74:C:N4	2.30	0.63
1:2A:2624:G:N7	61:2A:6351:HOH:O	2.30	0.63
5:2F:157:VAL:HB	5:2F:194:MET:HG2	1.80	0.63
20:2Y:86:ARG:HD2	20:2Y:100:ALA:HA	1.80	0.63
1:1A:822:U:OP2	61:1A:6645:HOH:O	2.15	0.63
1:1A:994:C:OP1	16:1U:53:ARG:NH2	2.31	0.63
6:1G:41:GLN:HB3	6:1G:43:LEU:HD13	1.79	0.63
32:1a:1074:G:O2'	32:1a:1101:A:N1	2.31	0.63
32:2a:78:G:O6	32:2a:91:C:N3	2.32	0.63
32:2a:1104:G:H4'	33:2b:111:ARG:HH21	1.62	0.63
32:1a:107:G:N7	51:1t:15:ARG:NH2	2.46	0.63
32:1a:1027:C:C4	32:1a:1034:G:C2	2.86	0.63
1:2A:1025:G:O2'	61:2A:5647:HOH:O	2.15	0.63
19:2X:53:LYS:HB3	19:2X:82:GLN:HB3	1.79	0.63
54:2w:4:C:N4	54:2w:69:G:H1	1.95	0.63
32:1a:1004:A:H5'	32:1a:1024:G:H1	1.63	0.63
32:2a:585:G:OP1	48:2q:37:LYS:NZ	2.30	0.63
32:2a:1007:C:O2	32:2a:1022:G:N1	2.27	0.63
33:2b:162:ILE:HD11	33:2b:184:VAL:HG22	1.79	0.63
36:2e:102:ALA:O	36:2e:107:ARG:NH2	2.32	0.63
39:2h:49:GLU:OE2	39:2h:62:TYR:OH	2.17	0.63
1:1A:882:G:H4'	54:1w:19:G:C6	2.33	0.63
29:17:8:ASN:HB3	29:17:11:LYS:HB3	1.79	0.63
1:2A:2839:G:H5'	13:2R:46:GLY:HA2	1.81	0.63
1:1A:1309:G:H4'	29:17:7:PRO:HB2	1.81	0.63
1:1A:1840:G:N7	61:1A:5163:HOH:O	2.31	0.63
32:1a:1305:G:N2	32:1a:1331:G:H1'	2.13	0.63
54:1y:19:G:N2	54:1y:56:C:N3	2.46	0.63
15:2T:39:ARG:NH2	32:2a:345:C:OP2	2.31	0.63
6:1G:18:GLU:OE2	6:1G:21:ARG:NH1	2.32	0.63
13:1R:97:VAL:HG22	13:1R:114:VAL:HG13	1.81	0.63
54:1w:29:G:H1	54:1w:41:C:N4	1.96	0.63
1:2A:2287:A:H62	1:2A:2344:U:H3	1.46	0.63
54:2w:9:A:OP2	54:2w:13:C:N4	2.31	0.63
1:1A:2328:A:H2'	1:1A:2329:G:C8	2.34	0.63
1:1A:2727:G:O2'	10:1O:70:LYS:NZ	2.30	0.63
1:1A:1048:A:OP2	1:1A:1109:C:N4	2.23	0.62
34:1c:131:ARG:HE	34:1c:135:LYS:HE3	1.64	0.62
40:1i:21:PRO:HA	40:1i:59:PHE:HA	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:21:51:VAL:HG11	23:21:74:VAL:HG21	1.80	0.62
1:1A:2140:C:N3	1:1A:2151:G:O6	2.32	0.62
33:1b:82:ARG:NH1	33:1b:92:TYR:OH	2.32	0.62
49:1r:32:ARG:HA	49:1r:69:THR:HG21	1.81	0.62
1:2A:1141:U:OP2	9:2N:63:THR:OG1	2.16	0.62
5:2F:143:ALA:HB1	5:2F:148:LEU:HB2	1.80	0.62
32:2a:67:C:H2'	32:2a:68:G:C8	2.33	0.62
32:2a:1020:U:H2'	32:2a:1021:G:H8	1.63	0.62
54:2y:26:A:N6	54:2y:44:G:C6	2.67	0.62
50:1s:77:THR:HG23	50:1s:78:ARG:HG3	1.81	0.62
1:2A:652(B):A:H61	1:2A:655:A:H1'	1.64	0.62
1:2A:2849:U:OP2	15:2T:95:ARG:NH1	2.32	0.62
32:1a:911:U:OP2	43:1l:97:ARG:NH2	2.24	0.62
32:2a:975:A:H5"	32:2a:1363(A):A:H62	1.65	0.62
32:2a:1145:C:H4'	32:2a:1146:A:H5'	1.81	0.62
54:2y:52:G:N2	54:2y:62:C:N3	2.46	0.62
17:1V:74:LYS:HB2	17:1V:83:ARG:HB2	1.80	0.62
32:1a:1006:C:N3	32:1a:1023:G:N2	2.47	0.62
1:2A:1378:A:O2'	1:2A:1380:G:N7	2.28	0.62
6:2G:15:VAL:HG22	6:2G:175:LEU:HB3	1.82	0.62
33:2b:166:ASP:HB3	33:2b:169:LYS:HB3	1.81	0.62
1:1A:1509(A):A:H3'	1:1A:1509(B):A:H8	1.65	0.62
6:1G:38:VAL:HG22	6:1G:93:THR:HG23	1.81	0.62
3:2D:108:PRO:HB3	3:2D:143:HIS:CE1	2.34	0.62
24:22:39:ALA:HB2	24:22:44:LEU:HD23	1.81	0.62
32:2a:405:U:O4	35:2d:2:GLY:N	2.33	0.62
36:2e:148:VAL:HG21	39:2h:107:LEU:HD22	1.81	0.62
39:2h:83:ILE:HB	39:2h:137:VAL:HG13	1.82	0.62
42:2k:51:LYS:HA	42:2k:55:LYS:HE3	1.81	0.62
6:1G:142:PRO:HB2	26:14:31:ILE:HD13	1.81	0.62
46:1o:11:VAL:HG21	46:1o:34:LEU:HD22	1.82	0.62
1:2A:531:C:OP1	1:2A:561:G:N1	2.31	0.62
5:2F:167:ALA:HB1	5:2F:173:VAL:HG11	1.81	0.62
18:2W:88:ARG:NH1	18:2W:94:ASP:OD2	2.33	0.62
32:2a:1368:G:OP1	40:2i:111:ARG:NH2	2.32	0.62
54:2w:12:U:H3'	54:2w:13:C:H5"	1.82	0.62
1:1A:1798:U:H5'	3:1D:259:THR:HG22	1.82	0.62
54:1w:51:U:H2'	54:1w:52:G:C8	2.35	0.62
5:2F:64:ILE:HG21	5:2F:78:ILE:HG23	1.80	0.62
35:2d:116:GLN:HE21	35:2d:157:LEU:HD21	1.65	0.62
3:1D:17:THR:O	3:1D:211:ARG:NH2	2.33	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1202:G:H1'	45:1n:29:ARG:HD2	1.81	0.62
1:2A:2317:C:N4	1:2A:2318:G:O6	2.33	0.62
26:14:58:ARG:HG3	50:1s:68:GLY:H	1.65	0.62
1:2A:1266:G:O5'	18:2W:15:ARG:NH2	2.33	0.62
32:2a:959:A:O2'	32:2a:984:C:O2'	2.17	0.62
34:2c:131:ARG:HH21	36:2e:50:GLU:HG3	1.65	0.62
1:2A:322:A:OP2	5:2F:169:ASN:HB2	2.00	0.61
1:2A:2136:C:H42	1:2A:2155:G:H1	1.45	0.61
3:2D:125:ILE:HB	37:2f:81:ILE:HD11	1.82	0.61
10:2O:63:VAL:HG11	10:2O:85:VAL:HG23	1.82	0.61
44:2m:82:MET:O	44:2m:93:ARG:NH2	2.33	0.61
1:1A:833:U:O2	11:1P:55:ARG:NH2	2.33	0.61
1:1A:1105:U:H2'	1:1A:1106:G:C8	2.35	0.61
34:1c:11:ARG:HB3	34:1c:15:THR:HB	1.81	0.61
51:1t:57:ARG:HH12	51:1t:100:ILE:HD12	1.65	0.61
1:2A:889:C:O2'	1:2A:890:A:O4'	2.17	0.61
1:2A:2134:A:OP2	1:2A:2135:A:N6	2.32	0.61
32:2a:420:U:O2'	32:2a:423:G:O6	2.09	0.61
32:2a:521:G:N7	43:2l:53:ARG:NH2	2.47	0.61
32:2a:1052:U:O2'	32:2a:1055:A:OP2	2.15	0.61
32:2a:1089:G:N2	32:2a:1096:C:N3	2.40	0.61
39:2h:51:VAL:HG11	39:2h:60:ARG:HH12	1.64	0.61
43:2l:124:LYS:HD2	43:2l:125:PRO:HD2	1.81	0.61
50:2s:27:GLU:HG3	50:2s:47:HIS:CE1	2.35	0.61
32:1a:67:C:H2'	32:1a:68:G:C8	2.34	0.61
1:2A:2657:A:O3'	7:2H:160:LYS:NZ	2.26	0.61
2:2B:48:A:H4'	14:2S:95:HIS:HD2	1.63	0.61
33:2b:55:PHE:O	33:2b:59:GLU:N	2.25	0.61
7:1H:149:ARG:NH1	7:1H:167:GLU:OE2	2.33	0.61
33:1b:77:ALA:HB2	33:1b:211:ILE:HD13	1.82	0.61
1:2A:764:A:H5'	3:2D:210:GLY:HA2	1.83	0.61
12:2Q:16:ARG:HE	12:2Q:18:LYS:HD3	1.65	0.61
33:2b:74:LYS:NZ	33:2b:205:ASP:O	2.33	0.61
1:1A:2142:C:N3	1:1A:2149:G:O6	2.32	0.61
1:1A:2801(A):A:H1'	1:1A:2895:U:H1'	1.83	0.61
12:1Q:35:VAL:HG13	12:1Q:130:LYS:HB3	1.82	0.61
32:1a:559:A:OP2	36:1e:126:ARG:NH2	2.34	0.61
1:2A:132:G:O6	61:2A:5539:HOH:O	2.15	0.61
9:2N:32:THR:HG23	9:2N:37:LYS:HB2	1.82	0.61
32:1a:1077:G:N2	32:1a:1080:A:OP2	2.33	0.61
1:2A:1434:A:H61	1:2A:1558:A:H62	1.48	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2022:U:O2'	1:2A:2617:C:H5'	2.00	0.61
1:2A:2151:G:H2'	1:2A:2152:G:C8	2.35	0.61
13:2R:2:ARG:NH1	13:2R:5:LYS:O	2.33	0.61
51:2t:50:GLU:HB2	51:2t:99:LEU:HD22	1.83	0.61
54:2w:68:C:N4	54:2w:69:G:O6	2.34	0.61
8:1I:130:TYR:HB3	8:1I:138:ILE:HB	1.82	0.61
32:1a:356:A:N3	32:1a:368:U:O2'	2.29	0.61
32:1a:1047:G:H5"	45:1n:4:LYS:HD3	1.82	0.61
1:2A:700:G:O2'	1:2A:1632:A:N3	2.31	0.61
1:2A:1507:A:O2'	1:2A:1508:A:O5'	2.18	0.61
1:2A:2336:A:H61	22:20:43:THR:HG22	1.66	0.61
33:2b:100:GLY:N	33:2b:176:GLU:OE2	2.32	0.61
35:2d:57:ARG:HD3	35:2d:205:GLU:HB3	1.82	0.61
44:2m:37:THR:O	44:2m:55:ARG:NH1	2.34	0.61
1:1A:859:G:O2'	1:1A:916:G:O6	2.17	0.61
1:1A:1176:G:N2	1:1A:1178:C:OP1	2.34	0.61
35:1d:187:ARG:NH1	35:1d:190:ASP:OD1	2.32	0.61
1:2A:18:C:O2'	1:2A:554:U:OP1	2.19	0.61
1:2A:276:A:H5"	1:2A:277:C:H5'	1.83	0.61
1:2A:2035:G:O6	61:2A:4288:HOH:O	2.15	0.61
1:2A:2316:C:O2'	6:2G:128:ARG:NH2	2.33	0.61
3:2D:108:PRO:HG2	3:2D:111:LEU:HB2	1.81	0.61
5:2F:156:LEU:HD21	5:2F:163:VAL:HG12	1.82	0.61
18:1W:11:ARG:NH1	18:1W:99:ARG:O	2.33	0.61
23:11:51:VAL:HG11	23:11:74:VAL:HG21	1.83	0.61
32:1a:1030:C:N4	32:1a:1030(A):G:N3	2.49	0.61
54:1w:23:A:H3'	54:1w:24:G:H8	1.65	0.61
1:2A:2127:G:C5	1:2A:2161:C:N4	2.68	0.61
32:2a:426:G:OP1	35:2d:38:TYR:OH	2.17	0.61
1:1A:1385:G:O2'	1:1A:1396:U:O2	2.19	0.60
29:27:2:LYS:NZ	61:27:201:HOH:O	2.34	0.60
32:2a:1367:C:OP2	40:2i:112:LYS:NZ	2.25	0.60
36:2e:7:GLU:OE1	36:2e:37:ARG:NE	2.31	0.60
47:2p:51:VAL:HG12	47:2p:53:VAL:H	1.64	0.60
1:1A:674:G:OP2	61:1A:7223:HOH:O	2.17	0.60
1:1A:2788:C:OP1	4:1E:61:ARG:NH2	2.34	0.60
32:1a:1030(A):G:O2'	32:1a:1031:G:N2	2.34	0.60
1:2A:458:G:O2'	1:2A:469:G:O6	2.19	0.60
5:2F:103:LYS:HA	5:2F:106:ARG:HG3	1.82	0.60
32:2a:437:U:O2	35:2d:119:GLN:NE2	2.35	0.60
33:2b:60:ASP:OD1	33:2b:64:ARG:NH1	2.34	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:1P:63:PRO:HD3	30:18:27:THR:HG22	1.83	0.60
2:2B:110:G:H2'	2:2B:111:G:H5'	1.82	0.60
32:2a:643:C:H2'	32:2a:644:G:H8	1.66	0.60
32:2a:1346:A:OP1	40:2i:120:ARG:NH1	2.31	0.60
2:1B:92:C:OP1	21:1Z:79:ARG:NH1	2.35	0.60
43:1l:124:LYS:HD2	43:1l:125:PRO:HD2	1.84	0.60
1:2A:2143:C:H2'	1:2A:2144:U:O4'	2.01	0.60
1:2A:2836:U:H2'	1:2A:2837:G:C8	2.36	0.60
5:2F:108:LYS:HG2	5:2F:112:MET:HE2	1.83	0.60
7:2H:149:ARG:NH1	7:2H:167:GLU:OE2	2.34	0.60
32:2a:1357:A:N6	32:2a:1363(A):A:N1	2.50	0.60
34:2c:131:ARG:NH2	36:2e:50:GLU:HG3	2.17	0.60
54:2w:6:G:O6	54:2w:67:C:N3	2.35	0.60
1:1A:586:A:H5'	5:1F:89:VAL:HG21	1.84	0.60
1:1A:1693:U:O2'	3:1D:14:ARG:NH2	2.34	0.60
18:1W:82:LEU:HB2	18:1W:98:LYS:HB2	1.83	0.60
32:1a:953:G:H5'	32:1a:965:A:H61	1.64	0.60
32:1a:1028:C:H42	32:1a:1033:G:H1	1.50	0.60
54:1y:58:A:O2'	54:1y:59:U:OP1	2.18	0.60
1:2A:568:U:H5'	1:2A:945:A:N1	2.16	0.60
1:2A:2882:A:OP1	13:2R:96:ARG:NH1	2.33	0.60
3:1D:242:ARG:HD2	3:1D:246:PRO:HG3	1.82	0.60
32:1a:1095:U:P	32:1a:1108:G:H1	2.24	0.60
37:1f:35:ALA:HB2	37:1f:67:MET:HE2	1.83	0.60
39:1h:10:LEU:HD22	39:1h:83:ILE:HD11	1.82	0.60
40:1i:111:ARG:O	40:1i:113:LYS:NZ	2.34	0.60
1:2A:223:A:O2'	1:2A:420:C:O2	2.18	0.60
32:2a:157:G:H1	32:2a:164:U:H3	1.50	0.60
32:2a:532:A:N6	32:2a:1206:G:O2'	2.34	0.60
1:1A:1754:C:OP1	15:1T:96:ARG:NH1	2.35	0.60
8:1I:5:LEU:HD11	8:1I:19:VAL:HG22	1.82	0.60
32:1a:972:C:O2'	41:1j:55:LYS:O	2.20	0.60
1:2A:2079:U:O3'	23:21:35:THR:OG1	2.19	0.60
25:23:7:LYS:HB2	25:23:34:GLU:HG3	1.82	0.60
32:2a:532:A:N1	34:2c:156:ARG:NH1	2.48	0.60
32:2a:1239:A:H4'	32:2a:1240:U:H5"	1.84	0.60
33:2b:74:LYS:HD2	33:2b:166:ASP:HB2	1.82	0.60
33:2b:158:LEU:HD21	33:2b:180:LEU:HD13	1.82	0.60
1:1A:1025:G:C4	1:1A:1135:C:H1'	2.36	0.60
1:1A:2596:U:OP1	61:1A:4205:HOH:O	2.17	0.60
11:1P:63:PRO:HG2	30:18:25:MET:HB2	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:328:C:H4'	32:1a:329:A:H5'	1.82	0.60
32:1a:1503:A:O2'	53:1v:13:A:N1	2.33	0.60
50:1s:27:GLU:OE1	50:1s:27:GLU:N	2.29	0.60
1:2A:666:G:H1'	30:28:4:MET:HE3	1.84	0.60
48:2q:9:VAL:HG12	48:2q:56:VAL:HG22	1.83	0.60
1:1A:581:C:OP1	16:1U:33:ARG:HG3	2.02	0.60
1:2A:1420:U:O2'	1:2A:1421:G:OP1	2.19	0.60
8:2I:3:VAL:HG12	8:2I:38:LEU:HA	1.83	0.60
34:2c:3:ASN:N	34:2c:3:ASN:OD1	2.32	0.60
54:2w:50:U:O2	54:2w:64:A:N1	2.35	0.60
10:1O:35:VAL:HG11	10:1O:103:ALA:HB3	1.82	0.60
36:1e:6:PHE:HB3	36:1e:34:VAL:HG22	1.83	0.60
4:2E:48:GLN:NE2	4:2E:78:LEU:HD23	2.17	0.60
11:2P:63:PRO:HD3	30:28:27:THR:HG22	1.84	0.60
32:1a:557:G:N7	61:1a:2490:HOH:O	2.30	0.59
1:2A:1652:A:OP1	13:2R:8:ARG:NH1	2.34	0.59
1:2A:1796:U:H2'	1:2A:1797:C:C6	2.37	0.59
1:2A:2126:A:H61	1:2A:2162:G:HO2'	1.49	0.59
32:2a:1048:G:N2	32:2a:1214:C:O2	2.31	0.59
32:2a:1147:C:O2	40:2i:16:ARG:NH1	2.36	0.59
1:1A:272(F):C:H42	1:1A:363(D):G:H1	1.51	0.59
1:1A:566:U:H5"	11:1P:29:LYS:HE3	1.85	0.59
1:1A:1165:U:H2'	1:1A:1166:C:C6	2.37	0.59
1:1A:1226:A:OP1	17:1V:84:LYS:NZ	2.26	0.59
1:1A:1359:A:H2'	1:1A:1360:A:H5'	1.84	0.59
1:2A:927:G:O6	1:2A:928:G:N2	2.36	0.59
1:2A:2537:U:H2'	1:2A:2538:C:C6	2.37	0.59
32:2a:45:U:H2'	32:2a:46:G:C8	2.37	0.59
32:2a:1027:C:N4	32:2a:1036:G:O6	2.35	0.59
32:2a:1239:A:H62	32:2a:1299:A:H62	1.49	0.59
35:2d:79:PHE:HE1	35:2d:204:ILE:HD13	1.66	0.59
3:1D:108:PRO:HB3	3:1D:143:HIS:CE1	2.37	0.59
12:1Q:60:ARG:NH1	54:1w:54:5MU:OP2	2.35	0.59
1:1A:1452:A:OP2	61:1A:4749:HOH:O	2.17	0.59
1:2A:1803:A:O2'	3:2D:259:THR:HG21	2.02	0.59
1:2A:2343:C:O2'	1:2A:2373:G:O2'	2.15	0.59
32:2a:656:C:O2'	46:2o:28:GLN:OE1	2.10	0.59
1:1A:2023:G:H5'	1:1A:2617:C:H4'	1.84	0.59
6:1G:131:TYR:HB3	6:1G:159:VAL:HG13	1.85	0.59
14:1S:11:LYS:HE2	14:1S:15:ARG:HH12	1.67	0.59
21:1Z:151:HIS:HA	21:1Z:170:THR:HA	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:1j:81:THR:HA	41:1j:84:GLN:HB3	1.83	0.59
1:2A:2136:C:O2'	1:2A:2137:C:O5'	2.21	0.59
12:2Q:60:ARG:NH1	54:2w:54:5MU:OP2	2.36	0.59
32:2a:54:C:N4	32:2a:353:A:OP2	2.35	0.59
50:2s:70:LYS:HB2	50:2s:73:GLU:HG3	1.85	0.59
32:1a:1002:G:H3'	32:1a:1003:G:H4'	1.84	0.59
36:1e:8:GLU:OE2	36:1e:63:ARG:NH2	2.35	0.59
48:1q:66:SER:O	48:1q:70:ARG:NH1	2.36	0.59
1:2A:860:U:H1'	1:2A:2268:A:H5'	1.83	0.59
1:2A:1169:G:H1	1:2A:1180:C:H42	1.51	0.59
10:2O:48:PRO:HB3	32:2a:1422:G:H5"	1.84	0.59
32:2a:1151:A:N3	41:2j:39:PRO:HG3	2.17	0.59
32:2a:1376:U:H2'	32:2a:1377:A:C8	2.37	0.59
34:2c:43:LEU:HD21	34:2c:91:LEU:HD13	1.85	0.59
1:1A:1153:C:OP2	61:1A:5679:HOH:O	2.17	0.59
32:2a:1315:U:O2'	32:2a:1360:A:N3	2.26	0.59
37:2f:97:PHE:HE2	49:2r:62:GLU:HG2	1.66	0.59
40:2i:85:LEU:HB3	40:2i:92:TYR:HD2	1.68	0.59
50:2s:19:VAL:O	50:2s:23:ASN:ND2	2.35	0.59
32:1a:8:A:N6	35:1d:205:GLU:O	2.35	0.59
1:2A:882:G:H1	1:2A:894:C:H42	1.50	0.59
1:2A:1865:G:OP1	61:2A:3902:HOH:O	2.17	0.59
21:2Z:4:ARG:HG2	21:2Z:58:VAL:HB	1.84	0.59
32:2a:450:G:H4'	47:2p:41:PRO:HB2	1.85	0.59
1:1A:2822:G:OP2	61:1A:6915:HOH:O	2.16	0.59
32:1a:53:A:N6	61:1a:2342:HOH:O	2.35	0.59
32:1a:343:U:O2'	32:1a:346:G:O6	2.18	0.59
1:2A:668:G:H5'	1:2A:669:G:OP2	2.03	0.59
20:2Y:64:GLU:OE1	20:2Y:64:GLU:N	2.29	0.59
32:2a:815:A:N7	32:2a:1509:C:O2'	2.36	0.59
32:2a:946:A:H2'	32:2a:947:G:C8	2.37	0.59
48:2q:53:LEU:HD23	48:2q:82:MET:HE1	1.85	0.59
10:1O:64:ARG:HB2	10:1O:79:PHE:CG	2.38	0.59
25:13:6:VAL:HG12	25:13:28:LEU:HD11	1.84	0.59
33:1b:88:ALA:HB2	33:1b:219:VAL:HG13	1.84	0.59
37:1f:99:ALA:HB1	49:1r:23:LYS:HE3	1.84	0.59
61:2A:6385:HOH:O	4:2E:127:ASP:OD2	2.17	0.59
32:2a:331:G:N7	61:2a:3368:HOH:O	2.32	0.59
32:2a:818:G:N2	32:2a:873:A:OP1	2.36	0.59
32:2a:1275:A:H3'	32:2a:1276:G:H8	1.67	0.59
32:2a:1338:G:H21	55:2x:41:C:H1'	1.67	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:2e:31:LEU:HD22	36:2e:43:LEU:HD11	1.85	0.59
37:2f:9:VAL:HB	37:2f:87:ARG:HB2	1.84	0.59
44:2m:58:GLU:O	44:2m:62:ASN:ND2	2.33	0.59
1:1A:624:C:O2'	1:1A:657:U:OP1	2.19	0.58
1:1A:1094:U:H1'	1:1A:1097:U:H5	1.68	0.58
8:1I:12:LEU:HD22	8:1I:19:VAL:HG21	1.85	0.58
1:2A:2880:C:O3'	13:2R:90:ARG:NH1	2.35	0.58
34:2c:152:ILE:HG13	34:2c:167:TRP:HB3	1.83	0.58
35:2d:31:CYS:CB	60:2d:302:SF4:S3	2.91	0.58
33:1b:62:ALA:HB1	33:1b:226:ARG:HG3	1.84	0.58
11:2P:121:LYS:HG2	11:2P:123:LEU:HG	1.85	0.58
1:1A:764:A:H5"	3:1D:210:GLY:HA2	1.83	0.58
4:1E:48:GLN:HE21	4:1E:78:LEU:HG	1.68	0.58
4:1E:128:SER:OG	4:1E:129:HIS:N	2.34	0.58
32:1a:890:G:O2'	32:1a:906:G:O6	2.20	0.58
32:1a:1353:G:OP1	52:1u:10:ARG:NH1	2.37	0.58
1:2A:2144:U:H1'	1:2A:2148:G:N2	2.17	0.58
12:2Q:111:GLU:O	12:2Q:115:MET:HG2	2.03	0.58
32:2a:592:G:H1	32:2a:647:C:H42	1.51	0.58
54:2w:8:4SU:S4	54:2w:13:C:O2'	2.61	0.58
1:1A:452:G:OP2	61:1A:7439:HOH:O	2.17	0.58
1:1A:878:A:N6	1:1A:899:A:O2'	2.34	0.58
4:1E:8:LYS:HG2	4:1E:192:ASN:HA	1.85	0.58
15:2T:50:ILE:HG22	15:2T:102:ILE:HD11	1.83	0.58
21:2Z:72:ARG:NH2	21:2Z:97:GLU:O	2.36	0.58
32:2a:717:C:H4'	42:2k:117:ASN:HD22	1.67	0.58
33:2b:78:GLN:NE2	33:2b:94:ASN:O	2.36	0.58
35:2d:31:CYS:HB2	60:2d:302:SF4:S3	2.42	0.58
44:1m:23:TYR:HB3	44:1m:67:GLU:HA	1.85	0.58
1:2A:90:U:H1'	1:2A:92:A:C8	2.37	0.58
1:2A:481:G:N7	61:2A:3913:HOH:O	2.32	0.58
15:2T:127:ALA:C	15:2T:129:ARG:H	2.12	0.58
21:2Z:91:LEU:HD11	21:2Z:96:VAL:HG11	1.83	0.58
1:1A:744:G:OP1	61:1A:5723:HOH:O	2.16	0.58
1:1A:2723:C:OP1	13:1R:3:HIS:ND1	2.33	0.58
32:1a:581:G:OP1	46:1o:65:ARG:NH2	2.36	0.58
32:1a:1467:G:O6	61:1a:2150:HOH:O	2.16	0.58
33:1b:60:ASP:HA	33:1b:63:MET:HE3	1.85	0.58
61:2A:5566:HOH:O	19:2X:44:GLU:OE2	2.17	0.58
2:2B:22:U:H3	2:2B:61:G:H1	1.51	0.58
1:1A:946:G:OP1	61:1A:5865:HOH:O	2.17	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1702:G:N7	61:1A:6157:HOH:O	2.32	0.58
32:1a:783:C:OP1	32:1a:1515:C:O2'	2.20	0.58
41:1j:54:PHE:O	41:1j:56:HIS:N	2.31	0.58
54:1w:7:A:N1	54:1w:66:U:O2	2.37	0.58
28:26:35:GLU:OE2	28:26:50:ARG:NH1	2.36	0.58
32:2a:748:C:H4'	32:2a:749:C:O5'	2.04	0.58
32:1a:1196:U:H3	34:1c:162:GLN:HE22	1.51	0.58
1:2A:1309:G:H4'	29:27:7:PRO:HB2	1.85	0.58
1:2A:1568:G:N7	61:2A:5809:HOH:O	2.32	0.58
15:2T:26:ASP:OD1	15:2T:120:ARG:NH2	2.26	0.58
21:2Z:151:HIS:HA	21:2Z:170:THR:HA	1.84	0.58
36:2e:18:ARG:HH11	36:2e:27:ARG:HH12	1.51	0.58
43:2l:71:PRO:HG2	43:2l:102:ARG:HG2	1.86	0.58
15:1T:127:ALA:C	15:1T:129:ARG:H	2.12	0.58
21:1Z:21:ALA:O	21:1Z:23:LYS:NZ	2.35	0.58
32:1a:1104:G:H4'	33:1b:111:ARG:HH21	1.68	0.58
32:2a:134:A:H61	47:2p:25:ARG:HH12	1.52	0.58
32:2a:390:C:H2'	32:2a:391:G:C8	2.39	0.58
32:2a:646:U:H2'	32:2a:647:C:C6	2.39	0.58
32:2a:1029:C:C4	32:2a:1032:G:N1	2.71	0.58
32:2a:1189:C:OP1	41:2j:51:ARG:NH2	2.35	0.58
1:1A:1429:G:H2'	1:1A:1430:C:C6	2.38	0.58
32:1a:390:C:H2'	32:1a:391:G:C8	2.39	0.58
32:1a:1411:C:N4	61:1a:2396:HOH:O	2.30	0.58
1:2A:111:A:O2'	24:22:65:ASN:ND2	2.37	0.58
1:2A:566:U:H5"	11:2P:29:LYS:HE3	1.86	0.58
1:2A:2010:G:H5"	18:2W:42:ARG:HB2	1.85	0.58
1:2A:2176:A:H2'	1:2A:2177:C:C6	2.39	0.58
12:2Q:38:GLU:HG3	12:2Q:127:ILE:HB	1.84	0.58
33:2b:101:MET:HG2	33:2b:108:ILE:HG21	1.85	0.58
18:1W:71:VAL:HA	18:1W:107:LEU:HD12	1.86	0.57
32:1a:1221:G:OP1	32:1a:1320:C:N4	2.37	0.57
32:2a:1077:G:N2	32:2a:1080:A:OP2	2.36	0.57
32:2a:1404:5MC:O2	32:2a:1519:MA6:O2'	2.19	0.57
33:2b:200:ILE:HG22	33:2b:202:PRO:HD3	1.87	0.57
44:2m:80:ARG:HH12	50:2s:69:HIS:CE1	2.16	0.57
55:2x:76:A:O2'	61:2x:201:HOH:O	2.17	0.57
1:1A:2038:G:O6	61:1A:5710:HOH:O	2.16	0.57
1:1A:2336:A:H61	22:10:43:THR:CG2	2.17	0.57
1:1A:2706:G:N7	61:1A:5748:HOH:O	2.32	0.57
22:10:70:GLN:OE1	22:10:80:HIS:NE2	2.36	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1c:78:GLY:HA3	34:1c:83:ARG:H	1.69	0.57
61:2A:4994:HOH:O	11:2P:54:GLY:O	2.17	0.57
32:2a:1004:A:N6	32:2a:1037:C:O2	2.34	0.57
32:2a:1305:G:N2	32:2a:1331:G:H1'	2.19	0.57
33:2b:15:VAL:HG21	33:2b:213:LEU:HD22	1.86	0.57
50:2s:27:GLU:HG2	50:2s:28:LYS:HD2	1.86	0.57
54:2y:55:PSU:N3	54:2y:57:G:H5'	2.17	0.57
1:1A:2105:C:H2'	1:1A:2106:G:C8	2.40	0.57
32:1a:532:A:N6	32:1a:1206:G:O2'	2.37	0.57
41:1j:30:SER:O	41:1j:81:THR:OG1	2.23	0.57
1:2A:140:G:H1'	1:2A:141:A:H2	1.68	0.57
1:2A:873:G:H1	1:2A:904:C:H42	1.50	0.57
16:2U:92:ARG:HA	16:2U:95:LEU:HB2	1.86	0.57
1:1A:570:G:O6	61:1A:6393:HOH:O	2.17	0.57
1:1A:588:U:H2'	1:1A:589:C:C6	2.39	0.57
1:1A:897:C:N3	1:1A:898:C:N4	2.52	0.57
1:1A:1913:A:H4'	1:1A:1914:C:H5"	1.86	0.57
44:1m:34:LEU:HD13	44:1m:41:PRO:HA	1.87	0.57
5:2F:154:VAL:HG22	5:2F:191:ARG:HB2	1.85	0.57
32:2a:9:G:H2'	32:2a:10:A:H8	1.68	0.57
32:2a:376:G:H5"	47:2p:5:ARG:HB2	1.87	0.57
32:2a:444:C:H2'	32:2a:445:G:H8	1.69	0.57
32:2a:501:C:H2'	32:2a:502:G:C8	2.38	0.57
32:2a:1000:U:H2'	32:2a:1001:A:C8	2.39	0.57
32:2a:1119:C:H2'	32:2a:1120:G:H8	1.66	0.57
32:2a:1273:G:H3'	32:2a:1274:G:C8	2.32	0.57
46:2o:11:VAL:HG21	46:2o:34:LEU:HD22	1.86	0.57
54:2w:72:C:H2'	54:2w:73:A:C8	2.39	0.57
1:1A:662:G:H5"	11:1P:16:ARG:HG2	1.85	0.57
1:1A:883:G:H22	1:1A:893:C:H42	1.51	0.57
1:1A:2331:G:O2'	1:1A:2336:A:N1	2.35	0.57
1:1A:2522:U:O2'	1:1A:2647:U:OP1	2.16	0.57
32:1a:7:G:O2'	36:1e:120:THR:O	2.23	0.57
32:1a:1027:C:N4	32:1a:1034:G:C6	2.73	0.57
1:2A:1021:A:H62	1:2A:1141:U:H3	1.52	0.57
1:2A:2630:G:H2'	1:2A:2631:G:C8	2.40	0.57
32:2a:67:C:H2'	32:2a:68:G:H8	1.69	0.57
51:2t:60:GLU:HG3	51:2t:81:LYS:HD2	1.85	0.57
1:1A:1199:U:OP1	61:1A:5824:HOH:O	2.17	0.57
1:1A:2430:A:N3	1:1A:2430:A:H2'	2.19	0.57
4:1E:11:MET:HG2	4:1E:24:THR:HB	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:1N:70:LYS:HD3	9:1N:87:LEU:HD12	1.87	0.57
32:1a:1236:A:H4'	32:1a:1304:G:H4'	1.86	0.57
36:1e:78:HIS:HE1	36:1e:143:ARG:H	1.51	0.57
39:1h:83:ILE:HB	39:1h:137:VAL:HG13	1.86	0.57
1:2A:1028:A:N6	1:2A:1125:G:H2'	2.20	0.57
3:2D:108:PRO:HD2	3:2D:111:LEU:HD22	1.85	0.57
5:2F:195:ASP:HB3	5:2F:198:ALA:H	1.69	0.57
32:2a:1183:A:O2'	32:2a:1184:G:OP1	2.23	0.57
38:2g:59:LEU:HG	38:2g:63:LYS:HE2	1.85	0.57
38:2g:69:VAL:HG21	38:2g:104:LEU:HD11	1.86	0.57
1:1A:2001:A:OP1	13:1R:9:LYS:NZ	2.38	0.57
1:1A:2112:G:H1'	54:1y:19:G:O2'	2.05	0.57
33:1b:124:SER:HB3	33:1b:125:PRO:HA	1.87	0.57
32:2a:1113:C:N4	32:2a:1187:G:H1	2.03	0.57
1:1A:441:U:O2	5:1F:46:ARG:NH2	2.34	0.57
5:1F:11:VAL:HB	5:1F:18:ARG:HG3	1.85	0.57
7:1H:17:VAL:HG22	7:1H:26:VAL:HG22	1.86	0.57
32:1a:164:U:H2'	32:1a:165:C:C6	2.40	0.57
32:1a:410:G:OP1	35:1d:30:LYS:NZ	2.36	0.57
1:2A:247:G:H4'	1:2A:386:G:C5	2.39	0.57
1:2A:1383:C:O2	61:2A:6037:HOH:O	2.17	0.57
13:2R:51:LEU:HD22	13:2R:66:VAL:HG13	1.86	0.57
32:2a:1314:C:N4	50:2s:2:PRO:O	2.31	0.57
36:2e:145:LYS:HA	36:2e:148:VAL:HB	1.86	0.57
38:2g:16:LEU:HD21	40:2i:45:ALA:HB2	1.86	0.57
54:2w:8:4SU:H1'	54:2w:48:C:H1'	1.86	0.57
2:1B:1:U:O2'	2:1B:2:C:OP1	2.20	0.57
32:1a:1136:U:H5"	32:1a:1137:C:C4	2.40	0.57
1:2A:686:G:N2	1:2A:788:A:H61	2.02	0.57
5:2F:101:LEU:O	5:2F:106:ARG:NH1	2.38	0.57
13:2R:44:LEU:HD22	13:2R:48:VAL:HG23	1.87	0.57
32:2a:1333:A:H3'	32:2a:1334:G:H8	1.69	0.57
1:1A:615:G:OP1	5:1F:40:GLN:NE2	2.38	0.57
1:1A:1406:U:H2'	1:1A:1407:C:C6	2.40	0.57
29:17:12:ARG:NH2	29:17:44:PRO:HB3	2.20	0.57
32:1a:68:G:H1	32:1a:101:A:H61	1.53	0.57
32:1a:1414:U:H3	32:1a:1486:G:H1	1.52	0.57
33:1b:166:ASP:HB3	33:1b:169:LYS:HB3	1.85	0.57
36:1e:152:ARG:NH2	39:1h:107:LEU:O	2.37	0.57
48:1q:75:ARG:NH1	48:1q:76:LEU:O	2.38	0.57
1:2A:1769:G:O2'	1:2A:1958:C:OP1	2.18	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1148:U:H2'	32:2a:1149:C:O4'	2.05	0.57
1:1A:560:C:H5'	16:1U:52:ARG:HH21	1.69	0.56
32:1a:1001(A):G:C2	32:1a:1002:G:H1'	2.40	0.56
32:1a:1118:C:OP1	40:1i:104:ARG:NH1	2.34	0.56
1:2A:1688:U:O2	1:2A:1700:A:H5'	2.04	0.56
8:2I:123:LEU:HD22	8:2I:144:VAL:HB	1.87	0.56
32:2a:719:C:H1'	49:2r:49:LYS:HB3	1.86	0.56
35:2d:11:LEU:HD23	35:2d:66:ARG:HB3	1.87	0.56
54:2w:8:4SU:HN3	54:2w:14:A:H62	1.51	0.56
2:1B:13:A:N1	2:1B:69:G:O2'	2.36	0.56
6:1G:7:LEU:HD11	6:1G:107:LEU:HD12	1.87	0.56
2:2B:51:G:N7	14:2S:62:LYS:NZ	2.52	0.56
33:2b:102:LEU:HD23	33:2b:182:ILE:HD12	1.85	0.56
1:1A:642:G:N2	1:1A:645:C:OP2	2.36	0.56
1:1A:2136:C:N4	1:1A:2155:G:N1	2.29	0.56
7:1H:3:ARG:HE	7:1H:54:ARG:HH12	1.53	0.56
20:1Y:20:TYR:CE2	20:1Y:43:ASN:HA	2.39	0.56
22:10:11:ARG:O	22:10:14:ARG:NH2	2.37	0.56
32:1a:1356:G:H2'	32:1a:1357:A:C8	2.41	0.56
32:1a:1445:C:O2'	32:1a:1447:A:N6	2.38	0.56
33:1b:19:HIS:NE2	33:1b:206:ASP:OD2	2.33	0.56
33:1b:52:GLU:HG2	33:1b:56:ARG:HH12	1.70	0.56
39:1h:121:ASP:OD2	39:1h:125:ARG:NH2	2.36	0.56
46:1o:29:VAL:HG13	46:1o:63:ARG:HG3	1.87	0.56
49:1r:52:PRO:HB2	49:1r:54:ARG:HG2	1.87	0.56
32:2a:328:C:H4'	32:2a:329:A:H5'	1.87	0.56
1:1A:1688:U:O2	1:1A:1700:A:H5'	2.05	0.56
20:1Y:102:CYS:SG	20:1Y:103:GLY:N	2.77	0.56
26:14:64:GLY:C	26:14:66:SER:H	2.13	0.56
32:1a:108:G:N1	51:1t:15:ARG:HG2	2.20	0.56
32:1a:978:A:O2'	32:1a:1322:C:N3	2.35	0.56
32:1a:1007:C:N3	32:1a:1022:G:O6	2.38	0.56
54:1w:4:C:H2'	54:1w:5:G:C8	2.39	0.56
1:2A:1645:G:H5"	1:2A:1646:C:H5'	1.87	0.56
1:2A:2206:G:H3'	1:2A:2207:G:H8	1.65	0.56
11:2P:36:LYS:O	61:2P:305:HOH:O	2.17	0.56
26:24:64:GLY:C	26:24:66:SER:H	2.13	0.56
32:2a:1030(A):G:N2	32:2a:1030(C):G:H3'	2.21	0.56
32:2a:1274:G:N2	32:2a:1275:A:N7	2.47	0.56
32:2a:1366:C:H2'	32:2a:1367:C:C6	2.41	0.56
50:2s:28:LYS:HB3	50:2s:29:ARG:CB	2.34	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:919:G:N2	1:1A:2269:A:OP2	2.39	0.56
1:1A:2022:U:O2'	1:1A:2617:C:H5'	2.06	0.56
1:1A:2853:C:H2'	1:1A:2854:G:C8	2.41	0.56
21:1Z:69:THR:HG22	21:1Z:90:VAL:HA	1.88	0.56
32:1a:929:G:H1	32:1a:1388:C:H42	1.52	0.56
32:1a:1021:G:O2'	32:1a:1022:G:O5'	2.24	0.56
33:1b:28:PHE:HD1	33:1b:194:PRO:HG3	1.70	0.56
1:2A:122:G:N3	61:2A:3915:HOH:O	2.33	0.56
2:2B:117:G:N7	61:2B:301:HOH:O	2.33	0.56
5:2F:53:THR:HG23	5:2F:55:GLY:H	1.69	0.56
12:2Q:125:LEU:HD12	12:2Q:129:THR:HG21	1.88	0.56
1:2A:2343:C:HO2'	1:2A:2373:G:HO2'	1.48	0.56
32:2a:174:C:H2'	32:2a:175:C:H6	1.70	0.56
32:2a:1062:U:H2'	32:2a:1063:C:C6	2.41	0.56
32:2a:1190:G:H5'	34:2c:176:HIS:CE1	2.40	0.56
32:2a:1479:C:H2'	32:2a:1480:G:H8	1.69	0.56
1:1A:668:G:H5'	1:1A:669:G:OP2	2.06	0.56
32:1a:1036:G:H5"	32:1a:1037:C:C5	2.41	0.56
15:2T:118:ARG:HG2	32:2a:1442(A):G:C8	2.41	0.56
21:2Z:33:LEU:HD11	21:2Z:90:VAL:HG21	1.88	0.56
32:2a:537:G:H5"	43:2l:113:ARG:NH1	2.21	0.56
1:1A:1796:U:H2'	1:1A:1797:C:C6	2.40	0.56
1:1A:2478:A:OP2	31:19:2:LYS:NZ	2.24	0.56
4:1E:111:ARG:HG3	4:1E:160:TYR:CD2	2.41	0.56
12:1Q:10:ARG:NH1	12:1Q:90:VAL:H	2.04	0.56
12:1Q:16:ARG:HG3	12:1Q:18:LYS:HG3	1.88	0.56
32:1a:790:A:OP1	55:1x:38:A:O2'	2.20	0.56
54:1w:2:C:N3	54:1w:71:G:N2	2.54	0.56
32:2a:1412:C:H2'	32:2a:1413:A:C8	2.41	0.56
43:2l:32:PHE:HB3	43:2l:84:LEU:HD11	1.86	0.56
1:1A:616:G:H5'	5:1F:205:ARG:HD3	1.88	0.56
1:1A:1113:U:H2'	1:1A:1114:G:C8	2.40	0.56
1:1A:1862:G:H2'	1:1A:1863:G:H8	1.71	0.56
5:1F:178:PRO:HB2	5:1F:201:VAL:HG21	1.88	0.56
32:1a:636:U:H2'	32:1a:637:G:H8	1.71	0.56
32:1a:1008:C:O2	32:1a:1021:G:N1	2.25	0.56
1:2A:581:C:H2'	1:2A:582:G:C8	2.41	0.56
1:2A:2693:A:H2'	1:2A:2694:G:H8	1.71	0.56
6:2G:44:GLY:N	6:2G:88:ILE:O	2.39	0.56
32:2a:28:G:O2'	32:2a:296:U:OP1	2.21	0.56
33:2b:80:ILE:HG12	33:2b:215:LEU:HD23	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2567:G:H2'	1:1A:2568:C:C6	2.41	0.56
33:1b:80:ILE:HG12	33:1b:215:LEU:HD23	1.87	0.56
1:2A:631:A:OP1	11:2P:65:ARG:NE	2.26	0.56
2:2B:14:U:O3'	2:2B:108:U:O2'	2.23	0.56
6:2G:122:PRO:HB3	6:2G:170:ARG:HH12	1.71	0.56
8:2I:130:TYR:HB3	8:2I:138:ILE:HB	1.87	0.56
32:2a:259:G:OP2	51:2t:83:ARG:NH1	2.39	0.56
32:2a:952:U:H2'	32:2a:953:G:C8	2.41	0.56
32:2a:1040:U:H2'	32:2a:1041:A:C8	2.41	0.56
35:2d:119:GLN:HE21	35:2d:123:HIS:CD2	2.24	0.56
35:2d:148:VAL:HB	35:2d:181:MET:HG3	1.87	0.56
50:2s:20:LEU:HA	50:2s:23:ASN:HD22	1.71	0.56
54:2w:8:4SU:S4	54:2w:14:A:N7	2.79	0.56
1:1A:740:U:OP2	61:1A:5734:HOH:O	2.18	0.55
1:1A:2243:U:H2'	1:1A:2244:U:C6	2.40	0.55
12:1Q:85:LYS:HG2	22:10:7:LEU:HB3	1.87	0.55
13:1R:28:LEU:HD23	13:1R:48:VAL:HG21	1.88	0.55
32:1a:1027:C:N3	32:1a:1034:G:N2	2.54	0.55
33:1b:15:VAL:HG23	33:1b:16:HIS:ND1	2.22	0.55
33:1b:158:LEU:HD21	33:1b:180:LEU:HD13	1.88	0.55
39:1h:21:LYS:O	39:1h:65:TYR:OH	2.20	0.55
1:2A:1839:G:C8	1:2A:1927:A:H1'	2.41	0.55
32:2a:1106:G:H5"	34:2c:172:ARG:HG2	1.88	0.55
33:2b:91:PRO:HG2	33:2b:155:LEU:HD13	1.87	0.55
15:1T:49:VAL:HG12	15:1T:63:VAL:HG22	1.88	0.55
32:1a:73:G:H1	32:1a:96:U:H3	1.55	0.55
32:1a:1060:C:H5"	41:1j:51:ARG:HG2	1.88	0.55
34:2c:32:LEU:HD23	34:2c:59:ARG:HD3	1.87	0.55
34:2c:77:ILE:HG13	34:2c:78:GLY:H	1.72	0.55
55:2x:23:C:H2'	55:2x:24:U:C6	2.40	0.55
1:1A:2390:U:P	30:18:35:GLN:HE22	2.29	0.55
19:1X:53:LYS:HB3	19:1X:82:GLN:HB3	1.89	0.55
34:1c:15:THR:HG22	34:1c:16:ARG:HG2	1.87	0.55
1:2A:2646:C:OP2	1:2A:2732:G:O2'	2.21	0.55
12:2Q:68:ILE:HG22	12:2Q:101:ARG:HE	1.71	0.55
20:2Y:97:ARG:NH1	20:2Y:107:ASP:O	2.40	0.55
32:2a:157:G:H2'	32:2a:158:G:H8	1.72	0.55
32:2a:515:G:H2'	32:2a:516:PSU:H6	1.71	0.55
32:2a:581:G:N1	32:2a:759:A:OP2	2.32	0.55
32:2a:1269:A:OP1	52:2u:24:ARG:NH2	2.37	0.55
33:2b:28:PHE:HD1	33:2b:194:PRO:HG3	1.71	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:2d:76:ARG:NE	35:2d:80:GLU:OE2	2.34	0.55
54:2w:27:G:H1	54:2w:43:C:N4	2.05	0.55
18:1W:77:ASP:OD1	61:1W:301:HOH:O	2.18	0.55
40:1i:20:ARG:O	40:1i:60:ASP:N	2.33	0.55
1:2A:236:C:H2'	1:2A:237:C:C6	2.42	0.55
32:2a:967:5MC:H2'	32:2a:968:A:C8	2.41	0.55
37:2f:67:MET:HE1	37:2f:75:LEU:HD22	1.89	0.55
1:1A:579:G:OP1	61:1A:7016:HOH:O	2.18	0.55
1:1A:2467:C:H4'	12:1Q:123:HIS:CD2	2.41	0.55
32:1a:576:G:O6	32:1a:880:C:O2'	2.23	0.55
32:1a:976:G:H5'	32:1a:1358:U:O2'	2.06	0.55
1:2A:1580:A:H3'	1:2A:1581:G:H8	1.71	0.55
32:2a:584:G:OP2	48:2q:87:LYS:NZ	2.39	0.55
32:2a:1033:G:H2'	32:2a:1034:G:H8	1.71	0.55
32:2a:1240:U:N3	38:2g:30:ILE:O	2.28	0.55
32:2a:1342:C:H2'	32:2a:1343:G:H8	1.71	0.55
42:2k:43:SER:HA	42:2k:47:VAL:HG21	1.88	0.55
1:1A:1507:A:O2'	1:1A:1509(A):A:N6	2.40	0.55
1:1A:1786:A:H1'	1:1A:1938:A:N6	2.21	0.55
1:1A:2128:C:H42	1:1A:2160:G:H1	1.55	0.55
1:1A:2787:C:H1'	4:1E:62:PRO:HG3	1.89	0.55
32:1a:1378:C:O2	38:1g:76:ARG:NH2	2.40	0.55
40:1i:17:VAL:HG11	40:1i:81:ILE:HA	1.89	0.55
54:1y:15:G:H22	54:1y:48:C:H42	1.52	0.55
1:2A:819:A:OP2	1:2A:1187:G:N2	2.30	0.55
1:2A:2104:G:H1	1:2A:2185:C:H42	1.54	0.55
2:2B:41:U:H5	6:2G:70:VAL:H	1.55	0.55
3:2D:108:PRO:HB3	3:2D:143:HIS:HE1	1.70	0.55
6:2G:106:LEU:HA	6:2G:110:ALA:HB3	1.88	0.55
32:2a:1406:U:O2	32:2a:1517:G:N2	2.40	0.55
32:2a:1517:G:N7	32:2a:1518:MA6:H103	2.21	0.55
39:2h:110:ALA:HB3	39:2h:121:ASP:HB3	1.88	0.55
1:1A:793:A:OP2	1:1A:2071:A:O2'	2.23	0.55
1:1A:1057:A:H61	1:1A:1081:U:H3	1.54	0.55
1:1A:1537:G:OP1	61:1A:4207:HOH:O	2.18	0.55
3:1D:274:ARG:NH1	61:1D:401:HOH:O	2.40	0.55
4:1E:181:LEU:HD11	15:1T:6:LEU:HD23	1.88	0.55
32:1a:103:C:OP2	51:1t:14:LYS:NZ	2.31	0.55
32:1a:430:A:OP1	35:1d:9:CYS:HB2	2.07	0.55
28:26:9:LEU:HD22	28:26:25:LYS:HD2	1.89	0.55
32:2a:662:G:H2'	32:2a:663:A:H8	1.72	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:2b:187:LEU:HA	33:2b:201:ILE:HB	1.88	0.55
35:2d:164:ALA:HB1	35:2d:168:ARG:HH11	1.71	0.55
39:2h:28:ALA:HB3	39:2h:57:PRO:HB2	1.88	0.55
44:2m:5:ALA:HB3	44:2m:22:ILE:HD13	1.88	0.55
1:1A:1779:U:H2'	61:1A:6221:HOH:O	2.06	0.55
1:1A:2537:U:H2'	1:1A:2538:C:C6	2.42	0.55
2:1B:106:G:H5'	21:1Z:31:ARG:HG2	1.88	0.55
31:19:17:ILE:HD13	31:19:26:ILE:HD13	1.89	0.55
32:1a:45:U:H2'	32:1a:46:G:C8	2.42	0.55
36:1e:144:THR:OG1	36:1e:147:ASP:OD2	2.21	0.55
50:1s:27:GLU:CB	50:1s:28:LYS:HA	2.35	0.55
1:2A:800:A:H8	1:2A:800:A:OP1	1.90	0.55
1:2A:981:A:N1	1:2A:2027:G:O2'	2.38	0.55
1:2A:1311:G:H2'	29:27:47:ARG:HH22	1.70	0.55
2:2B:113:G:N2	14:2S:45:GLY:O	2.26	0.55
32:2a:64:G:H4'	32:2a:65:U:H3'	1.88	0.55
32:2a:537:G:H2'	32:2a:538:G:C8	2.41	0.55
38:2g:78:ARG:HG2	38:2g:79:ARG:H	1.71	0.55
25:13:18:ASP:OD1	25:13:18:ASP:N	2.40	0.55
32:1a:452:A:O2'	32:1a:453:A:OP2	2.24	0.55
1:2A:2273:A:H2'	1:2A:2274:A:C8	2.42	0.55
5:2F:184:TYR:CE2	5:2F:188:ARG:HD2	2.42	0.55
21:2Z:98:MET:O	21:2Z:126:VAL:N	2.39	0.55
41:2j:65:LEU:HD13	45:2n:56:VAL:HG22	1.89	0.55
16:1U:52:ARG:HH11	16:1U:55:ARG:HH21	1.55	0.55
32:1a:453:A:O2'	47:1p:68:ASP:O	2.24	0.55
1:2A:2788:C:OP1	4:2E:61:ARG:NH2	2.40	0.55
32:2a:538:G:H5"	43:2l:114:LYS:HB2	1.89	0.55
34:2c:108:ASN:HB3	34:2c:111:LEU:HB2	1.88	0.55
44:2m:11:ARG:HA	44:2m:45:VAL:HB	1.88	0.55
24:12:32:LEU:HD22	24:12:36:ARG:HH11	1.72	0.54
25:13:6:VAL:HG13	25:13:54:VAL:HG11	1.89	0.54
25:13:37:LEU:HB3	25:13:43:ILE:HD13	1.89	0.54
34:1c:155:GLY:HA3	34:1c:196:LEU:HD22	1.88	0.54
54:1y:53:G:H1	54:1y:61:C:H42	1.56	0.54
1:2A:1113:U:H2'	1:2A:1114:G:C8	2.42	0.54
10:2O:73:ASP:OD2	15:2T:32:TYR:OH	2.20	0.54
29:27:5:TRP:NE1	29:27:7:PRO:HG3	2.22	0.54
38:2g:68:ASN:ND2	38:2g:127:ALA:O	2.38	0.54
1:1A:2125:G:N1	1:1A:2172:U:OP1	2.29	0.54
10:1O:64:ARG:HG2	10:1O:83:ALA:HB3	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:1h:81:HIS:N	39:1h:138:TRP:O	2.40	0.54
1:2A:740:U:H2'	1:2A:741:G:C8	2.43	0.54
1:2A:955:C:OP1	12:2Q:87:LYS:NZ	2.27	0.54
1:2A:2144:U:H1'	1:2A:2148:G:H22	1.73	0.54
32:2a:565:U:OP2	32:2a:566:G:O2'	2.22	0.54
32:2a:947:G:O3'	44:2m:109:THR:OG1	2.25	0.54
32:2a:1323:G:H4'	32:2a:1363:C:C2	2.42	0.54
1:1A:729:G:C6	3:1D:208:LYS:HB2	2.41	0.54
1:1A:857:C:H4'	22:10:23:VAL:HG21	1.88	0.54
1:1A:2377:A:H2'	1:1A:2378:A:C8	2.42	0.54
10:1O:35:VAL:HG21	10:1O:69:ILE:HD13	1.89	0.54
17:1V:76:LYS:HB2	17:1V:81:TYR:HB3	1.88	0.54
39:1h:11:THR:O	39:1h:15:ASN:ND2	2.41	0.54
39:1h:34:GLU:OE1	39:1h:37:ARG:NH2	2.41	0.54
50:1s:38:SER:HB2	50:1s:71:LEU:HD23	1.89	0.54
1:2A:136:G:H1	1:2A:143(A):C:H42	1.53	0.54
1:2A:2753:A:N3	31:29:15:LYS:NZ	2.55	0.54
15:2T:11:GLU:O	15:2T:15:VAL:HG23	2.07	0.54
32:2a:975:A:H5"	32:2a:1363(A):A:N6	2.21	0.54
54:2w:28:G:H2'	54:2w:29:G:O4'	2.06	0.54
1:1A:323:G:C8	5:1F:171:PRO:HG3	2.43	0.54
32:1a:1401:G:C2	32:1a:1402:4OC:H1'	2.43	0.54
51:1t:60:GLU:HG3	51:1t:81:LYS:HD2	1.88	0.54
1:2A:99:U:O4	20:2Y:8:LYS:NZ	2.40	0.54
1:2A:517:C:OP1	27:25:16:ARG:NH2	2.41	0.54
1:2A:551:G:O2'	1:2A:1220:A:N3	2.37	0.54
1:2A:2499:C:OP1	61:2A:6007:HOH:O	2.17	0.54
6:2G:11:TYR:HA	6:2G:15:VAL:HB	1.89	0.54
7:2H:28:GLY:HA3	7:2H:79:VAL:HB	1.88	0.54
12:2Q:85:LYS:HG2	22:20:7:LEU:HB3	1.88	0.54
19:2X:43:VAL:HG21	19:2X:81:VAL:HG11	1.89	0.54
32:2a:1007:C:N3	32:2a:1022:G:C6	2.76	0.54
32:2a:1239:A:H62	32:2a:1299:A:N6	2.05	0.54
45:2n:37:PHE:HZ	45:2n:56:VAL:HG21	1.71	0.54
1:1A:1750:G:O2'	1:1A:2860:A:N1	2.40	0.54
32:1a:1027:C:N4	32:1a:1034:G:N1	2.56	0.54
32:1a:1030:C:N3	32:1a:1031:G:C2	2.76	0.54
32:1a:1510:U:H2'	32:1a:1511:G:C8	2.43	0.54
50:1s:22:LEU:HB3	50:1s:27:GLU:HB3	1.90	0.54
32:2a:1387:G:H2'	32:2a:1388:C:C6	2.42	0.54
26:14:58:ARG:HE	50:1s:68:GLY:HA3	1.73	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:254:G:O2'	48:1q:16:GLN:O	2.25	0.54
44:1m:37:THR:O	44:1m:55:ARG:NH1	2.40	0.54
1:2A:441:U:O2	5:2F:46:ARG:NH2	2.36	0.54
1:2A:1159:U:H2'	1:2A:1160:G:H8	1.71	0.54
32:2a:396:G:O2'	32:2a:398:C:OP1	2.16	0.54
32:2a:1485:U:H2'	32:2a:1486:G:C8	2.43	0.54
33:2b:88:ALA:HB2	33:2b:219:VAL:HG13	1.89	0.54
35:2d:60:GLU:HG2	35:2d:202:LEU:HB2	1.89	0.54
35:2d:119:GLN:HG2	35:2d:123:HIS:CD2	2.42	0.54
41:2j:49:VAL:HG11	45:2n:45:ARG:HD2	1.90	0.54
51:2t:59:ALA:O	51:2t:63:ILE:HG13	2.07	0.54
1:1A:1094:U:H1'	1:1A:1097:U:C5	2.43	0.54
1:1A:1668:A:O2'	1:1A:1674:G:N7	2.38	0.54
1:1A:1937:A:H1'	1:1A:1939:5MU:H72	1.88	0.54
6:1G:43:LEU:HD11	6:1G:153:ARG:HD2	1.90	0.54
12:1Q:51:ARG:HD3	12:1Q:66:ILE:HD11	1.89	0.54
21:1Z:150:LEU:HB3	21:1Z:171:ILE:HD11	1.89	0.54
35:1d:61:LYS:NZ	35:1d:72:GLU:OE1	2.40	0.54
47:1p:22:THR:HA	47:1p:33:ILE:HG13	1.90	0.54
32:2a:274:A:N6	61:2a:3617:HOH:O	2.26	0.54
32:2a:707:C:H2'	32:2a:708:C:H6	1.72	0.54
32:2a:1030(A):G:H21	32:2a:1030(C):G:H3'	1.71	0.54
5:1F:167:ALA:HB1	5:1F:173:VAL:HG11	1.89	0.54
32:1a:1062:U:H2'	32:1a:1063:C:C6	2.42	0.54
41:1j:38:ILE:HG13	41:1j:71:LEU:HB3	1.89	0.54
54:1w:44:G:C5	54:1w:45:U:H1'	2.43	0.54
1:2A:223:A:N1	1:2A:407:G:O2'	2.41	0.54
1:2A:630:G:N2	1:2A:633:A:OP2	2.36	0.54
1:2A:900:A:O2'	1:2A:901:A:OP1	2.20	0.54
3:2D:3:VAL:HG13	3:2D:17:THR:HB	1.89	0.54
32:2a:782:A:OP1	61:2a:3642:HOH:O	2.18	0.54
36:2e:110:LEU:HD13	36:2e:118:ILE:HG21	1.90	0.54
38:2g:69:VAL:HG22	38:2g:135:VAL:HG22	1.90	0.54
1:1A:1069:A:H2'	1:1A:1073:A:N7	2.23	0.54
1:1A:2747:G:O6	1:1A:2755:C:H5"	2.08	0.54
1:1A:2815:C:H5'	27:15:29:THR:HG21	1.89	0.54
6:1G:67:LYS:HD3	26:14:5:ILE:HD12	1.90	0.54
8:1I:65:ALA:HB1	8:1I:136:VAL:HG11	1.89	0.54
32:1a:676:A:H1'	42:1k:115:PRO:HB3	1.90	0.54
1:2A:2127:G:N1	1:2A:2161:C:C5	2.75	0.54
4:2E:116:VAL:HG13	4:2E:122:PHE:HB2	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:2H:9:ILE:HB	7:2H:50:VAL:HB	1.90	0.54
32:2a:1142:G:H2'	32:2a:1143:G:O4'	2.08	0.54
32:2a:1203:C:H2'	32:2a:1204:A:C8	2.41	0.54
37:2f:70:ASP:OD1	37:2f:70:ASP:N	2.40	0.54
41:2j:47:PHE:HB2	41:2j:63:PHE:HB2	1.90	0.54
1:1A:576:U:H2'	1:1A:577:G:C8	2.42	0.54
7:1H:40:GLU:OE1	7:1H:61:HIS:NE2	2.40	0.54
33:1b:93:VAL:HG21	33:1b:97:TRP:HD1	1.73	0.54
34:1c:15:THR:HG21	34:1c:181:ASN:HA	1.90	0.54
35:1d:81:GLU:OE1	35:1d:139:ARG:NH2	2.40	0.54
36:1e:78:HIS:CE1	36:1e:143:ARG:H	2.26	0.54
46:1o:25:THR:HG21	46:1o:70:LEU:HB2	1.89	0.54
1:2A:789:A:N1	61:2A:4447:HOH:O	2.33	0.54
1:2A:882:G:H2'	1:2A:883:G:H8	1.73	0.54
1:2A:2619:C:OP1	4:2E:152:LYS:NZ	2.28	0.54
32:2a:375:U:OP1	47:2p:69:THR:HG21	2.07	0.54
32:2a:1005:A:OP1	32:2a:1006:C:N4	2.41	0.54
1:1A:721:C:H2'	1:1A:722:A:C8	2.43	0.53
1:1A:2130:U:H2'	1:1A:2158:A:N1	2.23	0.53
32:1a:662:G:H2'	32:1a:663:A:C8	2.43	0.53
32:1a:1133:G:N2	32:1a:1141:C:N3	2.57	0.53
33:1b:21:ARG:O	33:1b:23:ARG:N	2.35	0.53
33:1b:162:ILE:O	33:1b:185:ILE:HG12	2.07	0.53
50:1s:50:ALA:HB1	50:1s:57:HIS:HB3	1.89	0.53
1:2A:271(G):C:H2'	1:2A:271(H):G:C8	2.42	0.53
1:2A:1826:G:H4'	3:2D:242:ARG:NH1	2.23	0.53
32:2a:189(B):C:H42	32:2a:189(I):G:H1	1.56	0.53
32:2a:986:A:N3	50:2s:52:TYR:OH	2.40	0.53
32:2a:1330:U:H4'	44:2m:23:TYR:CE1	2.43	0.53
49:2r:32:ARG:HA	49:2r:69:THR:HG21	1.90	0.53
55:2x:40:C:H2'	55:2x:41:C:H6	1.73	0.53
32:1a:1033:G:H2'	32:1a:1034:G:H8	1.73	0.53
35:1d:26:CYS:SG	60:1d:302:SF4:S1	3.07	0.53
1:2A:686:G:H21	1:2A:788:A:H61	1.55	0.53
1:2A:2117:A:O2'	1:2A:2118:U:H5"	2.07	0.53
1:2A:2126:A:N6	1:2A:2162:G:HO2'	2.05	0.53
1:2A:2646:C:H2'	1:2A:2647:U:O4'	2.08	0.53
1:2A:2751:G:O2'	1:2A:2752:C:O4'	2.26	0.53
32:2a:447:G:O6	32:2a:485:G:O2'	2.24	0.53
32:2a:585:G:O2'	32:2a:879:C:OP1	2.23	0.53
32:2a:1435:G:H2'	32:2a:1436:U:C6	2.44	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:2b:15:VAL:HG11	33:2b:213:LEU:HD13	1.88	0.53
1:1A:84:A:H5"	20:1Y:8:LYS:HG2	1.90	0.53
34:1c:35:GLU:CD	34:1c:59:ARG:HH22	2.16	0.53
42:1k:15:ALA:HA	42:1k:76:GLY:O	2.09	0.53
1:2A:1991:U:H2'	1:2A:1992:G:H5"	1.90	0.53
32:2a:662:G:H1	32:2a:743:U:H3	1.55	0.53
32:2a:1456:G:O6	51:2t:54:LYS:NZ	2.32	0.53
1:1A:2305:A:H5"	6:1G:134:GLY:HA3	1.89	0.53
1:1A:2312:U:H5'	6:1G:88:ILE:HD11	1.91	0.53
30:18:15:LYS:NZ	61:18:211:HOH:O	2.37	0.53
32:1a:731:G:H5'	32:1a:766:A:H4'	1.89	0.53
1:2A:845:G:OP2	1:2A:845:G:N2	2.36	0.53
1:2A:1231:G:H2'	1:2A:1232:G:C8	2.43	0.53
5:2F:95:ARG:NH1	5:2F:97:TYR:OH	2.42	0.53
8:2I:14:ASP:OD1	8:2I:15:VAL:N	2.41	0.53
12:2Q:81:VAL:HG12	22:20:5:LYS:HD2	1.90	0.53
13:2R:33:ARG:NH1	13:2R:115:GLU:OE1	2.35	0.53
26:24:24:THR:OG1	26:24:25:TYR:N	2.33	0.53
32:2a:834:C:H2'	32:2a:835:U:H6	1.73	0.53
32:2a:1347:G:N2	32:2a:1373:G:H2'	2.23	0.53
32:2a:1492:A:H4'	43:2l:47:LYS:HE3	1.91	0.53
32:2a:1513:A:H2'	32:2a:1514:C:C6	2.44	0.53
45:2n:24:CYS:HB3	45:2n:29:ARG:H	1.73	0.53
1:1A:271(M):G:O2'	1:1A:271(N):U:H5"	2.08	0.53
1:1A:1264:G:OP1	27:15:19:ARG:NH2	2.29	0.53
1:1A:1619:G:N7	61:1A:6580:HOH:O	2.34	0.53
1:1A:2627:G:O2'	1:1A:2781:A:N1	2.30	0.53
7:1H:164:TYR:HB2	7:1H:167:GLU:HB2	1.89	0.53
8:1I:116:LEU:HD21	8:1I:119:PRO:HA	1.91	0.53
32:1a:262:A:H2'	32:1a:263:A:C8	2.43	0.53
32:1a:998:G:N2	32:1a:1043:C:N3	2.46	0.53
1:2A:400:G:N7	61:2A:5225:HOH:O	2.33	0.53
1:2A:577:G:O2'	1:2A:1254:A:OP1	2.25	0.53
1:2A:1204:A:H5'	1:2A:1206:G:H1'	1.90	0.53
1:2A:2168:G:H8	1:2A:2170:A:N7	2.07	0.53
4:2E:26:ILE:HD11	4:2E:188:VAL:HG21	1.91	0.53
10:2O:68:GLU:HB3	10:2O:78:ARG:HG3	1.90	0.53
26:24:48:ARG:HE	26:24:52:THR:HA	1.74	0.53
32:2a:17:U:H2'	32:2a:18:C:C6	2.43	0.53
54:2w:53:G:H1	54:2w:61:C:H42	1.56	0.53
1:1A:1426:G:O2'	1:1A:1572:A:N6	2.42	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1675:C:O2	4:1E:128:SER:OG	2.27	0.53
1:1A:2483:C:OP1	54:1w:64:A:H4'	2.08	0.53
61:1A:6915:HOH:O	13:1R:3:HIS:NE2	2.34	0.53
7:1H:24:VAL:HG22	7:1H:35:VAL:HB	1.89	0.53
28:16:8:LYS:HD3	30:18:34:TRP:CD2	2.44	0.53
1:2A:2408:U:H2'	1:2A:2409:G:C8	2.44	0.53
18:2W:17:VAL:HG11	18:2W:103:ILE:HD11	1.90	0.53
32:2a:9:G:H2'	32:2a:10:A:C8	2.43	0.53
35:2d:114:ARG:O	35:2d:118:ARG:N	2.35	0.53
35:2d:173:TRP:CD1	35:2d:174:LEU:HG	2.44	0.53
36:2e:33:VAL:HG22	36:2e:112:LEU:HD12	1.90	0.53
6:1G:106:LEU:HA	6:1G:110:ALA:HB3	1.91	0.53
12:1Q:30:GLY:HA2	12:1Q:107:ALA:HB2	1.90	0.53
32:1a:1412:C:H2'	32:1a:1413:A:C8	2.44	0.53
48:1q:24:GLU:HA	48:1q:39:SER:HA	1.91	0.53
1:2A:212:G:H2'	1:2A:213:A:O4'	2.09	0.53
1:2A:296:C:O3'	20:2Y:95:LYS:NZ	2.42	0.53
1:2A:851:U:H5'	25:23:49:LYS:HD2	1.91	0.53
1:2A:979:G:H5"	1:2A:980:A:H5"	1.90	0.53
1:2A:1188:U:H4'	17:2V:79:VAL:HG22	1.89	0.53
3:2D:17:THR:O	3:2D:211:ARG:NH2	2.42	0.53
20:2Y:28:LYS:HB3	20:2Y:38:ILE:HG22	1.91	0.53
37:2f:30:LEU:HD23	37:2f:75:LEU:HD11	1.91	0.53
40:2i:85:LEU:HB3	40:2i:92:TYR:CD2	2.44	0.53
1:1A:278:A:H2'	1:1A:279:C:C6	2.43	0.53
7:1H:98:LEU:HD13	7:1H:125:VAL:HG23	1.89	0.53
12:1Q:20:ALA:HB2	21:1Z:79:ARG:HG3	1.90	0.53
26:14:57:GLU:HG2	26:14:58:ARG:HH11	1.73	0.53
26:14:58:ARG:O	26:14:61:ARG:N	2.28	0.53
32:1a:1027:C:C4	32:1a:1034:G:N1	2.76	0.53
34:1c:22:TRP:NE1	34:1c:36:ASP:OD2	2.40	0.53
36:1e:33:VAL:HG21	36:1e:109:ILE:HA	1.91	0.53
39:1h:7:ALA:HB2	39:1h:85:ARG:HG3	1.90	0.53
39:1h:124:ALA:O	39:1h:128:GLY:N	2.42	0.53
1:2A:1567:A:OP2	3:2D:84:TYR:OH	2.18	0.53
1:2A:2572:A:OP1	1:2A:2574:G:O2'	2.27	0.53
7:2H:80:SER:OG	7:2H:81:GLU:OE1	2.26	0.53
32:1a:333:G:H4'	51:1t:16:HIS:CE1	2.44	0.53
33:1b:24:TRP:H	33:1b:24:TRP:HD1	1.56	0.53
33:1b:91:PRO:HG2	33:1b:155:LEU:HD13	1.91	0.53
42:1k:84:VAL:HG11	42:1k:91:ARG:HD2	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:2H:24:VAL:HG13	7:2H:37:VAL:HG21	1.90	0.53
32:2a:560:U:OP2	61:2a:3572:HOH:O	2.18	0.53
32:2a:1117:G:N2	32:2a:1180:A:O2'	2.42	0.53
40:2i:46:ALA:HA	40:2i:78:LYS:HB2	1.91	0.53
41:2j:21:GLN:O	41:2j:21:GLN:NE2	2.40	0.53
1:1A:2590:A:H2'	1:1A:2591:C:C6	2.42	0.53
1:1A:2791:C:H2'	1:1A:2792:G:C8	2.44	0.53
1:1A:2839:G:H5'	13:1R:46:GLY:HA2	1.90	0.53
32:1a:1277:C:O2'	32:1a:1279:A:H1'	2.09	0.53
3:2D:182:LEU:HB2	3:2D:272:ALA:HB3	1.91	0.53
13:2R:33:ARG:NH2	27:25:57:VAL:O	2.26	0.53
35:2d:63:LYS:HD2	35:2d:198:VAL:HG22	1.90	0.53
40:2i:9:ARG:HG2	40:2i:14:VAL:HG12	1.91	0.53
1:1A:910:A:N3	1:1A:2264:C:O2'	2.35	0.52
1:1A:2386:C:O2'	61:1A:4208:HOH:O	2.19	0.52
32:1a:1347:G:H5"	40:1i:107:ARG:HB3	1.91	0.52
1:2A:817:C:O2'	1:2A:839:U:H5"	2.09	0.52
1:2A:1899:G:H2'	1:2A:1899:G:N3	2.25	0.52
2:2B:110:G:C2'	2:2B:111:G:H5'	2.39	0.52
3:2D:26:LYS:HB3	3:2D:83:GLU:HG2	1.90	0.52
32:2a:1030:C:N3	32:2a:1031:G:N2	2.57	0.52
41:2j:81:THR:HA	41:2j:84:GLN:HB3	1.91	0.52
46:2o:26:GLU:N	46:2o:26:GLU:OE1	2.42	0.52
1:1A:800:A:H8	1:1A:800:A:OP1	1.92	0.52
1:1A:1420:U:O2'	1:1A:1421:G:O5'	2.21	0.52
1:1A:2728:U:H5'	10:1O:70:LYS:HZ3	1.73	0.52
5:1F:140:LEU:HD11	5:1F:170:LEU:HD11	1.91	0.52
32:1a:69:G:H2'	32:1a:70:G:C8	2.45	0.52
32:1a:183:G:N2	32:1a:223:U:O2'	2.37	0.52
32:1a:1030:C:C4	32:1a:1030(A):G:H1'	2.44	0.52
33:1b:60:ASP:O	33:1b:64:ARG:HG2	2.10	0.52
54:1w:13:C:H2'	54:1w:14:A:H5"	1.90	0.52
1:2A:642:G:H21	1:2A:646:A:H2	1.57	0.52
1:2A:856:C:H2'	1:2A:857:C:C6	2.44	0.52
1:2A:2114:A:N6	1:2A:2115:G:H21	2.07	0.52
1:2A:2773:C:OP1	4:2E:166:THR:OG1	2.21	0.52
32:2a:537:G:H2'	32:2a:538:G:H8	1.74	0.52
42:2k:43:SER:HB3	42:2k:68:ALA:HB2	1.91	0.52
43:2l:33:ARG:HG2	43:2l:60:LEU:HD23	1.92	0.52
1:1A:72:U:H5'	24:12:61:LEU:HD12	1.91	0.52
1:1A:124:G:OP1	1:1A:1376:C:O2'	2.24	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1148:U:H2'	32:1a:1149:C:O4'	2.09	0.52
38:1g:47:CYS:HA	38:1g:50:ILE:HG22	1.90	0.52
1:2A:796:C:H2'	1:2A:797:C:C6	2.44	0.52
5:2F:12:LEU:HB2	5:2F:124:LEU:HD11	1.92	0.52
36:2e:146:ALA:O	36:2e:150:ARG:HG2	2.09	0.52
1:1A:1453:U:OP1	13:1R:77:ARG:NH1	2.32	0.52
6:1G:179:PRO:HG3	26:14:43:TYR:OH	2.10	0.52
12:1Q:10:ARG:NH1	12:1Q:11:LYS:HE2	2.24	0.52
30:18:23:VAL:HG11	30:18:47:LYS:HD3	1.90	0.52
32:1a:192:U:H2'	32:1a:193:C:H6	1.75	0.52
32:1a:1286:A:H2'	32:1a:1287:A:H4'	1.92	0.52
32:1a:1376:U:OP1	38:1g:98:SER:HB3	2.09	0.52
41:1j:40:LEU:HD12	41:1j:69:ASN:HB3	1.92	0.52
1:2A:112:U:H5'	24:22:65:ASN:ND2	2.24	0.52
1:2A:492:A:H2'	1:2A:493:G:O4'	2.08	0.52
1:2A:538:G:H5'	9:2N:5:VAL:HG11	1.92	0.52
1:2A:2134:A:H2'	1:2A:2134:A:N3	2.24	0.52
1:2A:2712:U:OP1	1:2A:2714:G:H4'	2.10	0.52
10:2O:15:GLY:O	10:2O:47:ILE:HG12	2.10	0.52
32:2a:1353:G:H2'	32:2a:1354:C:C6	2.45	0.52
1:1A:534:U:H2'	1:1A:535:C:C6	2.44	0.52
1:1A:637:A:OP1	11:1P:133:SER:OG	2.26	0.52
1:1A:971:C:O2'	1:1A:983:A:N3	2.36	0.52
1:1A:2121:G:H1	1:1A:2177:C:N4	2.07	0.52
32:1a:811:C:O2'	32:1a:901:A:N1	2.40	0.52
32:1a:1346:A:N1	32:1a:1374:A:H5"	2.24	0.52
39:1h:11:THR:HG22	39:1h:15:ASN:HD21	1.74	0.52
1:2A:1462:C:H4'	1:2A:2703:C:H5'	1.91	0.52
1:2A:1693:U:H1'	3:2D:14:ARG:NH2	2.25	0.52
1:2A:2524:G:N7	61:2A:6346:HOH:O	2.34	0.52
1:1A:272(J):C:H2'	1:1A:274:G:C8	2.39	0.52
1:1A:1419:A:O2'	1:1A:1421:G:N7	2.33	0.52
1:1A:2171:A:O2'	1:1A:2172:U:H5"	2.09	0.52
1:1A:2271:G:OP1	22:10:18:ALA:HB1	2.10	0.52
13:1R:12:ARG:O	13:1R:17:ARG:NH1	2.42	0.52
20:1Y:99:CYS:HB2	20:1Y:106:LEU:HD21	1.91	0.52
26:14:58:ARG:HG3	50:1s:68:GLY:N	2.25	0.52
32:1a:1237:C:O2'	32:1a:1300:G:N2	2.41	0.52
1:2A:2478:A:OP2	31:29:2:LYS:NZ	2.34	0.52
7:2H:11:VAL:HG21	7:2H:50:VAL:HG23	1.90	0.52
25:23:7:LYS:NZ	25:23:32:GLN:O	2.42	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:857:C:H2'	32:2a:858:G:O4'	2.08	0.52
32:2a:1157:A:H5'	32:2a:1158:C:C6	2.45	0.52
33:2b:30:ARG:HH21	33:2b:194:PRO:HB2	1.74	0.52
35:2d:187:ARG:NH1	35:2d:190:ASP:OD1	2.42	0.52
51:2t:16:HIS:O	51:2t:19:SER:OG	2.25	0.52
1:1A:1045:A:H5'	1:1A:1046:A:H5'	1.91	0.52
1:1A:1358:G:O2'	1:1A:1373:A:N6	2.41	0.52
1:1A:2129:C:N4	1:1A:2159:G:H1	2.04	0.52
8:1I:75:LEU:HD22	8:1I:105:HIS:CD2	2.45	0.52
26:14:64:GLY:O	26:14:66:SER:N	2.42	0.52
32:1a:673:G:H2'	32:1a:674:G:C8	2.45	0.52
1:2A:1865:G:N2	1:2A:1877:A:OP2	2.38	0.52
1:2A:2061:G:N2	1:2A:2062:A:N1	2.57	0.52
1:2A:2162:G:H4'	1:2A:2172:U:H2'	1.91	0.52
1:1A:1292:U:H2'	1:1A:1293:C:C6	2.45	0.52
1:1A:2343:C:O2'	1:1A:2373:G:O2'	2.28	0.52
39:1h:82:HIS:NE2	39:1h:136:GLU:OE2	2.41	0.52
1:2A:861:A:N3	2:2B:79:C:O2'	2.37	0.52
10:2O:64:ARG:HB2	10:2O:79:PHE:CG	2.45	0.52
20:2Y:43:ASN:HD22	20:2Y:67:LEU:HD23	1.75	0.52
26:24:16:CYS:SG	26:24:17:GLY:N	2.83	0.52
32:2a:401:C:P	35:2d:73:ARG:HH21	2.33	0.52
32:2a:925:G:H1	32:2a:1391:U:H3	1.57	0.52
32:2a:1053:G:H4'	32:2a:1054:C:H3'	1.91	0.52
35:2d:173:TRP:CD1	35:2d:189:PRO:HG3	2.44	0.52
40:2i:3:GLN:HE21	40:2i:20:ARG:HE	1.57	0.52
43:2l:88:GLY:HA3	43:2l:99:HIS:HD2	1.75	0.52
1:1A:1022:G:N7	9:1N:66:LYS:HE2	2.25	0.52
1:1A:1653:G:H3'	13:1R:2:ARG:HD3	1.91	0.52
1:1A:1826:G:H4'	3:1D:242:ARG:CZ	2.39	0.52
6:1G:108:ASN:HD22	26:14:22:ILE:HG21	1.75	0.52
35:1d:111:ALA:HB2	35:1d:120:LEU:HD12	1.91	0.52
38:1g:69:VAL:HG21	38:1g:104:LEU:HD11	1.92	0.52
54:1w:2:C:N4	54:1w:71:G:N1	2.58	0.52
1:2A:860:U:OP2	61:2A:6253:HOH:O	2.19	0.52
1:2A:2129:C:H5'	1:2A:2130:U:OP2	2.10	0.52
1:2A:2392:A:OP2	30:28:31:HIS:NE2	2.42	0.52
14:2S:14:VAL:O	14:2S:18:ILE:HG12	2.10	0.52
31:29:29:ASN:HD22	31:29:32:HIS:CE1	2.28	0.52
32:2a:1226:C:H4'	50:2s:80:TYR:CZ	2.45	0.52
32:2a:1256:A:H5'	32:2a:1258:G:O4'	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:2c:70:VAL:HG12	34:2c:72:LYS:H	1.75	0.52
38:2g:27:ILE:HA	38:2g:30:ILE:HD12	1.92	0.52
42:2k:34:ASP:HB3	42:2k:40:ILE:HD11	1.92	0.52
1:1A:922:U:H2'	1:1A:923:C:C6	2.45	0.52
1:1A:1153:C:H2'	1:1A:1154:G:O4'	2.10	0.52
32:1a:69:G:H2'	32:1a:70:G:H8	1.75	0.52
34:1c:87:LEU:O	34:1c:91:LEU:N	2.41	0.52
1:2A:973:A:H8	1:2A:973:A:OP1	1.93	0.52
1:2A:2285:C:OP2	28:26:6:ARG:HD3	2.10	0.52
32:2a:421:U:O2'	32:2a:423:G:N7	2.42	0.52
44:2m:101:GLN:OE1	44:2m:101:GLN:N	2.42	0.52
54:2y:19:G:O4'	54:2y:57:G:N1	2.40	0.52
1:1A:1278:A:OP1	13:1R:36:THR:HG23	2.10	0.51
1:1A:2108:C:H2'	1:1A:2109:U:H6	1.74	0.51
3:1D:21:PHE:HB3	3:1D:24:ILE:HD12	1.91	0.51
11:1P:65:ARG:HD2	30:18:25:MET:SD	2.50	0.51
32:1a:192:U:H2'	32:1a:193:C:C6	2.45	0.51
32:1a:1359:C:OP1	45:1n:22:THR:OG1	2.25	0.51
35:1d:19:LEU:H	35:1d:19:LEU:HD12	1.75	0.51
36:1e:140:ARG:O	36:1e:143:ARG:NH1	2.40	0.51
1:2A:1658:C:OP1	4:2E:135:HIS:NE2	2.37	0.51
1:2A:2552:2MU:OP2	61:2A:5426:HOH:O	2.19	0.51
32:2a:966:M2G:HM22	55:2x:34:C:H5'	1.92	0.51
33:2b:115:LEU:HB2	33:2b:145:LEU:HD13	1.92	0.51
1:1A:1754:C:H5	15:1T:96:ARG:HH21	1.58	0.51
3:1D:26:LYS:HE2	3:1D:28:GLU:O	2.09	0.51
8:1I:38:LEU:HD13	8:1I:40:THR:HG23	1.92	0.51
12:1Q:42:ILE:HD11	12:1Q:127:ILE:HD13	1.92	0.51
32:1a:148:G:H2'	32:1a:149:A:C8	2.40	0.51
32:1a:438:G:O2'	32:1a:494:U:O4	2.22	0.51
32:1a:584:G:H5'	48:1q:91:ARG:NH2	2.24	0.51
32:1a:742:G:OP2	46:1o:35:ARG:NH2	2.37	0.51
1:2A:2121:G:N1	1:2A:2177:C:N4	2.42	0.51
6:2G:120:LEU:N	6:2G:179:PRO:O	2.32	0.51
9:2N:54:VAL:HB	9:2N:122:VAL:HG22	1.93	0.51
18:2W:71:VAL:HA	18:2W:107:LEU:HD12	1.92	0.51
32:2a:1067:A:O2'	32:2a:1093:A:O2'	2.24	0.51
32:2a:1173:G:H2'	32:2a:1174:G:H8	1.75	0.51
32:2a:1342:C:H2'	32:2a:1343:G:C8	2.44	0.51
33:2b:50:GLU:HB3	33:2b:200:ILE:O	2.11	0.51
36:2e:33:VAL:HG21	36:2e:109:ILE:HA	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:2j:38:ILE:HD11	41:2j:71:LEU:HD23	1.92	0.51
1:1A:1379:A:H4'	1:1A:1380:G:OP2	2.09	0.51
5:1F:117:ARG:NH2	5:1F:189:THR:O	2.41	0.51
6:1G:4:ASP:OD1	6:1G:9:ARG:NH1	2.41	0.51
9:1N:73:THR:HG23	9:1N:82:LEU:HD11	1.93	0.51
32:1a:407:G:H5"	35:1d:115:ARG:HG2	1.91	0.51
32:1a:674:G:H2'	32:1a:675:A:H8	1.75	0.51
32:1a:1070:U:H2'	32:1a:1071:C:C6	2.45	0.51
36:1e:31:LEU:HD11	36:1e:129:ILE:HA	1.93	0.51
1:2A:586:A:H5'	5:2F:89:VAL:HG21	1.93	0.51
1:2A:1128:A:N7	1:2A:2489:G:O2'	2.43	0.51
32:2a:862:C:H1'	32:2a:874:G:H5"	1.92	0.51
52:2u:3:LYS:HA	52:2u:10:ARG:HG3	1.92	0.51
1:1A:2286:A:H4'	1:1A:2287:A:O4'	2.10	0.51
5:1F:184:TYR:CE2	5:1F:188:ARG:HD2	2.45	0.51
32:1a:1002:G:H3'	32:1a:1003:G:C4'	2.40	0.51
35:1d:64:LEU:HB2	35:1d:198:VAL:HG11	1.92	0.51
39:1h:25:ASP:OD2	39:1h:60:ARG:NH2	2.43	0.51
48:1q:4:LYS:HG3	48:1q:6:LEU:HD13	1.92	0.51
1:2A:790:C:OP2	61:2A:4442:HOH:O	2.19	0.51
1:2A:2615:U:C2	27:25:7:PRO:HA	2.45	0.51
32:2a:1026:G:H5'	32:2a:1027:C:O5'	2.11	0.51
32:2a:1132:C:N3	32:2a:1142:G:N2	2.52	0.51
1:1A:1066:U:N3	1:1A:1069:A:OP2	2.43	0.51
1:1A:1256:G:H1'	5:1F:82:ILE:HD11	1.93	0.51
1:1A:2238:G:N3	1:1A:2238:G:H2'	2.25	0.51
5:1F:53:THR:CG2	5:1F:55:GLY:H	2.24	0.51
1:2A:340:A:H2'	1:2A:341:G:O4'	2.10	0.51
1:2A:2280:G:O2'	1:2A:2388:A:N1	2.43	0.51
41:2j:32:ALA:HB3	41:2j:76:ASN:H	1.75	0.51
1:1A:1899:G:N3	1:1A:1899:G:H2'	2.24	0.51
1:1A:2276:G:N7	61:1A:7102:HOH:O	2.33	0.51
2:1B:91:C:OP2	12:1Q:16:ARG:NH1	2.43	0.51
32:1a:748:C:H4'	32:1a:749:C:O5'	2.10	0.51
32:1a:750:G:O2'	46:1o:21:ASP:OD1	2.29	0.51
32:1a:1029:C:N3	32:1a:1032:G:O6	2.43	0.51
38:1g:78:ARG:HG2	38:1g:79:ARG:H	1.76	0.51
41:1j:65:LEU:HD13	45:1n:56:VAL:HG22	1.93	0.51
1:2A:1187:G:H5'	17:2V:81:TYR:CE1	2.46	0.51
32:2a:56:U:H2'	32:2a:57:G:H8	1.76	0.51
32:2a:148:G:H2'	32:2a:149:A:C8	2.45	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:582:U:H5"	46:2o:64:ARG:HH12	1.76	0.51
32:2a:1006:C:H2'	32:2a:1007:C:C6	2.45	0.51
32:2a:1058:G:H1	32:2a:1199:U:H3	1.58	0.51
32:2a:1510:U:H2'	32:2a:1511:G:C8	2.45	0.51
36:2e:83:GLU:HA	36:2e:88:LYS:HA	1.93	0.51
39:2h:19:VAL:HG23	39:2h:21:LYS:HG2	1.92	0.51
39:2h:60:ARG:HG2	39:2h:62:TYR:CZ	2.46	0.51
39:2h:91:ARG:HD3	48:2q:32:TYR:O	2.10	0.51
1:1A:1054:A:H3'	1:1A:1055:G:C8	2.46	0.51
1:1A:1405:U:H2'	1:1A:1406:U:C6	2.45	0.51
1:1A:1783:A:H5'	1:1A:2608:G:H4'	1.93	0.51
1:1A:2150:U:H2'	1:1A:2151:G:C8	2.46	0.51
1:1A:2168:G:O6	1:1A:2171:A:H5"	2.10	0.51
17:1V:60:GLU:HB2	17:1V:97:LYS:HE2	1.92	0.51
32:1a:401:C:O2'	32:1a:621:A:N3	2.41	0.51
32:1a:1104:G:H4'	33:1b:111:ARG:HE	1.76	0.51
33:1b:71:VAL:N	33:1b:163:PHE:O	2.39	0.51
34:1c:73:PRO:HB3	34:1c:103:VAL:HG11	1.92	0.51
1:2A:10:G:O2'	1:2A:2801(A):A:N7	2.40	0.51
1:2A:271(G):C:H2'	1:2A:271(H):G:H8	1.75	0.51
1:2A:2693:A:H2'	1:2A:2694:G:C8	2.46	0.51
1:2A:2870:C:H2'	1:2A:2871:C:O4'	2.11	0.51
13:2R:87:TYR:OH	13:2R:117:VAL:O	2.26	0.51
32:2a:1126:U:H3	41:2j:40:LEU:HD11	1.76	0.51
7:1H:51:ARG:NH2	7:1H:53:GLU:OE2	2.43	0.51
32:1a:200:G:H1	32:1a:217:C:H42	1.58	0.51
32:1a:973:G:H3'	32:1a:974:A:H5"	1.91	0.51
33:1b:174:VAL:HG13	33:1b:184:VAL:HG11	1.93	0.51
1:2A:2379:G:O2'	14:2S:17:ARG:NH2	2.44	0.51
32:2a:72:C:N3	32:2a:97:G:O6	2.43	0.51
32:2a:263:A:OP1	51:2t:79:ARG:NH1	2.43	0.51
33:2b:81:VAL:HA	33:2b:215:LEU:HD21	1.93	0.51
39:2h:7:ALA:HB2	39:2h:85:ARG:HG3	1.92	0.51
52:2u:5:ASP:O	52:2u:11:GLY:HA3	2.10	0.51
1:1A:1301:A:O2'	1:1A:1302:A:H3'	2.10	0.51
32:1a:1006:C:N4	32:1a:1023:G:N1	2.52	0.51
32:1a:1095:U:OP1	32:1a:1108:G:N1	2.42	0.51
32:1a:1442:G:H2'	32:1a:1442:G:N3	2.25	0.51
40:1i:7:THR:O	40:1i:83:ARG:NH1	2.44	0.51
41:1j:21:GLN:HE21	41:1j:25:GLU:HG3	1.76	0.51
1:2A:661:C:H2'	1:2A:662:G:C8	2.45	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:821:A:N1	61:2A:4694:HOH:O	2.33	0.51
1:2A:1604:C:OP2	61:2A:5432:HOH:O	2.20	0.51
1:2A:1697:G:OP2	1:2A:1698:A:O2'	2.18	0.51
32:2a:839:U:H3'	32:2a:840:C:C6	2.46	0.51
32:2a:1071:C:H2'	32:2a:1072:G:C8	2.46	0.51
32:2a:1189:C:H5'	34:2c:5:ILE:HD12	1.92	0.51
32:2a:1323:G:H4'	32:2a:1363:C:N3	2.26	0.51
35:2d:76:ARG:O	35:2d:80:GLU:HG2	2.11	0.51
1:1A:278:A:H4'	1:1A:279:C:OP1	2.11	0.51
1:1A:2848:G:C8	15:1T:97:ALA:HB2	2.45	0.51
9:1N:62:VAL:HG11	9:1N:66:LYS:HB2	1.93	0.51
13:1R:8:ARG:HG3	13:1R:43:GLU:OE2	2.11	0.51
18:1W:65:LEU:HD12	18:1W:68:ARG:HE	1.76	0.51
1:2A:1203:G:OP2	1:2A:1204:A:O2'	2.20	0.51
1:2A:1906:G:OP2	1:2A:1929:G:O2'	2.29	0.51
1:2A:1920:4OC:HM22	1:2A:1921:G:H5'	1.93	0.51
6:2G:126:ASP:OD2	6:2G:130:ASN:ND2	2.44	0.51
21:2Z:54:HIS:CD2	21:2Z:101:PRO:HG3	2.46	0.51
32:2a:539:A:H2'	32:2a:540:G:C8	2.46	0.51
32:2a:545:C:P	35:2d:65:ARG:HH12	2.33	0.51
39:2h:25:ASP:N	39:2h:25:ASP:OD1	2.44	0.51
1:1A:336:C:O2'	20:1Y:35:TYR:OH	2.28	0.50
3:1D:12:SER:HB3	3:1D:208:LYS:HB3	1.93	0.50
31:19:32:HIS:O	31:19:34:GLN:HG3	2.11	0.50
32:1a:176:C:H2'	32:1a:177:C:C6	2.46	0.50
32:1a:1458:G:H5"	51:1t:31:SER:HB2	1.93	0.50
48:1q:6:LEU:HG	48:1q:23:VAL:HG11	1.93	0.50
1:2A:2142:C:H2'	1:2A:2143:C:O4'	2.11	0.50
7:2H:35:VAL:HG13	7:2H:71:LEU:HD23	1.93	0.50
8:2I:43:ASN:ND2	23:21:75:GLU:OE1	2.44	0.50
21:2Z:153:SER:HB3	21:2Z:167:PRO:HB3	1.93	0.50
32:2a:56:U:H2'	32:2a:57:G:C8	2.46	0.50
32:2a:196:A:OP1	51:2t:68:LYS:NZ	2.42	0.50
32:2a:1182:G:H4'	32:2a:1183:A:H5"	1.93	0.50
39:2h:21:LYS:O	39:2h:65:TYR:OH	2.27	0.50
1:1A:365:C:OP2	61:1A:6825:HOH:O	2.20	0.50
1:1A:1427:A:H4'	1:1A:1428:C:O4'	2.11	0.50
1:1A:1448:G:H4'	1:1A:1542:A:OP1	2.11	0.50
5:1F:39:TRP:CZ2	5:1F:43:LYS:HE3	2.46	0.50
6:1G:3:LEU:O	6:1G:8:LYS:NZ	2.40	0.50
15:1T:24:PRO:HD3	15:1T:52:ILE:HD12	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:1W:78:GLU:OE2	18:1W:99:ARG:NH1	2.40	0.50
54:1w:23:A:H3'	54:1w:24:G:C8	2.45	0.50
1:2A:652(B):A:N6	1:2A:655:A:H1'	2.26	0.50
1:2A:1514:U:H2'	1:2A:1515:G:C8	2.44	0.50
32:2a:660:G:H1	32:2a:745:C:H42	1.58	0.50
32:2a:673:G:H5"	37:2f:87:ARG:CZ	2.41	0.50
32:2a:1001:A:H2'	32:2a:1001(A):G:C8	2.45	0.50
32:2a:1082:G:N7	61:2a:3305:HOH:O	2.35	0.50
33:2b:195:ASP:OD1	33:2b:195:ASP:N	2.44	0.50
1:1A:1498:C:OP1	61:1A:7295:HOH:O	2.19	0.50
20:1Y:98:VAL:HG12	20:1Y:105:ALA:HA	1.93	0.50
1:2A:144:C:H5'	19:2X:2:LYS:HZ2	1.76	0.50
1:2A:1316:U:H2'	1:2A:1317:A:C8	2.46	0.50
1:2A:2198:A:OP1	8:2I:33:ARG:NH2	2.44	0.50
12:2Q:17:LEU:HB3	12:2Q:39:PRO:HB2	1.92	0.50
32:2a:359:U:H2'	32:2a:360:A:C8	2.46	0.50
32:2a:770:C:O2'	32:2a:899:C:N3	2.37	0.50
32:2a:1001:A:H2'	32:2a:1001(A):G:H8	1.76	0.50
45:2n:48:ALA:HB2	45:2n:53:LEU:HD12	1.93	0.50
1:1A:55:G:O2'	1:1A:127:A:N1	2.42	0.50
1:1A:1210:A:H5"	1:1A:1212:G:O4'	2.11	0.50
21:1Z:125:LEU:HB3	21:1Z:165:VAL:HG13	1.94	0.50
31:19:16:VAL:HG22	31:19:25:VAL:HG22	1.93	0.50
1:2A:301:G:OP2	20:2Y:84:ARG:NH2	2.42	0.50
1:2A:659:C:H2'	1:2A:660:G:H8	1.75	0.50
1:2A:2404:C:O3'	11:2P:77:ARG:NH2	2.44	0.50
8:2I:72:LEU:HD21	8:2I:107:VAL:HG11	1.94	0.50
10:2O:86:ILE:HG22	10:2O:94:ARG:HD3	1.93	0.50
32:2a:284:G:H2'	32:2a:285:G:C8	2.47	0.50
32:2a:736:C:H2'	32:2a:737:A:C8	2.46	0.50
34:2c:55:VAL:HG22	34:2c:68:VAL:HG22	1.93	0.50
37:2f:62:TRP:CH2	37:2f:64:GLN:HB2	2.47	0.50
48:2q:67:LYS:O	48:2q:68:ARG:HB3	2.12	0.50
1:1A:184:C:H2'	1:1A:185:U:C6	2.46	0.50
1:1A:880:G:H2'	1:1A:881:G:C8	2.38	0.50
1:1A:1045:A:H1'	1:1A:1047:G:N3	2.26	0.50
1:1A:2273:A:H2'	1:1A:2274:A:C8	2.46	0.50
9:1N:4:TYR:CD2	16:1U:100:VAL:HG11	2.47	0.50
32:1a:983:A:H5'	32:1a:984:C:OP2	2.11	0.50
1:2A:818:G:OP2	61:2A:4377:HOH:O	2.19	0.50
1:2A:1415:U:O2'	1:2A:1417:C:OP1	2.26	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2206:G:H5"	1:2A:2207:G:N7	2.26	0.50
1:2A:2785:C:OP1	4:2E:41:LYS:NZ	2.41	0.50
15:2T:6:LEU:O	15:2T:10:VAL:HG23	2.12	0.50
32:2a:20:U:H2'	32:2a:21:G:O4'	2.11	0.50
32:2a:707:C:H2'	32:2a:708:C:C6	2.46	0.50
32:2a:975:A:N1	41:2j:48:THR:HB	2.26	0.50
46:2o:54:ARG:HG2	46:2o:58:MET:HE2	1.93	0.50
1:1A:831:G:N2	11:1P:53:GLY:O	2.44	0.50
1:1A:1999:C:H4'	1:1A:2723:C:O2	2.11	0.50
1:1A:2611:U:C4	27:15:3:LYS:HG2	2.46	0.50
5:1F:135:LYS:HB2	5:1F:138:GLU:CD	2.37	0.50
14:1S:8:GLU:HA	14:1S:11:LYS:HB2	1.92	0.50
14:1S:65:VAL:O	14:1S:69:VAL:HG12	2.12	0.50
29:17:5:TRP:NE1	29:17:7:PRO:HG3	2.26	0.50
32:1a:370:C:O2	32:1a:482:A:O2'	2.26	0.50
32:1a:509:A:H2'	32:1a:510:A:C8	2.46	0.50
32:1a:584:G:O6	61:1a:2029:HOH:O	2.15	0.50
33:1b:59:GLU:HG2	33:1b:63:MET:HE2	1.93	0.50
36:1e:152:ARG:O	39:1h:64:LYS:NZ	2.36	0.50
44:1m:3:ARG:NH2	44:1m:9:ILE:O	2.43	0.50
46:1o:26:GLU:OE1	46:1o:77:ARG:NH2	2.45	0.50
48:1q:32:TYR:O	48:1q:34:LYS:N	2.42	0.50
1:2A:407:G:H2'	1:2A:408:G:H8	1.77	0.50
6:2G:32:PRO:HB3	6:2G:163:ALA:HB2	1.91	0.50
10:2O:87:ILE:HD12	10:2O:91:LEU:HA	1.92	0.50
12:2Q:7:MET:HE3	12:2Q:10:ARG:HA	1.92	0.50
18:2W:64:MET:HE2	18:2W:109:GLU:HG3	1.93	0.50
32:2a:936:C:H2'	32:2a:937:A:O4'	2.12	0.50
32:2a:1272:G:C4	32:2a:1273:G:H1'	2.47	0.50
48:2q:61:GLU:HA	48:2q:71:PHE:CD1	2.47	0.50
1:1A:768:G:O2'	1:1A:1379:A:N1	2.41	0.50
1:1A:1053:C:N4	1:1A:1106:G:H1	2.07	0.50
1:1A:2128:C:H2'	1:1A:2129:C:O4'	2.11	0.50
30:18:33:ASN:HA	30:18:36:LYS:HD2	1.93	0.50
32:1a:1126:U:O2	32:1a:1280:A:H2'	2.10	0.50
35:1d:18:LYS:NZ	35:1d:33:MET:HB3	2.27	0.50
1:2A:854:G:H2'	1:2A:855:G:C8	2.43	0.50
1:2A:1300:U:H4'	1:2A:1301:A:H5"	1.92	0.50
1:2A:2334:G:H5'	14:2S:9:ARG:HG2	1.93	0.50
1:2A:2504:U:OP2	61:2A:4814:HOH:O	2.20	0.50
10:2O:21:CYS:HB2	10:2O:39:ILE:HD12	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:26:6:ARG:HH11	28:26:26:ASN:HB2	1.75	0.50
32:2a:35:G:O2'	43:2l:118:SER:O	2.29	0.50
32:2a:737:A:H2'	32:2a:738:C:C6	2.47	0.50
32:2a:946:A:O2'	32:2a:1333:A:N3	2.32	0.50
1:1A:1066:U:H2'	1:1A:1068:G:OP2	2.12	0.50
1:1A:1174:A:H1'	1:1A:1175:U:O5'	2.12	0.50
1:1A:1439:A:OP1	61:1A:6792:HOH:O	2.19	0.50
4:1E:56:PRO:HG3	4:1E:74:PRO:HG2	1.93	0.50
5:1F:123:LEU:HD13	5:1F:192:LEU:HB3	1.94	0.50
17:1V:43:GLU:OE1	17:1V:43:GLU:N	2.43	0.50
20:1Y:35:TYR:CE2	20:1Y:69:ALA:HB3	2.47	0.50
32:1a:123:C:OP1	32:1a:311:C:O2'	2.24	0.50
1:2A:27:G:N2	1:2A:512:G:H1'	2.27	0.50
8:2I:116:LEU:HD11	8:2I:120:ILE:HG13	1.93	0.50
11:2P:99:LEU:HD23	11:2P:102:ARG:HH21	1.76	0.50
25:23:6:VAL:HG22	25:23:56:VAL:HG22	1.94	0.50
32:2a:78:G:N1	32:2a:91:C:O2	2.38	0.50
32:2a:1191:A:H5"	34:2c:4:LYS:HE3	1.93	0.50
33:2b:149:LEU:HA	33:2b:152:PHE:HB3	1.94	0.50
54:2y:51:U:H3	54:2y:63:G:H1	1.59	0.50
1:1A:249:C:O2'	11:1P:64:LYS:NZ	2.31	0.50
1:1A:2110:G:OP1	1:1A:2118:U:N3	2.38	0.50
2:1B:91:C:H5'	12:1Q:18:LYS:HA	1.92	0.50
32:1a:17:U:H2'	32:1a:18:C:C6	2.47	0.50
35:1d:119:GLN:HG2	35:1d:123:HIS:CD2	2.47	0.50
37:1f:33:TYR:HB2	37:1f:75:LEU:HD12	1.94	0.50
38:1g:89:MET:SD	38:1g:155:ARG:HB2	2.52	0.50
39:1h:19:VAL:HG23	39:1h:21:LYS:HG2	1.94	0.50
43:1l:53:ARG:HB3	43:1l:69:TYR:HE1	1.77	0.50
1:2A:288:C:H2'	1:2A:289:A:H8	1.76	0.50
1:2A:743:G:OP1	4:2E:130:GLY:HA2	2.11	0.50
1:2A:2870:C:H5"	13:2R:65:LEU:HD21	1.94	0.50
4:2E:77:ILE:HG12	4:2E:195:LEU:HD12	1.93	0.50
10:2O:36:GLY:HA2	10:2O:106:LEU:HD23	1.94	0.50
15:2T:51:ARG:HB2	15:2T:98:LYS:HD2	1.93	0.50
32:2a:1187:G:H4'	40:2i:111:ARG:HH11	1.75	0.50
41:2j:49:VAL:HG12	41:2j:61:GLU:O	2.12	0.50
54:2y:9:A:H8	54:2y:11:C:H41	1.60	0.50
1:1A:191:A:H2'	1:1A:192:C:C6	2.47	0.49
1:1A:524:U:H2'	1:1A:525:U:C6	2.47	0.49
1:1A:769:G:N7	61:1A:7107:HOH:O	2.34	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:862:G:H2'	1:1A:863:A:O4'	2.12	0.49
1:1A:1108:U:H2'	1:1A:1109:C:O4'	2.11	0.49
1:1A:1996:C:H4'	1:1A:1997:G:OP1	2.12	0.49
1:1A:2185:C:H2'	1:1A:2186:G:H8	1.77	0.49
1:1A:2336:A:H61	22:10:43:THR:HG21	1.77	0.49
1:1A:2552:2MU:O5'	1:1A:2552:2MU:H6	2.12	0.49
5:1F:110:LEU:HD11	5:1F:181:LEU:HG	1.94	0.49
9:1N:75:TYR:CE2	9:1N:77:GLY:HA2	2.47	0.49
18:1W:80:PRO:O	18:1W:100:THR:OG1	2.29	0.49
32:1a:146:G:H2'	32:1a:147:G:O4'	2.12	0.49
51:1t:10:LEU:HB3	51:1t:12:ALA:H	1.75	0.49
1:2A:657:U:H2'	1:2A:658:C:C6	2.46	0.49
1:2A:879:G:H5'	1:2A:880:G:OP2	2.12	0.49
1:2A:1899:G:O2'	1:2A:1900:A:OP2	2.28	0.49
1:2A:2030:A:H4'	1:2A:2031:A:C8	2.47	0.49
1:2A:2070:G:H2'	1:2A:2071:A:C8	2.47	0.49
1:2A:2218:U:N3	23:21:55:GLY:O	2.45	0.49
1:2A:2360:A:H2'	1:2A:2361:A:O4'	2.12	0.49
1:2A:2473:U:O2	1:2A:2473:U:H2'	2.12	0.49
1:2A:2507:C:H4'	54:2w:75:C:O2'	2.11	0.49
1:2A:2564:A:OP1	1:2A:2648:C:H4'	2.11	0.49
4:2E:48:GLN:HA	4:2E:80:GLU:HA	1.93	0.49
32:2a:107:G:H2'	32:2a:108:G:O4'	2.12	0.49
32:2a:794:A:OP2	61:2a:3641:HOH:O	2.20	0.49
42:2k:48:ILE:O	42:2k:50:TYR:N	2.45	0.49
44:2m:85:GLY:HA2	44:2m:93:ARG:HH21	1.77	0.49
1:1A:1047:G:O2'	1:1A:1048:A:H8	1.95	0.49
32:1a:401:C:H2'	32:1a:402:G:C8	2.47	0.49
32:1a:601:C:H2'	32:1a:602:A:H8	1.78	0.49
35:1d:105:VAL:HG13	35:1d:110:PHE:HB2	1.94	0.49
48:1q:53:LEU:HD23	48:1q:82:MET:HE1	1.93	0.49
50:1s:48:THR:HG22	50:1s:61:TYR:HD1	1.76	0.49
1:2A:1292:U:H2'	1:2A:1293:C:C6	2.47	0.49
1:2A:1593:G:H2'	1:2A:1594:G:C8	2.47	0.49
1:2A:2033:A:O2'	1:2A:2035:G:OP2	2.25	0.49
1:2A:2498:C:OP1	61:2A:4156:HOH:O	2.20	0.49
1:2A:2641:G:H5"	9:2N:76:SER:HB3	1.93	0.49
4:2E:167:VAL:HG22	4:2E:170:LEU:HD11	1.94	0.49
6:2G:97:ASP:N	6:2G:97:ASP:OD1	2.43	0.49
7:2H:3:ARG:HH11	7:2H:4:ILE:H	1.58	0.49
9:2N:97:ARG:HA	9:2N:100:GLU:HB2	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:6:G:H4'	32:2a:298:A:H4'	1.94	0.49
32:2a:411:A:H2'	32:2a:412:A:H4'	1.94	0.49
32:2a:448:A:P	32:2a:485:G:H22	2.34	0.49
32:2a:728:A:H2'	32:2a:729:A:C8	2.47	0.49
32:2a:1328:C:H3'	52:2u:7:ARG:HH22	1.76	0.49
33:2b:98:LEU:HD12	33:2b:101:MET:HE3	1.94	0.49
41:2j:78:ASN:O	41:2j:80:LYS:N	2.46	0.49
1:1A:1082:U:C4	1:1A:1086:A:N1	2.75	0.49
32:1a:765:G:N1	32:1a:812:C:O2'	2.37	0.49
36:1e:99:GLY:N	36:1e:117:ASP:OD1	2.38	0.49
39:1h:11:THR:HG22	39:1h:15:ASN:ND2	2.27	0.49
46:1o:55:GLY:HA2	46:1o:58:MET:HE3	1.92	0.49
49:1r:58:LEU:HB3	49:1r:62:GLU:HB2	1.94	0.49
1:2A:184:C:H2'	1:2A:185:U:C6	2.47	0.49
1:2A:236:C:H2'	1:2A:237:C:H6	1.77	0.49
1:2A:484:C:H2'	1:2A:485:C:C6	2.47	0.49
1:2A:1507:A:O2'	1:2A:1508:A:O4'	2.29	0.49
2:2B:40:U:O2'	2:2B:43:C:OP2	2.24	0.49
2:2B:105:A:H5'	2:2B:106:G:OP2	2.12	0.49
7:2H:56:SER:HB3	7:2H:61:HIS:ND1	2.27	0.49
32:2a:34:C:H2'	32:2a:35:G:H8	1.77	0.49
32:2a:570:G:H1'	32:2a:820:U:C4	2.47	0.49
32:2a:576:G:O6	32:2a:880:C:O2'	2.23	0.49
32:2a:955:U:H2'	32:2a:956:U:O4'	2.11	0.49
32:2a:1299:A:H2'	32:2a:1299:A:N3	2.27	0.49
32:2a:1305:G:H22	32:2a:1331:G:H1'	1.76	0.49
36:2e:53:LEU:HA	36:2e:56:GLN:HG2	1.93	0.49
1:1A:438:G:H2'	1:1A:440:G:C8	2.47	0.49
1:1A:657:U:H2'	1:1A:658:C:C6	2.47	0.49
1:1A:1268:A:H2'	1:1A:1269:A:O4'	2.12	0.49
1:1A:2310:A:N1	6:1G:79:ASN:ND2	2.60	0.49
8:1I:129:THR:HG22	8:1I:139:GLN:HE22	1.78	0.49
11:1P:106:LEU:HD22	11:1P:112:LEU:HD13	1.94	0.49
13:1R:36:THR:HG22	13:1R:37:THR:H	1.77	0.49
15:1T:29:ARG:HG3	15:1T:46:GLU:HB2	1.94	0.49
33:1b:21:ARG:HB3	33:1b:39:ILE:HG13	1.95	0.49
37:1f:97:PHE:CD2	49:1r:31:LEU:HD11	2.47	0.49
1:2A:890:A:H2'	1:2A:892:G:H8	1.77	0.49
1:2A:1019:U:H3	1:2A:1142(A):A:H62	1.60	0.49
1:2A:1913:A:N6	54:2w:37:MIA:O2'	2.44	0.49
2:2B:50:G:OP1	14:2S:63:THR:N	2.40	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2G:11:TYR:OH	6:2G:16:ARG:NH1	2.46	0.49
19:2X:26:TYR:HB3	19:2X:92:LEU:HD22	1.94	0.49
32:2a:673:G:H2'	32:2a:674:G:H8	1.75	0.49
46:2o:3:ILE:HG12	46:2o:38:ARG:HE	1.77	0.49
1:1A:740:U:H2'	1:1A:741:G:C8	2.47	0.49
1:1A:848:G:H2'	1:1A:849:A:C8	2.48	0.49
1:1A:1593:G:H2'	1:1A:1594:G:C8	2.48	0.49
1:1A:2350:C:OP2	61:1A:6676:HOH:O	2.18	0.49
32:1a:486:U:H2'	32:1a:487:A:C8	2.46	0.49
32:1a:1030:C:O2'	32:1a:1030(D):A:N6	2.46	0.49
41:1j:13:HIS:HA	41:1j:16:LEU:HB3	1.95	0.49
41:1j:16:LEU:HD22	41:1j:68:HIS:HB2	1.93	0.49
43:1l:24:VAL:HB	43:1l:27:LEU:HD22	1.94	0.49
54:1y:36:A:H2'	54:1y:37:MIA:O4'	2.12	0.49
1:2A:65:C:O2'	1:2A:456:C:N3	2.36	0.49
1:2A:897:C:H1'	54:2w:56:C:C5	2.41	0.49
1:2A:2127:G:H2'	1:2A:2128:C:C6	2.47	0.49
32:2a:977:A:O2'	32:2a:979:C:OP2	2.24	0.49
33:2b:98:LEU:HB2	33:2b:101:MET:HG3	1.95	0.49
36:2e:78:HIS:HE1	36:2e:143:ARG:H	1.60	0.49
46:2o:33:THR:HG21	46:2o:85:LEU:HD22	1.94	0.49
54:2w:6:G:N1	54:2w:67:C:O2	2.39	0.49
1:1A:64:A:O3'	19:1X:71:GLY:HA3	2.12	0.49
1:1A:286:C:H2'	1:1A:287:C:C6	2.48	0.49
1:1A:1418:G:OP2	61:1A:5574:HOH:O	2.20	0.49
1:1A:1508:A:O2'	1:1A:1509:C:H5"	2.12	0.49
32:1a:909:A:H2'	32:1a:910:C:O4'	2.13	0.49
45:1n:4:LYS:HA	45:1n:7:ILE:HG22	1.94	0.49
1:2A:852:G:H2'	1:2A:853:G:C8	2.47	0.49
19:2X:4:ALA:HB1	19:2X:42:ALA:HA	1.94	0.49
32:2a:824:C:H2'	32:2a:825:G:C8	2.46	0.49
32:2a:954:G:H2'	32:2a:955:U:O4'	2.12	0.49
40:2i:50:LEU:HD13	40:2i:56:LEU:HA	1.94	0.49
44:2m:15:VAL:HG11	44:2m:48:LEU:HD11	1.95	0.49
47:2p:22:THR:HA	47:2p:33:ILE:HG13	1.94	0.49
54:2y:67:C:H2'	54:2y:68:C:H6	1.78	0.49
4:1E:24:THR:HG23	4:1E:184:VAL:HG12	1.94	0.49
15:1T:74:ARG:HG2	15:1T:76:PHE:CZ	2.47	0.49
21:1Z:153:SER:HA	21:1Z:167:PRO:HB3	1.95	0.49
32:1a:316:G:OP2	32:1a:351:G:O2'	2.28	0.49
32:1a:1142:G:H2'	32:1a:1143:G:O4'	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1c:116:VAL:HG21	34:1c:202:ILE:HD11	1.93	0.49
36:1e:78:HIS:HE1	36:1e:142:LEU:HA	1.77	0.49
44:1m:80:ARG:HH22	50:1s:69:HIS:CE1	2.31	0.49
1:2A:524:U:H2'	1:2A:525:U:C6	2.48	0.49
1:2A:912:C:OP1	12:2Q:8:LYS:NZ	2.38	0.49
1:2A:974:G:OP1	1:2A:1187:G:O2'	2.19	0.49
1:2A:1670:C:OP1	61:2A:6087:HOH:O	2.19	0.49
1:2A:2327:A:H2'	1:2A:2328:A:C8	2.48	0.49
1:2A:2781:A:H5"	1:2A:2782:G:H5'	1.95	0.49
9:2N:103:VAL:HG11	9:2N:120:LEU:HD22	1.95	0.49
14:2S:34:HIS:O	14:2S:97:ARG:NH2	2.45	0.49
23:21:2:SER:HB3	23:21:46:LEU:HD12	1.94	0.49
32:2a:790:A:H61	32:2a:1498:UR3:P	2.35	0.49
32:2a:833:U:H2'	32:2a:834:C:C6	2.47	0.49
1:1A:2127:G:H1	1:1A:2161:C:H42	1.60	0.49
1:1A:2176:A:H2'	1:1A:2177:C:C6	2.46	0.49
32:1a:1531:A:H8	32:1a:1531:A:O5'	1.95	0.49
44:1m:11:ARG:C	44:1m:13:LYS:H	2.21	0.49
1:2A:1022:G:H22	1:2A:1142(A):A:H2	1.60	0.49
1:2A:1412:A:H2'	1:2A:1413:G:C8	2.47	0.49
1:2A:1794:U:H2'	1:2A:1795:C:C6	2.48	0.49
6:2G:122:PRO:HB3	6:2G:170:ARG:NH1	2.28	0.49
15:2T:74:ARG:HG2	15:2T:76:PHE:CZ	2.48	0.49
32:2a:1320:C:H1'	50:2s:73:GLU:HG2	1.94	0.49
47:2p:52:ASP:O	47:2p:54:GLU:N	2.42	0.49
1:1A:639:U:H2'	1:1A:640:C:C6	2.47	0.49
1:1A:1364:G:N7	23:11:3:LYS:HD2	2.27	0.49
1:1A:1756:G:H4'	1:1A:1758:G:O4'	2.12	0.49
1:1A:2705:A:N3	61:1R:301:HOH:O	2.35	0.49
2:1B:21:G:N7	61:1B:302:HOH:O	2.35	0.49
10:1O:64:ARG:HD3	10:1O:79:PHE:CD1	2.48	0.49
32:1a:165:C:H2'	32:1a:166:G:H8	1.78	0.49
32:1a:184:G:H2'	32:1a:185:A:C8	2.44	0.49
32:1a:194:C:H2'	32:1a:195:A:H5"	1.95	0.49
50:1s:11:VAL:HG12	50:1s:13:ASP:H	1.78	0.49
1:2A:93:G:H2'	1:2A:94:C:H6	1.78	0.49
1:2A:2130:U:O2	1:2A:2134:A:O2'	2.22	0.49
1:2A:2343:C:O3'	1:2A:2373:G:H4'	2.12	0.49
1:2A:2590:A:H5"	3:2D:239:ARG:HG3	1.94	0.49
25:23:12:PRO:HB2	25:23:20:LYS:HG2	1.94	0.49
32:2a:742:G:OP2	46:2o:35:ARG:NH2	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1369:C:OP2	40:2i:112:LYS:N	2.37	0.49
39:2h:10:LEU:HD22	39:2h:83:ILE:HD11	1.95	0.49
55:2x:44:A:H2'	55:2x:45:G:C8	2.47	0.49
1:1A:414:C:H2'	1:1A:415:A:C8	2.47	0.49
1:1A:2506:U:O2'	54:1w:76:A:H4'	2.12	0.49
1:1A:2849:U:H4'	1:1A:2868:A:C2	2.48	0.49
15:1T:65:LYS:HE3	15:1T:67:SER:HB2	1.95	0.49
32:1a:636:U:H2'	32:1a:637:G:C8	2.47	0.49
34:1c:22:TRP:CE2	45:1n:54:PRO:HG2	2.47	0.49
41:1j:32:ALA:HB3	41:1j:76:ASN:H	1.76	0.49
46:1o:56:LEU:O	46:1o:60:VAL:HG23	2.13	0.49
1:2A:275:G:H2'	1:2A:276:A:O4'	2.13	0.49
1:2A:848:G:N3	1:2A:933:A:H1'	2.28	0.49
1:2A:1751:C:O2'	1:2A:2861:G:O2'	2.28	0.49
1:2A:1798:U:H5'	3:2D:259:THR:CG2	2.42	0.49
6:2G:173:LEU:HB3	6:2G:178:PHE:CD2	2.48	0.49
32:2a:590:C:H2'	32:2a:591:U:C6	2.48	0.49
32:2a:1118:C:H1'	32:2a:1179:A:C5	2.48	0.49
33:2b:12:GLU:O	33:2b:15:VAL:HG22	2.13	0.49
49:2r:53:ARG:HG2	49:2r:63:GLN:HE21	1.77	0.49
49:2r:58:LEU:HD11	49:2r:66:LEU:HD13	1.95	0.49
61:1A:6898:HOH:O	16:1U:16:LYS:HD3	2.13	0.48
6:1G:64:THR:HB	6:1G:94:LEU:HD21	1.94	0.48
18:1W:58:ALA:HB1	18:1W:64:MET:HB2	1.95	0.48
19:1X:43:VAL:HG21	19:1X:81:VAL:HG11	1.96	0.48
32:1a:509:A:H5"	35:1d:55:ALA:HB2	1.95	0.48
32:1a:1391:U:H2'	32:1a:1392:G:C8	2.48	0.48
33:1b:230:VAL:HG22	33:1b:232:PRO:HD2	1.95	0.48
1:2A:249:C:O2	30:28:12:LYS:NZ	2.38	0.48
1:2A:531:C:H4'	1:2A:532:A:H5"	1.95	0.48
1:2A:1023:U:O2'	1:2A:1122:G:H5'	2.14	0.48
1:2A:2110:G:H3'	1:2A:2111:C:H5'	1.95	0.48
1:2A:2526:G:O3'	31:29:33:LYS:NZ	2.46	0.48
3:2D:242:ARG:HH11	3:2D:242:ARG:HG3	1.79	0.48
4:2E:5:LEU:HD21	4:2E:79:ARG:HB2	1.94	0.48
5:2F:179:GLU:OE1	5:2F:179:GLU:N	2.45	0.48
8:2I:117:GLU:HG3	8:2I:118:LYS:H	1.77	0.48
9:2N:58:ASP:OD1	9:2N:58:ASP:N	2.41	0.48
11:2P:63:PRO:HG2	30:28:25:MET:HB2	1.94	0.48
21:2Z:74:VAL:HG22	21:2Z:86:VAL:HG12	1.95	0.48
32:2a:316:G:OP2	32:2a:351:G:O2'	2.28	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:920:U:H2'	32:2a:921:U:C6	2.48	0.48
32:2a:952:U:H2'	32:2a:953:G:H8	1.77	0.48
33:2b:93:VAL:HG21	33:2b:97:TRP:HD1	1.77	0.48
1:1A:1230:C:H2'	1:1A:1231:G:C8	2.49	0.48
1:1A:2096:U:H3	1:1A:2193:G:H1	1.61	0.48
1:1A:2804:C:H2'	1:1A:2805:G:O4'	2.12	0.48
12:1Q:31:ASP:OD1	12:1Q:134:ARG:NH1	2.43	0.48
32:1a:271:C:H2'	32:1a:272:C:C6	2.48	0.48
32:1a:330:C:O2	61:1a:2121:HOH:O	2.17	0.48
32:1a:1249:C:O2'	40:1i:73:GLN:NE2	2.46	0.48
33:1b:24:TRP:CZ3	33:1b:26:PRO:HA	2.48	0.48
50:1s:11:VAL:HG11	50:1s:16:LEU:HB2	1.95	0.48
1:2A:661:C:H2'	1:2A:662:G:H8	1.78	0.48
1:2A:1496:A:O2'	1:2A:1497:U:O2	2.25	0.48
1:2A:1711:C:H2'	1:2A:1712:C:C6	2.48	0.48
1:2A:1816:G:O6	3:2D:35:LYS:NZ	2.44	0.48
1:2A:2102:U:H2'	1:2A:2103:C:C6	2.47	0.48
2:2B:14:U:OP2	2:2B:70:C:O2'	2.25	0.48
2:2B:40:U:H2'	26:24:2:LYS:HE3	1.95	0.48
27:25:41:PRO:O	27:25:44:THR:OG1	2.23	0.48
29:27:12:ARG:NH2	29:27:44:PRO:HB3	2.27	0.48
30:28:30:ARG:HB3	30:28:31:HIS:HD2	1.78	0.48
32:2a:340:U:H2'	32:2a:341:C:C6	2.49	0.48
32:2a:560:U:H4'	32:2a:561:U:O5'	2.13	0.48
32:2a:596:C:OP2	61:2a:3425:HOH:O	2.20	0.48
33:2b:18:GLY:HA3	33:2b:42:ILE:H	1.77	0.48
1:1A:18:C:O2'	1:1A:554:U:OP1	2.29	0.48
2:1B:2:C:H2'	2:1B:3:C:C6	2.48	0.48
21:1Z:130:PRO:HA	21:1Z:133:ILE:HG13	1.96	0.48
32:1a:19:C:H2'	32:1a:20:U:C6	2.48	0.48
33:1b:178:ARG:HH22	39:1h:74:PRO:HB3	1.79	0.48
21:2Z:156:LYS:HE3	21:2Z:158:PRO:HD3	1.95	0.48
26:24:58:ARG:HG3	50:2s:68:GLY:H	1.77	0.48
32:2a:148:G:H2'	32:2a:149:A:H8	1.77	0.48
32:2a:181:G:H4'	32:2a:182:U:H5'	1.95	0.48
32:2a:442:C:H42	32:2a:492:G:H1	1.61	0.48
1:1A:1085:A:O2'	1:1A:1104:C:O2'	2.19	0.48
1:1A:1670:C:O2	4:1E:129:HIS:NE2	2.39	0.48
1:1A:2206:G:H5"	1:1A:2207:G:C5	2.48	0.48
1:1A:2364:C:H2'	1:1A:2365:G:O4'	2.14	0.48
2:1B:12:C:H2'	22:10:73:GLY:HA3	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1B:31:C:H4'	6:1G:29:TRP:CH2	2.48	0.48
4:1E:12:THR:HG22	4:1E:13:ARG:H	1.77	0.48
32:1a:128:G:O2'	48:1q:3:LYS:NZ	2.46	0.48
32:1a:452:A:H4'	47:1p:72:ARG:NH1	2.28	0.48
44:1m:50:GLU:HA	44:1m:53:VAL:HB	1.95	0.48
44:1m:87:TYR:CE2	44:1m:91:ARG:HD2	2.47	0.48
54:1y:38:A:H2'	54:1y:39:PSU:O4'	2.13	0.48
1:2A:140:G:N2	1:2A:1596:A:H4'	2.28	0.48
1:2A:251:A:C5	1:2A:252:G:H1'	2.48	0.48
1:2A:887:A:H4'	1:2A:888:C:C5	2.49	0.48
1:2A:1016:G:O6	1:2A:1147:C:N4	2.46	0.48
1:2A:1023:U:OP2	61:2A:5647:HOH:O	2.20	0.48
1:2A:1916:A:H2'	1:2A:1917:PSU:O4'	2.12	0.48
6:2G:97:ASP:HA	6:2G:100:TRP:HD1	1.79	0.48
21:2Z:28:MET:HE1	21:2Z:61:LEU:HD21	1.95	0.48
32:2a:109:A:C6	32:2a:326:G:C6	3.02	0.48
32:2a:324:G:N1	32:2a:327:A:OP2	2.47	0.48
32:2a:1016:A:C5	32:2a:1017:G:H1'	2.48	0.48
32:2a:1176:A:H2'	32:2a:1177:G:C8	2.49	0.48
32:2a:1306:A:H1'	32:2a:1332:A:C2	2.48	0.48
34:2c:47:LEU:HB2	34:2c:52:LEU:HD22	1.94	0.48
11:1P:98:GLU:O	11:1P:101:VAL:HG12	2.14	0.48
16:1U:49:HIS:HA	16:1U:52:ARG:HB3	1.94	0.48
18:1W:12:ILE:HD13	18:1W:17:VAL:HG13	1.95	0.48
19:1X:26:TYR:HB3	19:1X:92:LEU:HD22	1.95	0.48
32:1a:501:C:H2'	32:1a:502:G:H8	1.78	0.48
32:1a:659:U:H2'	32:1a:660:G:H8	1.78	0.48
32:1a:1260:C:O5'	32:1a:1284:C:H4'	2.13	0.48
33:1b:16:HIS:HB2	33:1b:204:ASN:HB3	1.96	0.48
36:1e:110:LEU:HD13	36:1e:118:ILE:HG21	1.95	0.48
1:2A:271(H):G:H2'	1:2A:271(I):G:C8	2.44	0.48
1:2A:2161:C:H2'	1:2A:2162:G:O4'	2.14	0.48
11:2P:120:ALA:HB2	11:2P:137:LYS:HB3	1.94	0.48
32:2a:228:A:H2'	32:2a:229:U:O4'	2.12	0.48
32:2a:429:U:H1'	32:2a:430:A:H5"	1.94	0.48
32:2a:1103:C:H5"	33:2b:98:LEU:HD22	1.95	0.48
32:2a:1264:C:N4	32:2a:1271:G:N1	2.39	0.48
34:2c:138:VAL:HG11	34:2c:169:ALA:HA	1.95	0.48
40:2i:26:VAL:HG13	40:2i:61:ALA:HB3	1.94	0.48
1:1A:301:G:OP2	20:1Y:84:ARG:NH2	2.46	0.48
1:1A:528:A:O2'	1:1A:529:A:H5'	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:796:C:H2'	1:1A:797:C:C6	2.48	0.48
32:1a:848:C:H2'	32:1a:849:C:C6	2.49	0.48
32:1a:1202:G:O4'	45:1n:29:ARG:NH1	2.45	0.48
33:1b:95:GLN:OE1	33:1b:147:LYS:HG2	2.13	0.48
36:1e:77:PRO:HD2	36:1e:142:LEU:HD13	1.94	0.48
45:1n:23:ARG:HD2	45:1n:28:GLY:O	2.14	0.48
51:1t:47:GLY:HA2	51:1t:48:LYS:C	2.38	0.48
1:2A:172:C:H2'	1:2A:173:G:H8	1.78	0.48
1:2A:855:G:O2'	22:20:27:GLU:OE2	2.31	0.48
11:2P:50:ARG:HD3	30:28:7:HIS:CD2	2.48	0.48
32:2a:235:C:N4	61:2a:3351:HOH:O	2.46	0.48
32:2a:1019:C:H2'	32:2a:1020:U:H4'	1.96	0.48
32:2a:1250:A:H4'	40:2i:68:GLY:N	2.29	0.48
32:2a:1423:G:H2'	32:2a:1424:C:H6	1.79	0.48
39:2h:51:VAL:HG11	39:2h:60:ARG:NH1	2.28	0.48
41:2j:16:LEU:HD21	41:2j:70:ARG:HG2	1.95	0.48
51:2t:18:GLN:O	51:2t:22:ARG:HG3	2.13	0.48
1:1A:883:G:H22	1:1A:893:C:N4	2.12	0.48
1:1A:2790:A:H5'	1:1A:2893:G:H21	1.78	0.48
2:1B:66:A:H61	2:1B:109:C:H5'	1.77	0.48
32:1a:848:C:H2'	32:1a:849:C:H6	1.79	0.48
32:1a:974:A:H8	32:1a:974:A:OP1	1.96	0.48
33:1b:74:LYS:HD2	33:1b:166:ASP:HB2	1.95	0.48
34:1c:5:ILE:HG12	34:1c:6:HIS:H	1.78	0.48
1:2A:118:A:N3	1:2A:178:G:H1'	2.28	0.48
1:2A:208:C:H2'	1:2A:209:C:C6	2.48	0.48
1:2A:582:G:H2'	1:2A:583:G:C8	2.49	0.48
1:2A:878:A:N6	1:2A:899:A:O2'	2.46	0.48
2:2B:90:A:C5	2:2B:91:C:H1'	2.48	0.48
3:2D:206:LEU:HA	3:2D:211:ARG:HE	1.79	0.48
7:2H:4:ILE:O	7:2H:69:ARG:HD2	2.14	0.48
32:2a:37:U:O2'	32:2a:500:G:H4'	2.14	0.48
32:2a:839:U:H3'	32:2a:840:C:H6	1.79	0.48
37:2f:69:GLU:CD	37:2f:69:GLU:H	2.21	0.48
32:1a:719:C:O2'	49:1r:49:LYS:HB3	2.13	0.48
32:1a:1317:C:O2	50:1s:37:ARG:NH2	2.46	0.48
54:1y:19:G:O4'	54:1y:57:G:N1	2.47	0.48
1:2A:645:C:H5"	1:2A:646:A:OP2	2.14	0.48
1:2A:832:G:H5'	11:2P:45:LEU:HD21	1.95	0.48
1:2A:1470:G:O2'	1:2A:1520:G:O6	2.31	0.48
1:2A:2849:U:H4'	1:2A:2868:A:C2	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:2P:59:LEU:HD22	11:2P:60:MET:HE2	1.95	0.48
30:28:31:HIS:ND1	30:28:32:LEU:HD13	2.28	0.48
32:2a:1060:C:H5"	41:2j:51:ARG:HG2	1.94	0.48
32:2a:1245:A:H2'	32:2a:1246:C:O4'	2.13	0.48
32:2a:1359:C:OP1	45:2n:22:THR:OG1	2.29	0.48
32:2a:1442:G:H2'	32:2a:1442:G:N3	2.27	0.48
32:2a:1518:MA6:N6	32:2a:1519:MA6:H103	2.29	0.48
34:2c:16:ARG:HH21	34:2c:54:ARG:NH1	2.12	0.48
36:2e:101:ILE:HG13	36:2e:119:LEU:HD23	1.96	0.48
37:2f:97:PHE:CE2	49:2r:62:GLU:HG2	2.46	0.48
1:1A:218:A:C2	1:1A:235:U:H4'	2.49	0.48
1:1A:297:C:OP1	20:1Y:87:LYS:NZ	2.42	0.48
1:1A:881:G:H3'	1:1A:882:G:H8	1.78	0.48
1:1A:1045:A:OP1	1:1A:1045:A:H4'	2.14	0.48
1:1A:1223:G:N2	1:1A:1226:A:OP2	2.37	0.48
1:1A:1300:U:H4'	1:1A:1301:A:H5"	1.95	0.48
1:1A:1766:U:H2'	1:1A:1767:C:H6	1.79	0.48
1:1A:2478:A:H5'	31:19:31:LYS:HD3	1.96	0.48
23:11:82:LEU:HD13	23:11:90:ILE:HG23	1.94	0.48
32:1a:769:G:H4'	32:1a:1513:A:H4'	1.94	0.48
32:1a:929:G:H1	32:1a:1388:C:N4	2.12	0.48
44:1m:80:ARG:HH22	50:1s:69:HIS:HE1	1.61	0.48
1:2A:857:C:H1'	22:20:26:TYR:CE1	2.49	0.48
1:2A:1747:G:H2'	1:2A:1747(A):G:H8	1.79	0.48
1:2A:2032:G:OP2	1:2A:2454:G:O2'	2.23	0.48
4:2E:181:LEU:HD11	15:2T:6:LEU:HD23	1.95	0.48
18:2W:18:ARG:HG2	18:2W:76:VAL:HB	1.96	0.48
20:2Y:9:LYS:HA	20:2Y:10:GLY:HA2	1.51	0.48
20:2Y:38:ILE:HD11	20:2Y:66:PRO:HG3	1.96	0.48
20:2Y:102:CYS:SG	20:2Y:103:GLY:N	2.87	0.48
30:28:26:LYS:HB2	30:28:44:LYS:O	2.14	0.48
32:2a:1029:C:C2	32:2a:1032:G:N2	2.78	0.48
33:2b:219:VAL:HG22	33:2b:222:ILE:HD12	1.96	0.48
38:2g:26:PHE:CE2	38:2g:30:ILE:HD11	2.48	0.48
1:1A:839:U:H2'	1:1A:840:C:C6	2.49	0.48
7:1H:56:SER:HB3	7:1H:61:HIS:ND1	2.28	0.48
35:1d:26:CYS:CB	60:1d:302:SF4:S1	3.01	0.48
39:1h:11:THR:HG23	39:1h:14:ARG:HH21	1.79	0.48
54:1w:5:G:H2'	54:1w:6:G:C8	2.49	0.48
1:2A:902:C:H2'	1:2A:903:C:C6	2.49	0.48
1:2A:2547:U:O2	10:2O:23:ARG:NH2	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2889:C:H2'	1:2A:2891:G:O4'	2.14	0.48
5:2F:187:VAL:HG12	11:2P:3:LEU:HD12	1.95	0.48
26:24:40:HIS:CD2	26:24:41:PRO:HD2	2.49	0.48
32:2a:237:C:H5"	48:2q:25:ARG:CZ	2.43	0.48
32:2a:1026:G:O6	32:2a:1036:G:N2	2.47	0.48
32:2a:1272:G:N3	32:2a:1273:G:H1'	2.29	0.48
38:2g:47:CYS:HA	38:2g:50:ILE:HG22	1.96	0.48
1:1A:324:A:N6	1:1A:338:G:O2'	2.47	0.47
1:1A:540:C:H2'	1:1A:541:C:C6	2.49	0.47
1:1A:1717:G:H2'	1:1A:1718:G:H8	1.79	0.47
1:1A:2137:C:H2'	1:1A:2138:C:C6	2.49	0.47
1:1A:2409:G:O2'	61:1A:6964:HOH:O	2.20	0.47
32:1a:319:G:H2'	32:1a:320:C:O4'	2.14	0.47
32:1a:736:C:H2'	32:1a:737:A:C8	2.49	0.47
45:1n:48:ALA:HB2	45:1n:53:LEU:HD12	1.95	0.47
50:1s:63:THR:OG1	50:1s:65:ASN:OD1	2.30	0.47
55:1x:13:C:H2'	55:1x:14:A:H5"	1.95	0.47
1:2A:947:G:H2'	1:2A:948:G:C8	2.49	0.47
1:2A:1973:G:OP2	61:2A:4871:HOH:O	2.19	0.47
1:2A:2062:A:H2'	1:2A:2062:A:N3	2.29	0.47
1:2A:2127:G:N3	1:2A:2161:C:N3	2.61	0.47
1:2A:2345:G:H1'	1:2A:2382:G:H5'	1.96	0.47
1:2A:2364:C:H2'	1:2A:2365:G:O4'	2.14	0.47
22:20:27:GLU:HG3	22:20:68:GLU:HA	1.96	0.47
28:26:9:LEU:HD13	28:26:51:GLU:HB2	1.95	0.47
32:2a:46:G:O2'	32:2a:365:U:H1'	2.14	0.47
32:2a:336:C:H2'	32:2a:337:C:C6	2.49	0.47
32:2a:434:U:H2'	32:2a:435:C:C6	2.48	0.47
33:2b:162:ILE:O	33:2b:185:ILE:HG12	2.14	0.47
1:1A:1057:A:N6	1:1A:1087:G:OP2	2.47	0.47
1:1A:1420:U:O2'	1:1A:1421:G:H8	1.97	0.47
1:1A:2228:G:OP1	3:1D:263:ARG:NH2	2.42	0.47
1:1A:2595:G:N2	1:1A:2598:A:OP2	2.45	0.47
19:1X:94:GLY:H	19:1X:95:LEU:HB2	1.79	0.47
32:1a:558:G:OP1	61:1a:2088:HOH:O	2.20	0.47
32:1a:741:G:H2'	32:1a:742:G:O4'	2.15	0.47
32:1a:1035:A:N3	32:1a:1036:G:N2	2.62	0.47
32:1a:1103:C:H2'	32:1a:1104:G:O4'	2.14	0.47
32:1a:1367:C:H2'	32:1a:1368:G:O4'	2.14	0.47
41:1j:5:ARG:O	41:1j:99:LYS:N	2.46	0.47
1:2A:196:A:N3	1:2A:196:A:H2'	2.29	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:893:C:H2'	1:2A:894:C:C5	2.49	0.47
1:2A:1237:A:OP2	61:2A:5390:HOH:O	2.20	0.47
1:2A:2658:C:P	7:2H:160:LYS:HZ1	2.35	0.47
5:2F:28:ILE:HG12	5:2F:112:MET:HG2	1.95	0.47
8:2I:5:LEU:HD11	8:2I:19:VAL:HG22	1.96	0.47
32:2a:137:C:H2'	32:2a:138:G:H8	1.77	0.47
33:2b:60:ASP:O	33:2b:64:ARG:HG2	2.14	0.47
35:2d:19:LEU:HG	35:2d:67:ILE:HG12	1.96	0.47
35:2d:57:ARG:NH2	36:2e:107:ARG:HD3	2.29	0.47
42:2k:48:ILE:C	42:2k:50:TYR:H	2.22	0.47
51:2t:10:LEU:HB3	51:2t:12:ALA:H	1.78	0.47
1:1A:747:U:H1'	18:1W:92:ARG:HH12	1.79	0.47
1:1A:1028:A:N6	1:1A:1125:G:H2'	2.29	0.47
1:1A:1062:G:P	1:1A:1070:A:H1'	2.54	0.47
1:1A:1372:U:H2'	1:1A:1373:A:O4'	2.14	0.47
1:1A:2532:G:O2'	1:1A:2657:A:N1	2.45	0.47
23:11:8:SER:HB3	23:11:66:HIS:CD2	2.49	0.47
32:1a:193:C:H2'	32:1a:194:C:C6	2.49	0.47
32:1a:789:U:O2'	32:1a:791:G:N7	2.40	0.47
32:1a:814:A:H2'	32:1a:816:A:H5"	1.97	0.47
32:1a:1038:C:O2'	32:1a:1039:C:H5'	2.13	0.47
32:1a:1497:G:N7	61:1a:2420:HOH:O	2.35	0.47
34:1c:22:TRP:CZ2	45:1n:54:PRO:HG2	2.50	0.47
37:1f:67:MET:HE1	37:1f:75:LEU:HD22	1.96	0.47
55:1x:75:C:H5"	55:1x:76:A:OP2	2.14	0.47
1:2A:93:G:H2'	1:2A:94:C:C6	2.49	0.47
1:2A:383:U:H2'	1:2A:385:C:H5	1.80	0.47
1:2A:629:G:H1'	1:2A:639:U:O2'	2.14	0.47
1:2A:827:U:O2'	1:2A:2068:U:C2	2.66	0.47
1:2A:1509(B):A:H2'	1:2A:1510:G:H8	1.79	0.47
1:2A:2822:G:O2'	1:2A:2824:C:OP2	2.23	0.47
12:2Q:81:VAL:HB	22:20:7:LEU:HD21	1.96	0.47
17:2V:43:GLU:OE1	17:2V:43:GLU:N	2.31	0.47
28:26:9:LEU:HA	28:26:54:ILE:HB	1.95	0.47
31:29:16:VAL:HG22	31:29:25:VAL:HG22	1.96	0.47
32:2a:974:A:O4'	45:2n:31:ARG:HD3	2.14	0.47
32:2a:1353:G:OP1	52:2u:10:ARG:NH1	2.46	0.47
33:2b:178:ARG:NH2	39:2h:74:PRO:HB3	2.29	0.47
34:2c:177:THR:HG22	34:2c:180:ALA:H	1.79	0.47
39:2h:25:ASP:OD2	39:2h:60:ARG:NH2	2.46	0.47
43:2l:84:LEU:HB2	43:2l:105:TYR:CE2	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2250:G:O2'	1:1A:2496:C:OP1	2.29	0.47
11:1P:82:GLY:HA2	11:1P:113:LYS:O	2.15	0.47
22:10:26:TYR:H	22:10:29:GLN:NE2	2.11	0.47
32:1a:78:G:C6	32:1a:91:C:N4	2.81	0.47
32:1a:1106:G:H2'	32:1a:1107:C:C6	2.49	0.47
45:1n:21:TYR:OH	45:1n:23:ARG:NH2	2.45	0.47
54:1w:4:C:H2'	54:1w:5:G:H8	1.78	0.47
1:2A:218:A:C2	1:2A:235:U:H4'	2.49	0.47
1:2A:479:A:N3	1:2A:481:G:H5"	2.29	0.47
1:2A:778:G:H5"	3:2D:48:ARG:HD2	1.96	0.47
1:2A:2680:C:H5'	4:2E:189:PRO:HA	1.96	0.47
2:2B:95:C:H2'	2:2B:96:U:C6	2.49	0.47
32:2a:1172:C:N4	32:2a:1173:G:O6	2.48	0.47
32:2a:1191:A:OP2	34:2c:3:ASN:ND2	2.48	0.47
35:2d:172:PRO:HD2	35:2d:173:TRP:CZ3	2.50	0.47
41:2j:9:ARG:NE	41:2j:69:ASN:OD1	2.46	0.47
50:2s:40:ILE:HB	50:2s:67:VAL:O	2.15	0.47
54:2w:7:A:N1	54:2w:66:U:O4	2.48	0.47
1:1A:2134:A:H4'	1:1A:2135:A:OP1	2.15	0.47
13:1R:59:ASP:OD1	13:1R:59:ASP:N	2.47	0.47
32:1a:266:G:O3'	48:1q:67:LYS:HB2	2.14	0.47
32:1a:625:G:H4'	47:1p:16:HIS:CD2	2.50	0.47
55:1x:8:4SU:O2	55:1x:21:A:H2	1.97	0.47
1:2A:866:A:H2	1:2A:867:C:C4	2.31	0.47
1:2A:1496:A:N3	1:2A:1577:C:O2'	2.46	0.47
1:2A:2498:C:H3'	61:2A:5660:HOH:O	2.14	0.47
7:2H:154:PRO:HB3	7:2H:163:TYR:CE1	2.50	0.47
8:2I:65:ALA:O	8:2I:69:LYS:N	2.45	0.47
9:2N:67:LEU:HA	9:2N:87:LEU:HD22	1.95	0.47
35:2d:64:LEU:HB2	35:2d:198:VAL:HG11	1.95	0.47
1:1A:1014:U:OP2	61:1A:6533:HOH:O	2.20	0.47
26:14:24:THR:OG1	26:14:25:TYR:N	2.48	0.47
32:1a:191:G:N2	51:1t:102:GLY:O	2.43	0.47
32:1a:234:C:H2'	32:1a:235:C:C6	2.50	0.47
33:1b:142:LEU:HA	33:1b:145:LEU:HD12	1.95	0.47
39:1h:91:ARG:HD3	48:1q:32:TYR:O	2.14	0.47
1:2A:322:A:OP1	5:2F:168:ARG:HD2	2.14	0.47
1:2A:526:A:N3	1:2A:2044:C:H1'	2.30	0.47
1:2A:1161:C:H2'	1:2A:1162:G:H8	1.78	0.47
2:2B:24:G:N3	2:2B:26:A:N6	2.62	0.47
21:2Z:48:PHE:CE1	21:2Z:52:SER:HA	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:2w:43:C:H2'	54:2w:44:G:C8	2.49	0.47
54:2y:10:G:H1	54:2y:25:C:H42	1.62	0.47
1:1A:34:C:H5"	1:1A:35:G:OP2	2.15	0.47
1:1A:247:G:H4'	1:1A:386:G:C5	2.49	0.47
1:1A:643:A:N1	1:1A:2369:A:O2'	2.43	0.47
1:1A:853:G:C2'	1:1A:854:G:H5'	2.44	0.47
1:1A:1075:C:H42	1:1A:1077:A:H62	1.62	0.47
1:1A:1190:G:OP1	11:1P:30:THR:OG1	2.28	0.47
1:1A:1641:A:H2'	1:1A:1642:G:O4'	2.15	0.47
1:1A:1712:C:H2'	1:1A:1713:U:O4'	2.15	0.47
1:1A:1803:A:O2'	3:1D:259:THR:HG21	2.14	0.47
1:1A:2126:A:N3	1:1A:2127:G:H1'	2.30	0.47
1:1A:2127:G:H1	1:1A:2161:C:N4	2.11	0.47
1:1A:2533:A:H2'	1:1A:2534:A:O4'	2.15	0.47
1:1A:2803:C:H2'	1:1A:2804:C:C6	2.49	0.47
32:1a:34:C:H2'	32:1a:35:G:C8	2.50	0.47
32:1a:40:C:H2'	32:1a:41:G:H8	1.78	0.47
32:1a:539:A:H2'	32:1a:540:G:C8	2.49	0.47
32:1a:1129:C:O2'	32:1a:1139:G:N7	2.39	0.47
38:1g:77:SER:HA	38:1g:85:TYR:O	2.15	0.47
50:1s:80:TYR:CZ	50:1s:82:GLY:HA2	2.49	0.47
51:1t:9:ASN:O	51:1t:10:LEU:HB2	2.14	0.47
51:1t:47:GLY:N	51:1t:48:LYS:HB2	2.30	0.47
1:2A:484:C:H2'	1:2A:485:C:H6	1.80	0.47
1:2A:848:G:H2'	1:2A:849:A:C8	2.49	0.47
1:2A:2127:G:N2	1:2A:2161:C:N1	2.63	0.47
1:2A:2291:U:H2'	1:2A:2292:C:C6	2.50	0.47
2:2B:91:C:OP1	12:2Q:16:ARG:HG3	2.14	0.47
6:2G:17:PRO:HA	6:2G:20:ILE:HD12	1.97	0.47
7:2H:127:GLU:OE1	7:2H:130:ARG:NE	2.46	0.47
7:2H:154:PRO:HB3	7:2H:163:TYR:CZ	2.49	0.47
9:2N:121:LYS:HD3	9:2N:130:HIS:CE1	2.50	0.47
13:2R:44:LEU:HD23	13:2R:44:LEU:HA	1.81	0.47
15:2T:1:MET:HE2	15:2T:3:ARG:HG2	1.97	0.47
19:2X:94:GLY:N	19:2X:95:LEU:HA	2.30	0.47
20:2Y:35:TYR:CE2	20:2Y:69:ALA:HB3	2.50	0.47
32:2a:76:C:H42	32:2a:93:G:H1	1.62	0.47
32:2a:909:A:N3	32:2a:1413:A:O2'	2.37	0.47
32:2a:942:G:H21	40:2i:124:GLN:NE2	2.12	0.47
32:2a:983:A:O2'	32:2a:1050:G:OP2	2.28	0.47
32:2a:1368:G:H5'	40:2i:112:LYS:HB3	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1376:U:H2'	32:2a:1377:A:H8	1.78	0.47
32:2a:1423:G:H2'	32:2a:1424:C:C6	2.49	0.47
32:2a:1479:C:H2'	32:2a:1480:G:C8	2.49	0.47
34:2c:58:GLU:O	34:2c:65:ALA:N	2.46	0.47
34:2c:77:ILE:HG13	34:2c:78:GLY:N	2.30	0.47
34:2c:117:ALA:HB2	34:2c:200:ALA:HB2	1.97	0.47
34:2c:142:MET:HG3	34:2c:170:GLN:HB3	1.95	0.47
38:2g:65:ALA:HB1	38:2g:127:ALA:HB3	1.96	0.47
40:2i:8:GLY:HA3	40:2i:76:ALA:O	2.14	0.47
42:2k:81:ASP:OD1	42:2k:107:SER:OG	2.30	0.47
48:2q:45:HIS:CD2	48:2q:47:PRO:HD3	2.50	0.47
48:2q:67:LYS:HA	48:2q:70:ARG:HH12	1.79	0.47
50:2s:64:GLU:CD	50:2s:64:GLU:H	2.22	0.47
50:2s:66:MET:HB2	50:2s:74:PHE:CZ	2.49	0.47
1:1A:56:A:H2'	1:1A:57:C:O4'	2.15	0.47
1:1A:614(C):A:C4	5:1F:180:GLY:HA2	2.50	0.47
1:1A:684:G:OP1	29:17:16:HIS:ND1	2.45	0.47
1:1A:1364:G:P	23:11:3:LYS:HG3	2.55	0.47
1:1A:1936:A:OP1	1:1A:1937:A:H5'	2.15	0.47
1:1A:2052:G:O2'	61:1A:4204:HOH:O	2.16	0.47
1:1A:2134:A:O2'	1:1A:2135:A:O5'	2.31	0.47
1:1A:2693:A:H2'	1:1A:2694:G:C8	2.50	0.47
3:1D:211:ARG:HG3	3:1D:214:TRP:CE3	2.50	0.47
5:1F:156:LEU:HD21	5:1F:163:VAL:HG12	1.97	0.47
32:1a:381:C:H2'	32:1a:382:A:O4'	2.14	0.47
32:1a:1035:A:C4	32:1a:1036:G:N2	2.82	0.47
49:1r:38:GLU:HA	49:1r:41:LYS:HE2	1.97	0.47
1:2A:888:C:H2'	1:2A:889:C:C4	2.50	0.47
1:2A:1932:A:H2'	1:2A:1933:G:O4'	2.15	0.47
6:2G:124:SER:HB2	6:2G:131:TYR:CE1	2.50	0.47
10:2O:68:GLU:OE1	10:2O:78:ARG:NH1	2.47	0.47
14:2S:7:TYR:CZ	14:2S:91:PRO:HG3	2.50	0.47
32:2a:417:C:H2'	32:2a:418:C:H6	1.80	0.47
32:2a:629:G:H2'	32:2a:630:G:O4'	2.14	0.47
32:2a:750:G:N3	46:2o:23:GLY:HA3	2.29	0.47
32:2a:977:A:N6	32:2a:1224:G:O5'	2.48	0.47
32:2a:1318:A:OP1	50:2s:3:ARG:NH1	2.29	0.47
34:2c:150:LYS:HG3	34:2c:169:ALA:HB2	1.96	0.47
40:2i:127:LYS:O	40:2i:128:ARG:HG2	2.15	0.47
1:1A:579:G:H2'	1:1A:580:C:C6	2.50	0.47
1:1A:1252:G:O4'	16:1U:33:ARG:HD2	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1Y:13:VAL:HB	20:1Y:72:VAL:HG22	1.96	0.47
24:12:32:LEU:HD11	24:12:54:LYS:HG2	1.97	0.47
25:13:10:LYS:HB3	25:13:53:LEU:HA	1.97	0.47
32:1a:35:G:O2'	43:1l:118:SER:O	2.29	0.47
32:1a:51:A:N7	32:1a:114:U:O2'	2.42	0.47
33:1b:17:PHE:HB3	33:1b:44:LEU:HD11	1.97	0.47
34:1c:124:ILE:HG22	34:1c:130:VAL:HG22	1.95	0.47
39:1h:81:HIS:HB2	39:1h:138:TRP:CD1	2.50	0.47
1:2A:839:U:H2'	1:2A:840:C:C6	2.50	0.47
1:2A:903:C:H2'	1:2A:904:C:C6	2.49	0.47
1:2A:2723:C:OP1	13:2R:3:HIS:ND1	2.38	0.47
1:2A:2751:G:H5'	7:2H:2:SER:HA	1.96	0.47
2:2B:24:G:N7	2:2B:56:G:H2'	2.29	0.47
7:2H:86:GLU:OE2	7:2H:132:ARG:NH2	2.47	0.47
8:2I:93:THR:HG22	8:2I:119:PRO:HB3	1.95	0.47
32:2a:646:U:H2'	32:2a:647:C:H6	1.79	0.47
32:2a:1370:G:C8	40:2i:109:VAL:HG11	2.50	0.47
39:2h:30:ARG:O	39:2h:34:GLU:HG2	2.15	0.47
41:2j:8:LEU:HB2	41:2j:70:ARG:HB2	1.97	0.47
1:1A:586:A:N1	1:1A:809:G:O2'	2.44	0.47
1:1A:625:G:O6	11:1P:107:LYS:NZ	2.44	0.47
1:1A:918:A:H5"	2:1B:98:G:O2'	2.15	0.47
1:1A:1091:G:C6	1:1A:1101:U:C2	3.03	0.47
1:1A:1432:C:H2'	1:1A:1433:U:O4'	2.15	0.47
1:1A:2108:C:H2'	1:1A:2109:U:C6	2.50	0.47
6:1G:56:ALA:O	6:1G:59:GLU:HG2	2.15	0.47
22:10:38:VAL:HB	22:10:59:LEU:HB2	1.96	0.47
32:1a:895:G:H2'	32:1a:896:C:C6	2.50	0.47
32:1a:1343:G:H1'	40:1i:121:ARG:NH1	2.29	0.47
36:1e:11:ILE:HG23	36:1e:105:VAL:HG22	1.97	0.47
36:1e:78:HIS:CE1	36:1e:142:LEU:HA	2.50	0.47
42:1k:18:ARG:HB2	42:1k:33:THR:OG1	2.15	0.47
44:1m:3:ARG:HH21	44:1m:9:ILE:HG13	1.80	0.47
1:2A:658:C:H2'	1:2A:659:C:C6	2.50	0.47
1:2A:1246:A:OP1	5:2F:38:ARG:NH2	2.39	0.47
1:2A:1509(B):A:H2'	1:2A:1510:G:C8	2.50	0.47
1:2A:2483:C:N3	12:2Q:124:LYS:HE3	2.30	0.47
1:2A:2705:A:O2'	1:2A:2852:G:OP1	2.20	0.47
7:2H:64:LEU:O	7:2H:68:THR:OG1	2.24	0.47
7:2H:137:ASP:HB3	7:2H:140:LYS:HB3	1.97	0.47
17:2V:62:LEU:HD21	17:2V:95:LEU:HB2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:70:G:H1	32:2a:99:U:H3	1.62	0.47
32:2a:1301:U:O2'	32:2a:1302:U:H5'	2.15	0.47
40:2i:42:ARG:HE	40:2i:42:ARG:HB3	1.42	0.47
53:2v:22:U:H2'	53:2v:23:A:H8	1.80	0.47
55:2x:14:A:N6	55:2x:21:A:H2	2.11	0.47
1:1A:264:C:O2'	1:1A:265:A:H2'	2.15	0.46
1:1A:1092:C:H2'	1:1A:1093:G:O4'	2.15	0.46
1:1A:1266:G:O2'	1:1A:2012:G:O6	2.26	0.46
16:1U:76:TYR:CZ	16:1U:80:ILE:HG13	2.50	0.46
17:1V:14:VAL:HB	17:1V:96:ILE:HG13	1.96	0.46
21:1Z:98:MET:O	21:1Z:125:LEU:HD12	2.15	0.46
32:1a:977:A:H1'	32:1a:982:U:O4	2.15	0.46
32:1a:1499:A:H3'	61:1a:2345:HOH:O	2.13	0.46
33:1b:93:VAL:HG21	33:1b:97:TRP:CD1	2.50	0.46
35:1d:31:CYS:SG	60:1d:302:SF4:S2	3.14	0.46
55:1x:8:4SU:O5'	55:1x:8:4SU:H6	2.16	0.46
1:2A:597:U:H2'	1:2A:598:G:C8	2.51	0.46
1:2A:968:G:H2'	1:2A:969:U:C6	2.49	0.46
1:2A:979:G:H5"	1:2A:980:A:C5'	2.46	0.46
6:2G:122:PRO:HG3	6:2G:182:LYS:H	1.80	0.46
7:2H:156:ALA:O	7:2H:172:LYS:HG2	2.15	0.46
22:20:53:MET:HG2	22:20:57:PHE:HA	1.95	0.46
29:27:34:ARG:NH2	29:27:39:ARG:HG2	2.30	0.46
32:2a:359:U:H2'	32:2a:360:A:H8	1.78	0.46
32:2a:429:U:H3'	35:2d:9:CYS:SG	2.54	0.46
32:2a:564:C:C4	48:2q:31:LEU:HD11	2.49	0.46
32:2a:1003:G:H2'	32:2a:1004:A:O4'	2.15	0.46
32:2a:1011:G:N2	32:2a:1018:C:C2	2.80	0.46
35:2d:175:SER:HB3	35:2d:184:LYS:HB3	1.97	0.46
38:2g:32:ARG:HH21	38:2g:109:ASN:ND2	2.13	0.46
41:2j:46:ARG:HG2	41:2j:64:GLU:HB3	1.97	0.46
43:2l:113:ARG:HD2	43:2l:114:LYS:H	1.80	0.46
51:2t:42:GLN:HE21	51:2t:46:GLU:HG3	1.80	0.46
1:1A:2066:C:H5"	61:1A:5237:HOH:O	2.15	0.46
1:1A:2252:G:N7	22:10:4:LYS:NZ	2.63	0.46
5:1F:33:LEU:HD13	5:1F:112:MET:HE3	1.96	0.46
16:1U:55:ARG:O	16:1U:59:ARG:HG3	2.15	0.46
32:1a:1118:C:H2'	32:1a:1119:C:C6	2.50	0.46
1:2A:1351:C:O3'	1:2A:1571:A:O2'	2.33	0.46
1:2A:1711:C:H2'	1:2A:1712:C:H6	1.80	0.46
32:2a:598:U:H4'	39:2h:94:TYR:CG	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:2c:22:TRP:CG	34:2c:59:ARG:HG3	2.50	0.46
39:2h:6:ILE:O	39:2h:10:LEU:HG	2.15	0.46
40:2i:6:GLY:HA3	40:2i:80:GLY:O	2.15	0.46
1:1A:784:A:O4'	3:1D:227:ASN:ND2	2.48	0.46
1:1A:1052:C:H2'	1:1A:1053:C:C6	2.50	0.46
1:1A:1792:G:O2'	1:1A:1830:C:OP1	2.32	0.46
1:1A:2687:U:H2'	1:1A:2688:U:O4'	2.16	0.46
1:1A:2785:C:OP1	4:1E:41:LYS:NZ	2.46	0.46
6:1G:18:GLU:HG3	6:1G:22:ARG:HD2	1.96	0.46
28:16:19:ARG:HD3	61:16:201:HOH:O	2.14	0.46
32:1a:921:U:O2	36:1e:19:MET:HB2	2.14	0.46
37:1f:100:ASN:HB2	49:1r:28:GLU:HA	1.97	0.46
41:1j:40:LEU:HB2	41:1j:69:ASN:HB2	1.97	0.46
46:1o:60:VAL:O	46:1o:64:ARG:HB2	2.15	0.46
1:2A:921:G:H4'	1:2A:2269:A:C5	2.49	0.46
1:2A:1275:A:N1	1:2A:1295:C:O2'	2.45	0.46
1:2A:1358:G:O2'	1:2A:1373:A:N6	2.45	0.46
1:2A:1578:U:C2'	1:2A:1579:A:H5'	2.46	0.46
1:2A:2061:G:H5"	1:2A:2503:2MA:C2	2.45	0.46
1:2A:2314:C:H2'	1:2A:2315:G:C8	2.50	0.46
4:2E:76:ARG:HB2	4:2E:77:ILE:HD12	1.97	0.46
5:2F:11:VAL:HG22	5:2F:125:LEU:HB2	1.97	0.46
6:2G:114:ILE:HB	6:2G:117:PHE:HD1	1.80	0.46
15:2T:94:ALA:HB1	15:2T:99:LEU:HD21	1.96	0.46
32:2a:108:G:N1	51:2t:15:ARG:HG2	2.31	0.46
32:2a:547:A:H4'	32:2a:548:G:O5'	2.14	0.46
32:2a:1129:C:H5'	32:2a:1130:A:OP1	2.15	0.46
35:2d:11:LEU:HG	35:2d:66:ARG:HD3	1.97	0.46
35:2d:38:TYR:OH	35:2d:45:GLN:NE2	2.48	0.46
36:2e:9:LYS:HD2	36:2e:9:LYS:HA	1.63	0.46
54:2w:12:U:H3'	54:2w:13:C:C5'	2.44	0.46
3:1D:69:ARG:HE	3:1D:130:ALA:HB2	1.81	0.46
6:1G:101:ILE:O	6:1G:105:LYS:NZ	2.49	0.46
11:1P:97:PRO:HD3	11:1P:126:VAL:O	2.15	0.46
26:14:58:ARG:N	26:14:58:ARG:HD2	2.29	0.46
32:1a:108:G:H1	51:1t:15:ARG:HG2	1.81	0.46
32:1a:1305:G:H22	32:1a:1331:G:H1'	1.79	0.46
34:1c:71:ALA:HB2	34:1c:115:LEU:HD21	1.98	0.46
41:1j:11:PHE:HE1	41:1j:67:THR:HG22	1.79	0.46
1:2A:289:A:H2'	1:2A:290:G:O4'	2.16	0.46
1:2A:900:A:HO2'	1:2A:901:A:P	2.37	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1264:G:H2'	1:2A:2014:A:N6	2.31	0.46
1:2A:1608:A:H1'	1:2A:1610:A:OP2	2.16	0.46
1:2A:2061:G:O6	57:2A:3888:CLM:H3	2.14	0.46
1:2A:2238:G:H2'	1:2A:2238:G:N3	2.29	0.46
1:2A:2398:U:H2'	1:2A:2399:G:H8	1.80	0.46
2:2B:75:G:H22	21:2Z:73:GLN:NE2	2.13	0.46
4:2E:174:ASP:OD1	4:2E:175:VAL:N	2.47	0.46
5:2F:102:PRO:HB2	5:2F:105:VAL:HG23	1.98	0.46
14:2S:35:ILE:HG23	14:2S:69:VAL:HG11	1.97	0.46
15:2T:60:THR:HG22	15:2T:77:PRO:HA	1.96	0.46
32:2a:1201:A:H4'	32:2a:1202:G:O5'	2.15	0.46
32:2a:1371:G:O3'	40:2i:69:GLY:HA3	2.15	0.46
33:2b:24:TRP:CD1	33:2b:24:TRP:H	2.34	0.46
36:2e:65:ASN:HD21	36:2e:140:ARG:NH2	2.13	0.46
1:1A:747:U:O2	1:1A:2014:A:H1'	2.16	0.46
1:1A:841:A:H2'	1:1A:842:G:C8	2.50	0.46
1:1A:1818:U:H2'	3:1D:157:ARG:HG3	1.98	0.46
1:1A:2090:G:N2	23:11:45:ASN:OD1	2.32	0.46
1:1A:2564:A:C2	1:1A:2647:U:H4'	2.50	0.46
1:1A:2689:U:OP2	1:1A:2719:G:N2	2.33	0.46
6:1G:11:TYR:HA	6:1G:15:VAL:HB	1.97	0.46
32:1a:824:C:H2'	32:1a:825:G:C8	2.51	0.46
32:1a:1038:C:H2'	32:1a:1039:C:H6	1.81	0.46
33:1b:18:GLY:HA3	33:1b:42:ILE:HG13	1.97	0.46
40:1i:5:TYR:HH	40:1i:7:THR:HG1	1.62	0.46
50:1s:27:GLU:HG2	50:1s:28:LYS:HD2	1.97	0.46
50:1s:64:GLU:HA	50:1s:67:VAL:HG23	1.98	0.46
1:2A:1031:G:H5"	31:29:8:LYS:HE3	1.98	0.46
1:2A:1156:A:O4'	16:2U:51:LYS:NZ	2.49	0.46
2:2B:25:A:H2'	2:2B:26:A:C8	2.51	0.46
2:2B:32:C:H42	2:2B:50:G:H1	1.61	0.46
3:2D:18:VAL:HG12	3:2D:211:ARG:HH12	1.80	0.46
3:2D:85:ASP:OD2	3:2D:88:ARG:NH1	2.42	0.46
4:2E:48:GLN:HE21	4:2E:78:LEU:HD23	1.78	0.46
9:2N:108:PRO:O	9:2N:113:GLY:HA3	2.15	0.46
16:2U:28:ARG:NH1	16:2U:38:THR:OG1	2.45	0.46
32:2a:34:C:H2'	32:2a:35:G:C8	2.51	0.46
32:2a:401:C:O2'	32:2a:621:A:N3	2.40	0.46
32:2a:1247:U:H1'	32:2a:1291:G:N2	2.30	0.46
32:2a:1250:A:OP1	40:2i:67:GLY:N	2.41	0.46
32:2a:1347:G:C8	40:2i:107:ARG:HB2	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:2c:24:ALA:HB3	34:2c:29:TYR:HD1	1.81	0.46
44:2m:65:LYS:O	44:2m:70:LEU:HD12	2.14	0.46
49:2r:47:THR:O	49:2r:47:THR:OG1	2.26	0.46
1:1A:97:C:OP1	24:12:2:LYS:HE2	2.16	0.46
1:1A:1035:U:H2'	1:1A:1036:G:C8	2.51	0.46
1:1A:1803:A:H4'	3:1D:259:THR:HG23	1.97	0.46
1:1A:1939:5MU:OP1	1:1A:2604:U:O2'	2.34	0.46
1:1A:2771:C:H2'	1:1A:2772:C:C6	2.50	0.46
11:1P:138:LEU:HD23	11:1P:145:PRO:HB3	1.98	0.46
16:1U:17:ILE:HG23	16:1U:39:LEU:HD12	1.98	0.46
20:1Y:13:VAL:HG12	20:1Y:74:PRO:HA	1.97	0.46
32:1a:542:G:H5'	35:1d:41:GLY:HA3	1.96	0.46
32:1a:1273:G:H3'	32:1a:1274:G:H8	1.80	0.46
38:1g:74:GLU:O	38:1g:88:PRO:HA	2.15	0.46
43:1l:7:ILE:HD13	43:1l:10:LEU:HD12	1.97	0.46
1:2A:191:A:H2'	1:2A:192:C:C6	2.50	0.46
1:2A:884:C:H3'	1:2A:885:C:C6	2.50	0.46
1:2A:1005:C:H2'	1:2A:1006:C:C6	2.51	0.46
1:2A:1818:U:H2'	3:2D:157:ARG:HG3	1.97	0.46
1:2A:2137:C:O2'	1:2A:2138:C:OP2	2.31	0.46
3:2D:134:ARG:HD2	3:2D:135:PHE:CZ	2.50	0.46
4:2E:1:MET:O	4:2E:84:PHE:HB2	2.15	0.46
12:2Q:36:ALA:HB2	12:2Q:103:MET:SD	2.56	0.46
32:2a:403:C:O2'	35:2d:122:ARG:NH2	2.48	0.46
