



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2026 – 06:15 AM EDT

PDB ID : 6OF1 / pdb_00006of1
Title : Crystal structure of the Thermus thermophilus 70S ribosome in complex with dirithromycin and bound to mRNA and A-, P-, and E-site tRNAs at 2.80Å resolution
Authors : Khabibullina, N.F.; Tereshchenkov, A.G.; Komarova, E.S.; Syroegin, E.A.; Shiriaev, D.I.; Paleskava, A.; Kartsev, V.G.; Bogdanov, A.A.; Konevega, A.L.; Dontsova, O.A.; Sergiev, P.V.; Osterman, I.A.; Polikanov, Y.S.
Deposited on : 2019-03-28
Resolution : 2.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

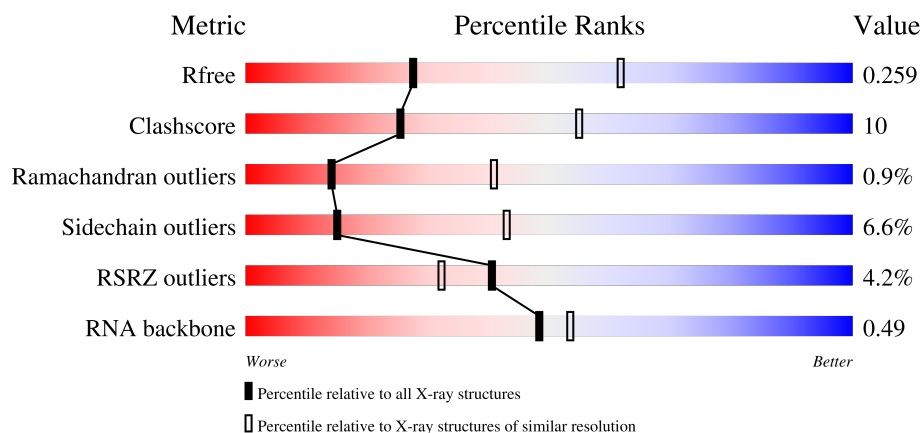
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)
RNA backbone	3983	1114 (3.00-2.60)

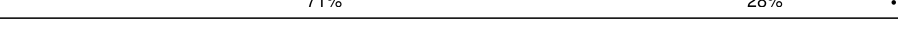
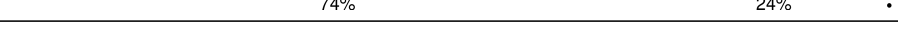
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$. 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	2% 61% 31% 7%
1	2A	2915	2% 55% 35% 7%

Continued on next page...

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

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
56	MG	1A	3862	-	-	-	X
56	MG	1A	4081	-	-	-	X
56	MG	1y	103	-	-	-	X
56	MG	1y	104	-	-	-	X
56	MG	2A	3392	-	-	-	X

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 300274 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
			276	124	48	91	13			
53	2v	13	Total	C	N	O	P	0	0	0
			276	124	48	91	13			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1w	73	Total 1568	C 700	N 282	O 512	P 73	S 1	0	0	0
54	1y	73	Total 1568	C 700	N 282	O 512	P 73	S 1	0	0	0
54	2w	73	Total 1568	C 700	N 282	O 512	P 73	S 1	0	0	0
54	2y	73	Total 1568	C 700	N 282	O 512	P 73	S 1	0	0	0

- 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	1148	Total	Mg	0	0
			1148	1148		
56	2A	860	Total	Mg	0	0
			860	860		
56	1B	37	Total	Mg	0	0
			37	37		
56	1D	13	Total	Mg	0	0
			13	13		
56	1E	8	Total	Mg	0	0
			8	8		
56	1F	9	Total	Mg	0	0
			9	9		
56	1G	5	Total	Mg	0	0
			5	5		
56	1H	1	Total	Mg	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	1I	1	Total Mg 1 1	0	0
56	1N	8	Total Mg 8 8	0	0
56	1O	5	Total Mg 5 5	0	0
56	1P	3	Total Mg 3 3	0	0
56	1Q	6	Total Mg 6 6	0	0
56	1R	2	Total Mg 2 2	0	0
56	1S	3	Total Mg 3 3	0	0
56	1T	2	Total Mg 2 2	0	0
56	1U	7	Total Mg 7 7	0	0
56	1V	2	Total Mg 2 2	0	0
56	1W	6	Total Mg 6 6	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	7	Total Mg 7 7	0	0
56	11	4	Total Mg 4 4	0	0
56	12	2	Total Mg 2 2	0	0
56	13	3	Total Mg 3 3	0	0
56	15	5	Total Mg 5 5	0	0
56	16	2	Total Mg 2 2	0	0
56	17	3	Total Mg 3 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	18	2	Total 2	Mg 2	0	0
56	1a	244	Total 244	Mg 244	0	0
56	1b	2	Total 2	Mg 2	0	0
56	1d	1	Total 1	Mg 1	0	0
56	1f	1	Total 1	Mg 1	0	0
56	1h	1	Total 1	Mg 1	0	0
56	1l	3	Total 3	Mg 3	0	0
56	1m	3	Total 3	Mg 3	0	0
56	1p	1	Total 1	Mg 1	0	0
56	1r	1	Total 1	Mg 1	0	0
56	1s	1	Total 1	Mg 1	0	0
56	1t	1	Total 1	Mg 1	0	0
56	1v	1	Total 1	Mg 1	0	0
56	1w	7	Total 7	Mg 7	0	0
56	1x	12	Total 12	Mg 12	0	0
56	1y	5	Total 5	Mg 5	0	0
56	2B	21	Total 21	Mg 21	0	0
56	2D	3	Total 3	Mg 3	0	0
56	2E	8	Total 8	Mg 8	0	0
56	2F	4	Total 4	Mg 4	0	0
56	2G	1	Total 1	Mg 1	0	0

Continued on next page...

Continued from previous page...

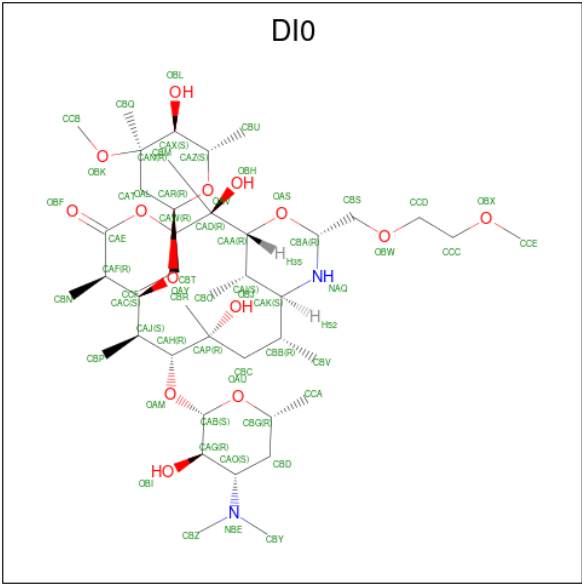
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2O	2	Total 2	Mg 2	0	0
56	2P	3	Total 3	Mg 3	0	0
56	2Q	3	Total 3	Mg 3	0	0
56	2R	2	Total 2	Mg 2	0	0
56	2T	3	Total 3	Mg 3	0	0
56	2U	4	Total 4	Mg 4	0	0
56	2V	2	Total 2	Mg 2	0	0
56	2W	2	Total 2	Mg 2	0	0
56	2X	2	Total 2	Mg 2	0	0
56	2Z	1	Total 1	Mg 1	0	0
56	20	2	Total 2	Mg 2	0	0
56	21	1	Total 1	Mg 1	0	0
56	23	1	Total 1	Mg 1	0	0
56	25	4	Total 4	Mg 4	0	0
56	27	1	Total 1	Mg 1	0	0
56	28	1	Total 1	Mg 1	0	0
56	2a	231	Total 231	Mg 231	0	0
56	2d	2	Total 2	Mg 2	0	0
56	2e	1	Total 1	Mg 1	0	0
56	2f	2	Total 2	Mg 2	0	0
56	2g	1	Total 1	Mg 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2i	1	Total	Mg	0	0
			1	1		
56	2j	2	Total	Mg	0	0
			2	2		
56	2l	2	Total	Mg	0	0
			2	2		
56	2q	3	Total	Mg	0	0
			3	3		
56	2r	1	Total	Mg	0	0
			1	1		
56	2t	1	Total	Mg	0	0
			1	1		
56	2v	3	Total	Mg	0	0
			3	3		
56	2w	1	Total	Mg	0	0
			1	1		
56	2x	5	Total	Mg	0	0
			5	5		
56	2y	7	Total	Mg	0	0
			7	7		

- Molecule 57 is Dirithromycin (CCD ID: DI0) (formula: C₄₂H₇₈N₂O₁₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
57	1A	1	Total	C	N	O	0	0
			58	42	2	14		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
57	2A	1	Total	C	N	O	0	0
			58	42	2	14		

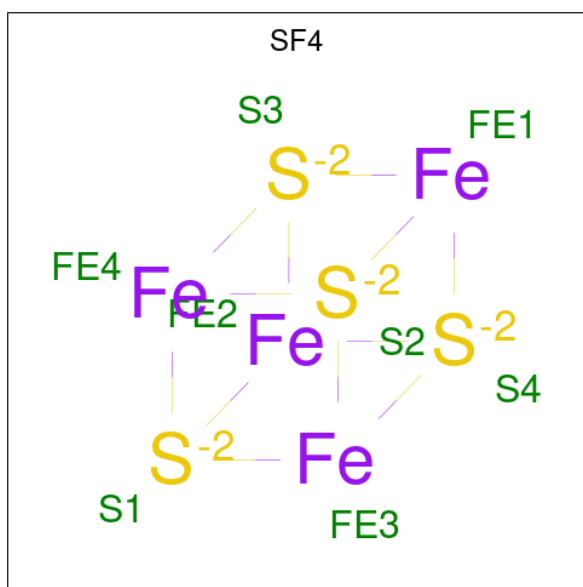
- Molecule 58 is POTASSIUM ION (CCD ID: K) (formula: K).

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		
59	1n	1	Total	Zn	0	0
			1	1		
59	2Y	1	Total	Zn	0	0
			1	1		
59	24	1	Total	Zn	0	0
			1	1		
59	25	1	Total	Zn	0	0
			1	1		
59	26	1	Total	Zn	0	0
			1	1		
59	29	1	Total	Zn	0	0
			1	1		
59	2n	1	Total	Zn	0	0
			1	1		

- Molecule 60 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



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

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	2034	Total	O	0	0
			2034	2034		
61	2A	1099	Total	O	0	0
			1099	1099		
61	1B	65	Total	O	0	0
			65	65		
61	1D	29	Total	O	0	0
			29	29		
61	1E	24	Total	O	0	0
			24	24		
61	1F	12	Total	O	0	0
			12	12		
61	1G	5	Total	O	0	0
			5	5		
61	1H	1	Total	O	0	0
			1	1		
61	1I	2	Total	O	0	0
			2	2		
61	1N	6	Total	O	0	0
			6	6		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1O	7	Total 7	O 7	0	0
61	1P	23	Total 23	O 23	0	0
61	1Q	7	Total 7	O 7	0	0
61	1R	14	Total 14	O 14	0	0
61	1S	3	Total 3	O 3	0	0
61	1T	10	Total 10	O 10	0	0
61	1U	12	Total 12	O 12	0	0
61	1V	8	Total 8	O 8	0	0
61	1W	10	Total 10	O 10	0	0
61	1X	4	Total 4	O 4	0	0
61	1Y	3	Total 3	O 3	0	0
61	10	11	Total 11	O 11	0	0
61	11	8	Total 8	O 8	0	0
61	12	4	Total 4	O 4	0	0
61	13	4	Total 4	O 4	0	0
61	15	3	Total 3	O 3	0	0
61	16	4	Total 4	O 4	0	0
61	17	6	Total 6	O 6	0	0
61	18	12	Total 12	O 12	0	0
61	19	1	Total 1	O 1	0	0
61	1a	439	Total 439	O 439	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1b	1	Total 1	O 1	0	0
61	1d	2	Total 2	O 2	0	0
61	1f	2	Total 2	O 2	0	0
61	1g	2	Total 2	O 2	0	0
61	1l	11	Total 11	O 11	0	0
61	1o	1	Total 1	O 1	0	0
61	1p	1	Total 1	O 1	0	0
61	1q	2	Total 2	O 2	0	0
61	1r	2	Total 2	O 2	0	0
61	1t	2	Total 2	O 2	0	0
61	1u	1	Total 1	O 1	0	0
61	1v	9	Total 9	O 9	0	0
61	1w	6	Total 6	O 6	0	0
61	1x	7	Total 7	O 7	0	0
61	1y	4	Total 4	O 4	0	0
61	2B	24	Total 24	O 24	0	0
61	2D	20	Total 20	O 20	0	0
61	2E	12	Total 12	O 12	0	0
61	2F	7	Total 7	O 7	0	0
61	2I	4	Total 4	O 4	0	0
61	2N	1	Total 1	O 1	0	0

Continued on next page...

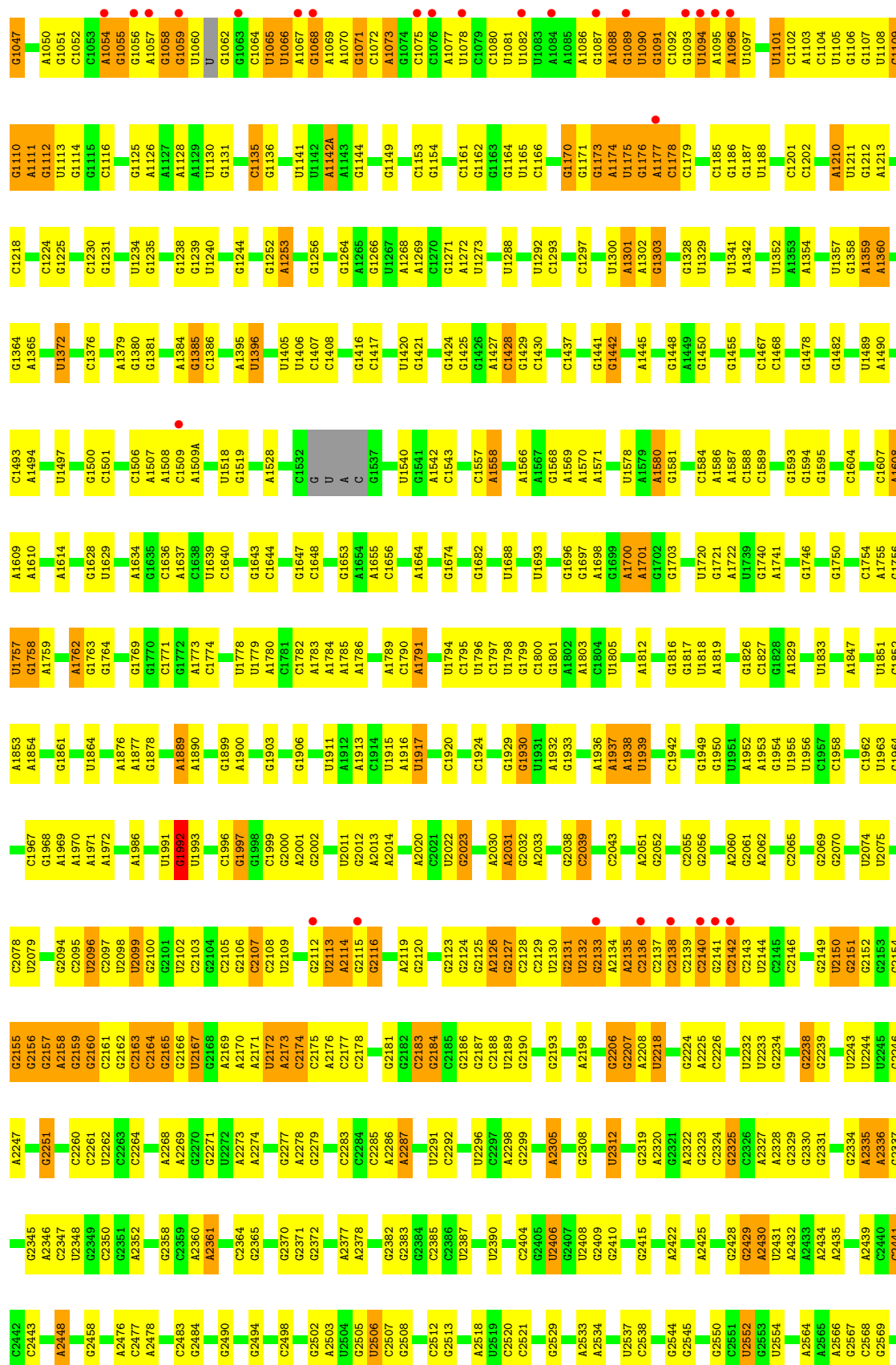
Continued from previous page...

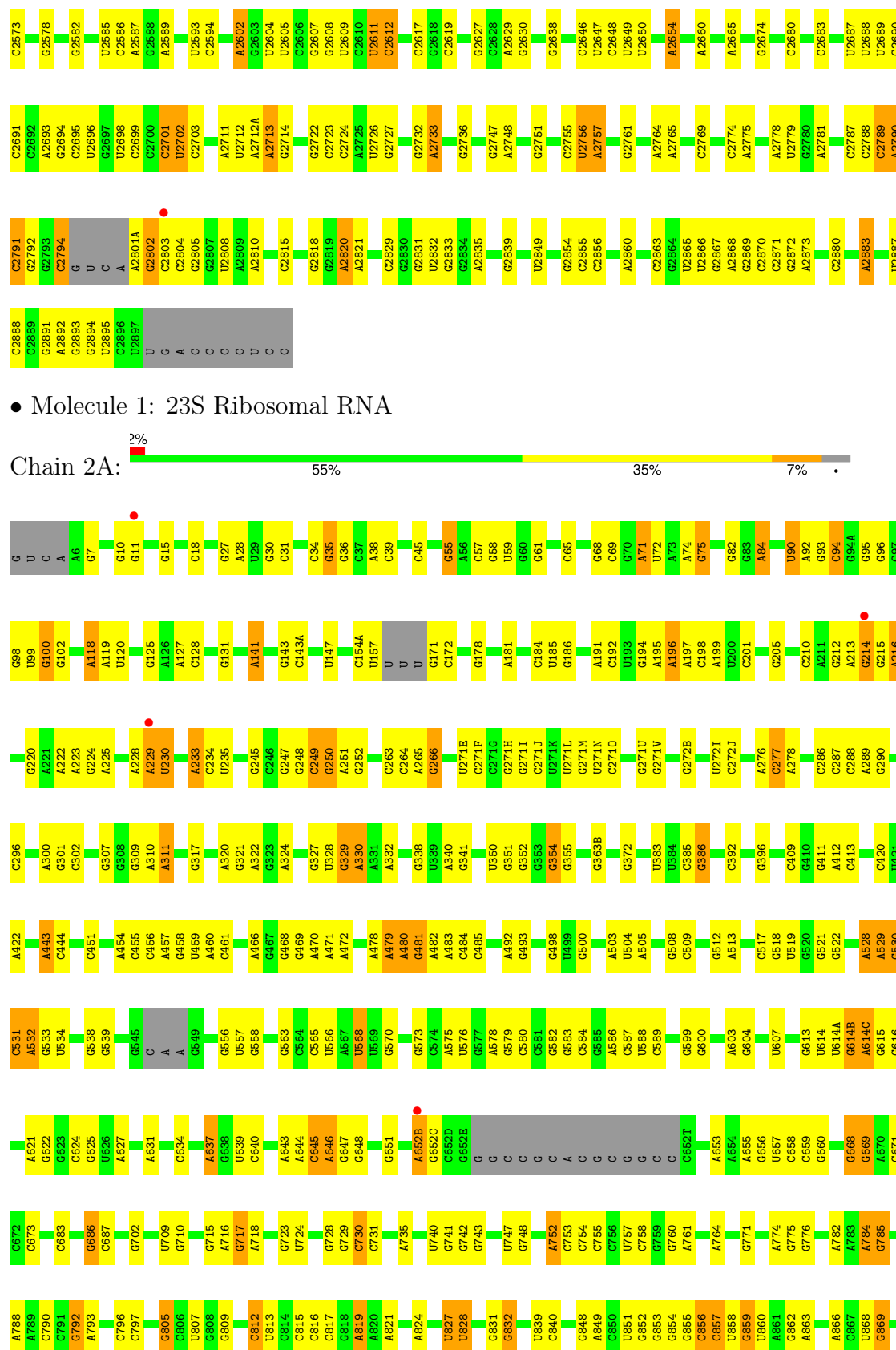
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2O	1	Total 1	O 1	0	0
61	2P	12	Total 12	O 12	0	0
61	2Q	2	Total 2	O 2	0	0
61	2R	2	Total 2	O 2	0	0
61	2T	4	Total 4	O 4	0	0
61	2U	4	Total 4	O 4	0	0
61	2V	1	Total 1	O 1	0	0
61	2W	4	Total 4	O 4	0	0
61	2X	5	Total 5	O 5	0	0
61	2Y	1	Total 1	O 1	0	0
61	2Z	1	Total 1	O 1	0	0
61	20	3	Total 3	O 3	0	0
61	21	6	Total 6	O 6	0	0
61	23	2	Total 2	O 2	0	0
61	25	1	Total 1	O 1	0	0
61	27	3	Total 3	O 3	0	0
61	28	4	Total 4	O 4	0	0
61	29	1	Total 1	O 1	0	0
61	2a	284	Total 284	O 284	0	0
61	2d	1	Total 1	O 1	0	0
61	2e	2	Total 2	O 2	0	0

Continued on next page...

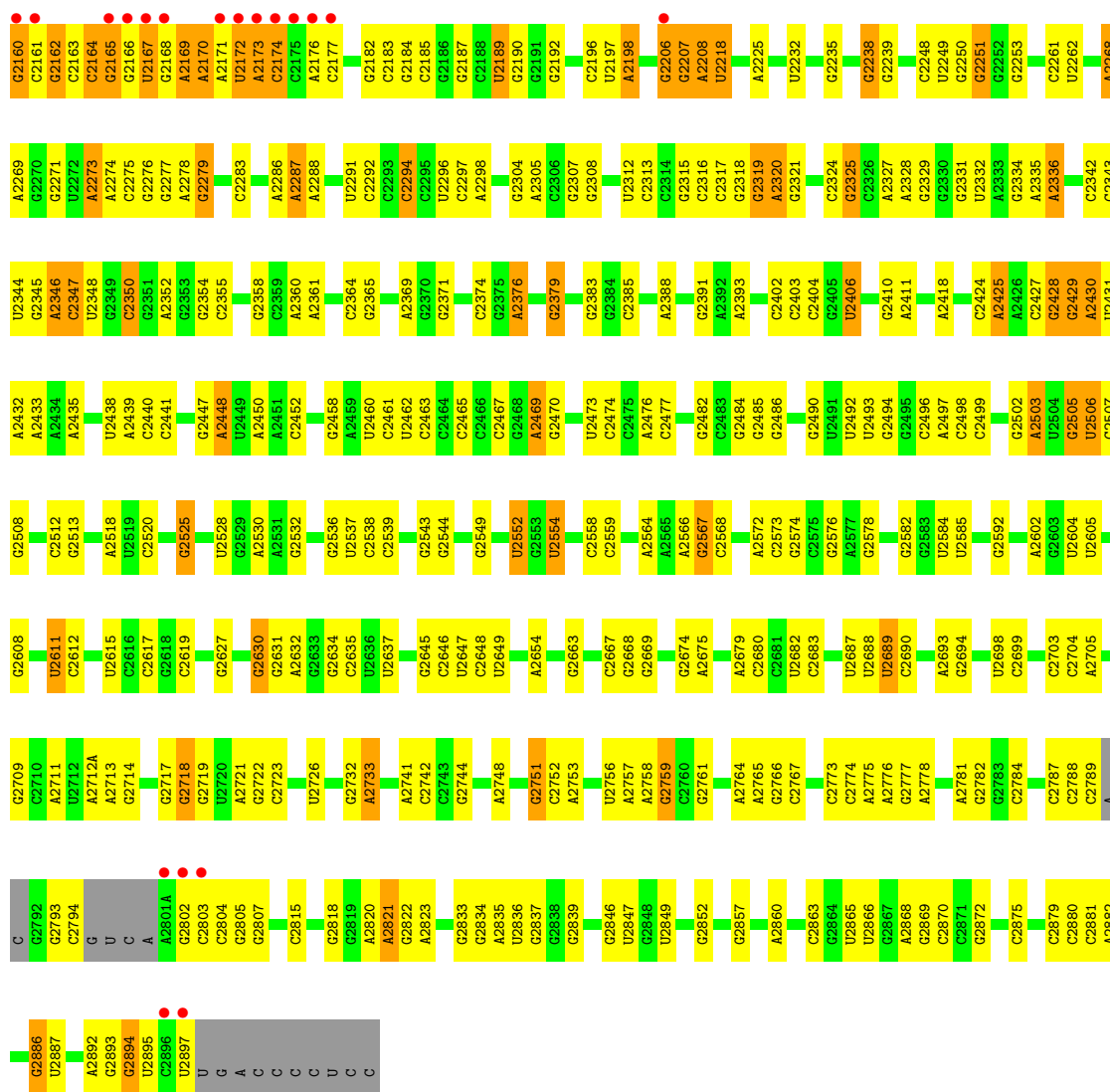
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2g	1	Total	O	0	0
			1	1		
61	2j	3	Total	O	0	0
			3	3		
61	2l	2	Total	O	0	0
			2	2		
61	2n	1	Total	O	0	0
			1	1		
61	2o	1	Total	O	0	0
			1	1		
61	2p	1	Total	O	0	0
			1	1		
61	2q	1	Total	O	0	0
			1	1		
61	2r	1	Total	O	0	0
			1	1		
61	2t	3	Total	O	0	0
			3	3		
61	2v	3	Total	O	0	0
			3	3		
61	2w	3	Total	O	0	0
			3	3		
61	2x	5	Total	O	0	0
			5	5		
61	2y	16	Total	O	0	0
			16	16		



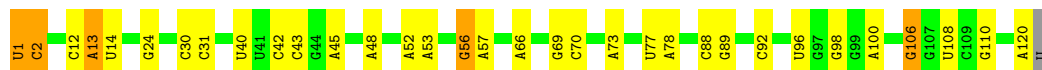


G2100	A2014	A1802	A1580	A1477	A1395	A1278	U	A	U1033	G948	G875
G2101	U2017	C1920	U1693	G1478	U1405	G1283	A	U	G1034	A953	U877
G2102	G2018	C1924	C1694	G1479	U1406	A1284	A	G	U1035	G954	G878
G2103	A2019		G1695	G1480	U1407	G1285	C	C	G1036	C955	A879
G2105		A1812	G1697	G1482	C1408	C1180	U	U	G1038	G956	G880
G2106	U2022	A1927	A1698		C1409	U1288		C		G981	G881
G2107	G2023	G1813	G1699	A1490	G1410	C1181	C	A	C1043	U957	G882
G2108	G2023	G1814	G1699	A1490	G1410	C1182	C	U	G	U958	G883
U2108		A1815	U1700	A1491	C1411	U1292	C	C	A	A959	G884
U2109	G2027	U1816	A1701	U1590	A1412	C1293		U	A	A960	G885
G2110		G1817	G1702	G1494	G1413			G	A	C961	G886
G2111		U1818	G1591	A1494		G1296		G	A	G962	
G2112	A2030	A1934	G1592	A1495		C1297		U	A	U963	A887
G2113	A2031	G1819	G1593	A1496	G1416			U	C	C964	C888
G2114	G2032	U1820	G1594	U1497	C1417	C1191	C	C	A		G889
A2114	A2033	A1821	G1595	U1497		U1300	C	C			
G2115		C1712		C1506	U1420	A1301	C	A		C971	A890
G2116	G2036	G1822	C1598		G1421	A1302	C	G	G1112	G892	
G2117	G2037	G1826	G1721	C1509		A1303		U	U1113	C	C893
G2118	G2038	A1939	A1722	C1509A		G1303		U	G1114	G974	G894
G2119	G2039	G1827	U1739	A1509A				A	A	C975	U895
G2120	C1942	G1828	G1740		A1427	C1314		G	G	G978	A896
G2121	G1945	C1837	C1607	U1512	C1428	C1315		G	A	G979	C897
U2041	U1946	U1848	A1608	C1513	C1429	U1211		G	G	G978	
A2042	U1946	C1837	A1609	U1514	C1430	C1316		G	G	A880	A898
C2043	C1947	U1849	A1610	U1514	U1431	A1317		G	A	A881	A899
		C1843	C1754	G1515	C1432	A1214		U	U	C982	A900
			A1755	U1433		G1328		G	U	A883	A901
A2051	U1955	A1847	A1614	U1518	A1434	A1220		U	G	C902	G902
G2125	A2126	A1848	G1756	G1519		A1336		U	G	G986	C903
G2127	G1958	G1849	A1762	C1437		G1337		C	C	G987	C904
G2128	G2055	G1850	G1763	G1525				U			
A2057	G1959		G1764		G1442	A1342					
G2129	G1960	A1853	C1636								
U2130	C1961		A1637	A1528		U1352				C994	U907
A2058	A1962	G1857	C1638	A1528A	A1445	A1352		U	A	C995	C908
A2059	C1962	G1857	U1639	G1529	C1446A	A1353		G	A	A996	A909
A2060	G1963	G1857	G1640	C1530	C1446	G1229		G	A		A910
G2133	G1964	G1858	G1640	C1531	G1447	G1355		A	A	A1000	A911
A2134	C1965		A1641	C1531	G1448	G1356		C	C	G1003	C912
A2135	A1966	G1865	G1642	C1532	G1449	G1239		G	G	A1005	A917
C2136	C1967		G1647	C1533	A1449	U1240		A	A	C1006	A918
C2137	U1970	A1877	G1647	U	G1450	A1241		C	C		G919
G2067	A1970	G1878	G1648	A		A1242		U	U		G920
U2068	A1971	G1780	G1649	C1536	A1452	A1360		C	C	G1011	G921
G2069	A1972	A1885	G1781		U1453			A	A	U1012	
			C1782	A1542		G1364		U	U	C1013	C925
U2074	G1984	A1889	A1783	A1542	C1488	A1365		C	C	U1014	A926
C2143	U2075	A1890	C1657	A1545	G1459	A1366		U	U	C1151	
U2144		G1891	C1658	C1546	A1367	G1256		C	C	G1152	G927
U2079			A1786	C1547	G1461	G1368		U	U	C1153	G928
G1982			G1787	C1462	G1369	G1257		U	U	G1016	
U1993			A1664	C1453	G1370	G115A		U	U	G1017	
			A1665	C1463				A	A	C1018	G932
C1986			G1666	A1558	G1371	A1265		C	C	G1160	A933
G1997			A1789	G1559	G1372	G1266		A	A	C1161	
G1907			G1667	G1559	U1267	G1162		A	A	U1019	G938
U1998			A1668		G1466	G1269		G	A	A1021	A939
C1908			C1669	A1566	C1467	A1268		U	U	G1022	G940
G2000			A1670	C1468	G1380	C1270		G	G	U1023	A941
				A1569	A1469	G1271		U	U	G1024	G942
U1911			G1674	A1572	A1471	C1384		C	C	U1025	
A1912			C1795	G1573	A1471	G1385		G	G	G1170	
A1913			C1796	A1572	A1471	A1272		U	U	A1027	A945
G2010			U1798	G1573	C1386	U1273		C	C	G1171	G946
G2011			C1686	G1573	C1386	A1274		U	U	A1028	C947
U1915			G1687	U1915	C1474			A	A		
G1799			U1688	U1570	G1475			G	G		
C1800			C1801	A1570	C1475	A1392		U	U	C1277	
A1916			A1680		C1476						
A1917			A1680		C1476						
A1918			A1680		C1476						
A1919			A1680		C1476						
A1920			A1680		C1476						
A1921			A1680		C1476						
A1922			A1680		C1476						
A1923			A1680		C1476						
A1924			A1680		C1476						
A1925			A1680		C1476						
A1926			A1680		C1476						
A1927			A1680		C1476						
A1928			A1680		C1476						
A1929			A1680		C1476						
A1930			A1680		C1476						
A1931			A1680		C1476						
A1932			A1680		C1476						
A1933			A1680		C1476						
A1934			A1680		C1476						
A1935			A1680		C1476						
A1936			A1680		C1476						
A1937			A1680		C1476						
A1938			A1680		C1476						
A1939			A1680		C1476						
A1940			A1680		C1476						
A1941			A1680		C1476						
A1942			A1680		C1476						
A1943			A1680		C1476						
A1944			A1680		C1476						
A1945			A1680		C1476						
A1946			A1680		C1476						
A1947			A1680		C1476						
A1948			A1680		C1476						
A1949			A1680		C1476						
A1950			A1680		C1476						
A1951			A1680		C1476						
A1952			A1680		C1476						
A1953			A1680		C1476						
A1954			A1680		C1476						
A1955			A1680		C1476						
A1956			A1680		C1476						
A1957			A1680		C1476						
A1958			A1680		C1476						
A1959			A1680		C1476						
A1960			A1680		C1476						
A1961			A1680		C1476						
A1962			A1680		C1476						
A1963			A1680		C1476						
A1964			A1680		C1476						
A1965			A1680		C1476						
A1966			A1680		C1476						
A1967			A1680		C1476						
A1968			A1680		C1476						
A1969			A1680		C1476						
A1970			A1680		C1476						
A1971			A1680		C1476						
A1972			A1680		C1476						
A1973			A1680		C1476						
A1974			A1680		C1476						
A1975			A1680		C1476						
A1976			A1680		C1476						
A1977			A1680		C1476						
A1978			A1680		C1476						
A1979			A1680		C1476						
A1980			A1680		C1476						
A1981			A1680		C1476						
A1982			A1680		C1476						
A1983			A1680		C1476						
A1984			A1680		C1476						
A1985			A1680		C1476						
A1986			A1680		C1476						
A1987			A1680		C1476						
A1988			A1680		C1476						
A1989			A1680		C1476						
A1990			A1680		C1476						
A1991			A1680		C1476						
A1992			A1680		C1476						
A1993			A1680		C1476						
A1994			A1680		C1476						
A1995			A1680		C1476						
A1996			A1680		C1476						
A1997			A1680		C1476						
A1998			A1680		C1476						
A1999			A1680		C1476						
A2000			A1680		C1476						
A2001			A1680		C1476						
A2002			A1680		C1476						
A2003			A1680		C1476						
A2004			A1680		C1476						
A2005			A1680		C1476						
A2006			A1680		C1476						



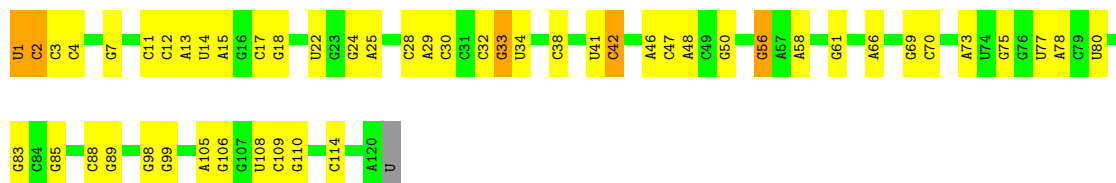
- Molecule 2: 5S Ribosomal RNA

Chain 1B: 72% 23%

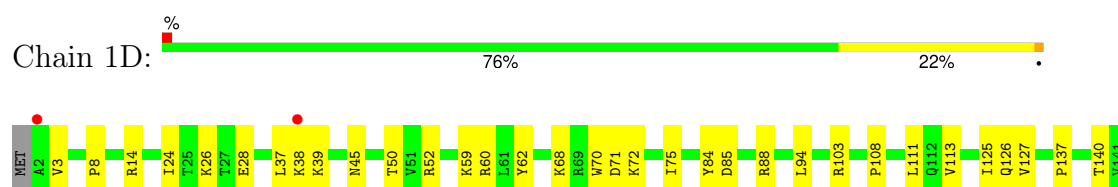


- Molecule 2: 5S Ribosomal RNA

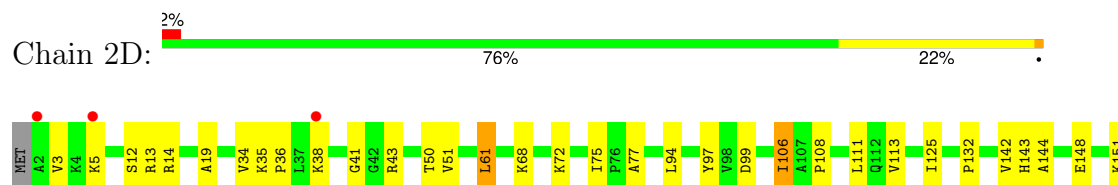
Chain 2B: 57% 38%



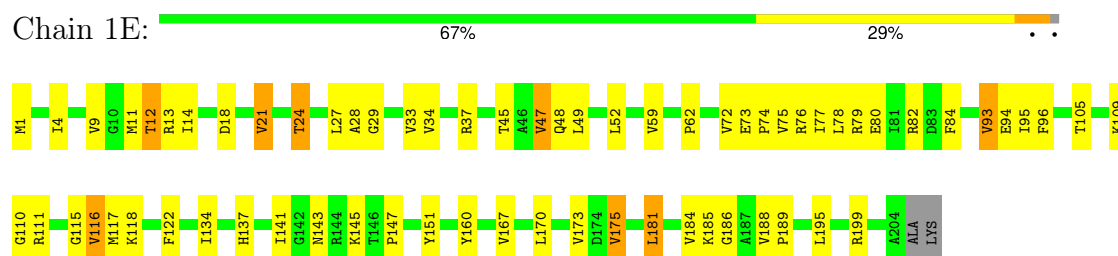
- Molecule 3: 50S ribosomal protein L2



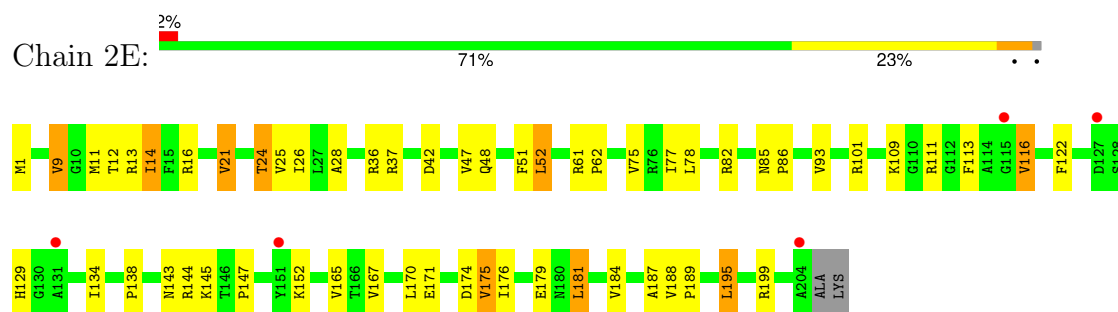
• Molecule 3: 50S ribosomal protein L2



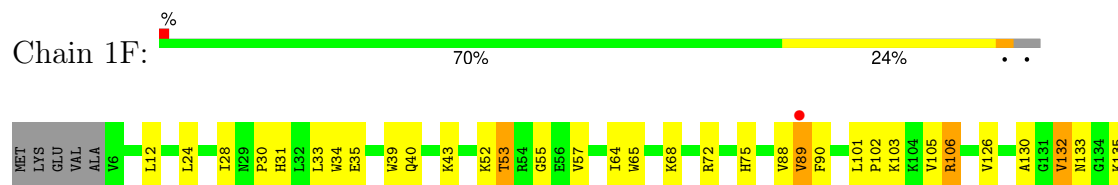
• Molecule 4: 50S ribosomal protein L3



• Molecule 4: 50S ribosomal protein L3

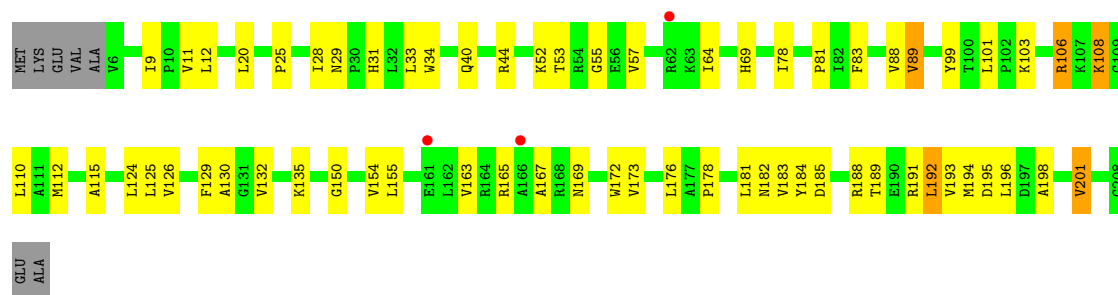


• Molecule 5: 50S ribosomal protein L4

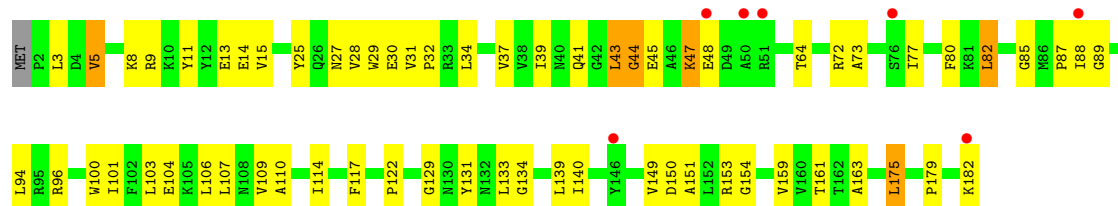




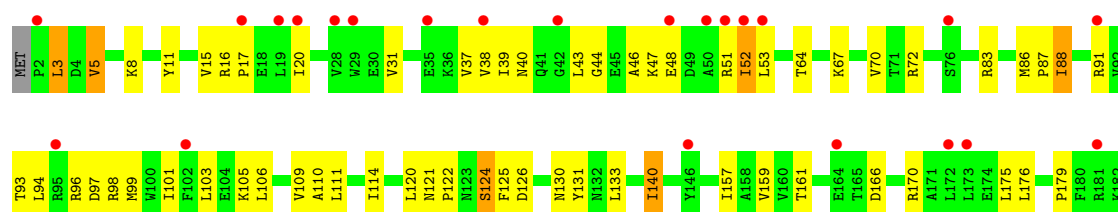
- Molecule 5: 50S ribosomal protein L4



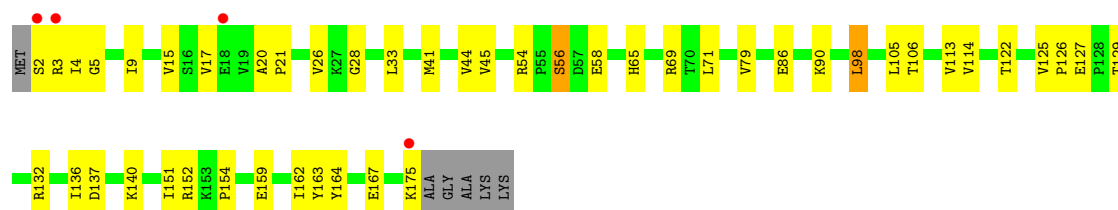
- Molecule 6: 50S ribosomal protein L5



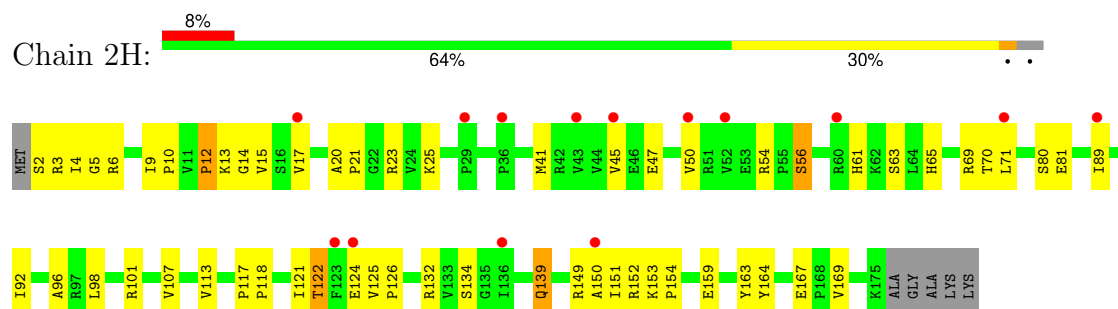
- Molecule 6: 50S ribosomal protein L5



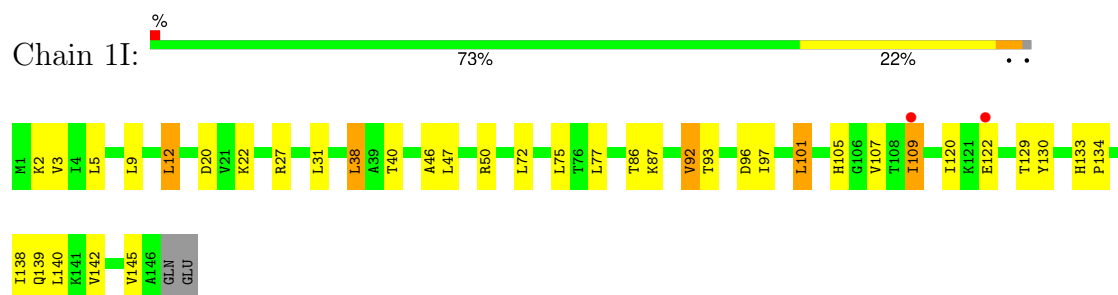
- Molecule 7: 50S ribosomal protein L6



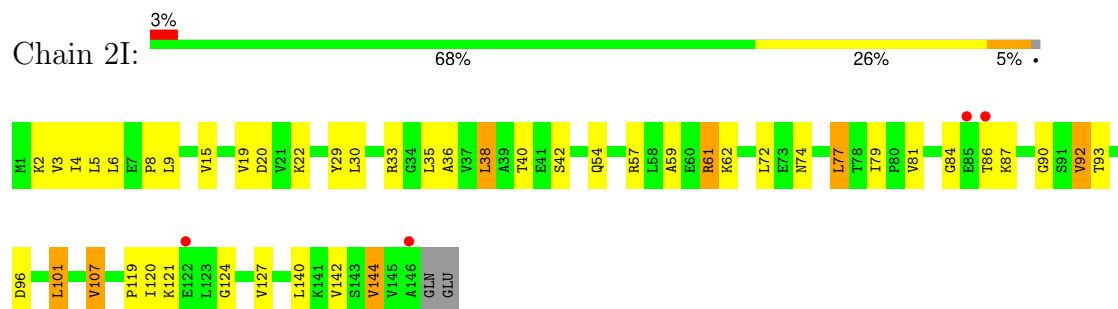
- Molecule 7: 50S ribosomal protein L6



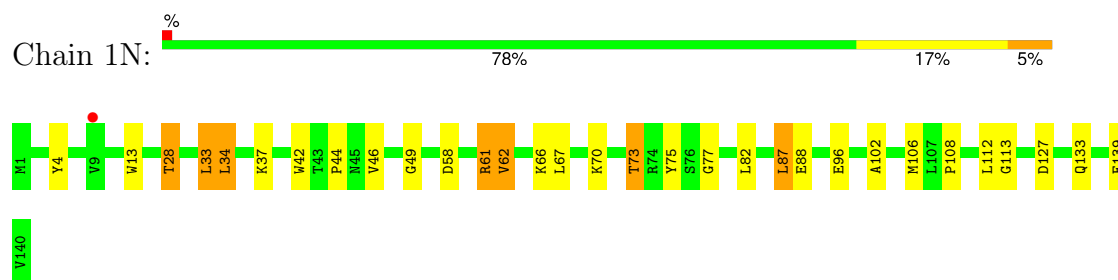
- Molecule 8: 50S ribosomal protein L9



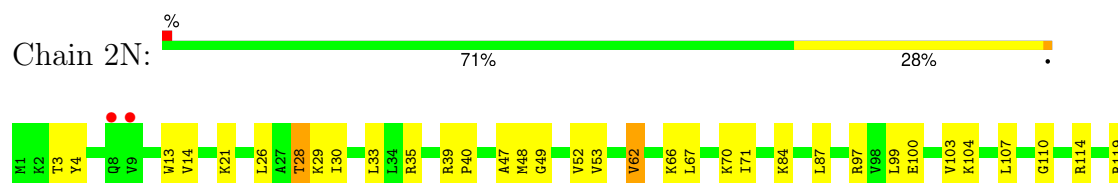
- Molecule 8: 50S ribosomal protein L9



- Molecule 9: 50S ribosomal protein L13



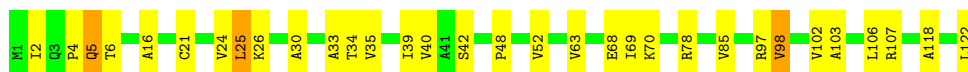
- Molecule 9: 50S ribosomal protein L13





- Molecule 10: 50S ribosomal protein L14

Chain 1O: 74% 24%



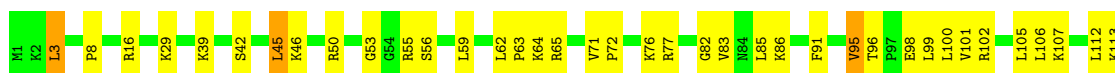
- Molecule 10: 50S ribosomal protein L14

Chain 2O: 72% 25%



- Molecule 11: 50S ribosomal protein L15

Chain 1P: 69% 28%



- Molecule 11: 50S ribosomal protein L15

Chain 2P: 71% 26%



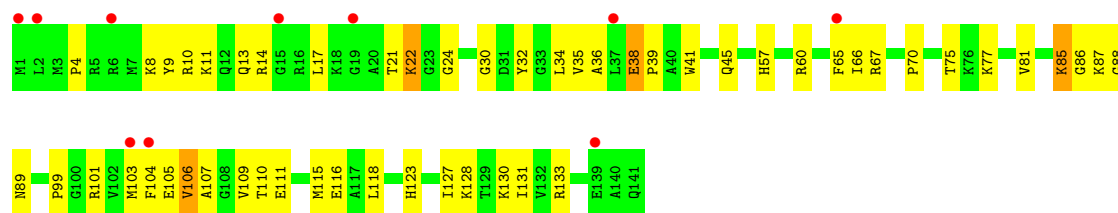
- Molecule 12: 50S ribosomal protein L16

Chain 1Q: 77% 20%



- Molecule 12: 50S ribosomal protein L16

Chain 2Q: 62% 35%



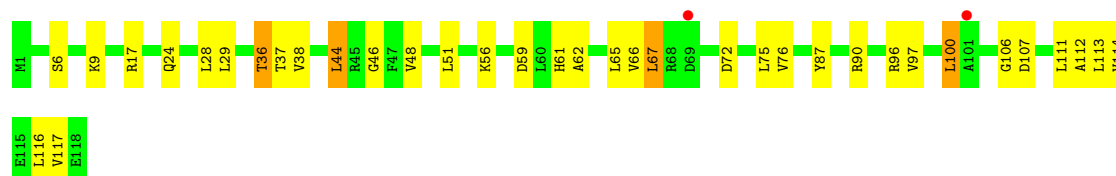
• Molecule 13: 50S ribosomal protein L17

Chain 1R: 73% 24%



• Molecule 13: 50S ribosomal protein L17

Chain 2R: 2% 69% 27%



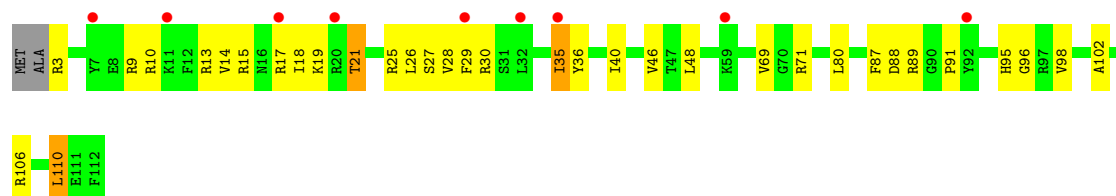
• Molecule 14: 50S ribosomal protein L18

Chain 1S: % 74% 21%



• Molecule 14: 50S ribosomal protein L18

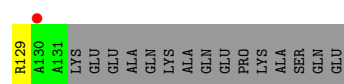
Chain 2S: 8% 68% 28%



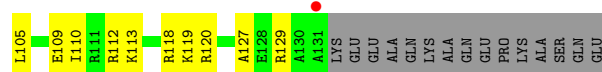
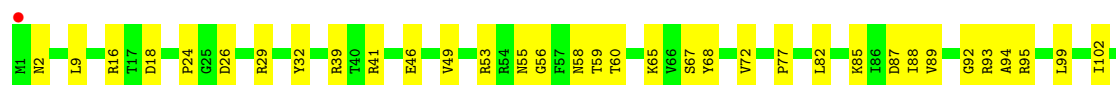
• Molecule 15: 50S ribosomal protein L19

Chain 1T: % 66% 22% 10%

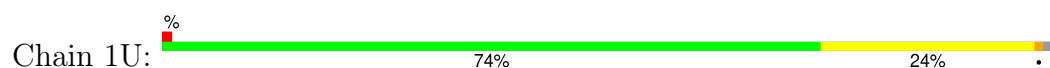




- Molecule 15: 50S ribosomal protein L19



- Molecule 16: 50S ribosomal protein L20



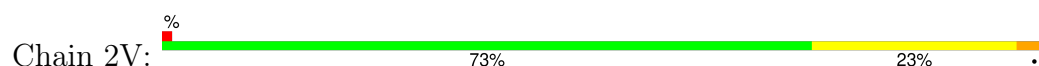
- Molecule 16: 50S ribosomal protein L20



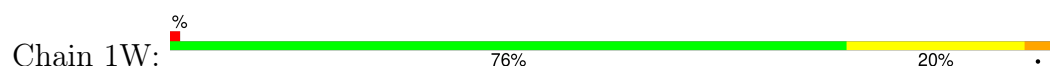
- Molecule 17: 50S ribosomal protein L21



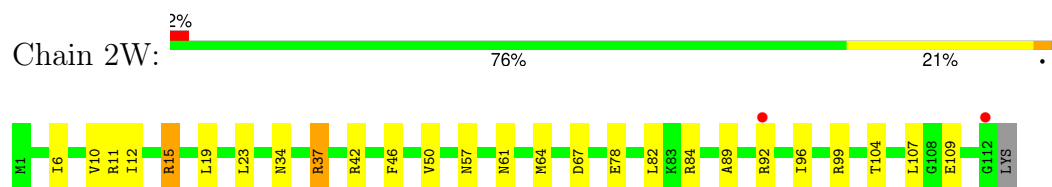
- Molecule 17: 50S ribosomal protein L21



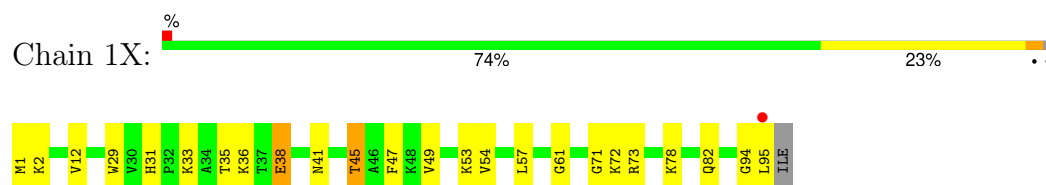
- Molecule 18: 50S ribosomal protein L22



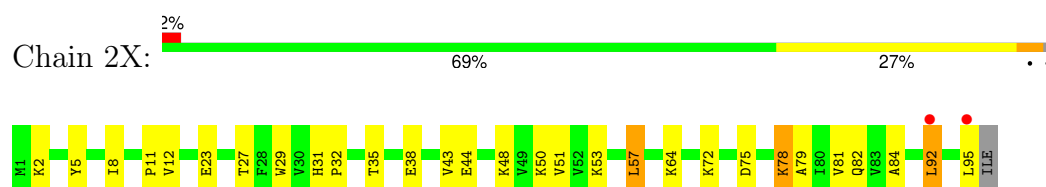
• Molecule 18: 50S ribosomal protein L22



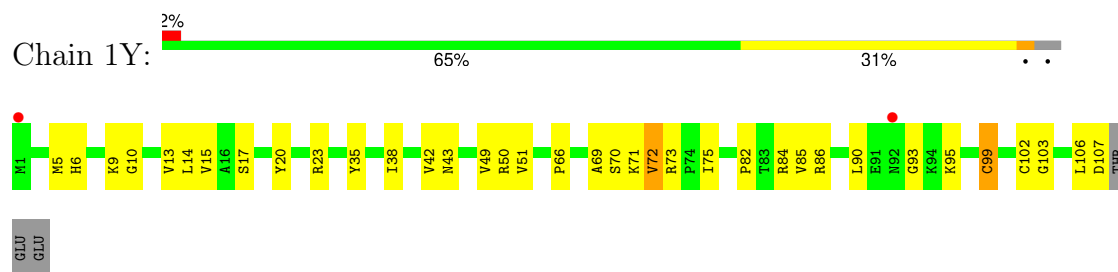
• Molecule 19: 50S ribosomal protein L23



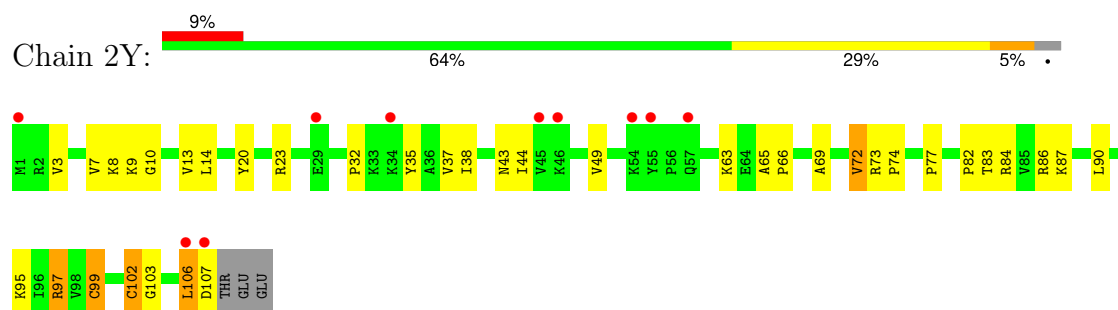
• Molecule 19: 50S ribosomal protein L23



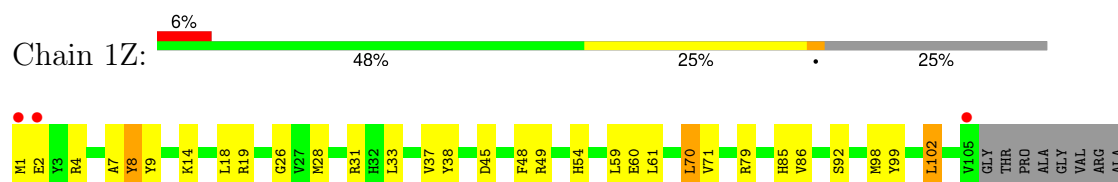
• Molecule 20: 50S ribosomal protein L24

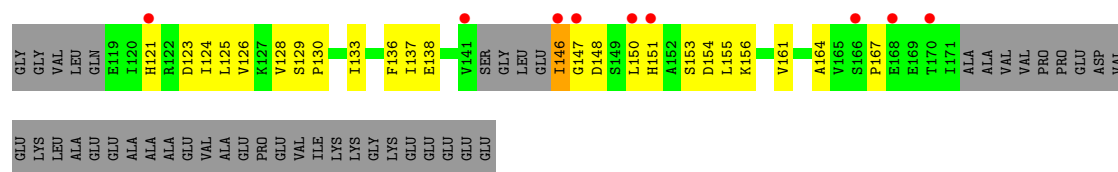


• Molecule 20: 50S ribosomal protein L24

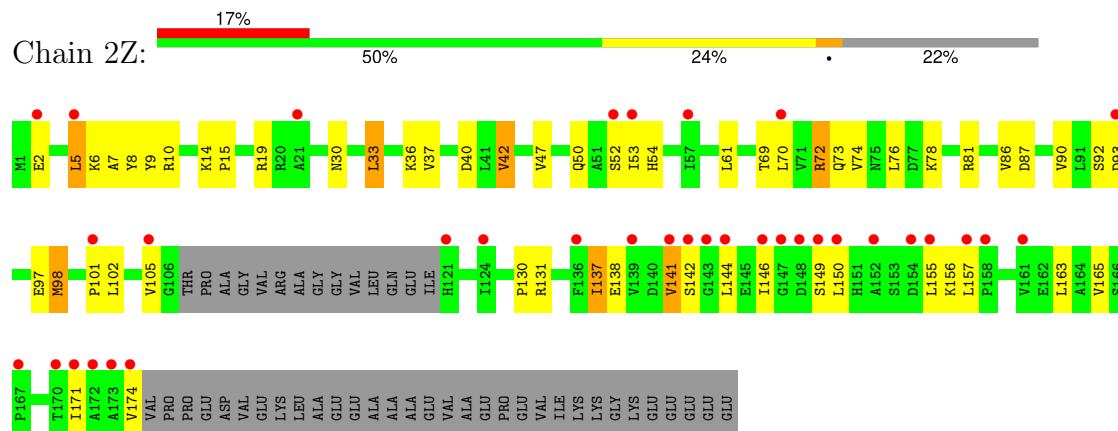


• Molecule 21: 50S ribosomal protein L25

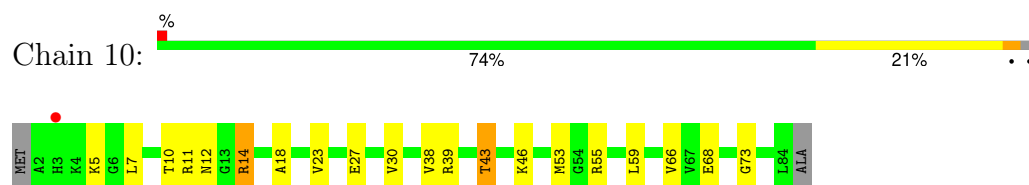




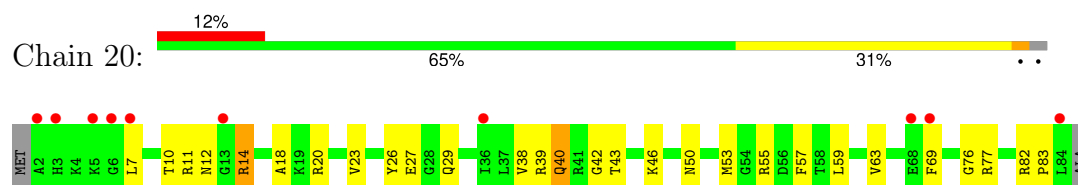
• Molecule 21: 50S ribosomal protein L25



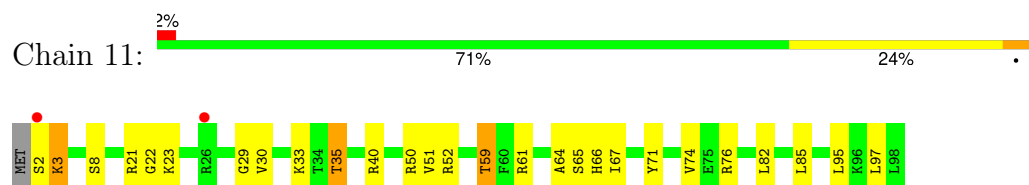
• Molecule 22: 50S ribosomal protein L27



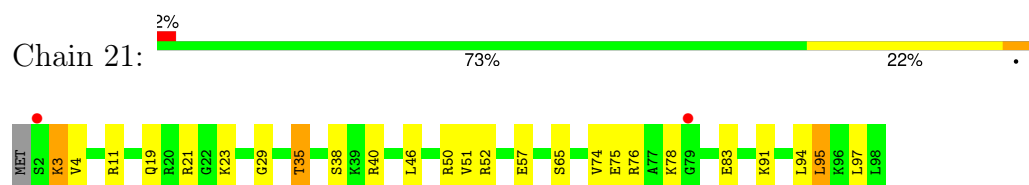
• Molecule 22: 50S ribosomal protein L27



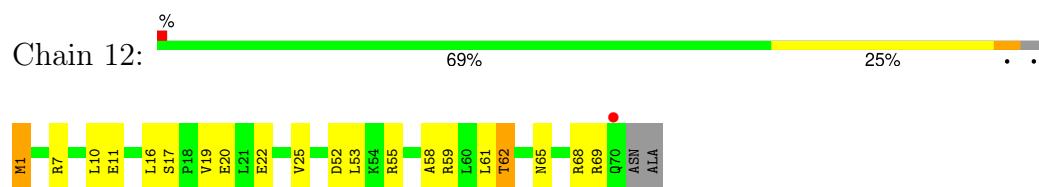
• Molecule 23: 50S ribosomal protein L28



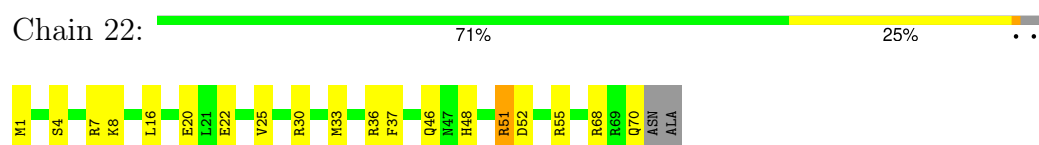
• Molecule 23: 50S ribosomal protein L28



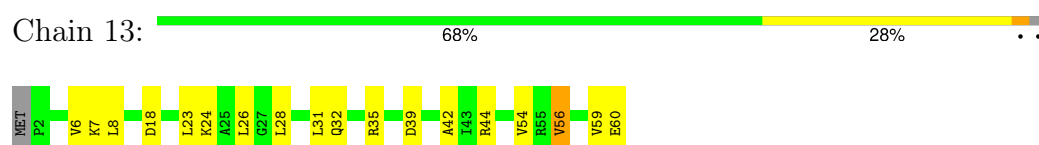
- Molecule 24: 50S ribosomal protein L29



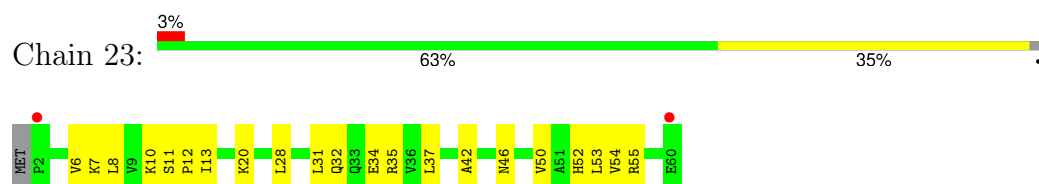
- Molecule 24: 50S ribosomal protein L29



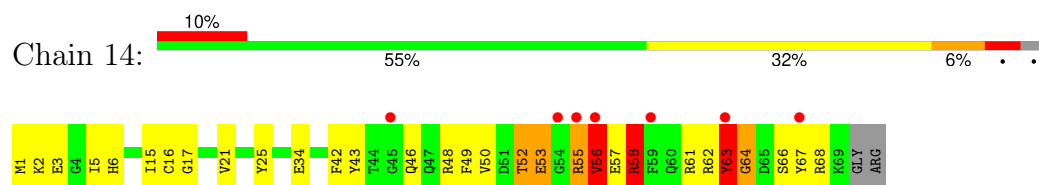
- Molecule 25: 50S ribosomal protein L30



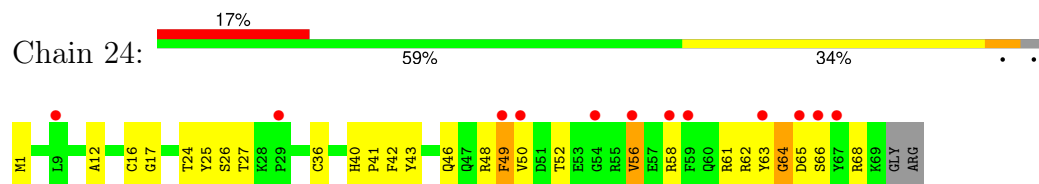
- Molecule 25: 50S ribosomal protein L30



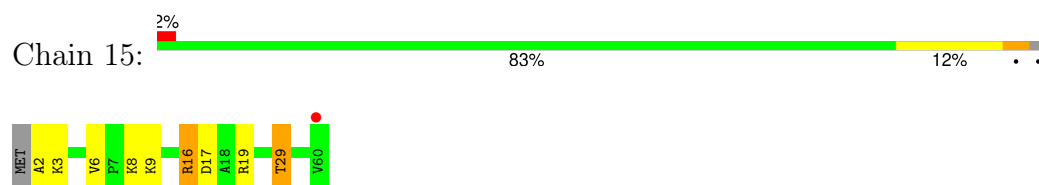
- Molecule 26: 50S ribosomal protein L31



- Molecule 26: 50S ribosomal protein L31



- Molecule 27: 50S ribosomal protein L32



- Molecule 27: 50S ribosomal protein L32

Chain 25:  83% 12% ..



- Molecule 28: 50S ribosomal protein L33

Chain 16:  69% 24% 6% ..



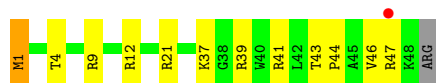
- Molecule 28: 50S ribosomal protein L33

Chain 26:  76% 19% ..



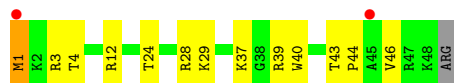
- Molecule 29: 50S ribosomal protein L34

Chain 17:  73% 22% ..



- Molecule 29: 50S ribosomal protein L34

Chain 27:  71% 24% ..



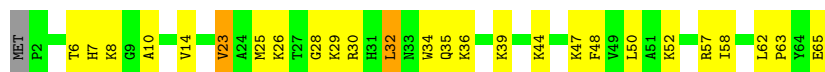
- Molecule 30: 50S ribosomal protein L35

Chain 18:  57% 40% ..



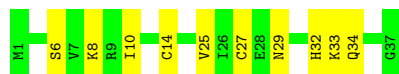
- Molecule 30: 50S ribosomal protein L35

Chain 28:  58% 37% ..



- Molecule 31: 50S ribosomal protein L36

Chain 19:  73% 27%



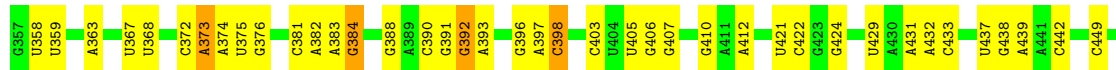
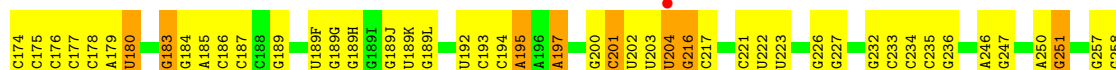
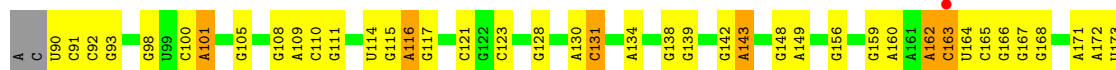
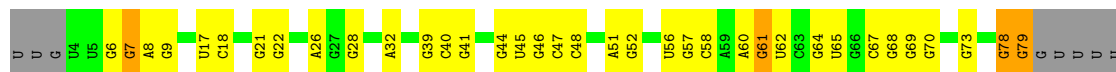
- Molecule 31: 50S ribosomal protein L36

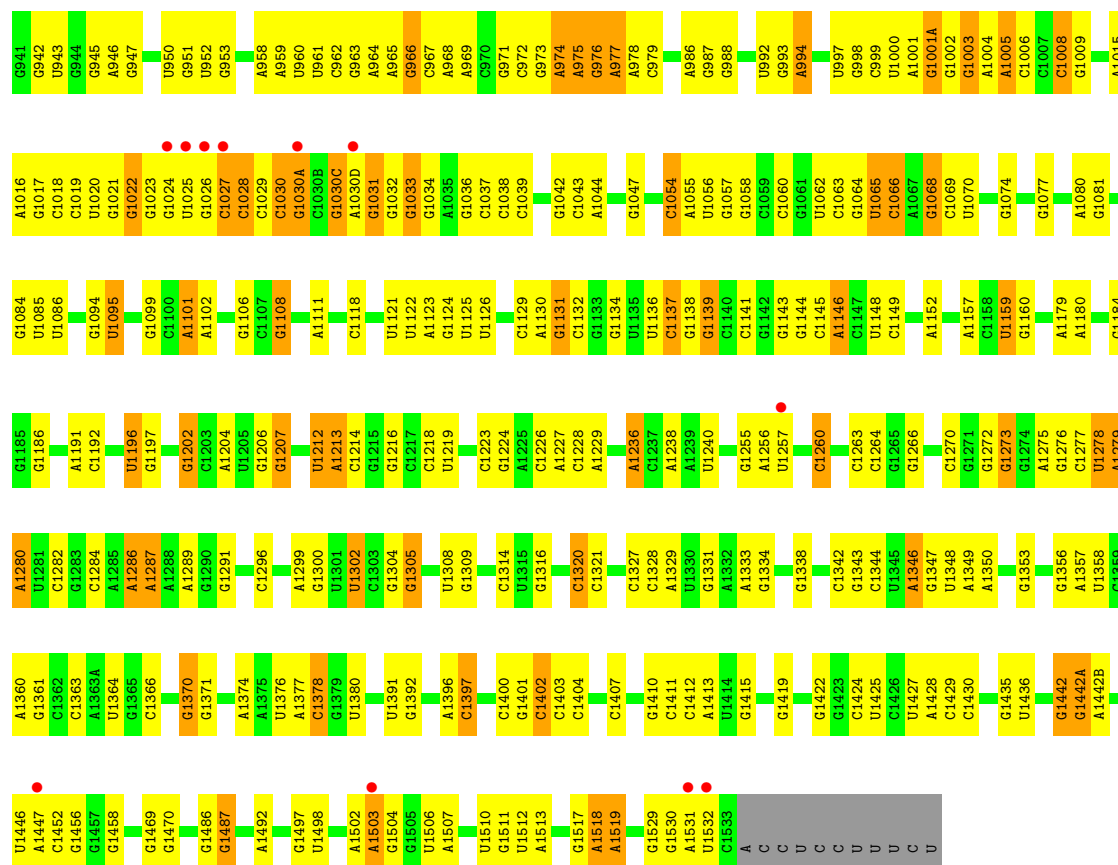
Chain 29:  3% 73% 24%



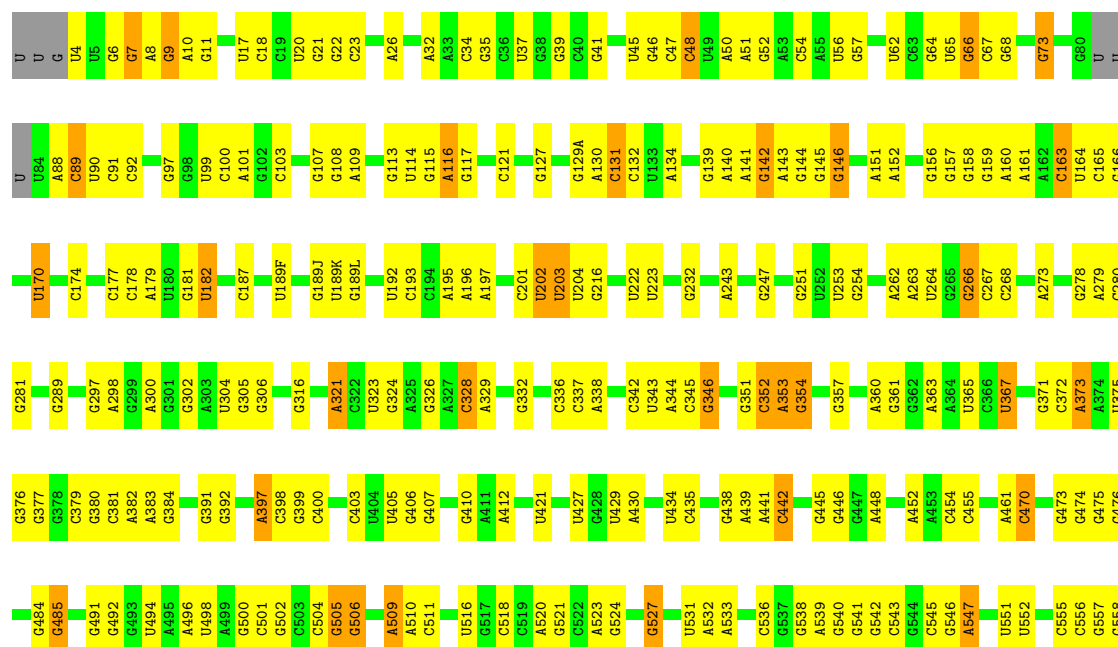
- Molecule 32: 16S Ribosomal RNA

Chain 1a:  52% 39% 7%

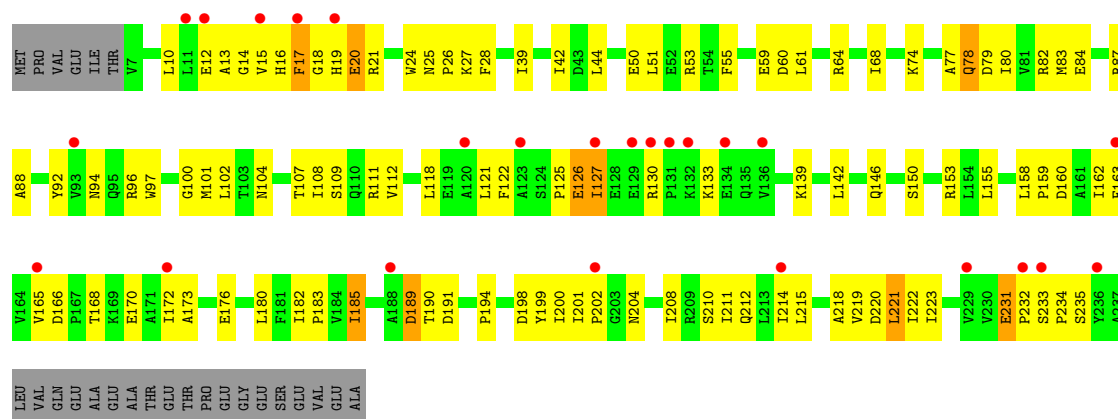




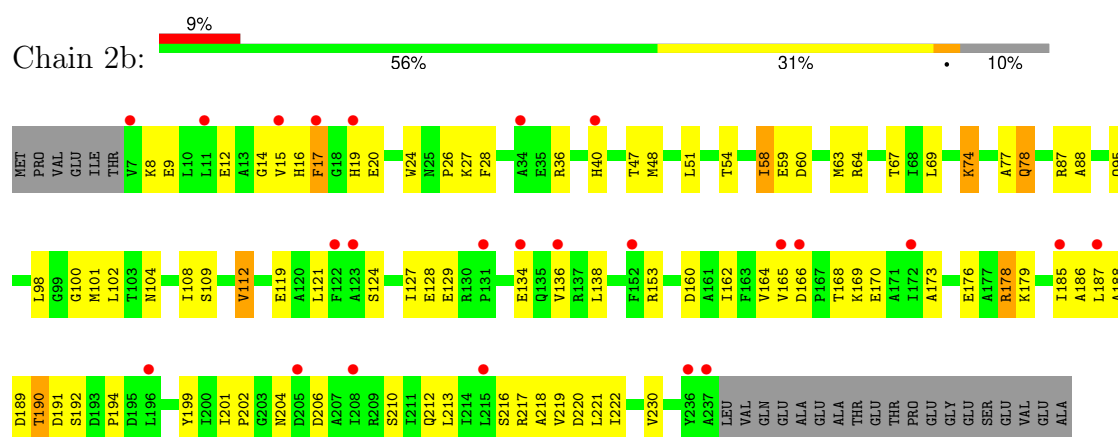
- Molecule 32: 16S Ribosomal RNA



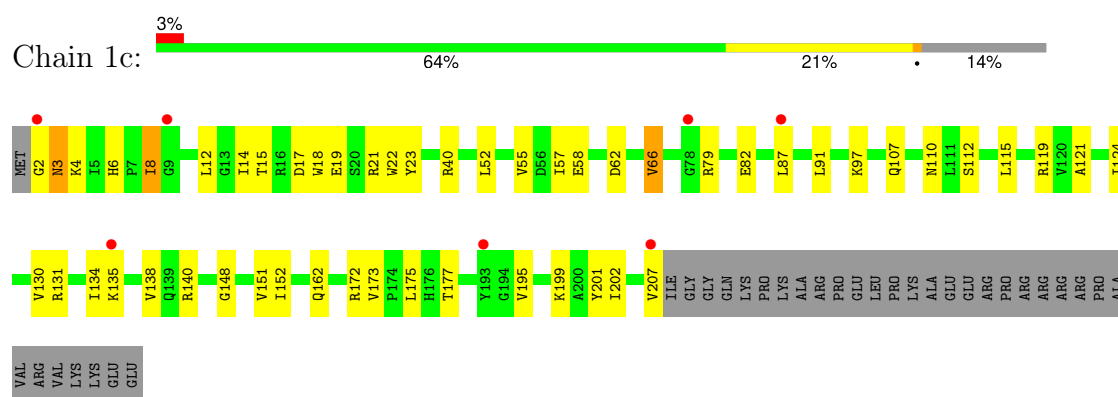




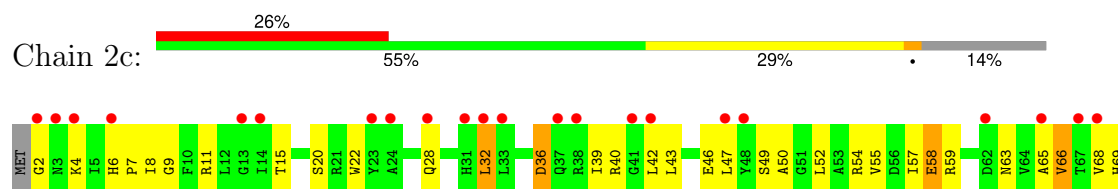
- Molecule 33: 30S ribosomal protein S2

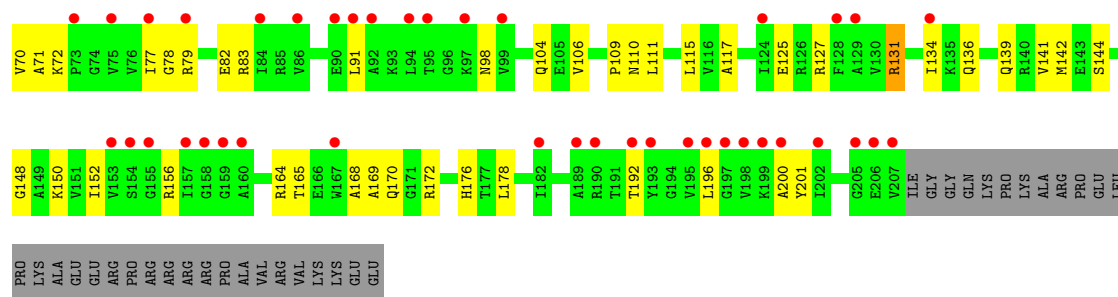


- Molecule 34: 30S ribosomal protein S3

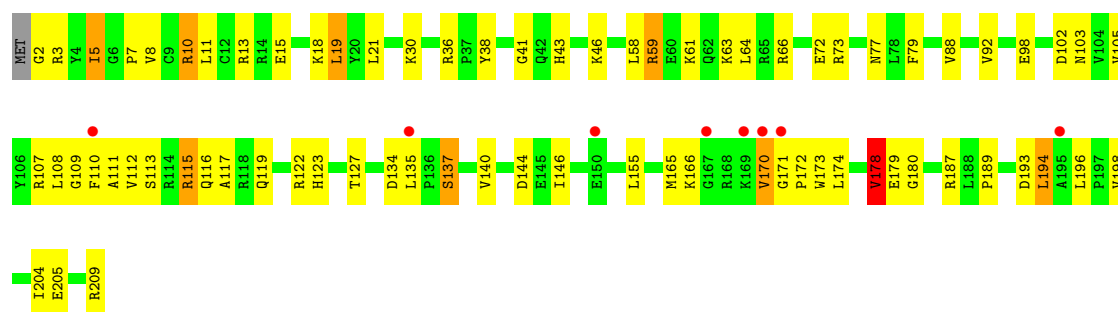


- Molecule 34: 30S ribosomal protein S3

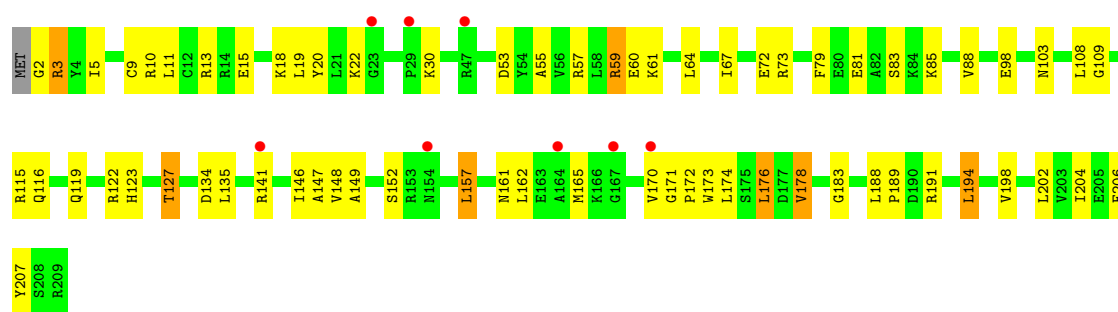




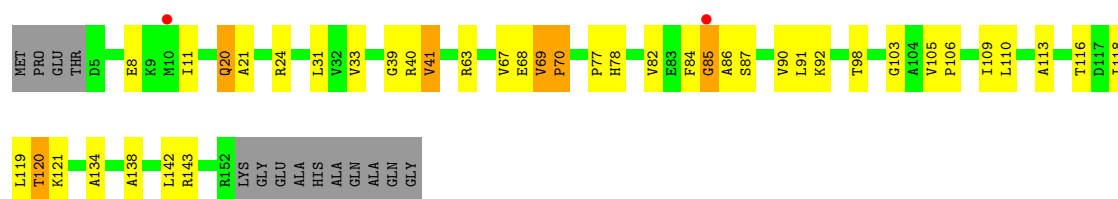
• Molecule 35: 30S ribosomal protein S4



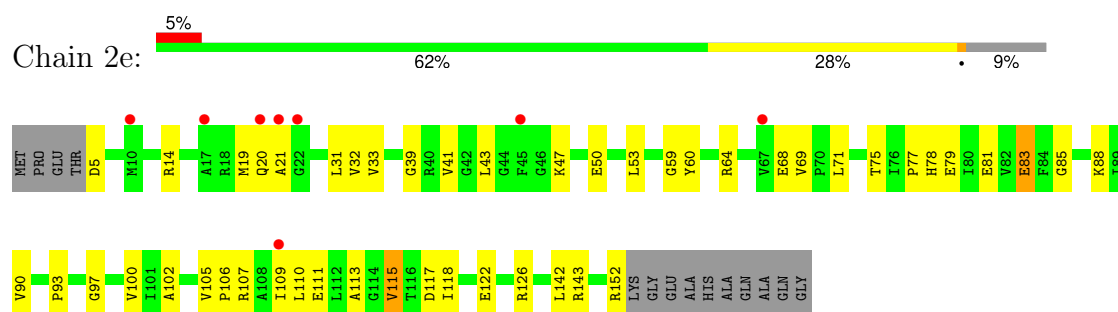
• Molecule 35: 30S ribosomal protein S4



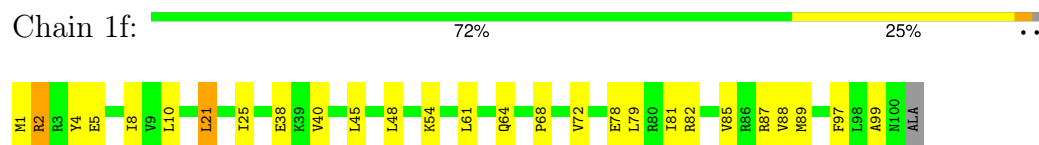
• Molecule 36: 30S ribosomal protein S5



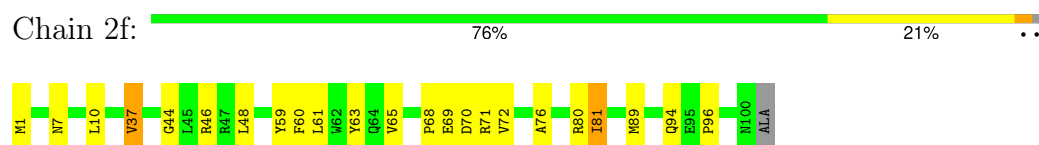
• Molecule 36: 30S ribosomal protein S5



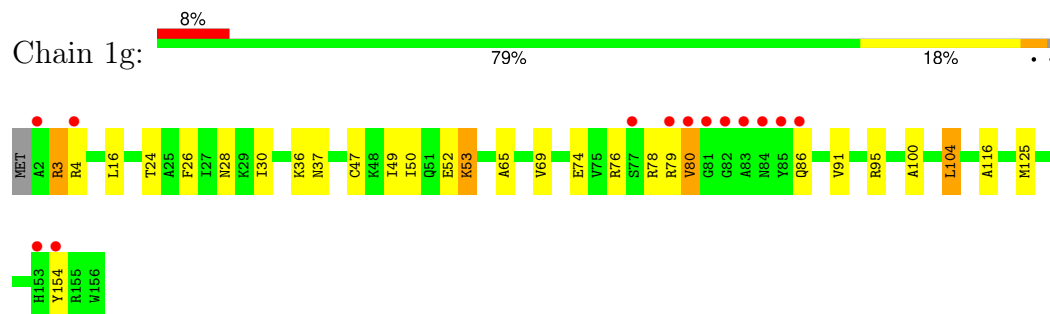
- Molecule 37: 30S ribosomal protein S6



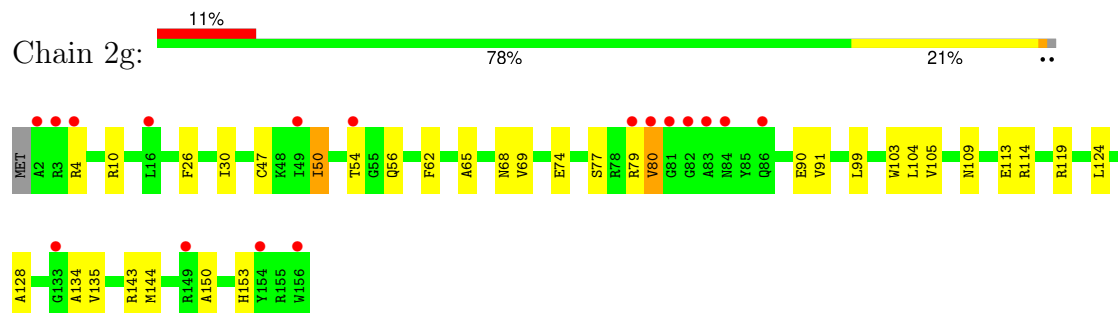
- Molecule 37: 30S ribosomal protein S6



- Molecule 38: 30S ribosomal protein S7

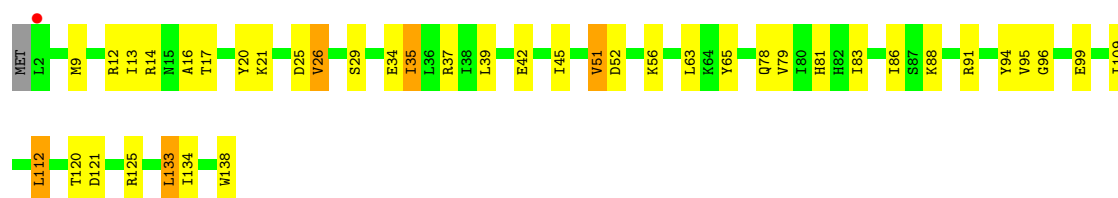


- Molecule 38: 30S ribosomal protein S7

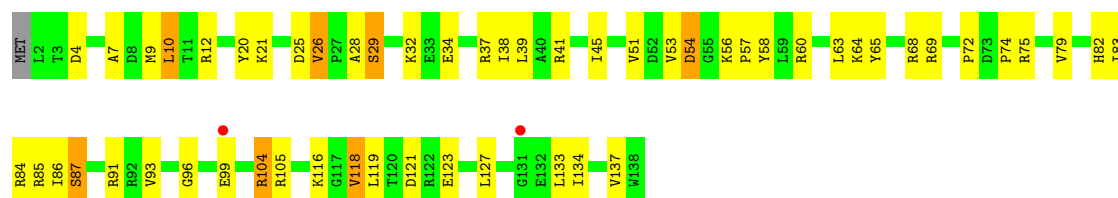


- Molecule 39: 30S ribosomal protein S8

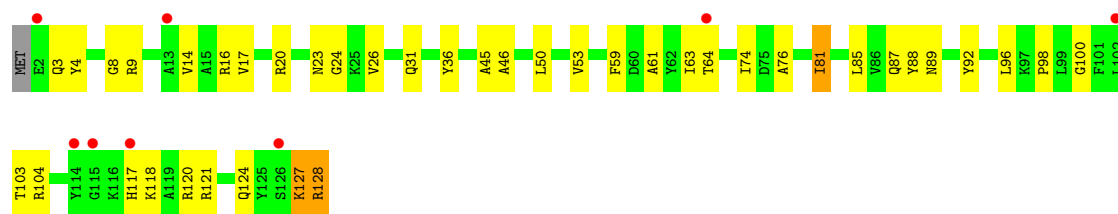




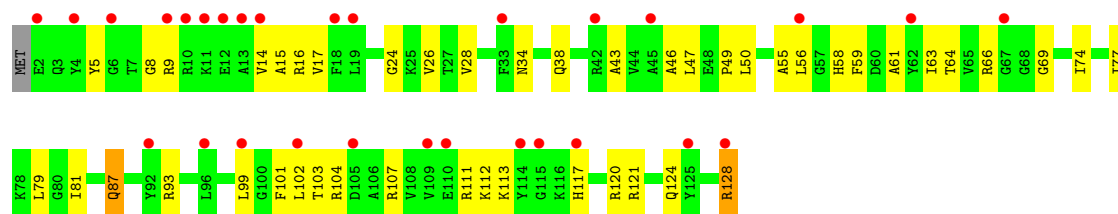
- Molecule 39: 30S ribosomal protein S8



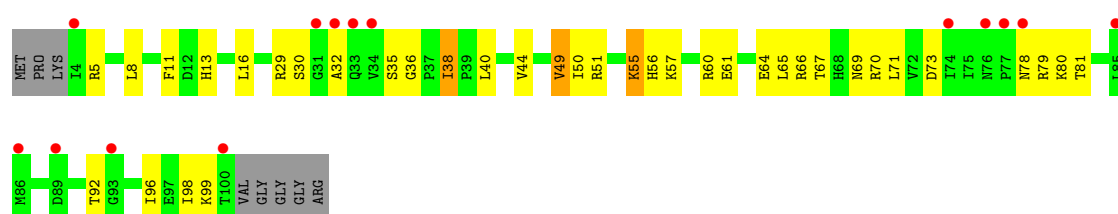
- Molecule 40: 30S ribosomal protein S9



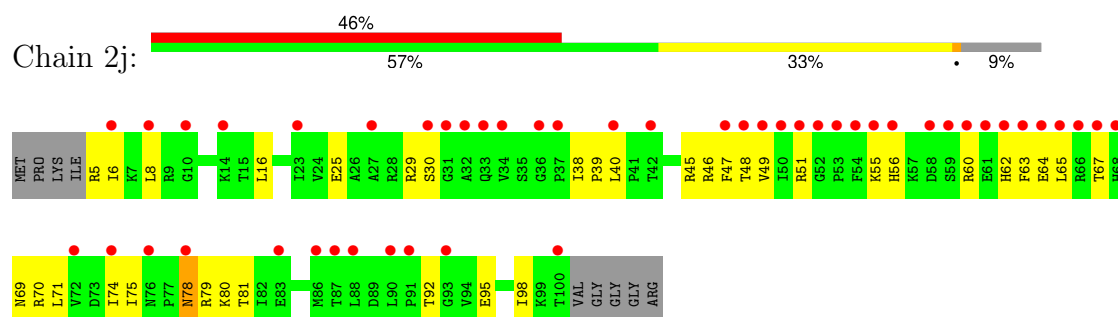
- Molecule 40: 30S ribosomal protein S9



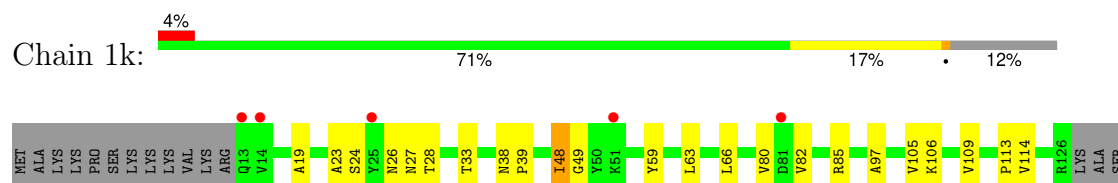
- Molecule 41: 30S ribosomal protein S10



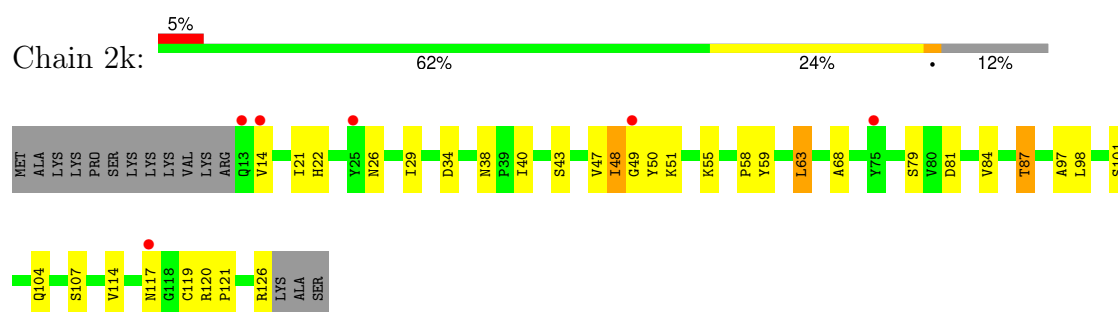
- Molecule 41: 30S ribosomal protein S10



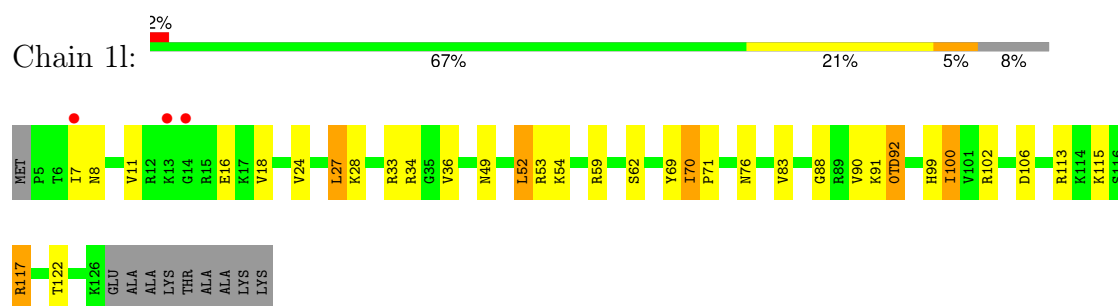
- Molecule 42: 30S ribosomal protein S11



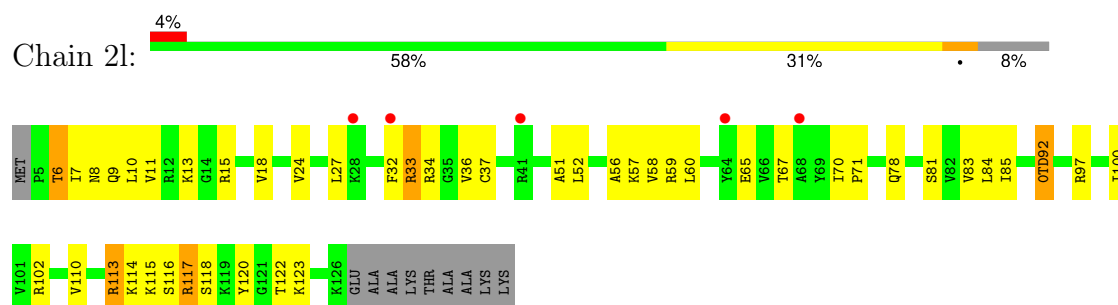
- Molecule 42: 30S ribosomal protein S11



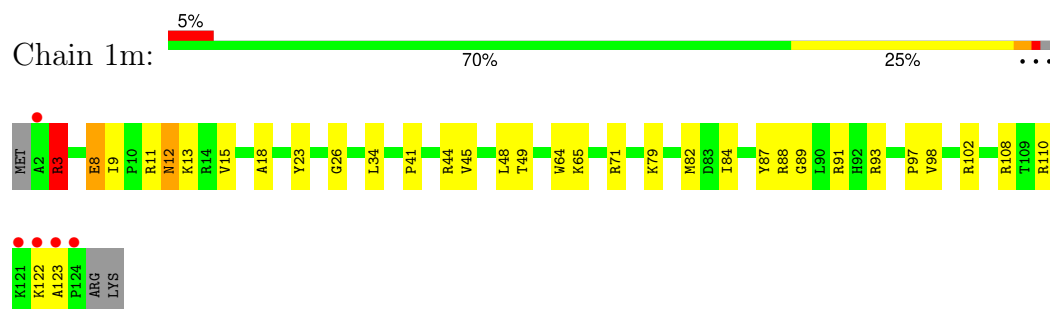
- Molecule 43: 30S ribosomal protein S12



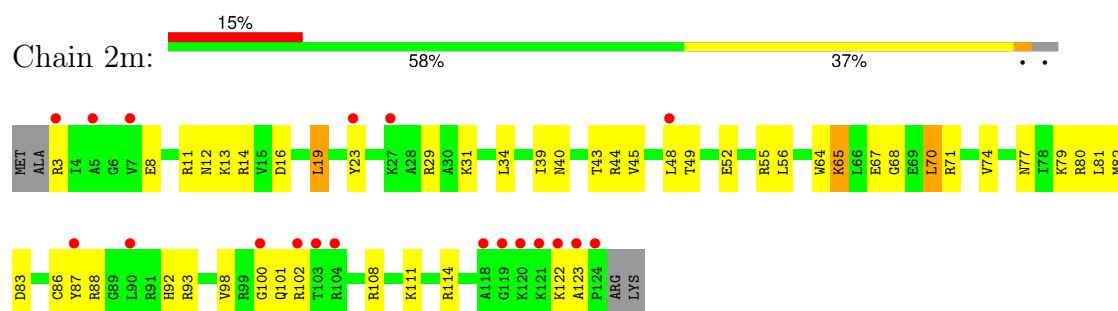
- Molecule 43: 30S ribosomal protein S12



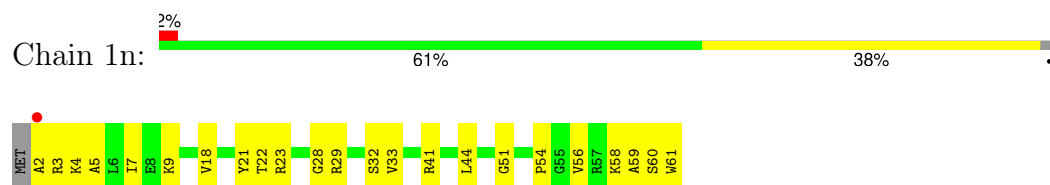
- Molecule 44: 30S ribosomal protein S13



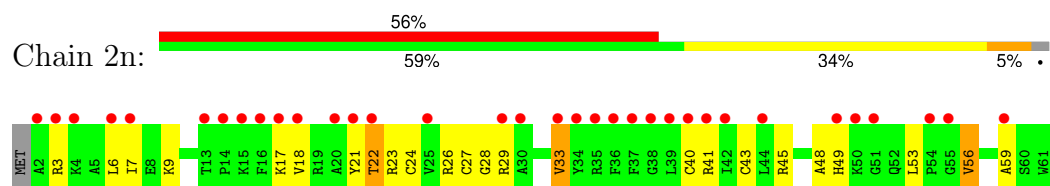
- Molecule 44: 30S ribosomal protein S13



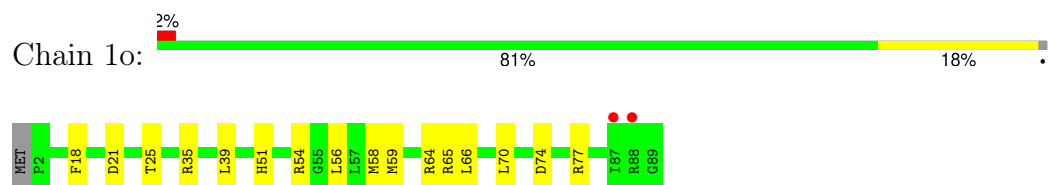
- Molecule 45: 30S ribosomal protein S14 type Z



- Molecule 45: 30S ribosomal protein S14 type Z



- Molecule 46: 30S ribosomal protein S15



- Molecule 46: 30S ribosomal protein S15

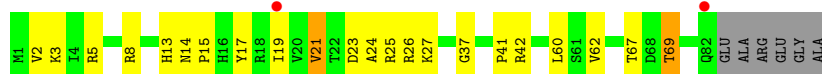




- Molecule 47: 30S ribosomal protein S16



- Molecule 47: 30S ribosomal protein S16



- Molecule 48: 30S ribosomal protein S17



- Molecule 48: 30S ribosomal protein S17

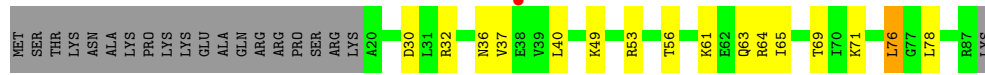


ALA

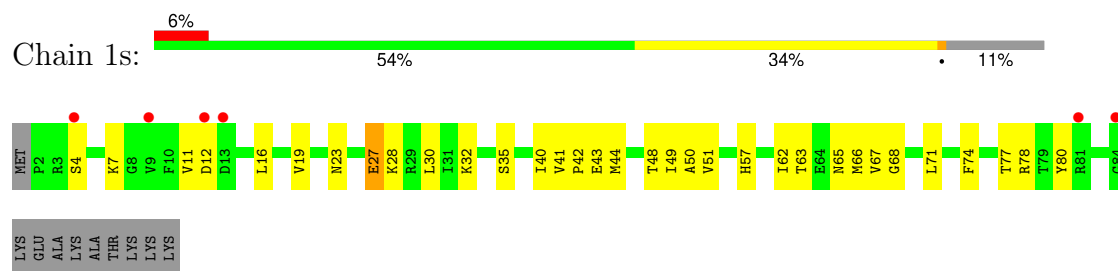
- Molecule 49: 30S ribosomal protein S18



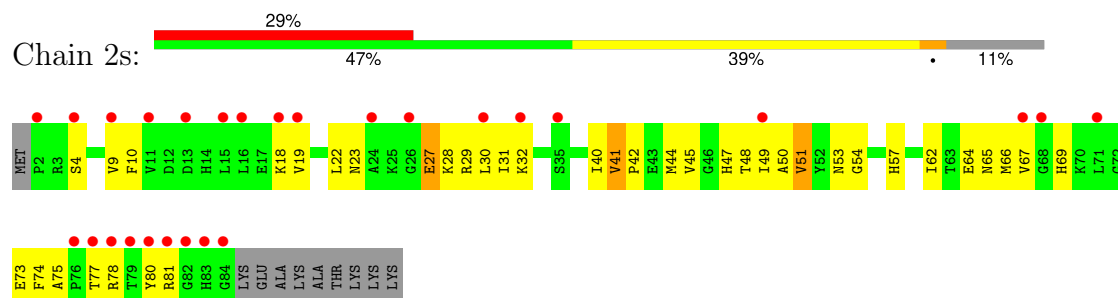
- Molecule 49: 30S ribosomal protein S18



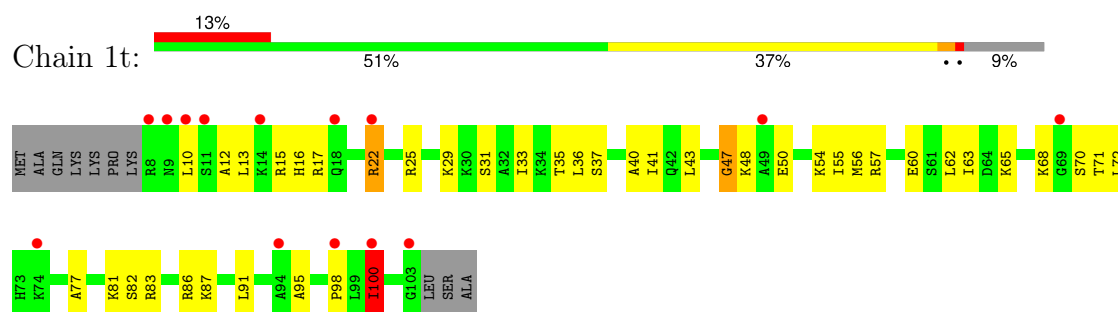
- Molecule 50: 30S ribosomal protein S19



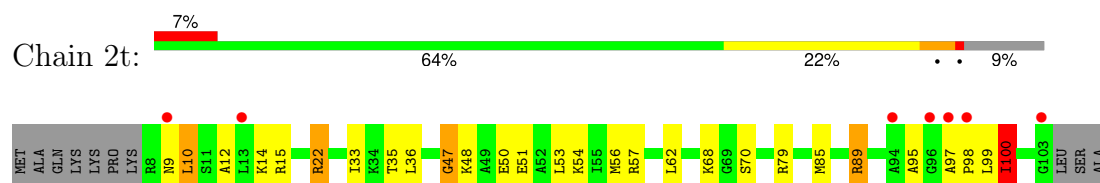
- Molecule 50: 30S ribosomal protein S19



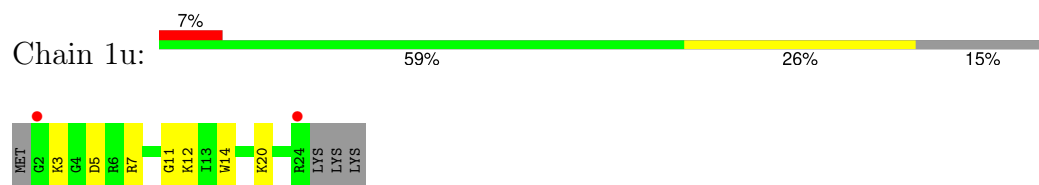
- Molecule 51: 30S ribosomal protein S20



- Molecule 51: 30S ribosomal protein S20

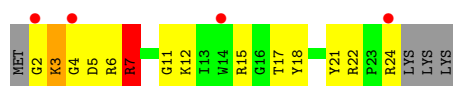


- Molecule 52: 30S ribosomal protein Thx

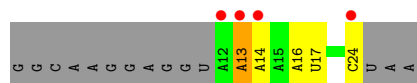
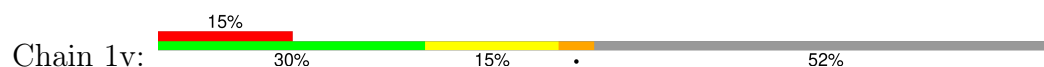


- Molecule 52: 30S ribosomal protein Thx

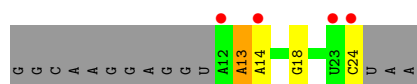
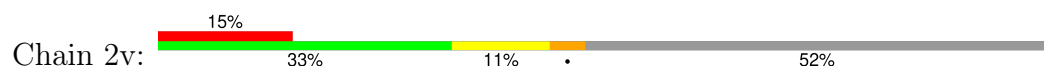