32:2a:984:C:H2'	32:2a:985:C:C6	2.50	0.46
55:2x:21:A:H62	55:2x:46:G:C2'	2.29	0.46
1:1A:119:A:H4'	1:1A:120:U:OP1	2.15	0.46
1:1A:286:C:H2'	1:1A:287:C:H6	1.81	0.46
1:1A:784:A:N6	3:1D:229:VAL:HG11	2.31	0.46
1:1A:2086:U:H2'	1:1A:2087:G:C8	2.50	0.46
1:1A:2291:U:H2'	1:1A:2292:C:C6	2.51	0.46
1:1A:2507:C:H4'	54:1w:75:C:O2'	2.16	0.46
1:1A:2508:G:H5'	54:1w:74:C:H42	1.79	0.46
3:1D:8:PRO:HB3	3:1D:14:ARG:HG2	1.97	0.46
5:1F:178:PRO:HB2	5:1F:201:VAL:CG2	2.46	0.46
7:1H:154:PRO:HB3	7:1H:163:TYR:CZ	2.51	0.46
28:16:9:LEU:HD13	28:16:51:GLU:HB2	1.98	0.46
32:1a:44:G:C2	32:1a:45:U:H1'	2.51	0.46
32:1a:392:G:OP1	47:1p:8:ARG:NH2	2.49	0.46
32:1a:555:C:H2'	32:1a:556:C:C6	2.50	0.46
32:1a:1127:G:H5'	32:1a:1280:A:O2'	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1233:G:H2'	32:1a:1234:C:C6	2.50	0.46
33:1b:112:VAL:O	33:1b:116:GLU:N	2.31	0.46
34:1c:180:ALA:HA	34:1c:206:GLU:HA	1.97	0.46
47:1p:50:LYS:HD2	47:1p:50:LYS:HA	1.74	0.46
49:1r:31:LEU:HD13	49:1r:65:ILE:HB	1.96	0.46
54:1w:5:G:H2'	54:1w:6:G:H8	1.81	0.46
54:1y:61:C:H2'	54:1y:62:C:C6	2.51	0.46
1:2A:774:A:H2'	1:2A:774:A:N3	2.31	0.46
1:2A:848:G:C2	1:2A:933:A:H1'	2.50	0.46
1:2A:1796:U:H2'	1:2A:1797:C:H6	1.81	0.46
1:2A:2019:A:OP2	27:25:9:LYS:NZ	2.39	0.46
1:2A:2683:C:OP1	15:2T:53:ARG:NH2	2.47	0.46
7:2H:3:ARG:HH21	7:2H:54:ARG:NH1	2.14	0.46
32:2a:407:G:H2'	32:2a:408:A:C8	2.51	0.46
32:2a:765:G:N1	32:2a:812:C:O2'	2.36	0.46
32:2a:834:C:H2'	32:2a:835:U:C6	2.49	0.46
32:2a:1179:A:H2'	32:2a:1180:A:O4'	2.16	0.46
37:2f:23:LYS:NZ	37:2f:42:GLU:OE1	2.34	0.46
50:2s:27:GLU:HB2	50:2s:28:LYS:HA	1.98	0.46
1:1A:458:G:O2'	1:1A:469:G:O6	2.30	0.46
1:1A:1047:G:O2'	1:1A:1048:A:O5'	2.33	0.46
1:1A:1930:G:O2'	1:1A:1968:G:O6	2.28	0.46
1:1A:2142:C:O2	1:1A:2149:G:N1	2.40	0.46
1:1A:2497:A:O2'	61:1A:5717:HOH:O	2.16	0.46
5:1F:13:SER:OG	5:1F:16:GLY:O	2.30	0.46
14:1S:10:ARG:O	14:1S:14:VAL:HG13	2.16	0.46
15:1T:39:ARG:HH21	32:1a:345:C:H5"	1.81	0.46
21:1Z:6:LYS:HE3	21:1Z:8:TYR:OH	2.15	0.46
32:1a:96:U:H2'	32:1a:97:G:C8	2.51	0.46
32:1a:431:A:H2'	32:1a:432:A:O4'	2.15	0.46
32:1a:859:A:H2'	32:1a:860:A:O4'	2.16	0.46
32:1a:1314:C:H2'	32:1a:1315:U:C6	2.51	0.46
1:2A:248:G:C2	1:2A:2431:U:H4'	2.50	0.46
1:2A:320:A:H4'	1:2A:322:A:C8	2.51	0.46
1:2A:350:U:H2'	1:2A:351:G:O4'	2.16	0.46
1:2A:1803:A:H4'	3:2D:259:THR:HG23	1.97	0.46
1:2A:2394:C:P	30:28:30:ARG:HH21	2.39	0.46
2:2B:28:C:H2'	2:2B:29:A:O4'	2.15	0.46
2:2B:107:G:H2'	2:2B:108:U:H5"	1.98	0.46
5:2F:164:ARG:O	5:2F:168:ARG:HB2	2.16	0.46
21:2Z:101:PRO:HA	21:2Z:123:ASP:HA	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:26:40:CYS:O	28:26:44:ARG:N	2.49	0.46
32:2a:160:A:H61	32:2a:347:G:H1'	1.81	0.46
32:2a:811:C:O2'	32:2a:901:A:N1	2.47	0.46
32:2a:1183:A:O2'	32:2a:1185:G:OP2	2.34	0.46
32:2a:1481:U:H2'	32:2a:1482:G:C8	2.51	0.46
34:2c:50:ALA:HB1	34:2c:70:VAL:HG11	1.98	0.46
43:2l:53:ARG:HB3	43:2l:69:TYR:HE1	1.81	0.46
1:1A:335:C:H4'	20:1Y:73:ARG:HD2	1.98	0.46
32:1a:1239:A:H62	32:1a:1299:A:N6	2.14	0.46
34:1c:52:LEU:HA	34:1c:70:VAL:HG22	1.97	0.46
36:1e:106:PRO:O	36:1e:110:LEU:HG	2.15	0.46
1:2A:359:A:H3'	1:2A:360:G:H8	1.80	0.46
1:2A:613:G:O2'	1:2A:614(C):A:N1	2.43	0.46
1:2A:1195:G:N7	11:2P:15:ARG:NH2	2.61	0.46
1:2A:1592:C:H2'	1:2A:1593:G:C8	2.50	0.46
1:2A:1919:A:O3'	32:2a:1517:G:H1'	2.16	0.46
1:2A:2432:A:C8	23:21:33:LYS:HD2	2.51	0.46
32:2a:554:C:O2'	61:2a:3302:HOH:O	2.21	0.46
32:2a:1030:C:N4	32:2a:1031:G:N1	2.62	0.46
32:2a:1057:G:H2'	32:2a:1058:G:O4'	2.16	0.46
32:2a:1107:C:O2	32:2a:1191:A:O2'	2.34	0.46
49:2r:26:LEU:HD21	49:2r:42:ARG:HE	1.80	0.46
51:2t:87:LYS:O	51:2t:91:LEU:HG	2.15	0.46
1:1A:330:A:H8	1:1A:1210:A:C4	2.34	0.46
1:1A:897:C:H4'	54:1w:55:PSU:O3'	2.15	0.46
1:1A:2111:C:N3	1:1A:2145:C:O2'	2.48	0.46
1:1A:2319:G:H22	14:1S:3:ARG:NH1	2.14	0.46
1:1A:2751:G:H4'	7:1H:4:ILE:HD11	1.97	0.46
8:1I:12:LEU:HD23	8:1I:12:LEU:HA	1.73	0.46
14:1S:14:VAL:O	14:1S:18:ILE:HG12	2.16	0.46
21:1Z:1:MET:HA	21:1Z:2:GLU:HA	1.53	0.46
21:1Z:24:LEU:HB2	21:1Z:41:LEU:HD12	1.98	0.46
21:1Z:123:ASP:OD1	21:1Z:123:ASP:N	2.47	0.46
32:1a:339:C:H2'	32:1a:340:U:C6	2.51	0.46
32:1a:604:G:H2'	32:1a:605:U:C6	2.51	0.46
32:1a:1218:C:H2'	32:1a:1219:U:C6	2.51	0.46
32:1a:1302:U:C6	44:1m:17:VAL:HG11	2.50	0.46
33:1b:71:VAL:HA	33:1b:93:VAL:HG23	1.98	0.46
39:1h:51:VAL:HG12	39:1h:52:ASP:H	1.81	0.46
44:1m:17:VAL:O	44:1m:20:THR:OG1	2.29	0.46
47:1p:14:ASN:HA	47:1p:42:ARG:NH2	2.31	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:380:U:H2'	1:2A:381:G:H8	1.81	0.46
1:2A:646:A:H2'	1:2A:647:G:O4'	2.16	0.46
1:2A:1845:G:OP1	3:2D:258:LYS:NZ	2.45	0.46
8:2I:92:VAL:HG13	8:2I:120:ILE:HB	1.97	0.46
32:2a:201:C:H42	32:2a:216:G:H1	1.64	0.46
32:2a:1218:C:H2'	32:2a:1219:U:C6	2.51	0.46
32:2a:1244:C:H42	32:2a:1293:G:H1	1.63	0.46
33:2b:157:ARG:NH2	33:2b:160:ASP:OD1	2.49	0.46
34:2c:135:LYS:NZ	36:2e:52:PRO:HG2	2.31	0.46
38:2g:26:PHE:HB2	38:2g:101:LEU:HD22	1.97	0.46
41:2j:44:VAL:HG22	41:2j:66:ARG:HG2	1.98	0.46
55:2x:43:A:H2'	55:2x:44:A:C8	2.50	0.46
1:1A:1354:A:H2'	1:1A:1355:G:O4'	2.17	0.45
1:1A:2790:A:H3'	1:1A:2790:A:N3	2.31	0.45
5:1F:32:LEU:HB3	5:1F:112:MET:HE1	1.97	0.45
5:1F:89:VAL:HG12	5:1F:90:PHE:CD2	2.51	0.45
8:1I:79:ILE:HG22	8:1I:81:VAL:HG13	1.98	0.45
12:1Q:54:MET:HG2	12:1Q:117:ALA:HB1	1.98	0.45
18:1W:92:ARG:NH1	61:1W:302:HOH:O	2.38	0.45
32:1a:186:C:H2'	32:1a:187:C:H6	1.81	0.45
32:1a:189(K):U:H2'	32:1a:189(L):G:C8	2.51	0.45
32:1a:606:G:N2	32:1a:631:G:N7	2.64	0.45
32:1a:755:G:OP2	46:1o:65:ARG:HD3	2.16	0.45
32:1a:1323:G:H2'	32:1a:1324:A:C8	2.51	0.45
32:1a:1348:U:H4'	40:1i:120:ARG:HD2	1.98	0.45
33:1b:52:GLU:O	33:1b:56:ARG:NH1	2.49	0.45
34:1c:56:ASP:O	34:1c:66:VAL:HA	2.16	0.45
43:1l:60:LEU:HD11	43:1l:85:ILE:HD13	1.97	0.45
54:1y:15:G:N2	54:1y:48:C:H42	2.14	0.45
1:2A:143:G:H2'	1:2A:143(A):C:C6	2.51	0.45
1:2A:185:U:H4'	1:2A:218:A:H4'	1.97	0.45
1:2A:299:A:H5"	20:2Y:86:ARG:NH2	2.30	0.45
1:2A:458:G:O2'	29:27:39:ARG:HD2	2.16	0.45
1:2A:1025:G:C4	1:2A:1135:C:H1'	2.51	0.45
1:2A:1456:G:N7	61:2A:5365:HOH:O	2.36	0.45
1:2A:1790:C:H5"	1:2A:1791:A:OP1	2.15	0.45
1:2A:1814:G:H4'	3:2D:51:VAL:HG21	1.98	0.45
1:2A:1853:A:N1	1:2A:2087:G:H1'	2.31	0.45
1:2A:1910:G:H22	1:2A:1920:4OC:C2	2.28	0.45
1:2A:2001:A:H2'	1:2A:2002:G:C8	2.51	0.45
1:2A:2110:G:OP2	1:2A:2149:G:O2'	2.27	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2744:G:N2	7:2H:143:GLN:OE1	2.48	0.45
5:2F:109:GLY:HA2	5:2F:112:MET:HE3	1.98	0.45
16:2U:76:TYR:OH	16:2U:92:ARG:NE	2.39	0.45
32:2a:229:U:H5"	47:2p:33:ILE:HD13	1.98	0.45
32:2a:1390:U:H2'	32:2a:1391:U:C6	2.51	0.45
33:2b:101:MET:HA	33:2b:108:ILE:HG21	1.98	0.45
1:1A:27:G:N2	1:1A:512:G:H1'	2.31	0.45
1:1A:1876:A:H2'	1:1A:1877:A:C8	2.51	0.45
5:1F:25:PRO:HD2	5:1F:115:ALA:HB2	1.97	0.45
5:1F:192:LEU:HD13	5:1F:194:MET:HE2	1.96	0.45
29:17:12:ARG:HH21	29:17:44:PRO:HB3	1.81	0.45
32:1a:407:G:H5"	35:1d:115:ARG:CG	2.46	0.45
32:1a:667:G:H4'	46:1o:51:HIS:ND1	2.31	0.45
32:1a:1048:G:O6	32:1a:1210:C:N4	2.50	0.45
35:1d:170:VAL:HG22	35:1d:171:GLY:H	1.81	0.45
35:1d:175:SER:HB3	35:1d:184:LYS:HB3	1.98	0.45
1:2A:1316:U:H2'	1:2A:1317:A:H8	1.80	0.45
1:2A:1814:G:OP1	3:2D:40:THR:OG1	2.33	0.45
1:2A:2307:G:H8	1:2A:2307:G:OP1	1.99	0.45
1:2A:2786:U:H2'	1:2A:2787:C:C6	2.51	0.45
4:2E:9:VAL:HG22	4:2E:25:VAL:HB	1.98	0.45
9:2N:15:LEU:HD23	9:2N:137:LYS:HG3	1.99	0.45
32:2a:130:A:H1'	32:2a:263:A:O2'	2.17	0.45
32:2a:524:G:H2'	32:2a:525:C:C6	2.50	0.45
32:2a:627:G:H2'	32:2a:628:G:C8	2.51	0.45
32:2a:828:A:H2'	32:2a:829:G:O4'	2.16	0.45
32:2a:1121:U:C2'	32:2a:1122:U:H5'	2.47	0.45
32:2a:1312:G:H1	32:2a:1325:C:N4	2.10	0.45
33:2b:52:GLU:O	33:2b:56:ARG:NH1	2.49	0.45
36:2e:57:LYS:HG2	36:2e:61:TYR:CE2	2.51	0.45
38:2g:144:MET:HE2	38:2g:144:MET:HB3	1.79	0.45
1:1A:323:G:H1'	1:1A:1205:U:O2	2.16	0.45
1:1A:825:C:O2'	11:1P:55:ARG:HD3	2.16	0.45
3:1D:145:VAL:HG11	3:1D:175:LEU:HD11	1.98	0.45
32:1a:216:G:H2'	32:1a:217:C:C6	2.51	0.45
32:1a:279:A:C5	48:1q:98:LEU:HD23	2.52	0.45
32:1a:976:G:OP2	32:1a:1358:U:O2'	2.32	0.45
35:1d:81:GLU:CD	35:1d:139:ARG:HH22	2.24	0.45
39:1h:25:ASP:N	39:1h:25:ASP:OD1	2.50	0.45
45:1n:23:ARG:NH1	45:1n:30:ALA:HB2	2.30	0.45
1:2A:971:C:H2'	1:2A:972:G:O4'	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1288:U:O2'	1:2A:1647:G:N2	2.50	0.45
7:2H:107:VAL:HG11	7:2H:162:ILE:HD11	1.98	0.45
13:2R:87:TYR:HD1	13:2R:90:ARG:HD2	1.82	0.45
16:2U:66:ASN:HD21	16:2U:70:ARG:HH21	1.64	0.45
21:2Z:75:ASN:O	21:2Z:84:GLU:N	2.37	0.45
32:2a:558:G:OP1	61:2a:3416:HOH:O	2.20	0.45
32:2a:1226:C:H6	44:2m:103:THR:HB	1.81	0.45
32:2a:1272:G:C2	32:2a:1273:G:H1'	2.52	0.45
32:2a:1323:G:N2	32:2a:1361:G:O2'	2.45	0.45
34:2c:131:ARG:NH2	34:2c:135:LYS:HE3	2.31	0.45
49:2r:76:LEU:HD12	49:2r:76:LEU:HA	1.83	0.45
55:2x:16:C:H5'	55:2x:59:A:N1	2.31	0.45
1:1A:570:G:H2'	1:1A:2030:A:N7	2.32	0.45
1:1A:952:G:OP1	12:1Q:16:ARG:NH2	2.45	0.45
1:1A:1044:G:H5'	1:1A:1045:A:OP2	2.16	0.45
1:1A:2155:G:H3'	1:1A:2156:G:C8	2.50	0.45
5:1F:161:GLU:HG2	5:1F:164:ARG:NH2	2.30	0.45
7:1H:83:TYR:CE2	7:1H:138:LYS:HB2	2.52	0.45
18:1W:73:ALA:HB3	18:1W:106:ILE:HB	1.98	0.45
21:1Z:91:LEU:HD12	21:1Z:91:LEU:HA	1.75	0.45
26:14:61:ARG:HH12	50:1s:9:VAL:HG11	1.81	0.45
32:1a:435:C:H2'	32:1a:436:C:H6	1.81	0.45
32:1a:598:U:H2'	32:1a:599:C:C6	2.51	0.45
32:1a:1060:C:OP1	45:1n:45:ARG:NH2	2.42	0.45
33:1b:16:HIS:CD2	33:1b:204:ASN:H	2.34	0.45
33:1b:163:PHE:CD1	33:1b:185:ILE:HG13	2.51	0.45
34:1c:18:TRP:O	34:1c:54:ARG:NH2	2.49	0.45
40:1i:11:LYS:C	40:1i:13:ALA:H	2.24	0.45
1:2A:839:U:H1'	1:2A:1191:G:H1'	1.98	0.45
1:2A:879:G:H3'	1:2A:880:G:C8	2.52	0.45
1:2A:2495:G:H5"	12:2Q:82:ARG:HG2	1.98	0.45
1:2A:2702:U:H4'	1:2A:2703:C:OP1	2.17	0.45
1:2A:2705:A:H2'	1:2A:2706:G:O4'	2.17	0.45
3:2D:68:LYS:C	3:2D:70:TRP:H	2.24	0.45
10:2O:26:LYS:O	10:2O:30:ALA:HB2	2.16	0.45
13:2R:57:ARG:HH22	13:2R:61:HIS:CD2	2.35	0.45
13:2R:63:ARG:O	13:2R:67:LEU:HB2	2.17	0.45
14:2S:87:PHE:CZ	14:2S:102:ALA:HB2	2.51	0.45
26:24:62:ARG:HD3	26:24:62:ARG:HA	1.72	0.45
28:26:15:GLU:OE1	28:26:45:LYS:NZ	2.50	0.45
30:28:14:VAL:HG22	30:28:24:ALA:HB2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:129(A):G:C6	32:2a:189(E):U:H4'	2.51	0.45
32:2a:986:A:H2'	32:2a:987:G:O4'	2.17	0.45
32:2a:1122:U:H3	32:2a:1151:A:H61	1.63	0.45
32:2a:1242:C:H2'	32:2a:1243:C:O4'	2.16	0.45
32:2a:1372:U:H2'	32:2a:1373:G:O4'	2.15	0.45
32:2a:1509:C:H2'	32:2a:1510:U:O4'	2.16	0.45
34:2c:119:ARG:HE	34:2c:140:ARG:CZ	2.30	0.45
42:2k:79:SER:HA	42:2k:104:GLN:HB3	1.98	0.45
45:2n:45:ARG:O	45:2n:49:HIS:HD2	2.00	0.45
55:2x:15:G:H2'	55:2x:59:A:N1	2.31	0.45
1:1A:363(A):A:H2'	1:1A:363(B):G:C8	2.51	0.45
1:1A:2649:U:H2'	1:1A:2650:U:C6	2.52	0.45
1:1A:2693:A:H2'	1:1A:2694:G:H8	1.81	0.45
8:1I:93:THR:H	8:1I:96:ASP:HB2	1.81	0.45
13:1R:22:ARG:HG2	13:1R:69:ASP:HB3	1.97	0.45
32:1a:202:U:H3'	32:1a:203:U:C5	2.52	0.45
32:1a:401:C:OP2	35:1d:73:ARG:NH2	2.49	0.45
32:1a:1289:A:N1	32:1a:1371:G:O2'	2.48	0.45
38:1g:57:GLU:O	38:1g:61:VAL:HG23	2.16	0.45
54:1w:2:C:N4	54:1w:71:G:H1	2.15	0.45
54:1y:19:G:N1	54:1y:56:C:N4	2.62	0.45
1:2A:892:G:H3'	1:2A:893:C:H5"	1.99	0.45
1:2A:2638:G:P	4:2E:82:ARG:HH12	2.39	0.45
3:2D:142:VAL:HG23	3:2D:193:VAL:HA	1.98	0.45
6:2G:129:GLY:O	6:2G:161:THR:OG1	2.29	0.45
31:29:7:VAL:HG12	31:29:34:GLN:HB3	1.99	0.45
32:2a:685:G:C2	32:2a:686:U:C4	3.05	0.45
32:2a:1075:C:OP1	33:2b:179:LYS:NZ	2.44	0.45
32:2a:1128:C:O2'	32:2a:1129:C:OP1	2.35	0.45
32:2a:1176:A:H2'	32:2a:1177:G:H8	1.82	0.45
32:2a:1288:A:H1'	32:2a:1353:G:H4'	1.99	0.45
37:2f:72:VAL:HG23	37:2f:90:VAL:HG11	1.99	0.45
1:1A:222:A:H5"	1:1A:421:U:OP1	2.15	0.45
1:1A:1174:A:H4'	1:1A:1175:U:OP1	2.16	0.45
1:1A:2864:G:OP1	15:1T:119:LYS:HD2	2.17	0.45
4:1E:12:THR:HG21	15:1T:11:GLU:HG2	1.98	0.45
8:1I:92:VAL:HG11	8:1I:144:VAL:HG11	1.98	0.45
13:1R:2:ARG:NH1	13:1R:5:LYS:O	2.50	0.45
16:1U:52:ARG:NH1	16:1U:55:ARG:HH21	2.14	0.45
32:1a:119:A:H4'	32:1a:120:A:C8	2.51	0.45
32:1a:219:C:H2'	32:1a:220:G:O4'	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:1f:21:LEU:O	37:1f:25:ILE:HG13	2.17	0.45
40:1i:110:GLU:HG2	40:1i:113:LYS:HZ1	1.81	0.45
1:2A:274:G:H2'	1:2A:275:G:C8	2.52	0.45
1:2A:1651:G:H2'	1:2A:1652:A:O4'	2.17	0.45
1:2A:2014:A:H4'	18:2W:92:ARG:HH11	1.81	0.45
1:2A:2261:C:OP1	22:20:19:LYS:NZ	2.46	0.45
1:2A:2507:C:H5"	1:2A:2573:C:N4	2.30	0.45
1:2A:2717:G:H2'	1:2A:2718:G:O4'	2.17	0.45
61:2A:3999:HOH:O	23:21:3:LYS:HE2	2.17	0.45
15:2T:16:ARG:NH2	15:2T:18:ASP:OD2	2.37	0.45
24:22:1:MET:SD	24:22:56:GLN:NE2	2.89	0.45
32:2a:441:A:H5'	32:2a:442:C:OP2	2.16	0.45
32:2a:822:C:H2'	32:2a:823:G:C8	2.52	0.45
32:2a:1329:A:OP2	52:2u:7:ARG:NH1	2.50	0.45
33:2b:95:GLN:HB2	33:2b:148:TYR:HD1	1.81	0.45
1:1A:715:G:C2	46:1o:56:LEU:HD21	2.51	0.45
1:1A:1826:G:H4'	3:1D:242:ARG:NH1	2.32	0.45
1:1A:2855:C:H2'	1:1A:2856:C:C6	2.52	0.45
5:1F:28:ILE:O	5:1F:30:PRO:HD3	2.16	0.45
6:1G:53:LEU:HD11	6:1G:87:PRO:HB2	1.98	0.45
9:1N:67:LEU:O	9:1N:88:GLU:HG3	2.16	0.45
32:1a:196:A:OP1	51:1t:68:LYS:NZ	2.46	0.45
32:1a:620:C:H2'	32:1a:621:A:O4'	2.17	0.45
32:1a:863:U:OP1	61:1a:2189:HOH:O	2.21	0.45
32:1a:1118:C:H1'	32:1a:1179:A:C4	2.52	0.45
44:1m:19:LEU:HD12	44:1m:19:LEU:HA	1.74	0.45
51:1t:74:LYS:HA	51:1t:74:LYS:HD2	1.71	0.45
1:2A:721:C:H2'	1:2A:722:A:C8	2.52	0.45
1:2A:2590:A:O3'	3:2D:239:ARG:NH2	2.50	0.45
12:2Q:37:LEU:HD21	12:2Q:130:LYS:HE2	1.99	0.45
21:2Z:93:ASP:HB3	21:2Z:131:ARG:HH22	1.81	0.45
32:2a:1050:G:H1'	32:2a:1214:C:O2	2.17	0.45
35:2d:114:ARG:HA	35:2d:117:ALA:HB3	1.99	0.45
39:2h:34:GLU:O	39:2h:38:ILE:HG12	2.16	0.45
40:2i:11:LYS:HA	40:2i:108:VAL:HG12	1.97	0.45
54:2w:11:C:N3	54:2w:24:G:N2	2.64	0.45
1:1A:2183:C:O2'	1:1A:2184:G:OP1	2.33	0.45
1:1A:2319:G:H22	14:1S:3:ARG:HA	1.82	0.45
1:1A:2334:G:H5'	14:1S:9:ARG:HG2	1.99	0.45
1:1A:2591:C:H2'	1:1A:2592:G:C8	2.51	0.45
1:1A:2630:G:H2'	1:1A:2631:G:C8	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1D:142:VAL:HG23	3:1D:193:VAL:HA	1.98	0.45
7:1H:127:GLU:H	7:1H:127:GLU:HG3	1.60	0.45
20:1Y:6:HIS:H	20:1Y:6:HIS:CD2	2.35	0.45
27:15:42:PRO:HB2	27:15:43:HIS:ND1	2.30	0.45
32:1a:1005:A:OP2	32:1a:1006:C:N4	2.49	0.45
32:1a:1109:C:H2'	32:1a:1110:A:O4'	2.17	0.45
35:1d:156:GLU:OE1	35:1d:156:GLU:N	2.39	0.45
40:1i:9:ARG:HD3	40:1i:14:VAL:HG12	1.98	0.45
44:1m:3:ARG:HG3	44:1m:4:ILE:N	2.31	0.45
54:1y:9:A:O3'	54:1y:45:U:O2'	2.32	0.45
1:2A:30:G:O2'	1:2A:1214:A:N3	2.46	0.45
1:2A:335:C:H4'	20:2Y:73:ARG:HD2	1.97	0.45
1:2A:1410:G:H2'	1:2A:1411:C:C6	2.52	0.45
1:2A:1592:C:H2'	1:2A:1593:G:H8	1.82	0.45
1:2A:1903:G:OP1	3:2D:241:PRO:HB2	2.17	0.45
1:2A:2271:G:OP1	22:20:18:ALA:HB1	2.17	0.45
1:2A:2507:C:O2'	54:2w:75:C:O2	2.32	0.45
4:2E:52:LEU:HB3	4:2E:76:ARG:HD3	1.98	0.45
9:2N:73:THR:HG23	9:2N:82:LEU:HD11	1.98	0.45
18:2W:33:ARG:NH2	18:2W:52:GLU:OE1	2.40	0.45
32:2a:966:M2G:HM23	32:2a:967:5MC:H1'	1.98	0.45
32:2a:980:C:H1'	45:2n:19:ARG:HA	1.99	0.45
32:2a:1406:U:C6	32:2a:1407:5MC:HM52	2.52	0.45
33:2b:16:HIS:HB2	33:2b:204:ASN:CB	2.40	0.45
34:2c:131:ARG:HH21	34:2c:135:LYS:HE3	1.82	0.45
47:2p:58:TYR:O	47:2p:61:SER:OG	2.23	0.45
51:2t:35:THR:O	51:2t:39:LYS:N	2.39	0.45
1:1A:2126:A:N6	1:1A:2162:G:O2'	2.50	0.45
3:1D:232:PRO:HB3	3:1D:244:ARG:CZ	2.46	0.45
7:1H:3:ARG:HH11	7:1H:4:ILE:H	1.65	0.45
10:1O:64:ARG:NH2	10:1O:99:PHE:O	2.50	0.45
32:1a:839:U:H3'	32:1a:840:C:H5'	1.99	0.45
32:1a:1499:A:OP2	61:1a:2345:HOH:O	2.21	0.45
49:1r:40:LEU:HD13	49:1r:79:LEU:HD11	1.98	0.45
1:2A:614(B):G:N3	5:2F:44:ARG:HG2	2.32	0.45
1:2A:1449:A:O2'	1:2A:1529:G:N2	2.24	0.45
1:2A:1821:A:H2'	1:2A:1822:G:C8	2.52	0.45
1:2A:1913:A:H4'	1:2A:1914:C:C5'	2.47	0.45
1:2A:2884:U:OP2	61:2A:4777:HOH:O	2.21	0.45
4:2E:7:VAL:HG12	4:2E:27:LEU:HB3	1.99	0.45
5:2F:185:ASP:HA	5:2F:188:ARG:HD3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:2P:52:GLU:HB3	11:2P:55:ARG:CZ	2.46	0.45
20:2Y:28:LYS:N	20:2Y:38:ILE:O	2.50	0.45
29:27:47:ARG:HD3	29:27:47:ARG:HA	1.61	0.45
32:2a:1057:G:O3'	34:2c:197:GLY:HA3	2.16	0.45
32:2a:1327:C:H2'	32:2a:1328:C:C6	2.52	0.45
34:2c:12:LEU:HD11	45:2n:51:GLY:HA2	1.99	0.45
39:2h:20:TYR:HA	39:2h:65:TYR:CZ	2.52	0.45
43:2l:24:VAL:HB	43:2l:27:LEU:HD22	1.98	0.45
1:1A:515:A:H1'	1:1A:581:C:H1'	1.99	0.45
1:1A:861:A:N3	2:1B:79:C:O2'	2.50	0.45
1:1A:1310:G:H1'	1:1A:1611:C:H5'	1.99	0.45
1:1A:1636:C:H2'	1:1A:1637:A:C8	2.52	0.45
4:1E:1:MET:HE3	4:1E:199:ARG:HB3	1.98	0.45
23:11:59:THR:O	23:11:91:LYS:NZ	2.50	0.45
28:16:13:CYS:SG	28:16:47:THR:HG21	2.57	0.45
32:1a:501:C:H2'	32:1a:502:G:C8	2.51	0.45
35:1d:60:GLU:HG2	35:1d:202:LEU:HB2	1.99	0.45
45:1n:33:VAL:HA	45:1n:40:CYS:HA	1.99	0.45
1:2A:445:C:OP1	16:2U:2:PRO:HA	2.17	0.45
1:2A:747:U:O2	1:2A:2014:A:H1'	2.17	0.45
1:2A:813:U:H2'	1:2A:814:C:C6	2.53	0.45
1:2A:1037:G:H1	1:2A:1118:C:H42	1.63	0.45
1:2A:1248:G:C5	16:2U:3:ARG:HB2	2.52	0.45
1:2A:1448:G:H4'	1:2A:1542:A:OP1	2.17	0.45
1:2A:1607:C:H5"	1:2A:1608:A:H5'	1.99	0.45
1:2A:1889:A:H2'	1:2A:1890:A:C8	2.52	0.45
1:2A:2630:G:H2'	1:2A:2631:G:H8	1.80	0.45
3:2D:75:ILE:HG21	3:2D:99:ASP:HB2	1.99	0.45
7:2H:164:TYR:HB2	7:2H:167:GLU:HB2	1.99	0.45
11:2P:95:VAL:HG13	11:2P:125:VAL:HA	1.98	0.45
16:2U:49:HIS:HA	16:2U:52:ARG:HB3	1.98	0.45
32:2a:743:U:H2'	32:2a:744:C:C6	2.52	0.45
32:2a:868:C:H2'	32:2a:869:G:O4'	2.16	0.45
32:2a:875:C:O2'	39:2h:15:ASN:ND2	2.47	0.45
32:2a:1002:G:H5'	32:2a:1003:G:OP2	2.16	0.45
32:2a:1137:C:H4'	32:2a:1138:G:O5'	2.17	0.45
32:2a:1456:G:N1	51:2t:51:GLU:OE2	2.45	0.45
37:2f:14:LEU:HD22	37:2f:18:GLN:HB3	1.99	0.45
50:2s:15:LEU:HD12	50:2s:18:LYS:HD2	1.98	0.45
54:2w:72:C:H2'	54:2w:73:A:H8	1.81	0.45
55:2x:25:C:H2'	55:2x:26: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:8:A:H2'	1:1A:9:U:C6	2.53	0.44
1:1A:944:G:N7	61:1A:4211:HOH:O	2.36	0.44
1:1A:1032:A:H2	1:1A:1122:G:H22	1.65	0.44
1:1A:1052:C:H2'	1:1A:1053:C:H6	1.82	0.44
1:1A:1218:C:H42	1:1A:1231:G:H1	1.66	0.44
1:1A:1935:G:H1'	1:1A:1964:G:N2	2.32	0.44
1:1A:1972:A:H2'	1:1A:1973:G:H8	1.81	0.44
1:1A:2155:G:H3'	1:1A:2156:G:H8	1.82	0.44
1:1A:2870:C:H2'	1:1A:2871:C:O4'	2.16	0.44
21:1Z:99:TYR:HA	21:1Z:124:ILE:O	2.16	0.44
32:1a:1317:C:OP2	45:1n:17:LYS:HE2	2.17	0.44
32:1a:1518:MA6:H93	32:1a:1519:MA6:H92	1.99	0.44
33:1b:28:PHE:CD2	33:1b:190:THR:HA	2.52	0.44
50:1s:31:ILE:HD12	50:1s:49:ILE:HG12	1.98	0.44
1:2A:581:C:H2'	1:2A:582:G:H8	1.82	0.44
1:2A:705:A:C2	1:2A:727:A:H1'	2.52	0.44
1:2A:820:A:N3	1:2A:943:U:H4'	2.32	0.44
1:2A:1579:A:H2'	1:2A:1580:A:C8	2.52	0.44
1:2A:1636:C:H2'	1:2A:1637:A:C8	2.52	0.44
32:2a:189(F):U:H3	48:2q:72:ARG:HH22	1.65	0.44
32:2a:997:U:O2	32:2a:1044:A:N1	2.50	0.44
33:2b:97:TRP:HZ3	33:2b:172:ILE:HG22	1.81	0.44
1:1A:271(A):A:N1	1:1A:272(D):G:O2'	2.42	0.44
1:1A:774:A:N3	1:1A:774:A:H2'	2.32	0.44
1:1A:1790:C:H5"	1:1A:1791:A:OP1	2.16	0.44
1:1A:2181:G:O2'	1:1A:2182:G:OP1	2.31	0.44
1:1A:2418:A:H2'	1:1A:2419:U:C6	2.52	0.44
1:1A:2712:U:O2'	1:1A:2713:A:H5'	2.17	0.44
3:1D:37:LEU:HB2	3:1D:62:TYR:HB2	1.99	0.44
14:1S:34:HIS:O	14:1S:97:ARG:NH2	2.50	0.44
15:1T:118:ARG:HG2	32:1a:1442(A):G:C8	2.52	0.44
32:1a:189(C):C:H2'	32:1a:189(D):C:O4'	2.17	0.44
32:1a:339:C:H2'	32:1a:340:U:H6	1.82	0.44
33:1b:55:PHE:HD1	33:1b:221:LEU:HD22	1.82	0.44
50:1s:20:LEU:HD21	50:1s:43:GLU:HG2	1.99	0.44
1:2A:71:A:H5"	1:2A:73:A:C8	2.52	0.44
1:2A:1843:C:H5'	3:2D:253:GLN:OE1	2.18	0.44
1:2A:2232:U:P	23:21:40:ARG:HH12	2.40	0.44
1:2A:2845:G:H2'	1:2A:2846:G:C8	2.52	0.44
7:2H:74:ASN:O	7:2H:78:GLY:N	2.50	0.44
9:2N:49:GLY:O	9:2N:119:ARG:NH1	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:2V:72:VAL:HG13	17:2V:85:LYS:HB3	1.99	0.44
32:2a:711:G:H2'	32:2a:712:A:H8	1.83	0.44
32:2a:1104:G:H4'	33:2b:111:ARG:HE	1.81	0.44
32:2a:1260:C:P	32:2a:1284:C:H4'	2.57	0.44
33:2b:16:HIS:CD2	33:2b:204:ASN:H	2.35	0.44
35:2d:116:GLN:HE22	35:2d:161:ASN:HD21	1.63	0.44
40:2i:128:ARG:HH21	55:2x:32:5MC:P	2.40	0.44
46:2o:5:LYS:HE2	46:2o:5:LYS:HB2	1.89	0.44
55:2x:66:C:H2'	55:2x:67:C:O4'	2.18	0.44
1:1A:272:G:N7	1:1A:421:U:H2'	2.33	0.44
1:1A:1364:G:C8	23:11:3:LYS:HD2	2.53	0.44
1:1A:2334:G:O6	22:10:74:ARG:NH1	2.44	0.44
1:1A:2557:G:H2'	1:1A:2558:C:C6	2.53	0.44
2:1B:66:A:H61	2:1B:108:U:H2'	1.82	0.44
6:1G:114:ILE:HG12	6:1G:140:ILE:HG12	1.99	0.44
24:12:14:ARG:O	24:12:67:LYS:NZ	2.49	0.44
32:1a:642:A:N3	39:1h:113:SER:OG	2.42	0.44
32:1a:1518:MA6:O5'	32:1a:1518:MA6:H8	2.17	0.44
33:1b:155:LEU:HD11	33:1b:159:PRO:HG3	1.99	0.44
35:1d:78:LEU:HD23	35:1d:97:LEU:HD23	2.00	0.44
1:2A:1116:C:H2'	1:2A:1117:G:C8	2.52	0.44
1:2A:1946:U:H2'	1:2A:1947:C:C6	2.52	0.44
1:2A:1952:A:N3	1:2A:2560:C:O2'	2.43	0.44
1:2A:2062:A:OP1	61:2A:4300:HOH:O	2.21	0.44
1:2A:2152:G:C2	1:2A:2153:G:H1'	2.52	0.44
1:2A:2390:U:P	30:28:35:GLN:HE22	2.39	0.44
2:2B:42:C:C4	2:2B:43:C:C4	3.06	0.44
3:2D:148:GLU:HB2	3:2D:151:LYS:HD2	1.98	0.44
5:2F:36:VAL:O	5:2F:40:GLN:HG3	2.17	0.44
7:2H:3:ARG:NH1	7:2H:4:ILE:H	2.15	0.44
12:2Q:2:LEU:HD12	12:2Q:69:PHE:HE1	1.82	0.44
15:2T:65:LYS:HE2	15:2T:65:LYS:HB3	1.78	0.44
32:2a:448:A:O5'	32:2a:485:G:N2	2.45	0.44
32:2a:1251:A:N6	32:2a:1285:A:N1	2.65	0.44
32:2a:1298:C:OP2	38:2g:114:ARG:NH2	2.50	0.44
38:2g:37:ASN:HD21	40:2i:40:LEU:HD23	1.82	0.44
40:2i:128:ARG:NH2	55:2x:33:U:OP2	2.47	0.44
1:1A:24:G:O2'	18:1W:78:GLU:O	2.26	0.44
2:1B:88:C:H2'	2:1B:89:G:O4'	2.18	0.44
4:1E:181:LEU:HD12	4:1E:181:LEU:HA	1.72	0.44
6:1G:170:ARG:NH2	6:1G:182:LYS:O	2.48	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1H:113:VAL:HG11	7:1H:151:ILE:HG21	1.98	0.44
28:16:14:THR:HG21	28:16:48:VAL:HG13	1.99	0.44
32:1a:835:U:OP1	49:1r:64:ARG:NH2	2.33	0.44
32:1a:881:G:P	43:1l:12:ARG:HH22	2.39	0.44
54:1y:58:A:HO2'	54:1y:59:U:P	2.37	0.44
1:2A:94(A):G:H2'	1:2A:95:G:O4'	2.17	0.44
1:2A:521:G:H2'	1:2A:522:G:H8	1.83	0.44
1:2A:607:U:OP1	5:2F:102:PRO:HA	2.18	0.44
1:2A:882:G:H1	1:2A:894:C:N4	2.14	0.44
1:2A:927:G:H2'	1:2A:928:G:O4'	2.16	0.44
1:2A:1657:C:H2'	1:2A:1658:C:C6	2.53	0.44
1:2A:2312:U:H5'	6:2G:88:ILE:HD11	1.98	0.44
3:2D:18:VAL:HG12	3:2D:211:ARG:NH1	2.32	0.44
9:2N:138:LEU:HD23	9:2N:138:LEU:HA	1.85	0.44
32:2a:671:G:H2'	32:2a:672:U:O4'	2.18	0.44
32:2a:876:G:OP1	39:2h:14:ARG:NH1	2.50	0.44
32:2a:1189:C:H2'	34:2c:176:HIS:CE1	2.53	0.44
38:2g:79:ARG:HH21	38:2g:80:VAL:H	1.65	0.44
54:2y:54:5MU:C4	54:2y:55:PSU:C2	3.05	0.44
1:1A:1401:G:H2'	1:1A:1402:C:O4'	2.17	0.44
1:1A:1406:U:H2'	1:1A:1407:C:H6	1.79	0.44
1:1A:1823:G:P	3:1D:54:ARG:HH21	2.40	0.44
1:1A:2102:U:H3	1:1A:2187:G:H1	1.65	0.44
1:1A:2336:A:H61	22:10:43:THR:HG22	1.82	0.44
3:1D:101:GLU:OE2	3:1D:103:ARG:NE	2.42	0.44
6:1G:43:LEU:HD12	6:1G:43:LEU:HA	1.81	0.44
12:1Q:134:ARG:NH1	21:1Z:122:ARG:HH21	2.15	0.44
26:14:49:PHE:HB3	26:14:50:VAL:H	1.51	0.44
32:1a:883:C:N4	32:1a:884:U:O4	2.51	0.44
32:1a:1223:C:P	50:1s:78:ARG:HH21	2.41	0.44
32:1a:1376:U:H2'	32:1a:1377:A:C8	2.52	0.44
38:1g:144:MET:HB3	38:1g:144:MET:HE2	1.66	0.44
40:1i:50:LEU:HD23	40:1i:81:ILE:HD11	2.00	0.44
1:2A:250:G:OP1	30:28:13:ARG:NH2	2.50	0.44
1:2A:571:A:O2'	17:2V:78:LYS:HE2	2.18	0.44
1:2A:1231:G:H2'	1:2A:1232:G:H8	1.82	0.44
1:2A:2875:C:H2'	1:2A:2876:G:O4'	2.18	0.44
9:2N:67:LEU:O	9:2N:88:GLU:HG3	2.17	0.44
17:2V:58:VAL:HB	17:2V:98:GLU:HG3	2.00	0.44
30:28:62:LEU:HB3	30:28:65:GLU:HG2	1.99	0.44
32:2a:19:C:H5"	36:2e:86:ALA:HB3	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1107:C:OP1	34:2c:173:VAL:N	2.50	0.44
32:2a:1228:C:H5"	44:2m:108:ARG:HH22	1.82	0.44
34:2c:112:SER:HB3	34:2c:115:LEU:HD22	1.99	0.44
35:2d:65:ARG:HG3	35:2d:75:PHE:CG	2.53	0.44
51:2t:47:GLY:HA2	51:2t:48:LYS:C	2.42	0.44
54:2w:27:G:N2	54:2w:43:C:N3	2.65	0.44
1:1A:551:G:O2'	1:1A:1220:A:N3	2.48	0.44
1:1A:614(B):G:N2	5:1F:44:ARG:O	2.46	0.44
1:1A:2121:G:H2'	1:1A:2122:U:C6	2.53	0.44
1:1A:2181:G:HO2'	1:1A:2182:G:P	2.39	0.44
20:1Y:9:LYS:HA	20:1Y:10:GLY:HA2	1.54	0.44
21:1Z:99:TYR:HB3	21:1Z:123:ASP:OD2	2.18	0.44
32:1a:11:G:O2'	32:1a:506:G:N2	2.49	0.44
32:1a:120:A:OP1	61:1a:1901:HOH:O	2.21	0.44
32:1a:405:U:O4	35:1d:2:GLY:N	2.51	0.44
33:1b:174:VAL:O	33:1b:178:ARG:HG3	2.18	0.44
40:1i:81:ILE:O	40:1i:85:LEU:HG	2.18	0.44
54:1y:20:U:O2'	54:1y:21:A:H4'	2.17	0.44
54:1y:28:G:H2'	54:1y:29:G:C8	2.52	0.44
1:2A:1155:A:H5"	16:2U:55:ARG:NE	2.32	0.44
1:2A:1637:A:H5'	1:2A:1760:A:O2'	2.18	0.44
1:2A:2516:G:C6	1:2A:2517:C:C4	3.06	0.44
1:2A:2689:U:P	1:2A:2719:G:H22	2.41	0.44
2:2B:34:U:O4	2:2B:44:G:O2'	2.33	0.44
12:2Q:50:ALA:HB1	12:2Q:121:ALA:HB1	1.99	0.44
16:2U:76:TYR:CZ	16:2U:80:ILE:HG13	2.52	0.44
32:2a:173:U:H5"	32:2a:197:A:O4'	2.17	0.44
32:2a:551:U:H2'	32:2a:552:U:C6	2.53	0.44
32:2a:858:G:O6	32:2a:869:G:H3'	2.17	0.44
32:2a:1025:U:N3	32:2a:1036:G:N1	2.50	0.44
55:2x:28:C:H2'	55:2x:29:G:C8	2.48	0.44
1:1A:234:C:H2'	1:1A:235:U:H6	1.82	0.44
1:1A:1566:A:OP1	3:1D:211:ARG:NH1	2.49	0.44
1:1A:2590:A:H2'	1:1A:2591:C:H6	1.82	0.44
1:1A:2887:U:H2'	1:1A:2888:C:C6	2.52	0.44
19:1X:35:THR:HG22	19:1X:37:THR:H	1.83	0.44
32:1a:40:C:H2'	32:1a:41:G:C8	2.53	0.44
32:1a:93:G:H2'	32:1a:96:U:O4'	2.16	0.44
32:1a:186:C:H2'	32:1a:187:C:C6	2.52	0.44
32:1a:286:G:N7	61:1a:2299:HOH:O	2.36	0.44
32:1a:540:G:H2'	32:1a:541:G:O4'	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:1b:47:THR:O	33:1b:51:LEU:HG	2.18	0.44
46:1o:18:PHE:O	46:1o:20:GLY:N	2.50	0.44
46:1o:29:VAL:HB	46:1o:81:LEU:HD21	2.00	0.44
1:2A:1007:C:P	9:2N:37:LYS:HZ2	2.41	0.44
1:2A:2125:G:N1	1:2A:2172:U:OP1	2.41	0.44
1:2A:2506:U:O2'	54:2w:76:A:H4'	2.18	0.44
3:2D:3:VAL:HG21	3:2D:203:ASN:HB2	2.00	0.44
3:2D:77:ALA:HA	3:2D:97:TYR:HA	2.00	0.44
17:2V:48:GLY:HA2	17:2V:52:VAL:HG13	1.99	0.44
32:2a:377:G:OP1	47:2p:3:LYS:HD3	2.17	0.44
32:2a:863:U:O2'	32:2a:865:A:N7	2.47	0.44
32:2a:1401:G:C2	32:2a:1402:4OC:H1'	2.52	0.44
33:2b:189:ASP:OD1	33:2b:189:ASP:N	2.44	0.44
43:2l:7:ILE:O	43:2l:11:VAL:HG23	2.17	0.44
44:2m:68:GLY:HA2	44:2m:71:ARG:HB2	1.99	0.44
48:2q:9:VAL:HA	48:2q:55:ASP:O	2.18	0.44
1:1A:407:G:H2'	1:1A:408:G:H8	1.83	0.44
1:1A:438:G:H2'	1:1A:440:G:H8	1.83	0.44
1:1A:1069:A:H2	1:1A:1095:A:O2'	2.01	0.44
1:1A:1166:C:H2'	1:1A:1167:U:C6	2.53	0.44
1:1A:1275:A:H4'	61:1A:7623:HOH:O	2.17	0.44
1:1A:2171:A:HO2'	1:1A:2172:U:H5"	1.82	0.44
1:1A:2179:C:H2'	1:1A:2180:U:C6	2.53	0.44
4:1E:143:ASN:HD22	4:1E:147:PRO:HD3	1.82	0.44
9:1N:36:GLY:HA2	9:1N:38:HIS:CE1	2.53	0.44
10:1O:64:ARG:HB2	10:1O:79:PHE:CD2	2.53	0.44
12:1Q:134:ARG:CZ	21:1Z:122:ARG:HH21	2.31	0.44
13:1R:54:LEU:HD12	13:1R:54:LEU:HA	1.83	0.44
16:1U:104:GLN:NE2	16:1U:105:VAL:HG23	2.33	0.44
28:16:18:ARG:HD2	28:16:42:TRP:CD1	2.53	0.44
32:1a:659:U:H2'	32:1a:660:G:C8	2.53	0.44
32:1a:1027:C:H5	32:1a:1028:C:C4	2.36	0.44
32:1a:1048:G:OP1	45:1n:3:ARG:HB3	2.17	0.44
33:1b:96:ARG:HH11	33:1b:98:LEU:HD22	1.83	0.44
33:1b:155:LEU:HD12	33:1b:155:LEU:HA	1.87	0.44
41:1j:38:ILE:HD11	41:1j:71:LEU:HD23	1.99	0.44
1:2A:35:G:H2'	1:2A:36:G:O4'	2.17	0.44
1:2A:271(R):G:OP1	23:21:76:ARG:NH1	2.51	0.44
1:2A:407:G:H2'	1:2A:408:G:C8	2.52	0.44
1:2A:489:G:H2'	1:2A:491:G:O4'	2.18	0.44
1:2A:1017:G:N7	61:2A:5060:HOH:O	2.46	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2364:C:OP1	22:20:55:ARG:NH1	2.47	0.44
7:2H:80:SER:OG	7:2H:81:GLU:N	2.51	0.44
21:2Z:91:LEU:HD12	21:2Z:91:LEU:HA	1.85	0.44
32:2a:423:G:H3'	32:2a:423:G:N3	2.33	0.44
32:2a:545:C:O2'	32:2a:549:C:OP1	2.29	0.44
32:2a:659:U:OP1	46:2o:9:GLN:NE2	2.50	0.44
32:2a:734:G:H21	49:2r:75:ILE:HD11	1.81	0.44
39:2h:20:TYR:HA	39:2h:65:TYR:CE1	2.52	0.44
55:2x:15:G:N2	55:2x:21:A:N3	2.66	0.44
1:1A:185:U:H2'	1:1A:186:G:H8	1.83	0.44
1:1A:911:A:H2'	12:1Q:9:TYR:OH	2.18	0.44
1:1A:1065:U:N3	1:1A:1070:A:OP1	2.42	0.44
1:1A:1420:U:H6	1:1A:1420:U:H2'	1.62	0.44
1:1A:1637:A:OP2	61:1A:7206:HOH:O	2.21	0.44
1:1A:2330:G:H2'	1:1A:2331:G:O4'	2.18	0.44
32:1a:50:A:H1'	32:1a:52:G:C8	2.52	0.44
32:1a:72:C:H2'	32:1a:73:G:C8	2.53	0.44
32:1a:160:A:H1'	32:1a:344:A:C8	2.53	0.44
32:1a:193:C:H2'	32:1a:194:C:H6	1.83	0.44
32:1a:674:G:H2'	32:1a:675:A:C8	2.53	0.44
35:1d:173:TRP:CD1	35:1d:174:LEU:HG	2.53	0.44
54:1w:11:C:H42	54:1w:24:G:H1	1.66	0.44
54:1w:66:U:H2'	54:1w:67:C:C6	2.53	0.44
1:2A:322:A:H5'	1:2A:340:A:H1'	1.99	0.44
1:2A:752:A:P	29:27:3:ARG:HH22	2.41	0.44
1:2A:892:G:H3'	1:2A:893:C:C5'	2.48	0.44
1:2A:1012:U:O4	9:2N:28:THR:HG21	2.18	0.44
1:2A:1239:G:H2'	1:2A:1240:U:O4'	2.18	0.44
1:2A:2562:U:H4'	10:2O:25:LEU:HD21	2.00	0.44
1:2A:2611:U:C4	27:25:3:LYS:HG2	2.53	0.44
1:2A:2820:A:OP1	13:2R:2:ARG:NH2	2.47	0.44
2:2B:41:U:H5	6:2G:70:VAL:N	2.16	0.44
5:2F:178:PRO:HB2	5:2F:201:VAL:HG21	1.99	0.44
32:2a:355:C:H1'	32:2a:388:G:H1'	1.99	0.44
32:2a:643:C:H2'	32:2a:644:G:C8	2.50	0.44
32:2a:973:G:H3'	32:2a:974:A:H5"	2.00	0.44
33:2b:16:HIS:HD2	33:2b:18:GLY:H	1.65	0.44
49:2r:73:ALA:HB1	49:2r:78:LEU:HB2	2.00	0.44
1:1A:242:G:C8	30:18:5:LYS:HG2	2.53	0.43
1:1A:271(K):U:H4'	1:1A:271(L):U:OP2	2.16	0.43
1:1A:1754:C:N3	1:1A:2716:U:O2'	2.44	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2441:C:OP2	1:1A:2586:C:O2'	2.31	0.43
10:1O:4:PRO:O	10:1O:5:GLN:HB2	2.18	0.43
11:1P:3:LEU:HD12	11:1P:3:LEU:HA	1.90	0.43
11:1P:124:LYS:HA	11:1P:144:GLU:HB3	1.98	0.43
12:1Q:25:ASP:OD1	12:1Q:25:ASP:N	2.50	0.43
20:1Y:5:MET:HE2	20:1Y:5:MET:HB2	1.81	0.43
32:1a:165:C:H2'	32:1a:166:G:C8	2.53	0.43
32:1a:266:G:H2'	32:1a:266:G:N3	2.32	0.43
32:1a:324:G:N2	32:1a:327:A:OP2	2.51	0.43
32:1a:580:U:H2'	32:1a:581:G:O4'	2.18	0.43
32:1a:1068:G:H8	32:1a:1068:G:OP2	2.01	0.43
32:1a:1191:A:OP1	34:1c:4:LYS:NZ	2.35	0.43
32:1a:1222:G:OP1	50:1s:77:THR:HG21	2.18	0.43
32:1a:1355:G:H2'	32:1a:1356:G:C8	2.53	0.43
35:1d:3:ARG:NH1	35:1d:5:ILE:HG13	2.33	0.43
35:1d:144:ASP:OD1	35:1d:144:ASP:N	2.51	0.43
1:2A:1028:A:H61	1:2A:1125:G:H2'	1.81	0.43
1:2A:1427:A:H4'	1:2A:1428:C:O5'	2.18	0.43
1:2A:2127:G:H2'	1:2A:2128:C:H6	1.82	0.43
1:2A:2547:U:H2'	1:2A:2548:G:C8	2.53	0.43
1:2A:2853:C:H2'	1:2A:2854:G:H8	1.82	0.43
2:2B:55:U:H1'	6:2G:29:TRP:CD1	2.53	0.43
5:2F:57:VAL:HG13	5:2F:59:TYR:H	1.83	0.43
8:2I:125:GLU:OE1	8:2I:143:SER:HB3	2.18	0.43
11:2P:52:GLU:HG3	30:28:57:ARG:HH22	1.82	0.43
13:2R:13:HIS:CE1	13:2R:16:HIS:HB2	2.53	0.43
32:2a:142:G:H2'	32:2a:143:A:C8	2.53	0.43
32:2a:1238:A:C2	32:2a:1303:C:H4'	2.53	0.43
32:2a:1500:A:H5"	32:2a:1508:G:H5"	1.99	0.43
36:2e:24:ARG:HD2	53:2v:24:A:OP2	2.18	0.43
38:2g:23:VAL:O	38:2g:27:ILE:HG13	2.18	0.43
42:2k:31:THR:HG22	42:2k:42:TRP:HB2	1.99	0.43
54:2w:9:A:H8	54:2w:11:C:H41	1.65	0.43
1:1A:118:A:C8	1:1A:119:A:C8	3.05	0.43
1:1A:324:A:H2'	1:1A:325:G:O4'	2.18	0.43
1:1A:1448:G:H5"	1:1A:1542:A:OP2	2.19	0.43
1:1A:1504:C:H2'	1:1A:1505:C:C6	2.54	0.43
1:1A:1754:C:H5	15:1T:96:ARG:NH2	2.16	0.43
1:1A:1799:G:O2'	3:1D:181:GLU:OE2	2.29	0.43
2:1B:74:U:H2'	2:1B:75:G:O4'	2.18	0.43
5:1F:106:ARG:H	5:1F:106:ARG:HG2	1.56	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1H:89:ILE:O	7:1H:129:THR:OG1	2.34	0.43
11:1P:3:LEU:HD12	11:1P:6:LEU:HD12	2.00	0.43
32:1a:58:C:O2'	32:1a:388:G:N7	2.37	0.43
32:1a:860:A:H3'	32:1a:861:G:H8	1.83	0.43
1:2A:362:U:O2'	1:2A:363:G:H5'	2.18	0.43
1:2A:567:A:OP2	11:2P:29:LYS:NZ	2.51	0.43
1:2A:625:G:O6	11:2P:107:LYS:NZ	2.46	0.43
1:2A:660:G:H5'	5:2F:99:TYR:CE1	2.53	0.43
1:2A:784:A:C6	3:2D:229:VAL:HG11	2.53	0.43
1:2A:1576:U:H2'	1:2A:1577:C:C6	2.53	0.43
1:2A:1754:C:N3	1:2A:2716:U:O2'	2.47	0.43
1:2A:2065:C:H4'	1:2A:2251:OMG:HM22	2.00	0.43
1:2A:2251:OMG:OP2	1:2A:2251:OMG:H8	2.01	0.43
1:2A:2695:C:H2'	1:2A:2696:U:C6	2.53	0.43
11:2P:70:GLN:O	11:2P:73:GLY:N	2.36	0.43
21:2Z:53:ILE:HG22	21:2Z:71:VAL:O	2.18	0.43
32:2a:992:U:H6	32:2a:992:U:H5'	1.83	0.43
32:2a:1356:G:H2'	32:2a:1357:A:C8	2.53	0.43
34:2c:120:VAL:HG21	34:2c:137:ALA:HB2	2.00	0.43
37:2f:100:ASN:ND2	49:2r:23:LYS:HE2	2.33	0.43
45:2n:23:ARG:NH1	45:2n:30:ALA:HB2	2.34	0.43
51:2t:10:LEU:HD23	51:2t:12:ALA:HB2	2.00	0.43
54:2w:50:U:H2'	54:2w:51:U:C6	2.53	0.43
1:1A:121:G:H4'	1:1A:149:A:H5'	2.00	0.43
1:1A:602:G:O2'	1:1A:655:A:N6	2.51	0.43
1:1A:1155:A:OP1	16:1U:55:ARG:HD2	2.19	0.43
1:1A:1692:U:O2'	1:1A:1693:U:H2'	2.18	0.43
1:1A:2120:G:C2'	1:1A:2121:G:H5'	2.48	0.43
1:1A:2788:C:O2'	1:1A:2809:A:N3	2.41	0.43
5:1F:185:ASP:HA	5:1F:188:ARG:HD3	2.00	0.43
7:1H:13:LYS:HA	7:1H:14:GLY:HA2	1.65	0.43
10:1O:115:VAL:HG13	10:1O:121:VAL:HG21	1.99	0.43
11:1P:50:ARG:HD3	30:18:7:HIS:HD2	1.79	0.43
26:14:63:TYR:N	26:14:63:TYR:CD1	2.85	0.43
32:1a:92:C:H2'	32:1a:93:G:H8	1.82	0.43
32:1a:657:G:H2'	32:1a:658:G:H8	1.84	0.43
33:1b:24:TRP:HZ3	33:1b:29:ALA:HB2	1.82	0.43
1:2A:208:C:H2'	1:2A:209:C:H6	1.83	0.43
1:2A:1364:G:P	23:21:3:LYS:HG3	2.58	0.43
1:2A:1598:C:H2'	1:2A:1599:C:C6	2.53	0.43
1:2A:1651:G:OP1	13:2R:37:THR:OG1	2.36	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2086:U:H2'	1:2A:2087:G:C8	2.53	0.43
1:2A:2108:C:H42	1:2A:2181:G:H1	1.64	0.43
1:2A:2441:C:OP2	1:2A:2586:C:O2'	2.32	0.43
1:2A:2526:G:H5'	1:2A:2742:C:O2'	2.18	0.43
2:2B:24:G:H4'	2:2B:25:A:C8	2.54	0.43
3:2D:9:TYR:CD1	3:2D:10:THR:HG23	2.53	0.43
3:2D:183:ARG:HG3	3:2D:270:ILE:HG12	2.01	0.43
6:2G:49:ASP:OD1	6:2G:49:ASP:N	2.48	0.43
8:2I:79:ILE:O	8:2I:144:VAL:HA	2.18	0.43
12:2Q:38:GLU:OE2	12:2Q:128:LYS:N	2.40	0.43
20:2Y:6:HIS:ND1	20:2Y:7:VAL:HG23	2.33	0.43
26:24:67:TYR:HD2	50:2s:9:VAL:HB	1.83	0.43
28:26:8:LYS:HD3	30:28:34:TRP:CD2	2.54	0.43
32:2a:41:G:H2'	32:2a:42:G:H8	1.83	0.43
32:2a:769:G:H4'	32:2a:1513:A:H4'	2.00	0.43
32:2a:865:A:H2	32:2a:918:A:H4'	1.83	0.43
32:2a:872:A:O2'	32:2a:873:A:H3'	2.18	0.43
44:2m:114:ARG:H	44:2m:114:ARG:HG2	1.62	0.43
48:2q:54:GLY:O	48:2q:81:ARG:N	2.32	0.43
1:1A:182:A:N3	1:1A:433:C:O2'	2.44	0.43
1:1A:1652:A:OP1	13:1R:8:ARG:NH1	2.51	0.43
1:1A:1796:U:H2'	1:1A:1797:C:H6	1.83	0.43
1:1A:1919:A:O2'	32:1a:1517:G:N3	2.40	0.43
1:1A:2206:G:OP2	1:1A:2206:G:H4'	2.17	0.43
1:1A:2691:C:O3'	1:1A:2871:C:H4'	2.18	0.43
1:1A:2820:A:OP2	13:1R:2:ARG:NH2	2.51	0.43
3:1D:218:ARG:HB3	3:1D:219:PRO:HD2	1.99	0.43
5:1F:129:PHE:HB3	5:1F:132:VAL:HG13	2.00	0.43
6:1G:41:GLN:HG2	6:1G:154:GLY:O	2.18	0.43
24:12:1:MET:N	24:12:52:ASP:OD2	2.40	0.43
30:18:63:PRO:HG2	30:18:64:TYR:CE2	2.53	0.43
32:1a:922:G:H4'	36:1e:20:GLN:HA	1.99	0.43
32:1a:1172:C:H2'	32:1a:1173:G:H8	1.83	0.43
39:1h:101:PRO:HG3	39:1h:133:LEU:HD11	2.01	0.43
41:1j:57:LYS:HE2	41:1j:60:ARG:NH2	2.34	0.43
54:1y:5:G:H1'	54:1y:69:G:N2	2.33	0.43
1:2A:284:U:H2'	1:2A:285:C:C6	2.54	0.43
1:2A:822:U:OP2	61:2A:5949:HOH:O	2.21	0.43
1:2A:1660:C:H2'	1:2A:1661:G:H8	1.83	0.43
1:2A:1794:U:H2'	1:2A:1795:C:H6	1.83	0.43
1:2A:2287:A:H2	1:2A:2346:A:H62	1.64	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:2A:4490:HOH:O	3:2D:237:GLU:OE2	2.20	0.43
6:2G:36:LYS:HD3	6:2G:95:ARG:NH1	2.33	0.43
8:2I:62:LYS:O	8:2I:66:GLU:HG2	2.18	0.43
19:2X:57:LEU:HD11	19:2X:78:LYS:HE2	1.99	0.43
20:2Y:13:VAL:HG12	20:2Y:74:PRO:HA	2.00	0.43
24:22:10:LEU:HD21	24:22:59:ARG:HG2	1.98	0.43
30:28:23:VAL:HG11	30:28:47:LYS:HD3	2.00	0.43
32:2a:41:G:H2'	32:2a:42:G:C8	2.53	0.43
32:2a:1004:A:N1	32:2a:1037:C:C2	2.86	0.43
32:2a:1004:A:C6	32:2a:1037:C:H1'	2.53	0.43
32:2a:1096:C:O2	32:2a:1170:A:O2'	2.33	0.43
32:2a:1251:A:H5"	40:2i:12:GLU:OE1	2.19	0.43
32:2a:1492:A:H2'	32:2a:1493:A:C8	2.53	0.43
32:2a:1517:G:H2'	32:2a:1518:MA6:H8	1.99	0.43
35:2d:187:ARG:NH2	35:2d:193:ASP:OD2	2.51	0.43
38:2g:77:SER:HA	38:2g:85:TYR:O	2.19	0.43
39:2h:39:LEU:HB3	39:2h:45:ILE:HG12	1.99	0.43
1:1A:26:G:H1'	1:1A:515:A:H61	1.84	0.43
1:1A:125:G:H1'	29:17:48:LYS:HD3	2.01	0.43
1:1A:747:U:H1'	18:1W:92:ARG:NH1	2.32	0.43
1:1A:1266:G:O5'	18:1W:15:ARG:NH2	2.51	0.43
7:1H:90:LYS:HD2	7:1H:159:GLU:HG2	1.99	0.43
15:1T:24:PRO:HA	15:1T:49:VAL:HG23	2.00	0.43
32:1a:826:C:H2'	32:1a:827:U:C6	2.54	0.43
32:1a:1206:G:O4'	34:1c:194:GLY:HA2	2.19	0.43
32:1a:1219:U:OP1	45:1n:19:ARG:NH1	2.40	0.43
38:1g:26:PHE:CE2	38:1g:30:ILE:HD11	2.53	0.43
46:1o:74:ASP:HB3	46:1o:77:ARG:HB2	2.00	0.43
52:1u:6:ARG:O	52:1u:12:LYS:HE3	2.18	0.43
1:2A:210:C:H2'	1:2A:211:A:C8	2.53	0.43
1:2A:565:C:H2'	1:2A:566:U:O4'	2.19	0.43
1:2A:589:C:H2'	1:2A:590:A:C8	2.53	0.43
1:2A:1537:G:H2'	1:2A:1538:G:C8	2.49	0.43
1:2A:1814:G:H2'	1:2A:1815:A:C8	2.54	0.43
1:2A:2322:A:H2'	1:2A:2323:G:O4'	2.18	0.43
2:2B:31:C:H4'	6:2G:29:TRP:CZ2	2.54	0.43
4:2E:59:VAL:HG21	4:2E:74:PRO:HB3	2.00	0.43
6:2G:135:LEU:O	6:2G:155:MET:N	2.40	0.43
13:2R:66:VAL:HG12	13:2R:70:LEU:HD12	1.99	0.43
15:2T:33:LYS:HB3	15:2T:82:LEU:HD22	2.00	0.43
15:2T:88:ILE:HG21	15:2T:91:ARG:NE	2.32	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:26:13:CYS:SG	28:26:47:THR:HG21	2.58	0.43
32:2a:65:U:H1'	32:2a:66:G:OP2	2.18	0.43
32:2a:309:G:O2'	32:2a:607:A:N1	2.49	0.43
41:2j:63:PHE:HE2	45:2n:45:ARG:HA	1.83	0.43
44:2m:16:ASP:O	44:2m:20:THR:HG23	2.18	0.43
44:2m:23:TYR:CZ	44:2m:71:ARG:HG3	2.54	0.43
1:1A:53:A:H2'	1:1A:54:G:O4'	2.19	0.43
1:1A:388:G:O2'	1:1A:389:G:N7	2.47	0.43
1:1A:1111:A:H4'	1:1A:1112:G:OP1	2.19	0.43
1:1A:1441:G:O6	61:1A:6075:HOH:O	2.21	0.43
1:1A:2049:G:N7	61:1A:6385:HOH:O	2.37	0.43
1:1A:2359:C:H2'	1:1A:2360:A:O4'	2.19	0.43
1:1A:2639:A:O2'	9:1N:97:ARG:NH2	2.52	0.43
32:1a:110:C:H2'	32:1a:111:G:O4'	2.18	0.43
32:1a:600:C:H2'	32:1a:601:C:C6	2.54	0.43
37:1f:69:GLU:H	37:1f:69:GLU:CD	2.26	0.43
47:1p:19:ILE:N	47:1p:37:GLY:O	2.51	0.43
1:2A:752:A:H4'	1:2A:753:C:H5'	1.99	0.43
1:2A:884:C:H3'	1:2A:885:C:H6	1.84	0.43
1:2A:1630:G:H2'	1:2A:1631:C:C6	2.53	0.43
1:2A:2563:U:H4'	10:2O:28:SER:HA	2.00	0.43
10:2O:29:ASN:N	10:2O:29:ASN:OD1	2.51	0.43
10:2O:49:ARG:NH1	32:2a:1422:G:O3'	2.51	0.43
13:2R:72:ASP:HB3	13:2R:75:LEU:HB3	2.00	0.43
16:2U:6:THR:HG21	16:2U:10:ARG:HH21	1.84	0.43
32:2a:4:U:O2	39:2h:105:ARG:NH2	2.51	0.43
32:2a:273:A:N7	61:2a:3622:HOH:O	2.37	0.43
32:2a:1401:G:OP1	53:2v:18:G:O2'	2.33	0.43
33:2b:97:TRP:CH2	33:2b:173:ALA:HA	2.53	0.43
38:2g:69:VAL:HG11	38:2g:134:ALA:HB1	2.01	0.43
40:2i:21:PRO:HA	40:2i:59:PHE:HA	2.00	0.43
47:2p:19:ILE:N	47:2p:37:GLY:O	2.51	0.43
1:1A:185:U:H2'	1:1A:186:G:C8	2.54	0.43
1:1A:1470:G:N2	1:1A:1520:G:OP2	2.34	0.43
1:1A:1952:A:C6	1:1A:1953:A:N1	2.86	0.43
1:1A:2168:G:C6	1:1A:2171:A:C8	3.07	0.43
1:1A:2188:C:H2'	1:1A:2189:U:O4'	2.18	0.43
1:1A:2718:G:O2'	1:1A:2847:U:OP1	2.32	0.43
4:1E:28:ALA:HB3	4:1E:93:VAL:HG12	2.01	0.43
7:1H:97:ARG:NE	7:1H:104:GLU:OE1	2.51	0.43
28:16:12:GLU:HA	28:16:19:ARG:HA	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:19:C:H4'	32:1a:864:A:O4'	2.18	0.43
32:1a:21:G:H2'	32:1a:22:G:C8	2.54	0.43
32:1a:44:G:O6	61:1a:2377:HOH:O	2.21	0.43
32:1a:269:C:H2'	32:1a:270:A:C8	2.54	0.43
32:1a:277:C:H5"	48:1q:68:ARG:NH2	2.33	0.43
32:1a:567:G:O6	43:1l:5:PRO:HD3	2.18	0.43
32:1a:743:U:H2'	32:1a:744:C:C6	2.54	0.43
32:1a:877:C:OP1	39:1h:88:LYS:NZ	2.35	0.43
32:1a:881:G:H2'	32:1a:882:C:O4'	2.19	0.43
32:1a:1006:C:N4	32:1a:1023:G:H1	2.11	0.43
32:1a:1009:G:O6	32:1a:1020:U:C2	2.72	0.43
32:1a:1244:C:H2'	32:1a:1245:A:C8	2.53	0.43
32:1a:1367:C:H5'	41:1j:60:ARG:NH1	2.33	0.43
35:1d:155:LEU:HD23	35:1d:155:LEU:HA	1.82	0.43
44:1m:123:ALA:HB2	54:1w:39:PSU:H1'	1.99	0.43
54:1y:15:G:H22	54:1y:48:C:N4	2.15	0.43
1:2A:469:G:N7	29:27:37:LYS:NZ	2.63	0.43
1:2A:684:G:N7	61:2A:3918:HOH:O	2.37	0.43
1:2A:855:G:H2'	1:2A:856:C:C6	2.53	0.43
1:2A:863:A:H2'	1:2A:864:G:C8	2.54	0.43
1:2A:1022:G:N2	1:2A:1023:U:O4	2.45	0.43
1:2A:1147:C:H2'	1:2A:1148:A:H8	1.84	0.43
1:2A:1423:G:H2'	1:2A:1424:G:H8	1.83	0.43
1:2A:2180:U:H2'	1:2A:2181:G:O4'	2.19	0.43
1:2A:2846:G:H2'	1:2A:2847:U:O4'	2.18	0.43
32:2a:160:A:H1'	32:2a:344:A:N7	2.33	0.43
32:2a:1081:G:H5'	36:2e:18:ARG:HB3	2.00	0.43
32:2a:1210:C:H3'	32:2a:1211:U:H5"	2.00	0.43
40:2i:77:ILE:O	40:2i:81:ILE:HG22	2.19	0.43
42:2k:15:ALA:HA	42:2k:76:GLY:O	2.19	0.43
46:2o:82:ILE:HB	46:2o:87:ILE:HB	2.00	0.43
49:2r:36:ASN:O	49:2r:40:LEU:HG	2.19	0.43
54:2w:68:C:H2'	54:2w:69:G:C8	2.54	0.43
1:1A:35:G:H2'	1:1A:36:G:O4'	2.19	0.43
1:1A:1638:C:H5"	1:1A:2710:C:O2'	2.18	0.43
9:1N:4:TYR:CE2	16:1U:100:VAL:HG11	2.53	0.43
21:1Z:136:PHE:O	21:1Z:137:ILE:HG13	2.18	0.43
32:1a:953:G:H2'	32:1a:954:G:O4'	2.18	0.43
32:1a:1118:C:H2'	32:1a:1119:C:H6	1.84	0.43
32:1a:1345:U:H4'	32:1a:1346:A:H5'	2.00	0.43
32:1a:1464:G:H2'	32:1a:1465:C:C6	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:1b:27:LYS:HB2	33:1b:194:PRO:HD2	2.00	0.43
44:1m:108:ARG:HD3	44:1m:108:ARG:HA	1.78	0.43
1:2A:458:G:C8	29:27:37:LYS:HG2	2.54	0.43
1:2A:848:G:O6	1:2A:928:G:H2'	2.18	0.43
1:2A:1131:G:O6	1:2A:2040:C:H1'	2.18	0.43
1:2A:1913:A:H4'	1:2A:1914:C:O5'	2.18	0.43
1:2A:2841:C:H2'	1:2A:2842:G:C8	2.53	0.43
2:2B:68:C:H2'	2:2B:69:G:H8	1.82	0.43
18:2W:46:PHE:O	18:2W:50:VAL:HG23	2.19	0.43
19:2X:12:VAL:HG22	19:2X:29:TRP:CE2	2.53	0.43
23:21:89:GLU:O	23:21:93:GLU:HG2	2.18	0.43
32:2a:229:U:O2'	47:2p:23:ASP:OD2	2.33	0.43
32:2a:338:A:H2	32:2a:351:G:H22	1.66	0.43
32:2a:741:G:H2'	32:2a:742:G:O4'	2.18	0.43
38:2g:80:VAL:HB	38:2g:85:TYR:HE2	1.84	0.43
44:2m:123:ALA:HB2	54:2w:39:PSU:H1'	2.01	0.43
48:2q:53:LEU:HB3	48:2q:82:MET:SD	2.58	0.43
1:1A:493:G:HO2'	18:1W:8:ARG:H	1.67	0.43
1:1A:1059:G:H2'	1:1A:1060:U:C5	2.54	0.43
1:1A:1783:A:C5'	1:1A:2608:G:H4'	2.49	0.43
1:1A:2001:A:H2'	1:1A:2002:G:C8	2.54	0.43
1:1A:2011:U:OP1	18:1W:42:ARG:NH1	2.51	0.43
1:1A:2135:A:H2	1:1A:2136:C:C2	2.37	0.43
1:1A:2156:G:H2'	1:1A:2157:G:C2	2.54	0.43
1:1A:2327:A:H2'	1:1A:2328:A:C8	2.54	0.43
2:1B:92:C:H5"	21:1Z:79:ARG:NH1	2.33	0.43
5:1F:53:THR:HG22	5:1F:55:GLY:H	1.83	0.43
11:1P:59:LEU:HD21	30:18:10:ALA:HA	2.01	0.43
32:1a:408:A:H2'	32:1a:409:G:O4'	2.18	0.43
32:1a:815:A:N7	32:1a:1509:C:O2'	2.50	0.43
32:1a:1025:U:O2	32:1a:1036:G:O6	2.37	0.43
32:1a:1144:G:H21	32:1a:1146:A:H62	1.67	0.43
44:1m:82:MET:O	44:1m:93:ARG:NH2	2.51	0.43
1:2A:729:G:C8	3:2D:208:LYS:HD2	2.54	0.43
1:2A:744:G:H2'	1:2A:745:G:O4'	2.18	0.43
1:2A:1504:C:H2'	1:2A:1505:C:H6	1.83	0.43
1:2A:1686:C:H2'	1:2A:1687:G:O4'	2.19	0.43
1:2A:2156:G:H2'	1:2A:2157:G:C2	2.54	0.43
1:2A:2394:C:N3	54:2y:76:A:O2'	2.41	0.43
1:2A:2840:C:H2'	1:2A:2841:C:C6	2.54	0.43
2:2B:11:C:H3'	2:2B:12:C:C6	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2B:66:A:H61	2:2B:108:U:H2'	1.84	0.43
6:2G:3:LEU:HD12	6:2G:8:LYS:NZ	2.34	0.43
17:2V:98:GLU:OE2	17:2V:100:ARG:NH1	2.52	0.43
21:2Z:50:GLN:OE1	21:2Z:50:GLN:N	2.51	0.43
32:2a:45:U:OP1	32:2a:307:C:O2'	2.36	0.43
32:2a:757:U:H2'	32:2a:758:G:O4'	2.18	0.43
32:2a:781:A:N6	61:2a:3307:HOH:O	2.45	0.43
32:2a:1032:G:H2'	32:2a:1033:G:C8	2.54	0.43
32:2a:1100:C:H2'	32:2a:1102:A:O5'	2.19	0.43
32:2a:1318:A:H4'	50:2s:10:PHE:CD2	2.53	0.43
32:2a:1380:U:C4	38:2g:3:ARG:HG2	2.54	0.43
36:2e:6:PHE:HB3	36:2e:34:VAL:HG22	2.00	0.43
36:2e:110:LEU:HB3	36:2e:115:VAL:HB	2.01	0.43
46:2o:82:ILE:HD12	46:2o:88:ARG:HB2	2.00	0.43
1:1A:234:C:H2'	1:1A:235:U:C6	2.54	0.43
1:1A:1010:A:N3	1:1A:1153:C:H1'	2.33	0.43
1:1A:1054:A:N6	1:1A:1105:U:N3	2.49	0.43
1:1A:1058:G:N1	1:1A:1080:C:N4	2.34	0.43
1:1A:1409:C:H2'	1:1A:1410:G:C8	2.54	0.43
1:1A:1418:G:O5'	1:1A:1418:G:H8	2.02	0.43
1:1A:1665:A:H2'	1:1A:1666:G:O4'	2.19	0.43
20:1Y:15:VAL:HG21	20:1Y:42:VAL:HG11	2.00	0.43
32:1a:171:A:H2'	32:1a:172:A:C8	2.54	0.43
32:1a:172:A:N6	32:1a:174:C:O2	2.52	0.43
32:1a:250:A:H4'	32:1a:251:G:O5'	2.18	0.43
32:1a:374:A:C6	32:1a:375:U:C4	3.07	0.43
32:1a:1229:A:O2'	55:1x:30:G:OP1	2.36	0.43
32:1a:1328:C:H2'	32:1a:1329:A:O4'	2.18	0.43
34:1c:6:HIS:CD2	34:1c:8:ILE:H	2.27	0.43
36:1e:69:VAL:O	36:1e:71:LEU:HD22	2.19	0.43
47:1p:58:TYR:O	47:1p:62:VAL:HG23	2.18	0.43
54:1w:37:MIA:H162	54:1w:37:MIA:H121	1.70	0.43
54:1w:63:G:H2'	54:1w:64:A:C8	2.54	0.43
1:2A:898:C:H2'	1:2A:899:A:H5'	2.01	0.43
1:2A:1568:G:H5"	3:2D:61:LEU:HD13	2.00	0.43
1:2A:2474:C:H5"	1:2A:2475:C:OP2	2.19	0.43
1:2A:2689:U:H4'	1:2A:2690:C:O5'	2.19	0.43
7:2H:122:THR:O	7:2H:134:SER:OG	2.33	0.43
10:2O:64:ARG:HG2	10:2O:83:ALA:HB3	2.01	0.43
32:2a:46:G:H2'	32:2a:366:C:C5	2.54	0.43
32:2a:892:A:O2'	32:2a:1415:G:H4'	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:922:G:N3	32:2a:1398:A:H2	2.17	0.43
32:2a:989:C:H2'	32:2a:990:C:C6	2.54	0.43
32:2a:1097:C:H1'	32:2a:1170:A:H1'	2.01	0.43
32:2a:1320:C:H2'	32:2a:1321:C:O4'	2.19	0.43
33:2b:16:HIS:CD2	33:2b:18:GLY:H	2.37	0.43
36:2e:33:VAL:HA	36:2e:42:GLY:O	2.19	0.43
39:2h:12:ARG:HD3	39:2h:26:VAL:HG12	2.00	0.43
40:2i:24:GLY:HA2	40:2i:59:PHE:O	2.19	0.43
45:2n:29:ARG:HD3	45:2n:40:CYS:SG	2.58	0.43
1:1A:143:G:H4'	19:1X:35:THR:HG21	2.00	0.42
1:1A:957:A:H4'	12:1Q:74:TYR:OH	2.19	0.42
1:1A:1430:C:H2'	1:1A:1431:U:C6	2.53	0.42
1:1A:2611:U:H5'	1:1A:2611:U:H6	1.84	0.42
1:1A:2801(A):A:H5"	1:1A:2802:G:C8	2.54	0.42
30:18:62:LEU:HB3	30:18:65:GLU:HG2	2.01	0.42
32:1a:562:C:H1'	43:1l:15:ARG:HB3	2.01	0.42
32:1a:1288:A:N3	32:1a:1352:C:O2'	2.48	0.42
32:1a:1347:G:N2	32:1a:1373:G:H2'	2.34	0.42
1:2A:139:G:H2'	1:2A:140:G:N7	2.34	0.42
1:2A:877:U:O2'	1:2A:900:A:N6	2.52	0.42
1:2A:923:C:H2'	1:2A:924:C:H6	1.84	0.42
1:2A:1263:U:C4	1:2A:1264:G:C6	3.06	0.42
1:2A:1354:A:O3'	3:2D:38:LYS:HE3	2.19	0.42
1:2A:1518:U:H2'	1:2A:1519:G:O4'	2.18	0.42
2:2B:19:G:H2'	2:2B:20:C:O4'	2.19	0.42
2:2B:42:C:O2'	6:2G:66:GLN:HG2	2.19	0.42
3:2D:70:TRP:CE2	3:2D:150:LYS:HG3	2.54	0.42
7:2H:3:ARG:NH1	7:2H:5:GLY:H	2.17	0.42
7:2H:43:VAL:HG13	7:2H:52:VAL:HG22	2.00	0.42
19:2X:5:TYR:CZ	24:22:30:ARG:HB2	2.53	0.42
32:2a:932:C:H4'	38:2g:4:ARG:CZ	2.49	0.42
32:2a:1352:C:H2'	32:2a:1353:G:C8	2.54	0.42
33:2b:31:TYR:CE2	33:2b:200:ILE:HG21	2.53	0.42
34:2c:123:GLN:HA	34:2c:126:ARG:HD2	2.01	0.42
35:2d:112:VAL:HG22	35:2d:116:GLN:OE1	2.19	0.42
36:2e:8:GLU:HG2	36:2e:34:VAL:HG23	2.01	0.42
42:2k:109:VAL:CG2	49:2r:84:LYS:HB3	2.49	0.42
51:2t:13:LEU:O	51:2t:17:ARG:HG3	2.19	0.42
1:1A:570:G:H2'	1:1A:2030:A:C5	2.54	0.42
1:1A:751:A:H5'	18:1W:90:ARG:HA	2.01	0.42
1:1A:2314:C:H2'	1:1A:2315:G:C8	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2478:A:O2'	1:1A:2536:G:N2	2.52	0.42
1:1A:2484:G:H1'	12:1Q:124:LYS:HD2	2.00	0.42
13:1R:72:ASP:HB3	13:1R:75:LEU:HB3	2.01	0.42
14:1S:34:HIS:HD1	14:1S:53:SER:HG	1.64	0.42
28:16:11:LEU:HD23	28:16:11:LEU:HA	1.91	0.42
32:1a:62:U:OP1	32:1a:385:C:O2'	2.31	0.42
32:1a:1111:A:N1	34:1c:177:THR:OG1	2.38	0.42
32:1a:1244:C:OP1	52:1u:9:ARG:HB2	2.19	0.42
37:1f:76:ALA:O	37:1f:80:ARG:HG3	2.19	0.42
38:1g:78:ARG:HD2	38:1g:156:TRP:CE3	2.53	0.42
42:1k:48:ILE:O	42:1k:50:TYR:N	2.48	0.42
44:1m:96:LEU:C	44:1m:110:ARG:HG2	2.44	0.42
1:2A:588:U:H2'	1:2A:589:C:C6	2.54	0.42
1:2A:2389:G:H5"	1:2A:2390:U:O4'	2.19	0.42
2:2B:55:U:O3'	6:2G:27:ASN:ND2	2.51	0.42
5:2F:32:LEU:HD13	5:2F:112:MET:HE1	2.00	0.42
10:2O:101:PRO:HD3	15:2T:68:TYR:HB2	2.00	0.42
12:2Q:20:ALA:HB2	21:2Z:79:ARG:HG2	2.00	0.42
12:2Q:57:HIS:NE2	12:2Q:116:GLU:HB3	2.34	0.42
21:2Z:30:ASN:HA	21:2Z:89:PHE:HE1	1.83	0.42
26:24:64:GLY:C	26:24:66:SER:N	2.77	0.42
33:2b:112:VAL:HG12	33:2b:149:LEU:HD22	2.02	0.42
1:1A:2224:G:H4'	1:1A:2226:C:C2	2.55	0.42
1:1A:2232:U:P	23:11:40:ARG:HH12	2.43	0.42
7:1H:56:SER:OG	7:1H:57:ASP:N	2.52	0.42
13:1R:67:LEU:HD13	13:1R:76:VAL:HG21	2.00	0.42
15:1T:94:ALA:HB1	15:1T:99:LEU:HD21	2.00	0.42
16:1U:27:LEU:HB3	16:1U:31:SER:HB3	1.99	0.42
24:12:53:LEU:HD23	24:12:53:LEU:HA	1.81	0.42
32:1a:97:G:H2'	32:1a:98:G:O4'	2.19	0.42
32:1a:472:A:H2'	32:1a:473:G:O4'	2.19	0.42
32:1a:812:C:N3	61:1a:2048:HOH:O	2.37	0.42
32:1a:1006:C:OP2	32:1a:1037:C:O2'	2.38	0.42
32:1a:1037:C:H2'	32:1a:1038:C:H6	1.83	0.42
32:1a:1530:G:H4'	32:1a:1530:G:OP1	2.20	0.42
34:1c:130:VAL:HG21	34:1c:157:ILE:HG23	2.00	0.42
40:1i:3:GLN:HE21	40:1i:20:ARG:HE	1.66	0.42
42:1k:34:ASP:OD1	42:1k:38:ASN:N	2.52	0.42
1:2A:598:G:H2'	1:2A:599:G:O4'	2.19	0.42
1:2A:996:A:H4'	16:2U:91:ASP:OD2	2.19	0.42
1:2A:1364:G:C8	23:21:3:LYS:HD2	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1580:A:H3'	1:2A:1581:G:C8	2.51	0.42
3:2D:69:ARG:HH11	3:2D:105:ILE:HG21	1.85	0.42
3:2D:242:ARG:HD2	3:2D:246:PRO:HG3	2.00	0.42
5:2F:184:TYR:CZ	5:2F:188:ARG:HD2	2.54	0.42
17:2V:85:LYS:HB2	17:2V:85:LYS:HE3	1.70	0.42
21:2Z:126:VAL:CG1	21:2Z:161:VAL:HG23	2.49	0.42
24:22:49:LYS:HE2	24:22:49:LYS:HB3	1.75	0.42
32:2a:397:A:H3'	32:2a:397:A:N3	2.34	0.42
32:2a:779:C:H2'	32:2a:780:A:O4'	2.18	0.42
32:2a:1321:C:H4'	44:2m:87:TYR:CE2	2.53	0.42
34:2c:180:ALA:HB1	34:2c:203:PHE:CE1	2.54	0.42
37:2f:3:ARG:HB3	37:2f:93:SER:HB2	2.01	0.42
40:2i:28:VAL:HG22	40:2i:63:ILE:HB	2.00	0.42
47:2p:51:VAL:HG12	47:2p:53:VAL:N	2.32	0.42
48:2q:82:MET:O	48:2q:86:GLU:HG2	2.19	0.42
50:2s:50:ALA:HA	50:2s:58:VAL:O	2.19	0.42
1:1A:478:A:N1	1:1A:500:G:H4'	2.33	0.42
1:1A:1178:C:O5'	1:1A:1178:C:H6	2.01	0.42
1:1A:1431:U:H2'	1:1A:1432:C:C6	2.55	0.42
1:1A:1769:G:O2'	1:1A:1958:C:OP1	2.28	0.42
1:1A:1798:U:H5'	3:1D:259:THR:CG2	2.47	0.42
9:1N:96:GLU:CD	9:1N:96:GLU:H	2.27	0.42
13:1R:98:LEU:HB2	13:1R:113:LEU:HD11	2.02	0.42
14:1S:10:ARG:HG3	14:1S:13:ARG:NH2	2.33	0.42
20:1Y:6:HIS:HE1	20:1Y:72:VAL:O	2.03	0.42
23:11:64:ALA:HA	23:11:67:ILE:HG13	2.00	0.42
32:1a:60:A:N1	32:1a:107:G:O2'	2.48	0.42
32:1a:92:C:H2'	32:1a:93:G:C8	2.54	0.42
32:1a:438:G:H4'	35:1d:123:HIS:CE1	2.54	0.42
32:1a:613:C:H2'	32:1a:614:A:C8	2.55	0.42
32:1a:841:U:OP2	32:1a:841:U:H6	2.01	0.42
43:1l:7:ILE:O	43:1l:11:VAL:HG23	2.18	0.42
46:1o:39:LEU:HD22	46:1o:56:LEU:HB2	2.00	0.42
1:2A:648:G:H2'	1:2A:649:G:C8	2.54	0.42
1:2A:807:U:O2'	1:2A:2060:A:N1	2.50	0.42
1:2A:2586:C:OP2	1:2A:2608:G:N1	2.42	0.42
1:2A:2792:G:H2'	1:2A:2792:G:N3	2.35	0.42
4:2E:11:MET:HG2	4:2E:24:THR:HB	2.00	0.42
10:2O:1:MET:HG3	10:2O:67:LYS:HG2	2.00	0.42
10:2O:64:ARG:HB2	10:2O:79:PHE:CD2	2.54	0.42
11:2P:101:VAL:HA	11:2P:106:LEU:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:2R:26:LYS:HE2	13:2R:70:LEU:O	2.19	0.42
21:2Z:54:HIS:HB3	21:2Z:101:PRO:HD3	2.02	0.42
26:24:34:GLU:HA	44:2m:57:ARG:NH1	2.34	0.42
27:25:16:ARG:NH1	27:25:17:ASP:OD1	2.52	0.42
32:2a:1359:C:O2'	32:2a:1361:G:N7	2.52	0.42
34:2c:9:GLY:HA3	45:2n:49:HIS:HA	2.01	0.42
35:2d:200:GLU:O	35:2d:204:ILE:HG12	2.19	0.42
46:2o:15:PHE:CE1	46:2o:84:LYS:HE3	2.54	0.42
54:2y:37:MIA:H2'	54:2y:38:A:O4'	2.20	0.42
1:1A:27:G:C2	1:1A:512:G:N3	2.87	0.42
1:1A:1027:A:C2	1:1A:2488:A:H5'	2.54	0.42
1:1A:1055:G:N2	1:1A:1104:C:N3	2.58	0.42
1:1A:2378:A:H2'	14:1S:21:THR:HG21	2.02	0.42
1:1A:2869:G:H2'	1:1A:2870:C:O4'	2.19	0.42
2:1B:42:C:O2'	6:1G:66:GLN:HG2	2.19	0.42
3:1D:208:LYS:HG3	3:1D:210:GLY:H	1.84	0.42
4:1E:9:VAL:HB	15:1T:3:ARG:HG2	2.02	0.42
10:1O:1:MET:HE2	10:1O:1:MET:HB3	1.81	0.42
15:1T:95:ARG:HB2	15:1T:96:ARG:HH12	1.84	0.42
17:1V:40:LEU:HB2	17:1V:46:VAL:HG22	2.01	0.42
26:14:55:ARG:H	26:14:56:VAL:HA	1.85	0.42
32:1a:253:U:H2'	32:1a:254:G:H8	1.85	0.42
32:1a:774:G:H2'	32:1a:775:G:O4'	2.19	0.42
32:1a:1028:C:N4	32:1a:1033:G:H1	2.15	0.42
32:1a:1053:G:O2'	61:1a:2107:HOH:O	2.22	0.42
32:1a:1488:G:H2'	32:1a:1489:G:C8	2.54	0.42
34:1c:122:GLU:O	34:1c:126:ARG:NH1	2.47	0.42
1:2A:250:G:C6	1:2A:251:A:C6	3.08	0.42
1:2A:320:A:H4'	1:2A:322:A:N7	2.34	0.42
1:2A:459:U:OP2	29:27:39:ARG:NH1	2.52	0.42
1:2A:729:G:C6	3:2D:208:LYS:HB2	2.54	0.42
1:2A:784:A:N6	3:2D:229:VAL:HG11	2.34	0.42
1:2A:1847:A:H3'	1:2A:1848:A:H5'	2.01	0.42
1:2A:2377:A:H2'	1:2A:2378:A:C8	2.54	0.42
1:2A:2494:G:OP1	22:20:3:HIS:N	2.43	0.42
1:2A:2612:C:OP2	27:25:2:ALA:N	2.52	0.42
1:2A:2748:A:H2	7:2H:63:SER:HB3	1.84	0.42
5:2F:32:LEU:O	5:2F:36:VAL:HG23	2.19	0.42
8:2I:26:ALA:O	8:2I:31:LEU:HB2	2.20	0.42
11:2P:83:VAL:HG22	11:2P:112:LEU:HD11	2.01	0.42
14:2S:62:LYS:O	14:2S:66:ALA:N	2.51	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:23:6:VAL:HG13	25:23:54:VAL:HG11	2.01	0.42
32:2a:476:G:H2'	32:2a:477:A:H8	1.85	0.42
32:2a:979:C:H41	32:2a:1360:A:N6	2.17	0.42
32:2a:1346:A:N1	32:2a:1374:A:H5"	2.34	0.42
32:2a:1387:G:H2'	32:2a:1388:C:H6	1.83	0.42
40:2i:4:TYR:CE1	40:2i:88:TYR:HA	2.55	0.42
45:2n:14:PRO:HB2	45:2n:19:ARG:HB2	2.01	0.42
52:2u:6:ARG:HG2	52:2u:15:ARG:HE	1.84	0.42
1:1A:573:G:O2'	1:1A:574:C:H3'	2.20	0.42
1:1A:744:G:OP1	4:1E:132:HIS:ND1	2.50	0.42
1:1A:817:C:H4'	1:1A:932:G:C5	2.55	0.42
1:1A:1057:A:N6	1:1A:1081:U:H3	2.15	0.42
1:1A:1187:G:H5"	17:1V:81:TYR:CE1	2.54	0.42
1:1A:1645:G:H5"	1:1A:1646:C:O4'	2.20	0.42
1:1A:1794:U:H2'	1:1A:1795:C:C6	2.55	0.42
1:1A:1821:A:H2'	1:1A:1822:G:C8	2.55	0.42
6:1G:25:TYR:CZ	6:1G:32:PRO:HD3	2.54	0.42
6:1G:49:ASP:OD1	6:1G:49:ASP:N	2.53	0.42
6:1G:142:PRO:HB2	26:14:31:ILE:HG21	2.01	0.42
9:1N:66:LYS:HB3	9:1N:70:LYS:HB2	2.00	0.42
11:1P:62:LEU:O	30:18:13:ARG:HD3	2.20	0.42
19:1X:28:PHE:CE1	19:1X:92:LEU:HD11	2.55	0.42
25:13:23:LEU:HD13	25:13:50:VAL:HG11	2.01	0.42
26:14:53:GLU:O	26:14:56:VAL:HG13	2.19	0.42
32:1a:194:C:C2'	32:1a:195:A:H5"	2.49	0.42
32:1a:390:C:H2'	32:1a:391:G:H8	1.83	0.42
32:1a:1425:U:H2'	32:1a:1426:C:C6	2.55	0.42
33:1b:111:ARG:HA	33:1b:111:ARG:HD3	1.82	0.42
47:1p:14:ASN:OD1	47:1p:42:ARG:NH2	2.53	0.42
47:1p:37:GLY:HA3	47:1p:50:LYS:O	2.19	0.42
54:1w:24:G:C6	54:1w:25:C:C4	3.08	0.42
54:1w:43:C:H2'	54:1w:44:G:C8	2.55	0.42
54:1w:70:G:C4	54:1w:71:G:H1'	2.54	0.42
1:2A:797:C:H2'	1:2A:798:G:O4'	2.20	0.42
1:2A:1027:A:C2	1:2A:2488:A:H5'	2.54	0.42
1:2A:1262:A:H2	27:25:10:LYS:HD2	1.83	0.42
1:2A:1405:U:H2'	1:2A:1406:U:C6	2.54	0.42
1:2A:1495:A:H2'	1:2A:1496:A:C8	2.53	0.42
1:2A:1540:U:H2'	1:2A:1541:G:O4'	2.20	0.42
1:2A:2278:A:OP2	22:20:12:ASN:ND2	2.43	0.42
1:2A:2305:A:H5"	6:2G:134:GLY:HA3	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2617:C:H2'	1:2A:2618:G:O4'	2.20	0.42
1:2A:2649:U:H2'	1:2A:2650:U:C6	2.54	0.42
7:2H:56:SER:OG	7:2H:57:ASP:N	2.53	0.42
10:2O:2:ILE:HD12	10:2O:6:THR:HG21	2.01	0.42
11:2P:138:LEU:HG	11:2P:143:GLY:HA3	2.00	0.42
13:2R:87:TYR:CD1	13:2R:90:ARG:HD2	2.55	0.42
20:2Y:14:LEU:HG	20:2Y:15:VAL:N	2.34	0.42
20:2Y:19:LYS:HB3	20:2Y:19:LYS:HE2	1.84	0.42
21:2Z:72:ARG:HD3	21:2Z:72:ARG:HA	1.73	0.42
32:2a:1287:A:H2	32:2a:1353:G:H1'	1.83	0.42
34:2c:22:TRP:CD2	34:2c:59:ARG:HD2	2.55	0.42
35:2d:180:GLY:O	35:2d:181:MET:HG2	2.19	0.42
45:2n:6:LEU:O	45:2n:10:ALA:N	2.50	0.42
49:2r:21:LYS:O	49:2r:25:THR:HG23	2.19	0.42
55:2x:8:4SU:O2	55:2x:21:A:C2	2.72	0.42
55:2x:47:U:H3'	55:2x:48:C:C5'	2.49	0.42
1:1A:762:U:OP1	61:1A:6670:HOH:O	2.22	0.42
1:1A:1047:G:H2'	1:1A:1110:G:H22	1.84	0.42
1:1A:1064:C:H2'	1:1A:1065:U:H5'	2.01	0.42
1:1A:1190:G:H5"	11:1P:32:THR:O	2.20	0.42
2:1B:83:G:OP1	25:13:19:GLN:NE2	2.49	0.42
4:1E:11:MET:HE2	4:1E:11:MET:HB3	1.90	0.42
19:1X:40:LYS:O	19:1X:44:GLU:HG3	2.19	0.42
21:1Z:154:ASP:C	21:1Z:155:LEU:HD12	2.44	0.42
25:13:39:ASP:OD1	25:13:44:ARG:NH1	2.52	0.42
32:1a:4:U:O4	39:1h:105:ARG:HG2	2.19	0.42
32:1a:234:C:H2'	32:1a:235:C:H6	1.83	0.42
33:1b:146:GLN:O	33:1b:150:SER:HB3	2.19	0.42
43:1l:60:LEU:HD21	43:1l:85:ILE:HD11	2.02	0.42
54:1y:46:7MG:O2'	54:1y:48:C:OP2	2.33	0.42
1:2A:746:A:H2'	1:2A:2612:C:H5"	2.00	0.42
1:2A:2116:G:N2	1:2A:2162:G:OP1	2.52	0.42
1:2A:2398:U:H2'	1:2A:2399:G:C8	2.55	0.42
1:2A:2512:C:H2'	1:2A:2513:G:O4'	2.19	0.42
5:2F:33:LEU:HD11	5:2F:112:MET:HB3	2.01	0.42
12:2Q:36:ALA:HA	12:2Q:129:THR:HG22	2.02	0.42
15:2T:51:ARG:HG2	15:2T:62:THR:HB	2.02	0.42
25:23:6:VAL:HG13	25:23:54:VAL:CG1	2.49	0.42
32:2a:93:G:C6	32:2a:96:U:C4	3.08	0.42
32:2a:259:G:H2'	32:2a:260:G:O4'	2.19	0.42
32:2a:620:C:H2'	32:2a:621:A:O4'	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1343:G:H1'	40:2i:121:ARG:HH11	1.84	0.42
38:2g:97:GLN:O	38:2g:101:LEU:HG	2.20	0.42
43:2l:53:ARG:HB2	43:2l:93:LEU:HD11	2.02	0.42
43:2l:58:VAL:HG12	43:2l:60:LEU:HD12	2.02	0.42
53:2v:22:U:H2'	53:2v:23:A:C8	2.54	0.42
54:2w:14:A:C2	54:2w:22:G:H1'	2.55	0.42
1:1A:27:G:O2'	1:1A:28:A:OP2	2.35	0.42
1:1A:686:G:N2	1:1A:788:A:H61	2.18	0.42
1:1A:1069:A:H1'	1:1A:1096:A:H4'	2.02	0.42
1:1A:1274:A:N3	1:1A:1297:C:H1'	2.35	0.42
1:1A:1465:G:O2'	1:1A:1545:A:N1	2.52	0.42
2:1B:28:C:H2'	2:1B:29:A:O4'	2.20	0.42
14:1S:10:ARG:HG3	14:1S:13:ARG:HH22	1.85	0.42
16:1U:47:TYR:HA	16:1U:50:ARG:NH2	2.34	0.42
18:1W:65:LEU:HB2	18:1W:68:ARG:HD2	2.01	0.42
20:1Y:28:LYS:HD2	20:1Y:40:GLU:OE1	2.20	0.42
20:1Y:106:LEU:O	20:1Y:107:ASP:HB2	2.19	0.42
32:1a:461:A:O2'	32:1a:470:C:H5'	2.20	0.42
32:1a:601:C:H2'	32:1a:602:A:C8	2.53	0.42
32:1a:629:G:H2'	32:1a:630:G:O4'	2.20	0.42
32:1a:1064:G:H4'	32:1a:1065:U:OP1	2.19	0.42
32:1a:1320:C:O2	50:1s:36:ARG:NH2	2.52	0.42
39:1h:110:ALA:HB3	39:1h:121:ASP:HB3	2.02	0.42
54:1y:18:G:N2	54:1y:57:G:C5	2.88	0.42
1:2A:297:C:H2'	1:2A:298:G:O4'	2.20	0.42
1:2A:729:G:O5'	3:2D:208:LYS:NZ	2.53	0.42
1:2A:1022:G:OP2	9:2N:69:GLN:NE2	2.46	0.42
1:2A:1832:C:H2'	1:2A:1833:U:O4'	2.20	0.42
1:2A:2133:G:C6	1:2A:2157:G:C6	3.08	0.42
1:2A:2758:A:C4	7:2H:67:LEU:HD21	2.55	0.42
2:2B:15:A:OP2	2:2B:69:G:N2	2.53	0.42
4:2E:101:ARG:CZ	4:2E:171:GLU:HB2	2.50	0.42
4:2E:181:LEU:HA	4:2E:181:LEU:HD12	1.74	0.42
10:2O:7:TYR:CZ	10:2O:44:LYS:HG3	2.55	0.42
15:2T:19:LEU:HD13	15:2T:86:ILE:HD12	2.02	0.42
16:2U:88:ILE:HG22	16:2U:90:VAL:HG23	2.01	0.42
21:2Z:149:SER:HG	21:2Z:170:THR:HG1	1.64	0.42
32:2a:156:G:H1	32:2a:165:C:H42	1.68	0.42
32:2a:779:C:O2'	42:2k:120:ARG:NH1	2.46	0.42
32:2a:1324:A:O4'	32:2a:1362:C:H4'	2.20	0.42
32:2a:1502:A:C8	32:2a:1505:G:N2	2.87	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:2b:111:ARG:HH11	33:2b:111:ARG:HA	1.84	0.42
36:2e:78:HIS:HB2	39:2h:104:ARG:HG2	2.02	0.42
38:2g:69:VAL:HA	38:2g:138:LYS:HD3	2.02	0.42
44:2m:87:TYR:CZ	44:2m:91:ARG:HD2	2.55	0.42
45:2n:21:TYR:OH	45:2n:23:ARG:NH2	2.45	0.42
54:2y:69:G:H2'	54:2y:70:G:O4'	2.19	0.42
1:1A:196:A:H2'	1:1A:196:A:N3	2.35	0.42
1:1A:271(E):U:H2'	1:1A:271(F):C:C6	2.55	0.42
1:1A:284:U:H2'	1:1A:285:C:C6	2.55	0.42
1:1A:1653:G:O3'	13:1R:2:ARG:HB2	2.19	0.42
61:1A:5688:HOH:O	11:1P:43:GLY:HA3	2.20	0.42
3:1D:147:LEU:HD13	3:1D:155:LEU:HD21	2.02	0.42
5:1F:125:LEU:HD21	5:1F:199:TRP:CD2	2.55	0.42
25:13:3:ARG:HB2	25:13:59:VAL:HG23	2.01	0.42
25:13:19:GLN:OE1	25:13:52:HIS:NE2	2.44	0.42
32:1a:134:A:H61	47:1p:25:ARG:HH12	1.67	0.42
32:1a:857:C:H2'	32:1a:858:G:O4'	2.20	0.42
32:1a:1004:A:C5'	32:1a:1024:G:H1	2.30	0.42
37:1f:97:PHE:HD2	49:1r:31:LEU:HD11	1.85	0.42
42:1k:99:GLN:HA	42:1k:105:VAL:HG21	2.02	0.42
44:1m:118:ALA:HB2	55:1x:28:C:H4'	2.01	0.42
54:1y:18:G:C2	54:1y:58:A:C5	3.08	0.42
1:2A:631:A:H1'	11:2P:66:GLY:HA2	2.02	0.42
1:2A:1429:G:H2'	1:2A:1430:C:C6	2.54	0.42
1:2A:1477:A:H2'	1:2A:1478:G:O4'	2.20	0.42
1:2A:2658:C:H5'	7:2H:160:LYS:HZ2	1.84	0.42
6:2G:27:ASN:HB3	6:2G:30:GLU:HB2	2.01	0.42
7:2H:152:ARG:HD3	7:2H:152:ARG:HA	1.86	0.42
14:2S:20:ARG:HA	14:2S:20:ARG:HD2	1.94	0.42
21:2Z:128:VAL:HG23	21:2Z:160:GLY:O	2.20	0.42
21:2Z:158:PRO:HA	21:2Z:159:PRO:HD3	1.97	0.42
32:2a:391:G:N7	61:2a:3610:HOH:O	2.37	0.42
32:2a:781:A:OP1	32:2a:1523:G:H5'	2.20	0.42
41:2j:27:ALA:HB3	41:2j:34:VAL:HG12	2.01	0.42
55:2x:61:C:H2'	55:2x:62:C:H6	1.84	0.42
1:1A:106:C:HO2'	1:1A:294:A:HO2'	1.66	0.42
1:1A:129:C:H2'	1:1A:130:C:H6	1.85	0.42
1:1A:251:A:C5	1:1A:252:G:H1'	2.54	0.42
1:1A:479:A:N3	1:1A:481:G:H5"	2.35	0.42
1:1A:607:U:OP1	5:1F:102:PRO:HA	2.20	0.42
1:1A:1156:A:OP1	16:1U:55:ARG:NH1	2.45	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1216:G:O6	61:1A:4803:HOH:O	2.21	0.42
1:1A:2040:C:H2'	1:1A:2041:U:O4'	2.20	0.42
1:1A:2141:G:C6	1:1A:2142:C:C2	3.07	0.42
1:1A:2846:G:H2'	1:1A:2847:U:O4'	2.20	0.42
6:1G:62:LEU:HA	26:14:27:THR:HG21	2.02	0.42
8:1I:26:ALA:O	8:1I:31:LEU:HB2	2.20	0.42
9:1N:62:VAL:CG1	9:1N:66:LYS:HB2	2.50	0.42
14:1S:15:ARG:C	14:1S:19:LYS:HZ3	2.27	0.42
18:1W:36:LEU:HD13	18:1W:48:ALA:HA	2.02	0.42
18:1W:46:PHE:O	18:1W:50:VAL:HG23	2.20	0.42
30:18:30:ARG:O	61:18:207:HOH:O	2.22	0.42
32:1a:524:G:H2'	32:1a:525:C:C6	2.54	0.42
32:1a:828:A:H2'	32:1a:829:G:O4'	2.19	0.42
32:1a:1008:C:N3	32:1a:1021:G:C6	2.87	0.42
32:1a:1295:G:O2'	44:1m:14:ARG:NH1	2.52	0.42
32:1a:1463:C:H2'	32:1a:1464:G:O4'	2.19	0.42
33:1b:178:ARG:NH2	39:1h:74:PRO:HB3	2.34	0.42
35:1d:200:GLU:O	35:1d:204:ILE:HG12	2.19	0.42
36:1e:82:VAL:HG21	36:1e:138:ALA:HA	2.02	0.42
53:1v:16:A:H2'	53:1v:17:U:O4'	2.20	0.42
1:2A:359:A:H2'	1:2A:360:G:O4'	2.20	0.42
1:2A:1639:U:H4'	1:2A:2699:C:H4'	2.02	0.42
1:2A:1713:U:H2'	1:2A:1714:G:H8	1.84	0.42
1:2A:1778:U:H2'	1:2A:1784:A:N6	2.35	0.42
1:2A:1902:C:H5'	3:2D:246:PRO:HD3	2.02	0.42
1:2A:2313:C:H2'	1:2A:2314:C:C6	2.55	0.42
6:2G:16:ARG:O	6:2G:20:ILE:HG13	2.19	0.42
26:24:18:CYS:SG	26:24:20:ASN:HB2	2.60	0.42
32:2a:72:C:H2'	32:2a:73:G:C8	2.55	0.42
32:2a:266:G:H2'	32:2a:266:G:N3	2.35	0.42
32:2a:986:A:O2'	50:2s:55:LYS:HA	2.19	0.42
32:2a:991:U:C4	32:2a:1212:U:H1'	2.54	0.42
32:2a:1128:C:O2'	32:2a:1147:C:N3	2.37	0.42
32:2a:1151:A:O2'	32:2a:1152:A:O5'	2.32	0.42
34:2c:52:LEU:HD12	34:2c:53:ALA:H	1.85	0.42
51:2t:50:GLU:O	51:2t:100:ILE:HD11	2.20	0.42
55:2x:37:A:H2'	55:2x:38:A:O4'	2.20	0.42
1:1A:669:G:N2	61:1A:4261:HOH:O	2.44	0.41
1:1A:1156:A:C8	16:1U:51:LYS:HD2	2.54	0.41
1:1A:1588:C:H2'	1:1A:1589:C:H6	1.84	0.41
1:1A:2032:G:OP2	1:1A:2454:G:O2'	2.29	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2849:U:OP2	15:1T:95:ARG:NH1	2.53	0.41
8:1I:50:ARG:CZ	8:1I:50:ARG:HB3	2.50	0.41
15:1T:33:LYS:HD3	15:1T:82:LEU:HD22	2.02	0.41
15:1T:95:ARG:HB2	15:1T:96:ARG:NH1	2.35	0.41
21:1Z:44:PHE:CZ	21:1Z:86:VAL:HG11	2.55	0.41
24:12:51:ARG:HD3	24:12:55:ARG:NH1	2.35	0.41
25:13:31:LEU:HD23	25:13:31:LEU:HA	1.92	0.41
27:15:16:ARG:NH1	27:15:17:ASP:OD1	2.53	0.41
32:1a:454:C:H3'	32:1a:455:C:C6	2.55	0.41
32:1a:629:G:H3'	32:1a:630:G:H5"	2.01	0.41
32:1a:688:G:H5'	42:1k:46:GLY:C	2.45	0.41
32:1a:926:G:O2'	53:1v:13:A:N3	2.50	0.41
32:1a:1429:C:H2'	32:1a:1430:C:C6	2.55	0.41
34:1c:131:ARG:NE	34:1c:135:LYS:HE3	2.33	0.41
40:1i:28:VAL:HG22	40:1i:63:ILE:HB	2.01	0.41
1:2A:784:A:OP1	1:2A:2588:G:H5"	2.19	0.41
1:2A:948:G:H21	1:2A:985:C:P	2.43	0.41
1:2A:2011:U:H2'	1:2A:2012:G:O4'	2.20	0.41
1:2A:2138:C:H2'	1:2A:2139:C:O4'	2.20	0.41
1:2A:2166:G:N7	1:2A:2168:G:N2	2.68	0.41
1:2A:2320:A:N3	1:2A:2320:A:H2'	2.34	0.41
1:2A:2533:A:OP1	1:2A:2665:A:O2'	2.37	0.41
2:2B:30:C:H2'	2:2B:31:C:H5'	2.02	0.41
2:2B:50:G:P	14:2S:62:LYS:HB2	2.60	0.41
5:2F:110:LEU:HD11	5:2F:181:LEU:HG	2.02	0.41
13:2R:29:LEU:HD12	13:2R:29:LEU:HA	1.85	0.41
20:2Y:87:LYS:HB3	20:2Y:95:LYS:HD2	2.01	0.41
32:2a:24:U:H2'	32:2a:25:C:C6	2.55	0.41
32:2a:742:G:P	46:2o:35:ARG:HH22	2.42	0.41
32:2a:1469:G:H2'	32:2a:1470:G:C8	2.55	0.41
33:2b:109:SER:O	33:2b:112:VAL:HG22	2.19	0.41
1:1A:271(H):G:H4'	23:11:81:LYS:HG2	2.02	0.41
1:1A:271(V):G:O6	61:1A:5975:HOH:O	2.22	0.41
1:1A:596:G:H2'	1:1A:597:U:O4'	2.20	0.41
1:1A:784:A:C6	3:1D:229:VAL:HG11	2.55	0.41
1:1A:996:A:O3'	16:1U:91:ASP:HB2	2.20	0.41
1:1A:2432:A:N9	23:11:33:LYS:HD3	2.35	0.41
6:1G:28:VAL:O	6:1G:31:VAL:HG12	2.20	0.41
8:1I:60:GLU:HG3	8:1I:61:ARG:NH1	2.35	0.41
11:1P:128:HIS:NE2	11:1P:148:LEU:HD11	2.35	0.41
26:14:49:PHE:HD1	26:14:49:PHE:HA	1.73	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:452:A:H4'	47:1p:72:ARG:CZ	2.50	0.41
32:1a:593:G:H2'	32:1a:594:G:O4'	2.19	0.41
32:1a:1065:U:H1'	32:1a:1066:C:OP2	2.20	0.41
32:1a:1221:G:O3'	50:1s:77:THR:OG1	2.34	0.41
32:1a:1429:C:H2'	32:1a:1430:C:H6	1.85	0.41
35:1d:18:LYS:CG	60:1d:302:SF4:S1	3.08	0.41
36:1e:12:LEU:HB3	36:1e:31:LEU:HB2	2.02	0.41
37:1f:55:ASP:HB2	37:1f:86:ARG:HH12	1.84	0.41
55:1x:50:U:H3	55:1x:64:G:H1	1.66	0.41
54:1y:47:U:O2'	54:1y:50:U:OP1	2.31	0.41
1:2A:56:A:H2'	1:2A:57:C:O4'	2.21	0.41
1:2A:1939:5MU:OP1	1:2A:2604:U:O2'	2.36	0.41
1:2A:2419:U:H2'	1:2A:2420:C:C6	2.56	0.41
1:2A:2558:C:H2'	1:2A:2559:C:O4'	2.20	0.41
1:2A:2643:G:H2'	1:2A:2644:G:O4'	2.19	0.41
1:2A:2697:G:H2'	1:2A:2698:U:O4'	2.21	0.41
2:2B:75:G:H1	21:2Z:73:GLN:NE2	2.19	0.41
7:2H:56:SER:HB3	7:2H:61:HIS:HD1	1.83	0.41
15:2T:73:GLU:OE2	15:2T:103:ARG:NE	2.53	0.41
26:24:40:HIS:O	26:24:44:THR:HG22	2.20	0.41
32:2a:434:U:H2'	32:2a:435:C:H6	1.85	0.41
32:2a:1061:G:H1'	41:2j:56:HIS:CE1	2.55	0.41
35:2d:149:ALA:HB3	35:2d:152:SER:HB2	2.01	0.41
44:2m:13:LYS:O	44:2m:45:VAL:HG23	2.21	0.41
48:2q:21:VAL:HG21	48:2q:59:ILE:HG21	2.01	0.41
49:2r:44:LEU:HD11	49:2r:79:LEU:HD13	2.02	0.41
53:2v:14:A:H2'	53:2v:14:A:N3	2.35	0.41
54:2w:31:A:H2'	54:2w:32:PSU:O4'	2.20	0.41
1:1A:1119:C:N4	61:1A:6713:HOH:O	2.53	0.41
1:1A:1866:C:H2'	1:1A:1876:A:O4'	2.20	0.41
1:1A:2206:G:H5"	1:1A:2207:G:N7	2.35	0.41
1:1A:2376:A:H2'	1:1A:2377:A:O4'	2.20	0.41
1:1A:2715:C:H2'	1:1A:2716:U:C6	2.56	0.41
32:1a:270:A:H2'	32:1a:271:C:O4'	2.20	0.41
32:1a:309:G:O2'	32:1a:607:A:N1	2.53	0.41
32:1a:375:U:OP1	47:1p:69:THR:HG21	2.19	0.41
32:1a:672:U:H2'	32:1a:673:G:C8	2.56	0.41
32:1a:749:C:H2'	32:1a:750:G:H8	1.85	0.41
32:1a:1060:C:H2'	32:1a:1061:G:H8	1.86	0.41
32:1a:1134:G:N3	32:1a:1134:G:H2'	2.35	0.41
32:1a:1519:MA6:H5"	32:1a:1520:G:OP2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:1p:48:TRP:HH2	47:1p:76:GLN:HE22	1.67	0.41
54:1y:28:G:N2	54:1y:42:C:N3	2.53	0.41
1:2A:288:C:H2'	1:2A:289:A:C8	2.54	0.41
1:2A:307:G:N2	1:2A:330:A:H62	2.16	0.41
1:2A:597:U:H2'	1:2A:598:G:H8	1.86	0.41
1:2A:1235:G:C6	1:2A:1236:G:N1	2.87	0.41
1:2A:1364:G:N7	23:21:3:LYS:HD2	2.36	0.41
1:2A:1510:G:H2'	1:2A:1511:C:O4'	2.20	0.41
1:2A:1619:G:N2	29:27:1:MET:O	2.47	0.41
1:2A:1770:G:H4'	1:2A:1938:A:OP1	2.20	0.41
1:2A:2185:C:H2'	1:2A:2186:G:O4'	2.21	0.41
1:2A:2419:U:H2'	1:2A:2420:C:H6	1.85	0.41
2:2B:43:C:O4'	6:2G:66:GLN:NE2	2.53	0.41
3:2D:159:ALA:HB1	3:2D:198:ASN:O	2.20	0.41
6:2G:5:VAL:HG22	6:2G:8:LYS:HE2	2.02	0.41
9:2N:99:LEU:HD23	9:2N:99:LEU:HA	1.84	0.41
32:2a:792:A:H4'	32:2a:793:U:H5"	2.01	0.41
32:2a:1084:G:H5'	32:2a:1102:A:OP2	2.21	0.41
32:2a:1286:A:H2	52:2u:18:TYR:OH	2.02	0.41
32:2a:1370:G:N7	40:2i:109:VAL:HG11	2.35	0.41
32:2a:1411:C:H2'	32:2a:1412:C:C6	2.55	0.41
33:2b:80:ILE:HD13	33:2b:211:ILE:HG22	2.02	0.41
33:2b:111:ARG:HA	33:2b:111:ARG:HD3	1.80	0.41
34:2c:54:ARG:H	34:2c:69:HIS:HB2	1.84	0.41
34:2c:111:LEU:HD21	34:2c:146:ALA:HB2	2.00	0.41
34:2c:122:GLU:O	34:2c:126:ARG:HG3	2.20	0.41
34:2c:164:ARG:NH2	34:2c:166:GLU:OE1	2.53	0.41
35:2d:92:VAL:O	35:2d:96:LEU:HD13	2.20	0.41
37:2f:91:VAL:HG11	49:2r:72:ARG:NH1	2.35	0.41
37:2f:100:ASN:HB2	49:2r:28:GLU:HA	2.01	0.41
41:2j:6:ILE:HB	41:2j:72:VAL:HG23	2.01	0.41
44:2m:85:GLY:HA2	44:2m:93:ARG:NH2	2.35	0.41
49:2r:22:VAL:HB	49:2r:56:THR:HA	2.02	0.41
54:2y:2:C:H2'	54:2y:3:C:H6	1.86	0.41
1:1A:129:C:H2'	1:1A:130:C:C6	2.55	0.41
1:1A:238:C:H2'	1:1A:239:U:O4'	2.21	0.41
1:1A:249:C:O2	30:18:12:LYS:NZ	2.36	0.41
1:1A:1178:C:H2'	1:1A:1179:C:C6	2.55	0.41
1:1A:1853:A:H2'	1:1A:1854:A:C8	2.55	0.41
1:1A:1913:A:C8	32:1a:1494:G:H4'	2.56	0.41
2:1B:1:U:HO2'	2:1B:2:C:P	2.42	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1D:146:GLU:HG2	3:1D:152:GLY:C	2.46	0.41
4:1E:52:LEU:HA	4:1E:53:PRO:HD3	1.91	0.41
13:1R:28:LEU:HD22	13:1R:44:LEU:HD13	2.03	0.41
26:14:16:CYS:SG	26:14:17:GLY:N	2.93	0.41
32:1a:1104:G:O2'	33:1b:111:ARG:NH2	2.53	0.41
32:1a:1346:A:O3'	32:1a:1347:G:H4'	2.20	0.41
33:1b:60:ASP:OD1	33:1b:64:ARG:NH2	2.53	0.41
34:1c:131:ARG:HH21	34:1c:135:LYS:HE3	1.85	0.41
38:1g:104:LEU:HD12	38:1g:134:ALA:HB1	2.01	0.41
47:1p:4:ILE:HG13	47:1p:64:ALA:HB1	2.02	0.41
54:1w:22:G:H5'	54:1w:23:A:OP2	2.21	0.41
54:1y:20:U:O3'	54:1y:21:A:H4'	2.21	0.41
1:2A:116:C:H2'	1:2A:117:G:O4'	2.21	0.41
1:2A:579:G:H2'	1:2A:580:C:C6	2.54	0.41
1:2A:896:A:H1'	54:2w:56:C:H5'	2.02	0.41
1:2A:1996:C:H4'	1:2A:1997:G:OP1	2.19	0.41
1:2A:2543:G:H2'	1:2A:2544:G:C8	2.56	0.41
1:2A:2679:A:H4'	4:2E:165:VAL:HG11	2.01	0.41
1:2A:2712:U:O2'	1:2A:2713:A:H5'	2.21	0.41
2:2B:42:C:O2	6:2G:93:THR:N	2.33	0.41
8:2I:93:THR:H	8:2I:96:ASP:HB2	1.85	0.41
9:2N:67:LEU:HD12	9:2N:87:LEU:HD22	2.02	0.41
14:2S:53:SER:O	14:2S:57:LYS:N	2.47	0.41
32:2a:751:U:H4'	46:2o:24:SER:HA	2.01	0.41
32:2a:1010:G:H2'	32:2a:1011:G:C8	2.55	0.41
32:2a:1375:A:O2'	38:2g:29:LYS:NZ	2.52	0.41
34:2c:135:LYS:HZ3	36:2e:52:PRO:HG2	1.86	0.41
40:2i:23:ASN:N	40:2i:60:ASP:OD1	2.53	0.41
44:2m:34:LEU:HD13	44:2m:41:PRO:HB3	2.02	0.41
47:2p:74:LEU:HG	47:2p:79:VAL:HG21	2.02	0.41
48:2q:12:SER:HB3	48:2q:20:THR:HB	2.02	0.41
1:1A:83:G:N7	61:1A:7268:HOH:O	2.37	0.41
1:1A:582:G:H2'	1:1A:583:G:C8	2.55	0.41
1:1A:1766:U:H2'	1:1A:1767:C:C6	2.55	0.41
1:1A:1837:C:OP1	32:1a:784:C:H4'	2.21	0.41
1:1A:1997:G:H5"	4:1E:117:MET:CE	2.51	0.41
4:1E:116:VAL:HG13	4:1E:122:PHE:HB2	2.02	0.41
5:1F:24:LEU:HD23	5:1F:115:ALA:HA	2.03	0.41
9:1N:14:VAL:HG11	9:1N:138:LEU:HD12	2.01	0.41
22:10:10:THR:HA	61:10:205:HOH:O	2.20	0.41
32:1a:250:A:H5'	32:1a:252:U:O4'	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:404:U:H2'	32:1a:405:U:C6	2.55	0.41
32:1a:413:G:H21	32:1a:428:G:H1'	1.86	0.41
32:1a:445:G:H2'	32:1a:446:G:C8	2.55	0.41
32:1a:769:G:N7	61:1a:2041:HOH:O	2.36	0.41
32:1a:1521:G:N3	61:1a:2054:HOH:O	2.37	0.41
33:1b:16:HIS:HB2	33:1b:204:ASN:CB	2.50	0.41
45:1n:24:CYS:HB3	45:1n:29:ARG:H	1.86	0.41
48:1q:64:PRO:HB3	48:1q:70:ARG:NH1	2.36	0.41
50:1s:80:TYR:O	50:1s:81:ARG:HG2	2.21	0.41
1:2A:265:A:C8	1:2A:266:G:H1'	2.55	0.41
1:2A:493:G:H2'	1:2A:494:G:O4'	2.21	0.41
1:2A:569:U:H1'	1:2A:947:G:O4'	2.21	0.41
1:2A:852:G:H2'	1:2A:853:G:H8	1.84	0.41
1:2A:1278:A:H2'	1:2A:1279:G:C8	2.56	0.41
1:2A:1471:A:OP2	1:2A:1519:G:N2	2.41	0.41
1:2A:2046:G:O5'	27:25:19:ARG:HA	2.19	0.41
1:2A:2690:C:N4	1:2A:2713:A:H1'	2.35	0.41
6:2G:3:LEU:HD12	6:2G:8:LYS:HZ1	1.85	0.41
13:2R:62:ALA:O	13:2R:66:VAL:HG23	2.21	0.41
16:2U:29:SER:OG	16:2U:30:LYS:NZ	2.44	0.41
20:2Y:20:TYR:CE2	20:2Y:43:ASN:HA	2.56	0.41
32:2a:683:G:H2'	32:2a:684:A:O4'	2.20	0.41
32:2a:737:A:H2'	32:2a:738:C:H6	1.84	0.41
32:2a:1023:G:H3'	32:2a:1024:G:H8	1.85	0.41
33:2b:163:PHE:HD1	33:2b:185:ILE:HG13	1.85	0.41
35:2d:33:MET:HB2	60:2d:302:SF4:S2	2.60	0.41
43:2l:92:0TD:H4	43:2l:92:0TD:H8	1.74	0.41
1:1A:38:A:H2'	1:1A:39:C:C6	2.55	0.41
1:1A:548:A:H61	17:1V:18:LEU:HA	1.86	0.41
1:1A:1862:G:H2'	1:1A:1863:G:C8	2.53	0.41
1:1A:2646:C:H2'	1:1A:2647:U:O4'	2.20	0.41
3:1D:80:ALA:HB3	3:1D:94:LEU:HD13	2.03	0.41
14:1S:43:GLU:OE2	22:10:49:LYS:HE3	2.20	0.41
24:12:2:LYS:O	24:12:6:VAL:HG23	2.21	0.41
24:12:51:ARG:O	24:12:55:ARG:HG2	2.20	0.41
32:1a:109:A:C6	32:1a:326:G:C6	3.08	0.41
33:1b:97:TRP:HZ2	33:1b:102:LEU:HD13	1.86	0.41
33:1b:114:ARG:NH1	33:1b:117:GLU:OE1	2.52	0.41
33:1b:158:LEU:HA	33:1b:159:PRO:HD3	1.96	0.41
34:1c:73:PRO:O	34:1c:77:ILE:HG12	2.21	0.41
34:1c:180:ALA:HB1	34:1c:203:PHE:CE1	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:1e:90:VAL:O	36:1e:120:THR:HA	2.19	0.41
54:1y:60:U:O2'	54:1y:61:C:H5'	2.21	0.41
1:2A:253:C:H2'	1:2A:254:G:O4'	2.21	0.41
1:2A:570:G:H2'	1:2A:2030:A:C5	2.55	0.41
1:2A:940:G:N3	1:2A:1191:G:H4'	2.36	0.41
1:2A:1368:G:OP1	29:27:28:ARG:NH2	2.53	0.41
1:2A:1783:A:H5'	1:2A:2608:G:H4'	2.03	0.41
1:2A:2165:G:H2'	1:2A:2166:G:O4'	2.20	0.41
1:2A:2313:C:H2'	1:2A:2314:C:H6	1.85	0.41
1:2A:2431:U:O2'	1:2A:2433:A:N7	2.46	0.41
1:2A:2648:C:H2'	1:2A:2649:U:C6	2.55	0.41
1:2A:2812:G:H2'	1:2A:2813:A:C8	2.55	0.41
3:2D:260:ARG:NH1	3:2D:267:SER:OG	2.54	0.41
9:2N:103:VAL:O	9:2N:107:LEU:HG	2.20	0.41
10:2O:2:ILE:HB	10:2O:33:ALA:HB3	2.01	0.41
32:2a:417:C:H2'	32:2a:418:C:C6	2.55	0.41
32:2a:953:G:H5'	32:2a:965:A:N6	2.25	0.41
32:2a:1347:G:H5"	40:2i:107:ARG:HB3	2.02	0.41
35:2d:100:ARG:O	35:2d:104:VAL:HG23	2.21	0.41
35:2d:150:GLU:OE1	35:2d:150:GLU:N	2.50	0.41
47:2p:37:GLY:HA3	47:2p:50:LYS:O	2.21	0.41
1:1A:620:G:N3	1:1A:620:G:H5'	2.36	0.41
1:1A:764:A:O4'	3:1D:213:ARG:HG3	2.21	0.41
1:1A:2695:C:H2'	1:1A:2696:U:C6	2.56	0.41
10:1O:76:ALA:HB3	15:1T:75:ILE:HD12	2.02	0.41
13:1R:24:GLN:HB3	13:1R:44:LEU:HD11	2.01	0.41
21:1Z:54:HIS:CG	21:1Z:101:PRO:HG3	2.56	0.41
28:16:25:LYS:HE3	28:16:27:LYS:HA	2.03	0.41
32:1a:192:U:O3'	51:1t:57:ARG:HD2	2.20	0.41
32:1a:510:A:H5"	35:1d:49:ARG:HH12	1.86	0.41
32:1a:544:G:OP2	35:1d:66:ARG:NH2	2.54	0.41
32:1a:944:G:O6	32:1a:1337:G:H8	2.03	0.41
32:1a:960:U:H2'	32:1a:1225:A:H62	1.86	0.41
32:1a:1003:G:C4	32:1a:1004:A:H2	2.38	0.41
32:1a:1123:A:O2'	41:1j:37:PRO:O	2.34	0.41
40:1i:18:PHE:HB2	40:1i:62:TYR:O	2.20	0.41
48:1q:28:PRO:HA	48:1q:35:VAL:HA	2.02	0.41
1:2A:199:A:OP1	61:2A:5372:HOH:O	2.22	0.41
1:2A:262:A:H2'	1:2A:263:C:O4'	2.20	0.41
1:2A:271(D):G:H2'	1:2A:271(E):U:C6	2.55	0.41
1:2A:921:G:C6	1:2A:922:U:C4	3.09	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:925:C:H2'	1:2A:926:A:H8	1.85	0.41
1:2A:2584:U:H2'	1:2A:2585:U:H2'	2.03	0.41
1:2A:2822:G:OP2	61:2A:6428:HOH:O	2.21	0.41
1:2A:2836:U:H2'	1:2A:2837:G:H8	1.82	0.41
2:2B:67:G:H2'	2:2B:68:C:C6	2.55	0.41
10:2O:107:ARG:HG3	10:2O:112:MET:HE1	2.02	0.41
15:2T:39:ARG:HH12	15:2T:41:ARG:HB3	1.86	0.41
19:2X:44:GLU:O	19:2X:48:LYS:N	2.50	0.41
32:2a:1003:G:C5	32:2a:1004:A:C2	3.09	0.41
32:2a:1086:U:H2'	32:2a:1087:G:H8	1.85	0.41
32:2a:1134:G:H1	32:2a:1140:C:H42	1.68	0.41
34:2c:120:VAL:HG13	34:2c:133:ALA:HB1	2.02	0.41
37:2f:50:TYR:CE2	49:2r:77:GLY:HA2	2.55	0.41
39:2h:17:THR:HA	39:2h:65:TYR:HE1	1.85	0.41
50:2s:28:LYS:HB3	50:2s:29:ARG:CA	2.51	0.41
1:1A:629:G:H1'	1:1A:639:U:H1'	2.03	0.41
1:1A:644:A:H4'	1:1A:645:C:H5	1.85	0.41
1:1A:646:A:H2'	1:1A:647:G:O4'	2.20	0.41
1:1A:755:C:H2'	1:1A:756:C:C6	2.55	0.41
1:1A:783:A:O2'	1:1A:785:G:OP1	2.30	0.41
1:1A:1086:A:H3'	1:1A:1086:A:N3	2.35	0.41
1:1A:1093:G:H3'	1:1A:1094:U:H5"	2.02	0.41
1:1A:1188:U:H4'	17:1V:79:VAL:HG22	2.02	0.41
1:1A:1288:U:O4	13:1R:106:GLY:HA3	2.21	0.41
1:1A:1310:G:OP2	29:17:9:ARG:NH2	2.54	0.41
1:1A:1957:C:H2'	1:1A:1958:C:C6	2.56	0.41
1:1A:2379:G:O2'	14:1S:17:ARG:NH2	2.54	0.41
61:1A:6401:HOH:O	25:13:13:ILE:O	2.22	0.41
61:1A:4469:HOH:O	55:1x:76:A:H1'	2.21	0.41
4:1E:37:ARG:HD2	4:1E:42:ASP:CG	2.45	0.41
15:1T:26:ASP:O	15:1T:49:VAL:HG22	2.21	0.41
15:1T:27:THR:HB	15:1T:90:GLN:HB3	2.03	0.41
26:14:64:GLY:C	26:14:66:SER:N	2.75	0.41
30:18:23:VAL:HG13	30:18:47:LYS:HB3	2.02	0.41
32:1a:78:G:C6	32:1a:91:C:C4	3.08	0.41
32:1a:156:G:H2'	32:1a:157:G:C8	2.56	0.41
32:1a:221:C:H2'	32:1a:222:U:H6	1.85	0.41
32:1a:1316:G:N1	32:1a:1319:A:OP2	2.53	0.41
33:1b:115:LEU:HD21	33:1b:153:ARG:NH1	2.36	0.41
33:1b:204:ASN:OD1	33:1b:206:ASP:N	2.44	0.41
36:1e:102:ALA:HB1	36:1e:106:PRO:HB2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:1g:27:ILE:HA	38:1g:30:ILE:HD12	2.02	0.41
42:1k:98:LEU:O	42:1k:101:SER:OG	2.25	0.41
55:1x:23:C:H2'	55:1x:24:U:C6	2.56	0.41
1:2A:26:G:C6	1:2A:27:G:N1	2.89	0.41
1:2A:747:U:O2'	18:2W:92:ARG:NH2	2.44	0.41
1:2A:984:A:H5"	1:2A:985:C:H5	1.86	0.41
1:2A:1031:G:H21	31:29:36:GLN:HE22	1.67	0.41
1:2A:1856:G:H1	1:2A:1886:C:H42	1.68	0.41
1:2A:1999:C:H5"	1:2A:2723:C:O2'	2.21	0.41
1:2A:2135:A:H5'	1:2A:2159:G:H1'	2.03	0.41
1:2A:2334:G:O6	22:20:74:ARG:NH1	2.46	0.41
1:2A:2745:C:C4	1:2A:2746:U:C4	3.09	0.41
61:2A:6160:HOH:O	19:2X:57:LEU:HA	2.20	0.41
4:2E:170:LEU:HB3	4:2E:184:VAL:CG2	2.51	0.41
6:2G:63:ILE:HD13	6:2G:141:PHE:CD2	2.55	0.41
6:2G:100:TRP:O	6:2G:104:GLU:HB2	2.20	0.41
23:21:64:ALA:HA	23:21:67:ILE:HG13	2.03	0.41
30:28:63:PRO:HG2	30:28:64:TYR:CE2	2.56	0.41
32:2a:63:C:H42	32:2a:104:G:H1	1.67	0.41
32:2a:473:G:H2'	32:2a:474:G:H8	1.86	0.41
32:2a:921:U:O2	36:2e:19:MET:HB2	2.20	0.41
33:2b:51:LEU:O	33:2b:55:PHE:HB2	2.20	0.41
34:2c:131:ARG:HH11	34:2c:166:GLU:HG3	1.85	0.41
35:2d:77:ASN:HD22	35:2d:77:ASN:HA	1.62	0.41
35:2d:156:GLU:HG3	35:2d:159:ARG:NH2	2.36	0.41
39:2h:20:TYR:CZ	39:2h:75:ARG:HB3	2.56	0.41
39:2h:119:LEU:HB3	39:2h:123:GLU:HB2	2.01	0.41
44:2m:82:MET:HG2	44:2m:89:GLY:O	2.21	0.41
1:1A:536:A:H2'	1:1A:537:C:C6	2.56	0.41
1:1A:589:C:H2'	1:1A:590:A:C8	2.56	0.41
1:1A:662:G:H5'	11:1P:14:LYS:O	2.21	0.41
1:1A:735:A:N7	1:1A:761:A:H2	2.19	0.41
1:1A:996:A:H4'	16:1U:91:ASP:OD2	2.21	0.41
1:1A:1183:G:O2'	25:13:29:ARG:NH1	2.54	0.41
1:1A:1239:G:H2'	1:1A:1240:U:O4'	2.21	0.41
1:1A:1889:A:H2'	1:1A:1890:A:C8	2.56	0.41
1:1A:1932:A:H2'	1:1A:1933:G:O4'	2.21	0.41
1:1A:2105:C:H2'	1:1A:2106:G:H8	1.83	0.41
1:1A:2140:C:H2'	1:1A:2141:G:C8	2.55	0.41
1:1A:2233:U:H2'	1:1A:2234:G:C8	2.56	0.41
1:1A:2352:A:N6	1:1A:2365:G:O2'	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2732:G:OP1	4:1E:203:LYS:NZ	2.48	0.41
61:1A:5688:HOH:O	11:1P:42:SER:O	2.21	0.41
11:1P:135:LEU:HD23	11:1P:135:LEU:HA	1.85	0.41
13:1R:2:ARG:HG2	13:1R:5:LYS:HB2	2.03	0.41
16:1U:8:VAL:HG23	16:1U:11:ARG:HH21	1.86	0.41
21:1Z:92:SER:O	21:1Z:130:PRO:HG2	2.20	0.41
30:18:26:LYS:HB2	30:18:44:LYS:O	2.21	0.41
32:1a:152:A:N6	32:1a:170:U:C2	2.88	0.41
32:1a:376:G:OP2	47:1p:67:THR:HG21	2.21	0.41
32:1a:413:G:O6	35:1d:35:ARG:HD3	2.21	0.41
32:1a:652:U:O4	32:1a:752:G:O2'	2.34	0.41
32:1a:739:C:O2'	46:1o:42:HIS:ND1	2.53	0.41
32:1a:888:G:H8	32:1a:888:G:O5'	2.04	0.41
32:1a:921:U:H2'	32:1a:922:G:O4'	2.21	0.41
32:1a:947:G:C6	32:1a:948:C:C4	3.09	0.41
32:1a:1026:G:C8	32:1a:1027:C:O2	2.73	0.41
32:1a:1201:A:H1'	32:1a:1202:G:OP2	2.21	0.41
32:1a:1350:A:O2'	38:1g:33:ASP:OD1	2.28	0.41
32:1a:1381:U:H1'	38:1g:79:ARG:HG2	2.02	0.41
32:1a:1510:U:H1'	32:1a:1526:G:N2	2.36	0.41
33:1b:128:GLU:HG3	33:1b:135:GLN:HE22	1.86	0.41
36:1e:59:GLY:O	36:1e:63:ARG:HG3	2.20	0.41
38:1g:18:TYR:CE1	38:1g:59:LEU:HB2	2.56	0.41
41:1j:13:HIS:O	41:1j:17:ASP:N	2.38	0.41
42:1k:86:GLY:O	42:1k:91:ARG:HD3	2.21	0.41
43:1l:54:LYS:HG2	43:1l:75:HIS:HD2	1.85	0.41
1:2A:355:G:H2'	1:2A:356:G:O4'	2.21	0.41
1:2A:656:G:H2'	1:2A:657:U:O4'	2.20	0.41
1:2A:723:G:H2'	1:2A:724:U:O4'	2.21	0.41
1:2A:1031:G:N2	31:29:36:GLN:HE22	2.18	0.41
1:2A:1599:C:H2'	1:2A:1600:C:C6	2.56	0.41
1:2A:2218:U:H1'	23:21:52:ARG:HH12	1.86	0.41
1:2A:2295:C:H41	14:2S:13:ARG:NH1	2.18	0.41
1:2A:2300:G:C6	1:2A:2301:C:C4	3.09	0.41
1:2A:2579:C:OP1	61:2A:3903:HOH:O	2.22	0.41
1:2A:2784:C:H2'	1:2A:2785:C:C6	2.55	0.41
2:2B:59:A:H2'	2:2B:60:C:O4'	2.21	0.41
3:2D:211:ARG:HG3	3:2D:214:TRP:CE3	2.55	0.41
4:2E:12:THR:HG21	15:2T:11:GLU:HG2	2.03	0.41
6:2G:51:ARG:HD3	6:2G:52:ILE:H	1.85	0.41
10:2O:70:LYS:HB3	10:2O:70:LYS:HE2	1.92	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:2T:102:ILE:HB	15:2T:110:ILE:HG12	2.03	0.41
17:2V:3:ALA:HB3	17:2V:14:VAL:HG23	2.03	0.41
17:2V:62:LEU:HD23	17:2V:93:GLU:HG2	2.03	0.41
23:21:83:GLU:OE1	23:21:83:GLU:N	2.54	0.41
24:22:1:MET:N	24:22:52:ASP:OD1	2.51	0.41
28:26:8:LYS:HG2	30:28:34:TRP:CD1	2.56	0.41
32:2a:14:U:H5"	61:2a:3452:HOH:O	2.19	0.41
32:2a:147:G:H1	32:2a:175:C:H42	1.69	0.41
32:2a:509:A:H2'	32:2a:510:A:C8	2.56	0.41
32:2a:577:G:C8	32:2a:816:A:C6	3.08	0.41
32:2a:612:C:N4	61:2a:3560:HOH:O	2.53	0.41
32:2a:664:G:N2	32:2a:741:G:H1	2.09	0.41
32:2a:714:G:H2'	32:2a:715:A:C8	2.56	0.41
32:2a:1094:G:O2'	32:2a:1108:G:N2	2.47	0.41
32:2a:1161:C:H2'	32:2a:1162:C:C6	2.56	0.41
32:2a:1251:A:H2'	32:2a:1252:A:C8	2.56	0.41
32:2a:1502:A:H5'	32:2a:1504:G:N7	2.36	0.41
33:2b:97:TRP:HZ2	33:2b:102:LEU:HD13	1.86	0.41
33:2b:168:THR:OG1	33:2b:191:ASP:O	2.34	0.41
35:2d:38:TYR:CE1	35:2d:45:GLN:HG3	2.56	0.41
37:2f:11:ASN:HB3	37:2f:14:LEU:HG	2.02	0.41
37:2f:97:PHE:CE1	49:2r:61:LYS:HE2	2.56	0.41
44:2m:91:ARG:HG2	44:2m:96:LEU:HB2	2.03	0.41
54:2w:10:G:N2	54:2w:11:C:C2	2.89	0.41
54:2w:56:C:H2'	54:2w:57:G:O4'	2.20	0.41
1:1A:969:U:H2'	1:1A:970:C:C6	2.56	0.41
1:1A:1063:G:C5	1:1A:1064:C:N4	2.89	0.41
1:1A:1286:A:C6	1:1A:1329:U:C2	3.09	0.41
1:1A:2364:C:OP1	22:10:55:ARG:NH1	2.54	0.41
1:1A:2448:A:OP1	61:1A:6393:HOH:O	2.22	0.41
61:1A:4208:HOH:O	22:10:41:ARG:HA	2.21	0.41
3:1D:168:ARG:HA	3:1D:173:VAL:HA	2.03	0.41
5:1F:150:GLY:HA2	5:1F:172:TRP:CD2	2.55	0.41
11:1P:88:LEU:HD11	11:1P:114:ILE:HD12	2.03	0.41
12:1Q:38:GLU:HG3	12:1Q:127:ILE:HB	2.02	0.41
14:1S:87:PHE:CZ	14:1S:102:ALA:HB2	2.55	0.41
32:1a:130:A:O2'	32:1a:131:C:O5'	2.33	0.41
32:1a:156:G:H2'	32:1a:157:G:H8	1.86	0.41
32:1a:840:C:H4'	32:1a:841:U:OP1	2.20	0.41
32:1a:1039:C:H2'	32:1a:1040:U:C6	2.56	0.41
32:1a:1151:A:O2'	32:1a:1152:A:H8	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1183:A:O2'	32:1a:1184:G:OP1	2.37	0.41
35:1d:11:LEU:HG	35:1d:66:ARG:HD3	2.03	0.41
43:1l:53:ARG:HB2	43:1l:93:LEU:HD11	2.02	0.41
44:1m:65:LYS:HB2	44:1m:65:LYS:HE3	1.91	0.41
48:1q:50:LYS:HE3	48:1q:51:TYR:CE2	2.56	0.41
50:1s:80:TYR:C	50:1s:82:GLY:H	2.29	0.41
54:1w:9:A:C6	54:1w:45:U:C4	3.09	0.41
54:1w:50:U:O4	54:1w:64:A:N1	2.54	0.41
55:1x:25:C:H2'	55:1x:26:G:O4'	2.20	0.41
55:1x:66:C:H2'	55:1x:67:C:O4'	2.20	0.41
1:2A:380:U:H2'	1:2A:381:G:C8	2.55	0.41
1:2A:2356:C:H2'	1:2A:2357:U:O4'	2.21	0.41
1:2A:2400:G:H2'	1:2A:2401:U:H6	1.86	0.41
4:2E:12:THR:HG22	4:2E:13:ARG:H	1.86	0.41
6:2G:41:GLN:HG2	6:2G:154:GLY:O	2.21	0.41
32:2a:528:C:H41	43:2l:49:ASN:ND2	2.20	0.41
32:2a:540:G:H2'	32:2a:541:G:O4'	2.21	0.41
32:2a:577:G:H2'	32:2a:578:C:H6	1.86	0.41
32:2a:826:C:H2'	32:2a:827:U:C6	2.55	0.41
32:2a:1030(A):G:C2	32:2a:1030(C):G:H5"	2.55	0.41
32:2a:1353:G:H2'	32:2a:1354:C:H6	1.86	0.41
33:2b:167:PRO:HD3	33:2b:187:LEU:O	2.20	0.41
35:2d:61:LYS:HD2	35:2d:207:TYR:OH	2.21	0.41
35:2d:110:PHE:N	35:2d:110:PHE:CD1	2.89	0.41
39:2h:26:VAL:O	39:2h:59:LEU:N	2.51	0.41
44:2m:25:ILE:HG13	44:2m:66:LEU:HD22	2.02	0.41
50:2s:20:LEU:HA	50:2s:20:LEU:HD23	1.86	0.41
54:2y:72:C:H2'	54:2y:73:A:O4'	2.21	0.41
1:1A:228:A:H3'	1:1A:229:A:C5'	2.49	0.40
1:1A:942:G:OP2	11:1P:39:LYS:HE2	2.21	0.40
1:1A:1336:A:H2'	1:1A:1337:G:C8	2.56	0.40
1:1A:1655:A:H3'	1:1A:1656:C:C6	2.56	0.40
1:1A:1789:A:H5"	3:1D:220:HIS:O	2.21	0.40
1:1A:1920:4OC:H6	1:1A:1920:4OC:O5'	2.21	0.40
1:1A:2408:U:H2'	1:1A:2409:G:C8	2.56	0.40
4:1E:9:VAL:HG13	4:1E:25:VAL:O	2.21	0.40
7:1H:3:ARG:NH2	7:1H:65:HIS:HB3	2.37	0.40
9:1N:108:PRO:O	9:1N:113:GLY:HA3	2.21	0.40
10:1O:86:ILE:HG22	10:1O:94:ARG:HD3	2.03	0.40
14:1S:5:THR:OG1	14:1S:8:GLU:HG2	2.21	0.40
18:1W:18:ARG:HG2	18:1W:76:VAL:HB	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:359:U:H2'	32:1a:360:A:C8	2.56	0.40
32:1a:993:G:H2'	32:1a:995:C:H41	1.86	0.40
32:1a:999:C:H42	32:1a:1042:G:H1	1.68	0.40
32:1a:1312:G:N7	50:1s:2:PRO:HD2	2.35	0.40
32:1a:1379:G:OP1	38:1g:6:ARG:NH1	2.55	0.40
32:1a:1509:C:H2'	32:1a:1510:U:O4'	2.21	0.40
40:1i:100:GLY:O	40:1i:103:THR:HG22	2.21	0.40
43:1l:113:ARG:HD2	43:1l:113:ARG:HA	1.93	0.40
54:1y:4:C:H2'	54:1y:5:G:O4'	2.21	0.40
1:2A:136:G:H2'	1:2A:137:C:C6	2.56	0.40
1:2A:271(Z):C:OP2	61:2A:6005:HOH:O	2.22	0.40
1:2A:1252:G:N2	16:2U:37:GLU:OE2	2.48	0.40
1:2A:1266:G:O2'	1:2A:2012:G:O6	2.19	0.40
1:2A:2053:G:OP2	61:2A:4832:HOH:O	2.22	0.40
12:2Q:2:LEU:HD12	12:2Q:69:PHE:CE1	2.57	0.40
12:2Q:34:LEU:HB2	12:2Q:118:LEU:HD22	2.03	0.40
15:2T:64:ARG:HB2	15:2T:73:GLU:HG2	2.02	0.40
15:2T:118:ARG:HB3	32:2a:1442(A):G:C5	2.57	0.40
32:2a:580:U:H5"	46:2o:58:MET:HG2	2.03	0.40
32:2a:1060:C:H2'	32:2a:1061:G:H8	1.87	0.40
32:2a:1068:G:H8	32:2a:1068:G:OP2	2.03	0.40
32:2a:1219:U:OP1	45:2n:19:ARG:NH1	2.30	0.40
33:2b:28:PHE:CD1	33:2b:194:PRO:HG3	2.55	0.40
34:2c:151:VAL:HG22	34:2c:200:ALA:HA	2.03	0.40
35:2d:4:TYR:O	35:2d:5:ILE:HG22	2.21	0.40
35:2d:61:LYS:HE3	35:2d:61:LYS:HB3	1.95	0.40
36:2e:78:HIS:HE1	36:2e:143:ARG:N	2.19	0.40
43:2l:10:LEU:HB3	48:2q:32:TYR:CE2	2.56	0.40
1:1A:30:G:H2'	1:1A:31:C:C6	2.56	0.40
1:1A:330:A:N7	1:1A:1210:A:O2'	2.35	0.40
1:1A:857:C:N4	1:1A:858:U:O4	2.55	0.40
1:1A:1106:G:H2'	1:1A:1107:G:O4'	2.21	0.40
1:1A:1156:A:OP2	61:1A:6455:HOH:O	2.21	0.40
1:1A:1570:A:H2'	1:1A:1571:A:C8	2.56	0.40
1:1A:1862:G:C2	1:1A:1881:C:C2	3.09	0.40
1:1A:2142:C:H2'	1:1A:2143:C:C6	2.56	0.40
1:1A:2280:G:O2'	1:1A:2388:A:N1	2.45	0.40
1:1A:2443:C:OP1	5:1F:68:LYS:HD3	2.21	0.40
5:1F:135:LYS:HE3	5:1F:135:LYS:HB3	1.90	0.40
7:1H:127:GLU:CD	7:1H:130:ARG:HE	2.29	0.40
9:1N:61:ARG:HD3	9:1N:61:ARG:HA	1.87	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1Y:19:LYS:HE2	20:1Y:19:LYS:HB3	1.78	0.40
32:1a:16:A:N1	32:1a:919:A:H2	2.19	0.40
32:1a:626:U:C2	32:1a:627:G:C8	3.10	0.40
32:1a:1139:G:H4'	32:1a:1140:C:H5'	2.03	0.40
32:1a:1241:G:H2'	32:1a:1242:C:C6	2.57	0.40
33:1b:9:GLU:HA	33:1b:48:MET:SD	2.61	0.40
34:1c:148:GLY:HA3	34:1c:172:ARG:O	2.22	0.40
55:1x:32:5MC:HM52	55:1x:33:U:O4	2.21	0.40
1:2A:271:A:N6	1:2A:271(X):G:H1'	2.37	0.40
1:2A:643:A:N1	1:2A:2369:A:O2'	2.50	0.40
1:2A:1353:A:H2'	1:2A:1354:A:C8	2.56	0.40
1:2A:1448:G:H2'	1:2A:1449:A:C8	2.57	0.40
1:2A:2119:A:H2	1:2A:2171:A:H5'	1.86	0.40
1:2A:2758:A:C2	1:2A:2759:G:H1'	2.56	0.40
5:2F:140:LEU:HD11	5:2F:170:LEU:HD11	2.03	0.40
9:2N:104:LYS:HA	9:2N:107:LEU:HD12	2.02	0.40
10:2O:4:PRO:HD3	10:2O:24:VAL:HG23	2.02	0.40
22:20:11:ARG:O	22:20:14:ARG:NH2	2.54	0.40
24:22:51:ARG:O	24:22:55:ARG:HG2	2.21	0.40
24:22:64:LEU:HD11	24:22:68:ARG:NH2	2.35	0.40
25:23:11:SER:HA	25:23:31:LEU:HD21	2.02	0.40
32:2a:113:G:O2'	32:2a:354:G:H5'	2.22	0.40
32:2a:860:A:H2'	32:2a:861:G:O4'	2.21	0.40
32:2a:1015:A:H1'	32:2a:1219:U:H5'	2.03	0.40
32:2a:1298:C:C5	38:2g:114:ARG:HD3	2.57	0.40
32:2a:1410:G:H2'	32:2a:1411:C:C6	2.56	0.40
34:2c:164:ARG:HG2	34:2c:165:THR:H	1.86	0.40
37:2f:37:VAL:HA	37:2f:65:VAL:HG12	2.04	0.40
41:2j:57:LYS:HE2	41:2j:60:ARG:NH2	2.35	0.40
46:2o:39:LEU:HD12	46:2o:59:MET:HE3	2.03	0.40
50:2s:27:GLU:OE1	50:2s:27:GLU:N	2.52	0.40
1:1A:580:C:H2'	1:1A:581:C:C6	2.56	0.40
1:1A:695:G:OP1	1:1A:1380:G:O2'	2.35	0.40
1:1A:781:A:OP1	3:1D:218:ARG:NH2	2.55	0.40
1:1A:858:U:O2	1:1A:2268:A:H2'	2.21	0.40
1:1A:1038:C:H42	1:1A:1117:G:H1	1.67	0.40
1:1A:1608:A:H1'	1:1A:1610:A:OP2	2.22	0.40
5:1F:197:ASP:O	5:1F:201:VAL:HG13	2.21	0.40
15:1T:127:ALA:C	15:1T:129:ARG:N	2.77	0.40
32:1a:34:C:H2'	32:1a:35:G:H8	1.87	0.40
32:1a:376:G:O3'	47:1p:5:ARG:NH1	2.43	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:803:G:OP1	61:1a:2104:HOH:O	2.21	0.40
32:1a:1376:U:H2'	32:1a:1377:A:H8	1.86	0.40
43:1l:54:LYS:N	43:1l:54:LYS:HD2	2.36	0.40
1:2A:109:G:H2'	1:2A:110:G:O4'	2.22	0.40
1:2A:297:C:OP1	20:2Y:87:LYS:HG3	2.20	0.40
1:2A:527:C:H4'	1:2A:528:A:O5'	2.21	0.40
1:2A:847:U:H5'	1:2A:848:G:OP2	2.21	0.40
1:2A:857:C:H4'	22:20:23:VAL:HG21	2.03	0.40
1:2A:902:C:H2'	1:2A:903:C:H6	1.86	0.40
1:2A:1027:A:N6	1:2A:1126:A:C4	2.90	0.40
1:2A:1147:C:H2'	1:2A:1148:A:C8	2.56	0.40
1:2A:1270:C:H5"	1:2A:1271:G:O5'	2.22	0.40
1:2A:1614:A:H8	1:2A:1614:A:P	2.44	0.40
1:2A:2324:C:H2'	1:2A:2385:C:H5	1.87	0.40
1:2A:2652:C:H42	1:2A:2668:G:H1	1.69	0.40
7:2H:25:LYS:HE2	7:2H:27:LYS:NZ	2.36	0.40
7:2H:143:GLN:NE2	7:2H:147:ASN:OD1	2.54	0.40
16:2U:65:ILE:HD13	16:2U:95:LEU:HD23	2.04	0.40
19:2X:84:ALA:HB3	19:2X:87:GLN:CD	2.46	0.40
21:2Z:80:ARG:HB3	21:2Z:82:ARG:HD3	2.04	0.40
32:2a:575:G:O4'	32:2a:881:G:N2	2.54	0.40
32:2a:701:C:OP1	32:2a:702:A:O2'	2.19	0.40
32:2a:783:C:H2'	32:2a:784:C:C6	2.55	0.40
32:2a:918:A:H2'	32:2a:919:A:O4'	2.22	0.40
32:2a:990:C:H2'	32:2a:991:U:C6	2.57	0.40
32:2a:1085:U:H3'	32:2a:1086:U:C5	2.57	0.40
32:2a:1177:G:H2'	32:2a:1178:G:O4'	2.21	0.40
32:2a:1359:C:OP2	45:2n:35:ARG:NH1	2.55	0.40
33:2b:63:MET:HG3	33:2b:225:ALA:HB1	2.02	0.40
33:2b:95:GLN:HB2	33:2b:148:TYR:CD1	2.56	0.40
33:2b:98:LEU:HD13	33:2b:108:ILE:HD12	2.02	0.40
33:2b:146:GLN:O	33:2b:150:SER:HB3	2.22	0.40
34:2c:22:TRP:HZ3	34:2c:24:ALA:HB2	1.85	0.40
36:2e:7:GLU:N	36:2e:35:GLY:O	2.39	0.40
36:2e:139:LEU:HA	36:2e:142:LEU:HD12	2.04	0.40
37:2f:37:VAL:HG13	37:2f:65:VAL:HG12	2.02	0.40
41:2j:40:LEU:HB2	41:2j:69:ASN:CB	2.46	0.40
45:2n:14:PRO:HG3	45:2n:20:ALA:HB2	2.03	0.40
55:2x:23:C:H2'	55:2x:24:U:H6	1.82	0.40
54:2y:48:C:C2	54:2y:59:U:H1'	2.56	0.40
54:2y:63:G:H2'	54:2y:64:A:O4'	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:86:C:H4'	1:1A:104:U:H1'	2.03	0.40
1:1A:1164:G:H2'	1:1A:1165:U:C6	2.57	0.40
1:1A:1923:U:H2'	1:1A:1924:C:C6	2.55	0.40
1:1A:2031:A:C6	1:1A:2498:C:H1'	2.57	0.40
1:1A:2065:C:H2'	1:1A:2066:C:C6	2.56	0.40
7:1H:3:ARG:NH1	7:1H:5:GLY:H	2.20	0.40
24:12:1:MET:HE2	24:12:6:VAL:HG22	2.03	0.40
25:13:6:VAL:HG13	25:13:54:VAL:CG1	2.50	0.40
28:16:9:LEU:HD11	28:16:34:LEU:HD12	2.04	0.40
32:1a:229:U:H2'	32:1a:230:G:C8	2.56	0.40
32:1a:625:G:H2'	32:1a:626:U:C6	2.57	0.40
32:1a:946:A:O2'	32:1a:1333:A:N3	2.45	0.40
32:1a:1044:A:C5	32:1a:1045:C:H1'	2.56	0.40
32:1a:1263:C:H2'	32:1a:1264:C:C6	2.55	0.40
32:1a:1333:A:H2'	32:1a:1334:G:O4'	2.22	0.40
34:1c:119:ARG:HE	34:1c:140:ARG:CZ	2.34	0.40
54:1w:35:A:H2'	54:1w:36:A:O4'	2.22	0.40
54:1y:35:A:H8	54:1y:35:A:OP2	2.04	0.40
1:2A:384:U:H2'	1:2A:385:C:H6	1.86	0.40
1:2A:797:C:OP1	5:2F:60:SER:OG	2.37	0.40
1:2A:863:A:P	12:2Q:22:LYS:HG3	2.61	0.40
1:2A:1019:U:OP1	1:2A:1035:U:O2'	2.30	0.40
1:2A:1541:G:H3'	1:2A:1542:A:H8	1.86	0.40
1:2A:1786:A:H1'	1:2A:1938:A:N6	2.37	0.40
1:2A:2843:G:H1	1:2A:2874:C:H42	1.69	0.40
4:2E:169:ASN:HB2	4:2E:203:LYS:HG3	2.03	0.40
15:2T:11:GLU:OE1	15:2T:57:PHE:HB3	2.21	0.40
15:2T:82:LEU:HA	15:2T:82:LEU:HD23	1.82	0.40
24:22:12:GLU:O	24:22:16:LEU:HG	2.22	0.40
27:25:16:ARG:HG3	27:25:17:ASP:N	2.37	0.40
32:2a:284:G:H2'	32:2a:285:G:H8	1.84	0.40
32:2a:690:G:O6	42:2k:55:LYS:NZ	2.54	0.40
32:2a:1169:A:H2'	32:2a:1170:A:C8	2.57	0.40
32:2a:1225:A:H2'	32:2a:1226:C:C5	2.56	0.40
32:2a:1275:A:H3'	32:2a:1276:G:C8	2.53	0.40
33:2b:133:LYS:HE3	33:2b:133:LYS:HB2	1.89	0.40
35:2d:3:ARG:NH1	35:2d:5:ILE:HG13	2.36	0.40
36:2e:89:ILE:HD12	36:2e:89:ILE:HA	1.83	0.40
37:2f:82:ARG:HB2	37:2f:85:VAL:HG23	2.02	0.40
1:1A:214:G:O2'	1:1A:216:A:O2'	2.31	0.40
2:1B:14:U:OP2	2:1B:70:C:O2'	2.39	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:1P:111:ARG:HB3	11:1P:128:HIS:CG	2.56	0.40
11:1P:120:ALA:HB2	11:1P:137:LYS:HB3	2.03	0.40
32:1a:115:G:H4'	32:1a:116:A:O5'	2.21	0.40
32:1a:1284:C:H3'	32:1a:1285:A:H8	1.86	0.40
33:1b:62:ALA:HB3	33:1b:225:ALA:HB3	2.03	0.40
33:1b:115:LEU:HD21	33:1b:153:ARG:HH11	1.86	0.40
38:1g:28:ASN:HD21	38:1g:36:LYS:NZ	2.19	0.40
41:1j:39:PRO:HA	41:1j:70:ARG:HD3	2.03	0.40
47:1p:60:LEU:HD12	47:1p:60:LEU:HA	1.90	0.40
1:2A:918:A:C5	1:2A:919:G:H1'	2.57	0.40
1:2A:1372:U:H2'	1:2A:1373:A:O4'	2.21	0.40
1:2A:1915:5MU:H2'	1:2A:1916:A:O4'	2.21	0.40
1:2A:1987:G:H2'	1:2A:1988:C:C6	2.56	0.40
1:2A:2050:C:N4	1:2A:2051:A:N1	2.70	0.40
3:2D:17:THR:HG1	3:2D:205:VAL:H	1.64	0.40
19:2X:5:TYR:CZ	24:22:30:ARG:HD2	2.57	0.40
21:2Z:71:VAL:HG22	21:2Z:88:PHE:CE1	2.57	0.40
32:2a:427:U:O2'	32:2a:541:G:OP1	2.27	0.40
32:2a:495:A:H1'	32:2a:496:A:H5"	2.04	0.40
32:2a:875:C:H1'	39:2h:15:ASN:HD21	1.86	0.40
32:2a:1347:G:H8	40:2i:107:ARG:HB2	1.85	0.40
32:2a:1353:G:C2	32:2a:1370:G:C2	3.09	0.40
35:2d:116:GLN:O	35:2d:120:LEU:HG	2.21	0.40
43:2l:59:ARG:HA	43:2l:65:GLU:HA	2.02	0.40
48:2q:40:LYS:HD3	48:2q:42:TYR:OH	2.22	0.40
51:2t:43:LEU:HD13	51:2t:51:GLU:HB3	2.04	0.40
54:2y:9:A:O5'	54:2y:46:7MG:N2	2.36	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%)	261 (96%)	11 (4%)	1 (0%)	30	51
3	2D	273/276 (99%)	261 (96%)	11 (4%)	1 (0%)	30	51
4	1E	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	24	46
4	2E	202/206 (98%)	195 (96%)	6 (3%)	1 (0%)	24	46
5	1F	201/210 (96%)	193 (96%)	7 (4%)	1 (0%)	24	46
5	2F	201/210 (96%)	197 (98%)	1 (0%)	3 (2%)	8	18
6	1G	179/182 (98%)	168 (94%)	10 (6%)	1 (1%)	21	42
6	2G	179/182 (98%)	159 (89%)	18 (10%)	2 (1%)	11	25
7	1H	172/180 (96%)	163 (95%)	8 (5%)	1 (1%)	21	42
7	2H	172/180 (96%)	160 (93%)	10 (6%)	2 (1%)	10	23
8	1I	144/148 (97%)	137 (95%)	7 (5%)	0	100	100
8	2I	144/148 (97%)	134 (93%)	10 (7%)	0	100	100
9	1N	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
9	2N	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
10	1O	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
10	2O	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
11	1P	147/150 (98%)	139 (95%)	8 (5%)	0	100	100
11	2P	147/150 (98%)	141 (96%)	6 (4%)	0	100	100
12	1Q	139/141 (99%)	129 (93%)	10 (7%)	0	100	100
12	2Q	139/141 (99%)	132 (95%)	7 (5%)	0	100	100
13	1R	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
13	2R	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
14	1S	108/112 (96%)	103 (95%)	5 (5%)	0	100	100
14	2S	108/112 (96%)	102 (94%)	6 (6%)	0	100	100
15	1T	129/146 (88%)	122 (95%)	7 (5%)	0	100	100
15	2T	129/146 (88%)	124 (96%)	5 (4%)	0	100	100
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
17	1V	99/101 (98%)	93 (94%)	5 (5%)	1 (1%)	12	28
17	2V	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	12	28
18	1W	110/113 (97%)	108 (98%)	2 (2%)	0	100	100
18	2W	110/113 (97%)	108 (98%)	2 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	1X	93/96 (97%)	90 (97%)	3 (3%)	0	100	100
19	2X	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
20	1Y	105/110 (96%)	101 (96%)	4 (4%)	0	100	100
20	2Y	105/110 (96%)	102 (97%)	3 (3%)	0	100	100
21	1Z	148/206 (72%)	140 (95%)	8 (5%)	0	100	100
21	2Z	156/206 (76%)	142 (91%)	14 (9%)	0	100	100
22	10	81/85 (95%)	80 (99%)	1 (1%)	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	25
23	21	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
25	13	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
25	23	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
26	14	67/71 (94%)	57 (85%)	7 (10%)	3 (4%)	2	2
26	24	67/71 (94%)	54 (81%)	11 (16%)	2 (3%)	3	6
27	15	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
27	25	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
28	16	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
28	26	51/54 (94%)	51 (100%)	0	0	100	100
29	17	46/49 (94%)	46 (100%)	0	0	100	100
29	27	46/49 (94%)	44 (96%)	2 (4%)	0	100	100
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
33	1b	229/256 (90%)	202 (88%)	20 (9%)	7 (3%)	3	5
33	2b	229/256 (90%)	203 (89%)	20 (9%)	6 (3%)	4	7
34	1c	204/239 (85%)	187 (92%)	15 (7%)	2 (1%)	12	28
34	2c	204/239 (85%)	187 (92%)	15 (7%)	2 (1%)	12	28
35	1d	206/209 (99%)	198 (96%)	7 (3%)	1 (0%)	24	46