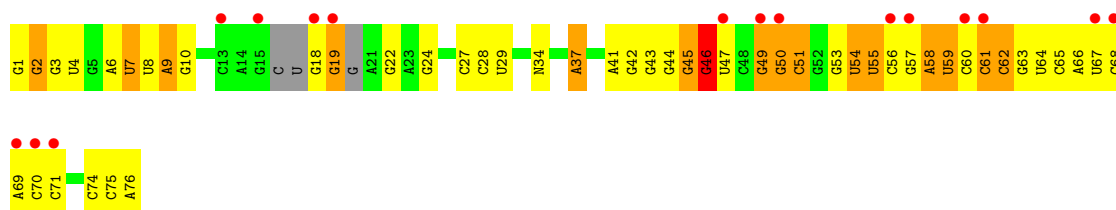
• Molecule 53: mRNA



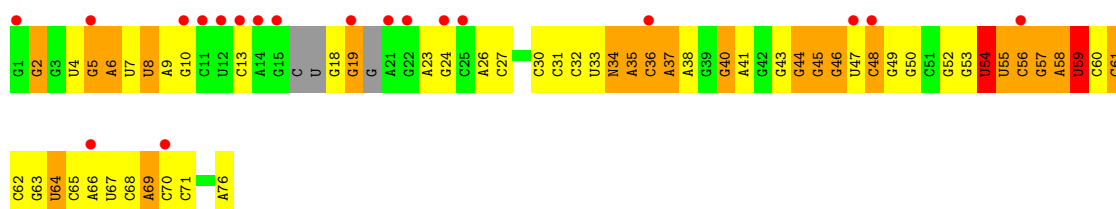
• Molecule 53: mRNA



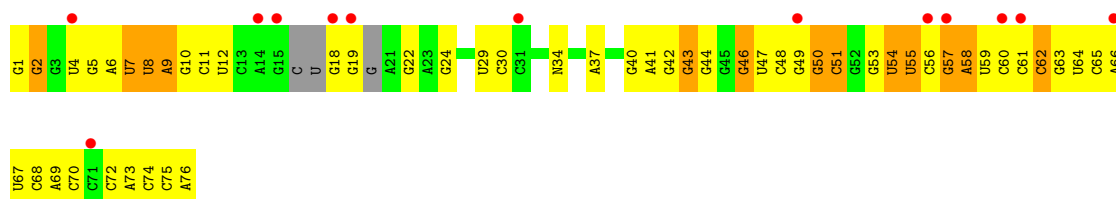
• Molecule 54: A-site and E-site tRNAs



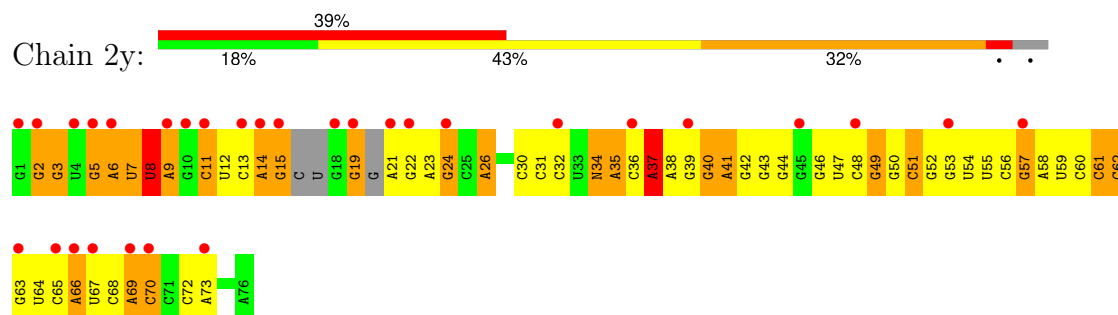
• Molecule 54: A-site and E-site tRNAs



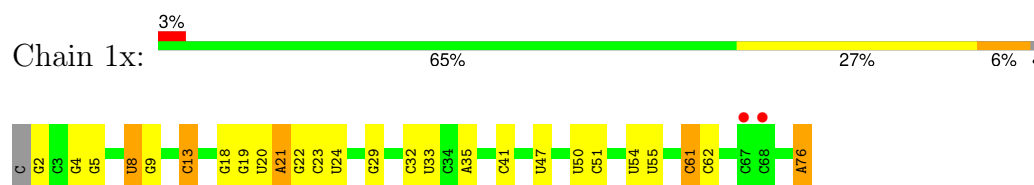
• Molecule 54: A-site and E-site tRNAs



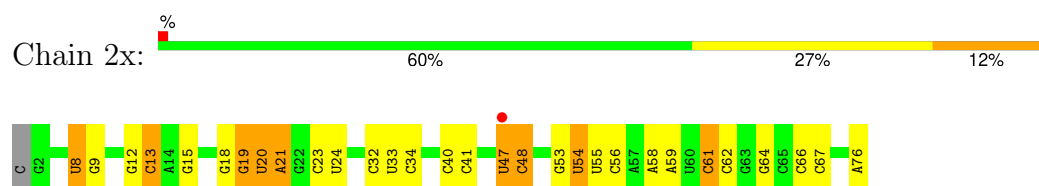
- Molecule 54: A-site and E-site tRNAs



- Molecule 55: P-site tRNA



- Molecule 55: P-site tRNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	208.15Å 446.40Å 615.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	253.38 – 2.80 253.38 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (253.38-2.80) 99.8 (253.38-2.80)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 2.82Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.215 , 0.263 0.213 , 0.259	Depositor DCC
R_{free} test set	69538 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	57.3	Xtriage
Anisotropy	0.245	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 71.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	300274	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: 5MC, MG, M2G, 2MU, MA6, PSU, 4OC, 0TD, OMG, 7MG, UR3, 2MG, 2MA, 5MU, DI0, K, 6MZ, 4SU, ZN, CM0, SF4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1A	0.30	0/69009	0.46	1/107712 (0.0%)
1	2A	0.23	0/67293	0.40	1/105034 (0.0%)
2	1B	0.23	0/2882	0.40	0/4494
2	2B	0.18	0/2879	0.36	0/4487
3	1D	0.29	0/2186	0.51	0/2944
3	2D	0.25	0/2186	0.49	0/2944
4	1E	0.32	0/1592	0.57	1/2149 (0.0%)
4	2E	0.22	0/1592	0.45	0/2149
5	1F	0.28	0/1619	0.51	0/2193
5	2F	0.21	0/1615	0.45	0/2188
6	1G	0.22	0/1448	0.49	1/1957 (0.1%)
6	2G	0.19	0/1453	0.41	0/1963
7	1H	0.24	0/1356	0.41	0/1834
7	2H	0.17	0/1356	0.37	0/1834
8	1I	0.18	0/1112	0.38	0/1514
8	2I	0.20	0/1079	0.40	0/1475
9	1N	0.27	0/1144	0.43	0/1543
9	2N	0.18	0/1144	0.40	0/1543
10	1O	0.28	0/943	0.48	0/1269
10	2O	0.22	0/943	0.45	0/1269
11	1P	0.29	0/1152	0.49	0/1533
11	2P	0.22	0/1152	0.45	0/1533
12	1Q	0.26	0/1143	0.44	0/1527
12	2Q	0.20	0/1143	0.41	0/1527
13	1R	0.29	0/982	0.49	0/1312
13	2R	0.21	0/982	0.44	0/1312
14	1S	0.23	0/883	0.47	0/1176
14	2S	0.20	0/880	0.44	0/1172
15	1T	0.26	0/1105	0.50	0/1477
15	2T	0.21	0/1097	0.42	0/1468
16	1U	0.32	0/977	0.46	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.21	0/977	0.41	0/1301
17	1V	0.30	0/782	0.49	0/1049
17	2V	0.19	0/782	0.40	0/1049
18	1W	0.29	0/897	0.46	0/1205
18	2W	0.23	0/897	0.41	0/1205
19	1X	0.28	0/764	0.49	0/1025
19	2X	0.20	0/764	0.38	0/1025
20	1Y	0.24	0/819	0.48	1/1095 (0.1%)
20	2Y	0.25	0/819	0.55	2/1095 (0.2%)
21	1Z	0.29	0/1267	0.49	0/1717
21	2Z	0.20	0/1299	0.46	0/1763
22	10	0.29	0/662	0.55	0/881
22	20	0.22	0/662	0.48	0/881
23	11	0.26	0/762	0.46	0/1014
23	21	0.23	0/762	0.42	0/1014
24	12	0.27	0/590	0.47	0/781
24	22	0.18	0/590	0.35	0/781
25	13	0.26	0/474	0.45	0/635
25	23	0.20	0/469	0.39	0/630
26	14	0.27	0/565	0.74	2/761 (0.3%)
26	24	0.26	0/545	0.59	0/737
27	15	0.29	0/469	0.52	0/635
27	25	0.28	0/469	0.42	0/635
28	16	0.30	0/460	0.51	0/613
28	26	0.21	0/456	0.46	0/608
29	17	0.31	0/426	0.51	0/561
29	27	0.27	0/426	0.52	0/561
30	18	0.30	0/525	0.50	0/691
30	28	0.21	0/525	0.41	0/691
31	19	0.28	0/310	0.53	0/407
31	29	0.20	0/310	0.46	0/407
32	1a	0.22	0/35795	0.40	0/55864
32	2a	0.19	0/35886	0.38	0/56005
33	1b	0.21	0/1881	0.45	0/2542
33	2b	0.22	0/1860	0.47	0/2518
34	1c	0.25	1/1572 (0.1%)	0.39	0/2126
34	2c	0.20	0/1566	0.44	1/2119 (0.0%)
35	1d	0.21	0/1685	0.45	0/2262
35	2d	0.20	0/1704	0.43	0/2284
36	1e	0.21	0/1145	0.44	0/1543
36	2e	0.21	0/1149	0.47	0/1548
37	1f	0.20	0/823	0.37	0/1115
37	2f	0.21	0/829	0.38	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.19	0/1250	0.39	0/1679
38	2g	0.18	0/1254	0.38	0/1683
39	1h	0.20	0/1108	0.41	0/1494
39	2h	0.18	0/1108	0.41	0/1494
40	1i	0.20	0/1002	0.49	0/1346
40	2i	0.20	0/997	0.42	0/1343
41	1j	0.19	0/722	0.48	0/982
41	2j	0.20	0/727	0.42	0/988
42	1k	0.20	0/844	0.41	0/1145
42	2k	0.19	0/848	0.44	0/1149
43	1l	0.21	0/937	0.42	0/1260
43	2l	0.19	0/937	0.41	0/1260
44	1m	0.21	0/969	0.46	0/1302
44	2m	0.20	0/961	0.40	0/1291
45	1n	0.20	0/501	0.46	0/664
45	2n	0.20	0/501	0.43	0/664
46	1o	0.21	0/739	0.41	0/985
46	2o	0.17	0/739	0.39	0/985
47	1p	0.22	0/697	0.50	0/939
47	2p	0.21	0/693	0.42	0/935
48	1q	0.19	0/836	0.39	0/1117
48	2q	0.17	0/836	0.37	0/1117
49	1r	0.20	0/560	0.43	0/746
49	2r	0.17	0/560	0.41	0/746
50	1s	0.22	0/667	0.51	0/900
50	2s	0.26	0/661	0.55	0/893
51	1t	0.20	0/730	0.47	0/965
51	2t	0.20	0/729	0.47	0/965
52	1u	0.23	0/203	0.44	0/266
52	2u	0.58	1/203 (0.5%)	0.54	0/266
53	1v	0.26	0/308	0.56	0/477
53	2v	0.26	0/308	0.40	0/477
54	1w	0.36	2/1600 (0.1%)	0.44	0/2482
54	1y	0.36	2/1600 (0.1%)	0.45	0/2482
54	2w	0.27	0/1600	0.38	0/2482
54	2y	0.34	1/1600 (0.1%)	0.46	0/2482
55	1x	0.26	0/1725	0.42	0/2689
55	2x	0.24	0/1725	0.38	0/2689
All	All	0.25	7/316731 (0.0%)	0.43	10/474164 (0.0%)

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
26	14	0	3
26	24	0	1
33	2b	0	1
All	All	0	5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	2u	7	ARG	CA-C	7.31	1.62	1.52
34	1c	173	VAL	C-N	6.54	1.49	1.33
54	2y	8	4SU	O3'-P	6.17	1.62	1.56
54	1y	8	4SU	O3'-P	5.66	1.61	1.56
54	1y	59	U	C4-O4	5.33	1.34	1.23
54	1w	59	U	C4-O4	5.29	1.34	1.23
54	1w	8	4SU	O3'-P	5.15	1.61	1.56

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	14	63	TYR	N-CA-C	-8.55	100.90	110.91
26	14	64	GLY	N-CA-C	7.89	131.89	113.18
20	2Y	102	CYS	CB-CA-C	-6.71	106.67	116.53
4	1E	95	ILE	N-CA-C	-6.35	105.04	112.98
1	2A	1992	G	C2'-C3'-O3'	6.26	118.88	109.50
1	1A	1992	G	C2'-C3'-O3'	6.18	118.78	109.50
20	2Y	102	CYS	CA-C-O	5.39	121.72	118.33
34	2c	8	ILE	N-CA-C	-5.25	106.68	111.67
20	1Y	93	GLY	N-CA-C	-5.17	108.33	114.48
6	1G	44	GLY	N-CA-C	-5.11	108.93	115.42

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	14	56	VAL	Peptide
26	14	63	TYR	Peptide
26	14	64	GLY	Peptide
26	24	56	VAL	Peptide
33	2b	124	SER	Peptide

5.2 Too-close contacts

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	31193	697	0
1	2A	60322	0	30423	754	0
2	1B	2577	0	1305	23	0
2	2B	2575	0	1303	34	0
3	1D	2136	0	2218	47	0
3	2D	2136	0	2217	48	0
4	1E	1559	0	1618	41	0
4	2E	1559	0	1618	43	0
5	1F	1584	0	1625	36	0
5	2F	1580	0	1619	42	0
6	1G	1423	0	1436	42	0
6	2G	1428	0	1438	47	0
7	1H	1330	0	1407	27	0
7	2H	1330	0	1407	33	0
8	1I	1097	0	1140	23	0
8	2I	1064	0	1082	27	0
9	1N	1117	0	1184	23	0
9	2N	1117	0	1184	23	0
10	1O	933	0	996	22	0
10	2O	933	0	996	23	0
11	1P	1135	0	1212	37	0
11	2P	1135	0	1211	38	0
12	1Q	1122	0	1179	22	0
12	2Q	1122	0	1179	39	0
13	1R	968	0	1033	21	0
13	2R	968	0	1033	20	0
14	1S	873	0	927	21	0
14	2S	870	0	923	28	0
15	1T	1091	0	1151	23	0
15	2T	1083	0	1136	36	0
16	1U	959	0	1019	18	0
16	2U	959	0	1019	26	0
17	1V	771	0	830	14	0
17	2V	771	0	830	14	0
18	1W	886	0	940	21	0
18	2W	886	0	940	12	0
19	1X	750	0	814	16	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	2X	750	0	814	18	0
20	1Y	806	0	881	19	0
20	2Y	806	0	881	22	0
21	1Z	1240	0	1240	30	0
21	2Z	1271	0	1273	36	0
22	10	653	0	674	17	0
22	20	653	0	674	28	0
23	11	755	0	826	21	0
23	21	755	0	826	17	0
24	12	588	0	643	15	0
24	22	588	0	643	13	0
25	13	469	0	518	11	0
25	23	464	0	514	13	0
26	14	552	0	533	23	0
26	24	532	0	503	17	0
27	15	455	0	465	8	0
27	25	455	0	465	7	0
28	16	453	0	473	9	0
28	26	449	0	469	6	0
29	17	418	0	467	6	0
29	27	418	0	467	9	0
30	18	517	0	582	22	0
30	28	517	0	582	22	0
31	19	307	0	335	5	0
31	29	307	0	335	8	0
32	1a	32246	0	16296	481	0
32	2a	32327	0	16340	564	0
33	1b	1846	0	1867	68	0
33	2b	1825	0	1828	64	0
34	1c	1548	0	1535	32	0
34	2c	1542	0	1517	52	0
35	1d	1655	0	1672	54	0
35	2d	1674	0	1714	49	0
36	1e	1129	0	1185	25	0
36	2e	1133	0	1191	31	0
37	1f	810	0	804	17	0
37	2f	816	0	808	14	0
38	1g	1231	0	1238	21	0
38	2g	1235	0	1249	26	0
39	1h	1088	0	1126	22	0
39	2h	1088	0	1126	42	0
40	1i	983	0	986	35	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	2i	978	0	966	34	0
41	1j	709	0	650	28	0
41	2j	714	0	672	29	0
42	1k	829	0	825	13	0
42	2k	833	0	836	20	0
43	1l	932	0	981	21	0
43	2l	932	0	981	32	0
44	1m	958	0	1002	22	0
44	2m	950	0	988	33	0
45	1n	492	0	529	18	0
45	2n	492	0	529	23	0
46	1o	728	0	760	11	0
46	2o	728	0	760	20	0
47	1p	681	0	697	23	0
47	2p	677	0	686	16	0
48	1q	823	0	891	18	0
48	2q	823	0	891	21	0
49	1r	555	0	618	7	0
49	2r	555	0	618	12	0
50	1s	652	0	662	25	0
50	2s	646	0	644	33	0
51	1t	728	0	798	29	0
51	2t	727	0	796	26	0
52	1u	199	0	208	7	0
52	2u	199	0	208	12	0
53	1v	276	0	139	2	0
53	2v	276	0	139	2	0
54	1w	1568	0	800	37	0
54	1y	1568	0	800	47	0
54	2w	1568	0	802	38	0
54	2y	1568	0	801	58	0
55	1x	1625	0	828	16	0
55	2x	1625	0	828	21	0
56	10	7	0	0	0	0
56	11	4	0	0	0	0
56	12	2	0	0	0	0
56	13	3	0	0	0	0
56	15	5	0	0	0	0
56	16	2	0	0	0	0
56	17	3	0	0	0	0
56	18	2	0	0	0	0
56	1A	1148	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	1B	37	0	0	0	0
56	1D	13	0	0	0	0
56	1E	8	0	0	0	0
56	1F	9	0	0	0	0
56	1G	5	0	0	0	0
56	1H	1	0	0	0	0
56	1I	1	0	0	0	0
56	1N	8	0	0	0	0
56	1O	5	0	0	0	0
56	1P	3	0	0	0	0
56	1Q	6	0	0	0	0
56	1R	2	0	0	0	0
56	1S	3	0	0	0	0
56	1T	2	0	0	0	0
56	1U	7	0	0	0	0
56	1V	2	0	0	0	0
56	1W	6	0	0	0	0
56	1X	5	0	0	0	0
56	1Y	3	0	0	0	0
56	1Z	3	0	0	0	0
56	1a	244	0	0	0	0
56	1b	2	0	0	0	0
56	1d	1	0	0	0	0
56	1f	1	0	0	0	0
56	1h	1	0	0	0	0
56	1l	3	0	0	0	0
56	1m	3	0	0	0	0
56	1p	1	0	0	0	0
56	1r	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	7	0	0	0	0
56	1x	12	0	0	0	0
56	1y	5	0	0	0	0
56	20	2	0	0	0	0
56	21	1	0	0	0	0
56	23	1	0	0	0	0
56	25	4	0	0	0	0
56	27	1	0	0	0	0
56	28	1	0	0	0	0
56	2A	860	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	2B	21	0	0	0	0
56	2D	3	0	0	0	0
56	2E	8	0	0	0	0
56	2F	4	0	0	0	0
56	2G	1	0	0	0	0
56	2O	2	0	0	0	0
56	2P	3	0	0	0	0
56	2Q	3	0	0	0	0
56	2R	2	0	0	0	0
56	2T	3	0	0	0	0
56	2U	4	0	0	0	0
56	2V	2	0	0	0	0
56	2W	2	0	0	0	0
56	2X	2	0	0	0	0
56	2Z	1	0	0	0	0
56	2a	231	0	0	0	0
56	2d	2	0	0	0	0
56	2e	1	0	0	0	0
56	2f	2	0	0	0	0
56	2g	1	0	0	0	0
56	2i	1	0	0	0	0
56	2j	2	0	0	0	0
56	2l	2	0	0	0	0
56	2q	3	0	0	0	0
56	2r	1	0	0	0	0
56	2t	1	0	0	0	0
56	2v	3	0	0	0	0
56	2w	1	0	0	0	0
56	2x	5	0	0	0	0
56	2y	7	0	0	0	0
57	1A	58	0	0	5	0
57	2A	58	0	0	0	0
58	1A	1	0	0	0	0
58	2A	1	0	0	0	0
59	14	1	0	0	0	0
59	15	1	0	0	0	0
59	16	1	0	0	0	0
59	19	1	0	0	0	0
59	1Y	1	0	0	0	0
59	1n	1	0	0	0	0
59	24	1	0	0	0	0
59	25	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	26	1	0	0	0	0
59	29	1	0	0	0	0
59	2Y	1	0	0	0	0
59	2n	1	0	0	0	0
60	1d	8	0	0	1	0
60	2d	8	0	0	1	0
61	10	11	0	0	0	0
61	11	8	0	0	0	0
61	12	4	0	0	1	0
61	13	4	0	0	0	0
61	15	3	0	0	0	0
61	16	4	0	0	0	0
61	17	6	0	0	1	0
61	18	12	0	0	0	0
61	19	1	0	0	0	0
61	1A	2034	0	0	65	0
61	1B	65	0	0	0	0
61	1D	29	0	0	3	0
61	1E	24	0	0	0	0
61	1F	12	0	0	1	0
61	1G	5	0	0	2	0
61	1H	1	0	0	0	0
61	1I	2	0	0	0	0
61	1N	6	0	0	0	0
61	1O	7	0	0	1	0
61	1P	23	0	0	1	0
61	1Q	7	0	0	0	0
61	1R	14	0	0	1	0
61	1S	3	0	0	0	0
61	1T	10	0	0	1	0
61	1U	12	0	0	0	0
61	1V	8	0	0	0	0
61	1W	10	0	0	0	0
61	1X	4	0	0	0	0
61	1Y	3	0	0	0	0
61	1a	439	0	0	21	0
61	1b	1	0	0	0	0
61	1d	2	0	0	0	0
61	1f	2	0	0	1	0
61	1g	2	0	0	0	0
61	1l	11	0	0	0	0
61	1o	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6l	1p	1	0	0	0	0
6l	1q	2	0	0	0	0
6l	1r	2	0	0	0	0
6l	1t	2	0	0	0	0
6l	1u	1	0	0	1	0
6l	1v	9	0	0	0	0
6l	1w	6	0	0	1	0
6l	1x	7	0	0	0	0
6l	1y	4	0	0	0	0
6l	20	3	0	0	0	0
6l	21	6	0	0	0	0
6l	23	2	0	0	1	0
6l	25	1	0	0	0	0
6l	27	3	0	0	0	0
6l	28	4	0	0	0	0
6l	29	1	0	0	0	0
6l	2A	1099	0	0	49	0
6l	2B	24	0	0	0	0
6l	2D	20	0	0	1	0
6l	2E	12	0	0	0	0
6l	2F	7	0	0	0	0
6l	2I	4	0	0	0	0
6l	2N	1	0	0	0	0
6l	2O	1	0	0	0	0
6l	2P	12	0	0	2	0
6l	2Q	2	0	0	0	0
6l	2R	2	0	0	0	0
6l	2T	4	0	0	0	0
6l	2U	4	0	0	1	0
6l	2V	1	0	0	0	0
6l	2W	4	0	0	0	0
6l	2X	5	0	0	0	0
6l	2Y	1	0	0	0	0
6l	2Z	1	0	0	0	0
6l	2a	284	0	0	16	0
6l	2d	1	0	0	0	0
6l	2e	2	0	0	0	0
6l	2g	1	0	0	0	0
6l	2j	3	0	0	2	0
6l	2l	2	0	0	0	0
6l	2n	1	0	0	0	0
6l	2o	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	2p	1	0	0	0	0
61	2q	1	0	0	0	0
61	2r	1	0	0	0	0
61	2t	3	0	0	0	0
61	2v	3	0	0	0	0
61	2w	3	0	0	1	0
61	2x	5	0	0	0	0
61	2y	16	0	0	0	0
All	All	300274	0	196683	4508	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 (4508) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1082:U:H3	1:1A:1086:A:N6	1.19	1.37
1:1A:2136:C:N4	1:1A:2155:G:H1	1.47	1.09
54:2y:30:C:N4	54:2y:40:G:H1	1.53	1.07
32:2a:997:U:H3	32:2a:1044:A:N6	1.52	1.07
32:2a:1002:G:H1	32:2a:1038:C:N4	1.54	1.04
1:1A:1082:U:O4	1:1A:1086:A:N1	1.92	1.02
1:2A:2138:C:N4	1:2A:2153:G:H1	1.59	0.98
54:2w:53:G:H1	54:2w:61:C:H42	0.98	0.98
54:1w:51:C:N4	54:1w:63:G:H1	1.60	0.98
32:2a:1029:C:N4	32:2a:1032:G:H1	1.60	0.97
1:2A:2104:G:H1	1:2A:2185:C:H42	1.07	0.97
1:1A:1058:G:H1	1:1A:1080:C:N4	1.63	0.97
1:1A:2099:U:H3	1:1A:2190:G:H1	1.12	0.96
1:2A:2129:C:H42	1:2A:2159:G:H1	1.14	0.94
32:1a:1030:C:H42	32:1a:1031:G:H1	1.15	0.94
32:2a:1089:G:H1	32:2a:1096:C:N4	1.66	0.93
1:2A:882:G:H1	1:2A:894:C:H42	1.05	0.92
33:1b:16:HIS:HB2	33:1b:204:ASN:HB3	1.52	0.92
1:1A:1071:G:N2	1:1A:1091:G:N7	2.18	0.92
54:1y:30:C:H42	54:1y:40:G:H1	1.12	0.92
55:1x:8:4SU:O2	55:1x:21:A:H2	1.52	0.92
54:1w:54:5MU:O2	54:1w:58:A:N7	2.03	0.92
1:2A:2138:C:H42	1:2A:2153:G:H1	0.93	0.92
32:2a:999:C:H42	32:2a:1042:G:H1	1.14	0.91
54:2w:50:G:H1	54:2w:64:U:H3	1.12	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1058:G:H1	1:1A:1080:C:H42	1.03	0.90
1:1A:2136:C:N3	1:1A:2155:G:N2	2.20	0.89
54:2w:53:G:H1	54:2w:61:C:N4	1.71	0.89
1:2A:784:A:OP2	61:2A:3901:HOH:O	1.90	0.89
32:2a:1089:G:H1	32:2a:1096:C:H42	0.94	0.89
1:2A:1204:A:H2	1:2A:1241:A:H62	1.21	0.89
1:2A:2137:C:H42	1:2A:2154:G:H1	1.18	0.88
1:1A:1264:G:OP1	27:15:19:ARG:NH2	2.07	0.87
1:1A:1082:U:N3	1:1A:1086:A:N6	2.01	0.87
1:2A:2137:C:N4	1:2A:2154:G:H1	1.73	0.86
11:2P:59:LEU:HD11	30:28:10:ALA:HB2	1.57	0.86
1:1A:2135:A:N6	1:1A:2156:G:O2'	2.06	0.86
1:1A:1054:A:H61	1:1A:1105:U:H3	1.22	0.86
32:2a:1029:C:H42	32:2a:1032:G:H1	1.22	0.86
54:1y:5:G:H1	54:1y:68:C:H42	1.23	0.85
33:2b:185:ILE:HG22	33:2b:199:TYR:HB2	1.58	0.85
54:1y:30:C:N4	54:1y:40:G:H1	1.73	0.85
1:2A:2104:G:H1	1:2A:2185:C:N4	1.74	0.85
1:1A:1062:G:H1	1:1A:1077:A:H61	1.25	0.84
54:2w:51:C:H42	54:2w:63:G:H1	1.25	0.84
1:1A:2124:G:H1	1:1A:2174:C:H42	1.26	0.84
1:2A:2138:C:N3	1:2A:2153:G:N2	2.23	0.84
54:1w:51:C:H42	54:1w:63:G:H1	0.86	0.84
49:2r:53:ARG:HG2	49:2r:63:GLN:HG3	1.60	0.84
1:2A:962:G:OP1	61:2A:3928:HOH:O	1.96	0.84
1:1A:1604:C:OP2	61:1A:4211:HOH:O	1.95	0.83
1:1A:1058:G:N2	1:1A:1080:C:N3	2.26	0.83
1:2A:1689:A:H62	1:2A:1698:A:H2	1.26	0.83
10:2O:48:PRO:HB3	32:2a:1422:G:H5''	1.61	0.83
54:1y:5:G:H1	54:1y:68:C:N4	1.77	0.83
43:1l:28:LYS:HD3	43:1l:62:SER:HB2	1.58	0.83
3:1D:125:ILE:HB	37:1f:81:ILE:HD11	1.59	0.82
1:2A:2129:C:N4	1:2A:2159:G:H1	1.76	0.82
5:1F:53:THR:HG23	5:1F:55:GLY:H	1.43	0.82
32:1a:266:G:H5''	32:1a:268:C:H41	1.42	0.82
1:1A:517:C:OP1	27:15:16:ARG:NH2	2.12	0.82
1:1A:511:U:OP2	61:1A:4206:HOH:O	1.97	0.82
1:1A:1065:U:O2	1:1A:1073:A:N6	2.12	0.82
1:2A:2807:G:N1	1:2A:2893:G:O6	2.12	0.81
32:1a:1036:G:H5''	32:1a:1037:C:H5	1.46	0.81
44:2m:80:ARG:HH12	50:2s:69:HIS:HE1	1.29	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:1w:2:G:O6	54:1w:71:C:N3	2.12	0.81
54:2y:30:C:N3	54:2y:40:G:N2	2.27	0.81
32:2a:975:A:H4'	32:2a:976:G:H5''	1.62	0.81
1:1A:762:U:OP1	61:1A:4275:HOH:O	2.00	0.80
54:1w:53:G:H1	54:1w:61:C:H42	1.25	0.80
19:1X:57:LEU:HD11	19:1X:78:LYS:HE2	1.62	0.80
22:10:11:ARG:O	22:10:14:ARG:NH2	2.14	0.80
8:2I:93:THR:H	8:2I:96:ASP:HB2	1.46	0.80
1:1A:2135:A:H61	1:1A:2156:G:HO2'	1.28	0.80
21:1Z:4:ARG:NH1	21:1Z:60:GLU:OE2	2.13	0.80
32:2a:157:G:H1	32:2a:164:U:H3	1.25	0.80
20:1Y:102:CYS:SG	20:1Y:103:GLY:N	2.49	0.80
32:2a:1002:G:N2	32:2a:1038:C:N3	2.27	0.80
54:2y:12:U:O4	54:2y:23:A:N1	2.15	0.80
1:2A:1818:U:H2'	3:2D:157:ARG:HD2	1.61	0.80
10:1O:48:PRO:HB3	32:1a:1422:G:H5''	1.64	0.80
32:2a:363:A:OP2	43:2l:34:ARG:NH1	2.15	0.80
13:1R:50:HIS:ND1	61:1R:301:HOH:O	2.14	0.80
54:1y:19:G:N2	54:1y:56:C:N3	2.29	0.79
50:2s:77:THR:HG23	50:2s:78:ARG:HG3	1.63	0.79
1:2A:994:C:OP1	16:2U:53:ARG:NH2	2.16	0.79
1:1A:250:G:OP2	30:18:13:ARG:NH2	2.15	0.78
11:1P:59:LEU:HD11	30:18:10:ALA:HB2	1.65	0.78
54:2w:54:5MU:O2	54:2w:58:A:N7	2.16	0.78
1:1A:272(J):C:H2'	1:1A:274:G:H8	1.48	0.78
32:1a:664:G:H22	32:1a:741:G:H1	1.30	0.78
54:2y:19:G:H1	54:2y:56:C:H42	1.32	0.78
1:1A:761:A:N7	61:1A:4293:HOH:O	2.16	0.78
33:1b:87:ARG:NH2	33:1b:220:ASP:OD1	2.15	0.78
1:1A:880:G:H2'	1:1A:881:G:H8	1.49	0.78
1:1A:1054:A:N6	1:1A:1105:U:H3	1.81	0.78
1:1A:2589:A:OP1	61:1A:4202:HOH:O	2.02	0.78
43:2l:57:LYS:HG2	43:2l:67:THR:HG22	1.65	0.78
15:1T:98:LYS:NZ	61:1T:301:HOH:O	2.15	0.78
32:2a:1030:C:N4	32:2a:1031:G:H1	1.81	0.78
1:1A:392:C:OP1	61:1A:4276:HOH:O	2.02	0.78
54:1w:4:U:H3	54:1w:69:A:H61	1.32	0.78
2:2B:22:U:H3	2:2B:61:G:H1	1.29	0.78
32:2a:64:G:H4'	32:2a:65:U:H3'	1.64	0.77
33:2b:88:ALA:HB2	33:2b:219:VAL:HG13	1.66	0.77
17:2V:72:VAL:HG13	17:2V:85:LYS:HB3	1.67	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:912:C:OP1	12:2Q:8:LYS:NZ	2.18	0.77
32:1a:975:A:H4'	32:1a:976:G:H5''	1.64	0.77
54:1y:2:G:O6	54:1y:71:C:N3	2.17	0.77
1:2A:2143:C:H42	1:2A:2148:G:H1	1.32	0.77
26:24:64:GLY:O	26:24:66:SER:N	2.17	0.77
57:1A:4098:DIO:OBJ	57:1A:4098:DIO:NAQ	2.17	0.77
54:1w:2:G:N1	54:1w:71:C:O2	2.16	0.77
9:2N:128:HIS:O	9:2N:131:GLN:NE2	2.18	0.77
1:2A:1434:A:H61	1:2A:1558:A:H62	1.32	0.76
32:1a:323:U:O3'	51:1t:22:ARG:NH1	2.18	0.76
32:2a:998:G:H1	32:2a:1043:C:H42	1.33	0.76
4:2E:47:VAL:HG11	4:2E:86:PRO:HD2	1.68	0.76
32:2a:1029:C:N3	32:2a:1032:G:N2	2.33	0.76
8:1I:92:VAL:HG13	8:1I:120:ILE:HB	1.67	0.76
32:1a:1027:C:C2	32:1a:1034:G:N2	2.53	0.76
32:2a:798:G:N7	61:2a:1929:HOH:O	2.18	0.76
15:2T:39:ARG:HH12	15:2T:41:ARG:HD3	1.49	0.76
54:2y:50:G:H1	54:2y:64:U:H3	1.32	0.76
1:1A:2312:U:H5'	6:1G:88:ILE:HD11	1.67	0.76
43:2l:32:PHE:HB3	43:2l:84:LEU:HD11	1.67	0.76
12:2Q:81:VAL:HB	22:20:7:LEU:HD21	1.68	0.76
1:2A:2171:A:N3	1:2A:2172:U:N3	2.33	0.76
33:1b:185:ILE:HG22	33:1b:199:TYR:HB2	1.68	0.75
32:2a:987:G:H1	32:2a:1218:C:H42	1.33	0.75
47:2p:13:HIS:O	47:2p:42:ARG:NH2	2.20	0.75
1:2A:2683:C:O2	10:2O:70:LYS:NZ	2.14	0.75
32:1a:1366:C:O2'	41:1j:60:ARG:NH1	2.18	0.75
54:2y:11:C:N3	54:2y:24:G:O6	2.19	0.75
23:21:51:VAL:HG11	23:21:74:VAL:HG21	1.67	0.75
34:1c:152:ILE:HB	34:1c:199:LYS:HB2	1.68	0.75
32:2a:999:C:N4	32:2a:1042:G:H1	1.85	0.75
41:2j:5:ARG:N	61:2j:301:HOH:O	2.18	0.75
1:2A:2287:A:H62	1:2A:2344:U:H3	1.35	0.75
33:2b:59:GLU:HG3	33:2b:221:LEU:HD21	1.68	0.75
1:2A:195:A:N7	61:2A:3908:HOH:O	2.20	0.74
1:2A:2355:C:H1'	22:20:39:ARG:HH21	1.52	0.74
1:2A:2404:C:O3'	11:2P:77:ARG:NH2	2.19	0.74
32:1a:405:U:O4	35:1d:2:GLY:N	2.20	0.74
1:2A:2345:G:H4'	1:2A:2346:A:H5''	1.69	0.74
40:2i:9:ARG:HG2	40:2i:14:VAL:HG12	1.66	0.74
40:2i:46:ALA:HB2	40:2i:74:ILE:HG23	1.68	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:2k:51:LYS:HA	42:2k:55:LYS:HE3	1.69	0.74
2:2B:66:A:H61	2:2B:109:C:H5''	1.52	0.74
33:2b:74:LYS:HD2	33:2b:166:ASP:HB2	1.68	0.74
1:1A:195:A:N7	61:1A:4303:HOH:O	2.19	0.74
1:1A:880:G:H2'	1:1A:881:G:C8	2.22	0.74
32:1a:142:G:H2'	32:1a:143:A:H8	1.52	0.74
32:1a:504:C:OP1	61:1a:1921:HOH:O	2.05	0.74
4:2E:36:ARG:NH1	4:2E:85:ASN:OD1	2.20	0.74
61:1A:4201:HOH:O	13:1R:3:HIS:NE2	2.21	0.74
54:1y:44:G:H3'	54:1y:45:G:H8	1.52	0.74
32:1a:1106:G:H5''	34:1c:172:ARG:HG2	1.70	0.74
40:2i:50:LEU:HD13	40:2i:56:LEU:HA	1.69	0.74
43:2l:117:ARG:HG2	43:2l:122:THR:HB	1.69	0.74
1:2A:1264:G:OP1	27:25:19:ARG:NH2	2.20	0.74
32:2a:139:G:H2'	32:2a:140:A:H8	1.53	0.73
54:2y:51:C:N3	54:2y:63:G:O6	2.21	0.73
1:1A:1798:U:H5'	3:1D:259:THR:HG22	1.71	0.73
54:1w:50:G:H1	54:1w:64:U:H3	1.34	0.73
32:2a:1187:G:H5'	40:2i:113:LYS:HE3	1.69	0.73
34:2c:150:LYS:HE3	34:2c:152:ILE:HD11	1.69	0.73
54:1w:18:G:N2	54:1w:58:A:OP2	2.21	0.73
32:1a:1008:C:N3	32:1a:1021:G:O6	2.21	0.73
8:2I:92:VAL:HG13	8:2I:120:ILE:HB	1.70	0.73
12:2Q:11:LYS:NZ	12:2Q:88:GLY:O	2.21	0.73
1:1A:2133:G:HO2'	1:1A:2157:G:H1	1.37	0.73
32:1a:1047:G:H5''	45:1n:4:LYS:HD3	1.70	0.73
1:2A:2805:G:H2'	1:2A:2807:G:C8	2.23	0.73
39:1h:112:LEU:HD22	39:1h:133:LEU:HA	1.70	0.73
31:29:25:VAL:HB	31:29:34:GLN:HB2	1.69	0.73
32:2a:1352:C:OP1	52:2u:3:LYS:NZ	2.20	0.73
22:10:27:GLU:HG3	22:10:68:GLU:HA	1.70	0.73
32:2a:953:G:H5'	32:2a:965:A:H61	1.53	0.73
41:2j:8:LEU:HB2	41:2j:70:ARG:HB2	1.69	0.73
1:2A:2154:G:N7	1:2A:2156:G:N2	2.36	0.72
32:2a:1002:G:H1	32:2a:1038:C:H42	0.78	0.72
33:2b:101:MET:HG2	33:2b:108:ILE:HG21	1.71	0.72
44:2m:31:LYS:HA	44:2m:34:LEU:HD12	1.71	0.72
10:2O:115:VAL:HG13	10:2O:121:VAL:HG21	1.71	0.72
33:1b:80:ILE:HG12	33:1b:215:LEU:HD23	1.68	0.72
40:2i:28:VAL:HG22	40:2i:63:ILE:HB	1.69	0.72
1:2A:614(A):U:H4'	1:2A:614(B):G:H5'	1.70	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2788:C:OP1	4:2E:61:ARG:NH2	2.23	0.72
7:1H:164:TYR:HB2	7:1H:167:GLU:HB2	1.71	0.72
34:1c:52:LEU:HD21	34:1c:55:VAL:HG23	1.70	0.72
5:1F:185:ASP:HA	5:1F:188:ARG:HD3	1.71	0.72
32:1a:953:G:H5'	32:1a:965:A:H61	1.53	0.72
1:1A:956:G:O6	61:1A:4277:HOH:O	2.06	0.72
1:1A:512:G:N7	61:1A:4206:HOH:O	2.22	0.71
1:1A:582:G:N7	61:1A:4313:HOH:O	2.22	0.71
54:1w:22:G:N7	54:1w:46:7MG:N2	2.35	0.71
1:2A:1693:U:O2'	3:2D:14:ARG:NH2	2.24	0.71
6:1G:77:ILE:HD12	6:1G:82:LEU:HD12	1.71	0.71
32:1a:116:A:OP1	61:1a:1922:HOH:O	2.08	0.71
10:2O:35:VAL:HG11	10:2O:103:ALA:HB3	1.72	0.71
11:2P:42:SER:O	61:2P:301:HOH:O	2.08	0.71
32:2a:922:G:H4'	36:2e:20:GLN:HA	1.73	0.71
1:1A:505:A:OP2	61:1A:4278:HOH:O	2.07	0.71
61:1A:4201:HOH:O	4:1E:110:GLY:O	2.08	0.71
1:2A:2206:G:H3'	1:2A:2207:G:C8	2.26	0.71
11:2P:95:VAL:HG13	11:2P:125:VAL:HA	1.73	0.71
17:1V:14:VAL:HB	17:1V:96:ILE:HG13	1.72	0.71
46:1o:74:ASP:HB3	46:1o:77:ARG:HB2	1.73	0.71
1:1A:1174:A:H4'	1:1A:1175:U:OP1	1.91	0.71
1:1A:1395:A:OP1	61:1A:4211:HOH:O	2.09	0.71
1:1A:2683:C:O2	10:1O:70:LYS:NZ	2.21	0.71
1:2A:2839:G:H5'	13:2R:46:GLY:HA2	1.73	0.71
43:1l:71:PRO:O	43:1l:102:ARG:NH1	2.24	0.71
6:1G:37:VAL:HG22	6:1G:159:VAL:HG12	1.73	0.71
1:1A:279:C:H42	1:1A:361:G:H1	1.39	0.70
54:2y:51:C:C2	54:2y:63:G:N1	2.58	0.70
1:2A:2365:G:N7	30:28:39:LYS:NZ	2.38	0.70
32:2a:997:U:H3	32:2a:1044:A:H61	0.76	0.70
54:2y:51:C:O2	54:2y:63:G:N1	2.24	0.70
22:10:23:VAL:HG22	22:10:38:VAL:HG22	1.71	0.70
3:2D:108:PRO:HB3	3:2D:143:HIS:HE1	1.56	0.70
32:2a:661:G:H1	32:2a:744:C:H42	1.39	0.70
1:1A:1468:C:OP1	61:1A:4281:HOH:O	2.09	0.70
52:1u:5:ASP:OD2	61:1u:101:HOH:O	2.09	0.70
32:2a:539:A:OP2	43:2l:115:LYS:NZ	2.24	0.70
11:2P:87:ASP:O	11:2P:90:ARG:NH1	2.23	0.70
32:2a:407:G:H5''	35:2d:115:ARG:HG2	1.73	0.70
1:2A:652(B):A:N6	1:2A:655:A:N3	2.39	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2297:C:O2	1:2A:2321:G:N2	2.16	0.70
33:1b:118:LEU:HB3	33:1b:142:LEU:HD12	1.72	0.70
35:1d:166:LYS:NZ	35:1d:179:GLU:OE2	2.22	0.70
48:2q:66:SER:O	48:2q:70:ARG:NH1	2.24	0.70
54:2w:51:C:N4	54:2w:63:G:H1	1.88	0.70
1:1A:2815:C:H5'	27:15:29:THR:HG21	1.72	0.70
32:2a:576:G:OP1	61:2a:1922:HOH:O	2.09	0.70
36:1e:78:HIS:HE1	36:1e:143:ARG:H	1.38	0.70
42:1k:48:ILE:HD12	42:1k:63:LEU:HB2	1.74	0.70
26:14:58:ARG:H	26:14:58:ARG:HD2	1.57	0.69
32:1a:200:G:H1	32:1a:217:C:H42	1.38	0.69
1:1A:578:A:OP2	61:1A:4279:HOH:O	2.09	0.69
1:1A:613:G:N2	1:1A:614(C):A:O2'	2.25	0.69
1:1A:2128:C:H42	1:1A:2160:G:H1	1.40	0.69
36:2e:20:GLN:NE2	36:2e:21:ALA:O	2.25	0.69
50:1s:27:GLU:HB2	50:1s:28:LYS:HD3	1.74	0.69
18:1W:57:ASN:HA	18:1W:61:ASN:HD22	1.56	0.69
32:1a:171:A:H2'	32:1a:172:A:C8	2.27	0.69
21:2Z:155:LEU:HB3	21:2Z:157:LEU:HG	1.73	0.69
22:20:11:ARG:O	22:20:14:ARG:NH2	2.25	0.69
32:2a:693:G:H21	54:2y:37:6MZ:H2	1.57	0.69
1:1A:588:U:OP2	61:1A:4280:HOH:O	2.09	0.69
1:1A:2839:G:H5'	13:1R:46:GLY:HA2	1.74	0.69
32:1a:1304:G:OP2	61:1a:1923:HOH:O	2.09	0.69
6:2G:15:VAL:HG22	6:2G:175:LEU:HB3	1.75	0.69
1:1A:2296:U:OP2	14:1S:9:ARG:NH2	2.24	0.69
1:1A:1041:C:H42	1:1A:1114:G:H1	1.39	0.69
1:1A:1170:G:N7	61:1A:4324:HOH:O	2.25	0.69
1:1A:1354:A:OP2	61:1A:4282:HOH:O	2.10	0.69
7:2H:124:GLU:HB2	7:2H:132:ARG:HB3	1.74	0.69
10:1O:35:VAL:HG11	10:1O:103:ALA:HB3	1.73	0.69
33:1b:84:GLU:OE1	33:1b:87:ARG:NH1	2.26	0.69
1:2A:2126:A:N6	1:2A:2162:G:O2'	2.26	0.69
33:1b:101:MET:HG2	33:1b:108:ILE:HG21	1.75	0.69
18:2W:57:ASN:HA	18:2W:61:ASN:HD22	1.57	0.69
25:23:12:PRO:HB2	25:23:20:LYS:HG2	1.74	0.69
32:2a:1089:G:N2	32:2a:1096:C:N3	2.36	0.69
1:2A:1816:G:O6	3:2D:35:LYS:NZ	2.21	0.68
32:1a:117:G:OP2	61:1a:1922:HOH:O	2.11	0.68
41:1j:40:LEU:HB2	41:1j:69:ASN:HB2	1.75	0.68
32:1a:1518:MA6:N6	32:1a:1519:MA6:H103	2.09	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1030:C:H42	32:2a:1031:G:H1	1.40	0.68
1:1A:1176:G:N2	1:1A:1178:C:OP2	2.26	0.68
1:2A:1798:U:H5'	3:2D:259:THR:HG22	1.74	0.68
38:1g:78:ARG:NH1	38:1g:154:TYR:O	2.25	0.68
6:2G:11:TYR:OH	6:2G:16:ARG:NH1	2.26	0.68
20:2Y:102:CYS:SG	20:2Y:103:GLY:N	2.63	0.68
26:14:61:ARG:HH21	50:1s:42:PRO:HD2	1.58	0.68
33:1b:82:ARG:NH1	33:1b:92:TYR:OH	2.27	0.68
26:24:16:CYS:SG	26:24:17:GLY:N	2.66	0.68
32:2a:547:A:OP1	61:2a:1923:HOH:O	2.12	0.68
54:2y:19:G:N2	54:2y:56:C:N3	2.39	0.68
1:1A:1381:G:N7	61:1A:4332:HOH:O	2.26	0.68
1:2A:854:G:H2'	1:2A:855:G:H8	1.58	0.68
35:1d:105:VAL:HG13	35:1d:110:PHE:HB2	1.75	0.68
42:2k:121:PRO:HG2	42:2k:126:ARG:HD2	1.76	0.68
32:2a:1274:G:N2	32:2a:1275:A:N7	2.41	0.68
46:2o:64:ARG:HH21	46:2o:68:ARG:HH21	1.41	0.68
1:1A:2125:G:N1	1:1A:2172:U:OP1	2.25	0.68
32:1a:812:C:N3	61:1a:1938:HOH:O	2.26	0.68
32:2a:1295:G:O2'	44:2m:14:ARG:NH1	2.26	0.68
35:2d:157:LEU:O	35:2d:161:ASN:ND2	2.26	0.68
46:2o:54:ARG:HG2	46:2o:58:MET:HE2	1.74	0.68
48:2q:5:VAL:HG22	48:2q:60:ILE:HG13	1.74	0.68
1:1A:2285:C:OP2	28:16:6:ARG:NH1	2.25	0.68
1:2A:730:C:OP2	61:2A:3902:HOH:O	2.12	0.68
11:2P:91:PHE:O	11:2P:121:LYS:NZ	2.25	0.68
1:2A:578:A:OP2	61:2A:3959:HOH:O	2.11	0.67
1:2A:2592:G:OP1	61:2A:3958:HOH:O	2.11	0.67
41:2j:30:SER:O	41:2j:81:THR:OG1	2.11	0.67
1:1A:882:G:H1	1:1A:894:C:H42	1.42	0.67
1:1A:2136:C:H42	1:1A:2155:G:H1	0.72	0.67
1:2A:1266:G:O5'	18:2W:15:ARG:NH2	2.27	0.67
32:2a:1226:C:O2'	44:2m:111:LYS:NZ	2.25	0.67
1:1A:1071:G:H1'	1:1A:1089:G:H2'	1.77	0.67
1:1A:1769:G:O2'	1:1A:1958:C:OP1	2.08	0.67
1:2A:2169:A:H2'	1:2A:2170:A:C8	2.28	0.67
32:2a:266:G:H5''	32:2a:268:C:H41	1.59	0.67
34:2c:11:ARG:HB3	34:2c:15:THR:HB	1.76	0.67
1:2A:907:U:O2'	12:2Q:101:ARG:NH2	2.23	0.67
32:2a:959:A:HO2'	32:2a:984:C:HO2'	1.37	0.67
51:2t:57:ARG:HH12	51:2t:100:ILE:HD12	1.59	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:272(J):C:H2'	1:1A:274:G:C8	2.29	0.67
1:1A:783:A:OP2	61:1A:4202:HOH:O	2.11	0.67
1:1A:2305:A:H5''	6:1G:134:GLY:HA3	1.75	0.67
1:1A:2430:A:OP1	61:1A:4283:HOH:O	2.12	0.67
1:1A:2736:G:N7	61:1A:4339:HOH:O	2.28	0.67
1:2A:2849:U:OP2	15:2T:95:ARG:NH1	2.28	0.67
17:1V:76:LYS:HB2	17:1V:81:TYR:HB3	1.77	0.67
32:1a:998:G:H1	32:1a:1043:C:H42	1.41	0.67
32:1a:1224:G:OP1	61:1a:1924:HOH:O	2.12	0.67
41:1j:38:ILE:HG12	41:1j:71:LEU:HB3	1.77	0.67
9:2N:67:LEU:HA	9:2N:87:LEU:HD22	1.77	0.67
12:2Q:30:GLY:HA2	12:2Q:107:ALA:HB2	1.77	0.67
1:1A:301:G:OP2	20:1Y:84:ARG:NH2	2.28	0.67
1:2A:2134:A:O2'	1:2A:2159:G:N2	2.28	0.67
25:13:8:LEU:HG	25:13:31:LEU:HD23	1.76	0.67
54:1y:18:G:H1	54:1y:55:PSU:H1'	1.59	0.67
32:2a:1286:A:C8	32:2a:1287:A:H4'	2.30	0.67
52:2u:17:THR:O	52:2u:22:ARG:NH1	2.28	0.67
1:2A:2110:G:H3'	1:2A:2111:C:H5'	1.76	0.67
54:1w:7:U:O2'	54:1w:49:G:OP2	2.12	0.67
54:1y:30:C:N3	54:1y:40:G:N2	2.41	0.67
12:2Q:85:LYS:HD3	22:20:7:LEU:HD13	1.76	0.67
36:2e:78:HIS:HE1	36:2e:143:ARG:H	1.43	0.67
1:2A:643:A:N1	1:2A:2369:A:O2'	2.27	0.67
1:2A:761:A:OP2	61:2A:3960:HOH:O	2.12	0.67
32:1a:1291:G:OP1	38:1g:37:ASN:ND2	2.28	0.67
39:1h:17:THR:O	39:1h:78:GLN:NE2	2.25	0.67
48:1q:53:LEU:HD23	48:1q:82:MET:HE1	1.75	0.67
1:1A:1818:U:H2'	3:1D:157:ARG:HD2	1.76	0.67
20:1Y:15:VAL:HG21	20:1Y:42:VAL:HG11	1.75	0.67
55:1x:8:4SU:O2	55:1x:21:A:C2	2.44	0.67
1:2A:2296:U:OP2	14:2S:9:ARG:NH2	2.29	0.66
47:1p:38:TYR:OH	47:1p:47:ASP:OD2	2.13	0.66
32:2a:1029:C:N4	32:2a:1032:G:N1	2.40	0.66
1:1A:1153:C:OP2	61:1A:4284:HOH:O	2.12	0.66
1:2A:2452:C:OP1	61:2A:3964:HOH:O	2.13	0.66
11:1P:42:SER:O	61:1P:301:HOH:O	2.14	0.66
12:2Q:11:LYS:HD3	12:2Q:87:LYS:HG2	1.77	0.66
1:2A:309:G:N3	1:2A:329:G:O2'	2.29	0.66
33:1b:80:ILE:HD13	33:1b:211:ILE:HG22	1.75	0.66
41:2j:62:HIS:HB3	45:2n:59:ALA:HB3	1.78	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1185:C:OP2	61:1A:4285:HOH:O	2.13	0.66
44:1m:12:ASN:O	44:1m:44:ARG:NH1	2.29	0.66
47:1p:13:HIS:O	47:1p:42:ARG:NH2	2.29	0.66
3:2D:108:PRO:HG2	3:2D:111:LEU:HB2	1.77	0.66
39:2h:87:SER:HB2	39:2h:93:VAL:H	1.59	0.66
1:2A:740:U:OP2	61:2A:3961:HOH:O	2.12	0.66
1:2A:1119:C:N4	61:2A:4002:HOH:O	2.23	0.66
1:2A:1778:U:OP1	61:2A:3962:HOH:O	2.12	0.66
32:1a:542:G:OP1	35:1d:10:ARG:NH2	2.29	0.66
32:2a:931:C:H42	32:2a:1386:G:H1	1.44	0.66
1:2A:2238:G:OP2	61:2A:3967:HOH:O	2.13	0.66
1:2A:2592:G:OP1	61:2A:3968:HOH:O	2.14	0.66
32:1a:1159:U:OP1	33:1b:133:LYS:NZ	2.29	0.66
21:2Z:141:VAL:HG13	21:2Z:142:SER:H	1.60	0.66
32:2a:741:G:H5'	46:2o:39:LEU:HD12	1.76	0.66
32:2a:1347:G:N2	32:2a:1373:G:H2'	2.10	0.66
33:2b:16:HIS:HB2	33:2b:204:ASN:HB3	1.75	0.66
1:1A:572:A:N7	61:1A:4350:HOH:O	2.29	0.66
1:2A:1603:A:OP1	61:2A:3965:HOH:O	2.13	0.66
1:2A:2723:C:OP2	4:2E:109:LYS:NZ	2.29	0.66
9:2N:123:TYR:OH	9:2N:130:HIS:NE2	2.24	0.66
1:1A:2124:G:H1	1:1A:2174:C:N4	1.94	0.66
1:2A:1242:A:N1	11:2P:2:LYS:NZ	2.43	0.66
1:2A:1828:G:OP2	61:2A:3966:HOH:O	2.13	0.66
32:1a:877:C:H5''	39:1h:88:LYS:HD3	1.78	0.66
5:2F:103:LYS:HA	5:2F:106:ARG:HG3	1.77	0.66
6:2G:47:LYS:HG3	6:2G:48:GLU:H	1.61	0.66
21:2Z:52:SER:OG	21:2Z:53:ILE:N	2.27	0.66
1:2A:2364:C:OP1	22:20:55:ARG:NH1	2.28	0.66
15:1T:16:ARG:NH1	15:1T:83:ILE:O	2.27	0.66
8:2I:92:VAL:HG11	8:2I:144:VAL:HG11	1.78	0.66
41:2j:49:VAL:HG23	45:2n:41:ARG:HB2	1.77	0.66
55:2x:8:4SU:O2	55:2x:21:A:H2	1.79	0.66
8:1I:27:ARG:HD3	23:11:71:TYR:CE2	2.32	0.65
32:1a:1350:A:N7	40:1i:118:LYS:NZ	2.44	0.65
54:2y:11:C:O2	54:2y:24:G:N1	2.29	0.65
1:1A:11:G:H2'	1:1A:12:U:H5''	1.79	0.65
1:1A:987:G:N7	61:1A:4351:HOH:O	2.29	0.65
1:2A:2166:G:H3'	1:2A:2167:U:H5''	1.78	0.65
32:1a:1031:G:H2'	32:1a:1032:G:C8	2.31	0.65
54:1w:51:C:N3	54:1w:63:G:N2	2.36	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:438:G:H4'	35:2d:123:HIS:HD1	1.61	0.65
32:2a:1142:G:H3'	32:2a:1143:G:H8	1.61	0.65
36:2e:79:GLU:O	39:2h:104:ARG:NH1	2.29	0.65
1:1A:933:A:OP1	25:13:24:LYS:NZ	2.29	0.65
1:1A:2163:C:OP1	1:1A:2165:G:N2	2.30	0.65
7:2H:101:ARG:HH12	7:2H:122:THR:HG23	1.61	0.65
13:2R:44:LEU:HD22	13:2R:48:VAL:HG23	1.78	0.65
32:2a:595:G:O2'	61:2a:1924:HOH:O	2.13	0.65
1:2A:2250:G:OP1	12:2Q:85:LYS:NZ	2.29	0.65
51:1t:57:ARG:HH12	51:1t:100:ILE:HD12	1.61	0.65
54:1w:53:G:H1	54:1w:61:C:N4	1.94	0.65
1:1A:2274:A:OP2	61:1A:4287:HOH:O	2.15	0.65
1:2A:2137:C:N3	1:2A:2154:G:N2	2.44	0.65
1:2A:2857:G:N2	1:2A:2860:A:OP2	2.28	0.65
41:1j:5:ARG:NE	41:1j:73:ASP:OD1	2.30	0.65
1:2A:1449:A:O2'	1:2A:1529:G:N2	2.30	0.65
11:1P:59:LEU:HD21	30:18:10:ALA:HA	1.79	0.65
48:1q:9:VAL:HG12	48:1q:56:VAL:HG22	1.78	0.65
11:2P:50:ARG:HH21	30:28:7:HIS:HD2	1.44	0.65
32:2a:1105:A:H2'	32:2a:1106:G:H8	1.61	0.65
50:2s:30:LEU:HD11	50:2s:50:ALA:HB2	1.77	0.65
1:1A:2000:G:OP1	13:1R:5:LYS:NZ	2.29	0.65
32:1a:1314:C:OP2	50:1s:4:SER:OG	2.10	0.65
32:2a:987:G:H1	32:2a:1218:C:N4	1.94	0.65
32:2a:1368:G:OP1	40:2i:111:ARG:NH2	2.29	0.65
55:2x:40:C:H2'	55:2x:41:C:H6	1.61	0.65
1:1A:2079:U:O3'	23:11:35:THR:OG1	2.13	0.65
1:2A:1022:G:H22	1:2A:1142(A):A:H2	1.45	0.65
4:2E:77:ILE:HD12	4:2E:195:LEU:HD22	1.78	0.65
17:2V:43:GLU:OE1	17:2V:43:GLU:N	2.30	0.65
21:2Z:138:GLU:HB2	21:2Z:156:LYS:HD3	1.78	0.65
32:2a:882:C:OP2	43:2l:13:LYS:NZ	2.29	0.65
1:1A:1235:G:OP1	61:1A:4278:HOH:O	2.13	0.65
1:2A:296:C:O3'	20:2Y:95:LYS:NZ	2.30	0.65
24:12:22:GLU:OE2	24:12:68:ARG:NH2	2.29	0.65
1:1A:2183:C:H2'	1:1A:2184:G:H8	1.62	0.65
1:2A:2584:U:O4	61:2A:3963:HOH:O	2.13	0.65
32:2a:48:C:OP2	61:2a:1925:HOH:O	2.15	0.65
54:2w:53:G:N2	54:2w:61:C:N3	2.39	0.65
32:1a:972:C:O2'	41:1j:55:LYS:O	2.15	0.64
50:1s:27:GLU:HB2	50:1s:28:LYS:HA	1.79	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2F:33:LEU:HD11	5:2F:112:MET:HB2	1.79	0.64
21:2Z:102:LEU:HD21	21:2Z:171:ILE:HD11	1.79	0.64
1:2A:792:G:OP2	61:2A:3970:HOH:O	2.15	0.64
1:2A:852:G:H2'	1:2A:853:G:H8	1.62	0.64
8:1I:72:LEU:HD21	8:1I:107:VAL:HG11	1.79	0.64
32:1a:505:G:N7	61:1a:1949:HOH:O	2.30	0.64
1:2A:1147:C:H2'	1:2A:1148:A:H8	1.62	0.64
1:2A:2129:C:N3	1:2A:2159:G:N2	2.39	0.64
1:2A:2206:G:OP1	3:2D:68:LYS:NZ	2.29	0.64
32:1a:1027:C:N3	32:1a:1034:G:N2	2.45	0.64
18:2W:78:GLU:OE2	18:2W:99:ARG:NH1	2.26	0.64
1:2A:521:G:H2'	1:2A:522:G:H8	1.62	0.64
7:1H:86:GLU:OE2	7:1H:132:ARG:NH2	2.30	0.64
54:2y:69:A:H3'	54:2y:70:C:H5''	1.77	0.64
32:1a:1027:C:C4	32:1a:1034:G:C2	2.86	0.64
2:2B:41:U:H5	6:2G:70:VAL:H	1.45	0.64
36:2e:77:PRO:HD2	36:2e:142:LEU:HD13	1.80	0.64
36:1e:20:GLN:NE2	36:1e:21:ALA:O	2.30	0.64
1:2A:1796:U:H2'	1:2A:1797:C:C6	2.33	0.64
32:1a:683:G:H21	42:1k:38:ASN:HD22	1.46	0.64
25:23:6:VAL:HG13	25:23:54:VAL:HG11	1.80	0.64
41:2j:47:PHE:N	41:2j:63:PHE:O	2.27	0.64
55:1x:61:C:H2'	55:1x:62:C:H6	1.62	0.64
40:2i:8:GLY:HA2	40:2i:79:LEU:HD23	1.80	0.64
1:1A:1007:C:OP2	61:1A:4288:HOH:O	2.15	0.64
1:1A:2243:U:OP1	61:1A:4286:HOH:O	2.14	0.64
1:2A:1452:A:OP2	61:2A:3972:HOH:O	2.15	0.64
26:24:24:THR:OG1	26:24:25:TYR:N	2.31	0.64
33:2b:8:LYS:HB2	33:2b:48:MET:HE3	1.78	0.64
33:2b:166:ASP:HB3	33:2b:169:LYS:HB3	1.80	0.64
32:1a:171:A:H2'	32:1a:172:A:H8	1.63	0.63
41:1j:50:ILE:HA	41:1j:60:ARG:HG2	1.80	0.63
45:1n:4:LYS:HA	45:1n:7:ILE:HG22	1.80	0.63
54:1y:44:G:H3'	54:1y:45:G:C8	2.32	0.63
1:1A:1009:A:OP2	9:1N:37:LYS:NZ	2.31	0.63
1:1A:2105:C:H2'	1:1A:2106:G:C8	2.33	0.63
21:1Z:126:VAL:HG13	21:1Z:161:VAL:HG23	1.79	0.63
32:1a:1129:C:O2'	32:1a:1139:G:N7	2.31	0.63
16:2U:29:SER:OG	16:2U:30:LYS:NZ	2.32	0.63
25:23:35:ARG:HE	25:23:37:LEU:HD21	1.62	0.63
1:1A:428:A:OP1	61:1A:4289:HOH:O	2.15	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:302:C:OP2	20:2Y:73:ARG:NH1	2.31	0.63
1:2A:1636:C:OP2	61:2A:3971:HOH:O	2.15	0.63
32:1a:619:U:N3	35:1d:134:ASP:OD1	2.28	0.63
36:1e:110:LEU:HD13	36:1e:118:ILE:HG21	1.79	0.63
41:1j:61:GLU:OE2	45:1n:58:LYS:NZ	2.28	0.63
32:2a:1010:G:N2	32:2a:1020:U:O2'	2.31	0.63
1:2A:1021:A:H62	1:2A:1141:U:H3	1.46	0.63
1:2A:1530:C:O2'	1:2A:1531:C:O5'	2.13	0.63
1:2A:2133:G:O2'	1:2A:2157:G:N2	2.31	0.63
32:1a:1027:C:N4	32:1a:1034:G:N1	2.46	0.63
54:1y:19:G:N1	54:1y:56:C:N4	2.45	0.63
2:1B:106:G:H5'	21:1Z:31:ARG:HG2	1.80	0.63
26:14:16:CYS:SG	26:14:17:GLY:N	2.71	0.63
32:1a:1036:G:H5''	32:1a:1037:C:C5	2.32	0.63
32:1a:1136:U:H5''	32:1a:1137:C:C2	2.33	0.63
54:1y:58:A:O2'	54:1y:59:U:OP1	2.12	0.63
11:2P:50:ARG:HD3	30:28:7:HIS:CD2	2.34	0.63
8:2I:3:VAL:HG12	8:2I:38:LEU:HA	1.80	0.63
19:2X:57:LEU:HD11	19:2X:78:LYS:HE2	1.79	0.63
32:2a:1376:U:H2'	32:2a:1377:A:C8	2.33	0.63
54:2w:76:A:OP1	61:2w:201:HOH:O	2.16	0.63
2:2B:75:G:H22	21:2Z:73:GLN:NE2	1.97	0.63
4:2E:28:ALA:HB3	4:2E:93:VAL:HG12	1.78	0.63
1:1A:1105:U:H2'	1:1A:1106:G:H8	1.63	0.63
1:1A:1173:G:O2'	1:1A:1174:A:O4'	2.16	0.63
1:2A:517:C:OP1	27:25:16:ARG:NH2	2.30	0.63
4:1E:48:GLN:HE21	4:1E:78:LEU:HD22	1.63	0.63
32:1a:1435:G:H2'	32:1a:1436:U:C6	2.34	0.63
6:2G:105:LYS:NZ	26:24:25:TYR:O	2.31	0.63
46:2o:11:VAL:HG21	46:2o:34:LEU:HD22	1.81	0.63
1:1A:2131:G:H5''	1:1A:2132:U:H3'	1.81	0.62
1:1A:2404:C:O3'	11:1P:77:ARG:NH2	2.28	0.62
1:2A:2131:G:H1	1:2A:2158:A:N6	1.96	0.62
10:1O:97:ARG:NH1	32:1a:339:C:OP2	2.32	0.62
32:1a:21:G:OP1	61:1a:1925:HOH:O	2.16	0.62
5:2F:53:THR:HG23	5:2F:55:GLY:H	1.64	0.62
32:2a:1348:U:H4'	40:2i:120:ARG:HD2	1.81	0.62
40:2i:16:ARG:HB2	40:2i:64:THR:HG22	1.81	0.62
33:1b:16:HIS:HB3	33:1b:210:SER:HB2	1.81	0.62
40:1i:46:ALA:HB2	40:1i:74:ILE:HG23	1.80	0.62
32:2a:972:C:O2'	41:2j:55:LYS:O	2.17	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1002:G:C2	32:2a:1003:G:H1'	2.33	0.62
32:2a:1295:G:O2'	32:2a:1302:U:O4	2.14	0.62
1:1A:583:G:OP2	16:1U:10:ARG:NH1	2.33	0.62
32:1a:1033:G:H2'	32:1a:1034:G:H8	1.65	0.62
10:2O:2:ILE:HD12	10:2O:6:THR:HG21	1.82	0.62
35:2d:170:VAL:HG21	35:2d:176:LEU:HD23	1.79	0.62
1:2A:307:G:N1	1:2A:310:A:OP2	2.31	0.62
1:2A:2572:A:N7	4:2E:145:LYS:HB2	2.14	0.62
14:1S:61:ASN:HB3	14:1S:64:GLU:HB2	1.81	0.62
1:2A:566:U:H5''	11:2P:29:LYS:HE3	1.82	0.62
32:1a:1402:4OC:HM22	32:1a:1403:C:H5'	1.81	0.62
7:2H:113:VAL:HG11	7:2H:151:ILE:HG21	1.80	0.62
21:2Z:146:ILE:HG12	21:2Z:174:VAL:HG13	1.81	0.62
47:2p:8:ARG:HH21	47:2p:15:PRO:HG3	1.65	0.62
49:2r:56:THR:OG1	49:2r:63:GLN:NE2	2.32	0.62
54:2y:30:C:H42	54:2y:40:G:H1	0.76	0.62
17:1V:40:LEU:HB2	17:1V:46:VAL:HG13	1.82	0.62
32:1a:17:U:H2'	32:1a:18:C:C6	2.35	0.62
32:1a:653:A:OP1	39:1h:56:LYS:NZ	2.29	0.62
22:20:40:GLN:HE21	22:20:57:PHE:HB3	1.64	0.62
32:2a:542:G:OP1	35:2d:10:ARG:NH2	2.30	0.62
32:2a:1030(A):G:N2	32:2a:1030(D):A:OP2	2.30	0.62
34:2c:36:ASP:HA	34:2c:39:ILE:HD12	1.81	0.62
1:1A:253:C:OP2	30:18:5:LYS:NZ	2.21	0.62
1:2A:1170:G:O6	1:2A:1180:C:N4	2.32	0.62
1:2A:2074:U:H2'	1:2A:2075:U:C6	2.34	0.62
27:15:16:ARG:NH1	27:15:17:ASP:OD1	2.32	0.62
42:2k:22:HIS:HB3	42:2k:29:ILE:HB	1.82	0.62
1:1A:1094:U:N3	1:1A:1097:U:OP2	2.33	0.62
50:1s:50:ALA:HB1	50:1s:57:HIS:HB3	1.80	0.62
3:2D:125:ILE:HB	37:2f:81:ILE:HD11	1.81	0.62
1:1A:278:A:H2'	1:1A:279:C:C6	2.35	0.62
1:1A:1693:U:O2'	3:1D:14:ARG:NH2	2.32	0.62
1:1A:2100:G:H1	1:1A:2189:U:H3	1.48	0.62
1:1A:2646:C:OP2	1:1A:2732:G:O2'	2.15	0.62
1:2A:728:G:H5''	3:2D:13:ARG:NH2	2.15	0.62
32:1a:1030:C:N4	32:1a:1031:G:H1	1.92	0.62
32:1a:1348:U:H4'	40:1i:120:ARG:HD2	1.82	0.62
34:1c:6:HIS:HD2	34:1c:8:ILE:H	1.48	0.62
47:1p:14:ASN:HA	47:1p:42:ARG:NH2	2.14	0.62
1:2A:2711:A:N3	61:2A:4026:HOH:O	2.31	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:1i:50:LEU:HA	40:1i:53:VAL:HG22	1.81	0.61
42:1k:27:ASN:OD1	42:1k:28:THR:N	2.33	0.61
1:2A:1939:5MU:OP1	1:2A:2604:U:O2'	2.16	0.61
33:1b:27:LYS:HG3	33:1b:194:PRO:HD2	1.81	0.61
35:1d:61:LYS:NZ	35:1d:72:GLU:OE1	2.32	0.61
32:2a:1007:C:N3	32:2a:1022:G:O6	2.34	0.61
1:1A:1071:G:H2'	1:1A:1072:C:C6	2.35	0.61
1:1A:1986:A:OP1	61:1A:4292:HOH:O	2.16	0.61
1:1A:2140:C:H42	1:1A:2150:U:H3	1.46	0.61
32:2a:1262:C:H42	32:2a:1273:G:H1	1.47	0.61
1:1A:323:G:C8	5:1F:171:PRO:HG3	2.35	0.61
1:2A:1579:A:H2'	1:2A:1580:A:C8	2.35	0.61
32:1a:1305:G:N2	32:1a:1331:G:H1'	2.16	0.61
40:1i:16:ARG:HH11	40:1i:64:THR:HG21	1.64	0.61
51:1t:10:LEU:HB3	51:1t:12:ALA:H	1.65	0.61
54:1w:62:C:H2'	54:1w:63:G:C8	2.35	0.61
3:2D:108:PRO:HB3	3:2D:143:HIS:CE1	2.36	0.61
13:2R:97:VAL:HG22	13:2R:114:VAL:HG22	1.82	0.61
35:2d:64:LEU:HB2	35:2d:198:VAL:HG11	1.81	0.61
36:2e:33:VAL:HG21	36:2e:109:ILE:HA	1.82	0.61
1:2A:2424:C:O2	1:2A:2429:G:O2'	2.16	0.61
12:1Q:85:LYS:HG2	22:10:7:LEU:HB3	1.83	0.61
24:12:1:MET:N	24:12:52:ASP:OD1	2.33	0.61
32:1a:165:C:H2'	32:1a:166:G:H8	1.65	0.61
32:1a:193:C:H2'	32:1a:194:C:H6	1.65	0.61
32:1a:1129:C:O2	32:1a:1130:A:N6	2.31	0.61
54:1w:4:U:H3	54:1w:69:A:N6	1.98	0.61
19:2X:43:VAL:HG21	19:2X:81:VAL:HG11	1.82	0.61
1:1A:1266:G:O5'	18:1W:15:ARG:NH2	2.34	0.61
1:1A:2162:G:H4'	1:1A:2172:U:H2'	1.82	0.61
1:2A:1019:U:H3	1:2A:1142(A):A:H62	1.48	0.61
11:1P:50:ARG:HD3	30:18:7:HIS:HD2	1.64	0.61
32:1a:45:U:H2'	32:1a:46:G:C8	2.36	0.61
32:1a:67:C:H2'	32:1a:68:G:C8	2.35	0.61
32:1a:142:G:H2'	32:1a:143:A:C8	2.36	0.61
32:2a:966:M2G:HM22	55:2x:34:C:H5'	1.83	0.61
34:2c:54:ARG:HB3	34:2c:69:HIS:HB2	1.82	0.61
34:2c:57:ILE:HD13	34:2c:66:VAL:HA	1.82	0.61
1:1A:672:C:OP1	61:1A:4291:HOH:O	2.16	0.61
16:2U:73:GLY:O	61:2U:301:HOH:O	2.16	0.61
32:2a:448:A:OP2	32:2a:485:G:N2	2.20	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:2i:49:PRO:HD2	40:2i:81:ILE:HD11	1.83	0.61
1:1A:2448:A:OP1	61:1A:4218:HOH:O	2.16	0.61
1:2A:1153:C:OP1	16:2U:92:ARG:NH2	2.30	0.61
33:1b:126:GLU:HG2	33:1b:127:ILE:HG12	1.81	0.61
33:1b:201:ILE:HG21	33:1b:214:ILE:HG21	1.82	0.61
32:2a:771:G:N7	61:2a:1952:HOH:O	2.31	0.61
32:2a:911:U:OP2	43:2l:97:ARG:NH2	2.32	0.61
5:1F:140:LEU:HD11	5:1F:170:LEU:HD11	1.83	0.61
32:1a:159:G:N2	32:1a:162:A:OP2	2.34	0.61
14:2S:14:VAL:O	14:2S:18:ILE:HG12	2.01	0.61
54:2y:11:C:N3	54:2y:24:G:C6	2.69	0.61
54:2y:40:G:H2'	54:2y:41:A:C8	2.35	0.61
1:2A:468:G:N7	29:27:39:ARG:NH2	2.45	0.61
1:2A:882:G:H1	1:2A:894:C:N4	1.89	0.61
32:1a:1027:C:N4	32:1a:1034:G:C6	2.69	0.61
32:1a:1458:G:H5''	51:1t:31:SER:HB2	1.83	0.61
47:1p:14:ASN:HA	47:1p:42:ARG:HH21	1.66	0.61
32:2a:859:A:OP2	32:2a:869:G:N2	2.34	0.61
32:2a:975:A:N1	41:2j:48:THR:HB	2.16	0.61
1:2A:752:A:H3'	29:27:1:MET:HE1	1.82	0.60
1:2A:1991:U:H2'	1:2A:1992:G:H5''	1.82	0.60
11:1P:98:GLU:OE2	11:1P:102:ARG:NH1	2.34	0.60
23:11:51:VAL:HG11	23:11:74:VAL:HG21	1.82	0.60
37:1f:48:LEU:HD22	49:1r:77:GLY:HA3	1.83	0.60
32:2a:1106:G:H5''	34:2c:172:ARG:HG2	1.82	0.60
38:2g:105:VAL:O	38:2g:109:ASN:ND2	2.34	0.60
54:2w:9:A:O2'	54:2w:10:G:N7	2.34	0.60
1:1A:2789:C:O2'	1:1A:2790:A:O4'	2.19	0.60
1:2A:2232:U:P	23:21:40:ARG:HH12	2.24	0.60
19:1X:41:ASN:O	19:1X:45:THR:HG23	2.01	0.60
32:1a:826:C:H4'	39:1h:12:ARG:HG3	1.82	0.60
54:1y:52:G:H1	54:1y:62:C:H42	1.48	0.60
38:2g:74:GLU:HG2	38:2g:91:VAL:HG22	1.82	0.60
32:1a:376:G:O3'	47:1p:5:ARG:NH1	2.32	0.60
32:2a:67:C:H2'	32:2a:68:G:C8	2.36	0.60
32:2a:1204:A:OP1	45:2n:3:ARG:NH2	2.33	0.60
1:2A:72:U:OP1	61:2A:3975:HOH:O	2.16	0.60
1:2A:1028:A:N6	1:2A:1125:G:H2'	2.15	0.60
32:1a:1068:G:H8	32:1a:1068:G:OP2	1.85	0.60
32:2a:1062:U:H2'	32:2a:1063:C:C6	2.36	0.60
40:2i:8:GLY:O	40:2i:15:ALA:N	2.34	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:576:U:H2'	1:1A:577:G:C8	2.35	0.60
1:2A:1786:A:H1'	1:2A:1938:A:N6	2.16	0.60
30:18:6:THR:HG22	30:18:63:PRO:HD2	1.83	0.60
33:1b:88:ALA:HB2	33:1b:219:VAL:HG13	1.83	0.60
2:2B:42:C:O2'	6:2G:67:LYS:O	2.14	0.60
32:1a:627:G:H2'	32:1a:628:G:H8	1.66	0.60
13:2R:67:LEU:HD13	13:2R:76:VAL:HG21	1.83	0.60
20:2Y:77:PRO:HD2	20:2Y:106:LEU:HD23	1.82	0.60
37:2f:46:ARG:HH22	49:2r:37:VAL:HG11	1.67	0.60
50:2s:19:VAL:O	50:2s:23:ASN:ND2	2.35	0.60
1:1A:249:C:O2	30:18:12:LYS:NZ	2.27	0.60
1:1A:2432:A:C4	23:11:33:LYS:HG2	2.37	0.60
1:2A:2143:C:N4	1:2A:2148:G:H1	1.99	0.60
14:1S:11:LYS:HG3	14:1S:91:PRO:HD3	1.82	0.60
31:19:8:LYS:H	31:19:34:GLN:HE22	1.49	0.60
4:2E:167:VAL:HG22	4:2E:170:LEU:HD11	1.84	0.60
9:2N:97:ARG:HA	9:2N:100:GLU:HB2	1.83	0.60
32:2a:1348:U:OP2	61:2a:1926:HOH:O	2.16	0.60
1:1A:607:U:OP1	5:1F:102:PRO:HA	2.01	0.60
1:1A:729:G:C6	3:1D:208:LYS:HB2	2.37	0.60
1:1A:2484:G:H1'	12:1Q:124:LYS:HG3	1.83	0.60
1:1A:2863:C:OP1	15:1T:93:ARG:NH1	2.34	0.60
1:2A:621:A:OP2	11:2P:108:LYS:NZ	2.35	0.60
1:2A:2140:C:H2'	1:2A:2141:G:H5''	1.82	0.60
5:1F:103:LYS:HA	5:1F:106:ARG:HG3	1.84	0.60
32:1a:1008:C:O2	32:1a:1021:G:N1	2.32	0.60
3:2D:148:GLU:HB2	3:2D:151:LYS:HD2	1.83	0.60
5:2F:124:LEU:HB3	5:2F:193:VAL:HG22	1.84	0.60
14:2S:27:SER:HA	14:2S:88:ASP:HB3	1.83	0.60
32:2a:67:C:H2'	32:2a:68:G:H8	1.66	0.60
54:2w:54:5MU:C2	54:2w:58:A:N7	2.69	0.60
1:1A:588:U:H2'	1:1A:589:C:C6	2.36	0.60
1:2A:184:C:H2'	1:2A:185:U:C6	2.37	0.60
1:2A:479:A:N3	1:2A:481:G:H5''	2.16	0.60
33:2b:12:GLU:O	33:2b:15:VAL:HG22	2.01	0.60
38:2g:69:VAL:HG22	38:2g:135:VAL:HG22	1.83	0.60
45:2n:23:ARG:HD2	45:2n:28:GLY:O	2.02	0.60
1:1A:2849:U:O2'	61:1A:4290:HOH:O	2.16	0.60
1:2A:2079:U:O3'	23:21:35:THR:OG1	2.19	0.60
1:2A:2499:C:OP2	61:2A:3974:HOH:O	2.16	0.60
11:1P:98:GLU:O	11:1P:101:VAL:HG12	2.01	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:1b:158:LEU:HD21	33:1b:180:LEU:HD13	1.84	0.60
54:1y:2:G:N1	54:1y:71:C:O2	2.23	0.60
5:2F:110:LEU:HD21	5:2F:181:LEU:HD23	1.84	0.60
1:2A:300:A:OP1	20:2Y:86:ARG:NH2	2.35	0.59
30:18:33:ASN:HA	30:18:36:LYS:HD2	1.83	0.59
32:1a:343:U:O2'	32:1a:346:G:O6	2.18	0.59
32:1a:976:G:H5'	32:1a:1358:U:O2'	2.01	0.59
35:1d:187:ARG:NH2	35:1d:193:ASP:OD2	2.34	0.59
41:1j:78:ASN:O	41:1j:80:LYS:N	2.35	0.59
32:2a:107:G:N7	51:2t:15:ARG:NH2	2.50	0.59
33:2b:119:GLU:HG3	33:2b:153:ARG:HH22	1.68	0.59
1:1A:1518:U:H2'	1:1A:1519:G:O4'	2.02	0.59
1:1A:2164:C:H2'	1:1A:2165:G:H5'	1.82	0.59
25:13:6:VAL:HG13	25:13:54:VAL:HG11	1.84	0.59
32:1a:1228:C:OP1	44:1m:115:LYS:NZ	2.33	0.59
32:2a:189(K):U:H2'	32:2a:189(L):G:C8	2.37	0.59
46:2o:16:ALA:HB1	46:2o:21:ASP:HB3	1.84	0.59
54:2w:43:G:H2'	54:2w:44:G:C8	2.38	0.59
1:1A:751:A:H5'	18:1W:90:ARG:HA	1.84	0.59
1:2A:859:G:N2	1:2A:917:A:OP2	2.28	0.59
32:1a:165:C:H2'	32:1a:166:G:C8	2.37	0.59
32:1a:1356:G:H2'	32:1a:1357:A:C8	2.35	0.59
32:2a:664:G:H22	32:2a:741:G:H1	1.49	0.59
32:2a:1256:A:H61	32:2a:1278:U:H2'	1.68	0.59
8:1I:109:ILE:HG13	8:1I:130:TYR:CZ	2.37	0.59
32:1a:584:G:H5'	48:1q:91:ARG:HH22	1.68	0.59
37:1f:1:MET:HE2	37:1f:68:PRO:HD3	1.85	0.59
5:2F:110:LEU:HD11	5:2F:181:LEU:HG	1.85	0.59
28:26:10:LEU:HG	28:26:54:ILE:HG13	1.85	0.59
38:2g:150:ALA:HA	42:2k:59:TYR:HB3	1.84	0.59
1:1A:881:G:C2	1:1A:882:G:H1'	2.37	0.59
1:2A:568:U:H5'	1:2A:945:A:N1	2.18	0.59
14:1S:68:GLN:HG3	14:1S:71:ARG:HH21	1.66	0.59
35:1d:119:GLN:HG3	35:1d:123:HIS:CD2	2.37	0.59
32:2a:34:C:H2'	32:2a:35:G:H8	1.67	0.59
54:2w:5:G:H2'	54:2w:6:A:H8	1.67	0.59
1:1A:881:G:N2	1:1A:897:C:N3	2.50	0.59
1:2A:220:G:O2'	1:2A:233:A:N3	2.29	0.59
5:1F:167:ALA:HB1	5:1F:173:VAL:HG11	1.84	0.59
32:1a:356:A:N3	32:1a:368:U:O2'	2.35	0.59
32:1a:742:G:OP2	46:1o:35:ARG:NH2	2.31	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:1s:63:THR:OG1	50:1s:65:ASN:OD1	2.18	0.59
28:26:9:LEU:HD13	28:26:51:GLU:HB2	1.84	0.59
32:2a:35:G:O2'	43:2l:118:SER:O	2.19	0.59
32:2a:1279:A:O2'	32:2a:1281:U:OP2	2.16	0.59
1:1A:606:U:H4'	1:1A:658:C:H4'	1.84	0.59
1:2A:784:A:H5'	1:2A:785:G:OP1	2.03	0.59
1:2A:1772:G:OP1	61:2A:3978:HOH:O	2.17	0.59
1:2A:2126:A:N3	1:2A:2127:G:H1'	2.18	0.59
7:1H:113:VAL:HG11	7:1H:151:ILE:HD13	1.83	0.59
21:1Z:45:ASP:CG	21:1Z:49:ARG:HE	2.10	0.59
32:1a:945:G:OP1	61:1a:1926:HOH:O	2.17	0.59
32:1a:1001:A:H2'	32:1a:1001(A):G:C8	2.38	0.59
32:1a:1030:C:H3'	32:1a:1030(A):G:H5''	1.85	0.59
34:2c:36:ASP:O	34:2c:40:ARG:HG2	2.02	0.59
1:1A:530:G:N1	1:1A:2023:G:OP1	2.33	0.59
1:1A:1007:C:OP1	9:1N:37:LYS:NZ	2.36	0.59
1:1A:2140:C:N3	1:1A:2151:G:O6	2.36	0.59
1:2A:600:G:O6	61:2A:3976:HOH:O	2.16	0.59
1:2A:974:G:OP1	1:2A:1187:G:O2'	2.17	0.59
1:2A:2163:C:C5	1:2A:2164:C:H1'	2.38	0.59
18:2W:10:VAL:HG12	18:2W:12:ILE:HG22	1.85	0.59
32:2a:1301:U:O2'	32:2a:1302:U:H5'	2.02	0.59
1:1A:2291:U:H2'	1:1A:2292:C:C6	2.38	0.59
1:1A:2422:A:O4'	54:1y:76:A:N6	2.36	0.59
1:2A:2022:U:O2'	1:2A:2617:C:H5'	2.03	0.59
1:2A:2196:C:OP2	61:2A:3977:HOH:O	2.17	0.59
26:14:58:ARG:HD2	26:14:58:ARG:N	2.17	0.59
51:1t:43:LEU:O	51:1t:47:GLY:N	2.25	0.59
4:2E:48:GLN:HE21	4:2E:78:LEU:HD22	1.68	0.59
1:1A:1268:A:OP1	61:1A:4294:HOH:O	2.17	0.59
1:2A:1015:G:H2'	1:2A:1016:G:H8	1.67	0.59
1:2A:2318:G:N2	14:2S:3:ARG:HE	2.01	0.59
28:26:23:THR:OG1	28:26:24:GLU:N	2.36	0.59
34:2c:156:ARG:H	34:2c:196:LEU:HD22	1.68	0.59
50:2s:32:LYS:HA	50:2s:50:ALA:HB3	1.84	0.59
1:1A:792:G:OP2	61:1A:4296:HOH:O	2.17	0.58
1:2A:2430:A:OP2	61:2A:3979:HOH:O	2.17	0.58
12:1Q:35:VAL:HG13	12:1Q:130:LYS:HB3	1.85	0.58
17:1V:55:ALA:HA	17:1V:101:GLY:HA2	1.84	0.58
33:2b:24:TRP:CD1	33:2b:24:TRP:H	2.20	0.58
51:2t:9:ASN:O	51:2t:10:LEU:HB2	2.02	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:212:G:H2'	1:2A:213:A:O4'	2.03	0.58
32:2a:920:U:H2'	32:2a:921:U:C6	2.38	0.58
32:2a:1004:A:H5''	32:2a:1024:G:H22	1.68	0.58
32:2a:1305:G:N2	32:2a:1331:G:H1'	2.17	0.58
45:2n:48:ALA:HB2	45:2n:53:LEU:HD12	1.85	0.58
1:2A:2317:C:N4	1:2A:2318:G:O6	2.36	0.58
18:1W:11:ARG:HH11	18:1W:11:ARG:C	2.11	0.58
32:1a:130:A:O2'	32:1a:131:C:O5'	2.19	0.58
32:2a:828:A:N6	32:2a:858:G:O2'	2.35	0.58
32:2a:1507:A:OP2	53:2v:13:A:N6	2.32	0.58
54:2y:7:U:O2'	54:2y:49:G:OP2	2.21	0.58
1:1A:226:G:H21	1:1A:228:A:H62	1.49	0.58
1:1A:1647:G:OP1	61:1A:4295:HOH:O	2.17	0.58
1:1A:1762:A:H2'	61:1A:5830:HOH:O	2.03	0.58
1:2A:2121:G:H1	1:2A:2177:C:H42	1.49	0.58
16:1U:81:HIS:CE1	16:1U:85:LYS:HD2	2.37	0.58
32:1a:405:U:OP2	35:1d:3:ARG:NH1	2.34	0.58
32:2a:1151:A:O2'	32:2a:1152:A:O5'	2.19	0.58
32:2a:1259:C:O2'	32:2a:1283:G:N3	2.36	0.58
1:2A:2010:G:H5''	18:2W:42:ARG:HB2	1.84	0.58
9:1N:73:THR:HG23	9:1N:82:LEU:HD11	1.84	0.58
32:1a:258:G:H2'	32:1a:259:G:H8	1.69	0.58
32:1a:1016:A:H2'	32:1a:1017:G:O4'	2.03	0.58
32:1a:1366:C:HO2'	41:1j:60:ARG:HH12	1.49	0.58
32:2a:542:G:P	35:2d:10:ARG:HH22	2.25	0.58
48:2q:9:VAL:HG11	48:2q:84:LEU:HD12	1.86	0.58
1:2A:910:A:N1	1:2A:2277:G:H1'	2.18	0.58
1:2A:1593:G:H2'	1:2A:1594:G:C8	2.38	0.58
1:2A:2815:C:H5'	27:25:29:THR:HG21	1.86	0.58
6:1G:27:ASN:HB3	6:1G:30:GLU:HG3	1.84	0.58
32:1a:673:G:H2'	32:1a:674:G:C8	2.38	0.58
32:1a:946:A:H2'	32:1a:947:G:C8	2.39	0.58
41:1j:30:SER:O	41:1j:81:THR:OG1	2.19	0.58
30:28:6:THR:HG22	30:28:63:PRO:HD2	1.84	0.58
35:2d:72:GLU:OE2	35:2d:207:TYR:OH	2.22	0.58
1:2A:2104:G:N2	1:2A:2185:C:N3	2.45	0.58
10:1O:63:VAL:HG12	10:1O:106:LEU:HD11	1.86	0.58
18:1W:11:ARG:HE	18:1W:98:LYS:HB3	1.69	0.58
32:1a:6:G:H4'	32:1a:298:A:H4'	1.86	0.58
50:1s:77:THR:HG23	50:1s:78:ARG:HG3	1.85	0.58
54:1w:54:5MU:C2	54:1w:58:A:N7	2.71	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:997:U:O2	32:2a:1044:A:N1	2.36	0.58
1:1A:409:C:OP1	61:1A:4276:HOH:O	2.17	0.58
1:1A:1086:A:O2'	1:1A:1087:G:N7	2.35	0.58
15:2T:118:ARG:HG2	32:2a:1442(A):G:C8	2.39	0.58
39:2h:119:LEU:HB3	39:2h:123:GLU:HB2	1.85	0.58
1:1A:2748:A:H5'	7:1H:4:ILE:HD12	1.84	0.58
21:1Z:7:ALA:HB2	21:1Z:59:LEU:HD22	1.85	0.58
32:1a:1329:A:N7	52:1u:7:ARG:NH2	2.51	0.58
32:2a:1456:G:O6	51:2t:54:LYS:NZ	2.32	0.58
32:2a:1518:MA6:N6	32:2a:1519:MA6:H103	2.19	0.58
36:2e:122:GLU:HB2	36:2e:126:ARG:HD3	1.86	0.58
1:1A:1406:U:H2'	1:1A:1407:C:C6	2.39	0.58
1:1A:1778:U:H2'	1:1A:1784:A:N6	2.19	0.58
1:2A:2150:U:H2'	1:2A:2151:G:C8	2.39	0.58
32:1a:1003:G:C4	32:1a:1004:A:H2	2.22	0.58
33:1b:189:ASP:OD1	33:1b:189:ASP:N	2.37	0.58
54:1y:59:U:H3'	54:1y:60:C:H6	1.69	0.58
1:1A:250:G:P	30:18:13:ARG:HH22	2.27	0.57
1:1A:782:A:N1	61:1A:4377:HOH:O	2.32	0.57
1:1A:1991:U:H2'	1:1A:1992:G:H5''	1.86	0.57
5:1F:178:PRO:O	5:1F:205:ARG:NH2	2.37	0.57
6:1G:11:TYR:HA	6:1G:15:VAL:HB	1.86	0.57
32:2a:1026:G:O6	32:2a:1036:G:N2	2.36	0.57
34:2c:22:TRP:CH2	34:2c:32:LEU:HB3	2.39	0.57
36:2e:71:LEU:HD21	36:2e:115:VAL:HG22	1.86	0.57
54:2y:19:G:H1	54:2y:56:C:N4	2.02	0.57
32:2a:562:C:H1'	43:2l:15:ARG:HB3	1.86	0.57
35:2d:119:GLN:HG2	35:2d:123:HIS:CD2	2.38	0.57
55:2x:8:4SU:O5'	55:2x:8:4SU:H6	2.04	0.57
1:1A:286:C:H2'	1:1A:287:C:C6	2.39	0.57
1:1A:2142:C:H2'	1:1A:2143:C:H6	1.69	0.57
1:2A:1019:U:OP1	1:2A:1035:U:O2'	2.13	0.57
2:2B:48:A:OP2	14:2S:30:ARG:NH2	2.37	0.57
6:2G:114:ILE:HG13	6:2G:140:ILE:HG12	1.85	0.57
7:2H:56:SER:HB3	7:2H:61:HIS:ND1	2.20	0.57
50:2s:22:LEU:HB3	50:2s:27:GLU:HB3	1.85	0.57
1:1A:1113:U:H2'	1:1A:1114:G:C8	2.40	0.57
49:1r:32:ARG:HA	49:1r:69:THR:HG21	1.85	0.57
54:1y:5:G:N2	54:1y:68:C:N3	2.42	0.57
19:2X:35:THR:HG22	19:2X:38:GLU:HB2	1.87	0.57
32:2a:1203:C:H2'	32:2a:1204:A:C8	2.39	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:2d:173:TRP:CD1	35:2d:189:PRO:HG3	2.40	0.57
54:2y:36:C:H2'	54:2y:37:6MZ:O4'	2.04	0.57
54:2y:51:C:N3	54:2y:63:G:C6	2.73	0.57
1:1A:286:C:H2'	1:1A:287:C:H6	1.69	0.57
1:2A:918:A:N3	2:2B:80:U:H4'	2.19	0.57
6:1G:45:GLU:OE2	61:1G:301:HOH:O	2.18	0.57
48:1q:76:LEU:HD21	48:1q:79:SER:HB2	1.86	0.57
1:1A:2336:A:H61	22:10:43:THR:HG22	1.69	0.57
1:2A:271(H):G:H2'	1:2A:271(I):G:C8	2.39	0.57
1:2A:1019:U:HO2'	1:2A:1021:A:H2	1.51	0.57
1:2A:2150:U:H2'	1:2A:2151:G:H8	1.68	0.57
12:1Q:37:LEU:HD21	12:1Q:130:LYS:HE3	1.87	0.57
32:1a:1060:C:H5''	41:1j:51:ARG:HG2	1.85	0.57
32:2a:107:G:H2'	32:2a:108:G:O4'	2.04	0.57
32:1a:674:G:H2'	32:1a:675:A:C8	2.40	0.57
33:1b:74:LYS:HD2	33:1b:166:ASP:HB2	1.86	0.57
15:2T:41:ARG:NH1	32:2a:346:G:OP1	2.36	0.57
15:2T:127:ALA:C	15:2T:129:ARG:H	2.13	0.57
32:2a:157:G:H2'	32:2a:158:G:H8	1.69	0.57
32:2a:557:G:OP1	61:2a:1927:HOH:O	2.18	0.57
33:2b:119:GLU:OE2	33:2b:153:ARG:NH1	2.38	0.57
54:2y:56:C:H2'	54:2y:57:G:O4'	2.04	0.57
1:1A:2552:2MU:O5'	1:1A:2552:2MU:H6	2.04	0.57
1:2A:2042:A:OP1	61:2A:3980:HOH:O	2.17	0.57
1:2A:2206:G:H3'	1:2A:2207:G:H8	1.69	0.57
12:1Q:138:ASP:N	12:1Q:138:ASP:OD1	2.35	0.57
32:1a:649:G:H2'	32:1a:650:G:H8	1.69	0.57
32:1a:674:G:H2'	32:1a:675:A:H8	1.68	0.57
32:1a:737:A:H2'	32:1a:738:C:C6	2.40	0.57
38:1g:16:LEU:HD21	40:1i:45:ALA:HB2	1.87	0.57
32:2a:1179:A:H2'	32:2a:1180:A:O4'	2.04	0.57
32:2a:1218:C:OP2	45:2n:9:LYS:NZ	2.30	0.57
34:2c:59:ARG:HG3	34:2c:63:ASN:O	2.05	0.57
1:1A:1817:G:OP1	3:1D:88:ARG:NH2	2.37	0.57
1:2A:2138:C:N4	1:2A:2153:G:N1	2.30	0.57
20:1Y:17:SER:OG	20:1Y:71:LYS:NZ	2.37	0.57
32:1a:341:C:H2'	32:1a:342:C:C6	2.40	0.57
54:1w:62:C:H2'	54:1w:63:G:H8	1.69	0.57
9:2N:103:VAL:HG11	9:2N:120:LEU:HD22	1.87	0.57
23:21:83:GLU:OE1	23:21:83:GLU:N	2.38	0.57
33:2b:98:LEU:H	33:2b:101:MET:HE2	1.69	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:2e:60:TYR:OH	36:2e:64:ARG:NH2	2.35	0.57
39:2h:10:LEU:HD22	39:2h:83:ILE:HD11	1.86	0.57
44:2m:11:ARG:HG3	44:2m:12:ASN:HD22	1.69	0.57
1:1A:1087:G:H2'	1:1A:1089:G:C8	2.40	0.57
1:2A:1220:A:OP2	16:2U:19:LYS:NZ	2.27	0.57
12:1Q:111:GLU:OE2	12:1Q:133:ARG:NH2	2.38	0.57
32:1a:1015:A:N3	32:1a:1218:C:O2'	2.36	0.57
35:1d:170:VAL:HG12	35:1d:171:GLY:H	1.69	0.57
55:1x:29:G:H1	55:1x:41:C:H42	1.51	0.57
32:2a:829:G:N7	61:2a:1953:HOH:O	2.33	0.57
33:2b:179:LYS:HA	39:2h:72:PRO:HG3	1.85	0.57
1:1A:363(F):A:N1	61:1A:4368:HOH:O	2.32	0.56
32:1a:1378:C:O2	38:1g:76:ARG:NH2	2.38	0.56
19:2X:8:ILE:O	24:22:36:ARG:NH2	2.36	0.56
20:2Y:87:LYS:HB3	20:2Y:95:LYS:HD2	1.85	0.56
25:23:8:LEU:HB2	25:23:28:LEU:HD13	1.87	0.56
32:2a:222:U:H2'	32:2a:223:U:C6	2.40	0.56
1:1A:1939:5MU:OP1	1:1A:2604:U:O2'	2.20	0.56
1:1A:2660:A:N7	7:1H:175:LYS:NZ	2.53	0.56
1:2A:75:G:H4'	24:22:55:ARG:NH1	2.19	0.56
1:2A:307:G:H21	1:2A:330:A:H62	1.54	0.56
35:1d:98:GLU:OE1	35:1d:103:ASN:ND2	2.33	0.56
12:2Q:36:ALA:HB2	12:2Q:103:MET:SD	2.44	0.56
1:1A:530:G:H4'	1:1A:531:C:OP1	2.05	0.56
1:1A:1039:G:H1	1:1A:1116:C:H42	1.51	0.56
1:1A:2849:U:H4'	1:1A:2868:A:C2	2.40	0.56
1:2A:900:A:O2'	1:2A:901:A:OP1	2.21	0.56
1:2A:2287:A:N6	1:2A:2344:U:H3	2.03	0.56
20:1Y:20:TYR:CE2	20:1Y:43:ASN:HA	2.39	0.56
32:1a:677:U:H3	32:1a:713:G:H22	1.53	0.56
32:1a:1316:G:N7	50:1s:7:LYS:NZ	2.53	0.56
54:1y:52:G:H1	54:1y:62:C:N4	2.04	0.56
5:2F:101:LEU:O	5:2F:106:ARG:NH1	2.38	0.56
12:2Q:111:GLU:O	12:2Q:115:MET:HG2	2.05	0.56
32:2a:321:A:N7	32:2a:328:C:O2'	2.30	0.56
32:2a:405:U:O4	35:2d:2:GLY:N	2.38	0.56
32:2a:1270:C:H2'	32:2a:1271:G:H8	1.70	0.56
35:2d:149:ALA:HB3	35:2d:152:SER:HB2	1.87	0.56
54:2y:2:G:N2	54:2y:72:C:O2	2.38	0.56
1:1A:2680:C:H5'	4:1E:189:PRO:HA	1.88	0.56
7:1H:154:PRO:HB3	7:1H:163:TYR:CZ	2.41	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:16:14:THR:OG1	28:16:48:VAL:O	2.23	0.56
3:2D:182:LEU:HB2	3:2D:272:ALA:HB3	1.88	0.56
1:1A:2364:C:OP1	22:10:55:ARG:NH1	2.38	0.56
1:1A:2432:A:C5	23:11:33:LYS:HG2	2.40	0.56
1:2A:1180:C:H2'	1:2A:1181:C:H6	1.71	0.56
32:1a:952:U:H2'	32:1a:953:G:H8	1.71	0.56
47:1p:17:TYR:HE2	47:1p:41:PRO:HG3	1.71	0.56
8:2I:124:GLY:H	8:2I:144:VAL:HG23	1.69	0.56
32:2a:297:G:N2	32:2a:300:A:OP2	2.38	0.56
32:2a:1060:C:H5''	41:2j:51:ARG:HG2	1.88	0.56
1:1A:1405:U:H2'	1:1A:1406:U:C6	2.41	0.56
1:1A:1750:G:O2'	1:1A:2860:A:N1	2.30	0.56
1:1A:1786:A:H1'	1:1A:1938:A:N6	2.21	0.56
1:2A:851:U:O2'	25:23:42:ALA:O	2.22	0.56
1:2A:857:C:H4'	22:20:23:VAL:HG21	1.88	0.56
1:2A:938:G:OP2	30:28:52:LYS:NZ	2.27	0.56
4:1E:24:THR:HG22	4:1E:186:GLY:O	2.05	0.56
32:1a:26:A:O2'	35:1d:209:ARG:NH1	2.38	0.56
35:1d:178:VAL:HG12	35:1d:179:GLU:H	1.71	0.56
33:2b:98:LEU:HB2	33:2b:101:MET:HG3	1.88	0.56
1:1A:1266:G:O2'	1:1A:2012:G:O6	2.19	0.56
1:1A:1364:G:OP2	23:11:3:LYS:HG3	2.06	0.56
1:1A:2790:A:H5''	1:1A:2791:C:H5'	1.87	0.56
1:2A:2646:C:H2'	1:2A:2647:U:O4'	2.06	0.56
32:1a:184:G:H2'	32:1a:185:A:H8	1.71	0.56
32:1a:727:G:N7	61:1a:1951:HOH:O	2.33	0.56
32:1a:814:A:H2'	32:1a:816:A:H5''	1.88	0.56
32:1a:1077:G:N2	32:1a:1080:A:OP2	2.38	0.56
36:1e:33:VAL:HG21	36:1e:109:ILE:HA	1.87	0.56
14:2S:30:ARG:HB3	14:2S:35:ILE:HD12	1.87	0.56
31:29:2:LYS:NZ	31:29:31:LYS:O	2.39	0.56
32:2a:323:U:O3'	51:2t:22:ARG:NH1	2.39	0.56
32:2a:942:G:H21	40:2i:124:GLN:NE2	2.03	0.56
7:1H:3:ARG:NH1	7:1H:5:GLY:H	2.03	0.56
41:1j:5:ARG:HD2	41:1j:71:LEU:HD11	1.88	0.56
12:2Q:10:ARG:NH2	55:2x:64:G:O2'	2.35	0.56
32:2a:998:G:H1	32:2a:1043:C:N4	2.02	0.56
32:2a:1264:C:H2'	32:2a:1265:G:H8	1.71	0.56
34:2c:63:ASN:HB3	34:2c:98:ASN:HD22	1.71	0.56
35:2d:170:VAL:HG12	35:2d:171:GLY:H	1.70	0.56
42:2k:48:ILE:HG21	42:2k:63:LEU:HB3	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:952:G:OP1	12:1Q:16:ARG:NH2	2.37	0.56
1:1A:2483:C:N3	12:1Q:124:LYS:HE3	2.21	0.56
15:2T:94:ALA:HB1	15:2T:99:LEU:HD21	1.88	0.56
37:2f:69:GLU:O	37:2f:72:VAL:HG12	2.06	0.56
8:1I:3:VAL:HG12	8:1I:38:LEU:HA	1.87	0.56
15:1T:127:ALA:C	15:1T:129:ARG:H	2.14	0.56
32:1a:69:G:H2'	32:1a:70:G:H8	1.71	0.56
22:20:18:ALA:O	22:20:20:ARG:NH1	2.39	0.56
32:2a:1152:A:OP1	41:2j:70:ARG:NH2	2.39	0.56
42:2k:48:ILE:O	42:2k:50:TYR:N	2.38	0.56
55:2x:23:C:H2'	55:2x:24:U:C6	2.41	0.56
1:2A:2113:U:H3	1:2A:2170:A:H61	1.54	0.55
32:1a:715:A:H2'	32:1a:716:A:C8	2.42	0.55
32:1a:943:U:H1'	40:1i:124:GLN:HE22	1.70	0.55
12:2Q:111:GLU:OE1	12:2Q:133:ARG:NH2	2.38	0.55
33:2b:48:MET:HA	33:2b:51:LEU:HB2	1.87	0.55
1:1A:910:A:N3	1:1A:2264:C:O2'	2.35	0.55
1:2A:479:A:H4'	1:2A:480:A:OP1	2.05	0.55
1:2A:728:G:H5''	3:2D:13:ARG:HH21	1.71	0.55
1:2A:2693:A:H2'	1:2A:2694:G:H8	1.70	0.55
8:1I:46:ALA:O	8:1I:50:ARG:HG2	2.06	0.55
37:1f:5:GLU:OE1	61:1f:301:HOH:O	2.18	0.55
43:1l:53:ARG:HB3	43:1l:69:TYR:HE1	1.71	0.55
32:2a:1298:C:OP2	38:2g:114:ARG:NH2	2.39	0.55
45:2n:26:ARG:HD3	45:2n:43:CYS:HB3	1.88	0.55
47:2p:17:TYR:HE2	47:2p:41:PRO:HG3	1.71	0.55
1:1A:582:G:H2'	1:1A:583:G:C8	2.41	0.55
1:1A:631:A:N3	1:1A:2415:G:O2'	2.34	0.55
1:1A:1376:C:OP1	61:1A:4297:HOH:O	2.18	0.55
2:1B:45:A:OP2	6:1G:96:ARG:NH2	2.31	0.55
32:1a:922:G:H4'	36:1e:20:GLN:HA	1.87	0.55
33:1b:24:TRP:CZ3	33:1b:26:PRO:HA	2.41	0.55
33:1b:162:ILE:O	33:1b:185:ILE:HG12	2.05	0.55
38:1g:74:GLU:HG2	38:1g:91:VAL:HG22	1.88	0.55
40:1i:17:VAL:HG11	40:1i:81:ILE:HG22	1.87	0.55
50:1s:19:VAL:O	50:1s:23:ASN:ND2	2.38	0.55
4:2E:116:VAL:HG21	4:2E:138:PRO:HB3	1.88	0.55
1:1A:2649:U:H2'	1:1A:2650:U:C6	2.41	0.55
1:1A:2747:G:O6	1:1A:2755:C:H5''	2.06	0.55
1:2A:857:C:OP2	22:20:77:ARG:NH2	2.39	0.55
21:1Z:138:GLU:HB2	21:1Z:156:LYS:HD3	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1118:C:H1'	32:1a:1179:A:C4	2.42	0.55
39:1h:121:ASP:OD2	39:1h:125:ARG:NH2	2.38	0.55
6:2G:114:ILE:HA	6:2G:140:ILE:HD11	1.88	0.55
32:2a:473:G:H2'	32:2a:474:G:H8	1.71	0.55
32:2a:736:C:H2'	32:2a:737:A:C8	2.41	0.55
32:2a:1442:G:H2'	32:2a:1442:G:N3	2.21	0.55
40:2i:9:ARG:H	40:2i:79:LEU:HD23	1.71	0.55
1:2A:2159:G:H2'	1:2A:2160:G:H8	1.71	0.55
14:1S:35:ILE:HG12	14:1S:101:LEU:HD12	1.87	0.55
32:1a:1030:C:N3	32:1a:1031:G:N2	2.54	0.55
33:2b:178:ARG:HH12	39:2h:68:ARG:HH22	1.53	0.55
34:2c:42:LEU:O	34:2c:46:GLU:HG2	2.06	0.55
1:1A:2319:G:H22	14:1S:3:ARG:NE	2.05	0.55
1:1A:2550:G:OP2	61:1A:4300:HOH:O	2.18	0.55
1:2A:1446:C:H42	1:2A:1465:G:H1	1.55	0.55
1:2A:2336:A:H61	22:20:43:THR:HG22	1.72	0.55
3:1D:85:ASP:OD2	3:1D:88:ARG:NH1	2.38	0.55
32:2a:660:G:H1	32:2a:745:C:H42	1.55	0.55
44:2m:13:LYS:HA	44:2m:44:ARG:HH11	1.71	0.55
45:2n:24:CYS:HB3	45:2n:29:ARG:H	1.71	0.55
1:1A:1187:G:H5''	17:1V:81:TYR:CE1	2.42	0.55
1:1A:2108:C:H2'	1:1A:2109:U:H6	1.71	0.55
1:1A:2114:A:N6	1:1A:2119:A:N7	2.54	0.55
1:2A:2781:A:H5''	1:2A:2782:G:H5'	1.89	0.55
13:1R:28:LEU:HD23	13:1R:48:VAL:HG21	1.88	0.55
32:1a:977:A:H2'	32:1a:978:A:H5''	1.89	0.55
11:2P:63:PRO:HG2	30:28:25:MET:HB2	1.87	0.55
22:20:26:TYR:O	22:20:29:GLN:HB2	2.07	0.55
48:2q:45:HIS:HB2	48:2q:65:ILE:HD13	1.89	0.55
51:2t:53:LEU:HA	51:2t:56:MET:HG2	1.88	0.55
1:1A:488:G:O2'	18:1W:49:LYS:NZ	2.40	0.55
1:1A:2001:A:H2'	1:1A:2002:G:C8	2.42	0.55
1:1A:2125:G:H1'	1:1A:2173:A:H61	1.72	0.55
20:1Y:20:TYR:HB3	20:1Y:23:ARG:HG3	1.89	0.55
32:1a:7:G:H5'	32:1a:298:A:O4'	2.05	0.55
22:20:40:GLN:HE22	22:20:43:THR:HA	1.72	0.55
32:2a:1226:C:H4'	50:2s:80:TYR:CZ	2.42	0.55
32:2a:1499:A:H1'	32:2a:1520:G:H5'	1.88	0.55
32:2a:1517:G:H3'	32:2a:1518:MA6:H8	1.89	0.55
1:1A:911:A:H2'	12:1Q:9:TYR:OH	2.06	0.55
1:1A:2097:C:H2'	1:1A:2098:U:O4'	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:8:A:N6	35:1d:205:GLU:O	2.40	0.55
33:1b:158:LEU:HG	33:1b:182:ILE:HD11	1.88	0.55
7:2H:3:ARG:NH1	7:2H:4:ILE:H	2.05	0.55
33:2b:69:LEU:HB3	33:2b:162:ILE:HG22	1.88	0.55
1:1A:2810:A:N6	1:1A:2891:G:O2'	2.34	0.55
1:2A:2630:G:H2'	1:2A:2631:G:C8	2.42	0.55
4:1E:59:VAL:HG21	4:1E:74:PRO:HB3	1.88	0.55
11:1P:63:PRO:HG2	30:18:25:MET:HB2	1.87	0.55
19:1X:94:GLY:HA2	19:1X:95:LEU:C	2.32	0.55
32:1a:590:C:H2'	32:1a:591:U:H6	1.72	0.55
32:1a:1036:G:H3'	32:1a:1037:C:H6	1.72	0.55
2:2B:15:A:OP2	2:2B:69:G:N2	2.38	0.55
10:2O:73:ASP:HB2	15:2T:82:LEU:HD12	1.89	0.55
15:2T:39:ARG:NH2	32:2a:345:C:OP2	2.40	0.55
24:22:51:ARG:HG3	24:22:55:ARG:NH2	2.21	0.55
32:2a:504:C:OP1	61:2a:1928:HOH:O	2.18	0.55
54:2w:64:U:H2'	54:2w:65:C:C6	2.42	0.55
1:1A:1025:G:C4	1:1A:1135:C:H1'	2.42	0.54
32:1a:246:A:N1	32:1a:278:G:O2'	2.38	0.54
36:1e:39:GLY:HA2	36:1e:69:VAL:HG13	1.88	0.54
38:1g:79:ARG:HG3	38:1g:80:VAL:H	1.71	0.54
38:1g:146:GLU:OE1	38:1g:149:ARG:NE	2.40	0.54
40:1i:9:ARG:HG2	40:1i:14:VAL:HG12	1.88	0.54
5:2F:167:ALA:HB1	5:2F:173:VAL:HG11	1.88	0.54
7:2H:122:THR:O	7:2H:134:SER:OG	2.24	0.54
25:23:6:VAL:HG12	25:23:28:LEU:HD11	1.88	0.54
32:2a:869:G:H8	32:2a:869:G:O5'	1.90	0.54
32:2a:1346:A:H2'	38:2g:10:ARG:HH22	1.71	0.54
34:2c:70:VAL:O	34:2c:106:VAL:N	2.39	0.54
34:2c:79:ARG:H	34:2c:82:GLU:HB3	1.72	0.54
39:2h:12:ARG:HD2	39:2h:26:VAL:HG12	1.89	0.54
41:2j:69:ASN:O	41:2j:70:ARG:NH1	2.38	0.54
1:1A:859:G:O2'	1:1A:916:G:O6	2.21	0.54
1:1A:993:G:OP1	16:1U:50:ARG:NH2	2.41	0.54
1:2A:1152:C:H2'	1:2A:1153:C:H6	1.71	0.54
1:2A:2206:G:H5''	1:2A:2207:G:N7	2.22	0.54
5:2F:155:LEU:HB2	5:2F:189:THR:HG21	1.88	0.54
15:2T:26:ASP:OD2	15:2T:120:ARG:NH1	2.37	0.54
32:2a:946:A:H2'	32:2a:947:G:C8	2.42	0.54
32:2a:1456:G:N1	51:2t:51:GLU:OE2	2.39	0.54
1:1A:2106:G:H1	1:1A:2183:C:H42	1.54	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2116:G:N2	1:1A:2162:G:OP1	2.39	0.54
1:1A:2206:G:H5''	1:1A:2207:G:C6	2.42	0.54
1:1A:2286:A:H4'	1:1A:2287:A:O4'	2.07	0.54
1:2A:340:A:H2'	1:2A:341:G:O4'	2.07	0.54
1:2A:492:A:H2'	1:2A:493:G:O4'	2.08	0.54
1:2A:586:A:N1	1:2A:809:G:O2'	2.37	0.54
1:2A:987:G:O2'	1:2A:1000:A:N3	2.36	0.54
1:2A:1125:G:H5'	31:29:37:GLY:HA2	1.90	0.54
1:2A:2152:G:C4	1:2A:2153:G:H1'	2.43	0.54
1:2A:2342:C:O2'	1:2A:2374:C:OP1	2.23	0.54
32:1a:148:G:H2'	32:1a:149:A:H8	1.72	0.54
38:2g:79:ARG:HG3	38:2g:80:VAL:H	1.72	0.54
46:2o:39:LEU:HD22	46:2o:56:LEU:HD13	1.89	0.54
1:1A:82:G:N1	1:1A:103:A:OP2	2.31	0.54
1:1A:994:C:OP1	16:1U:53:ARG:NH2	2.41	0.54
1:1A:2176:A:H2'	1:1A:2177:C:C6	2.42	0.54
1:1A:2278:A:OP2	22:10:12:ASN:ND2	2.39	0.54
1:1A:2727:G:O2'	10:1O:70:LYS:NZ	2.41	0.54
1:1A:2829:C:O3'	4:1E:76:ARG:NH2	2.39	0.54
1:2A:276:A:H5''	1:2A:277:C:H5'	1.89	0.54
1:2A:1223:G:N2	1:2A:1226:A:OP2	2.36	0.54
1:2A:1557:C:OP2	1:2A:1558:A:O2'	2.19	0.54
28:16:9:LEU:HD13	28:16:51:GLU:HB2	1.89	0.54
32:1a:204:U:H4'	32:1a:216:G:O5'	2.06	0.54
4:2E:116:VAL:HG13	4:2E:122:PHE:HB2	1.89	0.54
25:23:13:ILE:O	61:23:201:HOH:O	2.19	0.54
30:28:28:GLY:O	30:28:36:LYS:NZ	2.38	0.54
36:2e:31:LEU:HD22	36:2e:43:LEU:HD11	1.89	0.54
1:2A:686:G:N2	1:2A:788:A:H61	2.06	0.54
1:2A:2136:C:H1'	1:2A:2137:C:H5'	1.89	0.54
6:1G:9:ARG:NH1	6:1G:13:GLU:OE2	2.40	0.54
23:11:23:LYS:HB3	23:11:29:GLY:HA3	1.88	0.54
31:19:29:ASN:HD22	31:19:32:HIS:CE1	2.26	0.54
33:1b:172:ILE:H	33:1b:172:ILE:HD12	1.73	0.54
43:1l:24:VAL:HB	43:1l:27:LEU:HD22	1.88	0.54
7:2H:98:LEU:HD13	7:2H:125:VAL:HG23	1.89	0.54
8:2I:29:TYR:HD2	8:2I:30:LEU:HD23	1.71	0.54
13:2R:28:LEU:HD23	13:2R:48:VAL:HG21	1.89	0.54
32:2a:34:C:H2'	32:2a:35:G:C8	2.42	0.54
32:2a:976:G:H5'	32:2a:1358:U:O2'	2.08	0.54
32:2a:1310:G:H5'	44:2m:77:ASN:ND2	2.23	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:2q:45:HIS:HB3	48:2q:72:ARG:HG2	1.89	0.54
1:2A:2197:U:H1'	1:2A:2198:A:C8	2.43	0.54
5:1F:65:TRP:CZ2	5:1F:75:HIS:HD2	2.26	0.54
33:1b:155:LEU:HD21	33:1b:159:PRO:HD3	1.88	0.54
19:2X:12:VAL:HG22	19:2X:29:TRP:CE2	2.43	0.54
32:2a:377:G:OP1	47:2p:3:LYS:HD3	2.07	0.54
32:2a:719:C:O2'	49:2r:49:LYS:HB3	2.07	0.54
32:2a:748:C:H4'	32:2a:749:C:O5'	2.08	0.54
1:1A:801:G:O6	5:1F:53:THR:OG1	2.25	0.54
1:2A:2137:C:N4	1:2A:2154:G:N1	2.49	0.54
15:1T:74:ARG:HG2	15:1T:76:PHE:CZ	2.43	0.54
32:1a:974:A:H8	32:1a:974:A:OP1	1.91	0.54
39:1h:81:HIS:N	39:1h:138:TRP:O	2.41	0.54
32:2a:17:U:H2'	32:2a:18:C:C6	2.43	0.54
32:2a:815:A:N7	32:2a:1509:C:O2'	2.33	0.54
32:2a:885:G:O2'	32:2a:914:A:N1	2.37	0.54
37:2f:10:LEU:HD13	37:2f:61:LEU:HD13	1.89	0.54
1:1A:1359:A:H2	1:1A:1372:U:O4	1.91	0.54
1:1A:2070:G:OP2	61:1A:4302:HOH:O	2.19	0.54
1:1A:2887:U:H2'	1:1A:2888:C:C6	2.43	0.54
1:2A:503:A:H4'	1:2A:504:U:H5''	1.90	0.54
1:2A:2137:C:H1'	1:2A:2138:C:H5'	1.90	0.54
4:1E:12:THR:HG21	15:1T:11:GLU:HG2	1.90	0.54
21:1Z:126:VAL:HG12	21:1Z:128:VAL:HB	1.90	0.54
33:1b:51:LEU:HD22	33:1b:55:PHE:HE2	1.72	0.54
6:2G:72:ARG:NH1	6:2G:87:PRO:HG3	2.23	0.54
11:2P:36:LYS:O	61:2P:302:HOH:O	2.18	0.54
14:2S:25:ARG:HH21	14:2S:40:ILE:HG21	1.72	0.54
20:2Y:73:ARG:HD2	20:2Y:82:PRO:HB2	1.90	0.54
21:2Z:69:THR:HG22	21:2Z:90:VAL:HA	1.90	0.54
21:2Z:163:LEU:HD11	21:2Z:165:VAL:HG22	1.90	0.54
32:2a:108:G:N1	51:2t:15:ARG:HG2	2.23	0.54
33:2b:219:VAL:HA	33:2b:222:ILE:HD12	1.90	0.54
43:2l:59:ARG:HA	43:2l:65:GLU:HA	1.89	0.54
44:2m:40:ASN:HB3	44:2m:43:THR:HG23	1.89	0.54
1:1A:881:G:H1	1:1A:897:C:H42	1.54	0.54
15:1T:60:THR:HG22	15:1T:77:PRO:HA	1.89	0.54
43:1l:76:ASN:ND2	43:1l:106:ASP:O	2.41	0.54
10:2O:119:PRO:HB2	15:2T:68:TYR:CE2	2.43	0.54
14:2S:28:VAL:HG11	14:2S:98:VAL:HG13	1.90	0.54
30:28:26:LYS:HD2	30:28:48:PHE:CD2	2.43	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:501:C:H2'	32:2a:502:G:C8	2.43	0.54
32:2a:523:A:N1	43:2l:92:0TD:H6	2.23	0.54
40:2i:9:ARG:HB2	40:2i:104:ARG:HE	1.73	0.54
1:1A:1292:U:H2'	1:1A:1293:C:C6	2.42	0.54
1:2A:2751:G:H8	7:2H:2:SER:HA	1.72	0.54
6:1G:15:VAL:HG22	6:1G:175:LEU:HB3	1.88	0.54
32:1a:1366:C:N4	61:1a:1944:HOH:O	2.40	0.54
40:1i:26:VAL:HG13	40:1i:61:ALA:HB3	1.90	0.54
26:24:48:ARG:HG3	26:24:52:THR:HG23	1.90	0.54
32:2a:54:C:N4	32:2a:353:A:OP2	2.39	0.54
32:2a:1202:G:O4'	45:2n:29:ARG:NH1	2.41	0.54
32:2a:1275:A:H3'	32:2a:1276:G:H8	1.73	0.54
34:2c:70:VAL:HG22	34:2c:72:LYS:H	1.72	0.54
1:1A:184:C:H2'	1:1A:185:U:C6	2.43	0.53
1:1A:668:G:H5'	1:1A:669:G:OP2	2.08	0.53
1:1A:748:G:C8	18:1W:89:ALA:HB1	2.43	0.53
1:2A:848:G:H2'	1:2A:849:A:C8	2.42	0.53
1:2A:2058:A:N7	61:2A:4044:HOH:O	2.34	0.53
1:2A:2183:C:H2'	1:2A:2184:G:H8	1.72	0.53
43:1l:52:LEU:O	43:1l:54:LYS:NZ	2.38	0.53
6:2G:3:LEU:O	6:2G:8:LYS:NZ	2.27	0.53
19:2X:53:LYS:HB3	19:2X:82:GLN:HB3	1.89	0.53
32:2a:656:C:O2'	46:2o:28:GLN:OE1	2.22	0.53
33:2b:74:LYS:O	33:2b:78:GLN:HG2	2.07	0.53
34:2c:78:GLY:HA3	34:2c:83:ARG:H	1.72	0.53
1:2A:1790:C:H5''	1:2A:1791:A:OP1	2.08	0.53
1:2A:2327:A:H2'	1:2A:2328:A:C8	2.43	0.53
32:1a:1511:G:H2'	32:1a:1512:U:O4'	2.07	0.53
36:1e:85:GLY:C	36:1e:87:SER:H	2.17	0.53
36:1e:85:GLY:O	36:1e:87:SER:N	2.39	0.53
3:2D:166:GLN:NE2	32:2a:713:G:OP1	2.40	0.53
4:2E:179:GLU:HG3	15:2T:9:LEU:HD21	1.89	0.53
32:2a:947:G:H1	32:2a:1234:C:H42	1.54	0.53
32:2a:1135:U:H2'	32:2a:1137:C:C2	2.43	0.53
34:2c:43:LEU:HD21	34:2c:91:LEU:HD13	1.89	0.53
54:2w:61:C:H3'	54:2w:62:C:H5''	1.90	0.53
1:1A:875:G:H1	1:1A:902:C:H42	1.56	0.53
1:1A:1055:G:H1	1:1A:1104:C:H42	1.56	0.53
1:1A:1164:G:H2'	1:1A:1165:U:C6	2.44	0.53
1:2A:271(U):G:H2'	1:2A:271(V):G:H8	1.74	0.53
1:2A:1359:A:H2	1:2A:1372:U:O4	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1H:137:ASP:HB3	7:1H:140:LYS:HB3	1.91	0.53
8:1I:133:HIS:ND1	8:1I:134:PRO:O	2.39	0.53
23:11:82:LEU:HA	23:11:85:LEU:HD12	1.89	0.53
32:1a:573:A:OP1	61:1a:1927:HOH:O	2.18	0.53
32:1a:580:U:H2'	32:1a:581:G:O4'	2.08	0.53
35:1d:79:PHE:HE1	35:1d:204:ILE:HD13	1.72	0.53
6:2G:106:LEU:HA	6:2G:110:ALA:HB3	1.90	0.53
33:2b:60:ASP:O	33:2b:64:ARG:HG2	2.08	0.53
39:2h:28:ALA:HB3	39:2h:57:PRO:HB2	1.90	0.53
54:2w:72:C:H2'	54:2w:73:A:C8	2.44	0.53
1:1A:566:U:H5''	11:1P:29:LYS:HE3	1.90	0.53
1:1A:744:G:OP1	61:1A:4298:HOH:O	2.18	0.53
1:2A:646:A:H2'	1:2A:647:G:O4'	2.09	0.53
1:2A:1803:A:O2'	3:2D:259:THR:HG21	2.08	0.53
32:1a:316:G:OP2	32:1a:351:G:O2'	2.26	0.53
32:1a:376:G:H5''	47:1p:5:ARG:HD2	1.89	0.53
32:1a:1305:G:H22	32:1a:1331:G:H1'	1.72	0.53
39:1h:96:GLY:N	39:1h:99:GLU:OE1	2.35	0.53
54:1y:27:C:H42	54:1y:43:G:H1	1.54	0.53
5:2F:154:VAL:HG22	5:2F:191:ARG:HB2	1.91	0.53
10:2O:98:VAL:HG22	10:2O:118:ALA:HA	1.90	0.53
32:2a:407:G:OP1	35:2d:115:ARG:HD3	2.09	0.53
32:2a:551:U:H2'	32:2a:552:U:C6	2.43	0.53
32:2a:954:G:H2'	32:2a:955:U:O4'	2.08	0.53
33:2b:87:ARG:NH2	33:2b:220:ASP:OD1	2.35	0.53
40:2i:17:VAL:HG11	40:2i:81:ILE:HG22	1.90	0.53
43:2l:71:PRO:O	43:2l:102:ARG:NH1	2.35	0.53
54:2y:8:4SU:H1'	54:2y:48:C:H1'	1.91	0.53
4:1E:77:ILE:HD11	4:1E:195:LEU:HD13	1.91	0.53
11:1P:39:LYS:HB2	11:1P:45:LEU:HD21	1.91	0.53
19:1X:35:THR:HG22	19:1X:38:GLU:HB3	1.89	0.53
32:1a:381:C:H2'	32:1a:382:A:O4'	2.09	0.53
32:1a:975:A:H5'	32:1a:975:A:H8	1.74	0.53
32:1a:1123:A:H4'	41:1j:36:GLY:HA3	1.91	0.53
32:2a:410:G:OP1	35:2d:30:LYS:NZ	2.28	0.53
32:2a:750:G:N3	46:2o:23:GLY:HA3	2.22	0.53
33:2b:212:GLN:O	33:2b:216:SER:OG	2.20	0.53
1:2A:27:G:N2	1:2A:512:G:H1'	2.23	0.53
1:2A:1799:G:O2'	3:2D:181:GLU:OE2	2.17	0.53
1:2A:2125:G:N1	1:2A:2172:U:OP1	2.41	0.53
1:2A:2498:C:H3'	61:2A:3974:HOH:O	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:1O:122:LEU:HD13	15:1T:72:VAL:HG11	1.89	0.53
32:1a:109:A:H2'	32:1a:326:G:N2	2.24	0.53
32:1a:437:U:H5'	35:1d:155:LEU:HD21	1.91	0.53
32:1a:438:G:H4'	35:1d:123:HIS:CE1	2.44	0.53
32:1a:449:C:O2	47:1p:42:ARG:HD3	2.09	0.53
33:1b:10:LEU:H	33:1b:10:LEU:HD12	1.73	0.53
41:1j:8:LEU:HB2	41:1j:70:ARG:HB2	1.91	0.53
32:2a:767:A:H2'	32:2a:768:A:O4'	2.07	0.53
1:2A:2619:C:OP1	4:2E:152:LYS:NZ	2.36	0.53
10:1O:21:CYS:HB2	10:1O:39:ILE:HD12	1.90	0.53
51:1t:82:SER:OG	51:1t:86:ARG:NH1	2.40	0.53
7:2H:89:ILE:HD12	7:2H:96:ALA:HB2	1.90	0.53
32:2a:715:A:H2'	32:2a:716:A:C8	2.43	0.53
38:2g:62:PHE:HA	38:2g:124:LEU:HD22	1.88	0.53
51:2t:56:MET:HE1	51:2t:85:MET:HG2	1.91	0.53
1:1A:848:G:H2'	1:1A:849:A:C8	2.43	0.53
1:1A:1818:U:OP2	3:1D:157:ARG:HD3	2.09	0.53
16:1U:76:TYR:CZ	16:1U:80:ILE:HG13	2.44	0.53
32:1a:662:G:H2'	32:1a:663:A:C8	2.44	0.53
32:1a:1380:U:C4	38:1g:3:ARG:HG2	2.44	0.53
35:1d:63:LYS:HD2	35:1d:198:VAL:HG22	1.91	0.53
35:1d:64:LEU:HB2	35:1d:198:VAL:HG11	1.90	0.53
41:1j:35:SER:HB3	41:1j:73:ASP:HB2	1.90	0.53
48:1q:66:SER:O	48:1q:70:ARG:NH1	2.42	0.53
54:1y:37:6MZ:H2'	54:1y:38:A:C8	2.43	0.53
2:2B:14:U:OP2	2:2B:70:C:O2'	2.24	0.53
7:2H:149:ARG:HH21	7:2H:154:PRO:HG2	1.74	0.53
32:2a:1095:U:P	32:2a:1108:G:H1	2.31	0.53
32:2a:1103:C:H5''	33:2b:98:LEU:HD22	1.90	0.53
39:2h:96:GLY:N	39:2h:99:GLU:OE1	2.35	0.53
1:1A:1178:C:H2'	1:1A:1179:C:H6	1.73	0.53
1:1A:2390:U:P	30:18:35:GLN:HE22	2.32	0.53
1:2A:75:G:H4'	24:22:55:ARG:HH11	1.74	0.53
1:2A:171:G:H2'	1:2A:172:C:H6	1.74	0.53
1:2A:2693:A:H2'	1:2A:2694:G:C8	2.44	0.53
1:2A:2698:U:H2'	1:2A:2699:C:C6	2.44	0.53
3:1D:108:PRO:HG2	3:1D:111:LEU:HB2	1.90	0.53
5:1F:184:TYR:CE2	5:1F:188:ARG:HD2	2.44	0.53
4:2E:101:ARG:CZ	4:2E:171:GLU:HB2	2.38	0.53
5:2F:185:ASP:OD1	5:2F:188:ARG:NH1	2.41	0.53
32:2a:1347:G:H5''	40:2i:107:ARG:HB3	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:2h:41:ARG:NH2	39:2h:123:GLU:OE2	2.41	0.53
1:1A:839:U:H2'	1:1A:840:C:C6	2.43	0.53
1:1A:1066:U:N3	1:1A:1069:A:OP2	2.41	0.53
1:1A:1799:G:O2'	3:1D:181:GLU:OE2	2.18	0.53
1:1A:2105:C:H2'	1:1A:2106:G:H8	1.74	0.53
1:1A:2183:C:H2'	1:1A:2184:G:C8	2.43	0.53
1:1A:2430:A:N3	1:1A:2430:A:H2'	2.23	0.53
1:1A:2820:A:C8	4:1E:109:LYS:HE2	2.44	0.53
1:2A:1364:G:OP2	23:21:3:LYS:HG3	2.09	0.53
5:1F:187:VAL:HG12	11:1P:3:LEU:HD12	1.91	0.53
32:1a:403:C:OP1	35:1d:137:SER:OG	2.26	0.53
32:1a:1001:A:H2'	32:1a:1001(A):G:H8	1.72	0.53
15:2T:109:GLU:HG2	15:2T:112:ARG:HH22	1.73	0.53
20:2Y:8:LYS:HE3	20:2Y:97:ARG:CZ	2.39	0.53
26:24:61:ARG:HH21	50:2s:42:PRO:HD3	1.73	0.53
32:2a:1117:G:H5'	32:2a:1118:C:OP2	2.08	0.53
1:1A:486:C:O2'	18:1W:60:ASN:ND2	2.37	0.52
1:1A:1614:A:C2	18:1W:93:ALA:HB2	2.44	0.52
4:1E:116:VAL:HG13	4:1E:122:PHE:HB2	1.91	0.52
5:1F:101:LEU:HD12	5:1F:102:PRO:HD2	1.90	0.52
32:1a:1320:C:H2'	32:1a:1321:C:O4'	2.10	0.52
33:2b:16:HIS:HB2	33:2b:204:ASN:CB	2.38	0.52
44:2m:19:LEU:HD21	44:2m:56:LEU:HD21	1.91	0.52
57:1A:4098:DI0:NAQ	57:1A:4098:DI0:CCD	2.73	0.52
1:2A:1379:A:H4'	1:2A:1380:G:OP2	2.06	0.52
1:2A:1837:C:O2'	1:2A:1927:A:N3	2.37	0.52
1:2A:2567:G:H2'	1:2A:2568:C:C6	2.43	0.52
13:1R:44:LEU:HD22	13:1R:48:VAL:HG23	1.90	0.52
32:1a:562:C:O2	43:1l:16:GLU:N	2.43	0.52
32:1a:1074:G:O2'	32:1a:1101:A:N1	2.29	0.52
36:1e:82:VAL:HG21	36:1e:138:ALA:HA	1.90	0.52
41:1j:8:LEU:HD22	41:1j:96:ILE:HG22	1.90	0.52
4:2E:143:ASN:HD22	4:2E:147:PRO:HD3	1.74	0.52
6:2G:11:TYR:HA	6:2G:15:VAL:HB	1.91	0.52
7:2H:118:PRO:HD2	7:2H:121:ILE:HB	1.91	0.52
7:2H:159:GLU:HG3	7:2H:169:VAL:HG11	1.90	0.52
32:2a:501:C:H2'	32:2a:502:G:H8	1.73	0.52
32:2a:987:G:H2'	32:2a:988:G:C8	2.44	0.52
33:2b:40:HIS:HB2	33:2b:190:THR:HG21	1.91	0.52
41:2j:8:LEU:HB3	41:2j:16:LEU:HD11	1.91	0.52
1:1A:1876:A:H2'	1:1A:1877:A:C8	2.44	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2139:C:H2'	1:1A:2140:C:O4'	2.08	0.52
1:2A:251:A:C5	1:2A:252:G:H1'	2.45	0.52
8:1I:77:LEU:HD13	8:1I:101:LEU:HD13	1.92	0.52
12:1Q:34:LEU:HB2	12:1Q:118:LEU:HD22	1.90	0.52
15:1T:24:PRO:HA	15:1T:49:VAL:HG22	1.92	0.52
24:12:10:LEU:HD21	24:12:59:ARG:HG2	1.90	0.52
32:1a:201:C:H42	32:1a:216:G:H1	1.57	0.52
32:1a:473:G:H2'	32:1a:474:G:H8	1.75	0.52
23:21:76:ARG:HH22	23:21:97:LEU:HD22	1.74	0.52
25:23:7:LYS:HG3	25:23:34:GLU:HG3	1.91	0.52
32:2a:9:G:H2'	32:2a:10:A:H8	1.73	0.52
37:2f:61:LEU:HD23	37:2f:63:TYR:OH	2.09	0.52
38:2g:90:GLU:H	38:2g:90:GLU:CD	2.16	0.52
54:2y:51:C:O2	54:2y:63:G:C2	2.63	0.52
1:1A:154(A):C:H42	1:1A:171:G:H1	1.58	0.52
1:2A:1239:G:H2'	1:2A:1240:U:O4'	2.08	0.52
1:2A:1590:U:H2'	1:2A:1591:G:H8	1.75	0.52
5:1F:39:TRP:O	5:1F:43:LYS:HG2	2.09	0.52
6:1G:73:ALA:HB3	6:1G:85:GLY:H	1.74	0.52
32:1a:684:A:N6	61:1a:1960:HOH:O	2.36	0.52
32:1a:920:U:H2'	32:1a:921:U:C6	2.44	0.52
32:2a:1309:G:O2'	44:2m:77:ASN:ND2	2.40	0.52
35:2d:3:ARG:HG3	35:2d:5:ILE:HG23	1.90	0.52
55:2x:40:C:H2'	55:2x:41:C:C6	2.42	0.52
1:1A:363(A):A:H2'	1:1A:363(B):G:C8	2.44	0.52
1:2A:301:G:OP2	20:2Y:84:ARG:NH2	2.39	0.52
1:2A:981:A:N1	1:2A:2027:G:O2'	2.42	0.52
1:2A:1248:G:C5	16:2U:3:ARG:HB2	2.45	0.52
10:1O:2:ILE:HD12	10:1O:6:THR:HG21	1.90	0.52
23:11:76:ARG:HH22	23:11:97:LEU:HB3	1.75	0.52
32:1a:341:C:H2'	32:1a:342:C:H6	1.73	0.52
32:1a:664:G:N2	32:1a:741:G:H1	2.04	0.52
32:1a:925:G:H1'	32:1a:1502:A:C4	2.44	0.52
40:1i:16:ARG:HB2	40:1i:64:THR:HG22	1.91	0.52
48:1q:26:GLN:HE21	48:1q:37:LYS:HE2	1.74	0.52
5:2F:150:GLY:HA2	5:2F:172:TRP:CD2	2.44	0.52
50:2s:28:LYS:HB3	50:2s:29:ARG:HA	1.90	0.52
1:1A:2188:C:H2'	1:1A:2189:U:O4'	2.10	0.52
1:1A:2377:A:H2'	1:1A:2378:A:C8	2.44	0.52
1:2A:451:C:H4'	5:2F:52:LYS:HE3	1.91	0.52
1:2A:2143:C:H2'	1:2A:2144:U:O4'	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2261:C:H1'	1:2A:2388:A:N3	2.25	0.52
1:2A:2538:C:H2'	1:2A:2539:C:H6	1.74	0.52
32:1a:56:U:H2'	32:1a:57:G:C8	2.44	0.52
32:1a:160:A:H1'	32:1a:344:A:C5	2.44	0.52
41:1j:65:LEU:HD13	45:1n:56:VAL:HG22	1.91	0.52
3:2D:12:SER:HB3	3:2D:208:LYS:HB3	1.91	0.52
4:2E:16:ARG:NH1	4:2E:171:GLU:OE2	2.36	0.52
32:2a:1191:A:H5''	34:2c:4:LYS:HE3	1.92	0.52
41:2j:51:ARG:O	45:2n:45:ARG:NH1	2.43	0.52
48:2q:57:VAL:HG12	48:2q:76:LEU:HA	1.91	0.52
1:1A:814:C:H4'	1:1A:1224:C:O2	2.09	0.52
1:1A:944:G:O3'	61:1A:4301:HOH:O	2.19	0.52
1:1A:2135:A:H2'	1:1A:2136:C:C6	2.45	0.52
1:2A:534:U:O2'	16:2U:49:HIS:ND1	2.41	0.52
1:2A:2313:C:H5''	6:2G:91:ARG:HD3	1.91	0.52
11:1P:101:VAL:HG23	11:1P:106:LEU:O	2.10	0.52
14:1S:34:HIS:O	14:1S:97:ARG:NH2	2.42	0.52
43:1l:90:VAL:O	43:1l:92:OTD:N	2.43	0.52
45:1n:21:TYR:HE1	45:1n:23:ARG:HE	1.55	0.52
7:2H:164:TYR:HB2	7:2H:167:GLU:HB2	1.92	0.52
32:2a:20:U:H2'	32:2a:21:G:O4'	2.08	0.52
32:2a:673:G:H2'	32:2a:674:G:C8	2.45	0.52
32:2a:1084:G:H5'	32:2a:1102:A:OP2	2.10	0.52
52:2u:15:ARG:HB2	52:2u:15:ARG:HH11	1.75	0.52
1:1A:1213:A:N3	1:1A:1238:G:O2'	2.39	0.52
1:2A:324:A:N6	1:2A:338:G:O2'	2.43	0.52
1:2A:889:C:O2'	1:2A:890:A:O4'	2.24	0.52
1:2A:1891:G:O6	61:2A:3969:HOH:O	2.15	0.52
1:2A:2637:U:H5''	4:2E:82:ARG:NH1	2.25	0.52
19:1X:53:LYS:HB3	19:1X:82:GLN:HB3	1.92	0.52
32:1a:79:G:C2	32:1a:90:U:O2	2.63	0.52
51:1t:71:THR:HG22	51:1t:72:LEU:HG	1.92	0.52
10:2O:24:VAL:HG13	10:2O:33:ALA:HB2	1.90	0.52
32:2a:160:A:H2'	32:2a:161:A:C8	2.44	0.52
32:2a:1270:C:H2'	32:2a:1271:G:C8	2.44	0.52
39:2h:116:LYS:HD3	39:2h:127:LEU:HD23	1.91	0.52
49:2r:32:ARG:HA	49:2r:69:THR:HG21	1.91	0.52
1:1A:2791:C:H2'	1:1A:2792:G:H8	1.73	0.52
1:2A:223:A:O2'	1:2A:420:C:O2	2.27	0.52
32:1a:545:C:O2'	32:1a:549:C:OP1	2.28	0.52
32:1a:1277:C:O2'	32:1a:1279:A:H1'	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:1h:9:MET:HG3	39:1h:26:VAL:HG11	1.92	0.52
6:2G:166:ASP:O	6:2G:170:ARG:N	2.41	0.52
44:2m:16:ASP:HB3	44:2m:34:LEU:HD11	1.92	0.52
45:2n:29:ARG:HD3	45:2n:40:CYS:HB2	1.92	0.52
50:2s:51:VAL:HB	50:2s:75:ALA:HB2	1.91	0.52
1:1A:2151:G:H2'	1:1A:2152:G:C8	2.45	0.52
1:2A:2001:A:H2'	1:2A:2002:G:C8	2.45	0.52
1:2A:2173:A:H2'	1:2A:2174:C:O4'	2.10	0.52
11:1P:50:ARG:HD3	30:18:7:HIS:CD2	2.44	0.52
32:1a:110:C:O2'	47:1p:25:ARG:O	2.28	0.52
15:2T:29:ARG:NH2	15:2T:46:GLU:OE1	2.43	0.52
32:2a:475:G:H2'	32:2a:476:G:O4'	2.10	0.52
32:2a:1245:A:H2'	32:2a:1246:C:O4'	2.09	0.52
34:2c:142:MET:HG3	34:2c:170:GLN:HB3	1.92	0.52
40:2i:26:VAL:HG13	40:2i:61:ALA:HB3	1.92	0.52
54:2w:65:C:H2'	54:2w:66:A:C8	2.45	0.52
1:1A:615:G:OP1	5:1F:40:GLN:NE2	2.43	0.51
1:1A:1165:U:H2'	1:1A:1166:C:C6	2.45	0.51
1:1A:2123:G:H2'	1:1A:2124:G:C8	2.44	0.51
1:2A:521:G:H2'	1:2A:522:G:C8	2.45	0.51
1:2A:1181:C:H2'	1:2A:1182:A:C8	2.45	0.51
1:2A:1405:U:H2'	1:2A:1406:U:C6	2.46	0.51
1:2A:1769:G:O2'	1:2A:1958:C:OP1	2.28	0.51
3:1D:145:VAL:HG11	3:1D:175:LEU:HD11	1.92	0.51
32:1a:539:A:H2'	32:1a:540:G:C8	2.44	0.51
32:1a:1027:C:C4	32:1a:1034:G:N1	2.78	0.51
32:1a:1333:A:H2'	32:1a:1334:G:O4'	2.10	0.51
33:1b:24:TRP:CD1	33:1b:24:TRP:H	2.28	0.51
46:1o:25:THR:HG21	46:1o:70:LEU:HB2	1.91	0.51
6:2G:97:ASP:O	6:2G:101:ILE:HG13	2.10	0.51
12:2Q:39:PRO:HD3	12:2Q:99:PRO:HG3	1.91	0.51
32:2a:1009:G:H22	32:2a:1021:G:H1'	1.74	0.51
43:2l:113:ARG:HH21	43:2l:116:SER:HB2	1.75	0.51
1:1A:443:A:H1'	1:1A:1201:C:O4'	2.10	0.51
1:1A:2690:C:N4	1:1A:2713:A:H1'	2.25	0.51
1:2A:2371:G:O2'	28:26:46:HIS:ND1	2.42	0.51
1:2A:2438:U:O2'	1:2A:2440:C:OP1	2.26	0.51
7:1H:3:ARG:HH11	7:1H:4:ILE:H	1.55	0.51
11:1P:96:THR:HG23	11:1P:99:LEU:H	1.75	0.51
21:1Z:146:ILE:O	21:1Z:148:ASP:N	2.40	0.51
26:14:58:ARG:HH21	50:1s:68:GLY:HA3	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1021:G:O2'	32:1a:1022:G:O5'	2.28	0.51
32:1a:1028:C:H2'	32:1a:1029:C:O4'	2.10	0.51
32:1a:1503:A:O2'	53:1v:13:A:N1	2.43	0.51
34:1c:119:ARG:HE	34:1c:140:ARG:NH2	2.08	0.51
38:1g:28:ASN:HD21	38:1g:36:LYS:NZ	2.09	0.51
39:1h:86:ILE:HG13	39:1h:133:LEU:HD22	1.92	0.51
21:2Z:33:LEU:HD21	21:2Z:90:VAL:HG21	1.92	0.51
32:2a:1176:A:H2'	32:2a:1177:G:O4'	2.11	0.51
32:2a:1302:U:OP1	44:2m:13:LYS:NZ	2.35	0.51
38:2g:143:ARG:HH21	54:2y:42:G:H5'	1.76	0.51
50:2s:42:PRO:HA	50:2s:45:VAL:HG23	1.91	0.51
1:1A:1932:A:H2'	1:1A:1933:G:O4'	2.09	0.51
1:1A:2537:U:H2'	1:1A:2538:C:C6	2.45	0.51
1:1A:2820:A:P	13:1R:2:ARG:HH22	2.33	0.51
1:2A:902:C:H2'	1:2A:903:C:C6	2.46	0.51
1:2A:1598:C:O3'	19:2X:35:THR:OG1	2.29	0.51
1:2A:2059:A:O2'	5:2F:69:HIS:HD2	1.92	0.51
10:1O:68:GLU:HB3	10:1O:78:ARG:HB2	1.93	0.51
32:1a:658:G:H2'	32:1a:659:U:H6	1.75	0.51
40:1i:9:ARG:O	40:1i:104:ARG:HG3	2.10	0.51
2:2B:66:A:N6	2:2B:109:C:H5''	2.24	0.51
9:2N:104:LYS:HA	9:2N:107:LEU:HD12	1.92	0.51
12:2Q:34:LEU:HB2	12:2Q:118:LEU:HD22	1.91	0.51
32:2a:671:G:H2'	32:2a:672:U:O4'	2.10	0.51
32:2a:1318:A:H4'	50:2s:10:PHE:CE2	2.45	0.51
33:2b:24:TRP:H	33:2b:24:TRP:HD1	1.57	0.51
33:2b:98:LEU:N	33:2b:101:MET:HE2	2.25	0.51
1:1A:483:A:O2'	20:1Y:49:VAL:O	2.20	0.51
1:1A:580:C:H2'	1:1A:581:C:C6	2.45	0.51
1:1A:2161:C:O2'	1:1A:2162:G:H8	1.94	0.51
6:1G:106:LEU:HA	6:1G:110:ALA:HB3	1.93	0.51
28:16:28:ARG:NH2	28:16:29:ASN:OD1	2.44	0.51
32:1a:544:G:OP1	35:1d:59:ARG:NH2	2.39	0.51
32:1a:627:G:H2'	32:1a:628:G:C8	2.46	0.51
32:1a:1376:U:H2'	32:1a:1377:A:C8	2.45	0.51
40:1i:17:VAL:HG22	40:1i:63:ILE:HG12	1.93	0.51
44:1m:79:LYS:HA	44:1m:82:MET:HE2	1.92	0.51
13:2R:36:THR:OG1	13:2R:37:THR:N	2.43	0.51
13:2R:72:ASP:HB3	13:2R:75:LEU:HB3	1.93	0.51
32:2a:11:G:H1	32:2a:23:C:H42	1.58	0.51
48:2q:54:GLY:O	48:2q:81:ARG:N	2.43	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1826:G:H2'	1:1A:1827:C:O4'	2.10	0.51
1:2A:860:U:H1'	1:2A:2268:A:H5'	1.91	0.51
1:2A:1762:A:N1	61:2A:4052:HOH:O	2.35	0.51
1:2A:2176:A:H2'	1:2A:2177:C:C6	2.46	0.51
43:1l:54:LYS:HD2	43:1l:54:LYS:N	2.25	0.51
55:1x:23:C:H2'	55:1x:24:U:H6	1.74	0.51
3:2D:106:ILE:HD11	3:2D:144:ALA:HB2	1.93	0.51
12:2Q:17:LEU:HD21	12:2Q:41:TRP:HE1	1.75	0.51
32:2a:399:G:H2'	32:2a:400:C:C6	2.45	0.51
32:2a:1001(A):G:H3'	32:2a:1002:G:O4'	2.10	0.51
1:1A:883:G:N2	1:1A:893:C:H42	2.08	0.51
1:1A:2327:A:H2'	1:1A:2328:A:C8	2.46	0.51
1:2A:1805:U:O2	3:2D:50:THR:HB	2.11	0.51
4:1E:47:VAL:HG22	4:1E:84:PHE:O	2.10	0.51
33:1b:84:GLU:HB3	33:1b:219:VAL:HG21	1.92	0.51
34:1c:3:ASN:OD1	34:1c:3:ASN:N	2.44	0.51
36:1e:68:GLU:HG3	36:1e:70:PRO:HD3	1.92	0.51
38:1g:100:ALA:O	38:1g:104:LEU:HB2	2.11	0.51
44:1m:11:ARG:HA	44:1m:45:VAL:HB	1.91	0.51
4:2E:9:VAL:HG22	4:2E:25:VAL:HB	1.93	0.51
32:2a:1178:G:OP1	40:2i:93:ARG:NH1	2.44	0.51
35:2d:79:PHE:HE1	35:2d:204:ILE:HD13	1.75	0.51
39:2h:21:LYS:O	39:2h:65:TYR:OH	2.19	0.51
1:2A:1406:U:H2'	1:2A:1407:C:C6	2.45	0.51
5:1F:31:HIS:NE2	5:1F:35:GLU:OE2	2.39	0.51
32:1a:328:C:H4'	32:1a:329:A:H5'	1.93	0.51
32:1a:690:G:C6	32:1a:691:G:C6	2.98	0.51
40:1i:96:LEU:H	40:1i:98:PRO:HD2	1.74	0.51
2:2B:17:C:H2'	2:2B:18:G:O4'	2.10	0.51
11:2P:96:THR:HG23	11:2P:99:LEU:H	1.76	0.51
14:2S:15:ARG:HB3	14:2S:19:LYS:HE3	1.93	0.51
18:2W:34:ASN:OD1	18:2W:37:ARG:NH2	2.44	0.51
32:2a:1272:G:C2	32:2a:1273:G:H1'	2.45	0.51
32:2a:1402:4OC:HM22	32:2a:1403:C:H5'	1.93	0.51
32:2a:1411:C:H42	32:2a:1489:G:H1	1.59	0.51
1:1A:1071:G:H2'	1:1A:1072:C:H6	1.74	0.51
1:1A:1094:U:H3	1:1A:1096:A:H3'	1.76	0.51
1:1A:1936:A:OP1	1:1A:1937:A:H5'	2.11	0.51
1:1A:2787:C:H1'	4:1E:62:PRO:HG3	1.91	0.51
1:2A:1316:U:H2'	1:2A:1317:A:C8	2.46	0.51
9:1N:4:TYR:HB2	16:1U:101:ARG:NH1	2.26	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:10:38:VAL:HB	22:10:59:LEU:HB2	1.92	0.51
23:11:3:LYS:HB2	23:11:61:ARG:HH12	1.75	0.51
28:16:8:LYS:HD3	30:18:34:TRP:CD2	2.46	0.51
32:1a:186:C:H2'	32:1a:187:C:H6	1.75	0.51
33:1b:97:TRP:HZ2	33:1b:102:LEU:HD13	1.76	0.51
40:1i:31:GLN:HE21	40:1i:36:TYR:HD1	1.59	0.51
6:2G:16:ARG:O	6:2G:20:ILE:HG13	2.10	0.51
6:2G:72:ARG:HH12	6:2G:87:PRO:HG3	1.76	0.51
7:2H:41:MET:HE1	7:2H:54:ARG:HB3	1.92	0.51
32:2a:769:G:H4'	32:2a:1513:A:H4'	1.93	0.51
34:2c:127:ARG:NH2	34:2c:192:THR:OG1	2.44	0.51
36:2e:50:GLU:HB2	36:2e:53:LEU:HD12	1.91	0.51
44:2m:88:ARG:O	44:2m:92:HIS:ND1	2.43	0.51
44:2m:122:LYS:HG3	44:2m:123:ALA:H	1.76	0.51
1:1A:2136:C:N4	1:1A:2155:G:N1	2.25	0.51
1:2A:824:A:O2'	1:2A:2358:G:O6	2.25	0.51
2:1B:24:G:N7	2:1B:56:G:H2'	2.26	0.51
3:1D:108:PRO:HB3	3:1D:143:HIS:CE1	2.46	0.51
5:1F:64:ILE:HD11	5:1F:75:HIS:HB2	1.92	0.51
32:1a:1286:A:C8	32:1a:1287:A:H4'	2.45	0.51
7:2H:154:PRO:HB3	7:2H:163:TYR:CE1	2.46	0.51
32:2a:701:C:OP1	32:2a:702:A:O2'	2.20	0.51
32:2a:1070:U:H2'	32:2a:1071:C:H6	1.75	0.51
32:2a:1356:G:H2'	32:2a:1357:A:C8	2.45	0.51
52:2u:15:ARG:HB2	52:2u:15:ARG:NH1	2.25	0.51
54:2w:41:A:H2'	54:2w:42:G:C8	2.46	0.51
1:1A:1057:A:N6	1:1A:1087:G:OP2	2.43	0.51
1:1A:2627:G:O2'	1:1A:2781:A:N1	2.32	0.51
1:1A:2701:C:H2'	1:1A:2702:U:H2'	1.93	0.51
57:1A:4098:DI0:NAQ	57:1A:4098:DI0:CAP	2.73	0.51
1:2A:947:G:H2'	1:2A:948:G:C8	2.46	0.51
1:2A:1592:C:H2'	1:2A:1593:G:H8	1.75	0.51
1:2A:1688:U:O2	1:2A:1700:A:H5'	2.11	0.51
1:2A:2558:C:H2'	1:2A:2559:C:O4'	2.11	0.51
24:12:16:LEU:HB3	24:12:20:GLU:HB2	1.93	0.51
32:1a:1469:G:H2'	32:1a:1470:G:C8	2.46	0.51
33:1b:17:PHE:HB3	33:1b:44:LEU:HD11	1.93	0.51
33:1b:212:GLN:NE2	33:1b:234:PRO:O	2.44	0.51
34:1c:131:ARG:HE	34:1c:135:LYS:HE2	1.75	0.51
12:2Q:60:ARG:NH2	54:2w:54:5MU:H72	2.26	0.51
24:22:16:LEU:HD13	24:22:20:GLU:HB3	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:6:G:O2'	32:2a:7:G:H5'	2.11	0.51
32:2a:1327:C:OP1	52:2u:12:LYS:NZ	2.35	0.51
32:2a:1333:A:H2'	32:2a:1334:G:O4'	2.11	0.51
35:2d:88:VAL:HA	36:2e:97:GLY:HA3	1.93	0.51
39:2h:64:LYS:HG2	39:2h:79:VAL:HG21	1.92	0.51
1:1A:1047:G:H2'	1:1A:1110:G:H22	1.75	0.50
1:1A:1054:A:H3'	1:1A:1055:G:C8	2.46	0.50
1:1A:1342:A:OP2	61:1A:4249:HOH:O	2.19	0.50
1:1A:1783:A:H5'	1:1A:2608:G:H4'	1.92	0.50
1:1A:2867:G:OP2	15:1T:119:LYS:NZ	2.36	0.50
1:2A:350:U:H2'	1:2A:351:G:O4'	2.11	0.50
1:2A:468:G:OP2	29:27:37:LYS:NZ	2.43	0.50
1:2A:1899:G:H2'	1:2A:1899:G:N3	2.26	0.50
1:2A:2019:A:N7	27:25:9:LYS:HE2	2.25	0.50
1:2A:2126:A:H4'	1:2A:2127:G:OP1	2.11	0.50
1:2A:2645:G:N2	1:2A:2767:C:OP2	2.44	0.50
32:1a:193:C:H2'	32:1a:194:C:C6	2.44	0.50
32:1a:1309:G:OP1	44:1m:88:ARG:NH2	2.40	0.50
5:2F:132:VAL:HG21	5:2F:163:VAL:HG22	1.92	0.50
26:24:26:SER:OG	26:24:27:THR:N	2.43	0.50
32:2a:1513:A:H2'	32:2a:1514:C:C6	2.47	0.50
1:1A:1113:U:H2'	1:1A:1114:G:H8	1.76	0.50
1:1A:1186:G:OP1	61:1A:4299:HOH:O	2.18	0.50
1:1A:1864:U:OP1	1:1A:2410:G:O2'	2.22	0.50
1:1A:2693:A:H2'	1:1A:2694:G:C8	2.46	0.50
1:2A:229:A:H5'	1:2A:230:U:OP1	2.11	0.50
1:2A:2682:U:O2'	15:2T:58:ASN:ND2	2.45	0.50
8:1I:75:LEU:HD22	8:1I:105:HIS:CD2	2.46	0.50
21:1Z:9:TYR:OH	21:1Z:61:LEU:HD23	2.11	0.50
21:1Z:48:PHE:HE1	21:1Z:71:VAL:HG11	1.75	0.50
33:1b:200:ILE:HG22	33:1b:202:PRO:HD3	1.92	0.50
35:1d:178:VAL:O	35:1d:180:GLY:N	2.41	0.50
36:1e:90:VAL:O	36:1e:120:THR:HA	2.11	0.50
50:1s:43:GLU:OE1	50:1s:43:GLU:N	2.44	0.50
13:2R:56:LYS:NZ	13:2R:90:ARG:O	2.44	0.50
16:2U:49:HIS:HA	16:2U:52:ARG:HB2	1.93	0.50
32:2a:600:C:H2'	32:2a:601:C:C6	2.47	0.50
32:2a:1320:C:H2'	32:2a:1321:C:O4'	2.11	0.50
32:2a:1412:C:H2'	32:2a:1413:A:C8	2.46	0.50
32:2a:1469:G:H2'	32:2a:1470:G:H8	1.76	0.50
34:2c:28:GLN:HE21	34:2c:32:LEU:HD13	1.76	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:2m:67:GLU:HG3	44:2m:68:GLY:H	1.76	0.50
1:1A:2803:C:H2'	1:1A:2804:C:C6	2.47	0.50
1:2A:214:G:H1'	1:2A:216:A:O2'	2.11	0.50
1:2A:903:C:H2'	1:2A:904:C:C6	2.46	0.50
1:2A:2572:A:C8	4:2E:144:ARG:HD3	2.46	0.50
32:1a:1412:C:H2'	32:1a:1413:A:C8	2.46	0.50
39:1h:14:ARG:NH1	39:1h:83:ILE:O	2.44	0.50
44:1m:15:VAL:HG11	44:1m:48:LEU:HD21	1.94	0.50
50:1s:32:LYS:HA	50:1s:50:ALA:HB3	1.93	0.50
54:1w:75:C:H2'	54:1w:76:A:C8	2.47	0.50
32:2a:382:A:H2'	32:2a:383:A:C8	2.47	0.50
1:2A:392:C:H5''	1:2A:409:C:H5''	1.94	0.50
1:2A:1152:C:H2'	1:2A:1153:C:C6	2.46	0.50
1:2A:1430:C:H2'	1:2A:1431:U:C6	2.47	0.50
1:2A:2102:U:H2'	1:2A:2103:C:C6	2.47	0.50
1:2A:2278:A:H5''	22:20:12:ASN:HD21	1.77	0.50
4:1E:14:ILE:HG13	4:1E:21:VAL:HG13	1.93	0.50
32:1a:636:U:H2'	32:1a:637:G:H8	1.76	0.50
39:1h:16:ALA:HB1	39:1h:21:LYS:HB2	1.93	0.50
44:1m:11:ARG:C	44:1m:13:LYS:H	2.20	0.50
3:2D:159:ALA:HB1	3:2D:198:ASN:O	2.11	0.50
32:2a:1347:G:H22	32:2a:1373:G:H2'	1.77	0.50
33:2b:15:VAL:HG21	33:2b:213:LEU:HD13	1.92	0.50
34:2c:131:ARG:HH21	36:2e:50:GLU:HG3	1.76	0.50
45:2n:22:THR:HB	45:2n:33:VAL:HG21	1.92	0.50
50:2s:49:ILE:HG13	50:2s:62:ILE:HD11	1.92	0.50
54:2y:8:4SU:H5'	54:2y:9:A:OP2	2.11	0.50
1:1A:1999:C:H4'	1:1A:2723:C:O2	2.10	0.50
1:2A:2787:C:H1'	4:2E:62:PRO:HG3	1.93	0.50
14:1S:93:LYS:HG2	14:1S:95:HIS:HB2	1.93	0.50
32:1a:998:G:H1	32:1a:1043:C:N4	2.09	0.50
34:1c:148:GLY:HA3	34:1c:172:ARG:O	2.12	0.50
47:1p:20:VAL:HG21	47:1p:32:TYR:CD2	2.45	0.50
51:1t:40:ALA:HB2	51:1t:55:ILE:HG22	1.93	0.50
32:2a:619:U:N3	35:2d:134:ASP:OD1	2.35	0.50
36:2e:5:ASP:N	36:2e:5:ASP:OD1	2.44	0.50
36:2e:78:HIS:CD2	39:2h:104:ARG:HG3	2.47	0.50
38:2g:65:ALA:O	38:2g:69:VAL:HG23	2.11	0.50
52:2u:5:ASP:O	52:2u:11:GLY:HA3	2.11	0.50
1:1A:1047:G:H2'	1:1A:1110:G:N2	2.24	0.50
1:1A:2074:U:H2'	1:1A:2075:U:C6	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2721:A:OP1	61:2A:3982:HOH:O	2.19	0.50
13:1R:100:LEU:HD11	13:1R:113:LEU:HD23	1.93	0.50
20:1Y:35:TYR:CE2	20:1Y:69:ALA:HB3	2.46	0.50
7:2H:150:ALA:HA	7:2H:153:LYS:HG2	1.93	0.50
32:2a:939:G:H1	32:2a:1344:C:H42	1.60	0.50
34:2c:32:LEU:HD21	34:2c:59:ARG:HD2	1.94	0.50
43:2l:70:ILE:HG12	43:2l:100:ILE:HD12	1.94	0.50
47:2p:14:ASN:HA	47:2p:42:ARG:HH21	1.77	0.50
1:1A:774:A:N3	1:1A:774:A:H2'	2.25	0.50
1:1A:2292:C:OP1	14:1S:17:ARG:NH2	2.33	0.50
1:1A:2361:A:H5'	30:18:27:THR:OG1	2.11	0.50
1:1A:2693:A:H2'	1:1A:2694:G:H8	1.76	0.50
32:1a:1458:G:OP1	51:1t:35:THR:OG1	2.27	0.50
6:2G:125:PHE:HB3	6:2G:166:ASP:CG	2.36	0.50
8:2I:93:THR:HG22	8:2I:119:PRO:HB3	1.94	0.50
9:2N:21:LYS:HD3	9:2N:26:LEU:HD13	1.93	0.50
13:2R:51:LEU:HD22	13:2R:66:VAL:HG13	1.93	0.50
22:20:27:GLU:HB2	22:20:69:PHE:HD2	1.77	0.50
32:2a:1239:A:H62	32:2a:1299:A:N6	2.09	0.50
32:2a:1371:G:O3'	40:2i:69:GLY:HA3	2.12	0.50
38:2g:69:VAL:HG11	38:2g:134:ALA:HB1	1.94	0.50
39:2h:10:LEU:HD13	39:2h:83:ILE:HG12	1.93	0.50
47:2p:19:ILE:N	47:2p:37:GLY:O	2.45	0.50
54:2y:21:A:H2'	54:2y:21:A:N3	2.26	0.50
1:1A:1803:A:O2'	3:1D:259:THR:HG21	2.11	0.50
1:1A:2022:U:O2'	1:1A:2617:C:H5'	2.11	0.50
1:2A:668:G:H5'	1:2A:669:G:OP2	2.10	0.50
1:2A:673:C:H5''	5:2F:81:PRO:HD2	1.92	0.50
1:2A:821:A:N1	61:2A:4053:HOH:O	2.35	0.50
1:2A:2849:U:H4'	1:2A:2868:A:C2	2.47	0.50
32:1a:390:C:H2'	32:1a:391:G:C8	2.47	0.50
32:1a:458:C:H2'	32:1a:460:G:O4'	2.12	0.50
32:1a:523:A:N1	43:1l:92:OTD:H6	2.27	0.50
32:1a:757:U:H2'	32:1a:758:G:O4'	2.11	0.50
32:1a:1305:G:N7	61:1a:1952:HOH:O	2.33	0.50
54:1w:65:C:H2'	54:1w:66:A:C8	2.47	0.50
10:2O:68:GLU:OE1	10:2O:78:ARG:NH1	2.45	0.50
23:21:23:LYS:HB3	23:21:29:GLY:HA3	1.93	0.50
31:29:16:VAL:HG22	31:29:25:VAL:HG22	1.94	0.50
32:2a:1258:G:H2'	32:2a:1259:C:C6	2.47	0.50
32:2a:1435:G:H2'	32:2a:1436:U:C6	2.47	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:2b:100:GLY:N	33:2b:176:GLU:OE2	2.45	0.50
1:1A:1057:A:N1	1:1A:1081:U:O4	2.44	0.50
1:1A:1086:A:O3'	1:1A:1087:G:H8	1.94	0.50
1:1A:1178:C:H2'	1:1A:1179:C:C6	2.47	0.50
1:1A:1796:U:H2'	1:1A:1797:C:C6	2.46	0.50
1:2A:955:C:OP2	12:2Q:14:ARG:HG3	2.10	0.50
1:2A:1406:U:H2'	1:2A:1407:C:H6	1.77	0.50
1:2A:1865:G:OP1	61:2A:3984:HOH:O	2.20	0.50
1:2A:2803:C:H2'	1:2A:2804:C:C6	2.47	0.50
2:1B:92:C:H5''	21:1Z:79:ARG:NH1	2.27	0.50
3:1D:8:PRO:HB3	3:1D:14:ARG:HB2	1.92	0.50
19:1X:2:LYS:NZ	19:1X:38:GLU:OE2	2.43	0.50
44:1m:122:LYS:HG3	44:1m:123:ALA:H	1.76	0.50
4:2E:11:MET:HG2	4:2E:24:THR:HB	1.94	0.50
7:2H:92:ILE:H	7:2H:92:ILE:HD12	1.77	0.50
8:2I:72:LEU:HD21	8:2I:107:VAL:HG11	1.94	0.50
32:2a:302:G:N3	32:2a:556:C:H4'	2.26	0.50
32:2a:1007:C:O2	32:2a:1022:G:N1	2.41	0.50
32:2a:1030:C:N3	32:2a:1031:G:N2	2.53	0.50
43:2l:110:VAL:HG23	43:2l:120:TYR:HB3	1.93	0.50
1:2A:65:C:O2'	1:2A:456:C:N3	2.37	0.49
1:2A:932:G:H4'	1:2A:933:A:O5'	2.12	0.49
1:2A:1641:A:H2'	1:2A:1642:G:O4'	2.12	0.49
32:1a:1030:C:H3'	32:1a:1030(A):G:C5'	2.40	0.49
33:1b:25:ASN:OD1	33:1b:27:LYS:HG2	2.12	0.49
2:2B:14:U:O3'	2:2B:108:U:O2'	2.30	0.49
32:2a:139:G:H2'	32:2a:140:A:C8	2.41	0.49
32:2a:546:G:OP1	35:2d:73:ARG:HG2	2.11	0.49
32:2a:1080:A:OP1	36:2e:47:LYS:HD3	2.11	0.49
32:2a:1120:G:H2'	32:2a:1121:U:C6	2.47	0.49
32:2a:1252:A:H61	32:2a:1285:A:H61	1.58	0.49
33:2b:178:ARG:NH2	39:2h:74:PRO:HB3	2.27	0.49
38:2g:26:PHE:O	38:2g:30:ILE:HG13	2.12	0.49
54:2w:5:G:H2'	54:2w:6:A:C8	2.47	0.49
54:2w:54:5MU:H2'	54:2w:55:PSU:O4'	2.12	0.49
1:1A:2238:G:N3	1:1A:2238:G:H2'	2.26	0.49
1:2A:928:G:H8	1:2A:928:G:O5'	1.94	0.49
14:1S:10:ARG:O	14:1S:14:VAL:HG13	2.12	0.49
30:18:62:LEU:HB3	30:18:65:GLU:HG2	1.94	0.49
19:2X:72:LYS:NZ	19:2X:75:ASP:OD1	2.43	0.49
32:2a:646:U:H2'	32:2a:647:C:C6	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:921:U:O2	36:2e:19:MET:HB2	2.12	0.49
32:2a:1118:C:H1'	32:2a:1179:A:C4	2.47	0.49
32:2a:1182:G:H4'	32:2a:1183:A:H5''	1.94	0.49
32:2a:1262:C:N4	32:2a:1273:G:H1	2.10	0.49
39:2h:20:TYR:HE2	39:2h:75:ARG:HD2	1.77	0.49
1:1A:414:C:H2'	1:1A:415:A:C8	2.48	0.49
1:2A:1296:G:OP1	1:2A:2709:G:O2'	2.18	0.49
6:1G:5:VAL:HG22	6:1G:8:LYS:H	1.77	0.49
12:1Q:38:GLU:HA	12:1Q:99:PRO:HG3	1.95	0.49
32:1a:69:G:H2'	32:1a:70:G:C8	2.47	0.49
32:1a:222:U:H2'	32:1a:223:U:C6	2.47	0.49
32:1a:407:G:OP1	35:1d:115:ARG:NH2	2.45	0.49
32:1a:1005:A:OP2	32:1a:1024:G:N2	2.45	0.49
32:1a:1286:A:H2'	32:1a:1287:A:H4'	1.94	0.49
33:1b:92:TYR:CE1	33:1b:94:ASN:HB2	2.48	0.49
39:1h:51:VAL:HG12	39:1h:52:ASP:H	1.77	0.49
32:2a:1190:G:H5'	34:2c:176:HIS:CE1	2.47	0.49
55:2x:15:G:H2'	55:2x:59:A:N1	2.27	0.49
54:2y:61:C:H2'	54:2y:62:C:C6	2.47	0.49
1:1A:64:A:O3'	19:1X:71:GLY:HA3	2.12	0.49
1:1A:222:A:H5''	1:1A:421:U:OP1	2.13	0.49
1:1A:476:G:H4'	1:1A:502:A:N1	2.27	0.49
1:1A:918:A:H5''	2:1B:98:G:O2'	2.12	0.49
1:2A:90:U:H1'	1:2A:92:A:C8	2.47	0.49
1:2A:839:U:H2'	1:2A:840:C:C6	2.47	0.49
1:2A:1818:U:OP2	3:2D:157:ARG:HD3	2.12	0.49
1:2A:1935:G:H1'	1:2A:1964:G:N2	2.28	0.49
4:1E:77:ILE:HD12	4:1E:195:LEU:HD22	1.93	0.49
8:1I:86:THR:HG22	8:1I:122:GLU:OE1	2.13	0.49
33:1b:77:ALA:HB2	33:1b:165:VAL:HG11	1.94	0.49
47:1p:43:LYS:HG2	47:1p:48:TRP:CE2	2.48	0.49
4:2E:170:LEU:HB3	4:2E:184:VAL:HG22	1.94	0.49
32:2a:114:U:O2'	32:2a:115:G:H5'	2.13	0.49
32:2a:675:A:H2'	32:2a:676:A:O4'	2.12	0.49
32:2a:1328:C:OP1	52:2u:21:TYR:OH	2.27	0.49
33:2b:16:HIS:HB3	33:2b:210:SER:HB2	1.95	0.49
33:2b:16:HIS:CD2	33:2b:204:ASN:H	2.30	0.49
40:2i:99:LEU:HB3	40:2i:101:PHE:CE1	2.47	0.49
50:2s:18:LYS:HD2	50:2s:31:ILE:HG23	1.94	0.49
1:1A:253:C:O2'	61:1A:4304:HOH:O	2.19	0.49
1:1A:271(E):U:H2'	1:1A:271(F):C:C6	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2206:G:OP2	1:1A:2206:G:H4'	2.13	0.49
1:1A:2429:G:OP1	61:1A:4231:HOH:O	2.20	0.49
1:2A:817:C:O2'	1:2A:839:U:H5''	2.13	0.49
1:2A:1035:U:H2'	1:2A:1036:G:C8	2.47	0.49
1:2A:2507:C:H2'	1:2A:2508:G:O4'	2.11	0.49
1:2A:2802:G:H2'	1:2A:2803:C:O4'	2.11	0.49
4:1E:12:THR:HG22	4:1E:13:ARG:H	1.78	0.49
32:1a:250:A:H4'	32:1a:251:G:O5'	2.12	0.49
32:1a:410:G:OP1	35:1d:30:LYS:NZ	2.42	0.49
35:1d:173:TRP:CD1	35:1d:173:TRP:H	2.29	0.49
36:1e:105:VAL:HB	36:1e:106:PRO:HD3	1.94	0.49
4:2E:176:ILE:HB	4:2E:181:LEU:HB2	1.94	0.49
18:2W:46:PHE:O	18:2W:50:VAL:HG23	2.12	0.49
32:2a:263:A:OP1	51:2t:79:ARG:NH1	2.45	0.49
32:2a:1032:G:H2'	32:2a:1033:G:C8	2.46	0.49
32:2a:1064:G:OP1	32:2a:1386:G:H4'	2.13	0.49
55:2x:61:C:H2'	55:2x:62:C:H6	1.78	0.49
1:1A:269:U:C2'	1:1A:270:A:H5'	2.41	0.49
1:1A:2142:C:H2'	1:1A:2143:C:C6	2.46	0.49
1:1A:2218:U:O4'	23:11:52:ARG:NH2	2.45	0.49
1:2A:30:G:H2'	1:2A:31:C:C6	2.47	0.49
1:2A:311:A:C6	1:2A:328:U:C4	3.01	0.49
1:2A:625:G:N7	11:2P:107:LYS:NZ	2.52	0.49
1:2A:2136:C:O2'	1:2A:2137:C:H6	1.96	0.49
1:2A:2291:U:H2'	1:2A:2292:C:C6	2.46	0.49
14:1S:14:VAL:O	14:1S:18:ILE:HG12	2.13	0.49
25:13:59:VAL:O	25:13:60:GLU:HG2	2.13	0.49
32:1a:100:C:H2'	32:1a:101:A:C8	2.47	0.49
32:1a:1095:U:P	32:1a:1108:G:H1	2.36	0.49
40:1i:128:ARG:NH2	55:1x:33:U:OP2	2.46	0.49
6:2G:46:ALA:HB2	6:2G:53:LEU:HG	1.94	0.49
16:2U:8:VAL:O	16:2U:12:ARG:HG3	2.13	0.49
32:2a:1469:G:H2'	32:2a:1470:G:C8	2.47	0.49
50:2s:28:LYS:HB3	50:2s:29:ARG:CA	2.42	0.49
52:2u:2:GLY:O	52:2u:4:GLY:N	2.45	0.49
1:1A:34:C:H5''	1:1A:35:G:OP2	2.13	0.49
1:1A:1379:A:H4'	1:1A:1380:G:OP2	2.11	0.49
1:1A:1876:A:H2'	1:1A:1877:A:H8	1.78	0.49
1:1A:2328:A:H2'	1:1A:2329:G:C8	2.47	0.49
1:1A:2724:C:OP1	4:1E:118:LYS:NZ	2.41	0.49
1:2A:796:C:H2'	1:2A:797:C:C6	2.46	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1514:U:H2'	1:2A:1515:G:H8	1.78	0.49
1:2A:1614:A:P	1:2A:1614:A:H8	2.36	0.49
1:2A:1798:U:H5'	3:2D:259:THR:CG2	2.42	0.49
10:1O:25:LEU:HG	10:1O:40:VAL:HG23	1.94	0.49
10:1O:30:ALA:N	61:1O:302:HOH:O	2.44	0.49
32:1a:620:C:H2'	32:1a:621:A:O4'	2.12	0.49
32:1a:952:U:H2'	32:1a:953:G:C8	2.48	0.49
32:1a:1218:C:H2'	32:1a:1219:U:C6	2.47	0.49
33:1b:21:ARG:HB3	33:1b:39:ILE:HG12	1.94	0.49
36:1e:41:VAL:HG23	36:1e:67:VAL:HG12	1.95	0.49
37:1f:10:LEU:HD13	37:1f:61:LEU:HD13	1.94	0.49
54:1w:29:U:H3	54:1w:41:A:H61	1.60	0.49
54:1y:53:G:H2'	54:1y:54:5MU:H6	1.78	0.49
6:2G:5:VAL:HG13	6:2G:8:LYS:HE2	1.93	0.49
11:2P:50:ARG:HH21	30:28:7:HIS:CD2	2.29	0.49
12:2Q:66:ILE:HG12	12:2Q:104:PHE:CD1	2.48	0.49
32:2a:352:C:O2'	32:2a:354:G:OP1	2.27	0.49
33:2b:19:HIS:NE2	33:2b:206:ASP:OD2	2.38	0.49
33:2b:51:LEU:HD21	33:2b:201:ILE:HG23	1.95	0.49
48:2q:9:VAL:HG12	48:2q:56:VAL:HG22	1.95	0.49
1:1A:2169:A:N6	54:1y:19:G:H1	2.11	0.49
1:1A:2441:C:OP2	1:1A:2586:C:O2'	2.30	0.49
19:1X:12:VAL:HG22	19:1X:29:TRP:CE2	2.48	0.49
33:1b:127:ILE:HD12	33:1b:130:ARG:HD3	1.94	0.49
34:1c:87:LEU:O	34:1c:91:LEU:HB2	2.12	0.49
4:2E:48:GLN:NE2	4:2E:78:LEU:HD13	2.28	0.49
5:2F:64:ILE:HG21	5:2F:78:ILE:HG23	1.95	0.49
32:2a:678:U:H2'	32:2a:679:C:C6	2.47	0.49
32:2a:967:5MC:H2'	32:2a:968:A:C8	2.47	0.49
35:2d:162:LEU:HD22	35:2d:178:VAL:HG13	1.94	0.49
42:2k:34:ASP:HB3	42:2k:40:ILE:HD11	1.93	0.49
1:1A:300:A:OP1	20:1Y:86:ARG:NH2	2.45	0.49
1:1A:922:U:H2'	1:1A:923:C:C6	2.48	0.49
1:1A:1028:A:N6	1:1A:1125:G:H2'	2.28	0.49
1:1A:1268:A:H2'	1:1A:1269:A:O4'	2.12	0.49
1:2A:57:C:H2'	1:2A:58:G:O4'	2.13	0.49
1:2A:459:U:H5''	29:27:40:TRP:CD2	2.48	0.49
1:2A:1022:G:N2	1:2A:1023:U:O4	2.46	0.49
1:2A:1518:U:H2'	1:2A:1519:G:O4'	2.13	0.49
1:2A:2473:U:O2	1:2A:2473:U:H2'	2.13	0.49
1:2A:2630:G:H2'	1:2A:2631:G:H8	1.76	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1R:12:ARG:O	13:1R:17:ARG:NH1	2.46	0.49
32:1a:79:G:C6	32:1a:90:U:N3	2.79	0.49
32:1a:278:G:OP2	48:1q:92:ARG:NH2	2.46	0.49
32:1a:1064:G:H4'	32:1a:1065:U:OP1	2.13	0.49
35:1d:7:PRO:HB2	35:1d:10:ARG:HD2	1.94	0.49
42:1k:33:THR:HA	42:1k:39:PRO:HA	1.94	0.49
44:1m:87:TYR:O	44:1m:91:ARG:HG2	2.13	0.49
48:1q:45:HIS:NE2	48:1q:47:PRO:HB3	2.28	0.49
54:1y:66:A:H2'	54:1y:67:U:C6	2.47	0.49
6:2G:44:GLY:N	6:2G:88:ILE:O	2.44	0.49
11:2P:52:GLU:HG3	30:28:57:ARG:HH22	1.78	0.49
32:2a:1002:G:N1	32:2a:1003:G:H8	2.11	0.49
32:2a:1038:C:H2'	32:2a:1039:C:C5	2.48	0.49
32:2a:1376:U:H2'	32:2a:1377:A:H8	1.77	0.49
32:2a:1479:C:H2'	32:2a:1480:G:H8	1.78	0.49
34:2c:110:ASN:O	34:2c:141:VAL:HG22	2.13	0.49
35:2d:98:GLU:OE1	35:2d:103:ASN:ND2	2.42	0.49
51:2t:50:GLU:O	51:2t:100:ILE:HD11	2.11	0.49
1:1A:893:C:H2'	1:1A:894:C:C6	2.47	0.49
1:1A:1188:U:H4'	17:1V:79:VAL:HG22	1.95	0.49
1:1A:2612:C:OP2	27:15:2:ALA:N	2.46	0.49
1:2A:288:C:H2'	1:2A:289:A:H8	1.77	0.49
1:2A:1011:G:OP2	16:2U:66:ASN:ND2	2.39	0.49
5:1F:28:ILE:O	5:1F:30:PRO:HD3	2.12	0.49
32:1a:92:C:H2'	32:1a:93:G:C8	2.47	0.49
32:1a:262:A:H2'	32:1a:263:A:C8	2.48	0.49
32:1a:300:A:H2'	32:1a:301:G:O4'	2.12	0.49
32:1a:539:A:OP2	43:1l:115:LYS:NZ	2.46	0.49
32:1a:736:C:H2'	32:1a:737:A:C8	2.47	0.49
3:2D:206:LEU:O	3:2D:211:ARG:HD3	2.12	0.49
21:2Z:9:TYR:OH	21:2Z:61:LEU:HD23	2.13	0.49
32:2a:994:A:N7	32:2a:1216:G:H4'	2.28	0.49
32:2a:1255:G:OP1	41:2j:45:ARG:NH2	2.45	0.49
32:2a:1353:G:H2'	32:2a:1354:C:C6	2.48	0.49
32:2a:1381:U:O2'	38:2g:79:ARG:HD3	2.13	0.49
32:2a:1502:A:C8	32:2a:1505:G:N2	2.79	0.49
36:2e:81:GLU:HG2	36:2e:90:VAL:HG13	1.95	0.49
47:2p:3:LYS:O	47:2p:21:VAL:HA	2.13	0.49
1:1A:882:G:H4'	54:1w:19:G:O6	2.13	0.48
1:2A:1826:G:H4'	3:2D:242:ARG:CZ	2.42	0.48
1:2A:2646:C:OP2	1:2A:2732:G:O2'	2.28	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1F:12:LEU:HB3	5:1F:126:VAL:HG12	1.93	0.48
11:1P:62:LEU:O	30:18:13:ARG:HD3	2.13	0.48
32:1a:1370:G:N7	61:1a:1958:HOH:O	2.35	0.48
54:1w:1:G:H5''	61:1w:205:HOH:O	2.13	0.48
54:1w:9:A:O2'	54:1w:10:G:N7	2.46	0.48
17:2V:62:LEU:HD21	17:2V:95:LEU:HB2	1.95	0.48
26:24:46:GLN:NE2	26:24:48:ARG:HD3	2.28	0.48
32:2a:1126:U:O2	41:2j:40:LEU:HD21	2.13	0.48
34:2c:111:LEU:HG	34:2c:144:SER:HB3	1.94	0.48
35:2d:109:GLY:HA3	35:2d:165:MET:HG3	1.95	0.48
41:2j:6:ILE:HG12	41:2j:98:ILE:HG12	1.93	0.48
42:2k:87:THR:O	42:2k:87:THR:OG1	2.27	0.48
1:1A:71:A:N7	19:1X:31:HIS:HE1	2.11	0.48
1:1A:340:A:H2'	1:1A:341:G:O4'	2.13	0.48
1:1A:1903:G:OP1	3:1D:241:PRO:HB2	2.13	0.48
1:2A:38:A:H2'	1:2A:39:C:C6	2.48	0.48
1:2A:639:U:H2'	1:2A:640:C:C6	2.48	0.48
10:1O:34:THR:OG1	10:1O:35:VAL:N	2.47	0.48
23:11:21:ARG:HG2	23:11:22:GLY:N	2.28	0.48
24:12:65:ASN:HD22	24:12:69:ARG:HH11	1.60	0.48
32:1a:176:C:H2'	32:1a:177:C:C6	2.49	0.48
32:1a:544:G:P	35:1d:59:ARG:HH22	2.35	0.48
32:1a:946:A:O2'	32:1a:1333:A:N3	2.44	0.48
54:1w:43:G:H2'	54:1w:44:G:C8	2.47	0.48
5:2F:28:ILE:HG12	5:2F:112:MET:HB3	1.95	0.48
17:2V:16:PRO:HD3	17:2V:99:ILE:HD11	1.95	0.48
32:2a:520:A:N1	32:2a:536:C:H1'	2.27	0.48
32:2a:952:U:H2'	32:2a:953:G:C8	2.48	0.48
32:2a:1013:G:N2	32:2a:1016:A:OP2	2.41	0.48
33:2b:127:ILE:O	33:2b:129:GLU:N	2.46	0.48
34:2c:7:PRO:O	34:2c:11:ARG:NH1	2.46	0.48
55:2x:61:C:H2'	55:2x:62:C:C6	2.48	0.48
1:1A:747:U:O2	1:1A:2014:A:H1'	2.14	0.48
1:1A:1093:G:H3'	1:1A:1094:U:H5''	1.95	0.48
1:2A:1448:G:H1'	1:2A:1528:A:N1	2.29	0.48
1:2A:2741:A:H2'	1:2A:2742:C:O4'	2.12	0.48
5:1F:132:VAL:HA	5:1F:138:GLU:HB3	1.95	0.48
5:1F:161:GLU:HG2	5:1F:164:ARG:NH2	2.28	0.48
25:13:6:VAL:HG12	25:13:28:LEU:HD11	1.95	0.48
32:1a:134:A:H1'	32:1a:325:A:C5	2.48	0.48
32:1a:1346:A:N1	32:1a:1374:A:H5''	2.28	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:1b:18:GLY:HA3	33:1b:42:ILE:HG13	1.95	0.48
51:1t:50:GLU:O	51:1t:100:ILE:HD11	2.14	0.48
54:1y:5:G:H2'	54:1y:6:A:O4'	2.14	0.48
17:2V:69:LYS:HA	17:2V:88:ARG:HG2	1.95	0.48
32:2a:253:U:H2'	32:2a:254:G:C8	2.49	0.48
32:2a:434:U:H2'	32:2a:435:C:C6	2.48	0.48
32:2a:601:C:H2'	32:2a:602:A:C8	2.48	0.48
32:2a:1137:C:H5''	32:2a:1138:G:OP1	2.13	0.48
32:2a:1403:C:H2'	32:2a:1404:5MC:HM53	1.93	0.48
34:2c:117:ALA:HB2	34:2c:200:ALA:HB2	1.95	0.48
44:2m:23:TYR:CE2	44:2m:71:ARG:HG3	2.48	0.48
1:1A:1131:G:H21	9:1N:73:THR:HG21	1.79	0.48
1:1A:1441:G:H2'	1:1A:1442:G:H8	1.78	0.48
1:1A:2106:G:H2'	1:1A:2107:C:H6	1.79	0.48
1:2A:141:A:H8	1:2A:1408:C:HO2'	1.58	0.48
1:2A:443:A:H1'	1:2A:1201:C:O4'	2.12	0.48
1:2A:458:G:O2'	1:2A:469:G:O6	2.30	0.48
1:2A:856:C:H2'	1:2A:857:C:C6	2.48	0.48
2:1B:66:A:H61	2:1B:108:U:H2'	1.79	0.48
32:1a:721:G:H4'	32:1a:722:A:O4'	2.13	0.48
32:1a:1329:A:H5''	44:1m:26:GLY:H	1.77	0.48
38:1g:86:GLN:NE2	54:1y:32:C:O2'	2.46	0.48
2:2B:75:G:H22	21:2Z:73:GLN:HE21	1.59	0.48
6:2G:15:VAL:HG13	6:2G:175:LEU:HD23	1.94	0.48
32:2a:565:U:OP2	32:2a:566:G:O2'	2.30	0.48
32:2a:1286:A:H8	32:2a:1287:A:H4'	1.75	0.48
1:1A:226:G:N2	1:1A:228:A:H62	2.12	0.48
1:1A:729:G:C8	3:1D:208:LYS:HD2	2.47	0.48
1:1A:1634:A:H5''	61:1A:5613:HOH:O	2.13	0.48
1:1A:1851:U:H2'	1:1A:1852:C:O4'	2.13	0.48
1:1A:2233:U:H2'	1:1A:2234:G:C8	2.47	0.48
1:1A:2239:G:H5'	3:1D:251:GLY:HA3	1.95	0.48
1:2A:897:C:H2'	1:2A:898:C:C2	2.49	0.48
1:2A:964:C:O2'	1:2A:2273:A:N3	2.40	0.48
6:1G:39:ILE:HD12	6:1G:64:THR:HG21	1.95	0.48
12:1Q:137:TYR:O	12:1Q:141:GLN:HG2	2.13	0.48
32:1a:618:C:H5''	32:1a:619:U:H5''	1.95	0.48
32:1a:1002:G:H3'	32:1a:1003:G:H4'	1.96	0.48
32:1a:1397:C:OP2	36:1e:24:ARG:NH2	2.44	0.48
55:1x:23:C:H2'	55:1x:24:U:C6	2.48	0.48
2:2B:48:A:H4'	14:2S:95:HIS:HD2	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:2I:77:LEU:HD12	8:2I:101:LEU:HD13	1.96	0.48
8:2I:124:GLY:N	8:2I:144:VAL:HG23	2.28	0.48
16:2U:65:ILE:HD11	16:2U:95:LEU:HB3	1.95	0.48
32:2a:45:U:H2'	32:2a:46:G:C8	2.49	0.48
32:2a:573:A:N3	32:2a:883:C:O2'	2.47	0.48
32:2a:817:C:OP2	61:2a:1930:HOH:O	2.20	0.48
32:2a:881:G:H2'	32:2a:882:C:O4'	2.13	0.48
35:2d:127:THR:HG23	35:2d:147:ALA:HB3	1.94	0.48
36:2e:39:GLY:HA2	36:2e:69:VAL:HG13	1.94	0.48
36:2e:75:THR:OG1	36:2e:117:ASP:O	2.22	0.48
43:2l:7:ILE:O	43:2l:11:VAL:HG23	2.14	0.48
1:1A:93:G:H2'	1:1A:94:C:C6	2.48	0.48
1:1A:1357:U:H2'	1:1A:1358:G:O4'	2.14	0.48
1:1A:1639:U:O2'	1:1A:1640:C:H5'	2.13	0.48
1:2A:1187:G:H5'	17:2V:81:TYR:CE1	2.48	0.48
1:2A:1336:A:H2'	1:2A:1337:G:C8	2.49	0.48
1:2A:1477:A:H2'	1:2A:1478:G:O4'	2.13	0.48
20:1Y:9:LYS:HA	20:1Y:10:GLY:HA2	1.65	0.48
32:1a:848:C:H2'	32:1a:849:C:H6	1.78	0.48
32:1a:977:A:O2'	32:1a:979:C:OP2	2.32	0.48
34:1c:22:TRP:CZ2	45:1n:54:PRO:HG2	2.49	0.48
41:1j:55:LYS:O	41:1j:57:LYS:N	2.47	0.48
50:1s:40:ILE:HB	50:1s:67:VAL:O	2.13	0.48
54:1y:40:G:H2'	54:1y:41:A:H8	1.79	0.48
8:2I:5:LEU:HD23	8:2I:36:ALA:HB2	1.95	0.48
13:2R:96:ARG:NH2	13:2R:117:VAL:HG13	2.28	0.48
21:2Z:73:GLN:O	21:2Z:87:ASP:N	2.41	0.48
32:2a:1512:U:H2'	32:2a:1513:A:C8	2.49	0.48
34:2c:47:LEU:HD13	34:2c:68:VAL:HG11	1.96	0.48
1:1A:330:A:N7	1:1A:1210:A:O2'	2.34	0.48
1:1A:2133:G:O2'	1:1A:2157:G:N1	2.41	0.48
1:1A:2277:G:P	22:10:10:THR:HG21	2.54	0.48
1:2A:729:G:C6	3:2D:208:LYS:HB2	2.48	0.48
1:2A:774:A:H2'	1:2A:774:A:N3	2.29	0.48
1:2A:895:U:H2'	1:2A:897:C:C5	2.48	0.48
1:2A:2429:G:O6	11:2P:61:ARG:NE	2.46	0.48
1:2A:2627:G:O2'	1:2A:2781:A:N1	2.46	0.48
3:1D:26:LYS:HE2	3:1D:28:GLU:O	2.13	0.48
3:1D:206:LEU:HD22	3:1D:211:ARG:HG2	1.94	0.48
32:1a:189(K):U:H2'	32:1a:189(L):G:C8	2.49	0.48
32:1a:473:G:H2'	32:1a:474:G:C8	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:553:A:H5''	43:1l:24:VAL:HG21	1.96	0.48
32:1a:1216:G:OP1	45:1n:2:ALA:HA	2.13	0.48
32:1a:1278:U:H5'	32:1a:1279:A:O4'	2.13	0.48
33:1b:51:LEU:HD21	33:1b:201:ILE:HG23	1.95	0.48
3:2D:108:PRO:HD2	3:2D:111:LEU:HD22	1.95	0.48
12:2Q:4:PRO:HD3	12:2Q:70:PRO:O	2.13	0.48
12:2Q:35:VAL:HG12	12:2Q:130:LYS:O	2.13	0.48
15:2T:24:PRO:HA	15:2T:49:VAL:HG23	1.96	0.48
32:2a:1257:U:O4	45:2n:17:LYS:NZ	2.39	0.48
40:2i:79:LEU:HD22	40:2i:104:ARG:HB2	1.95	0.48
50:2s:50:ALA:HB1	50:2s:57:HIS:HB3	1.95	0.48
1:1A:536:A:H2'	1:1A:537:C:C6	2.49	0.48
1:1A:821:A:H2'	1:1A:946:G:H5''	1.94	0.48
1:1A:957:A:N1	1:1A:2458:G:H4'	2.29	0.48
1:1A:1006:C:H1'	9:1N:106:MET:HB3	1.96	0.48
1:1A:2365:G:O6	30:18:39:LYS:HE3	2.13	0.48
1:2A:747:U:O2	1:2A:2014:A:H1'	2.14	0.48
1:2A:815:C:H2'	1:2A:816:C:C6	2.49	0.48
1:2A:1857:G:O2'	1:2A:1885:A:N6	2.44	0.48
5:1F:65:TRP:HH2	5:1F:72:ARG:HH21	1.62	0.48
14:1S:34:HIS:ND1	14:1S:53:SER:OG	2.38	0.48
32:1a:67:C:H2'	32:1a:68:G:H8	1.79	0.48
32:1a:186:C:H2'	32:1a:187:C:C6	2.48	0.48
32:1a:1263:C:H2'	32:1a:1264:C:H6	1.77	0.48
54:1y:19:G:H5''	54:1y:57:G:H1	1.79	0.48
15:2T:65:LYS:HE3	15:2T:67:SER:HB2	1.96	0.48
18:2W:82:LEU:HD22	18:2W:84:ARG:NH2	2.28	0.48
32:2a:397:A:H3'	32:2a:397:A:N3	2.28	0.48
54:2y:6:A:N1	54:2y:66:A:N6	2.62	0.48
54:2y:36:C:O5'	54:2y:36:C:H6	1.96	0.48
54:2y:69:A:C6	54:2y:70:C:C2	3.02	0.48
1:1A:86:C:H4'	1:1A:104:U:H1'	1.96	0.48
1:1A:800:A:H8	1:1A:800:A:OP1	1.97	0.48
1:1A:1090:U:C2	1:1A:1102:C:H1'	2.48	0.48
1:1A:1916:A:H2'	1:1A:1917:PSU:O4'	2.14	0.48
1:2A:7:G:H4'	9:2N:13:TRP:CH2	2.49	0.48
15:1T:109:GLU:O	15:1T:113:LYS:HG2	2.14	0.48
24:12:1:MET:H1	24:12:52:ASP:CG	2.21	0.48
32:1a:636:U:H2'	32:1a:637:G:C8	2.47	0.48
32:1a:924:C:O2'	32:1a:1502:A:N1	2.43	0.48
39:1h:42:GLU:HG3	39:1h:109:ILE:HD13	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2D:274:ARG:O	3:2D:275:LYS:HD2	2.13	0.48
8:2I:90:GLY:O	8:2I:121:LYS:NZ	2.39	0.48
10:2O:71:ARG:HH22	10:2O:122:LEU:C	2.22	0.48
13:2R:38:VAL:HG22	13:2R:112:ALA:HB2	1.96	0.48
30:28:23:VAL:HG22	30:28:47:LYS:HB3	1.95	0.48
32:2a:977:A:O2'	32:2a:981:U:N3	2.46	0.48
32:2a:1096:C:O2	32:2a:1170:A:O2'	2.29	0.48
54:2w:18:G:H22	54:2w:57:G:H3'	1.78	0.48
1:1A:784:A:C5	3:1D:229:VAL:HG21	2.49	0.48
1:1A:1364:G:OP1	23:11:2:SER:HA	2.14	0.48
1:2A:460:A:H2'	1:2A:461:C:O4'	2.14	0.48
1:2A:579:G:H2'	1:2A:580:C:C6	2.48	0.48
1:2A:911:A:H2'	12:2Q:9:TYR:OH	2.14	0.48
1:2A:1005:C:H2'	1:2A:1006:C:C6	2.49	0.48
1:2A:2098:U:H2'	1:2A:2099:U:O4'	2.14	0.48
24:12:7:ARG:O	24:12:11:GLU:HG3	2.14	0.48
26:14:48:ARG:HG2	26:14:52:THR:HG23	1.96	0.48
32:1a:727:G:N2	32:1a:730:G:OP2	2.43	0.48
35:1d:5:ILE:HG13	35:1d:5:ILE:O	2.14	0.48
44:1m:3:ARG:H	44:1m:3:ARG:HG3	1.41	0.48
47:1p:23:ASP:OD1	47:1p:25:ARG:HG2	2.14	0.48
54:1w:55:PSU:O4	54:1w:57:G:H3'	2.14	0.48
3:2D:239:ARG:NE	61:2D:407:HOH:O	2.46	0.48
4:2E:14:ILE:HG13	4:2E:21:VAL:HG13	1.96	0.48
7:2H:13:LYS:HA	7:2H:14:GLY:HA2	1.58	0.48
22:20:40:GLN:NE2	22:20:43:THR:HA	2.28	0.48
26:24:62:ARG:HD3	26:24:62:ARG:HA	1.60	0.48
32:2a:192:U:H2'	32:2a:193:C:H6	1.78	0.48
32:2a:974:A:OP2	45:2n:29:ARG:NH2	2.27	0.48
32:2a:1005:A:H3'	32:2a:1006:C:C6	2.49	0.48
32:2a:1276:G:C2'	32:2a:1277:C:H5'	2.44	0.48
46:2o:36:ILE:HG23	46:2o:56:LEU:HD11	1.96	0.48
50:2s:41:VAL:HG12	50:2s:42:PRO:HD2	1.96	0.48
1:1A:1798:U:H5'	3:1D:259:THR:CG2	2.41	0.47
1:1A:2038:G:H2'	1:1A:2039:C:O4'	2.14	0.47
1:1A:2154:G:C2	1:1A:2155:G:H1'	2.48	0.47
1:1A:2638:G:P	4:1E:82:ARG:HH12	2.36	0.47
1:1A:2646:C:H2'	1:1A:2647:U:O4'	2.14	0.47
1:2A:570:G:H2'	1:2A:2030:A:C5	2.49	0.47
1:2A:576:U:OP1	61:2A:3983:HOH:O	2.19	0.47
1:2A:1037:G:H1	1:2A:1118:C:H42	1.61	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1364:G:P	23:21:3:LYS:HG3	2.54	0.47
1:2A:1665:A:H2'	1:2A:1666:G:O4'	2.14	0.47
1:2A:2278:A:OP2	22:20:12:ASN:ND2	2.46	0.47
4:1E:105:THR:OG1	4:1E:199:ARG:NH2	2.47	0.47
17:1V:72:VAL:HG22	17:1V:85:LYS:HB3	1.95	0.47
32:1a:1038:C:H2'	32:1a:1039:C:C6	2.49	0.47
32:1a:1086:U:H3	32:1a:1099:G:H22	1.61	0.47
2:2B:11:C:OP2	2:2B:12:C:N4	2.38	0.47
3:2D:19:ALA:HB2	3:2D:204:ILE:HD11	1.96	0.47
16:2U:85:LYS:HB2	16:2U:116:ALA:HB1	1.95	0.47
26:24:41:PRO:HG3	26:24:49:PHE:CZ	2.49	0.47
32:2a:89:C:H2'	32:2a:90:U:O4'	2.13	0.47
32:2a:253:U:H2'	32:2a:254:G:H8	1.78	0.47
32:2a:304:U:H2'	32:2a:305:G:C8	2.49	0.47
32:2a:1251:A:H2'	32:2a:1252:A:C8	2.50	0.47
32:2a:1346:A:N1	32:2a:1374:A:H5''	2.29	0.47
34:2c:9:GLY:HA3	45:2n:49:HIS:HA	1.95	0.47
41:2j:65:LEU:HD13	45:2n:56:VAL:HG22	1.95	0.47
44:2m:86:CYS:SG	44:2m:87:TYR:N	2.87	0.47
1:1A:1043:C:H2'	1:1A:1044:G:H5''	1.96	0.47
1:1A:2232:U:P	23:11:40:ARG:HH12	2.37	0.47
1:1A:2352:A:N6	1:1A:2365:G:O2'	2.48	0.47
1:1A:2428:G:OP1	61:1A:4231:HOH:O	2.20	0.47
1:2A:568:U:H5'	1:2A:945:A:C6	2.49	0.47
1:2A:1429:G:H2'	1:2A:1430:C:C6	2.49	0.47
1:2A:1794:U:H2'	1:2A:1795:C:C6	2.49	0.47
1:2A:2328:A:H2'	1:2A:2329:G:C8	2.50	0.47
9:1N:4:TYR:CD2	16:1U:100:VAL:HG11	2.49	0.47
11:1P:106:LEU:HD13	11:1P:112:LEU:HD13	1.96	0.47
13:1R:38:VAL:HG22	13:1R:112:ALA:HB2	1.96	0.47
32:1a:520:A:N1	32:1a:536:C:H1'	2.29	0.47
32:1a:1391:U:H2'	32:1a:1392:G:C8	2.49	0.47
35:1d:119:GLN:HG3	35:1d:123:HIS:HD2	1.78	0.47
40:1i:4:TYR:CG	40:1i:88:TYR:HB2	2.48	0.47
44:1m:23:TYR:CE2	44:1m:71:ARG:HG3	2.49	0.47
5:2F:40:GLN:NE2	5:2F:182:ASN:HB2	2.29	0.47
6:2G:179:PRO:HB2	26:24:42:PHE:HE2	1.79	0.47
30:28:26:LYS:HB2	30:28:44:LYS:O	2.15	0.47
32:2a:278:G:OP2	48:2q:41:LYS:HE2	2.13	0.47
32:2a:539:A:H2'	32:2a:540:G:C8	2.50	0.47
32:2a:1070:U:H2'	32:2a:1071:C:C6	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:2d:61:LYS:HD3	35:2d:206:PHE:CE2	2.49	0.47
1:1A:1268:A:C2	1:1A:2013:A:C4	3.02	0.47
1:1A:1580:A:OP2	1:1A:1580:A:H8	1.97	0.47
1:2A:1021:A:H2'	1:2A:1022:G:H4'	1.95	0.47
1:2A:2218:U:H1'	23:21:52:ARG:HH12	1.78	0.47
11:1P:91:PHE:O	11:1P:121:LYS:NZ	2.47	0.47
32:1a:881:G:H2'	32:1a:882:C:O4'	2.14	0.47
32:1a:1027:C:H3'	32:1a:1028:C:H5''	1.96	0.47
32:1a:1149:C:O2'	32:1a:1280:A:N1	2.40	0.47
33:1b:16:HIS:CG	33:1b:17:PHE:N	2.82	0.47
34:1c:17:ASP:OD2	34:1c:21:ARG:NE	2.40	0.47
32:2a:1031:G:H2'	32:2a:1032:G:C8	2.49	0.47
32:2a:1032:G:H2'	32:2a:1033:G:H8	1.80	0.47
32:2a:1270:C:OP2	52:2u:24:ARG:NH2	2.47	0.47
34:2c:58:GLU:HG2	34:2c:65:ALA:HB3	1.95	0.47
38:2g:77:SER:OG	54:2y:32:C:H4'	2.14	0.47
42:2k:43:SER:HA	42:2k:47:VAL:HG21	1.95	0.47
54:2y:62:C:H2'	54:2y:63:G:C8	2.49	0.47
1:1A:75:G:H4'	24:12:55:ARG:NH1	2.30	0.47
1:1A:882:G:H3'	1:1A:883:G:H8	1.77	0.47
1:1A:1429:G:H2'	1:1A:1430:C:C6	2.48	0.47
1:1A:2128:C:N4	1:1A:2160:G:H1	2.07	0.47
1:2A:195:A:H61	1:2A:198:C:H3'	1.80	0.47
1:2A:2482:G:O3'	54:2w:64:U:H4'	2.14	0.47
5:1F:75:HIS:ND1	61:1F:401:HOH:O	2.16	0.47
32:1a:22:G:H4'	32:1a:885:G:C8	2.49	0.47
32:1a:58:C:O2'	32:1a:388:G:N7	2.44	0.47
32:1a:1196:U:H3	34:1c:162:GLN:HE22	1.60	0.47
32:1a:1260:C:OP1	32:1a:1284:C:O2'	2.27	0.47
33:1b:150:SER:HA	33:1b:153:ARG:HH12	1.80	0.47
36:1e:69:VAL:HG11	36:1e:113:ALA:HB1	1.95	0.47
55:1x:4:G:H2'	55:1x:5:G:C8	2.50	0.47
5:2F:31:HIS:HB2	11:2P:9:ASN:OD1	2.14	0.47
5:2F:184:TYR:CE2	5:2F:188:ARG:HD2	2.50	0.47
6:2G:120:LEU:N	6:2G:179:PRO:O	2.42	0.47
8:2I:54:GLN:HG3	8:2I:57:ARG:NH2	2.29	0.47
10:2O:26:LYS:O	10:2O:30:ALA:HB2	2.14	0.47
32:2a:901:A:O2'	32:2a:1513:A:OP1	2.18	0.47
34:2c:136:GLN:O	34:2c:139:GLN:N	2.46	0.47
38:2g:26:PHE:CE2	38:2g:30:ILE:HD11	2.49	0.47
40:2i:117:HIS:HB2	40:2i:121:ARG:HG3	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:2k:79:SER:HA	42:2k:104:GLN:HB3	1.97	0.47
1:1A:1131:G:H21	9:1N:73:THR:CG2	2.27	0.47
1:1A:2123:G:H1	1:1A:2175:C:H42	1.62	0.47
1:1A:2712:U:O2'	1:1A:2713:A:H5'	2.15	0.47
1:2A:484:C:H2'	1:2A:485:C:C6	2.49	0.47
1:2A:854:G:H2'	1:2A:855:G:C8	2.44	0.47
1:2A:1152:C:H4'	16:2U:77:SER:HA	1.97	0.47
1:2A:1366:A:H2'	1:2A:1367:A:O4'	2.15	0.47
1:2A:1664:A:OP1	61:2A:3985:HOH:O	2.20	0.47
1:2A:2732:G:H3'	1:2A:2733:A:O4'	2.14	0.47
3:1D:230:ASP:OD1	61:1D:401:HOH:O	2.20	0.47
25:13:26:LEU:O	25:13:35:ARG:NE	2.47	0.47
28:16:13:CYS:SG	28:16:47:THR:HG21	2.54	0.47
33:1b:87:ARG:NE	33:1b:233:SER:HB3	2.29	0.47
33:1b:109:SER:O	33:1b:112:VAL:HG22	2.13	0.47
6:2G:179:PRO:HG3	26:24:43:TYR:OH	2.15	0.47
20:2Y:9:LYS:HA	20:2Y:10:GLY:HA2	1.58	0.47
25:23:8:LEU:O	25:23:32:GLN:N	2.42	0.47
32:2a:620:C:H2'	32:2a:621:A:O4'	2.14	0.47
32:2a:1365:G:H2'	32:2a:1366:C:O4'	2.15	0.47
1:1A:1899:G:N3	1:1A:1899:G:H2'	2.30	0.47
1:1A:2335:A:C8	1:1A:2337:G:C5	3.02	0.47
1:1A:2732:G:H3'	1:1A:2733:A:O4'	2.15	0.47
1:2A:96:G:H4'	24:22:48:HIS:CD2	2.49	0.47
1:2A:1131:G:O6	1:2A:2040:C:H1'	2.14	0.47
1:2A:2458:G:O2'	1:2A:2460:U:O4	2.27	0.47
8:1I:2:LYS:HG2	8:1I:20:ASP:OD1	2.14	0.47
10:1O:16:ALA:HB2	10:1O:52:VAL:HG21	1.95	0.47
20:1Y:6:HIS:H	20:1Y:6:HIS:CD2	2.32	0.47
8:2I:59:ALA:HA	8:2I:62:LYS:HB3	1.96	0.47
36:2e:102:ALA:HB1	36:2e:106:PRO:HB2	1.96	0.47
44:2m:80:ARG:HH12	50:2s:69:HIS:CE1	2.20	0.47
1:1A:548:A:O2'	1:1A:549:G:OP1	2.30	0.47
1:1A:582:G:H2'	1:1A:583:G:H8	1.79	0.47
1:1A:715:G:C2	46:1o:56:LEU:HD21	2.50	0.47
1:1A:1682:G:C2	1:1A:1757:U:H1'	2.50	0.47
1:1A:2126:A:H4'	1:1A:2127:G:H5'	1.96	0.47
1:1A:2869:G:H2'	1:1A:2870:C:O4'	2.15	0.47
1:2A:184:C:H2'	1:2A:185:U:H6	1.79	0.47
1:2A:740:U:H2'	1:2A:741:G:C8	2.50	0.47
1:2A:784:A:OP1	61:2A:3988:HOH:O	2.20	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1037:G:H2'	1:2A:1038:C:O4'	2.15	0.47
1:2A:1285:G:N2	1:2A:1328:G:H5''	2.30	0.47
1:2A:1464:C:H2'	1:2A:1465:G:C8	2.50	0.47
1:2A:1779:U:H2'	61:2A:4135:HOH:O	2.13	0.47
1:2A:1996:C:H4'	1:2A:1997:G:OP1	2.13	0.47
1:2A:2683:C:OP1	15:2T:53:ARG:NH2	2.43	0.47
1:2A:2753:A:N3	31:29:15:LYS:NZ	2.51	0.47
1:2A:2759:G:N2	7:2H:139:GLN:OE1	2.47	0.47
4:1E:111:ARG:HD2	4:1E:160:TYR:CD2	2.49	0.47
6:1G:77:ILE:HD13	6:1G:80:PHE:HD2	1.80	0.47
7:1H:98:LEU:HD13	7:1H:125:VAL:HG23	1.97	0.47
20:1Y:38:ILE:HD11	20:1Y:66:PRO:HG3	1.96	0.47
21:1Z:48:PHE:CE1	21:1Z:71:VAL:HG11	2.50	0.47
32:1a:7:G:H21	36:1e:121:LYS:HG2	1.80	0.47
32:1a:110:C:H2'	32:1a:111:G:O4'	2.14	0.47
32:1a:184:G:H2'	32:1a:185:A:C8	2.48	0.47
32:1a:532:A:N6	32:1a:1206:G:O2'	2.48	0.47
32:1a:679:C:H2'	32:1a:680:C:C6	2.50	0.47
32:1a:691:G:H2'	32:1a:692:U:C6	2.50	0.47
32:1a:1263:C:H2'	32:1a:1264:C:C6	2.49	0.47
33:1b:50:GLU:OE2	33:1b:53:ARG:NH1	2.47	0.47
37:1f:89:MET:SD	49:1r:76:LEU:HD11	2.54	0.47
47:1p:52:ASP:O	47:1p:54:GLU:N	2.46	0.47
50:1s:41:VAL:HG12	50:1s:43:GLU:H	1.79	0.47
4:2E:181:LEU:HD12	4:2E:181:LEU:HA	1.72	0.47
7:2H:4:ILE:O	7:2H:69:ARG:HD2	2.15	0.47
7:2H:152:ARG:HD3	7:2H:152:ARG:HA	1.77	0.47
21:2Z:5:LEU:HB2	21:2Z:47:VAL:HG21	1.97	0.47
21:2Z:10:ARG:NE	21:2Z:37:VAL:O	2.37	0.47
22:20:40:GLN:NE2	22:20:42:GLY:O	2.48	0.47
26:24:50:VAL:HG21	44:2m:65:LYS:HA	1.97	0.47
32:2a:202:U:H3'	32:2a:203:U:C5	2.50	0.47
32:2a:1128:C:H1'	32:2a:1147:C:H42	1.79	0.47
32:2a:1518:MA6:C6	32:2a:1519:MA6:H103	2.44	0.47
33:2b:60:ASP:HA	33:2b:63:MET:HE2	1.97	0.47
34:2c:148:GLY:HA3	34:2c:172:ARG:O	2.15	0.47
36:2e:100:VAL:HG22	36:2e:118:ILE:HG22	1.97	0.47
36:2e:110:LEU:HD13	36:2e:118:ILE:HG21	1.97	0.47
44:2m:3:ARG:HD2	44:2m:8:GLU:HG3	1.95	0.47
45:2n:45:ARG:O	45:2n:49:HIS:HD2	1.96	0.47
46:2o:25:THR:HG21	46:2o:70:LEU:HB2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:195:A:OP1	11:1P:46:LYS:HE2	2.15	0.47
1:1A:271(A):A:N1	1:1A:272(D):G:O2'	2.46	0.47
1:1A:1952:A:C6	1:1A:1953:A:N1	2.83	0.47
1:1A:2031:A:C6	1:1A:2498:C:H1'	2.50	0.47
1:1A:2602:A:N6	55:1x:76:A:H2'	2.29	0.47
1:2A:1711:C:H2'	1:2A:1712:C:C6	2.50	0.47
1:2A:1777:U:H2'	1:2A:1778:U:C6	2.50	0.47
1:2A:2100:G:H1	1:2A:2189:U:H3	1.62	0.47
4:1E:11:MET:HG2	4:1E:24:THR:HB	1.97	0.47
6:1G:122:PRO:HG2	6:1G:182:LYS:C	2.39	0.47
6:1G:131:TYR:HB3	6:1G:159:VAL:HG23	1.97	0.47
12:1Q:30:GLY:N	12:1Q:105:GLU:OE1	2.42	0.47
32:1a:262:A:C6	32:1a:263:A:C6	3.03	0.47
32:1a:1413:A:H2	32:1a:1487:G:H22	1.61	0.47
32:1a:1469:G:H2'	32:1a:1470:G:H8	1.80	0.47
37:1f:97:PHE:N	49:1r:30:ASP:OD1	2.47	0.47
54:1w:2:G:H2'	54:1w:3:G:O4'	2.15	0.47
54:1y:53:G:H2'	54:1y:54:5MU:C6	2.50	0.47
7:2H:54:ARG:HD2	7:2H:56:SER:O	2.15	0.47
13:2R:100:LEU:HD11	13:2R:113:LEU:HD23	1.95	0.47
20:2Y:3:VAL:HB	20:2Y:32:PRO:HB3	1.96	0.47
22:20:38:VAL:HG12	22:20:40:GLN:HG2	1.97	0.47
32:2a:1278:U:H5'	32:2a:1279:A:H5'	1.97	0.47
36:2e:105:VAL:HB	36:2e:106:PRO:HD3	1.97	0.47
39:2h:86:ILE:HG21	39:2h:133:LEU:HD13	1.97	0.47
1:1A:93:G:H2'	1:1A:94:C:H6	1.79	0.47
1:1A:570:G:H2'	1:1A:2030:A:C5	2.50	0.47
1:1A:1789:A:H5''	3:1D:220:HIS:O	2.15	0.47
1:2A:171:G:H2'	1:2A:172:C:C6	2.50	0.47
1:2A:717:G:H2'	1:2A:718:A:O4'	2.15	0.47
1:2A:815:C:H2'	1:2A:816:C:H6	1.80	0.47
1:2A:887:A:H2'	1:2A:887:A:N3	2.29	0.47
1:2A:2538:C:H2'	1:2A:2539:C:C6	2.49	0.47
4:1E:47:VAL:O	4:1E:80:GLU:HA	2.15	0.47
6:1G:131:TYR:HB3	6:1G:159:VAL:CG2	2.45	0.47
6:1G:150:ASP:N	6:1G:150:ASP:OD1	2.47	0.47
7:1H:17:VAL:HG22	7:1H:26:VAL:HG22	1.97	0.47
7:1H:33:LEU:HD21	7:1H:136:ILE:HG13	1.97	0.47
32:1a:167:G:H2'	32:1a:168:G:C8	2.50	0.47
32:1a:232:G:H1'	32:1a:262:A:N1	2.29	0.47
33:1b:12:GLU:C	33:1b:14:GLY:H	2.23	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:1i:3:GLN:HE21	40:1i:20:ARG:CZ	2.27	0.47
55:1x:2:G:H2'	55:1x:2:G:N3	2.29	0.47
2:2B:114:C:H4'	14:2S:46:VAL:HG22	1.97	0.47
7:2H:9:ILE:HD11	7:2H:69:ARG:HG2	1.97	0.47
9:2N:4:TYR:CD2	16:2U:100:VAL:HG11	2.50	0.47
13:2R:9:LYS:O	13:2R:17:ARG:HD3	2.15	0.47
16:2U:107:ALA:O	16:2U:111:GLU:HG2	2.14	0.47
21:2Z:74:VAL:HG13	21:2Z:86:VAL:HG22	1.97	0.47
32:2a:559:A:H4'	32:2a:560:U:H3'	1.97	0.47
32:2a:652:U:O4	32:2a:752:G:O2'	2.30	0.47
32:2a:1259:C:C4	32:2a:1260:C:H1'	2.50	0.47
32:2a:1329:A:OP2	52:2u:7:ARG:NH1	2.36	0.47
32:2a:1346:A:C2'	38:2g:10:ARG:HH22	2.28	0.47
39:2h:34:GLU:O	39:2h:38:ILE:HG12	2.13	0.47
54:2y:26:A:C6	54:2y:44:G:C6	3.03	0.47
1:1A:2206:G:H3'	1:1A:2207:G:C8	2.50	0.47
1:1A:2564:A:C2	1:1A:2647:U:H4'	2.50	0.47
17:1V:59:ALA:HB1	17:1V:94:LEU:HB3	1.97	0.47
32:1a:536:C:OP2	61:1a:1929:HOH:O	2.20	0.47
32:1a:933:G:O6	38:1g:3:ARG:NH2	2.48	0.47
32:1a:1101:A:H4'	32:1a:1102:A:O5'	2.15	0.47
35:1d:196:LEU:C	35:1d:198:VAL:H	2.23	0.47
55:1x:8:4SU:O5'	55:1x:8:4SU:H6	2.14	0.47
32:2a:545:C:H5'	35:2d:72:GLU:HB2	1.97	0.47
32:2a:1049:U:C6	32:2a:1201:A:H5'	2.49	0.47
32:2a:1093:A:C4	32:2a:1095:U:H5'	2.49	0.47
32:2a:1298:C:C5	38:2g:114:ARG:HD3	2.50	0.47
33:2b:218:ALA:O	33:2b:222:ILE:HG13	2.15	0.47
37:2f:70:ASP:OD1	37:2f:71:ARG:HG3	2.15	0.47
40:2i:128:ARG:NH2	55:2x:33:U:OP2	2.42	0.47
54:2w:7:U:O2'	54:2w:8:4SU:H5''	2.14	0.47
54:2y:66:A:H3'	54:2y:67:U:C6	2.50	0.47
1:1A:535:C:O3'	16:1U:53:ARG:NH1	2.47	0.46
1:1A:1069:A:H4'	1:1A:1070:A:H5''	1.96	0.46
1:1A:2330:G:H2'	1:1A:2331:G:O4'	2.15	0.46
1:2A:647:G:H21	1:2A:2350:C:H4'	1.80	0.46
1:2A:1495:A:H2'	1:2A:1496:A:C8	2.51	0.46
1:2A:2469:A:H5''	1:2A:2470:G:OP2	2.14	0.46
2:1B:1:U:O2'	2:1B:2:C:OP1	2.27	0.46
3:1D:146:GLU:HB2	3:1D:189:CYS:HB3	1.95	0.46
32:1a:28:G:O2'	32:1a:296:U:OP1	2.30	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:890:G:O2'	32:1a:906:G:O6	2.30	0.46
32:1a:1410:G:H2'	32:1a:1411:C:C6	2.50	0.46
32:1a:1442:G:H2'	32:1a:1442:G:N3	2.30	0.46
33:1b:212:GLN:NE2	33:1b:235:SER:HA	2.29	0.46
3:2D:218:ARG:HB3	3:2D:219:PRO:HD2	1.98	0.46
5:2F:25:PRO:HD2	5:2F:115:ALA:HB2	1.97	0.46
21:2Z:40:ASP:OD2	21:2Z:42:VAL:HG13	2.14	0.46
35:2d:9:CYS:O	35:2d:13:ARG:HG3	2.16	0.46
43:2l:78:GLN:O	43:2l:81:SER:OG	2.24	0.46
54:2y:69:A:H3'	54:2y:70:C:C5'	2.46	0.46
1:1A:884:C:H2'	1:1A:885:C:H4'	1.98	0.46
1:1A:1239:G:H2'	1:1A:1240:U:O4'	2.14	0.46
1:1A:1794:U:H2'	1:1A:1795:C:C6	2.50	0.46
1:2A:84:A:N1	1:2A:98:G:O2'	2.45	0.46
1:2A:483:A:O2'	20:2Y:49:VAL:O	2.28	0.46
1:2A:2875:C:O2'	15:2T:2:ASN:OD1	2.27	0.46
2:1B:13:A:N1	2:1B:69:G:O2'	2.37	0.46
13:1R:67:LEU:HD13	13:1R:76:VAL:HG21	1.97	0.46
18:1W:18:ARG:HG2	18:1W:76:VAL:HB	1.97	0.46
25:13:6:VAL:HG22	25:13:56:VAL:HG13	1.96	0.46
26:14:55:ARG:H	26:14:56:VAL:HA	1.79	0.46
32:1a:266:G:H2'	32:1a:266:G:N3	2.31	0.46
33:1b:19:HIS:CD2	33:1b:20:GLU:HG3	2.50	0.46
33:1b:97:TRP:CZ2	33:1b:102:LEU:HD13	2.50	0.46
35:1d:140:VAL:HG11	35:1d:146:ILE:HD11	1.97	0.46
36:1e:78:HIS:CE1	36:1e:143:ARG:H	2.26	0.46
37:1f:82:ARG:HB2	37:1f:85:VAL:HG23	1.97	0.46
4:2E:174:ASP:OD1	4:2E:175:VAL:N	2.46	0.46
9:2N:28:THR:HG22	9:2N:29:LYS:N	2.30	0.46
16:2U:89:GLU:O	17:2V:11:GLN:NE2	2.41	0.46
32:2a:26:A:N6	32:2a:558:G:O2'	2.47	0.46
32:2a:103:C:OP2	51:2t:14:LYS:HE2	2.16	0.46
32:2a:109:A:H2'	32:2a:326:G:N2	2.30	0.46
32:2a:375:U:OP1	47:2p:69:THR:HG21	2.15	0.46
32:2a:859:A:H2'	32:2a:860:A:O4'	2.15	0.46
32:2a:1073:U:H2'	32:2a:1074:G:H8	1.79	0.46
32:2a:1387:G:H2'	32:2a:1388:C:C6	2.51	0.46
33:2b:77:ALA:HB2	33:2b:165:VAL:HG11	1.97	0.46
34:2c:52:LEU:HD21	34:2c:55:VAL:HG23	1.95	0.46
35:2d:60:GLU:HG3	35:2d:202:LEU:HD12	1.98	0.46
36:2e:83:GLU:HA	36:2e:88:LYS:HA	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:2g:47:CYS:O	38:2g:50:ILE:HG22	2.14	0.46
55:2x:8:4SU:O2	55:2x:21:A:C2	2.64	0.46
1:1A:1771:C:OP1	61:1A:4308:HOH:O	2.21	0.46
1:1A:2336:A:H61	22:10:43:THR:CG2	2.28	0.46
1:1A:2587:A:N6	1:1A:2608:G:O2'	2.48	0.46
1:1A:2687:U:H2'	1:1A:2688:U:O4'	2.16	0.46
1:2A:819:A:OP2	1:2A:1187:G:N2	2.38	0.46
1:2A:995:C:O2	9:2N:3:THR:OG1	2.23	0.46
6:1G:114:ILE:HA	6:1G:140:ILE:HD11	1.97	0.46
15:1T:8:LYS:HE3	15:1T:8:LYS:HB3	1.70	0.46
26:14:61:ARG:HG3	26:14:62:ARG:N	2.30	0.46
32:1a:177:C:H2'	32:1a:178:C:H6	1.80	0.46
32:1a:1038:C:H2'	32:1a:1039:C:H6	1.80	0.46
32:1a:1069:C:O2'	32:1a:1192:C:HI'	2.15	0.46
38:1g:47:CYS:HA	38:1g:50:ILE:HG22	1.97	0.46
24:22:33:MET:HE3	24:22:37:PHE:CZ	2.51	0.46
32:2a:737:A:H2'	32:2a:738:C:C6	2.50	0.46
32:2a:939:G:H2'	32:2a:940:C:C6	2.51	0.46
32:2a:1326:C:H5''	52:2u:18:TYR:O	2.15	0.46
38:2g:99:LEU:HD22	38:2g:103:TRP:CZ2	2.51	0.46
41:2j:74:ILE:HG22	61:2j:301:HOH:O	2.16	0.46
1:1A:524:U:H2'	1:1A:525:U:C6	2.50	0.46
1:1A:631:A:OP1	11:1P:65:ARG:NE	2.36	0.46
1:1A:1853:A:H2'	1:1A:1854:A:C8	2.51	0.46
1:1A:2243:U:H2'	1:1A:2244:U:C6	2.50	0.46
1:2A:471:A:H2'	1:2A:472:A:O4'	2.16	0.46
1:2A:925:C:H2'	1:2A:926:A:H8	1.80	0.46
1:2A:974:G:O2'	1:2A:975:C:OP1	2.25	0.46
1:2A:1818:U:O2'	3:2D:154:LYS:O	2.29	0.46
1:2A:2126:A:H61	1:2A:2162:G:HO2'	1.62	0.46
18:1W:20:VAL:O	18:1W:23:LEU:HB2	2.15	0.46
30:18:15:LYS:HB3	30:18:23:VAL:HG12	1.96	0.46
32:1a:570:G:HI'	32:1a:820:U:C4	2.51	0.46
32:1a:828:A:H2'	32:1a:829:G:O4'	2.14	0.46
32:1a:1192:C:OP2	34:1c:4:LYS:NZ	2.34	0.46
44:1m:9:ILE:HB	44:1m:18:ALA:HB1	1.97	0.46
45:1n:23:ARG:HD2	45:1n:28:GLY:O	2.15	0.46
48:1q:43:LEU:HD12	48:1q:68:ARG:HB3	1.96	0.46
32:2a:1065:U:H3	32:2a:1109:C:H5''	1.80	0.46
32:2a:1095:U:OP1	32:2a:1108:G:N2	2.47	0.46
37:2f:68:PRO:HG2	37:2f:71:ARG:HD2	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:2j:78:ASN:O	41:2j:80:LYS:N	2.48	0.46
43:2l:8:ASN:HB2	48:2q:34:LYS:HZ2	1.80	0.46
54:2y:65:C:H2'	54:2y:66:A:H8	1.80	0.46
1:1A:269:U:H2'	1:1A:270:A:H5'	1.97	0.46
1:1A:1364:G:P	23:11:3:LYS:HG3	2.56	0.46
1:1A:2443:C:OP1	5:1F:68:LYS:HD3	2.15	0.46
1:2A:55:G:O2'	1:2A:127:A:N1	2.39	0.46
1:2A:686:G:H21	1:2A:788:A:H61	1.62	0.46
1:2A:1268:A:H2'	1:2A:1269:A:O4'	2.16	0.46
1:2A:2163:C:OP1	1:2A:2165:G:N2	2.48	0.46
1:2A:2262:U:H4'	1:2A:2328:A:C2	2.50	0.46
1:2A:2821:A:H2'	1:2A:2822:G:C8	2.51	0.46
3:1D:52:ARG:HG3	61:1D:422:HOH:O	2.15	0.46
3:1D:147:LEU:HD13	3:1D:155:LEU:HD21	1.97	0.46
24:12:65:ASN:HD22	24:12:69:ARG:NH1	2.14	0.46
26:14:55:ARG:N	26:14:56:VAL:HA	2.30	0.46
29:17:21:ARG:NH1	61:17:201:HOH:O	2.38	0.46
32:1a:1226:C:H4'	50:1s:80:TYR:OH	2.16	0.46
32:1a:1272:G:H2'	32:1a:1273:G:O4'	2.16	0.46
33:1b:28:PHE:CD2	33:1b:190:THR:HA	2.50	0.46
34:1c:121:ALA:O	34:1c:124:ILE:HG12	2.15	0.46
31:29:29:ASN:HD22	31:29:32:HIS:CE1	2.33	0.46
32:2a:689:C:H2'	32:2a:690:G:O4'	2.14	0.46
32:2a:1063:C:H3'	32:2a:1064:G:H2'	1.96	0.46
32:2a:1264:C:H2'	32:2a:1265:G:C8	2.49	0.46
32:2a:1508:G:H2'	32:2a:1509:C:C6	2.51	0.46
37:2f:60:PHE:CE2	49:2r:78:LEU:HD21	2.50	0.46
39:2h:37:ARG:HH21	39:2h:38:ILE:HD11	1.81	0.46
43:2l:113:ARG:NH2	43:2l:116:SER:HB2	2.31	0.46
54:2w:4:U:H3	54:2w:69:A:H61	1.62	0.46
1:1A:863:A:H2'	1:1A:864:G:C8	2.49	0.46
1:1A:1020:A:N1	1:1A:1141:U:O2'	2.38	0.46
1:1A:1051:G:H2'	1:1A:1052:C:O4'	2.15	0.46
1:1A:1790:C:H5''	1:1A:1791:A:OP1	2.16	0.46
1:1A:2127:G:H2'	1:1A:2128:C:C6	2.50	0.46
1:2A:287:C:H2'	1:2A:288:C:C6	2.51	0.46
1:2A:910:A:C5	12:2Q:13:GLN:HG3	2.50	0.46
1:2A:1356:G:OP2	61:2A:3989:HOH:O	2.21	0.46
1:2A:2144:U:O2'	1:2A:2147:G:O6	2.32	0.46
1:2A:2863:C:OP1	15:2T:93:ARG:NH1	2.49	0.46
7:1H:41:MET:HE2	7:1H:65:HIS:HA	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:1P:86:LYS:HB3	11:1P:118:GLY:HA3	1.97	0.46
12:1Q:81:VAL:HG12	22:10:5:LYS:HD3	1.98	0.46
28:16:25:LYS:NZ	28:16:51:GLU:OE2	2.30	0.46
32:1a:108:G:N1	51:1t:15:ARG:HG2	2.30	0.46
32:1a:130:A:H5'	48:1q:63:ARG:NH1	2.30	0.46
32:1a:767:A:H2'	32:1a:768:A:O4'	2.16	0.46
32:1a:869:G:OP2	61:1a:1928:HOH:O	2.20	0.46
32:1a:1255:G:H1	32:1a:1282:C:H42	1.62	0.46
35:1d:98:GLU:HG3	35:1d:194:LEU:HD21	1.98	0.46
40:1i:117:HIS:HB2	40:1i:121:ARG:HG3	1.97	0.46
50:1s:51:VAL:HG21	50:1s:71:LEU:HB3	1.98	0.46
4:2E:1:MET:HE3	4:2E:199:ARG:HB3	1.98	0.46
5:2F:178:PRO:HB3	5:2F:198:ALA:HA	1.96	0.46
6:2G:106:LEU:O	6:2G:111:LEU:HG	2.16	0.46
32:2a:587:G:N1	32:2a:754:C:OP2	2.42	0.46
32:2a:1030(A):G:C2	32:2a:1030(C):G:H8	2.34	0.46
33:2b:16:HIS:CG	33:2b:17:PHE:N	2.83	0.46
33:2b:164:VAL:HB	33:2b:186:ALA:HB2	1.97	0.46
39:2h:20:TYR:HA	39:2h:65:TYR:CZ	2.51	0.46
1:1A:383:U:H2'	1:1A:385:C:H5	1.80	0.46
1:1A:862:G:H2'	1:1A:863:A:O4'	2.16	0.46
1:1A:1427:A:H4'	1:1A:1428:C:O4'	2.16	0.46
1:1A:2103:C:H42	1:1A:2186:G:H1	1.63	0.46
1:2A:528:A:O2'	1:2A:529:A:H5'	2.16	0.46
1:2A:940:G:N3	1:2A:1191:G:H4'	2.30	0.46
1:2A:1357:U:H2'	1:2A:1358:G:O4'	2.16	0.46
1:2A:1448:G:H4'	1:2A:1542:A:OP1	2.16	0.46
1:2A:2572:A:OP1	1:2A:2574:G:O2'	2.29	0.46
1:2A:2680:C:H5'	4:2E:189:PRO:HA	1.98	0.46
26:14:48:ARG:HD3	26:14:48:ARG:HA	1.73	0.46
32:1a:667:G:H4'	46:1o:51:HIS:CE1	2.51	0.46
32:1a:857:C:H2'	32:1a:858:G:O4'	2.16	0.46
32:1a:994:A:N1	32:1a:1047:G:H4'	2.29	0.46
32:1a:1346:A:H5''	40:1i:120:ARG:NH1	2.30	0.46
32:1a:1349:A:OP1	40:1i:118:LYS:HB2	2.15	0.46
34:1c:40:ARG:NH1	34:1c:55:VAL:O	2.48	0.46
34:1c:134:ILE:HG23	34:1c:151:VAL:HB	1.96	0.46
40:1i:23:ASN:OD1	40:1i:23:ASN:N	2.48	0.46
54:1y:18:G:N1	54:1y:55:PSU:H1'	2.28	0.46
14:2S:26:LEU:HD22	14:2S:87:PHE:CD1	2.50	0.46
32:2a:131:C:H2'	32:2a:132:C:C6	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:427:U:OP1	35:2d:13:ARG:NH1	2.45	0.46
32:2a:834:C:H2'	32:2a:835:U:C6	2.51	0.46
32:2a:946:A:O2'	32:2a:1333:A:N3	2.44	0.46
32:2a:1479:C:H2'	32:2a:1480:G:C8	2.51	0.46
32:2a:1510:U:H2'	32:2a:1511:G:C8	2.50	0.46
33:2b:121:LEU:O	33:2b:127:ILE:HG23	2.15	0.46
44:2m:11:ARG:HA	44:2m:45:VAL:HB	1.97	0.46
1:1A:2648:C:H2'	1:1A:2649:U:C6	2.50	0.46
1:2A:197:A:N6	1:2A:2430:A:H2'	2.31	0.46
1:2A:263:C:H2'	1:2A:264:C:O4'	2.16	0.46
1:2A:764:A:H5'	3:2D:210:GLY:HA2	1.98	0.46
1:2A:852:G:H2'	1:2A:853:G:C8	2.46	0.46
1:2A:860:U:C2	1:2A:2268:A:C8	3.03	0.46
1:2A:1636:C:H2'	1:2A:1637:A:C8	2.51	0.46
32:1a:728:A:H2'	32:1a:729:A:C8	2.51	0.46
32:1a:924:C:H2'	32:1a:925:G:C8	2.51	0.46
37:1f:8:ILE:HG12	37:1f:88:VAL:HG22	1.98	0.46
44:1m:87:TYR:CZ	44:1m:91:ARG:HD3	2.51	0.46
48:1q:70:ARG:C	48:1q:71:PHE:HD1	2.23	0.46
55:1x:61:C:H2'	55:1x:62:C:C6	2.48	0.46
6:2G:38:VAL:HG22	6:2G:93:THR:HA	1.97	0.46
7:2H:80:SER:OG	7:2H:81:GLU:HG3	2.16	0.46
10:2O:49:ARG:HH12	32:2a:1423:G:P	2.38	0.46
19:2X:5:TYR:CE2	24:22:30:ARG:HB2	2.50	0.46
32:2a:360:A:H2'	32:2a:361:G:C8	2.50	0.46
32:2a:581:G:OP1	46:2o:61:GLY:HA3	2.16	0.46
32:2a:678:U:H2'	32:2a:679:C:H6	1.81	0.46
32:2a:1352:C:H2'	32:2a:1353:G:C8	2.51	0.46
33:2b:74:LYS:NZ	33:2b:206:ASP:OD1	2.38	0.46
43:2l:60:LEU:HD21	43:2l:85:ILE:HD11	1.98	0.46
48:2q:21:VAL:HG21	48:2q:59:ILE:HG21	1.98	0.46
54:2w:6:A:N6	54:2w:67:U:O4	2.48	0.46
54:2y:14:A:H5'	54:2y:15:G:OP2	2.16	0.46
1:1A:222:A:H3'	1:1A:421:U:H5'	1.97	0.46
1:1A:1082:U:C4	1:1A:1086:A:N1	2.80	0.46
1:1A:1697:G:OP2	1:1A:1698:A:O2'	2.31	0.46
1:1A:1700:A:H2'	1:1A:1701:A:H5'	1.97	0.46
1:1A:1790:C:H2'	1:1A:1791:A:C5	2.50	0.46
1:1A:1996:C:H4'	1:1A:1997:G:OP1	2.15	0.46
1:2A:251:A:C4	1:2A:252:G:H1'	2.50	0.46
1:2A:586:A:H5'	5:2F:89:VAL:HG21	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:868:U:C4	1:2A:869:G:N7	2.83	0.46
1:2A:1354:A:O3'	3:2D:38:LYS:HE3	2.16	0.46
1:2A:1364:G:N7	23:21:3:LYS:HD2	2.30	0.46
1:2A:1514:U:H2'	1:2A:1515:G:C8	2.51	0.46
1:2A:2687:U:H2'	1:2A:2688:U:O4'	2.16	0.46
4:1E:72:VAL:HG12	4:1E:73:GLU:O	2.15	0.46
4:1E:111:ARG:HD2	4:1E:160:TYR:CE2	2.51	0.46
7:1H:9:ILE:HD11	7:1H:69:ARG:HG2	1.97	0.46
32:1a:61:G:H2'	32:1a:62:U:O4'	2.16	0.46
32:1a:1401:G:C2	32:1a:1402:4OC:H1'	2.51	0.46
54:1y:60:C:H2'	54:1y:61:C:C5	2.51	0.46
12:2Q:85:LYS:HG2	22:20:7:LEU:HB3	1.98	0.46
17:2V:24:LYS:HE2	17:2V:24:LYS:HB3	1.82	0.46
30:28:32:LEU:O	30:28:36:LYS:HE3	2.16	0.46
32:2a:403:C:N4	61:2a:1923:HOH:O	2.42	0.46
32:2a:714:G:H2'	32:2a:715:A:C8	2.50	0.46
32:2a:741:G:H2'	32:2a:742:G:O4'	2.16	0.46
32:2a:1004:A:N3	32:2a:1038:C:C2	2.84	0.46
32:2a:1201:A:H4'	32:2a:1202:G:O5'	2.16	0.46
32:2a:1279:A:H5''	32:2a:1280:A:OP1	2.16	0.46
32:2a:1353:G:H2'	32:2a:1354:C:H6	1.81	0.46
38:2g:68:ASN:HD22	38:2g:128:ALA:HA	1.80	0.46
1:1A:244:A:C2	1:1A:255:A:C4	3.04	0.46
1:1A:1557:C:H5''	1:1A:1558:A:OP2	2.16	0.46
1:1A:1930:G:O2'	1:1A:1968:G:O6	2.29	0.46
1:1A:2128:C:N4	1:1A:2161:C:H42	2.14	0.46
1:1A:2791:C:H2'	1:1A:2792:G:C8	2.50	0.46
1:2A:147:U:O4	61:2A:3981:HOH:O	2.18	0.46
1:2A:286:C:H2'	1:2A:287:C:C6	2.51	0.46
1:2A:287:C:H2'	1:2A:288:C:H6	1.80	0.46
1:2A:832:G:H5'	11:2P:45:LEU:HD22	1.98	0.46
1:2A:2099:U:H3	1:2A:2190:G:H1	1.65	0.46
1:2A:2331:G:O2'	1:2A:2336:A:N1	2.39	0.46
1:2A:2447:G:N2	1:2A:2450:A:OP2	2.49	0.46
1:2A:2788:C:N4	1:2A:2789:C:H41	2.14	0.46
6:1G:179:PRO:HG3	26:14:43:TYR:OH	2.15	0.46
16:1U:17:ILE:HG23	16:1U:39:LEU:HD12	1.97	0.46
23:11:35:THR:OG1	23:11:35:THR:O	2.33	0.46
47:1p:8:ARG:C	47:1p:9:PHE:HD1	2.23	0.46
47:1p:42:ARG:HB3	47:1p:44:THR:HG23	1.97	0.46
50:1s:30:LEU:HD11	50:1s:50:ALA:HB2	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:1w:6:A:N6	54:1w:67:U:O4	2.49	0.46
6:2G:64:THR:HB	6:2G:94:LEU:HD21	1.96	0.46
32:2a:9:G:H2'	32:2a:10:A:C8	2.51	0.46
32:2a:113:G:O4'	32:2a:354:G:H4'	2.15	0.46
32:2a:942:G:C2	32:2a:1342:C:C2	3.04	0.46
32:2a:1305:G:O2'	32:2a:1331:G:N2	2.48	0.46
1:1A:1055:G:C2	1:1A:1056:G:H1'	2.51	0.45
1:1A:1406:U:H2'	1:1A:1407:C:H6	1.79	0.45
1:1A:1587:A:H2'	1:1A:1588:C:C6	2.51	0.45
1:1A:1720:U:H2'	1:1A:1721:G:O4'	2.16	0.45
1:1A:1805:U:O2	3:1D:50:THR:HB	2.15	0.45
1:2A:2121:G:H1	1:2A:2177:C:N4	2.14	0.45
1:2A:2704:C:H2'	1:2A:2705:A:O4'	2.16	0.45
1:2A:2784:C:H1'	4:2E:37:ARG:HH12	1.81	0.45
10:1O:4:PRO:O	10:1O:5:GLN:HB2	2.16	0.45
10:1O:48:PRO:CB	32:1a:1422:G:H5''	2.42	0.45
10:1O:63:VAL:HG11	10:1O:85:VAL:HG23	1.98	0.45
11:1P:85:LEU:HD13	11:1P:120:ALA:HB2	1.97	0.45
17:1V:14:VAL:HA	17:1V:18:LEU:HD23	1.97	0.45
39:1h:34:GLU:OE1	39:1h:37:ARG:NH1	2.49	0.45
9:2N:62:VAL:CG1	9:2N:66:LYS:HB2	2.46	0.45
11:2P:8:PRO:HB2	11:2P:12:ALA:HB3	1.98	0.45
11:2P:59:LEU:HD22	11:2P:60:MET:HE2	1.98	0.45
23:21:50:ARG:HD2	23:21:57:GLU:OE2	2.17	0.45
32:2a:1004:A:H1'	32:2a:1038:C:O2	2.16	0.45
32:2a:1050:G:H1'	32:2a:1214:C:O2	2.16	0.45
32:2a:1247:U:H1'	32:2a:1291:G:N2	2.30	0.45
34:2c:7:PRO:HG3	34:2c:201:TYR:HE1	1.80	0.45
39:2h:39:LEU:HB3	39:2h:45:ILE:HG12	1.97	0.45
43:2l:10:LEU:HB3	48:2q:32:TYR:CE2	2.51	0.45
55:2x:58:A:H4'	55:2x:59:A:OP1	2.16	0.45
1:1A:465:G:O6	61:1A:4305:HOH:O	2.19	0.45
1:1A:784:A:H5'	1:1A:785:G:OP1	2.16	0.45
1:1A:947:G:OP2	61:1A:4309:HOH:O	2.21	0.45
1:1A:1428:C:N4	1:1A:1570:A:OP2	2.36	0.45
1:1A:1952:A:OP1	10:1O:42:SER:OG	2.34	0.45
1:1A:2506:U:O2'	54:1w:76:A:H4'	2.16	0.45
1:2A:908:C:OP2	12:2Q:22:LYS:HD2	2.16	0.45
1:2A:958:U:OP2	12:2Q:14:ARG:NE	2.48	0.45
1:2A:2467:C:H4'	12:2Q:123:HIS:CD2	2.52	0.45
3:1D:68:LYS:C	3:1D:70:TRP:H	2.24	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1H:26:VAL:HG12	7:1H:79:VAL:HG21	1.98	0.45
9:1N:58:ASP:OD1	9:1N:58:ASP:N	2.47	0.45
14:1S:110:LEU:HD12	14:1S:110:LEU:HA	1.80	0.45
15:1T:57:PHE:HA	15:1T:79:HIS:CD2	2.51	0.45
32:1a:78:G:O2'	32:1a:79:G:H8	1.99	0.45
32:1a:431:A:H2'	32:1a:432:A:O4'	2.16	0.45
32:1a:452:A:O2'	32:1a:453:A:OP2	2.27	0.45
35:1d:15:GLU:OE2	35:1d:66:ARG:NH1	2.49	0.45
37:1f:78:GLU:O	37:1f:81:ILE:HG22	2.15	0.45
38:1g:49:ILE:O	38:1g:53:LYS:HG3	2.16	0.45
40:1i:8:GLY:HA3	40:1i:76:ALA:O	2.16	0.45
47:1p:56:ALA:O	47:1p:60:LEU:HD13	2.16	0.45
52:1u:3:LYS:HD2	52:1u:14:TRP:CD1	2.51	0.45
3:2D:106:ILE:H	3:2D:106:ILE:HG12	1.45	0.45
6:2G:96:ARG:H	6:2G:99:MET:HE2	1.81	0.45
8:2I:140:LEU:HD22	8:2I:142:VAL:HG22	1.99	0.45
9:2N:4:TYR:HB2	16:2U:101:ARG:NH1	2.32	0.45
10:2O:66:LYS:HA	10:2O:79:PHE:O	2.17	0.45
22:20:50:ASN:HB3	22:20:63:VAL:HG22	1.97	0.45
32:2a:115:G:H4'	32:2a:116:A:O5'	2.16	0.45
32:2a:232:G:H1'	32:2a:262:A:N1	2.30	0.45
32:2a:669:U:H2'	32:2a:670:G:O4'	2.15	0.45
32:2a:1118:C:H1'	32:2a:1179:A:C5	2.51	0.45
32:2a:1288:A:N1	32:2a:1371:G:H1'	2.32	0.45
42:2k:34:ASP:OD1	42:2k:38:ASN:N	2.47	0.45
1:1A:818:G:H4'	1:1A:838:C:O3'	2.16	0.45
1:1A:2568:C:H2'	1:1A:2569:G:O4'	2.16	0.45
1:2A:196:A:O2'	1:2A:805:G:O6	2.25	0.45
1:2A:383:U:H2'	1:2A:385:C:H5	1.82	0.45
1:2A:482:A:H1'	1:2A:498:G:N2	2.32	0.45
1:2A:647:G:H2'	1:2A:648:G:O4'	2.17	0.45
1:2A:962:G:H2'	1:2A:963:U:O4'	2.17	0.45
1:2A:1283:G:N2	1:2A:1285:G:H3'	2.31	0.45
1:2A:1647:G:OP1	61:2A:3924:HOH:O	2.21	0.45
1:2A:2121:G:H2'	1:2A:2122:U:O4'	2.16	0.45
1:2A:2482:G:H4'	54:2w:64:U:O2'	2.15	0.45
1:2A:2537:U:H2'	1:2A:2538:C:C6	2.51	0.45
1:2A:2836:U:H2'	1:2A:2837:G:C8	2.51	0.45
2:1B:48:A:H4'	14:1S:95:HIS:HD2	1.80	0.45
3:1D:108:PRO:HD2	3:1D:111:LEU:HD22	1.99	0.45
3:1D:126:GLN:NE2	3:1D:127:VAL:H	2.13	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1F:64:ILE:HD11	5:1F:75:HIS:CB	2.45	0.45
8:1I:130:TYR:HB3	8:1I:138:ILE:HB	1.98	0.45
29:17:12:ARG:NH2	29:17:44:PRO:HB3	2.31	0.45
32:1a:92:C:H2'	32:1a:93:G:H8	1.81	0.45
32:1a:502:G:H2'	32:1a:503:C:O4'	2.16	0.45
32:1a:911:U:H2'	32:1a:912:C:C6	2.52	0.45
32:1a:962:C:H2'	32:1a:963:G:O4'	2.16	0.45
32:1a:1260:C:O5'	32:1a:1284:C:H4'	2.16	0.45
33:1b:55:PHE:HE1	33:1b:218:ALA:HA	1.80	0.45
6:2G:11:TYR:O	6:2G:16:ARG:HG3	2.16	0.45
8:2I:84:GLY:C	8:2I:86:THR:H	2.23	0.45
32:2a:952:U:H4'	32:2a:964:A:N1	2.32	0.45
32:2a:1023:G:C6	32:2a:1024:G:H1'	2.52	0.45
32:2a:1346:A:H61	32:2a:1374:A:H3'	1.82	0.45
32:2a:1348:U:H2'	32:2a:1349:A:H8	1.80	0.45
34:2c:39:ILE:O	34:2c:43:LEU:HG	2.15	0.45
35:2d:55:ALA:O	35:2d:59:ARG:HB2	2.16	0.45
54:2y:8:4SU:H1'	54:2y:48:C:O2	2.16	0.45
1:1A:1054:A:H3'	1:1A:1055:G:H8	1.82	0.45
1:1A:1500:G:H2'	1:1A:1501:C:C6	2.52	0.45
1:1A:2156:G:H2'	1:1A:2157:G:C6	2.52	0.45
1:1A:2167:U:O2	1:1A:2167:U:H2'	2.14	0.45
1:1A:2619:C:H4'	4:1E:151:TYR:O	2.17	0.45
1:2A:942:G:H4'	1:2A:1190:G:H5'	1.98	0.45
1:2A:2532:G:H1'	1:2A:2663:G:N2	2.31	0.45
6:1G:43:LEU:C	6:1G:45:GLU:H	2.24	0.45
11:1P:91:PHE:CD1	11:1P:99:LEU:HD21	2.52	0.45
24:12:55:ARG:NH2	61:12:202:HOH:O	2.49	0.45
32:1a:21:G:H2'	32:1a:22:G:C8	2.52	0.45
32:1a:1145:C:H4'	32:1a:1146:A:H5'	1.97	0.45
32:1a:1186:G:H21	45:1n:61:TRP:C	2.24	0.45
38:1g:150:ALA:HA	42:1k:59:TYR:HB3	1.98	0.45
40:1i:127:LYS:O	40:1i:128:ARG:HG2	2.16	0.45
50:1s:11:VAL:HG11	50:1s:16:LEU:HB2	1.97	0.45
54:1w:19:G:OP2	54:1w:19:G:H8	2.00	0.45
4:2E:9:VAL:HG13	4:2E:25:VAL:O	2.16	0.45
8:2I:93:THR:N	8:2I:96:ASP:HB2	2.24	0.45
9:2N:49:GLY:O	9:2N:119:ARG:NH1	2.50	0.45
12:2Q:10:ARG:HH22	55:2x:64:G:HO2'	1.63	0.45
13:2R:62:ALA:O	13:2R:66:VAL:HG23	2.17	0.45
17:2V:12:TYR:CZ	17:2V:22:VAL:HG12	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:141:A:H2'	32:2a:142:G:O4'	2.16	0.45
32:2a:328:C:H4'	32:2a:329:A:H5'	1.99	0.45
32:2a:931:C:N4	32:2a:1386:G:H1	2.10	0.45
32:2a:1203:C:H2'	32:2a:1204:A:H8	1.79	0.45
32:2a:1221:G:H4'	50:2s:53:ASN:O	2.16	0.45
39:2h:20:TYR:CE2	39:2h:75:ARG:HD2	2.52	0.45
54:2y:38:A:H2'	54:2y:39:G:O4'	2.17	0.45
54:2y:68:C:H2'	54:2y:69:A:O4'	2.17	0.45
1:2A:2431:U:O2'	1:2A:2433:A:N7	2.42	0.45
4:1E:117:MET:HE2	4:1E:117:MET:HB3	1.81	0.45
6:1G:101:ILE:HD13	26:14:25:TYR:HB2	1.99	0.45
9:1N:42:TRP:CH2	9:1N:44:PRO:HB3	2.51	0.45
16:1U:104:GLN:NE2	16:1U:105:VAL:HG23	2.31	0.45
32:1a:233:C:H2'	32:1a:234:C:H6	1.81	0.45
32:1a:1018:C:H2'	32:1a:1019:C:O4'	2.16	0.45
32:1a:1030(D):A:H2'	32:1a:1031:G:H4'	1.98	0.45
32:1a:1060:C:C5	34:1c:2:GLY:HA3	2.51	0.45
32:1a:1148:U:H2'	32:1a:1149:C:O4'	2.16	0.45
41:1j:55:LYS:HE2	41:1j:56:HIS:CE1	2.50	0.45
11:2P:59:LEU:HD12	30:28:58:ILE:HG12	1.98	0.45
31:29:7:VAL:HG12	31:29:34:GLN:HB3	1.98	0.45
51:2t:10:LEU:HG	51:2t:12:ALA:H	1.82	0.45
1:1A:796:C:H2'	1:1A:797:C:C6	2.51	0.45
1:1A:1153:C:H2'	1:1A:1154:G:O4'	2.17	0.45
1:1A:1803:A:H4'	3:1D:259:THR:HG23	1.98	0.45
1:1A:2052:G:C8	4:1E:141:ILE:HD11	2.52	0.45
1:1A:2790:A:H5''	1:1A:2893:G:H21	1.81	0.45
1:2A:792:G:H5''	1:2A:793:A:H5'	1.98	0.45
1:2A:900:A:HO2'	1:2A:901:A:P	2.37	0.45
1:2A:1803:A:N1	1:2A:1822:G:O2'	2.46	0.45
1:2A:2679:A:H4'	4:2E:165:VAL:HG11	1.98	0.45
2:1B:30:C:H2'	2:1B:31:C:H5'	1.98	0.45
6:1G:114:ILE:HB	6:1G:117:PHE:HB2	1.98	0.45
32:1a:333:G:H4'	51:1t:16:HIS:CE1	2.52	0.45
33:1b:122:PHE:CE2	33:1b:139:LYS:HD3	2.52	0.45
51:1t:87:LYS:O	51:1t:91:LEU:HG	2.17	0.45
7:2H:3:ARG:CZ	7:2H:5:GLY:H	2.29	0.45
7:2H:10:PRO:O	7:2H:12:PRO:HD3	2.17	0.45
12:2Q:21:THR:O	21:2Z:78:LYS:HD2	2.17	0.45
15:2T:16:ARG:HB3	15:2T:18:ASP:OD1	2.16	0.45
32:2a:1007:C:N3	32:2a:1022:G:C6	2.85	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:2y:6:A:H62	54:2y:65:C:N4	2.15	0.45
1:1A:37:C:H4'	1:1A:451:C:OP1	2.17	0.45
1:1A:589:C:H2'	1:1A:590:A:C8	2.51	0.45
1:1A:657:U:H2'	1:1A:658:C:C6	2.52	0.45
1:1A:1328:G:O2'	1:1A:1329:U:H2'	2.16	0.45
1:1A:1506:C:H2'	1:1A:1507:A:C8	2.51	0.45
1:1A:1779:U:H2'	61:1A:4879:HOH:O	2.16	0.45
1:1A:2260:C:H2'	1:1A:2261:C:H6	1.82	0.45
1:1A:2779:U:H5'	1:1A:2781:A:O4'	2.17	0.45
1:2A:271(E):U:H2'	1:2A:271(F):C:C6	2.52	0.45
1:2A:271(H):G:H2'	1:2A:271(I):G:H8	1.82	0.45
1:2A:956:G:H2'	1:2A:957:A:H2'	1.99	0.45
15:1T:91:ARG:HD2	15:1T:120:ARG:HB3	1.97	0.45
32:1a:60:A:OP1	32:1a:111:G:N2	2.49	0.45
32:1a:540:G:H2'	32:1a:541:G:O4'	2.16	0.45
32:1a:576:G:O6	32:1a:880:C:O2'	2.32	0.45
32:1a:737:A:H2'	32:1a:738:C:H6	1.81	0.45
32:1a:755:G:OP2	46:1o:65:ARG:HD2	2.17	0.45
32:1a:1240:U:OP2	38:1g:116:ALA:N	2.40	0.45
39:1h:35:ILE:HD11	39:1h:134:ILE:HG21	1.98	0.45
46:1o:18:PHE:CZ	46:1o:21:ASP:HB2	2.52	0.45
51:1t:47:GLY:HA2	51:1t:48:LYS:C	2.42	0.45
7:2H:45:VAL:HG12	7:2H:50:VAL:HG22	1.98	0.45
23:21:19:GLN:HB3	23:21:35:THR:HG23	1.99	0.45
32:2a:376:G:H5''	47:2p:5:ARG:HB2	1.98	0.45
32:2a:984:C:H2'	32:2a:985:C:C6	2.52	0.45
32:2a:1024:G:C2'	32:2a:1025:U:H5''	2.46	0.45
32:2a:1112:C:N3	34:2c:178:LEU:HD12	2.31	0.45
32:2a:1235:U:O2'	32:2a:1305:G:O5'	2.34	0.45
32:2a:1518:MA6:H93	32:2a:1519:MA6:H92	1.97	0.45
33:2b:188:ALA:O	33:2b:202:PRO:HA	2.17	0.45
44:2m:108:ARG:HD3	44:2m:108:ARG:HA	1.75	0.45
50:2s:64:GLU:H	50:2s:64:GLU:CD	2.25	0.45
54:2w:11:C:H2'	54:2w:12:U:H6	1.81	0.45
1:1A:8:A:H2'	1:1A:9:U:C6	2.51	0.45
1:1A:1949:G:C6	1:1A:1950:G:C6	3.05	0.45
1:1A:2156:G:OP2	1:1A:2156:G:H8	2.00	0.45
1:1A:2364:C:H2'	1:1A:2365:G:O4'	2.17	0.45
1:2A:18:C:OP2	61:2A:3991:HOH:O	2.21	0.45
1:2A:71:A:N7	19:2X:31:HIS:HE1	2.15	0.45
1:2A:946:G:OP1	61:2A:3990:HOH:O	2.21	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1589:C:H2'	1:2A:1590:U:C6	2.52	0.45
1:2A:1794:U:H2'	1:2A:1795:C:H6	1.81	0.45
2:1B:31:C:H4'	6:1G:29:TRP:CH2	2.52	0.45
5:1F:102:PRO:O	5:1F:106:ARG:HG2	2.16	0.45
18:1W:71:VAL:HA	18:1W:107:LEU:HD12	1.98	0.45
20:1Y:5:MET:HE2	20:1Y:5:MET:HB2	1.71	0.45
32:1a:192:U:H2'	32:1a:193:C:H6	1.82	0.45
32:1a:353:A:H5'	32:1a:353:A:H8	1.81	0.45
32:1a:432:A:H3'	32:1a:433:C:C6	2.51	0.45
32:1a:688:G:H2'	32:1a:689:C:H6	1.82	0.45
32:1a:1328:C:OP1	52:1u:20:LYS:NZ	2.49	0.45
42:1k:59:TYR:CE2	42:1k:63:LEU:HD11	2.52	0.45
2:2B:1:U:O2'	2:2B:2:C:OP1	2.30	0.45
6:2G:124:SER:HB2	6:2G:131:TYR:CE1	2.52	0.45
8:2I:38:LEU:HB2	8:2I:40:THR:HG23	1.97	0.45
12:2Q:118:LEU:HD12	12:2Q:131:ILE:HG23	1.99	0.45
32:2a:583:A:H2'	32:2a:584:G:O4'	2.17	0.45
32:2a:701:C:O2	32:2a:703:G:N1	2.49	0.45
32:2a:1126:U:N3	41:2j:40:LEU:HD11	2.32	0.45
32:2a:1148:U:H2'	32:2a:1149:C:O4'	2.16	0.45
33:2b:187:LEU:HA	33:2b:201:ILE:HB	1.99	0.45
40:2i:24:GLY:HA2	40:2i:59:PHE:O	2.17	0.45
44:2m:98:VAL:C	44:2m:100:GLY:H	2.25	0.45
54:2w:29:U:H2'	54:2w:30:C:C6	2.52	0.45
54:2y:5:G:C2	54:2y:6:A:H1'	2.52	0.45
54:2y:41:A:H2'	54:2y:42:G:O4'	2.17	0.45
1:1A:388:G:O2'	1:1A:389:G:N7	2.48	0.45
1:1A:695:G:OP1	1:1A:1380:G:O2'	2.27	0.45
1:1A:719:C:H2'	1:1A:720:C:C6	2.52	0.45
1:1A:1924:C:H4'	55:1x:13:C:O2'	2.17	0.45
1:1A:2114:A:H2'	1:1A:2115:G:O4'	2.16	0.45
1:2A:754:C:H2'	1:2A:755:C:C6	2.51	0.45
1:2A:1358:G:O2'	1:2A:1359:A:H5''	2.16	0.45
1:2A:1462:C:H4'	1:2A:2703:C:H5'	1.98	0.45
1:2A:1945:G:O6	1:2A:1960:A:N6	2.49	0.45
1:2A:2066:C:OP1	61:2A:3992:HOH:O	2.21	0.45
1:2A:2298:A:N6	1:2A:2318:G:C8	2.85	0.45
2:1B:40:U:O4	26:14:1:MET:N	2.36	0.45
6:1G:41:GLN:HG2	6:1G:154:GLY:O	2.17	0.45
12:1Q:111:GLU:O	12:1Q:115:MET:HG2	2.17	0.45
20:1Y:99:CYS:HB2	20:1Y:106:LEU:HD21	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:156:G:H1	32:1a:165:C:N4	2.14	0.45
32:1a:555:C:H2'	32:1a:556:C:C6	2.52	0.45
32:1a:692:U:O2'	32:1a:694:A:N7	2.47	0.45
32:1a:741:G:H5''	46:1o:59:MET:HE1	1.99	0.45
32:1a:859:A:H2'	32:1a:860:A:O4'	2.16	0.45
32:1a:1002:G:C2	32:1a:1004:A:H1'	2.52	0.45
32:1a:1216:G:H5''	45:1n:5:ALA:HB2	1.98	0.45
33:1b:155:LEU:HD11	33:1b:159:PRO:HG3	1.99	0.45
33:1b:163:PHE:CD1	33:1b:185:ILE:HG13	2.52	0.45
34:1c:57:ILE:HD13	34:1c:66:VAL:HA	1.99	0.45
35:1d:173:TRP:CE3	35:1d:174:LEU:HG	2.52	0.45
50:1s:66:MET:HB2	50:1s:74:PHE:CZ	2.52	0.45
14:2S:18:ILE:O	14:2S:21:THR:HG23	2.16	0.45
16:2U:83:LEU:O	16:2U:87:GLY:N	2.50	0.45
32:2a:538:G:H5''	43:2l:114:LYS:HB2	1.97	0.45
32:2a:999:C:N3	32:2a:1042:G:N2	2.53	0.45
42:2k:81:ASP:OD1	42:2k:107:SER:OG	2.35	0.45
43:2l:36:VAL:O	43:2l:58:VAL:HA	2.17	0.45
43:2l:56:ALA:HB3	43:2l:100:ILE:HD11	1.99	0.45
1:1A:764:A:O4'	3:1D:213:ARG:HG3	2.17	0.45
1:1A:881:G:H1	1:1A:897:C:N4	2.14	0.45
1:1A:1607:C:H4'	1:1A:1608:A:O5'	2.17	0.45
1:2A:644:A:C2	1:2A:2369:A:H1'	2.51	0.45
1:2A:657:U:H2'	1:2A:658:C:C6	2.52	0.45
1:2A:890:A:H2'	1:2A:892:G:O4'	2.16	0.45
1:2A:1889:A:H2'	1:2A:1890:A:C8	2.52	0.45
1:2A:2037:G:H2'	1:2A:2038:G:C8	2.52	0.45
1:2A:2717:G:H2'	1:2A:2718:G:O4'	2.17	0.45
2:1B:14:U:OP2	2:1B:70:C:O2'	2.28	0.45
4:1E:24:THR:HG23	4:1E:184:VAL:HG13	1.99	0.45
8:1I:75:LEU:HD22	8:1I:105:HIS:CG	2.52	0.45
9:1N:67:LEU:HB3	9:1N:88:GLU:HG3	1.99	0.45
32:1a:1424:C:H2'	32:1a:1425:U:O4'	2.17	0.45
54:1y:33:U:O2'	54:1y:35:A:N7	2.43	0.45
54:1y:48:C:OP1	54:1y:48:C:H2'	2.17	0.45
5:2F:172:TRP:H	5:2F:172:TRP:CD1	2.34	0.45
6:2G:11:TYR:CE2	6:2G:16:ARG:HD2	2.51	0.45
15:2T:60:THR:HG22	15:2T:77:PRO:HA	1.99	0.45
18:2W:64:MET:HE2	18:2W:109:GLU:HG3	1.99	0.45
26:24:58:ARG:HG3	50:2s:65:ASN:O	2.17	0.45
32:2a:181:G:H4'	32:2a:182:U:H5'	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:371:G:O2'	32:2a:373:A:N7	2.49	0.45
32:2a:792:A:H4'	32:2a:793:U:H5''	1.99	0.45
32:2a:1198:G:H2'	32:2a:1199:U:C6	2.52	0.45
32:2a:1457:G:H5''	51:2t:35:THR:HG21	1.98	0.45
33:2b:47:THR:O	33:2b:51:LEU:N	2.42	0.45
33:2b:87:ARG:HH11	33:2b:219:VAL:HG12	1.82	0.45
34:2c:6:HIS:CG	45:2n:49:HIS:HB3	2.52	0.45
44:2m:39:ILE:HG12	44:2m:55:ARG:NH2	2.32	0.45
54:2w:51:C:N3	54:2w:63:G:N2	2.55	0.45
1:1A:272(I):U:H2'	1:1A:272(J):C:O4'	2.16	0.44
1:1A:2246:G:H2'	1:1A:2247:A:C8	2.53	0.44
1:2A:143:G:H2'	1:2A:143(A):C:C6	2.52	0.44
1:2A:2332:U:O2'	1:2A:2335:A:N3	2.43	0.44
16:1U:107:ALA:O	16:1U:111:GLU:HG2	2.18	0.44
32:1a:345:C:H5'	32:1a:346:G:C5	2.52	0.44
32:1a:598:U:H4'	39:1h:94:TYR:CD2	2.52	0.44
32:1a:836:G:OP1	49:1r:61:LYS:NZ	2.35	0.44
32:1a:973:G:H3'	32:1a:974:A:H5''	1.99	0.44
32:1a:976:G:OP1	45:1n:32:SER:N	2.44	0.44
32:1a:1144:G:N2	32:1a:1146:A:H62	2.15	0.44
32:1a:1442:G:O2'	32:1a:1442(A):G:H5'	2.18	0.44
32:1a:1510:U:H2'	32:1a:1511:G:C8	2.52	0.44
47:1p:27:LYS:HG3	47:1p:30:GLY:HA3	1.98	0.44
51:1t:36:LEU:HD12	51:1t:62:LEU:HD12	1.99	0.44
52:1u:3:LYS:HB3	52:1u:14:TRP:CD1	2.52	0.44
54:1y:36:C:H2'	54:1y:37:6MZ:O4'	2.16	0.44
54:1y:47:U:O2'	54:1y:50:G:OP1	2.19	0.44
2:2B:3:C:H2'	2:2B:4:C:C6	2.52	0.44
5:2F:126:VAL:HG21	5:2F:129:PHE:CZ	2.52	0.44
27:25:16:ARG:HG3	27:25:17:ASP:N	2.32	0.44
32:2a:134:A:H61	47:2p:25:ARG:NH1	2.15	0.44
33:2b:12:GLU:C	33:2b:14:GLY:H	2.25	0.44
37:2f:37:VAL:HA	37:2f:65:VAL:HG12	1.99	0.44
40:2i:17:VAL:HG11	40:2i:81:ILE:HA	1.99	0.44
50:2s:28:LYS:HD2	50:2s:47:HIS:HA	1.98	0.44
55:2x:66:C:H2'	55:2x:67:C:O4'	2.16	0.44
1:1A:26:G:C6	1:1A:27:G:N1	2.85	0.44
1:1A:863:A:H2'	1:1A:864:G:H8	1.82	0.44
1:1A:1588:C:H2'	1:1A:1589:C:C6	2.52	0.44
1:1A:1653:G:H3'	13:1R:2:ARG:HB2	1.98	0.44
1:1A:2406:U:H2'	1:1A:2406:U:OP2	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:500:G:N1	1:2A:503:A:OP2	2.49	0.44
1:2A:588:U:H2'	1:2A:589:C:C6	2.52	0.44
1:2A:1721:G:H5'	1:2A:1722:A:OP2	2.17	0.44
1:2A:2432:A:C6	1:2A:2433:A:C6	3.06	0.44
1:2A:2674:G:H2'	1:2A:2675:A:C8	2.53	0.44
3:1D:37:LEU:HD13	3:1D:62:TYR:HB2	1.99	0.44
5:1F:102:PRO:HB2	5:1F:105:VAL:HG23	1.98	0.44
21:1Z:153:SER:HA	21:1Z:167:PRO:HB3	1.98	0.44
23:11:64:ALA:HA	23:11:67:ILE:HG13	2.00	0.44
25:13:39:ASP:OD1	25:13:44:ARG:NH1	2.44	0.44
32:1a:78:G:C6	32:1a:91:C:N4	2.85	0.44
32:1a:200:G:H1	32:1a:217:C:N4	2.11	0.44
42:1k:85:ARG:HD3	42:1k:113:PRO:HD3	1.99	0.44
47:1p:5:ARG:HE	47:1p:22:THR:HG21	1.82	0.44
2:2B:38:C:O4'	14:2S:95:HIS:NE2	2.50	0.44
5:2F:178:PRO:HB2	5:2F:201:VAL:HG21	1.98	0.44
10:2O:79:PHE:CD1	15:2T:72:VAL:HG22	2.52	0.44
11:2P:52:GLU:CG	30:28:57:ARG:HH22	2.31	0.44
15:2T:119:LYS:HB2	32:2a:1442(A):G:N2	2.33	0.44
32:2a:336:C:H2'	32:2a:337:C:C6	2.52	0.44
32:2a:1287:A:N3	32:2a:1353:G:O2'	2.42	0.44
33:2b:27:LYS:HG3	33:2b:194:PRO:HD2	1.99	0.44
50:2s:40:ILE:HB	50:2s:67:VAL:O	2.17	0.44
54:2y:51:C:C2	54:2y:63:G:C6	3.05	0.44
1:1A:2094:G:P	8:1I:22:LYS:HD2	2.58	0.44
1:1A:2319:G:N1	14:1S:3:ARG:HA	2.31	0.44
1:1A:2854:G:H2'	1:1A:2855:C:C6	2.52	0.44
1:2A:247:G:H4'	1:2A:386:G:C5	2.53	0.44
1:2A:1316:U:H2'	1:2A:1317:A:H8	1.82	0.44
1:2A:2512:C:H2'	1:2A:2513:G:O4'	2.16	0.44
1:2A:2552:2MU:H2'	1:2A:2554:U:OP2	2.17	0.44
6:1G:179:PRO:HB2	26:14:42:PHE:HE2	1.81	0.44
21:1Z:124:ILE:HG23	21:1Z:126:VAL:HG23	1.99	0.44
21:1Z:125:LEU:HG	21:1Z:164:ALA:HB3	1.99	0.44
30:18:63:PRO:HG2	30:18:64:TYR:CE2	2.52	0.44
32:1a:313:A:H2'	32:1a:314:C:C6	2.52	0.44
32:1a:405:U:O2'	32:1a:498:U:H5'	2.17	0.44
32:1a:600:C:H2'	32:1a:601:C:C6	2.52	0.44
32:1a:848:C:H2'	32:1a:849:C:C6	2.52	0.44
32:1a:939:G:C6	32:1a:940:C:N4	2.84	0.44
34:1c:19:GLU:O	34:1c:40:ARG:NH2	2.49	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:1i:89:ASN:HB3	40:1i:92:TYR:CD2	2.53	0.44
42:1k:23:ALA:HB2	42:1k:28:THR:HG23	1.99	0.44
50:1s:12:ASP:OD2	50:1s:35:SER:OG	2.29	0.44
51:1t:60:GLU:HG3	51:1t:81:LYS:HD2	1.98	0.44
3:2D:72:LYS:NZ	3:2D:99:ASP:OD2	2.42	0.44
3:2D:132:PRO:HD3	3:2D:190:TYR:CZ	2.52	0.44
4:2E:12:THR:HG22	4:2E:13:ARG:H	1.82	0.44
32:2a:343:U:O2'	32:2a:344:A:H2'	2.16	0.44
32:2a:1242:C:H42	32:2a:1295:G:H1	1.65	0.44
32:2a:1401:G:OP1	53:2v:18:G:O2'	2.31	0.44
32:2a:1431:C:H2'	32:2a:1432:G:O4'	2.18	0.44
39:2h:54:ASP:OD1	39:2h:54:ASP:N	2.47	0.44
1:1A:252:G:OP1	11:1P:50:ARG:NH1	2.36	0.44
1:1A:832:G:N3	11:1P:53:GLY:HA3	2.32	0.44
1:1A:889:C:O2'	1:1A:890:A:O4'	2.36	0.44
1:1A:1062:G:C8	1:1A:1088:A:H2'	2.53	0.44
1:1A:1358:G:OP2	61:1A:4306:HOH:O	2.20	0.44
1:1A:1740:G:H2'	1:1A:1741:A:C8	2.52	0.44
1:1A:2593:U:H2'	1:1A:2594:C:C6	2.53	0.44
1:2A:224:G:H2'	1:2A:225:A:O4'	2.17	0.44
1:2A:538:G:H2'	1:2A:539:G:H8	1.82	0.44
1:2A:807:U:OP2	11:2P:41:ARG:NH2	2.51	0.44
1:2A:1608:A:H1'	1:2A:1610:A:OP2	2.18	0.44
1:2A:2155:G:N7	1:2A:2156:G:H1'	2.32	0.44
1:2A:2484:G:C2	1:2A:2485:G:C8	3.06	0.44
1:2A:2543:G:H2'	1:2A:2544:G:C8	2.52	0.44
2:1B:78:A:C2	2:1B:100:A:C4	3.05	0.44
6:1G:179:PRO:HG3	26:14:43:TYR:CZ	2.52	0.44
7:1H:3:ARG:HE	7:1H:54:ARG:HH12	1.65	0.44
11:1P:82:GLY:HA2	11:1P:113:LYS:O	2.17	0.44
28:16:6:ARG:NH1	28:16:26:ASN:HB2	2.32	0.44
32:1a:236:G:H5''	48:1q:42:TYR:OH	2.17	0.44
32:1a:710:G:H5''	37:1f:54:LYS:HE3	2.00	0.44
32:1a:942:G:H21	40:1i:124:GLN:NE2	2.15	0.44
32:1a:1029:C:N4	32:1a:1031:G:O6	2.50	0.44
39:1h:65:TYR:HA	39:1h:79:VAL:HG23	2.00	0.44
40:1i:96:LEU:N	40:1i:98:PRO:HD2	2.33	0.44
51:1t:83:ARG:HG2	51:1t:86:ARG:NH2	2.32	0.44
20:2Y:7:VAL:HG21	20:2Y:72:VAL:HG12	1.99	0.44
20:2Y:13:VAL:HB	20:2Y:72:VAL:HG13	1.98	0.44
20:2Y:38:ILE:HD11	20:2Y:66:PRO:HG3	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1020:U:H2'	32:2a:1021:G:C8	2.52	0.44
32:2a:1073:U:O2	33:2b:104:ASN:ND2	2.50	0.44
32:2a:1079:G:O3'	36:2e:14:ARG:NH2	2.50	0.44
32:2a:1304:G:O2'	32:2a:1333:A:N6	2.44	0.44
40:2i:55:ALA:HA	40:2i:58:HIS:HD2	1.82	0.44
1:1A:185:U:H4'	1:1A:218:A:H4'	1.98	0.44
1:1A:207:A:H2'	1:1A:208:C:O4'	2.16	0.44
1:1A:1070:A:N7	1:1A:1096:A:O2'	2.41	0.44
1:1A:2011:U:H2'	1:1A:2012:G:O4'	2.18	0.44
1:1A:2611:U:H5'	1:1A:2611:U:H6	1.82	0.44
1:2A:245:G:O6	30:28:8:LYS:HE3	2.17	0.44
1:2A:613:G:O2'	1:2A:614(C):A:N1	2.46	0.44
1:2A:660:G:H5'	5:2F:99:TYR:CE1	2.53	0.44
1:2A:892:G:H3'	1:2A:893:C:C5'	2.48	0.44
1:2A:1013:C:H2'	1:2A:1014:U:H6	1.82	0.44
1:2A:1315:C:O2'	1:2A:1392:A:N3	2.49	0.44
1:2A:2198:A:OP1	8:2I:33:ARG:NH2	2.50	0.44
1:2A:2667:C:H2'	1:2A:2668:G:O4'	2.16	0.44
2:1B:43:C:H5''	26:14:1:MET:HE3	2.00	0.44
4:1E:181:LEU:HD12	4:1E:181:LEU:HA	1.81	0.44
7:1H:152:ARG:HD3	7:1H:152:ARG:HA	1.68	0.44
8:1I:93:THR:OG1	8:1I:96:ASP:N	2.48	0.44
9:1N:62:VAL:CG1	9:1N:66:LYS:HB2	2.48	0.44
18:1W:11:ARG:HH21	18:1W:98:LYS:HG2	1.81	0.44
21:1Z:92:SER:O	21:1Z:130:PRO:HG2	2.18	0.44
24:12:17:SER:OG	24:12:20:GLU:HG3	2.18	0.44
32:1a:175:C:H4'	51:1t:25:ARG:HD3	2.00	0.44
32:1a:567:G:H2'	32:1a:568:G:O4'	2.16	0.44
32:1a:1202:G:O4'	45:1n:29:ARG:NH1	2.50	0.44
32:1a:1289:A:N1	32:1a:1371:G:O2'	2.38	0.44
32:1a:1346:A:OP1	40:1i:120:ARG:NH1	2.43	0.44
40:1i:3:GLN:HE21	40:1i:20:ARG:NH2	2.16	0.44
43:1l:117:ARG:HG2	43:1l:122:THR:HB	2.00	0.44
2:2B:24:G:N7	2:2B:56:G:H2'	2.32	0.44
5:2F:9:ILE:HG21	5:2F:125:LEU:HD13	1.98	0.44
12:2Q:38:GLU:OE2	12:2Q:128:LYS:N	2.44	0.44
21:2Z:70:LEU:HD23	21:2Z:70:LEU:HA	1.70	0.44
22:20:53:MET:HG3	22:20:59:LEU:HD23	1.99	0.44
32:2a:7:G:H5''	32:2a:298:A:O4'	2.17	0.44
32:2a:99:U:H2'	32:2a:100:C:C6	2.53	0.44
32:2a:604:G:H2'	32:2a:605:U:O4'	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1005:A:OP2	32:2a:1006:C:N4	2.47	0.44
32:2a:1161:C:H2'	32:2a:1162:C:C6	2.53	0.44
33:2b:189:ASP:OD1	33:2b:189:ASP:N	2.39	0.44
38:2g:153:HIS:ND1	42:2k:58:PRO:HD2	2.32	0.44
44:2m:39:ILE:HD13	44:2m:52:GLU:HB3	2.00	0.44
1:1A:143:G:H2'	1:1A:143(A):C:C6	2.53	0.44
1:1A:372:G:H8	23:11:65:SER:O	2.00	0.44
1:1A:1794:U:H2'	1:1A:1795:C:H6	1.82	0.44
1:1A:2106:G:H1	1:1A:2183:C:N4	2.16	0.44
1:2A:354:G:H2'	1:2A:355:G:C8	2.52	0.44
1:2A:1149:G:H2'	1:2A:1150:C:C6	2.52	0.44
1:2A:1266:G:O2'	1:2A:2012:G:O6	2.34	0.44
1:2A:1665:A:H4'	10:2O:67:LYS:HB2	1.99	0.44
32:1a:179:A:H2'	32:1a:180:U:C6	2.53	0.44
32:1a:933:G:OP2	38:1g:3:ARG:HB2	2.17	0.44
32:1a:1084:G:C5	32:1a:1085:U:C4	3.05	0.44
32:1a:1518:MA6:H93	32:1a:1519:MA6:H92	2.00	0.44
35:1d:73:ARG:HD2	35:1d:73:ARG:HA	1.87	0.44
37:1f:99:ALA:O	49:1r:28:GLU:HA	2.16	0.44
3:2D:260:ARG:NH2	3:2D:266:SER:OG	2.48	0.44
32:2a:151:A:H2'	32:2a:152:A:O4'	2.18	0.44
32:2a:1148:U:H1'	40:2i:66:ARG:HH22	1.83	0.44
35:2d:119:GLN:O	35:2d:123:HIS:HD2	2.01	0.44
36:2e:93:PRO:HG2	39:2h:105:ARG:NE	2.33	0.44
40:2i:112:LYS:HE2	40:2i:117:HIS:O	2.18	0.44
55:2x:47:U:H3'	55:2x:48:C:H5'	1.99	0.44
1:1A:26:G:H1'	1:1A:514:A:N6	2.31	0.44
1:1A:1045:A:OP1	1:1A:1046:A:H3'	2.18	0.44
1:1A:1095:A:C8	1:1A:1096:A:N7	2.86	0.44
1:1A:1176:G:H4'	1:1A:1177:A:OP1	2.16	0.44
1:1A:1570:A:H2'	1:1A:1571:A:C8	2.53	0.44
1:1A:2695:C:H2'	1:1A:2696:U:C6	2.53	0.44
1:1A:2722:G:H2'	1:1A:2723:C:C6	2.52	0.44
1:1A:2870:C:H2'	1:1A:2871:C:O4'	2.18	0.44
1:2A:565:C:H2'	1:2A:566:U:O4'	2.18	0.44
1:2A:855:G:C5	1:2A:856:C:C4	3.06	0.44
1:2A:1277:G:O2'	13:2R:24:GLN:HG2	2.18	0.44
1:2A:1420:U:O2'	1:2A:1421:G:H8	2.00	0.44
1:2A:1800:C:P	3:2D:183:ARG:HH12	2.41	0.44
30:18:63:PRO:HG2	30:18:64:TYR:CD2	2.53	0.44
32:1a:221:C:H2'	32:1a:222:U:H6	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:373:A:H1'	32:1a:481:G:N3	2.32	0.44
32:1a:565:U:H3'	32:1a:566:G:H2'	2.00	0.44
32:1a:926:G:H5''	32:1a:927:G:O5'	2.18	0.44
37:1f:21:LEU:O	37:1f:25:ILE:HG13	2.18	0.44
47:1p:51:VAL:HG12	47:1p:53:VAL:H	1.83	0.44
5:2F:11:VAL:HG22	5:2F:125:LEU:HB2	1.99	0.44
6:2G:111:LEU:HA	6:2G:114:ILE:HD12	2.00	0.44
14:2S:10:ARG:NE	14:2S:91:PRO:O	2.44	0.44
15:2T:82:LEU:HD23	15:2T:82:LEU:HA	1.77	0.44
15:2T:85:LYS:NZ	15:2T:87:ASP:OD2	2.49	0.44
15:2T:109:GLU:HG2	15:2T:112:ARG:NH2	2.33	0.44
32:2a:109:A:C6	32:2a:326:G:C6	3.05	0.44
32:2a:818:G:N2	32:2a:873:A:OP1	2.50	0.44
37:2f:76:ALA:O	37:2f:80:ARG:HG3	2.17	0.44
51:2t:47:GLY:HA2	51:2t:48:LYS:C	2.42	0.44
1:1A:288:C:H2'	1:1A:289:A:H8	1.82	0.44
1:1A:373:U:O2'	1:1A:423:A:H1'	2.18	0.44
1:1A:570:G:H5''	61:1A:5756:HOH:O	2.17	0.44
1:1A:1162:G:O2'	17:1V:90:PRO:HG2	2.17	0.44
1:1A:1210:A:H5''	1:1A:1212:G:O4'	2.18	0.44
1:2A:658:C:H2'	1:2A:659:C:C6	2.53	0.44
1:2A:1292:U:H2'	1:2A:1293:C:C6	2.52	0.44
1:2A:1469:A:H2'	1:2A:1470:G:O4'	2.18	0.44
1:2A:1572:A:H2'	1:2A:1573:G:O4'	2.17	0.44
2:1B:96:U:OP1	21:1Z:14:LYS:NZ	2.51	0.44
4:1E:170:LEU:HB3	4:1E:184:VAL:CG2	2.47	0.44
11:1P:100:LEU:HD22	11:1P:105:LEU:HD12	2.00	0.44
29:17:9:ARG:NH1	29:17:47:ARG:HB2	2.33	0.44
32:1a:271:C:H2'	32:1a:272:C:C6	2.53	0.44
32:1a:1057:G:H2'	32:1a:1058:G:O4'	2.18	0.44
32:1a:1429:C:H2'	32:1a:1430:C:C6	2.53	0.44
33:1b:59:GLU:HB2	33:1b:221:LEU:HD21	2.00	0.44
42:1k:19:ALA:HB3	42:1k:82:VAL:HG22	2.00	0.44
48:1q:83:ASP:N	48:1q:83:ASP:OD1	2.51	0.44
5:2F:195:ASP:OD1	5:2F:196:LEU:N	2.50	0.44
5:2F:196:LEU:HD23	5:2F:196:LEU:HA	1.81	0.44
25:23:46:ASN:O	25:23:50:VAL:HG22	2.18	0.44
32:2a:757:U:H2'	32:2a:758:G:O4'	2.18	0.44
32:2a:1261:A:H5'	32:2a:1283:G:O3'	2.17	0.44
33:2b:58:ILE:H	33:2b:58:ILE:HG13	1.57	0.44
43:2l:37:CYS:SG	43:2l:81:SER:HB2	2.58	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:2s:40:ILE:HA	50:2s:44:MET:SD	2.58	0.44
54:2y:40:G:H2'	54:2y:41:A:H8	1.80	0.44
1:1A:124:G:OP1	1:1A:1376:C:O2'	2.32	0.44
1:1A:296:C:H2'	1:1A:297:C:H6	1.82	0.44
1:1A:824:A:H1'	1:1A:2358:G:N7	2.33	0.44
1:1A:1252:G:N3	16:1U:33:ARG:HG2	2.33	0.44
1:1A:2094:G:OP1	8:1I:22:LYS:HD2	2.18	0.44
1:1A:2137:C:H2'	1:1A:2138:C:C6	2.53	0.44
1:1A:2224:G:H4'	1:1A:2226:C:C2	2.53	0.44
1:1A:2674:G:H5'	10:1O:26:LYS:HE2	1.99	0.44
1:2A:637:A:H2'	11:2P:117:GLU:OE1	2.18	0.44
1:2A:1695:G:N7	3:2D:14:ARG:NH2	2.65	0.44
1:2A:1814:G:H4'	3:2D:51:VAL:HG21	2.00	0.44
1:2A:2144:U:H1'	1:2A:2148:G:N2	2.33	0.44
1:2A:2320:A:N3	1:2A:2320:A:H2'	2.32	0.44
1:2A:2352:A:N6	1:2A:2365:G:O2'	2.51	0.44
13:1R:59:ASP:N	13:1R:59:ASP:OD1	2.45	0.44
32:1a:175:C:H2'	32:1a:176:C:C6	2.53	0.44
32:1a:363:A:OP2	43:1l:34:ARG:NH1	2.51	0.44
37:1f:8:ILE:HD11	37:1f:79:LEU:HD13	2.00	0.44
40:1i:53:VAL:HG21	40:1i:85:LEU:HD13	1.99	0.44
55:1x:50:U:H2'	55:1x:51:C:C6	2.53	0.44
54:1y:56:C:H2'	54:1y:57:G:O4'	2.18	0.44
6:2G:126:ASP:HB2	6:2G:130:ASN:O	2.17	0.44
7:2H:20:ALA:HB3	7:2H:23:ARG:HG3	1.99	0.44
12:2Q:24:GLY:HA2	12:2Q:67:ARG:NH2	2.33	0.44
16:2U:16:LYS:HB3	16:2U:16:LYS:HE2	1.75	0.44
21:2Z:6:LYS:HE2	21:2Z:8:TYR:HE2	1.82	0.44
26:24:36:CYS:O	26:24:40:HIS:HB2	2.18	0.44
32:2a:46:G:O2'	32:2a:365:U:H1'	2.17	0.44
32:2a:441:A:H3'	32:2a:442:C:C6	2.53	0.44
32:2a:1122:U:H2'	32:2a:1123:A:H8	1.82	0.44
32:2a:1299:A:H2'	32:2a:1299:A:N3	2.32	0.44
43:2l:24:VAL:HB	43:2l:27:LEU:HD22	2.00	0.44
43:2l:51:ALA:O	43:2l:52:LEU:HD12	2.18	0.44
54:2w:4:U:H3	54:2w:69:A:N6	2.16	0.44
1:1A:72:U:H3	24:12:62:THR:HG23	1.83	0.43
1:1A:620:G:N3	1:1A:620:G:H5'	2.32	0.43
1:1A:2065:C:H4'	1:1A:2251:OMG:HM22	2.00	0.43
1:2A:82:G:H5''	1:2A:296:C:H5'	1.99	0.43
1:2A:127:A:H5''	1:2A:128:C:C6	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:265:A:H1'	1:2A:266:G:O4'	2.18	0.43
1:2A:715:G:H2'	1:2A:716:A:O4'	2.18	0.43
1:2A:899:A:O2'	1:2A:900:A:H5''	2.18	0.43
1:2A:1013:C:H2'	1:2A:1014:U:C6	2.53	0.43
1:2A:1274:A:N3	1:2A:1297:C:H1'	2.33	0.43
5:1F:188:ARG:HA	11:1P:3:LEU:HD13	2.00	0.43
26:14:34:GLU:H	26:14:34:GLU:CD	2.26	0.43
32:1a:1126:U:O2	32:1a:1280:A:H2'	2.18	0.43
34:1c:12:LEU:HD11	45:1n:51:GLY:HA2	1.98	0.43
39:1h:39:LEU:O	39:1h:45:ILE:HG12	2.17	0.43
40:1i:128:ARG:NH1	55:1x:35:A:OP2	2.51	0.43
6:2G:101:ILE:HG22	6:2G:105:LYS:NZ	2.33	0.43
15:2T:56:GLY:O	15:2T:59:THR:HG22	2.18	0.43
24:22:22:GLU:OE2	24:22:68:ARG:NH2	2.51	0.43
30:28:32:LEU:HD12	30:28:32:LEU:HA	1.86	0.43
32:2a:1320:C:C1'	50:2s:73:GLU:HG3	2.48	0.43
32:2a:1465:C:H2'	32:2a:1466:C:O4'	2.18	0.43
36:2e:68:GLU:HG3	36:2e:69:VAL:N	2.32	0.43
39:2h:51:VAL:HG21	39:2h:60:ARG:HB2	2.00	0.43
43:2l:33:ARG:HD3	43:2l:33:ARG:HA	1.79	0.43
1:1A:1059:G:H2'	1:1A:1060:U:C6	2.52	0.43
1:1A:1230:C:H2'	1:1A:1231:G:C8	2.52	0.43
1:1A:1266:G:O6	18:1W:13:SER:OG	2.23	0.43
1:1A:2262:U:OP1	1:1A:2387:U:O2'	2.33	0.43
1:2A:531:C:H4'	1:2A:532:A:H5''	2.00	0.43
1:2A:827:U:O2'	1:2A:2068:U:C2	2.66	0.43
1:2A:919:G:H22	1:2A:2268:A:H3'	1.84	0.43
1:2A:1165:U:H2'	1:2A:1166:C:C6	2.53	0.43
1:2A:1264:G:H2'	1:2A:2014:A:N6	2.34	0.43
1:2A:2135:A:C8	1:2A:2136:C:H5	2.36	0.43
6:1G:47:LYS:HG3	6:1G:48:GLU:H	1.82	0.43
14:1S:32:LEU:HD23	14:1S:32:LEU:HA	1.82	0.43
32:1a:163:C:H2'	32:1a:164:U:C6	2.53	0.43
32:1a:660:G:H2'	32:1a:661:G:O4'	2.17	0.43
32:1a:880:C:OP1	43:1l:8:ASN:ND2	2.51	0.43
32:1a:945:G:OP2	61:1a:1931:HOH:O	2.21	0.43
33:1b:170:GLU:HG3	33:1b:173:ALA:HB3	1.99	0.43
53:1v:16:A:H2'	53:1v:17:U:O4'	2.18	0.43
12:2Q:65:PHE:HB2	12:2Q:105:GLU:HB2	2.00	0.43
12:2Q:75:THR:HA	12:2Q:89:ASN:O	2.18	0.43
21:2Z:54:HIS:CG	21:2Z:101:PRO:HG3	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:923:A:O2'	32:2a:1399:C:OP2	2.33	0.43
32:2a:987:G:H2'	32:2a:988:G:H8	1.82	0.43
32:2a:1005:A:H5''	32:2a:1006:C:H5	1.83	0.43
35:2d:122:ARG:HA	35:2d:122:ARG:HD2	1.93	0.43
39:2h:91:ARG:HD3	48:2q:32:TYR:O	2.18	0.43
55:2x:19:G:H3'	55:2x:20:U:C6	2.53	0.43
55:2x:19:G:H3'	55:2x:20:U:H6	1.82	0.43
54:2y:35:A:H2'	54:2y:36:C:C6	2.53	0.43
1:1A:271(M):G:O2'	1:1A:271(N):U:H5''	2.18	0.43
1:1A:2108:C:H2'	1:1A:2109:U:C6	2.52	0.43
1:1A:2112:G:C5	1:1A:2113:U:H1'	2.53	0.43
1:2A:321:G:OP1	5:2F:135:LYS:NZ	2.51	0.43
1:2A:2064:C:H2'	1:2A:2065:C:C6	2.53	0.43
1:2A:2108:C:H2'	1:2A:2109:U:H6	1.83	0.43
1:2A:2173:A:H3'	1:2A:2173:A:OP2	2.19	0.43
1:2A:2846:G:H2'	1:2A:2847:U:O4'	2.18	0.43
5:1F:183:VAL:O	5:1F:187:VAL:HG23	2.17	0.43
6:1G:129:GLY:O	6:1G:161:THR:OG1	2.31	0.43
8:1I:38:LEU:HD13	8:1I:40:THR:HG23	1.98	0.43
9:1N:61:ARG:HA	9:1N:61:ARG:HD3	1.58	0.43
13:1R:13:HIS:CE1	13:1R:16:HIS:HB2	2.53	0.43
32:1a:189:G:C6	32:1a:189(L):G:N1	2.87	0.43
32:1a:383:A:C5	32:1a:384:G:H1'	2.53	0.43
32:1a:701:C:OP1	32:1a:702:A:O2'	2.31	0.43
32:1a:922:G:C6	32:1a:923:A:C6	3.05	0.43
32:1a:1008:C:N3	32:1a:1021:G:C6	2.87	0.43
32:1a:1030:C:N4	32:1a:1031:G:N1	2.53	0.43
32:1a:1296:C:H4'	32:1a:1302:U:C4	2.53	0.43
35:1d:173:TRP:CD2	35:1d:189:PRO:HG3	2.52	0.43
37:1f:2:ARG:HD2	37:1f:4:TYR:OH	2.19	0.43
54:1w:59:U:H3'	54:1w:60:C:O2	2.18	0.43
7:2H:3:ARG:HG2	7:2H:6:ARG:NE	2.33	0.43
7:2H:20:ALA:HB1	7:2H:21:PRO:HD2	2.00	0.43
9:2N:30:ILE:HG23	9:2N:52:VAL:HG11	2.00	0.43
32:2a:127:G:N2	48:2q:61:GLU:OE2	2.49	0.43
32:2a:473:G:H2'	32:2a:474:G:C8	2.53	0.43
32:2a:922:G:N3	32:2a:1398:A:H2	2.15	0.43
32:2a:1362:C:H2'	32:2a:1363:C:H5''	1.99	0.43
32:2a:1427:U:H2'	32:2a:1428:A:C8	2.52	0.43
35:2d:157:LEU:HG	35:2d:161:ASN:ND2	2.33	0.43
1:1A:1010:A:N3	1:1A:1153:C:H1'	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1111:A:N3	1:1A:1112:G:H1'	2.33	0.43
1:1A:1628:G:H2'	1:1A:1629:U:C6	2.53	0.43
1:1A:1784:A:H4'	1:1A:1785:A:O5'	2.18	0.43
1:1A:2298:A:H2'	1:1A:2299:G:O4'	2.18	0.43
1:1A:2855:C:H2'	1:1A:2856:C:H6	1.83	0.43
1:2A:185:U:H2'	1:2A:186:G:H8	1.82	0.43
1:2A:191:A:H2'	1:2A:192:C:C6	2.53	0.43
1:2A:645:C:H5'	1:2A:646:A:OP2	2.18	0.43
1:2A:1278:A:OP1	13:2R:36:THR:HB	2.18	0.43
1:2A:1890:A:OP2	61:2A:3993:HOH:O	2.21	0.43
1:2A:2164:C:H3'	1:2A:2165:G:O4'	2.19	0.43
1:2A:2376:A:N3	14:2S:106:ARG:NH2	2.61	0.43
2:1B:77:U:OP1	21:1Z:19:ARG:NH2	2.52	0.43
5:1F:135:LYS:HB2	5:1F:138:GLU:CD	2.43	0.43
9:1N:102:ALA:O	9:1N:106:MET:HG3	2.19	0.43
10:1O:24:VAL:HG13	10:1O:33:ALA:HB2	1.99	0.43
32:1a:271:C:H2'	32:1a:272:C:H6	1.83	0.43
32:1a:652:U:O4	32:1a:752:G:O2'	2.32	0.43
32:1a:958:A:C6	32:1a:959:A:N1	2.86	0.43
54:1y:19:G:H1	54:1y:56:C:N4	2.17	0.43
2:2B:14:U:O2	2:2B:108:U:H4'	2.18	0.43
32:2a:56:U:H2'	32:2a:57:G:C8	2.53	0.43
32:2a:999:C:C4	32:2a:1000:U:C4	3.07	0.43
32:2a:1157:A:H5'	32:2a:1158:C:C6	2.54	0.43
33:2b:78:GLN:HE22	33:2b:95:GLN:CD	2.26	0.43
33:2b:134:GLU:O	33:2b:138:LEU:HG	2.17	0.43
34:2c:6:HIS:HB3	45:2n:49:HIS:ND1	2.33	0.43
36:2e:32:VAL:HG11	36:2e:59:GLY:HA2	2.00	0.43
46:2o:43:LEU:HD11	46:2o:53:HIS:HA	2.00	0.43
1:1A:107:C:H2'	1:1A:108:U:C6	2.53	0.43
1:1A:1055:G:H3'	1:1A:1056:G:H8	1.83	0.43
1:1A:1101:U:H2'	1:1A:1102:C:H6	1.82	0.43
1:1A:1759:A:H1'	1:1A:2711:A:C2	2.53	0.43
1:1A:2477:C:N4	31:19:10:ILE:HG23	2.33	0.43
1:1A:2683:C:OP1	15:1T:53:ARG:NH2	2.49	0.43
1:2A:27:G:O2'	1:2A:28:A:OP2	2.35	0.43
1:2A:289:A:H2'	1:2A:290:G:O4'	2.19	0.43
1:2A:2274:A:C5	1:2A:2276:G:C8	3.07	0.43
4:1E:18:ASP:HB3	15:1T:82:LEU:HD21	1.99	0.43
9:1N:13:TRP:CE2	9:1N:133:GLN:HG2	2.54	0.43
15:1T:26:ASP:O	15:1T:49:VAL:HG13	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:114:U:O2'	32:1a:115:G:H5'	2.19	0.43
32:1a:128:G:O3'	48:1q:3:LYS:NZ	2.50	0.43
32:1a:235:C:H2'	32:1a:236:G:H8	1.84	0.43
32:1a:382:A:H2'	32:1a:383:A:C8	2.54	0.43
32:1a:625:G:H4'	47:1p:16:HIS:CD2	2.54	0.43
32:1a:646:U:H2'	32:1a:647:C:C6	2.53	0.43
41:1j:5:ARG:O	41:1j:99:LYS:N	2.38	0.43
44:1m:108:ARG:HD3	44:1m:108:ARG:HA	1.71	0.43
8:2I:2:LYS:HA	8:2I:19:VAL:O	2.19	0.43
25:23:10:LYS:HB3	25:23:53:LEU:HA	2.00	0.43
32:2a:62:U:O2'	32:2a:379:C:O2	2.29	0.43
32:2a:677:U:H1'	42:2k:119:CYS:SG	2.58	0.43
32:2a:1142:G:H2'	32:2a:1143:G:O4'	2.18	0.43
34:2c:69:HIS:NE2	34:2c:104:GLN:HG2	2.33	0.43
46:2o:48:LYS:HA	46:2o:48:LYS:HD3	1.74	0.43
47:2p:23:ASP:OD1	47:2p:24:ALA:N	2.52	0.43
1:1A:296:C:H2'	1:1A:297:C:C6	2.54	0.43
1:1A:625:G:N7	11:1P:107:LYS:NZ	2.61	0.43
1:1A:851:U:O2'	25:13:42:ALA:O	2.36	0.43
1:1A:1489:U:O3'	1:1A:1490:A:H8	2.02	0.43
1:1A:1593:G:H2'	1:1A:1594:G:C8	2.53	0.43
1:1A:2051:A:H5'	1:1A:2578:G:O4'	2.18	0.43
1:1A:2370:G:C6	1:1A:2371:G:C6	3.06	0.43
1:2A:702:G:C2	1:2A:731:C:C2	3.07	0.43
1:2A:893:C:H2'	1:2A:894:C:C5	2.53	0.43
1:2A:945:A:C4	1:2A:2448:A:C2	3.06	0.43
1:2A:2012:G:OP1	18:2W:11:ARG:NH2	2.50	0.43
1:2A:2051:A:H5'	1:2A:2578:G:O4'	2.18	0.43
1:2A:2462:U:H2'	1:2A:2463:C:C6	2.54	0.43
1:2A:2893:G:H5''	1:2A:2894:G:O4'	2.19	0.43
2:1B:88:C:H2'	2:1B:89:G:O4'	2.18	0.43
4:1E:29:GLY:H	4:1E:93:VAL:HG12	1.82	0.43
7:1H:90:LYS:HD3	7:1H:159:GLU:HG2	2.00	0.43
7:1H:164:TYR:N	7:1H:167:GLU:OE1	2.34	0.43
9:1N:33:LEU:HD12	9:1N:33:LEU:HA	1.87	0.43
17:1V:64:HIS:ND1	17:1V:92:THR:OG1	2.45	0.43
18:1W:73:ALA:HB3	18:1W:106:ILE:HB	2.00	0.43
26:14:15:ILE:HD12	26:14:21:VAL:HG22	1.99	0.43
32:1a:1054:C:C4	32:1a:1196:U:H5	2.37	0.43
34:1c:130:VAL:O	34:1c:134:ILE:HG13	2.18	0.43
36:1e:77:PRO:HD2	36:1e:142:LEU:HD22	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2F:176:LEU:HD23	5:2F:176:LEU:HA	1.83	0.43
15:2T:92:GLY:O	15:2T:120:ARG:NH2	2.52	0.43
17:2V:10:LYS:HE2	17:2V:10:LYS:HB2	1.85	0.43
19:2X:35:THR:HG23	19:2X:38:GLU:H	1.84	0.43
20:2Y:83:THR:HG21	20:2Y:99:CYS:HB2	2.00	0.43
30:28:50:LEU:HA	30:28:50:LEU:HD23	1.68	0.43
32:2a:4:U:H3	39:2h:105:ARG:NH2	2.17	0.43
32:2a:357:G:OP1	32:2a:367:U:H5''	2.18	0.43
32:2a:660:G:H1	32:2a:745:C:N4	2.16	0.43
32:2a:925:G:H1'	32:2a:1502:A:C4	2.54	0.43
32:2a:975:A:H5'	32:2a:975:A:H8	1.84	0.43
32:2a:1030(A):G:N1	32:2a:1030(D):A:OP2	2.48	0.43
32:2a:1109:C:H2'	32:2a:1110:A:O4'	2.19	0.43
32:2a:1228:C:H2'	32:2a:1229:A:H8	1.83	0.43
34:2c:125:GLU:C	34:2c:127:ARG:H	2.27	0.43
35:2d:57:ARG:NH2	36:2e:107:ARG:HD3	2.33	0.43
50:2s:30:LEU:C	50:2s:31:ILE:HG13	2.44	0.43
1:1A:817:C:H4'	1:1A:932:G:C5	2.54	0.43
1:1A:1005:C:O2'	9:1N:28:THR:HG21	2.19	0.43
1:1A:2206:G:H8	1:1A:2207:G:N7	2.16	0.43
1:2A:723:G:H2'	1:2A:724:U:O4'	2.19	0.43
1:2A:1530:C:HO2'	1:2A:1531:C:P	2.41	0.43
1:2A:1803:A:H4'	3:2D:259:THR:HG23	2.00	0.43
1:2A:2095:C:H2'	1:2A:2096:U:O4'	2.18	0.43
1:2A:2360:A:H2'	1:2A:2361:A:O4'	2.18	0.43
5:1F:34:TRP:CH2	11:1P:8:PRO:HB3	2.53	0.43
31:19:14:CYS:HA	31:19:27:CYS:HB2	1.99	0.43
32:1a:963:G:H4'	61:1a:2261:HOH:O	2.19	0.43
32:1a:1223:C:P	50:1s:78:ARG:HH21	2.42	0.43
32:1a:1486:G:H2'	32:1a:1487:G:O4'	2.19	0.43
40:1i:100:GLY:O	40:1i:103:THR:HG22	2.18	0.43
43:1l:88:GLY:O	43:1l:99:HIS:HD2	2.02	0.43
16:2U:88:ILE:HG22	16:2U:90:VAL:HG23	2.01	0.43
19:2X:11:PRO:HB3	19:2X:92:LEU:HD11	2.01	0.43
20:2Y:35:TYR:CE2	20:2Y:69:ALA:HB3	2.53	0.43
21:2Z:7:ALA:HB3	21:2Z:61:LEU:HD12	2.00	0.43
23:21:4:VAL:HG11	23:21:11:ARG:NH2	2.33	0.43
32:2a:337:C:H2'	32:2a:338:A:C8	2.54	0.43
32:2a:742:G:P	46:2o:35:ARG:HH22	2.42	0.43
32:2a:841:U:O2	32:2a:841:U:H2'	2.17	0.43
32:2a:857:C:H2'	32:2a:858:G:O4'	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1062:U:H2'	32:2a:1063:C:C5	2.52	0.43
32:2a:1126:U:H6	32:2a:1281:U:C4	2.37	0.43
32:2a:1149:C:O2'	32:2a:1280:A:N1	2.42	0.43
32:2a:1320:C:O4'	50:2s:73:GLU:HG3	2.19	0.43
40:2i:101:PHE:N	40:2i:101:PHE:CD1	2.86	0.43
44:2m:82:MET:O	44:2m:93:ARG:NH2	2.51	0.43
46:2o:55:GLY:HA2	46:2o:58:MET:HE3	2.00	0.43
47:2p:3:LYS:HE3	47:2p:3:LYS:HB3	1.81	0.43
54:2y:3:G:H1	54:2y:70:C:H42	1.67	0.43
1:1A:234:C:H2'	1:1A:235:U:C6	2.54	0.43
1:1A:631:A:H2'	1:1A:632:A:O4'	2.18	0.43
1:2A:459:U:H2'	1:2A:460:A:H8	1.83	0.43
1:2A:2017:U:O2	27:25:10:LYS:HB2	2.19	0.43
3:1D:232:PRO:HB3	3:1D:244:ARG:CZ	2.48	0.43
8:1I:109:ILE:HA	8:1I:109:ILE:HD12	1.69	0.43
12:1Q:30:GLY:HA2	12:1Q:107:ALA:HB2	2.01	0.43
16:1U:76:TYR:CE2	16:1U:80:ILE:HG13	2.54	0.43
16:1U:83:LEU:CD1	16:1U:113:ALA:HB2	2.49	0.43
17:1V:85:LYS:HE2	17:1V:85:LYS:HB2	1.85	0.43
19:1X:31:HIS:CD2	19:1X:33:LYS:H	2.37	0.43
32:1a:194:C:H2'	32:1a:195:A:H5''	2.01	0.43
32:1a:455:C:H42	32:1a:476:G:H1	1.65	0.43
32:1a:1036:G:H3'	32:1a:1037:C:C6	2.53	0.43
33:1b:168:THR:OG1	33:1b:191:ASP:O	2.29	0.43
10:2O:2:ILE:HD11	10:2O:82:ASN:HB3	2.00	0.43
12:2Q:17:LEU:HD21	12:2Q:41:TRP:NE1	2.33	0.43
15:2T:105:LEU:HB2	15:2T:110:ILE:HG13	2.01	0.43
32:2a:37:U:O2'	32:2a:500:G:H4'	2.18	0.43
32:2a:145:G:H2'	32:2a:146:G:O4'	2.19	0.43
32:2a:178:C:H2'	32:2a:179:A:O4'	2.19	0.43
32:2a:580:U:H5''	46:2o:58:MET:HG2	2.00	0.43
32:2a:1005:A:H3'	32:2a:1006:C:H6	1.83	0.43
32:2a:1142:G:H3'	32:2a:1143:G:C8	2.49	0.43
35:2d:11:LEU:O	35:2d:15:GLU:HG2	2.19	0.43
39:2h:87:SER:HB3	39:2h:133:LEU:O	2.19	0.43
44:2m:81:LEU:HD22	44:2m:88:ARG:HB2	2.01	0.43
44:2m:101:GLN:OE1	44:2m:101:GLN:N	2.52	0.43
47:2p:8:ARG:NH2	47:2p:15:PRO:HG3	2.33	0.43
54:2y:60:C:H3'	54:2y:61:C:C6	2.53	0.43
1:1A:573:G:O2'	1:1A:574:C:H3'	2.19	0.43
1:1A:597:U:H2'	1:1A:598:G:C8	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1405:U:H2'	1:1A:1406:U:H6	1.82	0.43
1:1A:2102:U:H3	1:1A:2187:G:H1	1.67	0.43
1:1A:2319:G:C2	14:1S:3:ARG:HA	2.53	0.43
1:2A:185:U:H2'	1:2A:186:G:C8	2.54	0.43
1:2A:748:G:C8	18:2W:89:ALA:HB1	2.53	0.43
1:2A:1594:G:H2'	1:2A:1595:G:O4'	2.19	0.43
1:2A:2393:A:H5''	11:2P:63:PRO:HB3	2.00	0.43
1:2A:2788:C:P	4:2E:61:ARG:HH21	2.41	0.43
6:1G:104:GLU:HG3	61:1G:305:HOH:O	2.17	0.43
18:1W:6:ILE:HA	18:1W:103:ILE:O	2.19	0.43
32:1a:584:G:H2'	32:1a:585:G:C8	2.53	0.43
32:1a:1003:G:H2'	32:1a:1004:A:N3	2.33	0.43
32:1a:1342:C:O2'	40:1i:124:GLN:HG2	2.18	0.43
35:1d:18:LYS:HG2	60:1d:3102:SF4:S1	2.59	0.43
36:1e:84:PHE:HB3	36:1e:134:ALA:HB2	2.01	0.43
41:1j:35:SER:CB	41:1j:73:ASP:HB2	2.49	0.43
41:1j:49:VAL:HG21	45:1n:41:ARG:O	2.18	0.43
54:1y:60:C:H2'	54:1y:61:C:H5	1.83	0.43
5:2F:34:TRP:CZ3	11:2P:8:PRO:HB3	2.54	0.43
8:2I:9:LEU:HD21	8:2I:35:LEU:HD13	2.01	0.43
11:2P:2:LYS:O	11:2P:5:ASP:HB2	2.18	0.43
19:2X:50:LYS:HG2	19:2X:84:ALA:HB2	2.01	0.43
32:2a:718:G:H5'	42:2k:117:ASN:CG	2.44	0.43
32:2a:977:A:O2'	32:2a:979:C:OP2	2.32	0.43
32:2a:1060:C:C5	34:2c:2:GLY:HA3	2.53	0.43
32:2a:1097:C:H1'	32:2a:1170:A:H1'	2.01	0.43
35:2d:81:GLU:O	35:2d:85:LYS:HG3	2.19	0.43
41:2j:16:LEU:HD12	41:2j:16:LEU:HA	1.91	0.43
42:2k:43:SER:HB3	42:2k:68:ALA:HB2	2.01	0.43
54:2y:11:C:O5'	54:2y:11:C:H6	2.02	0.43
1:1A:311:A:C6	1:1A:328:U:C4	3.06	0.43
1:1A:1297:C:O2'	1:1A:1302:A:N1	2.42	0.43
1:1A:1954:G:O2'	1:1A:1956:U:O4	2.26	0.43
1:2A:2102:U:H3	1:2A:2187:G:H1	1.66	0.43
1:2A:2705:A:O2'	1:2A:2852:G:OP1	2.33	0.43
12:1Q:8:LYS:HG2	12:1Q:9:TYR:CE2	2.54	0.43
20:1Y:73:ARG:HD2	20:1Y:82:PRO:HB2	2.01	0.43
32:1a:192:U:H2'	32:1a:193:C:C6	2.54	0.43
32:1a:342:C:H2'	32:1a:343:U:C6	2.54	0.43
38:1g:26:PHE:O	38:1g:30:ILE:HG13	2.19	0.43
40:1i:24:GLY:HA2	40:1i:59:PHE:O	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:1m:84:ILE:HB	50:1s:66:MET:HE2	2.01	0.43
54:1y:34:CM0:H2'	54:1y:35:A:O4'	2.19	0.43
54:1y:63:G:N1	54:1y:64:U:O2	2.52	0.43
2:2B:105:A:H2'	2:2B:106:G:O4'	2.19	0.43
6:2G:83:ARG:N	6:2G:86:MET:SD	2.79	0.43
11:2P:120:ALA:HB2	11:2P:137:LYS:HG2	2.00	0.43
12:2Q:32:TYR:HB2	12:2Q:106:VAL:HG23	2.00	0.43
19:2X:44:GLU:O	19:2X:48:LYS:N	2.50	0.43
32:2a:826:C:H2'	32:2a:827:U:C6	2.53	0.43
32:2a:1022:G:N3	32:2a:1023:G:H1'	2.34	0.43
32:2a:1250:A:C6	32:2a:1287:A:C4	3.07	0.43
32:2a:1316:G:N1	32:2a:1319:A:OP2	2.48	0.43
37:2f:7:ASN:HB2	37:2f:89:MET:HB3	2.00	0.43
54:2w:1:G:C2'	54:2w:2:G:H5'	2.49	0.43
54:2y:26:A:N6	54:2y:44:G:C6	2.87	0.43
1:1A:153:C:H2'	1:1A:154:G:C8	2.54	0.42
1:1A:271(T):C:H2'	1:1A:271(U):G:H8	1.84	0.42
1:1A:511:U:O4	1:1A:512:G:N1	2.52	0.42
1:1A:969:U:H2'	1:1A:970:C:C6	2.54	0.42
1:1A:1224:C:H2'	1:1A:1225:G:O4'	2.18	0.42
1:1A:1812:A:O2'	3:1D:45:ASN:N	2.48	0.42
1:1A:2319:G:N2	14:1S:3:ARG:HA	2.34	0.42
1:1A:2324:C:H5''	1:1A:2325:G:H5'	2.01	0.42
1:1A:2521:C:O2'	1:1A:2564:A:N3	2.46	0.42
1:1A:2801(A):A:N3	1:1A:2895:U:H1'	2.34	0.42
1:2A:194:G:H2'	1:2A:195:A:O4'	2.19	0.42
1:2A:687:C:H5'	29:27:4:THR:O	2.18	0.42
1:2A:709:U:H2'	1:2A:710:G:C8	2.53	0.42
1:2A:1545:A:H2'	1:2A:1546:C:O4'	2.19	0.42
1:2A:1581:G:H2'	1:2A:1582:C:O4'	2.18	0.42
1:2A:1670:C:O2	4:2E:129:HIS:NE2	2.44	0.42
1:2A:1778:U:H2'	1:2A:1784:A:N6	2.33	0.42
1:2A:1946:U:H2'	1:2A:1947:C:C6	2.54	0.42
1:2A:2153:G:N2	1:2A:2154:G:H1'	2.34	0.42
1:2A:2506:U:O2'	54:2w:76:A:H4'	2.19	0.42
1:2A:2564:A:OP1	1:2A:2648:C:H4'	2.19	0.42
3:1D:72:LYS:HB3	3:1D:75:ILE:HD12	2.01	0.42
4:1E:28:ALA:HB3	4:1E:93:VAL:HG12	2.01	0.42
7:1H:3:ARG:NH1	7:1H:4:ILE:H	2.17	0.42
8:1I:12:LEU:HD23	8:1I:12:LEU:HA	1.83	0.42
9:1N:34:LEU:O	9:1N:49:GLY:HA3	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1Z:121:HIS:HB3	21:1Z:123:ASP:O	2.18	0.42
27:15:16:ARG:HG2	27:15:17:ASP:OD1	2.18	0.42
32:1a:123:C:OP1	32:1a:311:C:O2'	2.31	0.42
32:1a:865:A:H2	32:1a:918:A:H4'	1.83	0.42
32:1a:892:A:O2'	32:1a:1415:G:H4'	2.19	0.42
35:1d:172:PRO:C	35:1d:174:LEU:H	2.27	0.42
48:1q:25:ARG:HG2	48:1q:38:ARG:O	2.19	0.42
50:1s:40:ILE:HA	50:1s:44:MET:SD	2.59	0.42
51:1t:33:ILE:HG23	51:1t:63:ILE:HG12	2.01	0.42
11:2P:89:ALA:O	11:2P:121:LYS:NZ	2.48	0.42
11:2P:90:ARG:NH1	11:2P:105:LEU:HD11	2.33	0.42
20:2Y:43:ASN:O	20:2Y:65:ALA:N	2.40	0.42
20:2Y:44:ILE:HA	20:2Y:63:LYS:O	2.19	0.42
21:2Z:30:ASN:ND2	21:2Z:90:VAL:HB	2.34	0.42
32:2a:501:C:OP1	43:2l:117:ARG:NH2	2.43	0.42
32:2a:1105:A:H2'	32:2a:1106:G:C8	2.49	0.42
33:2b:28:PHE:CD2	33:2b:190:THR:HA	2.54	0.42
34:2c:134:ILE:HG22	34:2c:168:ALA:HB3	2.01	0.42
39:2h:9:MET:HG3	39:2h:26:VAL:HG11	2.01	0.42
39:2h:85:ARG:HH12	39:2h:134:ILE:HD12	1.83	0.42
48:2q:81:ARG:HH21	48:2q:84:LEU:HD21	1.84	0.42
51:2t:54:LYS:HA	51:2t:57:ARG:CZ	2.49	0.42
1:1A:300:A:P	20:1Y:86:ARG:HH21	2.42	0.42
1:1A:580:C:H2'	1:1A:581:C:H6	1.84	0.42
1:1A:1086:A:H4'	1:1A:1103:A:C2	2.54	0.42
1:1A:1341:U:O4'	19:1X:57:LEU:HD23	2.19	0.42
1:2A:828:U:H4'	1:2A:831:G:N1	2.34	0.42
1:2A:2082:A:H2'	1:2A:2083:G:O4'	2.18	0.42
1:2A:2336:A:H61	22:20:43:THR:CG2	2.30	0.42
1:2A:2635:C:H5''	4:2E:78:LEU:O	2.19	0.42
7:1H:28:GLY:HA3	7:1H:79:VAL:HB	2.01	0.42
26:14:46:GLN:O	26:14:46:GLN:HG2	2.19	0.42
32:1a:258:G:H2'	32:1a:259:G:C8	2.50	0.42
32:1a:499:A:H4'	32:1a:500:G:OP1	2.19	0.42
32:1a:999:C:H42	32:1a:1042:G:H1	1.67	0.42
33:1b:100:GLY:O	33:1b:104:ASN:N	2.45	0.42
34:1c:62:ASP:O	34:1c:97:LYS:HB3	2.18	0.42
54:1w:27:C:H42	54:1w:43:G:H1	1.68	0.42
54:1y:4:U:H2'	54:1y:5:G:O4'	2.19	0.42
9:2N:62:VAL:HG11	9:2N:66:LYS:HB2	2.01	0.42
9:2N:110:GLY:O	9:2N:114:ARG:HG3	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:2O:73:ASP:OD2	15:2T:32:TYR:OH	2.31	0.42
21:2Z:73:GLN:H	21:2Z:87:ASP:HB2	1.84	0.42
32:2a:91:C:H2'	32:2a:92:C:C6	2.54	0.42
32:2a:177:C:H2'	32:2a:178:C:C6	2.54	0.42
32:2a:243:A:N6	32:2a:281:G:H1'	2.34	0.42
32:2a:273:A:H1'	48:2q:16:GLN:NE2	2.34	0.42
32:2a:523:A:H61	43:2l:92:0TD:CG	2.32	0.42
32:2a:1023:G:C5	32:2a:1024:G:H1'	2.55	0.42
33:2b:217:ARG:HA	33:2b:220:ASP:HB2	2.01	0.42
42:2k:97:ALA:O	42:2k:101:SER:HB3	2.19	0.42
1:1A:385:C:O2	11:1P:71:VAL:HG21	2.19	0.42
1:1A:2012:G:OP1	18:1W:11:ARG:NH2	2.52	0.42
1:1A:2774:C:H2'	1:1A:2775:A:O4'	2.19	0.42
1:2A:35:G:H2'	1:2A:36:G:O4'	2.19	0.42
1:2A:757:U:H2'	1:2A:758:C:O4'	2.20	0.42
1:2A:848:G:C4	1:2A:933:A:H8	2.37	0.42
1:2A:1288:U:O2'	1:2A:1647:G:N2	2.52	0.42
1:2A:2108:C:C2'	1:2A:2109:U:H5'	2.50	0.42
1:2A:2251:OMG:HM23	1:2A:2251:OMG:H1'	1.84	0.42
1:2A:2752:C:H2'	1:2A:2753:A:O4'	2.20	0.42
9:1N:96:GLU:H	9:1N:96:GLU:CD	2.27	0.42
12:1Q:57:HIS:CD2	12:1Q:117:ALA:HB2	2.54	0.42
21:1Z:150:LEU:HD11	21:1Z:154:ASP:OD2	2.19	0.42
22:10:43:THR:OG1	22:10:46:LYS:HG2	2.19	0.42
32:1a:79:G:N1	32:1a:90:U:N3	2.67	0.42
32:1a:437:U:H5''	35:1d:155:LEU:HD11	2.01	0.42
32:1a:765:G:H5''	32:1a:766:A:OP1	2.19	0.42
32:1a:828:A:N3	33:1b:26:PRO:HG2	2.34	0.42
32:1a:1191:A:OP1	34:1c:4:LYS:NZ	2.44	0.42
33:1b:231:GLU:HB3	33:1b:232:PRO:HD3	2.01	0.42
35:1d:36:ARG:HB3	35:1d:38:TYR:CZ	2.54	0.42
54:1y:68:C:H2'	54:1y:69:A:O4'	2.19	0.42
3:2D:36:PRO:HA	3:2D:61:LEU:HD12	2.00	0.42
7:2H:54:ARG:HG2	7:2H:65:HIS:ND1	2.34	0.42
21:2Z:50:GLN:OE1	21:2Z:50:GLN:N	2.52	0.42
21:2Z:98:MET:HE3	21:2Z:98:MET:HB2	1.72	0.42
32:2a:66:G:H8	32:2a:66:G:OP1	2.02	0.42
32:2a:491:G:H2'	32:2a:492:G:O4'	2.20	0.42
32:2a:636:U:H2'	32:2a:637:G:C8	2.54	0.42
32:2a:693:G:H2'	32:2a:694:A:C8	2.54	0.42
32:2a:1402:4OC:H6	32:2a:1402:4OC:O5'	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:2j:51:ARG:H	41:2j:60:ARG:HA	1.84	0.42
43:2l:110:VAL:HB	43:2l:113:ARG:HG2	2.00	0.42
50:2s:27:GLU:HB2	50:2s:28:LYS:HA	2.01	0.42
1:1A:1354:A:O3'	3:1D:38:LYS:HE3	2.19	0.42
1:1A:2158:A:O2'	1:1A:2159:G:OP2	2.35	0.42
1:1A:2698:U:O4	61:1A:4307:HOH:O	2.20	0.42
1:1A:2788:C:H2'	1:1A:2789:C:O4'	2.19	0.42
1:2A:118:A:N3	1:2A:178:G:H1'	2.35	0.42
1:2A:320:A:H4'	1:2A:322:A:N7	2.33	0.42
1:2A:1011:G:C2	1:2A:1151:G:C2	3.07	0.42
1:2A:1999:C:H4'	1:2A:2723:C:O2	2.19	0.42
1:2A:2250:G:O2'	1:2A:2496:C:OP1	2.26	0.42
1:2A:2465:C:O2	1:2A:2486:G:C2	2.72	0.42
1:2A:2721:A:H2'	1:2A:2722:G:O4'	2.20	0.42
10:1O:102:VAL:HB	10:1O:106:LEU:HD12	2.01	0.42
25:13:18:ASP:OD1	25:13:18:ASP:N	2.50	0.42
32:1a:831:U:H2'	32:1a:832:C:C6	2.53	0.42
32:1a:859:A:OP2	32:1a:869:G:N1	2.42	0.42
32:1a:1218:C:OP2	45:1n:9:LYS:NZ	2.36	0.42
32:1a:1429:C:H2'	32:1a:1430:C:H6	1.83	0.42
36:1e:8:GLU:OE2	36:1e:63:ARG:NH2	2.38	0.42
38:1g:74:GLU:CD	38:1g:95:ARG:HH21	2.27	0.42
43:1l:70:ILE:HG12	43:1l:100:ILE:HD13	2.01	0.42
12:2Q:86:GLY:HA3	22:20:10:THR:HG23	2.02	0.42
19:2X:64:LYS:HD3	19:2X:64:LYS:HA	1.86	0.42
32:2a:21:G:O2'	32:2a:914:A:N6	2.46	0.42
32:2a:974:A:P	45:2n:29:ARG:HH21	2.39	0.42
49:2r:36:ASN:O	49:2r:40:LEU:HG	2.20	0.42
1:1A:30:G:H2'	1:1A:31:C:O4'	2.20	0.42
1:1A:1005:C:H5''	61:1A:4746:HOH:O	2.20	0.42
1:1A:1066:U:H2'	1:1A:1068:G:OP2	2.19	0.42
1:1A:1186:G:H2'	1:1A:1187:G:O4'	2.20	0.42
1:1A:1364:G:N7	23:11:3:LYS:HD2	2.34	0.42
1:1A:1588:C:H2'	1:1A:1589:C:H6	1.84	0.42
1:1A:2095:C:H2'	1:1A:2096:U:O4'	2.19	0.42
1:1A:2136:C:N3	1:1A:2155:G:C2	2.86	0.42
1:1A:2506:U:C2	1:1A:2585:U:O4	2.73	0.42
1:1A:2695:C:H2'	1:1A:2696:U:H6	1.84	0.42
1:2A:839:U:H2'	1:2A:840:C:H6	1.84	0.42
1:2A:921:G:H4'	1:2A:2269:A:C5	2.55	0.42
1:2A:1154:G:O5'	1:2A:1154:G:H8	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2318:G:H21	14:2S:3:ARG:HE	1.67	0.42
1:2A:2528:U:H2'	1:2A:2530:A:O5'	2.20	0.42
8:1I:5:LEU:HD21	8:1I:12:LEU:HD13	2.01	0.42
21:1Z:136:PHE:O	21:1Z:137:ILE:HG13	2.20	0.42
24:12:25:VAL:HG11	24:12:61:LEU:HD21	2.01	0.42
30:18:52:LYS:N	30:18:53:PRO:HD2	2.35	0.42
32:1a:297:G:H4'	32:1a:557:G:H4'	2.00	0.42
32:1a:373:A:H2'	32:1a:374:A:H8	1.83	0.42
32:1a:741:G:H2'	32:1a:742:G:O4'	2.19	0.42
32:1a:768:A:C5	32:1a:769:G:C8	3.08	0.42
32:1a:870:U:H4'	32:1a:871:U:H5''	2.01	0.42
33:1b:122:PHE:CZ	33:1b:139:LYS:HB2	2.54	0.42
35:1d:111:ALA:HB1	35:1d:116:GLN:HE21	1.84	0.42
35:1d:113:SER:O	35:1d:117:ALA:N	2.45	0.42
37:1f:38:GLU:HB2	37:1f:64:GLN:HG2	2.00	0.42
51:1t:29:LYS:O	51:1t:33:ILE:HG13	2.20	0.42
5:2F:108:LYS:O	5:2F:112:MET:HG3	2.19	0.42
12:2Q:38:GLU:HG3	12:2Q:127:ILE:HB	2.02	0.42
21:2Z:141:VAL:HG23	21:2Z:144:LEU:HB3	2.00	0.42
32:2a:957:U:H2'	32:2a:959:A:OP2	2.19	0.42
32:2a:994:A:C5	32:2a:1216:G:H4'	2.55	0.42
32:2a:1119:C:H2'	32:2a:1120:G:C8	2.54	0.42
32:2a:1183:A:O2'	32:2a:1185:G:OP2	2.36	0.42
32:2a:1347:G:O2'	32:2a:1348:U:OP2	2.36	0.42
35:2d:59:ARG:HA	35:2d:59:ARG:HD3	1.68	0.42
46:2o:40:SER:O	46:2o:44:LYS:HG3	2.19	0.42
54:2y:62:C:H2'	54:2y:63:G:H8	1.85	0.42
1:1A:218:A:C2	1:1A:235:U:H4'	2.54	0.42
1:1A:657:U:H2'	1:1A:658:C:H6	1.85	0.42
1:1A:752:A:H3'	29:17:1:MET:HE1	2.01	0.42
1:1A:1142(A):A:C4	1:1A:1144:G:N7	2.87	0.42
1:1A:1288:U:O4	13:1R:106:GLY:HA3	2.20	0.42
1:1A:1408:C:C2	1:1A:1595:G:N2	2.88	0.42
1:1A:1833:U:O2'	1:1A:1969:A:N1	2.40	0.42
1:1A:2322:A:H2'	1:1A:2323:G:O4'	2.19	0.42
1:1A:2691:C:O3'	1:1A:2871:C:H4'	2.19	0.42
1:2A:587:C:C5	1:2A:671:C:H1'	2.55	0.42
1:2A:631:A:OP1	11:2P:65:ARG:NE	2.44	0.42
1:2A:1820:U:H4'	1:2A:1821:A:OP2	2.19	0.42
1:2A:2142:C:H2'	1:2A:2143:C:C6	2.55	0.42
1:2A:2324:C:H5''	1:2A:2325:G:H5'	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:1P:95:VAL:HA	11:1P:99:LEU:HD23	2.01	0.42
14:1S:36:TYR:CD2	14:1S:36:TYR:N	2.87	0.42
15:1T:112:ARG:HG3	15:1T:115:ARG:NH2	2.34	0.42
16:1U:49:HIS:HA	16:1U:52:ARG:HB2	2.01	0.42
32:1a:226:G:H2'	32:1a:227:G:O4'	2.18	0.42
32:1a:1015:A:H2'	32:1a:1016:A:C8	2.54	0.42
32:1a:1206:G:C6	32:1a:1207:2MG:C5	3.07	0.42
32:1a:1212:U:H5'	32:1a:1213:A:H5'	1.99	0.42
36:1e:31:LEU:HD23	36:1e:31:LEU:HA	1.92	0.42
36:1e:40:ARG:HD3	36:1e:40:ARG:HA	1.89	0.42
39:1h:20:TYR:HA	39:1h:65:TYR:CZ	2.55	0.42
42:1k:66:LEU:HG	42:1k:97:ALA:HB1	2.02	0.42
51:1t:47:GLY:N	51:1t:48:LYS:HB2	2.35	0.42
54:1w:44:G:O2'	54:1w:45:G:OP1	2.25	0.42
12:2Q:57:HIS:CE1	12:2Q:116:GLU:HG2	2.55	0.42
19:2X:27:THR:HA	19:2X:79:ALA:O	2.20	0.42
22:20:43:THR:HG23	22:20:43:THR:O	2.20	0.42
32:2a:1417:G:O6	61:2a:1931:HOH:O	2.21	0.42
34:2c:150:LYS:HG3	34:2c:169:ALA:HB2	2.01	0.42
35:2d:61:LYS:HD2	35:2d:207:TYR:OH	2.20	0.42
52:2u:6:ARG:HG2	52:2u:15:ARG:NH1	2.35	0.42
54:2w:65:C:O5'	54:2w:65:C:H6	2.02	0.42
54:2y:65:C:H2'	54:2y:66:A:C8	2.54	0.42
1:1A:182:A:H2	1:1A:433:C:O2	2.03	0.42
1:1A:614:U:H2'	1:1A:614(A):U:O4'	2.20	0.42
1:1A:1041:C:N4	1:1A:1114:G:H1	2.11	0.42
1:1A:1068:G:O2'	1:1A:1070:A:N7	2.50	0.42
1:1A:1643:G:H2'	1:1A:1644:C:O4'	2.19	0.42
1:1A:2149:G:C6	1:1A:2150:U:C2	3.07	0.42
1:1A:2279:G:N7	22:10:14:ARG:NH1	2.67	0.42
1:1A:2756:U:H1'	1:1A:2757:A:H5''	2.01	0.42
1:2A:652(B):A:H62	1:2A:655:A:H1'	1.85	0.42
1:2A:947:G:N2	1:2A:971:C:C2	2.87	0.42
1:2A:1590:U:H2'	1:2A:1591:G:C8	2.53	0.42
1:2A:2279:G:N7	22:20:14:ARG:NH1	2.68	0.42
4:1E:48:GLN:NE2	4:1E:78:LEU:HD13	2.34	0.42
33:1b:12:GLU:O	33:1b:15:VAL:HG22	2.20	0.42
34:1c:62:ASP:HA	34:1c:97:LYS:HD3	2.02	0.42
36:1e:103:GLY:O	36:1e:106:PRO:HD2	2.19	0.42
46:1o:54:ARG:HG2	46:1o:58:MET:HE2	2.01	0.42
48:1q:22:LEU:HD11	48:1q:39:SER:HB2	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:23:11:SER:HA	25:23:31:LEU:HD21	2.01	0.42
32:2a:160:A:H1'	32:2a:344:A:N7	2.34	0.42
32:2a:264:U:O2	48:2q:64:PRO:HG2	2.20	0.42
32:2a:570:G:H1'	32:2a:820:U:C4	2.54	0.42
32:2a:778:G:H2'	32:2a:779:C:O4'	2.20	0.42
32:2a:1107:C:C4	32:2a:1108:G:C8	3.08	0.42
32:2a:1146:A:H2'	32:2a:1147:C:O4'	2.18	0.42
32:2a:1316:G:N2	32:2a:1318:A:H3'	2.35	0.42
35:2d:108:LEU:HD11	35:2d:174:LEU:HD22	2.01	0.42
38:2g:54:THR:O	38:2g:56:GLN:N	2.48	0.42
38:2g:113:GLU:HB2	38:2g:119:ARG:HG2	2.02	0.42
1:1A:27:G:N2	1:1A:512:G:H1'	2.35	0.42
1:1A:357:A:H2'	1:1A:358:U:C6	2.55	0.42
1:1A:646:A:H2'	1:1A:647:G:O4'	2.20	0.42
1:1A:760:G:H2'	1:1A:761:A:O4'	2.20	0.42
1:1A:1022:G:N7	9:1N:66:LYS:HE2	2.34	0.42
1:1A:1252:G:C2	1:1A:1253:A:C2	3.08	0.42
1:1A:1614:A:C6	18:1W:87:PRO:HB3	2.54	0.42
1:1A:1655:A:H4'	4:1E:115:GLY:N	2.35	0.42
1:2A:875:G:C6	1:2A:876:C:C2	3.07	0.42
1:2A:1028:A:H61	1:2A:1125:G:H2'	1.85	0.42
1:2A:1355:G:P	3:2D:38:LYS:HE3	2.59	0.42
1:2A:1452:A:O2'	1:2A:1453:U:H2'	2.19	0.42
1:2A:1529:G:O2'	1:2A:1530:C:H5'	2.19	0.42
1:2A:1853:A:N1	1:2A:2087:G:H1'	2.35	0.42
1:2A:1924:C:H4'	55:2x:13:C:O2'	2.19	0.42
1:2A:2183:C:H2'	1:2A:2184:G:C8	2.53	0.42
1:2A:2315:G:H2'	1:2A:2316:C:C6	2.54	0.42
7:1H:125:VAL:HG12	7:1H:127:GLU:O	2.19	0.42
32:1a:598:U:H2'	32:1a:599:C:H6	1.83	0.42
32:1a:718:G:N2	49:1r:81:PHE:O	2.51	0.42
33:1b:74:LYS:O	33:1b:78:GLN:HG2	2.19	0.42
35:1d:77:ASN:HD22	35:1d:77:ASN:HA	1.74	0.42
48:1q:9:VAL:HG11	48:1q:84:LEU:HD12	2.01	0.42
51:1t:65:LYS:HA	51:1t:68:LYS:HD3	2.01	0.42
54:1y:2:G:C6	54:1y:71:C:N3	2.88	0.42
3:2D:77:ALA:HB2	3:2D:97:TYR:CD1	2.54	0.42
8:2I:8:PRO:HD3	8:2I:15:VAL:HB	2.01	0.42
9:2N:39:ARG:HA	9:2N:40:PRO:HD3	1.91	0.42
9:2N:71:ILE:HG21	9:2N:84:LYS:HB3	2.02	0.42
14:2S:87:PHE:CE1	14:2S:102:ALA:HB2	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:2U:52:ARG:HA	16:2U:55:ARG:HG3	2.02	0.42
20:2Y:20:TYR:CE2	20:2Y:43:ASN:HA	2.55	0.42
21:2Z:150:LEU:HD12	21:2Z:150:LEU:HA	1.88	0.42
29:27:12:ARG:NH2	29:27:44:PRO:HB3	2.34	0.42
30:28:62:LEU:HB3	30:28:65:GLU:HG2	2.02	0.42
32:2a:625:G:H2'	32:2a:626:U:H6	1.85	0.42
32:2a:894:G:N7	61:2a:1957:HOH:O	2.37	0.42
32:2a:908:A:H2'	32:2a:909:A:C8	2.55	0.42
32:2a:951:G:OP2	44:2m:102:ARG:NH1	2.53	0.42
32:2a:983:A:N1	32:2a:1222:G:N2	2.68	0.42
32:2a:1112:C:C4	34:2c:178:LEU:HD12	2.55	0.42
32:2a:1217:C:H2'	32:2a:1218:C:O4'	2.20	0.42
32:2a:1228:C:H2'	32:2a:1229:A:C8	2.55	0.42
32:2a:1278:U:H5'	32:2a:1279:A:OP1	2.19	0.42
39:2h:29:SER:OG	39:2h:32:LYS:N	2.51	0.42
40:2i:77:ILE:O	40:2i:81:ILE:HG23	2.20	0.42
44:2m:65:LYS:HB3	44:2m:65:LYS:HE2	1.78	0.42
47:2p:14:ASN:HA	47:2p:42:ARG:NH2	2.34	0.42
54:2w:72:C:H2'	54:2w:73:A:H8	1.84	0.42
1:1A:142(A):C:H2'	1:1A:143:G:O4'	2.19	0.42
1:1A:265:A:N1	1:1A:427:U:O2'	2.40	0.42
1:1A:1819:A:H5''	3:1D:161:THR:HG21	2.01	0.42
1:1A:2533:A:H2'	1:1A:2534:A:O4'	2.19	0.42
1:1A:2794:C:N4	1:1A:2802:G:H22	2.18	0.42
1:1A:2855:C:H2'	1:1A:2856:C:C6	2.54	0.42
1:2A:320:A:H4'	1:2A:322:A:C8	2.55	0.42
1:2A:656:G:H2'	1:2A:657:U:O4'	2.19	0.42
1:2A:848:G:C2	1:2A:849:A:C5	3.08	0.42
1:2A:855:G:C6	1:2A:856:C:C4	3.08	0.42
1:2A:1686:C:H2'	1:2A:1687:G:O4'	2.19	0.42
1:2A:1908:C:O2'	55:2x:12:G:H5''	2.20	0.42
1:2A:2136:C:O2'	1:2A:2137:C:C6	2.72	0.42
1:2A:2505:G:O6	1:2A:2576:G:H2'	2.20	0.42
1:2A:2881:C:H2'	1:2A:2882:A:O4'	2.20	0.42
3:1D:127:VAL:HA	3:1D:193:VAL:HG22	2.02	0.42
6:1G:25:TYR:CZ	6:1G:32:PRO:HD3	2.55	0.42
6:1G:64:THR:HB	6:1G:94:LEU:HD21	2.02	0.42
6:1G:103:LEU:O	6:1G:107:LEU:HG	2.20	0.42
13:1R:28:LEU:HD22	13:1R:44:LEU:HD13	2.01	0.42
18:1W:58:ALA:HB1	18:1W:64:MET:HB2	2.02	0.42
21:1Z:8:TYR:HB2	21:1Z:38:TYR:CE2	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1Z:98:MET:O	21:1Z:125:LEU:HD12	2.20	0.42
26:14:1:MET:HG3	26:14:6:HIS:CD2	2.55	0.42
32:1a:183:G:H5'	32:1a:184:G:OP2	2.19	0.42
32:1a:392:G:OP1	47:1p:8:ARG:NH2	2.53	0.42
32:1a:1427:U:H2'	32:1a:1428:A:C8	2.55	0.42
33:1b:183:PRO:HA	33:1b:198:ASP:OD2	2.19	0.42
35:1d:102:ASP:OD1	35:1d:103:ASN:N	2.53	0.42
41:1j:64:GLU:OE2	41:1j:66:ARG:NE	2.40	0.42
41:1j:64:GLU:HB3	45:1n:59:ALA:HB2	2.02	0.42
51:1t:54:LYS:HG3	51:1t:57:ARG:NH2	2.35	0.42
51:1t:63:ILE:HG22	51:1t:77:ALA:HB1	2.02	0.42
2:2B:33:G:N3	2:2B:50:G:N2	2.68	0.42
9:2N:70:LYS:HD3	9:2N:87:LEU:HD12	2.02	0.42
10:2O:102:VAL:HB	10:2O:106:LEU:HD12	2.01	0.42
21:2Z:93:ASP:HA	21:2Z:130:PRO:HD2	2.01	0.42
21:2Z:105:VAL:O	21:2Z:141:VAL:HG12	2.19	0.42
32:2a:202:U:H3'	32:2a:203:U:C6	2.55	0.42
32:2a:1223:C:P	50:2s:78:ARG:HH21	2.43	0.42
32:2a:1512:U:H2'	32:2a:1513:A:H8	1.84	0.42
35:2d:18:LYS:HD2	35:2d:20:TYR:CZ	2.55	0.42
1:1A:270:A:OP2	1:1A:271(X):G:N2	2.47	0.42
1:1A:694:U:OP1	3:1D:59:LYS:NZ	2.51	0.42
1:1A:768:G:O2'	1:1A:1379:A:N1	2.45	0.42
1:1A:1086:A:H4'	1:1A:1103:A:H2	1.85	0.42
1:1A:2078:C:C4	1:1A:2079:U:C4	3.08	0.42
1:2A:68:G:H2'	1:2A:69:C:O4'	2.20	0.42
1:2A:1788:C:OP1	3:2D:222:ARG:NH2	2.53	0.42
1:2A:2286:A:H4'	1:2A:2287:A:O4'	2.20	0.42
1:2A:2552:2MU:H6	1:2A:2552:2MU:O5'	2.20	0.42
8:1I:77:LEU:HB3	8:1I:142:VAL:HG22	2.02	0.42
12:1Q:15:GLY:H	12:1Q:41:TRP:HZ2	1.67	0.42
15:1T:118:ARG:HA	15:1T:118:ARG:HD3	1.79	0.42
21:1Z:155:LEU:HD12	21:1Z:155:LEU:HA	1.90	0.42
31:19:25:VAL:O	31:19:33:LYS:HA	2.19	0.42
32:1a:257:G:C6	32:1a:258:G:C5	3.08	0.42
32:1a:438:G:H4'	35:1d:123:HIS:ND1	2.34	0.42
32:1a:501:C:H2'	32:1a:502:G:C8	2.55	0.42
32:1a:974:A:P	45:1n:29:ARG:HH21	2.43	0.42
32:1a:1266:G:N2	32:1a:1270:C:N3	2.68	0.42
32:1a:1503:A:OP1	32:1a:1531:A:O2'	2.37	0.42
36:1e:11:ILE:HB	36:1e:31:LEU:HB3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:1w:2:G:C6	54:1w:71:C:N3	2.85	0.42
2:2B:46:A:H2'	2:2B:47:C:C6	2.55	0.42
14:2S:71:ARG:HE	14:2S:71:ARG:HB2	1.71	0.42
19:2X:44:GLU:HG3	19:2X:51:VAL:HG23	2.02	0.42
23:21:91:LYS:HG2	23:21:95:LEU:HD22	2.02	0.42
32:2a:596:C:H3'	61:2a:1904:HOH:O	2.19	0.42
32:2a:1122:U:N3	32:2a:1123:A:N7	2.68	0.42
32:2a:1490:C:H2'	32:2a:1491:G:O4'	2.19	0.42
34:2c:71:ALA:HB2	34:2c:109:PRO:HB3	2.02	0.42
50:2s:66:MET:HB2	50:2s:74:PHE:CZ	2.55	0.42
54:2w:75:C:H2'	54:2w:76:A:C8	2.55	0.42
1:1A:732:C:OP2	61:1A:4310:HOH:O	2.22	0.41
1:1A:1062:G:N2	1:1A:1088:A:C6	2.88	0.41
1:1A:1359:A:H2'	1:1A:1360:A:H5'	2.02	0.41
1:1A:1587:A:H2'	1:1A:1588:C:H6	1.85	0.41
1:2A:484:C:H2'	1:2A:485:C:H6	1.85	0.41
1:2A:858:U:O2'	1:2A:2268:A:N3	2.51	0.41
1:2A:892:G:H2'	1:2A:892:G:N3	2.35	0.41
1:2A:1754:C:H5''	15:2T:113:LYS:HE2	2.01	0.41
1:2A:1782:C:O2	1:2A:2608:G:O2'	2.28	0.41
1:2A:2018:G:H2'	1:2A:2019:A:O4'	2.20	0.41
1:2A:2273:A:O2'	1:2A:2274:A:H5'	2.20	0.41
1:2A:2427:C:H5''	1:2A:2428:G:OP1	2.20	0.41
1:2A:2774:C:H2'	1:2A:2775:A:O4'	2.20	0.41
1:2A:2869:G:H2'	1:2A:2870:C:O4'	2.20	0.41
3:1D:126:GLN:HE21	3:1D:127:VAL:H	1.67	0.41
6:1G:32:PRO:HB3	6:1G:163:ALA:HB2	2.01	0.41
32:1a:176:C:H2'	32:1a:177:C:H6	1.85	0.41
32:1a:545:C:H2'	32:1a:546:G:O4'	2.20	0.41
33:1b:60:ASP:O	33:1b:64:ARG:HG2	2.20	0.41
40:1i:8:GLY:O	40:1i:76:ALA:HB1	2.19	0.41
46:1o:39:LEU:HD22	46:1o:56:LEU:HB2	2.02	0.41
51:1t:98:PRO:O	51:1t:100:ILE:N	2.48	0.41
2:2B:32:C:H2'	2:2B:33:G:O4'	2.20	0.41
4:2E:51:PHE:CD2	4:2E:52:LEU:HG	2.55	0.41
6:2G:96:ARG:N	6:2G:99:MET:HE2	2.35	0.41
15:2T:102:ILE:HA	15:2T:105:LEU:HD12	2.02	0.41
20:2Y:23:ARG:HD3	20:2Y:23:ARG:HA	1.80	0.41
26:24:49:PHE:HB3	26:24:50:VAL:H	1.64	0.41
32:2a:196:A:OP1	51:2t:68:LYS:NZ	2.28	0.41
32:2a:555:C:H2'	32:2a:556:C:C6	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:693:G:N2	54:2y:37:6MZ:H2	2.29	0.41
35:2d:22:LYS:HG3	60:2d:303:SF4:S4	2.60	0.41
37:2f:96:PRO:HB3	49:2r:30:ASP:CG	2.44	0.41
41:2j:6:ILE:O	41:2j:71:LEU:HD12	2.20	0.41
54:2y:50:G:H2'	54:2y:50:G:N3	2.33	0.41
1:1A:107:C:H2'	1:1A:108:U:H6	1.84	0.41
1:1A:468:G:N7	29:17:39:ARG:NH2	2.62	0.41
1:1A:695:G:H2'	1:1A:696:G:O4'	2.20	0.41
1:1A:1161:C:O2'	17:1V:8:GLY:HA2	2.20	0.41
1:1A:1754:C:H2'	1:1A:1755:A:O4'	2.19	0.41
1:1A:2156:G:H2'	1:1A:2157:G:N1	2.35	0.41
1:1A:2698:U:H2'	1:1A:2699:C:C6	2.55	0.41
1:2A:196:A:N3	1:2A:196:A:H2'	2.34	0.41
1:2A:234:C:H2'	1:2A:235:U:C6	2.54	0.41
1:2A:530:G:C5	1:2A:2022:U:H5''	2.55	0.41
1:2A:582:G:H2'	1:2A:583:G:C8	2.55	0.41
1:2A:892:G:H3'	1:2A:893:C:C4'	2.49	0.41
1:2A:1162:G:O2'	17:2V:90:PRO:HG2	2.20	0.41
1:2A:2249:U:N3	1:2A:2253:G:OP2	2.43	0.41
4:1E:37:ARG:O	4:1E:45:THR:HA	2.20	0.41
8:1I:129:THR:HG22	8:1I:139:GLN:HE22	1.86	0.41
9:1N:108:PRO:O	9:1N:113:GLY:HA3	2.20	0.41
12:1Q:86:GLY:HA3	22:10:10:THR:HG23	2.02	0.41
21:1Z:102:LEU:HD12	21:1Z:137:ILE:HB	2.02	0.41
26:14:2:LYS:HD2	26:14:5:ILE:HD13	2.02	0.41
32:1a:115:G:H4'	32:1a:116:A:O5'	2.20	0.41
32:1a:186:C:O4'	51:1t:81:LYS:HE3	2.19	0.41
32:1a:355:C:H2'	32:1a:356:A:O4'	2.20	0.41
32:1a:542:G:H5'	35:1d:41:GLY:HA3	2.02	0.41
32:1a:557:G:N7	61:1a:1962:HOH:O	2.36	0.41
32:1a:811:C:H4'	32:1a:900:A:N6	2.35	0.41
32:1a:1236:A:O2'	32:1a:1304:G:H4'	2.19	0.41
32:1a:1402:4OC:O5'	32:1a:1402:4OC:H6	2.20	0.41
34:1c:18:TRP:H	34:1c:18:TRP:HE3	1.67	0.41
35:1d:19:LEU:O	35:1d:21:LEU:HG	2.20	0.41
43:1l:7:ILE:O	43:1l:11:VAL:HG23	2.20	0.41
54:1y:4:U:H3	54:1y:69:A:H61	1.68	0.41
32:2a:165:C:H2'	32:2a:166:G:C8	2.55	0.41
32:2a:509:A:N3	32:2a:543:C:O2'	2.51	0.41
32:2a:586:C:O2'	32:2a:878:G:H4'	2.19	0.41
32:2a:892:A:O2'	32:2a:1415:G:H4'	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1305:G:H22	32:2a:1331:G:H1'	1.86	0.41
42:2k:98:LEU:O	42:2k:101:SER:OG	2.25	0.41
1:1A:1095:A:H2'	1:1A:1096:A:C8	2.54	0.41
1:1A:1424:G:H2'	1:1A:1425:G:O4'	2.20	0.41
1:1A:1756:G:H4'	1:1A:1758:G:O4'	2.20	0.41
1:1A:2271:G:OP1	22:10:18:ALA:HB1	2.20	0.41
1:2A:1431:U:H2'	1:2A:1432:C:C6	2.56	0.41
1:2A:1448:G:H2'	1:2A:1449:A:C8	2.55	0.41
1:2A:1474:C:H2'	1:2A:1475:G:C8	2.54	0.41
1:2A:1474:C:H2'	1:2A:1475:G:H8	1.84	0.41
1:2A:1786:A:H1'	1:2A:1938:A:H61	1.84	0.41
1:2A:2086:U:H2'	1:2A:2087:G:C8	2.55	0.41
1:2A:2751:G:H5'	7:2H:2:SER:HA	2.02	0.41
4:1E:4:ILE:HD13	4:1E:28:ALA:HB1	2.02	0.41
20:1Y:13:VAL:HB	20:1Y:72:VAL:HG13	2.02	0.41
36:1e:92:LYS:HB3	36:1e:119:LEU:HB2	2.03	0.41
39:1h:21:LYS:O	39:1h:65:TYR:OH	2.31	0.41
42:1k:24:SER:C	42:1k:26:ASN:H	2.27	0.41
43:1l:33:ARG:HD3	43:1l:33:ARG:HA	1.87	0.41
44:1m:89:GLY:O	44:1m:93:ARG:HG3	2.19	0.41
52:1u:5:ASP:O	52:1u:11:GLY:HA3	2.20	0.41
3:2D:5:LYS:HE3	3:2D:5:LYS:HB3	1.91	0.41
21:2Z:14:LYS:HA	21:2Z:15:PRO:HD3	1.94	0.41
24:22:4:SER:HA	24:22:7:ARG:HH21	1.84	0.41
29:27:24:THR:O	29:27:28:ARG:HG3	2.20	0.41
32:2a:381:C:H2'	32:2a:382:A:O4'	2.21	0.41
32:2a:445:G:H2'	32:2a:446:G:C8	2.56	0.41
33:2b:109:SER:O	33:2b:112:VAL:HG22	2.20	0.41
34:2c:71:ALA:HA	34:2c:106:VAL:HB	2.02	0.41
41:2j:38:ILE:HD11	41:2j:71:LEU:HB3	2.02	0.41
1:1A:412:A:H8	1:1A:412:A:O5'	2.03	0.41
1:1A:662:G:OP1	11:1P:16:ARG:NE	2.51	0.41
1:1A:892:G:C2'	1:1A:893:C:H5'	2.50	0.41
1:1A:895:U:O2'	1:1A:896:A:H5'	2.20	0.41
1:1A:1301:A:C8	1:1A:1303:G:C8	3.08	0.41
1:1A:1359:A:C2	1:1A:1372:U:N3	2.84	0.41
1:1A:1655:A:H3'	1:1A:1656:C:C6	2.55	0.41
1:1A:2112:G:C6	1:1A:2113:U:H1'	2.56	0.41
1:1A:2751:G:C4	7:1H:2:SER:HA	2.55	0.41
1:2A:210:C:OP1	29:27:29:LYS:HD2	2.19	0.41
1:2A:614:U:H2'	1:2A:614(A):U:O4'	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2319:G:N1	14:2S:3:ARG:HA	2.35	0.41
1:2A:2461:C:H2'	1:2A:2462:U:C6	2.55	0.41
1:2A:2637:U:H5''	4:2E:82:ARG:HH12	1.85	0.41
1:2A:2680:C:OP2	4:2E:111:ARG:NH2	2.38	0.41
4:1E:79:ARG:HA	4:1E:79:ARG:HD3	1.92	0.41
18:1W:57:ASN:HA	18:1W:61:ASN:ND2	2.29	0.41
19:1X:36:LYS:HG2	19:1X:54:VAL:HG12	2.02	0.41
19:1X:47:PHE:O	19:1X:49:VAL:HG13	2.21	0.41
32:1a:44:G:C2	32:1a:45:U:H1'	2.55	0.41
32:1a:109:A:C6	32:1a:326:G:C6	3.08	0.41
32:1a:166:G:H2'	32:1a:167:G:C8	2.56	0.41
32:1a:560:U:H5'	32:1a:566:G:N2	2.35	0.41
32:1a:986:A:H2'	32:1a:987:G:O4'	2.21	0.41
32:1a:1027:C:H5	32:1a:1028:C:N3	2.19	0.41
6:2G:131:TYR:HB3	6:2G:159:VAL:CG2	2.50	0.41
8:2I:29:TYR:O	8:2I:33:ARG:HD2	2.20	0.41
17:2V:76:LYS:HB2	17:2V:81:TYR:HB3	2.01	0.41
21:2Z:149:SER:OG	21:2Z:150:LEU:N	2.52	0.41
32:2a:280:C:N3	48:2q:39:SER:N	2.67	0.41
32:2a:391:G:C6	32:2a:392:G:C5	3.09	0.41
32:2a:461:A:O2'	32:2a:470:C:H5'	2.20	0.41
32:2a:719:C:N4	49:2r:71:LYS:HE2	2.36	0.41
32:2a:971:G:OP1	32:2a:971:G:H3'	2.21	0.41
32:2a:1084:G:C5	32:2a:1085:U:C4	3.09	0.41
32:2a:1122:U:C4	32:2a:1123:A:N7	2.88	0.41
38:2g:144:MET:HE1	54:2y:31:C:H1'	2.01	0.41
39:2h:82:HIS:HE2	39:2h:84:ARG:HB2	1.84	0.41
39:2h:121:ASP:N	39:2h:121:ASP:OD1	2.51	0.41
51:2t:97:ALA:O	51:2t:99:LEU:HD13	2.20	0.41
1:1A:102:G:OP1	24:12:7:ARG:NH1	2.53	0.41
1:1A:1913:A:N1	54:1w:37:6MZ:O2'	2.47	0.41
57:1A:4098:DI0:CBN	57:1A:4098:DI0:CAR	2.99	0.41
1:2A:249:C:H4'	1:2A:250:G:O5'	2.21	0.41
1:2A:460:A:C2	1:2A:470:A:C4	3.09	0.41
1:2A:478:A:N1	1:2A:500:G:H4'	2.35	0.41
1:2A:614(B):G:H2'	5:2F:44:ARG:HD2	2.02	0.41
1:2A:1160:G:C6	1:2A:1161:C:C4	3.08	0.41
1:2A:1288:U:O4	13:2R:106:GLY:HA3	2.20	0.41
1:2A:1467:C:C5	1:2A:1546:C:H2'	2.56	0.41
1:2A:2410:G:C2	1:2A:2411:A:H1'	2.55	0.41
1:2A:2758:A:C2	1:2A:2759:G:H1'	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1Y:14:LEU:HB2	20:1Y:75:ILE:HD11	2.02	0.41
32:1a:236:G:OP1	48:1q:40:LYS:NZ	2.51	0.41
32:1a:685:G:O2'	32:1a:686:U:H5'	2.20	0.41
32:1a:769:G:H4'	32:1a:1513:A:H4'	2.02	0.41
32:1a:892:A:OP2	61:1a:1932:HOH:O	2.22	0.41
33:1b:218:ALA:O	33:1b:222:ILE:HG13	2.20	0.41
35:1d:88:VAL:O	35:1d:92:VAL:HG23	2.21	0.41
41:1j:13:HIS:HA	41:1j:16:LEU:HB3	2.02	0.41
42:1k:80:VAL:O	42:1k:106:LYS:N	2.45	0.41
44:1m:97:PRO:HA	44:1m:110:ARG:HD3	2.03	0.41
54:1w:28:C:H2'	54:1w:29:U:C6	2.56	0.41
55:1x:29:G:H1	55:1x:41:C:N4	2.17	0.41
54:1y:8:4SU:H4'	54:1y:48:C:H4'	2.01	0.41
2:2B:28:C:H2'	2:2B:29:A:O4'	2.21	0.41
6:2G:51:ARG:O	6:2G:52:ILE:C	2.64	0.41
16:2U:65:ILE:CD1	16:2U:95:LEU:HB3	2.50	0.41
32:2a:266:G:N3	32:2a:266:G:H2'	2.34	0.41
32:2a:438:G:O2'	32:2a:494:U:O4	2.25	0.41
32:2a:505:G:H2'	32:2a:506:G:C8	2.56	0.41
32:2a:575:G:O2'	32:2a:821:G:H5'	2.20	0.41
32:2a:984:C:H2'	32:2a:985:C:H6	1.86	0.41
32:2a:1006:C:C4	32:2a:1007:C:C4	3.09	0.41
32:2a:1061:G:H1'	41:2j:56:HIS:CE1	2.56	0.41
32:2a:1068:G:H8	32:2a:1068:G:OP2	2.04	0.41
32:2a:1148:U:O2'	40:2i:66:ARG:NH2	2.51	0.41
33:2b:54:THR:O	33:2b:58:ILE:HG13	2.21	0.41
33:2b:74:LYS:H	33:2b:74:LYS:HG3	1.66	0.41
34:2c:59:ARG:O	41:2j:92:THR:HB	2.21	0.41
35:2d:19:LEU:HG	35:2d:67:ILE:HG12	2.01	0.41
36:2e:113:ALA:HB3	36:2e:115:VAL:HG23	2.03	0.41
37:2f:1:MET:HE2	37:2f:68:PRO:HD3	2.02	0.41
46:2o:39:LEU:HD23	46:2o:39:LEU:C	2.45	0.41
54:2w:61:C:H3'	54:2w:62:C:C5'	2.50	0.41
1:1A:971:C:H2'	1:1A:972:G:O4'	2.21	0.41
1:1A:1027:A:C6	1:1A:1126:A:C4	3.08	0.41
1:1A:1700:A:H2'	1:1A:1701:A:C5'	2.50	0.41
1:1A:1889:A:H2'	1:1A:1890:A:C8	2.56	0.41
1:1A:2135:A:H2'	1:1A:2136:C:C5	2.54	0.41
1:1A:2607:G:H2'	1:1A:2608:G:O4'	2.19	0.41
1:2A:28:A:C2	1:2A:513:A:C8	3.08	0.41
1:2A:584:C:OP2	16:2U:6:THR:OG1	2.34	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:622:G:OP2	11:2P:108:LYS:NZ	2.45	0.41
1:2A:1458:C:H4'	1:2A:1459:G:O4'	2.20	0.41
1:2A:2149:G:C6	1:2A:2150:U:N3	2.89	0.41
1:2A:2294:C:P	14:2S:89:ARG:HH22	2.43	0.41
1:2A:2406:U:H6	1:2A:2406:U:H2'	1.73	0.41
1:2A:2410:G:H2'	1:2A:2411:A:O4'	2.20	0.41
1:2A:2823:A:OP1	4:2E:113:PHE:HB2	2.21	0.41
6:1G:72:ARG:NH1	6:1G:87:PRO:HG3	2.36	0.41
11:1P:95:VAL:HG13	11:1P:125:VAL:HB	2.02	0.41
11:1P:121:LYS:O	11:1P:123:LEU:N	2.53	0.41
12:1Q:38:GLU:HB2	12:1Q:39:PRO:HD2	2.03	0.41
13:1R:118:GLU:H	13:1R:118:GLU:CD	2.28	0.41
32:1a:269:C:H2'	32:1a:270:A:C8	2.55	0.41
32:1a:1343:G:H2'	32:1a:1344:C:C6	2.56	0.41
33:1b:146:GLN:O	33:1b:150:SER:HB3	2.21	0.41
38:1g:65:ALA:O	38:1g:69:VAL:HG23	2.19	0.41
42:1k:38:ASN:HA	42:1k:39:PRO:HD3	1.95	0.41
50:1s:49:ILE:HG13	50:1s:62:ILE:HD11	2.03	0.41
54:1y:63:G:H2'	54:1y:64:U:O4'	2.21	0.41
3:2D:41:GLY:O	3:2D:43:ARG:NH1	2.53	0.41
6:2G:176:LEU:HD23	6:2G:176:LEU:HA	1.86	0.41
14:2S:110:LEU:HD12	14:2S:110:LEU:HA	1.90	0.41
23:21:46:LEU:HD23	23:21:46:LEU:HA	1.83	0.41
30:28:34:TRP:CG	30:28:35:GLN:N	2.89	0.41
32:2a:163:C:H2'	32:2a:164:U:O4'	2.21	0.41
32:2a:382:A:H2'	32:2a:383:A:H8	1.84	0.41
32:2a:685:G:C2	32:2a:686:U:C4	3.09	0.41
32:2a:1327:C:H2'	32:2a:1328:C:C6	2.55	0.41
32:2a:1330:U:H2'	32:2a:1331:G:H5'	2.03	0.41
35:2d:191:ARG:NH1	35:2d:194:LEU:O	2.54	0.41
51:2t:97:ALA:HB1	51:2t:98:PRO:HD2	2.01	0.41
55:2x:53:G:H3'	55:2x:54:5MU:H73	2.01	0.41
1:1A:247:G:H4'	1:1A:386:G:C5	2.56	0.41
1:1A:612:C:H2'	1:1A:613:G:O4'	2.21	0.41
1:1A:1568:G:H5'	3:1D:60:ARG:HA	2.03	0.41
1:1A:1614:A:P	1:1A:1614:A:H8	2.43	0.41
1:1A:2808:U:H5''	1:1A:2891:G:O6	2.21	0.41
1:2A:652(B):A:N3	1:2A:652(B):A:H2'	2.36	0.41
1:2A:735:A:N7	1:2A:761:A:H2	2.17	0.41
1:2A:862:G:O2'	2:2B:78:A:N3	2.53	0.41
1:2A:1412:A:H2'	1:2A:1413:G:C8	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1837:C:OP1	32:2a:784:C:H4'	2.19	0.41
1:2A:2061:G:H5''	1:2A:2503:2MA:C2	2.51	0.41
1:2A:2112:G:OP1	1:2A:2113:U:H5	2.02	0.41
1:2A:2161:C:H2'	1:2A:2162:G:O4'	2.21	0.41
4:1E:134:ILE:HA	4:1E:137:HIS:CD2	2.56	0.41
6:1G:43:LEU:HB3	6:1G:44:GLY:H	1.65	0.41
6:1G:106:LEU:HD12	6:1G:110:ALA:HB3	2.01	0.41
8:1I:77:LEU:HD22	8:1I:97:ILE:HG23	2.01	0.41
9:1N:75:TYR:CE2	9:1N:77:GLY:HA2	2.55	0.41
15:1T:127:ALA:O	15:1T:128:GLU:HG2	2.21	0.41
18:1W:70:TYR:O	18:1W:107:LEU:HD12	2.21	0.41
19:1X:61:GLY:HA3	19:1X:73:ARG:O	2.21	0.41
22:10:30:VAL:HG22	22:10:66:VAL:HG22	2.01	0.41
32:1a:841:U:C2	32:1a:848:C:H1'	2.56	0.41
35:1d:8:VAL:O	35:1d:11:LEU:HB2	2.21	0.41
35:1d:13:ARG:HB3	35:1d:38:TYR:O	2.21	0.41
35:1d:43:HIS:HB3	35:1d:46:LYS:HD2	2.01	0.41
35:1d:109:GLY:HA3	35:1d:165:MET:SD	2.60	0.41
38:1g:50:ILE:HG13	38:1g:125:MET:HG3	2.02	0.41
51:1t:37:SER:O	51:1t:41:ILE:HG13	2.20	0.41
5:2F:40:GLN:NE2	5:2F:182:ASN:OD1	2.54	0.41
6:2G:39:ILE:HG12	6:2G:157:ILE:HG12	2.02	0.41
13:2R:87:TYR:OH	13:2R:116:LEU:HB3	2.21	0.41
17:2V:55:ALA:HA	17:2V:101:GLY:HA2	2.03	0.41
22:20:82:ARG:HA	22:20:83:PRO:HD3	1.91	0.41
32:2a:99:U:H2'	32:2a:100:C:H6	1.86	0.41
32:2a:130:A:H5'	48:2q:63:ARG:NH1	2.35	0.41
32:2a:547:A:H5'	61:2a:1923:HOH:O	2.19	0.41
32:2a:664:G:P	49:2r:64:ARG:HH21	2.43	0.41
32:2a:751:U:H4'	46:2o:24:SER:HA	2.03	0.41
32:2a:814:A:N7	32:2a:816:A:C4	2.88	0.41
32:2a:986:A:H1'	50:2s:54:GLY:O	2.19	0.41
32:2a:1017:G:H2'	32:2a:1018:C:O4'	2.21	0.41
32:2a:1314:C:OP2	50:2s:4:SER:OG	2.30	0.41
32:2a:1524:C:OP1	42:2k:120:ARG:NH2	2.53	0.41
35:2d:146:ILE:HD12	35:2d:146:ILE:H	1.86	0.41
35:2d:176:LEU:HA	35:2d:183:GLY:HA2	2.02	0.41
39:2h:4:ASP:HB3	39:2h:7:ALA:HB3	2.02	0.41
39:2h:12:ARG:HD3	39:2h:25:ASP:O	2.19	0.41
49:2r:61:LYS:O	49:2r:65:ILE:HG12	2.21	0.41
54:2w:43:G:H2'	54:2w:44:G:H8	1.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1688:U:O2	1:1A:1700:A:H5'	2.20	0.41
1:1A:2030:A:H4'	1:1A:2031:A:C8	2.55	0.41
1:1A:2161:C:HO2'	1:1A:2162:G:H8	1.68	0.41
57:1A:4098:DI0:CAB	57:1A:4098:DI0:CBP	2.99	0.41
1:2A:93:G:H2'	1:2A:94:C:C6	2.56	0.41
1:2A:141:A:C8	1:2A:1408:C:O2'	2.66	0.41
1:2A:372:G:H8	23:21:65:SER:O	2.04	0.41
1:2A:978:G:C2	1:2A:986:C:C2	3.09	0.41
1:2A:1257:C:H4'	5:2F:83:PHE:CD1	2.56	0.41
1:2A:1592:C:H2'	1:2A:1593:G:C8	2.54	0.41
1:2A:1669:A:C8	10:2O:5:GLN:HG3	2.56	0.41
1:2A:1932:A:H2'	1:2A:1933:G:O4'	2.21	0.41
1:2A:2615:U:C2	27:25:7:PRO:HA	2.55	0.41
2:1B:12:C:H2'	22:10:73:GLY:HA3	2.03	0.41
6:1G:43:LEU:HB2	6:1G:89:GLY:HA2	2.03	0.41
13:1R:72:ASP:O	13:1R:76:VAL:HG23	2.20	0.41
15:1T:106:SER:O	15:1T:110:ILE:HG13	2.21	0.41
15:1T:127:ALA:C	15:1T:129:ARG:N	2.77	0.41
25:13:7:LYS:HE3	25:13:32:GLN:NE2	2.36	0.41
32:1a:396:G:O2'	32:1a:398:C:OP1	2.21	0.41
32:1a:502:G:C2	32:1a:503:C:C2	3.09	0.41
34:1c:22:TRP:CH2	45:1n:54:PRO:HG2	2.56	0.41
35:1d:122:ARG:HA	35:1d:122:ARG:HD2	1.74	0.41
2:2B:1:U:HO2'	2:2B:2:C:P	2.42	0.41
2:2B:98:G:H2'	2:2B:99:G:O4'	2.21	0.41
6:2G:37:VAL:HG21	6:2G:103:LEU:HD11	2.03	0.41
6:2G:101:ILE:HG22	6:2G:105:LYS:HZ3	1.86	0.41
8:2I:61:ARG:HE	8:2I:61:ARG:HB2	1.57	0.41
11:2P:120:ALA:HB1	11:2P:138:LEU:HA	2.02	0.41
21:2Z:72:ARG:NH2	21:2Z:97:GLU:O	2.54	0.41
22:20:46:LYS:HE3	22:20:76:GLY:HA3	2.02	0.41
23:21:75:GLU:O	23:21:78:LYS:HG3	2.21	0.41
24:22:8:LYS:HD2	24:22:8:LYS:HA	1.91	0.41
24:22:51:ARG:HE	24:22:51:ARG:HB2	1.50	0.41
32:2a:116:A:C4	32:2a:117:G:C8	3.08	0.41
32:2a:187:C:O2'	51:2t:89:ARG:NH2	2.54	0.41
32:2a:454:C:H3'	32:2a:455:C:H6	1.86	0.41
32:2a:455:C:H42	32:2a:476:G:H1	1.68	0.41
32:2a:738:C:H2'	32:2a:739:C:C6	2.55	0.41
32:2a:758:G:H4'	32:2a:880:C:H4'	2.03	0.41
32:2a:981:U:H5'	45:2n:21:TYR:CE2	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:989:C:H1'	32:2a:1016:A:H2	1.85	0.41
32:2a:1207:2MG:C6	32:2a:1208:C:C4	3.09	0.41
34:2c:164:ARG:HG2	34:2c:165:THR:H	1.86	0.41
35:2d:116:GLN:NE2	35:2d:157:LEU:HD11	2.35	0.41
39:2h:20:TYR:HA	39:2h:65:TYR:CE1	2.56	0.41
45:2n:17:LYS:HE2	45:2n:17:LYS:HB3	1.83	0.41
1:1A:192:C:H2'	1:1A:193:U:H5'	2.03	0.41
1:1A:335:C:H2'	1:1A:336:C:H6	1.86	0.41
1:1A:458:G:C8	29:17:37:LYS:HG2	2.56	0.41
1:1A:586:A:H5'	5:1F:89:VAL:HG21	2.02	0.41
1:1A:910:A:N1	1:1A:2277:G:H1'	2.36	0.41
1:1A:1001:A:H2'	1:1A:1002:G:O4'	2.21	0.41
1:1A:1059:G:H2'	1:1A:1060:U:C5	2.56	0.41
1:1A:1202:C:N4	61:1A:4222:HOH:O	2.53	0.41
1:1A:1385:G:O2'	1:1A:1396:U:O2	2.29	0.41
1:1A:2345:G:H4'	1:1A:2346:A:H5''	2.02	0.41
1:1A:2348:U:O4	1:1A:2382:G:N1	2.54	0.41
1:1A:2512:C:H2'	1:1A:2513:G:O4'	2.21	0.41
1:1A:2865:U:C4	1:1A:2866:U:C4	3.09	0.41
1:2A:466:A:N3	1:2A:683:C:H1'	2.36	0.41
1:2A:518:G:H2'	1:2A:519:U:C6	2.55	0.41
1:2A:752:A:P	29:27:3:ARG:HH22	2.44	0.41
1:2A:760:G:H2'	1:2A:761:A:O4'	2.20	0.41
1:2A:1022:G:C6	1:2A:1140:C:C4	3.09	0.41
1:2A:1180:C:H2'	1:2A:1181:C:C6	2.53	0.41
1:2A:1479:G:C6	1:2A:1480:G:C5	3.09	0.41
1:2A:1607:C:H5''	1:2A:1608:A:H5'	2.03	0.41
1:2A:1638:C:H2'	1:2A:1639:U:O4'	2.21	0.41
1:2A:2094:G:P	8:2I:22:LYS:HD2	2.61	0.41
1:2A:2347:C:H2'	1:2A:2348:U:C6	2.56	0.41
1:2A:2477:C:H2'	31:29:2:LYS:HE2	2.03	0.41
1:2A:2776:A:H4'	1:2A:2777:G:H5''	2.02	0.41
1:2A:2886:G:H2'	1:2A:2887:U:C6	2.56	0.41
3:1D:228:PRO:O	61:1D:402:HOH:O	2.21	0.41
9:1N:70:LYS:HB3	9:1N:87:LEU:HB2	2.03	0.41
11:1P:64:LYS:HE3	30:18:12:LYS:HD3	2.02	0.41
12:1Q:7:MET:HE3	12:1Q:7:MET:HB3	1.83	0.41
16:1U:113:ALA:O	16:1U:117:GLN:HG2	2.21	0.41
23:11:8:SER:HB3	23:11:66:HIS:CD2	2.56	0.41
26:14:53:GLU:OE2	44:1m:65:LYS:NZ	2.53	0.41
32:1a:64:G:H4'	32:1a:65:U:H5''	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:79:G:H1'	32:1a:91:C:O2	2.20	0.41
32:1a:173:U:C2	32:1a:197:A:N1	2.89	0.41
32:1a:358:U:H2'	32:1a:359:U:H6	1.86	0.41
32:1a:756:C:H2'	32:1a:757:U:O4'	2.21	0.41
32:1a:950:U:H2'	32:1a:951:G:C8	2.56	0.41
32:1a:987:G:H2'	32:1a:988:G:H8	1.85	0.41
32:1a:1002:G:N2	32:1a:1004:A:H1'	2.36	0.41
32:1a:1002:G:N7	32:1a:1003:G:H1'	2.36	0.41
34:1c:23:TYR:HA	41:1j:11:PHE:CE2	2.55	0.41
34:1c:138:VAL:HG23	34:1c:151:VAL:HG23	2.02	0.41
39:1h:13:ILE:O	39:1h:17:THR:HG23	2.21	0.41
5:2F:192:LEU:HD21	5:2F:194:MET:HE3	2.03	0.41
6:2G:17:PRO:HA	6:2G:20:ILE:HD12	2.02	0.41
6:2G:64:THR:HB	6:2G:94:LEU:HD11	2.03	0.41
8:2I:79:ILE:HG22	8:2I:81:VAL:HG13	2.02	0.41
10:2O:120:GLU:HB2	15:2T:68:TYR:HE2	1.85	0.41
11:2P:122:PRO:O	11:2P:123:LEU:HD23	2.21	0.41
14:2S:10:ARG:HG2	14:2S:91:PRO:HA	2.03	0.41
14:2S:25:ARG:HD2	14:2S:88:ASP:OD2	2.21	0.41
15:2T:55:ASN:H	15:2T:59:THR:HB	1.86	0.41
16:2U:91:ASP:O	16:2U:95:LEU:HB2	2.21	0.41
21:2Z:137:ILE:HA	21:2Z:156:LYS:HE2	2.03	0.41
24:22:1:MET:HG3	24:22:52:ASP:OD2	2.21	0.41
32:2a:157:G:H2'	32:2a:158:G:C8	2.52	0.41
32:2a:243:A:H62	32:2a:281:G:H1'	1.85	0.41
32:2a:324:G:OP1	51:2t:22:ARG:HD2	2.21	0.41
32:2a:509:A:C5'	35:2d:55:ALA:HB2	2.51	0.41
32:2a:540:G:H2'	32:2a:541:G:O4'	2.20	0.41
32:2a:576:G:O6	32:2a:880:C:O2'	2.24	0.41
32:2a:649:G:H2'	32:2a:650:G:O4'	2.21	0.41
32:2a:689:C:H4'	32:2a:705:U:H1'	2.03	0.41
32:2a:765:G:N1	32:2a:812:C:O2'	2.48	0.41
32:2a:922:G:H2'	32:2a:923:A:C8	2.56	0.41
32:2a:944:G:H1'	32:2a:1339:A:H61	1.85	0.41
32:2a:1004:A:H5''	32:2a:1024:G:N2	2.34	0.41
32:2a:1252:A:H61	32:2a:1285:A:N6	2.18	0.41
34:2c:20:SER:HA	34:2c:57:ILE:O	2.21	0.41
37:2f:44:GLY:HA2	37:2f:59:TYR:CE1	2.56	0.41
39:2h:56:LYS:HB2	39:2h:58:TYR:HE2	1.86	0.41
39:2h:72:PRO:O	39:2h:74:PRO:HD3	2.21	0.41
40:2i:5:TYR:H	40:2i:87:GLN:NE2	2.18	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:2i:34:ASN:O	40:2i:38:GLN:HB2	2.21	0.41
44:2m:79:LYS:HG2	44:2m:83:ASP:OD2	2.20	0.41
45:2n:27:CYS:SG	45:2n:29:ARG:HB2	2.60	0.41
54:2y:8:4SU:S4	54:2y:14:A:N7	2.94	0.41
1:1A:22:C:H2'	1:1A:23:G:O4'	2.21	0.41
1:1A:411:G:C5	11:1P:72:PRO:HB3	2.56	0.41
1:1A:887:A:H61	1:1A:890:A:H5''	1.86	0.41
1:1A:1072:C:O2	1:1A:1092:C:H5	2.04	0.41
1:1A:1173:G:H2'	1:1A:1173:G:OP2	2.21	0.41
1:1A:2831:G:H1'	1:1A:2883:A:H2'	2.02	0.41
1:2A:99:U:H4'	1:2A:100:G:H5'	2.03	0.41
1:2A:742:G:H2'	1:2A:743:G:H8	1.86	0.41
1:2A:1161:C:H2'	1:2A:1162:G:C8	2.56	0.41
1:2A:1649:G:O2'	13:2R:107:ASP:OD2	2.29	0.41
1:2A:1657:C:H2'	1:2A:1658:C:C6	2.56	0.41
1:2A:1900:A:OP2	61:2A:3996:HOH:O	2.22	0.41
1:2A:2391:G:O6	1:2A:2425:A:H8	2.04	0.41
1:2A:2525:G:N2	1:2A:2539:C:C2	2.89	0.41
2:1B:31:C:O2'	2:1B:53:A:N1	2.44	0.41
2:1B:57:A:H1'	6:1G:29:TRP:HB2	2.02	0.41
4:1E:143:ASN:HD22	4:1E:147:PRO:HD3	1.85	0.41
5:1F:157:VAL:HG21	5:1F:181:LEU:HD13	2.03	0.41
13:1R:41:ALA:HB1	13:1R:114:VAL:HG22	2.03	0.41
16:1U:105:VAL:HG11	17:1V:39:LEU:HD21	2.03	0.41
21:1Z:54:HIS:HD2	21:1Z:99:TYR:O	2.03	0.41
24:12:58:ALA:O	24:12:62:THR:OG1	2.39	0.41
32:1a:272:C:H2'	32:1a:273:A:H8	1.86	0.41
32:1a:582:U:H5''	46:1o:64:ARG:HH22	1.86	0.41
32:1a:841:U:OP2	32:1a:841:U:H6	2.04	0.41
32:1a:1003:G:N3	32:1a:1004:A:H2	2.19	0.41
32:1a:1062:U:H2'	32:1a:1063:C:C6	2.56	0.41
32:1a:1130:A:H2'	32:1a:1131:G:C8	2.56	0.41
51:1t:10:LEU:HD12	51:1t:10:LEU:HA	1.87	0.41
54:1w:54:5MU:H2'	54:1w:55:PSU:C6	2.56	0.41
10:2O:7:TYR:CE2	10:2O:20:MET:HB2	2.56	0.41
12:2Q:45:GLN:H	12:2Q:45:GLN:CD	2.29	0.41
13:2R:59:ASP:OD2	13:2R:61:HIS:HB3	2.21	0.41
14:2S:10:ARG:HG3	14:2S:13:ARG:HH21	1.86	0.41
14:2S:30:ARG:HG3	14:2S:30:ARG:O	2.21	0.41
15:2T:88:ILE:H	15:2T:88:ILE:HG12	1.70	0.41
16:2U:76:TYR:CZ	16:2U:80:ILE:HG13	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:130:A:H5'	48:2q:63:ARG:HH11	1.86	0.41
32:2a:152:A:N6	32:2a:170:U:C2	2.89	0.41
32:2a:1006:C:H2'	32:2a:1007:C:C6	2.56	0.41
32:2a:1124:G:N7	32:2a:1145:C:O2'	2.53	0.41
32:2a:1177:G:H3'	32:2a:1178:G:H8	1.86	0.41
33:2b:59:GLU:O	33:2b:63:MET:HG3	2.21	0.41
34:2c:63:ASN:CB	34:2c:98:ASN:HB2	2.52	0.41
38:2g:26:PHE:CD2	38:2g:62:PHE:HE1	2.39	0.41
1:1A:890:A:C2	1:1A:892:G:H1'	2.56	0.40
1:1A:973:A:OP1	1:1A:973:A:H8	2.04	0.40
1:1A:1108:U:H2'	1:1A:1109:C:C6	2.55	0.40
1:1A:1500:G:H2'	1:1A:1501:C:H6	1.85	0.40
1:1A:1636:C:H2'	1:1A:1637:A:C8	2.57	0.40
1:1A:2654:A:N1	1:1A:2665:A:H5''	2.36	0.40
1:2A:624:C:OP1	61:2A:3987:HOH:O	2.20	0.40
1:2A:647:G:N3	1:2A:2350:C:O2'	2.54	0.40
1:2A:812:C:H2'	1:2A:813:U:H6	1.86	0.40
1:2A:2379:G:O2'	14:2S:17:ARG:NH1	2.53	0.40
1:2A:2648:C:H2'	1:2A:2649:U:C6	2.56	0.40
1:2A:2773:C:H2'	1:2A:2774:C:H6	1.86	0.40
4:1E:96:PHE:O	4:1E:175:VAL:HG11	2.21	0.40
4:1E:173:VAL:CG2	4:1E:185:LYS:HB2	2.51	0.40
13:1R:26:LYS:HE2	13:1R:70:LEU:O	2.21	0.40
19:1X:72:LYS:HG2	19:1X:73:ARG:O	2.21	0.40
21:1Z:70:LEU:HD23	21:1Z:70:LEU:HA	1.85	0.40
21:1Z:130:PRO:HA	21:1Z:133:ILE:HD11	2.03	0.40
26:14:63:TYR:N	26:14:63:TYR:CD1	2.87	0.40
32:1a:938:A:C6	32:1a:939:G:C5	3.09	0.40
32:1a:1111:A:N1	34:1c:177:THR:OG1	2.50	0.40
33:1b:61:LEU:HD23	33:1b:68:ILE:HD11	2.03	0.40
33:1b:100:GLY:N	33:1b:176:GLU:OE2	2.51	0.40
41:1j:11:PHE:HE1	41:1j:67:THR:HG22	1.86	0.40
41:1j:44:VAL:HG22	41:1j:66:ARG:HG2	2.04	0.40
47:1p:50:LYS:HD2	47:1p:50:LYS:HA	1.65	0.40
10:2O:68:GLU:HB3	10:2O:78:ARG:HB3	2.03	0.40
19:2X:31:HIS:HA	19:2X:32:PRO:HD3	1.97	0.40
20:2Y:13:VAL:HG12	20:2Y:74:PRO:HA	2.03	0.40
26:24:12:ALA:HB2	26:24:26:SER:HB3	2.03	0.40
32:2a:73:G:C6	32:2a:97:G:C6	3.09	0.40
32:2a:1387:G:H2'	32:2a:1388:C:H6	1.86	0.40
35:2d:171:GLY:HA2	35:2d:172:PRO:HD3	1.92	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:2h:53:VAL:HB	39:2h:58:TYR:CD2	2.57	0.40
40:2i:43:ALA:HA	40:2i:74:ILE:HD13	2.03	0.40
41:2j:46:ARG:HA	41:2j:64:GLU:HA	2.02	0.40
47:2p:25:ARG:H	47:2p:25:ARG:HG2	1.71	0.40
48:2q:53:LEU:HD23	48:2q:82:MET:HE1	2.03	0.40
51:2t:36:LEU:HD12	51:2t:62:LEU:HD12	2.03	0.40
51:2t:54:LYS:HA	51:2t:57:ARG:NH2	2.36	0.40
1:1A:303:U:H2'	1:1A:304:G:C8	2.56	0.40
1:1A:588:U:H1'	5:1F:90:PHE:CG	2.57	0.40
1:1A:685:A:H1'	1:1A:688:U:O4	2.21	0.40
1:1A:759:G:OP1	61:1A:4311:HOH:O	2.22	0.40
1:2A:322:A:H2'	5:2F:169:ASN:HD21	1.86	0.40
1:2A:1015:G:H2'	1:2A:1016:G:C8	2.51	0.40
1:2A:1512:U:H2'	1:2A:1513:C:C6	2.56	0.40
1:2A:2418:A:OP1	30:28:29:LYS:NZ	2.53	0.40
1:2A:2833:G:H4'	1:2A:2834:G:OP2	2.20	0.40
3:1D:245:PRO:HA	3:1D:246:PRO:HD3	1.95	0.40
6:1G:34:LEU:HD12	6:1G:100:TRP:CZ3	2.57	0.40
6:1G:151:ALA:HB3	6:1G:153:ARG:NH1	2.36	0.40
7:1H:56:SER:HG	7:1H:58:GLU:H	1.67	0.40
7:1H:105:LEU:HD13	7:1H:162:ILE:HD11	2.04	0.40
15:1T:65:LYS:HE3	15:1T:67:SER:HB2	2.03	0.40
32:1a:393:A:OP2	47:1p:12:LYS:HD2	2.21	0.40
32:1a:598:U:H2'	32:1a:599:C:C6	2.56	0.40
32:1a:1391:U:O2'	32:1a:1532:U:OP1	2.32	0.40
34:1c:175:LEU:HD21	34:1c:201:TYR:CE1	2.56	0.40
35:1d:173:TRP:HB2	35:1d:187:ARG:O	2.21	0.40
50:1s:27:GLU:CB	50:1s:28:LYS:HA	2.46	0.40
54:1w:64:U:H2'	54:1w:65:C:C6	2.56	0.40
6:2G:16:ARG:HB2	6:2G:17:PRO:HD3	2.02	0.40
9:2N:13:TRP:CE2	9:2N:133:GLN:HG2	2.56	0.40
28:26:11:LEU:HB2	28:26:21:TYR:HB2	2.02	0.40
28:26:11:LEU:N	28:26:21:TYR:O	2.53	0.40
32:2a:142:G:H2'	32:2a:143:A:C8	2.56	0.40
32:2a:983:A:H2	32:2a:984:C:C6	2.39	0.40
32:2a:993:G:N3	32:2a:993:G:H2'	2.36	0.40
33:2b:24:TRP:CE3	33:2b:26:PRO:HA	2.56	0.40
44:2m:70:LEU:O	44:2m:74:VAL:HG23	2.21	0.40
49:2r:76:LEU:HD12	49:2r:76:LEU:HA	1.80	0.40
51:2t:98:PRO:O	51:2t:99:LEU:HB2	2.20	0.40
1:1A:817:C:O2'	1:1A:839:U:OP1	2.37	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1448:G:H1'	1:1A:1528:A:N1	2.36	0.40
1:1A:2260:C:H2'	1:1A:2261:C:C6	2.57	0.40
1:1A:2360:A:H2'	1:1A:2361:A:O4'	2.21	0.40
1:1A:2408:U:H2'	1:1A:2409:G:C8	2.55	0.40
1:2A:918:A:H5''	2:2B:98:G:O2'	2.21	0.40
1:2A:1213:A:H2'	1:2A:1214:A:O4'	2.22	0.40
1:2A:1221(A):C:C2	1:2A:1229:G:C2	3.10	0.40
1:2A:1530:C:O2'	1:2A:1531:C:H6	2.05	0.40
1:2A:1782:C:OP1	61:2A:3995:HOH:O	2.22	0.40
1:2A:2002:G:H1'	61:2A:4076:HOH:O	2.21	0.40
1:2A:2680:C:H1'	4:2E:187:ALA:HB1	2.03	0.40
3:1D:71:ASP:CG	3:1D:103:ARG:HH12	2.28	0.40
19:1X:1:MET:HE3	19:1X:1:MET:HB2	1.95	0.40
23:11:50:ARG:HG2	23:11:59:THR:HG22	2.03	0.40
28:16:18:ARG:HD2	28:16:42:TRP:CG	2.56	0.40
32:1a:138:G:H2'	32:1a:139:G:C8	2.57	0.40
32:1a:374:A:C6	32:1a:375:U:C4	3.09	0.40
32:1a:673:G:O3'	37:1f:87:ARG:NH2	2.54	0.40
32:1a:900:A:H2'	32:1a:901:A:C8	2.56	0.40
32:1a:938:A:N6	32:1a:939:G:C6	2.90	0.40
32:1a:1030(C):G:H2'	32:1a:1030(D):A:C8	2.56	0.40
32:1a:1360:A:H2'	32:1a:1361:G:O4'	2.21	0.40
44:1m:3:ARG:HG3	44:1m:8:GLU:HA	2.02	0.40
44:1m:34:LEU:HD13	44:1m:41:PRO:HA	2.04	0.40
54:1y:58:A:N6	54:1y:61:C:N3	2.70	0.40
4:2E:26:ILE:HD11	4:2E:188:VAL:HG21	2.03	0.40
4:2E:37:ARG:NH1	4:2E:42:ASP:OD1	2.52	0.40
7:2H:117:PRO:HA	7:2H:118:PRO:HD3	1.94	0.40
8:2I:6:LEU:H	8:2I:36:ALA:HA	1.86	0.40
11:2P:121:LYS:O	11:2P:123:LEU:N	2.54	0.40
18:2W:6:ILE:HG23	18:2W:104:THR:OG1	2.22	0.40
21:2Z:93:ASP:HB2	21:2Z:131:ARG:NH1	2.36	0.40
32:2a:108:G:H1	51:2t:15:ARG:HG2	1.83	0.40
32:2a:380:G:N1	32:2a:384:G:C6	2.89	0.40
32:2a:1104:G:C2	32:2a:1105:A:C4	3.09	0.40
32:2a:1272:G:C8	32:2a:1272:G:H5''	2.57	0.40
32:2a:1273:G:H3'	32:2a:1274:G:H8	1.87	0.40
32:2a:1452:C:OP2	32:2a:1452:C:H3'	2.21	0.40
35:2d:53:ASP:O	35:2d:57:ARG:HG3	2.21	0.40
42:2k:21:ILE:HD12	42:2k:84:VAL:HG22	2.04	0.40
43:2l:6:THR:HG23	43:2l:9:GLN:OE1	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:2o:39:LEU:CD2	46:2o:56:LEU:HB2	2.51	0.40
54:2y:50:G:N2	54:2y:64:U:O2	2.35	0.40
1:1A:251:A:C5	1:1A:252:G:H1'	2.56	0.40
1:1A:512:G:OP1	1:1A:1234:U:O2'	2.34	0.40
1:1A:603:A:H4'	1:1A:604:G:H5'	2.02	0.40
1:1A:825:C:O2	11:1P:55:ARG:NH1	2.53	0.40
1:1A:864:G:C6	1:1A:865:C:N4	2.89	0.40
1:1A:1050:A:H2'	1:1A:1051:G:O4'	2.20	0.40
1:1A:2183:C:HO2'	1:1A:2184:G:P	2.44	0.40
1:1A:2507:C:H2'	1:1A:2508:G:O4'	2.21	0.40
1:2A:7:G:H4'	9:2N:13:TRP:HH2	1.86	0.40
1:2A:557:U:H2'	1:2A:558:G:C8	2.57	0.40
1:2A:588:U:O5'	1:2A:588:U:H6	2.05	0.40
1:2A:862:G:H2'	1:2A:863:A:O4'	2.22	0.40
1:2A:996:A:O3'	16:2U:91:ASP:HB2	2.22	0.40
1:2A:1027:A:C6	1:2A:1126:A:C4	3.09	0.40
1:2A:1669:A:H4'	1:2A:2549:G:H5''	2.03	0.40
1:2A:1786:A:C4	1:2A:1938:A:C6	3.09	0.40
1:2A:1843:C:H5'	3:2D:253:GLN:OE1	2.21	0.40
1:2A:1849:G:H2'	1:2A:1850:G:H8	1.87	0.40
1:2A:2119:A:C5	1:2A:2170:A:C6	3.09	0.40
1:2A:2689:U:P	1:2A:2719:G:H22	2.44	0.40
2:1B:1:U:HO2'	2:1B:2:C:P	2.43	0.40
3:1D:137:PRO:HG2	3:1D:140:THR:OG1	2.22	0.40
5:1F:132:VAL:CG2	5:1F:163:VAL:HG22	2.51	0.40
7:1H:41:MET:HE1	7:1H:54:ARG:HB3	2.03	0.40
10:1O:98:VAL:HG22	10:1O:118:ALA:HA	2.04	0.40
13:1R:38:VAL:HG12	13:1R:42:LYS:HE3	2.02	0.40
20:1Y:95:LYS:HB3	20:1Y:95:LYS:HE2	1.95	0.40
27:15:8:LYS:O	27:15:9:LYS:HD2	2.21	0.40
32:1a:40:C:H2'	32:1a:41:G:C8	2.56	0.40
32:1a:868:C:H2'	32:1a:869:G:O4'	2.21	0.40
32:1a:1065:U:H1'	32:1a:1066:C:OP2	2.22	0.40
32:1a:1179:A:H2'	32:1a:1180:A:O4'	2.22	0.40
33:1b:79:ASP:O	33:1b:83:MET:HG2	2.21	0.40
2:2B:7:G:H5'	14:2S:29:PHE:CE2	2.57	0.40
2:2B:77:U:OP1	21:2Z:19:ARG:NH2	2.53	0.40
11:2P:21:ARG:HA	11:2P:21:ARG:HD3	1.79	0.40
15:2T:26:ASP:OD1	15:2T:120:ARG:NH2	2.54	0.40
17:2V:40:LEU:HB2	17:2V:46:VAL:HG22	2.03	0.40
32:2a:735:C:H2'	32:2a:736:C:H6	1.87	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1132:C:H42	32:2a:1142:G:H1	1.69	0.40
33:2b:168:THR:OG1	33:2b:191:ASP:O	2.36	0.40
33:2b:170:GLU:HG3	33:2b:173:ALA:HB3	2.03	0.40
39:2h:34:GLU:HB3	39:2h:118:VAL:HG21	2.03	0.40
41:2j:25:GLU:O	41:2j:29:ARG:HG2	2.21	0.40
47:2p:26:ARG:HG3	47:2p:27:LYS:N	2.37	0.40
51:2t:56:MET:CE	51:2t:85:MET:HG2	2.51	0.40
54:2w:41:A:H2'	54:2w:42:G:H8	1.86	0.40
1:1A:147:U:H2'	1:1A:148:C:C6	2.56	0.40
1:1A:671:C:H2'	1:1A:672:C:C6	2.56	0.40
1:1A:751:A:C6	1:1A:789:A:C5	3.10	0.40
1:1A:2544:G:H2'	1:1A:2545:G:O4'	2.20	0.40
1:1A:2611:U:C4	27:15:3:LYS:HG2	2.56	0.40
1:2A:201:C:O2'	1:2A:251:A:N1	2.51	0.40
1:2A:413:C:H6	1:2A:413:C:O5'	2.04	0.40
1:2A:1410:G:H2'	1:2A:1411:C:C6	2.56	0.40
1:2A:1587:A:H2'	1:2A:1588:C:C6	2.56	0.40
1:2A:2207:G:H3'	1:2A:2208:A:H5''	2.03	0.40
1:2A:2271:G:OP1	22:20:18:ALA:HB1	2.22	0.40
1:2A:2492:U:H2'	1:2A:2493:U:C6	2.57	0.40
1:2A:2611:U:H6	1:2A:2611:U:H5'	1.87	0.40
2:1B:48:A:H4'	14:1S:95:HIS:CD2	2.56	0.40
3:1D:24:ILE:HD13	3:1D:84:TYR:HB2	2.03	0.40
5:1F:133:ASN:N	5:1F:138:GLU:OE1	2.31	0.40
7:1H:20:ALA:HB1	7:1H:21:PRO:HD2	2.04	0.40
14:1S:30:ARG:HG2	14:1S:30:ARG:HH11	1.87	0.40
16:1U:54:LYS:H	16:1U:54:LYS:HG2	1.54	0.40
21:1Z:26:GLY:HA2	21:1Z:85:HIS:CD2	2.56	0.40
21:1Z:150:LEU:HG	21:1Z:151:HIS:N	2.37	0.40
32:1a:195:A:H1'	32:1a:222:U:O2'	2.21	0.40
32:1a:529:G:O6	43:1l:49:ASN:HA	2.22	0.40
32:1a:1121:U:H2'	32:1a:1122:U:H6	1.87	0.40
32:1a:1139:G:N2	32:1a:1143:G:C6	2.89	0.40
32:1a:1308:U:OP1	44:1m:98:VAL:N	2.48	0.40
32:1a:1327:C:OP1	52:1u:12:LYS:NZ	2.55	0.40
34:1c:79:ARG:O	34:1c:82:GLU:HG2	2.22	0.40
34:1c:110:ASN:HD22	34:1c:140:ARG:HB3	1.86	0.40
43:1l:117:ARG:CZ	43:1l:117:ARG:HB2	2.52	0.40
51:1t:13:LEU:O	51:1t:17:ARG:HG3	2.21	0.40
54:1y:52:G:H2'	54:1y:53:G:H8	1.86	0.40
2:2B:83:G:H5''	25:23:52:HIS:CD2	2.57	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2B:88:C:H2'	2:2B:89:G:O4'	2.21	0.40
5:2F:29:ASN:O	5:2F:33:LEU:HD13	2.22	0.40
6:2G:121:ASN:HA	6:2G:122:PRO:HD3	1.95	0.40
9:2N:53:VAL:HA	9:2N:121:LYS:O	2.22	0.40
32:2a:11:G:H1	32:2a:23:C:N4	2.19	0.40
32:2a:336:C:H2'	32:2a:337:C:H6	1.87	0.40
32:2a:1039:C:C2	32:2a:1040:U:H1'	2.57	0.40
32:2a:1306:A:H1'	32:2a:1332:A:C2	2.57	0.40
33:2b:192:SER:O	33:2b:194:PRO:HD3	2.22	0.40
34:2c:50:ALA:HB1	34:2c:70:VAL:HG21	2.03	0.40
39:2h:69:ARG:HD3	39:2h:75:ARG:O	2.22	0.40
41:2j:74:ILE:HD12	41:2j:74:ILE:HA	1.90	0.40
44:2m:29:ARG:HB3	44:2m:64:TRP:CZ2	2.56	0.40
50:2s:28:LYS:HE2	50:2s:47:HIS:CE1	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	256 (94%)	16 (6%)	1 (0%)	30	60
3	2D	273/276 (99%)	259 (95%)	13 (5%)	1 (0%)	30	60
4	1E	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	24	55
4	2E	202/206 (98%)	195 (96%)	6 (3%)	1 (0%)	24	55
5	1F	201/210 (96%)	194 (96%)	5 (2%)	2 (1%)	12	38
5	2F	201/210 (96%)	195 (97%)	4 (2%)	2 (1%)	12	38
6	1G	179/182 (98%)	168 (94%)	10 (6%)	1 (1%)	21	51
6	2G	179/182 (98%)	161 (90%)	16 (9%)	2 (1%)	11	36
7	1H	172/180 (96%)	160 (93%)	11 (6%)	1 (1%)	21	51