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
35	2d	206/209 (99%)	193 (94%)	11 (5%)	2 (1%)	12 28
36	1e	146/162 (90%)	140 (96%)	5 (3%)	1 (1%)	18 38
36	2e	146/162 (90%)	141 (97%)	5 (3%)	0	100 100
37	1f	98/101 (97%)	95 (97%)	3 (3%)	0	100 100
37	2f	98/101 (97%)	96 (98%)	2 (2%)	0	100 100
38	1g	153/156 (98%)	144 (94%)	7 (5%)	2 (1%)	9 21
38	2g	153/156 (98%)	140 (92%)	11 (7%)	2 (1%)	9 21
39	1h	135/138 (98%)	132 (98%)	3 (2%)	0	100 100
39	2h	135/138 (98%)	130 (96%)	5 (4%)	0	100 100
40	1i	125/128 (98%)	112 (90%)	13 (10%)	0	100 100
40	2i	125/128 (98%)	109 (87%)	16 (13%)	0	100 100
41	1j	95/105 (90%)	85 (90%)	6 (6%)	4 (4%)	2 3
41	2j	94/105 (90%)	81 (86%)	6 (6%)	7 (7%)	1 1
42	1k	112/129 (87%)	104 (93%)	6 (5%)	2 (2%)	6 14
42	2k	112/129 (87%)	104 (93%)	6 (5%)	2 (2%)	6 14
43	1l	119/132 (90%)	112 (94%)	6 (5%)	1 (1%)	16 34
43	2l	119/132 (90%)	112 (94%)	7 (6%)	0	100 100
44	1m	121/126 (96%)	112 (93%)	9 (7%)	0	100 100
44	2m	120/126 (95%)	111 (92%)	9 (8%)	0	100 100
45	1n	58/61 (95%)	56 (97%)	2 (3%)	0	100 100
45	2n	58/61 (95%)	54 (93%)	4 (7%)	0	100 100
46	1o	86/89 (97%)	84 (98%)	2 (2%)	0	100 100
46	2o	86/89 (97%)	84 (98%)	2 (2%)	0	100 100
47	1p	80/88 (91%)	74 (92%)	6 (8%)	0	100 100
47	2p	80/88 (91%)	77 (96%)	3 (4%)	0	100 100
48	1q	97/105 (92%)	94 (97%)	2 (2%)	1 (1%)	12 28
48	2q	97/105 (92%)	93 (96%)	3 (3%)	1 (1%)	12 28
49	1r	66/88 (75%)	64 (97%)	2 (3%)	0	100 100
49	2r	66/88 (75%)	64 (97%)	2 (3%)	0	100 100
50	1s	81/93 (87%)	72 (89%)	9 (11%)	0	100 100
50	2s	81/93 (87%)	72 (89%)	8 (10%)	1 (1%)	10 23