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	2H	172/180 (96%)	159 (92%)	10 (6%)	3 (2%)	7	25
8	1I	144/148 (97%)	127 (88%)	17 (12%)	0	100	100
8	2I	144/148 (97%)	130 (90%)	13 (9%)	1 (1%)	18	47
9	1N	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
9	2N	138/140 (99%)	133 (96%)	4 (3%)	1 (1%)	18	47
10	1O	120/122 (98%)	109 (91%)	10 (8%)	1 (1%)	16	44
10	2O	120/122 (98%)	112 (93%)	7 (6%)	1 (1%)	16	44
11	1P	147/150 (98%)	137 (93%)	9 (6%)	1 (1%)	18	47
11	2P	147/150 (98%)	138 (94%)	8 (5%)	1 (1%)	18	47
12	1Q	139/141 (99%)	133 (96%)	5 (4%)	1 (1%)	18	47
12	2Q	139/141 (99%)	130 (94%)	9 (6%)	0	100	100
13	1R	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
13	2R	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
14	1S	108/112 (96%)	99 (92%)	9 (8%)	0	100	100
14	2S	108/112 (96%)	105 (97%)	2 (2%)	1 (1%)	14	41
15	1T	129/146 (88%)	123 (95%)	6 (5%)	0	100	100
15	2T	129/146 (88%)	123 (95%)	6 (5%)	0	100	100
16	1U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
16	2U	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
17	1V	99/101 (98%)	93 (94%)	3 (3%)	3 (3%)	3	12
17	2V	99/101 (98%)	92 (93%)	5 (5%)	2 (2%)	6	21
18	1W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
18	2W	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
19	1X	93/96 (97%)	91 (98%)	2 (2%)	0	100	100
19	2X	93/96 (97%)	90 (97%)	3 (3%)	0	100	100
20	1Y	105/110 (96%)	98 (93%)	7 (7%)	0	100	100
20	2Y	105/110 (96%)	98 (93%)	7 (7%)	0	100	100
21	1Z	148/206 (72%)	130 (88%)	16 (11%)	2 (1%)	9	30
21	2Z	156/206 (76%)	135 (86%)	19 (12%)	2 (1%)	9	31
22	10	81/85 (95%)	78 (96%)	3 (4%)	0	100	100
22	20	81/85 (95%)	80 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	11	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	11	36
23	21	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	11	36
24	12	68/72 (94%)	68 (100%)	0	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%)	56 (98%)	1 (2%)	0	100	100
26	14	67/71 (94%)	52 (78%)	12 (18%)	3 (4%)	2	7
26	24	67/71 (94%)	53 (79%)	10 (15%)	4 (6%)	1	3
27	15	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
27	25	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
28	16	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
28	26	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
29	17	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
29	27	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	35 (100%)	0	0	100	100
33	1b	229/256 (90%)	201 (88%)	21 (9%)	7 (3%)	3	12
33	2b	229/256 (90%)	200 (87%)	24 (10%)	5 (2%)	5	19
34	1c	204/239 (85%)	188 (92%)	13 (6%)	3 (2%)	8	28
34	2c	204/239 (85%)	189 (93%)	14 (7%)	1 (0%)	24	55
35	1d	206/209 (99%)	195 (95%)	9 (4%)	2 (1%)	12	38
35	2d	206/209 (99%)	198 (96%)	7 (3%)	1 (0%)	24	55
36	1e	146/162 (90%)	138 (94%)	3 (2%)	5 (3%)	3	11
36	2e	146/162 (90%)	133 (91%)	12 (8%)	1 (1%)	18	47
37	1f	98/101 (97%)	94 (96%)	3 (3%)	1 (1%)	12	38
37	2f	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
38	1g	153/156 (98%)	141 (92%)	9 (6%)	3 (2%)	6	21
38	2g	153/156 (98%)	145 (95%)	6 (4%)	2 (1%)	9	31
39	1h	135/138 (98%)	131 (97%)	4 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	2h	135/138 (98%)	129 (96%)	6 (4%)	0	100	100
40	1i	125/128 (98%)	108 (86%)	17 (14%)	0	100	100
40	2i	125/128 (98%)	112 (90%)	13 (10%)	0	100	100
41	1j	95/105 (90%)	81 (85%)	11 (12%)	3 (3%)	3	11
41	2j	94/105 (90%)	84 (89%)	6 (6%)	4 (4%)	2	7
42	1k	112/129 (87%)	100 (89%)	10 (9%)	2 (2%)	6	23
42	2k	112/129 (87%)	99 (88%)	12 (11%)	1 (1%)	14	41
43	1l	119/132 (90%)	115 (97%)	3 (2%)	1 (1%)	16	44
43	2l	119/132 (90%)	115 (97%)	4 (3%)	0	100	100
44	1m	121/126 (96%)	110 (91%)	9 (7%)	2 (2%)	7	25
44	2m	120/126 (95%)	109 (91%)	11 (9%)	0	100	100
45	1n	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
45	2n	58/61 (95%)	53 (91%)	5 (9%)	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%)	76 (95%)	4 (5%)	0	100	100
47	2p	80/88 (91%)	75 (94%)	5 (6%)	0	100	100
48	1q	97/105 (92%)	89 (92%)	8 (8%)	0	100	100
48	2q	97/105 (92%)	93 (96%)	3 (3%)	1 (1%)	12	38
49	1r	66/88 (75%)	63 (96%)	3 (4%)	0	100	100
49	2r	66/88 (75%)	63 (96%)	3 (4%)	0	100	100
50	1s	81/93 (87%)	71 (88%)	9 (11%)	1 (1%)	10	34
50	2s	81/93 (87%)	66 (82%)	13 (16%)	2 (2%)	4	16
51	1t	94/106 (89%)	85 (90%)	6 (6%)	3 (3%)	3	11
51	2t	94/106 (89%)	86 (92%)	4 (4%)	4 (4%)	2	7
52	1u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
52	2u	21/27 (78%)	18 (86%)	1 (5%)	2 (10%)	0	1
All	All	11370/12128 (94%)	10640 (94%)	632 (6%)	98 (1%)	14	41