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
51	1t	94/106 (89%)	86 (92%)	5 (5%)	3 (3%)	3 5
51	2t	94/106 (89%)	85 (90%)	6 (6%)	3 (3%)	3 5
52	1u	21/27 (78%)	20 (95%)	1 (5%)	0	100 100
52	2u	21/27 (78%)	20 (95%)	1 (5%)	0	100 100
All	All	11370/12128 (94%)	10749 (94%)	549 (5%)	72 (1%)	21 42

All (72) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
7	1H	126	PRO
23	11	3	LYS
26	14	58	ARG
33	1b	10	LEU
33	1b	22	LYS
7	2H	126	PRO
26	24	55	ARG
26	24	65	ASP
33	2b	10	LEU
41	2j	75	ILE
51	2t	10	LEU
33	1b	9	GLU
41	1j	55	LYS
41	1j	75	ILE
35	2d	181	MET
38	2g	7	ALA
41	2j	33	GLN
42	2k	49	GLY
3	1D	3	VAL
6	1G	43	LEU
26	14	65	ASP
35	1d	5	ILE
48	1q	33	GLY
51	1t	10	LEU
51	1t	97	ALA
34	2c	156	ARG
41	2j	29	ARG
41	2j	78	ASN
41	2j	79	ARG
4	1E	52	LEU
33	1b	20	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	1b	125	PRO
34	1c	107	GLN
38	1g	114	ARG
41	1j	33	GLN
41	1j	78	ASN
4	2E	52	LEU
5	2F	130	ALA
7	2H	47	GLU
17	2V	79	VAL
33	2b	16	HIS
33	2b	20	GLU
34	2c	85	ARG
51	2t	97	ALA
17	1V	79	VAL
33	1b	17	PHE
33	1b	37	ASN
38	1g	80	VAL
43	1l	91	LYS
3	2D	3	VAL
5	2F	26	ALA
6	2G	49	ASP
6	2G	52	ILE
33	2b	17	PHE
35	2d	5	ILE
38	2g	80	VAL
48	2q	68	ARG
51	2t	47	GLY
34	1c	66	VAL
51	1t	47	GLY
5	2F	89	VAL
33	2b	9	GLU
50	2s	9	VAL
26	14	64	GLY
42	1k	105	VAL
33	2b	127	ILE
42	2k	105	VAL
36	1e	69	VAL
41	2j	24	VAL
41	2j	39	PRO
42	1k	49	GLY

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%)	198 (92%)	17 (8%)	11 26
3	2D	215/218 (99%)	201 (94%)	14 (6%)	15 35
4	1E	164/166 (99%)	148 (90%)	16 (10%)	7 17
4	2E	164/166 (99%)	155 (94%)	9 (6%)	19 41
5	1F	160/166 (96%)	146 (91%)	14 (9%)	9 21
5	2F	159/166 (96%)	148 (93%)	11 (7%)	14 32
6	1G	143/156 (92%)	134 (94%)	9 (6%)	16 36
6	2G	143/156 (92%)	129 (90%)	14 (10%)	7 17
7	1H	144/148 (97%)	136 (94%)	8 (6%)	19 40
7	2H	144/148 (97%)	138 (96%)	6 (4%)	26 52
8	1I	113/124 (91%)	107 (95%)	6 (5%)	20 43
8	2I	105/124 (85%)	95 (90%)	10 (10%)	8 18
9	1N	118/119 (99%)	108 (92%)	10 (8%)	10 22
9	2N	118/119 (99%)	110 (93%)	8 (7%)	14 32
10	1O	100/100 (100%)	96 (96%)	4 (4%)	28 55
10	2O	100/100 (100%)	97 (97%)	3 (3%)	36 64
11	1P	115/116 (99%)	109 (95%)	6 (5%)	21 44
11	2P	115/116 (99%)	110 (96%)	5 (4%)	26 51
12	1Q	111/111 (100%)	106 (96%)	5 (4%)	24 50
12	2Q	111/111 (100%)	107 (96%)	4 (4%)	31 58
13	1R	101/101 (100%)	88 (87%)	13 (13%)	4 8
13	2R	101/101 (100%)	90 (89%)	11 (11%)	6 13
14	1S	86/88 (98%)	82 (95%)	4 (5%)	23 48
14	2S	85/88 (97%)	83 (98%)	2 (2%)	43 70
15	1T	115/127 (91%)	111 (96%)	4 (4%)	32 59
15	2T	113/127 (89%)	112 (99%)	1 (1%)	70 87

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
16	1U	93/94 (99%)	90 (97%)	3 (3%)	34 62
16	2U	93/94 (99%)	89 (96%)	4 (4%)	26 51
17	1V	80/82 (98%)	70 (88%)	10 (12%)	4 9
17	2V	80/82 (98%)	70 (88%)	10 (12%)	4 9
18	1W	90/92 (98%)	81 (90%)	9 (10%)	7 16
18	2W	90/92 (98%)	84 (93%)	6 (7%)	15 33
19	1X	77/78 (99%)	73 (95%)	4 (5%)	21 44
19	2X	77/78 (99%)	75 (97%)	2 (3%)	40 68
20	1Y	85/91 (93%)	78 (92%)	7 (8%)	10 24
20	2Y	85/91 (93%)	76 (89%)	9 (11%)	6 14
21	1Z	135/179 (75%)	124 (92%)	11 (8%)	11 24
21	2Z	137/179 (76%)	131 (96%)	6 (4%)	25 50
22	10	65/67 (97%)	63 (97%)	2 (3%)	35 63
22	20	65/67 (97%)	64 (98%)	1 (2%)	57 80
23	11	80/83 (96%)	76 (95%)	4 (5%)	22 46
23	21	80/83 (96%)	77 (96%)	3 (4%)	29 56
24	12	65/67 (97%)	62 (95%)	3 (5%)	24 49
24	22	65/67 (97%)	65 (100%)	0	100 100
25	13	51/52 (98%)	48 (94%)	3 (6%)	18 38
25	23	50/52 (96%)	48 (96%)	2 (4%)	28 55
26	14	59/63 (94%)	53 (90%)	6 (10%)	7 15
26	24	53/63 (84%)	52 (98%)	1 (2%)	50 75
27	15	50/52 (96%)	47 (94%)	3 (6%)	17 37
27	25	50/52 (96%)	47 (94%)	3 (6%)	17 37
28	16	51/52 (98%)	49 (96%)	2 (4%)	28 55
28	26	50/52 (96%)	47 (94%)	3 (6%)	17 37
29	17	41/42 (98%)	36 (88%)	5 (12%)	5 10
29	27	41/42 (98%)	36 (88%)	5 (12%)	5 10
30	18	54/55 (98%)	49 (91%)	5 (9%)	8 18
30	28	54/55 (98%)	52 (96%)	2 (4%)	30 57
31	19	34/34 (100%)	33 (97%)	1 (3%)	37 65

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
31	29	34/34 (100%)	30 (88%)	4 (12%)	5 10
33	1b	192/220 (87%)	183 (95%)	9 (5%)	23 48
33	2b	187/220 (85%)	177 (95%)	10 (5%)	20 43
34	1c	142/188 (76%)	135 (95%)	7 (5%)	22 47
34	2c	140/188 (74%)	133 (95%)	7 (5%)	22 46
35	1d	169/181 (93%)	157 (93%)	12 (7%)	13 31
35	2d	173/181 (96%)	159 (92%)	14 (8%)	11 24
36	1e	113/123 (92%)	103 (91%)	10 (9%)	9 21
36	2e	114/123 (93%)	110 (96%)	4 (4%)	32 59
37	1f	84/90 (93%)	79 (94%)	5 (6%)	17 37
37	2f	85/90 (94%)	82 (96%)	3 (4%)	32 59
38	1g	119/127 (94%)	113 (95%)	6 (5%)	22 46
38	2g	120/127 (94%)	116 (97%)	4 (3%)	33 61
39	1h	114/119 (96%)	104 (91%)	10 (9%)	9 21
39	2h	114/119 (96%)	107 (94%)	7 (6%)	17 37
40	1i	90/99 (91%)	86 (96%)	4 (4%)	25 50
40	2i	89/99 (90%)	81 (91%)	8 (9%)	9 20
41	1j	66/92 (72%)	63 (96%)	3 (4%)	24 50
41	2j	69/92 (75%)	66 (96%)	3 (4%)	26 51
42	1k	82/99 (83%)	80 (98%)	2 (2%)	43 70
42	2k	83/99 (84%)	81 (98%)	2 (2%)	43 70
43	1l	96/108 (89%)	91 (95%)	5 (5%)	21 44
43	2l	96/108 (89%)	92 (96%)	4 (4%)	26 52
44	1m	93/101 (92%)	90 (97%)	3 (3%)	34 62
44	2m	92/101 (91%)	87 (95%)	5 (5%)	20 42
45	1n	49/50 (98%)	44 (90%)	5 (10%)	7 15
45	2n	49/50 (98%)	42 (86%)	7 (14%)	3 6
46	1o	78/80 (98%)	76 (97%)	2 (3%)	40 68
46	2o	78/80 (98%)	77 (99%)	1 (1%)	61 82
47	1p	69/74 (93%)	66 (96%)	3 (4%)	26 51
47	2p	68/74 (92%)	61 (90%)	7 (10%)	7 15

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
48	1q	94/97 (97%)	90 (96%)	4 (4%)	26 51
48	2q	94/97 (97%)	94 (100%)	0	100 100
49	1r	59/77 (77%)	55 (93%)	4 (7%)	14 32
49	2r	59/77 (77%)	55 (93%)	4 (7%)	14 32
50	1s	69/80 (86%)	68 (99%)	1 (1%)	59 81
50	2s	67/80 (84%)	63 (94%)	4 (6%)	17 37
51	1t	70/82 (85%)	65 (93%)	5 (7%)	13 31
51	2t	70/82 (85%)	69 (99%)	1 (1%)	59 81
52	1u	18/22 (82%)	17 (94%)	1 (6%)	19 40
52	2u	18/22 (82%)	18 (100%)	0	100 100
All	All	9303/10064 (92%)	8754 (94%)	549 (6%)	18 38

All (549) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	14	ARG
3	1D	22	SER
3	1D	32	SER
3	1D	37	LEU
3	1D	94	LEU
3	1D	113	VAL
3	1D	142	VAL
3	1D	155	LEU
3	1D	157	ARG
3	1D	162	SER
3	1D	168	ARG
3	1D	193	VAL
3	1D	211	ARG
3	1D	217	ARG
3	1D	221	VAL
3	1D	229	VAL
3	1D	242	ARG
4	1E	9	VAL
4	1E	21	VAL
4	1E	24	THR
4	1E	34	VAL
4	1E	47	VAL
4	1E	73	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	1E	75	VAL
4	1E	77	ILE
4	1E	78	LEU
4	1E	90	THR
4	1E	111	ARG
4	1E	116	VAL
4	1E	170	LEU
4	1E	175	VAL
4	1E	181	LEU
4	1E	184	VAL
5	1F	24	LEU
5	1F	33	LEU
5	1F	44	ARG
5	1F	53	THR
5	1F	57	VAL
5	1F	88	VAL
5	1F	106	ARG
5	1F	132	VAL
5	1F	140	LEU
5	1F	162	LEU
5	1F	170	LEU
5	1F	183	VAL
5	1F	192	LEU
5	1F	201	VAL
6	1G	3	LEU
6	1G	5	VAL
6	1G	43	LEU
6	1G	49	ASP
6	1G	70	VAL
6	1G	82	LEU
6	1G	140	ILE
6	1G	159	VAL
6	1G	175	LEU
7	1H	15	VAL
7	1H	23	ARG
7	1H	24	VAL
7	1H	51	ARG
7	1H	71	LEU
7	1H	84	SER
7	1H	122	THR
7	1H	124	GLU
8	1I	9	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	1I	38	LEU
8	1I	92	VAL
8	1I	109	ILE
8	1I	116	LEU
8	1I	129	THR
9	1N	14	VAL
9	1N	28	THR
9	1N	32	THR
9	1N	33	LEU
9	1N	34	LEU
9	1N	46	VAL
9	1N	62	VAL
9	1N	73	THR
9	1N	99	LEU
9	1N	121	LYS
10	1O	9	GLU
10	1O	10	VAL
10	1O	35	VAL
10	1O	98	VAL
11	1P	3	LEU
11	1P	83	VAL
11	1P	95	VAL
11	1P	101	VAL
11	1P	125	VAL
11	1P	147	LEU
12	1Q	6	ARG
12	1Q	7	MET
12	1Q	35	VAL
12	1Q	75	THR
12	1Q	101	ARG
13	1R	15	SER
13	1R	29	LEU
13	1R	33	ARG
13	1R	36	THR
13	1R	44	LEU
13	1R	54	LEU
13	1R	65	LEU
13	1R	67	LEU
13	1R	91	GLN
13	1R	96	ARG
13	1R	100	LEU
13	1R	111	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	1R	114	VAL
14	1S	14	VAL
14	1S	17	ARG
14	1S	69	VAL
14	1S	110	LEU
15	1T	28	VAL
15	1T	89	VAL
15	1T	96	ARG
15	1T	128	GLU
16	1U	59	ARG
16	1U	83	LEU
16	1U	95	LEU
17	1V	1	MET
17	1V	46	VAL
17	1V	51	VAL
17	1V	52	VAL
17	1V	61	VAL
17	1V	62	LEU
17	1V	72	VAL
17	1V	73	SER
17	1V	79	VAL
17	1V	82	ARG
18	1W	6	ILE
18	1W	11	ARG
18	1W	15	ARG
18	1W	17	VAL
18	1W	19	LEU
18	1W	23	LEU
18	1W	95	ILE
18	1W	100	THR
18	1W	107	LEU
19	1X	35	THR
19	1X	38	GLU
19	1X	72	LYS
19	1X	81	VAL
20	1Y	7	VAL
20	1Y	31	LEU
20	1Y	63	LYS
20	1Y	64	GLU
20	1Y	72	VAL
20	1Y	97	ARG
20	1Y	99	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	1Z	41	LEU
21	1Z	42	VAL
21	1Z	53	ILE
21	1Z	61	LEU
21	1Z	91	LEU
21	1Z	126	VAL
21	1Z	136	PHE
21	1Z	137	ILE
21	1Z	154	ASP
21	1Z	161	VAL
21	1Z	170	THR
22	10	39	ARG
22	10	74	ARG
23	11	11	ARG
23	11	30	VAL
23	11	80	LEU
23	11	95	LEU
24	12	3	LEU
24	12	30	ARG
24	12	41	ILE
25	13	23	LEU
25	13	34	GLU
25	13	60	GLU
26	14	31	ILE
26	14	49	PHE
26	14	53	GLU
26	14	56	VAL
26	14	58	ARG
26	14	63	TYR
27	15	6	VAL
27	15	16	ARG
27	15	29	THR
28	16	9	LEU
28	16	48	VAL
29	17	9	ARG
29	17	29	LYS
29	17	39	ARG
29	17	43	THR
29	17	46	VAL
30	18	14	VAL
30	18	23	VAL
30	18	29	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	18	30	ARG
30	18	32	LEU
31	19	4	ARG
33	1b	80	ILE
33	1b	93	VAL
33	1b	107	THR
33	1b	112	VAL
33	1b	115	LEU
33	1b	121	LEU
33	1b	142	LEU
33	1b	160	ASP
33	1b	162	ILE
34	1c	3	ASN
34	1c	57	ILE
34	1c	70	VAL
34	1c	89	GLU
34	1c	112	SER
34	1c	116	VAL
34	1c	196	LEU
35	1d	5	ILE
35	1d	8	VAL
35	1d	10	ARG
35	1d	49	ARG
35	1d	53	ASP
35	1d	56	VAL
35	1d	135	LEU
35	1d	140	VAL
35	1d	144	ASP
35	1d	175	SER
35	1d	182	LYS
35	1d	194	LEU
36	1e	16	THR
36	1e	20	GLN
36	1e	41	VAL
36	1e	51	VAL
36	1e	64	ARG
36	1e	71	LEU
36	1e	81	GLU
36	1e	91	LEU
36	1e	120	THR
36	1e	131	ILE
37	1f	17	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	1f	19	LEU
37	1f	25	ILE
37	1f	55	ASP
37	1f	72	VAL
38	1g	6	ARG
38	1g	9	VAL
38	1g	24	THR
38	1g	50	ILE
38	1g	79	ARG
38	1g	98	SER
39	1h	13	ILE
39	1h	25	ASP
39	1h	26	VAL
39	1h	51	VAL
39	1h	52	ASP
39	1h	63	LEU
39	1h	82	HIS
39	1h	104	ARG
39	1h	112	LEU
39	1h	137	VAL
40	1i	64	THR
40	1i	86	VAL
40	1i	108	VAL
40	1i	128	ARG
41	1j	19	SER
41	1j	81	THR
41	1j	92	THR
42	1k	48	ILE
42	1k	120	ARG
43	1l	18	VAL
43	1l	27	LEU
43	1l	33	ARG
43	1l	57	LYS
43	1l	83	VAL
44	1m	19	LEU
44	1m	43	THR
44	1m	70	LEU
45	1n	6	LEU
45	1n	13	THR
45	1n	18	VAL
45	1n	22	THR
45	1n	33	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
46	1o	5	LYS
46	1o	66	LEU
47	1p	20	VAL
47	1p	21	VAL
47	1p	62	VAL
48	1q	6	LEU
48	1q	9	VAL
48	1q	35	VAL
48	1q	63	ARG
49	1r	35	ARG
49	1r	37	VAL
49	1r	47	THR
49	1r	76	LEU
50	1s	12	ASP
51	1t	10	LEU
51	1t	13	LEU
51	1t	20	LEU
51	1t	31	SER
51	1t	84	LEU
52	1u	17	THR
3	2D	14	ARG
3	2D	54	ARG
3	2D	94	LEU
3	2D	99	ASP
3	2D	113	VAL
3	2D	116	GLN
3	2D	138	VAL
3	2D	141	VAL
3	2D	142	VAL
3	2D	157	ARG
3	2D	169	GLU
3	2D	204	ILE
3	2D	211	ARG
3	2D	221	VAL
4	2E	7	VAL
4	2E	9	VAL
4	2E	12	THR
4	2E	21	VAL
4	2E	38	THR
4	2E	75	VAL
4	2E	116	VAL
4	2E	175	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	2E	181	LEU
5	2F	12	LEU
5	2F	57	VAL
5	2F	70	THR
5	2F	88	VAL
5	2F	106	ARG
5	2F	132	VAL
5	2F	170	LEU
5	2F	183	VAL
5	2F	192	LEU
5	2F	195	ASP
5	2F	201	VAL
6	2G	9	ARG
6	2G	28	VAL
6	2G	31	VAL
6	2G	43	LEU
6	2G	49	ASP
6	2G	70	VAL
6	2G	79	ASN
6	2G	92	VAL
6	2G	97	ASP
6	2G	109	VAL
6	2G	130	ASN
6	2G	140	ILE
6	2G	145	THR
6	2G	159	VAL
7	2H	15	VAL
7	2H	70	THR
7	2H	71	LEU
7	2H	134	SER
7	2H	139	GLN
7	2H	148	ILE
8	2I	3	VAL
8	2I	31	LEU
8	2I	38	LEU
8	2I	47	LEU
8	2I	77	LEU
8	2I	92	VAL
8	2I	123	LEU
8	2I	127	VAL
8	2I	142	VAL
8	2I	144	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	2N	9	VAL
9	2N	14	VAL
9	2N	33	LEU
9	2N	34	LEU
9	2N	46	VAL
9	2N	62	VAL
9	2N	67	LEU
9	2N	99	LEU
10	2O	63	VAL
10	2O	69	ILE
10	2O	98	VAL
11	2P	95	VAL
11	2P	105	LEU
11	2P	131	SER
11	2P	133	SER
11	2P	148	LEU
12	2Q	1	MET
12	2Q	2	LEU
12	2Q	38	GLU
12	2Q	75	THR
13	2R	24	GLN
13	2R	29	LEU
13	2R	33	ARG
13	2R	36	THR
13	2R	44	LEU
13	2R	54	LEU
13	2R	65	LEU
13	2R	91	GLN
13	2R	96	ARG
13	2R	111	LEU
13	2R	114	VAL
14	2S	8	GLU
14	2S	48	LEU
15	2T	96	ARG
16	2U	8	VAL
16	2U	55	ARG
16	2U	95	LEU
16	2U	100	VAL
17	2V	14	VAL
17	2V	52	VAL
17	2V	57	VAL
17	2V	61	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	2V	62	LEU
17	2V	72	VAL
17	2V	79	VAL
17	2V	82	ARG
17	2V	95	LEU
17	2V	98	GLU
18	2W	11	ARG
18	2W	15	ARG
18	2W	17	VAL
18	2W	23	LEU
18	2W	39	THR
18	2W	107	LEU
19	2X	62	LYS
19	2X	81	VAL
20	2Y	19	LYS
20	2Y	21	LYS
20	2Y	55	TYR
20	2Y	61	ILE
20	2Y	72	VAL
20	2Y	88	LYS
20	2Y	90	LEU
20	2Y	99	CYS
20	2Y	107	ASP
21	2Z	42	VAL
21	2Z	96	VAL
21	2Z	126	VAL
21	2Z	154	ASP
21	2Z	155	LEU
21	2Z	171	ILE
22	20	14	ARG
23	21	4	VAL
23	21	35	THR
23	21	38	SER
25	23	30	ARG
25	23	57	GLU
26	24	50	VAL
27	25	6	VAL
27	25	29	THR
27	25	58	LEU
28	26	9	LEU
28	26	25	LYS
28	26	48	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
29	27	39	ARG
29	27	41	ARG
29	27	43	THR
29	27	46	VAL
29	27	48	LYS
30	28	14	VAL
30	28	41	ILE
31	29	4	ARG
31	29	7	VAL
31	29	17	ILE
31	29	26	ILE
33	2b	93	VAL
33	2b	111	ARG
33	2b	112	VAL
33	2b	115	LEU
33	2b	124	SER
33	2b	127	ILE
33	2b	154	LEU
33	2b	189	ASP
33	2b	195	ASP
33	2b	213	LEU
34	2c	3	ASN
34	2c	59	ARG
34	2c	68	VAL
34	2c	103	VAL
34	2c	115	LEU
34	2c	154	SER
34	2c	196	LEU
35	2d	8	VAL
35	2d	10	ARG
35	2d	17	VAL
35	2d	19	LEU
35	2d	31	CYS
35	2d	34	GLU
35	2d	83	SER
35	2d	108	LEU
35	2d	112	VAL
35	2d	119	GLN
35	2d	135	LEU
35	2d	170	VAL
35	2d	194	LEU
35	2d	205	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	2e	41	VAL
36	2e	53	LEU
36	2e	83	GLU
36	2e	149	GLU
37	2f	61	LEU
37	2f	72	VAL
37	2f	81	ILE
38	2g	52	GLU
38	2g	61	VAL
38	2g	79	ARG
38	2g	113	GLU
39	2h	2	LEU
39	2h	8	ASP
39	2h	25	ASP
39	2h	51	VAL
39	2h	69	ARG
39	2h	114	THR
39	2h	137	VAL
40	2i	23	ASN
40	2i	27	THR
40	2i	64	THR
40	2i	81	ILE
40	2i	102	LEU
40	2i	107	ARG
40	2i	108	VAL
40	2i	128	ARG
41	2j	16	LEU
41	2j	72	VAL
41	2j	81	THR
42	2k	48	ILE
42	2k	109	VAL
43	2l	18	VAL
43	2l	27	LEU
43	2l	113	ARG
43	2l	117	ARG
44	2m	3	ARG
44	2m	15	VAL
44	2m	60	VAL
44	2m	103	THR
44	2m	117	VAL
45	2n	3	ARG
45	2n	6	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
45	2n	7	ILE
45	2n	18	VAL
45	2n	22	THR
45	2n	31	ARG
45	2n	33	VAL
46	2o	39	LEU
47	2p	2	VAL
47	2p	20	VAL
47	2p	21	VAL
47	2p	44	THR
47	2p	60	LEU
47	2p	62	VAL
47	2p	67	THR
49	2r	21	LYS
49	2r	47	THR
49	2r	76	LEU
49	2r	85	LEU
50	2s	5	LEU
50	2s	33	THR
50	2s	77	THR
50	2s	83	HIS
51	2t	51	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (115) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	87	ASN
3	1D	166	GLN
4	1E	48	GLN
4	1E	121	ASN
5	1F	69	HIS
5	1F	203	GLN
5	1F	204	ASN
6	1G	26	GLN
6	1G	108	ASN
8	1I	11	ASN
9	1N	69	GLN
12	1Q	113	GLN
12	1Q	123	HIS
13	1R	31	HIS
13	1R	61	HIS
13	1R	71	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	1T	58	ASN
16	1U	72	HIS
19	1X	31	HIS
19	1X	82	GLN
20	1Y	6	HIS
21	1Z	54	HIS
22	10	29	GLN
24	12	46	GLN
24	12	56	GLN
26	14	47	GLN
28	16	20	ASN
33	1b	78	GLN
34	1c	6	HIS
34	1c	104	GLN
34	1c	108	ASN
34	1c	162	GLN
35	1d	74	GLN
35	1d	77	ASN
35	1d	116	GLN
35	1d	123	HIS
35	1d	125	HIS
36	1e	78	HIS
37	1f	100	ASN
38	1g	28	ASN
38	1g	148	ASN
40	1i	3	GLN
40	1i	73	GLN
41	1j	21	GLN
41	1j	56	HIS
43	1l	80	HIS
43	1l	99	HIS
44	1m	62	ASN
46	1o	46	HIS
47	1p	16	HIS
50	1s	57	HIS
50	1s	69	HIS
51	1t	16	HIS
3	2D	116	GLN
5	2F	69	HIS
5	2F	75	HIS
5	2F	204	ASN
8	2I	104	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	2I	105	HIS
8	2I	139	GLN
9	2N	128	HIS
11	2P	35	HIS
12	2Q	89	ASN
13	2R	13	HIS
13	2R	31	HIS
13	2R	71	GLN
15	2T	58	ASN
15	2T	90	GLN
16	2U	81	HIS
16	2U	94	ASN
17	2V	80	GLN
18	2W	62	HIS
19	2X	31	HIS
19	2X	82	GLN
20	2Y	43	ASN
21	2Z	73	GLN
22	20	29	GLN
24	22	56	GLN
24	22	65	ASN
26	24	46	GLN
33	2b	40	HIS
33	2b	78	GLN
33	2b	94	ASN
34	2c	108	ASN
34	2c	139	GLN
34	2c	176	HIS
35	2d	74	GLN
35	2d	77	ASN
35	2d	116	GLN
35	2d	125	HIS
36	2e	78	HIS
37	2f	73	ASN
37	2f	100	ASN
38	2g	13	GLN
38	2g	28	ASN
38	2g	37	ASN
38	2g	86	GLN
38	2g	109	ASN
40	2i	3	GLN
40	2i	58	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	2j	56	HIS
42	2k	22	HIS
42	2k	117	ASN
43	2l	99	HIS
46	2o	50	HIS
46	2o	62	GLN
47	2p	16	HIS
48	2q	45	HIS
49	2r	63	GLN
50	2s	23	ASN
50	2s	47	HIS
50	2s	57	HIS
50	2s	69	HIS
50	2s	83	HIS
51	2t	42	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	431 (15%)	29 (1%)
1	2A	2791/2915 (95%)	482 (17%)	24 (0%)
2	1B	120/121 (99%)	11 (9%)	1 (0%)
2	2B	118/121 (97%)	33 (27%)	0
32	1a	1497/1521 (98%)	240 (16%)	0
32	2a	1501/1521 (98%)	286 (19%)	0
53	1v	12/24 (50%)	2 (16%)	0
53	2v	12/24 (50%)	4 (33%)	0
54	1w	72/76 (94%)	23 (31%)	0
54	1y	72/76 (94%)	19 (26%)	0
54	2w	69/76 (90%)	22 (31%)	0
54	2y	70/76 (92%)	21 (30%)	0
55	1x	75/77 (97%)	10 (13%)	0
55	2x	75/77 (97%)	13 (17%)	0
All	All	9348/9620 (97%)	1597 (17%)	54 (0%)

All (1597) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	9	U
1	1A	12	U
1	1A	13	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	27	G
1	1A	34	C
1	1A	36	G
1	1A	45	C
1	1A	51	G
1	1A	55	G
1	1A	58	G
1	1A	71	A
1	1A	72	U
1	1A	74	A
1	1A	75	G
1	1A	84	A
1	1A	95	G
1	1A	102	G
1	1A	118	A
1	1A	119	A
1	1A	120	U
1	1A	125	G
1	1A	136	G
1	1A	139(A)	G
1	1A	182	A
1	1A	196	A
1	1A	199	A
1	1A	200	U
1	1A	205	G
1	1A	215	G
1	1A	216	A
1	1A	222	A
1	1A	225	A
1	1A	228	A
1	1A	229	A
1	1A	232	G
1	1A	248	G
1	1A	269	U
1	1A	271(E)	U
1	1A	271(K)	U
1	1A	271(L)	U
1	1A	271(M)	G
1	1A	271(N)	U
1	1A	271(O)	C
1	1A	271(S)	G
1	1A	271(U)	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	272(A)	U
1	1A	272(B)	G
1	1A	279	C
1	1A	311	A
1	1A	329	G
1	1A	330	A
1	1A	352	G
1	1A	363	G
1	1A	380	U
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	457	A
1	1A	481	G
1	1A	504	U
1	1A	505	A
1	1A	509	C
1	1A	510	C
1	1A	528	A
1	1A	530	G
1	1A	531	C
1	1A	532	A
1	1A	533	G
1	1A	545	G
1	1A	549	G
1	1A	563	G
1	1A	573	G
1	1A	574	C
1	1A	575	A
1	1A	587	C
1	1A	603	A
1	1A	604	G
1	1A	607	U
1	1A	614(B)	G
1	1A	615	G
1	1A	621	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	627	A
1	1A	637	A
1	1A	645	C
1	1A	646	A
1	1A	652(E)	G
1	1A	652(T)	C
1	1A	669	G
1	1A	686	G
1	1A	730	C
1	1A	740	U
1	1A	765	G
1	1A	775	G
1	1A	776	G
1	1A	782	A
1	1A	784	A
1	1A	785	G
1	1A	790	C
1	1A	792	G
1	1A	805	G
1	1A	812	C
1	1A	819	A
1	1A	827	U
1	1A	828	U
1	1A	854	G
1	1A	859	G
1	1A	866	A
1	1A	877	U
1	1A	879	G
1	1A	880	G
1	1A	882	G
1	1A	883	G
1	1A	884	C
1	1A	885	C
1	1A	886	C
1	1A	887	A
1	1A	888	C
1	1A	890	A
1	1A	895	U
1	1A	896	A
1	1A	897	C
1	1A	898	C
1	1A	907	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	910	A
1	1A	932	G
1	1A	945	A
1	1A	946	G
1	1A	953	A
1	1A	958	U
1	1A	959	A
1	1A	961	C
1	1A	974	G
1	1A	975	C
1	1A	983	A
1	1A	996	A
1	1A	1012	U
1	1A	1013	C
1	1A	1022	G
1	1A	1026	U
1	1A	1033	U
1	1A	1038	C
1	1A	1041	C
1	1A	1044	G
1	1A	1045	A
1	1A	1046	A
1	1A	1047	G
1	1A	1048	A
1	1A	1054	A
1	1A	1055	G
1	1A	1058	G
1	1A	1063	G
1	1A	1068	G
1	1A	1071	G
1	1A	1073	A
1	1A	1074	G
1	1A	1075	C
1	1A	1076	C
1	1A	1077	A
1	1A	1078	U
1	1A	1079	C
1	1A	1082	U
1	1A	1083	U
1	1A	1084	A
1	1A	1088	A
1	1A	1089	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1090	U
1	1A	1091	G
1	1A	1093	G
1	1A	1094	U
1	1A	1101	U
1	1A	1102	C
1	1A	1103	A
1	1A	1110	G
1	1A	1111	A
1	1A	1112	G
1	1A	1115	G
1	1A	1116	C
1	1A	1128	A
1	1A	1130	U
1	1A	1135	C
1	1A	1136	G
1	1A	1171	G
1	1A	1173	G
1	1A	1174	A
1	1A	1175	U
1	1A	1176	G
1	1A	1177	A
1	1A	1178	C
1	1A	1211	U
1	1A	1220	A
1	1A	1244	G
1	1A	1247	A
1	1A	1250	G
1	1A	1253	A
1	1A	1256	G
1	1A	1271	G
1	1A	1272	A
1	1A	1273	U
1	1A	1275	A
1	1A	1276	A
1	1A	1300	U
1	1A	1301	A
1	1A	1303	G
1	1A	1313	U
1	1A	1352	U
1	1A	1359	A
1	1A	1360	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1365	A
1	1A	1380	G
1	1A	1384	A
1	1A	1385	G
1	1A	1386	C
1	1A	1416	G
1	1A	1417	C
1	1A	1421	G
1	1A	1428	C
1	1A	1439	A
1	1A	1445	A
1	1A	1450	G
1	1A	1455	G
1	1A	1467	C
1	1A	1478	G
1	1A	1482	G
1	1A	1490	A
1	1A	1493	C
1	1A	1494	A
1	1A	1509	C
1	1A	1509(A)	A
1	1A	1558	A
1	1A	1559	G
1	1A	1566	A
1	1A	1569	A
1	1A	1578	U
1	1A	1581	G
1	1A	1584	C
1	1A	1586	A
1	1A	1608	A
1	1A	1610	A
1	1A	1648	C
1	1A	1654	A
1	1A	1664	A
1	1A	1669	A
1	1A	1674	G
1	1A	1696	G
1	1A	1700	A
1	1A	1701	A
1	1A	1703	G
1	1A	1722	A
1	1A	1746	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	1786	A
1	1A	1791	A
1	1A	1800	C
1	1A	1801	G
1	1A	1816	G
1	1A	1847	A
1	1A	1858	G
1	1A	1861	G
1	1A	1877	A
1	1A	1878	G
1	1A	1889	A
1	1A	1900	A
1	1A	1906	G
1	1A	1915	5MU
1	1A	1929	G
1	1A	1930	G
1	1A	1937	A
1	1A	1938	A
1	1A	1955	U
1	1A	1963	U
1	1A	1965	C
1	1A	1967	C
1	1A	1970	A
1	1A	1971	A
1	1A	1972	A
1	1A	1993	U
1	1A	1997	G
1	1A	2020	A
1	1A	2023	G
1	1A	2031	A
1	1A	2032	G
1	1A	2033	A
1	1A	2043	C
1	1A	2055	C
1	1A	2056	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2060	A
1	1A	2061	G
1	1A	2069	G
1	1A	2110	G
1	1A	2111	C
1	1A	2113	U
1	1A	2118	U
1	1A	2119	A
1	1A	2121	G
1	1A	2126	A
1	1A	2127	G
1	1A	2129	C
1	1A	2130	U
1	1A	2131	G
1	1A	2132	U
1	1A	2133	G
1	1A	2134	A
1	1A	2135	A
1	1A	2140	C
1	1A	2141	G
1	1A	2142	C
1	1A	2144	U
1	1A	2147	G
1	1A	2150	U
1	1A	2151	G
1	1A	2157	G
1	1A	2158	A
1	1A	2159	G
1	1A	2162	G
1	1A	2165	G
1	1A	2166	G
1	1A	2168	G
1	1A	2171	A
1	1A	2172	U
1	1A	2173	A
1	1A	2181	G
1	1A	2182	G
1	1A	2184	G
1	1A	2192	G
1	1A	2198	A
1	1A	2206	G
1	1A	2207	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2208	A
1	1A	2219	G
1	1A	2225	A
1	1A	2238	G
1	1A	2239	G
1	1A	2268	A
1	1A	2269	A
1	1A	2273	A
1	1A	2283	C
1	1A	2287	A
1	1A	2305	A
1	1A	2308	G
1	1A	2309	A
1	1A	2320	A
1	1A	2325	G
1	1A	2334	G
1	1A	2336	A
1	1A	2347	C
1	1A	2361	A
1	1A	2372	G
1	1A	2383	G
1	1A	2385	C
1	1A	2396	G
1	1A	2400	G
1	1A	2406	U
1	1A	2408	U
1	1A	2410	G
1	1A	2425	A
1	1A	2429	G
1	1A	2430	A
1	1A	2435	A
1	1A	2439	A
1	1A	2441	C
1	1A	2448	A
1	1A	2449	U
1	1A	2474	C
1	1A	2476	A
1	1A	2484	G
1	1A	2491	U
1	1A	2498	C
1	1A	2502	G
1	1A	2505	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2518	A
1	1A	2520	C
1	1A	2529	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	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	2757	A
1	1A	2758	A
1	1A	2761	G
1	1A	2764	A
1	1A	2765	A
1	1A	2766	G
1	1A	2769	C
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	2805	G
1	1A	2818	G
1	1A	2820	A
1	1A	2821	A
1	1A	2834	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2835	A
1	1A	2858	C
1	1A	2872	G
1	1A	2873	A
1	1A	2876	G
1	1A	2880	C
1	1A	2892	A
1	1A	2894	G
2	1B	2	C
2	1B	12	C
2	1B	21	G
2	1B	25	A
2	1B	35	U
2	1B	50	G
2	1B	56	G
2	1B	73	A
2	1B	85	G
2	1B	109	C
2	1B	110	G
32	1a	7	G
32	1a	9	G
32	1a	32	A
32	1a	33	A
32	1a	39	G
32	1a	47	C
32	1a	48	C
32	1a	50	A
32	1a	51	A
32	1a	52	G
32	1a	61	G
32	1a	65	U
32	1a	91	C
32	1a	98	G
32	1a	116	A
32	1a	120	A
32	1a	121	C
32	1a	131	C
32	1a	163	C
32	1a	174	C
32	1a	180	U
32	1a	183	G
32	1a	189(D)	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	189(F)	U
32	1a	189(G)	G
32	1a	189(J)	G
32	1a	195	A
32	1a	197	A
32	1a	199	G
32	1a	201	C
32	1a	202	U
32	1a	203	U
32	1a	204	U
32	1a	216	G
32	1a	217	C
32	1a	219	C
32	1a	222	U
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	321	A
32	1a	328	C
32	1a	332	G
32	1a	344	A
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	384	G
32	1a	397	A
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	423	G
32	1a	424	G
32	1a	429	U
32	1a	439	A
32	1a	452	A
32	1a	453	A
32	1a	461	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	470	C
32	1a	471	G
32	1a	485	G
32	1a	496	A
32	1a	498	U
32	1a	505	G
32	1a	509	A
32	1a	510	A
32	1a	511	C
32	1a	518	C
32	1a	528	C
32	1a	531	U
32	1a	532	A
32	1a	547	A
32	1a	559	A
32	1a	561	U
32	1a	568	G
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	577	G
32	1a	596	C
32	1a	629	G
32	1a	630	G
32	1a	653	A
32	1a	665	A
32	1a	686	U
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	792	A
32	1a	793	U
32	1a	794	A
32	1a	815	A
32	1a	816	A
32	1a	817	C
32	1a	821	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	828	A
32	1a	840	C
32	1a	841	U
32	1a	851	G
32	1a	853	G
32	1a	859	A
32	1a	870	U
32	1a	872	A
32	1a	902	G
32	1a	914	A
32	1a	926	G
32	1a	927	G
32	1a	932	C
32	1a	934	C
32	1a	955	U
32	1a	960	U
32	1a	961	U
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	982	U
32	1a	992	U
32	1a	993	G
32	1a	997	U
32	1a	1000	U
32	1a	1003	G
32	1a	1005	A
32	1a	1006	C
32	1a	1009	G
32	1a	1020	U
32	1a	1022	G
32	1a	1023	G
32	1a	1024	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C
32	1a	1029	C
32	1a	1030(A)	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	1030(B)	C
32	1a	1030(C)	G
32	1a	1031	G
32	1a	1032	G
32	1a	1033	G
32	1a	1039	C
32	1a	1045	C
32	1a	1054	C
32	1a	1065	U
32	1a	1066	C
32	1a	1068	G
32	1a	1070	U
32	1a	1081	G
32	1a	1087	G
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1104	G
32	1a	1108	G
32	1a	1121	U
32	1a	1125	U
32	1a	1132	C
32	1a	1134	G
32	1a	1136	U
32	1a	1137	C
32	1a	1138	G
32	1a	1139	G
32	1a	1140	C
32	1a	1146	A
32	1a	1152	A
32	1a	1156	G
32	1a	1157	A
32	1a	1159	U
32	1a	1160	G
32	1a	1166	G
32	1a	1184	G
32	1a	1193	G
32	1a	1196	U
32	1a	1197	G
32	1a	1202	G
32	1a	1212	U
32	1a	1213	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	1222	G
32	1a	1226	C
32	1a	1227	A
32	1a	1236	A
32	1a	1238	A
32	1a	1246	C
32	1a	1256	A
32	1a	1257	U
32	1a	1260	C
32	1a	1270	C
32	1a	1275	A
32	1a	1276	G
32	1a	1278	U
32	1a	1279	A
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1320	C
32	1a	1338	G
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1363(A)	A
32	1a	1368	G
32	1a	1370	G
32	1a	1378	C
32	1a	1394	A
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	1487	G
32	1a	1492	A
32	1a	1494	G
32	1a	1503	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	1504	G
32	1a	1506	U
32	1a	1517	G
32	1a	1519	MA6
32	1a	1520	G
32	1a	1529	G
32	1a	1530	G
53	1v	13	A
53	1v	24	A
54	1w	2	C
54	1w	3	C
54	1w	6	G
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	23	A
54	1w	24	G
54	1w	25	C
54	1w	45	U
54	1w	46	7MG
54	1w	47	U
54	1w	48	C
54	1w	50	U
54	1w	63	G
54	1w	68	C
54	1w	70	G
54	1w	71	G
54	1w	73	A
54	1w	74	C
55	1x	6	G
55	1x	9	G
55	1x	14	A
55	1x	19	G
55	1x	21	A
55	1x	22	G
55	1x	47	U
55	1x	63	G
55	1x	64	G
55	1x	76	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	1y	6	G
54	1y	8	4SU
54	1y	9	A
54	1y	11	C
54	1y	13	C
54	1y	14	A
54	1y	19	G
54	1y	20	U
54	1y	21	A
54	1y	22	G
54	1y	35	A
54	1y	44	G
54	1y	45	U
54	1y	46	7MG
54	1y	47	U
54	1y	57	G
54	1y	59	U
54	1y	61	C
54	1y	70	G
1	2A	10	G
1	2A	11	G
1	2A	15	G
1	2A	35	G
1	2A	45	C
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	79	G
1	2A	83	G
1	2A	84	A
1	2A	90	U
1	2A	95	G
1	2A	96	G
1	2A	100	G
1	2A	102	G
1	2A	118	A
1	2A	120	U
1	2A	131	G
1	2A	141	A
1	2A	154(A)	C
1	2A	157	U
1	2A	173	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	181	A
1	2A	196	A
1	2A	199	A
1	2A	205	G
1	2A	214	G
1	2A	215	G
1	2A	216	A
1	2A	221	A
1	2A	222	A
1	2A	225	A
1	2A	228	A
1	2A	229	A
1	2A	233	A
1	2A	248	G
1	2A	249	C
1	2A	266	G
1	2A	271(J)	C
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	271(O)	C
1	2A	272(B)	G
1	2A	277	C
1	2A	278	A
1	2A	294	A
1	2A	304	G
1	2A	311	A
1	2A	324	A
1	2A	327	G
1	2A	329	G
1	2A	330	A
1	2A	342	G
1	2A	352	G
1	2A	362	U
1	2A	363	G
1	2A	363(B)	G
1	2A	363(D)	G
1	2A	386	G
1	2A	389	G
1	2A	396	G
1	2A	411	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	412	A
1	2A	422	A
1	2A	435	C
1	2A	444	C
1	2A	454	A
1	2A	455	C
1	2A	457	A
1	2A	481	G
1	2A	505	A
1	2A	508	G
1	2A	509	C
1	2A	528	A
1	2A	529	A
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	545	G
1	2A	551	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	592	G
1	2A	595	C
1	2A	599	G
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	614(A)	U
1	2A	614(B)	G
1	2A	615	G
1	2A	616	G
1	2A	627	A
1	2A	637	A
1	2A	645	C
1	2A	652(B)	A
1	2A	652(U)	G
1	2A	653	A
1	2A	661	C
1	2A	669	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	686	G
1	2A	701	G
1	2A	712	G
1	2A	717	G
1	2A	726	G
1	2A	730	C
1	2A	753	C
1	2A	771	G
1	2A	775	G
1	2A	776	G
1	2A	778	G
1	2A	782	A
1	2A	783	A
1	2A	784	A
1	2A	785	G
1	2A	790	C
1	2A	792	G
1	2A	805	G
1	2A	806	C
1	2A	811	U
1	2A	812	C
1	2A	819	A
1	2A	827	U
1	2A	828	U
1	2A	832	G
1	2A	847	U
1	2A	854	G
1	2A	856	C
1	2A	857	C
1	2A	859	G
1	2A	866	A
1	2A	869	G
1	2A	873	G
1	2A	874	G
1	2A	875	G
1	2A	879	G
1	2A	880	G
1	2A	884	C
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	889	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	890	A
1	2A	892	G
1	2A	893	C
1	2A	894	C
1	2A	895	U
1	2A	896	A
1	2A	900	A
1	2A	901	A
1	2A	910	A
1	2A	914	C
1	2A	917	A
1	2A	932	G
1	2A	933	A
1	2A	936	C
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	953	A
1	2A	958	U
1	2A	959	A
1	2A	961	C
1	2A	974	G
1	2A	975	C
1	2A	979	G
1	2A	980	A
1	2A	983	A
1	2A	996	A
1	2A	997	G
1	2A	1012	U
1	2A	1013	C
1	2A	1017	G
1	2A	1020	A
1	2A	1022	G
1	2A	1025	G
1	2A	1027	A
1	2A	1033	U
1	2A	1038	C
1	2A	1039	G
1	2A	1043	C
1	2A	1114	G
1	2A	1116	C
1	2A	1130	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1135	C
1	2A	1136	G
1	2A	1139	G
1	2A	1166	C
1	2A	1167	U
1	2A	1171	G
1	2A	1188	U
1	2A	1195	G
1	2A	1206	G
1	2A	1210	A
1	2A	1211	U
1	2A	1220	A
1	2A	1229	G
1	2A	1237	A
1	2A	1248	G
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1273	U
1	2A	1284	A
1	2A	1287	A
1	2A	1300	U
1	2A	1301	A
1	2A	1309	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	1373	A
1	2A	1376	C
1	2A	1380	G
1	2A	1384	A
1	2A	1385	G
1	2A	1386	C
1	2A	1416	G
1	2A	1417	C
1	2A	1420	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1421	G
1	2A	1427	A
1	2A	1428	C
1	2A	1437	C
1	2A	1444	G
1	2A	1445	A
1	2A	1449	A
1	2A	1450	G
1	2A	1460	A
1	2A	1463	C
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	1496	A
1	2A	1497	U
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1525	G
1	2A	1531	C
1	2A	1532	C
1	2A	1533	G
1	2A	1537	G
1	2A	1543	C
1	2A	1544	A
1	2A	1547	C
1	2A	1558	A
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1579	A
1	2A	1580	A
1	2A	1584	C
1	2A	1586	A
1	2A	1608	A
1	2A	1609	A
1	2A	1610	A
1	2A	1640	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1648	C
1	2A	1654	A
1	2A	1663	C
1	2A	1674	G
1	2A	1696	G
1	2A	1700	A
1	2A	1701	A
1	2A	1703	G
1	2A	1721	G
1	2A	1722	A
1	2A	1739	U
1	2A	1740	G
1	2A	1746	G
1	2A	1756	G
1	2A	1758	G
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A
1	2A	1780	A
1	2A	1782	C
1	2A	1786	A
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1811	G
1	2A	1812	A
1	2A	1816	G
1	2A	1835	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1963	U
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1992	G
1	2A	1993	U
1	2A	1997	G
1	2A	2020	A
1	2A	2023	G
1	2A	2027	G
1	2A	2031	A
1	2A	2032	G
1	2A	2033	A
1	2A	2043	C
1	2A	2050	C
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2062	A
1	2A	2069	G
1	2A	2093	G
1	2A	2096	U
1	2A	2103	C
1	2A	2111	C
1	2A	2113	U
1	2A	2116	G
1	2A	2117	A
1	2A	2119	A
1	2A	2120	G
1	2A	2122	U
1	2A	2124	G
1	2A	2125	G
1	2A	2126	A
1	2A	2127	G
1	2A	2129	C
1	2A	2131	G
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2135	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2137	C
1	2A	2138	C
1	2A	2140	C
1	2A	2142	C
1	2A	2146	C
1	2A	2148	G
1	2A	2150	U
1	2A	2153	G
1	2A	2157	G
1	2A	2158	A
1	2A	2161	C
1	2A	2166	G
1	2A	2167	U
1	2A	2168	G
1	2A	2169	A
1	2A	2172	U
1	2A	2174	C
1	2A	2178	C
1	2A	2180	U
1	2A	2185	C
1	2A	2189	U
1	2A	2192	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2225	A
1	2A	2239	G
1	2A	2273	A
1	2A	2275	C
1	2A	2278	A
1	2A	2283	C
1	2A	2287	A
1	2A	2289	G
1	2A	2294	C
1	2A	2305	A
1	2A	2308	G
1	2A	2311	A
1	2A	2319	G
1	2A	2320	A
1	2A	2325	G
1	2A	2327	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2334	G
1	2A	2336	A
1	2A	2347	C
1	2A	2350	C
1	2A	2352	A
1	2A	2353	G
1	2A	2361	A
1	2A	2376	A
1	2A	2377	A
1	2A	2383	G
1	2A	2385	C
1	2A	2403	C
1	2A	2406	U
1	2A	2410	G
1	2A	2425	A
1	2A	2429	G
1	2A	2430	A
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2445	G
1	2A	2448	A
1	2A	2468	G
1	2A	2474	C
1	2A	2476	A
1	2A	2477	C
1	2A	2478	A
1	2A	2480	C
1	2A	2487	G
1	2A	2490	G
1	2A	2491	U
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	2554	U
1	2A	2566	A
1	2A	2567	G
1	2A	2586	C
1	2A	2602	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2609	U
1	2A	2610	C
1	2A	2611	U
1	2A	2612	C
1	2A	2623	G
1	2A	2629	A
1	2A	2630	G
1	2A	2654	A
1	2A	2662	A
1	2A	2689	U
1	2A	2690	C
1	2A	2691	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	2758	A
1	2A	2759	G
1	2A	2764	A
1	2A	2765	A
1	2A	2766	G
1	2A	2778	A
1	2A	2779	U
1	2A	2780	G
1	2A	2789	C
1	2A	2802	G
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2833	G
1	2A	2835	A
1	2A	2850	A
1	2A	2872	G
1	2A	2880	C
1	2A	2894	G
1	2A	2897	U
2	2B	2	C
2	2B	4	C
2	2B	5	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2B	8	U
2	2B	13	A
2	2B	19	G
2	2B	20	C
2	2B	25	A
2	2B	30	C
2	2B	34	U
2	2B	42	C
2	2B	52	A
2	2B	53	A
2	2B	56	G
2	2B	63	G
2	2B	64	C
2	2B	65	C
2	2B	66	A
2	2B	67	G
2	2B	72	G
2	2B	73	A
2	2B	74	U
2	2B	75	G
2	2B	85	G
2	2B	94	C
2	2B	106	G
2	2B	108	U
2	2B	110	G
2	2B	111	G
2	2B	114	C
2	2B	116	G
2	2B	119	G
2	2B	120	A
32	2a	6	G
32	2a	9	G
32	2a	32	A
32	2a	39	G
32	2a	47	C
32	2a	48	C
32	2a	51	A
32	2a	52	G
32	2a	66	G
32	2a	73	G
32	2a	79	G
32	2a	88	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	89	C
32	2a	101	A
32	2a	105	G
32	2a	116	A
32	2a	117	G
32	2a	121	C
32	2a	124	G
32	2a	131	C
32	2a	142	G
32	2a	144	G
32	2a	146	G
32	2a	159	G
32	2a	163	C
32	2a	174	C
32	2a	180	U
32	2a	182	U
32	2a	184	G
32	2a	189(E)	U
32	2a	189(F)	U
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	247	G
32	2a	251	G
32	2a	258	G
32	2a	266	G
32	2a	267	C
32	2a	269	C
32	2a	281	G
32	2a	289	G
32	2a	318	G
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	350	G
32	2a	351	G
32	2a	352	C
32	2a	353	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	354	G
32	2a	367	U
32	2a	372	C
32	2a	373	A
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	412	A
32	2a	415	A
32	2a	421	U
32	2a	423	G
32	2a	429	U
32	2a	430	A
32	2a	441	A
32	2a	442	C
32	2a	452	A
32	2a	461	A
32	2a	470	C
32	2a	484	G
32	2a	485	G
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	509	A
32	2a	510	A
32	2a	511	C
32	2a	517	G
32	2a	518	C
32	2a	528	C
32	2a	531	U
32	2a	532	A
32	2a	547	A
32	2a	559	A
32	2a	560	U
32	2a	561	U
32	2a	564	C
32	2a	572	A
32	2a	573	A
32	2a	574	A
32	2a	576	G
32	2a	577	G
32	2a	596	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	598	U
32	2a	618	C
32	2a	630	G
32	2a	653	A
32	2a	657	G
32	2a	665	A
32	2a	687	A
32	2a	688	G
32	2a	694	A
32	2a	695	A
32	2a	703	G
32	2a	721	G
32	2a	723	U
32	2a	724	G
32	2a	731	G
32	2a	749	C
32	2a	755	G
32	2a	777	A
32	2a	792	A
32	2a	793	U
32	2a	794	A
32	2a	815	A
32	2a	817	C
32	2a	821	G
32	2a	828	A
32	2a	834	C
32	2a	840	C
32	2a	841	U
32	2a	851	G
32	2a	853	G
32	2a	859	A
32	2a	874	G
32	2a	880	C
32	2a	885	G
32	2a	902	G
32	2a	914	A
32	2a	926	G
32	2a	927	G
32	2a	932	C
32	2a	934	C
32	2a	935	A
32	2a	959	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	960	U
32	2a	961	U
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	983	A
32	2a	984	C
32	2a	989	C
32	2a	992	U
32	2a	993	G
32	2a	995	C
32	2a	997	U
32	2a	999	C
32	2a	1001(A)	G
32	2a	1002	G
32	2a	1003	G
32	2a	1004	A
32	2a	1005	A
32	2a	1006	C
32	2a	1009	G
32	2a	1011	G
32	2a	1013	G
32	2a	1017	G
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	1029	C
32	2a	1030(A)	G
32	2a	1030(B)	C
32	2a	1030(D)	A
32	2a	1031	G
32	2a	1033	G
32	2a	1035	A
32	2a	1038	C
32	2a	1039	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1040	U
32	2a	1044	A
32	2a	1045	C
32	2a	1046	A
32	2a	1051	C
32	2a	1053	G
32	2a	1064	G
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1077	G
32	2a	1079	G
32	2a	1081	G
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A
32	2a	1103	C
32	2a	1113	C
32	2a	1115	C
32	2a	1116	C
32	2a	1117	G
32	2a	1122	U
32	2a	1125	U
32	2a	1129	C
32	2a	1130	A
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1145	C
32	2a	1146	A
32	2a	1152	A
32	2a	1157	A
32	2a	1159	U
32	2a	1160	G
32	2a	1171	G
32	2a	1172	C
32	2a	1182	G
32	2a	1183	A
32	2a	1184	G
32	2a	1189	C
32	2a	1196	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1197	G
32	2a	1202	G
32	2a	1209	C
32	2a	1211	U
32	2a	1212	U
32	2a	1213	A
32	2a	1228	C
32	2a	1233	G
32	2a	1236	A
32	2a	1238	A
32	2a	1240	U
32	2a	1241	G
32	2a	1248	A
32	2a	1255	G
32	2a	1256	A
32	2a	1257	U
32	2a	1260	C
32	2a	1264	C
32	2a	1270	C
32	2a	1273	G
32	2a	1275	A
32	2a	1276	G
32	2a	1278	U
32	2a	1279	A
32	2a	1280	A
32	2a	1285	A
32	2a	1286	A
32	2a	1287	A
32	2a	1299	A
32	2a	1300	G
32	2a	1302	U
32	2a	1303	C
32	2a	1305	G
32	2a	1312	G
32	2a	1319	A
32	2a	1320	C
32	2a	1347	G
32	2a	1363	C
32	2a	1364	U
32	2a	1368	G
32	2a	1370	G
32	2a	1397	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1402	4OC
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1442(B)	A
32	2a	1447	A
32	2a	1452	C
32	2a	1456	G
32	2a	1492	A
32	2a	1494	G
32	2a	1496	C
32	2a	1497	G
32	2a	1503	A
32	2a	1504	G
32	2a	1506	U
32	2a	1517	G
32	2a	1519	MA6
32	2a	1520	G
32	2a	1529	G
32	2a	1530	G
32	2a	1531	A
32	2a	1532	U
53	2v	13	A
53	2v	14	A
53	2v	18	G
53	2v	24	A
54	2w	3	C
54	2w	4	C
54	2w	5	G
54	2w	13	C
54	2w	14	A
54	2w	19	G
54	2w	22	G
54	2w	29	G
54	2w	36	A
54	2w	38	A
54	2w	46	7MG
54	2w	47	U
54	2w	48	C
54	2w	56	C
54	2w	59	U
54	2w	62	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	2w	63	G
54	2w	65	G
54	2w	68	C
54	2w	69	G
54	2w	72	C
54	2w	74	C
55	2x	9	G
55	2x	18	G
55	2x	21	A
55	2x	22	G
55	2x	46	G
55	2x	47	U
55	2x	48	C
55	2x	52	G
55	2x	56	C
55	2x	63	G
55	2x	67	C
55	2x	68	C
55	2x	76	A
54	2y	5	G
54	2y	6	G
54	2y	8	4SU
54	2y	11	C
54	2y	12	U
54	2y	13	C
54	2y	19	G
54	2y	35	A
54	2y	41	C
54	2y	44	G
54	2y	45	U
54	2y	46	7MG
54	2y	48	C
54	2y	52	G
54	2y	53	G
54	2y	57	G
54	2y	59	U
54	2y	61	C
54	2y	65	G
54	2y	70	G
54	2y	73	A