All (98) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	1V	53	GLU
33	1b	17	PHE
36	1e	98	THR
41	1j	79	ARG
50	1s	27	GLU
5	2F	130	ALA
6	2G	52	ILE
23	2I	3	LYS
26	24	65	ASP
33	2b	78	GLN
51	2t	47	GLY
5	1F	89	VAL
6	1G	47	LYS
21	1Z	2	GLU
21	1Z	147	GLY
26	14	55	ARG
33	1b	13	ALA
34	1c	107	GLN
36	1e	85	GLY
43	1l	91	LYS
5	2F	89	VAL
7	2H	47	GLU
21	2Z	2	GLU
21	2Z	141	VAL
33	2b	17	PHE
36	2e	85	GLY
41	2j	75	ILE
42	2k	49	GLY
51	2t	10	LEU
52	2u	7	ARG
7	1H	126	PRO
17	1V	43	GLU
26	14	58	ARG
26	14	68	ARG
33	1b	78	GLN
33	1b	125	PRO
41	1j	32	ALA
44	1m	3	ARG
51	1t	95	ALA
7	2H	126	PRO
33	2b	20	GLU
52	2u	3	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	1V	100	ARG
23	1l	3	LYS
33	1b	20	GLU
33	1b	126	GLU
36	1e	86	ALA
38	1g	4	ARG
41	1j	29	ARG
51	1t	47	GLY
8	2I	42	SER
10	2O	5	GLN
17	2V	100	ARG
26	24	64	GLY
26	24	68	ARG
33	2b	9	GLU
41	2j	39	PRO
50	2s	81	ARG
51	2t	95	ALA
3	1D	3	VAL
4	1E	52	LEU
12	1Q	16	ARG
33	1b	231	GLU
34	1c	14	ILE
38	1g	52	GLU
38	1g	80	VAL
44	1m	12	ASN
3	2D	3	VAL
4	2E	52	LEU
6	2G	124	SER
9	2N	47	ALA
33	2b	36	ARG
41	2j	78	ASN
41	2j	79	ARG
48	2q	99	SER
10	1O	5	GLN
36	1e	69	VAL
11	2P	122	PRO
35	2d	3	ARG
38	2g	4	ARG
34	1c	66	VAL
35	1d	5	ILE
42	1k	49	GLY
11	1P	122	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	2S	96	GLY
17	2V	79	VAL
34	2c	66	VAL
51	2t	100	ILE
35	1d	178	VAL
37	1f	40	VAL
42	1k	105	VAL
51	1t	100	ILE
7	2H	12	PRO
26	24	56	VAL
38	2g	80	VAL
50	2s	9	VAL
36	1e	70	PRO

5.3.2 Protein sidechains ⓘ

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%)	203 (94%)	12 (6%)	19	50
3	2D	215/218 (99%)	200 (93%)	15 (7%)	14	40
4	1E	164/166 (99%)	145 (88%)	19 (12%)	5	18
4	2E	164/166 (99%)	154 (94%)	10 (6%)	17	46
5	1F	160/166 (96%)	147 (92%)	13 (8%)	11	33
5	2F	159/166 (96%)	149 (94%)	10 (6%)	16	45
6	1G	143/156 (92%)	131 (92%)	12 (8%)	10	32
6	2G	143/156 (92%)	132 (92%)	11 (8%)	12	36
7	1H	144/148 (97%)	134 (93%)	10 (7%)	14	41
7	2H	144/148 (97%)	134 (93%)	10 (7%)	14	41
8	1I	113/124 (91%)	102 (90%)	11 (10%)	8	25
8	2I	105/124 (85%)	93 (89%)	12 (11%)	5	19
9	1N	118/119 (99%)	107 (91%)	11 (9%)	8	27
9	2N	118/119 (99%)	111 (94%)	7 (6%)	18	48

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	1O	100/100 (100%)	96 (96%)	4 (4%)	28	63
10	2O	100/100 (100%)	95 (95%)	5 (5%)	22	54
11	1P	115/116 (99%)	106 (92%)	9 (8%)	11	35
11	2P	115/116 (99%)	108 (94%)	7 (6%)	17	46
12	1Q	111/111 (100%)	103 (93%)	8 (7%)	13	39
12	2Q	111/111 (100%)	104 (94%)	7 (6%)	16	45
13	1R	101/101 (100%)	92 (91%)	9 (9%)	9	29
13	2R	101/101 (100%)	93 (92%)	8 (8%)	11	35
14	1S	86/88 (98%)	78 (91%)	8 (9%)	8	27
14	2S	85/88 (97%)	78 (92%)	7 (8%)	10	33
15	1T	115/127 (91%)	112 (97%)	3 (3%)	40	75
15	2T	113/127 (89%)	112 (99%)	1 (1%)	70	89
16	1U	93/94 (99%)	85 (91%)	8 (9%)	10	31
16	2U	93/94 (99%)	89 (96%)	4 (4%)	26	60
17	1V	80/82 (98%)	70 (88%)	10 (12%)	4	15
17	2V	80/82 (98%)	72 (90%)	8 (10%)	7	24
18	1W	90/92 (98%)	86 (96%)	4 (4%)	25	59
18	2W	90/92 (98%)	82 (91%)	8 (9%)	9	29
19	1X	77/78 (99%)	75 (97%)	2 (3%)	40	75
19	2X	77/78 (99%)	71 (92%)	6 (8%)	11	35
20	1Y	85/91 (93%)	77 (91%)	8 (9%)	8	27
20	2Y	85/91 (93%)	77 (91%)	8 (9%)	8	27
21	1Z	135/179 (75%)	124 (92%)	11 (8%)	11	33
21	2Z	137/179 (76%)	127 (93%)	10 (7%)	13	38
22	10	65/67 (97%)	61 (94%)	4 (6%)	16	45
22	20	65/67 (97%)	63 (97%)	2 (3%)	35	70
23	11	80/83 (96%)	76 (95%)	4 (5%)	22	54
23	21	80/83 (96%)	75 (94%)	5 (6%)	16	45
24	12	65/67 (97%)	61 (94%)	4 (6%)	16	45
24	22	65/67 (97%)	61 (94%)	4 (6%)	16	45
25	13	51/52 (98%)	49 (96%)	2 (4%)	28	64

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	23	50/52 (96%)	49 (98%)	1 (2%)	48	80
26	14	59/63 (94%)	49 (83%)	10 (17%)	2	7
26	24	53/63 (84%)	50 (94%)	3 (6%)	18	49
27	15	50/52 (96%)	47 (94%)	3 (6%)	17	47
27	25	50/52 (96%)	46 (92%)	4 (8%)	11	34
28	16	51/52 (98%)	46 (90%)	5 (10%)	7	25
28	26	50/52 (96%)	45 (90%)	5 (10%)	7	24
29	17	41/42 (98%)	36 (88%)	5 (12%)	5	16
29	27	41/42 (98%)	38 (93%)	3 (7%)	13	38
30	18	54/55 (98%)	47 (87%)	7 (13%)	4	14
30	28	54/55 (98%)	50 (93%)	4 (7%)	13	37
31	19	34/34 (100%)	33 (97%)	1 (3%)	37	73
31	29	34/34 (100%)	33 (97%)	1 (3%)	37	73
33	1b	192/220 (87%)	181 (94%)	11 (6%)	18	49
33	2b	187/220 (85%)	176 (94%)	11 (6%)	18	48
34	1c	142/188 (76%)	133 (94%)	9 (6%)	16	45
34	2c	140/188 (74%)	133 (95%)	7 (5%)	22	54
35	1d	169/181 (93%)	154 (91%)	15 (9%)	9	29
35	2d	173/181 (96%)	162 (94%)	11 (6%)	16	44
36	1e	113/123 (92%)	108 (96%)	5 (4%)	25	59
36	2e	114/123 (93%)	109 (96%)	5 (4%)	25	59
37	1f	84/90 (93%)	80 (95%)	4 (5%)	23	56
37	2f	85/90 (94%)	81 (95%)	4 (5%)	23	57
38	1g	119/127 (94%)	115 (97%)	4 (3%)	32	68
38	2g	120/127 (94%)	118 (98%)	2 (2%)	53	83
39	1h	114/119 (96%)	103 (90%)	11 (10%)	8	26
39	2h	114/119 (96%)	105 (92%)	9 (8%)	11	35
40	1i	90/99 (91%)	86 (96%)	4 (4%)	25	59
40	2i	89/99 (90%)	84 (94%)	5 (6%)	19	50
41	1j	66/92 (72%)	61 (92%)	5 (8%)	12	36
41	2j	69/92 (75%)	67 (97%)	2 (3%)	37	73

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	1k	82/99 (83%)	79 (96%)	3 (4%)	30	65
42	2k	83/99 (84%)	77 (93%)	6 (7%)	13	39
43	1l	96/108 (89%)	86 (90%)	10 (10%)	7	22
43	2l	96/108 (89%)	89 (93%)	7 (7%)	13	38
44	1m	93/101 (92%)	88 (95%)	5 (5%)	20	51
44	2m	92/101 (91%)	86 (94%)	6 (6%)	15	43
45	1n	49/50 (98%)	43 (88%)	6 (12%)	5	16
45	2n	49/50 (98%)	43 (88%)	6 (12%)	5	16
46	1o	78/80 (98%)	77 (99%)	1 (1%)	61	86
46	2o	78/80 (98%)	77 (99%)	1 (1%)	61	86
47	1p	69/74 (93%)	61 (88%)	8 (12%)	5	18
47	2p	68/74 (92%)	62 (91%)	6 (9%)	9	29
48	1q	94/97 (97%)	93 (99%)	1 (1%)	65	87
48	2q	94/97 (97%)	90 (96%)	4 (4%)	26	60
49	1r	59/77 (77%)	55 (93%)	4 (7%)	14	42
49	2r	59/77 (77%)	58 (98%)	1 (2%)	53	83
50	1s	69/80 (86%)	68 (99%)	1 (1%)	59	85
50	2s	67/80 (84%)	63 (94%)	4 (6%)	17	47
51	1t	70/82 (85%)	66 (94%)	4 (6%)	18	49
51	2t	70/82 (85%)	65 (93%)	5 (7%)	13	39
52	1u	18/22 (82%)	18 (100%)	0	100	100
52	2u	18/22 (82%)	18 (100%)	0	100	100
All	All	9303/10064 (92%)	8687 (93%)	616 (7%)	15	43

All (616) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	39	LYS
3	1D	94	LEU
3	1D	113	VAL
3	1D	142	VAL
3	1D	155	LEU
3	1D	157	ARG
3	1D	173	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	1D	193	VAL
3	1D	221	VAL
3	1D	229	VAL
3	1D	242	ARG
3	1D	260	ARG
4	1E	1	MET
4	1E	9	VAL
4	1E	12	THR
4	1E	21	VAL
4	1E	24	THR
4	1E	27	LEU
4	1E	33	VAL
4	1E	34	VAL
4	1E	47	VAL
4	1E	49	LEU
4	1E	75	VAL
4	1E	93	VAL
4	1E	94	GLU
4	1E	116	VAL
4	1E	145	LYS
4	1E	167	VAL
4	1E	175	VAL
4	1E	181	LEU
4	1E	188	VAL
5	1F	24	LEU
5	1F	33	LEU
5	1F	52	LYS
5	1F	53	THR
5	1F	57	VAL
5	1F	88	VAL
5	1F	106	ARG
5	1F	132	VAL
5	1F	158	THR
5	1F	183	VAL
5	1F	192	LEU
5	1F	197	ASP
5	1F	201	VAL
6	1G	3	LEU
6	1G	5	VAL
6	1G	14	GLU
6	1G	28	VAL
6	1G	31	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	1G	43	LEU
6	1G	82	LEU
6	1G	109	VAL
6	1G	133	LEU
6	1G	139	LEU
6	1G	149	VAL
6	1G	175	LEU
7	1H	15	VAL
7	1H	44	VAL
7	1H	45	VAL
7	1H	56	SER
7	1H	71	LEU
7	1H	98	LEU
7	1H	106	THR
7	1H	114	VAL
7	1H	122	THR
7	1H	129	THR
8	1I	9	LEU
8	1I	12	LEU
8	1I	31	LEU
8	1I	38	LEU
8	1I	47	LEU
8	1I	87	LYS
8	1I	92	VAL
8	1I	101	LEU
8	1I	109	ILE
8	1I	140	LEU
8	1I	145	VAL
9	1N	28	THR
9	1N	33	LEU
9	1N	34	LEU
9	1N	46	VAL
9	1N	61	ARG
9	1N	62	VAL
9	1N	73	THR
9	1N	87	LEU
9	1N	112	LEU
9	1N	127	ASP
9	1N	139	GLU
10	1O	25	LEU
10	1O	69	ILE
10	1O	98	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	1O	107	ARG
11	1P	3	LEU
11	1P	45	LEU
11	1P	56	SER
11	1P	76	LYS
11	1P	83	VAL
11	1P	95	VAL
11	1P	125	VAL
11	1P	135	LEU
11	1P	148	LEU
12	1Q	8	LYS
12	1Q	35	VAL
12	1Q	37	LEU
12	1Q	60	ARG
12	1Q	109	VAL
12	1Q	110	THR
12	1Q	112	GLU
12	1Q	138	ASP
13	1R	6	SER
13	1R	29	LEU
13	1R	44	LEU
13	1R	54	LEU
13	1R	65	LEU
13	1R	67	LEU
13	1R	100	LEU
13	1R	111	LEU
13	1R	114	VAL
14	1S	8	GLU
14	1S	14	VAL
14	1S	35	ILE
14	1S	36	TYR
14	1S	46	VAL
14	1S	50	SER
14	1S	69	VAL
14	1S	110	LEU
15	1T	28	VAL
15	1T	49	VAL
15	1T	67	SER
16	1U	5	LYS
16	1U	8	VAL
16	1U	9	VAL
16	1U	36	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	1U	54	LYS
16	1U	74	LEU
16	1U	77	SER
16	1U	95	LEU
17	1V	35	LEU
17	1V	38	LEU
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	79	VAL
17	1V	82	ARG
18	1W	17	VAL
18	1W	23	LEU
18	1W	103	ILE
18	1W	107	LEU
19	1X	38	GLU
19	1X	45	THR
20	1Y	50	ARG
20	1Y	51	VAL
20	1Y	70	SER
20	1Y	72	VAL
20	1Y	85	VAL
20	1Y	90	LEU
20	1Y	99	CYS
20	1Y	107	ASP
21	1Z	1	MET
21	1Z	8	TYR
21	1Z	18	LEU
21	1Z	28	MET
21	1Z	33	LEU
21	1Z	37	VAL
21	1Z	70	LEU
21	1Z	86	VAL
21	1Z	102	LEU
21	1Z	129	SER
21	1Z	146	ILE
22	10	14	ARG
22	10	39	ARG
22	10	43	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	10	53	MET
23	11	30	VAL
23	11	35	THR
23	11	59	THR
23	11	95	LEU
24	12	1	MET
24	12	19	VAL
24	12	53	LEU
24	12	62	THR
25	13	23	LEU
25	13	56	VAL
26	14	3	GLU
26	14	49	PHE
26	14	50	VAL
26	14	52	THR
26	14	53	GLU
26	14	56	VAL
26	14	57	GLU
26	14	58	ARG
26	14	66	SER
26	14	67	TYR
27	15	6	VAL
27	15	16	ARG
27	15	29	THR
28	16	14	THR
28	16	19	ARG
28	16	24	GLU
28	16	29	ASN
28	16	51	GLU
29	17	1	MET
29	17	4	THR
29	17	41	ARG
29	17	43	THR
29	17	46	VAL
30	18	14	VAL
30	18	23	VAL
30	18	29	LYS
30	18	30	ARG
30	18	32	LEU
30	18	37	SER
30	18	42	ARG
31	19	6	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	1b	96	ARG
33	1b	107	THR
33	1b	111	ARG
33	1b	121	LEU
33	1b	127	ILE
33	1b	160	ASP
33	1b	185	ILE
33	1b	189	ASP
33	1b	208	ILE
33	1b	221	LEU
33	1b	223	ILE
34	1c	3	ASN
34	1c	8	ILE
34	1c	15	THR
34	1c	58	GLU
34	1c	112	SER
34	1c	115	LEU
34	1c	195	VAL
34	1c	202	ILE
34	1c	207	VAL
35	1d	10	ARG
35	1d	19	LEU
35	1d	58	LEU
35	1d	59	ARG
35	1d	107	ARG
35	1d	108	LEU
35	1d	112	VAL
35	1d	115	ARG
35	1d	127	THR
35	1d	135	LEU
35	1d	137	SER
35	1d	144	ASP
35	1d	170	VAL
35	1d	178	VAL
35	1d	194	LEU
36	1e	20	GLN
36	1e	41	VAL
36	1e	91	LEU
36	1e	116	THR
36	1e	120	THR
37	1f	2	ARG
37	1f	21	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	1f	45	LEU
37	1f	72	VAL
38	1g	3	ARG
38	1g	24	THR
38	1g	53	LYS
38	1g	104	LEU
39	1h	25	ASP
39	1h	26	VAL
39	1h	29	SER
39	1h	35	ILE
39	1h	51	VAL
39	1h	63	LEU
39	1h	91	ARG
39	1h	95	VAL
39	1h	112	LEU
39	1h	120	THR
39	1h	133	LEU
40	1i	81	ILE
40	1i	87	GLN
40	1i	127	LYS
40	1i	128	ARG
41	1j	38	ILE
41	1j	49	VAL
41	1j	55	LYS
41	1j	92	THR
41	1j	98	ILE
42	1k	48	ILE
42	1k	109	VAL
42	1k	114	VAL
43	1l	18	VAL
43	1l	27	LEU
43	1l	36	VAL
43	1l	52	LEU
43	1l	59	ARG
43	1l	70	ILE
43	1l	83	VAL
43	1l	100	ILE
43	1l	113	ARG
43	1l	117	ARG
44	1m	3	ARG
44	1m	8	GLU
44	1m	49	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
44	1m	64	TRP
44	1m	102	ARG
45	1n	3	ARG
45	1n	18	VAL
45	1n	22	THR
45	1n	33	VAL
45	1n	44	LEU
45	1n	60	SER
46	1o	66	LEU
47	1p	2	VAL
47	1p	6	LEU
47	1p	20	VAL
47	1p	21	VAL
47	1p	25	ARG
47	1p	45	THR
47	1p	50	LYS
47	1p	62	VAL
48	1q	85	VAL
49	1r	35	ARG
49	1r	37	VAL
49	1r	47	THR
49	1r	86	VAL
50	1s	48	THR
51	1t	22	ARG
51	1t	56	MET
51	1t	70	SER
51	1t	100	ILE
3	2D	34	VAL
3	2D	61	LEU
3	2D	75	ILE
3	2D	94	LEU
3	2D	106	ILE
3	2D	113	VAL
3	2D	142	VAL
3	2D	155	LEU
3	2D	157	ARG
3	2D	173	VAL
3	2D	193	VAL
3	2D	212	SER
3	2D	221	VAL
3	2D	229	VAL
3	2D	242	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	2E	9	VAL
4	2E	14	ILE
4	2E	21	VAL
4	2E	24	THR
4	2E	75	VAL
4	2E	116	VAL
4	2E	134	ILE
4	2E	175	VAL
4	2E	181	LEU
4	2E	195	LEU
5	2F	12	LEU
5	2F	20	LEU
5	2F	57	VAL
5	2F	88	VAL
5	2F	106	ARG
5	2F	108	LYS
5	2F	165	ARG
5	2F	183	VAL
5	2F	192	LEU
5	2F	201	VAL
6	2G	3	LEU
6	2G	5	VAL
6	2G	31	VAL
6	2G	40	ASN
6	2G	43	LEU
6	2G	88	ILE
6	2G	98	ARG
6	2G	109	VAL
6	2G	133	LEU
6	2G	140	ILE
6	2G	161	THR
7	2H	15	VAL
7	2H	17	VAL
7	2H	25	LYS
7	2H	56	SER
7	2H	63	SER
7	2H	70	THR
7	2H	71	LEU
7	2H	107	VAL
7	2H	122	THR
7	2H	139	GLN
8	2I	4	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	2I	20	ASP
8	2I	38	LEU
8	2I	61	ARG
8	2I	74	ASN
8	2I	77	LEU
8	2I	87	LYS
8	2I	92	VAL
8	2I	101	LEU
8	2I	107	VAL
8	2I	127	VAL
8	2I	144	VAL
9	2N	14	VAL
9	2N	28	THR
9	2N	33	LEU
9	2N	35	ARG
9	2N	48	MET
9	2N	62	VAL
9	2N	99	LEU
10	2O	28	SER
10	2O	42	SER
10	2O	52	VAL
10	2O	78	ARG
10	2O	98	VAL
11	2P	3	LEU
11	2P	58	THR
11	2P	83	VAL
11	2P	95	VAL
11	2P	96	THR
11	2P	106	LEU
11	2P	148	LEU
12	2Q	22	LYS
12	2Q	38	GLU
12	2Q	77	LYS
12	2Q	85	LYS
12	2Q	106	VAL
12	2Q	109	VAL
12	2Q	110	THR
13	2R	6	SER
13	2R	29	LEU
13	2R	36	THR
13	2R	44	LEU
13	2R	65	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	2R	67	LEU
13	2R	100	LEU
13	2R	111	LEU
14	2S	21	THR
14	2S	35	ILE
14	2S	36	TYR
14	2S	48	LEU
14	2S	69	VAL
14	2S	80	LEU
14	2S	110	LEU
15	2T	89	VAL
16	2U	5	LYS
16	2U	8	VAL
16	2U	74	LEU
16	2U	95	LEU
17	2V	7	THR
17	2V	38	LEU
17	2V	46	VAL
17	2V	52	VAL
17	2V	61	VAL
17	2V	62	LEU
17	2V	72	VAL
17	2V	79	VAL
18	2W	15	ARG
18	2W	19	LEU
18	2W	23	LEU
18	2W	37	ARG
18	2W	67	ASP
18	2W	92	ARG
18	2W	96	ILE
18	2W	107	LEU
19	2X	2	LYS
19	2X	23	GLU
19	2X	57	LEU
19	2X	78	LYS
19	2X	92	LEU
19	2X	95	LEU
20	2Y	14	LEU
20	2Y	37	VAL
20	2Y	72	VAL
20	2Y	90	LEU
20	2Y	97	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	2Y	99	CYS
20	2Y	106	LEU
20	2Y	107	ASP
21	2Z	5	LEU
21	2Z	33	LEU
21	2Z	36	LYS
21	2Z	42	VAL
21	2Z	72	ARG
21	2Z	76	LEU
21	2Z	81	ARG
21	2Z	92	SER
21	2Z	98	MET
21	2Z	137	ILE
22	20	14	ARG
22	20	40	GLN
23	21	21	ARG
23	21	35	THR
23	21	38	SER
23	21	94	LEU
23	21	95	LEU
24	22	25	VAL
24	22	46	GLN
24	22	51	ARG
24	22	70	GLN
25	23	55	ARG
26	24	1	MET
26	24	49	PHE
26	24	63	TYR
27	25	6	VAL
27	25	16	ARG
27	25	29	THR
27	25	58	LEU
28	26	14	THR
28	26	23	THR
28	26	30	THR
28	26	48	VAL
28	26	51	GLU
29	27	1	MET
29	27	43	THR
29	27	46	VAL
30	28	14	VAL
30	28	23	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	28	30	ARG
30	28	32	LEU
31	29	7	VAL
33	2b	58	ILE
33	2b	67	THR
33	2b	74	LYS
33	2b	102	LEU
33	2b	112	VAL
33	2b	128	GLU
33	2b	136	VAL
33	2b	160	ASP
33	2b	178	ARG
33	2b	190	THR
33	2b	230	VAL
34	2c	32	LEU
34	2c	36	ASP
34	2c	49	SER
34	2c	58	GLU
34	2c	77	ILE
34	2c	115	LEU
34	2c	131	ARG
35	2d	59	ARG
35	2d	83	SER
35	2d	127	THR
35	2d	135	LEU
35	2d	141	ARG
35	2d	148	VAL
35	2d	157	LEU
35	2d	176	LEU
35	2d	178	VAL
35	2d	188	LEU
35	2d	194	LEU
36	2e	41	VAL
36	2e	83	GLU
36	2e	111	GLU
36	2e	115	VAL
36	2e	152	ARG
37	2f	37	VAL
37	2f	48	LEU
37	2f	81	ILE
37	2f	94	GLN
38	2g	50	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	2g	104	LEU
39	2h	10	LEU
39	2h	26	VAL
39	2h	29	SER
39	2h	54	ASP
39	2h	63	LEU
39	2h	87	SER
39	2h	104	ARG
39	2h	118	VAL
39	2h	137	VAL
40	2i	47	LEU
40	2i	87	GLN
40	2i	102	LEU
40	2i	103	THR
40	2i	128	ARG
41	2j	67	THR
41	2j	95	GLU
42	2k	14	VAL
42	2k	26	ASN
42	2k	48	ILE
42	2k	63	LEU
42	2k	87	THR
42	2k	114	VAL
43	2l	6	THR
43	2l	18	VAL
43	2l	33	ARG
43	2l	83	VAL
43	2l	113	ARG
43	2l	117	ARG
43	2l	123	LYS
44	2m	19	LEU
44	2m	48	LEU
44	2m	49	THR
44	2m	65	LYS
44	2m	70	LEU
44	2m	114	ARG
45	2n	6	LEU
45	2n	7	ILE
45	2n	18	VAL
45	2n	22	THR
45	2n	33	VAL
45	2n	56	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
46	2o	87	ILE
47	2p	2	VAL
47	2p	21	VAL
47	2p	60	LEU
47	2p	62	VAL
47	2p	67	THR
47	2p	69	THR
48	2q	19	VAL
48	2q	56	VAL
48	2q	77	VAL
48	2q	87	LYS
49	2r	76	LEU
50	2s	27	GLU
50	2s	41	VAL
50	2s	48	THR
50	2s	51	VAL
51	2t	22	ARG
51	2t	33	ILE
51	2t	70	SER
51	2t	89	ARG
51	2t	100	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (140) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	116	GLN
3	1D	126	GLN
4	1E	48	GLN
4	1E	180	ASN
5	1F	8	GLN
5	1F	69	HIS
5	1F	203	GLN
6	1G	26	GLN
6	1G	108	ASN
8	1I	11	ASN
8	1I	74	ASN
10	1O	3	GLN
10	1O	5	GLN
12	1Q	57	HIS
12	1Q	141	GLN
15	1T	58	ASN
15	1T	79	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	1T	90	GLN
16	1U	81	HIS
19	1X	31	HIS
19	1X	82	GLN
20	1Y	6	HIS
21	1Z	32	HIS
21	1Z	34	ASN
21	1Z	54	HIS
21	1Z	151	HIS
23	11	47	GLN
23	11	56	GLN
24	12	65	ASN
25	13	32	GLN
26	14	60	GLN
30	18	35	GLN
31	19	29	ASN
31	19	34	GLN
33	1b	135	GLN
34	1c	6	HIS
34	1c	31	HIS
34	1c	37	GLN
34	1c	104	GLN
34	1c	162	GLN
35	1d	77	ASN
35	1d	116	GLN
35	1d	119	GLN
35	1d	123	HIS
36	1e	20	GLN
36	1e	78	HIS
37	1f	18	GLN
37	1f	100	ASN
38	1g	28	ASN
38	1g	86	GLN
38	1g	96	GLN
38	1g	148	ASN
40	1i	3	GLN
40	1i	73	GLN
40	1i	124	GLN
41	1j	56	HIS
42	1k	38	ASN
42	1k	93	GLN
42	1k	116	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
43	1l	80	HIS
44	1m	62	ASN
44	1m	92	HIS
45	1n	52	GLN
47	1p	13	HIS
47	1p	14	ASN
47	1p	16	HIS
48	1q	26	GLN
49	1r	63	GLN
50	1s	47	HIS
50	1s	57	HIS
50	1s	69	HIS
50	1s	83	HIS
51	1t	42	GLN
51	1t	73	HIS
3	2D	87	ASN
4	2E	48	GLN
5	2F	40	GLN
5	2F	69	HIS
5	2F	203	GLN
6	2G	66	GLN
6	2G	108	ASN
6	2G	132	ASN
8	2I	74	ASN
8	2I	133	HIS
9	2N	38	HIS
9	2N	94	HIS
10	2O	5	GLN
11	2P	35	HIS
12	2Q	89	ASN
12	2Q	123	HIS
13	2R	13	HIS
13	2R	71	GLN
13	2R	91	GLN
15	2T	58	ASN
19	2X	31	HIS
21	2Z	73	GLN
22	20	40	GLN
24	22	56	GLN
24	22	65	ASN
26	24	46	GLN
28	26	20	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	28	35	GLN
33	2b	78	GLN
33	2b	135	GLN
33	2b	212	GLN
34	2c	28	GLN
34	2c	31	HIS
34	2c	98	ASN
34	2c	102	ASN
34	2c	170	GLN
34	2c	181	ASN
35	2d	77	ASN
35	2d	119	GLN
35	2d	125	HIS
35	2d	161	ASN
36	2e	78	HIS
37	2f	73	ASN
37	2f	84	ASN
37	2f	100	ASN
38	2g	28	ASN
38	2g	106	GLN
38	2g	148	ASN
40	2i	38	GLN
40	2i	58	HIS
40	2i	87	GLN
40	2i	117	HIS
40	2i	124	GLN
41	2j	56	HIS
42	2k	22	HIS
42	2k	38	ASN
43	2l	8	ASN
44	2m	12	ASN
44	2m	77	ASN
46	2o	53	HIS
46	2o	62	GLN
47	2p	13	HIS
49	2r	63	GLN
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	2863/2915 (98%)	431 (15%)	28 (0%)
1	2A	2791/2915 (95%)	466 (16%)	20 (0%)
2	1B	120/121 (99%)	9 (7%)	1 (0%)
2	2B	119/121 (98%)	12 (10%)	1 (0%)
32	1a	1497/1521 (98%)	249 (16%)	0
32	2a	1501/1521 (98%)	283 (18%)	0
53	1v	12/27 (44%)	3 (25%)	0
53	2v	12/27 (44%)	3 (25%)	0
54	1w	70/76 (92%)	19 (27%)	0
54	1y	70/76 (92%)	30 (42%)	0
54	2w	70/76 (92%)	23 (32%)	0
54	2y	70/76 (92%)	35 (50%)	0
55	1x	75/77 (97%)	10 (13%)	0
55	2x	75/77 (97%)	11 (14%)	0
All	All	9345/9626 (97%)	1584 (16%)	50 (0%)