All (54) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	90	U
1	1A	195	A
1	1A	196	A
1	1A	266	G
1	1A	271(K)	U
1	1A	278	A
1	1A	548	A
1	1A	746	A
1	1A	895	U
1	1A	1047	G
1	1A	1065	U
1	1A	1067	A
1	1A	1174	A
1	1A	1176	G
1	1A	1210	A
1	1A	1275	A
1	1A	1379	A
1	1A	1420	U
1	1A	1442	G
1	1A	1508	A
1	1A	1653	G
1	1A	2134	A
1	1A	2170	A
1	1A	2181	G
1	1A	2183	C
1	1A	2406	U
1	1A	2430	A
1	1A	2689	U
1	1A	2756	U
2	1B	1	U
1	2A	34	C
1	2A	228	A
1	2A	266	G
1	2A	271(K)	U
1	2A	271(M)	G
1	2A	277	C
1	2A	528	A
1	2A	752	A
1	2A	827	U
1	2A	856	C
1	2A	900	A
1	2A	1210	A
1	2A	1379	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1420	U
1	2A	1442	G
1	2A	1493	C
1	2A	1530	C
1	2A	1653	G
1	2A	1913	A
1	2A	1992	G
1	2A	2119	A
1	2A	2126	A
1	2A	2351	G
1	2A	2689	U

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

84 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	$\#\|Z\| > 2$
43	0TD	1l	92	43	8,9,10	4.56	1 (12%)	6,11,13	4.80	3 (50%)
54	4SU	1w	8	54	18,21,22	1.81	5 (27%)	25,30,33	1.89	5 (20%)
1	5MC	2A	1942	1	19,22,23	1.65	3 (15%)	26,32,35	1.11	2 (7%)
54	MIA	2y	37	54	21,24,32	1.59	4 (19%)	30,35,47	2.05	7 (23%)
32	MA6	2a	1519	32	23,26,27	1.59	4 (17%)	33,38,41	2.28	11 (33%)
1	PSU	1A	1911	1	18,21,22	1.39	2 (11%)	21,30,33	2.07	4 (19%)
1	2MU	1A	2552	56,1	19,22,24	1.19	2 (10%)	25,31,36	2.00	6 (24%)
32	5MC	1a	1400	32	19,22,23	1.68	3 (15%)	26,32,35	1.13	3 (11%)
55	5MC	1x	32	55	19,22,23	1.72	3 (15%)	26,32,35	1.22	2 (7%)
54	PSU	1y	55	54	18,21,22	1.35	2 (11%)	21,30,33	2.03	3 (14%)
32	MA6	1a	1518	32	23,26,27	1.51	4 (17%)	33,38,41	2.31	13 (39%)
54	MIA	1y	37	54	21,24,32	1.59	4 (19%)	30,35,47	2.00	8 (26%)
54	PSU	2y	32	54	18,21,22	1.37	2 (11%)	21,30,33	2.02	4 (19%)
1	5MC	1A	1942	1	19,22,23	1.60	3 (15%)	26,32,35	1.12	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
54	4SU	2y	8	54	18,21,22	1.87	5 (27%)	25,30,33	2.03	5 (20%)
32	UR3	2a	1498	32	19,22,23	1.04	2 (10%)	26,32,35	1.78	3 (11%)
32	2MG	2a	1207	32	23,26,27	1.24	3 (13%)	33,38,41	2.18	7 (21%)
1	OMG	2A	2251	55,56,1	23,26,27	1.21	3 (13%)	32,38,41	1.97	6 (18%)
1	4OC	1A	1920	1	19,22,24	0.80	0	25,31,35	0.95	1 (4%)
32	5MC	2a	967	32	19,22,23	1.71	3 (15%)	26,32,35	1.13	3 (11%)
32	4OC	2a	1402	32,56	20,23,24	0.77	0	25,32,35	0.97	1 (4%)
54	PSU	1y	39	54	18,21,22	1.33	2 (11%)	21,30,33	2.07	4 (19%)
1	5MU	1A	1939	56,1	19,22,23	1.40	6 (31%)	27,32,35	2.15	6 (22%)
54	PSU	2w	39	54	18,21,22	1.37	2 (11%)	21,30,33	1.84	3 (14%)
32	PSU	2a	516	32	18,21,22	1.38	2 (11%)	21,30,33	1.91	3 (14%)
54	7MG	1w	46	54	23,26,27	1.42	4 (17%)	27,39,42	2.55	8 (29%)
54	7MG	2y	46	54	23,26,27	1.34	3 (13%)	27,39,42	2.74	6 (22%)
32	7MG	1a	527	32,56	23,26,27	1.36	4 (17%)	27,39,42	2.61	7 (25%)
32	5MC	1a	1407	32	19,22,23	1.65	3 (15%)	26,32,35	1.14	2 (7%)
54	7MG	1y	46	54	23,26,27	1.34	4 (17%)	27,39,42	2.62	7 (25%)
55	PSU	2x	55	55	18,21,22	1.38	2 (11%)	21,30,33	2.03	4 (19%)
55	5MC	2x	32	55	19,22,23	1.69	3 (15%)	26,32,35	1.16	3 (11%)
1	2MA	2A	2503	56,1	22,25,26	1.50	4 (18%)	32,37,40	2.27	7 (21%)
32	5MC	1a	967	32	19,22,23	1.62	3 (15%)	26,32,35	1.14	2 (7%)
32	M2G	2a	966	32	24,27,28	1.31	4 (16%)	33,40,43	1.87	6 (18%)
32	4OC	1a	1402	32	20,23,24	0.77	0	25,32,35	0.95	1 (4%)
1	PSU	1A	1917	1	18,21,22	1.36	2 (11%)	21,30,33	2.02	4 (19%)
32	MA6	1a	1519	32	23,26,27	1.56	4 (17%)	33,38,41	2.31	13 (39%)
54	PSU	2y	55	54	18,21,22	1.34	2 (11%)	21,30,33	2.03	4 (19%)
55	PSU	1x	55	55,56	18,21,22	1.37	2 (11%)	21,30,33	2.02	4 (19%)
55	5MU	2x	54	55	19,22,23	1.41	6 (31%)	27,32,35	2.03	6 (22%)
1	PSU	2A	1917	1	18,21,22	1.36	2 (11%)	21,30,33	2.05	4 (19%)
54	5MU	2y	54	54	19,22,23	1.44	6 (31%)	27,32,35	1.85	7 (25%)
1	5MU	1A	1915	1	19,22,23	1.44	5 (26%)	27,32,35	2.08	6 (22%)
32	PSU	1a	516	32	18,21,22	1.37	2 (11%)	21,30,33	1.96	3 (14%)
54	MIA	1w	37	54	28,31,32	2.33	6 (21%)	38,44,47	2.73	13 (34%)
55	5MU	1x	54	55,56	19,22,23	1.42	5 (26%)	27,32,35	1.98	6 (22%)
1	4OC	2A	1920	1	19,22,24	0.78	0	25,31,35	0.90	1 (4%)
32	UR3	1a	1498	32	19,22,23	1.02	1 (5%)	26,32,35	1.73	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
54	PSU	1w	55	54	18,21,22	1.43	2 (11%)	21,30,33	2.11	3 (14%)
1	5MC	2A	1962	56,1	19,22,23	1.65	3 (15%)	26,32,35	1.11	2 (7%)
32	MA6	2a	1518	32	23,26,27	1.57	5 (21%)	33,38,41	2.28	12 (36%)
1	5MU	2A	1939	56,1	19,22,23	1.42	6 (31%)	27,32,35	2.23	6 (22%)
54	PSU	1w	32	54	18,21,22	1.37	2 (11%)	21,30,33	1.94	3 (14%)
1	PSU	2A	1911	1	18,21,22	1.36	2 (11%)	21,30,33	2.00	3 (14%)
1	2MU	2A	2552	56,1	19,22,24	1.30	3 (15%)	25,31,36	1.88	6 (24%)
54	4SU	2w	8	54	18,21,22	1.80	4 (22%)	25,30,33	2.67	6 (24%)
32	5MC	2a	1404	32	19,22,23	1.74	3 (15%)	26,32,35	1.19	3 (11%)
32	2MG	1a	1207	32	23,26,27	1.25	4 (17%)	33,38,41	2.15	6 (18%)
54	PSU	1w	39	54	18,21,22	1.37	2 (11%)	21,30,33	2.01	4 (19%)
1	PSU	1A	2605	56,1	18,21,22	1.37	2 (11%)	21,30,33	1.92	3 (14%)
54	4SU	1y	8	54	18,21,22	1.76	4 (22%)	25,30,33	2.01	4 (16%)
54	PSU	2y	39	54	18,21,22	1.34	2 (11%)	21,30,33	2.00	4 (19%)
54	PSU	2w	55	54	18,21,22	1.39	2 (11%)	21,30,33	2.02	3 (14%)
54	5MU	1w	54	54	19,22,23	1.37	6 (31%)	27,32,35	2.17	7 (25%)
32	5MC	2a	1400	32	19,22,23	1.64	3 (15%)	26,32,35	1.10	2 (7%)
32	5MC	1a	1404	32	19,22,23	1.71	3 (15%)	26,32,35	1.14	3 (11%)
54	5MU	2w	54	54	19,22,23	1.37	5 (26%)	27,32,35	1.86	7 (25%)
54	MIA	2w	37	54	24,27,32	2.05	5 (20%)	32,39,47	2.42	10 (31%)
1	OMG	1A	2251	55,56,1	23,26,27	1.17	3 (13%)	32,38,41	1.98	6 (18%)
43	0TD	2l	92	43	8,9,10	4.51	1 (12%)	6,11,13	3.45	3 (50%)
1	5MU	2A	1915	1	19,22,23	1.44	5 (26%)	27,32,35	2.06	6 (22%)
32	M2G	1a	966	32	24,27,28	1.30	3 (12%)	33,40,43	1.82	5 (15%)
32	5MC	2a	1407	32	19,22,23	1.56	3 (15%)	26,32,35	1.11	3 (11%)
54	PSU	2w	32	54	18,21,22	1.35	2 (11%)	21,30,33	1.99	3 (14%)
54	PSU	1y	32	54	18,21,22	1.37	2 (11%)	21,30,33	1.99	3 (14%)
1	PSU	2A	2605	1	18,21,22	1.38	3 (16%)	21,30,33	2.03	4 (19%)
55	4SU	1x	8	55	18,21,22	2.15	6 (33%)	25,30,33	1.61	5 (20%)
55	4SU	2x	8	55,56	18,21,22	2.04	5 (27%)	25,30,33	1.79	7 (28%)
32	7MG	2a	527	32,56	23,26,27	1.33	3 (13%)	27,39,42	2.62	7 (25%)
1	2MA	1A	2503	56,1	22,25,26	1.49	5 (22%)	32,37,40	2.26	9 (28%)
54	7MG	2w	46	54	23,26,27	1.36	4 (17%)	27,39,42	2.56	7 (25%)
54	5MU	1y	54	54	19,22,23	1.41	5 (26%)	27,32,35	2.13	6 (22%)
1	5MC	1A	1962	56,1	19,22,23	1.63	3 (15%)	26,32,35	1.10	2 (7%)

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
43	0TD	1l	92	43	-	1/7/12/14	-
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
54	MIA	2y	37	54	-	0/7/25/34	0/3/3/3
32	MA6	2a	1519	32	-	6/11/29/30	0/3/3/3
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
1	2MU	1A	2552	56,1	-	0/9/27/28	0/2/2/2
32	5MC	1a	1400	32	-	2/7/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
54	PSU	1y	55	54	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	2/11/29/30	0/3/3/3
54	MIA	1y	37	54	-	0/7/25/34	0/3/3/3
54	PSU	2y	32	54	-	0/7/25/26	0/2/2/2
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
54	4SU	2y	8	54	-	2/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	0/9/27/28	0/3/3/3
1	OMG	2A	2251	55,56,1	-	1/9/27/28	0/3/3/3
1	4OC	1A	1920	1	-	1/9/27/30	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32,56	-	2/9/29/30	0/2/2/2
54	PSU	1y	39	54	-	0/7/25/26	0/2/2/2
1	5MU	1A	1939	56,1	-	0/7/25/26	0/2/2/2
54	PSU	2w	39	54	-	2/7/25/26	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
54	7MG	1w	46	54	-	2/7/37/38	0/3/3/3
54	7MG	2y	46	54	-	3/7/37/38	0/3/3/3
32	7MG	1a	527	32,56	-	3/7/37/38	0/3/3/3
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
54	7MG	1y	46	54	-	3/7/37/38	0/3/3/3
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
1	2MA	2A	2503	56,1	-	0/7/25/26	0/3/3/3
32	5MC	1a	967	32	-	1/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	4/11/29/30	0/3/3/3
54	PSU	2y	55	54	-	0/7/25/26	0/2/2/2
55	PSU	1x	55	55,56	-	0/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
54	5MU	2y	54	54	-	0/7/25/26	0/2/2/2
1	5MU	1A	1915	1	-	2/7/25/26	0/2/2/2
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
54	MIA	1w	37	54	-	1/15/33/34	0/3/3/3
55	5MU	1x	54	55,56	-	0/7/25/26	0/2/2/2
1	4OC	2A	1920	1	-	0/9/27/30	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	56,1	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	2/11/29/30	0/3/3/3
1	5MU	2A	1939	56,1	-	0/7/25/26	0/2/2/2
54	PSU	1w	32	54	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
1	2MU	2A	2552	56,1	-	0/9/27/28	0/2/2/2
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/9/27/28	0/3/3/3
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
1	PSU	1A	2605	56,1	-	0/7/25/26	0/2/2/2
54	4SU	1y	8	54	-	3/7/25/26	0/2/2/2
54	PSU	2y	39	54	-	0/7/25/26	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	1/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
54	MIA	2w	37	54	-	0/11/29/34	0/3/3/3
1	OMG	1A	2251	55,56,1	-	0/9/27/28	0/3/3/3
43	0TD	2l	92	43	-	2/7/12/14	-
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
54	PSU	1y	32	54	-	0/7/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
55	4SU	2x	8	55,56	-	1/7/25/26	0/2/2/2
32	7MG	2a	527	32,56	-	1/7/37/38	0/3/3/3
1	2MA	1A	2503	56,1	-	1/7/25/26	0/3/3/3
54	7MG	2w	46	54	-	2/7/37/38	0/3/3/3
54	5MU	1y	54	54	-	1/7/25/26	0/2/2/2
1	5MC	1A	1962	56,1	-	0/7/25/26	0/2/2/2

All (268) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-12.49	1.69	1.82
43	2l	92	0TD	CB-SB	-12.35	1.69	1.82
54	1w	37	MIA	C13-C14	6.84	1.52	1.32
54	1w	37	MIA	C2-S10	-6.74	1.70	1.75
54	2w	37	MIA	C2-S10	-6.47	1.70	1.75
32	2a	1404	5MC	C5-C4	6.33	1.48	1.44
32	2a	967	5MC	C5-C4	6.25	1.48	1.44
55	1x	32	5MC	C5-C4	6.25	1.48	1.44
32	1a	1404	5MC	C5-C4	6.24	1.48	1.44
55	2x	32	5MC	C5-C4	6.11	1.48	1.44
32	1a	1400	5MC	C5-C4	6.06	1.48	1.44
32	1a	1407	5MC	C5-C4	6.05	1.48	1.44
1	1A	1962	5MC	C5-C4	6.03	1.48	1.44
1	2A	1962	5MC	C5-C4	6.03	1.48	1.44
1	2A	1942	5MC	C5-C4	5.95	1.48	1.44
32	2a	1400	5MC	C5-C4	5.93	1.48	1.44
32	1a	967	5MC	C5-C4	5.81	1.48	1.44
1	1A	1942	5MC	C5-C4	5.72	1.48	1.44
32	2a	1407	5MC	C5-C4	5.57	1.48	1.44
32	2a	1519	MA6	C5-C4	5.01	1.48	1.39
54	2w	37	MIA	C5-C4	4.99	1.48	1.39
54	2w	8	4SU	C4-S4	-4.99	1.59	1.68
54	2y	8	4SU	C4-S4	-4.95	1.59	1.68
54	2y	37	MIA	C5-C4	4.94	1.47	1.39
55	2x	8	4SU	C4-S4	-4.94	1.59	1.68
54	1y	37	MIA	C5-C4	4.91	1.47	1.39
32	2a	1518	MA6	C5-C4	4.90	1.47	1.39
54	1w	37	MIA	C5-C4	4.90	1.47	1.39
55	1x	8	4SU	C4-S4	-4.81	1.60	1.68
32	1a	1519	MA6	C5-C4	4.73	1.47	1.39
32	1a	1518	MA6	C5-C4	4.71	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	8	4SU	C4-S4	-4.71	1.60	1.68
54	1y	8	4SU	C4-S4	-4.71	1.60	1.68
55	1x	8	4SU	C4-N3	-4.65	1.32	1.37
1	1A	2503	2MA	C5-C4	4.59	1.47	1.39
1	2A	2503	2MA	C5-C4	4.53	1.47	1.39
55	2x	8	4SU	C4-N3	-4.35	1.33	1.37
54	1w	55	PSU	C6-C5	3.88	1.39	1.35
54	2w	55	PSU	C6-C5	3.77	1.39	1.35
54	2y	32	PSU	C6-C5	3.77	1.39	1.35
54	2w	39	PSU	C6-C5	3.72	1.39	1.35
54	1y	32	PSU	C6-C5	3.70	1.39	1.35
55	2x	55	PSU	C6-C5	3.67	1.39	1.35
32	2a	516	PSU	C6-C5	3.58	1.39	1.35
55	1x	55	PSU	C6-C5	3.54	1.39	1.35
54	2y	55	PSU	C6-C5	3.54	1.39	1.35
54	2w	32	PSU	C6-C5	3.53	1.39	1.35
54	2y	46	7MG	C5-C4	3.52	1.48	1.37
54	1y	55	PSU	C6-C5	3.51	1.39	1.35
1	2A	1917	PSU	C6-C5	3.49	1.39	1.35
1	2A	1911	PSU	C6-C5	3.48	1.39	1.35
54	1y	39	PSU	C6-C5	3.48	1.39	1.35
1	2A	2605	PSU	C6-C5	3.45	1.39	1.35
54	1w	46	7MG	C4-N9	-3.44	1.33	1.37
54	1y	46	7MG	C5-C4	3.44	1.48	1.37
54	1w	32	PSU	C6-C5	3.42	1.39	1.35
54	1w	39	PSU	C6-C5	3.42	1.39	1.35
1	1A	1917	PSU	C6-C5	3.40	1.39	1.35
54	2y	8	4SU	C4-N3	-3.39	1.34	1.37
54	1w	46	7MG	C5-C4	3.39	1.48	1.37
1	1A	2605	PSU	C6-C5	3.39	1.39	1.35
54	2y	39	PSU	C6-C5	3.37	1.39	1.35
32	1a	516	PSU	C6-C5	3.36	1.39	1.35
55	1x	8	4SU	C5-C4	-3.36	1.38	1.42
54	2w	46	7MG	C4-N9	-3.35	1.33	1.37
1	1A	1911	PSU	C6-C5	3.34	1.39	1.35
32	2a	527	7MG	C5-C4	3.34	1.47	1.37
55	1x	8	4SU	C2-N3	-3.34	1.32	1.38
32	1a	527	7MG	C5-C4	3.33	1.47	1.37
54	2w	46	7MG	C5-C4	3.32	1.47	1.37
54	1w	8	4SU	C4-N3	-3.24	1.34	1.37
32	1a	527	7MG	C4-N9	-3.21	1.33	1.37
32	2a	1207	2MG	C5-C4	3.19	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2a	1519	MA6	C5-C6	3.17	1.49	1.41
32	2a	966	M2G	C5-C4	3.16	1.47	1.38
1	2A	2251	OMG	C5-C4	3.16	1.47	1.38
32	2a	1518	MA6	C5-C6	3.14	1.49	1.41
54	1y	8	4SU	C4-N3	-3.14	1.34	1.37
32	1a	1207	2MG	C5-C4	3.10	1.47	1.38
32	1a	966	M2G	C5-C4	3.10	1.47	1.38
55	2x	8	4SU	C5-C4	-3.09	1.38	1.42
1	1A	2251	OMG	C5-C4	3.09	1.47	1.38
32	2a	1404	5MC	C6-C5	3.06	1.39	1.34
32	1a	1519	MA6	C5-C6	3.02	1.49	1.41
55	1x	32	5MC	C6-C5	3.00	1.39	1.34
32	1a	1518	MA6	C5-C6	2.99	1.49	1.41
32	2a	966	M2G	C2-N2	2.98	1.40	1.35
1	2A	1915	5MU	C6-C5	2.97	1.39	1.34
1	1A	1915	5MU	C6-C5	2.96	1.39	1.34
55	2x	32	5MC	C6-C5	2.92	1.39	1.34
32	1a	1404	5MC	C6-C5	2.92	1.39	1.34
54	2w	8	4SU	C5-C4	-2.92	1.39	1.42
32	2a	967	5MC	C6-C5	2.91	1.39	1.34
54	1w	37	MIA	C5-C6	2.89	1.48	1.41
1	2A	1939	5MU	C6-C5	2.88	1.39	1.34
32	1a	966	M2G	C2-N2	2.88	1.40	1.35
54	1y	54	5MU	C6-C5	2.88	1.39	1.34
32	1a	1400	5MC	C6-C5	2.87	1.39	1.34
54	2w	8	4SU	C4-N3	-2.87	1.34	1.37
54	2w	37	MIA	C5-C6	2.86	1.48	1.41
54	1y	37	MIA	C5-C6	2.85	1.48	1.41
55	2x	54	5MU	C6-C5	2.85	1.39	1.34
1	2A	2552	2MU	C4-N3	-2.84	1.33	1.38
1	2A	1942	5MC	C6-C5	2.83	1.39	1.34
1	1A	1939	5MU	C6-C5	2.83	1.39	1.34
1	1A	1942	5MC	C6-C5	2.81	1.39	1.34
54	2y	37	MIA	C5-C6	2.80	1.48	1.41
32	2a	1400	5MC	C6-C5	2.79	1.39	1.34
55	2x	8	4SU	C2-N3	-2.79	1.33	1.38
55	1x	54	5MU	C6-C5	2.78	1.39	1.34
1	1A	2605	PSU	C4-N3	-2.75	1.33	1.38
54	2w	54	5MU	C6-C5	2.74	1.39	1.34
32	1a	1407	5MC	C6-C5	2.74	1.39	1.34
1	1A	1911	PSU	C4-N3	-2.73	1.33	1.38
54	2y	54	5MU	C6-C5	2.71	1.39	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	2605	PSU	C4-N3	-2.70	1.33	1.38
1	2A	1939	5MU	C4-N3	-2.70	1.33	1.38
32	2a	527	7MG	C4-N9	-2.68	1.34	1.37
54	2y	8	4SU	C5-C4	-2.67	1.39	1.42
32	2a	1407	5MC	C6-C5	2.66	1.38	1.34
1	1A	2503	2MA	C5-C6	2.66	1.48	1.41
54	1w	39	PSU	C4-N3	-2.66	1.33	1.38
1	2A	1962	5MC	C6-C5	2.65	1.38	1.34
1	1A	1939	5MU	C4-N3	-2.64	1.33	1.38
1	2A	2503	2MA	C5-C6	2.64	1.48	1.41
54	1w	8	4SU	C5-C4	-2.64	1.39	1.42
1	1A	1915	5MU	C4-N3	-2.63	1.33	1.38
55	1x	54	5MU	C4-N3	-2.63	1.33	1.38
54	2y	55	PSU	C4-N3	-2.62	1.33	1.38
1	1A	1917	PSU	C4-N3	-2.61	1.34	1.38
55	2x	54	5MU	C4-N3	-2.61	1.34	1.38
1	2A	1911	PSU	C4-N3	-2.61	1.34	1.38
32	1a	966	M2G	C6-N1	-2.60	1.34	1.38
54	2w	54	5MU	C4-N3	-2.59	1.34	1.38
1	1A	2552	2MU	C4-N3	-2.59	1.34	1.38
54	2y	54	5MU	C4-N3	-2.58	1.34	1.38
54	1w	54	5MU	C6-C5	2.58	1.38	1.34
1	1A	1915	5MU	C2-N1	2.58	1.42	1.38
32	1a	967	5MC	C6-C5	2.58	1.38	1.34
54	2w	39	PSU	C4-N3	-2.57	1.34	1.38
1	2A	1917	PSU	C4-N3	-2.57	1.34	1.38
1	2A	2251	OMG	C6-N1	-2.57	1.34	1.38
54	1y	8	4SU	C5-C4	-2.56	1.39	1.42
54	2y	39	PSU	C4-N3	-2.56	1.34	1.38
1	2A	1915	5MU	C4-C5	2.55	1.49	1.44
1	1A	1962	5MC	C6-C5	2.54	1.38	1.34
1	2A	1915	5MU	C4-N3	-2.54	1.34	1.38
54	1w	32	PSU	C4-N3	-2.53	1.34	1.38
54	1w	55	PSU	C4-N3	-2.53	1.34	1.38
54	2w	8	4SU	C2-N1	2.53	1.42	1.38
54	1y	54	5MU	C4-N3	-2.51	1.34	1.38
32	1a	516	PSU	C4-N3	-2.51	1.34	1.38
54	1w	54	5MU	C4-C5	2.50	1.48	1.44
55	2x	55	PSU	C4-N3	-2.49	1.34	1.38
32	1a	1207	2MG	C6-N1	-2.48	1.34	1.38
54	2w	55	PSU	C4-N3	-2.47	1.34	1.38
54	2y	54	5MU	C2-N1	2.47	1.42	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1x	55	PSU	C4-N3	-2.47	1.34	1.38
54	1y	32	PSU	C4-N3	-2.47	1.34	1.38
54	1y	46	7MG	C4-N9	-2.46	1.34	1.37
54	2y	46	7MG	C6-N1	-2.46	1.34	1.38
54	1w	46	7MG	C6-N1	-2.46	1.34	1.38
54	1y	37	MIA	C8-N7	2.46	1.36	1.31
54	1y	39	PSU	C4-N3	-2.45	1.34	1.38
54	1y	55	PSU	C4-N3	-2.45	1.34	1.38
1	2A	2552	2MU	C5-C4	2.43	1.49	1.43
54	2w	32	PSU	C4-N3	-2.42	1.34	1.38
55	2x	54	5MU	C4-C5	2.42	1.48	1.44
54	2y	37	MIA	C8-N7	2.40	1.36	1.31
54	1w	54	5MU	C4-N3	-2.39	1.34	1.38
54	1y	54	5MU	C4-C5	2.38	1.48	1.44
32	2a	516	PSU	C4-N3	-2.38	1.34	1.38
55	1x	54	5MU	C4-C5	2.38	1.48	1.44
54	1y	54	5MU	C2-N1	2.37	1.42	1.38
1	2A	2503	2MA	C5-N7	-2.36	1.34	1.39
32	2a	527	7MG	C6-N1	-2.36	1.34	1.38
54	2y	8	4SU	C2-N1	2.35	1.42	1.38
54	1w	8	4SU	C2-N1	2.35	1.42	1.38
32	2a	966	M2G	C6-N1	-2.35	1.34	1.38
32	1a	967	5MC	C6-N1	-2.35	1.34	1.38
1	1A	2251	OMG	C6-N1	-2.34	1.34	1.38
1	2A	1939	5MU	C4-C5	2.34	1.48	1.44
54	2y	32	PSU	C4-N3	-2.34	1.34	1.38
55	2x	8	4SU	C2-N1	2.34	1.42	1.38
1	1A	2503	2MA	C8-N7	2.33	1.36	1.31
54	2w	37	MIA	C8-N7	2.33	1.36	1.31
54	1w	37	MIA	C8-N7	2.33	1.36	1.31
32	2a	1207	2MG	C6-N1	-2.32	1.34	1.38
1	2A	1939	5MU	C6-N1	-2.32	1.34	1.38
54	2y	54	5MU	C2-N3	-2.31	1.33	1.38
1	1A	1942	5MC	C6-N1	-2.30	1.34	1.38
54	2w	54	5MU	C4-C5	2.30	1.48	1.44
1	2A	1915	5MU	C2-N1	2.30	1.42	1.38
55	1x	8	4SU	O2-C2	2.29	1.27	1.23
1	1A	1915	5MU	C4-C5	2.29	1.48	1.44
55	1x	54	5MU	C2-N1	2.28	1.42	1.38
54	2y	54	5MU	C4-C5	2.28	1.48	1.44
54	1y	46	7MG	C6-N1	-2.28	1.34	1.38
1	2A	1962	5MC	C6-N1	-2.28	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	8	4SU	C2-N3	-2.28	1.34	1.38
1	2A	2503	2MA	C8-N7	2.27	1.36	1.31
54	2y	8	4SU	C2-N3	-2.26	1.34	1.38
32	1a	1519	MA6	C8-N7	2.26	1.36	1.31
32	1a	1519	MA6	C5-N7	-2.26	1.35	1.39
32	1a	1518	MA6	C8-N7	2.25	1.36	1.31
1	1A	1939	5MU	C6-N1	-2.25	1.34	1.38
1	1A	1962	5MC	C6-N1	-2.24	1.34	1.38
54	2w	46	7MG	C6-N1	-2.24	1.34	1.38
54	2w	37	MIA	C5-N7	-2.23	1.35	1.39
32	1a	527	7MG	C6-N1	-2.23	1.34	1.38
1	1A	1939	5MU	C2-N3	-2.21	1.34	1.38
32	2a	1519	MA6	C8-N7	2.19	1.35	1.31
54	1w	54	5MU	C2-N1	2.19	1.41	1.38
54	1w	37	MIA	C5-N7	-2.19	1.35	1.39
32	1a	1498	UR3	C2-N1	2.19	1.41	1.38
55	1x	32	5MC	C6-N1	-2.19	1.34	1.38
1	2A	2251	OMG	C5-N7	-2.18	1.34	1.39
54	1y	54	5MU	C6-N1	-2.18	1.34	1.38
1	2A	1939	5MU	C2-N3	-2.18	1.34	1.38
54	1w	54	5MU	C6-N1	-2.18	1.34	1.38
32	2a	1518	MA6	C8-N7	2.18	1.35	1.31
1	2A	1915	5MU	C6-N1	-2.17	1.34	1.38
1	1A	2503	2MA	C5-N7	-2.17	1.35	1.39
32	2a	1498	UR3	C2-N1	2.16	1.41	1.38
54	2y	37	MIA	C5-N7	-2.16	1.35	1.39
32	1a	1400	5MC	C6-N1	-2.16	1.34	1.38
32	2a	1498	UR3	C6-C5	2.15	1.40	1.35
55	2x	54	5MU	C2-N1	2.15	1.41	1.38
1	1A	1939	5MU	C4-C5	2.14	1.48	1.44
32	2a	1404	5MC	C6-N1	-2.14	1.34	1.38
1	2A	1942	5MC	C6-N1	-2.14	1.34	1.38
1	1A	2251	OMG	C5-N7	-2.13	1.34	1.39
32	2a	1407	5MC	C6-N1	-2.13	1.34	1.38
32	2a	1400	5MC	C6-N1	-2.13	1.34	1.38
55	2x	54	5MU	C2-N3	-2.12	1.34	1.38
54	1y	37	MIA	C5-N7	-2.11	1.35	1.39
55	1x	8	4SU	C2-N1	2.11	1.41	1.38
55	1x	54	5MU	C6-N1	-2.11	1.34	1.38
1	2A	2605	PSU	C2-N3	-2.11	1.34	1.37
32	2a	1518	MA6	C4-N9	-2.11	1.33	1.37
32	2a	1519	MA6	C5-N7	-2.10	1.35	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1939	5MU	C2-N1	2.10	1.41	1.38
54	1w	46	7MG	C8-N9	2.10	1.47	1.45
32	1a	1207	2MG	C2-N3	2.10	1.36	1.32
54	1y	46	7MG	C8-N9	2.09	1.47	1.45
32	1a	1404	5MC	C6-N1	-2.09	1.34	1.38
1	2A	2552	2MU	C2-N3	-2.08	1.34	1.38
55	2x	32	5MC	C6-N1	-2.07	1.34	1.38
54	2w	54	5MU	C2-N3	-2.07	1.34	1.38
1	1A	2552	2MU	C5-C4	2.06	1.48	1.43
54	2y	54	5MU	C6-N1	-2.06	1.34	1.38
32	2a	1518	MA6	C5-N7	-2.06	1.35	1.39
1	1A	2503	2MA	C4-N9	-2.06	1.33	1.37
32	1a	1407	5MC	C6-N1	-2.05	1.34	1.38
32	1a	527	7MG	C8-N9	2.05	1.47	1.45
32	1a	1207	2MG	C5-N7	-2.04	1.35	1.39
1	1A	1915	5MU	C6-N1	-2.04	1.34	1.38
54	2w	54	5MU	C2-N1	2.04	1.41	1.38
1	2A	1939	5MU	C2-N1	2.04	1.41	1.38
32	2a	966	M2G	C5-N7	-2.04	1.35	1.39
32	1a	1518	MA6	C5-N7	-2.03	1.35	1.39
55	2x	54	5MU	C6-N1	-2.03	1.34	1.38
54	2w	46	7MG	C8-N9	2.03	1.47	1.45
54	1w	54	5MU	C2-N3	-2.01	1.34	1.38
32	2a	1207	2MG	C2-N3	2.01	1.35	1.32
54	2y	46	7MG	C8-N9	2.01	1.47	1.45
54	1y	8	4SU	C2-N3	-2.01	1.34	1.38
32	2a	967	5MC	C6-N1	-2.00	1.34	1.38

All (415) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	1l	92	0TD	CSB-SB-CB	-11.01	82.57	102.36
54	2y	46	7MG	N9-C4-N3	9.82	139.84	125.46
54	1y	46	7MG	N9-C4-N3	9.20	138.94	125.46
32	2a	527	7MG	N9-C4-N3	9.09	138.78	125.46
54	1w	37	MIA	C12-C13-C14	-9.05	110.76	127.01
32	1a	527	7MG	N9-C4-N3	8.89	138.49	125.46
54	1w	46	7MG	N9-C4-N3	8.78	138.33	125.46
54	2w	46	7MG	N9-C4-N3	8.54	137.97	125.46
54	2w	37	MIA	C5-C4-N3	-8.33	118.41	127.18
1	2A	2503	2MA	C5-C4-N3	-8.13	118.61	127.18
54	2w	8	4SU	C4-N3-C2	-8.09	119.56	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	1w	37	MIA	C5-C4-N3	-7.78	118.99	127.18
1	1A	2503	2MA	C5-C4-N3	-7.73	119.03	127.18
32	2a	1498	UR3	C4-N3-C2	-7.16	118.82	124.58
43	2l	92	0TD	CSB-SB-CB	-7.11	89.59	102.36
32	2a	1207	2MG	C2-N3-C4	7.06	120.84	112.00
32	1a	1207	2MG	C2-N3-C4	6.95	120.70	112.00
32	1a	1498	UR3	C4-N3-C2	-6.82	119.09	124.58
54	2w	37	MIA	N3-C4-N9	6.74	135.54	126.99
55	2x	55	PSU	N1-C2-N3	6.42	121.94	115.17
1	2A	2503	2MA	N3-C4-N9	6.41	135.13	126.99
54	1w	55	PSU	N1-C2-N3	6.41	121.93	115.17
1	1A	1911	PSU	N1-C2-N3	6.39	121.91	115.17
1	2A	1917	PSU	N1-C2-N3	6.39	121.91	115.17
54	1y	39	PSU	N1-C2-N3	6.37	121.88	115.17
54	2y	55	PSU	N1-C2-N3	6.33	121.85	115.17
54	1w	39	PSU	N1-C2-N3	6.33	121.84	115.17
1	2A	2605	PSU	N1-C2-N3	6.32	121.84	115.17
54	2y	32	PSU	N1-C2-N3	6.30	121.81	115.17
55	1x	55	PSU	N1-C2-N3	6.26	121.78	115.17
54	2w	32	PSU	N1-C2-N3	6.26	121.77	115.17
1	2A	1911	PSU	N1-C2-N3	6.26	121.77	115.17
54	1y	55	PSU	N1-C2-N3	6.25	121.77	115.17
1	2A	2251	OMG	C5-C4-N3	-6.24	118.45	128.39
54	2y	39	PSU	N1-C2-N3	6.24	121.75	115.17
1	1A	1917	PSU	N1-C2-N3	6.24	121.75	115.17
54	2w	55	PSU	N1-C2-N3	6.20	121.71	115.17
54	1y	32	PSU	N1-C2-N3	6.20	121.70	115.17
54	2w	8	4SU	C5-C4-N3	6.15	120.47	114.75
1	1A	2503	2MA	N3-C4-N9	6.13	134.78	126.99
54	1w	32	PSU	N1-C2-N3	6.12	121.62	115.17
32	2a	966	M2G	C5-C4-N3	-6.10	118.68	128.39
54	1w	37	MIA	N3-C4-N9	6.05	134.67	126.99
32	1a	516	PSU	N1-C2-N3	6.05	121.55	115.17
1	1A	2605	PSU	N1-C2-N3	6.02	121.52	115.17
32	2a	516	PSU	N1-C2-N3	6.02	121.52	115.17
1	1A	2251	OMG	C5-C4-N3	-5.99	118.86	128.39
54	1y	8	4SU	C4-N3-C2	-5.95	121.61	127.31
54	2y	46	7MG	C5-C4-N3	-5.94	116.99	128.13
32	1a	1207	2MG	C5-C4-N3	-5.93	118.96	128.39
32	1a	966	M2G	C5-C4-N3	-5.90	119.00	128.39
54	2y	37	MIA	C5-C4-N3	-5.85	118.66	126.72
32	2a	1207	2MG	C5-C4-N3	-5.79	119.18	128.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	2w	39	PSU	N1-C2-N3	5.73	121.22	115.17
54	2y	8	4SU	C4-N3-C2	-5.73	121.82	127.31
32	1a	1519	MA6	C5-C4-N3	-5.69	118.88	126.72
32	2a	1519	MA6	C5-C4-N3	-5.66	118.93	126.72
32	2a	527	7MG	C5-C4-N3	-5.59	117.64	128.13
1	2A	1939	5MU	C4-N3-C2	-5.59	120.02	127.34
54	1y	37	MIA	C5-C4-N3	-5.56	119.06	126.72
54	2y	8	4SU	C5-C4-N3	5.55	119.92	114.75
54	1y	46	7MG	C5-C4-N3	-5.53	117.74	128.13
32	1a	1518	MA6	C5-C4-N3	-5.44	119.23	126.72
1	2A	1939	5MU	N3-C2-N1	5.44	121.97	114.89
54	2w	46	7MG	N9-C8-N7	-5.38	95.75	103.37
1	1A	1939	5MU	C4-N3-C2	-5.31	120.38	127.34
54	1w	54	5MU	C4-N3-C2	-5.29	120.41	127.34
32	1a	527	7MG	C5-C4-N3	-5.29	118.20	128.13
54	1w	46	7MG	N9-C8-N7	-5.28	95.89	103.37
54	2w	8	4SU	C5-C4-S4	-5.26	118.30	124.31
32	1a	527	7MG	N9-C8-N7	-5.25	95.94	103.37
1	1A	1915	5MU	N3-C2-N1	5.24	121.71	114.89
54	1y	54	5MU	C4-N3-C2	-5.22	120.49	127.34
54	1y	8	4SU	C5-C4-N3	5.21	119.59	114.75
54	1w	54	5MU	N3-C2-N1	5.16	121.61	114.89
54	1y	54	5MU	N3-C2-N1	5.16	121.61	114.89
1	2A	2552	2MU	N3-C2-N1	5.16	121.60	114.89
54	1w	8	4SU	C5-C4-N3	5.15	119.54	114.75
1	1A	2552	2MU	N3-C2-N1	5.13	121.56	114.89
1	2A	1915	5MU	N3-C2-N1	5.13	121.56	114.89
54	1w	8	4SU	C4-N3-C2	-5.11	122.42	127.31
32	2a	527	7MG	N9-C8-N7	-5.11	96.14	103.37
1	1A	2251	OMG	C2-N3-C4	5.09	121.06	112.30
32	2a	1518	MA6	C5-C4-N3	-5.08	119.72	126.72
1	2A	1915	5MU	C4-N3-C2	-5.01	120.77	127.34
32	2a	1518	MA6	C9-N6-C6	-5.00	107.80	120.52
1	1A	1915	5MU	C4-N3-C2	-5.00	120.78	127.34
54	2w	46	7MG	C5-C4-N3	-4.97	118.80	128.13
55	1x	54	5MU	N3-C2-N1	4.97	121.36	114.89
55	2x	54	5MU	N3-C2-N1	4.96	121.34	114.89
54	1y	46	7MG	N9-C8-N7	-4.96	96.36	103.37
1	1A	1939	5MU	N3-C2-N1	4.93	121.31	114.89
1	2A	2251	OMG	C2-N3-C4	4.92	120.78	112.30
54	2y	46	7MG	N9-C8-N7	-4.91	96.42	103.37
1	1A	2552	2MU	C4-N3-C2	-4.88	120.55	126.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	2x	54	5MU	C4-N3-C2	-4.88	120.94	127.34
1	1A	1939	5MU	C5-C4-N3	4.87	119.56	115.32
1	2A	2251	OMG	N9-C4-N3	4.86	135.66	125.95
55	2x	8	4SU	C5-C4-N3	4.78	119.20	114.75
54	1w	46	7MG	C5-C4-N3	-4.77	119.17	128.13
1	2A	2552	2MU	C4-N3-C2	-4.77	120.69	126.61
54	2y	37	MIA	N3-C4-N9	4.73	135.21	127.17
55	1x	54	5MU	C4-N3-C2	-4.71	121.16	127.34
1	2A	1939	5MU	C5-C4-N3	4.67	119.38	115.32
54	2y	46	7MG	C2-N3-C4	4.63	120.28	112.30
54	2w	8	4SU	N3-C2-N1	4.60	120.88	114.89
32	2a	1518	MA6	C2-N1-C6	4.56	122.97	111.83
32	2a	966	M2G	N9-C4-N3	4.54	135.04	125.95
32	2a	966	M2G	C2-N3-C4	4.51	120.85	112.51
1	1A	2251	OMG	N9-C4-N3	4.48	134.92	125.95
54	1w	54	5MU	C5-C4-N3	4.48	119.22	115.32
32	1a	966	M2G	C2-N3-C4	4.48	120.79	112.51
54	2w	54	5MU	N3-C2-N1	4.46	120.69	114.89
54	1y	46	7MG	C2-N3-C4	4.45	119.97	112.30
32	1a	1518	MA6	C9-N6-C6	-4.45	109.21	120.52
32	2a	1518	MA6	C4-C5-N7	-4.40	105.55	110.58
54	1y	54	5MU	C5-C4-N3	4.40	119.15	115.32
54	1y	37	MIA	N3-C4-N9	4.40	134.65	127.17
32	2a	527	7MG	C2-N3-C4	4.40	119.88	112.30
32	2a	1519	MA6	C2-N1-C6	4.37	122.50	111.83
32	1a	1518	MA6	C2-N1-C6	4.36	122.48	111.83
1	1A	1939	5MU	O4-C4-C5	-4.36	119.93	124.92
32	1a	1519	MA6	C9-N6-C6	-4.34	109.47	120.52
32	1a	966	M2G	N9-C4-N3	4.34	134.63	125.95
32	2a	1519	MA6	N3-C4-N9	4.32	134.52	127.17
32	1a	527	7MG	C2-N3-C4	4.32	119.74	112.30
55	2x	54	5MU	C5-C4-N3	4.28	119.04	115.32
1	1A	1915	5MU	C5-C4-N3	4.27	119.03	115.32
32	1a	1207	2MG	N9-C4-N3	4.26	134.47	125.95
54	2w	46	7MG	C2-N3-C4	4.26	119.63	112.30
54	1y	39	PSU	C4-N3-C2	-4.26	120.51	126.37
54	2w	54	5MU	C4-N3-C2	-4.26	121.76	127.34
32	2a	1519	MA6	C9-N6-C6	-4.24	109.73	120.52
32	1a	1519	MA6	N3-C4-N9	4.23	134.37	127.17
32	1a	1519	MA6	C4-C5-N7	-4.20	105.78	110.58
55	1x	8	4SU	C5-C4-N3	4.19	118.65	114.75
1	2A	2605	PSU	C4-N3-C2	-4.19	120.60	126.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	1a	1519	MA6	C2-N1-C6	4.15	121.97	111.83
1	2A	1917	PSU	C4-N3-C2	-4.13	120.67	126.37
54	2y	55	PSU	C4-N3-C2	-4.13	120.68	126.37
32	2a	1519	MA6	C4-C5-N7	-4.13	105.86	110.58
1	1A	1911	PSU	C4-N3-C2	-4.13	120.69	126.37
1	2A	1915	5MU	C5-C4-N3	4.12	118.91	115.32
54	2y	54	5MU	C5-C4-N3	4.12	118.90	115.32
54	1w	54	5MU	O4-C4-C5	-4.12	120.21	124.92
54	1y	54	5MU	O4-C4-C5	-4.11	120.21	124.92
55	2x	8	4SU	C1'-N1-C2	4.11	124.97	117.59
54	1w	46	7MG	C2-N3-C4	4.10	119.37	112.30
1	1A	1917	PSU	C4-N3-C2	-4.09	120.74	126.37
32	1a	1518	MA6	C4-C5-N7	-4.07	105.92	110.58
54	2y	39	PSU	C4-N3-C2	-4.07	120.77	126.37
54	1y	55	PSU	C4-N3-C2	-4.06	120.78	126.37
1	1A	1915	5MU	O4-C4-C5	-4.06	120.28	124.92
55	1x	55	PSU	C4-N3-C2	-4.04	120.81	126.37
1	2A	1939	5MU	C5-C6-N1	-4.04	118.93	123.31
1	2A	1939	5MU	O4-C4-C5	-4.03	120.30	124.92
1	2A	1911	PSU	C4-N3-C2	-4.03	120.81	126.37
32	1a	1518	MA6	N3-C4-N9	4.03	134.02	127.17
54	1w	55	PSU	O2-C2-N1	-4.01	118.65	122.79
55	2x	55	PSU	C4-N3-C2	-4.00	120.85	126.37
54	1w	39	PSU	C4-N3-C2	-3.99	120.87	126.37
54	2y	54	5MU	C4-N3-C2	-3.99	122.11	127.34
1	1A	1911	PSU	O2-C2-N1	-3.99	118.68	122.79
54	2y	32	PSU	C4-N3-C2	-3.96	120.91	126.37
54	1w	37	MIA	C15-C14-C13	-3.95	110.79	122.66
54	1y	32	PSU	C4-N3-C2	-3.94	120.94	126.37
54	1w	55	PSU	C4-N3-C2	-3.93	120.96	126.37
54	2w	54	5MU	C5-C4-N3	3.93	118.74	115.32
54	2w	32	PSU	C4-N3-C2	-3.91	120.99	126.37
1	1A	1939	5MU	C5-C6-N1	-3.90	119.08	123.31
54	2y	54	5MU	O4-C4-C5	-3.90	120.46	124.92
54	2y	54	5MU	N3-C2-N1	3.88	119.94	114.89
32	2a	1207	2MG	N9-C4-N3	3.87	133.70	125.95
55	1x	54	5MU	C5-C4-N3	3.87	118.69	115.32
54	2w	55	PSU	C4-N3-C2	-3.87	121.04	126.37
1	1A	2605	PSU	C4-N3-C2	-3.85	121.06	126.37
32	1a	516	PSU	C4-N3-C2	-3.83	121.10	126.37
55	2x	54	5MU	O4-C4-C5	-3.81	120.56	124.92
54	1y	39	PSU	O2-C2-N1	-3.78	118.89	122.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	1y	55	PSU	O2-C2-N1	-3.76	118.91	122.79
55	1x	32	5MC	C5-C6-N1	-3.76	119.23	123.31
54	1w	32	PSU	C4-N3-C2	-3.75	121.20	126.37
54	1w	37	MIA	C16-C14-C13	-3.75	111.40	122.66
1	2A	1915	5MU	O4-C4-C5	-3.74	120.64	124.92
32	2a	1207	2MG	C6-C5-N7	3.73	137.07	130.29
54	2w	55	PSU	O2-C2-N1	-3.71	118.97	122.79
32	1a	516	PSU	O2-C2-N1	-3.70	118.97	122.79
54	2y	37	MIA	C2-N3-C4	3.70	120.86	111.83
1	2A	1962	5MC	C5-C6-N1	-3.69	119.30	123.31
32	1a	1518	MA6	C2-N3-C4	3.69	120.84	111.83
32	2a	1518	MA6	N3-C4-N9	3.68	133.43	127.17
54	1y	8	4SU	N3-C2-N1	3.68	119.69	114.89
55	1x	54	5MU	O4-C4-C5	-3.68	120.70	124.92
32	2a	516	PSU	C4-N3-C2	-3.67	121.31	126.37
32	2a	1519	MA6	C2-N3-C4	3.66	120.76	111.83
54	1y	37	MIA	C2-N3-C4	3.65	120.75	111.83
54	2w	39	PSU	C4-N3-C2	-3.65	121.34	126.37
55	2x	55	PSU	O2-C2-N1	-3.63	119.04	122.79
54	1y	8	4SU	C5-C4-S4	-3.63	120.16	124.31
32	1a	1519	MA6	C2-N3-C4	3.63	120.69	111.83
1	2A	1917	PSU	O2-C2-N1	-3.62	119.05	122.79
54	2w	32	PSU	O2-C2-N1	-3.62	119.05	122.79
1	1A	1917	PSU	O2-C2-N1	-3.61	119.07	122.79
54	2y	32	PSU	O2-C2-N1	-3.60	119.08	122.79
54	1y	37	MIA	N3-C2-N1	-3.60	123.14	128.58
1	1A	1942	5MC	C5-C6-N1	-3.59	119.42	123.31
54	1w	32	PSU	O2-C2-N1	-3.58	119.10	122.79
55	1x	55	PSU	O2-C2-N1	-3.57	119.11	122.79
54	1w	39	PSU	O2-C2-N1	-3.56	119.12	122.79
54	2y	8	4SU	C5-C4-S4	-3.52	120.28	124.31
32	2a	1518	MA6	C2-N3-C4	3.52	120.43	111.83
54	1y	37	MIA	C4-C5-N7	-3.51	106.57	110.58
54	2w	54	5MU	O4-C4-C5	-3.51	120.90	124.92
54	2w	37	MIA	C2-N3-C4	3.51	121.48	112.29
54	2y	8	4SU	N3-C2-N1	3.51	119.46	114.89
54	2y	37	MIA	N3-C2-N1	-3.50	123.28	128.58
1	2A	1911	PSU	O2-C2-N1	-3.50	119.18	122.79
54	2y	37	MIA	C4-C5-N7	-3.49	106.59	110.58
54	1y	32	PSU	O2-C2-N1	-3.49	119.19	122.79
32	2a	516	PSU	O2-C2-N1	-3.49	119.19	122.79
54	2y	39	PSU	O2-C2-N1	-3.48	119.20	122.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	1a	1518	MA6	N1-C2-N3	-3.48	123.32	128.58
54	1y	54	5MU	C5-C6-N1	-3.47	119.54	123.31
43	2l	92	0TD	OD2-CG-CB	3.47	120.65	113.15
32	1a	1404	5MC	C5-C6-N1	-3.46	119.55	123.31
32	2a	1404	5MC	C5-C6-N1	-3.43	119.59	123.31
1	2A	1915	5MU	C5-C6-N1	-3.43	119.59	123.31
54	1w	37	MIA	C2-N3-C4	3.42	121.26	112.29
32	2a	1518	MA6	N1-C2-N3	-3.42	123.41	128.58
54	1w	8	4SU	N3-C2-N1	3.42	119.34	114.89
32	1a	1207	2MG	C6-C5-N7	3.40	136.47	130.29
55	1x	8	4SU	C6-C5-C4	-3.39	117.02	119.95
54	1w	37	MIA	C6-C5-N7	3.38	136.12	132.43
55	2x	54	5MU	C5-C6-N1	-3.38	119.64	123.31
1	1A	2503	2MA	C4-C5-N7	-3.37	106.72	110.58
1	2A	2503	2MA	C4-C5-N7	-3.34	106.76	110.58
54	1w	37	MIA	C4-C5-N7	-3.33	106.77	110.58
54	1w	8	4SU	C5-C4-S4	-3.33	120.50	124.31
1	1A	2552	2MU	O2-C2-N1	-3.32	118.47	122.80
1	2A	1942	5MC	C5-C6-N1	-3.31	119.72	123.31
32	2a	967	5MC	C5-C6-N1	-3.29	119.73	123.31
54	2w	37	MIA	C4-C5-N7	-3.28	106.83	110.58
32	1a	966	M2G	C6-C5-N7	3.28	136.25	130.29
32	1a	1498	UR3	C5-C4-N3	3.26	119.33	115.04
32	2a	1519	MA6	N1-C2-N3	-3.26	123.65	128.58
54	2y	55	PSU	O2-C2-N1	-3.25	119.44	122.79
1	1A	2251	OMG	C6-C5-N7	3.23	136.16	130.29
32	1a	967	5MC	C5-C6-N1	-3.22	119.81	123.31
1	1A	1962	5MC	C5-C6-N1	-3.18	119.86	123.31
54	1w	54	5MU	C5-C6-N1	-3.18	119.86	123.31
1	2A	2605	PSU	O2-C2-N1	-3.17	119.52	122.79
1	1A	2552	2MU	O4-C4-C5	-3.17	119.69	125.16
32	2a	966	M2G	C6-C5-N7	3.16	136.05	130.29
32	1a	1400	5MC	C5-C6-N1	-3.14	119.91	123.31
55	1x	54	5MU	C5-C6-N1	-3.12	119.92	123.31
1	1A	1915	5MU	C5-C6-N1	-3.12	119.92	123.31
1	1A	2552	2MU	C5-C4-N3	3.11	119.16	114.80
1	1A	2552	2MU	C2'-C1'-N1	-3.11	108.35	114.24
32	2a	1498	UR3	C5-C4-N3	3.09	119.11	115.04
32	2a	1400	5MC	C5-C6-N1	-3.08	119.96	123.31
1	2A	2552	2MU	C5-C4-N3	3.08	119.11	114.80
43	1l	92	0TD	OD2-CG-CB	3.07	119.78	113.15
32	1a	1519	MA6	N1-C2-N3	-3.07	123.94	128.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	1x	32	5MC	C5-C4-N3	-3.05	118.63	121.75
55	1x	8	4SU	O2-C2-N1	3.04	126.75	122.80
32	2a	1407	5MC	C5-C4-N3	-3.03	118.65	121.75
55	2x	32	5MC	C5-C6-N1	-3.03	120.03	123.31
32	1a	1407	5MC	C5-C6-N1	-3.01	120.04	123.31
54	2y	54	5MU	C5-C6-N1	-3.01	120.05	123.31
54	1w	46	7MG	C5-C4-N9	-3.00	102.50	106.33
54	2w	8	4SU	C1'-N1-C2	2.99	122.97	117.59
32	2a	1518	MA6	C5-N7-C8	2.99	108.14	103.45
32	1a	1518	MA6	C10-N6-C6	-2.98	112.93	120.52
55	1x	8	4SU	C1'-N1-C2	2.98	122.95	117.59
32	2a	1207	2MG	C4-C5-N7	-2.98	105.95	110.67
32	2a	1404	5MC	C5-C4-N3	-2.97	118.71	121.75
1	1A	2503	2MA	C4-N9-C8	2.97	108.86	105.74
1	2A	2503	2MA	N6-C6-N1	2.95	121.01	117.03
1	1A	2503	2MA	N6-C6-N1	2.94	120.99	117.03
1	2A	1939	5MU	O2-C2-N1	-2.93	118.98	122.80
32	1a	1519	MA6	C5-N7-C8	2.93	108.05	103.45
32	2a	1519	MA6	C5-N7-C8	2.88	107.98	103.45
55	2x	32	5MC	C5-C4-N3	-2.88	118.81	121.75
1	2A	2251	OMG	C6-C5-N7	2.86	135.49	130.29
1	2A	1942	5MC	C5-C4-N3	-2.84	118.85	121.75
32	1a	1518	MA6	C5-N7-C8	2.84	107.91	103.45
32	1a	1407	5MC	C5-C4-N3	-2.84	118.85	121.75
54	2w	37	MIA	C6-C5-N7	2.82	135.51	132.43
1	2A	2552	2MU	O2-C2-N1	-2.82	119.13	122.80
32	1a	527	7MG	C5-C6-N1	2.80	115.87	110.94
1	1A	2605	PSU	O2-C2-N1	-2.79	119.91	122.79
1	1A	1962	5MC	C5-C4-N3	-2.79	118.90	121.75
32	2a	1407	5MC	C5-C6-N1	-2.77	120.30	123.31
32	1a	1400	5MC	C5-C4-N3	-2.77	118.91	121.75
1	1A	2503	2MA	C2-N1-C6	2.77	122.36	118.10
32	2a	1400	5MC	C5-C4-N3	-2.76	118.92	121.75
54	2w	54	5MU	C5-C6-N1	-2.76	120.31	123.31
32	2a	1518	MA6	C4-N9-C8	2.74	108.61	105.74
55	2x	8	4SU	C4-N3-C2	-2.74	124.69	127.31
32	2a	1518	MA6	C6-C5-N7	2.73	137.79	133.43
32	1a	1207	2MG	C4-C5-N7	-2.73	106.35	110.67
32	2a	1207	2MG	N1-C2-N2	2.73	119.34	116.56
32	2a	967	5MC	C5-C4-N3	-2.72	118.97	121.75
32	1a	1404	5MC	C5-C4-N3	-2.71	118.97	121.75
54	1y	54	5MU	O2-C2-N1	-2.71	119.27	122.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	2y	37	MIA	C4-N9-C8	2.70	108.58	105.74
32	2a	527	7MG	C5-C6-N1	2.70	115.70	110.94
54	2w	37	MIA	C12-N6-C6	-2.70	120.35	122.85
1	1A	1942	5MC	C5-C4-N3	-2.67	119.02	121.75
1	2A	2503	2MA	C4-N9-C8	2.66	108.53	105.74
54	1w	54	5MU	O2-C2-N1	-2.66	119.33	122.80
32	1a	1518	MA6	C4-N9-C8	2.65	108.52	105.74
54	2w	39	PSU	O2-C2-N1	-2.64	120.07	122.79
32	1a	1519	MA6	C4-N9-C8	2.64	108.50	105.74
54	2y	37	MIA	C5-N7-C8	2.63	107.58	103.45
32	2a	966	M2G	C4-C5-N7	-2.61	106.53	110.67
1	1A	1939	5MU	O2-C2-N1	-2.61	119.39	122.80
54	2y	46	7MG	C5-C6-N1	2.61	115.54	110.94
54	2w	8	4SU	O2-C2-N1	-2.61	119.40	122.80
54	1y	37	MIA	C4-N9-C8	2.60	108.47	105.74
54	1y	37	MIA	C5-N7-C8	2.58	107.51	103.45
32	2a	1519	MA6	C4-N9-C8	2.57	108.43	105.74
43	2l	92	0TD	OD1-CG-CB	-2.55	117.09	122.44
1	2A	2503	2MA	C2-N1-C6	2.54	122.00	118.10
32	1a	967	5MC	C5-C4-N3	-2.54	119.15	121.75
54	1w	37	MIA	C2-N1-C6	2.53	122.34	117.54
54	1w	37	MIA	N3-C2-N1	-2.52	122.39	127.00
1	2A	1962	5MC	C5-C4-N3	-2.52	119.17	121.75
54	1y	46	7MG	C5-C6-N1	2.52	115.37	110.94
54	1w	54	5MU	C5M-C5-C4	2.51	121.46	118.78
54	2w	46	7MG	C5-C6-N1	2.50	115.34	110.94
32	1a	1519	MA6	C10-N6-C6	-2.50	114.17	120.52
54	2y	46	7MG	C5-C4-N9	-2.48	103.15	106.33
1	1A	2503	2MA	C5-N7-C8	2.48	107.35	103.45
54	2w	37	MIA	N3-C2-N1	-2.48	122.48	127.00
1	1A	2251	OMG	C4-C5-N7	-2.48	106.75	110.67
55	2x	54	5MU	O2-C2-N1	-2.47	119.58	122.80
54	2w	37	MIA	C5-N7-C8	2.46	107.32	103.45
1	2A	2503	2MA	C5-N7-C8	2.44	107.29	103.45
54	2w	37	MIA	C4-N9-C8	2.44	108.30	105.74
54	2w	46	7MG	C5-C4-N9	-2.43	103.22	106.33
32	1a	966	M2G	C4-C5-N7	-2.41	106.86	110.67
32	1a	1518	MA6	C6-C5-N7	2.40	137.27	133.43
54	2w	37	MIA	C2-N1-C6	2.40	122.09	117.54
32	1a	527	7MG	C5-C4-N9	-2.38	103.28	106.33
32	2a	1519	MA6	C10-N6-C6	-2.38	114.47	120.52
1	1A	2251	OMG	O6-C6-C5	-2.38	120.26	126.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	1a	1518	MA6	C10-N6-C9	-2.37	108.58	116.18
54	1y	46	7MG	C5-C4-N9	-2.36	103.31	106.33
32	2a	1404	5MC	O2-C2-N3	-2.35	118.62	122.33
1	2A	2552	2MU	C2'-C1'-N1	-2.35	109.78	114.24
1	2A	1915	5MU	O2-C2-N1	-2.35	119.74	122.80
1	2A	2251	OMG	C4-C5-N7	-2.34	106.96	110.67
55	2x	32	5MC	O2-C2-N3	-2.34	118.65	122.33
54	1w	37	MIA	C4-N9-C8	2.33	108.19	105.74
32	2a	1518	MA6	C10-N6-C9	-2.33	108.71	116.18
32	2a	1498	UR3	C3U-N3-C4	2.32	121.09	117.87
55	2x	8	4SU	C6-C5-C4	-2.31	117.95	119.95
55	2x	8	4SU	C1'-N1-C6	-2.30	115.87	120.78
54	1w	37	MIA	C5-N7-C8	2.29	107.05	103.45
32	1a	1498	UR3	C3U-N3-C4	2.29	121.05	117.87
55	1x	54	5MU	O2-C2-N1	-2.29	119.82	122.80
1	1A	1920	4OC	O2-C2-N3	-2.29	118.73	122.33
54	2w	54	5MU	C5M-C5-C4	2.28	121.22	118.78
54	2y	55	PSU	C5-C6-N1	-2.28	118.97	122.14
55	1x	8	4SU	O2-C2-N3	-2.28	117.29	121.49
1	1A	2503	2MA	C6-C5-N7	2.27	136.47	132.09
54	1w	37	MIA	C11-S10-C2	-2.26	100.55	102.25
1	2A	2552	2MU	O4-C4-C5	-2.26	121.26	125.16
32	1a	527	7MG	O6-C6-C5	-2.25	122.10	127.62
55	2x	8	4SU	O2-C2-N3	-2.23	117.37	121.49
54	2y	39	PSU	C5-C6-N1	-2.21	119.07	122.14
32	1a	1402	4OC	C6-C5-C4	2.21	119.66	117.00
1	2A	1920	4OC	O2-C2-N3	-2.20	118.86	122.33
32	1a	1400	5MC	O2-C2-N3	-2.20	118.86	122.33
1	2A	2251	OMG	O6-C6-C5	-2.19	120.75	126.53
1	2A	2605	PSU	C5-C6-N1	-2.19	119.10	122.14
43	1l	92	0TD	OD1-CG-CB	-2.19	117.86	122.44
54	1w	8	4SU	C1'-N1-C2	2.19	121.52	117.59
32	1a	1404	5MC	O2-C2-N3	-2.18	118.89	122.33
32	1a	1519	MA6	C6-C5-N7	2.18	136.91	133.43
32	2a	1518	MA6	N9-C8-N7	-2.18	110.85	113.94
54	1w	46	7MG	C5-C6-N1	2.17	114.77	110.94
32	2a	967	5MC	O2-C2-N3	-2.17	118.91	122.33
54	2y	54	5MU	C5M-C5-C4	2.17	121.10	118.78
32	2a	1519	MA6	C6-C5-N7	2.17	136.89	133.43
32	2a	527	7MG	C5-C4-N9	-2.16	103.57	106.33
1	1A	1911	PSU	C5-C6-N1	-2.16	119.15	122.14
1	1A	2503	2MA	N9-C8-N7	-2.15	110.88	113.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	1a	1518	MA6	N9-C8-N7	-2.14	110.89	113.94
32	1a	1519	MA6	N9-C8-N7	-2.14	110.90	113.94
54	2w	54	5MU	O2-C2-N1	-2.13	120.02	122.80
54	2y	8	4SU	C1'-N1-C2	2.13	121.42	117.59
55	1x	55	PSU	C5-C6-N1	-2.13	119.18	122.14
55	2x	8	4SU	C5-C4-S4	-2.12	121.88	124.31
32	1a	1207	2MG	N1-C2-N2	2.12	118.72	116.56
54	1y	37	MIA	C6-C5-N7	2.12	136.17	132.09
32	2a	1402	4OC	C6-C5-C4	2.10	119.53	117.00
54	1w	39	PSU	C5-C6-N1	-2.09	119.24	122.14
32	1a	1519	MA6	N1-C6-N6	2.09	119.40	116.86
32	2a	966	M2G	O6-C6-C5	-2.07	121.08	126.53
1	2A	1917	PSU	C5-C6-N1	-2.06	119.28	122.14
54	1y	39	PSU	C5-C6-N1	-2.06	119.28	122.14
54	2w	46	7MG	O6-C6-C5	-2.06	122.57	127.62
32	2a	527	7MG	O6-C6-C5	-2.05	122.59	127.62
32	2a	1207	2MG	N2-C2-N3	-2.05	117.90	120.51
1	1A	1917	PSU	C5-C6-N1	-2.04	119.31	122.14
1	1A	1915	5MU	O2-C2-N1	-2.04	120.15	122.80
55	2x	55	PSU	C5-C6-N1	-2.03	119.32	122.14
54	1w	46	7MG	C4-C5-N7	2.03	107.77	105.38
54	2y	32	PSU	O4'-C1'-C2'	2.02	107.94	105.15
32	2a	1407	5MC	O2-C2-N3	-2.02	119.15	122.33
54	1y	46	7MG	O6-C6-C5	-2.01	122.67	127.62
54	1w	46	7MG	O6-C6-C5	-2.00	122.70	127.62
54	2y	54	5MU	C1'-N1-C6	-2.00	117.85	121.15

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1402	4OC	O4'-C4'-C5'-O5'
32	2a	1518	MA6	C5-C6-N6-C9
32	2a	1519	MA6	O4'-C4'-C5'-O5'
43	2l	92	0TD	O-C-CA-CB
54	2y	8	4SU	O4'-C4'-C5'-O5'
54	1w	37	MIA	C12-C13-C14-C16
54	1y	46	7MG	C4'-C5'-O5'-P
54	2y	46	7MG	C4'-C5'-O5'-P
32	1a	1402	4OC	O4'-C4'-C5'-O5'
1	1A	1915	5MU	C3'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	1A	1915	5MU	O4'-C4'-C5'-O5'
54	2y	8	4SU	C3'-C4'-C5'-O5'
54	1y	8	4SU	C3'-C4'-C5'-O5'
54	1y	8	4SU	O4'-C4'-C5'-O5'
32	2a	1518	MA6	N1-C6-N6-C9
32	1a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	1402	4OC	C3'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
32	1a	527	7MG	C3'-C4'-C5'-O5'
32	2a	1519	MA6	N1-C6-N6-C9
32	1a	1402	4OC	C3'-C4'-C5'-O5'
32	1a	1518	MA6	C5-C6-N6-C10
32	1a	1519	MA6	C5-C6-N6-C10
32	2a	1519	MA6	C5-C6-N6-C9
32	1a	1400	5MC	O4'-C4'-C5'-O5'
54	2w	46	7MG	C2'-C1'-N9-C8
54	2y	46	7MG	C2'-C1'-N9-C8
54	1w	46	7MG	C2'-C1'-N9-C8
54	1y	46	7MG	C2'-C1'-N9-C8
43	2l	92	0TD	CG-CB-SB-CSB
32	1a	527	7MG	O4'-C4'-C5'-O5'
54	2w	39	PSU	O4'-C1'-C5-C4
32	1a	1400	5MC	C3'-C4'-C5'-O5'
32	1a	1518	MA6	C5-C6-N6-C9
32	2a	1519	MA6	C5-C6-N6-C10
32	2a	1519	MA6	C4'-C5'-O5'-P
1	1A	2503	2MA	C4'-C5'-O5'-P
54	1y	54	5MU	O4'-C4'-C5'-O5'
32	2a	527	7MG	C4'-C5'-O5'-P
54	1w	46	7MG	O4'-C1'-N9-C8
54	2w	39	PSU	O4'-C1'-C5-C6
32	1a	967	5MC	O4'-C4'-C5'-O5'
54	1y	46	7MG	O4'-C1'-N9-C8
54	2w	46	7MG	O4'-C1'-N9-C8
54	2y	46	7MG	O4'-C1'-N9-C8
43	1l	92	0TD	CG-CB-SB-CSB
32	2a	1400	5MC	O4'-C4'-C5'-O5'
32	1a	527	7MG	C4'-C5'-O5'-P
32	1a	1519	MA6	C4'-C5'-O5'-P
1	2A	2251	OMG	C4'-C5'-O5'-P
54	1y	8	4SU	C4'-C5'-O5'-P
1	1A	1920	4OC	C2'-C1'-N1-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
55	2x	8	4SU	C2'-C1'-N1-C2

There are no ring outliers.

46 monomers are involved in 63 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	2y	37	MIA	1	0
32	2a	1519	MA6	2	0
1	1A	2552	2MU	1	0
55	1x	32	5MC	1	0
32	1a	1518	MA6	3	0
54	1y	37	MIA	1	0
32	2a	1498	UR3	2	0
1	2A	2251	OMG	2	0
1	1A	1920	4OC	1	0
32	2a	967	5MC	2	0
32	2a	1402	4OC	2	0
54	1y	39	PSU	1	0
1	1A	1939	5MU	2	0
54	2w	39	PSU	1	0
32	2a	516	PSU	1	0
54	1w	46	7MG	1	0
54	2y	46	7MG	2	0
54	1y	46	7MG	1	0
55	2x	32	5MC	1	0
1	2A	2503	2MA	1	0
32	2a	966	M2G	2	0
32	1a	1402	4OC	2	0
32	1a	1519	MA6	3	0
54	2y	55	PSU	2	0
1	2A	1917	PSU	1	0
54	2y	54	5MU	1	0
54	1w	37	MIA	1	0
1	2A	1920	4OC	2	0
54	1w	55	PSU	1	0
32	2a	1518	MA6	3	0
1	2A	1939	5MU	1	0
1	2A	2552	2MU	1	0
54	2w	8	4SU	5	0
32	2a	1404	5MC	1	0
54	1w	39	PSU	1	0
54	1y	8	4SU	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	2y	39	PSU	1	0
54	1w	54	5MU	1	0
54	2w	54	5MU	1	0
54	2w	37	MIA	1	0
43	2l	92	0TD	1	0
1	2A	1915	5MU	1	0
32	2a	1407	5MC	1	0
54	2w	32	PSU	1	0
55	1x	8	4SU	2	0
55	2x	8	4SU	2	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2840 ligands modelled in this entry, 2836 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
60	SF4	1d	302	35	0,12,12	-	-	-		
57	CLM	2A	3888	-	20,20,20	0.93	2 (10%)	23,27,27	1.00	1 (4%)
60	SF4	2d	302	35	0,12,12	-	-	-		
57	CLM	1A	4102	-	20,20,20	0.91	2 (10%)	23,27,27	0.74	0

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

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	CLM	2A	3888	-	-	6/20/22/22	0/1/1/1
60	SF4	2d	302	35	-	-	0/6/5/5
57	CLM	1A	4102	-	-	7/20/22/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	2A	3888	CLM	C6-C5	-2.44	1.48	1.51
57	2A	3888	CLM	C9-N9	-2.15	1.40	1.45
57	1A	4102	CLM	C6-C5	-2.12	1.48	1.51
57	1A	4102	CLM	C9-N9	-2.02	1.40	1.45

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	2A	3888	CLM	C6-C5-C3	-2.82	106.66	111.72

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	2A	3888	CLM	C1-C2-N2-C3
57	2A	3888	CLM	O2-C2-N2-C3
57	2A	3888	CLM	C4-C3-N2-C2
57	2A	3888	CLM	N2-C3-C4-O4
57	2A	3888	CLM	C5-C3-C4-O4
57	1A	4102	CLM	O2-C2-N2-C3
57	1A	4102	CLM	C1-C2-N2-C3
57	1A	4102	CLM	C5-C3-C4-O4
57	1A	4102	CLM	N2-C3-C4-O4
57	1A	4102	CLM	C5-C3-N2-C2
57	1A	4102	CLM	C4-C3-N2-C2
57	1A	4102	CLM	C4-C3-C5-O5
57	2A	3888	CLM	C4-C3-C5-O5

There are no ring outliers.

3 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	1d	302	SF4	11	0

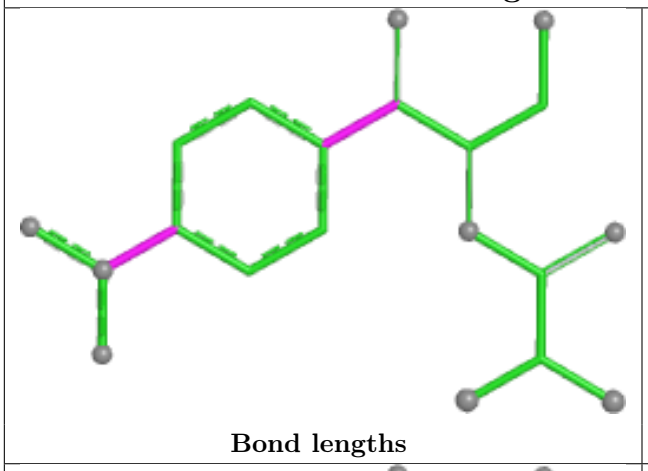
Continued on next page...

Continued from previous page...

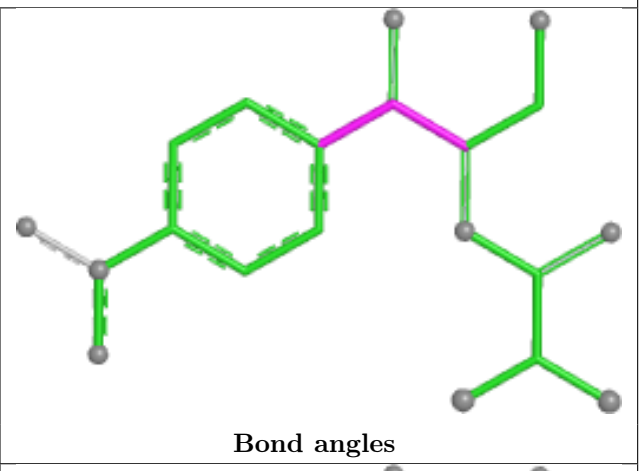
Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	2A	3888	CLM	1	0
60	2d	302	SF4	3	0

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.

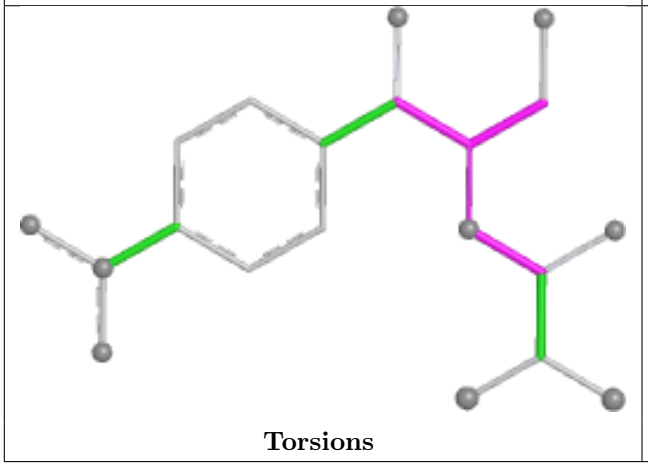
Ligand CLM 2A 3888



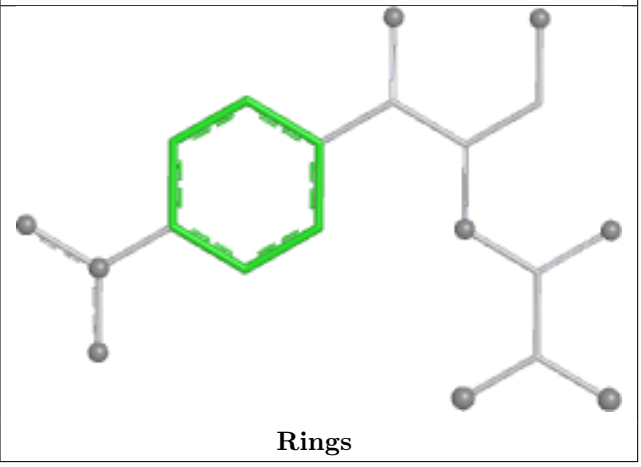
Bond lengths



Bond angles

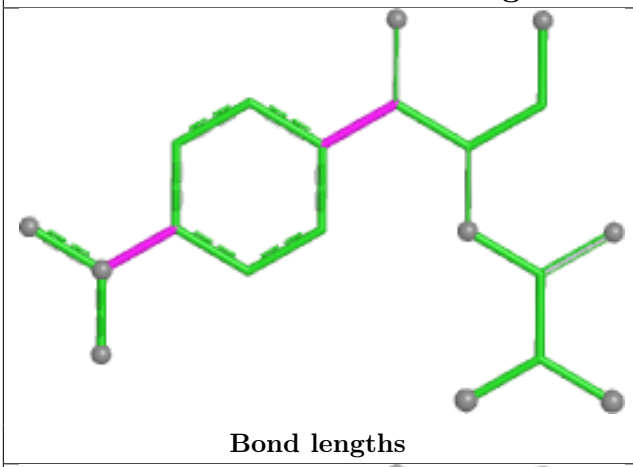


Torsions

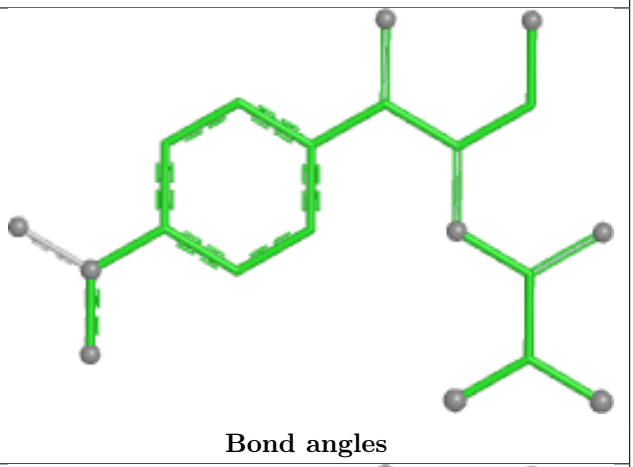


Rings

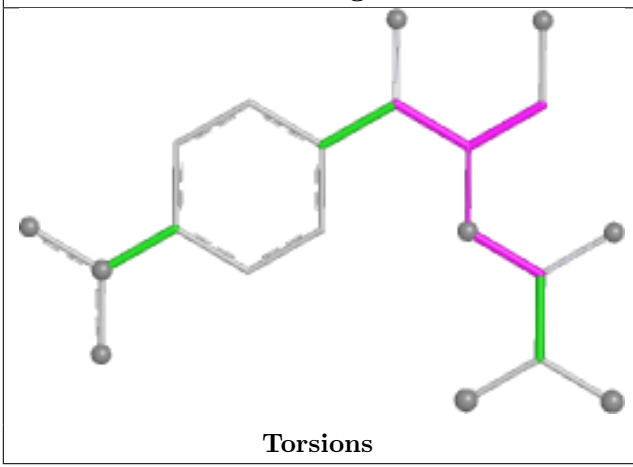
Ligand CLM 1A 4102



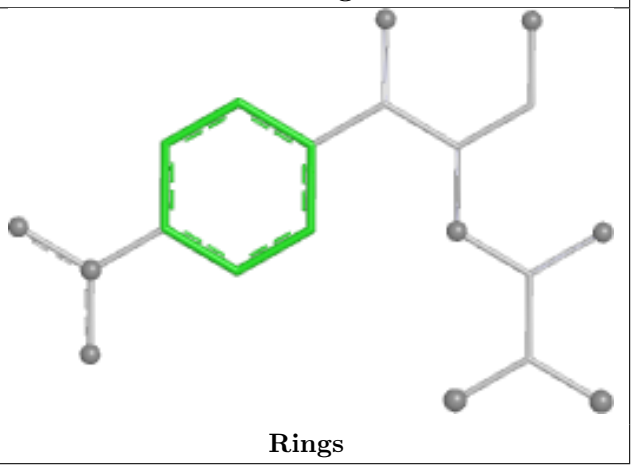
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.41	102 (3%) 46 40	17, 34, 87, 101	0
1	2A	2789/2915 (95%)	0.13	94 (3%) 48 42	34, 57, 87, 102	0
2	1B	120/121 (99%)	-0.29	0 100 100	27, 48, 58, 79	0
2	2B	120/121 (99%)	1.04	9 (7%) 20 16	58, 78, 85, 87	0
3	1D	275/276 (99%)	-0.01	4 (1%) 72 68	20, 35, 50, 73	0
3	2D	275/276 (99%)	0.44	2 (0%) 84 82	33, 51, 62, 73	0
4	1E	204/206 (99%)	-0.04	1 (0%) 87 85	18, 40, 57, 73	0
4	2E	204/206 (99%)	0.55	9 (4%) 39 33	35, 58, 69, 79	0
5	1F	203/210 (96%)	-0.01	2 (0%) 79 76	16, 41, 63, 80	0
5	2F	203/210 (96%)	0.64	6 (2%) 52 47	37, 64, 77, 83	0
6	1G	181/182 (99%)	0.55	8 (4%) 39 33	39, 56, 69, 78	0
6	2G	181/182 (99%)	1.21	23 (12%) 8 6	68, 77, 85, 93	0
7	1H	174/180 (96%)	0.30	3 (1%) 69 64	37, 50, 62, 71	0
7	2H	174/180 (96%)	1.38	39 (22%) 2 2	67, 78, 84, 91	0
8	1I	146/148 (98%)	0.89	4 (2%) 56 50	45, 70, 77, 81	0
8	2I	146/148 (98%)	1.13	16 (10%) 10 8	53, 70, 80, 85	0
9	1N	140/140 (100%)	0.01	1 (0%) 84 82	26, 38, 54, 72	0
9	2N	140/140 (100%)	0.64	4 (2%) 53 48	46, 64, 75, 80	0
10	1O	122/122 (100%)	-0.03	0 100 100	26, 40, 55, 61	0
10	2O	122/122 (100%)	0.58	1 (0%) 82 80	44, 57, 68, 73	0
11	1P	149/150 (99%)	0.10	0 100 100	17, 44, 64, 72	0
11	2P	149/150 (99%)	0.66	1 (0%) 84 82	38, 64, 77, 83	0
12	1Q	141/141 (100%)	0.10	1 (0%) 84 82	27, 41, 54, 74	0
12	2Q	141/141 (100%)	1.01	12 (8%) 16 13	52, 65, 74, 80	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%)	-0.23	0 100 100	22, 34, 47, 55	0
13	2R	118/118 (100%)	0.29	0 100 100	38, 51, 59, 67	0
14	1S	110/112 (98%)	0.25	0 100 100	37, 49, 61, 65	0
14	2S	110/112 (98%)	1.56	35 (31%) 1 1	63, 73, 80, 84	0
15	1T	131/146 (89%)	0.18	2 (1%) 72 68	33, 43, 64, 70	0
15	2T	131/146 (89%)	0.65	4 (3%) 51 45	49, 59, 74, 79	0
16	1U	116/118 (98%)	-0.21	1 (0%) 81 78	20, 29, 47, 60	0
16	2U	116/118 (98%)	0.84	5 (4%) 40 34	47, 61, 74, 80	0
17	1V	101/101 (100%)	-0.19	0 100 100	20, 39, 56, 69	0
17	2V	101/101 (100%)	0.75	1 (0%) 79 76	42, 68, 76, 82	0
18	1W	112/113 (99%)	-0.23	2 (1%) 67 63	21, 30, 46, 75	0
18	2W	112/113 (99%)	0.55	1 (0%) 81 78	38, 50, 66, 88	0
19	1X	95/96 (98%)	-0.04	2 (2%) 63 58	24, 36, 55, 72	0
19	2X	95/96 (98%)	0.80	4 (4%) 40 35	44, 58, 70, 81	0
20	1Y	107/110 (97%)	0.41	1 (0%) 81 78	33, 48, 66, 74	0
20	2Y	107/110 (97%)	0.92	5 (4%) 36 30	59, 68, 75, 84	0
21	1Z	154/206 (74%)	0.67	9 (5%) 29 23	41, 60, 77, 85	0
21	2Z	160/206 (77%)	1.71	51 (31%) 1 1	66, 78, 86, 88	0
22	10	83/85 (97%)	0.40	7 (8%) 17 13	27, 37, 60, 72	0
22	20	83/85 (97%)	1.32	12 (14%) 6 4	53, 64, 74, 83	0
23	11	97/98 (98%)	0.22	2 (2%) 63 58	24, 43, 63, 68	0
23	21	97/98 (98%)	0.71	5 (5%) 33 27	40, 56, 71, 73	0
24	12	70/72 (97%)	0.19	2 (2%) 53 48	32, 46, 57, 65	0
24	22	70/72 (97%)	0.97	5 (7%) 22 17	54, 68, 73, 76	0
25	13	59/60 (98%)	-0.04	1 (1%) 69 64	25, 36, 58, 78	0
25	23	59/60 (98%)	0.64	1 (1%) 69 64	53, 64, 77, 79	0
26	14	69/71 (97%)	1.04	11 (15%) 5 4	49, 71, 81, 85	0
26	24	69/71 (97%)	1.50	18 (26%) 1 1	76, 82, 88, 91	0
27	15	59/60 (98%)	-0.32	1 (1%) 69 64	18, 29, 45, 63	0
27	25	59/60 (98%)	0.32	2 (3%) 48 42	38, 50, 63, 67	0
28	16	53/54 (98%)	0.07	0 100 100	30, 41, 55, 61	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	26	53/54 (98%)	1.17	6 (11%) 10 8	49, 61, 68, 75	0
29	17	48/49 (97%)	-0.12	0 100 100	18, 24, 52, 58	0
29	27	48/49 (97%)	0.23	4 (8%) 17 13	32, 41, 60, 68	0
30	18	64/65 (98%)	-0.03	1 (1%) 70 66	26, 31, 38, 54	0
30	28	64/65 (98%)	0.67	2 (3%) 51 45	45, 54, 60, 71	0
31	19	37/37 (100%)	-0.13	0 100 100	27, 38, 54, 57	0
31	29	37/37 (100%)	1.15	3 (8%) 18 14	59, 66, 73, 76	0
32	1a	1488/1521 (97%)	0.39	45 (3%) 52 47	33, 65, 87, 100	0
32	2a	1491/1521 (98%)	0.90	157 (10%) 11 9	50, 75, 91, 99	0
33	1b	231/256 (90%)	1.35	44 (19%) 3 2	63, 74, 82, 87	0
33	2b	231/256 (90%)	1.53	60 (25%) 1 1	71, 83, 88, 92	0
34	1c	206/239 (86%)	0.91	15 (7%) 21 17	59, 70, 78, 83	0
34	2c	206/239 (86%)	2.08	102 (49%) 0 0	72, 82, 87, 91	0
35	1d	208/209 (99%)	1.10	24 (11%) 9 7	56, 69, 80, 84	0
35	2d	208/209 (99%)	0.97	13 (6%) 26 20	57, 67, 75, 82	0
36	1e	148/162 (91%)	0.66	4 (2%) 56 50	49, 63, 70, 76	0
36	2e	148/162 (91%)	1.30	23 (15%) 5 4	67, 76, 81, 88	0
37	1f	100/101 (99%)	0.64	2 (2%) 65 60	50, 64, 70, 73	0
37	2f	100/101 (99%)	1.19	13 (13%) 7 5	60, 70, 77, 81	0
38	1g	155/156 (99%)	1.01	17 (10%) 10 8	50, 67, 76, 87	0
38	2g	155/156 (99%)	1.31	27 (17%) 4 3	66, 75, 82, 88	0
39	1h	137/138 (99%)	0.50	2 (1%) 72 68	56, 64, 71, 75	0
39	2h	137/138 (99%)	1.20	17 (12%) 8 6	67, 75, 80, 86	0
40	1i	127/128 (99%)	1.32	26 (20%) 2 2	52, 72, 77, 79	0
40	2i	127/128 (99%)	2.05	67 (52%) 0 0	68, 80, 86, 89	0
41	1j	97/105 (92%)	1.29	22 (22%) 2 1	58, 76, 83, 89	0
41	2j	96/105 (91%)	2.67	74 (77%) 0 0	71, 82, 88, 96	0
42	1k	114/129 (88%)	0.69	4 (3%) 47 41	38, 61, 70, 74	0
42	2k	114/129 (88%)	1.17	19 (16%) 4 3	56, 72, 77, 82	0
43	1l	121/132 (91%)	0.70	10 (8%) 17 13	42, 56, 66, 69	0
43	2l	121/132 (91%)	1.44	24 (19%) 3 2	58, 69, 76, 80	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	1m	123/126 (97%)	0.98	10 (8%) 18 14	55, 67, 75, 81	0
44	2m	122/126 (96%)	1.94	47 (38%) 1 0	71, 79, 85, 88	0
45	1n	60/61 (98%)	1.28	8 (13%) 7 5	60, 68, 73, 76	0
45	2n	60/61 (98%)	2.55	44 (73%) 0 0	74, 82, 86, 90	0
46	1o	88/89 (98%)	0.81	5 (5%) 29 24	48, 60, 70, 74	0
46	2o	88/89 (98%)	1.14	15 (17%) 4 3	60, 70, 78, 82	0
47	1p	82/88 (93%)	1.33	12 (14%) 6 4	56, 70, 76, 79	0
47	2p	82/88 (93%)	1.11	6 (7%) 21 17	58, 65, 74, 80	0
48	1q	99/105 (94%)	1.23	16 (16%) 4 3	50, 63, 71, 73	0
48	2q	99/105 (94%)	0.99	8 (8%) 18 14	62, 69, 77, 81	0
49	1r	68/88 (77%)	0.75	6 (8%) 15 12	55, 64, 73, 75	0
49	2r	68/88 (77%)	1.04	3 (4%) 39 33	62, 71, 78, 82	0
50	1s	83/93 (89%)	1.06	9 (10%) 11 8	60, 70, 77, 80	0
50	2s	83/93 (89%)	2.47	58 (69%) 0 0	75, 82, 87, 91	0
51	1t	96/106 (90%)	1.06	8 (8%) 17 13	58, 68, 76, 81	0
51	2t	96/106 (90%)	1.28	17 (17%) 4 3	57, 69, 76, 79	0
52	1u	23/27 (85%)	1.42	4 (17%) 4 3	59, 64, 69, 71	0
52	2u	23/27 (85%)	2.10	12 (52%) 0 0	74, 77, 81, 85	0
53	1v	13/24 (54%)	0.80	1 (7%) 19 15	47, 66, 80, 86	0
53	2v	13/24 (54%)	2.51	8 (61%) 0 0	69, 82, 92, 92	0
54	1w	67/76 (88%)	1.56	15 (22%) 2 2	59, 87, 94, 98	0
54	1y	67/76 (88%)	0.83	3 (4%) 38 32	38, 86, 93, 96	0
54	2w	65/76 (85%)	1.76	23 (35%) 1 1	74, 91, 96, 101	0
54	2y	66/76 (86%)	1.41	10 (15%) 5 4	57, 92, 96, 99	0
55	1x	72/77 (93%)	0.42	3 (4%) 40 35	37, 62, 77, 85	0
55	2x	72/77 (93%)	0.84	2 (2%) 55 49	55, 78, 86, 89	0
All	All	20875/21748 (95%)	0.53	1712 (8%) 17 14	16, 62, 85, 102	0