All (1584) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	13	A
1	1A	15	G
1	1A	34	C
1	1A	36	G
1	1A	45	C
1	1A	63	U
1	1A	71	A
1	1A	74	A
1	1A	75	G
1	1A	84	A
1	1A	95	G
1	1A	118	A
1	1A	119	A
1	1A	120	U
1	1A	125	G
1	1A	139(A)	G
1	1A	182	A
1	1A	196	A
1	1A	197	A
1	1A	199	A
1	1A	205	G
1	1A	215	G
1	1A	216	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	222	A
1	1A	225	A
1	1A	228	A
1	1A	229	A
1	1A	230	U
1	1A	233	A
1	1A	248	G
1	1A	250	G
1	1A	266	G
1	1A	270	A
1	1A	271(K)	U
1	1A	271(L)	U
1	1A	271(M)	G
1	1A	271(N)	U
1	1A	271(O)	C
1	1A	272(A)	U
1	1A	272(B)	G
1	1A	279	C
1	1A	311	A
1	1A	324	A
1	1A	329	G
1	1A	330	A
1	1A	345	A
1	1A	352	G
1	1A	363	G
1	1A	363(B)	G
1	1A	386	G
1	1A	389	G
1	1A	396	G
1	1A	405	U
1	1A	411	G
1	1A	418	G
1	1A	421	U
1	1A	428	A
1	1A	443	A
1	1A	444	C
1	1A	448	U
1	1A	456	C
1	1A	457	A
1	1A	481	G
1	1A	504	U
1	1A	505	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	509	C
1	1A	528	A
1	1A	529	A
1	1A	530	G
1	1A	531	C
1	1A	532	A
1	1A	533	G
1	1A	545	G
1	1A	549	G
1	1A	563	G
1	1A	573	G
1	1A	575	A
1	1A	603	A
1	1A	604	G
1	1A	607	U
1	1A	614(B)	G
1	1A	614(C)	A
1	1A	615	G
1	1A	616	G
1	1A	619	G
1	1A	627	A
1	1A	637	A
1	1A	645	C
1	1A	646	A
1	1A	652(A)	A
1	1A	652(E)	G
1	1A	652(T)	C
1	1A	669	G
1	1A	677	A
1	1A	686	G
1	1A	730	C
1	1A	775	G
1	1A	776	G
1	1A	779	U
1	1A	782	A
1	1A	783	A
1	1A	784	A
1	1A	785	G
1	1A	792	G
1	1A	802	A
1	1A	805	G
1	1A	812	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	819	A
1	1A	827	U
1	1A	828	U
1	1A	859	G
1	1A	879	G
1	1A	880	G
1	1A	883	G
1	1A	884	C
1	1A	885	C
1	1A	886	C
1	1A	887	A
1	1A	888	C
1	1A	889	C
1	1A	890	A
1	1A	893	C
1	1A	894	C
1	1A	895	U
1	1A	896	A
1	1A	897	C
1	1A	898	C
1	1A	907	U
1	1A	910	A
1	1A	932	G
1	1A	945	A
1	1A	946	G
1	1A	953	A
1	1A	958	U
1	1A	959	A
1	1A	961	C
1	1A	963	U
1	1A	974	G
1	1A	975	C
1	1A	983	A
1	1A	996	A
1	1A	1012	U
1	1A	1013	C
1	1A	1025	G
1	1A	1026	U
1	1A	1033	U
1	1A	1039	G
1	1A	1041	C
1	1A	1044	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1046	A
1	1A	1047	G
1	1A	1054	A
1	1A	1055	G
1	1A	1058	G
1	1A	1059	G
1	1A	1064	C
1	1A	1066	U
1	1A	1068	G
1	1A	1071	G
1	1A	1073	A
1	1A	1075	C
1	1A	1078	U
1	1A	1088	A
1	1A	1089	G
1	1A	1090	U
1	1A	1091	G
1	1A	1094	U
1	1A	1096	A
1	1A	1101	U
1	1A	1107	G
1	1A	1109	C
1	1A	1110	G
1	1A	1111	A
1	1A	1112	G
1	1A	1128	A
1	1A	1130	U
1	1A	1135	C
1	1A	1136	G
1	1A	1149	G
1	1A	1170	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	1218	C
1	1A	1244	G
1	1A	1253	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1256	G
1	1A	1271	G
1	1A	1272	A
1	1A	1273	U
1	1A	1300	U
1	1A	1301	A
1	1A	1303	G
1	1A	1352	U
1	1A	1359	A
1	1A	1360	A
1	1A	1365	A
1	1A	1372	U
1	1A	1384	A
1	1A	1385	G
1	1A	1386	C
1	1A	1396	U
1	1A	1416	G
1	1A	1417	C
1	1A	1420	U
1	1A	1421	G
1	1A	1428	C
1	1A	1437	C
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	1493	C
1	1A	1494	A
1	1A	1497	U
1	1A	1508	A
1	1A	1509	C
1	1A	1509(A)	A
1	1A	1540	U
1	1A	1542	A
1	1A	1543	C
1	1A	1558	A
1	1A	1566	A
1	1A	1569	A
1	1A	1578	U
1	1A	1580	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1581	G
1	1A	1584	C
1	1A	1586	A
1	1A	1608	A
1	1A	1609	A
1	1A	1610	A
1	1A	1648	C
1	1A	1664	A
1	1A	1674	G
1	1A	1696	G
1	1A	1700	A
1	1A	1701	A
1	1A	1703	G
1	1A	1722	A
1	1A	1746	G
1	1A	1757	U
1	1A	1758	G
1	1A	1762	A
1	1A	1763	G
1	1A	1764	G
1	1A	1773	A
1	1A	1774	C
1	1A	1780	A
1	1A	1782	C
1	1A	1791	A
1	1A	1800	C
1	1A	1801	G
1	1A	1816	G
1	1A	1829	A
1	1A	1847	A
1	1A	1861	G
1	1A	1878	G
1	1A	1889	A
1	1A	1900	A
1	1A	1906	G
1	1A	1929	G
1	1A	1930	G
1	1A	1937	A
1	1A	1938	A
1	1A	1955	U
1	1A	1963	U
1	1A	1964	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1967	C
1	1A	1970	A
1	1A	1971	A
1	1A	1972	A
1	1A	1992	G
1	1A	1993	U
1	1A	1997	G
1	1A	2020	A
1	1A	2023	G
1	1A	2031	A
1	1A	2032	G
1	1A	2033	A
1	1A	2039	C
1	1A	2043	C
1	1A	2055	C
1	1A	2056	G
1	1A	2060	A
1	1A	2061	G
1	1A	2062	A
1	1A	2069	G
1	1A	2096	U
1	1A	2099	U
1	1A	2107	C
1	1A	2113	U
1	1A	2114	A
1	1A	2116	G
1	1A	2120	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	2136	C
1	1A	2138	C
1	1A	2140	C
1	1A	2141	G
1	1A	2142	C
1	1A	2144	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2146	C
1	1A	2150	U
1	1A	2151	G
1	1A	2155	G
1	1A	2156	G
1	1A	2157	G
1	1A	2158	A
1	1A	2159	G
1	1A	2160	G
1	1A	2163	C
1	1A	2164	C
1	1A	2165	G
1	1A	2166	G
1	1A	2167	U
1	1A	2171	A
1	1A	2172	U
1	1A	2173	A
1	1A	2174	C
1	1A	2178	C
1	1A	2181	G
1	1A	2184	G
1	1A	2193	G
1	1A	2198	A
1	1A	2206	G
1	1A	2207	G
1	1A	2208	A
1	1A	2218	U
1	1A	2225	A
1	1A	2238	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	2312	U
1	1A	2320	A
1	1A	2325	G
1	1A	2334	G
1	1A	2335	A
1	1A	2336	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2347	C
1	1A	2350	C
1	1A	2361	A
1	1A	2372	G
1	1A	2383	G
1	1A	2385	C
1	1A	2406	U
1	1A	2425	A
1	1A	2429	G
1	1A	2430	A
1	1A	2431	U
1	1A	2434	A
1	1A	2435	A
1	1A	2439	A
1	1A	2441	C
1	1A	2448	A
1	1A	2476	A
1	1A	2478	A
1	1A	2490	G
1	1A	2494	G
1	1A	2502	G
1	1A	2505	G
1	1A	2506	U
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	2582	G
1	1A	2602	A
1	1A	2609	U
1	1A	2611	U
1	1A	2612	C
1	1A	2629	A
1	1A	2630	G
1	1A	2654	A
1	1A	2689	U
1	1A	2701	C
1	1A	2702	U
1	1A	2703	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	2761	G
1	1A	2764	A
1	1A	2765	A
1	1A	2769	C
1	1A	2778	A
1	1A	2789	C
1	1A	2790	A
1	1A	2791	C
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	2832	U
1	1A	2833	G
1	1A	2835	A
1	1A	2872	G
1	1A	2873	A
1	1A	2880	C
1	1A	2883	A
1	1A	2892	A
1	1A	2894	G
1	2A	10	G
1	2A	11	G
1	2A	15	G
1	2A	34	C
1	2A	35	G
1	2A	45	C
1	2A	55	G
1	2A	59	U
1	2A	61	G
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	84	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	90	U
1	2A	94	C
1	2A	95	G
1	2A	100	G
1	2A	102	G
1	2A	118	A
1	2A	119	A
1	2A	120	U
1	2A	125	G
1	2A	131	G
1	2A	141	A
1	2A	154(A)	C
1	2A	157	U
1	2A	181	A
1	2A	196	A
1	2A	199	A
1	2A	205	G
1	2A	214	G
1	2A	215	G
1	2A	216	A
1	2A	222	A
1	2A	228	A
1	2A	229	A
1	2A	230	U
1	2A	233	A
1	2A	248	G
1	2A	249	C
1	2A	250	G
1	2A	266	G
1	2A	271(J)	C
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	272(I)	U
1	2A	272(J)	C
1	2A	277	C
1	2A	278	A
1	2A	311	A
1	2A	317	G
1	2A	327	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	329	G
1	2A	330	A
1	2A	332	A
1	2A	352	G
1	2A	354	G
1	2A	363(B)	G
1	2A	386	G
1	2A	396	G
1	2A	411	G
1	2A	412	A
1	2A	422	A
1	2A	443	A
1	2A	444	C
1	2A	454	A
1	2A	455	C
1	2A	457	A
1	2A	480	A
1	2A	481	G
1	2A	505	A
1	2A	508	G
1	2A	509	C
1	2A	529	A
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	556	G
1	2A	563	G
1	2A	568	U
1	2A	573	G
1	2A	575	A
1	2A	599	G
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	614(B)	G
1	2A	614(C)	A
1	2A	615	G
1	2A	616	G
1	2A	627	A
1	2A	634	C
1	2A	637	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	645	C
1	2A	646	A
1	2A	651	G
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	653	A
1	2A	668	G
1	2A	669	G
1	2A	686	G
1	2A	717	G
1	2A	730	C
1	2A	752	A
1	2A	753	C
1	2A	771	G
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	790	C
1	2A	792	G
1	2A	805	G
1	2A	812	C
1	2A	819	A
1	2A	827	U
1	2A	828	U
1	2A	832	G
1	2A	857	C
1	2A	859	G
1	2A	866	A
1	2A	869	G
1	2A	875	G
1	2A	878	A
1	2A	879	G
1	2A	881	G
1	2A	884	C
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	893	C
1	2A	894	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	895	U
1	2A	896	A
1	2A	900	A
1	2A	901	A
1	2A	910	A
1	2A	917	A
1	2A	932	G
1	2A	933	A
1	2A	938	G
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	980	A
1	2A	983	A
1	2A	996	A
1	2A	1003	G
1	2A	1012	U
1	2A	1013	C
1	2A	1017	G
1	2A	1022	G
1	2A	1023	U
1	2A	1025	G
1	2A	1033	U
1	2A	1038	C
1	2A	1043	C
1	2A	1114	G
1	2A	1117	G
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1139	G
1	2A	1142(A)	A
1	2A	1167	U
1	2A	1170	G
1	2A	1171	G
1	2A	1188	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1210	A
1	2A	1211	U
1	2A	1220	A
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1273	U
1	2A	1300	U
1	2A	1301	A
1	2A	1303	G
1	2A	1314	C
1	2A	1342	A
1	2A	1352	U
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1368	G
1	2A	1370	C
1	2A	1380	G
1	2A	1384	A
1	2A	1385	G
1	2A	1386	C
1	2A	1395	A
1	2A	1416	G
1	2A	1417	C
1	2A	1420	U
1	2A	1421	G
1	2A	1427	A
1	2A	1428	C
1	2A	1437	C
1	2A	1445	A
1	2A	1449	A
1	2A	1450	G
1	2A	1461	G
1	2A	1467	C
1	2A	1471	A
1	2A	1482	G
1	2A	1490	A
1	2A	1493	C
1	2A	1494	A
1	2A	1496	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1497	U
1	2A	1506	C
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1525	G
1	2A	1531	C
1	2A	1532	C
1	2A	1545	A
1	2A	1547	C
1	2A	1558	A
1	2A	1559	G
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1584	C
1	2A	1586	A
1	2A	1608	A
1	2A	1609	A
1	2A	1610	A
1	2A	1634	A
1	2A	1639	U
1	2A	1647	G
1	2A	1648	C
1	2A	1654	A
1	2A	1664	A
1	2A	1667	G
1	2A	1674	G
1	2A	1696	G
1	2A	1700	A
1	2A	1701	A
1	2A	1703	G
1	2A	1721	G
1	2A	1722	A
1	2A	1740	G
1	2A	1746	G
1	2A	1756	G
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A
1	2A	1780	A
1	2A	1782	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1812	A
1	2A	1816	G
1	2A	1820	U
1	2A	1847	A
1	2A	1848	A
1	2A	1858	G
1	2A	1877	A
1	2A	1878	G
1	2A	1900	A
1	2A	1906	G
1	2A	1913	A
1	2A	1914	C
1	2A	1929	G
1	2A	1930	G
1	2A	1936	A
1	2A	1938	A
1	2A	1955	U
1	2A	1963	U
1	2A	1966	A
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1984	G
1	2A	1992	G
1	2A	1993	U
1	2A	1997	G
1	2A	2023	G
1	2A	2031	A
1	2A	2032	G
1	2A	2033	A
1	2A	2036	C
1	2A	2043	C
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2069	G
1	2A	2093	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2099	U
1	2A	2106	G
1	2A	2108	C
1	2A	2109	U
1	2A	2110	G
1	2A	2111	C
1	2A	2115	G
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
1	2A	2136	C
1	2A	2137	C
1	2A	2138	C
1	2A	2140	C
1	2A	2141	G
1	2A	2143	C
1	2A	2146	C
1	2A	2150	U
1	2A	2153	G
1	2A	2154	G
1	2A	2155	G
1	2A	2156	G
1	2A	2157	G
1	2A	2158	A
1	2A	2160	G
1	2A	2162	G
1	2A	2164	C
1	2A	2165	G
1	2A	2167	U
1	2A	2168	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2169	A
1	2A	2170	A
1	2A	2172	U
1	2A	2173	A
1	2A	2174	C
1	2A	2182	G
1	2A	2189	U
1	2A	2192	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2218	U
1	2A	2225	A
1	2A	2235	G
1	2A	2238	G
1	2A	2239	G
1	2A	2248	C
1	2A	2268	A
1	2A	2273	A
1	2A	2275	C
1	2A	2279	G
1	2A	2283	C
1	2A	2287	A
1	2A	2288	A
1	2A	2294	C
1	2A	2304	G
1	2A	2305	A
1	2A	2307	G
1	2A	2308	G
1	2A	2312	U
1	2A	2319	G
1	2A	2320	A
1	2A	2325	G
1	2A	2334	G
1	2A	2336	A
1	2A	2343	C
1	2A	2346	A
1	2A	2347	C
1	2A	2350	C
1	2A	2354	G
1	2A	2376	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2379	G
1	2A	2383	G
1	2A	2385	C
1	2A	2402	C
1	2A	2403	C
1	2A	2406	U
1	2A	2425	A
1	2A	2428	G
1	2A	2429	G
1	2A	2430	A
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2448	A
1	2A	2469	A
1	2A	2474	C
1	2A	2476	A
1	2A	2490	G
1	2A	2494	G
1	2A	2497	A
1	2A	2502	G
1	2A	2505	G
1	2A	2506	U
1	2A	2518	A
1	2A	2520	C
1	2A	2525	G
1	2A	2536	G
1	2A	2554	U
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2582	G
1	2A	2585	U
1	2A	2602	A
1	2A	2611	U
1	2A	2612	C
1	2A	2630	G
1	2A	2632	A
1	2A	2634	G
1	2A	2654	A
1	2A	2669	G
1	2A	2689	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2690	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	2744	G
1	2A	2748	A
1	2A	2751	G
1	2A	2757	A
1	2A	2759	G
1	2A	2761	G
1	2A	2764	A
1	2A	2765	A
1	2A	2766	G
1	2A	2778	A
1	2A	2793	G
1	2A	2794	C
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2835	A
1	2A	2865	U
1	2A	2866	U
1	2A	2872	G
1	2A	2879	C
1	2A	2880	C
1	2A	2886	G
1	2A	2892	A
1	2A	2894	G
1	2A	2895	U
1	2A	2897	U
2	1B	2	C
2	1B	13	A
2	1B	42	C
2	1B	52	A
2	1B	56	G
2	1B	73	A
2	1B	106	G
2	1B	110	G
2	1B	120	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	7	G
32	1a	9	G
32	1a	32	A
32	1a	39	G
32	1a	47	C
32	1a	48	C
32	1a	51	A
32	1a	52	G
32	1a	61	G
32	1a	73	G
32	1a	78	G
32	1a	79	G
32	1a	98	G
32	1a	101	A
32	1a	105	G
32	1a	116	A
32	1a	121	C
32	1a	131	C
32	1a	143	A
32	1a	162	A
32	1a	163	C
32	1a	174	C
32	1a	180	U
32	1a	183	G
32	1a	189(F)	U
32	1a	189(G)	G
32	1a	189(H)	G
32	1a	189(J)	G
32	1a	195	A
32	1a	197	A
32	1a	201	C
32	1a	202	U
32	1a	203	U
32	1a	204	U
32	1a	216	G
32	1a	247	G
32	1a	251	G
32	1a	266	G
32	1a	267	C
32	1a	289	G
32	1a	301	G
32	1a	321	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	328	C
32	1a	332	G
32	1a	342	C
32	1a	345	C
32	1a	346	G
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	384	G
32	1a	392	G
32	1a	397	A
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	421	U
32	1a	422	C
32	1a	424	G
32	1a	429	U
32	1a	439	A
32	1a	442	C
32	1a	452	A
32	1a	457	C
32	1a	458	C
32	1a	461	A
32	1a	470	C
32	1a	485	G
32	1a	496	A
32	1a	498	U
32	1a	508	C
32	1a	510	A
32	1a	511	C
32	1a	518	C
32	1a	519	C
32	1a	531	U
32	1a	532	A
32	1a	536	C
32	1a	547	A
32	1a	559	A
32	1a	560	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	561	U
32	1a	562	C
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	619	U
32	1a	630	G
32	1a	631	G
32	1a	653	A
32	1a	661	G
32	1a	665	A
32	1a	680	C
32	1a	687	A
32	1a	688	G
32	1a	717	C
32	1a	723	U
32	1a	724	G
32	1a	734	G
32	1a	749	C
32	1a	755	G
32	1a	766	A
32	1a	774	G
32	1a	777	A
32	1a	792	A
32	1a	793	U
32	1a	794	A
32	1a	816	A
32	1a	817	C
32	1a	821	G
32	1a	828	A
32	1a	840	C
32	1a	841	U
32	1a	851	G
32	1a	859	A
32	1a	870	U
32	1a	873	A
32	1a	876	G
32	1a	885	G
32	1a	902	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	913	A
32	1a	914	A
32	1a	926	G
32	1a	927	G
32	1a	934	C
32	1a	939	G
32	1a	960	U
32	1a	961	U
32	1a	964	A
32	1a	966	M2G
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	992	U
32	1a	993	G
32	1a	994	A
32	1a	997	U
32	1a	1000	U
32	1a	1001(A)	G
32	1a	1003	G
32	1a	1005	A
32	1a	1006	C
32	1a	1008	C
32	1a	1009	G
32	1a	1020	U
32	1a	1022	G
32	1a	1023	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C
32	1a	1028	C
32	1a	1030	C
32	1a	1030(A)	G
32	1a	1030(C)	G
32	1a	1031	G
32	1a	1033	G
32	1a	1044	A
32	1a	1054	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	1055	A
32	1a	1056	U
32	1a	1065	U
32	1a	1066	C
32	1a	1068	G
32	1a	1070	U
32	1a	1081	G
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1108	G
32	1a	1124	G
32	1a	1125	U
32	1a	1131	G
32	1a	1132	C
32	1a	1134	G
32	1a	1137	C
32	1a	1138	G
32	1a	1139	G
32	1a	1141	C
32	1a	1146	A
32	1a	1152	A
32	1a	1157	A
32	1a	1159	U
32	1a	1160	G
32	1a	1184	G
32	1a	1196	U
32	1a	1197	G
32	1a	1202	G
32	1a	1204	A
32	1a	1212	U
32	1a	1213	A
32	1a	1214	C
32	1a	1227	A
32	1a	1229	A
32	1a	1236	A
32	1a	1238	A
32	1a	1256	A
32	1a	1257	U
32	1a	1260	C
32	1a	1273	G
32	1a	1275	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	1305	G
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	1364	U
32	1a	1370	G
32	1a	1378	C
32	1a	1396	A
32	1a	1397	C
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1442(B)	A
32	1a	1446	U
32	1a	1447	A
32	1a	1452	C
32	1a	1456	G
32	1a	1487	G
32	1a	1492	A
32	1a	1497	G
32	1a	1503	A
32	1a	1504	G
32	1a	1506	U
32	1a	1507	A
32	1a	1517	G
32	1a	1529	G
32	1a	1530	G
53	1v	13	A
53	1v	14	A
53	1v	24	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	1w	2	G
54	1w	7	U
54	1w	9	A
54	1w	19	G
54	1w	24	G
54	1w	42	G
54	1w	45	G
54	1w	46	7MG
54	1w	47	U
54	1w	49	G
54	1w	50	G
54	1w	51	C
54	1w	56	C
54	1w	58	A
54	1w	61	C
54	1w	62	C
54	1w	68	C
54	1w	70	C
54	1w	74	C
55	1x	9	G
55	1x	13	C
55	1x	18	G
55	1x	19	G
55	1x	20	U
55	1x	21	A
55	1x	22	G
55	1x	47	U
55	1x	61	C
55	1x	76	A
54	1y	2	G
54	1y	5	G
54	1y	6	A
54	1y	7	U
54	1y	9	A
54	1y	10	G
54	1y	13	C
54	1y	19	G
54	1y	23	A
54	1y	24	G
54	1y	26	A
54	1y	31	C
54	1y	35	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	1y	36	C
54	1y	40	G
54	1y	44	G
54	1y	45	G
54	1y	46	7MG
54	1y	48	C
54	1y	49	G
54	1y	54	5MU
54	1y	56	C
54	1y	57	G
54	1y	58	A
54	1y	59	U
54	1y	61	C
54	1y	64	U
54	1y	65	C
54	1y	69	A
54	1y	70	C
2	2B	2	C
2	2B	13	A
2	2B	25	A
2	2B	30	C
2	2B	33	G
2	2B	34	U
2	2B	42	C
2	2B	56	G
2	2B	58	A
2	2B	73	A
2	2B	85	G
2	2B	110	G
32	2a	7	G
32	2a	8	A
32	2a	9	G
32	2a	22	G
32	2a	32	A
32	2a	39	G
32	2a	41	G
32	2a	47	C
32	2a	48	C
32	2a	50	A
32	2a	51	A
32	2a	52	G
32	2a	66	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	73	G
32	2a	88	A
32	2a	89	C
32	2a	101	A
32	2a	116	A
32	2a	121	C
32	2a	129(A)	G
32	2a	131	C
32	2a	142	G
32	2a	144	G
32	2a	146	G
32	2a	156	G
32	2a	159	G
32	2a	163	C
32	2a	170	U
32	2a	174	C
32	2a	182	U
32	2a	189(F)	U
32	2a	189(J)	G
32	2a	195	A
32	2a	197	A
32	2a	201	C
32	2a	202	U
32	2a	203	U
32	2a	204	U
32	2a	216	G
32	2a	247	G
32	2a	251	G
32	2a	266	G
32	2a	267	C
32	2a	279	A
32	2a	289	G
32	2a	306	G
32	2a	316	G
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	342	C
32	2a	346	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	421	U
32	2a	429	U
32	2a	430	A
32	2a	439	A
32	2a	442	C
32	2a	452	A
32	2a	470	C
32	2a	484	G
32	2a	485	G
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	506	G
32	2a	509	A
32	2a	510	A
32	2a	511	C
32	2a	518	C
32	2a	521	G
32	2a	524	G
32	2a	527	7MG
32	2a	531	U
32	2a	532	A
32	2a	533	A
32	2a	547	A
32	2a	559	A
32	2a	560	U
32	2a	561	U
32	2a	564	C
32	2a	568	G
32	2a	572	A
32	2a	573	A
32	2a	574	A
32	2a	576	G
32	2a	577	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	596	C
32	2a	601	C
32	2a	619	U
32	2a	630	G
32	2a	650	G
32	2a	653	A
32	2a	665	A
32	2a	666	G
32	2a	687	A
32	2a	688	G
32	2a	695	A
32	2a	723	U
32	2a	729	A
32	2a	731	G
32	2a	733	A
32	2a	734	G
32	2a	746	A
32	2a	749	C
32	2a	755	G
32	2a	763	G
32	2a	777	A
32	2a	792	A
32	2a	793	U
32	2a	794	A
32	2a	805	C
32	2a	815	A
32	2a	816	A
32	2a	817	C
32	2a	821	G
32	2a	828	A
32	2a	840	C
32	2a	841	U
32	2a	851	G
32	2a	853	G
32	2a	859	A
32	2a	873	A
32	2a	891	U
32	2a	902	G
32	2a	914	A
32	2a	916	G
32	2a	926	G
32	2a	927	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	931	C
32	2a	933	G
32	2a	934	C
32	2a	935	A
32	2a	960	U
32	2a	961	U
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	982	U
32	2a	983	A
32	2a	984	C
32	2a	992	U
32	2a	993	G
32	2a	994	A
32	2a	997	U
32	2a	998	G
32	2a	999	C
32	2a	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	1020	U
32	2a	1022	G
32	2a	1023	G
32	2a	1024	G
32	2a	1026	G
32	2a	1027	C
32	2a	1028	C
32	2a	1030(A)	G
32	2a	1030(C)	G
32	2a	1036	G
32	2a	1037	C
32	2a	1039	C
32	2a	1040	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1045	C
32	2a	1046	A
32	2a	1053	G
32	2a	1056	U
32	2a	1064	G
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1077	G
32	2a	1081	G
32	2a	1085	U
32	2a	1086	U
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A
32	2a	1103	C
32	2a	1108	G
32	2a	1117	G
32	2a	1118	C
32	2a	1122	U
32	2a	1125	U
32	2a	1129	C
32	2a	1130	A
32	2a	1132	C
32	2a	1136	U
32	2a	1138	G
32	2a	1139	G
32	2a	1141	C
32	2a	1146	A
32	2a	1152	A
32	2a	1157	A
32	2a	1159	U
32	2a	1181	G
32	2a	1182	G
32	2a	1183	A
32	2a	1184	G
32	2a	1196	U
32	2a	1197	G
32	2a	1202	G
32	2a	1204	A
32	2a	1207	2MG
32	2a	1208	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1210	C
32	2a	1211	U
32	2a	1212	U
32	2a	1213	A
32	2a	1214	C
32	2a	1220	G
32	2a	1222	G
32	2a	1227	A
32	2a	1238	A
32	2a	1240	U
32	2a	1241	G
32	2a	1256	A
32	2a	1257	U
32	2a	1258	G
32	2a	1260	C
32	2a	1270	C
32	2a	1272	G
32	2a	1273	G
32	2a	1275	A
32	2a	1277	C
32	2a	1278	U
32	2a	1279	A
32	2a	1280	A
32	2a	1281	U
32	2a	1282	C
32	2a	1286	A
32	2a	1287	A
32	2a	1293	G
32	2a	1294	G
32	2a	1299	A
32	2a	1302	U
32	2a	1303	C
32	2a	1305	G
32	2a	1320	C
32	2a	1340	A
32	2a	1346	A
32	2a	1347	G
32	2a	1353	G
32	2a	1363	C
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	1404	5MC
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1446	U
32	2a	1447	A
32	2a	1452	C
32	2a	1456	G
32	2a	1492	A
32	2a	1493	A
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
53	2v	13	A
53	2v	14	A
53	2v	24	C
54	2w	2	G
54	2w	7	U
54	2w	9	A
54	2w	19	G
54	2w	22	G
54	2w	24	G
54	2w	40	G
54	2w	43	G
54	2w	46	7MG
54	2w	47	U
54	2w	48	C
54	2w	49	G
54	2w	50	G
54	2w	51	C
54	2w	56	C
54	2w	57	G
54	2w	58	A
54	2w	59	U
54	2w	60	C
54	2w	62	C
54	2w	68	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	2w	70	C
54	2w	74	C
55	2x	9	G
55	2x	13	C
55	2x	18	G
55	2x	19	G
55	2x	20	U
55	2x	21	A
55	2x	47	U
55	2x	48	C
55	2x	56	C
55	2x	61	C
55	2x	76	A
54	2y	2	G
54	2y	3	G
54	2y	5	G
54	2y	6	A
54	2y	7	U
54	2y	8	4SU
54	2y	9	A
54	2y	11	C
54	2y	13	C
54	2y	14	A
54	2y	15	G
54	2y	19	G
54	2y	22	G
54	2y	24	G
54	2y	26	A
54	2y	34	CM0
54	2y	35	A
54	2y	37	6MZ
54	2y	40	G
54	2y	41	A
54	2y	43	G
54	2y	47	U
54	2y	49	G
54	2y	51	C
54	2y	52	G
54	2y	53	G
54	2y	57	G
54	2y	58	A
54	2y	59	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	2y	61	C
54	2y	62	C
54	2y	66	A
54	2y	69	A
54	2y	70	C
54	2y	73	A

All (50) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	196	A
1	1A	266	G
1	1A	271(K)	U
1	1A	278	A
1	1A	746	A
1	1A	764	A
1	1A	774	A
1	1A	895	U
1	1A	974	G
1	1A	1065	U
1	1A	1067	A
1	1A	1142(A)	A
1	1A	1174	A
1	1A	1175	U
1	1A	1176	G
1	1A	1210	A
1	1A	1442	G
1	1A	1508	A
1	1A	1608	A
1	1A	1992	G
1	1A	2134	A
1	1A	2170	A
1	1A	2183	C
1	1A	2238	G
1	1A	2406	U
1	1A	2430	A
1	1A	2439	A
1	1A	2756	U
1	2A	228	A
1	2A	266	G
1	2A	271(M)	G
1	2A	277	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	479	A
1	2A	528	A
1	2A	752	A
1	2A	827	U
1	2A	856	C
1	2A	893	C
1	2A	900	A
1	2A	1210	A
1	2A	1379	A
1	2A	1420	U
1	2A	1442	G
1	2A	1608	A
1	2A	1913	A
1	2A	1992	G
1	2A	2689	U
1	2A	2756	U
2	1B	1	U
2	2B	1	U

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

80 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MC	1A	1962	56,1	19,22,23	1.75	3 (15%)	26,32,35	1.15	2 (7%)
55	5MC	1x	32	55,56	19,22,23	1.58	3 (15%)	26,32,35	1.25	3 (11%)
55	4SU	2x	8	55	18,21,22	2.04	4 (22%)	25,30,33	1.43	5 (20%)
54	CM0	2y	34	54,53	21,26,27	1.15	1 (4%)	26,37,40	2.00	4 (15%)
32	UR3	2a	1498	32	19,22,23	1.04	1 (5%)	26,32,35	1.76	3 (11%)
54	4SU	2y	8	54	18,21,22	1.80	4 (22%)	25,30,33	2.41	6 (24%)
1	PSU	1A	1911	1	18,21,22	1.41	2 (11%)	21,30,33	1.90	3 (14%)
1	OMG	1A	2251	55,56,1	23,26,27	1.28	3 (13%)	32,38,41	2.10	7 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	5MU	2y	54	54	19,22,23	1.37	6 (31%)	27,32,35	2.03	7 (25%)
55	4SU	1x	8	55	18,21,22	2.11	4 (22%)	25,30,33	1.50	4 (16%)
1	5MU	1A	1915	1	19,22,23	1.44	5 (26%)	27,32,35	2.12	7 (25%)
32	MA6	1a	1518	32	23,26,27	1.54	5 (21%)	33,38,41	2.23	14 (42%)
1	2MA	2A	2503	1	22,25,26	1.51	5 (22%)	32,37,40	2.37	8 (25%)
1	2MA	1A	2503	56,1	22,25,26	1.43	5 (22%)	32,37,40	2.33	10 (31%)
32	7MG	2a	527	32,56	23,26,27	1.38	4 (17%)	27,39,42	2.50	5 (18%)
54	PSU	2w	55	54	18,21,22	1.41	1 (5%)	21,30,33	2.03	4 (19%)
54	5MU	1y	54	54	19,22,23	1.42	5 (26%)	27,32,35	2.07	6 (22%)
32	2MG	2a	1207	32,56	23,26,27	1.24	3 (13%)	33,38,41	2.15	7 (21%)
54	6MZ	1w	37	54	22,25,26	1.52	4 (18%)	29,36,39	2.20	9 (31%)
32	5MC	1a	1400	32	19,22,23	1.52	3 (15%)	26,32,35	1.15	2 (7%)
54	PSU	2y	55	54	18,21,22	1.37	2 (11%)	21,30,33	1.97	4 (19%)
32	PSU	1a	516	32	18,21,22	1.36	3 (16%)	21,30,33	1.98	5 (23%)
43	0TD	1l	92	43	8,9,10	4.63	1 (12%)	6,11,13	4.14	3 (50%)
1	5MU	1A	1939	1	19,22,23	1.41	5 (26%)	27,32,35	2.20	6 (22%)
54	PSU	1y	55	54	18,21,22	1.36	2 (11%)	21,30,33	2.14	4 (19%)
54	CM0	1w	34	54	21,26,27	1.15	2 (9%)	26,37,40	1.68	4 (15%)
54	5MU	2w	54	54	19,22,23	1.40	4 (21%)	27,32,35	1.95	6 (22%)
54	6MZ	2w	37	54	22,25,26	1.49	4 (18%)	29,36,39	2.21	10 (34%)
54	PSU	1w	55	54	18,21,22	1.44	1 (5%)	21,30,33	2.06	5 (23%)
1	PSU	2A	1917	1	18,21,22	1.38	2 (11%)	21,30,33	2.02	4 (19%)
1	5MC	2A	1962	56,1	19,22,23	1.52	3 (15%)	26,32,35	1.16	2 (7%)
32	MA6	1a	1519	32	23,26,27	1.53	4 (17%)	33,38,41	2.30	13 (39%)
55	5MU	2x	54	55	19,22,23	1.37	5 (26%)	27,32,35	2.14	7 (25%)
32	5MC	2a	1400	32	19,22,23	1.62	3 (15%)	26,32,35	1.18	3 (11%)
54	6MZ	2y	37	32,54	22,25,26	1.57	4 (18%)	29,36,39	2.19	9 (31%)
1	PSU	2A	1911	1	18,21,22	1.39	2 (11%)	21,30,33	1.96	3 (14%)
55	5MU	1x	54	55,56	19,22,23	1.40	5 (26%)	27,32,35	1.99	6 (22%)
1	4OC	2A	1920	1	19,22,24	0.82	0	25,31,35	1.00	1 (4%)
32	5MC	2a	1407	32,56	19,22,23	1.52	3 (15%)	26,32,35	1.16	3 (11%)
32	5MC	1a	1407	32	19,22,23	1.50	3 (15%)	26,32,35	1.10	2 (7%)
54	4SU	2w	8	54	18,21,22	1.71	4 (22%)	25,30,33	2.12	5 (20%)
54	CM0	1y	34	54	21,26,27	1.29	3 (14%)	26,37,40	2.08	4 (15%)
54	7MG	1y	46	54	23,26,27	1.39	3 (13%)	27,39,42	2.76	7 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	MA6	2a	1518	32	23,26,27	1.63	5 (21%)	33,38,41	2.28	12 (36%)
54	5MU	1w	54	54	19,22,23	1.45	6 (31%)	27,32,35	2.36	6 (22%)
32	M2G	1a	966	32	24,27,28	1.31	4 (16%)	33,40,43	1.89	6 (18%)
1	5MU	2A	1915	1	19,22,23	1.47	5 (26%)	27,32,35	2.18	6 (22%)
1	PSU	1A	2605	56,1	18,21,22	1.38	3 (16%)	21,30,33	2.10	4 (19%)
54	CM0	2w	34	54	21,26,27	1.15	3 (14%)	26,37,40	1.71	4 (15%)
32	M2G	2a	966	32	24,27,28	1.32	3 (12%)	33,40,43	1.89	5 (15%)
1	PSU	2A	2605	1	18,21,22	1.38	3 (16%)	21,30,33	2.10	4 (19%)
55	PSU	2x	55	55	18,21,22	1.34	2 (11%)	21,30,33	1.99	4 (19%)
32	5MC	1a	967	32	19,22,23	1.33	3 (15%)	26,32,35	1.10	2 (7%)
32	7MG	1a	527	32,56	23,26,27	1.35	3 (13%)	27,39,42	2.56	6 (22%)
54	4SU	1w	8	54	18,21,22	1.77	5 (27%)	25,30,33	2.02	4 (16%)
32	4OC	2a	1402	32,56	20,23,24	0.74	0	25,32,35	1.03	2 (8%)
32	2MG	1a	1207	32	23,26,27	1.26	3 (13%)	33,38,41	2.20	8 (24%)
54	6MZ	1y	37	54	22,25,26	1.61	3 (13%)	29,36,39	2.29	10 (34%)
1	2MU	2A	2552	56,1	19,22,24	1.26	3 (15%)	25,31,36	2.02	6 (24%)
32	5MC	2a	967	32	19,22,23	1.71	3 (15%)	26,32,35	1.09	2 (7%)
54	7MG	1w	46	54	23,26,27	1.37	3 (13%)	27,39,42	2.58	6 (22%)
1	5MC	2A	1942	1	19,22,23	1.59	3 (15%)	26,32,35	1.12	2 (7%)
43	0TD	2l	92	43	8,9,10	4.56	1 (12%)	6,11,13	2.69	3 (50%)
55	PSU	1x	55	55	18,21,22	1.34	2 (11%)	21,30,33	2.13	4 (19%)
1	5MC	1A	1942	1	19,22,23	1.47	3 (15%)	26,32,35	1.15	2 (7%)
1	OMG	2A	2251	55,56,1	23,26,27	1.23	3 (13%)	32,38,41	1.98	7 (21%)
1	PSU	1A	1917	1	18,21,22	1.41	3 (16%)	21,30,33	2.03	4 (19%)
32	5MC	1a	1404	32	19,22,23	1.63	3 (15%)	26,32,35	1.19	3 (11%)
32	MA6	2a	1519	32	23,26,27	1.59	4 (17%)	33,38,41	2.26	12 (36%)
1	4OC	1A	1920	1	19,22,24	0.75	0	25,31,35	0.96	2 (8%)
54	7MG	2w	46	54	23,26,27	1.34	4 (17%)	27,39,42	2.67	7 (25%)
1	2MU	1A	2552	56,1	19,22,24	1.24	2 (10%)	25,31,36	2.07	6 (24%)
32	PSU	2a	516	32,56	18,21,22	1.35	2 (11%)	21,30,33	1.98	5 (23%)
54	7MG	2y	46	54	23,26,27	1.35	3 (13%)	27,39,42	2.91	7 (25%)
54	4SU	1y	8	54	18,21,22	1.81	6 (33%)	25,30,33	2.01	5 (20%)
1	5MU	2A	1939	1	19,22,23	1.45	6 (31%)	27,32,35	2.31	8 (29%)
32	4OC	1a	1402	32,56	20,23,24	0.73	0	25,32,35	1.04	1 (4%)
32	UR3	1a	1498	32	19,22,23	1.11	1 (5%)	26,32,35	1.76	4 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	5MC	2a	1404	32	19,22,23	1.69	3 (15%)	26,32,35	1.16	3 (11%)
55	5MC	2x	32	55	19,22,23	1.73	3 (15%)	26,32,35	1.29	3 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	1A	1962	56,1	-	0/7/25/26	0/2/2/2
55	5MC	1x	32	55,56	-	0/7/25/26	0/2/2/2
55	4SU	2x	8	55	-	0/7/25/26	0/2/2/2
54	CM0	2y	34	54,53	-	1/12/30/31	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
54	4SU	2y	8	54	-	1/7/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
1	OMG	1A	2251	55,56,1	-	0/9/27/28	0/3/3/3
54	5MU	2y	54	54	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
1	5MU	1A	1915	1	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	1/11/29/30	0/3/3/3
1	2MA	2A	2503	1	-	0/7/25/26	0/3/3/3
1	2MA	1A	2503	56,1	-	1/7/25/26	0/3/3/3
32	7MG	2a	527	32,56	-	3/7/37/38	0/3/3/3
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
54	5MU	1y	54	54	-	2/7/25/26	0/2/2/2
32	2MG	2a	1207	32,56	-	2/9/27/28	0/3/3/3
54	6MZ	1w	37	54	-	0/9/27/28	0/3/3/3
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
54	PSU	2y	55	54	-	2/7/25/26	0/2/2/2
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
43	0TD	1l	92	43	-	3/7/12/14	-
1	5MU	1A	1939	1	-	0/7/25/26	0/2/2/2
54	PSU	1y	55	54	-	0/7/25/26	0/2/2/2
54	CM0	1w	34	54	-	1/12/30/31	0/2/2/2
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
54	6MZ	2w	37	54	-	0/9/27/28	0/3/3/3
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	56,1	-	2/7/25/26	0/2/2/2
32	MA6	1a	1519	32	-	3/11/29/30	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	4/7/25/26	0/2/2/2
54	6MZ	2y	37	32,54	-	3/9/27/28	0/3/3/3
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
55	5MU	1x	54	55,56	-	0/7/25/26	0/2/2/2
1	4OC	2A	1920	1	-	1/9/27/30	0/2/2/2
32	5MC	2a	1407	32,56	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
54	4SU	2w	8	54	-	0/7/25/26	0/2/2/2
54	CM0	1y	34	54	-	2/12/30/31	0/2/2/2
54	7MG	1y	46	54	-	4/7/37/38	0/3/3/3
32	MA6	2a	1518	32	-	3/11/29/30	0/3/3/3
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	2605	56,1	-	0/7/25/26	0/2/2/2
54	CM0	2w	34	54	-	5/12/30/31	0/2/2/2
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
32	7MG	1a	527	32,56	-	3/7/37/38	0/3/3/3
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32,56	-	1/9/29/30	0/2/2/2
32	2MG	1a	1207	32	-	0/9/27/28	0/3/3/3
54	6MZ	1y	37	54	-	0/9/27/28	0/3/3/3
1	2MU	2A	2552	56,1	-	1/9/27/28	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
54	7MG	1w	46	54	-	2/7/37/38	0/3/3/3
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	1/7/12/14	-
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
1	5MC	1A	1942	1	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	55,56,1	-	0/9/27/28	0/3/3/3
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	4/11/29/30	0/3/3/3
1	4OC	1A	1920	1	-	1/9/27/30	0/2/2/2
54	7MG	2w	46	54	-	2/7/37/38	0/3/3/3
1	2MU	1A	2552	56,1	-	0/9/27/28	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	PSU	2a	516	32,56	-	0/7/25/26	0/2/2/2
54	7MG	2y	46	54	-	2/7/37/38	0/3/3/3
54	4SU	1y	8	54	-	1/7/25/26	0/2/2/2
1	5MU	2A	1939	1	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32,56	-	2/9/29/30	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	2/7/25/26	0/2/2/2
55	5MC	2x	32	55	-	1/7/25/26	0/2/2/2

All (251) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-12.74	1.69	1.82
43	2l	92	0TD	CB-SB	-12.59	1.69	1.82
1	1A	1962	5MC	C5-C4	6.59	1.49	1.44
55	2x	32	5MC	C5-C4	6.26	1.48	1.44
32	2a	1404	5MC	C5-C4	6.24	1.48	1.44
32	2a	967	5MC	C5-C4	6.21	1.48	1.44
32	2a	1400	5MC	C5-C4	5.89	1.48	1.44
32	1a	1404	5MC	C5-C4	5.75	1.48	1.44
1	2A	1942	5MC	C5-C4	5.59	1.48	1.44
55	1x	32	5MC	C5-C4	5.46	1.48	1.44
32	1a	1400	5MC	C5-C4	5.38	1.48	1.44
32	1a	1407	5MC	C5-C4	5.34	1.48	1.44
1	2A	1962	5MC	C5-C4	5.27	1.48	1.44
32	2a	1407	5MC	C5-C4	5.25	1.48	1.44
54	2y	37	6MZ	C5-C4	5.10	1.48	1.39
1	1A	1942	5MC	C5-C4	5.10	1.48	1.44
32	2a	1518	MA6	C5-C4	5.09	1.48	1.39
54	1y	37	6MZ	C5-C4	5.08	1.48	1.39
32	2a	1519	MA6	C5-C4	4.96	1.47	1.39
54	1w	8	4SU	C4-S4	-4.82	1.60	1.68
54	2y	8	4SU	C4-S4	-4.78	1.60	1.68
32	1a	1518	MA6	C5-C4	4.75	1.47	1.39
54	2w	37	6MZ	C5-C4	4.75	1.47	1.39
55	1x	8	4SU	C4-S4	-4.74	1.60	1.68
54	1w	55	PSU	C6-C5	4.73	1.40	1.35
32	1a	1519	MA6	C5-C4	4.69	1.47	1.39
54	1y	8	4SU	C4-S4	-4.69	1.60	1.68
54	1w	37	6MZ	C5-C4	4.67	1.47	1.39
54	2w	8	4SU	C4-S4	-4.66	1.60	1.68
55	2x	8	4SU	C4-N3	-4.65	1.32	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1x	8	4SU	C4-N3	-4.61	1.32	1.37
54	2w	55	PSU	C6-C5	4.55	1.40	1.35
1	2A	2503	2MA	C5-C4	4.54	1.47	1.39
55	2x	8	4SU	C4-S4	-4.53	1.60	1.68
32	1a	967	5MC	C5-C4	4.35	1.47	1.44
55	1x	8	4SU	C2-N3	-3.94	1.31	1.38
1	1A	2503	2MA	C5-C4	3.85	1.45	1.39
54	1y	55	PSU	C6-C5	3.77	1.39	1.35
32	2a	527	7MG	C4-N9	-3.70	1.33	1.37
55	2x	55	PSU	C6-C5	3.66	1.39	1.35
54	2y	55	PSU	C6-C5	3.63	1.39	1.35
54	1y	46	7MG	C5-C4	3.62	1.48	1.37
55	2x	8	4SU	C2-N3	-3.59	1.31	1.38
32	1a	527	7MG	C4-N9	-3.56	1.33	1.37
1	2A	1911	PSU	C6-C5	3.55	1.39	1.35
32	2a	516	PSU	C6-C5	3.52	1.39	1.35
54	2w	46	7MG	C5-C4	3.51	1.48	1.37
54	2y	46	7MG	C5-C4	3.50	1.48	1.37
1	1A	1911	PSU	C6-C5	3.50	1.39	1.35
1	2A	1917	PSU	C6-C5	3.45	1.39	1.35
1	1A	1917	PSU	C6-C5	3.39	1.39	1.35
54	1y	8	4SU	C4-N3	-3.39	1.34	1.37
32	2a	966	M2G	C5-C4	3.38	1.48	1.38
55	1x	55	PSU	C6-C5	3.36	1.39	1.35
55	1x	8	4SU	C5-C4	-3.36	1.38	1.42
54	1w	46	7MG	C5-C4	3.34	1.47	1.37
32	2a	1518	MA6	C5-C6	3.33	1.49	1.41
54	1w	46	7MG	C4-N9	-3.33	1.33	1.37
1	2A	2605	PSU	C6-C5	3.32	1.39	1.35
54	1y	37	6MZ	C5-C6	3.28	1.49	1.41
32	2a	1207	2MG	C5-C4	3.27	1.47	1.38
1	1A	2552	2MU	C4-N3	-3.27	1.33	1.38
54	1w	54	5MU	C6-C5	3.24	1.39	1.34
54	1y	34	CM0	C2-N1	3.23	1.43	1.38
32	1a	516	PSU	C6-C5	3.19	1.38	1.35
32	2a	527	7MG	C5-C4	3.17	1.47	1.37
32	1a	527	7MG	C5-C4	3.16	1.47	1.37
55	1x	32	5MC	C6-C5	3.12	1.39	1.34
32	1a	966	M2G	C5-C4	3.09	1.47	1.38
1	1A	2251	OMG	C5-C4	3.09	1.47	1.38
54	1w	8	4SU	C4-N3	-3.08	1.34	1.37
54	2y	8	4SU	C5-C4	-3.07	1.38	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2a	1519	MA6	C5-C6	3.05	1.49	1.41
54	1y	54	5MU	C6-C5	3.05	1.39	1.34
55	2x	8	4SU	C5-C4	-3.04	1.38	1.42
54	2y	34	CM0	C2-N1	3.03	1.43	1.38
1	2A	2251	OMG	C5-C4	3.02	1.47	1.38
32	1a	966	M2G	C2-N2	3.02	1.40	1.35
54	2y	37	6MZ	C5-C6	3.01	1.49	1.41
1	1A	2251	OMG	C6-N1	-2.98	1.33	1.38
54	2w	54	5MU	C6-C5	2.96	1.39	1.34
32	2a	1404	5MC	C6-C5	2.94	1.39	1.34
32	1a	1207	2MG	C5-C4	2.91	1.46	1.38
1	2A	2251	OMG	C6-N1	-2.88	1.33	1.38
1	2A	1915	5MU	C4-N3	-2.86	1.33	1.38
1	2A	1942	5MC	C6-C5	2.86	1.39	1.34
54	2w	37	6MZ	C5-C6	2.84	1.48	1.41
32	2a	966	M2G	C2-N2	2.83	1.40	1.35
32	2a	1407	5MC	C6-C5	2.83	1.39	1.34
32	1a	1518	MA6	C5-C6	2.83	1.48	1.41
32	2a	967	5MC	C6-C5	2.83	1.39	1.34
1	2A	2552	2MU	C4-N3	-2.81	1.33	1.38
54	1w	37	6MZ	C5-C6	2.81	1.48	1.41
55	2x	32	5MC	C6-C5	2.81	1.39	1.34
1	1A	2605	PSU	C4-N3	-2.80	1.33	1.38
1	2A	1915	5MU	C6-C5	2.79	1.39	1.34
1	2A	1917	PSU	C4-N3	-2.76	1.33	1.38
1	2A	1939	5MU	C4-N3	-2.76	1.33	1.38
55	1x	54	5MU	C6-C5	2.76	1.39	1.34
1	2A	1939	5MU	C6-N1	-2.72	1.33	1.38
54	2y	8	4SU	C2-N1	2.72	1.42	1.38
54	2w	34	CM0	C4-N3	-2.71	1.33	1.38
1	2A	1911	PSU	C4-N3	-2.71	1.33	1.38
54	2w	8	4SU	C4-N3	-2.71	1.34	1.37
55	2x	54	5MU	C6-C5	2.70	1.39	1.34
32	1a	1519	MA6	C5-C6	2.70	1.48	1.41
32	1a	1207	2MG	C6-N1	-2.69	1.33	1.38
1	2A	1962	5MC	C6-C5	2.68	1.39	1.34
1	2A	2605	PSU	C4-N3	-2.68	1.33	1.38
1	1A	1915	5MU	C6-C5	2.68	1.39	1.34
1	1A	1915	5MU	C4-N3	-2.67	1.33	1.38
54	1y	34	CM0	C4-N3	-2.67	1.33	1.38
54	1w	34	CM0	C4-N3	-2.67	1.33	1.38
55	1x	55	PSU	C4-N3	-2.65	1.33	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1y	8	4SU	C2-N1	2.64	1.42	1.38
32	2a	1400	5MC	C6-C5	2.63	1.38	1.34
32	1a	1498	UR3	C2-N1	2.61	1.42	1.38
1	1A	1939	5MU	C4-N3	-2.61	1.34	1.38
32	1a	967	5MC	C6-C5	2.61	1.38	1.34
32	1a	516	PSU	C4-N3	-2.61	1.34	1.38
32	1a	1404	5MC	C6-C5	2.60	1.38	1.34
32	1a	1400	5MC	C6-C5	2.60	1.38	1.34
1	1A	1911	PSU	C4-N3	-2.60	1.34	1.38
54	2w	46	7MG	C4-N9	-2.60	1.34	1.37
54	1y	46	7MG	C8-N9	2.59	1.47	1.45
55	1x	54	5MU	C4-N3	-2.59	1.34	1.38
54	1y	54	5MU	C4-C5	2.58	1.49	1.44
1	1A	2503	2MA	C5-N7	-2.57	1.34	1.39
54	1w	54	5MU	C4-C5	2.56	1.49	1.44
1	1A	1939	5MU	C6-N1	-2.56	1.33	1.38
1	2A	1915	5MU	C2-N1	2.56	1.42	1.38
1	1A	1939	5MU	C6-C5	2.56	1.38	1.34
1	1A	1917	PSU	C4-N3	-2.56	1.34	1.38
54	1y	37	6MZ	C8-N7	2.55	1.36	1.31
32	1a	1404	5MC	C6-N1	-2.55	1.33	1.38
1	1A	2605	PSU	C2-N1	-2.54	1.33	1.36
54	2y	54	5MU	C6-C5	2.53	1.38	1.34
54	2w	54	5MU	C4-N3	-2.51	1.34	1.38
55	2x	54	5MU	C4-N3	-2.51	1.34	1.38
54	2y	8	4SU	C4-N3	-2.51	1.35	1.37
54	1w	37	6MZ	C5-N7	-2.50	1.34	1.39
54	1w	8	4SU	C5-C4	-2.50	1.39	1.42
32	1a	966	M2G	C6-N1	-2.50	1.34	1.38
1	1A	1915	5MU	C4-C5	2.48	1.48	1.44
32	1a	1407	5MC	C6-C5	2.48	1.38	1.34
55	2x	54	5MU	C4-C5	2.48	1.48	1.44
54	2y	54	5MU	C4-C5	2.48	1.48	1.44
1	2A	1939	5MU	C4-C5	2.48	1.48	1.44
32	1a	1519	MA6	C5-N7	-2.47	1.34	1.39
1	1A	1962	5MC	C6-C5	2.45	1.38	1.34
54	2y	55	PSU	C4-N3	-2.45	1.34	1.38
32	2a	527	7MG	C6-N1	-2.45	1.34	1.38
55	2x	55	PSU	C4-N3	-2.45	1.34	1.38
54	1y	46	7MG	C6-N1	-2.44	1.34	1.38
32	2a	516	PSU	C4-N3	-2.44	1.34	1.38
1	1A	2503	2MA	C5-C6	2.44	1.47	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1942	5MC	C6-N1	-2.43	1.33	1.38
1	2A	1939	5MU	C2-N3	-2.43	1.33	1.38
1	2A	2503	2MA	C5-N7	-2.41	1.34	1.39
1	1A	1915	5MU	C2-N1	2.41	1.42	1.38
54	1y	54	5MU	C4-N3	-2.40	1.34	1.38
1	2A	1939	5MU	C6-C5	2.40	1.38	1.34
54	1y	55	PSU	C4-N3	-2.40	1.34	1.38
1	1A	2605	PSU	C2-N3	-2.40	1.33	1.37
32	2a	966	M2G	C6-N1	-2.39	1.34	1.38
54	2y	46	7MG	C6-N1	-2.39	1.34	1.38
1	1A	1942	5MC	C6-C5	2.39	1.38	1.34
55	1x	54	5MU	C2-N1	2.39	1.42	1.38
54	2w	8	4SU	C2-N1	2.39	1.42	1.38
1	1A	2552	2MU	C2-N3	-2.39	1.33	1.38
1	2A	1915	5MU	C4-C5	2.39	1.48	1.44
1	2A	1962	5MC	C6-N1	-2.39	1.33	1.38
32	2a	1519	MA6	C8-N7	2.38	1.36	1.31
32	2a	1207	2MG	C6-N1	-2.38	1.34	1.38
54	2w	8	4SU	C5-C4	-2.37	1.39	1.42
54	2w	37	6MZ	C8-N7	2.37	1.36	1.31
1	2A	2251	OMG	C5-N7	-2.36	1.34	1.39
54	2y	54	5MU	C4-N3	-2.34	1.34	1.38
54	1y	8	4SU	C5-C4	-2.34	1.39	1.42
1	1A	2251	OMG	C5-N7	-2.33	1.34	1.39
1	2A	2503	2MA	C5-C6	2.32	1.47	1.41
32	1a	967	5MC	C6-N1	-2.31	1.34	1.38
54	2y	37	6MZ	C8-N7	2.30	1.36	1.31
32	2a	1518	MA6	C8-N7	2.29	1.36	1.31
1	2A	1915	5MU	C6-N1	-2.29	1.34	1.38
32	1a	1518	MA6	C5-N7	-2.29	1.34	1.39
55	1x	54	5MU	C4-C5	2.29	1.48	1.44
1	1A	1962	5MC	C6-N1	-2.28	1.34	1.38
54	2y	54	5MU	C2-N1	2.27	1.42	1.38
54	1w	37	6MZ	C8-N7	2.26	1.36	1.31
32	1a	1519	MA6	C8-N7	2.26	1.36	1.31
1	1A	2503	2MA	C4-N9	-2.25	1.33	1.37
54	2y	46	7MG	C8-N9	2.24	1.47	1.45
32	1a	1400	5MC	C6-N1	-2.24	1.34	1.38
1	2A	2552	2MU	C5-C4	2.23	1.48	1.43
54	2w	54	5MU	C2-N1	2.23	1.42	1.38
32	2a	1498	UR3	C2-N1	2.23	1.41	1.38
32	1a	1407	5MC	C6-N1	-2.23	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	-2.22	1.34	1.38
54	1y	54	5MU	C2-N1	2.22	1.41	1.38
54	2w	34	CM0	C2-N1	2.22	1.41	1.38
32	2a	1400	5MC	C6-N1	-2.21	1.34	1.38
32	2a	967	5MC	C6-N1	-2.20	1.34	1.38
32	1a	1518	MA6	C8-N7	2.20	1.35	1.31
1	1A	1939	5MU	C4-C5	2.19	1.48	1.44
32	1a	516	PSU	C2-N3	-2.19	1.33	1.37
1	1A	1939	5MU	C2-N3	-2.19	1.34	1.38
32	2a	1519	MA6	C5-N7	-2.18	1.35	1.39
55	1x	32	5MC	C6-N1	-2.18	1.34	1.38
54	1w	34	CM0	C2-N3	-2.18	1.34	1.38
1	2A	1942	5MC	C6-N1	-2.18	1.34	1.38
1	2A	2605	PSU	C2-N3	-2.17	1.33	1.37
32	1a	1207	2MG	C5-N7	-2.16	1.34	1.39
1	1A	2503	2MA	C8-N7	2.16	1.35	1.31
54	2y	37	6MZ	C5-N7	-2.14	1.35	1.39
54	1w	54	5MU	C4-N3	-2.14	1.34	1.38
54	2w	54	5MU	C4-C5	2.14	1.48	1.44
54	2w	46	7MG	C8-N9	2.13	1.47	1.45
1	1A	1915	5MU	C6-N1	-2.13	1.34	1.38
55	2x	54	5MU	C2-N1	2.12	1.41	1.38
54	2y	54	5MU	C2-N3	-2.12	1.34	1.38
54	2y	54	5MU	C6-N1	-2.12	1.34	1.38
1	2A	2503	2MA	C4-N9	-2.12	1.33	1.37
54	1w	54	5MU	C6-N1	-2.12	1.34	1.38
54	1w	46	7MG	C6-N1	-2.12	1.34	1.38
32	1a	1518	MA6	C4-N9	-2.11	1.33	1.37
1	2A	2552	2MU	C2-N3	-2.11	1.34	1.38
54	2w	37	6MZ	C5-N7	-2.10	1.35	1.39
54	1w	54	5MU	C2-N1	2.10	1.41	1.38
32	2a	527	7MG	C5-C6	2.09	1.48	1.43
32	1a	966	M2G	C5-N7	-2.09	1.34	1.39
54	1y	54	5MU	C6-N1	-2.08	1.34	1.38
1	2A	2503	2MA	C8-N7	2.08	1.35	1.31
55	2x	54	5MU	C6-N1	-2.08	1.34	1.38
54	2w	46	7MG	C6-N1	-2.08	1.35	1.38
55	1x	54	5MU	C6-N1	-2.08	1.34	1.38
32	2a	1404	5MC	C6-N1	-2.07	1.34	1.38
54	1w	8	4SU	C2-N1	2.06	1.41	1.38
55	2x	32	5MC	C6-N1	-2.06	1.34	1.38
32	2a	1518	MA6	C4-N9	-2.06	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2a	1207	2MG	C5-N7	-2.06	1.34	1.39
54	1w	54	5MU	C2-N3	-2.06	1.34	1.38
32	2a	1407	5MC	C6-N1	-2.05	1.34	1.38
54	1y	8	4SU	C6-C5	2.04	1.39	1.35
32	1a	527	7MG	C6-N1	-2.04	1.35	1.38
54	1y	8	4SU	C2-N3	-2.04	1.34	1.38
54	1y	34	CM0	C2-N3	-2.01	1.34	1.38
1	2A	1939	5MU	C2-N1	2.01	1.41	1.38
32	2a	1518	MA6	C5-N7	-2.01	1.35	1.39
54	2w	34	CM0	C2-N3	-2.00	1.34	1.38
1	1A	1917	PSU	C2-N3	-2.00	1.34	1.37

All (417) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2y	46	7MG	N9-C4-N3	10.47	140.81	125.46
54	1y	46	7MG	N9-C4-N3	9.85	139.90	125.46
43	1l	92	0TD	CSB-SB-CB	9.19	118.88	102.36
54	2w	46	7MG	N9-C4-N3	9.17	138.89	125.46
54	1w	46	7MG	N9-C4-N3	8.71	138.23	125.46
32	1a	527	7MG	N9-C4-N3	8.27	137.57	125.46
32	2a	527	7MG	N9-C4-N3	8.17	137.43	125.46
1	2A	2503	2MA	C5-C4-N3	-8.05	118.70	127.18
1	1A	2503	2MA	C5-C4-N3	-7.93	118.82	127.18
1	2A	2503	2MA	N3-C4-N9	7.04	135.92	126.99
32	2a	1498	UR3	C4-N3-C2	-6.90	119.03	124.58
32	1a	1207	2MG	C2-N3-C4	6.84	120.56	112.00
1	1A	2251	OMG	C5-C4-N3	-6.68	117.75	128.39
32	2a	1207	2MG	C2-N3-C4	6.65	120.32	112.00
54	1y	55	PSU	N1-C2-N3	6.63	122.16	115.17
32	1a	1498	UR3	C4-N3-C2	-6.63	119.25	124.58
55	1x	55	PSU	N1-C2-N3	6.51	122.04	115.17
32	2a	966	M2G	C5-C4-N3	-6.49	118.06	128.39
1	1A	2605	PSU	N1-C2-N3	6.37	121.88	115.17
1	2A	1917	PSU	N1-C2-N3	6.37	121.88	115.17
1	1A	1917	PSU	N1-C2-N3	6.32	121.84	115.17
54	2y	46	7MG	C5-C4-N3	-6.32	116.26	128.13
54	2w	8	4SU	C4-N3-C2	-6.32	121.26	127.31
54	2y	34	CM0	C4-N3-C2	-6.29	119.10	127.34
1	2A	2605	PSU	N1-C2-N3	6.28	121.80	115.17
1	2A	2251	OMG	C5-C4-N3	-6.27	118.41	128.39
54	2y	55	PSU	N1-C2-N3	6.27	121.78	115.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1911	PSU	N1-C2-N3	6.15	121.65	115.17
32	1a	966	M2G	C5-C4-N3	-6.09	118.70	128.39
54	1w	37	6MZ	C5-C4-N3	-6.07	118.35	126.72
32	2a	516	PSU	N1-C2-N3	6.06	121.56	115.17
1	1A	2503	2MA	N3-C4-N9	6.04	134.65	126.99
55	2x	55	PSU	N1-C2-N3	6.03	121.53	115.17
32	1a	516	PSU	N1-C2-N3	6.02	121.52	115.17
54	2y	37	6MZ	C5-C4-N3	-6.01	118.44	126.72
54	2w	37	6MZ	C5-C4-N3	-5.92	118.57	126.72
54	2w	55	PSU	N1-C2-N3	5.89	121.39	115.17
54	1y	34	CM0	C7-O5-C5	5.88	124.97	117.48
1	1A	1911	PSU	N1-C2-N3	5.85	121.33	115.17
54	1y	37	6MZ	C5-C4-N3	-5.84	118.68	126.72
54	1w	55	PSU	N1-C2-N3	5.82	121.31	115.17
1	2A	1939	5MU	C4-N3-C2	-5.82	119.71	127.34
54	1w	8	4SU	C4-N3-C2	-5.81	121.75	127.31
54	1w	8	4SU	C5-C4-N3	5.75	120.10	114.75
54	1w	54	5MU	C4-N3-C2	-5.74	119.82	127.34
32	1a	1207	2MG	C5-C4-N3	-5.72	119.29	128.39
54	1w	46	7MG	N9-C8-N7	-5.70	95.31	103.37
1	1A	2552	2MU	N3-C2-N1	5.67	122.27	114.89
32	2a	527	7MG	N9-C8-N7	-5.60	95.44	103.37
32	2a	1207	2MG	C5-C4-N3	-5.59	119.49	128.39
32	1a	1519	MA6	C5-C4-N3	-5.57	119.05	126.72
54	1y	34	CM0	N3-C2-N1	5.56	122.13	114.89
32	2a	1519	MA6	C5-C4-N3	-5.52	119.12	126.72
32	2a	1518	MA6	C5-C4-N3	-5.51	119.13	126.72
1	1A	2251	OMG	C2-N3-C4	5.50	121.78	112.30
54	2w	8	4SU	C5-C4-N3	5.45	119.82	114.75
54	2w	46	7MG	C5-C4-N3	-5.42	117.95	128.13
54	2y	8	4SU	C5-C4-N3	5.41	119.78	114.75
54	1y	8	4SU	C4-N3-C2	-5.40	122.14	127.31
1	2A	1915	5MU	C4-N3-C2	-5.40	120.26	127.34
54	2y	34	CM0	N3-C2-N1	5.39	121.90	114.89
1	1A	1939	5MU	C4-N3-C2	-5.37	120.30	127.34
32	1a	527	7MG	N9-C8-N7	-5.37	95.77	103.37
54	1y	46	7MG	C5-C4-N3	-5.37	118.06	128.13
54	1w	54	5MU	N3-C2-N1	5.35	121.86	114.89
55	2x	54	5MU	N3-C2-N1	5.31	121.80	114.89
1	2A	1939	5MU	N3-C2-N1	5.28	121.77	114.89
54	1w	34	CM0	N3-C2-N1	5.26	121.74	114.89
54	1y	54	5MU	N3-C2-N1	5.26	121.74	114.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1518	MA6	C5-C4-N3	-5.23	119.51	126.72
55	2x	54	5MU	C4-N3-C2	-5.20	120.52	127.34
54	2y	8	4SU	C4-N3-C2	-5.20	122.33	127.31
1	1A	1915	5MU	C4-N3-C2	-5.19	120.54	127.34
1	2A	2552	2MU	N3-C2-N1	5.16	121.61	114.89
54	2y	8	4SU	C5-C4-S4	-5.16	118.42	124.31
54	2w	34	CM0	C4-N3-C2	-5.14	120.61	127.34
54	2w	46	7MG	N9-C8-N7	-5.13	96.11	103.37
32	1a	527	7MG	C5-C4-N3	-5.11	118.53	128.13
1	1A	1915	5MU	N3-C2-N1	5.11	121.54	114.89
54	2y	46	7MG	C2-N3-C4	5.07	121.04	112.30
43	2l	92	0TD	CSB-SB-CB	-5.07	93.25	102.36
54	2w	34	CM0	N3-C2-N1	5.07	121.49	114.89
54	1y	54	5MU	C4-N3-C2	-5.05	120.72	127.34
54	1w	46	7MG	C5-C4-N3	-5.03	118.69	128.13
54	2y	8	4SU	C1'-N1-C2	5.02	126.61	117.59
1	2A	1915	5MU	N3-C2-N1	5.01	121.42	114.89
32	2a	527	7MG	C5-C4-N3	-4.99	118.77	128.13
1	2A	2552	2MU	C4-N3-C2	-4.99	120.42	126.61
55	1x	54	5MU	N3-C2-N1	4.95	121.34	114.89
54	1y	8	4SU	C5-C4-N3	4.93	119.33	114.75
1	2A	2251	OMG	C2-N3-C4	4.90	120.74	112.30
54	1w	34	CM0	C4-N3-C2	-4.89	120.93	127.34
54	1y	46	7MG	N9-C8-N7	-4.88	96.47	103.37
54	1y	34	CM0	C4-N3-C2	-4.86	120.96	127.34
1	2A	1915	5MU	C5-C4-N3	4.84	119.53	115.32
32	2a	966	M2G	N9-C4-N3	4.82	135.58	125.95
1	2A	1939	5MU	C5-C4-N3	4.81	119.51	115.32
1	2A	2251	OMG	N9-C4-N3	4.81	135.58	125.95
1	1A	2251	OMG	N9-C4-N3	4.81	135.57	125.95
1	1A	1939	5MU	C5-C4-N3	4.80	119.49	115.32
1	1A	1939	5MU	O4-C4-C5	-4.78	119.45	124.92
54	2y	54	5MU	C4-N3-C2	-4.77	121.09	127.34
54	2y	37	6MZ	N3-C4-N9	4.75	135.24	127.17
54	1w	54	5MU	C5-C4-N3	4.72	119.42	115.32
54	1w	54	5MU	O4-C4-C5	-4.70	119.54	124.92
32	1a	1519	MA6	C9-N6-C6	-4.67	108.63	120.52
54	2w	37	6MZ	N3-C4-N9	4.67	135.11	127.17
32	1a	966	M2G	C2-N3-C4	4.65	121.11	112.51
1	1A	1915	5MU	C5-C4-N3	4.65	119.36	115.32
1	1A	1939	5MU	N3-C2-N1	4.64	120.94	114.89
54	2y	54	5MU	N3-C2-N1	4.63	120.92	114.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	1x	54	5MU	C4-N3-C2	-4.63	121.27	127.34
32	2a	966	M2G	C2-N3-C4	4.60	121.02	112.51
54	2w	54	5MU	N3-C2-N1	4.59	120.87	114.89
54	2y	46	7MG	N9-C8-N7	-4.59	96.87	103.37
54	1w	37	6MZ	N3-C4-N9	4.59	134.97	127.17
32	2a	1518	MA6	C9-N6-C6	-4.56	108.91	120.52
32	1a	966	M2G	N9-C4-N3	4.53	135.01	125.95
54	2w	54	5MU	C4-N3-C2	-4.53	121.41	127.34
54	1y	46	7MG	C2-N3-C4	4.51	120.07	112.30
32	1a	527	7MG	C2-N3-C4	4.51	120.06	112.30
32	2a	1518	MA6	C4-C5-N7	-4.48	105.46	110.58
54	1w	54	5MU	C5-C6-N1	-4.47	118.45	123.31
1	1A	2552	2MU	C4-N3-C2	-4.47	121.06	126.61
54	1y	37	6MZ	N3-C4-N9	4.47	134.76	127.17
55	1x	55	PSU	C4-N3-C2	-4.44	120.26	126.37
32	1a	1518	MA6	C2-N1-C6	4.43	122.65	111.83
1	2A	1939	5MU	C5-C6-N1	-4.41	118.52	123.31
1	2A	2605	PSU	C4-N3-C2	-4.41	120.30	126.37
1	1A	2605	PSU	C4-N3-C2	-4.40	120.31	126.37
32	1a	1519	MA6	N3-C4-N9	4.39	134.63	127.17
54	2w	46	7MG	C2-N3-C4	4.37	119.83	112.30
32	2a	1518	MA6	C2-N1-C6	4.36	122.47	111.83
32	2a	1519	MA6	C2-N1-C6	4.32	122.37	111.83
54	1y	54	5MU	C5-C4-N3	4.27	119.04	115.32
1	1A	1939	5MU	C5-C6-N1	-4.26	118.69	123.31
55	2x	54	5MU	C5-C4-N3	4.25	119.02	115.32
54	1y	55	PSU	O2-C2-N1	-4.23	118.42	122.79
55	2x	55	PSU	C4-N3-C2	-4.23	120.55	126.37
54	2y	54	5MU	C5-C4-N3	4.23	119.00	115.32
32	2a	1519	MA6	C9-N6-C6	-4.20	109.82	120.52
32	2a	527	7MG	C2-N3-C4	4.20	119.54	112.30
54	1y	37	6MZ	C6-C5-N7	4.20	137.00	132.43
54	1w	46	7MG	C2-N3-C4	4.16	119.46	112.30
32	2a	1519	MA6	N3-C4-N9	4.15	134.22	127.17
54	2y	34	CM0	C7-O5-C5	4.13	122.74	117.48
32	1a	516	PSU	C4-N3-C2	-4.13	120.69	126.37
32	2a	516	PSU	C4-N3-C2	-4.11	120.71	126.37
1	1A	1917	PSU	C4-N3-C2	-4.09	120.73	126.37
54	2w	55	PSU	O2-C2-N1	-4.09	118.57	122.79
32	2a	1519	MA6	C4-C5-N7	-4.09	105.90	110.58
32	1a	1519	MA6	C2-N1-C6	4.07	121.77	111.83
1	1A	2552	2MU	O2-C2-N1	-4.03	117.56	122.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1y	55	PSU	C4-N3-C2	-3.99	120.88	126.37
1	2A	1915	5MU	C5-C6-N1	-3.99	118.98	123.31
54	1y	37	6MZ	C4-C5-N7	-3.99	106.02	110.58
54	2w	54	5MU	O4-C4-C5	-3.99	120.36	124.92
1	2A	1939	5MU	O4-C4-C5	-3.96	120.39	124.92
54	1y	54	5MU	O4-C4-C5	-3.96	120.39	124.92
1	1A	1915	5MU	O4-C4-C5	-3.96	120.39	124.92
1	2A	2503	2MA	N6-C6-N1	3.95	122.35	117.03
55	1x	8	4SU	C6-C5-C4	-3.95	116.53	119.95
32	1a	1518	MA6	C4-C5-N7	-3.94	106.08	110.58
55	1x	8	4SU	C5-C4-N3	3.93	118.41	114.75
32	1a	1518	MA6	N3-C4-N9	3.92	133.84	127.17
55	2x	54	5MU	O4-C4-C5	-3.91	120.44	124.92
1	2A	1917	PSU	C4-N3-C2	-3.91	120.99	126.37
54	2y	54	5MU	O4-C4-C5	-3.89	120.47	124.92
1	2A	1911	PSU	C4-N3-C2	-3.89	121.01	126.37
54	1w	55	PSU	C4-N3-C2	-3.88	121.02	126.37
32	2a	1518	MA6	N3-C4-N9	3.88	133.76	127.17
1	1A	2552	2MU	C2'-C1'-N1	-3.88	106.88	114.24
55	1x	32	5MC	C5-C6-N1	-3.87	119.11	123.31
54	1y	8	4SU	N3-C2-N1	3.84	119.89	114.89
54	1w	55	PSU	O2-C2-N1	-3.83	118.84	122.79
54	2y	55	PSU	C4-N3-C2	-3.82	121.10	126.37
1	1A	1962	5MC	C5-C6-N1	-3.81	119.17	123.31
54	2w	8	4SU	C5-C4-S4	-3.81	119.96	124.31
54	1y	37	6MZ	C2-N3-C4	3.79	121.10	111.83
54	2w	54	5MU	C5-C4-N3	3.79	118.62	115.32
32	1a	1207	2MG	N9-C4-N3	3.78	133.50	125.95
54	2y	37	6MZ	C4-C5-N7	-3.77	106.28	110.58
55	1x	54	5MU	C5-C4-N3	3.76	118.59	115.32
54	2w	8	4SU	N3-C2-N1	3.76	119.79	114.89
55	1x	54	5MU	O4-C4-C5	-3.76	120.62	124.92
54	1w	37	6MZ	C9-N6-C6	-3.75	119.37	122.85
1	2A	1915	5MU	O4-C4-C5	-3.75	120.63	124.92
32	1a	1207	2MG	C6-C5-N7	3.75	137.11	130.29
54	2w	37	6MZ	C9-N6-C6	-3.74	119.38	122.85
32	2a	1207	2MG	N9-C4-N3	3.73	133.41	125.95
54	1w	37	6MZ	C2-N3-C4	3.72	120.91	111.83
54	2w	55	PSU	C4-N3-C2	-3.72	121.25	126.37
1	1A	2605	PSU	O2-C2-N1	-3.71	118.96	122.79
55	2x	32	5MC	C5-C6-N1	-3.68	119.32	123.31
1	1A	1911	PSU	C4-N3-C2	-3.67	121.31	126.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2503	2MA	C4-C5-N7	-3.65	106.40	110.58
1	2A	1917	PSU	O2-C2-N1	-3.65	119.03	122.79
54	1w	37	6MZ	C4-C5-N7	-3.64	106.42	110.58
32	2a	1207	2MG	C6-C5-N7	3.64	136.91	130.29
32	1a	1519	MA6	C2-N3-C4	3.62	120.68	111.83
55	1x	55	PSU	O2-C2-N1	-3.62	119.05	122.79
1	2A	2552	2MU	O2-C2-N1	-3.62	118.08	122.80
32	2a	1519	MA6	C2-N3-C4	3.61	120.64	111.83
32	2a	1518	MA6	C2-N3-C4	3.60	120.62	111.83
54	2w	37	6MZ	C2-N3-C4	3.59	120.61	111.83
32	1a	1400	5MC	C5-C6-N1	-3.59	119.42	123.31
32	1a	1518	MA6	C9-N6-C6	-3.59	111.40	120.52
54	2w	37	6MZ	C4-C5-N7	-3.57	106.50	110.58
32	1a	1519	MA6	C4-C5-N7	-3.54	106.54	110.58
54	2y	55	PSU	O2-C2-N1	-3.54	119.14	122.79
54	1w	54	5MU	O2-C2-N1	-3.53	118.21	122.80
1	1A	1917	PSU	O2-C2-N1	-3.49	119.19	122.79
54	2y	37	6MZ	C2-N3-C4	3.49	120.34	111.83
32	2a	1407	5MC	C5-C6-N1	-3.44	119.58	123.31
54	1w	8	4SU	C5-C4-S4	-3.43	120.39	124.31
54	1y	8	4SU	C1'-N1-C2	3.43	123.75	117.59
32	1a	1498	UR3	C5-C4-N3	3.43	119.55	115.04
1	2A	1911	PSU	O2-C2-N1	-3.42	119.26	122.79
32	2a	1498	UR3	C5-C4-N3	3.41	119.54	115.04
1	1A	1911	PSU	O2-C2-N1	-3.38	119.30	122.79
32	1a	1518	MA6	C2-N3-C4	3.37	120.06	111.83
54	2w	37	6MZ	C6-C5-N7	3.36	136.09	132.43
54	2w	54	5MU	C5-C6-N1	-3.35	119.67	123.31
54	1y	46	7MG	C5-C4-N9	-3.35	102.04	106.33
1	2A	2503	2MA	C4-N9-C8	3.35	109.25	105.74
55	2x	8	4SU	C5-C4-N3	3.35	117.86	114.75
32	2a	1400	5MC	C5-C6-N1	-3.33	119.69	123.31
54	1w	8	4SU	N3-C2-N1	3.33	119.22	114.89
32	2a	1207	2MG	N1-C2-N2	3.31	119.94	116.56
32	1a	966	M2G	C6-C5-N7	3.31	136.32	130.29
32	2a	967	5MC	C5-C6-N1	-3.31	119.72	123.31
54	1y	37	6MZ	N1-C2-N3	-3.30	123.59	128.58
54	1y	37	6MZ	C9-N6-C6	-3.27	119.82	122.85
32	1a	1519	MA6	N1-C2-N3	-3.27	123.63	128.58
32	2a	1519	MA6	N1-C2-N3	-3.25	123.66	128.58
43	1l	92	0TD	OD2-CG-CB	3.25	120.17	113.15
55	2x	54	5MU	C5-C6-N1	-3.24	119.79	123.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	2x	32	5MC	O2-C2-N3	-3.24	117.22	122.33
1	1A	1942	5MC	C5-C6-N1	-3.24	119.80	123.31
1	1A	2251	OMG	C6-C5-N7	3.23	136.16	130.29
1	2A	2605	PSU	O2-C2-N1	-3.22	119.47	122.79
43	2l	92	0TD	OD2-CG-CB	3.20	120.07	113.15
32	1a	1518	MA6	N1-C2-N3	-3.18	123.77	128.58
1	1A	1915	5MU	C5-C6-N1	-3.16	119.88	123.31
1	2A	2552	2MU	C5-C4-N3	3.16	119.22	114.80
54	1w	37	6MZ	C6-C5-N7	3.16	135.87	132.43
54	2y	8	4SU	C1'-N1-C6	-3.15	114.04	120.78
55	2x	54	5MU	O2-C2-N1	-3.13	118.72	122.80
32	2a	1518	MA6	N1-C2-N3	-3.13	123.85	128.58
54	2y	37	6MZ	C9-N6-C6	-3.13	119.95	122.85
54	2y	37	6MZ	C6-C5-N7	3.12	135.82	132.43
55	2x	8	4SU	C6-C5-C4	-3.11	117.25	119.95
32	2a	1404	5MC	C5-C6-N1	-3.11	119.93	123.31
54	2w	54	5MU	O2-C2-N1	-3.11	118.75	122.80
54	1w	37	6MZ	N1-C2-N3	-3.10	123.89	128.58
1	2A	1942	5MC	C5-C6-N1	-3.09	119.95	123.31
32	1a	1207	2MG	N1-C2-N2	3.08	119.71	116.56
54	2y	54	5MU	C5-C6-N1	-3.08	119.97	123.31
32	1a	1207	2MG	C4-C5-N7	-3.05	105.84	110.67
1	2A	1962	5MC	C5-C4-N3	-3.04	118.64	121.75
32	1a	967	5MC	C5-C6-N1	-3.01	120.04	123.31
1	2A	2552	2MU	C2'-C1'-N1	-3.01	108.53	114.24
54	1y	54	5MU	C5-C6-N1	-3.00	120.06	123.31
1	1A	2503	2MA	C4-N9-C8	3.00	108.89	105.74
32	1a	1404	5MC	C5-C6-N1	-2.99	120.06	123.31
55	1x	54	5MU	C5-C6-N1	-2.99	120.06	123.31
55	1x	32	5MC	C5-C4-N3	-2.99	118.69	121.75
32	2a	516	PSU	O2-C2-N1	-2.99	119.71	122.79
32	1a	1518	MA6	C10-N6-C6	-2.96	112.99	120.52
1	1A	1939	5MU	O2-C2-N1	-2.95	118.96	122.80
1	2A	1962	5MC	C5-C6-N1	-2.91	120.16	123.31
55	1x	8	4SU	O2-C2-N1	2.91	126.58	122.80
32	2a	1407	5MC	C5-C4-N3	-2.89	118.80	121.75
55	2x	55	PSU	O2-C2-N1	-2.88	119.82	122.79
32	1a	1407	5MC	C5-C4-N3	-2.88	118.80	121.75
32	2a	966	M2G	C6-C5-N7	2.88	135.52	130.29
32	2a	1207	2MG	N2-C2-N3	-2.87	116.85	120.51
54	2w	37	6MZ	N1-C2-N3	-2.86	124.25	128.58
1	2A	2251	OMG	C6-C5-N7	2.86	135.49	130.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1518	MA6	C5-N7-C8	2.86	107.94	103.45
54	1y	37	6MZ	C5-N7-C8	2.86	107.94	103.45
54	1w	34	CM0	C7-O5-C5	2.86	121.12	117.48
54	2y	46	7MG	C5-C6-N1	2.85	115.96	110.94
32	2a	1207	2MG	C4-C5-N7	-2.83	106.19	110.67
1	2A	1939	5MU	O2-C2-N1	-2.82	119.12	122.80
1	1A	2503	2MA	C2-N1-C6	2.82	122.44	118.10
32	2a	1519	MA6	C5-N7-C8	2.81	107.87	103.45
54	2w	34	CM0	C7-O5-C5	2.81	121.06	117.48
54	2y	8	4SU	N3-C2-N1	2.79	118.53	114.89
54	2y	37	6MZ	C5-N7-C8	2.79	107.84	103.45
1	2A	2503	2MA	C4-C5-N7	-2.79	107.39	110.58
1	1A	2503	2MA	N6-C6-N1	2.79	120.79	117.03
32	1a	516	PSU	O2-C2-N1	-2.79	119.91	122.79
1	2A	2552	2MU	O4-C4-C5	-2.79	120.36	125.16
1	1A	2503	2MA	C5-N7-C8	2.78	107.81	103.45
32	1a	1404	5MC	C5-C4-N3	-2.78	118.91	121.75
32	1a	527	7MG	C5-C6-N1	2.77	115.82	110.94
54	2y	34	CM0	O2-C2-N1	-2.77	119.19	122.80
54	2w	37	6MZ	C4-N9-C8	2.74	108.61	105.74
32	2a	967	5MC	C5-C4-N3	-2.74	118.95	121.75
1	1A	1942	5MC	C5-C4-N3	-2.74	118.95	121.75
32	1a	1402	4OC	C6-C5-C4	2.73	120.29	117.00
32	1a	1518	MA6	C5-N7-C8	2.72	107.73	103.45
32	1a	967	5MC	C5-C4-N3	-2.72	118.97	121.75
32	2a	1404	5MC	C5-C4-N3	-2.70	118.99	121.75
54	2w	34	CM0	O2-C2-N1	-2.69	119.30	122.80
32	1a	1518	MA6	N1-C6-N6	2.67	120.11	116.86
54	1y	37	6MZ	C4-N9-C8	2.67	108.54	105.74
32	1a	1519	MA6	C10-N6-C6	-2.66	113.75	120.52
54	2y	46	7MG	C5-C4-N9	-2.66	102.93	106.33
1	2A	1942	5MC	C5-C4-N3	-2.65	119.04	121.75
32	2a	527	7MG	C5-C6-N1	2.65	115.60	110.94
1	1A	2251	OMG	C4-C5-N7	-2.65	106.48	110.67
32	2a	1518	MA6	C10-N6-C9	-2.64	107.69	116.18
55	2x	8	4SU	C1'-N1-C2	2.64	122.33	117.59
54	1y	54	5MU	O2-C2-N1	-2.64	119.36	122.80
32	2a	1519	MA6	C4-N9-C8	2.64	108.50	105.74
32	1a	1407	5MC	C5-C6-N1	-2.62	120.47	123.31
32	1a	1519	MA6	C4-N9-C8	2.62	108.49	105.74
54	2y	37	6MZ	N1-C2-N3	-2.62	124.62	128.58
54	2w	37	6MZ	C5-N7-C8	2.61	107.56	103.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	2x	32	5MC	C5-C4-N3	-2.61	119.08	121.75
32	1a	1519	MA6	C5-N7-C8	2.61	107.55	103.45
32	1a	1518	MA6	C4-N9-C8	2.60	108.46	105.74
32	1a	1498	UR3	C1'-N1-C2	2.60	121.29	117.04
54	2w	46	7MG	C5-C6-N1	2.59	115.51	110.94
32	1a	1519	MA6	N1-C6-N6	2.59	120.01	116.86
1	1A	1915	5MU	O2-C2-N1	-2.59	119.43	122.80
32	1a	966	M2G	C4-C5-N7	-2.58	106.58	110.67
54	1w	55	PSU	C6-C5-C4	-2.55	116.45	118.17
54	1w	37	6MZ	C5-N7-C8	2.54	107.45	103.45
54	1w	46	7MG	C5-C4-N9	-2.54	103.08	106.33
54	1y	8	4SU	C5-C4-S4	-2.54	121.41	124.31
55	2x	8	4SU	O2-C2-N1	2.53	126.09	122.80
1	1A	2552	2MU	C5-C4-N3	2.53	118.34	114.80
1	1A	2503	2MA	N9-C8-N7	-2.51	110.37	113.94
54	2y	54	5MU	C5M-C5-C4	2.50	121.45	118.78
54	1w	34	CM0	O2-C2-N1	-2.49	119.55	122.80
1	2A	2605	PSU	C5-C6-N1	-2.48	118.69	122.14
54	2w	46	7MG	C5-C4-N9	-2.48	103.16	106.33
32	1a	1207	2MG	N2-C2-N3	-2.47	117.36	120.51
54	2y	37	6MZ	C4-N9-C8	2.47	108.33	105.74
32	2a	966	M2G	C4-C5-N7	-2.47	106.76	110.67
32	2a	1518	MA6	C6-C5-N7	2.46	137.36	133.43
54	2y	46	7MG	O6-C6-C5	-2.44	121.64	127.62
1	1A	2552	2MU	O4-C4-C5	-2.43	120.97	125.16
1	2A	2503	2MA	C2-N1-C6	2.41	121.81	118.10
32	1a	1400	5MC	C5-C4-N3	-2.40	119.30	121.75
55	2x	55	PSU	C5-C6-N1	-2.39	118.82	122.14
1	2A	2251	OMG	O6-C6-C5	-2.39	120.22	126.53
54	1y	34	CM0	O2-C2-N3	-2.38	117.09	121.49
43	2l	92	0TD	OD1-CG-CB	-2.38	117.45	122.44
55	1x	55	PSU	C5-C6-N1	-2.38	118.84	122.14
32	2a	1402	4OC	C6-C5-C4	2.38	119.86	117.00
32	2a	1404	5MC	O2-C2-N3	-2.37	118.59	122.33
32	2a	1518	MA6	C4-N9-C8	2.36	108.22	105.74
1	1A	2503	2MA	C6-C5-N7	2.36	136.65	132.09
54	1w	46	7MG	C5-C6-N1	2.36	115.10	110.94
55	2x	8	4SU	O2-C2-N3	-2.36	117.13	121.49
32	2a	1518	MA6	C10-N6-C6	-2.36	114.52	120.52
32	1a	527	7MG	O6-C6-C5	-2.35	121.84	127.62
32	2a	1402	4OC	CM4-N4-C4	-2.34	117.88	122.45
32	2a	1519	MA6	C10-N6-C6	-2.34	114.57	120.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1y	46	7MG	C5-C6-N1	2.33	115.04	110.94
54	1y	46	7MG	C4-C5-N7	2.32	108.11	105.38
32	2a	1519	MA6	C6-C5-N7	2.31	137.12	133.43
1	2A	2251	OMG	C4-C5-N7	-2.29	107.05	110.67
1	1A	2605	PSU	C5-C6-N1	-2.27	118.98	122.14
32	1a	1404	5MC	O2-C2-N3	-2.27	118.75	122.33
32	1a	1518	MA6	C10-N6-C9	-2.26	108.92	116.18
32	2a	1400	5MC	C5-C4-N3	-2.26	119.44	121.75
1	2A	1920	4OC	O2-C2-N3	-2.26	118.77	122.33
32	1a	1498	UR3	C3U-N3-C2	2.26	121.26	117.33
54	2w	55	PSU	O4-C4-C5	-2.25	118.42	124.01
1	2A	1915	5MU	O2-C2-N1	-2.24	119.89	122.80
1	2A	2503	2MA	C5-N7-C8	2.22	106.94	103.45
54	2w	8	4SU	C1'-N1-C2	2.20	121.54	117.59
55	1x	32	5MC	O2-C2-N3	-2.19	118.88	122.33
54	1w	55	PSU	O4-C4-C5	-2.19	118.58	124.01
43	1l	92	0TD	OD1-CG-CB	-2.18	117.88	122.44
1	1A	1920	4OC	CM2-O2'-C2'	-2.18	108.89	114.47
54	2y	54	5MU	O2-C2-N1	-2.17	119.97	122.80
54	2w	46	7MG	O6-C6-C5	-2.15	122.34	127.62
32	1a	1519	MA6	C5-C6-N6	-2.13	121.97	125.33
1	1A	1915	5MU	C5M-C5-C4	2.13	121.05	118.78
1	1A	2251	OMG	O6-C6-C5	-2.12	120.92	126.53
32	1a	516	PSU	O4'-C1'-C2'	2.12	108.09	105.15
32	1a	516	PSU	C5-C6-N1	-2.12	119.20	122.14
54	1y	37	6MZ	N9-C8-N7	-2.11	110.94	113.94
1	1A	2251	OMG	C5-C6-N1	2.11	118.61	113.25
55	2x	54	5MU	C5M-C5-C4	2.10	121.02	118.78
32	1a	966	M2G	O6-C6-C5	-2.10	121.00	126.53
1	1A	1917	PSU	C5-C6-N1	-2.09	119.24	122.14
55	1x	54	5MU	O2-C2-N1	-2.09	120.07	122.80
32	2a	516	PSU	O4'-C1'-C2'	2.09	108.04	105.15
32	1a	1207	2MG	C8-N7-C5	2.09	107.97	104.26
54	2w	37	6MZ	N9-C8-N7	-2.07	111.00	113.94
1	2A	2251	OMG	C5-C6-N1	2.06	118.50	113.25
1	1A	2503	2MA	N3-C2-N1	-2.06	122.13	125.77
54	1w	37	6MZ	C4-N9-C8	2.06	107.90	105.74
32	1a	1518	MA6	C6-C5-N7	2.06	136.72	133.43
1	2A	2503	2MA	N9-C8-N7	-2.06	111.02	113.94
1	2A	1917	PSU	C5-C6-N1	-2.05	119.30	122.14
32	2a	1407	5MC	O2-C2-N3	-2.05	119.10	122.33
54	1y	55	PSU	O4'-C1'-C2'	2.05	107.98	105.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	1x	8	4SU	C1'-N1-C2	2.04	121.26	117.59
32	2a	1519	MA6	N9-C8-N7	-2.04	111.04	113.94
32	2a	1498	UR3	C1'-N1-C2	2.04	120.38	117.04
54	2y	55	PSU	O4'-C1'-C2'	2.03	107.96	105.15
1	2A	1939	5MU	C5M-C5-C4	2.02	120.94	118.78
32	1a	1518	MA6	N9-C8-N7	-2.02	111.07	113.94
1	2A	1939	5MU	C5M-C5-C6	-2.02	120.12	122.85
32	2a	1400	5MC	O2-C2-N3	-2.02	119.15	122.33
32	1a	1519	MA6	N9-C8-N7	-2.02	111.08	113.94
1	1A	1920	4OC	O2-C2-N3	-2.01	119.16	122.33
1	1A	1962	5MC	C5-C4-N3	-2.01	119.70	121.75
32	2a	516	PSU	C5-C6-N1	-2.01	119.36	122.14

There are no chirality outliers.

All (67) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
43	1l	92	0TD	O-C-CA-CB
43	1l	92	0TD	CG-CB-SB-CSB
32	2a	1518	MA6	C5-C6-N6-C9
32	2a	1519	MA6	O4'-C4'-C5'-O5'
54	1w	46	7MG	O4'-C4'-C5'-O5'
54	1y	46	7MG	C4'-C5'-O5'-P
54	2y	46	7MG	C2'-C1'-N9-C8
54	1y	54	5MU	O4'-C4'-C5'-O5'
32	1a	1402	4OC	O4'-C4'-C5'-O5'
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1207	2MG	O4'-C4'-C5'-O5'
32	2a	1207	2MG	C3'-C4'-C5'-O5'
54	1y	54	5MU	C3'-C4'-C5'-O5'
32	2a	527	7MG	C3'-C4'-C5'-O5'
54	2w	46	7MG	O4'-C4'-C5'-O5'
32	2a	1518	MA6	N1-C6-N6-C9
54	1w	46	7MG	C3'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
54	2w	46	7MG	C3'-C4'-C5'-O5'
54	2w	34	CM0	O5-C7-C8-O9
32	1a	527	7MG	C3'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	527	7MG	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C5-C6-N6-C10
54	2w	34	CM0	O5-C7-C8-O8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
54	2w	34	CM0	C6-C5-O5-C7
54	1y	46	7MG	C3'-C4'-C5'-O5'
54	2w	34	CM0	C4-C5-O5-C7
54	1y	34	CM0	O5-C7-C8-O8
32	1a	1402	4OC	C3'-C4'-C5'-O5'
32	2a	1402	4OC	O4'-C4'-C5'-O5'
54	2w	34	CM0	C8-C7-O5-C5
54	2y	34	CM0	C8-C7-O5-C5
54	1y	34	CM0	O5-C7-C8-O9
32	2a	1400	5MC	C2'-C1'-N1-C6
32	1a	1518	MA6	C5-C6-N6-C10
32	1a	1519	MA6	C5-C6-N6-C10
54	1y	46	7MG	C2'-C1'-N9-C8
32	2a	1404	5MC	C3'-C4'-C5'-O5'
43	2l	92	0TD	CG-CB-SB-CSB
54	2y	37	6MZ	C3'-C4'-C5'-O5'
32	1a	527	7MG	O4'-C4'-C5'-O5'
1	2A	2552	2MU	O4'-C4'-C5'-O5'
54	2y	55	PSU	O4'-C1'-C5-C4
32	2a	1400	5MC	O4'-C1'-N1-C6
32	1a	527	7MG	C4'-C5'-O5'-P
32	2a	1519	MA6	C4'-C5'-O5'-P
54	2y	37	6MZ	C4'-C5'-O5'-P
32	2a	1404	5MC	O4'-C4'-C5'-O5'
54	1y	46	7MG	O4'-C1'-N9-C8
54	2y	46	7MG	C2'-C1'-N9-C4
43	1l	92	0TD	CA-CB-SB-CSB
54	2y	55	PSU	O4'-C1'-C5-C6
32	2a	1400	5MC	O4'-C1'-N1-C2
54	1y	8	4SU	C2'-C1'-N1-C6
54	2y	8	4SU	C2'-C1'-N1-C6
32	2a	1400	5MC	C2'-C1'-N1-C2
32	2a	1518	MA6	C5-C6-N6-C10
54	2y	37	6MZ	O4'-C4'-C5'-O5'
54	1w	34	CM0	O5-C7-C8-O8
1	1A	2503	2MA	C4'-C5'-O5'-P
1	2A	1962	5MC	C2'-C1'-N1-C6
32	2a	527	7MG	C4'-C5'-O5'-P
1	2A	1920	4OC	C2'-C1'-N1-C2
1	1A	1920	4OC	C2'-C1'-N1-C2
55	2x	32	5MC	C2'-C1'-N1-C2
1	2A	1962	5MC	O4'-C1'-N1-C6

There are no ring outliers.

38 monomers are involved in 62 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	2x	8	4SU	3	0
54	2y	8	4SU	4	0
1	1A	2251	OMG	1	0
55	1x	8	4SU	3	0
32	1a	1518	MA6	2	0
1	2A	2503	2MA	1	0
54	2w	55	PSU	1	0
54	1y	54	5MU	2	0
32	2a	1207	2MG	1	0
54	1w	37	6MZ	1	0
43	1l	92	0TD	2	0
1	1A	1939	5MU	1	0
54	1y	55	PSU	2	0
54	2w	54	5MU	4	0
54	1w	55	PSU	2	0
32	1a	1519	MA6	2	0
55	2x	54	5MU	1	0
54	2y	37	6MZ	3	0
54	2w	8	4SU	1	0
54	1y	34	CM0	1	0
32	2a	1518	MA6	4	0
54	1w	54	5MU	3	0
32	2a	966	M2G	1	0
32	2a	1402	4OC	2	0
32	1a	1207	2MG	1	0
54	1y	37	6MZ	2	0
1	2A	2552	2MU	2	0
32	2a	967	5MC	1	0
54	1w	46	7MG	1	0
43	2l	92	0TD	2	0
1	2A	2251	OMG	1	0
1	1A	1917	PSU	1	0
32	2a	1519	MA6	3	0
1	1A	2552	2MU	1	0
54	1y	8	4SU	1	0
1	2A	1939	5MU	1	0
32	1a	1402	4OC	3	0
32	2a	1404	5MC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2801 ligands modelled in this entry, 2797 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$
57	DI0	1A	4098	-	58,61,61	2.52	23 (39%)	78,92,92	2.14	26 (33%)
57	DI0	2A	3846	-	58,61,61	1.09	4 (6%)	78,92,92	1.62	16 (20%)
60	SF4	1d	3102	35	0,12,12	-	-	-	-	-
60	SF4	2d	303	35	0,12,12	-	-	-	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	DI0	1A	4098	-	-	10/70/121/121	0/3/4/4
57	DI0	2A	3846	-	-	8/70/121/121	0/3/4/4
60	SF4	1d	3102	35	-	-	0/6/5/5
60	SF4	2d	303	35	-	-	0/6/5/5

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	1A	4098	DI0	CAF-CAE	-6.64	1.37	1.51
57	1A	4098	DI0	OBJ-CAP	-5.84	1.35	1.44
57	2A	3846	DI0	CAF-CAE	-5.49	1.39	1.51
57	1A	4098	DI0	OBH-CAD	-4.72	1.36	1.44
57	1A	4098	DI0	OBK-CAN	-4.51	1.35	1.44
57	1A	4098	DI0	OAU-CBG	-4.33	1.36	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	1A	4098	DI0	CBC-CBB	-4.17	1.48	1.54
57	1A	4098	DI0	CAP-CAH	-4.01	1.47	1.55
57	1A	4098	DI0	OAL-CAW	-3.93	1.39	1.46
57	1A	4098	DI0	CBD-CBG	-3.79	1.45	1.52
57	1A	4098	DI0	OAY-CAR	-3.76	1.31	1.41
57	1A	4098	DI0	OAS-CBA	3.62	1.49	1.45
57	1A	4098	DI0	OAM-CAH	-3.49	1.35	1.44
57	1A	4098	DI0	OAM-CAB	-3.43	1.32	1.41
57	1A	4098	DI0	CAZ-CAX	-3.09	1.46	1.53
57	1A	4098	DI0	CBC-CAP	-3.02	1.49	1.54
57	1A	4098	DI0	OBL-CAX	-2.80	1.37	1.42
57	1A	4098	DI0	CAD-CAW	-2.70	1.50	1.55
57	1A	4098	DI0	CBQ-CAN	-2.66	1.46	1.52
57	1A	4098	DI0	OBI-CAG	-2.65	1.36	1.43
57	1A	4098	DI0	CAD-CAA	-2.46	1.49	1.54
57	1A	4098	DI0	OAV-CAZ	-2.14	1.39	1.44
57	2A	3846	DI0	OAM-CAB	2.14	1.47	1.41
57	1A	4098	DI0	OAS-CAA	-2.07	1.39	1.43
57	2A	3846	DI0	OAU-CBG	-2.06	1.40	1.44
57	2A	3846	DI0	CAD-CAW	-2.02	1.51	1.55
57	1A	4098	DI0	OAV-CAR	-2.00	1.37	1.42

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	1A	4098	DI0	CCA-CBG-CBD	-5.63	104.75	113.27
57	1A	4098	DI0	OAM-CAB-OAU	-5.05	97.41	110.69
57	1A	4098	DI0	CBU-CAZ-CAX	-5.02	104.26	112.58
57	1A	4098	DI0	CBO-CAI-CAK	-4.59	106.58	112.02
57	1A	4098	DI0	CBY-NBE-CBZ	-4.55	97.12	110.49
57	2A	3846	DI0	CAW-OAL-CAE	-4.42	110.48	118.20
57	1A	4098	DI0	CBT-CAW-CAD	-4.28	107.36	115.20
57	2A	3846	DI0	CAP-CAH-CAJ	-3.66	108.58	113.89
57	1A	4098	DI0	CAT-CAN-CAX	3.64	113.87	107.64
57	2A	3846	DI0	CBT-CAW-CAD	-3.60	108.61	115.20
57	1A	4098	DI0	CBZ-NBE-CAO	-3.59	102.82	113.15
57	1A	4098	DI0	OBK-CAN-CBQ	-3.55	101.59	110.77
57	1A	4098	DI0	CBD-CAO-NBE	-3.31	106.28	115.59
57	2A	3846	DI0	OBK-CAN-CAX	3.29	108.63	103.86
57	1A	4098	DI0	CBB-CAK-NAQ	-3.27	104.46	110.36
57	1A	4098	DI0	OBK-CAN-CAX	3.23	108.54	103.86
57	2A	3846	DI0	CBV-CBB-CBC	-3.22	105.13	112.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	2A	3846	DI0	CBB-CAK-NAQ	3.03	115.84	110.36
57	1A	4098	DI0	OAY-CAR-OAV	-2.94	100.48	109.97
57	2A	3846	DI0	CBO-CAI-CAK	-2.89	108.59	112.02
57	1A	4098	DI0	CBQ-CAN-CAT	-2.86	105.65	110.64
57	1A	4098	DI0	OAS-CAA-CAI	-2.84	104.57	109.99
57	2A	3846	DI0	CCA-CBG-CBD	-2.84	108.98	113.27
57	2A	3846	DI0	CAN-CAT-CAR	-2.78	110.29	114.99
57	1A	4098	DI0	OBL-CAX-CAZ	-2.78	104.67	109.46
57	1A	4098	DI0	OBW-CBS-CBA	-2.75	102.77	109.28
57	2A	3846	DI0	CBP-CAJ-CAC	-2.67	106.70	111.40
57	2A	3846	DI0	CBD-CAO-NBE	-2.67	108.10	115.59
57	2A	3846	DI0	CBM-CAD-CAW	-2.66	107.67	111.26
57	1A	4098	DI0	CBM-CAD-CAW	-2.64	107.69	111.26
57	1A	4098	DI0	OBJ-CAP-CAH	2.58	112.36	107.60
57	1A	4098	DI0	OBH-CAD-CAW	2.56	111.16	107.24
57	1A	4098	DI0	OBK-CAN-CAT	2.41	116.66	112.95
57	2A	3846	DI0	OAL-CAE-CAF	2.40	116.66	111.53
57	1A	4098	DI0	CAB-OAU-CBG	2.37	116.57	112.91
57	1A	4098	DI0	CAR-OAV-CAZ	2.34	120.23	113.82
57	2A	3846	DI0	OAM-CAH-CAP	2.33	109.18	106.40
57	2A	3846	DI0	CAR-OAY-CAC	-2.30	110.14	114.72
57	1A	4098	DI0	CBP-CAJ-CAC	-2.29	107.38	111.40
57	1A	4098	DI0	OAY-CAR-CAT	-2.26	105.21	108.99
57	2A	3846	DI0	CCB-OBK-CAN	-2.24	112.95	117.51
57	1A	4098	DI0	OBJ-CAP-CBR	-2.02	103.81	108.48

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	1A	4098	DI0	CAT-CAN-OBK-CCB
57	1A	4098	DI0	CBR-CAP-CBC-CBB
57	2A	3846	DI0	CBR-CAP-CBC-CBB
57	1A	4098	DI0	CBD-CAO-NBE-CBY
57	2A	3846	DI0	CBD-CAO-NBE-CBY
57	2A	3846	DI0	CAJ-CAH-CAP-OBJ
57	1A	4098	DI0	OAL-CAW-CBT-CCF
57	2A	3846	DI0	CCC-CCD-OBW-CBS
57	1A	4098	DI0	NAQ-CBA-CBS-OBW
57	2A	3846	DI0	OAL-CAW-CBT-CCF
57	1A	4098	DI0	CBV-CBB-CBC-CAP
57	1A	4098	DI0	CAJ-CAH-CAP-OBJ

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
57	1A	4098	DI0	OAS-CBA-CBS-OBW
57	1A	4098	DI0	OBJ-CAP-CBC-CBB
57	2A	3846	DI0	OBJ-CAP-CBC-CBB
57	1A	4098	DI0	CAD-CAW-CBT-CCF
57	2A	3846	DI0	CAD-CAW-CBT-CCF
57	2A	3846	DI0	CAG-CAO-NBE-CBZ

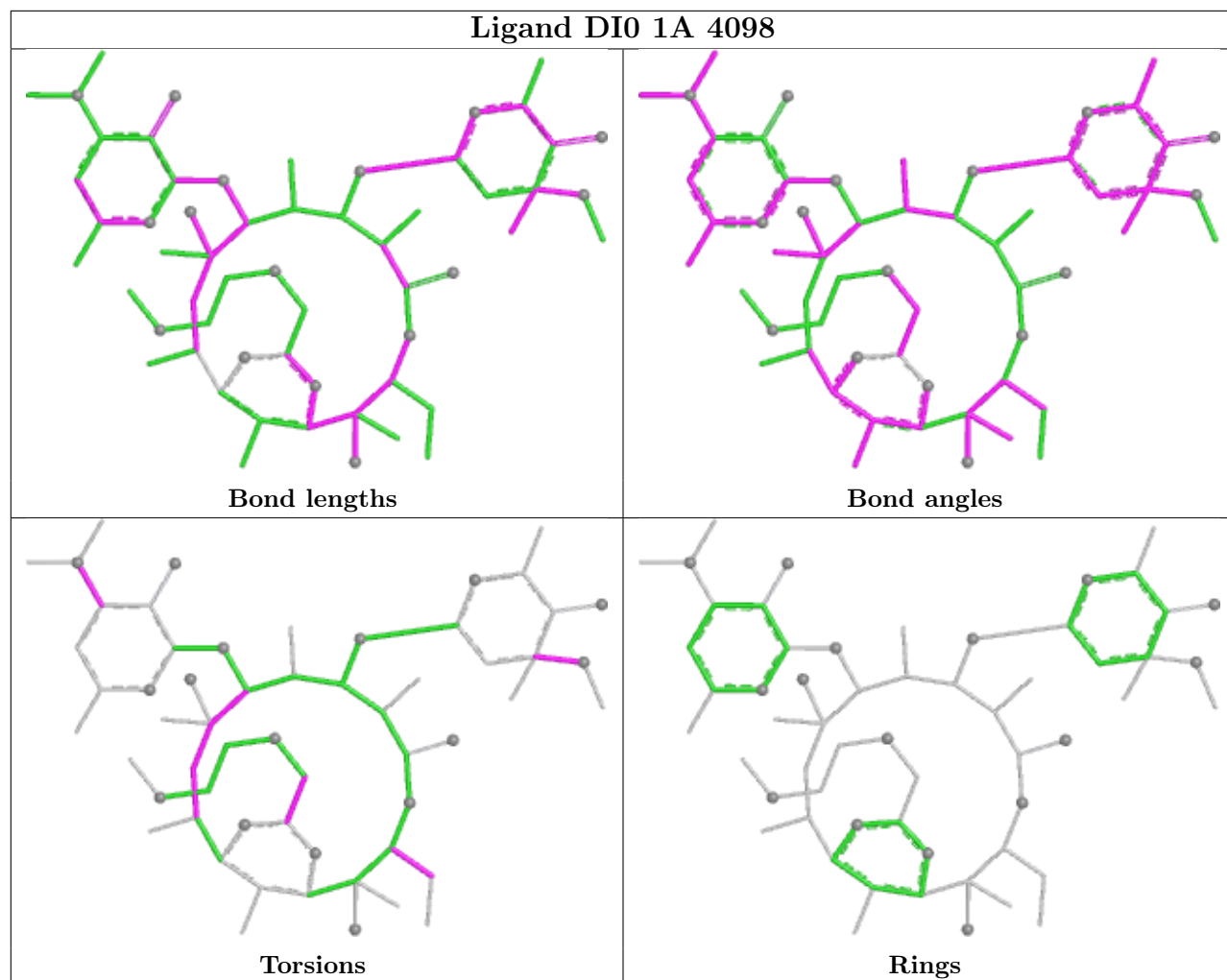
There are no ring outliers.

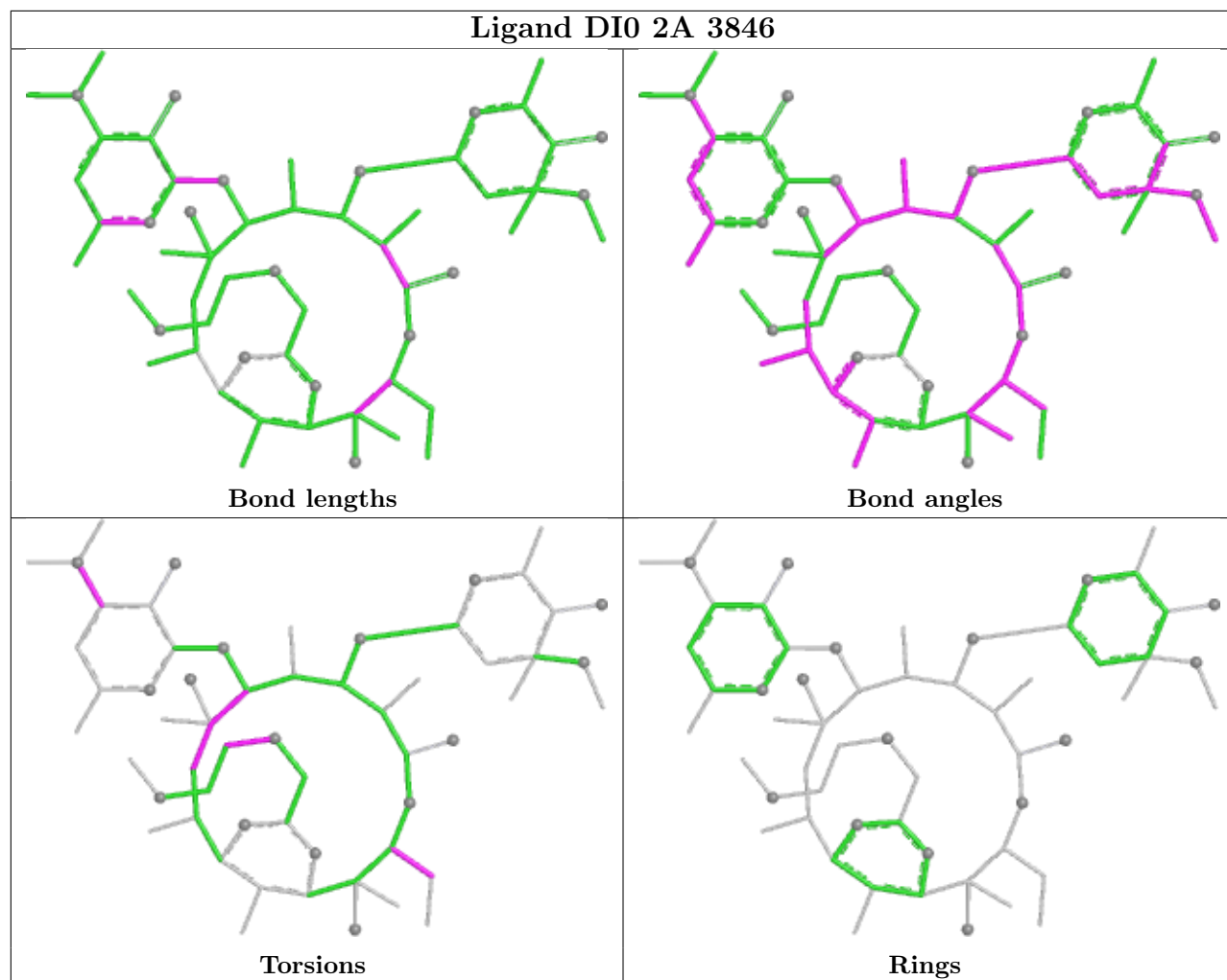
3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	1A	4098	DI0	5	0
60	1d	3102	SF4	1	0
60	2d	303	SF4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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 DI0 1A 4098





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1A	2860/2915 (98%)	-0.54	44 (1%) 72 63	18, 35, 99, 114	0
1	2A	2789/2915 (95%)	-0.10	60 (2%) 62 52	30, 56, 97, 114	0
2	1B	120/121 (99%)	-0.52	0 100 100	28, 48, 63, 92	0
2	2B	120/121 (99%)	0.47	0 100 100	62, 77, 88, 98	0
3	1D	275/276 (99%)	-0.23	3 (1%) 78 70	20, 35, 50, 87	0
3	2D	275/276 (99%)	0.15	5 (1%) 67 58	31, 47, 64, 83	0
4	1E	204/206 (99%)	-0.21	0 100 100	21, 40, 59, 79	0
4	2E	204/206 (99%)	0.27	5 (2%) 58 48	33, 58, 73, 86	0
5	1F	203/210 (96%)	-0.13	2 (0%) 79 72	20, 41, 71, 89	0
5	2F	203/210 (96%)	0.46	3 (1%) 72 63	35, 66, 82, 94	0
6	1G	181/182 (99%)	0.45	7 (3%) 43 34	40, 59, 76, 86	0
6	2G	181/182 (99%)	1.29	23 (12%) 8 6	70, 81, 90, 102	0
7	1H	174/180 (96%)	0.02	4 (2%) 61 51	38, 53, 68, 74	0
7	2H	174/180 (96%)	1.10	14 (8%) 18 13	70, 84, 94, 98	0
8	1I	146/148 (98%)	0.41	2 (1%) 73 64	40, 73, 82, 88	0
8	2I	146/148 (98%)	0.62	4 (2%) 56 46	54, 72, 85, 90	0
9	1N	140/140 (100%)	-0.12	1 (0%) 84 77	27, 37, 62, 74	0
9	2N	140/140 (100%)	0.53	2 (1%) 73 64	45, 64, 81, 85	0
10	1O	122/122 (100%)	-0.13	0 100 100	26, 38, 56, 65	0
10	2O	122/122 (100%)	0.19	0 100 100	42, 57, 71, 78	0
11	1P	149/150 (99%)	0.06	2 (1%) 75 66	20, 45, 73, 84	0
11	2P	149/150 (99%)	0.64	5 (3%) 48 39	34, 69, 83, 94	0
12	1Q	141/141 (100%)	-0.10	0 100 100	25, 40, 56, 76	0
12	2Q	141/141 (100%)	0.84	10 (7%) 22 16	46, 66, 78, 84	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1R	118/118 (100%)	-0.25	0 100 100	23, 33, 48, 59	0
13	2R	118/118 (100%)	0.08	2 (1%) 69 60	39, 51, 62, 73	0
14	1S	110/112 (98%)	-0.11	1 (0%) 81 74	35, 48, 61, 66	0
14	2S	110/112 (98%)	0.98	9 (8%) 17 13	62, 72, 82, 85	0
15	1T	131/146 (89%)	0.08	2 (1%) 72 63	30, 43, 71, 80	0
15	2T	131/146 (89%)	0.41	2 (1%) 72 63	52, 61, 80, 87	0
16	1U	116/118 (98%)	-0.32	1 (0%) 81 74	22, 30, 49, 63	0
16	2U	116/118 (98%)	0.32	0 100 100	42, 61, 76, 84	0
17	1V	101/101 (100%)	-0.21	1 (0%) 79 72	25, 39, 55, 68	0
17	2V	101/101 (100%)	0.46	1 (0%) 79 72	42, 71, 83, 90	0
18	1W	112/113 (99%)	-0.30	1 (0%) 81 74	22, 31, 52, 84	0
18	2W	112/113 (99%)	0.18	2 (1%) 67 58	39, 47, 69, 89	0
19	1X	95/96 (98%)	-0.06	1 (1%) 78 70	20, 38, 61, 75	0
19	2X	95/96 (98%)	0.35	2 (2%) 63 54	41, 58, 73, 80	0
20	1Y	107/110 (97%)	0.13	2 (1%) 66 57	34, 49, 70, 81	0
20	2Y	107/110 (97%)	0.97	10 (9%) 14 10	59, 72, 83, 89	0
21	1Z	154/206 (74%)	0.68	12 (7%) 19 14	44, 66, 92, 100	0
21	2Z	160/206 (77%)	1.48	35 (21%) 2 2	64, 85, 100, 105	0
22	10	83/85 (97%)	-0.21	1 (1%) 76 68	25, 36, 54, 74	0
22	20	83/85 (97%)	0.97	10 (12%) 9 6	45, 62, 73, 86	0
23	11	97/98 (98%)	0.19	2 (2%) 63 54	27, 43, 72, 76	0
23	21	97/98 (98%)	0.47	2 (2%) 63 54	35, 53, 77, 85	0
24	12	70/72 (97%)	0.09	1 (1%) 73 64	35, 46, 59, 81	0
24	22	70/72 (97%)	0.25	0 100 100	55, 69, 80, 81	0
25	13	59/60 (98%)	-0.22	0 100 100	25, 34, 59, 79	0
25	23	59/60 (98%)	0.73	2 (3%) 48 39	49, 66, 82, 90	0
26	14	69/71 (97%)	0.84	7 (10%) 12 9	53, 73, 91, 98	0
26	24	69/71 (97%)	1.50	12 (17%) 4 3	80, 88, 97, 103	0
27	15	59/60 (98%)	-0.32	1 (1%) 69 60	19, 31, 48, 67	0
27	25	59/60 (98%)	0.00	0 100 100	36, 51, 66, 77	0
28	16	53/54 (98%)	-0.34	0 100 100	28, 40, 53, 62	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	26	53/54 (98%)	0.62	0 100 100	50, 60, 72, 76	0
29	17	48/49 (97%)	-0.31	1 (2%) 63 54	21, 27, 55, 64	0
29	27	48/49 (97%)	-0.01	2 (4%) 40 32	31, 37, 64, 71	0
30	18	64/65 (98%)	-0.15	0 100 100	26, 33, 43, 58	0
30	28	64/65 (98%)	0.53	0 100 100	43, 54, 62, 70	0
31	19	37/37 (100%)	-0.31	0 100 100	30, 39, 59, 61	0
31	29	37/37 (100%)	0.89	1 (2%) 56 46	59, 67, 78, 79	0
32	1a	1488/1521 (97%)	0.02	16 (1%) 78 70	31, 63, 95, 110	0
32	2a	1491/1521 (98%)	0.27	28 (1%) 66 57	49, 77, 99, 114	0
33	1b	231/256 (90%)	1.00	25 (10%) 11 8	61, 80, 93, 96	0
33	2b	231/256 (90%)	1.12	24 (10%) 11 8	74, 89, 97, 102	0
34	1c	206/239 (86%)	0.67	7 (3%) 48 39	56, 69, 83, 91	0
34	2c	206/239 (86%)	1.65	62 (30%) 1 1	76, 86, 93, 99	0
35	1d	208/209 (99%)	0.56	8 (3%) 44 35	51, 66, 79, 87	0
35	2d	208/209 (99%)	0.70	8 (3%) 44 35	63, 73, 84, 89	0
36	1e	148/162 (91%)	0.36	2 (1%) 73 64	49, 63, 75, 87	0
36	2e	148/162 (91%)	0.92	8 (5%) 31 24	68, 78, 87, 90	0
37	1f	100/101 (99%)	0.41	0 100 100	50, 65, 76, 81	0
37	2f	100/101 (99%)	0.45	0 100 100	55, 68, 79, 81	0
38	1g	155/156 (99%)	0.70	13 (8%) 17 12	56, 70, 87, 93	0
38	2g	155/156 (99%)	1.07	17 (10%) 10 8	71, 79, 90, 94	0
39	1h	137/138 (99%)	0.42	1 (0%) 84 77	52, 65, 72, 78	0
39	2h	137/138 (99%)	0.72	2 (1%) 72 63	67, 79, 85, 90	0
40	1i	127/128 (99%)	0.83	8 (6%) 26 19	50, 77, 86, 89	0
40	2i	127/128 (99%)	1.44	29 (22%) 2 1	76, 86, 93, 98	0
41	1j	97/105 (92%)	1.06	14 (14%) 6 5	52, 77, 92, 99	0
41	2j	96/105 (91%)	2.03	48 (50%) 0 0	79, 89, 96, 102	0
42	1k	114/129 (88%)	0.52	5 (4%) 39 31	43, 64, 77, 85	0
42	2k	114/129 (88%)	0.79	6 (5%) 32 24	51, 72, 83, 89	0
43	1l	121/132 (91%)	0.20	3 (2%) 58 48	39, 50, 65, 71	0
43	2l	121/132 (91%)	0.69	5 (4%) 41 33	50, 67, 77, 83	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%)	0.76	6 (4%) 35 27	56, 69, 81, 101	0
44	2m	122/126 (96%)	1.49	19 (15%) 5 4	72, 84, 90, 101	0
45	1n	60/61 (98%)	0.66	1 (1%) 69 60	54, 66, 73, 76	0
45	2n	60/61 (98%)	2.25	34 (56%) 0 0	75, 86, 91, 95	0
46	1o	88/89 (98%)	0.36	2 (2%) 61 51	47, 62, 74, 77	0
46	2o	88/89 (98%)	0.52	3 (3%) 48 39	58, 71, 81, 90	0
47	1p	82/88 (93%)	0.93	4 (4%) 35 27	57, 66, 78, 84	0
47	2p	82/88 (93%)	0.67	2 (2%) 59 49	60, 68, 78, 82	0
48	1q	99/105 (94%)	0.62	1 (1%) 79 72	51, 65, 76, 82	0
48	2q	99/105 (94%)	0.71	1 (1%) 79 72	60, 73, 81, 85	0
49	1r	68/88 (77%)	0.34	1 (1%) 72 63	53, 64, 76, 78	0
49	2r	68/88 (77%)	0.53	1 (1%) 72 63	58, 71, 84, 89	0
50	1s	83/93 (89%)	0.83	6 (7%) 21 16	59, 72, 83, 86	0
50	2s	83/93 (89%)	1.83	27 (32%) 1 1	81, 89, 96, 99	0
51	1t	96/106 (90%)	0.98	14 (14%) 6 4	57, 69, 81, 85	0
51	2t	96/106 (90%)	0.73	7 (7%) 21 15	61, 70, 84, 86	0
52	1u	23/27 (85%)	0.83	2 (8%) 16 11	59, 64, 74, 75	0
52	2u	23/27 (85%)	1.51	4 (17%) 4 3	77, 82, 87, 90	0
53	1v	13/27 (48%)	0.85	4 (30%) 1 1	45, 56, 94, 105	0
53	2v	13/27 (48%)	1.41	4 (30%) 1 1	63, 82, 101, 101	0
54	1w	67/76 (88%)	1.25	16 (23%) 2 1	41, 90, 101, 106	0
54	1y	67/76 (88%)	1.62	19 (28%) 1 1	35, 101, 108, 112	0
54	2w	67/76 (88%)	1.33	13 (19%) 3 2	55, 99, 105, 111	0
54	2y	67/76 (88%)	1.80	30 (44%) 0 0	53, 103, 107, 110	0
55	1x	72/77 (93%)	0.39	2 (2%) 55 45	36, 69, 89, 93	0
55	2x	72/77 (93%)	0.53	1 (1%) 73 64	51, 81, 94, 102	0
All	All	20878/21754 (95%)	0.25	885 (4%) 40 32	18, 62, 93, 114	0