All (1712) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	2m	124	PRO	8.5
45	1n	2	ALA	8.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
38	2g	80	VAL	7.6
34	2c	2	GLY	7.4
38	1g	80	VAL	7.0
44	2m	6	GLY	6.7
50	2s	79	THR	6.1
44	2m	5	ALA	6.0
32	2a	1034	G	5.9
32	1a	1036	G	5.5
44	2m	102	ARG	5.5
23	21	2	SER	5.5
44	1m	124	PRO	5.3
32	2a	1033	G	5.3
1	1A	2159	G	5.1
21	2Z	174	VAL	5.1
50	2s	9	VAL	5.1
45	2n	7	ILE	5.0
44	1m	2	ALA	5.0
47	1p	82	GLN	5.0
44	2m	121	LYS	4.8
41	2j	49	VAL	4.8
36	2e	22	GLY	4.8
34	2c	187	ALA	4.7
53	2v	24	A	4.7
44	2m	123	ALA	4.7
54	1w	73	A	4.7
33	2b	187	LEU	4.6
41	2j	40	LEU	4.6
41	2j	65	LEU	4.6
43	2l	13	LYS	4.6
1	1A	2112	G	4.6
32	2a	1030(B)	C	4.5
15	1T	130	ALA	4.5
41	2j	27	ALA	4.5
38	2g	84	ASN	4.5
38	2g	81	GLY	4.5
21	2Z	172	ALA	4.5
41	2j	34	VAL	4.5
52	2u	14	TRP	4.5
32	2a	1036	G	4.5
45	2n	3	ARG	4.5
22	10	7	LEU	4.4
33	2b	237	ALA	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
38	1g	85	TYR	4.4
45	2n	44	LEU	4.4
1	2A	1536	C	4.4
22	10	6	GLY	4.4
26	14	56	VAL	4.4
40	2i	14	VAL	4.4
40	2i	102	LEU	4.4
45	2n	25	VAL	4.4
45	2n	39	LEU	4.3
33	1b	237	ALA	4.3
45	2n	47	LEU	4.3
15	1T	131	ALA	4.3
50	2s	76	PRO	4.3
1	2A	883	G	4.3
41	2j	76	ASN	4.3
33	1b	202	PRO	4.2
6	2G	20	ILE	4.2
41	2j	47	PHE	4.2
1	1A	2115	G	4.2
12	2Q	104	PHE	4.2
7	2H	45	VAL	4.2
5	2F	166	ALA	4.2
21	1Z	146	ILE	4.2
41	2j	50	ILE	4.2
40	2i	41	VAL	4.2
41	2j	85	LEU	4.2
1	1A	2113	U	4.2
1	2A	2146	C	4.2
34	2c	77	ILE	4.2
22	10	3	HIS	4.2
1	1A	1059	G	4.2
41	2j	32	ALA	4.1
45	2n	2	ALA	4.1
33	2b	185	ILE	4.1
34	1c	39	ILE	4.1
34	2c	4	LYS	4.1
44	2m	122	LYS	4.1
51	2t	103	GLY	4.1
33	1b	127	ILE	4.1
1	1A	1078	U	4.1
32	1a	1531	A	4.1
44	2m	66	LEU	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
41	2j	55	LYS	4.1
21	2Z	171	ILE	4.1
40	2i	126	SER	4.1
50	2s	11	VAL	4.1
54	1w	1	G	4.0
15	2T	131	ALA	4.0
34	2c	67	THR	4.0
1	2A	2133	G	4.0
3	2D	2	ALA	4.0
36	2e	109	ILE	4.0
40	2i	36	TYR	4.0
42	2k	25	TYR	4.0
1	2A	2155	G	4.0
50	2s	53	ASN	4.0
43	1l	14	GLY	4.0
45	2n	6	LEU	4.0
22	10	5	LYS	4.0
32	2a	1220	G	3.9
32	2a	1310	G	3.9
34	2c	5	ILE	3.9
34	2c	3	ASN	3.9
32	1a	1532	U	3.9
32	2a	1224	G	3.9
34	2c	52	LEU	3.9
19	1X	95	LEU	3.9
43	2l	56	ALA	3.9
50	2s	15	LEU	3.9
32	2a	1222	G	3.9
45	2n	33	VAL	3.9
22	10	4	LYS	3.9
1	1A	1064	C	3.9
33	1b	230	VAL	3.9
40	2i	105	ASP	3.9
32	2a	1001(A)	G	3.8
53	2v	13	A	3.8
34	2c	9	GLY	3.8
54	2w	3	C	3.8
43	2l	9	GLN	3.8
50	2s	14	HIS	3.8
21	2Z	21	ALA	3.8
34	2c	129	ALA	3.8
26	24	65	ASP	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
52	2u	5	ASP	3.8
34	2c	167	TRP	3.8
34	2c	149	ALA	3.8
21	2Z	146	ILE	3.8
34	2c	189	ALA	3.8
33	2b	71	VAL	3.8
34	2c	153	VAL	3.8
33	1b	129	GLU	3.7
41	2j	42	THR	3.7
33	1b	229	VAL	3.7
53	2v	12	A	3.7
5	2F	131	GLY	3.7
1	2A	2118	U	3.7
14	2S	3	ARG	3.7
1	1A	1058	G	3.7
54	1w	71	G	3.7
38	1g	154	TYR	3.7
40	2i	125	TYR	3.7
31	29	37	GLY	3.7
34	2c	53	ALA	3.7
40	2i	82	ALA	3.7
45	2n	38	GLY	3.7
1	1A	1057	A	3.7
41	2j	44	VAL	3.7
32	2a	1030(A)	G	3.7
50	2s	13	ASP	3.7
26	24	63	TYR	3.7
33	2b	165	VAL	3.7
32	2a	1035	A	3.6
38	2g	16	LEU	3.6
50	2s	22	LEU	3.6
1	2A	2112	G	3.6
32	2a	1032	G	3.6
35	2d	183	GLY	3.6
50	2s	82	GLY	3.6
26	24	50	VAL	3.6
34	1c	12	LEU	3.6
34	2c	192	THR	3.6
45	1n	7	ILE	3.6
32	2a	1001	A	3.6
21	2Z	173	ALA	3.6
7	2H	21	PRO	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	1094	U	3.6
32	2a	1225	A	3.6
33	1b	17	PHE	3.6
50	1s	9	VAL	3.6
1	2A	2145	C	3.6
1	1A	2116	G	3.6
32	2a	1002	G	3.6
32	2a	1221	G	3.6
45	2n	22	THR	3.6
34	2c	168	ALA	3.6
41	2j	91	PRO	3.6
35	1d	150	GLU	3.6
43	2l	16	GLU	3.6
51	1t	14	LYS	3.6
34	2c	134	ILE	3.5
50	2s	63	THR	3.5
1	2A	2174	C	3.5
32	1a	1002	G	3.5
34	2c	145	GLY	3.5
38	2g	83	ALA	3.5
40	2i	127	LYS	3.5
1	1A	1081	U	3.5
35	1d	135	LEU	3.5
40	2i	64	THR	3.5
54	1w	72	C	3.5
1	1A	1087	G	3.5
1	2A	2159	G	3.5
50	2s	80	TYR	3.5
32	2a	239	U	3.5
32	1a	1035	A	3.5
32	2a	1286	A	3.5
22	10	8	GLY	3.5
33	2b	161	ALA	3.5
34	2c	65	ALA	3.5
44	1m	123	ALA	3.5
50	1s	84	GLY	3.5
33	2b	7	VAL	3.5
38	1g	153	HIS	3.5
45	2n	21	TYR	3.5
32	1a	1257	U	3.5
44	1m	122	LYS	3.5
6	1G	51	ARG	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	1097	U	3.4
1	2A	2156	G	3.4
1	2A	2319	G	3.4
8	2I	20	ASP	3.4
1	1A	2158	A	3.4
26	14	50	VAL	3.4
44	1m	3	ARG	3.4
44	2m	60	VAL	3.4
42	2k	50	TYR	3.4
51	1t	103	GLY	3.4
19	2X	92	LEU	3.4
22	20	84	LEU	3.4
34	2c	188	LEU	3.4
1	2A	2144	U	3.4
33	1b	28	PHE	3.4
40	2i	10	ARG	3.4
32	2a	1003	G	3.4
1	1A	2117	A	3.4
7	2H	2	SER	3.4
22	20	2	ALA	3.4
34	2c	200	ALA	3.4
36	2e	17	ALA	3.4
50	2s	2	PRO	3.4
34	2c	207	VAL	3.4
1	1A	1060	U	3.4
54	1w	70	G	3.4
41	2j	87	THR	3.4
21	2Z	164	ALA	3.4
44	2m	90	LEU	3.4
34	1c	207	VAL	3.4
1	1A	1065	U	3.3
32	1a	1037	C	3.3
32	2a	1219	U	3.3
33	2b	196	LEU	3.3
34	2c	12	LEU	3.3
41	2j	36	GLY	3.3
51	2t	22	ARG	3.3
14	2S	34	HIS	3.3
33	2b	186	ALA	3.3
33	2b	122	PHE	3.3
41	2j	89	ASP	3.3
43	2l	18	VAL	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	1509	C	3.3
24	12	69	ARG	3.3
32	2a	1321	C	3.3
54	1w	2	C	3.3
44	2m	100	GLY	3.3
46	1o	89	GLY	3.3
6	2G	160	VAL	3.3
9	1N	140	VAL	3.3
34	2c	68	VAL	3.3
34	2c	70	VAL	3.3
34	2c	76	VAL	3.3
32	2a	1016	A	3.3
32	2a	1236	A	3.3
1	1A	2160	G	3.3
32	2a	238	G	3.3
23	11	2	SER	3.3
42	2k	126	ARG	3.3
41	2j	13	HIS	3.3
41	2j	93	GLY	3.3
1	1A	2145	C	3.3
1	2A	2166	G	3.3
21	2Z	33	LEU	3.3
21	2Z	149	SER	3.3
41	2j	18	ALA	3.3
26	24	59	PHE	3.3
41	2j	96	ILE	3.3
33	1b	24	TRP	3.2
32	2a	965	A	3.2
51	2t	24	LEU	3.2
1	2A	2125	G	3.2
26	24	56	VAL	3.2
34	2c	55	VAL	3.2
41	2j	66	ARG	3.2
14	2S	58	LEU	3.2
41	1j	77	PRO	3.2
41	2j	41	PRO	3.2
41	2j	83	GLU	3.2
50	2s	71	LEU	3.2
7	1H	2	SER	3.2
41	2j	59	SER	3.2
52	2u	16	GLY	3.2
1	2A	2119	A	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	2169	A	3.2
40	1i	106	ALA	3.2
6	2G	28	VAL	3.2
7	2H	24	VAL	3.2
41	2j	74	ILE	3.2
50	2s	40	ILE	3.2
44	2m	88	ARG	3.2
1	1A	1026	U	3.2
26	14	57	GLU	3.2
50	1s	5	LEU	3.2
7	2H	55	PRO	3.2
27	25	29	THR	3.2
38	2g	82	GLY	3.2
32	2a	1038	C	3.2
32	2a	1226	C	3.2
41	2j	30	SER	3.2
40	2i	114	TYR	3.2
41	1j	65	LEU	3.2
32	2a	1017	G	3.2
12	2Q	61	GLY	3.2
39	2h	90	GLY	3.2
34	2c	160	ALA	3.2
41	2j	23	ILE	3.2
7	2H	44	VAL	3.2
40	2i	28	VAL	3.2
1	2A	2111	C	3.1
32	2a	1030	C	3.1
50	1s	13	ASP	3.1
50	2s	70	LYS	3.1
6	1G	139	LEU	3.1
40	2i	19	LEU	3.1
53	1v	12	A	3.1
26	14	52	THR	3.1
26	14	54	GLY	3.1
45	2n	61	TRP	3.1
50	2s	84	GLY	3.1
8	1I	146	ALA	3.1
26	24	49	PHE	3.1
34	2c	198	VAL	3.1
41	2j	54	PHE	3.1
26	14	67	TYR	3.1
32	1a	1034	G	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	2a	1190	G	3.1
50	2s	52	TYR	3.1
54	1w	65	G	3.1
36	2e	25	ARG	3.1
41	2j	99	LYS	3.1
32	2a	995	C	3.1
41	2j	39	PRO	3.1
32	2a	1183	A	3.1
33	1b	7	VAL	3.1
41	2j	35	SER	3.1
50	2s	60	VAL	3.1
14	2S	57	LYS	3.1
45	2n	34	TYR	3.1
33	2b	10	LEU	3.1
36	2e	31	LEU	3.1
41	2j	88	LEU	3.1
1	2A	2318	G	3.1
40	2i	124	GLN	3.1
34	2c	8	ILE	3.1
49	2r	60	ALA	3.1
21	2Z	71	VAL	3.1
41	2j	72	VAL	3.1
14	2S	32	LEU	3.1
32	2a	1196	U	3.1
32	2a	1532	U	3.1
34	2c	17	ASP	3.1
21	2Z	106	GLY	3.1
41	2j	75	ILE	3.1
43	2l	15	ARG	3.1
1	1A	886	C	3.1
1	1A	1100	C	3.1
1	2A	885	C	3.1
32	2a	1059	C	3.1
40	1i	59	PHE	3.1
54	2w	13	C	3.1
36	2e	133	TYR	3.0
38	2g	85	TYR	3.0
41	2j	71	LEU	3.0
33	1b	167	PRO	3.0
41	2j	37	PRO	3.0
41	1j	48	THR	3.0
35	1d	5	ILE	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
40	2i	9	ARG	3.0
51	2t	8	ARG	3.0
1	2A	2157	G	3.0
1	1A	34	C	3.0
32	2a	824	C	3.0
32	2a	1118	C	3.0
32	2a	1119	C	3.0
34	2c	69	HIS	3.0
40	1i	2	GLU	3.0
43	2l	8	ASN	3.0
51	2t	9	ASN	3.0
1	2A	2173	A	3.0
47	2p	76	GLN	3.0
3	1D	276	LYS	3.0
22	20	5	LYS	3.0
40	2i	11	LYS	3.0
42	1k	123	LYS	3.0
14	2S	20	ARG	3.0
14	2S	35	ILE	3.0
44	2m	78	ILE	3.0
44	2m	103	THR	3.0
49	2r	65	ILE	3.0
35	1d	195	ALA	3.0
40	2i	13	ALA	3.0
5	2F	6	VAL	3.0
33	1b	163	PHE	3.0
33	2b	112	VAL	3.0
4	2E	195	LEU	3.0
6	2G	19	LEU	3.0
14	2S	92	TYR	3.0
40	2i	123	PRO	3.0
1	1A	1093	G	3.0
7	2H	175	LYS	3.0
1	1A	2138	C	3.0
32	2a	1054	C	3.0
26	14	58	ARG	3.0
52	1u	24	ARG	3.0
53	2v	14	A	3.0
21	1Z	147	GLY	3.0
40	2i	81	ILE	3.0
50	2s	49	ILE	3.0
45	2n	10	ALA	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	2a	1040	U	3.0
21	2Z	141	VAL	3.0
45	1n	56	VAL	3.0
21	2Z	125	LEU	3.0
40	1i	126	SER	3.0
50	2s	4	SER	3.0
34	2c	72	LYS	3.0
1	1A	2190	G	3.0
1	2A	2154	G	3.0
1	2A	645	C	3.0
6	2G	50	ALA	3.0
34	2c	71	ALA	3.0
50	2s	24	ALA	3.0
54	2w	34	G	3.0
32	2a	1322	C	3.0
33	2b	163	PHE	3.0
33	1b	11	LEU	2.9
48	2q	98	LEU	2.9
1	1A	271(K)	U	2.9
33	1b	19	HIS	2.9
50	2s	66	MET	2.9
36	2e	85	GLY	2.9
52	2u	11	GLY	2.9
40	2i	7	THR	2.9
8	2I	146	ALA	2.9
40	1i	43	ALA	2.9
7	2H	19	VAL	2.9
40	2i	99	LEU	2.9
1	1A	1062	G	2.9
1	1A	2141	G	2.9
32	2a	972	C	2.9
32	2a	979	C	2.9
32	2a	1027	C	2.9
1	2A	229	A	2.9
32	2a	1061	G	2.9
32	2a	1114	C	2.9
32	2a	1216	G	2.9
33	1b	134	GLU	2.9
32	2a	1285	A	2.9
45	2n	17	LYS	2.9
53	2v	23	A	2.9
54	2w	76	A	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
50	2s	78	ARG	2.9
47	2p	38	TYR	2.9
12	2Q	33	GLY	2.9
51	1t	69	GLY	2.9
50	2s	33	THR	2.9
5	2F	89	VAL	2.9
41	1j	40	LEU	2.9
41	2j	16	LEU	2.9
41	2j	90	LEU	2.9
8	2I	64	GLU	2.9
8	2I	85	GLU	2.9
21	2Z	166	SER	2.9
26	24	66	SER	2.9
34	2c	144	SER	2.9
1	1A	1080	C	2.9
28	26	37	ARG	2.9
34	2c	190	ARG	2.9
54	2w	4	C	2.9
1	1A	1089	G	2.9
1	2A	2131	G	2.9
1	2A	2149	G	2.9
1	2A	2893	G	2.9
32	1a	1026	G	2.9
38	1g	37	ASN	2.9
41	2j	6	ILE	2.9
4	2E	167	VAL	2.9
33	2b	184	VAL	2.9
33	2b	215	LEU	2.9
34	2c	33	LEU	2.9
35	1d	194	LEU	2.9
45	2n	56	VAL	2.9
40	2i	2	GLU	2.9
21	2Z	57	ILE	2.9
1	1A	1054	A	2.9
1	1A	2129	C	2.9
1	1A	2132	U	2.9
5	2F	208	GLY	2.9
26	24	64	GLY	2.9
32	1a	344	A	2.9
32	2a	948	C	2.9
33	2b	31	TYR	2.9
40	1i	67	GLY	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	1099	G	2.9
1	1A	2165	G	2.9
1	2A	2751	G	2.9
12	2Q	121	ALA	2.9
15	2T	130	ALA	2.9
33	1b	133	LYS	2.9
33	2b	11	LEU	2.9
34	2c	47	LEU	2.9
34	2c	138	VAL	2.9
39	2h	112	LEU	2.9
51	1t	74	LYS	2.9
40	2i	117	HIS	2.9
45	2n	49	HIS	2.9
51	2t	80	ARG	2.8
35	1d	173	TRP	2.8
50	2s	38	SER	2.8
33	2b	201	ILE	2.8
38	1g	84	ASN	2.8
51	2t	26	ASN	2.8
50	2s	61	TYR	2.8
29	27	45	ALA	2.8
33	2b	138	LEU	2.8
36	2e	108	ALA	2.8
1	1A	1066	U	2.8
16	2U	90	VAL	2.8
34	2c	75	VAL	2.8
34	2c	106	VAL	2.8
34	2c	195	VAL	2.8
32	2a	1110	A	2.8
32	2a	1019	C	2.8
32	2a	1116	C	2.8
32	2a	1214	C	2.8
32	2a	1260	C	2.8
52	2u	23	PRO	2.8
1	2A	1533	G	2.8
32	1a	1030(A)	G	2.8
38	1g	5	ARG	2.8
34	2c	170	GLN	2.8
34	2c	124	ILE	2.8
44	2m	4	ILE	2.8
48	1q	62	SER	2.8
50	2s	54	GLY	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
52	1u	2	GLY	2.8
33	1b	236	TYR	2.8
41	2j	8	LEU	2.8
38	2g	152	ALA	2.8
40	2i	4	TYR	2.8
40	2i	56	LEU	2.8
50	2s	5	LEU	2.8
50	2s	16	LEU	2.8
44	2m	105	THR	2.8
7	2H	107	VAL	2.8
21	2Z	96	VAL	2.8
43	2l	32	PHE	2.8
33	1b	12	GLU	2.8
38	1g	79	ARG	2.8
40	2i	49	PRO	2.8
1	1A	1095	A	2.8
1	2A	2170	A	2.8
16	1U	117	GLN	2.8
32	1a	1001	A	2.8
32	2a	974	A	2.8
41	2j	38	ILE	2.8
47	2p	3	LYS	2.8
32	2a	954	G	2.8
32	2a	971	G	2.8
35	2d	154	ASN	2.8
44	2m	106	ASN	2.8
54	2w	70	G	2.8
14	2S	56	LEU	2.8
33	2b	152	PHE	2.8
41	2j	86	MET	2.8
44	2m	99	ARG	2.8
50	2s	36	ARG	2.8
38	2g	86	GLN	2.8
1	1A	2130	U	2.8
32	2a	1235	U	2.8
1	1A	1092	C	2.8
1	2A	1043	C	2.8
32	2a	1066	C	2.8
45	2n	60	SER	2.8
48	2q	99	SER	2.8
21	2Z	150	LEU	2.8
36	2e	23	GLY	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
38	1g	82	GLY	2.8
41	2j	52	GLY	2.8
51	2t	73	HIS	2.8
21	1Z	168	GLU	2.8
22	20	68	GLU	2.8
28	26	52	VAL	2.8
34	2c	120	VAL	2.8
1	1A	1176	G	2.8
33	2b	199	TYR	2.8
4	1E	56	PRO	2.7
33	1b	131	PRO	2.7
8	2I	17	GLN	2.7
6	2G	157	ILE	2.7
33	2b	127	ILE	2.7
33	2b	214	ILE	2.7
44	2m	96	LEU	2.7
1	2A	2171	A	2.7
32	2a	983	A	2.7
1	1A	888	C	2.7
1	2A	2128	C	2.7
1	2A	2164	C	2.7
7	2H	43	VAL	2.7
8	2I	3	VAL	2.7
21	2Z	152	ALA	2.7
33	2b	123	ALA	2.7
26	14	59	PHE	2.7
32	2a	984	C	2.7
40	2i	128	ARG	2.7
41	2j	43	ARG	2.7
50	2s	67	VAL	2.7
23	21	68	PRO	2.7
44	2m	21	TYR	2.7
1	1A	2162	G	2.7
54	1y	18	G	2.7
33	1b	214	ILE	2.7
34	2c	202	ILE	2.7
47	1p	19	ILE	2.7
8	2I	12	LEU	2.7
33	1b	10	LEU	2.7
40	2i	96	LEU	2.7
8	2I	1	MET	2.7
20	2Y	5	MET	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	2c	6	HIS	2.7
40	2i	39	GLY	2.7
44	2m	64	TRP	2.7
44	2m	95	GLY	2.7
1	1A	2167	U	2.7
35	1d	192	GLU	2.7
35	2d	3	ARG	2.7
43	1l	16	GLU	2.7
3	1D	2	ALA	2.7
33	2b	164	VAL	2.7
38	1g	2	ALA	2.7
44	2m	104	ARG	2.7
45	2n	13	THR	2.7
48	1q	68	ARG	2.7
49	1r	24	ALA	2.7
1	1A	1084	A	2.7
1	2A	896	A	2.7
6	2G	2	PRO	2.7
33	2b	236	TYR	2.7
38	2g	154	TYR	2.7
42	2k	124	LYS	2.7
1	2A	2175	C	2.7
32	2a	1223	C	2.7
45	2n	53	LEU	2.7
49	1r	78	LEU	2.7
21	2Z	26	GLY	2.7
21	2Z	121	HIS	2.7
26	14	64	GLY	2.7
32	2a	973	G	2.7
32	2a	1026	G	2.7
54	2y	18	G	2.7
55	2x	70	G	2.7
41	1j	78	ASN	2.7
22	20	69	PHE	2.7
36	1e	67	VAL	2.7
37	2f	6	VAL	2.7
40	2i	18	PHE	2.7
40	2i	43	ALA	2.7
41	2j	94	VAL	2.7
1	1A	1101	U	2.7
1	2A	2113	U	2.7
52	1u	23	PRO	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
54	1y	20	U	2.7
1	1A	2119	A	2.7
1	2A	1847	A	2.7
34	2c	182	ILE	2.7
41	1j	74	ILE	2.7
1	1A	885	C	2.7
32	2a	1203	C	2.7
54	1w	74	C	2.7
44	2m	70	LEU	2.7
14	2S	45	GLY	2.7
26	24	61	ARG	2.7
41	1j	79	ARG	2.7
45	2n	29	ARG	2.7
46	2o	20	GLY	2.7
46	2o	68	ARG	2.7
7	2H	123	PHE	2.7
43	2l	104	VAL	2.7
50	2s	7	LYS	2.7
52	2u	3	LYS	2.7
39	2h	4	ASP	2.7
1	2A	2160	G	2.6
32	1a	1001(A)	G	2.6
32	1a	1003	G	2.6
32	2a	951	G	2.6
40	2i	73	GLN	2.6
26	24	67	TYR	2.6
32	2a	1126	U	2.6
44	2m	22	ILE	2.6
21	2Z	144	LEU	2.6
32	2a	1333	A	2.6
33	1b	196	LEU	2.6
1	1A	2161	C	2.6
3	1D	38	LYS	2.6
32	1a	345	C	2.6
54	1w	4	C	2.6
54	2w	74	C	2.6
55	1x	69	C	2.6
22	20	12	ASN	2.6
41	2j	78	ASN	2.6
21	1Z	141	VAL	2.6
21	2Z	88	PHE	2.6
21	2Z	139	VAL	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
21	2Z	167	PRO	2.6
26	24	42	PHE	2.6
51	2t	98	PRO	2.6
6	2G	146	TYR	2.6
1	1A	1082	U	2.6
55	2x	47	U	2.6
22	20	7	LEU	2.6
33	2b	121	LEU	2.6
34	2c	101	LEU	2.6
43	2l	10	LEU	2.6
7	2H	60	ARG	2.6
41	2j	68	HIS	2.6
8	1I	70	GLU	2.6
33	1b	228	GLY	2.6
34	2c	13	GLY	2.6
35	1d	169	LYS	2.6
40	2i	115	GLY	2.6
45	2n	4	LYS	2.6
45	2n	55	GLY	2.6
2	2B	59	A	2.6
32	2a	1306	A	2.6
8	2I	19	VAL	2.6
33	1b	25	ASN	2.6
14	2S	12	PHE	2.6
37	1f	90	VAL	2.6
38	2g	7	ALA	2.6
40	1i	15	ALA	2.6
50	2s	41	VAL	2.6
33	2b	97	TRP	2.6
1	1A	2111	C	2.6
32	1a	1027	C	2.6
32	2a	1045	C	2.6
32	2a	1249	C	2.6
47	1p	1	MET	2.6
47	2p	19	ILE	2.6
43	2l	19	ARG	2.6
46	1o	88	ARG	2.6
52	1u	6	ARG	2.6
32	2a	1308	U	2.6
41	2j	22	LYS	2.6
51	2t	74	LYS	2.6
44	2m	67	GLU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	2H	174	GLY	2.6
18	1W	112	GLY	2.6
34	2c	41	GLY	2.6
45	1n	51	GLY	2.6
50	1s	8	GLY	2.6
32	1a	1024	G	2.6
32	2a	1047	G	2.6
32	2a	1202	G	2.6
32	2a	1331	G	2.6
54	2w	15	G	2.6
34	2c	137	ALA	2.6
42	2k	89	ALA	2.6
46	2o	19	PRO	2.6
34	2c	107	GLN	2.6
1	1A	548	A	2.6
32	1a	1005	A	2.6
32	2a	949	A	2.6
6	2G	52	ILE	2.6
33	2b	200	ILE	2.6
46	1o	87	ILE	2.6
50	2s	31	ILE	2.6
32	1a	221	C	2.6
32	2a	985	C	2.6
32	2a	1384	C	2.6
40	2i	47	LEU	2.6
54	2w	2	C	2.6
12	2Q	60	ARG	2.6
34	2c	79	ARG	2.6
45	2n	12	ARG	2.6
48	2q	32	TYR	2.6
12	2Q	22	LYS	2.6
21	2Z	143	GLY	2.6
43	2l	63	GLY	2.6
7	2H	52	VAL	2.6
32	2a	960	U	2.6
45	2n	40	CYS	2.6
34	2c	73	PRO	2.6
41	1j	32	ALA	2.6
41	1j	47	PHE	2.6
45	2n	16	PHE	2.6
41	1j	100	THR	2.5
41	2j	100	THR	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	2165	G	2.5
32	1a	1023	G	2.5
32	2a	1253	G	2.5
54	2y	5	G	2.5
1	1A	2135	A	2.5
32	1a	1447	A	2.5
44	2m	19	LEU	2.5
14	2S	17	ARG	2.5
34	2c	176	HIS	2.5
34	2c	48	TYR	2.5
40	2i	62	TYR	2.5
1	2A	884	C	2.5
50	2s	26	GLY	2.5
21	2Z	165	VAL	2.5
41	2j	77	PRO	2.5
42	1k	14	VAL	2.5
50	2s	42	PRO	2.5
24	12	70	GLN	2.5
40	1i	13	ALA	2.5
42	1k	97	ALA	2.5
43	1l	6	THR	2.5
54	2y	45	U	2.5
21	2Z	157	LEU	2.5
34	2c	172	ARG	2.5
45	1n	3	ARG	2.5
48	2q	100	LYS	2.5
1	1A	1055	G	2.5
1	1A	1068	G	2.5
32	2a	1031	G	2.5
1	2A	1913	A	2.5
26	24	57	GLU	2.5
32	2a	1251	A	2.5
32	2a	1447	A	2.5
33	1b	31	TYR	2.5
33	1b	33	TYR	2.5
45	2n	28	GLY	2.5
46	1o	19	PRO	2.5
34	2c	128	PHE	2.5
38	1g	7	ALA	2.5
40	2i	106	ALA	2.5
41	2j	63	PHE	2.5
45	2n	59	ALA	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	889	C	2.5
1	1A	2164	C	2.5
1	2A	886	C	2.5
2	2B	6	C	2.5
32	1a	1030(B)	C	2.5
32	2a	1149	C	2.5
46	2o	4	THR	2.5
43	2l	52	LEU	2.5
44	2m	34	LEU	2.5
45	2n	23	ARG	2.5
46	2o	3	ILE	2.5
50	2s	32	LYS	2.5
7	2H	51	ARG	2.5
21	2Z	102	LEU	2.5
37	2f	45	LEU	2.5
26	14	63	TYR	2.5
38	2g	133	GLY	2.5
33	2b	125	PRO	2.5
1	1A	1098	A	2.5
1	2A	2062	A	2.5
1	2A	2117	A	2.5
32	2a	1064	G	2.5
32	2a	1117	G	2.5
32	2a	1357	A	2.5
32	2a	1370	G	2.5
33	1b	136	VAL	2.5
40	2i	53	VAL	2.5
50	2s	45	VAL	2.5
55	1x	70	G	2.5
4	2E	51	PHE	2.5
10	2O	99	PHE	2.5
41	2j	26	ALA	2.5
43	2l	68	ALA	2.5
45	2n	37	PHE	2.5
51	1t	12	ALA	2.5
14	2S	19	LYS	2.5
39	2h	135	CYS	2.5
44	1m	121	LYS	2.5
48	1q	87	LYS	2.5
51	2t	30	LYS	2.5
6	2G	133	LEU	2.5
33	2b	130	ARG	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	2c	119	ARG	2.5
34	2c	157	ILE	2.5
34	2c	56	ASP	2.5
6	2G	24	GLY	2.5
33	2b	91	PRO	2.5
28	26	48	VAL	2.5
35	2d	198	VAL	2.5
40	1i	14	VAL	2.5
44	2m	7	VAL	2.5
51	1t	18	GLN	2.5
12	2Q	58	PHE	2.5
50	2s	10	PHE	2.5
50	2s	6	LYS	2.4
40	1i	7	THR	2.4
1	1A	1069	A	2.4
32	2a	1363(A)	A	2.4
35	2d	49	ARG	2.4
16	2U	62	ILE	2.4
21	2Z	91	LEU	2.4
33	2b	208	ILE	2.4
34	2c	57	ILE	2.4
1	1A	2133	G	2.4
1	2A	2110	G	2.4
32	2a	953	G	2.4
32	2a	1233	G	2.4
33	2b	109	SER	2.4
54	1y	19	G	2.4
54	2w	10	G	2.4
54	2w	71	G	2.4
54	2y	6	G	2.4
47	2p	48	TRP	2.4
1	1A	2794	C	2.4
32	1a	1006	C	2.4
1	2A	2132	U	2.4
32	1a	1025	U	2.4
32	2a	950	U	2.4
32	2a	1150	U	2.4
21	2Z	95	PRO	2.4
34	2c	171	GLY	2.4
36	2e	114	GLY	2.4
39	2h	106	GLY	2.4
40	1i	8	GLY	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
21	1Z	100	VAL	2.4
34	2c	199	LYS	2.4
37	2f	90	VAL	2.4
38	2g	75	VAL	2.4
14	2S	29	PHE	2.4
21	2Z	136	PHE	2.4
44	2m	31	LYS	2.4
42	2k	60	ALA	2.4
35	1d	3	ARG	2.4
35	1d	153	ARG	2.4
36	2e	18	ARG	2.4
38	1g	41	ARG	2.4
41	2j	15	THR	2.4
52	2u	8	THR	2.4
7	2H	72	ILE	2.4
33	1b	200	ILE	2.4
34	1c	188	LEU	2.4
34	2c	91	LEU	2.4
34	2c	152	ILE	2.4
35	1d	21	LEU	2.4
39	2h	83	ILE	2.4
41	1j	76	ASN	2.4
43	2l	7	ILE	2.4
44	2m	48	LEU	2.4
49	2r	66	LEU	2.4
41	2j	56	HIS	2.4
48	1q	66	SER	2.4
1	1A	2114	A	2.4
1	1A	614(B)	G	2.4
2	2B	118	G	2.4
32	2a	947	G	2.4
32	2a	1048	G	2.4
32	2a	1057	G	2.4
32	2a	1283	G	2.4
33	1b	125	PRO	2.4
38	2g	112	PRO	2.4
1	1A	1076	C	2.4
1	1A	2146	C	2.4
2	2B	88	C	2.4
27	15	60	VAL	2.4
32	1a	1028	C	2.4
32	2a	980	C	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	2a	1069	C	2.4
33	1b	165	VAL	2.4
34	2c	141	VAL	2.4
35	1d	20	TYR	2.4
44	2m	117	VAL	2.4
54	2y	48	C	2.4
1	2A	2167	U	2.4
53	2v	17	U	2.4
21	2Z	131	ARG	2.4
38	2g	4	ARG	2.4
41	2j	46	ARG	2.4
45	2n	31	ARG	2.4
21	2Z	137	ILE	2.4
34	2c	191	THR	2.4
40	2i	79	LEU	2.4
7	2H	56	SER	2.4
21	2Z	168	GLU	2.4
26	24	51	ASP	2.4
41	2j	64	GLU	2.4
41	2j	73	ASP	2.4
45	2n	8	GLU	2.4
1	2A	2114	A	2.4
32	1a	1503	A	2.4
32	2a	1280	A	2.4
33	2b	234	PRO	2.4
34	2c	148	GLY	2.4
43	1l	63	GLY	2.4
50	2s	8	GLY	2.4
6	2G	15	VAL	2.4
46	2o	60	VAL	2.4
1	1A	1063	G	2.4
1	2A	2127	G	2.4
6	1G	80	PHE	2.4
14	2S	7	TYR	2.4
14	2S	66	ALA	2.4
32	2a	1127	G	2.4
38	2g	149	ARG	2.4
47	1p	81	ARG	2.4
28	26	11	LEU	2.4
38	2g	12	LEU	2.4
50	2s	48	THR	2.4
1	2A	277	C	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
6	1G	48	GLU	2.4
14	2S	8	GLU	2.4
23	11	75	GLU	2.4
33	2b	231	GLU	2.4
36	2e	81	GLU	2.4
42	1k	92	GLU	2.4
44	2m	73	GLU	2.4
34	1c	45	LYS	2.4
44	2m	120	LYS	2.4
50	2s	28	LYS	2.4
46	2o	89	GLY	2.4
3	2D	217	ARG	2.4
7	2H	76	VAL	2.4
16	2U	105	VAL	2.4
19	2X	68	ARG	2.4
24	22	7	ARG	2.4
40	1i	66	ARG	2.4
41	1j	43	ARG	2.4
1	1A	878	A	2.4
32	2a	969	A	2.4
32	2a	1044	A	2.4
47	1p	7	ALA	2.4
47	1p	80	PHE	2.4
6	2G	34	LEU	2.3
21	2Z	9	TYR	2.3
27	25	58	LEU	2.3
40	2i	92	TYR	2.3
44	1m	87	TYR	2.3
51	1t	13	LEU	2.3
33	2b	39	ILE	2.3
42	2k	32	ILE	2.3
50	2s	62	ILE	2.3
1	2A	882	G	2.3
1	2A	2109	U	2.3
1	2A	2802	G	2.3
32	2a	1030(C)	G	2.3
54	2w	5	G	2.3
16	2U	89	GLU	2.3
1	1A	898	C	2.3
1	2A	2143	C	2.3
1	2A	2896	C	2.3
3	1D	275	LYS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
17	2V	85	LYS	2.3
52	2u	20	LYS	2.3
28	26	42	TRP	2.3
38	2g	156	TRP	2.3
40	1i	90	PRO	2.3
50	2s	59	PRO	2.3
4	2E	6	GLY	2.3
40	2i	72	GLY	2.3
40	2i	66	ARG	2.3
45	2n	26	ARG	2.3
52	2u	24	ARG	2.3
43	1l	18	VAL	2.3
48	1q	23	VAL	2.3
49	1r	86	VAL	2.3
21	1Z	150	LEU	2.3
33	1b	29	ALA	2.3
33	2b	17	PHE	2.3
34	2c	50	ALA	2.3
34	2c	178	LEU	2.3
33	1b	201	ILE	2.3
35	1d	158	ILE	2.3
37	2f	52	ILE	2.3
51	2t	63	ILE	2.3
19	2X	18	TYR	2.3
34	2c	23	TYR	2.3
35	1d	4	TYR	2.3
42	2k	75	TYR	2.3
1	2A	2126	A	2.3
14	2S	5	THR	2.3
32	2a	1531	A	2.3
40	2i	103	THR	2.3
21	2Z	28	MET	2.3
34	2c	19	GLU	2.3
34	2c	161	GLU	2.3
37	2f	95	GLU	2.3
39	2h	9	MET	2.3
7	2H	62	LYS	2.3
32	2a	1000	U	2.3
41	2j	58	ASP	2.3
1	2A	1537	G	2.3
1	2A	2147	G	2.3
1	2A	2148	G	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	2168	G	2.3
7	2H	10	PRO	2.3
32	2a	976	G	2.3
32	2a	1309	G	2.3
39	2h	67	PRO	2.3
1	1A	2128	C	2.3
1	1A	2143	C	2.3
1	2A	2297	C	2.3
30	28	46	ARG	2.3
32	1a	1038	C	2.3
41	2j	84	GLN	2.3
44	2m	29	ARG	2.3
44	2m	91	ARG	2.3
14	2S	65	VAL	2.3
40	2i	65	VAL	2.3
43	2l	39	VAL	2.3
4	2E	28	ALA	2.3
6	1G	50	ALA	2.3
7	2H	33	LEU	2.3
23	21	46	LEU	2.3
40	2i	59	PHE	2.3
42	2k	19	ALA	2.3
50	1s	71	LEU	2.3
34	1c	84	ILE	2.3
41	1j	75	ILE	2.3
6	1G	146	TYR	2.3
21	2Z	69	THR	2.3
22	20	26	TYR	2.3
34	2c	193	TYR	2.3
39	2h	24	THR	2.3
40	2i	27	THR	2.3
50	2s	77	THR	2.3
12	2Q	103	MET	2.3
33	1b	126	GLU	2.3
41	2j	7	LYS	2.3
51	2t	27	LYS	2.3
1	1A	1096	A	2.3
32	2a	120	A	2.3
32	2a	1398	A	2.3
54	2w	36	A	2.3
54	2y	36	A	2.3
41	1j	30	SER	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	1c	38	ARG	2.3
38	1g	156	TRP	2.3
38	2g	78	ARG	2.3
40	1i	9	ARG	2.3
40	2i	83	ARG	2.3
44	2m	113	PRO	2.3
52	2u	6	ARG	2.3
12	2Q	24	GLY	2.3
34	2c	37	GLN	2.3
34	2c	78	GLY	2.3
41	1j	31	GLY	2.3
44	2m	68	GLY	2.3
50	2s	72	GLY	2.3
1	1A	895	U	2.3
1	1A	2109	U	2.3
7	2H	50	VAL	2.3
21	2Z	90	VAL	2.3
34	2c	116	VAL	2.3
35	1d	170	VAL	2.3
6	2G	102	PHE	2.3
39	1h	2	LEU	2.3
39	2h	2	LEU	2.3
40	2i	101	PHE	2.3
1	1A	1071	G	2.3
1	1A	2100	G	2.3
1	2A	2108	C	2.3
1	2A	2115	G	2.3
1	2A	2116	G	2.3
6	2G	39	ILE	2.3
36	2e	21	ALA	2.3
36	2e	54	ALA	2.3
40	2i	61	ALA	2.3
18	1W	111	HIS	2.3
32	2a	926	G	2.3
32	2a	1115	C	2.3
54	2w	24	G	2.3
54	2y	25	C	2.3
29	27	48	LYS	2.3
35	2d	184	LYS	2.3
6	2G	11	TYR	2.3
8	2I	48	GLU	2.3
51	1t	75	ASN	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
21	2Z	31	ARG	2.3
34	2c	131	ARG	2.3
40	2i	42	ARG	2.3
41	2j	5	ARG	2.3
41	2j	19	SER	2.3
50	2s	81	ARG	2.3
52	2u	15	ARG	2.3
1	1A	896	A	2.3
1	1A	1847	A	2.3
5	1F	208	GLY	2.3
22	20	13	GLY	2.3
32	1a	134	A	2.3
34	2c	155	GLY	2.3
35	2d	130	GLY	2.3
7	2H	17	VAL	2.3
8	2I	123	LEU	2.3
11	2P	105	LEU	2.3
21	2Z	105	VAL	2.3
34	2c	32	LEU	2.3
35	1d	105	VAL	2.3
39	2h	61	VAL	2.3
48	1q	35	VAL	2.3
21	1Z	136	PHE	2.3
1	2A	362	U	2.2
1	2A	614(A)	U	2.2
1	2A	1026	U	2.2
22	10	2	ALA	2.2
33	1b	172	ILE	2.2
33	2b	162	ILE	2.2
35	2d	32	ALA	2.2
41	1j	38	ILE	2.2
44	1m	4	ILE	2.2
45	2n	24	CYS	2.2
50	2s	75	ALA	2.2
51	2t	97	ALA	2.2
50	1s	14	HIS	2.2
36	2e	10	MET	2.2
45	2n	58	LYS	2.2
38	2g	24	THR	2.2
41	2j	48	THR	2.2
12	1Q	80	GLU	2.2
36	2e	60	TYR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	2137	C	2.2
32	2a	970	C	2.2
32	2a	1039	C	2.2
32	2a	1336	C	2.2
1	1A	2131	G	2.2
1	2A	2100	G	2.2
2	2B	23	G	2.2
32	2a	587	G	2.2
32	2a	823	G	2.2
32	2a	987	G	2.2
32	2a	1365	G	2.2
54	1w	24	G	2.2
6	2G	51	ARG	2.2
14	2S	97	ARG	2.2
33	2b	21	ARG	2.2
40	2i	111	ARG	2.2
46	1o	65	ARG	2.2
26	24	29	PRO	2.2
41	2j	21	GLN	2.2
21	2Z	147	GLY	2.2
33	2b	18	GLY	2.2
50	2s	46	GLY	2.2
31	29	25	VAL	2.2
33	1b	215	LEU	2.2
33	2b	158	LEU	2.2
35	2d	148	VAL	2.2
1	1A	1070	A	2.2
1	2A	2158	A	2.2
14	2S	93	LYS	2.2
32	2a	946	A	2.2
34	2c	163	ALA	2.2
40	2i	119	ALA	2.2
44	2m	28	ALA	2.2
53	2v	15	A	2.2
54	2w	73	A	2.2
42	2k	119	CYS	2.2
21	1Z	119	GLU	2.2
32	2a	1281	U	2.2
9	2N	115	ARG	2.2
37	2f	46	ARG	2.2
40	2i	120	ARG	2.2
46	2o	88	ARG	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
47	1p	75	ARG	2.2
49	1r	87	ARG	2.2
33	1b	234	PRO	2.2
40	2i	21	PRO	2.2
1	1A	2174	C	2.2
1	2A	2136	C	2.2
2	2B	5	C	2.2
32	1a	1008	C	2.2
32	2a	877	C	2.2
32	2a	1029	C	2.2
54	1w	75	C	2.2
31	29	12	ASP	2.2
40	2i	67	GLY	2.2
40	2i	69	GLY	2.2
50	2s	12	ASP	2.2
1	1A	275	G	2.2
1	2A	1171	G	2.2
8	2I	68	LEU	2.2
20	2Y	31	LEU	2.2
32	1a	230	G	2.2
32	2a	945	G	2.2
6	2G	29	TRP	2.2
14	2S	11	LYS	2.2
14	2S	33	LYS	2.2
14	2S	59	LYS	2.2
23	21	69	LYS	2.2
34	2c	173	VAL	2.2
36	2e	115	VAL	2.2
38	2g	141	VAL	2.2
43	2l	40	VAL	2.2
44	2m	53	VAL	2.2
6	1G	52	ILE	2.2
15	2T	1	MET	2.2
34	1c	14	ILE	2.2
43	2l	100	ILE	2.2
34	2c	121	ALA	2.2
36	2e	86	ALA	2.2
38	1g	83	ALA	2.2
40	2i	45	ALA	2.2
40	2i	122	ALA	2.2
41	2j	20	ALA	2.2
1	1A	1067	A	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	1077	A	2.2
2	2B	25	A	2.2
8	2I	86	THR	2.2
26	24	52	THR	2.2
32	1a	101	A	2.2
32	1a	160	A	2.2
32	2a	975	A	2.2
32	2a	1250	A	2.2
34	1c	15	THR	2.2
41	2j	97	GLU	2.2
54	2w	23	A	2.2
54	2y	23	A	2.2
6	2G	33	ARG	2.2
14	2S	13	ARG	2.2
32	2a	952	U	2.2
32	2a	957	U	2.2
32	2a	961	U	2.2
32	2a	1049	U	2.2
37	2f	87	ARG	2.2
48	1q	92	ARG	2.2
54	1w	20	U	2.2
37	2f	7	ASN	2.2
38	2g	37	ASN	2.2
7	2H	36	PRO	2.2
34	2c	7	PRO	2.2
48	1q	28	PRO	2.2
48	2q	47	PRO	2.2
6	2G	41	GLN	2.2
35	2d	45	GLN	2.2
46	2o	62	GLN	2.2
22	20	37	LEU	2.2
24	22	60	LEU	2.2
33	1b	44	LEU	2.2
33	2b	98	LEU	2.2
35	1d	120	LEU	2.2
35	1d	188	LEU	2.2
43	1l	60	LEU	2.2
50	2s	20	LEU	2.2
51	2t	10	LEU	2.2
51	2t	64	ASP	2.2
26	24	35	VAL	2.2
33	2b	15	VAL	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	2c	151	VAL	2.2
40	2i	86	VAL	2.2
1	2A	2294	C	2.2
22	20	45	PHE	2.2
32	2a	1018	C	2.2
32	2a	1189	C	2.2
32	2a	1209	C	2.2
43	1l	7	ILE	2.2
45	2n	36	PHE	2.2
20	2Y	16	ALA	2.2
33	2b	207	ALA	2.2
1	2A	2123	G	2.2
1	2A	2182	G	2.2
30	18	65	GLU	2.2
32	1a	1033	G	2.2
7	2H	106	THR	2.2
41	2j	92	THR	2.2
24	22	51	ARG	2.2
39	2h	92	ARG	2.2
40	1i	10	ARG	2.2
1	1A	1045	A	2.2
1	1A	1073	A	2.2
1	1A	1088	A	2.2
1	2A	2176	A	2.2
2	2B	26	A	2.2
21	2Z	34	ASN	2.2
32	2a	1229	A	2.2
38	2g	88	PRO	2.2
39	2h	15	ASN	2.2
39	2h	72	PRO	2.2
44	2m	23	TYR	2.2
54	2w	14	A	2.2
54	2w	35	A	2.2
1	2A	2172	U	2.2
6	2G	74	LYS	2.2
4	2E	10	GLY	2.2
7	2H	103	LEU	2.2
34	2c	197	GLY	2.2
35	2d	196	LEU	2.2
38	1g	81	GLY	2.2
40	2i	57	GLY	2.2
41	1j	8	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
48	1q	33	GLY	2.2
48	1q	74	LEU	2.2
50	1s	20	LEU	2.2
37	2f	89	MET	2.2
7	2H	35	VAL	2.2
7	2H	38	SER	2.2
8	2I	109	ILE	2.2
33	2b	81	VAL	2.2
35	1d	83	SER	2.2
34	2c	14	ILE	2.2
36	2e	69	VAL	2.2
40	1i	117	HIS	2.2
43	2l	55	VAL	2.2
21	2Z	89	PHE	2.2
34	2c	10	PHE	2.2
7	2H	102	ALA	2.1
44	2m	76	ALA	2.1
1	1A	1079	C	2.1
1	2A	888	C	2.1
1	2A	2139	C	2.1
7	2H	101	ARG	2.1
20	1Y	50	ARG	2.1
26	24	68	ARG	2.1
29	27	23	ARG	2.1
32	1a	163	C	2.1
32	1a	1029	C	2.1
32	1a	1030	C	2.1
41	2j	60	ARG	2.1
42	2k	31	THR	2.1
1	1A	1056	G	2.1
1	1A	2168	G	2.1
1	2A	2153	G	2.1
25	23	2	PRO	2.1
32	1a	1032	G	2.1
32	2a	630	G	2.1
54	1w	15	G	2.1
54	2w	65	G	2.1
16	2U	84	LYS	2.1
34	2c	135	LYS	2.1
34	2c	201	TYR	2.1
40	1i	78	LYS	2.1
7	2H	88	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
9	2N	112	LEU	2.1
37	1f	19	LEU	2.1
49	1r	79	LEU	2.1
7	2H	5	GLY	2.1
32	2a	964	A	2.1
32	2a	1004	A	2.1
34	2c	205	GLY	2.1
40	1i	39	GLY	2.1
54	1w	7	A	2.1
1	1A	2172	U	2.1
7	2H	79	VAL	2.1
24	22	52	ASP	2.1
26	14	51	ASP	2.1
18	2W	13	SER	2.1
33	2b	42	ILE	2.1
33	2b	136	VAL	2.1
33	2b	172	ILE	2.1
34	1c	66	VAL	2.1
45	2n	32	SER	2.1
46	2o	27	VAL	2.1
53	2v	22	U	2.1
34	2c	100	ALA	2.1
45	2n	30	ALA	2.1
46	2o	14	GLU	2.1
50	1s	27	GLU	2.1
5	1F	17	ARG	2.1
7	2H	6	ARG	2.1
12	2Q	6	ARG	2.1
35	2d	122	ARG	2.1
43	1l	19	ARG	2.1
44	1m	102	ARG	2.1
45	1n	29	ARG	2.1
46	2o	54	ARG	2.1
8	2I	134	PRO	2.1
33	1b	132	LYS	2.1
33	2b	167	PRO	2.1
39	2h	89	PRO	2.1
43	2l	47	LYS	2.1
1	1A	1052	C	2.1
1	1A	2136	C	2.1
1	1A	2140	C	2.1
32	2a	1109	C	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	2a	1277	C	2.1
32	2a	1314	C	2.1
42	2k	13	GLN	2.1
33	1b	187	LEU	2.1
33	2b	101	MET	2.1
33	2b	154	LEU	2.1
35	1d	19	LEU	2.1
40	2i	50	LEU	2.1
42	2k	117	ASN	2.1
48	1q	51	TYR	2.1
48	1q	98	LEU	2.1
43	2l	103	GLY	2.1
52	2u	4	GLY	2.1
41	2j	62	HIS	2.1
1	2A	859	G	2.1
14	2S	14	VAL	2.1
32	1a	112	G	2.1
32	2a	1184	G	2.1
32	2a	1491	G	2.1
36	2e	90	VAL	2.1
40	1i	75	ASP	2.1
40	1i	91	ASP	2.1
48	1q	9	VAL	2.1
37	2f	93	SER	2.1
1	2A	528	A	2.1
1	2A	2122	U	2.1
32	1a	374	A	2.1
32	1a	608	A	2.1
32	2a	414	A	2.1
7	2H	34	GLU	2.1
32	2a	982	U	2.1
36	1e	134	ALA	2.1
40	2i	84	ALA	2.1
43	2l	51	ALA	2.1
46	2o	80	ALA	2.1
54	2y	35	A	2.1
50	2s	73	GLU	2.1
35	1d	118	ARG	2.1
38	2g	79	ARG	2.1
51	2t	25	ARG	2.1
21	1Z	156	LYS	2.1
50	2s	18	LYS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	2H	173	PRO	2.1
21	2Z	25	PRO	2.1
25	13	2	PRO	2.1
40	2i	3	GLN	2.1
34	2c	34	LEU	2.1
37	2f	98	LEU	2.1
39	2h	39	LEU	2.1
47	2p	6	LEU	2.1
48	2q	76	LEU	2.1
8	1I	106	GLY	2.1
19	1X	94	GLY	2.1
19	2X	69	TYR	2.1
21	2Z	99	TYR	2.1
33	1b	16	HIS	2.1
34	1c	185	GLY	2.1
40	2i	88	TYR	2.1
41	1j	36	GLY	2.1
42	2k	86	GLY	2.1
1	1A	897	C	2.1
1	1A	1075	C	2.1
1	2A	897	C	2.1
1	2A	2138	C	2.1
7	1H	92	ILE	2.1
32	2a	931	C	2.1
34	1c	55	VAL	2.1
40	2i	109	VAL	2.1
41	2j	24	VAL	2.1
48	2q	90	ILE	2.1
54	2w	11	C	2.1
38	1g	26	PHE	2.1
40	1i	105	ASP	2.1
14	2S	55	ALA	2.1
21	2Z	103	ARG	2.1
24	22	66	GLU	2.1
29	27	47	ARG	2.1
33	1b	9	GLU	2.1
33	2b	34	ALA	2.1
33	2b	129	GLU	2.1
36	1e	81	GLU	2.1
36	2e	27	ARG	2.1
40	2i	55	ALA	2.1
45	1n	5	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	2B	75	G	2.1
32	1a	111	G	2.1
32	2a	1305	G	2.1
42	2k	42	TRP	2.1
37	2f	54	LYS	2.1
40	1i	113	LYS	2.1
43	1l	46	LYS	2.1
43	1l	126	LYS	2.1
48	1q	14	LYS	2.1
54	2w	28	G	2.1
1	2A	271(L)	U	2.1
32	1a	149	A	2.1
32	2a	997	U	2.1
32	2a	1015	A	2.1
32	2a	1252	A	2.1
36	2e	16	THR	2.1
54	2y	47	U	2.1
33	2b	83	MET	2.1
9	2N	69	GLN	2.1
34	2c	118	GLN	2.1
34	2c	162	GLN	2.1
8	2I	35	LEU	2.1
14	2S	80	LEU	2.1
34	1c	52	LEU	2.1
46	2o	31	LEU	2.1
4	2E	121	ASN	2.1
47	1p	14	ASN	2.1
14	2S	90	GLY	2.1
14	2S	36	TYR	2.1
33	2b	33	TYR	2.1
37	2f	63	TYR	2.1
40	2i	63	ILE	2.1
41	1j	4	ILE	2.1
47	1p	38	TYR	2.1
48	1q	95	TYR	2.1
21	2Z	56	VAL	2.1
34	1c	99	VAL	2.1
45	2n	18	VAL	2.1
6	2G	23	PHE	2.1
6	1G	59	GLU	2.0
7	1H	3	ARG	2.0
38	2g	5	ARG	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
40	1i	42	ARG	2.0
42	2k	36	ASP	2.0
44	2m	94	ARG	2.0
50	2s	29	ARG	2.0
21	2Z	142	SER	2.0
34	2c	92	ALA	2.0
38	2g	2	ALA	2.0
45	2n	20	ALA	2.0
1	1A	2142	C	2.0
1	2A	2803	C	2.0
32	2a	1037	C	2.0
32	2a	1362	C	2.0
33	2b	22	LYS	2.0
45	2n	11	LYS	2.0
54	2w	67	C	2.0
47	1p	69	THR	2.0
39	1h	72	PRO	2.0
1	1A	2189	U	2.0
6	2G	53	LEU	2.0
14	2S	101	LEU	2.0
21	2Z	76	LEU	2.0
32	2a	1313	U	2.0
32	2a	1358	U	2.0
33	1b	154	LEU	2.0
33	2b	44	LEU	2.0
34	1c	107	GLN	2.0
34	2c	175	LEU	2.0
35	1d	101	LEU	2.0
35	2d	155	LEU	2.0
47	1p	49	LEU	2.0
50	2s	30	LEU	2.0
1	1A	1177	A	2.0
1	2A	614(B)	G	2.0
1	2A	1125	G	2.0
1	2A	2320	A	2.0
1	2A	2805	G	2.0
32	1a	1166	G	2.0
32	2a	994	A	2.0
32	2a	1356	G	2.0
20	2Y	92	ASN	2.0
44	2m	92	HIS	2.0
14	2S	96	GLY	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	2c	80	GLY	2.0
41	1j	52	GLY	2.0
41	2j	31	GLY	2.0
44	1m	39	ILE	2.0
46	2o	87	ILE	2.0
21	2Z	27	VAL	2.0
26	24	32	TYR	2.0
33	2b	93	VAL	2.0
36	2e	82	VAL	2.0
44	2m	87	TYR	2.0
12	2Q	16	ARG	2.0
34	2c	59	ARG	2.0
39	2h	30	ARG	2.0
42	2k	54	ARG	2.0
44	2m	3	ARG	2.0
48	2q	27	PHE	2.0
33	1b	207	ALA	2.0
38	2g	40	ALA	2.0
40	1i	70	LYS	2.0
45	1n	59	ALA	2.0
45	2n	5	ALA	2.0
49	1r	73	ALA	2.0
22	20	9	SER	2.0
33	2b	48	MET	2.0
4	2E	56	PRO	2.0
7	2H	8	PRO	2.0
8	1I	108	THR	2.0
9	2N	48	MET	2.0
36	1e	120	THR	2.0
41	1j	86	MET	2.0
20	2Y	53	PRO	2.0
33	1b	232	PRO	2.0
41	1j	39	PRO	2.0
41	2j	53	PRO	2.0
41	2j	67	THR	2.0
45	2n	14	PRO	2.0
47	1p	41	PRO	2.0
14	2S	73	LEU	2.0
21	2Z	155	LEU	2.0
32	2a	1218	C	2.0
38	1g	38	LEU	2.0
43	2l	84	LEU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
54	2w	72	C	2.0
14	2S	95	HIS	2.0
32	1a	204	U	2.0
32	1a	841	U	2.0
32	2a	1257	U	2.0
5	2F	16	GLY	2.0
12	2Q	23	GLY	2.0
15	2T	104	ASN	2.0
54	1w	47	U	2.0
23	21	28	GLY	2.0
30	28	16	ILE	2.0
35	1d	16	GLY	2.0
40	1i	69	GLY	2.0
40	1i	72	GLY	2.0
42	2k	48	ILE	2.0
42	2k	49	GLY	2.0
44	2m	112	GLY	2.0
50	2s	68	GLY	2.0
1	1A	229	A	2.0
1	1A	2170	A	2.0
1	2A	901	A	2.0
7	2H	49	VAL	2.0
14	2S	28	VAL	2.0
28	26	5	VAL	2.0
35	1d	139	ARG	2.0
43	2l	11	VAL	2.0
55	1x	76	A	2.0
4	2E	151	TYR	2.0
7	2H	157	TYR	2.0
48	1q	88	TYR	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	7MG	2w	46	24/25	0.51	0.16	80,93,101,121	0
54	7MG	1w	46	24/25	0.58	0.16	77,89,99,107	0
54	4SU	2w	8	20/21	0.60	0.15	83,93,104,117	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
54	7MG	2y	46	24/25	0.60	0.17	86,95,102,123	0
54	PSU	2w	55	20/21	0.67	0.13	81,91,96,98	0
54	PSU	2y	55	20/21	0.67	0.18	90,96,107,107	0
54	4SU	2y	8	20/21	0.69	0.13	88,93,99,104	0
54	7MG	1y	46	24/25	0.69	0.14	79,90,98,101	0
54	MIA	2y	37	22/30	0.72	0.14	75,87,99,109	0
54	5MU	2y	54	21/22	0.72	0.15	84,91,99,112	0
54	5MU	1y	54	21/22	0.73	0.13	79,85,91,97	0
54	PSU	2y	32	20/21	0.75	0.14	79,85,93,102	0
54	4SU	1w	8	20/21	0.75	0.14	80,85,93,94	0
54	4SU	1y	8	20/21	0.79	0.12	81,89,98,99	0
54	PSU	1y	55	20/21	0.79	0.12	80,89,98,103	0
32	2MG	2a	1207	24/25	0.80	0.14	63,83,92,95	0
1	5MU	2A	1915	21/22	0.80	0.16	74,78,84,94	0
54	PSU	2w	39	20/21	0.81	0.14	81,86,88,92	0
54	MIA	2w	37	25/30	0.81	0.17	75,82,88,103	0
54	PSU	1y	32	20/21	0.81	0.12	78,82,87,88	0
54	5MU	2w	54	21/22	0.81	0.11	67,82,87,93	0
54	PSU	1w	55	20/21	0.82	0.11	74,83,92,95	0
54	PSU	2y	39	20/21	0.82	0.13	79,84,92,96	0
55	4SU	2x	8	20/21	0.83	0.14	73,79,87,90	0
55	PSU	2x	55	20/21	0.83	0.11	72,80,82,85	0
55	5MU	2x	54	21/22	0.84	0.12	68,77,82,94	0
32	PSU	2a	516	20/21	0.86	0.12	70,77,83,85	0
1	PSU	2A	1917	20/21	0.86	0.12	62,71,81,87	0
54	MIA	1y	37	22/30	0.86	0.11	74,78,84,85	0
32	M2G	2a	966	25/26	0.87	0.20	60,69,84,86	0
54	PSU	1y	39	20/21	0.87	0.09	74,76,80,80	0
43	0TD	2l	92	10/11	0.87	0.14	67,71,72,79	0
55	5MU	1x	54	21/22	0.88	0.11	51,64,70,76	0
54	PSU	2w	32	20/21	0.89	0.13	78,85,93,97	0
54	PSU	1w	32	20/21	0.89	0.13	65,76,82,84	0
54	MIA	1w	37	29/30	0.89	0.16	56,65,72,74	0
1	4OC	2A	1920	21/23	0.90	0.13	61,65,67,71	0
43	0TD	1l	92	10/11	0.90	0.12	47,55,60,75	0
1	PSU	2A	1911	20/21	0.90	0.11	60,66,73,75	0
32	5MC	2a	967	21/22	0.90	0.16	61,70,78,82	0
55	4SU	1x	8	20/21	0.92	0.11	51,59,65,71	0
54	5MU	1w	54	21/22	0.92	0.09	64,72,79,82	0
55	5MC	2x	32	21/22	0.92	0.13	60,73,78,82	0
32	5MC	2a	1400	21/22	0.92	0.16	60,69,76,83	0
54	PSU	1w	39	20/21	0.92	0.11	67,74,85,85	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
55	PSU	1x	55	20/21	0.92	0.10	49,63,70,73	0
32	5MC	2a	1404	21/22	0.92	0.13	56,60,65,68	0
1	5MU	1A	1915	21/22	0.93	0.10	56,61,68,71	0
55	5MC	1x	32	21/22	0.93	0.13	46,54,60,74	0
32	4OC	2a	1402	22/23	0.93	0.13	53,65,69,70	0
32	PSU	1a	516	20/21	0.93	0.10	60,66,71,71	0
32	UR3	2a	1498	21/22	0.93	0.13	55,61,65,66	0
32	MA6	2a	1518	24/25	0.93	0.12	55,65,68,71	0
32	7MG	2a	527	24/25	0.93	0.12	63,66,72,76	0
32	MA6	2a	1519	24/25	0.94	0.12	52,63,67,69	0
32	2MG	1a	1207	24/25	0.94	0.10	59,67,73,75	0
32	5MC	1a	967	21/22	0.94	0.11	52,59,63,64	0
1	PSU	1A	1917	20/21	0.94	0.10	48,57,62,63	0
1	5MC	2A	1962	21/22	0.95	0.10	40,52,59,68	0
1	2MA	2A	2503	23/24	0.95	0.11	32,36,43,45	0
32	5MC	2a	1407	21/22	0.95	0.13	53,59,63,64	0
1	5MU	2A	1939	21/22	0.95	0.11	36,44,49,51	0
1	5MC	2A	1942	21/22	0.95	0.10	54,60,66,68	0
32	5MC	1a	1404	21/22	0.96	0.08	35,41,44,44	0
32	5MC	1a	1407	21/22	0.96	0.09	36,41,43,45	0
32	MA6	1a	1519	24/25	0.96	0.10	38,42,47,50	0
1	PSU	1A	1911	20/21	0.96	0.09	40,49,57,57	0
32	7MG	1a	527	24/25	0.96	0.09	42,49,57,58	0
1	OMG	2A	2251	24/25	0.96	0.09	42,45,51,56	0
1	5MC	1A	1942	21/22	0.96	0.09	31,40,43,49	0
1	2MU	2A	2552	21/23	0.96	0.09	35,42,46,62	0
32	M2G	1a	966	25/26	0.96	0.09	49,55,59,66	0
32	5MC	1a	1400	21/22	0.96	0.09	39,50,54,59	0
32	4OC	1a	1402	22/23	0.96	0.09	37,45,51,57	0
32	MA6	1a	1518	24/25	0.97	0.08	34,41,45,49	0
1	5MC	1A	1962	21/22	0.97	0.07	29,36,41,44	0
1	2MU	1A	2552	21/23	0.97	0.08	21,29,33,39	0
1	PSU	2A	2605	20/21	0.97	0.07	34,42,47,47	0
1	4OC	1A	1920	21/23	0.97	0.07	37,44,48,53	0
1	2MA	1A	2503	23/24	0.98	0.06	14,21,24,31	0
32	UR3	1a	1498	21/22	0.98	0.07	39,43,46,48	0
1	5MU	1A	1939	21/22	0.98	0.06	23,29,33,40	0
1	PSU	1A	2605	20/21	0.98	0.07	19,26,35,35	0
1	OMG	1A	2251	24/25	0.98	0.06	19,25,28,29	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3982	1/1	0.54	0.32	77,77,77,77	0
56	MG	1P	206	1/1	0.57	0.20	62,62,62,62	0
56	MG	2a	3225	1/1	0.57	0.40	73,73,73,73	0
56	MG	2A	3698	1/1	0.63	0.16	56,56,56,56	0
56	MG	2A	3762	1/1	0.64	0.20	59,59,59,59	0
56	MG	2A	3650	1/1	0.66	0.18	67,67,67,67	0
56	MG	2a	3199	1/1	0.66	0.27	70,70,70,70	0
56	MG	1A	3402	1/1	0.66	0.16	85,85,85,85	0
56	MG	1a	1784	1/1	0.67	0.21	56,56,56,56	0
56	MG	2a	3227	1/1	0.67	0.16	78,78,78,78	0
56	MG	2a	3209	1/1	0.68	0.31	73,73,73,73	0
56	MG	2A	3516	1/1	0.68	0.26	74,74,74,74	0
56	MG	2A	3636	1/1	0.68	0.28	55,55,55,55	0
56	MG	1A	3771	1/1	0.69	0.13	19,19,19,19	0
56	MG	1A	4083	1/1	0.70	0.14	51,51,51,51	0
56	MG	1a	1755	1/1	0.70	0.21	88,88,88,88	0
56	MG	2A	3687	1/1	0.70	0.17	71,71,71,71	0
56	MG	2a	3239	1/1	0.70	0.24	66,66,66,66	0
56	MG	2A	3817	1/1	0.71	0.21	75,75,75,75	0
56	MG	2B	216	1/1	0.71	0.17	65,65,65,65	0
56	MG	2a	3193	1/1	0.71	0.40	82,82,82,82	0
56	MG	2A	3405	1/1	0.71	0.28	64,64,64,64	0
56	MG	2A	3048	1/1	0.72	0.16	65,65,65,65	0
56	MG	2A	3809	1/1	0.72	0.21	60,60,60,60	0
56	MG	2A	3674	1/1	0.72	0.20	63,63,63,63	0
56	MG	2A	3620	1/1	0.72	0.15	64,64,64,64	0
56	MG	1a	1790	1/1	0.72	0.14	74,74,74,74	0
56	MG	2A	3678	1/1	0.73	0.28	76,76,76,76	0
56	MG	1a	1772	1/1	0.73	0.31	60,60,60,60	0
56	MG	1A	3800	1/1	0.73	0.12	60,60,60,60	0
56	MG	2A	3731	1/1	0.73	0.25	60,60,60,60	0
56	MG	2a	3031	1/1	0.73	0.23	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
56	MG	2a	3107	1/1	0.73	0.39	74,74,74,74	0
56	MG	2v	101	1/1	0.73	0.25	78,78,78,78	0
56	MG	2A	3688	1/1	0.74	0.23	57,57,57,57	0
56	MG	1x	111	1/1	0.74	0.27	71,71,71,71	0
56	MG	2a	3003	1/1	0.74	0.21	63,63,63,63	0
56	MG	1A	3341	1/1	0.74	0.18	50,50,50,50	0
56	MG	2A	3285	1/1	0.74	0.14	62,62,62,62	0
56	MG	2A	3334	1/1	0.74	0.19	74,74,74,74	0
56	MG	2A	3773	1/1	0.75	0.13	73,73,73,73	0
56	MG	2A	3396	1/1	0.75	0.20	63,63,63,63	0
56	MG	2A	3709	1/1	0.75	0.17	48,48,48,48	0
56	MG	2A	3712	1/1	0.75	0.20	70,70,70,70	0
56	MG	2A	3713	1/1	0.75	0.17	48,48,48,48	0
56	MG	2A	3040	1/1	0.75	0.26	88,88,88,88	0
56	MG	2j	201	1/1	0.75	0.20	76,76,76,76	0
56	MG	2A	3623	1/1	0.75	0.19	60,60,60,60	0
56	MG	2A	3069	1/1	0.76	0.15	54,54,54,54	0
56	MG	1A	4006	1/1	0.76	0.15	29,29,29,29	0
56	MG	2A	3665	1/1	0.76	0.12	61,61,61,61	0
56	MG	1a	1655	1/1	0.76	0.23	76,76,76,76	0
56	MG	2a	3070	1/1	0.76	0.21	68,68,68,68	0
56	MG	2A	3796	1/1	0.76	0.16	77,77,77,77	0
56	MG	1w	104	1/1	0.76	0.23	72,72,72,72	0
56	MG	2A	3602	1/1	0.77	0.20	55,55,55,55	0
56	MG	1A	3667	1/1	0.77	0.14	28,28,28,28	0
56	MG	2A	3333	1/1	0.77	0.15	65,65,65,65	0
56	MG	1A	3852	1/1	0.77	0.21	39,39,39,39	0
56	MG	2A	3828	1/1	0.77	0.14	59,59,59,59	0
56	MG	1A	3930	1/1	0.77	0.13	30,30,30,30	0
56	MG	1A	3425	1/1	0.77	0.20	60,60,60,60	0
56	MG	1s	101	1/1	0.77	0.17	71,71,71,71	0
56	MG	2A	3585	1/1	0.77	0.18	77,77,77,77	0
56	MG	1A	3968	1/1	0.78	0.26	43,43,43,43	0
56	MG	1A	3979	1/1	0.78	0.15	69,69,69,69	0
56	MG	2a	3053	1/1	0.78	0.31	70,70,70,70	0
56	MG	2a	3057	1/1	0.78	0.19	65,65,65,65	0
56	MG	18	105	1/1	0.78	0.23	45,45,45,45	0
56	MG	2A	3715	1/1	0.78	0.21	68,68,68,68	0
56	MG	1A	3801	1/1	0.78	0.11	53,53,53,53	0
56	MG	2a	3196	1/1	0.78	0.20	76,76,76,76	0
56	MG	2A	3350	1/1	0.78	0.31	68,68,68,68	0
56	MG	1a	1700	1/1	0.78	0.23	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
56	MG	1x	117	1/1	0.78	0.12	71,71,71,71	0
56	MG	2A	3452	1/1	0.78	0.37	70,70,70,70	0
56	MG	1A	3948	1/1	0.78	0.14	36,36,36,36	0
56	MG	2A	3532	1/1	0.78	0.27	61,61,61,61	0
56	MG	1A	4043	1/1	0.78	0.20	66,66,66,66	0
56	MG	2A	3171	1/1	0.79	0.32	74,74,74,74	0
56	MG	2a	3036	1/1	0.79	0.24	72,72,72,72	0
56	MG	2A	3661	1/1	0.79	0.15	59,59,59,59	0
56	MG	1A	3626	1/1	0.79	0.15	47,47,47,47	0
56	MG	2A	3750	1/1	0.79	0.16	55,55,55,55	0
56	MG	2A	3671	1/1	0.79	0.13	59,59,59,59	0
56	MG	2a	3170	1/1	0.79	0.14	73,73,73,73	0
56	MG	1a	1693	1/1	0.79	0.28	69,69,69,69	0
56	MG	2A	3543	1/1	0.79	0.13	45,45,45,45	0
56	MG	1A	3791	1/1	0.79	0.20	63,63,63,63	0
56	MG	1a	1739	1/1	0.79	0.14	77,77,77,77	0
56	MG	2A	3823	1/1	0.79	0.11	50,50,50,50	0
56	MG	1A	4060	1/1	0.79	0.27	52,52,52,52	0
56	MG	2A	3402	1/1	0.79	0.15	65,65,65,65	0
56	MG	2G	201	1/1	0.79	0.19	65,65,65,65	0
56	MG	2A	3088	1/1	0.79	0.30	78,78,78,78	0
56	MG	2B	220	1/1	0.80	0.20	65,65,65,65	0
56	MG	1a	1767	1/1	0.80	0.20	67,67,67,67	0
56	MG	14	101	1/1	0.80	0.16	69,69,69,69	0
56	MG	1A	3661	1/1	0.80	0.12	29,29,29,29	0
56	MG	2A	3736	1/1	0.80	0.11	57,57,57,57	0
56	MG	2a	3049	1/1	0.80	0.29	64,64,64,64	0
56	MG	1a	1642	1/1	0.80	0.13	57,57,57,57	0
56	MG	2A	3754	1/1	0.80	0.21	67,67,67,67	0
56	MG	2a	3064	1/1	0.80	0.15	64,64,64,64	0
56	MG	2a	3068	1/1	0.80	0.14	74,74,74,74	0
56	MG	1A	4032	1/1	0.80	0.20	57,57,57,57	0
56	MG	1A	4058	1/1	0.81	0.14	28,28,28,28	0
56	MG	2A	3595	1/1	0.81	0.22	65,65,65,65	0
56	MG	2A	3152	1/1	0.81	0.20	71,71,71,71	0
56	MG	1A	3699	1/1	0.81	0.13	37,37,37,37	0
56	MG	2A	3734	1/1	0.81	0.09	52,52,52,52	0
56	MG	2A	3261	1/1	0.81	0.14	59,59,59,59	0
56	MG	2a	3060	1/1	0.81	0.10	71,71,71,71	0
56	MG	1A	4067	1/1	0.81	0.14	55,55,55,55	0
56	MG	1A	3767	1/1	0.81	0.12	30,30,30,30	0
56	MG	1A	3061	1/1	0.81	0.20	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
56	MG	1A	3103	1/1	0.81	0.17	60,60,60,60	0
56	MG	1A	3317	1/1	0.81	0.28	65,65,65,65	0
56	MG	2A	3804	1/1	0.81	0.14	53,53,53,53	0
56	MG	1A	4000	1/1	0.81	0.18	62,62,62,62	0
56	MG	2A	3676	1/1	0.81	0.13	61,61,61,61	0
56	MG	2A	3819	1/1	0.81	0.19	69,69,69,69	0
56	MG	1A	3693	1/1	0.81	0.20	42,42,42,42	0
56	MG	1A	3808	1/1	0.81	0.25	65,65,65,65	0
56	MG	1A	3697	1/1	0.81	0.15	38,38,38,38	0
56	MG	1a	1721	1/1	0.81	0.34	54,54,54,54	0
56	MG	1a	1731	1/1	0.81	0.40	69,69,69,69	0
56	MG	1A	3263	1/1	0.82	0.22	64,64,64,64	0
56	MG	2D	309	1/1	0.82	0.15	35,35,35,35	0
56	MG	1a	1606	1/1	0.82	0.24	71,71,71,71	0
56	MG	2Q	204	1/1	0.82	0.18	62,62,62,62	0
56	MG	2A	3094	1/1	0.82	0.12	62,62,62,62	0
56	MG	2a	3027	1/1	0.82	0.21	70,70,70,70	0
56	MG	1A	3991	1/1	0.82	0.10	22,22,22,22	0
56	MG	1A	3498	1/1	0.82	0.29	59,59,59,59	0
56	MG	2A	3198	1/1	0.82	0.34	68,68,68,68	0
56	MG	2A	3228	1/1	0.82	0.16	72,72,72,72	0
56	MG	2A	3247	1/1	0.82	0.23	70,70,70,70	0
56	MG	2A	3748	1/1	0.82	0.19	68,68,68,68	0
56	MG	1a	1659	1/1	0.82	0.18	55,55,55,55	0
56	MG	2A	3637	1/1	0.82	0.16	47,47,47,47	0
56	MG	2A	3759	1/1	0.82	0.16	62,62,62,62	0
56	MG	2a	3100	1/1	0.82	0.20	77,77,77,77	0
56	MG	2A	3640	1/1	0.82	0.11	64,64,64,64	0
56	MG	1b	302	1/1	0.82	0.20	71,71,71,71	0
56	MG	2A	3315	1/1	0.82	0.16	62,62,62,62	0
56	MG	1A	3551	1/1	0.82	0.18	50,50,50,50	0
56	MG	2A	3805	1/1	0.82	0.10	67,67,67,67	0
56	MG	1w	102	1/1	0.82	0.09	75,75,75,75	0
56	MG	1A	4100	1/1	0.82	0.19	85,85,85,85	0
56	MG	1B	237	1/1	0.82	0.16	68,68,68,68	0
56	MG	2a	3233	1/1	0.82	0.21	67,67,67,67	0
56	MG	1A	3605	1/1	0.82	0.12	37,37,37,37	0
56	MG	2a	3240	1/1	0.82	0.17	67,67,67,67	0
56	MG	1A	3845	1/1	0.82	0.23	57,57,57,57	0
56	MG	1a	1753	1/1	0.82	0.17	53,53,53,53	0
56	MG	2w	102	1/1	0.82	0.20	72,72,72,72	0
56	MG	1A	3686	1/1	0.83	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
56	MG	1a	1779	1/1	0.83	0.12	88,88,88,88	0
56	MG	2A	3493	1/1	0.83	0.11	61,61,61,61	0
56	MG	1A	3532	1/1	0.83	0.20	52,52,52,52	0
56	MG	1a	1666	1/1	0.83	0.22	63,63,63,63	0
56	MG	2a	3017	1/1	0.83	0.21	71,71,71,71	0
56	MG	2a	3021	1/1	0.83	0.23	69,69,69,69	0
56	MG	2a	3023	1/1	0.83	0.24	76,76,76,76	0
56	MG	2A	3173	1/1	0.83	0.21	72,72,72,72	0
56	MG	2A	3729	1/1	0.83	0.20	68,68,68,68	0
56	MG	1a	1800	1/1	0.83	0.11	50,50,50,50	0
56	MG	2a	3041	1/1	0.83	0.28	66,66,66,66	0
56	MG	2a	3046	1/1	0.83	0.24	66,66,66,66	0
56	MG	2A	3214	1/1	0.83	0.13	62,62,62,62	0
56	MG	2A	3599	1/1	0.83	0.23	68,68,68,68	0
56	MG	2a	3054	1/1	0.83	0.19	71,71,71,71	0
56	MG	2A	3739	1/1	0.83	0.20	59,59,59,59	0
56	MG	1a	1692	1/1	0.83	0.23	70,70,70,70	0
56	MG	2A	3609	1/1	0.83	0.12	29,29,29,29	0
56	MG	1E	313	1/1	0.83	0.15	54,54,54,54	0
56	MG	1A	3838	1/1	0.83	0.22	60,60,60,60	0
56	MG	2a	3077	1/1	0.83	0.22	59,59,59,59	0
56	MG	1S	201	1/1	0.83	0.26	40,40,40,40	0
56	MG	2a	3101	1/1	0.83	0.27	68,68,68,68	0
56	MG	2A	3302	1/1	0.83	0.19	61,61,61,61	0
56	MG	2A	3310	1/1	0.83	0.28	65,65,65,65	0
56	MG	2a	3173	1/1	0.83	0.17	70,70,70,70	0
56	MG	2a	3174	1/1	0.83	0.14	75,75,75,75	0
56	MG	1x	110	1/1	0.83	0.28	61,61,61,61	0
56	MG	1A	3459	1/1	0.83	0.13	49,49,49,49	0
56	MG	2a	3197	1/1	0.83	0.14	73,73,73,73	0
56	MG	1A	3306	1/1	0.83	0.17	41,41,41,41	0
56	MG	2A	3816	1/1	0.83	0.18	68,68,68,68	0
56	MG	2A	3339	1/1	0.83	0.17	64,64,64,64	0
56	MG	1A	3876	1/1	0.83	0.16	34,34,34,34	0
56	MG	2A	3391	1/1	0.83	0.13	68,68,68,68	0
56	MG	2a	3238	1/1	0.83	0.18	72,72,72,72	0
56	MG	1A	3897	1/1	0.83	0.19	56,56,56,56	0
56	MG	2A	3830	1/1	0.83	0.11	77,77,77,77	0
56	MG	2d	301	1/1	0.83	0.13	65,65,65,65	0
56	MG	2A	3869	1/1	0.83	0.13	45,45,45,45	0
56	MG	1a	1654	1/1	0.83	0.25	71,71,71,71	0
56	MG	2B	218	1/1	0.83	0.22	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3224	1/1	0.84	0.14	45,45,45,45	0
56	MG	1a	1609	1/1	0.84	0.17	65,65,65,65	0
56	MG	1a	1611	1/1	0.84	0.13	68,68,68,68	0
56	MG	1B	233	1/1	0.84	0.13	63,63,63,63	0
56	MG	2A	3257	1/1	0.84	0.17	62,62,62,62	0
56	MG	2A	3538	1/1	0.84	0.10	38,38,38,38	0
56	MG	2A	3702	1/1	0.84	0.13	31,31,31,31	0
56	MG	2a	3092	1/1	0.84	0.18	77,77,77,77	0
56	MG	1A	3195	1/1	0.84	0.10	55,55,55,55	0
56	MG	2A	3570	1/1	0.84	0.13	48,48,48,48	0
56	MG	2A	3873	1/1	0.84	0.17	75,75,75,75	0
56	MG	2a	3162	1/1	0.84	0.10	82,82,82,82	0
56	MG	2a	3163	1/1	0.84	0.14	68,68,68,68	0
56	MG	2A	3027	1/1	0.84	0.17	71,71,71,71	0
56	MG	2A	3297	1/1	0.84	0.29	72,72,72,72	0
56	MG	2A	3029	1/1	0.84	0.28	62,62,62,62	0
56	MG	2a	3178	1/1	0.84	0.12	91,91,91,91	0
56	MG	1A	3411	1/1	0.84	0.20	57,57,57,57	0
56	MG	1A	3329	1/1	0.84	0.17	51,51,51,51	0
56	MG	2A	3612	1/1	0.84	0.11	41,41,41,41	0
56	MG	1A	3689	1/1	0.84	0.14	26,26,26,26	0
56	MG	2a	3201	1/1	0.84	0.16	60,60,60,60	0
56	MG	1Y	202	1/1	0.84	0.09	68,68,68,68	0
56	MG	2a	3220	1/1	0.84	0.15	63,63,63,63	0
56	MG	2a	3020	1/1	0.84	0.27	71,71,71,71	0
56	MG	1A	3797	1/1	0.84	0.14	27,27,27,27	0
56	MG	2A	3120	1/1	0.84	0.14	62,62,62,62	0
56	MG	2A	3757	1/1	0.84	0.15	66,66,66,66	0
56	MG	2A	3352	1/1	0.84	0.26	72,72,72,72	0
56	MG	2A	3368	1/1	0.84	0.16	65,65,65,65	0
56	MG	2A	3770	1/1	0.84	0.12	54,54,54,54	0
56	MG	1A	3458	1/1	0.84	0.22	62,62,62,62	0
56	MG	2l	203	1/1	0.84	0.21	61,61,61,61	0
56	MG	1e	201	1/1	0.84	0.10	73,73,73,73	0
56	MG	1a	1604	1/1	0.84	0.11	55,55,55,55	0
56	MG	2x	105	1/1	0.84	0.20	67,67,67,67	0
56	MG	2A	3191	1/1	0.85	0.18	70,70,70,70	0
56	MG	2A	3353	1/1	0.85	0.10	71,71,71,71	0
56	MG	2A	3624	1/1	0.85	0.17	40,40,40,40	0
56	MG	2A	3364	1/1	0.85	0.33	66,66,66,66	0
56	MG	1A	3665	1/1	0.85	0.09	30,30,30,30	0
56	MG	2A	3210	1/1	0.85	0.12	61,61,61,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1a	1818	1/1	0.85	0.11	71,71,71,71	0
56	MG	1a	1827	1/1	0.85	0.21	52,52,52,52	0
56	MG	2A	3234	1/1	0.85	0.21	60,60,60,60	0
56	MG	2A	3433	1/1	0.85	0.36	49,49,49,49	0
56	MG	2a	3080	1/1	0.85	0.23	62,62,62,62	0
56	MG	2A	3444	1/1	0.85	0.28	57,57,57,57	0
56	MG	2a	3096	1/1	0.85	0.20	67,67,67,67	0
56	MG	1B	207	1/1	0.85	0.31	70,70,70,70	0
56	MG	2A	3467	1/1	0.85	0.22	74,74,74,74	0
56	MG	2A	3679	1/1	0.85	0.11	52,52,52,52	0
56	MG	2a	3135	1/1	0.85	0.18	59,59,59,59	0
56	MG	2A	3686	1/1	0.85	0.14	53,53,53,53	0
56	MG	2A	3853	1/1	0.85	0.13	49,49,49,49	0
56	MG	2A	3858	1/1	0.85	0.12	64,64,64,64	0
56	MG	2A	3484	1/1	0.85	0.12	58,58,58,58	0
56	MG	2A	3491	1/1	0.85	0.18	50,50,50,50	0
56	MG	2A	3881	1/1	0.85	0.16	62,62,62,62	0
56	MG	2a	3188	1/1	0.85	0.15	59,59,59,59	0
56	MG	2A	3058	1/1	0.85	0.13	52,52,52,52	0
56	MG	2B	217	1/1	0.85	0.14	84,84,84,84	0
56	MG	2A	3059	1/1	0.85	0.13	58,58,58,58	0
56	MG	2A	3531	1/1	0.85	0.20	55,55,55,55	0
56	MG	2A	3711	1/1	0.85	0.12	54,54,54,54	0
56	MG	2A	3062	1/1	0.85	0.14	66,66,66,66	0
56	MG	2A	3065	1/1	0.85	0.25	68,68,68,68	0
56	MG	20	101	1/1	0.85	0.24	67,67,67,67	0
56	MG	1A	3739	1/1	0.85	0.13	51,51,51,51	0
56	MG	2a	3228	1/1	0.85	0.29	62,62,62,62	0
56	MG	2a	3005	1/1	0.85	0.25	66,66,66,66	0
56	MG	2a	3012	1/1	0.85	0.25	70,70,70,70	0
56	MG	1A	3766	1/1	0.85	0.10	26,26,26,26	0
56	MG	1A	3512	1/1	0.85	0.17	60,60,60,60	0
56	MG	1A	3270	1/1	0.85	0.12	55,55,55,55	0
56	MG	1a	1780	1/1	0.85	0.10	58,58,58,58	0
56	MG	2A	3601	1/1	0.85	0.17	58,58,58,58	0
56	MG	2q	202	1/1	0.85	0.16	72,72,72,72	0
56	MG	1A	3913	1/1	0.85	0.29	34,34,34,34	0
56	MG	2A	3341	1/1	0.85	0.11	66,66,66,66	0
56	MG	2w	104	1/1	0.85	0.10	69,69,69,69	0
56	MG	1A	3921	1/1	0.85	0.12	41,41,41,41	0
56	MG	2A	3718	1/1	0.86	0.09	41,41,41,41	0
56	MG	1B	222	1/1	0.86	0.16	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3502	1/1	0.86	0.12	55,55,55,55	0
56	MG	2A	3514	1/1	0.86	0.18	67,67,67,67	0
56	MG	2a	3043	1/1	0.86	0.28	66,66,66,66	0
56	MG	1B	230	1/1	0.86	0.08	61,61,61,61	0
56	MG	2A	3225	1/1	0.86	0.28	62,62,62,62	0
56	MG	1a	1691	1/1	0.86	0.26	64,64,64,64	0
56	MG	1A	3131	1/1	0.86	0.09	63,63,63,63	0
56	MG	1A	3428	1/1	0.86	0.09	56,56,56,56	0
56	MG	1a	1698	1/1	0.86	0.30	62,62,62,62	0
56	MG	1A	3577	1/1	0.86	0.22	47,47,47,47	0
56	MG	2A	3761	1/1	0.86	0.16	62,62,62,62	0
56	MG	1x	112	1/1	0.86	0.16	58,58,58,58	0
56	MG	2A	3596	1/1	0.86	0.09	40,40,40,40	0
56	MG	2A	3287	1/1	0.86	0.24	67,67,67,67	0
56	MG	2a	3082	1/1	0.86	0.20	65,65,65,65	0
56	MG	2a	3085	1/1	0.86	0.32	73,73,73,73	0
56	MG	1x	113	1/1	0.86	0.23	65,65,65,65	0
56	MG	2a	3095	1/1	0.86	0.16	79,79,79,79	0
56	MG	2A	3299	1/1	0.86	0.12	49,49,49,49	0
56	MG	1a	1715	1/1	0.86	0.11	53,53,53,53	0
56	MG	2A	3308	1/1	0.86	0.16	56,56,56,56	0
56	MG	2a	3106	1/1	0.86	0.19	65,65,65,65	0
56	MG	2A	3008	1/1	0.86	0.10	60,60,60,60	0
56	MG	2a	3121	1/1	0.86	0.17	54,54,54,54	0
56	MG	1A	3901	1/1	0.86	0.10	53,53,53,53	0
56	MG	2a	3147	1/1	0.86	0.11	80,80,80,80	0
56	MG	2a	3160	1/1	0.86	0.13	84,84,84,84	0
56	MG	2A	3321	1/1	0.86	0.14	65,65,65,65	0
56	MG	1A	3911	1/1	0.86	0.18	55,55,55,55	0
56	MG	2a	3165	1/1	0.86	0.09	78,78,78,78	0
56	MG	1U	201	1/1	0.86	0.18	51,51,51,51	0
56	MG	1A	4039	1/1	0.86	0.11	61,61,61,61	0
56	MG	2A	3831	1/1	0.86	0.15	56,56,56,56	0
56	MG	2A	3645	1/1	0.86	0.10	37,37,37,37	0
56	MG	1A	3798	1/1	0.86	0.10	39,39,39,39	0
56	MG	2A	3347	1/1	0.86	0.13	66,66,66,66	0
56	MG	1a	1763	1/1	0.86	0.18	62,62,62,62	0
56	MG	1A	4047	1/1	0.86	0.12	47,47,47,47	0
56	MG	2B	211	1/1	0.86	0.26	75,75,75,75	0
56	MG	1A	4056	1/1	0.86	0.10	45,45,45,45	0
56	MG	1A	3917	1/1	0.86	0.13	34,34,34,34	0
56	MG	2a	3216	1/1	0.86	0.13	72,72,72,72	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3086	1/1	0.86	0.23	66,66,66,66	0
56	MG	2A	3377	1/1	0.86	0.10	65,65,65,65	0
56	MG	1A	3446	1/1	0.86	0.11	52,52,52,52	0
56	MG	1A	3004	1/1	0.86	0.10	22,22,22,22	0
56	MG	1a	1634	1/1	0.86	0.29	66,66,66,66	0
56	MG	2a	3235	1/1	0.86	0.12	66,66,66,66	0
56	MG	2a	3236	1/1	0.86	0.28	73,73,73,73	0
56	MG	2R	201	1/1	0.86	0.14	65,65,65,65	0
56	MG	2Z	301	1/1	0.86	0.12	72,72,72,72	0
56	MG	2A	3123	1/1	0.86	0.33	59,59,59,59	0
56	MG	27	101	1/1	0.86	0.11	46,46,46,46	0
56	MG	2f	202	1/1	0.86	0.18	65,65,65,65	0
56	MG	2g	201	1/1	0.86	0.11	81,81,81,81	0
56	MG	2A	3124	1/1	0.86	0.09	66,66,66,66	0
56	MG	1a	1793	1/1	0.86	0.10	78,78,78,78	0
56	MG	1A	3214	1/1	0.86	0.15	57,57,57,57	0
56	MG	1A	3121	1/1	0.86	0.13	46,46,46,46	0
56	MG	1a	1826	1/1	0.86	0.19	58,58,58,58	0
56	MG	2A	3714	1/1	0.86	0.11	57,57,57,57	0
56	MG	2x	103	1/1	0.86	0.10	60,60,60,60	0
56	MG	2x	104	1/1	0.86	0.17	62,62,62,62	0
56	MG	1A	3422	1/1	0.86	0.12	58,58,58,58	0
56	MG	2y	106	1/1	0.86	0.16	83,83,83,83	0
56	MG	1A	3302	1/1	0.87	0.26	52,52,52,52	0
56	MG	2A	3330	1/1	0.87	0.20	60,60,60,60	0
56	MG	2a	3013	1/1	0.87	0.18	58,58,58,58	0
56	MG	1A	3928	1/1	0.87	0.15	69,69,69,69	0
56	MG	1A	3417	1/1	0.87	0.14	48,48,48,48	0
56	MG	1A	3932	1/1	0.87	0.12	48,48,48,48	0
56	MG	1A	3165	1/1	0.87	0.15	39,39,39,39	0
56	MG	2A	3346	1/1	0.87	0.13	67,67,67,67	0
56	MG	1B	234	1/1	0.87	0.16	56,56,56,56	0
56	MG	2A	3349	1/1	0.87	0.19	59,59,59,59	0
56	MG	2a	3039	1/1	0.87	0.22	55,55,55,55	0
56	MG	1A	3817	1/1	0.87	0.46	39,39,39,39	0
56	MG	1D	312	1/1	0.87	0.16	37,37,37,37	0
56	MG	1A	3822	1/1	0.87	0.14	25,25,25,25	0
56	MG	2A	3361	1/1	0.87	0.19	61,61,61,61	0
56	MG	1N	205	1/1	0.87	0.10	57,57,57,57	0
56	MG	1O	205	1/1	0.87	0.14	72,72,72,72	0
56	MG	1A	3471	1/1	0.87	0.17	51,51,51,51	0
56	MG	2A	3380	1/1	0.87	0.14	75,75,75,75	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	3062	1/1	0.87	0.23	71,71,71,71	0
56	MG	2A	3089	1/1	0.87	0.27	61,61,61,61	0
56	MG	1Q	208	1/1	0.87	0.16	47,47,47,47	0
56	MG	2A	3397	1/1	0.87	0.16	72,72,72,72	0
56	MG	2A	3099	1/1	0.87	0.28	68,68,68,68	0
56	MG	2A	3721	1/1	0.87	0.13	62,62,62,62	0
56	MG	1A	3483	1/1	0.87	0.18	59,59,59,59	0
56	MG	2A	3416	1/1	0.87	0.16	64,64,64,64	0
56	MG	2A	3418	1/1	0.87	0.10	66,66,66,66	0
56	MG	1A	3993	1/1	0.87	0.09	27,27,27,27	0
56	MG	2A	3737	1/1	0.87	0.08	70,70,70,70	0
56	MG	2A	3440	1/1	0.87	0.21	61,61,61,61	0
56	MG	2A	3443	1/1	0.87	0.22	59,59,59,59	0
56	MG	1A	3643	1/1	0.87	0.14	56,56,56,56	0
56	MG	2A	3753	1/1	0.87	0.12	42,42,42,42	0
56	MG	2a	3112	1/1	0.87	0.20	62,62,62,62	0
56	MG	2a	3117	1/1	0.87	0.19	65,65,65,65	0
56	MG	1A	3866	1/1	0.87	0.09	22,22,22,22	0
56	MG	2A	3155	1/1	0.87	0.16	55,55,55,55	0
56	MG	2a	3136	1/1	0.87	0.15	78,78,78,78	0
56	MG	2A	3474	1/1	0.87	0.07	61,61,61,61	0
56	MG	2a	3150	1/1	0.87	0.10	76,76,76,76	0
56	MG	1A	4028	1/1	0.87	0.09	61,61,61,61	0
56	MG	1A	3869	1/1	0.87	0.17	45,45,45,45	0
56	MG	1A	3360	1/1	0.87	0.17	65,65,65,65	0
56	MG	1A	3888	1/1	0.87	0.18	44,44,44,44	0
56	MG	2A	3205	1/1	0.87	0.09	63,63,63,63	0
56	MG	2A	3802	1/1	0.87	0.11	57,57,57,57	0
56	MG	2A	3207	1/1	0.87	0.19	64,64,64,64	0
56	MG	1a	1832	1/1	0.87	0.15	55,55,55,55	0
56	MG	2a	3186	1/1	0.87	0.16	54,54,54,54	0
56	MG	1a	1833	1/1	0.87	0.19	43,43,43,43	0
56	MG	2A	3533	1/1	0.87	0.10	60,60,60,60	0
56	MG	1A	3894	1/1	0.87	0.07	21,21,21,21	0
56	MG	1d	301	1/1	0.87	0.17	48,48,48,48	0
56	MG	2A	3562	1/1	0.87	0.13	35,35,35,35	0
56	MG	2A	3563	1/1	0.87	0.10	36,36,36,36	0
56	MG	2a	3202	1/1	0.87	0.26	75,75,75,75	0
56	MG	2A	3568	1/1	0.87	0.10	47,47,47,47	0
56	MG	1A	4049	1/1	0.87	0.11	54,54,54,54	0
56	MG	2A	3838	1/1	0.87	0.17	43,43,43,43	0
56	MG	1A	3143	1/1	0.87	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
56	MG	2A	3586	1/1	0.87	0.11	60,60,60,60	0
56	MG	2A	3860	1/1	0.87	0.11	73,73,73,73	0
56	MG	2A	3254	1/1	0.87	0.28	63,63,63,63	0
56	MG	1A	3514	1/1	0.87	0.21	64,64,64,64	0
56	MG	1A	3793	1/1	0.87	0.14	56,56,56,56	0
56	MG	2A	3884	1/1	0.87	0.38	61,61,61,61	0
56	MG	2A	3886	1/1	0.87	0.17	71,71,71,71	0
56	MG	2A	3280	1/1	0.87	0.15	57,57,57,57	0
56	MG	2B	215	1/1	0.87	0.19	69,69,69,69	0
56	MG	1w	106	1/1	0.87	0.12	61,61,61,61	0
56	MG	1x	104	1/1	0.87	0.34	56,56,56,56	0
56	MG	1x	109	1/1	0.87	0.17	61,61,61,61	0
56	MG	2A	3614	1/1	0.87	0.14	45,45,45,45	0
56	MG	2m	201	1/1	0.87	0.27	73,73,73,73	0
56	MG	2A	3618	1/1	0.87	0.10	49,49,49,49	0
56	MG	1A	3682	1/1	0.87	0.14	61,61,61,61	0
56	MG	2A	3300	1/1	0.87	0.17	52,52,52,52	0
56	MG	1a	1662	1/1	0.87	0.20	60,60,60,60	0
56	MG	1A	3531	1/1	0.87	0.15	47,47,47,47	0
56	MG	1A	4084	1/1	0.87	0.14	14,14,14,14	0
56	MG	1A	4093	1/1	0.87	0.10	38,38,38,38	0
56	MG	2A	3643	1/1	0.87	0.12	62,62,62,62	0
56	MG	1A	4081	1/1	0.88	0.10	44,44,44,44	0
56	MG	1A	3784	1/1	0.88	0.08	66,66,66,66	0
56	MG	2T	202	1/1	0.88	0.14	61,61,61,61	0
56	MG	2U	201	1/1	0.88	0.12	54,54,54,54	0
56	MG	2A	3615	1/1	0.88	0.16	60,60,60,60	0
56	MG	2A	3303	1/1	0.88	0.25	71,71,71,71	0
56	MG	1A	3650	1/1	0.88	0.09	49,49,49,49	0
56	MG	1a	1667	1/1	0.88	0.26	58,58,58,58	0
56	MG	1a	1669	1/1	0.88	0.11	75,75,75,75	0
56	MG	2a	3007	1/1	0.88	0.19	63,63,63,63	0
56	MG	1a	1674	1/1	0.88	0.10	53,53,53,53	0
56	MG	2A	3323	1/1	0.88	0.10	57,57,57,57	0
56	MG	2A	3324	1/1	0.88	0.16	49,49,49,49	0
56	MG	2A	3329	1/1	0.88	0.20	60,60,60,60	0
56	MG	1x	115	1/1	0.88	0.24	64,64,64,64	0
56	MG	1a	1688	1/1	0.88	0.27	63,63,63,63	0
56	MG	1A	3399	1/1	0.88	0.09	48,48,48,48	0
56	MG	1A	3513	1/1	0.88	0.23	63,63,63,63	0
56	MG	2a	3032	1/1	0.88	0.43	65,65,65,65	0
56	MG	2a	3034	1/1	0.88	0.12	72,72,72,72	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3124	1/1	0.88	0.13	46,46,46,46	0
56	MG	2A	3343	1/1	0.88	0.20	57,57,57,57	0
56	MG	2A	3039	1/1	0.88	0.33	65,65,65,65	0
56	MG	1A	3675	1/1	0.88	0.09	24,24,24,24	0
56	MG	2a	3045	1/1	0.88	0.33	72,72,72,72	0
56	MG	1A	3339	1/1	0.88	0.12	42,42,42,42	0
56	MG	2A	3684	1/1	0.88	0.22	56,56,56,56	0
56	MG	1a	1707	1/1	0.88	0.14	57,57,57,57	0
56	MG	1A	3955	1/1	0.88	0.09	65,65,65,65	0
56	MG	1A	3208	1/1	0.88	0.11	61,61,61,61	0
56	MG	1a	1730	1/1	0.88	0.22	65,65,65,65	0
56	MG	2A	3066	1/1	0.88	0.08	51,51,51,51	0
56	MG	2A	3703	1/1	0.88	0.12	59,59,59,59	0
56	MG	1A	3533	1/1	0.88	0.12	55,55,55,55	0
56	MG	2A	3373	1/1	0.88	0.17	67,67,67,67	0
56	MG	1A	3548	1/1	0.88	0.24	46,46,46,46	0
56	MG	1A	3823	1/1	0.88	0.17	50,50,50,50	0
56	MG	2A	3387	1/1	0.88	0.27	62,62,62,62	0
56	MG	1A	3461	1/1	0.88	0.14	61,61,61,61	0
56	MG	1a	1759	1/1	0.88	0.14	61,61,61,61	0
56	MG	1A	3563	1/1	0.88	0.12	53,53,53,53	0
56	MG	1A	3709	1/1	0.88	0.09	41,41,41,41	0
56	MG	2A	3121	1/1	0.88	0.14	48,48,48,48	0
56	MG	1A	4016	1/1	0.88	0.09	25,25,25,25	0
56	MG	2a	3102	1/1	0.88	0.12	54,54,54,54	0
56	MG	1a	1774	1/1	0.88	0.16	61,61,61,61	0
56	MG	1A	4018	1/1	0.88	0.10	35,35,35,35	0
56	MG	1T	201	1/1	0.88	0.09	47,47,47,47	0
56	MG	2a	3113	1/1	0.88	0.10	56,56,56,56	0
56	MG	1A	3855	1/1	0.88	0.10	20,20,20,20	0
56	MG	2a	3120	1/1	0.88	0.25	66,66,66,66	0
56	MG	1X	104	1/1	0.88	0.19	61,61,61,61	0
56	MG	2a	3124	1/1	0.88	0.20	55,55,55,55	0
56	MG	2A	3751	1/1	0.88	0.10	67,67,67,67	0
56	MG	1A	3722	1/1	0.88	0.15	59,59,59,59	0
56	MG	2A	3455	1/1	0.88	0.29	61,61,61,61	0
56	MG	2A	3457	1/1	0.88	0.13	50,50,50,50	0
56	MG	2a	3151	1/1	0.88	0.08	91,91,91,91	0
56	MG	2a	3153	1/1	0.88	0.13	73,73,73,73	0
56	MG	2A	3460	1/1	0.88	0.19	57,57,57,57	0
56	MG	10	102	1/1	0.88	0.08	41,41,41,41	0
56	MG	2A	3204	1/1	0.88	0.12	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
56	MG	2A	3475	1/1	0.88	0.18	56,56,56,56	0
56	MG	10	104	1/1	0.88	0.14	59,59,59,59	0
56	MG	2A	3490	1/1	0.88	0.28	53,53,53,53	0
56	MG	1A	3725	1/1	0.88	0.15	66,66,66,66	0
56	MG	16	102	1/1	0.88	0.22	40,40,40,40	0
56	MG	2a	3183	1/1	0.88	0.14	60,60,60,60	0
56	MG	2A	3498	1/1	0.88	0.16	58,58,58,58	0
56	MG	1a	1831	1/1	0.88	0.21	43,43,43,43	0
56	MG	2a	3190	1/1	0.88	0.18	77,77,77,77	0
56	MG	2A	3812	1/1	0.88	0.22	76,76,76,76	0
56	MG	2A	3216	1/1	0.88	0.21	65,65,65,65	0
56	MG	2A	3222	1/1	0.88	0.10	61,61,61,61	0
56	MG	2A	3525	1/1	0.88	0.15	60,60,60,60	0
56	MG	2a	3200	1/1	0.88	0.16	77,77,77,77	0
56	MG	1A	3726	1/1	0.88	0.09	53,53,53,53	0
56	MG	2A	3826	1/1	0.88	0.16	55,55,55,55	0
56	MG	1A	3420	1/1	0.88	0.20	51,51,51,51	0
56	MG	1A	3892	1/1	0.88	0.11	30,30,30,30	0
56	MG	2A	3237	1/1	0.88	0.21	44,44,44,44	0
56	MG	2A	3239	1/1	0.88	0.17	56,56,56,56	0
56	MG	1A	4053	1/1	0.88	0.09	34,34,34,34	0
56	MG	2A	3251	1/1	0.88	0.19	62,62,62,62	0
56	MG	2A	3566	1/1	0.88	0.11	44,44,44,44	0
56	MG	2A	3253	1/1	0.88	0.16	64,64,64,64	0
56	MG	1A	3053	1/1	0.88	0.15	62,62,62,62	0
56	MG	2A	3875	1/1	0.88	0.18	74,74,74,74	0
56	MG	2A	3878	1/1	0.88	0.16	38,38,38,38	0
56	MG	2A	3575	1/1	0.88	0.20	65,65,65,65	0
56	MG	2a	3241	1/1	0.88	0.24	63,63,63,63	0
56	MG	1f	202	1/1	0.88	0.21	70,70,70,70	0
56	MG	2A	3259	1/1	0.88	0.09	60,60,60,60	0
56	MG	2B	203	1/1	0.88	0.19	60,60,60,60	0
56	MG	2A	3587	1/1	0.88	0.22	56,56,56,56	0
56	MG	2B	212	1/1	0.88	0.14	57,57,57,57	0
56	MG	2B	213	1/1	0.88	0.18	56,56,56,56	0
56	MG	2q	201	1/1	0.88	0.16	68,68,68,68	0
56	MG	1A	3494	1/1	0.88	0.13	56,56,56,56	0
56	MG	1A	4059	1/1	0.88	0.12	27,27,27,27	0
56	MG	1A	3372	1/1	0.88	0.14	43,43,43,43	0
56	MG	2w	103	1/1	0.88	0.10	64,64,64,64	0
56	MG	2A	3600	1/1	0.88	0.11	56,56,56,56	0
56	MG	1w	105	1/1	0.88	0.15	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2D	308	1/1	0.88	0.08	39,39,39,39	0
56	MG	1A	3772	1/1	0.88	0.09	28,28,28,28	0
56	MG	1w	110	1/1	0.88	0.20	74,74,74,74	0
56	MG	2A	3250	1/1	0.89	0.12	64,64,64,64	0
56	MG	1a	1625	1/1	0.89	0.12	55,55,55,55	0
56	MG	2A	3252	1/1	0.89	0.13	48,48,48,48	0
56	MG	1a	1626	1/1	0.89	0.18	52,52,52,52	0
56	MG	2A	3572	1/1	0.89	0.18	51,51,51,51	0
56	MG	1A	3676	1/1	0.89	0.09	16,16,16,16	0
56	MG	1a	1640	1/1	0.89	0.26	69,69,69,69	0
56	MG	1A	3789	1/1	0.89	0.10	43,43,43,43	0
56	MG	1A	3561	1/1	0.89	0.29	62,62,62,62	0
56	MG	2R	202	1/1	0.89	0.12	47,47,47,47	0
56	MG	2A	3594	1/1	0.89	0.18	66,66,66,66	0
56	MG	2A	3262	1/1	0.89	0.11	60,60,60,60	0
56	MG	2W	201	1/1	0.89	0.07	57,57,57,57	0
56	MG	1A	4068	1/1	0.89	0.10	61,61,61,61	0
56	MG	2A	3281	1/1	0.89	0.13	70,70,70,70	0
56	MG	1A	4076	1/1	0.89	0.15	36,36,36,36	0
56	MG	2a	3002	1/1	0.89	0.07	63,63,63,63	0
56	MG	1A	3292	1/1	0.89	0.13	57,57,57,57	0
56	MG	2A	3295	1/1	0.89	0.09	58,58,58,58	0
56	MG	2a	3006	1/1	0.89	0.17	61,61,61,61	0
56	MG	2A	3605	1/1	0.89	0.10	51,51,51,51	0
56	MG	2a	3009	1/1	0.89	0.13	72,72,72,72	0
56	MG	2a	3010	1/1	0.89	0.18	60,60,60,60	0
56	MG	2a	3011	1/1	0.89	0.23	66,66,66,66	0
56	MG	2A	3608	1/1	0.89	0.10	34,34,34,34	0
56	MG	1w	109	1/1	0.89	0.24	77,77,77,77	0
56	MG	2a	3015	1/1	0.89	0.32	69,69,69,69	0
56	MG	1A	3796	1/1	0.89	0.15	20,20,20,20	0
56	MG	1w	112	1/1	0.89	0.13	53,53,53,53	0
56	MG	1A	3924	1/1	0.89	0.11	71,71,71,71	0
56	MG	1A	3574	1/1	0.89	0.22	40,40,40,40	0
56	MG	1a	1673	1/1	0.89	0.14	63,63,63,63	0
56	MG	1A	3691	1/1	0.89	0.12	24,24,24,24	0
56	MG	1a	1675	1/1	0.89	0.23	64,64,64,64	0
56	MG	1B	202	1/1	0.89	0.18	47,47,47,47	0
56	MG	1A	3331	1/1	0.89	0.10	43,43,43,43	0
56	MG	1B	208	1/1	0.89	0.16	57,57,57,57	0
56	MG	2A	3002	1/1	0.89	0.23	53,53,53,53	0
56	MG	1A	3602	1/1	0.89	0.13	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
56	MG	2a	3044	1/1	0.89	0.22	56,56,56,56	0
56	MG	1A	3251	1/1	0.89	0.17	69,69,69,69	0
56	MG	2A	3652	1/1	0.89	0.13	50,50,50,50	0
56	MG	2A	3657	1/1	0.89	0.12	84,84,84,84	0
56	MG	1A	3966	1/1	0.89	0.12	36,36,36,36	0
56	MG	2A	3337	1/1	0.89	0.10	49,49,49,49	0
56	MG	2A	3034	1/1	0.89	0.11	56,56,56,56	0
56	MG	1A	3703	1/1	0.89	0.14	48,48,48,48	0
56	MG	1a	1709	1/1	0.89	0.20	50,50,50,50	0
56	MG	1A	3971	1/1	0.89	0.15	32,32,32,32	0
56	MG	2A	3054	1/1	0.89	0.19	63,63,63,63	0
56	MG	2A	3680	1/1	0.89	0.12	54,54,54,54	0
56	MG	2A	3348	1/1	0.89	0.08	65,65,65,65	0
56	MG	1A	3706	1/1	0.89	0.12	53,53,53,53	0
56	MG	1A	3708	1/1	0.89	0.09	45,45,45,45	0
56	MG	1F	308	1/1	0.89	0.13	49,49,49,49	0
56	MG	2a	3086	1/1	0.89	0.20	63,63,63,63	0
56	MG	2A	3693	1/1	0.89	0.21	62,62,62,62	0
56	MG	1a	1734	1/1	0.89	0.16	53,53,53,53	0
56	MG	1F	309	1/1	0.89	0.12	53,53,53,53	0
56	MG	1a	1746	1/1	0.89	0.11	59,59,59,59	0
56	MG	2A	3704	1/1	0.89	0.13	44,44,44,44	0
56	MG	2A	3365	1/1	0.89	0.11	54,54,54,54	0
56	MG	2A	3710	1/1	0.89	0.13	42,42,42,42	0
56	MG	2A	3367	1/1	0.89	0.15	54,54,54,54	0
56	MG	2a	3108	1/1	0.89	0.30	65,65,65,65	0
56	MG	2A	3085	1/1	0.89	0.18	55,55,55,55	0
56	MG	1a	1751	1/1	0.89	0.15	52,52,52,52	0
56	MG	2a	3116	1/1	0.89	0.23	53,53,53,53	0
56	MG	2A	3087	1/1	0.89	0.13	48,48,48,48	0
56	MG	1A	3988	1/1	0.89	0.15	21,21,21,21	0
56	MG	2A	3383	1/1	0.89	0.16	66,66,66,66	0
56	MG	1A	3989	1/1	0.89	0.12	31,31,31,31	0
56	MG	2a	3127	1/1	0.89	0.19	63,63,63,63	0
56	MG	2a	3132	1/1	0.89	0.10	54,54,54,54	0
56	MG	2a	3133	1/1	0.89	0.20	66,66,66,66	0
56	MG	1A	3826	1/1	0.89	0.11	45,45,45,45	0
56	MG	1A	3835	1/1	0.89	0.09	33,33,33,33	0
56	MG	2A	3108	1/1	0.89	0.29	65,65,65,65	0
56	MG	1a	1766	1/1	0.89	0.08	61,61,61,61	0
56	MG	1A	3098	1/1	0.89	0.09	44,44,44,44	0
56	MG	2A	3408	1/1	0.89	0.27	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
56	MG	2A	3746	1/1	0.89	0.19	57,57,57,57	0
56	MG	2A	3414	1/1	0.89	0.09	59,59,59,59	0
56	MG	1A	3712	1/1	0.89	0.08	54,54,54,54	0
56	MG	2a	3164	1/1	0.89	0.10	58,58,58,58	0
56	MG	1A	3359	1/1	0.89	0.22	58,58,58,58	0
56	MG	2A	3424	1/1	0.89	0.21	49,49,49,49	0
56	MG	2A	3431	1/1	0.89	0.21	49,49,49,49	0
56	MG	2A	3138	1/1	0.89	0.20	70,70,70,70	0
56	MG	2A	3437	1/1	0.89	0.17	56,56,56,56	0
56	MG	2A	3140	1/1	0.89	0.16	57,57,57,57	0
56	MG	1A	4017	1/1	0.89	0.09	39,39,39,39	0
56	MG	1A	3644	1/1	0.89	0.09	58,58,58,58	0
56	MG	2A	3169	1/1	0.89	0.09	57,57,57,57	0
56	MG	2A	3781	1/1	0.89	0.09	57,57,57,57	0
56	MG	1A	3534	1/1	0.89	0.17	63,63,63,63	0
56	MG	2A	3799	1/1	0.89	0.12	75,75,75,75	0
56	MG	2A	3801	1/1	0.89	0.09	80,80,80,80	0
56	MG	1a	1785	1/1	0.89	0.08	65,65,65,65	0
56	MG	2A	3189	1/1	0.89	0.11	60,60,60,60	0
56	MG	2A	3463	1/1	0.89	0.23	55,55,55,55	0
56	MG	2A	3466	1/1	0.89	0.10	47,47,47,47	0
56	MG	2A	3810	1/1	0.89	0.11	78,78,78,78	0
56	MG	1a	1786	1/1	0.89	0.09	73,73,73,73	0
56	MG	2A	3815	1/1	0.89	0.10	73,73,73,73	0
56	MG	2A	3196	1/1	0.89	0.16	62,62,62,62	0
56	MG	1a	1787	1/1	0.89	0.12	66,66,66,66	0
56	MG	1A	3654	1/1	0.89	0.10	37,37,37,37	0
56	MG	2A	3821	1/1	0.89	0.09	55,55,55,55	0
56	MG	2A	3485	1/1	0.89	0.26	44,44,44,44	0
56	MG	1A	3547	1/1	0.89	0.09	42,42,42,42	0
56	MG	1a	1795	1/1	0.89	0.11	64,64,64,64	0
56	MG	1A	3877	1/1	0.89	0.18	30,30,30,30	0
56	MG	2A	3497	1/1	0.89	0.13	51,51,51,51	0
56	MG	2A	3212	1/1	0.89	0.24	66,66,66,66	0
56	MG	1a	1807	1/1	0.89	0.10	66,66,66,66	0
56	MG	2A	3503	1/1	0.89	0.16	39,39,39,39	0
56	MG	2A	3509	1/1	0.89	0.11	41,41,41,41	0
56	MG	1a	1809	1/1	0.89	0.11	72,72,72,72	0
56	MG	1a	1812	1/1	0.89	0.10	62,62,62,62	0
56	MG	1A	3503	1/1	0.89	0.15	57,57,57,57	0
56	MG	1A	3891	1/1	0.89	0.12	21,21,21,21	0
56	MG	1A	3240	1/1	0.89	0.12	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
56	MG	1A	3559	1/1	0.89	0.21	54,54,54,54	0
56	MG	1A	3774	1/1	0.89	0.10	19,19,19,19	0
56	MG	2A	3540	1/1	0.89	0.10	35,35,35,35	0
56	MG	2A	3541	1/1	0.89	0.12	49,49,49,49	0
56	MG	1a	1617	1/1	0.89	0.09	53,53,53,53	0
56	MG	2A	3556	1/1	0.89	0.22	50,50,50,50	0
56	MG	2A	3248	1/1	0.89	0.23	65,65,65,65	0
56	MG	1a	1799	1/1	0.90	0.15	46,46,46,46	0
56	MG	2B	201	1/1	0.90	0.18	66,66,66,66	0
56	MG	2A	3227	1/1	0.90	0.15	56,56,56,56	0
56	MG	2B	204	1/1	0.90	0.10	61,61,61,61	0
56	MG	1A	3238	1/1	0.90	0.29	56,56,56,56	0
56	MG	1Z	301	1/1	0.90	0.11	48,48,48,48	0
56	MG	1Z	302	1/1	0.90	0.08	60,60,60,60	0
56	MG	2B	214	1/1	0.90	0.21	62,62,62,62	0
56	MG	1A	3809	1/1	0.90	0.12	39,39,39,39	0
56	MG	2A	3240	1/1	0.90	0.12	51,51,51,51	0
56	MG	2A	3551	1/1	0.90	0.12	43,43,43,43	0
56	MG	1A	3990	1/1	0.90	0.09	33,33,33,33	0
56	MG	1A	3816	1/1	0.90	0.15	54,54,54,54	0
56	MG	1A	3189	1/1	0.90	0.25	47,47,47,47	0
56	MG	2A	3564	1/1	0.90	0.13	53,53,53,53	0
56	MG	1A	3819	1/1	0.90	0.08	44,44,44,44	0
56	MG	1A	3136	1/1	0.90	0.09	41,41,41,41	0
56	MG	1A	3467	1/1	0.90	0.12	46,46,46,46	0
56	MG	1A	3253	1/1	0.90	0.12	54,54,54,54	0
56	MG	1A	3700	1/1	0.90	0.10	25,25,25,25	0
56	MG	1A	3836	1/1	0.90	0.10	50,50,50,50	0
56	MG	1A	3473	1/1	0.90	0.16	65,65,65,65	0
56	MG	1A	3705	1/1	0.90	0.12	28,28,28,28	0
56	MG	2A	3264	1/1	0.90	0.15	56,56,56,56	0
56	MG	25	104	1/1	0.90	0.14	54,54,54,54	0
56	MG	25	105	1/1	0.90	0.12	49,49,49,49	0
56	MG	2A	3265	1/1	0.90	0.17	57,57,57,57	0
56	MG	2a	3001	1/1	0.90	0.14	57,57,57,57	0
56	MG	2A	3274	1/1	0.90	0.15	59,59,59,59	0
56	MG	2A	3276	1/1	0.90	0.09	51,51,51,51	0
56	MG	2A	3278	1/1	0.90	0.18	65,65,65,65	0
56	MG	1a	1630	1/1	0.90	0.15	60,60,60,60	0
56	MG	1A	3847	1/1	0.90	0.14	51,51,51,51	0
56	MG	1A	3481	1/1	0.90	0.12	40,40,40,40	0
56	MG	2A	3606	1/1	0.90	0.10	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3575	1/1	0.90	0.24	55,55,55,55	0
56	MG	2A	3291	1/1	0.90	0.15	57,57,57,57	0
56	MG	2A	3610	1/1	0.90	0.09	41,41,41,41	0
56	MG	2a	3014	1/1	0.90	0.19	63,63,63,63	0
56	MG	2A	3294	1/1	0.90	0.09	67,67,67,67	0
56	MG	1A	3858	1/1	0.90	0.09	43,43,43,43	0
56	MG	1A	3083	1/1	0.90	0.23	37,37,37,37	0
56	MG	1a	1657	1/1	0.90	0.09	68,68,68,68	0
56	MG	1A	3867	1/1	0.90	0.13	55,55,55,55	0
56	MG	1a	1660	1/1	0.90	0.20	72,72,72,72	0
56	MG	2a	3030	1/1	0.90	0.38	63,63,63,63	0
56	MG	1A	3404	1/1	0.90	0.25	60,60,60,60	0
56	MG	2A	3630	1/1	0.90	0.20	42,42,42,42	0
56	MG	1A	3018	1/1	0.90	0.09	30,30,30,30	0
56	MG	1A	4061	1/1	0.90	0.17	68,68,68,68	0
56	MG	2A	3314	1/1	0.90	0.08	60,60,60,60	0
56	MG	1A	3724	1/1	0.90	0.14	53,53,53,53	0
56	MG	2a	3042	1/1	0.90	0.20	60,60,60,60	0
56	MG	1A	3885	1/1	0.90	0.07	25,25,25,25	0
56	MG	1A	4075	1/1	0.90	0.15	48,48,48,48	0
56	MG	1A	3609	1/1	0.90	0.14	25,25,25,25	0
56	MG	2A	3003	1/1	0.90	0.24	44,44,44,44	0
56	MG	2A	3006	1/1	0.90	0.27	54,54,54,54	0
56	MG	2A	3662	1/1	0.90	0.08	59,59,59,59	0
56	MG	2A	3664	1/1	0.90	0.15	57,57,57,57	0
56	MG	1a	1687	1/1	0.90	0.14	50,50,50,50	0
56	MG	1A	3611	1/1	0.90	0.12	36,36,36,36	0
56	MG	2A	3673	1/1	0.90	0.12	57,57,57,57	0
56	MG	1A	3624	1/1	0.90	0.17	46,46,46,46	0
56	MG	2a	3066	1/1	0.90	0.17	60,60,60,60	0
56	MG	1A	3741	1/1	0.90	0.12	37,37,37,37	0
56	MG	1A	4088	1/1	0.90	0.12	21,21,21,21	0
56	MG	1a	1694	1/1	0.90	0.06	56,56,56,56	0
56	MG	1a	1697	1/1	0.90	0.25	49,49,49,49	0
56	MG	2A	3681	1/1	0.90	0.10	54,54,54,54	0
56	MG	2A	3049	1/1	0.90	0.13	54,54,54,54	0
56	MG	2A	3052	1/1	0.90	0.21	63,63,63,63	0
56	MG	2A	3053	1/1	0.90	0.36	64,64,64,64	0
56	MG	2a	3094	1/1	0.90	0.26	62,62,62,62	0
56	MG	1A	3748	1/1	0.90	0.10	47,47,47,47	0
56	MG	1A	3756	1/1	0.90	0.14	45,45,45,45	0
56	MG	2A	3697	1/1	0.90	0.16	72,72,72,72	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3762	1/1	0.90	0.14	21,21,21,21	0
56	MG	2A	3356	1/1	0.90	0.10	62,62,62,62	0
56	MG	2a	3104	1/1	0.90	0.15	54,54,54,54	0
56	MG	2A	3357	1/1	0.90	0.09	50,50,50,50	0
56	MG	1A	3340	1/1	0.90	0.14	50,50,50,50	0
56	MG	1a	1714	1/1	0.90	0.16	62,62,62,62	0
56	MG	1A	3916	1/1	0.90	0.10	22,22,22,22	0
56	MG	1a	1716	1/1	0.90	0.08	49,49,49,49	0
56	MG	2A	3074	1/1	0.90	0.13	41,41,41,41	0
56	MG	2A	3083	1/1	0.90	0.13	57,57,57,57	0
56	MG	1a	1720	1/1	0.90	0.28	51,51,51,51	0
56	MG	2A	3378	1/1	0.90	0.15	55,55,55,55	0
56	MG	1B	221	1/1	0.90	0.12	56,56,56,56	0
56	MG	2A	3381	1/1	0.90	0.10	57,57,57,57	0
56	MG	2A	3722	1/1	0.90	0.11	40,40,40,40	0
56	MG	1a	1728	1/1	0.90	0.26	51,51,51,51	0
56	MG	2A	3730	1/1	0.90	0.07	41,41,41,41	0
56	MG	1A	3632	1/1	0.90	0.08	34,34,34,34	0
56	MG	1A	3188	1/1	0.90	0.06	37,37,37,37	0
56	MG	2A	3735	1/1	0.90	0.09	62,62,62,62	0
56	MG	1a	1732	1/1	0.90	0.25	64,64,64,64	0
56	MG	1A	3344	1/1	0.90	0.13	53,53,53,53	0
56	MG	2a	3154	1/1	0.90	0.09	69,69,69,69	0
56	MG	2A	3107	1/1	0.90	0.09	65,65,65,65	0
56	MG	2A	3742	1/1	0.90	0.08	72,72,72,72	0
56	MG	2A	3743	1/1	0.90	0.11	59,59,59,59	0
56	MG	1A	3349	1/1	0.90	0.15	56,56,56,56	0
56	MG	2A	3406	1/1	0.90	0.11	66,66,66,66	0
56	MG	2A	3112	1/1	0.90	0.16	51,51,51,51	0
56	MG	1a	1743	1/1	0.90	0.14	61,61,61,61	0
56	MG	1A	3515	1/1	0.90	0.09	47,47,47,47	0
56	MG	2a	3175	1/1	0.90	0.08	73,73,73,73	0
56	MG	2a	3176	1/1	0.90	0.09	72,72,72,72	0
56	MG	1A	3522	1/1	0.90	0.18	53,53,53,53	0
56	MG	2A	3421	1/1	0.90	0.29	69,69,69,69	0
56	MG	1A	3937	1/1	0.90	0.10	60,60,60,60	0
56	MG	2A	3131	1/1	0.90	0.21	75,75,75,75	0
56	MG	1A	3942	1/1	0.90	0.09	51,51,51,51	0
56	MG	1A	3524	1/1	0.90	0.12	51,51,51,51	0
56	MG	2A	3771	1/1	0.90	0.11	62,62,62,62	0
56	MG	2A	3439	1/1	0.90	0.32	55,55,55,55	0
56	MG	2A	3149	1/1	0.90	0.17	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
56	MG	2A	3442	1/1	0.90	0.13	57,57,57,57	0
56	MG	2A	3150	1/1	0.90	0.13	53,53,53,53	0
56	MG	2A	3151	1/1	0.90	0.27	60,60,60,60	0
56	MG	2a	3204	1/1	0.90	0.29	65,65,65,65	0
56	MG	2a	3208	1/1	0.90	0.19	69,69,69,69	0
56	MG	2A	3448	1/1	0.90	0.38	64,64,64,64	0
56	MG	1G	203	1/1	0.90	0.07	63,63,63,63	0
56	MG	1A	3526	1/1	0.90	0.32	42,42,42,42	0
56	MG	2a	3224	1/1	0.90	0.16	61,61,61,61	0
56	MG	2A	3808	1/1	0.90	0.15	63,63,63,63	0
56	MG	1A	3962	1/1	0.90	0.11	48,48,48,48	0
56	MG	1A	3964	1/1	0.90	0.09	33,33,33,33	0
56	MG	2a	3229	1/1	0.90	0.10	61,61,61,61	0
56	MG	2A	3462	1/1	0.90	0.33	60,60,60,60	0
56	MG	1A	3353	1/1	0.90	0.16	33,33,33,33	0
56	MG	2A	3176	1/1	0.90	0.11	59,59,59,59	0
56	MG	2a	3237	1/1	0.90	0.23	61,61,61,61	0
56	MG	2A	3179	1/1	0.90	0.18	65,65,65,65	0
56	MG	2A	3469	1/1	0.90	0.28	64,64,64,64	0
56	MG	2A	3472	1/1	0.90	0.10	64,64,64,64	0
56	MG	1a	1775	1/1	0.90	0.12	65,65,65,65	0
56	MG	2A	3190	1/1	0.90	0.37	67,67,67,67	0
56	MG	1A	3438	1/1	0.90	0.10	50,50,50,50	0
56	MG	2A	3194	1/1	0.90	0.09	60,60,60,60	0
56	MG	1S	202	1/1	0.90	0.16	51,51,51,51	0
56	MG	2k	201	1/1	0.90	0.16	55,55,55,55	0
56	MG	1a	1782	1/1	0.90	0.07	79,79,79,79	0
56	MG	2A	3839	1/1	0.90	0.10	35,35,35,35	0
56	MG	1S	203	1/1	0.90	0.09	66,66,66,66	0
56	MG	1A	3356	1/1	0.90	0.09	53,53,53,53	0
56	MG	1T	204	1/1	0.90	0.13	59,59,59,59	0
56	MG	2A	3868	1/1	0.90	0.16	70,70,70,70	0
56	MG	1A	3685	1/1	0.90	0.17	31,31,31,31	0
56	MG	1a	1789	1/1	0.90	0.16	77,77,77,77	0
56	MG	2x	102	1/1	0.90	0.19	70,70,70,70	0
56	MG	1V	202	1/1	0.90	0.14	39,39,39,39	0
56	MG	1A	3450	1/1	0.90	0.14	50,50,50,50	0
56	MG	2A	3217	1/1	0.90	0.28	67,67,67,67	0
56	MG	2y	102	1/1	0.90	0.10	74,74,74,74	0
56	MG	2y	103	1/1	0.90	0.11	76,76,76,76	0
56	MG	1Y	201	1/1	0.90	0.09	32,32,32,32	0
56	MG	2A	3293	1/1	0.91	0.07	52,52,52,52	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3046	1/1	0.91	0.12	48,48,48,48	0
56	MG	1A	3039	1/1	0.91	0.14	54,54,54,54	0
56	MG	1A	3380	1/1	0.91	0.09	48,48,48,48	0
56	MG	2A	3051	1/1	0.91	0.30	72,72,72,72	0
56	MG	1A	3844	1/1	0.91	0.08	57,57,57,57	0
56	MG	2A	3301	1/1	0.91	0.08	57,57,57,57	0
56	MG	1A	3394	1/1	0.91	0.11	50,50,50,50	0
56	MG	2P	202	1/1	0.91	0.07	47,47,47,47	0
56	MG	2Q	203	1/1	0.91	0.11	56,56,56,56	0
56	MG	1a	1722	1/1	0.91	0.16	50,50,50,50	0
56	MG	2A	3597	1/1	0.91	0.18	58,58,58,58	0
56	MG	1a	1726	1/1	0.91	0.15	61,61,61,61	0
56	MG	1A	3733	1/1	0.91	0.11	45,45,45,45	0
56	MG	2A	3311	1/1	0.91	0.16	59,59,59,59	0
56	MG	2V	202	1/1	0.91	0.27	48,48,48,48	0
56	MG	1a	1729	1/1	0.91	0.25	54,54,54,54	0
56	MG	1A	3191	1/1	0.91	0.09	43,43,43,43	0
56	MG	1A	3646	1/1	0.91	0.09	30,30,30,30	0
56	MG	1A	3254	1/1	0.91	0.11	36,36,36,36	0
56	MG	2A	3071	1/1	0.91	0.07	40,40,40,40	0
56	MG	1a	1733	1/1	0.91	0.31	53,53,53,53	0
56	MG	2A	3611	1/1	0.91	0.11	51,51,51,51	0
56	MG	1A	3992	1/1	0.91	0.08	25,25,25,25	0
56	MG	1A	3865	1/1	0.91	0.11	65,65,65,65	0
56	MG	1A	3998	1/1	0.91	0.18	67,67,67,67	0
56	MG	1A	3346	1/1	0.91	0.12	52,52,52,52	0
56	MG	1A	4005	1/1	0.91	0.07	26,26,26,26	0
56	MG	2a	3008	1/1	0.91	0.14	57,57,57,57	0
56	MG	1A	3759	1/1	0.91	0.08	15,15,15,15	0
56	MG	1A	3324	1/1	0.91	0.10	39,39,39,39	0
56	MG	2A	3095	1/1	0.91	0.08	59,59,59,59	0
56	MG	2A	3631	1/1	0.91	0.12	39,39,39,39	0
56	MG	2A	3634	1/1	0.91	0.14	56,56,56,56	0
56	MG	2A	3096	1/1	0.91	0.13	52,52,52,52	0
56	MG	2A	3097	1/1	0.91	0.11	45,45,45,45	0
56	MG	2A	3098	1/1	0.91	0.20	61,61,61,61	0
56	MG	1A	3662	1/1	0.91	0.09	19,19,19,19	0
56	MG	1A	3538	1/1	0.91	0.10	50,50,50,50	0
56	MG	1A	3880	1/1	0.91	0.16	60,60,60,60	0
56	MG	1A	3883	1/1	0.91	0.28	66,66,66,66	0
56	MG	2A	3113	1/1	0.91	0.24	59,59,59,59	0
56	MG	2A	3359	1/1	0.91	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
56	MG	2A	3116	1/1	0.91	0.30	60,60,60,60	0
56	MG	1A	3541	1/1	0.91	0.14	43,43,43,43	0
56	MG	1A	4042	1/1	0.91	0.10	40,40,40,40	0
56	MG	2a	3037	1/1	0.91	0.18	48,48,48,48	0
56	MG	1A	3414	1/1	0.91	0.15	43,43,43,43	0
56	MG	11	104	1/1	0.91	0.14	48,48,48,48	0
56	MG	2A	3372	1/1	0.91	0.12	50,50,50,50	0
56	MG	12	101	1/1	0.91	0.09	54,54,54,54	0
56	MG	2A	3376	1/1	0.91	0.10	53,53,53,53	0
56	MG	1A	3477	1/1	0.91	0.09	53,53,53,53	0
56	MG	15	103	1/1	0.91	0.16	33,33,33,33	0
56	MG	1A	3680	1/1	0.91	0.14	38,38,38,38	0
56	MG	2A	3683	1/1	0.91	0.16	64,64,64,64	0
56	MG	1A	4052	1/1	0.91	0.12	48,48,48,48	0
56	MG	2A	3382	1/1	0.91	0.23	47,47,47,47	0
56	MG	2a	3059	1/1	0.91	0.18	80,80,80,80	0
56	MG	18	107	1/1	0.91	0.14	56,56,56,56	0
56	MG	1A	3480	1/1	0.91	0.12	54,54,54,54	0
56	MG	2a	3063	1/1	0.91	0.10	63,63,63,63	0
56	MG	1A	3232	1/1	0.91	0.25	56,56,56,56	0
56	MG	2a	3065	1/1	0.91	0.10	77,77,77,77	0
56	MG	2A	3395	1/1	0.91	0.24	66,66,66,66	0
56	MG	2A	3156	1/1	0.91	0.28	54,54,54,54	0
56	MG	2A	3699	1/1	0.91	0.11	70,70,70,70	0
56	MG	2A	3160	1/1	0.91	0.15	57,57,57,57	0
56	MG	2A	3399	1/1	0.91	0.18	69,69,69,69	0
56	MG	2A	3166	1/1	0.91	0.18	50,50,50,50	0
56	MG	2a	3083	1/1	0.91	0.22	65,65,65,65	0
56	MG	1a	1607	1/1	0.91	0.09	55,55,55,55	0
56	MG	2A	3170	1/1	0.91	0.14	52,52,52,52	0
56	MG	2a	3089	1/1	0.91	0.15	69,69,69,69	0
56	MG	1A	4057	1/1	0.91	0.10	23,23,23,23	0
56	MG	2A	3410	1/1	0.91	0.11	70,70,70,70	0
56	MG	2A	3412	1/1	0.91	0.10	53,53,53,53	0
56	MG	1A	3898	1/1	0.91	0.14	32,32,32,32	0
56	MG	1A	3418	1/1	0.91	0.11	55,55,55,55	0
56	MG	1a	1619	1/1	0.91	0.19	52,52,52,52	0
56	MG	2A	3419	1/1	0.91	0.13	62,62,62,62	0
56	MG	2A	3420	1/1	0.91	0.12	60,60,60,60	0
56	MG	2A	3723	1/1	0.91	0.12	51,51,51,51	0
56	MG	2A	3182	1/1	0.91	0.15	49,49,49,49	0
56	MG	2A	3186	1/1	0.91	0.24	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
56	MG	2A	3428	1/1	0.91	0.21	50,50,50,50	0
56	MG	1A	3904	1/1	0.91	0.10	32,32,32,32	0
56	MG	2a	3115	1/1	0.91	0.20	61,61,61,61	0
56	MG	2A	3432	1/1	0.91	0.26	40,40,40,40	0
56	MG	1A	3909	1/1	0.91	0.13	49,49,49,49	0
56	MG	1A	3486	1/1	0.91	0.13	44,44,44,44	0
56	MG	2A	3438	1/1	0.91	0.31	56,56,56,56	0
56	MG	2a	3122	1/1	0.91	0.33	73,73,73,73	0
56	MG	2a	3123	1/1	0.91	0.27	68,68,68,68	0
56	MG	2A	3741	1/1	0.91	0.12	42,42,42,42	0
56	MG	1A	3690	1/1	0.91	0.12	19,19,19,19	0
56	MG	1A	3565	1/1	0.91	0.10	58,58,58,58	0
56	MG	2A	3745	1/1	0.91	0.07	50,50,50,50	0
56	MG	2a	3134	1/1	0.91	0.18	58,58,58,58	0
56	MG	2A	3441	1/1	0.91	0.19	60,60,60,60	0
56	MG	1a	1641	1/1	0.91	0.09	57,57,57,57	0
56	MG	2a	3138	1/1	0.91	0.09	67,67,67,67	0
56	MG	2A	3201	1/1	0.91	0.32	70,70,70,70	0
56	MG	1A	3572	1/1	0.91	0.25	39,39,39,39	0
56	MG	2A	3447	1/1	0.91	0.28	55,55,55,55	0
56	MG	1A	4078	1/1	0.91	0.07	24,24,24,24	0
56	MG	1A	3491	1/1	0.91	0.09	38,38,38,38	0
56	MG	2a	3155	1/1	0.91	0.07	70,70,70,70	0
56	MG	1A	3807	1/1	0.91	0.32	27,27,27,27	0
56	MG	1A	3133	1/1	0.91	0.14	35,35,35,35	0
56	MG	2A	3458	1/1	0.91	0.08	53,53,53,53	0
56	MG	2A	3764	1/1	0.91	0.10	44,44,44,44	0
56	MG	2A	3765	1/1	0.91	0.13	53,53,53,53	0
56	MG	2A	3768	1/1	0.91	0.08	42,42,42,42	0
56	MG	1A	3357	1/1	0.91	0.20	48,48,48,48	0
56	MG	1a	1661	1/1	0.91	0.12	58,58,58,58	0
56	MG	1t	201	1/1	0.91	0.13	59,59,59,59	0
56	MG	2A	3775	1/1	0.91	0.16	66,66,66,66	0
56	MG	1A	4089	1/1	0.91	0.15	65,65,65,65	0
56	MG	2A	3792	1/1	0.91	0.14	63,63,63,63	0
56	MG	2A	3795	1/1	0.91	0.09	55,55,55,55	0
56	MG	1w	103	1/1	0.91	0.24	64,64,64,64	0
56	MG	1A	3815	1/1	0.91	0.08	28,28,28,28	0
56	MG	2a	3192	1/1	0.91	0.11	56,56,56,56	0
56	MG	1A	3933	1/1	0.91	0.08	49,49,49,49	0
56	MG	1A	3585	1/1	0.91	0.16	35,35,35,35	0
56	MG	1w	107	1/1	0.91	0.20	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
56	MG	2A	3479	1/1	0.91	0.13	52,52,52,52	0
56	MG	2A	3806	1/1	0.91	0.12	50,50,50,50	0
56	MG	1A	3601	1/1	0.91	0.23	43,43,43,43	0
56	MG	1A	3947	1/1	0.91	0.08	27,27,27,27	0
56	MG	1B	212	1/1	0.91	0.09	40,40,40,40	0
56	MG	1a	1676	1/1	0.91	0.17	72,72,72,72	0
56	MG	1x	108	1/1	0.91	0.26	62,62,62,62	0
56	MG	2A	3495	1/1	0.91	0.10	57,57,57,57	0
56	MG	2a	3217	1/1	0.91	0.13	72,72,72,72	0
56	MG	1a	1685	1/1	0.91	0.28	65,65,65,65	0
56	MG	1a	1686	1/1	0.91	0.14	62,62,62,62	0
56	MG	1A	3358	1/1	0.91	0.08	45,45,45,45	0
56	MG	1A	3336	1/1	0.91	0.12	60,60,60,60	0
56	MG	2A	3255	1/1	0.91	0.13	69,69,69,69	0
56	MG	2A	3513	1/1	0.91	0.10	50,50,50,50	0
56	MG	2a	3231	1/1	0.91	0.10	58,58,58,58	0
56	MG	1a	1690	1/1	0.91	0.08	56,56,56,56	0
56	MG	1B	226	1/1	0.91	0.08	69,69,69,69	0
56	MG	2A	3517	1/1	0.91	0.08	46,46,46,46	0
56	MG	2A	3524	1/1	0.91	0.18	69,69,69,69	0
56	MG	1B	229	1/1	0.91	0.07	38,38,38,38	0
56	MG	2A	3527	1/1	0.91	0.12	44,44,44,44	0
56	MG	2A	3859	1/1	0.91	0.09	60,60,60,60	0
56	MG	1A	3958	1/1	0.91	0.09	50,50,50,50	0
56	MG	2A	3864	1/1	0.91	0.11	69,69,69,69	0
56	MG	1A	3431	1/1	0.91	0.14	54,54,54,54	0
56	MG	1a	1695	1/1	0.91	0.20	52,52,52,52	0
56	MG	2A	3267	1/1	0.91	0.17	67,67,67,67	0
56	MG	2A	3271	1/1	0.91	0.20	58,58,58,58	0
56	MG	1A	3963	1/1	0.91	0.09	33,33,33,33	0
56	MG	1B	236	1/1	0.91	0.10	49,49,49,49	0
56	MG	2A	3547	1/1	0.91	0.11	34,34,34,34	0
56	MG	2A	3550	1/1	0.91	0.15	57,57,57,57	0
56	MG	2t	201	1/1	0.91	0.14	47,47,47,47	0
56	MG	2A	3887	1/1	0.91	0.11	56,56,56,56	0
56	MG	2w	101	1/1	0.91	0.32	69,69,69,69	0
56	MG	1A	3433	1/1	0.91	0.07	31,31,31,31	0
56	MG	2B	202	1/1	0.91	0.08	63,63,63,63	0
56	MG	2A	3033	1/1	0.91	0.13	36,36,36,36	0
56	MG	1A	3091	1/1	0.91	0.26	50,50,50,50	0
56	MG	2B	205	1/1	0.91	0.11	66,66,66,66	0
56	MG	2B	207	1/1	0.91	0.12	61,61,61,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3282	1/1	0.91	0.14	63,63,63,63	0
56	MG	2A	3037	1/1	0.91	0.29	68,68,68,68	0
56	MG	1E	303	1/1	0.91	0.13	38,38,38,38	0
56	MG	1E	309	1/1	0.91	0.13	47,47,47,47	0
56	MG	1a	1710	1/1	0.92	0.15	53,53,53,53	0
56	MG	1A	3123	1/1	0.92	0.12	41,41,41,41	0
56	MG	2D	302	1/1	0.92	0.19	55,55,55,55	0
56	MG	2D	304	1/1	0.92	0.18	57,57,57,57	0
56	MG	2A	3326	1/1	0.92	0.12	61,61,61,61	0
56	MG	1A	3954	1/1	0.92	0.11	75,75,75,75	0
56	MG	1A	3663	1/1	0.92	0.07	21,21,21,21	0
56	MG	1F	304	1/1	0.92	0.07	34,34,34,34	0
56	MG	1A	3002	1/1	0.92	0.13	51,51,51,51	0
56	MG	1A	3342	1/1	0.92	0.25	60,60,60,60	0
56	MG	1A	3089	1/1	0.92	0.10	41,41,41,41	0
56	MG	1G	204	1/1	0.92	0.07	52,52,52,52	0
56	MG	1N	201	1/1	0.92	0.30	51,51,51,51	0
56	MG	2A	3613	1/1	0.92	0.10	46,46,46,46	0
56	MG	2U	203	1/1	0.92	0.14	54,54,54,54	0
56	MG	1A	3530	1/1	0.92	0.09	40,40,40,40	0
56	MG	1O	201	1/1	0.92	0.08	57,57,57,57	0
56	MG	2A	3617	1/1	0.92	0.22	59,59,59,59	0
56	MG	1A	3813	1/1	0.92	0.13	40,40,40,40	0
56	MG	20	103	1/1	0.92	0.14	66,66,66,66	0
56	MG	2A	3619	1/1	0.92	0.08	36,36,36,36	0
56	MG	1A	3814	1/1	0.92	0.16	63,63,63,63	0
56	MG	2A	3621	1/1	0.92	0.19	63,63,63,63	0
56	MG	2A	3622	1/1	0.92	0.08	38,38,38,38	0
56	MG	1P	209	1/1	0.92	0.09	40,40,40,40	0
56	MG	1a	1736	1/1	0.92	0.20	46,46,46,46	0
56	MG	1a	1737	1/1	0.92	0.31	62,62,62,62	0
56	MG	2A	3110	1/1	0.92	0.21	61,61,61,61	0
56	MG	1A	3345	1/1	0.92	0.08	46,46,46,46	0
56	MG	1A	3973	1/1	0.92	0.11	50,50,50,50	0
56	MG	1A	3256	1/1	0.92	0.10	53,53,53,53	0
56	MG	1A	3684	1/1	0.92	0.09	36,36,36,36	0
56	MG	1A	3986	1/1	0.92	0.16	70,70,70,70	0
56	MG	1A	3261	1/1	0.92	0.15	52,52,52,52	0
56	MG	2A	3648	1/1	0.92	0.21	47,47,47,47	0
56	MG	1A	3444	1/1	0.92	0.14	43,43,43,43	0
56	MG	2A	3371	1/1	0.92	0.16	64,64,64,64	0
56	MG	1a	1760	1/1	0.92	0.11	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3658	1/1	0.92	0.19	69,69,69,69	0
56	MG	2A	3135	1/1	0.92	0.19	51,51,51,51	0
56	MG	1A	3535	1/1	0.92	0.15	57,57,57,57	0
56	MG	1W	204	1/1	0.92	0.11	34,34,34,34	0
56	MG	2a	3028	1/1	0.92	0.13	62,62,62,62	0
56	MG	1A	3536	1/1	0.92	0.13	69,69,69,69	0
56	MG	1A	3832	1/1	0.92	0.21	59,59,59,59	0
56	MG	1A	3834	1/1	0.92	0.18	32,32,32,32	0
56	MG	1A	3048	1/1	0.92	0.08	20,20,20,20	0
56	MG	1A	3205	1/1	0.92	0.10	46,46,46,46	0
56	MG	1A	3696	1/1	0.92	0.06	20,20,20,20	0
56	MG	2A	3390	1/1	0.92	0.18	54,54,54,54	0
56	MG	2a	3040	1/1	0.92	0.12	77,77,77,77	0
56	MG	2A	3159	1/1	0.92	0.17	66,66,66,66	0
56	MG	1A	3840	1/1	0.92	0.07	22,22,22,22	0
56	MG	2A	3164	1/1	0.92	0.13	48,48,48,48	0
56	MG	1A	3283	1/1	0.92	0.21	33,33,33,33	0
56	MG	1A	3207	1/1	0.92	0.10	47,47,47,47	0
56	MG	1A	3062	1/1	0.92	0.25	51,51,51,51	0
56	MG	2a	3048	1/1	0.92	0.19	58,58,58,58	0
56	MG	2A	3404	1/1	0.92	0.15	45,45,45,45	0
56	MG	2a	3050	1/1	0.92	0.10	47,47,47,47	0
56	MG	2a	3052	1/1	0.92	0.17	56,56,56,56	0
56	MG	15	102	1/1	0.92	0.14	42,42,42,42	0
56	MG	2A	3172	1/1	0.92	0.12	50,50,50,50	0
56	MG	1A	3848	1/1	0.92	0.15	54,54,54,54	0
56	MG	2a	3058	1/1	0.92	0.12	74,74,74,74	0
56	MG	2A	3175	1/1	0.92	0.13	50,50,50,50	0
56	MG	15	105	1/1	0.92	0.11	49,49,49,49	0
56	MG	1A	4030	1/1	0.92	0.10	61,61,61,61	0
56	MG	2A	3181	1/1	0.92	0.15	44,44,44,44	0
56	MG	2A	3417	1/1	0.92	0.20	68,68,68,68	0
56	MG	18	103	1/1	0.92	0.07	22,22,22,22	0
56	MG	1A	3463	1/1	0.92	0.12	47,47,47,47	0
56	MG	1A	4033	1/1	0.92	0.14	55,55,55,55	0
56	MG	1a	1602	1/1	0.92	0.16	61,61,61,61	0
56	MG	2a	3071	1/1	0.92	0.21	62,62,62,62	0
56	MG	2a	3072	1/1	0.92	0.17	51,51,51,51	0
56	MG	1A	3464	1/1	0.92	0.07	46,46,46,46	0
56	MG	2A	3425	1/1	0.92	0.20	43,43,43,43	0
56	MG	1a	1605	1/1	0.92	0.10	55,55,55,55	0
56	MG	2A	3429	1/1	0.92	0.29	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
56	MG	1A	3065	1/1	0.92	0.10	51,51,51,51	0
56	MG	1A	3468	1/1	0.92	0.17	57,57,57,57	0
56	MG	2A	3724	1/1	0.92	0.20	56,56,56,56	0
56	MG	1A	3367	1/1	0.92	0.16	57,57,57,57	0
56	MG	2a	3093	1/1	0.92	0.18	53,53,53,53	0
56	MG	2A	3202	1/1	0.92	0.12	47,47,47,47	0
56	MG	1A	3711	1/1	0.92	0.15	48,48,48,48	0
56	MG	1a	1616	1/1	0.92	0.07	55,55,55,55	0
56	MG	2a	3098	1/1	0.92	0.22	62,62,62,62	0
56	MG	2A	3206	1/1	0.92	0.15	53,53,53,53	0
56	MG	1A	3162	1/1	0.92	0.38	31,31,31,31	0
56	MG	1b	301	1/1	0.92	0.07	74,74,74,74	0
56	MG	2A	3738	1/1	0.92	0.08	48,48,48,48	0
56	MG	1A	3713	1/1	0.92	0.17	63,63,63,63	0
56	MG	2A	3213	1/1	0.92	0.21	61,61,61,61	0
56	MG	1A	3714	1/1	0.92	0.06	14,14,14,14	0
56	MG	2a	3109	1/1	0.92	0.08	72,72,72,72	0
56	MG	1A	3323	1/1	0.92	0.10	50,50,50,50	0
56	MG	2A	3744	1/1	0.92	0.10	44,44,44,44	0
56	MG	2A	3449	1/1	0.92	0.22	56,56,56,56	0
56	MG	1a	1627	1/1	0.92	0.08	55,55,55,55	0
56	MG	1A	3478	1/1	0.92	0.15	41,41,41,41	0
56	MG	2A	3749	1/1	0.92	0.10	58,58,58,58	0
56	MG	1a	1632	1/1	0.92	0.15	58,58,58,58	0
56	MG	1a	1633	1/1	0.92	0.14	52,52,52,52	0
56	MG	1A	3479	1/1	0.92	0.11	53,53,53,53	0
56	MG	2A	3461	1/1	0.92	0.18	44,44,44,44	0
56	MG	2a	3126	1/1	0.92	0.26	66,66,66,66	0
56	MG	2A	3755	1/1	0.92	0.19	54,54,54,54	0
56	MG	1A	3592	1/1	0.92	0.10	22,22,22,22	0
56	MG	2A	3758	1/1	0.92	0.18	64,64,64,64	0
56	MG	1A	3382	1/1	0.92	0.12	46,46,46,46	0
56	MG	1A	3163	1/1	0.92	0.27	48,48,48,48	0
56	MG	1a	1651	1/1	0.92	0.12	61,61,61,61	0
56	MG	2A	3243	1/1	0.92	0.15	64,64,64,64	0
56	MG	2a	3145	1/1	0.92	0.09	79,79,79,79	0
56	MG	1A	3893	1/1	0.92	0.10	21,21,21,21	0
56	MG	2A	3766	1/1	0.92	0.13	68,68,68,68	0
56	MG	2A	3767	1/1	0.92	0.15	51,51,51,51	0
56	MG	1A	4073	1/1	0.92	0.15	59,59,59,59	0
56	MG	1a	1656	1/1	0.92	0.15	62,62,62,62	0
56	MG	2A	3476	1/1	0.92	0.10	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3478	1/1	0.92	0.08	43,43,43,43	0
56	MG	1A	3482	1/1	0.92	0.08	43,43,43,43	0
56	MG	2A	3483	1/1	0.92	0.12	68,68,68,68	0
56	MG	2A	3788	1/1	0.92	0.07	51,51,51,51	0
56	MG	2A	3789	1/1	0.92	0.10	44,44,44,44	0
56	MG	1A	3895	1/1	0.92	0.08	18,18,18,18	0
56	MG	1A	3742	1/1	0.92	0.10	17,17,17,17	0
56	MG	2A	3486	1/1	0.92	0.13	62,62,62,62	0
56	MG	2A	3489	1/1	0.92	0.34	62,62,62,62	0
56	MG	1A	3397	1/1	0.92	0.20	30,30,30,30	0
56	MG	1A	3398	1/1	0.92	0.22	23,23,23,23	0
56	MG	2a	3179	1/1	0.92	0.07	69,69,69,69	0
56	MG	2A	3492	1/1	0.92	0.34	58,58,58,58	0
56	MG	2A	3256	1/1	0.92	0.21	68,68,68,68	0
56	MG	1a	1664	1/1	0.92	0.08	60,60,60,60	0
56	MG	1A	3613	1/1	0.92	0.14	42,42,42,42	0
56	MG	1A	3905	1/1	0.92	0.23	23,23,23,23	0
56	MG	1A	3623	1/1	0.92	0.09	26,26,26,26	0
56	MG	2a	3194	1/1	0.92	0.09	55,55,55,55	0
56	MG	2A	3811	1/1	0.92	0.09	54,54,54,54	0
56	MG	1a	1671	1/1	0.92	0.08	49,49,49,49	0
56	MG	2a	3198	1/1	0.92	0.12	62,62,62,62	0
56	MG	1A	3074	1/1	0.92	0.25	55,55,55,55	0
56	MG	2A	3511	1/1	0.92	0.10	58,58,58,58	0
56	MG	1A	4099	1/1	0.92	0.10	40,40,40,40	0
56	MG	2A	3269	1/1	0.92	0.12	53,53,53,53	0
56	MG	2A	3515	1/1	0.92	0.10	36,36,36,36	0
56	MG	1A	3493	1/1	0.92	0.10	48,48,48,48	0
56	MG	2A	3011	1/1	0.92	0.10	53,53,53,53	0
56	MG	2a	3215	1/1	0.92	0.12	59,59,59,59	0
56	MG	2A	3016	1/1	0.92	0.29	57,57,57,57	0
56	MG	1A	3770	1/1	0.92	0.06	32,32,32,32	0
56	MG	2a	3218	1/1	0.92	0.20	74,74,74,74	0
56	MG	1a	1678	1/1	0.92	0.08	59,59,59,59	0
56	MG	2A	3833	1/1	0.92	0.11	53,53,53,53	0
56	MG	1A	3184	1/1	0.92	0.15	64,64,64,64	0
56	MG	1A	3918	1/1	0.92	0.11	28,28,28,28	0
56	MG	2A	3844	1/1	0.92	0.09	72,72,72,72	0
56	MG	1A	3640	1/1	0.92	0.15	49,49,49,49	0
56	MG	2A	3855	1/1	0.92	0.11	74,74,74,74	0
56	MG	2A	3536	1/1	0.92	0.09	57,57,57,57	0
56	MG	1B	215	1/1	0.92	0.10	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3332	1/1	0.92	0.09	57,57,57,57	0
56	MG	1A	3775	1/1	0.92	0.09	21,21,21,21	0
56	MG	2A	3867	1/1	0.92	0.10	35,35,35,35	0
56	MG	2A	3047	1/1	0.92	0.06	24,24,24,24	0
56	MG	1B	224	1/1	0.92	0.13	52,52,52,52	0
56	MG	1A	3929	1/1	0.92	0.09	39,39,39,39	0
56	MG	2A	3050	1/1	0.92	0.14	57,57,57,57	0
56	MG	2e	201	1/1	0.92	0.12	64,64,64,64	0
56	MG	1A	3333	1/1	0.92	0.27	56,56,56,56	0
56	MG	1A	3504	1/1	0.92	0.12	54,54,54,54	0
56	MG	1A	3647	1/1	0.92	0.09	30,30,30,30	0
56	MG	2A	3885	1/1	0.92	0.08	59,59,59,59	0
56	MG	1A	3934	1/1	0.92	0.09	55,55,55,55	0
56	MG	2l	204	1/1	0.92	0.16	72,72,72,72	0
56	MG	2A	3304	1/1	0.92	0.11	44,44,44,44	0
56	MG	2A	3306	1/1	0.92	0.14	50,50,50,50	0
56	MG	2A	3569	1/1	0.92	0.09	46,46,46,46	0
56	MG	1A	3245	1/1	0.92	0.09	43,43,43,43	0
56	MG	1a	1701	1/1	0.92	0.29	53,53,53,53	0
56	MG	1a	1703	1/1	0.92	0.28	60,60,60,60	0
56	MG	2B	206	1/1	0.92	0.17	60,60,60,60	0
56	MG	2A	3583	1/1	0.92	0.08	61,61,61,61	0
56	MG	2B	210	1/1	0.92	0.14	67,67,67,67	0
56	MG	2A	3313	1/1	0.92	0.09	57,57,57,57	0
56	MG	2A	3063	1/1	0.92	0.15	58,58,58,58	0
56	MG	1A	3338	1/1	0.92	0.17	48,48,48,48	0
56	MG	2A	3317	1/1	0.92	0.24	49,49,49,49	0
56	MG	2A	3318	1/1	0.92	0.15	50,50,50,50	0
56	MG	2A	3319	1/1	0.92	0.16	53,53,53,53	0
56	MG	1A	3247	1/1	0.92	0.12	53,53,53,53	0
56	MG	2A	3529	1/1	0.93	0.20	52,52,52,52	0
56	MG	1a	1646	1/1	0.93	0.14	56,56,56,56	0
56	MG	1A	3499	1/1	0.93	0.07	44,44,44,44	0
56	MG	2A	3268	1/1	0.93	0.27	57,57,57,57	0
56	MG	1A	3116	1/1	0.93	0.08	36,36,36,36	0
56	MG	1A	3289	1/1	0.93	0.06	49,49,49,49	0
56	MG	1A	3506	1/1	0.93	0.08	47,47,47,47	0
56	MG	2A	3275	1/1	0.93	0.08	59,59,59,59	0
56	MG	2A	3542	1/1	0.93	0.07	46,46,46,46	0
56	MG	2B	208	1/1	0.93	0.11	59,59,59,59	0
56	MG	1A	3760	1/1	0.93	0.18	45,45,45,45	0
56	MG	1A	3117	1/1	0.93	0.10	35,35,35,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3279	1/1	0.93	0.16	62,62,62,62	0
56	MG	1A	4090	1/1	0.93	0.12	53,53,53,53	0
56	MG	1A	3296	1/1	0.93	0.06	32,32,32,32	0
56	MG	2A	3005	1/1	0.93	0.22	55,55,55,55	0
56	MG	2A	3283	1/1	0.93	0.07	57,57,57,57	0
56	MG	1A	3297	1/1	0.93	0.10	50,50,50,50	0
56	MG	2A	3565	1/1	0.93	0.20	68,68,68,68	0
56	MG	2B	219	1/1	0.93	0.13	62,62,62,62	0
56	MG	2A	3286	1/1	0.93	0.19	56,56,56,56	0
56	MG	2A	3567	1/1	0.93	0.08	54,54,54,54	0
56	MG	1A	3768	1/1	0.93	0.09	38,38,38,38	0
56	MG	2A	3289	1/1	0.93	0.14	61,61,61,61	0
56	MG	1a	1665	1/1	0.93	0.16	51,51,51,51	0
56	MG	2D	310	1/1	0.93	0.09	56,56,56,56	0
56	MG	2F	304	1/1	0.93	0.10	54,54,54,54	0
56	MG	2A	3014	1/1	0.93	0.13	55,55,55,55	0
56	MG	2O	8400	1/1	0.93	0.11	64,64,64,64	0
56	MG	1B	201	1/1	0.93	0.20	48,48,48,48	0
56	MG	2P	203	1/1	0.93	0.08	38,38,38,38	0
56	MG	2P	204	1/1	0.93	0.13	57,57,57,57	0
56	MG	2A	3576	1/1	0.93	0.07	26,26,26,26	0
56	MG	2A	3578	1/1	0.93	0.18	54,54,54,54	0
56	MG	2A	3020	1/1	0.93	0.18	39,39,39,39	0
56	MG	2A	3022	1/1	0.93	0.10	56,56,56,56	0
56	MG	2T	201	1/1	0.93	0.12	54,54,54,54	0
56	MG	1A	3769	1/1	0.93	0.09	25,25,25,25	0
56	MG	2T	204	1/1	0.93	0.13	54,54,54,54	0
56	MG	1a	1668	1/1	0.93	0.09	66,66,66,66	0
56	MG	1B	203	1/1	0.93	0.06	33,33,33,33	0
56	MG	2V	201	1/1	0.93	0.21	69,69,69,69	0
56	MG	1a	1670	1/1	0.93	0.20	60,60,60,60	0
56	MG	2V	203	1/1	0.93	0.07	57,57,57,57	0
56	MG	1A	3634	1/1	0.93	0.09	52,52,52,52	0
56	MG	1A	3639	1/1	0.93	0.07	36,36,36,36	0
56	MG	2A	3305	1/1	0.93	0.10	54,54,54,54	0
56	MG	1B	211	1/1	0.93	0.17	51,51,51,51	0
56	MG	25	103	1/1	0.93	0.11	45,45,45,45	0
56	MG	2A	3043	1/1	0.93	0.15	57,57,57,57	0
56	MG	2A	3309	1/1	0.93	0.35	55,55,55,55	0
56	MG	1A	3440	1/1	0.93	0.06	36,36,36,36	0
56	MG	28	101	1/1	0.93	0.13	66,66,66,66	0
56	MG	1B	213	1/1	0.93	0.09	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1a	1677	1/1	0.93	0.15	57,57,57,57	0
56	MG	1A	3920	1/1	0.93	0.22	65,65,65,65	0
56	MG	1a	1679	1/1	0.93	0.18	66,66,66,66	0
56	MG	2A	3316	1/1	0.93	0.18	53,53,53,53	0
56	MG	1A	3518	1/1	0.93	0.12	54,54,54,54	0
56	MG	1A	3234	1/1	0.93	0.12	54,54,54,54	0
56	MG	1B	223	1/1	0.93	0.15	51,51,51,51	0
56	MG	1A	3776	1/1	0.93	0.06	31,31,31,31	0
56	MG	1B	225	1/1	0.93	0.10	53,53,53,53	0
56	MG	1A	3783	1/1	0.93	0.07	17,17,17,17	0
56	MG	2A	3325	1/1	0.93	0.11	57,57,57,57	0
56	MG	2A	3060	1/1	0.93	0.10	46,46,46,46	0
56	MG	2A	3327	1/1	0.93	0.07	51,51,51,51	0
56	MG	1A	3303	1/1	0.93	0.29	55,55,55,55	0
56	MG	2a	3018	1/1	0.93	0.30	61,61,61,61	0
56	MG	1A	3931	1/1	0.93	0.07	40,40,40,40	0
56	MG	2A	3331	1/1	0.93	0.14	72,72,72,72	0
56	MG	2A	3628	1/1	0.93	0.14	55,55,55,55	0
56	MG	2a	3024	1/1	0.93	0.19	59,59,59,59	0
56	MG	2a	3025	1/1	0.93	0.12	59,59,59,59	0
56	MG	2a	3026	1/1	0.93	0.15	60,60,60,60	0
56	MG	2A	3332	1/1	0.93	0.07	46,46,46,46	0
56	MG	1B	232	1/1	0.93	0.09	50,50,50,50	0
56	MG	1A	3447	1/1	0.93	0.17	51,51,51,51	0
56	MG	2A	3068	1/1	0.93	0.18	61,61,61,61	0
56	MG	1A	3528	1/1	0.93	0.11	47,47,47,47	0
56	MG	2A	3639	1/1	0.93	0.13	42,42,42,42	0
56	MG	1A	3651	1/1	0.93	0.08	37,37,37,37	0
56	MG	2A	3072	1/1	0.93	0.09	61,61,61,61	0
56	MG	2A	3644	1/1	0.93	0.20	43,43,43,43	0
56	MG	1A	3653	1/1	0.93	0.10	35,35,35,35	0
56	MG	2A	3075	1/1	0.93	0.07	48,48,48,48	0
56	MG	2A	3649	1/1	0.93	0.12	68,68,68,68	0
56	MG	2A	3077	1/1	0.93	0.10	57,57,57,57	0
56	MG	2A	3078	1/1	0.93	0.24	59,59,59,59	0
56	MG	2A	3656	1/1	0.93	0.14	59,59,59,59	0
56	MG	1A	3941	1/1	0.93	0.06	35,35,35,35	0
56	MG	1A	3096	1/1	0.93	0.13	57,57,57,57	0
56	MG	1A	3945	1/1	0.93	0.12	56,56,56,56	0
56	MG	1a	1708	1/1	0.93	0.24	58,58,58,58	0
56	MG	1E	310	1/1	0.93	0.21	61,61,61,61	0
56	MG	1A	3309	1/1	0.93	0.11	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3093	1/1	0.93	0.08	37,37,37,37	0
56	MG	1A	3312	1/1	0.93	0.07	34,34,34,34	0
56	MG	1A	3361	1/1	0.93	0.12	56,56,56,56	0
56	MG	1A	3802	1/1	0.93	0.10	60,60,60,60	0
56	MG	1a	1718	1/1	0.93	0.16	53,53,53,53	0
56	MG	1A	3365	1/1	0.93	0.16	55,55,55,55	0
56	MG	1A	3366	1/1	0.93	0.09	40,40,40,40	0
56	MG	1A	3674	1/1	0.93	0.08	22,22,22,22	0
56	MG	1A	3314	1/1	0.93	0.17	48,48,48,48	0
56	MG	1A	3537	1/1	0.93	0.08	61,61,61,61	0
56	MG	2a	3067	1/1	0.93	0.12	47,47,47,47	0
56	MG	1A	3678	1/1	0.93	0.08	23,23,23,23	0
56	MG	2a	3069	1/1	0.93	0.09	62,62,62,62	0
56	MG	1A	3969	1/1	0.93	0.10	42,42,42,42	0
56	MG	2A	3114	1/1	0.93	0.37	64,64,64,64	0
56	MG	1P	207	1/1	0.93	0.11	51,51,51,51	0
56	MG	2a	3074	1/1	0.93	0.21	52,52,52,52	0
56	MG	2A	3694	1/1	0.93	0.12	50,50,50,50	0
56	MG	2a	3078	1/1	0.93	0.18	50,50,50,50	0
56	MG	2A	3695	1/1	0.93	0.07	60,60,60,60	0
56	MG	2a	3081	1/1	0.93	0.28	60,60,60,60	0
56	MG	2A	3696	1/1	0.93	0.08	55,55,55,55	0
56	MG	2A	3117	1/1	0.93	0.10	55,55,55,55	0
56	MG	2a	3084	1/1	0.93	0.28	58,58,58,58	0
56	MG	2A	3384	1/1	0.93	0.09	62,62,62,62	0
56	MG	1A	3016	1/1	0.93	0.16	45,45,45,45	0
56	MG	2a	3088	1/1	0.93	0.11	55,55,55,55	0
56	MG	2A	3701	1/1	0.93	0.08	58,58,58,58	0
56	MG	1Q	205	1/1	0.93	0.06	55,55,55,55	0
56	MG	1A	3539	1/1	0.93	0.22	45,45,45,45	0
56	MG	2A	3392	1/1	0.93	0.15	58,58,58,58	0
56	MG	1a	1735	1/1	0.93	0.22	53,53,53,53	0
56	MG	1R	203	1/1	0.93	0.23	46,46,46,46	0
56	MG	2a	3097	1/1	0.93	0.29	49,49,49,49	0
56	MG	1A	3320	1/1	0.93	0.18	46,46,46,46	0
56	MG	1A	3544	1/1	0.93	0.14	37,37,37,37	0
56	MG	2A	3400	1/1	0.93	0.13	59,59,59,59	0
56	MG	1A	3984	1/1	0.93	0.08	71,71,71,71	0
56	MG	2A	3148	1/1	0.93	0.13	51,51,51,51	0
56	MG	2a	3105	1/1	0.93	0.12	45,45,45,45	0
56	MG	2A	3717	1/1	0.93	0.07	51,51,51,51	0
56	MG	1A	3546	1/1	0.93	0.17	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
56	MG	1a	1748	1/1	0.93	0.06	36,36,36,36	0
56	MG	1A	3194	1/1	0.93	0.25	33,33,33,33	0
56	MG	2a	3110	1/1	0.93	0.15	62,62,62,62	0
56	MG	2a	3111	1/1	0.93	0.13	63,63,63,63	0
56	MG	1a	1752	1/1	0.93	0.10	74,74,74,74	0
56	MG	2A	3154	1/1	0.93	0.17	52,52,52,52	0
56	MG	2a	3114	1/1	0.93	0.12	65,65,65,65	0
56	MG	1A	3026	1/1	0.93	0.07	45,45,45,45	0
56	MG	2A	3415	1/1	0.93	0.15	62,62,62,62	0
56	MG	1a	1754	1/1	0.93	0.11	57,57,57,57	0
56	MG	2a	3118	1/1	0.93	0.28	62,62,62,62	0
56	MG	2A	3732	1/1	0.93	0.19	72,72,72,72	0
56	MG	1A	3202	1/1	0.93	0.08	40,40,40,40	0
56	MG	1V	205	1/1	0.93	0.07	29,29,29,29	0
56	MG	2A	3163	1/1	0.93	0.14	57,57,57,57	0
56	MG	1V	207	1/1	0.93	0.07	52,52,52,52	0
56	MG	1A	3556	1/1	0.93	0.21	41,41,41,41	0
56	MG	2A	3422	1/1	0.93	0.07	42,42,42,42	0
56	MG	2A	3167	1/1	0.93	0.08	39,39,39,39	0
56	MG	1a	1765	1/1	0.93	0.13	51,51,51,51	0
56	MG	2A	3426	1/1	0.93	0.23	42,42,42,42	0
56	MG	2A	3427	1/1	0.93	0.20	42,42,42,42	0
56	MG	1A	3330	1/1	0.93	0.12	46,46,46,46	0
56	MG	1A	3164	1/1	0.93	0.15	52,52,52,52	0
56	MG	2a	3140	1/1	0.93	0.08	57,57,57,57	0
56	MG	1a	1768	1/1	0.93	0.17	64,64,64,64	0
56	MG	1A	3996	1/1	0.93	0.16	51,51,51,51	0
56	MG	1A	3107	1/1	0.93	0.07	27,27,27,27	0
56	MG	1A	3843	1/1	0.93	0.07	51,51,51,51	0
56	MG	1a	1776	1/1	0.93	0.12	58,58,58,58	0
56	MG	10	101	1/1	0.93	0.07	38,38,38,38	0
56	MG	1A	4001	1/1	0.93	0.12	48,48,48,48	0
56	MG	1A	3180	1/1	0.93	0.12	35,35,35,35	0
56	MG	2A	3187	1/1	0.93	0.19	56,56,56,56	0
56	MG	11	102	1/1	0.93	0.12	42,42,42,42	0
56	MG	1A	3566	1/1	0.93	0.22	52,52,52,52	0
56	MG	2A	3446	1/1	0.93	0.30	63,63,63,63	0
56	MG	2A	3763	1/1	0.93	0.12	60,60,60,60	0
56	MG	11	105	1/1	0.93	0.09	53,53,53,53	0
56	MG	1A	4008	1/1	0.93	0.33	33,33,33,33	0
56	MG	1A	3212	1/1	0.93	0.08	35,35,35,35	0
56	MG	2A	3450	1/1	0.93	0.21	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3484	1/1	0.93	0.13	59,59,59,59	0
56	MG	2A	3453	1/1	0.93	0.14	52,52,52,52	0
56	MG	2a	3182	1/1	0.93	0.09	83,83,83,83	0
56	MG	2A	3454	1/1	0.93	0.24	50,50,50,50	0
56	MG	2a	3185	1/1	0.93	0.14	52,52,52,52	0
56	MG	2A	3200	1/1	0.93	0.23	48,48,48,48	0
56	MG	1A	3183	1/1	0.93	0.08	48,48,48,48	0
56	MG	2A	3777	1/1	0.93	0.09	47,47,47,47	0
56	MG	1A	3853	1/1	0.93	0.13	55,55,55,55	0
56	MG	2A	3784	1/1	0.93	0.11	64,64,64,64	0
56	MG	2A	3785	1/1	0.93	0.08	53,53,53,53	0
56	MG	1a	1797	1/1	0.93	0.08	65,65,65,65	0
56	MG	1a	1798	1/1	0.93	0.09	76,76,76,76	0
56	MG	2A	3791	1/1	0.93	0.13	56,56,56,56	0
56	MG	1A	3576	1/1	0.93	0.20	43,43,43,43	0
56	MG	1A	3487	1/1	0.93	0.10	44,44,44,44	0
56	MG	1A	3861	1/1	0.93	0.10	61,61,61,61	0
56	MG	2A	3798	1/1	0.93	0.09	51,51,51,51	0
56	MG	2a	3203	1/1	0.93	0.07	63,63,63,63	0
56	MG	1A	3864	1/1	0.93	0.13	52,52,52,52	0
56	MG	1A	3584	1/1	0.93	0.07	32,32,32,32	0
56	MG	2A	3470	1/1	0.93	0.16	62,62,62,62	0
56	MG	2A	3803	1/1	0.93	0.08	81,81,81,81	0
56	MG	1a	1603	1/1	0.93	0.08	61,61,61,61	0
56	MG	2A	3215	1/1	0.93	0.15	56,56,56,56	0
56	MG	1A	3265	1/1	0.93	0.12	43,43,43,43	0
56	MG	2a	3219	1/1	0.93	0.14	68,68,68,68	0
56	MG	1A	3587	1/1	0.93	0.23	35,35,35,35	0
56	MG	2a	3223	1/1	0.93	0.15	64,64,64,64	0
56	MG	2A	3221	1/1	0.93	0.10	57,57,57,57	0
56	MG	1a	1830	1/1	0.93	0.17	42,42,42,42	0
56	MG	1A	3589	1/1	0.93	0.10	35,35,35,35	0
56	MG	1A	4051	1/1	0.93	0.13	58,58,58,58	0
56	MG	1A	3871	1/1	0.93	0.07	32,32,32,32	0
56	MG	2a	3230	1/1	0.93	0.09	65,65,65,65	0
56	MG	2A	3230	1/1	0.93	0.16	67,67,67,67	0
56	MG	2a	3232	1/1	0.93	0.07	63,63,63,63	0
56	MG	2A	3487	1/1	0.93	0.27	48,48,48,48	0
56	MG	2A	3818	1/1	0.93	0.08	64,64,64,64	0
56	MG	1A	3221	1/1	0.93	0.09	46,46,46,46	0
56	MG	1a	1613	1/1	0.93	0.15	49,49,49,49	0
56	MG	1A	4054	1/1	0.93	0.17	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
56	MG	1A	3594	1/1	0.93	0.15	55,55,55,55	0
56	MG	2A	3241	1/1	0.93	0.23	62,62,62,62	0
56	MG	1a	1618	1/1	0.93	0.10	49,49,49,49	0
56	MG	1A	3271	1/1	0.93	0.23	44,44,44,44	0
56	MG	2A	3832	1/1	0.93	0.09	38,38,38,38	0
56	MG	1A	3881	1/1	0.93	0.13	36,36,36,36	0
56	MG	2A	3834	1/1	0.93	0.12	48,48,48,48	0
56	MG	2i	201	1/1	0.93	0.08	62,62,62,62	0
56	MG	2A	3836	1/1	0.93	0.10	62,62,62,62	0
56	MG	2A	3499	1/1	0.93	0.09	47,47,47,47	0
56	MG	2A	3501	1/1	0.93	0.07	58,58,58,58	0
56	MG	1w	101	1/1	0.93	0.21	65,65,65,65	0
56	MG	1A	3727	1/1	0.93	0.07	39,39,39,39	0
56	MG	2A	3505	1/1	0.93	0.21	57,57,57,57	0
56	MG	1A	3884	1/1	0.93	0.17	28,28,28,28	0
56	MG	1a	1629	1/1	0.93	0.19	54,54,54,54	0
56	MG	2A	3512	1/1	0.93	0.16	58,58,58,58	0
56	MG	1A	3728	1/1	0.93	0.10	44,44,44,44	0
56	MG	1A	3887	1/1	0.93	0.09	31,31,31,31	0
56	MG	1A	3497	1/1	0.93	0.09	50,50,50,50	0
56	MG	1A	3734	1/1	0.93	0.10	49,49,49,49	0
56	MG	2x	101	1/1	0.93	0.10	60,60,60,60	0
56	MG	1a	1638	1/1	0.93	0.19	61,61,61,61	0
56	MG	2A	3518	1/1	0.93	0.11	53,53,53,53	0
56	MG	1A	4074	1/1	0.93	0.08	48,48,48,48	0
56	MG	2A	3880	1/1	0.93	0.11	52,52,52,52	0
56	MG	1A	3279	1/1	0.93	0.18	39,39,39,39	0
56	MG	2A	3526	1/1	0.93	0.08	30,30,30,30	0
56	MG	2y	104	1/1	0.93	0.08	50,50,50,50	0
56	MG	1A	3607	1/1	0.93	0.10	27,27,27,27	0
56	MG	1A	3704	1/1	0.94	0.06	21,21,21,21	0
56	MG	1x	118	1/1	0.94	0.09	58,58,58,58	0
56	MG	1A	3558	1/1	0.94	0.21	54,54,54,54	0
56	MG	2A	3292	1/1	0.94	0.22	57,57,57,57	0
56	MG	2A	3571	1/1	0.94	0.09	42,42,42,42	0
56	MG	1A	3868	1/1	0.94	0.08	35,35,35,35	0
56	MG	2A	3573	1/1	0.94	0.10	62,62,62,62	0
56	MG	2D	306	1/1	0.94	0.32	47,47,47,47	0
56	MG	2D	307	1/1	0.94	0.27	47,47,47,47	0
56	MG	2A	3574	1/1	0.94	0.13	46,46,46,46	0
56	MG	1A	3462	1/1	0.94	0.14	54,54,54,54	0
56	MG	1a	1643	1/1	0.94	0.07	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
56	MG	2E	301	1/1	0.94	0.10	49,49,49,49	0
56	MG	2E	302	1/1	0.94	0.13	61,61,61,61	0
56	MG	2F	302	1/1	0.94	0.17	64,64,64,64	0
56	MG	1A	3870	1/1	0.94	0.10	30,30,30,30	0
56	MG	2A	3298	1/1	0.94	0.16	57,57,57,57	0
56	MG	1a	1647	1/1	0.94	0.20	55,55,55,55	0
56	MG	1A	3111	1/1	0.94	0.10	37,37,37,37	0
56	MG	1A	3304	1/1	0.94	0.15	21,21,21,21	0
56	MG	2A	3590	1/1	0.94	0.10	64,64,64,64	0
56	MG	2Q	201	1/1	0.94	0.06	49,49,49,49	0
56	MG	2Q	202	1/1	0.94	0.10	53,53,53,53	0
56	MG	2A	3592	1/1	0.94	0.09	46,46,46,46	0
56	MG	1A	3564	1/1	0.94	0.12	49,49,49,49	0
56	MG	2A	3021	1/1	0.94	0.24	55,55,55,55	0
56	MG	1A	3050	1/1	0.94	0.09	21,21,21,21	0
56	MG	2A	3024	1/1	0.94	0.18	48,48,48,48	0
56	MG	2A	3025	1/1	0.94	0.06	44,44,44,44	0
56	MG	2A	3026	1/1	0.94	0.23	53,53,53,53	0
56	MG	1A	3182	1/1	0.94	0.16	49,49,49,49	0
56	MG	2U	202	1/1	0.94	0.28	58,58,58,58	0
56	MG	1a	1658	1/1	0.94	0.10	63,63,63,63	0
56	MG	1A	3470	1/1	0.94	0.18	49,49,49,49	0
56	MG	2A	3312	1/1	0.94	0.10	50,50,50,50	0
56	MG	1A	3717	1/1	0.94	0.08	41,41,41,41	0
56	MG	1A	3310	1/1	0.94	0.24	40,40,40,40	0
56	MG	2W	202	1/1	0.94	0.08	45,45,45,45	0
56	MG	2W	203	1/1	0.94	0.08	51,51,51,51	0
56	MG	2X	101	1/1	0.94	0.08	56,56,56,56	0
56	MG	1A	3243	1/1	0.94	0.17	33,33,33,33	0
56	MG	1A	3474	1/1	0.94	0.23	32,32,32,32	0
56	MG	1A	3889	1/1	0.94	0.10	44,44,44,44	0
56	MG	21	101	1/1	0.94	0.28	55,55,55,55	0
56	MG	23	101	1/1	0.94	0.10	54,54,54,54	0
56	MG	23	102	1/1	0.94	0.09	45,45,45,45	0
56	MG	25	101	1/1	0.94	0.37	58,58,58,58	0
56	MG	1A	3051	1/1	0.94	0.15	31,31,31,31	0
56	MG	1A	3578	1/1	0.94	0.08	43,43,43,43	0
56	MG	2A	3320	1/1	0.94	0.22	54,54,54,54	0
56	MG	1A	4092	1/1	0.94	0.10	54,54,54,54	0
56	MG	27	102	1/1	0.94	0.16	34,34,34,34	0
56	MG	1A	3581	1/1	0.94	0.06	15,15,15,15	0
56	MG	28	102	1/1	0.94	0.10	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3378	1/1	0.94	0.10	42,42,42,42	0
56	MG	1A	3379	1/1	0.94	0.13	48,48,48,48	0
56	MG	1a	1672	1/1	0.94	0.07	44,44,44,44	0
56	MG	1A	3896	1/1	0.94	0.08	60,60,60,60	0
56	MG	1A	3737	1/1	0.94	0.06	41,41,41,41	0
56	MG	1A	3084	1/1	0.94	0.11	33,33,33,33	0
56	MG	1B	206	1/1	0.94	0.12	40,40,40,40	0
56	MG	2A	3629	1/1	0.94	0.10	36,36,36,36	0
56	MG	1A	3381	1/1	0.94	0.19	52,52,52,52	0
56	MG	1A	3318	1/1	0.94	0.20	43,43,43,43	0
56	MG	2A	3633	1/1	0.94	0.12	40,40,40,40	0
56	MG	1A	3746	1/1	0.94	0.12	46,46,46,46	0
56	MG	1a	1680	1/1	0.94	0.20	63,63,63,63	0
56	MG	2A	3338	1/1	0.94	0.14	62,62,62,62	0
56	MG	2A	3638	1/1	0.94	0.15	55,55,55,55	0
56	MG	1a	1683	1/1	0.94	0.10	43,43,43,43	0
56	MG	1a	1684	1/1	0.94	0.28	63,63,63,63	0
56	MG	2A	3641	1/1	0.94	0.09	38,38,38,38	0
56	MG	1A	3906	1/1	0.94	0.10	49,49,49,49	0
56	MG	1A	3747	1/1	0.94	0.06	54,54,54,54	0
56	MG	1A	3910	1/1	0.94	0.11	51,51,51,51	0
56	MG	1A	3388	1/1	0.94	0.12	44,44,44,44	0
56	MG	1a	1689	1/1	0.94	0.07	59,59,59,59	0
56	MG	2A	3076	1/1	0.94	0.12	31,31,31,31	0
56	MG	1A	3600	1/1	0.94	0.12	39,39,39,39	0
56	MG	2A	3653	1/1	0.94	0.17	61,61,61,61	0
56	MG	1A	3757	1/1	0.94	0.11	50,50,50,50	0
56	MG	2A	3079	1/1	0.94	0.12	46,46,46,46	0
56	MG	1A	3390	1/1	0.94	0.13	36,36,36,36	0
56	MG	2A	3358	1/1	0.94	0.17	56,56,56,56	0
56	MG	1A	3391	1/1	0.94	0.07	42,42,42,42	0
56	MG	1A	3392	1/1	0.94	0.08	45,45,45,45	0
56	MG	2A	3363	1/1	0.94	0.11	51,51,51,51	0
56	MG	2A	3668	1/1	0.94	0.15	54,54,54,54	0
56	MG	2A	3670	1/1	0.94	0.16	47,47,47,47	0
56	MG	1A	3763	1/1	0.94	0.08	22,22,22,22	0
56	MG	1a	1696	1/1	0.94	0.23	44,44,44,44	0
56	MG	1A	3923	1/1	0.94	0.11	59,59,59,59	0
56	MG	2a	3047	1/1	0.94	0.14	55,55,55,55	0
56	MG	2A	3675	1/1	0.94	0.12	57,57,57,57	0
56	MG	1A	3490	1/1	0.94	0.09	35,35,35,35	0
56	MG	2A	3369	1/1	0.94	0.12	64,64,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	3051	1/1	0.94	0.13	62,62,62,62	0
56	MG	2A	3370	1/1	0.94	0.16	64,64,64,64	0
56	MG	1a	1699	1/1	0.94	0.29	47,47,47,47	0
56	MG	1A	3052	1/1	0.94	0.08	40,40,40,40	0
56	MG	2A	3682	1/1	0.94	0.15	74,74,74,74	0
56	MG	1A	3034	1/1	0.94	0.20	23,23,23,23	0
56	MG	1A	3130	1/1	0.94	0.09	29,29,29,29	0
56	MG	1a	1706	1/1	0.94	0.23	59,59,59,59	0
56	MG	1A	3621	1/1	0.94	0.09	27,27,27,27	0
56	MG	2A	3379	1/1	0.94	0.15	56,56,56,56	0
56	MG	2A	3690	1/1	0.94	0.07	40,40,40,40	0
56	MG	1B	239	1/1	0.94	0.07	30,30,30,30	0
56	MG	1D	306	1/1	0.94	0.12	33,33,33,33	0
56	MG	1D	310	1/1	0.94	0.09	24,24,24,24	0
56	MG	1a	1712	1/1	0.94	0.09	53,53,53,53	0
56	MG	1A	3328	1/1	0.94	0.15	48,48,48,48	0
56	MG	1D	313	1/1	0.94	0.18	34,34,34,34	0
56	MG	2A	3115	1/1	0.94	0.08	41,41,41,41	0
56	MG	1A	3400	1/1	0.94	0.33	42,42,42,42	0
56	MG	1a	1717	1/1	0.94	0.15	64,64,64,64	0
56	MG	2a	3075	1/1	0.94	0.16	57,57,57,57	0
56	MG	2a	3076	1/1	0.94	0.07	53,53,53,53	0
56	MG	2A	3394	1/1	0.94	0.25	51,51,51,51	0
56	MG	2A	3118	1/1	0.94	0.15	43,43,43,43	0
56	MG	2A	3706	1/1	0.94	0.08	68,68,68,68	0
56	MG	1E	308	1/1	0.94	0.06	31,31,31,31	0
56	MG	1A	3401	1/1	0.94	0.20	35,35,35,35	0
56	MG	2A	3122	1/1	0.94	0.24	53,53,53,53	0
56	MG	1A	3627	1/1	0.94	0.08	18,18,18,18	0
56	MG	2A	3401	1/1	0.94	0.10	54,54,54,54	0
56	MG	1A	3095	1/1	0.94	0.18	44,44,44,44	0
56	MG	2A	3403	1/1	0.94	0.09	57,57,57,57	0
56	MG	1a	1724	1/1	0.94	0.21	49,49,49,49	0
56	MG	2a	3090	1/1	0.94	0.15	66,66,66,66	0
56	MG	1A	3780	1/1	0.94	0.09	34,34,34,34	0
56	MG	1F	305	1/1	0.94	0.07	45,45,45,45	0
56	MG	1A	3781	1/1	0.94	0.07	41,41,41,41	0
56	MG	2A	3409	1/1	0.94	0.26	66,66,66,66	0
56	MG	2A	3144	1/1	0.94	0.19	54,54,54,54	0
56	MG	2A	3726	1/1	0.94	0.07	50,50,50,50	0
56	MG	1A	3403	1/1	0.94	0.08	53,53,53,53	0
56	MG	1A	3635	1/1	0.94	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
56	MG	1A	3505	1/1	0.94	0.08	39,39,39,39	0
56	MG	1A	3257	1/1	0.94	0.15	58,58,58,58	0
56	MG	1N	204	1/1	0.94	0.17	42,42,42,42	0
56	MG	1A	3641	1/1	0.94	0.07	22,22,22,22	0
56	MG	1A	3961	1/1	0.94	0.07	56,56,56,56	0
56	MG	1A	3794	1/1	0.94	0.16	48,48,48,48	0
56	MG	2A	3158	1/1	0.94	0.28	56,56,56,56	0
56	MG	1P	202	1/1	0.94	0.14	23,23,23,23	0
56	MG	1P	205	1/1	0.94	0.07	16,16,16,16	0
56	MG	2A	3161	1/1	0.94	0.15	64,64,64,64	0
56	MG	2A	3162	1/1	0.94	0.19	64,64,64,64	0
56	MG	1a	1744	1/1	0.94	0.15	54,54,54,54	0
56	MG	1A	3642	1/1	0.94	0.06	14,14,14,14	0
56	MG	2A	3165	1/1	0.94	0.30	65,65,65,65	0
56	MG	1A	3510	1/1	0.94	0.06	41,41,41,41	0
56	MG	1A	3408	1/1	0.94	0.18	32,32,32,32	0
56	MG	1Q	204	1/1	0.94	0.08	44,44,44,44	0
56	MG	2a	3119	1/1	0.94	0.11	69,69,69,69	0
56	MG	1A	3258	1/1	0.94	0.17	25,25,25,25	0
56	MG	1A	3054	1/1	0.94	0.07	42,42,42,42	0
56	MG	1A	3416	1/1	0.94	0.12	36,36,36,36	0
56	MG	1A	3972	1/1	0.94	0.08	43,43,43,43	0
56	MG	1A	3020	1/1	0.94	0.07	33,33,33,33	0
56	MG	1a	1762	1/1	0.94	0.10	61,61,61,61	0
56	MG	2A	3178	1/1	0.94	0.14	48,48,48,48	0
56	MG	2a	3129	1/1	0.94	0.07	49,49,49,49	0
56	MG	1A	3976	1/1	0.94	0.09	47,47,47,47	0
56	MG	1A	3519	1/1	0.94	0.10	45,45,45,45	0
56	MG	1A	3980	1/1	0.94	0.08	62,62,62,62	0
56	MG	1A	3981	1/1	0.94	0.08	60,60,60,60	0
56	MG	1U	209	1/1	0.94	0.30	44,44,44,44	0
56	MG	1A	3100	1/1	0.94	0.15	41,41,41,41	0
56	MG	1A	3660	1/1	0.94	0.06	31,31,31,31	0
56	MG	2a	3144	1/1	0.94	0.09	65,65,65,65	0
56	MG	1A	3985	1/1	0.94	0.11	61,61,61,61	0
56	MG	1A	3523	1/1	0.94	0.11	53,53,53,53	0
56	MG	1a	1777	1/1	0.94	0.11	59,59,59,59	0
56	MG	2A	3772	1/1	0.94	0.12	66,66,66,66	0
56	MG	1A	3268	1/1	0.94	0.15	35,35,35,35	0
56	MG	1A	3147	1/1	0.94	0.11	39,39,39,39	0
56	MG	2A	3459	1/1	0.94	0.13	41,41,41,41	0
56	MG	2A	3779	1/1	0.94	0.07	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
56	MG	1A	3664	1/1	0.94	0.07	40,40,40,40	0
56	MG	1A	3424	1/1	0.94	0.09	48,48,48,48	0
56	MG	2A	3203	1/1	0.94	0.20	48,48,48,48	0
56	MG	1A	3148	1/1	0.94	0.16	35,35,35,35	0
56	MG	2a	3167	1/1	0.94	0.06	75,75,75,75	0
56	MG	1A	3668	1/1	0.94	0.06	21,21,21,21	0
56	MG	2a	3172	1/1	0.94	0.08	62,62,62,62	0
56	MG	1A	3825	1/1	0.94	0.12	34,34,34,34	0
56	MG	2A	3468	1/1	0.94	0.32	51,51,51,51	0
56	MG	2A	3793	1/1	0.94	0.15	77,77,77,77	0
56	MG	1a	1788	1/1	0.94	0.07	61,61,61,61	0
56	MG	2a	3177	1/1	0.94	0.14	65,65,65,65	0
56	MG	1A	3997	1/1	0.94	0.15	45,45,45,45	0
56	MG	1A	3276	1/1	0.94	0.09	45,45,45,45	0
56	MG	2a	3180	1/1	0.94	0.08	71,71,71,71	0
56	MG	2a	3181	1/1	0.94	0.12	64,64,64,64	0
56	MG	2A	3473	1/1	0.94	0.21	60,60,60,60	0
56	MG	11	103	1/1	0.94	0.07	36,36,36,36	0
56	MG	1A	3999	1/1	0.94	0.08	39,39,39,39	0
56	MG	1A	3278	1/1	0.94	0.07	41,41,41,41	0
56	MG	1A	3209	1/1	0.94	0.10	38,38,38,38	0
56	MG	12	102	1/1	0.94	0.09	39,39,39,39	0
56	MG	2A	3480	1/1	0.94	0.11	46,46,46,46	0
56	MG	2A	3219	1/1	0.94	0.16	52,52,52,52	0
56	MG	13	103	1/1	0.94	0.06	39,39,39,39	0
56	MG	1a	1803	1/1	0.94	0.09	61,61,61,61	0
56	MG	1A	4002	1/1	0.94	0.07	31,31,31,31	0
56	MG	2A	3226	1/1	0.94	0.10	57,57,57,57	0
56	MG	1A	3435	1/1	0.94	0.08	42,42,42,42	0
56	MG	1A	3436	1/1	0.94	0.07	49,49,49,49	0
56	MG	1A	4007	1/1	0.94	0.07	15,15,15,15	0
56	MG	1A	3837	1/1	0.94	0.11	51,51,51,51	0
56	MG	2A	3235	1/1	0.94	0.12	44,44,44,44	0
56	MG	2A	3236	1/1	0.94	0.10	45,45,45,45	0
56	MG	2a	3206	1/1	0.94	0.15	62,62,62,62	0
56	MG	17	104	1/1	0.94	0.07	37,37,37,37	0
56	MG	2A	3824	1/1	0.94	0.11	66,66,66,66	0
56	MG	1a	1829	1/1	0.94	0.14	43,43,43,43	0
56	MG	2A	3827	1/1	0.94	0.07	62,62,62,62	0
56	MG	18	101	1/1	0.94	0.11	37,37,37,37	0
56	MG	1A	4009	1/1	0.94	0.16	23,23,23,23	0
56	MG	2A	3242	1/1	0.94	0.08	64,64,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	18	104	1/1	0.94	0.12	49,49,49,49	0
56	MG	2a	3221	1/1	0.94	0.10	55,55,55,55	0
56	MG	2A	3245	1/1	0.94	0.09	47,47,47,47	0
56	MG	1A	4011	1/1	0.94	0.08	65,65,65,65	0
56	MG	1A	4012	1/1	0.94	0.09	68,68,68,68	0
56	MG	1A	4015	1/1	0.94	0.05	29,29,29,29	0
56	MG	1A	3437	1/1	0.94	0.18	53,53,53,53	0
56	MG	2A	3841	1/1	0.94	0.09	47,47,47,47	0
56	MG	1A	3151	1/1	0.94	0.12	42,42,42,42	0
56	MG	2A	3848	1/1	0.94	0.07	74,74,74,74	0
56	MG	1e	202	1/1	0.94	0.14	59,59,59,59	0
56	MG	1A	3155	1/1	0.94	0.11	43,43,43,43	0
56	MG	2a	3234	1/1	0.94	0.11	60,60,60,60	0
56	MG	1A	4019	1/1	0.94	0.06	22,22,22,22	0
56	MG	1A	4022	1/1	0.94	0.08	31,31,31,31	0
56	MG	1v	101	1/1	0.94	0.12	65,65,65,65	0
56	MG	1A	3291	1/1	0.94	0.09	32,32,32,32	0
56	MG	1A	3350	1/1	0.94	0.23	51,51,51,51	0
56	MG	1A	3846	1/1	0.94	0.07	39,39,39,39	0
56	MG	1A	3351	1/1	0.94	0.30	47,47,47,47	0
56	MG	1A	4037	1/1	0.94	0.07	68,68,68,68	0
56	MG	2A	3874	1/1	0.94	0.12	66,66,66,66	0
56	MG	2f	201	1/1	0.94	0.10	48,48,48,48	0
56	MG	1A	3545	1/1	0.94	0.09	46,46,46,46	0
56	MG	2A	3876	1/1	0.94	0.14	47,47,47,47	0
56	MG	1A	3217	1/1	0.94	0.06	39,39,39,39	0
56	MG	1a	1621	1/1	0.94	0.13	51,51,51,51	0
56	MG	1a	1622	1/1	0.94	0.07	40,40,40,40	0
56	MG	2A	3883	1/1	0.94	0.11	68,68,68,68	0
56	MG	2A	3272	1/1	0.94	0.12	56,56,56,56	0
56	MG	1a	1623	1/1	0.94	0.17	55,55,55,55	0
56	MG	1x	101	1/1	0.94	0.12	38,38,38,38	0
56	MG	1A	3454	1/1	0.94	0.19	39,39,39,39	0
56	MG	2r	101	1/1	0.94	0.09	65,65,65,65	0
56	MG	2A	3546	1/1	0.94	0.12	65,65,65,65	0
56	MG	1x	107	1/1	0.94	0.15	49,49,49,49	0
56	MG	2A	3549	1/1	0.94	0.17	47,47,47,47	0
56	MG	1A	3854	1/1	0.94	0.07	60,60,60,60	0
56	MG	1A	3101	1/1	0.94	0.18	56,56,56,56	0
56	MG	2A	3552	1/1	0.94	0.10	43,43,43,43	0
56	MG	2A	3555	1/1	0.94	0.09	27,27,27,27	0
56	MG	1A	3857	1/1	0.94	0.15	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
56	MG	2B	209	1/1	0.94	0.23	59,59,59,59	0
56	MG	2A	3557	1/1	0.94	0.10	59,59,59,59	0
56	MG	1A	3046	1/1	0.94	0.10	28,28,28,28	0
56	MG	1A	3019	1/1	0.94	0.15	41,41,41,41	0
56	MG	2A	3284	1/1	0.94	0.07	59,59,59,59	0
56	MG	1A	3701	1/1	0.94	0.08	23,23,23,23	0
56	MG	1A	3557	1/1	0.94	0.08	47,47,47,47	0
59	ZN	24	501	1/1	0.94	0.07	117,117,117,117	0
56	MG	2A	3001	1/1	0.95	0.23	55,55,55,55	0
56	MG	1A	4064	1/1	0.95	0.06	34,34,34,34	0
56	MG	2E	304	1/1	0.95	0.09	43,43,43,43	0
56	MG	2A	3581	1/1	0.95	0.10	46,46,46,46	0
56	MG	2F	303	1/1	0.95	0.09	48,48,48,48	0
56	MG	1A	3873	1/1	0.95	0.10	35,35,35,35	0
56	MG	2A	3004	1/1	0.95	0.24	58,58,58,58	0
56	MG	1a	1635	1/1	0.95	0.09	55,55,55,55	0
56	MG	2P	201	1/1	0.95	0.23	58,58,58,58	0
56	MG	1A	3041	1/1	0.95	0.30	34,34,34,34	0
56	MG	2A	3007	1/1	0.95	0.15	49,49,49,49	0
56	MG	1a	1639	1/1	0.95	0.19	56,56,56,56	0
56	MG	1A	4071	1/1	0.95	0.07	51,51,51,51	0
56	MG	2A	3012	1/1	0.95	0.06	40,40,40,40	0
56	MG	1A	3448	1/1	0.95	0.07	36,36,36,36	0
56	MG	2A	3015	1/1	0.95	0.11	39,39,39,39	0
56	MG	2A	3598	1/1	0.95	0.08	42,42,42,42	0
56	MG	1A	3707	1/1	0.95	0.08	25,25,25,25	0
56	MG	2A	3018	1/1	0.95	0.11	49,49,49,49	0
56	MG	1A	3449	1/1	0.95	0.15	32,32,32,32	0
56	MG	1A	3882	1/1	0.95	0.12	44,44,44,44	0
56	MG	1A	3262	1/1	0.95	0.18	59,59,59,59	0
56	MG	1a	1650	1/1	0.95	0.07	56,56,56,56	0
56	MG	1A	4079	1/1	0.95	0.08	53,53,53,53	0
56	MG	1A	3710	1/1	0.95	0.10	51,51,51,51	0
56	MG	1A	3348	1/1	0.95	0.14	41,41,41,41	0
56	MG	1A	3456	1/1	0.95	0.09	49,49,49,49	0
56	MG	2A	3030	1/1	0.95	0.07	46,46,46,46	0
56	MG	1A	4087	1/1	0.95	0.10	53,53,53,53	0
56	MG	1A	3192	1/1	0.95	0.11	25,25,25,25	0
56	MG	1A	3193	1/1	0.95	0.27	30,30,30,30	0
56	MG	2A	3616	1/1	0.95	0.07	63,63,63,63	0
56	MG	2A	3038	1/1	0.95	0.06	48,48,48,48	0
56	MG	20	102	1/1	0.95	0.06	65,65,65,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3460	1/1	0.95	0.07	40,40,40,40	0
56	MG	1A	3718	1/1	0.95	0.06	31,31,31,31	0
56	MG	2A	3041	1/1	0.95	0.12	70,70,70,70	0
56	MG	1A	3088	1/1	0.95	0.13	37,37,37,37	0
56	MG	1A	4095	1/1	0.95	0.06	38,38,38,38	0
56	MG	1A	4096	1/1	0.95	0.09	46,46,46,46	0
56	MG	1A	4098	1/1	0.95	0.06	50,50,50,50	0
56	MG	2A	3627	1/1	0.95	0.06	44,44,44,44	0
56	MG	1A	3573	1/1	0.95	0.09	34,34,34,34	0
56	MG	1A	3044	1/1	0.95	0.06	29,29,29,29	0
56	MG	1A	3198	1/1	0.95	0.12	35,35,35,35	0
56	MG	1A	3055	1/1	0.95	0.05	23,23,23,23	0
56	MG	28	103	1/1	0.95	0.08	42,42,42,42	0
56	MG	2A	3632	1/1	0.95	0.13	39,39,39,39	0
56	MG	1A	3465	1/1	0.95	0.28	48,48,48,48	0
56	MG	1A	3277	1/1	0.95	0.18	44,44,44,44	0
56	MG	1A	3580	1/1	0.95	0.19	29,29,29,29	0
56	MG	1A	3735	1/1	0.95	0.07	45,45,45,45	0
56	MG	1B	209	1/1	0.95	0.09	47,47,47,47	0
56	MG	1A	3203	1/1	0.95	0.12	24,24,24,24	0
56	MG	1A	3907	1/1	0.95	0.05	48,48,48,48	0
56	MG	2A	3335	1/1	0.95	0.19	47,47,47,47	0
56	MG	2A	3064	1/1	0.95	0.16	48,48,48,48	0
56	MG	1A	3582	1/1	0.95	0.10	30,30,30,30	0
56	MG	1B	214	1/1	0.95	0.08	46,46,46,46	0
56	MG	2A	3646	1/1	0.95	0.07	59,59,59,59	0
56	MG	1A	3092	1/1	0.95	0.17	45,45,45,45	0
56	MG	1B	219	1/1	0.95	0.14	34,34,34,34	0
56	MG	2A	3070	1/1	0.95	0.06	56,56,56,56	0
56	MG	2a	3019	1/1	0.95	0.13	54,54,54,54	0
56	MG	1A	3093	1/1	0.95	0.14	51,51,51,51	0
56	MG	1A	3472	1/1	0.95	0.13	33,33,33,33	0
56	MG	2A	3654	1/1	0.95	0.17	57,57,57,57	0
56	MG	2A	3073	1/1	0.95	0.14	52,52,52,52	0
56	MG	1A	3363	1/1	0.95	0.08	51,51,51,51	0
56	MG	2A	3351	1/1	0.95	0.26	59,59,59,59	0
56	MG	1A	3591	1/1	0.95	0.17	35,35,35,35	0
56	MG	1A	3364	1/1	0.95	0.08	37,37,37,37	0
56	MG	2a	3029	1/1	0.95	0.09	40,40,40,40	0
56	MG	2A	3354	1/1	0.95	0.09	62,62,62,62	0
56	MG	1A	3919	1/1	0.95	0.11	30,30,30,30	0
56	MG	1B	227	1/1	0.95	0.07	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
56	MG	2a	3033	1/1	0.95	0.09	81,81,81,81	0
56	MG	1A	3475	1/1	0.95	0.10	48,48,48,48	0
56	MG	2a	3035	1/1	0.95	0.08	76,76,76,76	0
56	MG	2A	3081	1/1	0.95	0.16	52,52,52,52	0
56	MG	2A	3360	1/1	0.95	0.06	56,56,56,56	0
56	MG	2a	3038	1/1	0.95	0.23	53,53,53,53	0
56	MG	1A	3596	1/1	0.95	0.06	29,29,29,29	0
56	MG	1A	3597	1/1	0.95	0.07	49,49,49,49	0
56	MG	1A	3284	1/1	0.95	0.39	35,35,35,35	0
56	MG	1A	3926	1/1	0.95	0.05	28,28,28,28	0
56	MG	1B	235	1/1	0.95	0.12	47,47,47,47	0
56	MG	1A	3288	1/1	0.95	0.11	34,34,34,34	0
56	MG	2A	3090	1/1	0.95	0.09	45,45,45,45	0
56	MG	2A	3091	1/1	0.95	0.11	48,48,48,48	0
56	MG	1A	3765	1/1	0.95	0.12	43,43,43,43	0
56	MG	1A	3140	1/1	0.95	0.14	40,40,40,40	0
56	MG	1A	3370	1/1	0.95	0.11	40,40,40,40	0
56	MG	2A	3374	1/1	0.95	0.24	57,57,57,57	0
56	MG	1D	308	1/1	0.95	0.05	36,36,36,36	0
56	MG	1a	1702	1/1	0.95	0.23	53,53,53,53	0
56	MG	2A	3691	1/1	0.95	0.10	71,71,71,71	0
56	MG	1A	3371	1/1	0.95	0.13	46,46,46,46	0
56	MG	2a	3056	1/1	0.95	0.28	57,57,57,57	0
56	MG	1a	1704	1/1	0.95	0.27	60,60,60,60	0
56	MG	2A	3100	1/1	0.95	0.12	53,53,53,53	0
56	MG	2A	3101	1/1	0.95	0.10	35,35,35,35	0
56	MG	2A	3103	1/1	0.95	0.16	58,58,58,58	0
56	MG	2A	3104	1/1	0.95	0.08	51,51,51,51	0
56	MG	1a	1705	1/1	0.95	0.14	56,56,56,56	0
56	MG	1A	3608	1/1	0.95	0.07	39,39,39,39	0
56	MG	2A	3109	1/1	0.95	0.13	39,39,39,39	0
56	MG	1A	3290	1/1	0.95	0.10	40,40,40,40	0
56	MG	1A	3610	1/1	0.95	0.09	44,44,44,44	0
56	MG	1E	307	1/1	0.95	0.13	57,57,57,57	0
56	MG	1A	3377	1/1	0.95	0.07	47,47,47,47	0
56	MG	1a	1711	1/1	0.95	0.08	39,39,39,39	0
56	MG	1A	3612	1/1	0.95	0.12	51,51,51,51	0
56	MG	2A	3398	1/1	0.95	0.18	58,58,58,58	0
56	MG	1A	3056	1/1	0.95	0.21	45,45,45,45	0
56	MG	1A	3616	1/1	0.95	0.09	19,19,19,19	0
56	MG	1E	314	1/1	0.95	0.14	30,30,30,30	0
56	MG	1A	3485	1/1	0.95	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
56	MG	1A	3950	1/1	0.95	0.08	55,55,55,55	0
56	MG	1a	1719	1/1	0.95	0.09	41,41,41,41	0
56	MG	1A	3058	1/1	0.95	0.06	32,32,32,32	0
56	MG	1A	3213	1/1	0.95	0.09	44,44,44,44	0
56	MG	2A	3132	1/1	0.95	0.06	36,36,36,36	0
56	MG	1F	310	1/1	0.95	0.11	41,41,41,41	0
56	MG	2A	3728	1/1	0.95	0.07	64,64,64,64	0
56	MG	1G	202	1/1	0.95	0.15	51,51,51,51	0
56	MG	2A	3411	1/1	0.95	0.06	46,46,46,46	0
56	MG	1A	3956	1/1	0.95	0.13	45,45,45,45	0
56	MG	2A	3141	1/1	0.95	0.23	39,39,39,39	0
56	MG	2a	3091	1/1	0.95	0.17	62,62,62,62	0
56	MG	1A	3488	1/1	0.95	0.07	33,33,33,33	0
56	MG	2A	3145	1/1	0.95	0.23	66,66,66,66	0
56	MG	2A	3147	1/1	0.95	0.22	31,31,31,31	0
56	MG	1A	3959	1/1	0.95	0.09	46,46,46,46	0
56	MG	1N	203	1/1	0.95	0.06	46,46,46,46	0
56	MG	1A	3787	1/1	0.95	0.06	44,44,44,44	0
56	MG	1A	3489	1/1	0.95	0.25	48,48,48,48	0
56	MG	1A	3060	1/1	0.95	0.09	39,39,39,39	0
56	MG	1A	3300	1/1	0.95	0.08	44,44,44,44	0
56	MG	1A	3965	1/1	0.95	0.06	49,49,49,49	0
56	MG	2a	3103	1/1	0.95	0.16	62,62,62,62	0
56	MG	1A	3387	1/1	0.95	0.12	48,48,48,48	0
56	MG	2A	3157	1/1	0.95	0.34	44,44,44,44	0
56	MG	2A	3747	1/1	0.95	0.11	66,66,66,66	0
56	MG	1A	3027	1/1	0.95	0.14	71,71,71,71	0
56	MG	1A	3005	1/1	0.95	0.08	37,37,37,37	0
56	MG	1a	1741	1/1	0.95	0.25	60,60,60,60	0
56	MG	1A	3157	1/1	0.95	0.10	40,40,40,40	0
56	MG	2A	3752	1/1	0.95	0.10	54,54,54,54	0
56	MG	1A	3228	1/1	0.95	0.10	32,32,32,32	0
56	MG	1A	3063	1/1	0.95	0.11	43,43,43,43	0
56	MG	1A	3395	1/1	0.95	0.13	40,40,40,40	0
56	MG	1A	3803	1/1	0.95	0.05	26,26,26,26	0
56	MG	1A	3038	1/1	0.95	0.13	30,30,30,30	0
56	MG	1A	3235	1/1	0.95	0.07	59,59,59,59	0
56	MG	2A	3168	1/1	0.95	0.08	53,53,53,53	0
56	MG	1A	3508	1/1	0.95	0.16	23,23,23,23	0
56	MG	1A	3983	1/1	0.95	0.06	64,64,64,64	0
56	MG	1T	202	1/1	0.95	0.10	45,45,45,45	0
56	MG	1T	203	1/1	0.95	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
56	MG	1A	3811	1/1	0.95	0.10	49,49,49,49	0
56	MG	1A	3313	1/1	0.95	0.09	39,39,39,39	0
56	MG	2a	3125	1/1	0.95	0.10	64,64,64,64	0
56	MG	1U	202	1/1	0.95	0.11	27,27,27,27	0
56	MG	2A	3451	1/1	0.95	0.21	37,37,37,37	0
56	MG	1U	206	1/1	0.95	0.07	33,33,33,33	0
56	MG	1A	3652	1/1	0.95	0.09	31,31,31,31	0
56	MG	1U	212	1/1	0.95	0.10	37,37,37,37	0
56	MG	1A	3987	1/1	0.95	0.08	50,50,50,50	0
56	MG	2A	3456	1/1	0.95	0.14	61,61,61,61	0
56	MG	2A	3183	1/1	0.95	0.12	52,52,52,52	0
56	MG	2A	3780	1/1	0.95	0.07	69,69,69,69	0
56	MG	2A	3184	1/1	0.95	0.09	41,41,41,41	0
56	MG	2a	3142	1/1	0.95	0.06	68,68,68,68	0
56	MG	1A	3110	1/1	0.95	0.13	26,26,26,26	0
56	MG	1A	3315	1/1	0.95	0.08	51,51,51,51	0
56	MG	1W	201	1/1	0.95	0.18	49,49,49,49	0
56	MG	2a	3148	1/1	0.95	0.07	63,63,63,63	0
56	MG	1A	3655	1/1	0.95	0.07	58,58,58,58	0
56	MG	1X	103	1/1	0.95	0.13	37,37,37,37	0
56	MG	2A	3464	1/1	0.95	0.23	63,63,63,63	0
56	MG	1A	3239	1/1	0.95	0.14	25,25,25,25	0
56	MG	1A	3821	1/1	0.95	0.06	26,26,26,26	0
56	MG	2a	3157	1/1	0.95	0.08	57,57,57,57	0
56	MG	1A	3069	1/1	0.95	0.11	28,28,28,28	0
56	MG	2A	3797	1/1	0.95	0.05	40,40,40,40	0
56	MG	1A	3166	1/1	0.95	0.16	34,34,34,34	0
56	MG	1A	3321	1/1	0.95	0.17	48,48,48,48	0
56	MG	1A	3520	1/1	0.95	0.11	56,56,56,56	0
56	MG	1A	3829	1/1	0.95	0.11	32,32,32,32	0
56	MG	10	103	1/1	0.95	0.07	32,32,32,32	0
56	MG	1A	3831	1/1	0.95	0.08	37,37,37,37	0
56	MG	10	105	1/1	0.95	0.09	53,53,53,53	0
56	MG	1A	3322	1/1	0.95	0.05	43,43,43,43	0
56	MG	2A	3208	1/1	0.95	0.08	53,53,53,53	0
56	MG	1A	3833	1/1	0.95	0.07	55,55,55,55	0
56	MG	2A	3481	1/1	0.95	0.22	60,60,60,60	0
56	MG	2A	3482	1/1	0.95	0.22	42,42,42,42	0
56	MG	1A	3168	1/1	0.95	0.24	40,40,40,40	0
56	MG	1A	3415	1/1	0.95	0.07	40,40,40,40	0
56	MG	1A	3670	1/1	0.95	0.09	28,28,28,28	0
56	MG	1A	3671	1/1	0.95	0.06	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
56	MG	1a	1806	1/1	0.95	0.09	59,59,59,59	0
56	MG	2A	3488	1/1	0.95	0.08	56,56,56,56	0
56	MG	1A	3246	1/1	0.95	0.16	50,50,50,50	0
56	MG	2A	3218	1/1	0.95	0.23	35,35,35,35	0
56	MG	1A	3326	1/1	0.95	0.06	48,48,48,48	0
56	MG	1A	3841	1/1	0.95	0.09	39,39,39,39	0
56	MG	1a	1817	1/1	0.95	0.07	58,58,58,58	0
56	MG	2A	3224	1/1	0.95	0.13	49,49,49,49	0
56	MG	1A	4014	1/1	0.95	0.06	46,46,46,46	0
56	MG	1a	1819	1/1	0.95	0.09	68,68,68,68	0
56	MG	15	104	1/1	0.95	0.08	42,42,42,42	0
56	MG	2A	3500	1/1	0.95	0.07	55,55,55,55	0
56	MG	1A	3327	1/1	0.95	0.19	36,36,36,36	0
56	MG	2A	3835	1/1	0.95	0.08	34,34,34,34	0
56	MG	1A	3174	1/1	0.95	0.20	27,27,27,27	0
56	MG	16	103	1/1	0.95	0.07	51,51,51,51	0
56	MG	1A	3679	1/1	0.95	0.07	34,34,34,34	0
56	MG	2A	3506	1/1	0.95	0.08	36,36,36,36	0
56	MG	2a	3207	1/1	0.95	0.09	62,62,62,62	0
56	MG	2A	3842	1/1	0.95	0.07	42,42,42,42	0
56	MG	17	107	1/1	0.95	0.16	49,49,49,49	0
56	MG	2a	3213	1/1	0.95	0.13	75,75,75,75	0
56	MG	2a	3214	1/1	0.95	0.16	74,74,74,74	0
56	MG	2A	3846	1/1	0.95	0.09	62,62,62,62	0
56	MG	1A	3248	1/1	0.95	0.19	51,51,51,51	0
56	MG	2A	3850	1/1	0.95	0.11	55,55,55,55	0
56	MG	2A	3851	1/1	0.95	0.10	39,39,39,39	0
56	MG	2A	3238	1/1	0.95	0.11	45,45,45,45	0
56	MG	18	102	1/1	0.95	0.19	41,41,41,41	0
56	MG	1A	3681	1/1	0.95	0.10	47,47,47,47	0
56	MG	2a	3222	1/1	0.95	0.19	55,55,55,55	0
56	MG	1A	4021	1/1	0.95	0.06	32,32,32,32	0
56	MG	1A	3249	1/1	0.95	0.19	42,42,42,42	0
56	MG	1A	4024	1/1	0.95	0.11	70,70,70,70	0
56	MG	2A	3244	1/1	0.95	0.10	43,43,43,43	0
56	MG	2A	3519	1/1	0.95	0.09	33,33,33,33	0
56	MG	1f	201	1/1	0.95	0.15	44,44,44,44	0
56	MG	2A	3872	1/1	0.95	0.10	48,48,48,48	0
56	MG	2A	3246	1/1	0.95	0.11	49,49,49,49	0
56	MG	19	101	1/1	0.95	0.06	34,34,34,34	0
56	MG	1h	201	1/1	0.95	0.07	58,58,58,58	0
56	MG	2A	3528	1/1	0.95	0.08	59,59,59,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2A	3249	1/1	0.95	0.08	55,55,55,55	0
56	MG	2A	3879	1/1	0.95	0.16	47,47,47,47	0
56	MG	1m	3002	1/1	0.95	0.09	56,56,56,56	0
56	MG	1n	101	1/1	0.95	0.09	54,54,54,54	0
56	MG	1a	1601	1/1	0.95	0.08	42,42,42,42	0
56	MG	2A	3535	1/1	0.95	0.11	51,51,51,51	0
56	MG	1A	3850	1/1	0.95	0.16	47,47,47,47	0
56	MG	1A	3250	1/1	0.95	0.11	36,36,36,36	0
56	MG	1A	3112	1/1	0.95	0.16	35,35,35,35	0
56	MG	1A	3114	1/1	0.95	0.08	32,32,32,32	0
56	MG	1A	3001	1/1	0.95	0.17	39,39,39,39	0
56	MG	2A	3258	1/1	0.95	0.06	67,67,67,67	0
56	MG	1A	4038	1/1	0.95	0.07	52,52,52,52	0
56	MG	1A	3337	1/1	0.95	0.18	37,37,37,37	0
56	MG	1A	3255	1/1	0.95	0.07	29,29,29,29	0
56	MG	2l	201	1/1	0.95	0.09	55,55,55,55	0
56	MG	2l	202	1/1	0.95	0.07	64,64,64,64	0
56	MG	2A	3263	1/1	0.95	0.39	71,71,71,71	0
56	MG	1a	1612	1/1	0.95	0.08	62,62,62,62	0
56	MG	1A	3859	1/1	0.95	0.24	38,38,38,38	0
56	MG	2A	3266	1/1	0.95	0.10	59,59,59,59	0
56	MG	1A	3860	1/1	0.95	0.17	36,36,36,36	0
56	MG	1A	3082	1/1	0.95	0.16	33,33,33,33	0
56	MG	2A	3559	1/1	0.95	0.10	53,53,53,53	0
56	MG	1A	3863	1/1	0.95	0.07	34,34,34,34	0
56	MG	2A	3270	1/1	0.95	0.19	57,57,57,57	0
56	MG	1A	3120	1/1	0.95	0.09	36,36,36,36	0
56	MG	1a	1620	1/1	0.95	0.19	55,55,55,55	0
56	MG	1A	3439	1/1	0.95	0.09	44,44,44,44	0
56	MG	1A	3698	1/1	0.95	0.13	28,28,28,28	0
56	MG	1A	4055	1/1	0.95	0.07	41,41,41,41	0
56	MG	2A	3277	1/1	0.95	0.06	58,58,58,58	0
56	MG	2D	303	1/1	0.95	0.18	42,42,42,42	0
56	MG	1A	3040	1/1	0.95	0.05	30,30,30,30	0
56	MG	2y	101	1/1	0.95	0.26	60,60,60,60	0
56	MG	1A	3443	1/1	0.95	0.10	49,49,49,49	0
56	MG	1A	3259	1/1	0.95	0.06	38,38,38,38	0
56	MG	1A	3260	1/1	0.95	0.09	47,47,47,47	0
56	MG	1A	3553	1/1	0.95	0.22	45,45,45,45	0
57	CLM	1A	4102	20/20	0.95	0.09	18,29,44,60	0
57	CLM	2A	3888	20/20	0.95	0.10	38,45,57,61	0
56	MG	1A	3872	1/1	0.95	0.15	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	ZN	2n	501	1/1	0.95	0.07	107,107,107,107	0
56	MG	1A	3569	1/1	0.96	0.11	42,42,42,42	0
56	MG	1A	3571	1/1	0.96	0.27	29,29,29,29	0
56	MG	1A	3842	1/1	0.96	0.08	31,31,31,31	0
56	MG	1A	3389	1/1	0.96	0.14	23,23,23,23	0
56	MG	1A	3138	1/1	0.96	0.15	28,28,28,28	0
56	MG	1A	3476	1/1	0.96	0.05	40,40,40,40	0
56	MG	1A	3080	1/1	0.96	0.14	47,47,47,47	0
56	MG	1A	3196	1/1	0.96	0.07	38,38,38,38	0
56	MG	1P	208	1/1	0.96	0.17	42,42,42,42	0
56	MG	1A	3393	1/1	0.96	0.07	43,43,43,43	0
56	MG	1Q	201	1/1	0.96	0.29	42,42,42,42	0
56	MG	2A	3082	1/1	0.96	0.06	43,43,43,43	0
56	MG	2A	3336	1/1	0.96	0.14	62,62,62,62	0
56	MG	1A	4003	1/1	0.96	0.08	42,42,42,42	0
56	MG	2A	3084	1/1	0.96	0.06	46,46,46,46	0
56	MG	1a	1713	1/1	0.96	0.07	50,50,50,50	0
56	MG	2A	3340	1/1	0.96	0.09	53,53,53,53	0
56	MG	1A	3849	1/1	0.96	0.07	52,52,52,52	0
56	MG	2A	3625	1/1	0.96	0.12	57,57,57,57	0
56	MG	2A	3626	1/1	0.96	0.10	33,33,33,33	0
56	MG	2A	3342	1/1	0.96	0.17	55,55,55,55	0
56	MG	1Q	206	1/1	0.96	0.06	51,51,51,51	0
56	MG	2A	3344	1/1	0.96	0.12	48,48,48,48	0
56	MG	2A	3345	1/1	0.96	0.07	39,39,39,39	0
56	MG	1A	3197	1/1	0.96	0.22	38,38,38,38	0
56	MG	1R	201	1/1	0.96	0.15	32,32,32,32	0
56	MG	1A	3579	1/1	0.96	0.10	21,21,21,21	0
56	MG	1A	3325	1/1	0.96	0.22	26,26,26,26	0
56	MG	2A	3635	1/1	0.96	0.07	61,61,61,61	0
56	MG	1A	3105	1/1	0.96	0.18	30,30,30,30	0
56	MG	1A	3029	1/1	0.96	0.09	23,23,23,23	0
56	MG	25	102	1/1	0.96	0.27	50,50,50,50	0
56	MG	1A	3856	1/1	0.96	0.05	16,16,16,16	0
56	MG	1A	3583	1/1	0.96	0.07	44,44,44,44	0
56	MG	1a	1725	1/1	0.96	0.12	42,42,42,42	0
56	MG	1A	3108	1/1	0.96	0.13	36,36,36,36	0
56	MG	1A	3149	1/1	0.96	0.15	29,29,29,29	0
56	MG	1A	3109	1/1	0.96	0.27	31,31,31,31	0
56	MG	1A	3588	1/1	0.96	0.33	36,36,36,36	0
56	MG	2A	3102	1/1	0.96	0.10	59,59,59,59	0
56	MG	1U	205	1/1	0.96	0.40	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
56	MG	1A	3059	1/1	0.96	0.16	47,47,47,47	0
56	MG	2A	3105	1/1	0.96	0.10	57,57,57,57	0
56	MG	2a	3004	1/1	0.96	0.24	51,51,51,51	0
56	MG	1A	3715	1/1	0.96	0.09	48,48,48,48	0
56	MG	2A	3366	1/1	0.96	0.19	60,60,60,60	0
56	MG	1A	3590	1/1	0.96	0.10	26,26,26,26	0
56	MG	2A	3655	1/1	0.96	0.15	56,56,56,56	0
56	MG	1A	4023	1/1	0.96	0.05	30,30,30,30	0
56	MG	1A	3030	1/1	0.96	0.25	32,32,32,32	0
56	MG	2A	3111	1/1	0.96	0.11	59,59,59,59	0
56	MG	2A	3660	1/1	0.96	0.06	33,33,33,33	0
56	MG	1A	4027	1/1	0.96	0.18	65,65,65,65	0
56	MG	1a	1738	1/1	0.96	0.07	57,57,57,57	0
56	MG	1A	3720	1/1	0.96	0.15	44,44,44,44	0
56	MG	1a	1740	1/1	0.96	0.15	43,43,43,43	0
56	MG	2A	3667	1/1	0.96	0.13	57,57,57,57	0
56	MG	2A	3375	1/1	0.96	0.09	64,64,64,64	0
56	MG	1W	202	1/1	0.96	0.15	50,50,50,50	0
56	MG	1A	3210	1/1	0.96	0.08	35,35,35,35	0
56	MG	2A	3672	1/1	0.96	0.06	51,51,51,51	0
56	MG	1W	205	1/1	0.96	0.05	39,39,39,39	0
56	MG	1A	3405	1/1	0.96	0.07	52,52,52,52	0
56	MG	1A	3334	1/1	0.96	0.18	43,43,43,43	0
56	MG	1a	1749	1/1	0.96	0.10	33,33,33,33	0
56	MG	2A	3677	1/1	0.96	0.05	51,51,51,51	0
56	MG	1a	1750	1/1	0.96	0.05	39,39,39,39	0
56	MG	1A	4035	1/1	0.96	0.06	64,64,64,64	0
56	MG	2A	3126	1/1	0.96	0.11	44,44,44,44	0
56	MG	2A	3385	1/1	0.96	0.17	53,53,53,53	0
56	MG	2A	3129	1/1	0.96	0.09	54,54,54,54	0
56	MG	2A	3388	1/1	0.96	0.09	62,62,62,62	0
56	MG	2A	3130	1/1	0.96	0.09	54,54,54,54	0
56	MG	1A	4036	1/1	0.96	0.09	41,41,41,41	0
56	MG	1Y	203	1/1	0.96	0.13	47,47,47,47	0
56	MG	2A	3134	1/1	0.96	0.05	39,39,39,39	0
56	MG	2A	3689	1/1	0.96	0.06	59,59,59,59	0
56	MG	1A	3211	1/1	0.96	0.18	34,34,34,34	0
56	MG	2A	3136	1/1	0.96	0.10	38,38,38,38	0
56	MG	1A	3598	1/1	0.96	0.11	35,35,35,35	0
56	MG	1a	1756	1/1	0.96	0.11	54,54,54,54	0
56	MG	1A	3412	1/1	0.96	0.07	38,38,38,38	0
56	MG	2A	3143	1/1	0.96	0.12	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
56	MG	1A	4040	1/1	0.96	0.12	47,47,47,47	0
56	MG	1a	1761	1/1	0.96	0.10	51,51,51,51	0
56	MG	2A	3146	1/1	0.96	0.17	38,38,38,38	0
56	MG	1A	3732	1/1	0.96	0.08	61,61,61,61	0
56	MG	1A	3495	1/1	0.96	0.18	47,47,47,47	0
56	MG	1a	1764	1/1	0.96	0.07	58,58,58,58	0
56	MG	2A	3407	1/1	0.96	0.09	57,57,57,57	0
56	MG	1A	3878	1/1	0.96	0.22	30,30,30,30	0
56	MG	10	106	1/1	0.96	0.06	49,49,49,49	0
56	MG	2a	3055	1/1	0.96	0.07	60,60,60,60	0
56	MG	11	101	1/1	0.96	0.21	33,33,33,33	0
56	MG	1A	3879	1/1	0.96	0.10	36,36,36,36	0
56	MG	1a	1771	1/1	0.96	0.07	40,40,40,40	0
56	MG	2A	3413	1/1	0.96	0.11	55,55,55,55	0
56	MG	1A	3413	1/1	0.96	0.06	37,37,37,37	0
56	MG	2a	3061	1/1	0.96	0.04	53,53,53,53	0
56	MG	1A	3158	1/1	0.96	0.12	60,60,60,60	0
56	MG	1A	3606	1/1	0.96	0.05	36,36,36,36	0
56	MG	1A	3738	1/1	0.96	0.09	45,45,45,45	0
56	MG	2A	3719	1/1	0.96	0.06	60,60,60,60	0
56	MG	1A	3273	1/1	0.96	0.26	35,35,35,35	0
56	MG	13	101	1/1	0.96	0.09	26,26,26,26	0
56	MG	13	102	1/1	0.96	0.07	38,38,38,38	0
56	MG	1A	3500	1/1	0.96	0.17	37,37,37,37	0
56	MG	1A	3502	1/1	0.96	0.07	47,47,47,47	0
56	MG	2A	3727	1/1	0.96	0.16	61,61,61,61	0
56	MG	15	101	1/1	0.96	0.18	31,31,31,31	0
56	MG	1A	3743	1/1	0.96	0.07	22,22,22,22	0
56	MG	1A	3744	1/1	0.96	0.07	50,50,50,50	0
56	MG	1A	3745	1/1	0.96	0.05	14,14,14,14	0
56	MG	1A	3043	1/1	0.96	0.13	33,33,33,33	0
56	MG	1A	4062	1/1	0.96	0.06	32,32,32,32	0
56	MG	1a	1791	1/1	0.96	0.06	64,64,64,64	0
56	MG	1A	3113	1/1	0.96	0.10	37,37,37,37	0
56	MG	1a	1794	1/1	0.96	0.07	60,60,60,60	0
56	MG	2A	3436	1/1	0.96	0.06	41,41,41,41	0
56	MG	2A	3174	1/1	0.96	0.25	56,56,56,56	0
56	MG	2A	3740	1/1	0.96	0.05	67,67,67,67	0
56	MG	17	101	1/1	0.96	0.09	31,31,31,31	0
56	MG	17	102	1/1	0.96	0.07	32,32,32,32	0
56	MG	1A	4066	1/1	0.96	0.05	24,24,24,24	0
56	MG	17	105	1/1	0.96	0.12	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
56	MG	2A	3180	1/1	0.96	0.19	47,47,47,47	0
56	MG	1A	3024	1/1	0.96	0.08	43,43,43,43	0
56	MG	1A	3749	1/1	0.96	0.05	30,30,30,30	0
56	MG	2A	3445	1/1	0.96	0.32	60,60,60,60	0
56	MG	1A	4069	1/1	0.96	0.05	20,20,20,20	0
56	MG	1A	4070	1/1	0.96	0.05	52,52,52,52	0
56	MG	1a	1808	1/1	0.96	0.06	50,50,50,50	0
56	MG	1A	3750	1/1	0.96	0.07	34,34,34,34	0
56	MG	2a	3099	1/1	0.96	0.09	52,52,52,52	0
56	MG	1a	1810	1/1	0.96	0.06	59,59,59,59	0
56	MG	1A	4072	1/1	0.96	0.07	48,48,48,48	0
56	MG	1a	1815	1/1	0.96	0.11	66,66,66,66	0
56	MG	2A	3193	1/1	0.96	0.31	63,63,63,63	0
56	MG	1A	3751	1/1	0.96	0.10	42,42,42,42	0
56	MG	2A	3195	1/1	0.96	0.05	44,44,44,44	0
56	MG	2A	3760	1/1	0.96	0.13	54,54,54,54	0
56	MG	1A	3219	1/1	0.96	0.11	32,32,32,32	0
56	MG	1A	3507	1/1	0.96	0.15	42,42,42,42	0
56	MG	1a	1821	1/1	0.96	0.05	53,53,53,53	0
56	MG	1A	3903	1/1	0.96	0.10	45,45,45,45	0
56	MG	1A	3617	1/1	0.96	0.05	36,36,36,36	0
56	MG	1A	3619	1/1	0.96	0.11	41,41,41,41	0
56	MG	1A	3620	1/1	0.96	0.08	52,52,52,52	0
56	MG	1A	3343	1/1	0.96	0.14	47,47,47,47	0
56	MG	2A	3769	1/1	0.96	0.10	39,39,39,39	0
56	MG	1A	3423	1/1	0.96	0.14	42,42,42,42	0
56	MG	2A	3465	1/1	0.96	0.13	48,48,48,48	0
56	MG	1a	1608	1/1	0.96	0.17	45,45,45,45	0
56	MG	1A	4085	1/1	0.96	0.08	17,17,17,17	0
56	MG	1a	1610	1/1	0.96	0.06	23,23,23,23	0
56	MG	1A	3511	1/1	0.96	0.06	36,36,36,36	0
56	MG	1A	3282	1/1	0.96	0.26	38,38,38,38	0
56	MG	2A	3471	1/1	0.96	0.06	32,32,32,32	0
56	MG	1A	3912	1/1	0.96	0.16	31,31,31,31	0
56	MG	2A	3783	1/1	0.96	0.08	58,58,58,58	0
56	MG	1a	1614	1/1	0.96	0.11	58,58,58,58	0
56	MG	1a	1615	1/1	0.96	0.06	43,43,43,43	0
56	MG	2A	3787	1/1	0.96	0.06	72,72,72,72	0
56	MG	2a	3131	1/1	0.96	0.35	60,60,60,60	0
56	MG	1A	3003	1/1	0.96	0.04	19,19,19,19	0
56	MG	1m	3001	1/1	0.96	0.09	54,54,54,54	0
56	MG	2A	3790	1/1	0.96	0.07	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
56	MG	1A	3426	1/1	0.96	0.14	44,44,44,44	0
56	MG	1A	3427	1/1	0.96	0.10	43,43,43,43	0
56	MG	2a	3137	1/1	0.96	0.11	75,75,75,75	0
56	MG	1A	4094	1/1	0.96	0.12	47,47,47,47	0
56	MG	2a	3139	1/1	0.96	0.07	70,70,70,70	0
56	MG	2A	3223	1/1	0.96	0.15	45,45,45,45	0
56	MG	1A	3516	1/1	0.96	0.11	40,40,40,40	0
56	MG	2a	3143	1/1	0.96	0.06	75,75,75,75	0
56	MG	1A	3636	1/1	0.96	0.06	16,16,16,16	0
56	MG	1A	3638	1/1	0.96	0.07	40,40,40,40	0
56	MG	1A	3223	1/1	0.96	0.16	46,46,46,46	0
56	MG	2A	3800	1/1	0.96	0.05	78,78,78,78	0
56	MG	2a	3149	1/1	0.96	0.06	76,76,76,76	0
56	MG	1A	3429	1/1	0.96	0.05	44,44,44,44	0
56	MG	1A	4101	1/1	0.96	0.07	53,53,53,53	0
56	MG	1A	3777	1/1	0.96	0.06	46,46,46,46	0
56	MG	1a	1628	1/1	0.96	0.15	47,47,47,47	0
56	MG	1A	3925	1/1	0.96	0.07	39,39,39,39	0
56	MG	1A	3778	1/1	0.96	0.10	20,20,20,20	0
56	MG	2A	3807	1/1	0.96	0.07	65,65,65,65	0
56	MG	1B	204	1/1	0.96	0.18	42,42,42,42	0
56	MG	1B	205	1/1	0.96	0.05	47,47,47,47	0
56	MG	1A	3286	1/1	0.96	0.15	42,42,42,42	0
56	MG	1x	102	1/1	0.96	0.16	46,46,46,46	0
56	MG	1x	103	1/1	0.96	0.16	48,48,48,48	0
56	MG	2a	3169	1/1	0.96	0.09	77,77,77,77	0
56	MG	2A	3814	1/1	0.96	0.10	60,60,60,60	0
56	MG	1A	3022	1/1	0.96	0.08	34,34,34,34	0
56	MG	1x	105	1/1	0.96	0.04	49,49,49,49	0
56	MG	1a	1636	1/1	0.96	0.10	49,49,49,49	0
56	MG	1A	3434	1/1	0.96	0.13	40,40,40,40	0
56	MG	1A	3227	1/1	0.96	0.13	37,37,37,37	0
56	MG	2A	3820	1/1	0.96	0.08	73,73,73,73	0
56	MG	2A	3504	1/1	0.96	0.16	49,49,49,49	0
56	MG	1B	210	1/1	0.96	0.23	51,51,51,51	0
56	MG	1A	3786	1/1	0.96	0.06	24,24,24,24	0
56	MG	1A	3167	1/1	0.96	0.07	38,38,38,38	0
56	MG	1A	3352	1/1	0.96	0.35	41,41,41,41	0
56	MG	1a	1645	1/1	0.96	0.17	52,52,52,52	0
56	MG	1A	3790	1/1	0.96	0.08	19,19,19,19	0
56	MG	1A	3648	1/1	0.96	0.07	30,30,30,30	0
56	MG	1B	218	1/1	0.96	0.08	39,39,39,39	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	2a	3189	1/1	0.96	0.15	57,57,57,57	0
56	MG	1A	3230	1/1	0.96	0.07	36,36,36,36	0
56	MG	2a	3191	1/1	0.96	0.18	71,71,71,71	0
56	MG	1a	1652	1/1	0.96	0.07	48,48,48,48	0
56	MG	1A	3943	1/1	0.96	0.05	38,38,38,38	0
56	MG	1A	3066	1/1	0.96	0.06	29,29,29,29	0
56	MG	2a	3195	1/1	0.96	0.17	52,52,52,52	0
56	MG	2A	3521	1/1	0.96	0.08	38,38,38,38	0
56	MG	2A	3522	1/1	0.96	0.06	41,41,41,41	0
56	MG	2A	3523	1/1	0.96	0.09	42,42,42,42	0
56	MG	1A	3293	1/1	0.96	0.19	42,42,42,42	0
56	MG	1A	3169	1/1	0.96	0.14	49,49,49,49	0
56	MG	1A	3170	1/1	0.96	0.07	47,47,47,47	0
56	MG	1A	3799	1/1	0.96	0.05	38,38,38,38	0
56	MG	2A	3849	1/1	0.96	0.07	63,63,63,63	0
56	MG	1A	3236	1/1	0.96	0.20	30,30,30,30	0
56	MG	2A	3013	1/1	0.96	0.11	50,50,50,50	0
56	MG	2A	3852	1/1	0.96	0.06	53,53,53,53	0
56	MG	1A	3657	1/1	0.96	0.05	44,44,44,44	0
56	MG	1A	3659	1/1	0.96	0.08	24,24,24,24	0
56	MG	1a	1663	1/1	0.96	0.10	52,52,52,52	0
56	MG	1B	231	1/1	0.96	0.08	39,39,39,39	0
56	MG	1A	3237	1/1	0.96	0.14	30,30,30,30	0
56	MG	2A	3861	1/1	0.96	0.06	62,62,62,62	0
56	MG	1A	3960	1/1	0.96	0.11	50,50,50,50	0
56	MG	2A	3866	1/1	0.96	0.13	38,38,38,38	0
56	MG	2A	3273	1/1	0.96	0.10	49,49,49,49	0
56	MG	1A	3172	1/1	0.96	0.05	36,36,36,36	0
56	MG	2A	3023	1/1	0.96	0.22	51,51,51,51	0
56	MG	2A	3870	1/1	0.96	0.10	42,42,42,42	0
56	MG	2A	3871	1/1	0.96	0.07	39,39,39,39	0
56	MG	1A	3067	1/1	0.96	0.04	32,32,32,32	0
56	MG	2A	3544	1/1	0.96	0.07	35,35,35,35	0
56	MG	2A	3545	1/1	0.96	0.12	35,35,35,35	0
56	MG	1A	3049	1/1	0.96	0.20	39,39,39,39	0
56	MG	1A	3451	1/1	0.96	0.17	42,42,42,42	0
56	MG	1A	3543	1/1	0.96	0.20	34,34,34,34	0
56	MG	2A	3028	1/1	0.96	0.24	48,48,48,48	0
56	MG	1D	301	1/1	0.96	0.06	34,34,34,34	0
56	MG	1A	3308	1/1	0.96	0.14	32,32,32,32	0
56	MG	2A	3554	1/1	0.96	0.07	49,49,49,49	0
56	MG	2A	3032	1/1	0.96	0.08	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
56	MG	1A	3097	1/1	0.96	0.14	35,35,35,35	0
56	MG	1A	3368	1/1	0.96	0.06	37,37,37,37	0
56	MG	2A	3036	1/1	0.96	0.05	28,28,28,28	0
56	MG	2A	3560	1/1	0.96	0.10	38,38,38,38	0
56	MG	1D	311	1/1	0.96	0.06	50,50,50,50	0
56	MG	1A	3970	1/1	0.96	0.07	20,20,20,20	0
56	MG	1A	3369	1/1	0.96	0.10	44,44,44,44	0
56	MG	1E	302	1/1	0.96	0.16	47,47,47,47	0
56	MG	1A	3818	1/1	0.96	0.07	42,42,42,42	0
56	MG	1a	1681	1/1	0.96	0.08	56,56,56,56	0
56	MG	2A	3044	1/1	0.96	0.12	59,59,59,59	0
56	MG	2A	3296	1/1	0.96	0.10	50,50,50,50	0
56	MG	1a	1682	1/1	0.96	0.20	40,40,40,40	0
56	MG	1A	3673	1/1	0.96	0.09	17,17,17,17	0
56	MG	1A	3129	1/1	0.96	0.17	47,47,47,47	0
56	MG	1A	3978	1/1	0.96	0.09	36,36,36,36	0
56	MG	1A	3550	1/1	0.96	0.18	40,40,40,40	0
56	MG	1A	3311	1/1	0.96	0.15	40,40,40,40	0
56	MG	1A	3552	1/1	0.96	0.14	27,27,27,27	0
56	MG	1A	3072	1/1	0.96	0.22	31,31,31,31	0
56	MG	2A	3579	1/1	0.96	0.07	45,45,45,45	0
56	MG	1A	3375	1/1	0.96	0.14	42,42,42,42	0
56	MG	2A	3055	1/1	0.96	0.21	53,53,53,53	0
56	MG	2D	301	1/1	0.96	0.10	47,47,47,47	0
56	MG	2A	3056	1/1	0.96	0.21	59,59,59,59	0
56	MG	2A	3057	1/1	0.96	0.15	46,46,46,46	0
56	MG	1A	3185	1/1	0.96	0.06	37,37,37,37	0
56	MG	1A	3057	1/1	0.96	0.06	28,28,28,28	0
56	MG	1A	3078	1/1	0.96	0.08	31,31,31,31	0
56	MG	2A	3593	1/1	0.96	0.09	46,46,46,46	0
56	MG	2A	3061	1/1	0.96	0.08	63,63,63,63	0
56	MG	1A	3316	1/1	0.96	0.06	40,40,40,40	0
56	MG	1A	3134	1/1	0.96	0.07	41,41,41,41	0
56	MG	1A	3102	1/1	0.96	0.07	46,46,46,46	0
56	MG	1I	201	1/1	0.96	0.07	61,61,61,61	0
56	MG	2F	301	1/1	0.96	0.08	46,46,46,46	0
56	MG	1A	3319	1/1	0.96	0.16	51,51,51,51	0
56	MG	2A	3067	1/1	0.96	0.09	30,30,30,30	0
56	MG	1N	202	1/1	0.96	0.07	42,42,42,42	0
56	MG	2F	305	1/1	0.96	0.08	43,43,43,43	0
56	MG	1A	3137	1/1	0.96	0.09	27,27,27,27	0
56	MG	2A	3322	1/1	0.96	0.14	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3242	1/1	0.97	0.15	22,22,22,22	0
56	MG	1A	3025	1/1	0.97	0.06	30,30,30,30	0
56	MG	2a	3016	1/1	0.97	0.06	52,52,52,52	0
56	MG	1A	3244	1/1	0.97	0.10	42,42,42,42	0
56	MG	1A	3077	1/1	0.97	0.11	35,35,35,35	0
56	MG	17	106	1/1	0.97	0.13	25,25,25,25	0
56	MG	1A	3492	1/1	0.97	0.05	33,33,33,33	0
56	MG	17	108	1/1	0.97	0.06	45,45,45,45	0
56	MG	1A	3820	1/1	0.97	0.04	18,18,18,18	0
56	MG	1A	3421	1/1	0.97	0.14	32,32,32,32	0
56	MG	2A	3494	1/1	0.97	0.06	67,67,67,67	0
56	MG	2A	3080	1/1	0.97	0.15	56,56,56,56	0
56	MG	1A	3299	1/1	0.97	0.05	30,30,30,30	0
56	MG	2A	3288	1/1	0.97	0.08	36,36,36,36	0
56	MG	1A	3692	1/1	0.97	0.08	55,55,55,55	0
56	MG	2A	3290	1/1	0.97	0.08	36,36,36,36	0
56	MG	1A	3824	1/1	0.97	0.05	30,30,30,30	0
56	MG	1A	3094	1/1	0.97	0.07	20,20,20,20	0
56	MG	1A	3695	1/1	0.97	0.03	25,25,25,25	0
56	MG	1A	3828	1/1	0.97	0.10	45,45,45,45	0
56	MG	1a	1770	1/1	0.97	0.05	49,49,49,49	0
56	MG	1A	3301	1/1	0.97	0.05	24,24,24,24	0
56	MG	1B	220	1/1	0.97	0.05	32,32,32,32	0
56	MG	1a	1773	1/1	0.97	0.09	54,54,54,54	0
56	MG	1A	3135	1/1	0.97	0.09	23,23,23,23	0
56	MG	1A	3206	1/1	0.97	0.10	42,42,42,42	0
56	MG	1A	3045	1/1	0.97	0.04	28,28,28,28	0
56	MG	1A	3037	1/1	0.97	0.09	32,32,32,32	0
56	MG	1a	1778	1/1	0.97	0.09	55,55,55,55	0
56	MG	1A	3362	1/1	0.97	0.06	35,35,35,35	0
56	MG	1A	3430	1/1	0.97	0.06	47,47,47,47	0
56	MG	1a	1781	1/1	0.97	0.10	75,75,75,75	0
56	MG	2A	3520	1/1	0.97	0.09	49,49,49,49	0
56	MG	1A	3013	1/1	0.97	0.12	26,26,26,26	0
56	MG	1a	1783	1/1	0.97	0.10	57,57,57,57	0
56	MG	1B	228	1/1	0.97	0.05	42,42,42,42	0
56	MG	1A	3432	1/1	0.97	0.19	36,36,36,36	0
56	MG	1A	3593	1/1	0.97	0.25	27,27,27,27	0
56	MG	1A	3252	1/1	0.97	0.12	37,37,37,37	0
56	MG	1A	3595	1/1	0.97	0.07	34,34,34,34	0
56	MG	1A	3171	1/1	0.97	0.08	44,44,44,44	0
56	MG	1A	3509	1/1	0.97	0.12	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
56	MG	2A	3530	1/1	0.97	0.10	49,49,49,49	0
56	MG	2A	3774	1/1	0.97	0.09	64,64,64,64	0
56	MG	1A	3006	1/1	0.97	0.14	47,47,47,47	0
56	MG	1A	3599	1/1	0.97	0.12	42,42,42,42	0
56	MG	2A	3778	1/1	0.97	0.10	58,58,58,58	0
56	MG	1A	3173	1/1	0.97	0.17	34,34,34,34	0
56	MG	1A	3017	1/1	0.97	0.18	50,50,50,50	0
56	MG	1A	3179	1/1	0.97	0.05	29,29,29,29	0
56	MG	2A	3537	1/1	0.97	0.06	56,56,56,56	0
56	MG	1D	302	1/1	0.97	0.08	36,36,36,36	0
56	MG	2A	3539	1/1	0.97	0.06	48,48,48,48	0
56	MG	1a	1624	1/1	0.97	0.13	62,62,62,62	0
56	MG	1D	303	1/1	0.97	0.08	17,17,17,17	0
56	MG	1a	1801	1/1	0.97	0.07	64,64,64,64	0
56	MG	1a	1802	1/1	0.97	0.09	63,63,63,63	0
56	MG	1D	304	1/1	0.97	0.05	35,35,35,35	0
56	MG	2a	3073	1/1	0.97	0.11	50,50,50,50	0
56	MG	2A	3328	1/1	0.97	0.07	41,41,41,41	0
56	MG	1D	305	1/1	0.97	0.16	29,29,29,29	0
56	MG	1A	3603	1/1	0.97	0.09	39,39,39,39	0
56	MG	2A	3548	1/1	0.97	0.13	35,35,35,35	0
56	MG	1A	3994	1/1	0.97	0.05	70,70,70,70	0
56	MG	2a	3079	1/1	0.97	0.15	56,56,56,56	0
56	MG	2A	3125	1/1	0.97	0.05	58,58,58,58	0
56	MG	1D	309	1/1	0.97	0.17	20,20,20,20	0
56	MG	2A	3127	1/1	0.97	0.16	65,65,65,65	0
56	MG	2A	3553	1/1	0.97	0.11	49,49,49,49	0
56	MG	2A	3128	1/1	0.97	0.04	42,42,42,42	0
56	MG	1a	1631	1/1	0.97	0.05	33,33,33,33	0
56	MG	1A	3851	1/1	0.97	0.06	11,11,11,11	0
56	MG	2a	3087	1/1	0.97	0.13	59,59,59,59	0
56	MG	1a	1813	1/1	0.97	0.06	53,53,53,53	0
56	MG	2A	3558	1/1	0.97	0.08	52,52,52,52	0
56	MG	1A	3604	1/1	0.97	0.08	27,27,27,27	0
56	MG	2A	3133	1/1	0.97	0.07	55,55,55,55	0
56	MG	2A	3561	1/1	0.97	0.07	36,36,36,36	0
56	MG	1a	1816	1/1	0.97	0.09	53,53,53,53	0
56	MG	1A	3215	1/1	0.97	0.08	39,39,39,39	0
56	MG	1A	3146	1/1	0.97	0.18	25,25,25,25	0
56	MG	2A	3813	1/1	0.97	0.07	53,53,53,53	0
56	MG	1E	301	1/1	0.97	0.28	28,28,28,28	0
56	MG	1A	3723	1/1	0.97	0.07	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
56	MG	1a	1822	1/1	0.97	0.06	69,69,69,69	0
56	MG	2A	3142	1/1	0.97	0.10	43,43,43,43	0
56	MG	1a	1824	1/1	0.97	0.05	60,60,60,60	0
56	MG	1A	3441	1/1	0.97	0.07	41,41,41,41	0
56	MG	1E	305	1/1	0.97	0.08	32,32,32,32	0
56	MG	1a	1828	1/1	0.97	0.17	42,42,42,42	0
56	MG	2A	3822	1/1	0.97	0.06	61,61,61,61	0
56	MG	1E	306	1/1	0.97	0.13	26,26,26,26	0
56	MG	1A	3442	1/1	0.97	0.08	36,36,36,36	0
56	MG	1A	3218	1/1	0.97	0.13	34,34,34,34	0
56	MG	2A	3355	1/1	0.97	0.07	51,51,51,51	0
56	MG	2A	3577	1/1	0.97	0.15	57,57,57,57	0
56	MG	1A	4004	1/1	0.97	0.05	51,51,51,51	0
56	MG	1A	3181	1/1	0.97	0.08	39,39,39,39	0
56	MG	1E	312	1/1	0.97	0.12	39,39,39,39	0
56	MG	1a	1649	1/1	0.97	0.14	44,44,44,44	0
56	MG	1A	3521	1/1	0.97	0.05	47,47,47,47	0
56	MG	1A	3445	1/1	0.97	0.10	36,36,36,36	0
56	MG	2A	3362	1/1	0.97	0.10	43,43,43,43	0
56	MG	1E	315	1/1	0.97	0.05	40,40,40,40	0
56	MG	1a	1653	1/1	0.97	0.14	56,56,56,56	0
56	MG	2A	3840	1/1	0.97	0.05	51,51,51,51	0
56	MG	1F	302	1/1	0.97	0.08	30,30,30,30	0
56	MG	1A	3376	1/1	0.97	0.10	44,44,44,44	0
56	MG	1l	201	1/1	0.97	0.08	56,56,56,56	0
56	MG	1l	202	1/1	0.97	0.09	41,41,41,41	0
56	MG	2A	3847	1/1	0.97	0.06	47,47,47,47	0
56	MG	1A	3614	1/1	0.97	0.12	35,35,35,35	0
56	MG	1F	306	1/1	0.97	0.10	23,23,23,23	0
56	MG	2a	3128	1/1	0.97	0.12	44,44,44,44	0
56	MG	1A	3220	1/1	0.97	0.12	49,49,49,49	0
56	MG	1A	3736	1/1	0.97	0.06	38,38,38,38	0
56	MG	1A	3525	1/1	0.97	0.13	31,31,31,31	0
56	MG	1G	201	1/1	0.97	0.10	43,43,43,43	0
56	MG	1A	3087	1/1	0.97	0.14	35,35,35,35	0
56	MG	2A	3857	1/1	0.97	0.06	66,66,66,66	0
56	MG	1A	3527	1/1	0.97	0.13	32,32,32,32	0
56	MG	2A	3607	1/1	0.97	0.08	57,57,57,57	0
56	MG	1A	3264	1/1	0.97	0.05	36,36,36,36	0
56	MG	1A	3622	1/1	0.97	0.05	22,22,22,22	0
56	MG	2A	3862	1/1	0.97	0.05	57,57,57,57	0
56	MG	2A	3863	1/1	0.97	0.06	28,28,28,28	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1A	3529	1/1	0.97	0.19	28,28,28,28	0
56	MG	2A	3865	1/1	0.97	0.04	51,51,51,51	0
56	MG	1A	3119	1/1	0.97	0.10	23,23,23,23	0
56	MG	1A	3874	1/1	0.97	0.14	27,27,27,27	0
56	MG	1w	108	1/1	0.97	0.06	74,74,74,74	0
56	MG	1A	3625	1/1	0.97	0.11	53,53,53,53	0
56	MG	1A	3266	1/1	0.97	0.15	40,40,40,40	0
56	MG	1N	206	1/1	0.97	0.08	37,37,37,37	0
56	MG	2a	3152	1/1	0.97	0.06	70,70,70,70	0
56	MG	2A	3386	1/1	0.97	0.39	55,55,55,55	0
56	MG	1A	4025	1/1	0.97	0.09	40,40,40,40	0
56	MG	1O	204	1/1	0.97	0.08	46,46,46,46	0
56	MG	2a	3156	1/1	0.97	0.06	72,72,72,72	0
56	MG	2A	3389	1/1	0.97	0.15	36,36,36,36	0
56	MG	1A	3452	1/1	0.97	0.08	38,38,38,38	0
56	MG	2A	3877	1/1	0.97	0.07	49,49,49,49	0
56	MG	1P	201	1/1	0.97	0.14	25,25,25,25	0
56	MG	1A	3629	1/1	0.97	0.04	29,29,29,29	0
56	MG	2A	3393	1/1	0.97	0.17	40,40,40,40	0
56	MG	1x	106	1/1	0.97	0.17	52,52,52,52	0
56	MG	1A	3630	1/1	0.97	0.06	29,29,29,29	0
56	MG	1A	3631	1/1	0.97	0.04	14,14,14,14	0
56	MG	2a	3171	1/1	0.97	0.09	64,64,64,64	0
56	MG	1A	3453	1/1	0.97	0.20	31,31,31,31	0
56	MG	2A	3192	1/1	0.97	0.12	60,60,60,60	0
56	MG	1A	4034	1/1	0.97	0.09	61,61,61,61	0
56	MG	1A	3753	1/1	0.97	0.06	34,34,34,34	0
56	MG	1A	3755	1/1	0.97	0.05	46,46,46,46	0
56	MG	1Q	202	1/1	0.97	0.19	34,34,34,34	0
56	MG	2A	3197	1/1	0.97	0.15	55,55,55,55	0
56	MG	1A	3267	1/1	0.97	0.14	40,40,40,40	0
56	MG	1x	116	1/1	0.97	0.12	65,65,65,65	0
56	MG	1A	3455	1/1	0.97	0.11	28,28,28,28	0
56	MG	1A	3758	1/1	0.97	0.06	40,40,40,40	0
56	MG	1A	3384	1/1	0.97	0.08	41,41,41,41	0
56	MG	2a	3184	1/1	0.97	0.15	57,57,57,57	0
56	MG	1A	3637	1/1	0.97	0.09	48,48,48,48	0
56	MG	1R	202	1/1	0.97	0.21	36,36,36,36	0
56	MG	1A	3385	1/1	0.97	0.05	27,27,27,27	0
56	MG	1A	4046	1/1	0.97	0.06	44,44,44,44	0
56	MG	1A	3068	1/1	0.97	0.09	48,48,48,48	0
56	MG	2A	3209	1/1	0.97	0.13	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
56	MG	2A	3647	1/1	0.97	0.32	64,64,64,64	0
56	MG	1A	3269	1/1	0.97	0.05	29,29,29,29	0
56	MG	2A	3211	1/1	0.97	0.07	45,45,45,45	0
56	MG	1A	3540	1/1	0.97	0.06	45,45,45,45	0
56	MG	2A	3010	1/1	0.97	0.16	46,46,46,46	0
56	MG	1A	3225	1/1	0.97	0.06	39,39,39,39	0
56	MG	1A	3542	1/1	0.97	0.11	37,37,37,37	0
56	MG	1A	3226	1/1	0.97	0.11	43,43,43,43	0
56	MG	1A	3645	1/1	0.97	0.10	20,20,20,20	0
56	MG	2A	3423	1/1	0.97	0.13	35,35,35,35	0
56	MG	1A	3902	1/1	0.97	0.10	43,43,43,43	0
56	MG	2A	3659	1/1	0.97	0.11	58,58,58,58	0
56	MG	1A	3272	1/1	0.97	0.13	22,22,22,22	0
56	MG	2a	3205	1/1	0.97	0.07	60,60,60,60	0
56	MG	2A	3220	1/1	0.97	0.07	52,52,52,52	0
56	MG	1A	3150	1/1	0.97	0.08	31,31,31,31	0
56	MG	1A	3275	1/1	0.97	0.17	31,31,31,31	0
56	MG	1U	210	1/1	0.97	0.19	25,25,25,25	0
56	MG	2A	3666	1/1	0.97	0.06	44,44,44,44	0
56	MG	2A	3430	1/1	0.97	0.15	31,31,31,31	0
56	MG	1A	3186	1/1	0.97	0.12	37,37,37,37	0
56	MG	2A	3669	1/1	0.97	0.10	59,59,59,59	0
56	MG	1V	201	1/1	0.97	0.25	30,30,30,30	0
56	MG	2F	306	1/1	0.97	0.17	51,51,51,51	0
56	MG	1A	3229	1/1	0.97	0.18	32,32,32,32	0
56	MG	2N	201	1/1	0.97	0.05	35,35,35,35	0
56	MG	2A	3434	1/1	0.97	0.24	46,46,46,46	0
56	MG	1V	204	1/1	0.97	0.17	32,32,32,32	0
56	MG	1A	3009	1/1	0.97	0.05	17,17,17,17	0
56	MG	1V	206	1/1	0.97	0.06	29,29,29,29	0
56	MG	2A	3231	1/1	0.97	0.20	50,50,50,50	0
56	MG	2a	3226	1/1	0.97	0.12	50,50,50,50	0
56	MG	2A	3232	1/1	0.97	0.07	60,60,60,60	0
56	MG	2A	3233	1/1	0.97	0.07	33,33,33,33	0
56	MG	1A	4063	1/1	0.97	0.07	46,46,46,46	0
56	MG	1A	3335	1/1	0.97	0.07	36,36,36,36	0
56	MG	1A	3231	1/1	0.97	0.16	33,33,33,33	0
56	MG	2A	3031	1/1	0.97	0.05	48,48,48,48	0
56	MG	1A	3281	1/1	0.97	0.21	31,31,31,31	0
56	MG	1A	3782	1/1	0.97	0.07	48,48,48,48	0
56	MG	2T	203	1/1	0.97	0.12	50,50,50,50	0
56	MG	2A	3685	1/1	0.97	0.06	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
56	MG	1A	3656	1/1	0.97	0.07	34,34,34,34	0
56	MG	2A	3035	1/1	0.97	0.08	36,36,36,36	0
56	MG	1A	3554	1/1	0.97	0.26	41,41,41,41	0
56	MG	1A	3658	1/1	0.97	0.08	42,42,42,42	0
56	MG	1A	3555	1/1	0.97	0.05	23,23,23,23	0
56	MG	1A	3788	1/1	0.97	0.05	35,35,35,35	0
56	MG	2A	3692	1/1	0.97	0.06	66,66,66,66	0
56	MG	1A	3154	1/1	0.97	0.15	39,39,39,39	0
56	MG	1A	3922	1/1	0.97	0.04	70,70,70,70	0
56	MG	2A	3042	1/1	0.97	0.08	44,44,44,44	0
56	MG	1A	3122	1/1	0.97	0.11	37,37,37,37	0
56	MG	1A	3156	1/1	0.97	0.23	39,39,39,39	0
56	MG	1A	3792	1/1	0.97	0.06	45,45,45,45	0
56	MG	1A	3285	1/1	0.97	0.25	26,26,26,26	0
56	MG	1A	4082	1/1	0.97	0.07	35,35,35,35	0
56	MG	1A	3560	1/1	0.97	0.07	51,51,51,51	0
56	MG	1A	3104	1/1	0.97	0.04	25,25,25,25	0
56	MG	23	103	1/1	0.97	0.06	55,55,55,55	0
56	MG	1A	3562	1/1	0.97	0.06	43,43,43,43	0
56	MG	2A	3705	1/1	0.97	0.15	51,51,51,51	0
56	MG	1A	3406	1/1	0.97	0.13	43,43,43,43	0
56	MG	1A	3407	1/1	0.97	0.07	36,36,36,36	0
56	MG	1A	3287	1/1	0.97	0.06	43,43,43,43	0
56	MG	1A	3672	1/1	0.97	0.04	35,35,35,35	0
56	MG	1A	3410	1/1	0.97	0.06	39,39,39,39	0
56	MG	1A	3940	1/1	0.97	0.04	28,28,28,28	0
56	MG	1A	3567	1/1	0.97	0.12	29,29,29,29	0
56	MG	1A	3804	1/1	0.97	0.06	22,22,22,22	0
56	MG	2A	3716	1/1	0.97	0.05	51,51,51,51	0
56	MG	1A	3568	1/1	0.97	0.14	30,30,30,30	0
56	MG	1A	3090	1/1	0.97	0.09	30,30,30,30	0
56	MG	1A	3159	1/1	0.97	0.17	30,30,30,30	0
56	MG	2A	3720	1/1	0.97	0.06	48,48,48,48	0
56	MG	1A	3106	1/1	0.97	0.06	26,26,26,26	0
56	MG	1a	1745	1/1	0.97	0.06	54,54,54,54	0
56	MG	1A	3812	1/1	0.97	0.05	54,54,54,54	0
56	MG	1a	1747	1/1	0.97	0.06	52,52,52,52	0
56	MG	1A	3951	1/1	0.97	0.05	42,42,42,42	0
56	MG	16	101	1/1	0.97	0.06	41,41,41,41	0
59	ZN	14	102	1/1	0.97	0.04	87,87,87,87	0
56	MG	1A	3347	1/1	0.97	0.20	41,41,41,41	0
56	MG	1A	3033	1/1	0.97	0.30	24,24,24,24	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
60	SF4	1d	302	8/8	0.97	0.06	68,78,85,86	0
60	SF4	2d	302	8/8	0.97	0.05	59,73,81,82	0
56	MG	1B	216	1/1	0.98	0.05	47,47,47,47	0
56	MG	2A	3534	1/1	0.98	0.05	41,41,41,41	0
56	MG	1B	217	1/1	0.98	0.13	47,47,47,47	0
56	MG	1A	3729	1/1	0.98	0.04	32,32,32,32	0
56	MG	1A	3731	1/1	0.98	0.05	24,24,24,24	0
56	MG	2A	3707	1/1	0.98	0.07	36,36,36,36	0
56	MG	2A	3229	1/1	0.98	0.16	33,33,33,33	0
56	MG	1A	3419	1/1	0.98	0.10	32,32,32,32	0
56	MG	1W	203	1/1	0.98	0.06	31,31,31,31	0
56	MG	1a	1814	1/1	0.98	0.05	67,67,67,67	0
56	MG	1A	3153	1/1	0.98	0.07	26,26,26,26	0
56	MG	1A	3081	1/1	0.98	0.08	27,27,27,27	0
56	MG	1X	101	1/1	0.98	0.06	32,32,32,32	0
56	MG	1X	102	1/1	0.98	0.10	35,35,35,35	0
56	MG	1A	4013	1/1	0.98	0.06	62,62,62,62	0
56	MG	1A	3015	1/1	0.98	0.05	39,39,39,39	0
56	MG	1A	3023	1/1	0.98	0.03	15,15,15,15	0
56	MG	1a	1823	1/1	0.98	0.04	59,59,59,59	0
56	MG	1A	3035	1/1	0.98	0.03	39,39,39,39	0
56	MG	1a	1825	1/1	0.98	0.14	43,43,43,43	0
56	MG	1A	3280	1/1	0.98	0.06	21,21,21,21	0
56	MG	2A	3092	1/1	0.98	0.15	48,48,48,48	0
56	MG	1A	3373	1/1	0.98	0.12	43,43,43,43	0
56	MG	1A	3125	1/1	0.98	0.18	34,34,34,34	0
56	MG	1Z	303	1/1	0.98	0.07	42,42,42,42	0
56	MG	1A	3241	1/1	0.98	0.23	30,30,30,30	0
56	MG	1A	3126	1/1	0.98	0.16	34,34,34,34	0
56	MG	2D	305	1/1	0.98	0.05	33,33,33,33	0
56	MG	1A	3827	1/1	0.98	0.06	39,39,39,39	0
56	MG	1A	3200	1/1	0.98	0.05	33,33,33,33	0
56	MG	2A	3733	1/1	0.98	0.05	51,51,51,51	0
56	MG	1A	3160	1/1	0.98	0.21	26,26,26,26	0
56	MG	1A	3669	1/1	0.98	0.05	19,19,19,19	0
56	MG	1A	3127	1/1	0.98	0.07	42,42,42,42	0
56	MG	1A	3204	1/1	0.98	0.04	29,29,29,29	0
56	MG	1B	238	1/1	0.98	0.06	37,37,37,37	0
56	MG	1A	3128	1/1	0.98	0.15	36,36,36,36	0
56	MG	2A	3106	1/1	0.98	0.07	36,36,36,36	0
56	MG	2a	3130	1/1	0.98	0.05	68,68,68,68	0
56	MG	1A	3383	1/1	0.98	0.17	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
56	MG	2A	3260	1/1	0.98	0.06	57,57,57,57	0
56	MG	1A	3927	1/1	0.98	0.06	55,55,55,55	0
56	MG	1A	3549	1/1	0.98	0.12	30,30,30,30	0
56	MG	1A	3752	1/1	0.98	0.04	37,37,37,37	0
56	MG	1A	3085	1/1	0.98	0.07	23,23,23,23	0
56	MG	1A	3086	1/1	0.98	0.15	28,28,28,28	0
56	MG	1D	307	1/1	0.98	0.10	44,44,44,44	0
56	MG	1A	3386	1/1	0.98	0.07	30,30,30,30	0
56	MG	1A	3010	1/1	0.98	0.07	36,36,36,36	0
56	MG	2a	3141	1/1	0.98	0.06	68,68,68,68	0
56	MG	1A	3132	1/1	0.98	0.06	33,33,33,33	0
56	MG	1A	3936	1/1	0.98	0.06	14,14,14,14	0
56	MG	2A	3580	1/1	0.98	0.09	45,45,45,45	0
56	MG	1A	4044	1/1	0.98	0.04	43,43,43,43	0
56	MG	2a	3146	1/1	0.98	0.07	68,68,68,68	0
56	MG	1A	3011	1/1	0.98	0.10	31,31,31,31	0
56	MG	2A	3756	1/1	0.98	0.14	55,55,55,55	0
56	MG	1A	3938	1/1	0.98	0.04	54,54,54,54	0
56	MG	1A	3615	1/1	0.98	0.05	33,33,33,33	0
56	MG	1A	4050	1/1	0.98	0.09	46,46,46,46	0
56	MG	2A	3588	1/1	0.98	0.07	37,37,37,37	0
56	MG	2A	3589	1/1	0.98	0.05	44,44,44,44	0
56	MG	1A	3761	1/1	0.98	0.06	36,36,36,36	0
56	MG	2A	3591	1/1	0.98	0.07	46,46,46,46	0
56	MG	1A	3683	1/1	0.98	0.10	20,20,20,20	0
56	MG	1A	3294	1/1	0.98	0.06	41,41,41,41	0
56	MG	2a	3158	1/1	0.98	0.10	54,54,54,54	0
56	MG	1A	3764	1/1	0.98	0.05	14,14,14,14	0
56	MG	2a	3161	1/1	0.98	0.04	67,67,67,67	0
56	MG	1A	3295	1/1	0.98	0.04	22,22,22,22	0
56	MG	1A	3012	1/1	0.98	0.06	28,28,28,28	0
56	MG	1E	311	1/1	0.98	0.06	52,52,52,52	0
56	MG	1A	3949	1/1	0.98	0.07	54,54,54,54	0
56	MG	2a	3166	1/1	0.98	0.04	67,67,67,67	0
56	MG	2A	3435	1/1	0.98	0.07	28,28,28,28	0
56	MG	2a	3168	1/1	0.98	0.06	51,51,51,51	0
56	MG	1A	3688	1/1	0.98	0.07	33,33,33,33	0
56	MG	1a	1723	1/1	0.98	0.23	46,46,46,46	0
56	MG	1A	3007	1/1	0.98	0.05	26,26,26,26	0
56	MG	2A	3603	1/1	0.98	0.04	60,60,60,60	0
56	MG	2A	3604	1/1	0.98	0.10	44,44,44,44	0
56	MG	1A	3298	1/1	0.98	0.06	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
56	MG	18	106	1/1	0.98	0.05	26,26,26,26	0
56	MG	1a	1727	1/1	0.98	0.13	36,36,36,36	0
56	MG	1F	301	1/1	0.98	0.04	27,27,27,27	0
56	MG	2A	3782	1/1	0.98	0.06	55,55,55,55	0
56	MG	1A	3028	1/1	0.98	0.13	21,21,21,21	0
56	MG	1F	303	1/1	0.98	0.09	28,28,28,28	0
56	MG	1A	3396	1/1	0.98	0.17	26,26,26,26	0
56	MG	2A	3786	1/1	0.98	0.08	51,51,51,51	0
56	MG	1A	3957	1/1	0.98	0.09	50,50,50,50	0
56	MG	1A	3071	1/1	0.98	0.09	29,29,29,29	0
56	MG	1F	307	1/1	0.98	0.13	30,30,30,30	0
56	MG	1A	4065	1/1	0.98	0.08	36,36,36,36	0
56	MG	2a	3187	1/1	0.98	0.06	70,70,70,70	0
56	MG	1A	3773	1/1	0.98	0.04	46,46,46,46	0
56	MG	1A	3694	1/1	0.98	0.08	41,41,41,41	0
56	MG	1A	3042	1/1	0.98	0.18	22,22,22,22	0
56	MG	2A	3794	1/1	0.98	0.04	65,65,65,65	0
56	MG	1A	3139	1/1	0.98	0.11	36,36,36,36	0
56	MG	1A	3862	1/1	0.98	0.11	36,36,36,36	0
56	MG	2A	3153	1/1	0.98	0.06	41,41,41,41	0
56	MG	1A	3175	1/1	0.98	0.17	30,30,30,30	0
56	MG	1a	1742	1/1	0.98	0.06	55,55,55,55	0
56	MG	1A	3628	1/1	0.98	0.04	51,51,51,51	0
56	MG	2A	3307	1/1	0.98	0.05	54,54,54,54	0
56	MG	2A	3009	1/1	0.98	0.05	38,38,38,38	0
56	MG	1A	3176	1/1	0.98	0.10	27,27,27,27	0
56	MG	1A	3177	1/1	0.98	0.12	25,25,25,25	0
56	MG	1A	3178	1/1	0.98	0.05	17,17,17,17	0
56	MG	1A	3702	1/1	0.98	0.03	8,8,8,8	0
56	MG	1A	4077	1/1	0.98	0.06	27,27,27,27	0
56	MG	1A	3570	1/1	0.98	0.12	29,29,29,29	0
56	MG	1A	3785	1/1	0.98	0.06	37,37,37,37	0
56	MG	2A	3017	1/1	0.98	0.04	36,36,36,36	0
56	MG	1O	202	1/1	0.98	0.15	47,47,47,47	0
56	MG	1O	203	1/1	0.98	0.09	40,40,40,40	0
56	MG	2a	3210	1/1	0.98	0.09	57,57,57,57	0
56	MG	2a	3211	1/1	0.98	0.07	50,50,50,50	0
56	MG	2a	3212	1/1	0.98	0.10	59,59,59,59	0
56	MG	1A	3633	1/1	0.98	0.05	28,28,28,28	0
56	MG	1A	3975	1/1	0.98	0.06	50,50,50,50	0
56	MG	1A	3014	1/1	0.98	0.06	22,22,22,22	0
56	MG	1A	3977	1/1	0.98	0.13	59,59,59,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1a	1758	1/1	0.98	0.05	32,32,32,32	0
56	MG	1P	203	1/1	0.98	0.10	25,25,25,25	0
56	MG	2A	3477	1/1	0.98	0.12	23,23,23,23	0
56	MG	1P	204	1/1	0.98	0.18	23,23,23,23	0
56	MG	1A	3457	1/1	0.98	0.05	25,25,25,25	0
56	MG	1A	3354	1/1	0.98	0.06	34,34,34,34	0
56	MG	2A	3177	1/1	0.98	0.14	35,35,35,35	0
56	MG	1A	3875	1/1	0.98	0.25	35,35,35,35	0
56	MG	2A	3825	1/1	0.98	0.03	43,43,43,43	0
56	MG	1A	3355	1/1	0.98	0.26	25,25,25,25	0
56	MG	2A	3651	1/1	0.98	0.07	44,44,44,44	0
56	MG	1A	3517	1/1	0.98	0.06	44,44,44,44	0
56	MG	1A	4091	1/1	0.98	0.05	31,31,31,31	0
56	MG	1A	3142	1/1	0.98	0.05	14,14,14,14	0
56	MG	1Q	203	1/1	0.98	0.09	24,24,24,24	0
56	MG	1a	1637	1/1	0.98	0.13	54,54,54,54	0
56	MG	2A	3185	1/1	0.98	0.12	47,47,47,47	0
56	MG	1A	3075	1/1	0.98	0.04	21,21,21,21	0
56	MG	1A	3409	1/1	0.98	0.12	41,41,41,41	0
56	MG	2A	3837	1/1	0.98	0.09	66,66,66,66	0
56	MG	2A	3188	1/1	0.98	0.06	43,43,43,43	0
56	MG	1A	3795	1/1	0.98	0.06	19,19,19,19	0
56	MG	1Q	207	1/1	0.98	0.05	44,44,44,44	0
56	MG	2A	3663	1/1	0.98	0.05	54,54,54,54	0
56	MG	1A	3145	1/1	0.98	0.18	21,21,21,21	0
56	MG	2A	3496	1/1	0.98	0.05	55,55,55,55	0
56	MG	1A	4097	1/1	0.98	0.06	35,35,35,35	0
56	MG	1a	1644	1/1	0.98	0.09	39,39,39,39	0
56	MG	1A	3115	1/1	0.98	0.04	32,32,32,32	0
56	MG	2A	3045	1/1	0.98	0.20	53,53,53,53	0
56	MG	1A	3021	1/1	0.98	0.04	21,21,21,21	0
56	MG	1A	3716	1/1	0.98	0.06	31,31,31,31	0
56	MG	1a	1648	1/1	0.98	0.05	48,48,48,48	0
56	MG	2A	3199	1/1	0.98	0.18	50,50,50,50	0
56	MG	1A	3886	1/1	0.98	0.04	23,23,23,23	0
56	MG	2A	3856	1/1	0.98	0.05	58,58,58,58	0
56	MG	1A	3466	1/1	0.98	0.07	36,36,36,36	0
56	MG	2A	3507	1/1	0.98	0.10	44,44,44,44	0
56	MG	1A	3031	1/1	0.98	0.16	31,31,31,31	0
56	MG	2A	3510	1/1	0.98	0.06	41,41,41,41	0
56	MG	1A	3118	1/1	0.98	0.14	22,22,22,22	0
56	MG	1A	3995	1/1	0.98	0.05	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
56	MG	1A	3890	1/1	0.98	0.03	33,33,33,33	0
56	MG	1A	3721	1/1	0.98	0.07	27,27,27,27	0
56	MG	1A	3469	1/1	0.98	0.05	33,33,33,33	0
56	MG	1U	203	1/1	0.98	0.26	28,28,28,28	0
56	MG	1A	3806	1/1	0.98	0.05	26,26,26,26	0
56	MG	1a	1792	1/1	0.98	0.06	60,60,60,60	0
56	MG	1A	3649	1/1	0.98	0.04	29,29,29,29	0
56	MG	1U	207	1/1	0.98	0.14	29,29,29,29	0
56	MG	1U	208	1/1	0.98	0.19	30,30,30,30	0
56	MG	1a	1796	1/1	0.98	0.06	59,59,59,59	0
56	MG	1A	3586	1/1	0.98	0.17	31,31,31,31	0
56	MG	1A	3032	1/1	0.98	0.12	26,26,26,26	0
56	MG	1U	211	1/1	0.98	0.11	28,28,28,28	0
56	MG	1A	3810	1/1	0.98	0.06	25,25,25,25	0
56	MG	1A	3099	1/1	0.98	0.10	16,16,16,16	0
56	MG	1A	3152	1/1	0.98	0.03	29,29,29,29	0
56	MG	1V	203	1/1	0.98	0.18	26,26,26,26	0
56	MG	1a	1804	1/1	0.98	0.05	53,53,53,53	0
59	ZN	2Y	501	1/1	0.98	0.04	81,81,81,81	0
56	MG	1a	1805	1/1	0.98	0.08	55,55,55,55	0
56	MG	2A	3882	1/1	0.98	0.06	42,42,42,42	0
56	MG	2A	3700	1/1	0.98	0.04	58,58,58,58	0
56	MG	1A	3274	1/1	0.98	0.11	38,38,38,38	0
56	MG	2A	3776	1/1	0.99	0.04	56,56,56,56	0
56	MG	2A	3854	1/1	0.99	0.06	35,35,35,35	0
56	MG	1A	3305	1/1	0.99	0.18	34,34,34,34	0
56	MG	1A	3233	1/1	0.99	0.03	30,30,30,30	0
56	MG	2A	3019	1/1	0.99	0.04	30,30,30,30	0
56	MG	1A	3307	1/1	0.99	0.08	26,26,26,26	0
56	MG	1A	3974	1/1	0.99	0.04	54,54,54,54	0
56	MG	1A	4020	1/1	0.99	0.04	33,33,33,33	0
56	MG	1A	3216	1/1	0.99	0.15	32,32,32,32	0
56	MG	1A	3201	1/1	0.99	0.03	22,22,22,22	0
56	MG	1A	3496	1/1	0.99	0.06	25,25,25,25	0
56	MG	1A	3187	1/1	0.99	0.05	31,31,31,31	0
56	MG	1A	3830	1/1	0.99	0.19	48,48,48,48	0
56	MG	1A	4026	1/1	0.99	0.04	35,35,35,35	0
56	MG	2A	3642	1/1	0.99	0.04	41,41,41,41	0
56	MG	1A	3144	1/1	0.99	0.10	42,42,42,42	0
56	MG	1A	4080	1/1	0.99	0.04	39,39,39,39	0
56	MG	1A	3740	1/1	0.99	0.04	49,49,49,49	0
56	MG	1A	4029	1/1	0.99	0.05	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
56	MG	1A	3899	1/1	0.99	0.04	38,38,38,38	0
56	MG	1A	4031	1/1	0.99	0.07	60,60,60,60	0
56	MG	2A	3508	1/1	0.99	0.05	64,64,64,64	0
56	MG	1X	105	1/1	0.99	0.06	29,29,29,29	0
56	MG	1A	3939	1/1	0.99	0.08	21,21,21,21	0
56	MG	2A	3725	1/1	0.99	0.06	34,34,34,34	0
56	MG	1A	4086	1/1	0.99	0.08	28,28,28,28	0
56	MG	1A	3900	1/1	0.99	0.03	20,20,20,20	0
56	MG	2A	3582	1/1	0.99	0.06	39,39,39,39	0
56	MG	1A	3079	1/1	0.99	0.15	26,26,26,26	0
56	MG	2A	3584	1/1	0.99	0.05	59,59,59,59	0
56	MG	1A	3687	1/1	0.99	0.08	27,27,27,27	0
56	MG	1A	3190	1/1	0.99	0.15	25,25,25,25	0
56	MG	1A	3944	1/1	0.99	0.05	44,44,44,44	0
56	MG	1A	3501	1/1	0.99	0.07	28,28,28,28	0
56	MG	1A	3946	1/1	0.99	0.03	40,40,40,40	0
56	MG	1A	3805	1/1	0.99	0.03	35,35,35,35	0
56	MG	1w	111	1/1	0.99	0.06	69,69,69,69	0
56	MG	1A	4041	1/1	0.99	0.02	42,42,42,42	0
56	MG	1A	3374	1/1	0.99	0.03	30,30,30,30	0
56	MG	2a	3159	1/1	0.99	0.03	56,56,56,56	0
56	MG	1A	3839	1/1	0.99	0.07	43,43,43,43	0
56	MG	1A	3908	1/1	0.99	0.04	32,32,32,32	0
56	MG	1A	4045	1/1	0.99	0.03	17,17,17,17	0
56	MG	1A	3222	1/1	0.99	0.16	29,29,29,29	0
56	MG	1A	3952	1/1	0.99	0.04	39,39,39,39	0
56	MG	2A	3119	1/1	0.99	0.11	36,36,36,36	0
56	MG	1A	4048	1/1	0.99	0.05	34,34,34,34	0
56	MG	1E	304	1/1	0.99	0.11	34,34,34,34	0
56	MG	1A	3953	1/1	0.99	0.03	50,50,50,50	0
56	MG	1A	3666	1/1	0.99	0.05	35,35,35,35	0
56	MG	1A	3719	1/1	0.99	0.09	47,47,47,47	0
56	MG	1A	3779	1/1	0.99	0.03	18,18,18,18	0
56	MG	1a	1811	1/1	0.99	0.05	38,38,38,38	0
56	MG	1x	114	1/1	0.99	0.05	51,51,51,51	0
56	MG	1A	3008	1/1	0.99	0.08	26,26,26,26	0
56	MG	2A	3829	1/1	0.99	0.04	45,45,45,45	0
56	MG	1A	3914	1/1	0.99	0.04	19,19,19,19	0
56	MG	1A	3073	1/1	0.99	0.07	14,14,14,14	0
56	MG	1A	3064	1/1	0.99	0.06	32,32,32,32	0
56	MG	1A	3036	1/1	0.99	0.05	15,15,15,15	0
56	MG	1A	3076	1/1	0.99	0.10	20,20,20,20	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
56	MG	1a	1757	1/1	0.99	0.04	35,35,35,35	0
56	MG	1A	3161	1/1	0.99	0.12	22,22,22,22	0
56	MG	2a	3022	1/1	0.99	0.11	43,43,43,43	0
56	MG	1a	1820	1/1	0.99	0.03	68,68,68,68	0
56	MG	2A	3137	1/1	0.99	0.14	40,40,40,40	0
56	MG	1A	3141	1/1	0.99	0.10	26,26,26,26	0
56	MG	2A	3139	1/1	0.99	0.12	34,34,34,34	0
56	MG	1U	204	1/1	0.99	0.04	22,22,22,22	0
56	MG	2E	303	1/1	0.99	0.11	36,36,36,36	0
56	MG	1A	3070	1/1	0.99	0.06	12,12,12,12	0
56	MG	2A	3843	1/1	0.99	0.11	35,35,35,35	0
56	MG	2y	105	1/1	0.99	0.03	76,76,76,76	0
56	MG	17	103	1/1	0.99	0.03	22,22,22,22	0
56	MG	2A	3845	1/1	0.99	0.04	44,44,44,44	0
56	MG	1A	4010	1/1	0.99	0.06	28,28,28,28	0
58	K	1A	4103	1/1	0.99	0.02	21,21,21,21	0
58	K	2A	3889	1/1	0.99	0.02	36,36,36,36	0
59	ZN	1Y	204	1/1	0.99	0.02	53,53,53,53	0
56	MG	1A	3199	1/1	0.99	0.14	20,20,20,20	0
59	ZN	16	104	1/1	0.99	0.04	37,37,37,37	0
59	ZN	1n	102	1/1	0.99	0.03	66,66,66,66	0
56	MG	1A	3967	1/1	0.99	0.04	46,46,46,46	0
56	MG	1A	3047	1/1	0.99	0.07	23,23,23,23	0
59	ZN	25	106	1/1	0.99	0.04	57,57,57,57	0
59	ZN	26	501	1/1	0.99	0.06	64,64,64,64	0
59	ZN	29	501	1/1	0.99	0.04	72,72,72,72	0
56	MG	1A	3730	1/1	0.99	0.04	19,19,19,19	0
56	MG	1A	3677	1/1	0.99	0.04	23,23,23,23	0
56	MG	1a	1769	1/1	0.99	0.11	52,52,52,52	0
56	MG	1A	3618	1/1	1.00	0.06	26,26,26,26	0
56	MG	1A	3935	1/1	1.00	0.02	40,40,40,40	0
59	ZN	15	106	1/1	1.00	0.03	38,38,38,38	0
56	MG	2A	3708	1/1	1.00	0.04	31,31,31,31	0
59	ZN	19	102	1/1	1.00	0.04	40,40,40,40	0
56	MG	1A	3754	1/1	1.00	0.04	18,18,18,18	0
56	MG	1A	3915	1/1	1.00	0.02	26,26,26,26	0

6.5 Other polymers (i)

There are no such residues in this entry.