All (885) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	1m	124	PRO	14.4
44	2m	124	PRO	12.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
44	2m	123	ALA	12.2
44	1m	123	ALA	10.4
44	2m	122	LYS	10.1
23	2l	2	SER	8.0
44	1m	122	LYS	6.4
45	1n	2	ALA	5.9
44	2m	102	ARG	5.8
34	2c	155	GLY	5.8
3	1D	276	LYS	5.7
51	1t	103	GLY	5.6
21	1Z	141	VAL	5.5
22	20	3	HIS	5.5
38	2g	80	VAL	5.1
41	2j	58	ASP	5.1
44	2m	119	GLY	4.9
45	2n	2	ALA	4.9
45	2n	39	LEU	4.8
41	2j	55	LYS	4.7
21	2Z	149	SER	4.7
40	2i	102	LEU	4.6
50	2s	13	ASP	4.6
34	2c	158	GLY	4.6
50	2s	68	GLY	4.6
53	1v	12	A	4.5
44	1m	121	LYS	4.5
45	2n	34	TYR	4.5
38	2g	79	ARG	4.5
50	2s	80	TYR	4.4
6	2G	28	VAL	4.4
21	1Z	168	GLU	4.4
41	2j	47	PHE	4.4
53	2v	24	C	4.4
27	15	60	VAL	4.3
38	2g	82	GLY	4.3
54	1w	56	C	4.3
44	2m	121	LYS	4.3
21	2Z	170	THR	4.3
21	2Z	144	LEU	4.2
41	2j	65	LEU	4.2
38	1g	84	ASN	4.2
6	2G	146	TYR	4.2
32	1a	1531	A	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
50	2s	82	GLY	4.2
22	10	3	HIS	4.1
23	11	2	SER	4.0
50	2s	11	VAL	4.0
21	2Z	146	ILE	4.0
26	24	49	PHE	4.0
50	2s	79	THR	4.0
15	1T	130	ALA	3.9
26	24	65	ASP	3.9
50	1s	84	GLY	3.9
25	23	60	GLU	3.9
41	2j	62	HIS	3.9
34	2c	193	TYR	3.9
24	12	70	GLN	3.9
54	2w	56	C	3.9
33	1b	127	ILE	3.9
40	1i	126	SER	3.9
41	2j	59	SER	3.9
34	2c	2	GLY	3.8
6	2G	53	LEU	3.8
41	2j	76	ASN	3.8
38	2g	81	GLY	3.8
54	2w	61	C	3.8
31	29	37	GLY	3.8
38	1g	79	ARG	3.8
47	1p	82	GLN	3.8
38	2g	84	ASN	3.8
34	2c	160	ALA	3.8
19	1X	95	LEU	3.7
38	2g	4	ARG	3.7
26	14	56	VAL	3.7
34	2c	198	VAL	3.7
21	1Z	146	ILE	3.7
52	2u	14	TRP	3.7
1	2A	2115	G	3.7
33	2b	165	VAL	3.7
40	2i	11	LYS	3.7
34	2c	65	ALA	3.7
21	2Z	147	GLY	3.7
26	24	56	VAL	3.7
1	2A	2133	G	3.6
34	2c	197	GLY	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	2c	13	GLY	3.6
42	2k	13	GLN	3.6
6	1G	48	GLU	3.6
54	1w	49	G	3.6
51	2t	9	ASN	3.6
34	1c	2	GLY	3.5
38	1g	85	TYR	3.5
42	2k	117	ASN	3.5
4	2E	204	ALA	3.5
42	1k	13	GLN	3.5
7	2H	136	ILE	3.5
43	2l	32	PHE	3.5
1	2A	2173	A	3.5
34	2c	159	GLY	3.5
1	2A	2896	C	3.4
25	23	2	PRO	3.4
22	20	2	ALA	3.4
26	14	63	TYR	3.4
33	2b	15	VAL	3.4
45	2n	33	VAL	3.4
34	2c	28	GLN	3.4
40	2i	125	TYR	3.4
50	2s	9	VAL	3.4
51	1t	22	ARG	3.4
38	2g	49	ILE	3.4
42	1k	25	TYR	3.4
1	2A	2116	G	3.3
1	2A	2125	G	3.3
1	2A	2168	G	3.3
3	1D	2	ALA	3.3
33	2b	237	ALA	3.3
21	2Z	174	VAL	3.3
45	2n	3	ARG	3.3
45	2n	21	TYR	3.3
51	1t	94	ALA	3.3
1	1A	880	G	3.3
32	2a	1202	G	3.3
45	2n	25	VAL	3.3
21	2Z	148	ASP	3.3
1	1A	896	A	3.3
50	2s	83	HIS	3.3
42	2k	75	TYR	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	2c	206	GLU	3.2
41	2j	32	ALA	3.2
50	2s	15	LEU	3.2
1	2A	2114	A	3.2
45	2n	13	THR	3.2
3	2D	38	LYS	3.2
45	2n	15	LYS	3.2
50	2s	2	PRO	3.2
54	2w	19	G	3.2
34	2c	157	ILE	3.2
40	2i	10	ARG	3.2
34	1c	193	TYR	3.2
54	1y	13	C	3.2
1	2A	2160	G	3.2
54	1y	15	G	3.2
45	2n	18	VAL	3.2
1	1A	548	A	3.2
1	1A	885	C	3.2
54	1w	61	C	3.2
1	1A	1078	U	3.2
20	2Y	54	LYS	3.2
44	2m	120	LYS	3.2
1	2A	2155	G	3.2
38	2g	156	TRP	3.2
33	1b	130	ARG	3.1
33	1b	19	HIS	3.1
5	1F	208	GLY	3.1
40	2i	2	GLU	3.1
1	2A	2166	G	3.1
34	2c	196	LEU	3.1
44	1m	2	ALA	3.1
1	1A	1076	C	3.1
45	2n	30	ALA	3.1
21	2Z	136	PHE	3.1
1	1A	1068	G	3.1
1	2A	2802	G	3.1
45	2n	41	ARG	3.1
54	2w	71	C	3.1
34	2c	199	LYS	3.1
15	2T	131	ALA	3.1
29	27	45	ALA	3.1
21	2Z	139	VAL	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	1b	17	PHE	3.1
40	1i	114	TYR	3.1
38	1g	80	VAL	3.1
44	2m	7	VAL	3.1
50	1s	13	ASP	3.1
33	2b	134	GLU	3.1
40	2i	9	ARG	3.1
45	2n	22	THR	3.1
51	1t	9	ASN	3.0
21	2Z	172	ALA	3.0
41	2j	63	PHE	3.0
1	2A	888	C	3.0
1	2A	1536	C	3.0
54	1y	36	C	3.0
26	14	55	ARG	3.0
51	1t	14	LYS	3.0
12	2Q	2	LEU	3.0
41	2j	40	LEU	3.0
41	2j	53	PRO	3.0
35	2d	164	ALA	3.0
21	2Z	141	VAL	3.0
36	2e	67	VAL	3.0
14	2S	92	TYR	3.0
34	2c	205	GLY	3.0
43	1l	14	GLY	3.0
45	2n	29	ARG	3.0
54	1w	60	C	3.0
6	2G	50	ALA	3.0
38	2g	2	ALA	3.0
53	2v	14	A	3.0
34	2c	182	ILE	3.0
41	2j	88	LEU	3.0
54	1w	57	G	3.0
21	2Z	142	SER	3.0
6	2G	48	GLU	3.0
54	1w	70	C	3.0
45	2n	42	ILE	2.9
42	2k	25	TYR	2.9
54	2y	21	A	2.9
35	2d	154	ASN	2.9
1	1A	2141	G	2.9
32	2a	1030(B)	C	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
9	2N	9	VAL	2.9
22	20	69	PHE	2.9
34	2c	167	TRP	2.9
32	2a	1256	A	2.9
53	2v	12	A	2.9
33	1b	15	VAL	2.9
33	2b	123	ALA	2.9
50	2s	19	VAL	2.9
1	1A	2133	G	2.9
1	2A	2154	G	2.9
54	2y	10	G	2.9
26	24	9	LEU	2.9
1	2A	896	A	2.9
54	2y	6	A	2.9
44	1m	120	LYS	2.9
34	2c	124	ILE	2.9
41	2j	74	ILE	2.9
34	2c	33	LEU	2.9
50	2s	84	GLY	2.9
51	2t	103	GLY	2.9
1	1A	614(B)	G	2.9
1	2A	883	G	2.9
1	2A	2159	G	2.9
32	2a	1024	G	2.9
33	2b	236	TYR	2.9
41	2j	78	ASN	2.9
13	2R	101	ALA	2.9
34	2c	195	VAL	2.9
1	2A	2126	A	2.9
32	1a	1447	A	2.9
14	2S	32	LEU	2.9
50	2s	16	LEU	2.9
1	1A	889	C	2.8
20	2Y	29	GLU	2.8
32	1a	163	C	2.8
45	2n	4	LYS	2.8
54	1y	10	G	2.8
40	2i	99	LEU	2.8
26	14	54	GLY	2.8
36	2e	22	GLY	2.8
50	2s	18	LYS	2.8
26	14	67	TYR	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
42	1k	14	VAL	2.8
53	1v	24	C	2.8
54	2y	36	C	2.8
21	2Z	155	LEU	2.8
6	2G	76	SER	2.8
1	2A	2124	G	2.8
32	2a	1030(A)	G	2.8
54	2y	19	G	2.8
26	14	45	GLY	2.8
38	1g	86	GLN	2.8
51	1t	18	GLN	2.8
6	2G	35	GLU	2.8
6	1G	146	TYR	2.8
32	1a	1257	U	2.8
21	2Z	53	ILE	2.8
38	2g	16	LEU	2.8
1	1A	884	C	2.8
32	1a	345	C	2.8
34	2c	62	ASP	2.8
3	2D	276	LYS	2.8
23	2l	79	GLY	2.8
45	2n	38	GLY	2.8
1	1A	881	G	2.8
41	2j	91	PRO	2.8
54	2y	15	G	2.8
21	2Z	2	GLU	2.8
34	2c	79	ARG	2.8
40	2i	14	VAL	2.8
12	2Q	104	PHE	2.8
49	1r	78	LEU	2.8
6	1G	182	LYS	2.8
18	1W	112	GLY	2.8
38	1g	81	GLY	2.8
42	2k	49	GLY	2.8
47	2p	82	GLN	2.7
8	2l	85	GLU	2.7
11	2P	74	GLU	2.7
41	2j	72	VAL	2.7
46	2o	60	VAL	2.7
40	2i	114	TYR	2.7
44	2m	87	TYR	2.7
41	2j	48	THR	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
6	2G	2	PRO	2.7
5	2F	161	GLU	2.7
33	1b	129	GLU	2.7
34	1c	207	VAL	2.7
34	2c	200	ALA	2.7
44	2m	5	ALA	2.7
45	2n	44	LEU	2.7
21	1Z	151	HIS	2.7
41	2j	56	HIS	2.7
54	1w	19	G	2.7
54	1w	50	G	2.7
41	2j	31	GLY	2.7
50	1s	12	ASP	2.7
41	2j	37	PRO	2.7
14	2S	35	ILE	2.7
32	2a	1277	C	2.7
18	2W	112	GLY	2.7
35	2d	141	ARG	2.7
38	2g	149	ARG	2.7
52	2u	24	ARG	2.7
16	1U	117	GLN	2.7
54	1w	18	G	2.7
22	20	68	GLU	2.7
34	2c	86	VAL	2.7
41	2j	64	GLU	2.7
21	2Z	21	ALA	2.7
22	20	5	LYS	2.7
45	2n	17	LYS	2.7
1	1A	2142	C	2.7
1	2A	2177	C	2.7
1	2A	229	A	2.7
32	2a	1532	U	2.7
20	2Y	107	ASP	2.7
7	2H	45	VAL	2.7
33	1b	165	VAL	2.7
6	2G	20	ILE	2.6
41	1j	4	ILE	2.6
41	2j	8	LEU	2.7
33	1b	132	LYS	2.6
35	1d	195	ALA	2.6
43	2l	68	ALA	2.6
45	2n	20	ALA	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	1089	G	2.6
40	2i	4	TYR	2.6
1	1A	1075	C	2.6
26	24	54	GLY	2.6
1	1A	1094	U	2.6
1	2A	2897	U	2.6
11	1P	119	GLU	2.6
14	2S	11	LYS	2.6
21	2Z	124	ILE	2.6
43	1l	13	LYS	2.6
45	2n	7	ILE	2.6
50	2s	32	LYS	2.6
54	2y	66	A	2.6
26	24	59	PHE	2.6
12	2Q	6	ARG	2.6
44	2m	104	ARG	2.6
50	2s	76	PRO	2.6
1	2A	885	C	2.6
26	24	50	VAL	2.6
41	1j	34	VAL	2.6
42	2k	14	VAL	2.6
54	1w	68	C	2.6
33	2b	166	ASP	2.6
45	2n	36	PHE	2.6
12	2Q	15	GLY	2.6
45	2n	54	PRO	2.6
51	1t	98	PRO	2.6
45	2n	40	CYS	2.6
1	1A	1056	G	2.6
1	2A	2156	G	2.6
21	2Z	5	LEU	2.6
33	2b	187	LEU	2.6
40	2i	110	GLU	2.6
43	1l	7	ILE	2.6
54	2y	2	G	2.6
45	2n	16	PHE	2.6
54	2y	73	A	2.6
7	2H	36	PRO	2.6
26	24	67	TYR	2.6
33	1b	202	PRO	2.6
34	2c	23	TYR	2.6
44	2m	90	LEU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	1F	89	VAL	2.6
8	1I	122	GLU	2.6
41	2j	61	GLU	2.6
1	2A	1533	G	2.5
54	1y	1	G	2.5
54	1y	24	G	2.5
54	2y	22	G	2.5
6	2G	95	ARG	2.5
51	1t	8	ARG	2.5
54	1w	13	C	2.5
3	2D	5	LYS	2.5
1	2A	2119	A	2.5
32	1a	344	A	2.5
33	2b	131	PRO	2.5
54	2y	9	A	2.5
45	2n	55	GLY	2.5
33	1b	236	TYR	2.5
21	2Z	171	ILE	2.5
34	2c	68	VAL	2.5
26	14	59	PHE	2.5
33	2b	122	PHE	2.5
34	2c	189	ALA	2.5
41	2j	60	ARG	2.5
34	2c	6	HIS	2.5
21	1Z	166	SER	2.5
32	1a	1025	U	2.5
54	1y	12	U	2.5
1	2A	2153	G	2.5
32	1a	1030(A)	G	2.5
54	1w	15	G	2.5
54	2w	18	G	2.5
1	2A	886	C	2.5
1	2A	2175	C	2.5
19	2X	92	LEU	2.5
21	2Z	57	ILE	2.5
34	2c	48	TYR	2.5
32	1a	1503	A	2.5
21	1Z	170	THR	2.5
41	1j	100	THR	2.5
33	1b	188	ALA	2.5
50	2s	24	ALA	2.5
14	1S	3	ARG	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
15	1T	112	ARG	2.5
47	1p	81	ARG	2.5
38	1g	153	HIS	2.5
41	2j	14	LYS	2.5
32	1a	204	U	2.5
33	1b	11	LEU	2.5
39	1h	2	LEU	2.5
40	2i	56	LEU	2.5
51	1t	10	LEU	2.5
36	2e	109	ILE	2.5
41	2j	10	GLY	2.5
41	2j	93	GLY	2.5
1	1A	888	C	2.5
1	1A	898	C	2.5
1	1A	1509	C	2.5
38	2g	154	TYR	2.5
54	2y	65	C	2.5
54	2w	57	G	2.5
33	1b	134	GLU	2.5
9	2N	8	GLN	2.5
36	2e	20	GLN	2.5
36	2e	21	ALA	2.5
1	2A	2117	A	2.5
6	2G	51	ARG	2.5
34	1c	87	LEU	2.5
51	2t	13	LEU	2.5
34	2c	73	PRO	2.5
21	1Z	147	GLY	2.5
34	2c	207	VAL	2.5
40	2i	109	VAL	2.5
34	2c	90	GLU	2.5
21	2Z	173	ALA	2.5
41	2j	33	GLN	2.5
1	2A	2174	C	2.5
42	1k	51	LYS	2.5
54	1w	71	C	2.5
54	1y	5	G	2.5
1	2A	2158	A	2.5
32	2a	1035	A	2.5
7	2H	71	LEU	2.4
20	2Y	1	MET	2.4
21	1Z	150	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	1026	U	2.4
29	17	47	ARG	2.4
38	2g	3	ARG	2.4
1	2A	2803	C	2.4
12	2Q	1	MET	2.4
34	2c	94	LEU	2.4
1	1A	1067	A	2.4
53	1v	13	A	2.4
1	1A	1087	G	2.4
21	2Z	93	ASP	2.4
54	1y	19	G	2.4
54	2y	24	G	2.4
21	2Z	52	SER	2.4
34	2c	154	SER	2.4
1	2A	2113	U	2.4
6	2G	29	TRP	2.4
33	2b	34	ALA	2.4
34	2c	24	ALA	2.4
34	2c	32	LEU	2.4
41	2j	34	VAL	2.4
41	2j	49	VAL	2.4
32	2a	1531	A	2.4
1	1A	1063	G	2.4
26	24	66	SER	2.4
32	1a	1024	G	2.4
54	2w	15	G	2.4
54	2y	18	G	2.4
6	1G	50	ALA	2.4
8	2I	146	ALA	2.4
33	1b	120	ALA	2.4
41	2j	27	ALA	2.4
41	2j	87	THR	2.4
33	2b	19	HIS	2.4
34	2c	31	HIS	2.4
40	1i	102	LEU	2.4
41	2j	90	LEU	2.4
50	2s	71	LEU	2.4
6	2G	52	ILE	2.4
41	1j	76	ASN	2.4
38	1g	82	GLY	2.4
35	2d	47	ARG	2.4
1	1A	1095	A	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	2b	17	PHE	2.4
41	2j	54	PHE	2.4
33	1b	12	GLU	2.4
38	1g	83	ALA	2.4
40	2i	13	ALA	2.4
40	2i	45	ALA	2.4
6	1G	76	SER	2.4
41	2j	30	SER	2.4
1	2A	2127	G	2.4
32	2a	976	G	2.4
54	1y	47	U	2.4
54	2y	53	G	2.4
54	2y	57	G	2.4
6	2G	173	LEU	2.4
35	1d	135	LEU	2.4
33	1b	172	ILE	2.4
41	2j	6	ILE	2.4
50	2s	49	ILE	2.4
6	2G	91	ARG	2.3
7	2H	52	VAL	2.3
20	2Y	34	LYS	2.3
33	2b	136	VAL	2.3
38	1g	4	ARG	2.3
41	2j	66	ARG	2.3
52	1u	2	GLY	2.3
52	1u	24	ARG	2.3
33	2b	205	ASP	2.3
12	2Q	139	GLU	2.3
41	1j	32	ALA	2.3
32	2a	1030	C	2.3
1	1A	1057	A	2.3
1	2A	2176	A	2.3
50	2s	35	SER	2.3
34	2c	47	LEU	2.3
41	2j	100	THR	2.3
1	2A	2172	U	2.3
32	2a	1257	U	2.3
34	2c	134	ILE	2.3
20	2Y	46	LYS	2.3
51	1t	74	LYS	2.3
1	2A	1171	G	2.3
7	2H	43	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	2H	60	ARG	2.3
32	2a	1034	G	2.3
45	2n	35	ARG	2.3
50	2s	81	ARG	2.3
54	2y	5	G	2.3
4	2E	115	GLY	2.3
40	2i	33	PHE	2.3
21	2Z	152	ALA	2.3
35	1d	150	GLU	2.3
40	1i	2	GLU	2.3
12	2Q	103	MET	2.3
20	1Y	1	MET	2.3
33	1b	233	SER	2.3
33	2b	40	HIS	2.3
1	1A	1054	A	2.3
6	1G	51	ARG	2.3
26	24	58	ARG	2.3
21	2Z	161	VAL	2.3
34	2c	75	VAL	2.3
35	2d	170	VAL	2.3
52	2u	2	GLY	2.3
1	2A	882	G	2.3
1	2A	2131	G	2.3
1	2A	2165	G	2.3
1	2A	2206	G	2.3
32	2a	1002	G	2.3
32	2a	1003	G	2.3
38	1g	2	ALA	2.3
54	2y	1	G	2.3
11	2P	45	LEU	2.3
34	2c	91	LEU	2.3
33	2b	208	ILE	2.3
34	1c	135	LYS	2.3
34	2c	4	LYS	2.3
47	2p	19	ILE	2.3
34	2c	192	THR	2.3
40	2i	62	TYR	2.3
7	2H	29	PRO	2.3
54	2y	14	A	2.3
55	1x	68	C	2.3
1	2A	2132	U	2.3
54	1w	67	U	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	2c	41	GLY	2.3
38	2g	133	GLY	2.3
41	1j	31	GLY	2.3
5	2F	166	ALA	2.3
7	2H	124	GLU	2.3
11	1P	149	GLU	2.3
6	2G	19	LEU	2.3
21	2Z	70	LEU	2.3
21	2Z	150	LEU	2.3
7	1H	175	LYS	2.3
34	2c	97	LYS	2.3
1	2A	2112	G	2.3
1	2A	2121	G	2.3
32	2a	1058	G	2.3
33	1b	214	ILE	2.3
41	1j	74	ILE	2.3
7	1H	2	SER	2.3
14	2S	17	ARG	2.3
20	2Y	45	VAL	2.3
21	2Z	167	PRO	2.3
34	2c	153	VAL	2.3
35	1d	167	GLY	2.3
44	2m	100	GLY	2.3
1	1A	1177	A	2.2
1	2A	884	C	2.2
32	2a	1116	C	2.2
54	1w	69	A	2.2
54	1y	70	C	2.2
41	2j	86	MET	2.2
3	2D	2	ALA	2.2
6	2G	164	GLU	2.2
11	2P	149	GLU	2.2
40	2i	12	GLU	2.2
22	20	84	LEU	2.2
45	2n	6	LEU	2.2
34	2c	77	ILE	2.2
45	2n	49	HIS	2.2
6	2G	38	VAL	2.2
21	1Z	105	VAL	2.2
33	2b	7	VAL	2.2
44	2m	23	TYR	2.2
40	1i	115	GLY	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	2130	U	2.2
1	2A	2167	U	2.2
33	2b	11	LEU	2.2
32	1a	1027	C	2.2
32	2a	1114	C	2.2
32	2a	1115	C	2.2
34	2c	14	ILE	2.2
34	2c	84	ILE	2.2
48	1q	36	ILE	2.2
34	2c	190	ARG	2.2
7	2H	17	VAL	2.2
17	1V	49	THR	2.2
33	1b	229	VAL	2.2
34	2c	67	THR	2.2
38	2g	54	THR	2.2
26	24	63	TYR	2.2
51	1t	11	SER	2.2
41	2j	52	GLY	2.2
45	2n	37	PHE	2.2
1	1A	1093	G	2.2
1	1A	2112	G	2.2
34	2c	92	ALA	2.2
39	2h	99	GLU	2.2
40	2i	19	LEU	2.2
40	2i	96	LEU	2.2
47	1p	49	LEU	2.2
54	1w	47	U	2.2
20	2Y	57	GLN	2.2
41	1j	33	GLN	2.2
41	2j	50	ILE	2.2
32	2a	1447	A	2.2
54	1y	21	A	2.2
1	2A	1509	C	2.2
54	1y	25	C	2.2
54	2w	31	C	2.2
40	2i	105	ASP	2.2
21	2Z	105	VAL	2.2
33	1b	136	VAL	2.2
33	1b	232	PRO	2.2
34	2c	99	VAL	2.2
50	1s	9	VAL	2.2
41	2j	42	THR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
41	2j	36	GLY	2.2
43	2l	64	TYR	2.2
45	2n	51	GLY	2.2
50	2s	4	SER	2.2
50	2s	26	GLY	2.2
51	2t	96	GLY	2.2
33	1b	163	PHE	2.2
34	2c	42	LEU	2.2
48	2q	74	LEU	2.2
51	2t	97	ALA	2.2
6	2G	181	ARG	2.2
7	1H	3	ARG	2.2
33	2b	172	ILE	2.2
50	2s	78	ARG	2.2
34	2c	3	ASN	2.2
54	2y	4	U	2.2
1	1A	879	G	2.2
1	1A	2115	G	2.2
1	2A	214	G	2.2
32	2a	993	G	2.2
1	1A	1084	A	2.2
1	2A	2171	A	2.2
21	2Z	154	ASP	2.2
32	1a	1030(D)	A	2.2
32	2a	1357	A	2.2
41	1j	89	ASP	2.2
1	1A	2803	C	2.2
54	1y	56	C	2.2
54	2y	13	C	2.2
35	2d	167	GLY	2.2
20	2Y	55	TYR	2.2
33	2b	152	PHE	2.2
35	1d	110	PHE	2.2
36	2e	45	PHE	2.2
21	2Z	157	LEU	2.2
33	2b	215	LEU	2.2
50	1s	4	SER	2.2
44	2m	118	ALA	2.2
46	2o	88	ARG	2.1
32	1a	1532	U	2.1
33	1b	93	VAL	2.1
35	2d	29	PRO	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
41	1j	86	MET	2.1
42	1k	81	ASP	2.1
1	2A	2157	G	2.1
3	2D	259	THR	2.1
32	2a	1001(A)	G	2.1
34	1c	78	GLY	2.1
35	1d	171	GLY	2.1
40	2i	115	GLY	2.1
44	2m	103	THR	2.1
50	2s	77	THR	2.1
53	1v	14	A	2.1
1	2A	2161	C	2.1
6	2G	102	PHE	2.1
12	2Q	37	LEU	2.1
4	2E	151	TYR	2.1
32	2a	1029	C	2.1
32	2a	1359	C	2.1
47	1p	38	TYR	2.1
55	1x	67	C	2.1
38	2g	83	ALA	2.1
45	2n	59	ALA	2.1
5	2F	62	ARG	2.1
43	2l	41	ARG	2.1
7	2H	89	ILE	2.1
33	2b	185	ILE	2.1
40	2i	117	HIS	2.1
20	1Y	92	ASN	2.1
1	2A	2122	U	2.1
51	2t	98	PRO	2.1
11	2P	109	GLY	2.1
21	2Z	143	GLY	2.1
35	2d	23	GLY	2.1
46	2o	89	GLY	2.1
19	2X	95	LEU	2.1
1	1A	1096	A	2.1
40	2i	128	ARG	2.1
54	1y	66	A	2.1
8	2I	122	GLU	2.1
22	20	36	ILE	2.1
32	1a	346	G	2.1
32	2a	962	C	2.1
54	1y	48	C	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	2H	50	VAL	2.1
6	2G	17	PRO	2.1
21	2Z	101	PRO	2.1
55	2x	47	U	2.1
6	2G	42	GLY	2.1
6	2G	172	LEU	2.1
33	2b	196	LEU	2.1
34	1c	9	GLY	2.1
40	2i	67	GLY	2.1
52	2u	4	GLY	2.1
34	2c	95	THR	2.1
40	1i	64	THR	2.1
40	2i	18	PHE	2.1
11	2P	15	ARG	2.1
14	2S	20	ARG	2.1
41	2j	51	ARG	2.1
46	1o	88	ARG	2.1
6	1G	88	ILE	2.1
34	2c	129	ALA	2.1
36	2e	17	ALA	2.1
40	1i	13	ALA	2.1
1	1A	529	A	2.1
1	2A	652(B)	A	2.1
1	2A	2801(A)	A	2.1
34	2c	37	GLN	2.1
1	1A	883	G	2.1
1	1A	897	C	2.1
1	1A	2136	C	2.1
1	2A	11	G	2.1
32	2a	1038	C	2.1
35	1d	169	LYS	2.1
40	1i	117	HIS	2.1
41	2j	68	HIS	2.1
32	2a	1272	G	2.1
35	1d	170	VAL	2.1
43	2l	28	LYS	2.1
45	2n	50	LYS	2.1
54	1y	11	C	2.1
54	2y	32	C	2.1
54	2y	63	G	2.1
33	1b	131	PRO	2.1
41	1j	77	PRO	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
22	20	6	GLY	2.1
36	1e	85	GLY	2.1
39	2h	131	GLY	2.1
51	1t	69	GLY	2.1
4	2E	127	ASP	2.1
17	2V	26	ASP	2.1
23	11	26	ARG	2.1
34	2c	38	ARG	2.1
44	2m	3	ARG	2.1
4	2E	131	ALA	2.1
41	2j	23	ILE	2.1
38	1g	154	TYR	2.1
15	2T	1	MET	2.0
29	27	1	MET	2.0
36	1e	10	MET	2.0
38	1g	77	SER	2.0
9	1N	9	VAL	2.0
50	2s	67	VAL	2.0
54	1y	14	A	2.0
54	2w	14	A	2.0
54	2w	66	A	2.0
1	1A	886	C	2.0
1	1A	2138	C	2.0
1	1A	2140	C	2.0
41	1j	85	LEU	2.0
54	2y	48	C	2.0
54	2y	70	C	2.0
1	1A	1059	G	2.0
40	2i	6	GLY	2.0
40	2i	42	ARG	2.0
54	2w	49	G	2.0
54	2y	39	G	2.0
8	1I	109	ILE	2.0
34	2c	202	ILE	2.0
46	1o	87	ILE	2.0
51	1t	100	ILE	2.0
54	2y	67	U	2.0
33	1b	123	ALA	2.0
51	1t	49	ALA	2.0
7	1H	18	GLU	2.0
21	1Z	2	GLU	2.0
14	2S	7	TYR	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
40	2i	92	TYR	2.0
44	2m	27	LYS	2.0
21	1Z	121	HIS	2.0
21	2Z	121	HIS	2.0
38	2g	86	GLN	2.0
21	2Z	158	PRO	2.0
26	24	29	PRO	2.0
45	2n	14	PRO	2.0
20	2Y	106	LEU	2.0
22	20	7	LEU	2.0
44	2m	48	LEU	2.0
50	2s	30	LEU	2.0
54	2y	69	A	2.0
18	2W	92	ARG	2.0
41	1j	78	ASN	2.0
50	1s	81	ARG	2.0
7	2H	123	PHE	2.0
12	2Q	19	GLY	2.0
12	2Q	65	PHE	2.0
14	2S	29	PHE	2.0
22	20	13	GLY	2.0
34	2c	128	PHE	2.0
41	1j	93	GLY	2.0
1	2A	2146	C	2.0
54	2w	60	C	2.0
54	2y	11	C	2.0
7	2H	150	ALA	2.0
8	2I	86	THR	2.0
41	2j	67	THR	2.0
51	2t	94	ALA	2.0
1	1A	1082	U	2.0
13	2R	69	ASP	2.0
41	2j	83	GLU	2.0
49	2r	38	GLU	2.0
53	2v	23	U	2.0
54	2w	4	U	2.0
3	1D	38	LYS	2.0
14	2S	59	LYS	2.0
32	1a	1026	G	2.0
54	1y	22	G	2.0
54	2y	45	G	2.0
21	1Z	1	MET	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
36	2e	10	MET	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
54	PSU	1y	55	20/21	0.51	0.16	95,103,109,120	0
54	CM0	1y	34	25/26	0.53	0.20	89,95,104,121	0
54	4SU	1y	8	20/21	0.53	0.15	97,103,115,130	0
54	PSU	2y	55	20/21	0.53	0.17	96,103,116,128	0
54	PSU	2w	55	20/21	0.55	0.16	80,102,110,113	0
54	7MG	1y	46	24/25	0.57	0.16	88,104,109,121	0
54	6MZ	1y	37	23/24	0.57	0.20	89,97,110,126	0
54	7MG	2y	46	24/25	0.58	0.15	95,105,113,128	0
54	4SU	2y	8	20/21	0.62	0.14	94,102,118,127	0
54	4SU	2w	8	20/21	0.64	0.15	91,103,115,116	0
54	CM0	2y	34	25/26	0.64	0.23	85,101,107,121	0
54	5MU	2y	54	21/22	0.65	0.17	91,100,114,130	0
54	5MU	2w	54	21/22	0.66	0.15	81,87,94,98	0
54	PSU	1w	55	20/21	0.68	0.19	64,91,100,110	0
54	5MU	1y	54	21/22	0.68	0.14	88,98,107,120	0
54	7MG	2w	46	24/25	0.69	0.14	87,98,108,119	0
54	7MG	1w	46	24/25	0.69	0.15	83,93,101,112	0
54	6MZ	2y	37	23/24	0.69	0.17	92,100,114,137	0
54	4SU	1w	8	20/21	0.80	0.12	84,89,100,104	0
54	5MU	1w	54	21/22	0.81	0.14	57,74,84,89	0
55	PSU	2x	55	20/21	0.81	0.12	75,82,88,93	0
55	4SU	2x	8	20/21	0.83	0.12	78,85,92,96	0
32	2MG	2a	1207	24/25	0.84	0.13	74,89,97,103	0
54	CM0	2w	34	25/26	0.87	0.13	65,79,90,95	0
32	M2G	2a	966	25/26	0.87	0.15	58,66,80,85	0
55	5MU	2x	54	21/22	0.89	0.10	83,87,89,95	0
55	4SU	1x	8	20/21	0.90	0.12	55,64,84,86	0
55	PSU	1x	55	20/21	0.90	0.09	60,66,75,78	0
43	0TD	1l	92	10/11	0.90	0.10	39,46,49,68	0
55	5MC	2x	32	21/22	0.91	0.15	65,72,78,84	0
55	5MU	1x	54	21/22	0.91	0.09	59,71,76,78	0
43	0TD	2l	92	10/11	0.91	0.14	60,65,68,82	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	PSU	2a	516	20/21	0.91	0.09	61,75,81,85	0
32	7MG	2a	527	24/25	0.91	0.12	58,65,72,84	0
32	5MC	2a	1400	21/22	0.92	0.15	60,68,71,76	0
1	5MU	2A	1915	21/22	0.92	0.10	66,73,79,85	0
1	5MU	1A	1915	21/22	0.93	0.10	51,57,61,65	0
1	PSU	2A	1911	20/21	0.93	0.09	57,63,65,75	0
1	PSU	2A	1917	20/21	0.93	0.09	61,65,74,75	0
32	5MC	2a	1404	21/22	0.93	0.10	47,55,64,66	0
32	5MC	2a	967	21/22	0.93	0.11	64,70,78,82	0
54	CM0	1w	34	25/26	0.93	0.10	49,64,67,70	0
55	5MC	1x	32	21/22	0.94	0.11	41,54,60,62	0
32	4OC	2a	1402	22/23	0.94	0.10	56,62,65,70	0
32	2MG	1a	1207	24/25	0.94	0.08	59,66,72,74	0
32	PSU	1a	516	20/21	0.95	0.08	52,57,61,61	0
32	7MG	1a	527	24/25	0.95	0.08	38,45,51,54	0
32	5MC	2a	1407	21/22	0.95	0.09	48,54,58,62	0
32	UR3	2a	1498	21/22	0.95	0.11	54,58,63,70	0
32	MA6	2a	1518	24/25	0.95	0.10	49,61,66,66	0
1	4OC	2A	1920	21/23	0.95	0.09	48,59,64,66	0
1	5MC	2A	1942	21/22	0.95	0.10	51,59,66,73	0
1	PSU	1A	1917	20/21	0.95	0.09	43,49,56,60	0
54	6MZ	2w	37	23/24	0.95	0.08	67,78,83,85	0
1	5MC	2A	1962	21/22	0.95	0.09	43,50,58,67	0
32	MA6	2a	1519	24/25	0.96	0.12	53,59,63,64	0
32	4OC	1a	1402	22/23	0.96	0.09	41,46,52,60	0
32	MA6	1a	1519	24/25	0.96	0.09	32,39,42,47	0
1	PSU	2A	2605	20/21	0.96	0.07	30,37,44,45	0
1	4OC	1A	1920	21/23	0.96	0.08	37,45,50,56	0
32	M2G	1a	966	25/26	0.96	0.09	46,50,58,65	0
32	5MC	1a	967	21/22	0.96	0.10	43,50,56,60	0
1	OMG	2A	2251	24/25	0.96	0.08	35,40,44,44	0
32	5MC	1a	1400	21/22	0.96	0.10	37,50,53,57	0
1	5MC	1A	1962	21/22	0.97	0.07	32,36,42,52	0
1	PSU	1A	2605	20/21	0.97	0.07	22,26,35,35	0
32	5MC	1a	1407	21/22	0.97	0.07	27,39,42,43	0
32	UR3	1a	1498	21/22	0.97	0.09	29,39,43,45	0
32	MA6	1a	1518	24/25	0.97	0.08	30,38,41,42	0
1	2MU	2A	2552	21/23	0.97	0.09	35,39,47,49	0
1	PSU	1A	1911	20/21	0.97	0.07	39,49,52,56	0
1	5MU	2A	1939	21/22	0.97	0.08	35,38,45,46	0
1	2MA	2A	2503	23/24	0.97	0.08	28,36,40,41	0
32	5MC	1a	1404	21/22	0.97	0.10	32,41,49,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	5MC	1A	1942	21/22	0.97	0.09	37,42,47,53	0
1	5MU	1A	1939	21/22	0.98	0.06	20,28,32,37	0
54	6MZ	1w	37	23/24	0.98	0.06	39,48,57,60	0
1	OMG	1A	2251	24/25	0.98	0.06	19,25,27,29	0
1	2MA	1A	2503	23/24	0.98	0.06	17,21,25,28	0
1	2MU	1A	2552	21/23	0.98	0.07	23,27,33,35	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2y	107	1/1	0.40	0.29	95,95,95,95	0
56	MG	2y	106	1/1	0.44	0.35	84,84,84,84	0
56	MG	2a	1649	1/1	0.45	0.12	69,69,69,69	0
56	MG	1A	3394	1/1	0.47	0.16	78,78,78,78	0
56	MG	2A	3684	1/1	0.47	0.17	77,77,77,77	0
56	MG	1B	235	1/1	0.47	0.26	81,81,81,81	0
56	MG	2A	3774	1/1	0.48	0.26	71,71,71,71	0
56	MG	2i	201	1/1	0.48	0.15	78,78,78,78	0
56	MG	2a	1804	1/1	0.49	0.20	79,79,79,79	0
56	MG	2A	3711	1/1	0.50	0.21	62,62,62,62	0
56	MG	2j	202	1/1	0.51	0.20	79,79,79,79	0
56	MG	1A	3282	1/1	0.54	0.20	53,53,53,53	0
56	MG	2F	301	1/1	0.54	0.20	71,71,71,71	0
56	MG	2A	3039	1/1	0.55	0.20	88,88,88,88	0
56	MG	1B	230	1/1	0.55	0.22	83,83,83,83	0
56	MG	2B	221	1/1	0.56	0.32	82,82,82,82	0
56	MG	2A	3639	1/1	0.56	0.24	62,62,62,62	0
56	MG	1A	3848	1/1	0.57	0.30	37,37,37,37	0
56	MG	2A	3781	1/1	0.58	0.25	60,60,60,60	0
56	MG	1a	1828	1/1	0.58	0.21	57,57,57,57	0
56	MG	2a	1756	1/1	0.58	0.18	72,72,72,72	0
56	MG	1A	4008	1/1	0.58	0.16	79,79,79,79	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3574	1/1	0.59	0.19	66,66,66,66	0
56	MG	2a	1831	1/1	0.59	0.38	80,80,80,80	0
56	MG	1A	3736	1/1	0.60	0.20	76,76,76,76	0
56	MG	1A	3511	1/1	0.61	0.23	67,67,67,67	0
56	MG	2A	3391	1/1	0.61	0.15	79,79,79,79	0
56	MG	2a	1652	1/1	0.61	0.27	82,82,82,82	0
56	MG	2y	105	1/1	0.61	0.36	93,93,93,93	0
56	MG	1y	104	1/1	0.61	0.47	87,87,87,87	0
56	MG	1A	4072	1/1	0.61	0.27	71,71,71,71	0
56	MG	2A	3056	1/1	0.62	0.21	74,74,74,74	0
56	MG	2a	1815	1/1	0.62	0.18	75,75,75,75	0
56	MG	2A	3606	1/1	0.62	0.26	79,79,79,79	0
56	MG	1y	103	1/1	0.62	0.43	76,76,76,76	0
56	MG	2a	1671	1/1	0.63	0.14	68,68,68,68	0
56	MG	2a	1733	1/1	0.63	0.16	96,96,96,96	0
56	MG	2A	3317	1/1	0.63	0.32	74,74,74,74	0
56	MG	2v	102	1/1	0.63	0.18	79,79,79,79	0
56	MG	2A	3136	1/1	0.63	0.30	63,63,63,63	0
56	MG	2A	3256	1/1	0.63	0.24	71,71,71,71	0
56	MG	2a	1821	1/1	0.63	0.27	72,72,72,72	0
56	MG	1A	4086	1/1	0.64	0.17	62,62,62,62	0
56	MG	1A	4081	1/1	0.64	0.83	92,92,92,92	0
56	MG	2A	3331	1/1	0.64	0.23	66,66,66,66	0
56	MG	2a	1703	1/1	0.64	0.29	81,81,81,81	0
56	MG	2a	1625	1/1	0.65	0.14	74,74,74,74	0
56	MG	2B	201	1/1	0.66	0.30	81,81,81,81	0
56	MG	1A	3979	1/1	0.66	0.23	92,92,92,92	0
56	MG	2a	1819	1/1	0.66	0.27	69,69,69,69	0
56	MG	1A	3822	1/1	0.66	0.17	77,77,77,77	0
56	MG	2a	1826	1/1	0.66	0.17	75,75,75,75	0
56	MG	2a	1653	1/1	0.66	0.18	87,87,87,87	0
56	MG	2A	3191	1/1	0.67	0.35	72,72,72,72	0
56	MG	2a	1630	1/1	0.67	0.17	71,71,71,71	0
56	MG	2a	1778	1/1	0.67	0.22	67,67,67,67	0
56	MG	1A	3678	1/1	0.67	0.15	64,64,64,64	0
56	MG	2a	1651	1/1	0.67	0.33	85,85,85,85	0
56	MG	2A	3162	1/1	0.68	0.29	70,70,70,70	0
56	MG	2A	3119	1/1	0.68	0.23	70,70,70,70	0
56	MG	1A	3002	1/1	0.68	0.23	57,57,57,57	0
56	MG	2B	206	1/1	0.68	0.15	76,76,76,76	0
56	MG	2A	3395	1/1	0.68	0.15	75,75,75,75	0
56	MG	2A	3402	1/1	0.68	0.38	76,76,76,76	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1w	102	1/1	0.68	0.18	63,63,63,63	0
56	MG	2a	1825	1/1	0.68	0.23	72,72,72,72	0
56	MG	2A	3561	1/1	0.69	0.29	64,64,64,64	0
56	MG	2A	3719	1/1	0.69	0.11	90,90,90,90	0
56	MG	1A	3639	1/1	0.69	0.13	70,70,70,70	0
56	MG	1A	3779	1/1	0.69	0.25	80,80,80,80	0
56	MG	2a	1714	1/1	0.69	0.25	81,81,81,81	0
56	MG	2A	3376	1/1	0.69	0.20	73,73,73,73	0
56	MG	2A	3547	1/1	0.69	0.20	73,73,73,73	0
56	MG	2a	1808	1/1	0.70	0.27	75,75,75,75	0
56	MG	1x	111	1/1	0.70	0.23	62,62,62,62	0
56	MG	2A	3004	1/1	0.70	0.32	82,82,82,82	0
56	MG	2A	3632	1/1	0.70	0.24	68,68,68,68	0
56	MG	1y	105	1/1	0.70	0.20	63,63,63,63	0
56	MG	1A	3834	1/1	0.70	0.21	51,51,51,51	0
56	MG	2A	3653	1/1	0.70	0.26	60,60,60,60	0
56	MG	2a	1708	1/1	0.70	0.24	70,70,70,70	0
56	MG	2A	3678	1/1	0.70	0.15	85,85,85,85	0
56	MG	1a	1658	1/1	0.70	0.11	61,61,61,61	0
56	MG	2a	1617	1/1	0.70	0.16	73,73,73,73	0
56	MG	2A	3285	1/1	0.70	0.18	64,64,64,64	0
56	MG	1A	4146	1/1	0.70	0.29	45,45,45,45	0
56	MG	1H	201	1/1	0.71	0.18	69,69,69,69	0
56	MG	2a	1800	1/1	0.71	0.22	71,71,71,71	0
56	MG	1U	202	1/1	0.71	0.16	56,56,56,56	0
56	MG	2A	3630	1/1	0.71	0.15	73,73,73,73	0
56	MG	1a	1686	1/1	0.71	0.16	62,62,62,62	0
56	MG	1a	1719	1/1	0.71	0.23	85,85,85,85	0
56	MG	1A	4061	1/1	0.71	0.23	65,65,65,65	0
56	MG	2A	3228	1/1	0.71	0.31	68,68,68,68	0
56	MG	2B	218	1/1	0.72	0.17	76,76,76,76	0
56	MG	2a	1627	1/1	0.72	0.21	63,63,63,63	0
56	MG	2a	1810	1/1	0.72	0.19	76,76,76,76	0
56	MG	2A	3369	1/1	0.72	0.22	68,68,68,68	0
56	MG	1v	101	1/1	0.72	0.24	67,67,67,67	0
56	MG	2a	1780	1/1	0.72	0.20	67,67,67,67	0
56	MG	2a	1824	1/1	0.72	0.24	71,71,71,71	0
56	MG	1A	3622	1/1	0.72	0.19	68,68,68,68	0
56	MG	1A	4003	1/1	0.73	0.15	84,84,84,84	0
56	MG	1A	3586	1/1	0.73	0.19	76,76,76,76	0
56	MG	2A	3283	1/1	0.73	0.16	75,75,75,75	0
56	MG	2a	1806	1/1	0.73	0.22	76,76,76,76	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1693	1/1	0.73	0.20	62,62,62,62	0
56	MG	1a	1706	1/1	0.73	0.20	59,59,59,59	0
56	MG	2A	3436	1/1	0.73	0.19	71,71,71,71	0
56	MG	1a	1813	1/1	0.73	0.17	63,63,63,63	0
56	MG	2A	3128	1/1	0.73	0.21	70,70,70,70	0
56	MG	2A	3304	1/1	0.73	0.26	66,66,66,66	0
56	MG	1w	101	1/1	0.73	0.23	67,67,67,67	0
56	MG	2A	3724	1/1	0.73	0.21	86,86,86,86	0
56	MG	1x	108	1/1	0.73	0.26	73,73,73,73	0
56	MG	1A	3810	1/1	0.73	0.17	61,61,61,61	0
56	MG	2A	3159	1/1	0.73	0.22	71,71,71,71	0
56	MG	2A	3625	1/1	0.73	0.20	72,72,72,72	0
56	MG	1A	4063	1/1	0.73	0.18	54,54,54,54	0
56	MG	1D	303	1/1	0.73	0.17	45,45,45,45	0
56	MG	1A	3672	1/1	0.73	0.12	49,49,49,49	0
56	MG	2A	3163	1/1	0.74	0.31	76,76,76,76	0
56	MG	2A	3355	1/1	0.74	0.12	67,67,67,67	0
56	MG	2B	208	1/1	0.74	0.14	64,64,64,64	0
56	MG	2A	3164	1/1	0.74	0.20	66,66,66,66	0
56	MG	1a	1834	1/1	0.74	0.19	73,73,73,73	0
56	MG	2A	3129	1/1	0.74	0.21	71,71,71,71	0
56	MG	2A	3699	1/1	0.74	0.15	81,81,81,81	0
56	MG	2a	1830	1/1	0.74	0.25	60,60,60,60	0
56	MG	1A	3862	1/1	0.74	0.44	44,44,44,44	0
56	MG	15	103	1/1	0.74	0.23	60,60,60,60	0
56	MG	2a	1792	1/1	0.74	0.14	82,82,82,82	0
56	MG	2A	3392	1/1	0.74	0.44	72,72,72,72	0
56	MG	2A	3312	1/1	0.74	0.21	71,71,71,71	0
56	MG	2A	3734	1/1	0.74	0.14	51,51,51,51	0
56	MG	2A	3246	1/1	0.74	0.29	75,75,75,75	0
56	MG	1A	4017	1/1	0.75	0.11	70,70,70,70	0
56	MG	1E	306	1/1	0.75	0.16	59,59,59,59	0
56	MG	1A	3817	1/1	0.75	0.22	56,56,56,56	0
56	MG	2A	3605	1/1	0.75	0.24	62,62,62,62	0
56	MG	1A	3230	1/1	0.75	0.16	50,50,50,50	0
56	MG	2A	3721	1/1	0.75	0.21	69,69,69,69	0
56	MG	1a	1664	1/1	0.75	0.29	64,64,64,64	0
56	MG	1A	3607	1/1	0.75	0.20	61,61,61,61	0
56	MG	2A	3054	1/1	0.75	0.19	82,82,82,82	0
56	MG	2A	3252	1/1	0.75	0.19	71,71,71,71	0
56	MG	2A	3353	1/1	0.75	0.10	66,66,66,66	0
56	MG	1a	1738	1/1	0.75	0.18	59,59,59,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3785	1/1	0.75	0.16	65,65,65,65	0
56	MG	2A	3457	1/1	0.75	0.09	66,66,66,66	0
56	MG	2v	103	1/1	0.75	0.22	78,78,78,78	0
56	MG	2a	1603	1/1	0.75	0.16	63,63,63,63	0
56	MG	1A	3289	1/1	0.75	0.17	46,46,46,46	0
56	MG	1b	302	1/1	0.75	0.17	86,86,86,86	0
56	MG	2A	3152	1/1	0.76	0.31	73,73,73,73	0
56	MG	2A	3258	1/1	0.76	0.17	61,61,61,61	0
56	MG	2a	1763	1/1	0.76	0.16	85,85,85,85	0
56	MG	2A	3377	1/1	0.76	0.24	70,70,70,70	0
56	MG	2A	3275	1/1	0.76	0.16	58,58,58,58	0
56	MG	1A	4009	1/1	0.76	0.12	74,74,74,74	0
56	MG	1A	3504	1/1	0.76	0.12	57,57,57,57	0
56	MG	2B	217	1/1	0.76	0.18	58,58,58,58	0
56	MG	2A	3397	1/1	0.76	0.18	67,67,67,67	0
56	MG	2a	1807	1/1	0.76	0.12	64,64,64,64	0
56	MG	2A	3089	1/1	0.76	0.20	69,69,69,69	0
56	MG	2A	3411	1/1	0.76	0.11	65,65,65,65	0
56	MG	2a	1812	1/1	0.76	0.14	74,74,74,74	0
56	MG	2a	1814	1/1	0.76	0.25	59,59,59,59	0
56	MG	1A	3364	1/1	0.76	0.18	55,55,55,55	0
56	MG	2A	3439	1/1	0.76	0.22	65,65,65,65	0
56	MG	2a	1620	1/1	0.76	0.15	80,80,80,80	0
56	MG	2A	3122	1/1	0.76	0.21	73,73,73,73	0
56	MG	2A	3328	1/1	0.76	0.19	70,70,70,70	0
56	MG	2A	3765	1/1	0.76	0.23	54,54,54,54	0
56	MG	2a	1829	1/1	0.76	0.18	69,69,69,69	0
56	MG	2a	1648	1/1	0.76	0.12	81,81,81,81	0
56	MG	2A	3772	1/1	0.76	0.21	65,65,65,65	0
56	MG	1A	3842	1/1	0.76	0.25	70,70,70,70	0
56	MG	2A	3345	1/1	0.76	0.32	73,73,73,73	0
56	MG	1A	3206	1/1	0.76	0.13	54,54,54,54	0
56	MG	1B	223	1/1	0.76	0.17	57,57,57,57	0
56	MG	2w	101	1/1	0.76	0.17	70,70,70,70	0
56	MG	2A	3040	1/1	0.76	0.16	68,68,68,68	0
56	MG	2A	3614	1/1	0.76	0.23	66,66,66,66	0
56	MG	1x	112	1/1	0.76	0.20	65,65,65,65	0
56	MG	2A	3549	1/1	0.77	0.23	58,58,58,58	0
56	MG	1s	3701	1/1	0.77	0.23	61,61,61,61	0
56	MG	2A	3703	1/1	0.77	0.14	57,57,57,57	0
56	MG	1A	3413	1/1	0.77	0.16	56,56,56,56	0
56	MG	1A	3872	1/1	0.77	0.31	64,64,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3896	1/1	0.77	0.14	52,52,52,52	0
56	MG	1A	3964	1/1	0.77	0.19	77,77,77,77	0
56	MG	2A	3121	1/1	0.77	0.17	54,54,54,54	0
56	MG	2A	3739	1/1	0.77	0.12	68,68,68,68	0
56	MG	2A	3746	1/1	0.77	0.14	65,65,65,65	0
56	MG	2A	3325	1/1	0.77	0.19	69,69,69,69	0
56	MG	2A	3445	1/1	0.77	0.24	67,67,67,67	0
56	MG	2A	3453	1/1	0.77	0.11	77,77,77,77	0
56	MG	2a	1719	1/1	0.77	0.20	75,75,75,75	0
56	MG	2a	1728	1/1	0.77	0.27	74,74,74,74	0
56	MG	2e	201	1/1	0.77	0.11	79,79,79,79	0
56	MG	1A	3467	1/1	0.77	0.24	67,67,67,67	0
56	MG	1a	1742	1/1	0.77	0.20	77,77,77,77	0
56	MG	1a	1808	1/1	0.77	0.20	61,61,61,61	0
56	MG	2A	3460	1/1	0.77	0.20	68,68,68,68	0
56	MG	2A	3480	1/1	0.77	0.23	66,66,66,66	0
56	MG	2y	103	1/1	0.77	0.18	79,79,79,79	0
56	MG	1A	3125	1/1	0.77	0.26	34,34,34,34	0
56	MG	2a	1606	1/1	0.77	0.17	61,61,61,61	0
56	MG	1a	1839	1/1	0.77	0.14	76,76,76,76	0
56	MG	2A	3166	1/1	0.78	0.20	67,67,67,67	0
56	MG	1a	1671	1/1	0.78	0.17	53,53,53,53	0
56	MG	1a	1674	1/1	0.78	0.28	61,61,61,61	0
56	MG	2A	3424	1/1	0.78	0.21	69,69,69,69	0
56	MG	2A	3617	1/1	0.78	0.27	74,74,74,74	0
56	MG	2A	3753	1/1	0.78	0.17	50,50,50,50	0
56	MG	1a	1717	1/1	0.78	0.08	48,48,48,48	0
56	MG	2A	3426	1/1	0.78	0.14	63,63,63,63	0
56	MG	2A	3167	1/1	0.78	0.23	80,80,80,80	0
56	MG	1A	3905	1/1	0.78	0.29	55,55,55,55	0
56	MG	1a	1771	1/1	0.78	0.14	59,59,59,59	0
56	MG	1A	3502	1/1	0.78	0.17	55,55,55,55	0
56	MG	2A	3233	1/1	0.78	0.12	78,78,78,78	0
56	MG	2A	3838	1/1	0.78	0.23	83,83,83,83	0
56	MG	1a	1832	1/1	0.78	0.27	66,66,66,66	0
56	MG	2A	3845	1/1	0.78	0.14	66,66,66,66	0
56	MG	1B	209	1/1	0.78	0.28	57,57,57,57	0
56	MG	1B	217	1/1	0.78	0.16	50,50,50,50	0
56	MG	2A	3235	1/1	0.78	0.19	79,79,79,79	0
56	MG	1t	201	1/1	0.78	0.21	56,56,56,56	0
56	MG	2a	1661	1/1	0.78	0.19	83,83,83,83	0
56	MG	2A	3380	1/1	0.78	0.14	57,57,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	1702	1/1	0.78	0.18	69,69,69,69	0
56	MG	2A	3236	1/1	0.78	0.15	59,59,59,59	0
56	MG	2q	201	1/1	0.78	0.14	63,63,63,63	0
56	MG	2q	203	1/1	0.78	0.17	75,75,75,75	0
56	MG	1A	3966	1/1	0.78	0.22	67,67,67,67	0
56	MG	2A	3031	1/1	0.78	0.19	64,64,64,64	0
56	MG	2a	1718	1/1	0.78	0.31	72,72,72,72	0
56	MG	2x	104	1/1	0.78	0.27	72,72,72,72	0
56	MG	2A	3712	1/1	0.78	0.11	79,79,79,79	0
56	MG	1A	3468	1/1	0.78	0.21	82,82,82,82	0
56	MG	2A	3340	1/1	0.78	0.11	69,69,69,69	0
56	MG	2A	3410	1/1	0.78	0.23	70,70,70,70	0
56	MG	1B	233	1/1	0.79	0.14	57,57,57,57	0
56	MG	2a	1811	1/1	0.79	0.11	72,72,72,72	0
56	MG	1A	4041	1/1	0.79	0.11	25,25,25,25	0
56	MG	1A	3260	1/1	0.79	0.12	44,44,44,44	0
56	MG	2a	1659	1/1	0.79	0.14	73,73,73,73	0
56	MG	1A	3505	1/1	0.79	0.21	75,75,75,75	0
56	MG	2A	3685	1/1	0.79	0.16	63,63,63,63	0
56	MG	2A	3691	1/1	0.79	0.14	79,79,79,79	0
56	MG	12	101	1/1	0.79	0.16	56,56,56,56	0
56	MG	2a	1707	1/1	0.79	0.21	76,76,76,76	0
56	MG	1A	3760	1/1	0.79	0.13	25,25,25,25	0
56	MG	1a	1644	1/1	0.79	0.15	60,60,60,60	0
56	MG	1a	1657	1/1	0.79	0.19	69,69,69,69	0
56	MG	2A	3456	1/1	0.79	0.16	70,70,70,70	0
56	MG	2A	3706	1/1	0.79	0.18	66,66,66,66	0
56	MG	2j	201	1/1	0.79	0.15	58,58,58,58	0
56	MG	2a	1614	1/1	0.79	0.17	67,67,67,67	0
56	MG	2A	3044	1/1	0.79	0.18	74,74,74,74	0
56	MG	1A	3291	1/1	0.79	0.27	66,66,66,66	0
56	MG	2a	1622	1/1	0.79	0.12	72,72,72,72	0
56	MG	2a	1624	1/1	0.79	0.15	70,70,70,70	0
56	MG	1A	3952	1/1	0.79	0.15	41,41,41,41	0
56	MG	1A	3293	1/1	0.79	0.19	56,56,56,56	0
56	MG	1a	1704	1/1	0.79	0.18	62,62,62,62	0
56	MG	2a	1641	1/1	0.79	0.27	70,70,70,70	0
56	MG	2A	3435	1/1	0.79	0.33	54,54,54,54	0
56	MG	2A	3640	1/1	0.79	0.15	48,48,48,48	0
56	MG	2a	1737	1/1	0.80	0.14	84,84,84,84	0
56	MG	2B	216	1/1	0.80	0.25	69,69,69,69	0
56	MG	2A	3650	1/1	0.80	0.23	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3822	1/1	0.80	0.17	63,63,63,63	0
56	MG	2A	3057	1/1	0.80	0.21	71,71,71,71	0
56	MG	2A	3675	1/1	0.80	0.23	55,55,55,55	0
56	MG	2P	201	1/1	0.80	0.19	63,63,63,63	0
56	MG	25	104	1/1	0.80	0.18	65,65,65,65	0
56	MG	1A	3425	1/1	0.80	0.30	57,57,57,57	0
56	MG	1a	1760	1/1	0.80	0.16	58,58,58,58	0
56	MG	2a	1609	1/1	0.80	0.18	76,76,76,76	0
56	MG	1a	1767	1/1	0.80	0.09	91,91,91,91	0
56	MG	2A	3362	1/1	0.80	0.10	69,69,69,69	0
56	MG	2A	3455	1/1	0.80	0.13	79,79,79,79	0
56	MG	2A	3262	1/1	0.80	0.14	54,54,54,54	0
56	MG	1A	3459	1/1	0.80	0.17	62,62,62,62	0
56	MG	2A	3280	1/1	0.80	0.19	59,59,59,59	0
56	MG	1A	3466	1/1	0.80	0.29	66,66,66,66	0
56	MG	2A	3389	1/1	0.80	0.16	69,69,69,69	0
56	MG	2A	3030	1/1	0.80	0.27	68,68,68,68	0
56	MG	1P	202	1/1	0.80	0.14	57,57,57,57	0
56	MG	2A	3199	1/1	0.80	0.25	61,61,61,61	0
56	MG	2a	1650	1/1	0.80	0.14	69,69,69,69	0
56	MG	2A	3305	1/1	0.80	0.16	68,68,68,68	0
56	MG	1A	3789	1/1	0.80	0.11	53,53,53,53	0
56	MG	2f	202	1/1	0.80	0.23	68,68,68,68	0
56	MG	2A	3232	1/1	0.80	0.17	61,61,61,61	0
56	MG	2A	3406	1/1	0.80	0.12	63,63,63,63	0
56	MG	1A	4067	1/1	0.80	0.28	83,83,83,83	0
56	MG	2l	202	1/1	0.80	0.09	60,60,60,60	0
56	MG	1A	4068	1/1	0.80	0.14	54,54,54,54	0
56	MG	2A	3755	1/1	0.80	0.15	54,54,54,54	0
56	MG	1A	3801	1/1	0.80	0.14	48,48,48,48	0
56	MG	1A	3843	1/1	0.80	0.13	65,65,65,65	0
56	MG	1a	1688	1/1	0.80	0.29	63,63,63,63	0
56	MG	1A	4083	1/1	0.80	0.17	55,55,55,55	0
56	MG	2B	207	1/1	0.80	0.20	69,69,69,69	0
56	MG	2A	3350	1/1	0.80	0.14	63,63,63,63	0
56	MG	2B	209	1/1	0.80	0.21	66,66,66,66	0
56	MG	2B	212	1/1	0.80	0.18	69,69,69,69	0
56	MG	2A	3624	1/1	0.81	0.17	74,74,74,74	0
56	MG	2A	3764	1/1	0.81	0.19	60,60,60,60	0
56	MG	1a	1684	1/1	0.81	0.19	67,67,67,67	0
56	MG	1A	4035	1/1	0.81	0.13	31,31,31,31	0
56	MG	2B	214	1/1	0.81	0.26	71,71,71,71	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3869	1/1	0.81	0.18	61,61,61,61	0
56	MG	2A	3346	1/1	0.81	0.27	60,60,60,60	0
56	MG	2A	3776	1/1	0.81	0.15	61,61,61,61	0
56	MG	2a	1782	1/1	0.81	0.12	72,72,72,72	0
56	MG	1A	3972	1/1	0.81	0.12	20,20,20,20	0
56	MG	2A	3260	1/1	0.81	0.17	51,51,51,51	0
56	MG	2A	3801	1/1	0.81	0.11	86,86,86,86	0
56	MG	1a	1723	1/1	0.81	0.31	60,60,60,60	0
56	MG	2A	3094	1/1	0.81	0.20	67,67,67,67	0
56	MG	2A	3357	1/1	0.81	0.29	59,59,59,59	0
56	MG	2A	3269	1/1	0.81	0.33	71,71,71,71	0
56	MG	2A	3367	1/1	0.81	0.19	65,65,65,65	0
56	MG	1a	1770	1/1	0.81	0.10	93,93,93,93	0
56	MG	2A	3095	1/1	0.81	0.28	44,44,44,44	0
56	MG	1A	3283	1/1	0.81	0.14	55,55,55,55	0
56	MG	2A	3688	1/1	0.81	0.14	53,53,53,53	0
56	MG	1A	3223	1/1	0.81	0.14	56,56,56,56	0
56	MG	2a	1823	1/1	0.81	0.14	61,61,61,61	0
56	MG	1a	1831	1/1	0.81	0.12	69,69,69,69	0
56	MG	2a	1628	1/1	0.81	0.18	65,65,65,65	0
56	MG	2A	3461	1/1	0.81	0.15	65,65,65,65	0
56	MG	2a	1633	1/1	0.81	0.26	68,68,68,68	0
56	MG	1A	3334	1/1	0.81	0.16	43,43,43,43	0
56	MG	2A	3514	1/1	0.81	0.09	58,58,58,58	0
56	MG	1A	3821	1/1	0.81	0.20	64,64,64,64	0
56	MG	1O	201	1/1	0.81	0.13	60,60,60,60	0
56	MG	1A	3717	1/1	0.81	0.13	74,74,74,74	0
56	MG	2A	3133	1/1	0.81	0.17	57,57,57,57	0
56	MG	1U	206	1/1	0.81	0.63	70,70,70,70	0
56	MG	1V	202	1/1	0.81	0.14	68,68,68,68	0
56	MG	2A	3053	1/1	0.81	0.20	69,69,69,69	0
56	MG	2A	3588	1/1	0.81	0.21	71,71,71,71	0
56	MG	2a	1696	1/1	0.81	0.25	73,73,73,73	0
56	MG	2a	1697	1/1	0.81	0.18	76,76,76,76	0
56	MG	2A	3146	1/1	0.81	0.21	52,52,52,52	0
56	MG	1a	1650	1/1	0.81	0.19	57,57,57,57	0
56	MG	2A	3327	1/1	0.81	0.17	67,67,67,67	0
56	MG	2A	3239	1/1	0.81	0.08	52,52,52,52	0
56	MG	1a	1661	1/1	0.81	0.18	72,72,72,72	0
56	MG	1A	4020	1/1	0.81	0.23	78,78,78,78	0
56	MG	2a	1611	1/1	0.82	0.15	69,69,69,69	0
56	MG	1a	1836	1/1	0.82	0.13	64,64,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	1787	1/1	0.82	0.27	63,63,63,63	0
56	MG	2A	3390	1/1	0.82	0.08	76,76,76,76	0
56	MG	1A	3388	1/1	0.82	0.23	72,72,72,72	0
56	MG	1A	3186	1/1	0.82	0.19	58,58,58,58	0
56	MG	1A	3095	1/1	0.82	0.22	54,54,54,54	0
56	MG	1A	3674	1/1	0.82	0.14	64,64,64,64	0
56	MG	2A	3805	1/1	0.82	0.11	54,54,54,54	0
56	MG	1A	3951	1/1	0.82	0.08	15,15,15,15	0
56	MG	1w	103	1/1	0.82	0.21	75,75,75,75	0
56	MG	1A	3054	1/1	0.82	0.09	61,61,61,61	0
56	MG	1A	3825	1/1	0.82	0.13	52,52,52,52	0
56	MG	2A	3705	1/1	0.82	0.18	69,69,69,69	0
56	MG	1A	3355	1/1	0.82	0.10	61,61,61,61	0
56	MG	1B	220	1/1	0.82	0.14	65,65,65,65	0
56	MG	1A	3526	1/1	0.82	0.21	50,50,50,50	0
56	MG	1B	225	1/1	0.82	0.11	56,56,56,56	0
56	MG	2B	202	1/1	0.82	0.29	84,84,84,84	0
56	MG	1A	3548	1/1	0.82	0.30	47,47,47,47	0
56	MG	1A	3982	1/1	0.82	0.12	42,42,42,42	0
56	MG	1A	3362	1/1	0.82	0.25	47,47,47,47	0
56	MG	2a	1688	1/1	0.82	0.17	66,66,66,66	0
56	MG	2A	3177	1/1	0.82	0.35	59,59,59,59	0
56	MG	2A	3733	1/1	0.82	0.19	66,66,66,66	0
56	MG	2A	3627	1/1	0.82	0.17	52,52,52,52	0
56	MG	2A	3282	1/1	0.82	0.24	68,68,68,68	0
56	MG	2A	3096	1/1	0.82	0.13	55,55,55,55	0
56	MG	1A	4143	1/1	0.82	0.15	51,51,51,51	0
56	MG	2a	1712	1/1	0.82	0.13	68,68,68,68	0
56	MG	1a	1786	1/1	0.82	0.13	53,53,53,53	0
56	MG	2A	3227	1/1	0.82	0.15	56,56,56,56	0
56	MG	1A	3855	1/1	0.82	0.14	34,34,34,34	0
56	MG	2Q	201	1/1	0.82	0.20	72,72,72,72	0
56	MG	2R	201	1/1	0.82	0.21	78,78,78,78	0
56	MG	10	102	1/1	0.82	0.21	56,56,56,56	0
56	MG	1A	3178	1/1	0.82	0.39	47,47,47,47	0
56	MG	2A	3673	1/1	0.82	0.14	71,71,71,71	0
56	MG	17	101	1/1	0.82	0.15	34,34,34,34	0
56	MG	2a	1692	1/1	0.83	0.15	65,65,65,65	0
56	MG	1A	3348	1/1	0.83	0.14	54,54,54,54	0
56	MG	2A	3466	1/1	0.83	0.32	59,59,59,59	0
56	MG	2a	1698	1/1	0.83	0.17	62,62,62,62	0
56	MG	1x	102	1/1	0.83	0.33	57,57,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1Y	202	1/1	0.83	0.07	65,65,65,65	0
56	MG	1A	3529	1/1	0.83	0.25	60,60,60,60	0
56	MG	2A	3493	1/1	0.83	0.20	49,49,49,49	0
56	MG	2a	1709	1/1	0.83	0.17	71,71,71,71	0
56	MG	2A	3502	1/1	0.83	0.22	52,52,52,52	0
56	MG	2A	3176	1/1	0.83	0.21	61,61,61,61	0
56	MG	1a	1631	1/1	0.83	0.24	71,71,71,71	0
56	MG	1a	1637	1/1	0.83	0.20	60,60,60,60	0
56	MG	2A	3518	1/1	0.83	0.14	61,61,61,61	0
56	MG	1A	3391	1/1	0.83	0.12	56,56,56,56	0
56	MG	2A	3745	1/1	0.83	0.12	65,65,65,65	0
56	MG	2A	3181	1/1	0.83	0.16	63,63,63,63	0
56	MG	1A	3580	1/1	0.83	0.10	41,41,41,41	0
56	MG	2A	3387	1/1	0.83	0.32	61,61,61,61	0
56	MG	1A	3987	1/1	0.83	0.23	47,47,47,47	0
56	MG	2A	3600	1/1	0.83	0.10	37,37,37,37	0
56	MG	2A	3770	1/1	0.83	0.12	69,69,69,69	0
56	MG	1A	3582	1/1	0.83	0.14	63,63,63,63	0
56	MG	2A	3310	1/1	0.83	0.14	80,80,80,80	0
56	MG	1a	1692	1/1	0.83	0.12	52,52,52,52	0
56	MG	1A	3063	1/1	0.83	0.27	55,55,55,55	0
56	MG	2A	3127	1/1	0.83	0.11	53,53,53,53	0
56	MG	2A	3396	1/1	0.83	0.07	62,62,62,62	0
56	MG	2R	202	1/1	0.83	0.16	59,59,59,59	0
56	MG	1a	1708	1/1	0.83	0.23	64,64,64,64	0
56	MG	2A	3799	1/1	0.83	0.16	63,63,63,63	0
56	MG	2a	1605	1/1	0.83	0.25	72,72,72,72	0
56	MG	2A	3800	1/1	0.83	0.15	63,63,63,63	0
56	MG	2A	3320	1/1	0.83	0.19	75,75,75,75	0
56	MG	1A	3359	1/1	0.83	0.21	50,50,50,50	0
56	MG	2a	1822	1/1	0.83	0.21	74,74,74,74	0
56	MG	1a	1739	1/1	0.83	0.18	69,69,69,69	0
56	MG	2A	3405	1/1	0.83	0.13	68,68,68,68	0
56	MG	2A	3326	1/1	0.83	0.11	56,56,56,56	0
56	MG	1A	3808	1/1	0.83	0.10	57,57,57,57	0
56	MG	1B	203	1/1	0.83	0.15	48,48,48,48	0
56	MG	1A	3888	1/1	0.83	0.10	68,68,68,68	0
56	MG	1A	3418	1/1	0.83	0.14	42,42,42,42	0
56	MG	2A	3425	1/1	0.83	0.23	69,69,69,69	0
56	MG	2A	3332	1/1	0.83	0.14	71,71,71,71	0
56	MG	1a	1821	1/1	0.83	0.12	87,87,87,87	0
56	MG	2A	3433	1/1	0.83	0.11	62,62,62,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	1642	1/1	0.83	0.22	74,74,74,74	0
56	MG	1A	3638	1/1	0.83	0.20	69,69,69,69	0
56	MG	2A	3343	1/1	0.83	0.22	66,66,66,66	0
56	MG	2A	3051	1/1	0.83	0.13	73,73,73,73	0
56	MG	1A	3302	1/1	0.83	0.32	61,61,61,61	0
56	MG	2A	3347	1/1	0.83	0.27	64,64,64,64	0
56	MG	1A	3064	1/1	0.83	0.33	57,57,57,57	0
56	MG	1N	203	1/1	0.83	0.13	41,41,41,41	0
56	MG	1A	3956	1/1	0.83	0.14	49,49,49,49	0
56	MG	1A	3518	1/1	0.83	0.48	53,53,53,53	0
56	MG	2a	1675	1/1	0.83	0.22	61,61,61,61	0
56	MG	2A	3268	1/1	0.83	0.16	53,53,53,53	0
56	MG	2A	3385	1/1	0.84	0.15	70,70,70,70	0
56	MG	2a	1691	1/1	0.84	0.22	74,74,74,74	0
56	MG	1A	3257	1/1	0.84	0.26	62,62,62,62	0
56	MG	2A	3537	1/1	0.84	0.19	69,69,69,69	0
56	MG	1a	1607	1/1	0.84	0.11	64,64,64,64	0
56	MG	1y	102	1/1	0.84	0.26	63,63,63,63	0
56	MG	1A	3706	1/1	0.84	0.11	53,53,53,53	0
56	MG	1a	1634	1/1	0.84	0.25	54,54,54,54	0
56	MG	1A	3709	1/1	0.84	0.12	46,46,46,46	0
56	MG	2A	3750	1/1	0.84	0.13	64,64,64,64	0
56	MG	2A	3560	1/1	0.84	0.13	54,54,54,54	0
56	MG	2B	203	1/1	0.84	0.12	62,62,62,62	0
56	MG	2A	3174	1/1	0.84	0.23	63,63,63,63	0
56	MG	2A	3052	1/1	0.84	0.13	60,60,60,60	0
56	MG	1A	3850	1/1	0.84	0.13	54,54,54,54	0
56	MG	2a	1721	1/1	0.84	0.23	72,72,72,72	0
56	MG	2a	1725	1/1	0.84	0.18	48,48,48,48	0
56	MG	2A	3599	1/1	0.84	0.15	66,66,66,66	0
56	MG	1a	1668	1/1	0.84	0.27	68,68,68,68	0
56	MG	2B	213	1/1	0.84	0.24	69,69,69,69	0
56	MG	1A	3390	1/1	0.84	0.32	38,38,38,38	0
56	MG	1A	3236	1/1	0.84	0.13	59,59,59,59	0
56	MG	2A	3198	1/1	0.84	0.23	53,53,53,53	0
56	MG	2a	1779	1/1	0.84	0.11	79,79,79,79	0
56	MG	1A	3357	1/1	0.84	0.33	72,72,72,72	0
56	MG	2A	3216	1/1	0.84	0.13	61,61,61,61	0
56	MG	2a	1786	1/1	0.84	0.18	65,65,65,65	0
56	MG	2A	3792	1/1	0.84	0.08	90,90,90,90	0
56	MG	1A	3775	1/1	0.84	0.11	35,35,35,35	0
56	MG	2a	1795	1/1	0.84	0.21	70,70,70,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3482	1/1	0.84	0.13	51,51,51,51	0
56	MG	2A	3414	1/1	0.84	0.20	66,66,66,66	0
56	MG	2A	3802	1/1	0.84	0.11	76,76,76,76	0
56	MG	2V	201	1/1	0.84	0.26	57,57,57,57	0
56	MG	20	102	1/1	0.84	0.15	65,65,65,65	0
56	MG	2A	3422	1/1	0.84	0.11	63,63,63,63	0
56	MG	2A	3814	1/1	0.84	0.13	64,64,64,64	0
56	MG	1A	3406	1/1	0.84	0.16	54,54,54,54	0
56	MG	2A	3635	1/1	0.84	0.13	56,56,56,56	0
56	MG	1A	3412	1/1	0.84	0.14	70,70,70,70	0
56	MG	1a	1740	1/1	0.84	0.12	54,54,54,54	0
56	MG	2A	3849	1/1	0.84	0.32	49,49,49,49	0
56	MG	2a	1615	1/1	0.84	0.17	60,60,60,60	0
56	MG	1A	3803	1/1	0.84	0.20	60,60,60,60	0
56	MG	1A	4079	1/1	0.84	0.18	69,69,69,69	0
56	MG	2a	1621	1/1	0.84	0.09	64,64,64,64	0
56	MG	1A	3308	1/1	0.84	0.25	64,64,64,64	0
56	MG	1A	3247	1/1	0.84	0.15	67,67,67,67	0
56	MG	1A	3515	1/1	0.84	0.18	75,75,75,75	0
56	MG	1A	4092	1/1	0.84	0.18	60,60,60,60	0
56	MG	2A	3680	1/1	0.84	0.13	53,53,53,53	0
56	MG	1A	4099	1/1	0.84	0.13	63,63,63,63	0
56	MG	1A	3820	1/1	0.84	0.16	59,59,59,59	0
56	MG	2A	3358	1/1	0.84	0.13	53,53,53,53	0
56	MG	1A	3641	1/1	0.84	0.10	32,32,32,32	0
56	MG	2A	3459	1/1	0.84	0.09	62,62,62,62	0
56	MG	1A	3516	1/1	0.84	0.10	45,45,45,45	0
56	MG	1N	208	1/1	0.84	0.15	37,37,37,37	0
56	MG	2A	3368	1/1	0.84	0.25	74,74,74,74	0
56	MG	2A	3158	1/1	0.84	0.16	60,60,60,60	0
56	MG	1A	3980	1/1	0.84	0.10	52,52,52,52	0
56	MG	1A	3347	1/1	0.84	0.34	67,67,67,67	0
56	MG	2y	102	1/1	0.84	0.16	76,76,76,76	0
56	MG	2A	3498	1/1	0.84	0.33	59,59,59,59	0
56	MG	2a	1670	1/1	0.84	0.17	63,63,63,63	0
56	MG	2A	3500	1/1	0.84	0.21	49,49,49,49	0
56	MG	1A	3676	1/1	0.84	0.12	50,50,50,50	0
56	MG	1A	3349	1/1	0.85	0.23	65,65,65,65	0
56	MG	2B	204	1/1	0.85	0.19	75,75,75,75	0
56	MG	1A	3465	1/1	0.85	0.13	64,64,64,64	0
56	MG	2A	3309	1/1	0.85	0.25	75,75,75,75	0
56	MG	2A	3182	1/1	0.85	0.13	37,37,37,37	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	1713	1/1	0.85	0.22	86,86,86,86	0
56	MG	1A	3595	1/1	0.85	0.21	46,46,46,46	0
56	MG	2B	210	1/1	0.85	0.22	61,61,61,61	0
56	MG	2A	3193	1/1	0.85	0.15	53,53,53,53	0
56	MG	2A	3194	1/1	0.85	0.13	61,61,61,61	0
56	MG	1A	3133	1/1	0.85	0.13	46,46,46,46	0
56	MG	2B	215	1/1	0.85	0.29	75,75,75,75	0
56	MG	2a	1730	1/1	0.85	0.29	66,66,66,66	0
56	MG	2A	3788	1/1	0.85	0.11	64,64,64,64	0
56	MG	2A	3114	1/1	0.85	0.24	41,41,41,41	0
56	MG	2A	3116	1/1	0.85	0.27	70,70,70,70	0
56	MG	2a	1762	1/1	0.85	0.12	104,104,104,104	0
56	MG	1A	4141	1/1	0.85	0.13	44,44,44,44	0
56	MG	2a	1767	1/1	0.85	0.19	61,61,61,61	0
56	MG	1A	3907	1/1	0.85	0.25	67,67,67,67	0
56	MG	1A	3944	1/1	0.85	0.17	82,82,82,82	0
56	MG	2A	3803	1/1	0.85	0.10	71,71,71,71	0
56	MG	1a	1715	1/1	0.85	0.36	66,66,66,66	0
56	MG	1A	4149	1/1	0.85	0.14	32,32,32,32	0
56	MG	1A	3797	1/1	0.85	0.20	59,59,59,59	0
56	MG	2A	3427	1/1	0.85	0.20	64,64,64,64	0
56	MG	2A	3009	1/1	0.85	0.15	60,60,60,60	0
56	MG	1A	3682	1/1	0.85	0.10	33,33,33,33	0
56	MG	1A	3705	1/1	0.85	0.09	70,70,70,70	0
56	MG	2A	3144	1/1	0.85	0.18	62,62,62,62	0
56	MG	2A	3444	1/1	0.85	0.33	57,57,57,57	0
56	MG	2A	3669	1/1	0.85	0.14	55,55,55,55	0
56	MG	1A	3957	1/1	0.85	0.11	61,61,61,61	0
56	MG	2A	3446	1/1	0.85	0.12	72,72,72,72	0
56	MG	1a	1781	1/1	0.85	0.12	66,66,66,66	0
56	MG	2A	3677	1/1	0.85	0.15	57,57,57,57	0
56	MG	1a	1797	1/1	0.85	0.15	62,62,62,62	0
56	MG	1A	3419	1/1	0.85	0.17	61,61,61,61	0
56	MG	1A	4066	1/1	0.85	0.16	30,30,30,30	0
56	MG	1A	3207	1/1	0.85	0.14	66,66,66,66	0
56	MG	2A	3267	1/1	0.85	0.16	64,64,64,64	0
56	MG	2A	3364	1/1	0.85	0.13	51,51,51,51	0
56	MG	2A	3365	1/1	0.85	0.21	45,45,45,45	0
56	MG	1A	3861	1/1	0.85	0.30	54,54,54,54	0
56	MG	1A	4070	1/1	0.85	0.15	51,51,51,51	0
56	MG	2A	3271	1/1	0.85	0.22	60,60,60,60	0
56	MG	2A	3482	1/1	0.85	0.28	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3492	1/1	0.85	0.25	49,49,49,49	0
56	MG	1A	3978	1/1	0.85	0.19	78,78,78,78	0
56	MG	2A	3718	1/1	0.85	0.15	70,70,70,70	0
56	MG	1A	3565	1/1	0.85	0.24	46,46,46,46	0
56	MG	2A	3499	1/1	0.85	0.14	50,50,50,50	0
56	MG	1A	3471	1/1	0.85	0.20	61,61,61,61	0
56	MG	13	101	1/1	0.85	0.13	56,56,56,56	0
56	MG	2A	3061	1/1	0.85	0.21	48,48,48,48	0
56	MG	1x	109	1/1	0.85	0.39	65,65,65,65	0
56	MG	2A	3506	1/1	0.85	0.22	77,77,77,77	0
56	MG	2A	3509	1/1	0.85	0.30	53,53,53,53	0
56	MG	2x	103	1/1	0.85	0.20	78,78,78,78	0
56	MG	2A	3386	1/1	0.85	0.22	61,61,61,61	0
56	MG	2A	3284	1/1	0.85	0.38	48,48,48,48	0
56	MG	2A	3067	1/1	0.85	0.33	60,60,60,60	0
56	MG	2A	3546	1/1	0.85	0.15	66,66,66,66	0
56	MG	2A	3295	1/1	0.85	0.17	70,70,70,70	0
56	MG	1a	1654	1/1	0.85	0.28	68,68,68,68	0
56	MG	1A	3629	1/1	0.86	0.18	53,53,53,53	0
56	MG	2A	3795	1/1	0.86	0.10	51,51,51,51	0
56	MG	2a	1643	1/1	0.86	0.18	75,75,75,75	0
56	MG	1A	3451	1/1	0.86	0.14	57,57,57,57	0
56	MG	1a	1746	1/1	0.86	0.21	62,62,62,62	0
56	MG	1A	3404	1/1	0.86	0.21	53,53,53,53	0
56	MG	1A	3216	1/1	0.86	0.09	46,46,46,46	0
56	MG	1A	3409	1/1	0.86	0.37	63,63,63,63	0
56	MG	2A	3138	1/1	0.86	0.24	68,68,68,68	0
56	MG	2a	1656	1/1	0.86	0.12	71,71,71,71	0
56	MG	1A	3523	1/1	0.86	0.21	65,65,65,65	0
56	MG	1A	3266	1/1	0.86	0.21	59,59,59,59	0
56	MG	2A	3604	1/1	0.86	0.11	52,52,52,52	0
56	MG	1A	3129	1/1	0.86	0.18	60,60,60,60	0
56	MG	1A	3536	1/1	0.86	0.15	56,56,56,56	0
56	MG	1a	1816	1/1	0.86	0.10	52,52,52,52	0
56	MG	1A	3827	1/1	0.86	0.14	48,48,48,48	0
56	MG	2A	3852	1/1	0.86	0.42	50,50,50,50	0
56	MG	2A	3020	1/1	0.86	0.16	54,54,54,54	0
56	MG	2A	3290	1/1	0.86	0.23	53,53,53,53	0
56	MG	2A	3294	1/1	0.86	0.26	61,61,61,61	0
56	MG	2A	3409	1/1	0.86	0.18	67,67,67,67	0
56	MG	1a	1838	1/1	0.86	0.19	58,58,58,58	0
56	MG	1B	221	1/1	0.86	0.16	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3629	1/1	0.86	0.22	49,49,49,49	0
56	MG	2A	3023	1/1	0.86	0.15	42,42,42,42	0
56	MG	1B	226	1/1	0.86	0.11	60,60,60,60	0
56	MG	2A	3296	1/1	0.86	0.19	50,50,50,50	0
56	MG	1A	3540	1/1	0.86	0.08	53,53,53,53	0
56	MG	2a	1716	1/1	0.86	0.19	70,70,70,70	0
56	MG	2A	3419	1/1	0.86	0.09	69,69,69,69	0
56	MG	1A	3981	1/1	0.86	0.20	51,51,51,51	0
56	MG	1A	3469	1/1	0.86	0.19	66,66,66,66	0
56	MG	1F	302	1/1	0.86	0.15	53,53,53,53	0
56	MG	1G	202	1/1	0.86	0.15	61,61,61,61	0
56	MG	1A	3090	1/1	0.86	0.17	46,46,46,46	0
56	MG	1A	3477	1/1	0.86	0.12	59,59,59,59	0
56	MG	2A	3050	1/1	0.86	0.19	56,56,56,56	0
56	MG	2a	1739	1/1	0.86	0.10	76,76,76,76	0
56	MG	1A	3731	1/1	0.86	0.13	33,33,33,33	0
56	MG	1O	205	1/1	0.86	0.10	58,58,58,58	0
56	MG	2A	3323	1/1	0.86	0.09	54,54,54,54	0
56	MG	1A	3321	1/1	0.86	0.17	51,51,51,51	0
56	MG	2A	3438	1/1	0.86	0.13	68,68,68,68	0
56	MG	1A	3583	1/1	0.86	0.25	65,65,65,65	0
56	MG	2A	3192	1/1	0.86	0.13	59,59,59,59	0
56	MG	1A	3489	1/1	0.86	0.29	55,55,55,55	0
56	MG	1A	3258	1/1	0.86	0.11	52,52,52,52	0
56	MG	2A	3696	1/1	0.86	0.12	70,70,70,70	0
56	MG	2A	3448	1/1	0.86	0.31	64,64,64,64	0
56	MG	2A	3452	1/1	0.86	0.11	67,67,67,67	0
56	MG	2a	1796	1/1	0.86	0.12	66,66,66,66	0
56	MG	2a	1797	1/1	0.86	0.12	62,62,62,62	0
56	MG	2A	3704	1/1	0.86	0.13	70,70,70,70	0
56	MG	1A	3781	1/1	0.86	0.21	42,42,42,42	0
56	MG	1A	4048	1/1	0.86	0.21	48,48,48,48	0
56	MG	2A	3213	1/1	0.86	0.18	60,60,60,60	0
56	MG	2A	3215	1/1	0.86	0.28	60,60,60,60	0
56	MG	2A	3062	1/1	0.86	0.17	63,63,63,63	0
56	MG	1a	1653	1/1	0.86	0.27	50,50,50,50	0
56	MG	2A	3225	1/1	0.86	0.32	63,63,63,63	0
56	MG	2E	308	1/1	0.86	0.14	65,65,65,65	0
56	MG	1A	4055	1/1	0.86	0.19	67,67,67,67	0
56	MG	1A	3432	1/1	0.86	0.34	52,52,52,52	0
56	MG	2A	3475	1/1	0.86	0.15	51,51,51,51	0
56	MG	1A	3793	1/1	0.86	0.16	24,24,24,24	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1665	1/1	0.86	0.14	65,65,65,65	0
56	MG	2A	3356	1/1	0.86	0.17	64,64,64,64	0
56	MG	2Z	301	1/1	0.86	0.24	74,74,74,74	0
56	MG	2A	3485	1/1	0.86	0.31	61,61,61,61	0
56	MG	23	101	1/1	0.86	0.15	66,66,66,66	0
56	MG	1A	3449	1/1	0.86	0.17	51,51,51,51	0
56	MG	1a	1675	1/1	0.86	0.11	63,63,63,63	0
56	MG	2A	3749	1/1	0.86	0.11	55,55,55,55	0
56	MG	2A	3234	1/1	0.86	0.15	60,60,60,60	0
56	MG	2A	3359	1/1	0.86	0.12	58,58,58,58	0
56	MG	1A	3799	1/1	0.86	0.11	52,52,52,52	0
56	MG	1A	3910	1/1	0.86	0.10	72,72,72,72	0
56	MG	2A	3237	1/1	0.86	0.15	68,68,68,68	0
56	MG	1A	3914	1/1	0.86	0.13	71,71,71,71	0
56	MG	2a	1619	1/1	0.86	0.26	76,76,76,76	0
56	MG	2A	3508	1/1	0.86	0.17	64,64,64,64	0
56	MG	1a	1710	1/1	0.86	0.14	70,70,70,70	0
56	MG	1a	1713	1/1	0.86	0.29	58,58,58,58	0
56	MG	1A	3928	1/1	0.86	0.11	60,60,60,60	0
56	MG	2A	3120	1/1	0.86	0.14	59,59,59,59	0
56	MG	2A	3370	1/1	0.86	0.10	59,59,59,59	0
56	MG	1A	3934	1/1	0.86	0.10	33,33,33,33	0
56	MG	1a	1726	1/1	0.86	0.25	62,62,62,62	0
56	MG	1A	3939	1/1	0.86	0.14	84,84,84,84	0
56	MG	2a	1637	1/1	0.86	0.10	68,68,68,68	0
58	K	2A	3515	1/1	0.86	0.14	66,66,66,66	0
56	MG	2a	1638	1/1	0.87	0.20	62,62,62,62	0
56	MG	1A	3352	1/1	0.87	0.07	39,39,39,39	0
56	MG	1a	1757	1/1	0.87	0.11	56,56,56,56	0
56	MG	1A	3805	1/1	0.87	0.13	55,55,55,55	0
56	MG	2A	3841	1/1	0.87	0.13	39,39,39,39	0
56	MG	1A	3456	1/1	0.87	0.21	56,56,56,56	0
56	MG	2A	3330	1/1	0.87	0.32	60,60,60,60	0
56	MG	1A	3285	1/1	0.87	0.23	41,41,41,41	0
56	MG	1A	3401	1/1	0.87	0.10	48,48,48,48	0
56	MG	1a	1789	1/1	0.87	0.14	47,47,47,47	0
56	MG	1a	1790	1/1	0.87	0.10	54,54,54,54	0
56	MG	2A	3231	1/1	0.87	0.09	60,60,60,60	0
56	MG	2a	1660	1/1	0.87	0.15	66,66,66,66	0
56	MG	1A	3648	1/1	0.87	0.12	62,62,62,62	0
56	MG	1A	4119	1/1	0.87	0.18	35,35,35,35	0
56	MG	1A	3316	1/1	0.87	0.55	44,44,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3647	1/1	0.87	0.17	60,60,60,60	0
56	MG	2A	3123	1/1	0.87	0.10	48,48,48,48	0
56	MG	2A	3348	1/1	0.87	0.30	62,62,62,62	0
56	MG	2A	3668	1/1	0.87	0.13	49,49,49,49	0
56	MG	2a	1695	1/1	0.87	0.21	65,65,65,65	0
56	MG	1A	3062	1/1	0.87	0.24	53,53,53,53	0
56	MG	2A	3671	1/1	0.87	0.12	63,63,63,63	0
56	MG	1A	3181	1/1	0.87	0.13	51,51,51,51	0
56	MG	1A	4147	1/1	0.87	0.11	27,27,27,27	0
56	MG	2A	3130	1/1	0.87	0.14	63,63,63,63	0
56	MG	2a	1705	1/1	0.87	0.09	78,78,78,78	0
56	MG	1m	203	1/1	0.87	0.21	49,49,49,49	0
56	MG	2A	3454	1/1	0.87	0.07	65,65,65,65	0
56	MG	1G	203	1/1	0.87	0.10	64,64,64,64	0
56	MG	1A	3025	1/1	0.87	0.18	42,42,42,42	0
56	MG	2A	3003	1/1	0.87	0.20	61,61,61,61	0
56	MG	1A	3537	1/1	0.87	0.25	56,56,56,56	0
56	MG	2A	3259	1/1	0.87	0.29	61,61,61,61	0
56	MG	2A	3363	1/1	0.87	0.09	55,55,55,55	0
56	MG	1x	104	1/1	0.87	0.24	67,67,67,67	0
56	MG	2A	3695	1/1	0.87	0.11	52,52,52,52	0
56	MG	1T	202	1/1	0.87	0.11	45,45,45,45	0
56	MG	2A	3007	1/1	0.87	0.27	64,64,64,64	0
56	MG	1A	3835	1/1	0.87	0.13	53,53,53,53	0
56	MG	2A	3470	1/1	0.87	0.22	44,44,44,44	0
56	MG	1X	101	1/1	0.87	0.21	34,34,34,34	0
56	MG	2A	3018	1/1	0.87	0.23	60,60,60,60	0
56	MG	2a	1743	1/1	0.87	0.09	96,96,96,96	0
56	MG	1Z	303	1/1	0.87	0.15	54,54,54,54	0
56	MG	1A	3837	1/1	0.87	0.17	54,54,54,54	0
56	MG	1A	3365	1/1	0.87	0.08	38,38,38,38	0
56	MG	2A	3710	1/1	0.87	0.15	61,61,61,61	0
56	MG	2a	1777	1/1	0.87	0.14	68,68,68,68	0
56	MG	2A	3483	1/1	0.87	0.25	49,49,49,49	0
56	MG	1A	3544	1/1	0.87	0.21	49,49,49,49	0
56	MG	1a	1605	1/1	0.87	0.18	56,56,56,56	0
56	MG	2A	3713	1/1	0.87	0.12	40,40,40,40	0
56	MG	2a	1784	1/1	0.87	0.12	74,74,74,74	0
56	MG	2A	3490	1/1	0.87	0.11	40,40,40,40	0
56	MG	1A	3369	1/1	0.87	0.16	44,44,44,44	0
56	MG	1A	3549	1/1	0.87	0.17	46,46,46,46	0
56	MG	2A	3378	1/1	0.87	0.20	68,68,68,68	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1645	1/1	0.87	0.16	59,59,59,59	0
56	MG	2A	3731	1/1	0.87	0.16	45,45,45,45	0
56	MG	1A	3725	1/1	0.87	0.12	53,53,53,53	0
56	MG	2a	1801	1/1	0.87	0.10	65,65,65,65	0
56	MG	2A	3382	1/1	0.87	0.26	67,67,67,67	0
56	MG	1A	3478	1/1	0.87	0.14	57,57,57,57	0
56	MG	2A	3504	1/1	0.87	0.35	66,66,66,66	0
56	MG	2A	3171	1/1	0.87	0.16	55,55,55,55	0
56	MG	1a	1662	1/1	0.87	0.18	62,62,62,62	0
56	MG	2F	302	1/1	0.87	0.35	59,59,59,59	0
56	MG	2O	201	1/1	0.87	0.14	64,64,64,64	0
56	MG	1A	3569	1/1	0.87	0.14	59,59,59,59	0
56	MG	1A	3754	1/1	0.87	0.16	45,45,45,45	0
56	MG	2a	1818	1/1	0.87	0.09	77,77,77,77	0
56	MG	1a	1666	1/1	0.87	0.20	65,65,65,65	0
56	MG	1A	3577	1/1	0.87	0.08	46,46,46,46	0
56	MG	2T	203	1/1	0.87	0.16	52,52,52,52	0
56	MG	1A	3481	1/1	0.87	0.11	51,51,51,51	0
56	MG	2W	201	1/1	0.87	0.12	60,60,60,60	0
56	MG	1A	3371	1/1	0.87	0.10	46,46,46,46	0
56	MG	2A	3545	1/1	0.87	0.10	47,47,47,47	0
56	MG	1a	1677	1/1	0.87	0.30	44,44,44,44	0
56	MG	1a	1681	1/1	0.87	0.21	42,42,42,42	0
56	MG	2A	3769	1/1	0.87	0.11	60,60,60,60	0
56	MG	2A	3393	1/1	0.87	0.31	76,76,76,76	0
56	MG	2A	3394	1/1	0.87	0.24	78,78,78,78	0
56	MG	2A	3299	1/1	0.87	0.20	69,69,69,69	0
56	MG	2A	3775	1/1	0.87	0.17	59,59,59,59	0
56	MG	2A	3183	1/1	0.87	0.14	54,54,54,54	0
56	MG	1A	3376	1/1	0.87	0.13	51,51,51,51	0
56	MG	2a	1616	1/1	0.87	0.25	75,75,75,75	0
56	MG	2A	3563	1/1	0.87	0.14	45,45,45,45	0
56	MG	2r	101	1/1	0.87	0.35	66,66,66,66	0
56	MG	2t	201	1/1	0.87	0.16	56,56,56,56	0
56	MG	2A	3307	1/1	0.87	0.28	59,59,59,59	0
56	MG	2A	3582	1/1	0.87	0.10	39,39,39,39	0
56	MG	1A	3496	1/1	0.87	0.15	54,54,54,54	0
56	MG	1A	3296	1/1	0.87	0.24	29,29,29,29	0
56	MG	1A	3911	1/1	0.87	0.10	73,73,73,73	0
56	MG	2y	101	1/1	0.87	0.25	61,61,61,61	0
56	MG	1A	3433	1/1	0.87	0.15	62,62,62,62	0
56	MG	1A	3620	1/1	0.87	0.18	44,44,44,44	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3210	1/1	0.87	0.21	59,59,59,59	0
56	MG	2A	3610	1/1	0.87	0.13	47,47,47,47	0
56	MG	1A	3162	1/1	0.87	0.28	63,63,63,63	0
56	MG	2A	3817	1/1	0.87	0.10	53,53,53,53	0
56	MG	1a	1721	1/1	0.88	0.14	54,54,54,54	0
56	MG	1a	1722	1/1	0.88	0.34	59,59,59,59	0
56	MG	2A	3273	1/1	0.88	0.14	47,47,47,47	0
56	MG	2A	3593	1/1	0.88	0.11	35,35,35,35	0
56	MG	2A	3274	1/1	0.88	0.09	44,44,44,44	0
56	MG	2a	1640	1/1	0.88	0.22	62,62,62,62	0
56	MG	1A	3222	1/1	0.88	0.11	49,49,49,49	0
56	MG	1A	3060	1/1	0.88	0.15	41,41,41,41	0
56	MG	2A	3815	1/1	0.88	0.12	80,80,80,80	0
56	MG	1A	3029	1/1	0.88	0.31	39,39,39,39	0
56	MG	1A	3849	1/1	0.88	0.25	48,48,48,48	0
56	MG	1A	3594	1/1	0.88	0.12	48,48,48,48	0
56	MG	1a	1761	1/1	0.88	0.20	60,60,60,60	0
56	MG	2A	3019	1/1	0.88	0.19	65,65,65,65	0
56	MG	2A	3408	1/1	0.88	0.10	62,62,62,62	0
56	MG	1A	3985	1/1	0.88	0.10	24,24,24,24	0
56	MG	1a	1773	1/1	0.88	0.14	56,56,56,56	0
56	MG	1A	3101	1/1	0.88	0.24	62,62,62,62	0
56	MG	2A	3024	1/1	0.88	0.20	65,65,65,65	0
56	MG	2a	1668	1/1	0.88	0.20	55,55,55,55	0
56	MG	1B	208	1/1	0.88	0.21	56,56,56,56	0
56	MG	2A	3029	1/1	0.88	0.41	56,56,56,56	0
56	MG	1B	214	1/1	0.88	0.07	50,50,50,50	0
56	MG	1a	1804	1/1	0.88	0.20	66,66,66,66	0
56	MG	1A	3605	1/1	0.88	0.08	47,47,47,47	0
56	MG	1A	3462	1/1	0.88	0.14	54,54,54,54	0
56	MG	2A	3423	1/1	0.88	0.13	70,70,70,70	0
56	MG	1A	3865	1/1	0.88	0.23	54,54,54,54	0
56	MG	2A	3306	1/1	0.88	0.35	70,70,70,70	0
56	MG	1a	1829	1/1	0.88	0.12	62,62,62,62	0
56	MG	2a	1699	1/1	0.88	0.16	65,65,65,65	0
56	MG	2A	3178	1/1	0.88	0.13	44,44,44,44	0
56	MG	2A	3308	1/1	0.88	0.12	69,69,69,69	0
56	MG	1a	1833	1/1	0.88	0.10	68,68,68,68	0
56	MG	1A	4011	1/1	0.88	0.14	58,58,58,58	0
56	MG	2A	3041	1/1	0.88	0.10	68,68,68,68	0
56	MG	1A	3616	1/1	0.88	0.12	61,61,61,61	0
56	MG	2a	1711	1/1	0.88	0.14	76,76,76,76	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1D	311	1/1	0.88	0.22	41,41,41,41	0
56	MG	2A	3670	1/1	0.88	0.14	43,43,43,43	0
56	MG	1d	3101	1/1	0.88	0.20	54,54,54,54	0
56	MG	2A	3184	1/1	0.88	0.12	72,72,72,72	0
56	MG	2A	3189	1/1	0.88	0.13	69,69,69,69	0
56	MG	1A	3463	1/1	0.88	0.15	53,53,53,53	0
56	MG	2A	3676	1/1	0.88	0.19	53,53,53,53	0
56	MG	2A	3324	1/1	0.88	0.19	73,73,73,73	0
56	MG	2a	1726	1/1	0.88	0.20	51,51,51,51	0
56	MG	1A	3873	1/1	0.88	0.09	22,22,22,22	0
56	MG	2a	1729	1/1	0.88	0.14	78,78,78,78	0
56	MG	2A	3679	1/1	0.88	0.17	55,55,55,55	0
56	MG	1w	105	1/1	0.88	0.21	64,64,64,64	0
56	MG	1A	3877	1/1	0.88	0.19	45,45,45,45	0
56	MG	1A	3883	1/1	0.88	0.11	31,31,31,31	0
56	MG	1x	105	1/1	0.88	0.32	65,65,65,65	0
56	MG	2a	1746	1/1	0.88	0.09	51,51,51,51	0
56	MG	2A	3195	1/1	0.88	0.17	71,71,71,71	0
56	MG	2A	3329	1/1	0.88	0.11	68,68,68,68	0
56	MG	1A	4054	1/1	0.88	0.12	25,25,25,25	0
56	MG	2A	3694	1/1	0.88	0.20	44,44,44,44	0
56	MG	2a	1770	1/1	0.88	0.10	58,58,58,58	0
56	MG	2a	1773	1/1	0.88	0.18	73,73,73,73	0
56	MG	1A	3885	1/1	0.88	0.17	61,61,61,61	0
56	MG	2A	3202	1/1	0.88	0.16	63,63,63,63	0
56	MG	1A	3353	1/1	0.88	0.16	55,55,55,55	0
56	MG	1A	3245	1/1	0.88	0.12	43,43,43,43	0
56	MG	1A	3068	1/1	0.88	0.18	64,64,64,64	0
56	MG	2A	3064	1/1	0.88	0.25	66,66,66,66	0
56	MG	13	103	1/1	0.88	0.20	59,59,59,59	0
56	MG	2A	3219	1/1	0.88	0.20	57,57,57,57	0
56	MG	2a	1788	1/1	0.88	0.10	60,60,60,60	0
56	MG	1A	3251	1/1	0.88	0.13	60,60,60,60	0
56	MG	2A	3478	1/1	0.88	0.31	62,62,62,62	0
56	MG	2A	3072	1/1	0.88	0.33	57,57,57,57	0
56	MG	1a	1608	1/1	0.88	0.18	56,56,56,56	0
56	MG	1a	1616	1/1	0.88	0.11	55,55,55,55	0
56	MG	1a	1621	1/1	0.88	0.28	64,64,64,64	0
56	MG	1A	3194	1/1	0.88	0.09	55,55,55,55	0
56	MG	2A	3714	1/1	0.88	0.09	71,71,71,71	0
56	MG	2A	3093	1/1	0.88	0.65	52,52,52,52	0
56	MG	1A	3083	1/1	0.88	0.17	52,52,52,52	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3720	1/1	0.88	0.13	69,69,69,69	0
56	MG	2A	3487	1/1	0.88	0.17	49,49,49,49	0
56	MG	1A	3650	1/1	0.88	0.09	36,36,36,36	0
56	MG	2a	1813	1/1	0.88	0.15	74,74,74,74	0
56	MG	2A	3728	1/1	0.88	0.14	52,52,52,52	0
56	MG	1A	4073	1/1	0.88	0.13	34,34,34,34	0
56	MG	1A	3923	1/1	0.88	0.09	52,52,52,52	0
56	MG	1a	1659	1/1	0.88	0.21	62,62,62,62	0
56	MG	1a	1660	1/1	0.88	0.15	43,43,43,43	0
56	MG	1A	3668	1/1	0.88	0.11	28,28,28,28	0
56	MG	1A	3472	1/1	0.88	0.13	44,44,44,44	0
56	MG	1A	3414	1/1	0.88	0.12	44,44,44,44	0
56	MG	2A	3240	1/1	0.88	0.15	65,65,65,65	0
56	MG	1A	3084	1/1	0.88	0.16	38,38,38,38	0
56	MG	2A	3250	1/1	0.88	0.31	67,67,67,67	0
56	MG	2W	202	1/1	0.88	0.13	66,66,66,66	0
56	MG	1A	3264	1/1	0.88	0.15	56,56,56,56	0
56	MG	2A	3253	1/1	0.88	0.16	38,38,38,38	0
56	MG	2A	3512	1/1	0.88	0.27	56,56,56,56	0
56	MG	2g	201	1/1	0.88	0.23	62,62,62,62	0
56	MG	2A	3254	1/1	0.88	0.28	59,59,59,59	0
56	MG	28	101	1/1	0.88	0.23	49,49,49,49	0
56	MG	2A	3768	1/1	0.88	0.43	46,46,46,46	0
56	MG	2a	1604	1/1	0.88	0.14	50,50,50,50	0
56	MG	1a	1683	1/1	0.88	0.16	54,54,54,54	0
56	MG	1A	4115	1/1	0.88	0.17	72,72,72,72	0
56	MG	2A	3534	1/1	0.88	0.10	45,45,45,45	0
56	MG	1A	3333	1/1	0.88	0.14	53,53,53,53	0
56	MG	1A	4127	1/1	0.88	0.17	40,40,40,40	0
56	MG	1A	3688	1/1	0.88	0.10	35,35,35,35	0
56	MG	1a	1694	1/1	0.88	0.25	59,59,59,59	0
56	MG	1A	4142	1/1	0.88	0.11	65,65,65,65	0
56	MG	2a	1618	1/1	0.88	0.09	72,72,72,72	0
56	MG	2A	3266	1/1	0.88	0.10	45,45,45,45	0
56	MG	2A	3552	1/1	0.88	0.08	42,42,42,42	0
56	MG	1A	3161	1/1	0.88	0.75	38,38,38,38	0
56	MG	1A	3495	1/1	0.88	0.15	52,52,52,52	0
56	MG	1A	3708	1/1	0.88	0.17	56,56,56,56	0
56	MG	2A	3270	1/1	0.88	0.23	57,57,57,57	0
56	MG	1A	3384	1/1	0.88	0.09	41,41,41,41	0
56	MG	1A	3728	1/1	0.89	0.13	45,45,45,45	0
56	MG	1A	3228	1/1	0.89	0.24	25,25,25,25	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3027	1/1	0.89	0.09	50,50,50,50	0
56	MG	2T	202	1/1	0.89	0.12	51,51,51,51	0
56	MG	2A	3276	1/1	0.89	0.20	64,64,64,64	0
56	MG	2A	3134	1/1	0.89	0.07	32,32,32,32	0
56	MG	2V	202	1/1	0.89	0.14	51,51,51,51	0
56	MG	2A	3674	1/1	0.89	0.24	49,49,49,49	0
56	MG	2A	3420	1/1	0.89	0.40	55,55,55,55	0
56	MG	1A	3105	1/1	0.89	0.38	37,37,37,37	0
56	MG	20	101	1/1	0.89	0.18	53,53,53,53	0
56	MG	1A	4091	1/1	0.89	0.14	61,61,61,61	0
56	MG	2I	101	1/1	0.89	0.17	62,62,62,62	0
56	MG	2A	3139	1/1	0.89	0.14	51,51,51,51	0
56	MG	1A	3483	1/1	0.89	0.18	61,61,61,61	0
56	MG	1a	1613	1/1	0.89	0.12	68,68,68,68	0
56	MG	2A	3145	1/1	0.89	0.13	57,57,57,57	0
56	MG	1A	3900	1/1	0.89	0.33	36,36,36,36	0
56	MG	1a	1622	1/1	0.89	0.21	59,59,59,59	0
56	MG	1a	1624	1/1	0.89	0.22	47,47,47,47	0
56	MG	1A	4110	1/1	0.89	0.20	36,36,36,36	0
56	MG	2a	1610	1/1	0.89	0.22	61,61,61,61	0
56	MG	2A	3687	1/1	0.89	0.08	28,28,28,28	0
56	MG	2a	1612	1/1	0.89	0.23	71,71,71,71	0
56	MG	2A	3155	1/1	0.89	0.29	47,47,47,47	0
56	MG	1a	1640	1/1	0.89	0.13	66,66,66,66	0
56	MG	1a	1642	1/1	0.89	0.13	58,58,58,58	0
56	MG	1A	3766	1/1	0.89	0.10	38,38,38,38	0
56	MG	2A	3437	1/1	0.89	0.10	66,66,66,66	0
56	MG	2A	3302	1/1	0.89	0.13	61,61,61,61	0
56	MG	1a	1651	1/1	0.89	0.19	40,40,40,40	0
56	MG	1A	3423	1/1	0.89	0.21	47,47,47,47	0
56	MG	2A	3442	1/1	0.89	0.09	59,59,59,59	0
56	MG	2A	3700	1/1	0.89	0.20	65,65,65,65	0
56	MG	2A	3702	1/1	0.89	0.17	73,73,73,73	0
56	MG	1A	3909	1/1	0.89	0.19	78,78,78,78	0
56	MG	1A	3592	1/1	0.89	0.13	34,34,34,34	0
56	MG	1A	3269	1/1	0.89	0.15	43,43,43,43	0
56	MG	2A	3447	1/1	0.89	0.12	71,71,71,71	0
56	MG	2a	1636	1/1	0.89	0.25	49,49,49,49	0
56	MG	2A	3709	1/1	0.89	0.10	52,52,52,52	0
56	MG	1A	3782	1/1	0.89	0.20	59,59,59,59	0
56	MG	2A	3450	1/1	0.89	0.15	65,65,65,65	0
56	MG	1A	3920	1/1	0.89	0.10	41,41,41,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3431	1/1	0.89	0.18	57,57,57,57	0
56	MG	1A	4148	1/1	0.89	0.15	59,59,59,59	0
56	MG	2a	1646	1/1	0.89	0.10	57,57,57,57	0
56	MG	2A	3313	1/1	0.89	0.18	62,62,62,62	0
56	MG	1A	3498	1/1	0.89	0.13	61,61,61,61	0
56	MG	2A	3319	1/1	0.89	0.07	58,58,58,58	0
56	MG	1A	3606	1/1	0.89	0.09	28,28,28,28	0
56	MG	2A	3321	1/1	0.89	0.08	48,48,48,48	0
56	MG	2A	3727	1/1	0.89	0.11	56,56,56,56	0
56	MG	1a	1687	1/1	0.89	0.11	57,57,57,57	0
56	MG	1A	3273	1/1	0.89	0.20	42,42,42,42	0
56	MG	2A	3730	1/1	0.89	0.12	32,32,32,32	0
56	MG	1A	3940	1/1	0.89	0.07	76,76,76,76	0
56	MG	2a	1664	1/1	0.89	0.21	62,62,62,62	0
56	MG	1A	3327	1/1	0.89	0.31	55,55,55,55	0
56	MG	2A	3473	1/1	0.89	0.30	54,54,54,54	0
56	MG	1a	1705	1/1	0.89	0.23	63,63,63,63	0
56	MG	2A	3736	1/1	0.89	0.10	59,59,59,59	0
56	MG	2a	1683	1/1	0.89	0.20	72,72,72,72	0
56	MG	1A	3802	1/1	0.89	0.24	53,53,53,53	0
56	MG	1A	3617	1/1	0.89	0.15	33,33,33,33	0
56	MG	1a	1712	1/1	0.89	0.41	52,52,52,52	0
56	MG	1A	3804	1/1	0.89	0.13	40,40,40,40	0
56	MG	1a	1714	1/1	0.89	0.07	71,71,71,71	0
56	MG	2A	3747	1/1	0.89	0.09	59,59,59,59	0
56	MG	1A	3434	1/1	0.89	0.15	63,63,63,63	0
56	MG	1A	3962	1/1	0.89	0.10	72,72,72,72	0
56	MG	1A	3446	1/1	0.89	0.12	59,59,59,59	0
56	MG	2A	3754	1/1	0.89	0.10	67,67,67,67	0
56	MG	2a	1704	1/1	0.89	0.21	66,66,66,66	0
56	MG	1A	3275	1/1	0.89	0.13	38,38,38,38	0
56	MG	2A	3489	1/1	0.89	0.25	41,41,41,41	0
56	MG	1a	1728	1/1	0.89	0.26	55,55,55,55	0
56	MG	1A	3967	1/1	0.89	0.15	66,66,66,66	0
56	MG	2a	1710	1/1	0.89	0.18	62,62,62,62	0
56	MG	1A	3815	1/1	0.89	0.08	42,42,42,42	0
56	MG	2A	3344	1/1	0.89	0.25	67,67,67,67	0
56	MG	1a	1741	1/1	0.89	0.09	48,48,48,48	0
56	MG	2A	3496	1/1	0.89	0.10	50,50,50,50	0
56	MG	1A	3634	1/1	0.89	0.09	38,38,38,38	0
56	MG	2A	3773	1/1	0.89	0.09	59,59,59,59	0
56	MG	1A	3635	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($\text{\AA}^2$)	Q<0.9
56	MG	2a	1720	1/1	0.89	0.17	55,55,55,55	0
56	MG	1A	3211	1/1	0.89	0.24	56,56,56,56	0
56	MG	2A	3046	1/1	0.89	0.16	49,49,49,49	0
56	MG	1A	3517	1/1	0.89	0.12	58,58,58,58	0
56	MG	2A	3352	1/1	0.89	0.14	66,66,66,66	0
56	MG	1A	3823	1/1	0.89	0.12	40,40,40,40	0
56	MG	2A	3790	1/1	0.89	0.08	82,82,82,82	0
56	MG	1a	1782	1/1	0.89	0.09	59,59,59,59	0
56	MG	2A	3354	1/1	0.89	0.11	60,60,60,60	0
56	MG	2A	3217	1/1	0.89	0.15	62,62,62,62	0
56	MG	1A	3984	1/1	0.89	0.11	40,40,40,40	0
56	MG	1A	3344	1/1	0.89	0.20	48,48,48,48	0
56	MG	2A	3522	1/1	0.89	0.14	62,62,62,62	0
56	MG	2A	3524	1/1	0.89	0.14	69,69,69,69	0
56	MG	2A	3525	1/1	0.89	0.07	62,62,62,62	0
56	MG	2A	3530	1/1	0.89	0.15	55,55,55,55	0
56	MG	2a	1769	1/1	0.89	0.08	56,56,56,56	0
56	MG	1a	1818	1/1	0.89	0.17	53,53,53,53	0
56	MG	2A	3811	1/1	0.89	0.08	45,45,45,45	0
56	MG	2A	3812	1/1	0.89	0.15	61,61,61,61	0
56	MG	1A	3519	1/1	0.89	0.18	45,45,45,45	0
56	MG	2A	3055	1/1	0.89	0.09	44,44,44,44	0
56	MG	1A	3345	1/1	0.89	0.15	56,56,56,56	0
56	MG	1A	3132	1/1	0.89	0.18	52,52,52,52	0
56	MG	2A	3829	1/1	0.89	0.10	61,61,61,61	0
56	MG	2A	3836	1/1	0.89	0.08	91,91,91,91	0
56	MG	2A	3058	1/1	0.89	0.11	54,54,54,54	0
56	MG	1A	3193	1/1	0.89	0.43	41,41,41,41	0
56	MG	2a	1791	1/1	0.89	0.22	71,71,71,71	0
56	MG	1a	1841	1/1	0.89	0.09	62,62,62,62	0
56	MG	1b	301	1/1	0.89	0.08	82,82,82,82	0
56	MG	1A	3397	1/1	0.89	0.15	33,33,33,33	0
56	MG	1A	3288	1/1	0.89	0.13	55,55,55,55	0
56	MG	1h	201	1/1	0.89	0.12	64,64,64,64	0
56	MG	1A	3846	1/1	0.89	0.10	35,35,35,35	0
56	MG	2A	3859	1/1	0.89	0.20	47,47,47,47	0
56	MG	2A	3070	1/1	0.89	0.23	58,58,58,58	0
56	MG	1B	204	1/1	0.89	0.17	52,52,52,52	0
56	MG	2A	3374	1/1	0.89	0.11	61,61,61,61	0
56	MG	2A	3575	1/1	0.89	0.09	35,35,35,35	0
56	MG	1B	211	1/1	0.89	0.11	57,57,57,57	0
56	MG	1w	104	1/1	0.89	0.29	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3255	1/1	0.89	0.20	53,53,53,53	0
56	MG	2A	3587	1/1	0.89	0.15	52,52,52,52	0
56	MG	2A	3241	1/1	0.89	0.10	61,61,61,61	0
56	MG	2a	1816	1/1	0.89	0.16	67,67,67,67	0
56	MG	2A	3590	1/1	0.89	0.10	54,54,54,54	0
56	MG	1x	106	1/1	0.89	0.19	66,66,66,66	0
56	MG	2A	3074	1/1	0.89	0.16	60,60,60,60	0
56	MG	2A	3249	1/1	0.89	0.23	64,64,64,64	0
56	MG	1A	3541	1/1	0.89	0.10	53,53,53,53	0
56	MG	1B	229	1/1	0.89	0.09	62,62,62,62	0
56	MG	1A	3685	1/1	0.89	0.10	66,66,66,66	0
56	MG	1B	231	1/1	0.89	0.12	64,64,64,64	0
56	MG	2a	1827	1/1	0.89	0.16	68,68,68,68	0
56	MG	1A	3852	1/1	0.89	0.17	54,54,54,54	0
56	MG	1B	234	1/1	0.89	0.11	67,67,67,67	0
56	MG	1A	3167	1/1	0.89	0.12	36,36,36,36	0
56	MG	1A	3545	1/1	0.89	0.16	53,53,53,53	0
56	MG	1A	3408	1/1	0.89	0.10	53,53,53,53	0
56	MG	1D	312	1/1	0.89	0.16	23,23,23,23	0
56	MG	1A	4065	1/1	0.89	0.32	52,52,52,52	0
56	MG	2A	3117	1/1	0.89	0.14	54,54,54,54	0
56	MG	1A	3863	1/1	0.89	0.19	29,29,29,29	0
56	MG	2A	3263	1/1	0.89	0.07	60,60,60,60	0
56	MG	1G	205	1/1	0.89	0.08	54,54,54,54	0
56	MG	2A	3264	1/1	0.89	0.11	66,66,66,66	0
56	MG	1A	3354	1/1	0.89	0.26	59,59,59,59	0
56	MG	1A	3562	1/1	0.89	0.20	48,48,48,48	0
56	MG	2A	3399	1/1	0.89	0.15	43,43,43,43	0
56	MG	1O	202	1/1	0.89	0.26	62,62,62,62	0
56	MG	2A	3636	1/1	0.89	0.15	62,62,62,62	0
56	MG	2x	102	1/1	0.89	0.20	75,75,75,75	0
56	MG	1A	3870	1/1	0.89	0.10	44,44,44,44	0
56	MG	1Q	204	1/1	0.89	0.07	52,52,52,52	0
56	MG	2E	302	1/1	0.89	0.23	39,39,39,39	0
56	MG	2A	3404	1/1	0.89	0.20	58,58,58,58	0
56	MG	1A	3224	1/1	0.89	0.17	46,46,46,46	0
56	MG	1A	3295	1/1	0.89	0.31	64,64,64,64	0
56	MG	2F	303	1/1	0.89	0.10	49,49,49,49	0
56	MG	1A	4077	1/1	0.89	0.20	56,56,56,56	0
56	MG	2A	3661	1/1	0.89	0.17	44,44,44,44	0
56	MG	1B	222	1/1	0.90	0.15	51,51,51,51	0
56	MG	1A	4062	1/1	0.90	0.17	61,61,61,61	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3613	1/1	0.90	0.09	12,12,12,12	0
56	MG	2A	3335	1/1	0.90	0.09	61,61,61,61	0
56	MG	1A	3889	1/1	0.90	0.11	58,58,58,58	0
56	MG	2A	3681	1/1	0.90	0.11	55,55,55,55	0
56	MG	1a	1772	1/1	0.90	0.10	53,53,53,53	0
56	MG	2A	3065	1/1	0.90	0.24	54,54,54,54	0
56	MG	1a	1775	1/1	0.90	0.09	59,59,59,59	0
56	MG	1a	1779	1/1	0.90	0.10	72,72,72,72	0
56	MG	2A	3222	1/1	0.90	0.22	63,63,63,63	0
56	MG	1A	3892	1/1	0.90	0.14	43,43,43,43	0
56	MG	1A	3040	1/1	0.90	0.20	57,57,57,57	0
56	MG	2A	3689	1/1	0.90	0.07	59,59,59,59	0
56	MG	2a	1655	1/1	0.90	0.22	63,63,63,63	0
56	MG	2A	3071	1/1	0.90	0.27	61,61,61,61	0
56	MG	2a	1657	1/1	0.90	0.24	53,53,53,53	0
56	MG	1A	3182	1/1	0.90	0.07	68,68,68,68	0
56	MG	2A	3472	1/1	0.90	0.29	56,56,56,56	0
56	MG	2A	3349	1/1	0.90	0.14	69,69,69,69	0
56	MG	1A	3904	1/1	0.90	0.10	43,43,43,43	0
56	MG	1a	1814	1/1	0.90	0.10	84,84,84,84	0
56	MG	2A	3477	1/1	0.90	0.43	56,56,56,56	0
56	MG	1G	204	1/1	0.90	0.07	42,42,42,42	0
56	MG	2A	3701	1/1	0.90	0.07	54,54,54,54	0
56	MG	2a	1676	1/1	0.90	0.22	66,66,66,66	0
56	MG	2a	1681	1/1	0.90	0.14	62,62,62,62	0
56	MG	1a	1827	1/1	0.90	0.19	70,70,70,70	0
56	MG	2a	1685	1/1	0.90	0.14	60,60,60,60	0
56	MG	2A	3078	1/1	0.90	0.10	51,51,51,51	0
56	MG	2A	3082	1/1	0.90	0.24	59,59,59,59	0
56	MG	1N	205	1/1	0.90	0.20	44,44,44,44	0
56	MG	1A	3618	1/1	0.90	0.09	29,29,29,29	0
56	MG	1A	3183	1/1	0.90	0.07	39,39,39,39	0
56	MG	1A	3250	1/1	0.90	0.21	52,52,52,52	0
56	MG	2A	3707	1/1	0.90	0.09	44,44,44,44	0
56	MG	1A	3367	1/1	0.90	0.12	51,51,51,51	0
56	MG	1A	3448	1/1	0.90	0.32	65,65,65,65	0
56	MG	2A	3103	1/1	0.90	0.13	27,27,27,27	0
56	MG	2A	3107	1/1	0.90	0.20	62,62,62,62	0
56	MG	2A	3113	1/1	0.90	0.12	50,50,50,50	0
56	MG	1A	3298	1/1	0.90	0.27	51,51,51,51	0
56	MG	2A	3717	1/1	0.90	0.15	69,69,69,69	0
56	MG	1m	202	1/1	0.90	0.23	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3497	1/1	0.90	0.19	47,47,47,47	0
56	MG	1A	3918	1/1	0.90	0.10	53,53,53,53	0
56	MG	2A	3366	1/1	0.90	0.11	59,59,59,59	0
56	MG	10	103	1/1	0.90	0.13	42,42,42,42	0
56	MG	11	103	1/1	0.90	0.13	67,67,67,67	0
56	MG	1A	3636	1/1	0.90	0.10	21,21,21,21	0
56	MG	1A	3123	1/1	0.90	0.12	42,42,42,42	0
56	MG	2A	3725	1/1	0.90	0.06	49,49,49,49	0
56	MG	1A	4097	1/1	0.90	0.14	60,60,60,60	0
56	MG	1A	3452	1/1	0.90	0.12	40,40,40,40	0
56	MG	2a	1723	1/1	0.90	0.20	66,66,66,66	0
56	MG	2A	3373	1/1	0.90	0.18	65,65,65,65	0
56	MG	1A	3811	1/1	0.90	0.10	39,39,39,39	0
56	MG	2A	3732	1/1	0.90	0.09	62,62,62,62	0
56	MG	1A	3528	1/1	0.90	0.31	43,43,43,43	0
56	MG	1A	3001	1/1	0.90	0.09	34,34,34,34	0
56	MG	2a	1732	1/1	0.90	0.10	62,62,62,62	0
56	MG	1A	4126	1/1	0.90	0.44	41,41,41,41	0
56	MG	2A	3379	1/1	0.90	0.13	58,58,58,58	0
56	MG	1A	3819	1/1	0.90	0.14	49,49,49,49	0
56	MG	1a	1625	1/1	0.90	0.28	57,57,57,57	0
56	MG	1a	1626	1/1	0.90	0.08	44,44,44,44	0
56	MG	1a	1629	1/1	0.90	0.13	59,59,59,59	0
56	MG	2a	1760	1/1	0.90	0.09	81,81,81,81	0
56	MG	1A	3457	1/1	0.90	0.14	40,40,40,40	0
56	MG	1A	3652	1/1	0.90	0.14	37,37,37,37	0
56	MG	2a	1765	1/1	0.90	0.13	69,69,69,69	0
56	MG	1A	3311	1/1	0.90	0.10	41,41,41,41	0
56	MG	1A	3026	1/1	0.90	0.19	43,43,43,43	0
56	MG	2B	205	1/1	0.90	0.19	69,69,69,69	0
56	MG	1A	3958	1/1	0.90	0.09	73,73,73,73	0
56	MG	1A	3203	1/1	0.90	0.11	26,26,26,26	0
56	MG	2A	3272	1/1	0.90	0.23	64,64,64,64	0
56	MG	2A	3761	1/1	0.90	0.16	63,63,63,63	0
56	MG	2A	3140	1/1	0.90	0.23	41,41,41,41	0
56	MG	2B	211	1/1	0.90	0.08	61,61,61,61	0
56	MG	1A	3088	1/1	0.90	0.29	38,38,38,38	0
56	MG	2A	3766	1/1	0.90	0.10	64,64,64,64	0
56	MG	1a	1656	1/1	0.90	0.07	54,54,54,54	0
56	MG	2A	3558	1/1	0.90	0.08	51,51,51,51	0
56	MG	1A	3261	1/1	0.90	0.15	40,40,40,40	0
56	MG	1A	3005	1/1	0.90	0.10	47,47,47,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2a	1793	1/1	0.90	0.10	74,74,74,74	0
56	MG	2A	3006	1/1	0.90	0.16	62,62,62,62	0
56	MG	1A	3400	1/1	0.90	0.17	53,53,53,53	0
56	MG	1A	3975	1/1	0.90	0.07	113,113,113,113	0
56	MG	2E	305	1/1	0.90	0.17	64,64,64,64	0
56	MG	2A	3014	1/1	0.90	0.15	50,50,50,50	0
56	MG	2a	1802	1/1	0.90	0.20	75,75,75,75	0
56	MG	2A	3403	1/1	0.90	0.08	45,45,45,45	0
56	MG	2A	3160	1/1	0.90	0.16	49,49,49,49	0
56	MG	2A	3589	1/1	0.90	0.08	62,62,62,62	0
56	MG	1a	1669	1/1	0.90	0.18	52,52,52,52	0
56	MG	1A	3558	1/1	0.90	0.17	53,53,53,53	0
56	MG	1a	1673	1/1	0.90	0.17	49,49,49,49	0
56	MG	1A	3689	1/1	0.90	0.08	25,25,25,25	0
56	MG	1A	3700	1/1	0.90	0.16	34,34,34,34	0
56	MG	1A	3561	1/1	0.90	0.13	34,34,34,34	0
56	MG	1a	1679	1/1	0.90	0.32	47,47,47,47	0
56	MG	2U	201	1/1	0.90	0.18	44,44,44,44	0
56	MG	1A	3342	1/1	0.90	0.32	37,37,37,37	0
56	MG	2A	3028	1/1	0.90	0.17	52,52,52,52	0
56	MG	1A	3146	1/1	0.90	0.10	39,39,39,39	0
56	MG	2A	3608	1/1	0.90	0.10	47,47,47,47	0
56	MG	2A	3175	1/1	0.90	0.31	59,59,59,59	0
56	MG	1A	3148	1/1	0.90	0.24	27,27,27,27	0
56	MG	1A	3091	1/1	0.90	0.22	51,51,51,51	0
56	MG	2A	3033	1/1	0.90	0.38	54,54,54,54	0
56	MG	1A	3990	1/1	0.90	0.20	65,65,65,65	0
56	MG	1a	1696	1/1	0.90	0.23	39,39,39,39	0
56	MG	1a	1698	1/1	0.90	0.13	42,42,42,42	0
56	MG	2a	1601	1/1	0.90	0.10	57,57,57,57	0
56	MG	1A	3274	1/1	0.90	0.36	37,37,37,37	0
56	MG	1A	3007	1/1	0.90	0.10	37,37,37,37	0
56	MG	1A	3351	1/1	0.90	0.11	53,53,53,53	0
56	MG	2A	3428	1/1	0.90	0.28	58,58,58,58	0
56	MG	1A	3166	1/1	0.90	0.24	51,51,51,51	0
56	MG	2A	3318	1/1	0.90	0.25	62,62,62,62	0
56	MG	2A	3048	1/1	0.90	0.15	52,52,52,52	0
56	MG	1A	3867	1/1	0.90	0.26	38,38,38,38	0
56	MG	1A	3737	1/1	0.90	0.15	66,66,66,66	0
56	MG	2A	3322	1/1	0.90	0.13	59,59,59,59	0
56	MG	2A	3440	1/1	0.90	0.22	50,50,50,50	0
56	MG	2v	101	1/1	0.90	0.16	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1B	201	1/1	0.90	0.09	53,53,53,53	0
56	MG	1B	202	1/1	0.90	0.15	59,59,59,59	0
56	MG	1A	3035	1/1	0.90	0.09	41,41,41,41	0
56	MG	1A	4037	1/1	0.90	0.10	42,42,42,42	0
56	MG	1A	3103	1/1	0.90	0.14	60,60,60,60	0
56	MG	1A	3231	1/1	0.90	0.13	51,51,51,51	0
56	MG	1A	3233	1/1	0.90	0.10	65,65,65,65	0
56	MG	2A	3204	1/1	0.90	0.19	53,53,53,53	0
56	MG	2a	1626	1/1	0.90	0.12	64,64,64,64	0
56	MG	1A	3427	1/1	0.90	0.12	52,52,52,52	0
56	MG	2A	3451	1/1	0.90	0.07	61,61,61,61	0
56	MG	1A	3428	1/1	0.90	0.11	41,41,41,41	0
56	MG	1a	1747	1/1	0.90	0.12	49,49,49,49	0
56	MG	1a	1711	1/1	0.91	0.18	39,39,39,39	0
56	MG	2A	3034	1/1	0.91	0.28	34,34,34,34	0
56	MG	1A	3858	1/1	0.91	0.14	30,30,30,30	0
56	MG	1A	3212	1/1	0.91	0.28	54,54,54,54	0
56	MG	1A	3047	1/1	0.91	0.16	31,31,31,31	0
56	MG	1A	3608	1/1	0.91	0.10	36,36,36,36	0
56	MG	2a	1623	1/1	0.91	0.21	56,56,56,56	0
56	MG	2A	3631	1/1	0.91	0.16	53,53,53,53	0
56	MG	1a	1720	1/1	0.91	0.20	51,51,51,51	0
56	MG	1A	3864	1/1	0.91	0.37	41,41,41,41	0
56	MG	2A	3858	1/1	0.91	0.06	66,66,66,66	0
56	MG	1A	4016	1/1	0.91	0.12	58,58,58,58	0
56	MG	2A	3860	1/1	0.91	0.11	36,36,36,36	0
56	MG	2A	3188	1/1	0.91	0.06	72,72,72,72	0
56	MG	2a	1635	1/1	0.91	0.27	51,51,51,51	0
56	MG	1A	3757	1/1	0.91	0.11	40,40,40,40	0
56	MG	1A	3361	1/1	0.91	0.12	57,57,57,57	0
56	MG	2A	3644	1/1	0.91	0.12	53,53,53,53	0
56	MG	1B	205	1/1	0.91	0.24	57,57,57,57	0
56	MG	1A	3765	1/1	0.91	0.09	58,58,58,58	0
56	MG	2A	3443	1/1	0.91	0.09	48,48,48,48	0
56	MG	1A	3248	1/1	0.91	0.08	41,41,41,41	0
56	MG	2a	1644	1/1	0.91	0.14	55,55,55,55	0
56	MG	1a	1754	1/1	0.91	0.16	58,58,58,58	0
56	MG	1A	3770	1/1	0.91	0.09	39,39,39,39	0
56	MG	1A	3521	1/1	0.91	0.35	44,44,44,44	0
56	MG	1B	218	1/1	0.91	0.12	42,42,42,42	0
56	MG	1a	1765	1/1	0.91	0.10	60,60,60,60	0
56	MG	1a	1766	1/1	0.91	0.09	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3197	1/1	0.91	0.15	40,40,40,40	0
56	MG	1A	3522	1/1	0.91	0.25	43,43,43,43	0
56	MG	2A	3449	1/1	0.91	0.26	57,57,57,57	0
56	MG	1A	3188	1/1	0.91	0.13	30,30,30,30	0
56	MG	1A	4056	1/1	0.91	0.10	48,48,48,48	0
56	MG	1A	3884	1/1	0.91	0.09	22,22,22,22	0
56	MG	1A	3464	1/1	0.91	0.27	65,65,65,65	0
56	MG	2a	1662	1/1	0.91	0.17	51,51,51,51	0
56	MG	1A	3785	1/1	0.91	0.13	17,17,17,17	0
56	MG	2a	1665	1/1	0.91	0.24	55,55,55,55	0
56	MG	2a	1666	1/1	0.91	0.09	60,60,60,60	0
56	MG	2A	3214	1/1	0.91	0.10	49,49,49,49	0
56	MG	1A	3527	1/1	0.91	0.20	37,37,37,37	0
56	MG	1A	3791	1/1	0.91	0.13	40,40,40,40	0
56	MG	2a	1673	1/1	0.91	0.18	53,53,53,53	0
56	MG	2A	3458	1/1	0.91	0.14	58,58,58,58	0
56	MG	2A	3683	1/1	0.91	0.09	78,78,78,78	0
56	MG	1A	3893	1/1	0.91	0.17	48,48,48,48	0
56	MG	2a	1682	1/1	0.91	0.27	68,68,68,68	0
56	MG	1A	3159	1/1	0.91	0.19	33,33,33,33	0
56	MG	2A	3686	1/1	0.91	0.13	64,64,64,64	0
56	MG	1A	3366	1/1	0.91	0.26	78,78,78,78	0
56	MG	2A	3463	1/1	0.91	0.22	54,54,54,54	0
56	MG	2A	3073	1/1	0.91	0.18	55,55,55,55	0
56	MG	1A	3903	1/1	0.91	0.09	20,20,20,20	0
56	MG	1a	1823	1/1	0.91	0.08	43,43,43,43	0
56	MG	1a	1826	1/1	0.91	0.17	62,62,62,62	0
56	MG	2A	3693	1/1	0.91	0.20	63,63,63,63	0
56	MG	1A	3170	1/1	0.91	0.07	43,43,43,43	0
56	MG	1I	201	1/1	0.91	0.10	60,60,60,60	0
56	MG	2A	3351	1/1	0.91	0.25	64,64,64,64	0
56	MG	1A	3368	1/1	0.91	0.17	53,53,53,53	0
56	MG	2A	3697	1/1	0.91	0.09	65,65,65,65	0
56	MG	2A	3084	1/1	0.91	0.15	48,48,48,48	0
56	MG	1A	4078	1/1	0.91	0.14	45,45,45,45	0
56	MG	1A	3906	1/1	0.91	0.10	58,58,58,58	0
56	MG	1A	4080	1/1	0.91	0.14	58,58,58,58	0
56	MG	1a	1840	1/1	0.91	0.09	54,54,54,54	0
56	MG	1Q	201	1/1	0.91	0.17	37,37,37,37	0
56	MG	1a	1842	1/1	0.91	0.25	58,58,58,58	0
56	MG	1A	3256	1/1	0.91	0.20	64,64,64,64	0
56	MG	1T	201	1/1	0.91	0.12	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3142	1/1	0.91	0.12	43,43,43,43	0
56	MG	2A	3102	1/1	0.91	0.19	43,43,43,43	0
56	MG	1U	205	1/1	0.91	0.18	49,49,49,49	0
56	MG	2A	3361	1/1	0.91	0.13	49,49,49,49	0
56	MG	1r	101	1/1	0.91	0.09	70,70,70,70	0
56	MG	1A	3374	1/1	0.91	0.10	43,43,43,43	0
56	MG	2A	3708	1/1	0.91	0.11	59,59,59,59	0
56	MG	2A	3105	1/1	0.91	0.13	57,57,57,57	0
56	MG	1Z	302	1/1	0.91	0.11	52,52,52,52	0
56	MG	1A	3204	1/1	0.91	0.11	49,49,49,49	0
56	MG	2A	3108	1/1	0.91	0.15	61,61,61,61	0
56	MG	1A	3807	1/1	0.91	0.08	41,41,41,41	0
56	MG	10	106	1/1	0.91	0.07	44,44,44,44	0
56	MG	2A	3251	1/1	0.91	0.35	64,64,64,64	0
56	MG	1A	3429	1/1	0.91	0.21	53,53,53,53	0
56	MG	2a	1745	1/1	0.91	0.10	54,54,54,54	0
56	MG	1A	3663	1/1	0.91	0.12	61,61,61,61	0
56	MG	1A	3115	1/1	0.91	0.07	41,41,41,41	0
56	MG	1x	107	1/1	0.91	0.24	54,54,54,54	0
56	MG	2A	3118	1/1	0.91	0.16	56,56,56,56	0
56	MG	1A	3813	1/1	0.91	0.08	27,27,27,27	0
56	MG	1A	3550	1/1	0.91	0.20	51,51,51,51	0
56	MG	1A	4122	1/1	0.91	0.08	35,35,35,35	0
56	MG	1A	3163	1/1	0.91	0.10	44,44,44,44	0
56	MG	2A	3726	1/1	0.91	0.08	70,70,70,70	0
56	MG	2A	3513	1/1	0.91	0.06	61,61,61,61	0
56	MG	1A	3389	1/1	0.91	0.56	45,45,45,45	0
56	MG	1A	3487	1/1	0.91	0.10	45,45,45,45	0
56	MG	2A	3265	1/1	0.91	0.06	53,53,53,53	0
56	MG	2A	3523	1/1	0.91	0.27	36,36,36,36	0
56	MG	1A	3164	1/1	0.91	0.13	32,32,32,32	0
56	MG	1a	1628	1/1	0.91	0.30	55,55,55,55	0
56	MG	1A	3490	1/1	0.91	0.12	45,45,45,45	0
56	MG	2A	3526	1/1	0.91	0.17	61,61,61,61	0
56	MG	1a	1632	1/1	0.91	0.28	62,62,62,62	0
56	MG	1A	4144	1/1	0.91	0.11	46,46,46,46	0
56	MG	1a	1636	1/1	0.91	0.19	51,51,51,51	0
56	MG	2A	3740	1/1	0.91	0.10	50,50,50,50	0
56	MG	1A	3442	1/1	0.91	0.13	40,40,40,40	0
56	MG	1A	3445	1/1	0.91	0.11	51,51,51,51	0
56	MG	2A	3539	1/1	0.91	0.11	50,50,50,50	0
56	MG	1A	3826	1/1	0.91	0.14	57,57,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3959	1/1	0.91	0.09	69,69,69,69	0
56	MG	1A	3960	1/1	0.91	0.10	38,38,38,38	0
56	MG	1A	3692	1/1	0.91	0.17	53,53,53,53	0
56	MG	2B	219	1/1	0.91	0.10	77,77,77,77	0
56	MG	2B	220	1/1	0.91	0.24	63,63,63,63	0
56	MG	2A	3550	1/1	0.91	0.09	52,52,52,52	0
56	MG	2D	303	1/1	0.91	0.12	67,67,67,67	0
56	MG	2A	3760	1/1	0.91	0.24	52,52,52,52	0
56	MG	2E	304	1/1	0.91	0.08	58,58,58,58	0
56	MG	1A	3830	1/1	0.91	0.18	53,53,53,53	0
56	MG	2E	306	1/1	0.91	0.14	47,47,47,47	0
56	MG	2A	3557	1/1	0.91	0.11	56,56,56,56	0
56	MG	1A	3832	1/1	0.91	0.09	60,60,60,60	0
56	MG	2A	3008	1/1	0.91	0.08	38,38,38,38	0
56	MG	2A	3398	1/1	0.91	0.14	56,56,56,56	0
56	MG	2a	1820	1/1	0.91	0.19	57,57,57,57	0
56	MG	2F	304	1/1	0.91	0.14	58,58,58,58	0
56	MG	2A	3151	1/1	0.91	0.12	51,51,51,51	0
56	MG	2A	3565	1/1	0.91	0.20	56,56,56,56	0
56	MG	2A	3568	1/1	0.91	0.16	57,57,57,57	0
56	MG	2A	3400	1/1	0.91	0.09	44,44,44,44	0
56	MG	1a	1667	1/1	0.91	0.20	73,73,73,73	0
56	MG	1A	3265	1/1	0.91	0.31	48,48,48,48	0
56	MG	2A	3578	1/1	0.91	0.10	55,55,55,55	0
56	MG	1A	3969	1/1	0.91	0.10	20,20,20,20	0
56	MG	2U	202	1/1	0.91	0.05	50,50,50,50	0
56	MG	2d	301	1/1	0.91	0.22	43,43,43,43	0
56	MG	2A	3777	1/1	0.91	0.12	66,66,66,66	0
56	MG	2A	3583	1/1	0.91	0.08	37,37,37,37	0
56	MG	2A	3784	1/1	0.91	0.08	47,47,47,47	0
56	MG	2A	3156	1/1	0.91	0.22	51,51,51,51	0
56	MG	2A	3286	1/1	0.91	0.10	46,46,46,46	0
56	MG	1A	3703	1/1	0.91	0.11	39,39,39,39	0
56	MG	2A	3291	1/1	0.91	0.22	47,47,47,47	0
56	MG	2A	3794	1/1	0.91	0.16	79,79,79,79	0
56	MG	1A	3500	1/1	0.91	0.20	58,58,58,58	0
56	MG	25	101	1/1	0.91	0.15	64,64,64,64	0
56	MG	2A	3597	1/1	0.91	0.11	66,66,66,66	0
56	MG	1A	3238	1/1	0.91	0.18	43,43,43,43	0
56	MG	1a	1690	1/1	0.91	0.21	40,40,40,40	0
56	MG	1a	1691	1/1	0.91	0.15	62,62,62,62	0
56	MG	1A	3589	1/1	0.91	0.18	32,32,32,32	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3601	1/1	0.91	0.13	45,45,45,45	0
56	MG	1A	3268	1/1	0.91	0.15	43,43,43,43	0
56	MG	2a	1608	1/1	0.91	0.06	74,74,74,74	0
56	MG	2A	3027	1/1	0.91	0.26	45,45,45,45	0
56	MG	1A	3711	1/1	0.91	0.13	39,39,39,39	0
56	MG	1A	3242	1/1	0.91	0.10	47,47,47,47	0
56	MG	1A	3356	1/1	0.91	0.10	46,46,46,46	0
56	MG	1A	3596	1/1	0.91	0.10	37,37,37,37	0
56	MG	1A	3453	1/1	0.91	0.14	49,49,49,49	0
56	MG	2A	3620	1/1	0.91	0.09	56,56,56,56	0
56	MG	1a	1680	1/1	0.92	0.24	48,48,48,48	0
56	MG	1A	3507	1/1	0.92	0.16	32,32,32,32	0
56	MG	2A	3782	1/1	0.92	0.09	67,67,67,67	0
56	MG	1A	3150	1/1	0.92	0.23	34,34,34,34	0
56	MG	1A	3151	1/1	0.92	0.16	44,44,44,44	0
56	MG	1A	3267	1/1	0.92	0.10	38,38,38,38	0
56	MG	2A	3789	1/1	0.92	0.07	43,43,43,43	0
56	MG	1a	1689	1/1	0.92	0.31	67,67,67,67	0
56	MG	2A	3566	1/1	0.92	0.10	51,51,51,51	0
56	MG	2A	3066	1/1	0.92	0.25	51,51,51,51	0
56	MG	2A	3573	1/1	0.92	0.09	46,46,46,46	0
56	MG	1A	3232	1/1	0.92	0.16	44,44,44,44	0
56	MG	1A	4021	1/1	0.92	0.09	69,69,69,69	0
56	MG	1A	4028	1/1	0.92	0.07	31,31,31,31	0
56	MG	2A	3245	1/1	0.92	0.19	59,59,59,59	0
56	MG	1a	1702	1/1	0.92	0.28	56,56,56,56	0
56	MG	1A	3157	1/1	0.92	0.08	63,63,63,63	0
56	MG	1A	3847	1/1	0.92	0.08	46,46,46,46	0
56	MG	1A	4040	1/1	0.92	0.10	54,54,54,54	0
56	MG	2A	3806	1/1	0.92	0.08	74,74,74,74	0
56	MG	1a	1709	1/1	0.92	0.22	41,41,41,41	0
56	MG	2A	3076	1/1	0.92	0.10	40,40,40,40	0
56	MG	1A	3271	1/1	0.92	0.20	49,49,49,49	0
56	MG	1A	3272	1/1	0.92	0.27	54,54,54,54	0
56	MG	2A	3594	1/1	0.92	0.11	38,38,38,38	0
56	MG	2a	1629	1/1	0.92	0.12	62,62,62,62	0
56	MG	1A	3074	1/1	0.92	0.25	58,58,58,58	0
56	MG	2A	3820	1/1	0.92	0.07	49,49,49,49	0
56	MG	2a	1634	1/1	0.92	0.17	47,47,47,47	0
56	MG	1A	3078	1/1	0.92	0.20	31,31,31,31	0
56	MG	1A	3854	1/1	0.92	0.10	57,57,57,57	0
56	MG	2A	3830	1/1	0.92	0.12	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3525	1/1	0.92	0.16	40,40,40,40	0
56	MG	2a	1639	1/1	0.92	0.17	63,63,63,63	0
56	MG	1A	3240	1/1	0.92	0.23	41,41,41,41	0
56	MG	1A	3436	1/1	0.92	0.34	38,38,38,38	0
56	MG	2A	3844	1/1	0.92	0.08	51,51,51,51	0
56	MG	2A	3101	1/1	0.92	0.21	57,57,57,57	0
56	MG	1a	1735	1/1	0.92	0.08	35,35,35,35	0
56	MG	1A	3691	1/1	0.92	0.14	24,24,24,24	0
56	MG	1A	3438	1/1	0.92	0.19	37,37,37,37	0
56	MG	2A	3855	1/1	0.92	0.29	49,49,49,49	0
56	MG	1A	3277	1/1	0.92	0.23	31,31,31,31	0
56	MG	2A	3616	1/1	0.92	0.07	47,47,47,47	0
56	MG	1A	3535	1/1	0.92	0.22	56,56,56,56	0
56	MG	1A	4069	1/1	0.92	0.19	30,30,30,30	0
56	MG	1a	1749	1/1	0.92	0.09	53,53,53,53	0
56	MG	2A	3622	1/1	0.92	0.15	61,61,61,61	0
56	MG	2A	3413	1/1	0.92	0.16	55,55,55,55	0
56	MG	2a	1658	1/1	0.92	0.14	73,73,73,73	0
56	MG	2A	3112	1/1	0.92	0.24	56,56,56,56	0
56	MG	2A	3418	1/1	0.92	0.17	66,66,66,66	0
56	MG	1A	3281	1/1	0.92	0.18	46,46,46,46	0
56	MG	1A	3241	1/1	0.92	0.11	47,47,47,47	0
56	MG	2a	1663	1/1	0.92	0.10	77,77,77,77	0
56	MG	1B	210	1/1	0.92	0.09	48,48,48,48	0
56	MG	2A	3421	1/1	0.92	0.10	61,61,61,61	0
56	MG	1A	3197	1/1	0.92	0.13	37,37,37,37	0
56	MG	1A	3363	1/1	0.92	0.11	61,61,61,61	0
56	MG	1A	3543	1/1	0.92	0.29	46,46,46,46	0
56	MG	1A	3243	1/1	0.92	0.27	51,51,51,51	0
56	MG	1A	3286	1/1	0.92	0.25	59,59,59,59	0
56	MG	1A	3287	1/1	0.92	0.15	54,54,54,54	0
56	MG	2A	3281	1/1	0.92	0.17	55,55,55,55	0
56	MG	2a	1678	1/1	0.92	0.18	57,57,57,57	0
56	MG	2A	3429	1/1	0.92	0.15	52,52,52,52	0
56	MG	1a	1788	1/1	0.92	0.10	57,57,57,57	0
56	MG	1A	3244	1/1	0.92	0.14	60,60,60,60	0
56	MG	1A	3019	1/1	0.92	0.27	48,48,48,48	0
56	MG	2a	1687	1/1	0.92	0.29	70,70,70,70	0
56	MG	1a	1794	1/1	0.92	0.18	83,83,83,83	0
56	MG	2A	3665	1/1	0.92	0.13	53,53,53,53	0
56	MG	1A	3553	1/1	0.92	0.11	46,46,46,46	0
56	MG	2a	1693	1/1	0.92	0.16	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1B	232	1/1	0.92	0.06	65,65,65,65	0
56	MG	1A	3752	1/1	0.92	0.08	35,35,35,35	0
56	MG	1A	4095	1/1	0.92	0.24	54,54,54,54	0
56	MG	1A	3554	1/1	0.92	0.23	48,48,48,48	0
56	MG	2A	3132	1/1	0.92	0.29	54,54,54,54	0
56	MG	2a	1700	1/1	0.92	0.10	62,62,62,62	0
56	MG	1D	310	1/1	0.92	0.21	47,47,47,47	0
56	MG	1a	1822	1/1	0.92	0.10	69,69,69,69	0
56	MG	1A	3755	1/1	0.92	0.10	31,31,31,31	0
56	MG	1a	1825	1/1	0.92	0.06	74,74,74,74	0
56	MG	2a	1706	1/1	0.92	0.14	65,65,65,65	0
56	MG	1A	3290	1/1	0.92	0.22	49,49,49,49	0
56	MG	1A	3759	1/1	0.92	0.08	27,27,27,27	0
56	MG	2A	3137	1/1	0.92	0.07	55,55,55,55	0
56	MG	1F	304	1/1	0.92	0.10	52,52,52,52	0
56	MG	1A	3370	1/1	0.92	0.15	46,46,46,46	0
56	MG	1A	3762	1/1	0.92	0.14	29,29,29,29	0
56	MG	1A	3246	1/1	0.92	0.22	42,42,42,42	0
56	MG	1A	3059	1/1	0.92	0.16	48,48,48,48	0
56	MG	2a	1715	1/1	0.92	0.07	46,46,46,46	0
56	MG	1A	4130	1/1	0.92	0.64	39,39,39,39	0
56	MG	1a	1837	1/1	0.92	0.13	79,79,79,79	0
56	MG	1A	4135	1/1	0.92	0.14	42,42,42,42	0
56	MG	1A	3043	1/1	0.92	0.23	27,27,27,27	0
56	MG	1A	3572	1/1	0.92	0.19	37,37,37,37	0
56	MG	2a	1722	1/1	0.92	0.10	49,49,49,49	0
56	MG	2A	3311	1/1	0.92	0.09	61,61,61,61	0
56	MG	2a	1724	1/1	0.92	0.22	57,57,57,57	0
56	MG	2A	3154	1/1	0.92	0.27	63,63,63,63	0
56	MG	1a	1844	1/1	0.92	0.17	46,46,46,46	0
56	MG	1A	3574	1/1	0.92	0.10	33,33,33,33	0
56	MG	2A	3316	1/1	0.92	0.21	66,66,66,66	0
56	MG	1A	3130	1/1	0.92	0.10	35,35,35,35	0
56	MG	2a	1731	1/1	0.92	0.17	72,72,72,72	0
56	MG	1A	3916	1/1	0.92	0.10	22,22,22,22	0
56	MG	1l	201	1/1	0.92	0.18	42,42,42,42	0
56	MG	2a	1735	1/1	0.92	0.09	66,66,66,66	0
56	MG	1A	3044	1/1	0.92	0.30	38,38,38,38	0
56	MG	1A	3252	1/1	0.92	0.15	33,33,33,33	0
56	MG	2a	1740	1/1	0.92	0.08	69,69,69,69	0
56	MG	1A	3788	1/1	0.92	0.07	38,38,38,38	0
56	MG	2A	3698	1/1	0.92	0.08	52,52,52,52	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3465	1/1	0.92	0.23	33,33,33,33	0
56	MG	2a	1751	1/1	0.92	0.09	58,58,58,58	0
56	MG	1A	3169	1/1	0.92	0.10	50,50,50,50	0
56	MG	1A	3933	1/1	0.92	0.13	37,37,37,37	0
56	MG	1A	3470	1/1	0.92	0.10	54,54,54,54	0
56	MG	1A	3792	1/1	0.92	0.06	29,29,29,29	0
56	MG	1Y	203	1/1	0.92	0.37	57,57,57,57	0
56	MG	2a	1766	1/1	0.92	0.13	60,60,60,60	0
56	MG	2A	3168	1/1	0.92	0.09	51,51,51,51	0
56	MG	1A	3587	1/1	0.92	0.10	51,51,51,51	0
56	MG	2A	3172	1/1	0.92	0.22	49,49,49,49	0
56	MG	1A	3943	1/1	0.92	0.10	58,58,58,58	0
56	MG	2A	3011	1/1	0.92	0.07	47,47,47,47	0
56	MG	10	107	1/1	0.92	0.20	67,67,67,67	0
56	MG	1A	3310	1/1	0.92	0.17	41,41,41,41	0
56	MG	2A	3484	1/1	0.92	0.26	54,54,54,54	0
56	MG	1x	110	1/1	0.92	0.20	49,49,49,49	0
56	MG	2A	3016	1/1	0.92	0.27	53,53,53,53	0
56	MG	2a	1785	1/1	0.92	0.12	53,53,53,53	0
56	MG	2A	3333	1/1	0.92	0.13	59,59,59,59	0
56	MG	1A	3798	1/1	0.92	0.09	52,52,52,52	0
56	MG	15	105	1/1	0.92	0.09	36,36,36,36	0
56	MG	1A	3215	1/1	0.92	0.17	44,44,44,44	0
56	MG	17	102	1/1	0.92	0.15	57,57,57,57	0
56	MG	18	102	1/1	0.92	0.13	38,38,38,38	0
56	MG	2a	1794	1/1	0.92	0.10	74,74,74,74	0
56	MG	1a	1602	1/1	0.92	0.17	42,42,42,42	0
56	MG	2A	3342	1/1	0.92	0.17	41,41,41,41	0
56	MG	1a	1606	1/1	0.92	0.14	50,50,50,50	0
56	MG	1A	3476	1/1	0.92	0.09	38,38,38,38	0
56	MG	2A	3495	1/1	0.92	0.23	51,51,51,51	0
56	MG	1A	3396	1/1	0.92	0.21	36,36,36,36	0
56	MG	1a	1614	1/1	0.92	0.26	43,43,43,43	0
56	MG	2a	1805	1/1	0.92	0.23	63,63,63,63	0
56	MG	1A	3028	1/1	0.92	0.22	68,68,68,68	0
56	MG	1A	3604	1/1	0.92	0.08	27,27,27,27	0
56	MG	1A	3480	1/1	0.92	0.23	44,44,44,44	0
56	MG	1A	3319	1/1	0.92	0.16	55,55,55,55	0
56	MG	1A	3320	1/1	0.92	0.24	51,51,51,51	0
56	MG	2A	3503	1/1	0.92	0.29	60,60,60,60	0
56	MG	1A	3809	1/1	0.92	0.07	23,23,23,23	0
56	MG	2A	3505	1/1	0.92	0.18	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3402	1/1	0.92	0.11	43,43,43,43	0
56	MG	2A	3507	1/1	0.92	0.13	50,50,50,50	0
56	MG	1A	3609	1/1	0.92	0.16	45,45,45,45	0
56	MG	2A	3196	1/1	0.92	0.06	40,40,40,40	0
56	MG	2A	3035	1/1	0.92	0.30	39,39,39,39	0
56	MG	1a	1639	1/1	0.92	0.22	60,60,60,60	0
56	MG	2E	301	1/1	0.92	0.14	51,51,51,51	0
56	MG	1A	3052	1/1	0.92	0.20	36,36,36,36	0
56	MG	2A	3741	1/1	0.92	0.07	49,49,49,49	0
56	MG	1a	1643	1/1	0.92	0.13	60,60,60,60	0
56	MG	1A	3488	1/1	0.92	0.20	43,43,43,43	0
56	MG	2A	3201	1/1	0.92	0.28	43,43,43,43	0
56	MG	1a	1646	1/1	0.92	0.24	50,50,50,50	0
56	MG	2A	3519	1/1	0.92	0.14	50,50,50,50	0
56	MG	1A	3259	1/1	0.92	0.11	60,60,60,60	0
56	MG	2A	3043	1/1	0.92	0.10	63,63,63,63	0
56	MG	2d	302	1/1	0.92	0.06	57,57,57,57	0
56	MG	2A	3208	1/1	0.92	0.37	70,70,70,70	0
56	MG	2A	3209	1/1	0.92	0.15	49,49,49,49	0
56	MG	2P	202	1/1	0.92	0.26	47,47,47,47	0
56	MG	1A	3407	1/1	0.92	0.09	45,45,45,45	0
56	MG	2A	3756	1/1	0.92	0.09	71,71,71,71	0
56	MG	2A	3529	1/1	0.92	0.09	67,67,67,67	0
56	MG	2A	3045	1/1	0.92	0.10	64,64,64,64	0
56	MG	1A	3494	1/1	0.92	0.08	58,58,58,58	0
56	MG	2A	3535	1/1	0.92	0.12	35,35,35,35	0
56	MG	1A	3328	1/1	0.92	0.24	56,56,56,56	0
56	MG	2U	204	1/1	0.92	0.15	57,57,57,57	0
56	MG	2A	3767	1/1	0.92	0.08	34,34,34,34	0
56	MG	1A	3179	1/1	0.92	0.11	44,44,44,44	0
56	MG	1A	3053	1/1	0.92	0.07	51,51,51,51	0
56	MG	1A	3499	1/1	0.92	0.15	42,42,42,42	0
56	MG	1A	3337	1/1	0.92	0.17	35,35,35,35	0
56	MG	1a	1670	1/1	0.92	0.19	49,49,49,49	0
56	MG	1A	3263	1/1	0.92	0.17	59,59,59,59	0
56	MG	1A	3415	1/1	0.92	0.19	59,59,59,59	0
56	MG	1A	4004	1/1	0.92	0.09	38,38,38,38	0
56	MG	1A	4006	1/1	0.92	0.09	74,74,74,74	0
56	MG	25	102	1/1	0.92	0.30	43,43,43,43	0
56	MG	25	103	1/1	0.92	0.17	51,51,51,51	0
56	MG	1A	3073	1/1	0.92	0.18	30,30,30,30	0
56	MG	2A	3780	1/1	0.92	0.11	35,35,35,35	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1703	1/1	0.93	0.12	38,38,38,38	0
56	MG	2A	3850	1/1	0.93	0.12	51,51,51,51	0
56	MG	2A	3851	1/1	0.93	0.10	73,73,73,73	0
56	MG	1A	3740	1/1	0.93	0.08	44,44,44,44	0
56	MG	1A	3745	1/1	0.93	0.09	57,57,57,57	0
56	MG	2A	3857	1/1	0.93	0.20	50,50,50,50	0
56	MG	1A	3988	1/1	0.93	0.11	23,23,23,23	0
56	MG	2A	3646	1/1	0.93	0.10	42,42,42,42	0
56	MG	1A	3749	1/1	0.93	0.14	37,37,37,37	0
56	MG	1A	3998	1/1	0.93	0.08	24,24,24,24	0
56	MG	1A	4001	1/1	0.93	0.07	30,30,30,30	0
56	MG	2A	3654	1/1	0.93	0.09	36,36,36,36	0
56	MG	1a	1716	1/1	0.93	0.18	56,56,56,56	0
56	MG	2A	3656	1/1	0.93	0.08	33,33,33,33	0
56	MG	1a	1718	1/1	0.93	0.08	56,56,56,56	0
56	MG	1A	3180	1/1	0.93	0.14	47,47,47,47	0
56	MG	2A	3663	1/1	0.93	0.17	34,34,34,34	0
56	MG	2A	3032	1/1	0.93	0.22	36,36,36,36	0
56	MG	2A	3666	1/1	0.93	0.11	37,37,37,37	0
56	MG	2A	3667	1/1	0.93	0.10	45,45,45,45	0
56	MG	1A	3420	1/1	0.93	0.20	49,49,49,49	0
56	MG	1A	3859	1/1	0.93	0.13	28,28,28,28	0
56	MG	1a	1730	1/1	0.93	0.13	55,55,55,55	0
56	MG	1a	1731	1/1	0.93	0.08	60,60,60,60	0
56	MG	2A	3180	1/1	0.93	0.12	42,42,42,42	0
56	MG	1A	3300	1/1	0.93	0.08	32,32,32,32	0
56	MG	1A	3756	1/1	0.93	0.12	26,26,26,26	0
56	MG	1A	3375	1/1	0.93	0.38	37,37,37,37	0
56	MG	1A	3113	1/1	0.93	0.10	31,31,31,31	0
56	MG	1B	224	1/1	0.93	0.10	59,59,59,59	0
56	MG	1A	3381	1/1	0.93	0.07	52,52,52,52	0
56	MG	1A	3866	1/1	0.93	0.17	28,28,28,28	0
56	MG	1A	3533	1/1	0.93	0.13	28,28,28,28	0
56	MG	2A	3469	1/1	0.93	0.20	39,39,39,39	0
56	MG	1a	1756	1/1	0.93	0.26	66,66,66,66	0
56	MG	1A	3382	1/1	0.93	0.08	48,48,48,48	0
56	MG	2a	1654	1/1	0.93	0.10	79,79,79,79	0
56	MG	1A	4033	1/1	0.93	0.14	24,24,24,24	0
56	MG	2A	3682	1/1	0.93	0.16	55,55,55,55	0
56	MG	1a	1762	1/1	0.93	0.09	62,62,62,62	0
56	MG	2A	3049	1/1	0.93	0.15	60,60,60,60	0
56	MG	1A	3017	1/1	0.93	0.10	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1B	237	1/1	0.93	0.06	37,37,37,37	0
56	MG	2A	3476	1/1	0.93	0.11	47,47,47,47	0
56	MG	1A	3309	1/1	0.93	0.26	48,48,48,48	0
56	MG	1A	3539	1/1	0.93	0.07	61,61,61,61	0
56	MG	2A	3479	1/1	0.93	0.30	54,54,54,54	0
56	MG	1E	302	1/1	0.93	0.37	36,36,36,36	0
56	MG	1a	1776	1/1	0.93	0.10	80,80,80,80	0
56	MG	1A	3625	1/1	0.93	0.07	39,39,39,39	0
56	MG	2a	1669	1/1	0.93	0.18	63,63,63,63	0
56	MG	2A	3481	1/1	0.93	0.34	65,65,65,65	0
56	MG	1A	4043	1/1	0.93	0.07	44,44,44,44	0
56	MG	1a	1785	1/1	0.93	0.06	64,64,64,64	0
56	MG	1F	305	1/1	0.93	0.14	43,43,43,43	0
56	MG	1A	3881	1/1	0.93	0.07	20,20,20,20	0
56	MG	1A	4049	1/1	0.93	0.07	39,39,39,39	0
56	MG	1A	3780	1/1	0.93	0.15	56,56,56,56	0
56	MG	1a	1791	1/1	0.93	0.11	75,75,75,75	0
56	MG	2A	3486	1/1	0.93	0.41	53,53,53,53	0
56	MG	1A	3116	1/1	0.93	0.22	34,34,34,34	0
56	MG	2a	1686	1/1	0.93	0.14	55,55,55,55	0
56	MG	1A	3633	1/1	0.93	0.05	43,43,43,43	0
56	MG	1a	1805	1/1	0.93	0.07	60,60,60,60	0
56	MG	1A	4060	1/1	0.93	0.10	46,46,46,46	0
56	MG	1A	3249	1/1	0.93	0.07	51,51,51,51	0
56	MG	1A	3542	1/1	0.93	0.20	49,49,49,49	0
56	MG	2A	3494	1/1	0.93	0.18	66,66,66,66	0
56	MG	1a	1817	1/1	0.93	0.17	54,54,54,54	0
56	MG	1A	3312	1/1	0.93	0.15	42,42,42,42	0
56	MG	1a	1820	1/1	0.93	0.12	61,61,61,61	0
56	MG	1A	3790	1/1	0.93	0.08	52,52,52,52	0
56	MG	1P	201	1/1	0.93	0.06	36,36,36,36	0
56	MG	1A	3485	1/1	0.93	0.11	38,38,38,38	0
56	MG	1A	3899	1/1	0.93	0.13	37,37,37,37	0
56	MG	1Q	203	1/1	0.93	0.12	57,57,57,57	0
56	MG	2A	3220	1/1	0.93	0.19	48,48,48,48	0
56	MG	1Q	205	1/1	0.93	0.13	44,44,44,44	0
56	MG	1Q	206	1/1	0.93	0.08	25,25,25,25	0
56	MG	1a	1830	1/1	0.93	0.10	65,65,65,65	0
56	MG	1A	3314	1/1	0.93	0.11	48,48,48,48	0
56	MG	2A	3501	1/1	0.93	0.23	48,48,48,48	0
56	MG	1A	3139	1/1	0.93	0.08	43,43,43,43	0
56	MG	1U	203	1/1	0.93	0.25	42,42,42,42	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3646	1/1	0.93	0.06	44,44,44,44	0
56	MG	1A	3443	1/1	0.93	0.13	48,48,48,48	0
56	MG	1A	3187	1/1	0.93	0.22	42,42,42,42	0
56	MG	1W	201	1/1	0.93	0.19	44,44,44,44	0
56	MG	1A	3651	1/1	0.93	0.17	55,55,55,55	0
56	MG	1Y	201	1/1	0.93	0.10	44,44,44,44	0
56	MG	1A	3551	1/1	0.93	0.22	46,46,46,46	0
56	MG	2A	3086	1/1	0.93	0.07	58,58,58,58	0
56	MG	1Z	301	1/1	0.93	0.08	48,48,48,48	0
56	MG	1A	3654	1/1	0.93	0.07	24,24,24,24	0
56	MG	2A	3090	1/1	0.93	0.11	49,49,49,49	0
56	MG	2A	3722	1/1	0.93	0.11	60,60,60,60	0
56	MG	1A	3659	1/1	0.93	0.12	17,17,17,17	0
56	MG	10	104	1/1	0.93	0.22	41,41,41,41	0
56	MG	10	105	1/1	0.93	0.07	50,50,50,50	0
56	MG	1p	101	1/1	0.93	0.23	44,44,44,44	0
56	MG	1A	3660	1/1	0.93	0.07	21,21,21,21	0
56	MG	1A	3915	1/1	0.93	0.09	52,52,52,52	0
56	MG	1A	4085	1/1	0.93	0.10	50,50,50,50	0
56	MG	1A	3018	1/1	0.93	0.17	24,24,24,24	0
56	MG	12	102	1/1	0.93	0.13	39,39,39,39	0
56	MG	1A	4088	1/1	0.93	0.09	50,50,50,50	0
56	MG	13	102	1/1	0.93	0.12	41,41,41,41	0
56	MG	2A	3247	1/1	0.93	0.15	56,56,56,56	0
56	MG	2A	3248	1/1	0.93	0.06	69,69,69,69	0
56	MG	1A	3254	1/1	0.93	0.14	47,47,47,47	0
56	MG	2a	1749	1/1	0.93	0.08	85,85,85,85	0
56	MG	1x	103	1/1	0.93	0.22	66,66,66,66	0
56	MG	2A	3527	1/1	0.93	0.16	66,66,66,66	0
56	MG	2a	1757	1/1	0.93	0.07	76,76,76,76	0
56	MG	2a	1758	1/1	0.93	0.07	64,64,64,64	0
56	MG	2A	3735	1/1	0.93	0.12	68,68,68,68	0
56	MG	2a	1761	1/1	0.93	0.11	61,61,61,61	0
56	MG	2A	3384	1/1	0.93	0.15	41,41,41,41	0
56	MG	1A	3322	1/1	0.93	0.17	41,41,41,41	0
56	MG	1a	1603	1/1	0.93	0.21	50,50,50,50	0
56	MG	1a	1604	1/1	0.93	0.18	53,53,53,53	0
56	MG	1A	4094	1/1	0.93	0.15	42,42,42,42	0
56	MG	2a	1768	1/1	0.93	0.10	60,60,60,60	0
56	MG	1A	3450	1/1	0.93	0.17	56,56,56,56	0
56	MG	2A	3109	1/1	0.93	0.10	52,52,52,52	0
56	MG	2A	3110	1/1	0.93	0.23	70,70,70,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1609	1/1	0.93	0.10	49,49,49,49	0
56	MG	1a	1610	1/1	0.93	0.20	46,46,46,46	0
56	MG	2A	3544	1/1	0.93	0.10	64,64,64,64	0
56	MG	2A	3748	1/1	0.93	0.21	68,68,68,68	0
56	MG	2A	3111	1/1	0.93	0.05	55,55,55,55	0
56	MG	1a	1618	1/1	0.93	0.06	45,45,45,45	0
56	MG	1a	1619	1/1	0.93	0.06	48,48,48,48	0
56	MG	1A	3926	1/1	0.93	0.07	37,37,37,37	0
56	MG	1A	3326	1/1	0.93	0.12	52,52,52,52	0
56	MG	1A	3172	1/1	0.93	0.54	40,40,40,40	0
56	MG	1A	3219	1/1	0.93	0.08	48,48,48,48	0
56	MG	2A	3551	1/1	0.93	0.08	59,59,59,59	0
56	MG	1a	1627	1/1	0.93	0.14	49,49,49,49	0
56	MG	2A	3757	1/1	0.93	0.14	39,39,39,39	0
56	MG	2A	3758	1/1	0.93	0.08	66,66,66,66	0
56	MG	1A	3503	1/1	0.93	0.12	56,56,56,56	0
56	MG	1A	3818	1/1	0.93	0.16	43,43,43,43	0
56	MG	2a	1798	1/1	0.93	0.05	62,62,62,62	0
56	MG	2a	1799	1/1	0.93	0.21	56,56,56,56	0
56	MG	1A	3329	1/1	0.93	0.17	50,50,50,50	0
56	MG	1A	3332	1/1	0.93	0.14	43,43,43,43	0
56	MG	1A	3410	1/1	0.93	0.21	44,44,44,44	0
56	MG	1A	4131	1/1	0.93	0.35	42,42,42,42	0
56	MG	1A	3581	1/1	0.93	0.13	42,42,42,42	0
56	MG	2A	3125	1/1	0.93	0.20	60,60,60,60	0
56	MG	1A	4136	1/1	0.93	0.08	31,31,31,31	0
56	MG	2A	3771	1/1	0.93	0.17	55,55,55,55	0
56	MG	2a	1809	1/1	0.93	0.11	66,66,66,66	0
56	MG	2A	3570	1/1	0.93	0.08	32,32,32,32	0
56	MG	1A	3510	1/1	0.93	0.10	54,54,54,54	0
56	MG	1a	1648	1/1	0.93	0.13	42,42,42,42	0
56	MG	1a	1649	1/1	0.93	0.09	54,54,54,54	0
56	MG	1A	3460	1/1	0.93	0.34	43,43,43,43	0
56	MG	1A	3585	1/1	0.93	0.10	38,38,38,38	0
56	MG	1A	3514	1/1	0.93	0.14	56,56,56,56	0
56	MG	1A	3829	1/1	0.93	0.08	39,39,39,39	0
56	MG	2A	3278	1/1	0.93	0.22	54,54,54,54	0
56	MG	1A	3461	1/1	0.93	0.10	42,42,42,42	0
56	MG	2A	3416	1/1	0.93	0.24	58,58,58,58	0
56	MG	2A	3417	1/1	0.93	0.13	57,57,57,57	0
56	MG	1A	3831	1/1	0.93	0.10	34,34,34,34	0
56	MG	1A	3588	1/1	0.93	0.22	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2Q	203	1/1	0.93	0.11	61,61,61,61	0
56	MG	2A	3001	1/1	0.93	0.10	46,46,46,46	0
56	MG	1a	1663	1/1	0.93	0.19	45,45,45,45	0
56	MG	2A	3595	1/1	0.93	0.08	28,28,28,28	0
56	MG	2A	3002	1/1	0.93	0.16	57,57,57,57	0
56	MG	1A	3055	1/1	0.93	0.08	33,33,33,33	0
56	MG	1A	3712	1/1	0.93	0.11	46,46,46,46	0
56	MG	2A	3798	1/1	0.93	0.10	82,82,82,82	0
56	MG	2A	3005	1/1	0.93	0.10	49,49,49,49	0
56	MG	1A	3970	1/1	0.93	0.11	24,24,24,24	0
56	MG	2A	3293	1/1	0.93	0.11	64,64,64,64	0
56	MG	2A	3147	1/1	0.93	0.13	48,48,48,48	0
56	MG	2A	3607	1/1	0.93	0.09	27,27,27,27	0
56	MG	2A	3149	1/1	0.93	0.09	58,58,58,58	0
56	MG	1A	3836	1/1	0.93	0.13	62,62,62,62	0
56	MG	2A	3431	1/1	0.93	0.20	52,52,52,52	0
56	MG	2A	3297	1/1	0.93	0.19	38,38,38,38	0
56	MG	2A	3298	1/1	0.93	0.18	50,50,50,50	0
56	MG	1A	3974	1/1	0.93	0.09	37,37,37,37	0
56	MG	1A	3714	1/1	0.93	0.20	46,46,46,46	0
56	MG	2A	3623	1/1	0.93	0.09	64,64,64,64	0
56	MG	2A	3010	1/1	0.93	0.32	62,62,62,62	0
56	MG	1A	3070	1/1	0.93	0.16	19,19,19,19	0
56	MG	2x	101	1/1	0.93	0.19	57,57,57,57	0
56	MG	1A	3335	1/1	0.93	0.17	46,46,46,46	0
56	MG	2A	3441	1/1	0.93	0.15	56,56,56,56	0
56	MG	1A	3198	1/1	0.93	0.11	21,21,21,21	0
56	MG	2A	3839	1/1	0.93	0.09	64,64,64,64	0
56	MG	2a	1607	1/1	0.93	0.29	64,64,64,64	0
56	MG	1A	3416	1/1	0.93	0.09	55,55,55,55	0
56	MG	2A	3843	1/1	0.93	0.11	46,46,46,46	0
56	MG	1A	3598	1/1	0.93	0.12	39,39,39,39	0
56	MG	1A	3339	1/1	0.93	0.11	57,57,57,57	0
57	DI0	2A	3846	58/58	0.93	0.14	33,44,84,93	0
56	MG	2A	3021	1/1	0.93	0.35	48,48,48,48	0
56	MG	1A	3508	1/1	0.94	0.23	35,35,35,35	0
56	MG	2A	3068	1/1	0.94	0.30	51,51,51,51	0
56	MG	2A	3609	1/1	0.94	0.18	46,46,46,46	0
56	MG	1A	3509	1/1	0.94	0.31	34,34,34,34	0
56	MG	2a	1613	1/1	0.94	0.22	52,52,52,52	0
56	MG	1A	3751	1/1	0.94	0.09	21,21,21,21	0
56	MG	1a	1699	1/1	0.94	0.27	47,47,47,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1700	1/1	0.94	0.35	59,59,59,59	0
56	MG	2A	3615	1/1	0.94	0.08	57,57,57,57	0
56	MG	1A	3868	1/1	0.94	0.24	38,38,38,38	0
56	MG	2A	3847	1/1	0.94	0.15	48,48,48,48	0
56	MG	1A	3378	1/1	0.94	0.19	40,40,40,40	0
56	MG	1A	3380	1/1	0.94	0.17	38,38,38,38	0
56	MG	1A	3602	1/1	0.94	0.10	32,32,32,32	0
56	MG	1A	3201	1/1	0.94	0.05	35,35,35,35	0
56	MG	2A	3854	1/1	0.94	0.08	55,55,55,55	0
56	MG	2A	3079	1/1	0.94	0.09	45,45,45,45	0
56	MG	1A	3121	1/1	0.94	0.07	31,31,31,31	0
56	MG	2A	3626	1/1	0.94	0.07	31,31,31,31	0
56	MG	1A	3880	1/1	0.94	0.12	19,19,19,19	0
56	MG	1A	3122	1/1	0.94	0.13	41,41,41,41	0
56	MG	1A	3386	1/1	0.94	0.27	29,29,29,29	0
56	MG	2a	1632	1/1	0.94	0.06	87,87,87,87	0
56	MG	1A	3165	1/1	0.94	0.18	35,35,35,35	0
56	MG	2A	3091	1/1	0.94	0.24	44,44,44,44	0
56	MG	1A	3004	1/1	0.94	0.06	24,24,24,24	0
56	MG	1A	3520	1/1	0.94	0.19	47,47,47,47	0
56	MG	2A	3637	1/1	0.94	0.10	57,57,57,57	0
56	MG	1A	3455	1/1	0.94	0.13	49,49,49,49	0
56	MG	1A	3336	1/1	0.94	0.08	52,52,52,52	0
56	MG	2A	3642	1/1	0.94	0.12	32,32,32,32	0
56	MG	2A	3098	1/1	0.94	0.07	44,44,44,44	0
56	MG	2A	3645	1/1	0.94	0.13	55,55,55,55	0
56	MG	2A	3100	1/1	0.94	0.12	36,36,36,36	0
56	MG	1A	3776	1/1	0.94	0.07	54,54,54,54	0
56	MG	2a	1645	1/1	0.94	0.11	57,57,57,57	0
56	MG	2A	3648	1/1	0.94	0.08	31,31,31,31	0
56	MG	2A	3649	1/1	0.94	0.08	33,33,33,33	0
56	MG	1A	4071	1/1	0.94	0.09	55,55,55,55	0
56	MG	2A	3651	1/1	0.94	0.10	48,48,48,48	0
56	MG	1A	3894	1/1	0.94	0.12	53,53,53,53	0
56	MG	1A	3041	1/1	0.94	0.09	31,31,31,31	0
56	MG	1B	228	1/1	0.94	0.06	39,39,39,39	0
56	MG	2A	3106	1/1	0.94	0.20	49,49,49,49	0
56	MG	1a	1751	1/1	0.94	0.09	55,55,55,55	0
56	MG	2A	3657	1/1	0.94	0.08	45,45,45,45	0
56	MG	1a	1755	1/1	0.94	0.05	51,51,51,51	0
56	MG	2A	3659	1/1	0.94	0.06	31,31,31,31	0
56	MG	1A	3898	1/1	0.94	0.19	63,63,63,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3662	1/1	0.94	0.06	40,40,40,40	0
56	MG	1A	3338	1/1	0.94	0.14	34,34,34,34	0
56	MG	1A	3098	1/1	0.94	0.15	34,34,34,34	0
56	MG	1a	1764	1/1	0.94	0.08	58,58,58,58	0
56	MG	1B	236	1/1	0.94	0.07	37,37,37,37	0
56	MG	1A	3340	1/1	0.94	0.16	59,59,59,59	0
56	MG	1A	3253	1/1	0.94	0.09	36,36,36,36	0
56	MG	1D	307	1/1	0.94	0.19	37,37,37,37	0
56	MG	1A	3787	1/1	0.94	0.11	36,36,36,36	0
56	MG	1A	4084	1/1	0.94	0.10	61,61,61,61	0
56	MG	1A	3011	1/1	0.94	0.11	38,38,38,38	0
56	MG	1A	3171	1/1	0.94	0.13	41,41,41,41	0
56	MG	1E	305	1/1	0.94	0.21	37,37,37,37	0
56	MG	1a	1777	1/1	0.94	0.07	59,59,59,59	0
56	MG	2a	1677	1/1	0.94	0.19	59,59,59,59	0
56	MG	1a	1778	1/1	0.94	0.07	67,67,67,67	0
56	MG	2a	1679	1/1	0.94	0.12	64,64,64,64	0
56	MG	2a	1680	1/1	0.94	0.07	58,58,58,58	0
56	MG	1A	3534	1/1	0.94	0.19	34,34,34,34	0
56	MG	2A	3289	1/1	0.94	0.32	53,53,53,53	0
56	MG	1A	3217	1/1	0.94	0.25	46,46,46,46	0
56	MG	1A	3405	1/1	0.94	0.21	36,36,36,36	0
56	MG	1F	308	1/1	0.94	0.08	45,45,45,45	0
56	MG	1A	4093	1/1	0.94	0.19	42,42,42,42	0
56	MG	1A	3912	1/1	0.94	0.07	49,49,49,49	0
56	MG	2a	1690	1/1	0.94	0.24	53,53,53,53	0
56	MG	1A	3913	1/1	0.94	0.07	70,70,70,70	0
56	MG	1A	3102	1/1	0.94	0.10	41,41,41,41	0
56	MG	1a	1792	1/1	0.94	0.08	58,58,58,58	0
56	MG	1A	3794	1/1	0.94	0.06	37,37,37,37	0
56	MG	2A	3126	1/1	0.94	0.10	47,47,47,47	0
56	MG	1A	4100	1/1	0.94	0.06	29,29,29,29	0
56	MG	2A	3300	1/1	0.94	0.13	63,63,63,63	0
56	MG	1a	1806	1/1	0.94	0.07	67,67,67,67	0
56	MG	2A	3462	1/1	0.94	0.14	40,40,40,40	0
56	MG	1A	4104	1/1	0.94	0.21	31,31,31,31	0
56	MG	1A	4108	1/1	0.94	0.29	30,30,30,30	0
56	MG	1A	3174	1/1	0.94	0.09	37,37,37,37	0
56	MG	2A	3468	1/1	0.94	0.24	41,41,41,41	0
56	MG	2A	3690	1/1	0.94	0.10	54,54,54,54	0
56	MG	1A	4114	1/1	0.94	0.22	42,42,42,42	0
56	MG	1Q	202	1/1	0.94	0.12	37,37,37,37	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3917	1/1	0.94	0.09	31,31,31,31	0
56	MG	1A	3643	1/1	0.94	0.07	37,37,37,37	0
56	MG	2A	3135	1/1	0.94	0.07	43,43,43,43	0
56	MG	2A	3474	1/1	0.94	0.13	34,34,34,34	0
56	MG	1R	201	1/1	0.94	0.16	51,51,51,51	0
56	MG	1R	202	1/1	0.94	0.14	35,35,35,35	0
56	MG	1S	201	1/1	0.94	0.22	50,50,50,50	0
56	MG	1A	4120	1/1	0.94	0.44	39,39,39,39	0
56	MG	1A	3175	1/1	0.94	0.16	37,37,37,37	0
56	MG	1A	4124	1/1	0.94	0.10	35,35,35,35	0
56	MG	1A	4125	1/1	0.94	0.16	35,35,35,35	0
56	MG	1A	3016	1/1	0.94	0.22	50,50,50,50	0
56	MG	2A	3141	1/1	0.94	0.08	50,50,50,50	0
56	MG	1U	207	1/1	0.94	0.19	38,38,38,38	0
56	MG	1A	3104	1/1	0.94	0.09	33,33,33,33	0
56	MG	1A	3303	1/1	0.94	0.22	40,40,40,40	0
56	MG	1W	203	1/1	0.94	0.29	31,31,31,31	0
56	MG	2a	1727	1/1	0.94	0.23	63,63,63,63	0
56	MG	1A	3304	1/1	0.94	0.06	39,39,39,39	0
56	MG	1X	105	1/1	0.94	0.16	52,52,52,52	0
56	MG	1A	3307	1/1	0.94	0.09	42,42,42,42	0
56	MG	1A	3937	1/1	0.94	0.07	55,55,55,55	0
56	MG	1A	4138	1/1	0.94	0.14	36,36,36,36	0
56	MG	1A	3656	1/1	0.94	0.07	23,23,23,23	0
56	MG	1A	3546	1/1	0.94	0.16	38,38,38,38	0
56	MG	1A	3057	1/1	0.94	0.25	46,46,46,46	0
56	MG	1l	202	1/1	0.94	0.10	83,83,83,83	0
56	MG	1l	203	1/1	0.94	0.06	49,49,49,49	0
56	MG	1m	201	1/1	0.94	0.18	42,42,42,42	0
56	MG	2a	1744	1/1	0.94	0.09	65,65,65,65	0
56	MG	1A	3358	1/1	0.94	0.10	62,62,62,62	0
56	MG	2A	3157	1/1	0.94	0.06	28,28,28,28	0
56	MG	1A	3945	1/1	0.94	0.12	55,55,55,55	0
56	MG	1A	3949	1/1	0.94	0.08	29,29,29,29	0
56	MG	2a	1752	1/1	0.94	0.07	76,76,76,76	0
56	MG	2a	1755	1/1	0.94	0.07	78,78,78,78	0
56	MG	1A	3106	1/1	0.94	0.13	34,34,34,34	0
56	MG	1A	3107	1/1	0.94	0.07	28,28,28,28	0
56	MG	1A	3955	1/1	0.94	0.12	33,33,33,33	0
56	MG	2a	1759	1/1	0.94	0.07	61,61,61,61	0
56	MG	1A	3149	1/1	0.94	0.16	43,43,43,43	0
56	MG	2A	3339	1/1	0.94	0.18	58,58,58,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3816	1/1	0.94	0.08	52,52,52,52	0
56	MG	1A	3111	1/1	0.94	0.05	38,38,38,38	0
56	MG	1A	3486	1/1	0.94	0.16	47,47,47,47	0
56	MG	2A	3170	1/1	0.94	0.18	43,43,43,43	0
56	MG	1A	3679	1/1	0.94	0.07	34,34,34,34	0
56	MG	1A	3680	1/1	0.94	0.07	21,21,21,21	0
56	MG	2A	3173	1/1	0.94	0.20	45,45,45,45	0
56	MG	1A	3424	1/1	0.94	0.20	53,53,53,53	0
56	MG	2a	1772	1/1	0.94	0.07	59,59,59,59	0
56	MG	1A	3684	1/1	0.94	0.10	23,23,23,23	0
56	MG	2A	3510	1/1	0.94	0.10	65,65,65,65	0
56	MG	1A	3237	1/1	0.94	0.13	40,40,40,40	0
56	MG	1A	3686	1/1	0.94	0.06	17,17,17,17	0
56	MG	2A	3738	1/1	0.94	0.06	55,55,55,55	0
56	MG	2A	3012	1/1	0.94	0.10	36,36,36,36	0
56	MG	2A	3516	1/1	0.94	0.16	49,49,49,49	0
56	MG	1A	3563	1/1	0.94	0.07	47,47,47,47	0
56	MG	2A	3742	1/1	0.94	0.10	58,58,58,58	0
56	MG	1a	1612	1/1	0.94	0.09	59,59,59,59	0
56	MG	2A	3743	1/1	0.94	0.09	35,35,35,35	0
56	MG	2A	3744	1/1	0.94	0.09	35,35,35,35	0
56	MG	1a	1615	1/1	0.94	0.09	57,57,57,57	0
56	MG	2A	3015	1/1	0.94	0.16	52,52,52,52	0
56	MG	1A	3564	1/1	0.94	0.23	35,35,35,35	0
56	MG	1A	3690	1/1	0.94	0.11	34,34,34,34	0
56	MG	1A	3426	1/1	0.94	0.18	58,58,58,58	0
56	MG	1A	3568	1/1	0.94	0.27	31,31,31,31	0
56	MG	1A	3698	1/1	0.94	0.09	28,28,28,28	0
56	MG	2A	3751	1/1	0.94	0.07	66,66,66,66	0
56	MG	2A	3752	1/1	0.94	0.06	46,46,46,46	0
56	MG	2A	3360	1/1	0.94	0.10	51,51,51,51	0
56	MG	1A	3087	1/1	0.94	0.33	42,42,42,42	0
56	MG	2a	1803	1/1	0.94	0.16	66,66,66,66	0
56	MG	1A	3701	1/1	0.94	0.11	44,44,44,44	0
56	MG	2A	3025	1/1	0.94	0.32	57,57,57,57	0
56	MG	2A	3026	1/1	0.94	0.38	53,53,53,53	0
56	MG	2A	3536	1/1	0.94	0.10	42,42,42,42	0
56	MG	1A	3570	1/1	0.94	0.08	44,44,44,44	0
56	MG	1A	3492	1/1	0.94	0.07	40,40,40,40	0
56	MG	1a	1638	1/1	0.94	0.23	59,59,59,59	0
56	MG	2A	3762	1/1	0.94	0.17	69,69,69,69	0
56	MG	2D	302	1/1	0.94	0.31	47,47,47,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3542	1/1	0.94	0.11	44,44,44,44	0
56	MG	1A	3840	1/1	0.94	0.08	22,22,22,22	0
56	MG	1A	3986	1/1	0.94	0.11	21,21,21,21	0
56	MG	1A	3573	1/1	0.94	0.11	49,49,49,49	0
56	MG	2a	1817	1/1	0.94	0.06	95,95,95,95	0
56	MG	1A	3493	1/1	0.94	0.15	42,42,42,42	0
56	MG	2A	3372	1/1	0.94	0.10	50,50,50,50	0
56	MG	2E	307	1/1	0.94	0.16	49,49,49,49	0
56	MG	1A	3844	1/1	0.94	0.08	16,16,16,16	0
56	MG	1A	3996	1/1	0.94	0.07	20,20,20,20	0
56	MG	1A	3155	1/1	0.94	0.27	40,40,40,40	0
56	MG	2A	3553	1/1	0.94	0.10	42,42,42,42	0
56	MG	2A	3555	1/1	0.94	0.09	55,55,55,55	0
56	MG	1A	3190	1/1	0.94	0.08	44,44,44,44	0
56	MG	1A	3006	1/1	0.94	0.17	51,51,51,51	0
56	MG	1A	3072	1/1	0.94	0.42	36,36,36,36	0
56	MG	1A	3716	1/1	0.94	0.14	51,51,51,51	0
56	MG	1A	3324	1/1	0.94	0.24	55,55,55,55	0
56	MG	2A	3383	1/1	0.94	0.07	51,51,51,51	0
56	MG	1A	3853	1/1	0.94	0.07	45,45,45,45	0
56	MG	2T	201	1/1	0.94	0.08	58,58,58,58	0
56	MG	2f	201	1/1	0.94	0.12	51,51,51,51	0
56	MG	2A	3567	1/1	0.94	0.08	48,48,48,48	0
56	MG	1A	4010	1/1	0.94	0.09	63,63,63,63	0
56	MG	1A	3719	1/1	0.94	0.12	53,53,53,53	0
56	MG	1A	4012	1/1	0.94	0.07	84,84,84,84	0
56	MG	1A	4013	1/1	0.94	0.09	65,65,65,65	0
56	MG	2A	3223	1/1	0.94	0.10	60,60,60,60	0
56	MG	2A	3224	1/1	0.94	0.20	68,68,68,68	0
56	MG	2A	3581	1/1	0.94	0.10	43,43,43,43	0
56	MG	1A	3325	1/1	0.94	0.13	45,45,45,45	0
56	MG	1A	3856	1/1	0.94	0.08	41,41,41,41	0
56	MG	1a	1672	1/1	0.94	0.23	49,49,49,49	0
56	MG	1A	3373	1/1	0.94	0.20	46,46,46,46	0
56	MG	2A	3229	1/1	0.94	0.26	56,56,56,56	0
56	MG	1A	3118	1/1	0.94	0.33	28,28,28,28	0
56	MG	1A	4024	1/1	0.94	0.12	66,66,66,66	0
56	MG	1A	4026	1/1	0.94	0.10	56,56,56,56	0
56	MG	2A	3808	1/1	0.94	0.09	72,72,72,72	0
56	MG	1A	4027	1/1	0.94	0.12	58,58,58,58	0
56	MG	2x	105	1/1	0.94	0.12	56,56,56,56	0
56	MG	1A	3735	1/1	0.94	0.07	20,20,20,20	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	4029	1/1	0.94	0.06	38,38,38,38	0
56	MG	1A	4031	1/1	0.94	0.07	38,38,38,38	0
56	MG	2y	104	1/1	0.94	0.23	52,52,52,52	0
56	MG	1A	3441	1/1	0.94	0.10	40,40,40,40	0
56	MG	1A	3119	1/1	0.94	0.32	39,39,39,39	0
56	MG	1A	3280	1/1	0.94	0.20	45,45,45,45	0
56	MG	2A	3407	1/1	0.94	0.08	51,51,51,51	0
58	K	1A	4145	1/1	0.94	0.08	55,55,55,55	0
56	MG	2A	3242	1/1	0.94	0.21	71,71,71,71	0
59	ZN	24	501	1/1	0.94	0.08	128,128,128,128	0
56	MG	1l	102	1/1	0.95	0.10	42,42,42,42	0
56	MG	1a	1795	1/1	0.95	0.07	71,71,71,71	0
56	MG	2A	3778	1/1	0.95	0.10	49,49,49,49	0
56	MG	1a	1800	1/1	0.95	0.09	74,74,74,74	0
56	MG	1A	4112	1/1	0.95	0.25	36,36,36,36	0
56	MG	1A	3403	1/1	0.95	0.30	46,46,46,46	0
56	MG	2A	3471	1/1	0.95	0.25	40,40,40,40	0
56	MG	1A	3591	1/1	0.95	0.17	31,31,31,31	0
56	MG	1a	1809	1/1	0.95	0.08	45,45,45,45	0
56	MG	1a	1812	1/1	0.95	0.09	55,55,55,55	0
56	MG	1A	4116	1/1	0.95	0.25	33,33,33,33	0
56	MG	1A	3214	1/1	0.95	0.14	48,48,48,48	0
56	MG	15	104	1/1	0.95	0.24	42,42,42,42	0
56	MG	2A	3643	1/1	0.95	0.09	29,29,29,29	0
56	MG	16	101	1/1	0.95	0.08	52,52,52,52	0
56	MG	1A	3066	1/1	0.95	0.11	53,53,53,53	0
56	MG	1A	3447	1/1	0.95	0.11	36,36,36,36	0
56	MG	1A	3270	1/1	0.95	0.06	39,39,39,39	0
56	MG	1a	1601	1/1	0.95	0.10	51,51,51,51	0
56	MG	1A	3137	1/1	0.95	0.22	40,40,40,40	0
56	MG	1A	3599	1/1	0.95	0.10	23,23,23,23	0
56	MG	2A	3097	1/1	0.95	0.09	42,42,42,42	0
56	MG	1A	3600	1/1	0.95	0.07	42,42,42,42	0
56	MG	2A	3099	1/1	0.95	0.11	46,46,46,46	0
56	MG	2A	3226	1/1	0.95	0.10	47,47,47,47	0
56	MG	1A	4129	1/1	0.95	0.23	41,41,41,41	0
56	MG	2A	3655	1/1	0.95	0.10	59,59,59,59	0
56	MG	1A	3997	1/1	0.95	0.10	37,37,37,37	0
56	MG	1A	3185	1/1	0.95	0.16	39,39,39,39	0
56	MG	1a	1835	1/1	0.95	0.08	47,47,47,47	0
56	MG	2A	3230	1/1	0.95	0.10	55,55,55,55	0
56	MG	2A	3660	1/1	0.95	0.14	37,37,37,37	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3488	1/1	0.95	0.31	48,48,48,48	0
56	MG	1A	4133	1/1	0.95	0.53	28,28,28,28	0
56	MG	1A	3306	1/1	0.95	0.11	54,54,54,54	0
56	MG	2A	3819	1/1	0.95	0.07	31,31,31,31	0
56	MG	2A	3664	1/1	0.95	0.10	37,37,37,37	0
56	MG	1A	3887	1/1	0.95	0.07	31,31,31,31	0
56	MG	1a	1623	1/1	0.95	0.10	54,54,54,54	0
56	MG	2A	3823	1/1	0.95	0.08	43,43,43,43	0
56	MG	2A	3824	1/1	0.95	0.06	34,34,34,34	0
56	MG	1f	201	1/1	0.95	0.17	46,46,46,46	0
56	MG	1A	4137	1/1	0.95	0.12	28,28,28,28	0
56	MG	1A	3030	1/1	0.95	0.06	34,34,34,34	0
56	MG	2A	3833	1/1	0.95	0.08	38,38,38,38	0
56	MG	2a	1701	1/1	0.95	0.07	56,56,56,56	0
56	MG	1A	3696	1/1	0.95	0.07	37,37,37,37	0
56	MG	1A	3890	1/1	0.95	0.08	43,43,43,43	0
56	MG	1A	3051	1/1	0.95	0.07	26,26,26,26	0
56	MG	1a	1633	1/1	0.95	0.09	41,41,41,41	0
56	MG	1A	3454	1/1	0.95	0.31	37,37,37,37	0
56	MG	1A	3497	1/1	0.95	0.08	53,53,53,53	0
56	MG	1A	3372	1/1	0.95	0.12	51,51,51,51	0
56	MG	2A	3244	1/1	0.95	0.13	41,41,41,41	0
56	MG	1A	3897	1/1	0.95	0.08	40,40,40,40	0
56	MG	1A	3612	1/1	0.95	0.07	35,35,35,35	0
56	MG	1a	1641	1/1	0.95	0.11	52,52,52,52	0
56	MG	1A	3143	1/1	0.95	0.13	38,38,38,38	0
56	MG	1A	4018	1/1	0.95	0.07	47,47,47,47	0
56	MG	1A	3145	1/1	0.95	0.20	24,24,24,24	0
56	MG	1x	101	1/1	0.95	0.06	54,54,54,54	0
56	MG	2a	1717	1/1	0.95	0.09	52,52,52,52	0
56	MG	1A	3458	1/1	0.95	0.07	39,39,39,39	0
56	MG	1A	3812	1/1	0.95	0.06	25,25,25,25	0
56	MG	1A	3279	1/1	0.95	0.28	34,34,34,34	0
56	MG	1A	3346	1/1	0.95	0.27	50,50,50,50	0
56	MG	1A	3225	1/1	0.95	0.14	45,45,45,45	0
56	MG	1A	3313	1/1	0.95	0.08	47,47,47,47	0
56	MG	1a	1652	1/1	0.95	0.17	48,48,48,48	0
56	MG	2A	3862	1/1	0.95	0.11	52,52,52,52	0
56	MG	2A	3257	1/1	0.95	0.08	55,55,55,55	0
56	MG	1a	1655	1/1	0.95	0.10	53,53,53,53	0
56	MG	1A	3627	1/1	0.95	0.08	29,29,29,29	0
56	MG	1A	4032	1/1	0.95	0.07	47,47,47,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3388	1/1	0.95	0.09	50,50,50,50	0
56	MG	1A	3422	1/1	0.95	0.11	35,35,35,35	0
56	MG	2A	3692	1/1	0.95	0.07	40,40,40,40	0
56	MG	2A	3261	1/1	0.95	0.12	41,41,41,41	0
56	MG	2A	3131	1/1	0.95	0.20	44,44,44,44	0
56	MG	1A	4034	1/1	0.95	0.13	25,25,25,25	0
56	MG	1B	213	1/1	0.95	0.21	49,49,49,49	0
56	MG	1A	3721	1/1	0.95	0.05	30,30,30,30	0
56	MG	2a	1741	1/1	0.95	0.07	80,80,80,80	0
56	MG	2a	1742	1/1	0.95	0.12	77,77,77,77	0
56	MG	1A	4036	1/1	0.95	0.06	35,35,35,35	0
56	MG	1A	3071	1/1	0.95	0.18	31,31,31,31	0
56	MG	1B	219	1/1	0.95	0.10	31,31,31,31	0
56	MG	1A	4038	1/1	0.95	0.07	40,40,40,40	0
56	MG	2A	3532	1/1	0.95	0.10	56,56,56,56	0
56	MG	2a	1750	1/1	0.95	0.09	61,61,61,61	0
56	MG	1A	3727	1/1	0.95	0.06	36,36,36,36	0
56	MG	1A	3350	1/1	0.95	0.09	59,59,59,59	0
56	MG	1A	3147	1/1	0.95	0.11	45,45,45,45	0
56	MG	1A	4044	1/1	0.95	0.10	52,52,52,52	0
56	MG	1A	3733	1/1	0.95	0.20	31,31,31,31	0
56	MG	2A	3143	1/1	0.95	0.09	57,57,57,57	0
56	MG	1a	1678	1/1	0.95	0.21	35,35,35,35	0
56	MG	1A	3734	1/1	0.95	0.07	31,31,31,31	0
56	MG	1A	4051	1/1	0.95	0.10	11,11,11,11	0
56	MG	1A	3196	1/1	0.95	0.07	36,36,36,36	0
56	MG	2A	3277	1/1	0.95	0.13	58,58,58,58	0
56	MG	1A	3922	1/1	0.95	0.05	20,20,20,20	0
56	MG	1A	3566	1/1	0.95	0.06	40,40,40,40	0
56	MG	1A	3387	1/1	0.95	0.26	34,34,34,34	0
56	MG	1A	3927	1/1	0.95	0.06	37,37,37,37	0
56	MG	2E	303	1/1	0.95	0.24	51,51,51,51	0
56	MG	2A	3715	1/1	0.95	0.06	54,54,54,54	0
56	MG	1D	301	1/1	0.95	0.19	28,28,28,28	0
56	MG	2A	3716	1/1	0.95	0.09	41,41,41,41	0
56	MG	1D	305	1/1	0.95	0.27	34,34,34,34	0
56	MG	1A	3640	1/1	0.95	0.17	25,25,25,25	0
56	MG	1A	3034	1/1	0.95	0.16	35,35,35,35	0
56	MG	1a	1695	1/1	0.95	0.23	43,43,43,43	0
56	MG	2A	3415	1/1	0.95	0.08	54,54,54,54	0
56	MG	1a	1697	1/1	0.95	0.17	41,41,41,41	0
56	MG	1A	3746	1/1	0.95	0.19	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2O	202	1/1	0.95	0.07	55,55,55,55	0
56	MG	2A	3036	1/1	0.95	0.18	40,40,40,40	0
56	MG	1E	304	1/1	0.95	0.18	51,51,51,51	0
56	MG	2A	3287	1/1	0.95	0.17	47,47,47,47	0
56	MG	2A	3037	1/1	0.95	0.20	35,35,35,35	0
56	MG	1E	307	1/1	0.95	0.28	37,37,37,37	0
56	MG	1A	3747	1/1	0.95	0.09	47,47,47,47	0
56	MG	1A	3020	1/1	0.95	0.07	38,38,38,38	0
56	MG	1A	3838	1/1	0.95	0.09	46,46,46,46	0
56	MG	1F	306	1/1	0.95	0.24	27,27,27,27	0
56	MG	2A	3042	1/1	0.95	0.24	56,56,56,56	0
56	MG	1F	309	1/1	0.95	0.23	48,48,48,48	0
56	MG	1G	201	1/1	0.95	0.13	37,37,37,37	0
56	MG	1A	3644	1/1	0.95	0.04	35,35,35,35	0
56	MG	2A	3165	1/1	0.95	0.09	38,38,38,38	0
56	MG	1A	3841	1/1	0.95	0.23	47,47,47,47	0
56	MG	1A	3571	1/1	0.95	0.09	35,35,35,35	0
56	MG	2X	102	1/1	0.95	0.10	57,57,57,57	0
56	MG	2A	3577	1/1	0.95	0.09	31,31,31,31	0
56	MG	1A	3108	1/1	0.95	0.30	35,35,35,35	0
56	MG	1N	202	1/1	0.95	0.15	43,43,43,43	0
56	MG	2A	3169	1/1	0.95	0.22	53,53,53,53	0
56	MG	1A	3950	1/1	0.95	0.07	62,62,62,62	0
56	MG	1N	206	1/1	0.95	0.11	34,34,34,34	0
56	MG	1N	207	1/1	0.95	0.09	59,59,59,59	0
56	MG	2A	3303	1/1	0.95	0.17	55,55,55,55	0
56	MG	2A	3434	1/1	0.95	0.20	41,41,41,41	0
56	MG	1A	3649	1/1	0.95	0.08	33,33,33,33	0
56	MG	1A	3039	1/1	0.95	0.18	38,38,38,38	0
56	MG	2a	1602	1/1	0.95	0.08	62,62,62,62	0
56	MG	1a	1734	1/1	0.95	0.09	54,54,54,54	0
56	MG	1A	3954	1/1	0.95	0.08	35,35,35,35	0
56	MG	1A	3475	1/1	0.95	0.10	49,49,49,49	0
56	MG	1A	3576	1/1	0.95	0.10	40,40,40,40	0
56	MG	1A	4082	1/1	0.95	0.09	55,55,55,55	0
56	MG	1A	3653	1/1	0.95	0.06	24,24,24,24	0
56	MG	1A	3045	1/1	0.95	0.06	33,33,33,33	0
56	MG	1a	1743	1/1	0.95	0.09	49,49,49,49	0
56	MG	1A	3764	1/1	0.95	0.05	36,36,36,36	0
56	MG	1A	3156	1/1	0.95	0.06	30,30,30,30	0
56	MG	2A	3315	1/1	0.95	0.07	49,49,49,49	0
56	MG	1A	4087	1/1	0.95	0.07	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1753	1/1	0.95	0.06	47,47,47,47	0
56	MG	1A	3131	1/1	0.95	0.13	62,62,62,62	0
56	MG	1S	203	1/1	0.95	0.11	67,67,67,67	0
56	MG	2A	3063	1/1	0.95	0.15	48,48,48,48	0
56	MG	2A	3187	1/1	0.95	0.07	45,45,45,45	0
56	MG	1A	3209	1/1	0.95	0.09	42,42,42,42	0
56	MG	1A	3771	1/1	0.95	0.07	41,41,41,41	0
56	MG	1U	204	1/1	0.95	0.20	34,34,34,34	0
56	MG	2A	3612	1/1	0.95	0.11	68,68,68,68	0
56	MG	2A	3759	1/1	0.95	0.10	54,54,54,54	0
56	MG	1A	3440	1/1	0.95	0.17	42,42,42,42	0
56	MG	1V	201	1/1	0.95	0.19	38,38,38,38	0
56	MG	2q	202	1/1	0.95	0.05	67,67,67,67	0
56	MG	1a	1768	1/1	0.95	0.12	54,54,54,54	0
56	MG	1A	3158	1/1	0.95	0.17	27,27,27,27	0
56	MG	1A	3777	1/1	0.95	0.07	46,46,46,46	0
56	MG	2A	3763	1/1	0.95	0.11	59,59,59,59	0
56	MG	2a	1631	1/1	0.95	0.24	50,50,50,50	0
56	MG	1W	205	1/1	0.95	0.18	39,39,39,39	0
56	MG	1a	1774	1/1	0.95	0.10	67,67,67,67	0
56	MG	2A	3069	1/1	0.95	0.26	49,49,49,49	0
56	MG	1A	4096	1/1	0.95	0.22	56,56,56,56	0
56	MG	2A	3621	1/1	0.95	0.19	55,55,55,55	0
56	MG	1A	3670	1/1	0.95	0.06	18,18,18,18	0
56	MG	1A	3671	1/1	0.95	0.06	18,18,18,18	0
56	MG	1A	3082	1/1	0.95	0.18	35,35,35,35	0
56	MG	1A	4103	1/1	0.95	0.21	28,28,28,28	0
56	MG	1a	1784	1/1	0.95	0.05	58,58,58,58	0
56	MG	1A	3484	1/1	0.95	0.20	47,47,47,47	0
56	MG	2A	3077	1/1	0.95	0.13	44,44,44,44	0
56	MG	1A	3531	1/1	0.95	0.32	61,61,61,61	0
56	MG	2A	3334	1/1	0.95	0.08	52,52,52,52	0
57	DI0	1A	4098	58/58	0.95	0.11	17,33,66,81	0
56	MG	2A	3207	1/1	0.95	0.18	34,34,34,34	0
56	MG	2a	1647	1/1	0.95	0.16	56,56,56,56	0
56	MG	1A	3786	1/1	0.95	0.08	19,19,19,19	0
56	MG	2A	3634	1/1	0.95	0.08	41,41,41,41	0
56	MG	2A	3124	1/1	0.96	0.15	44,44,44,44	0
56	MG	1A	3642	1/1	0.96	0.07	33,33,33,33	0
56	MG	1A	3135	1/1	0.96	0.08	30,30,30,30	0
56	MG	1A	4139	1/1	0.96	0.22	35,35,35,35	0
56	MG	1A	3993	1/1	0.96	0.06	68,68,68,68	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1802	1/1	0.96	0.06	83,83,83,83	0
56	MG	1A	3994	1/1	0.96	0.06	33,33,33,33	0
56	MG	2A	3611	1/1	0.96	0.11	48,48,48,48	0
56	MG	1A	3136	1/1	0.96	0.06	36,36,36,36	0
56	MG	1A	3645	1/1	0.96	0.07	37,37,37,37	0
56	MG	15	102	1/1	0.96	0.19	38,38,38,38	0
56	MG	1a	1811	1/1	0.96	0.06	60,60,60,60	0
56	MG	1A	3444	1/1	0.96	0.10	38,38,38,38	0
56	MG	1A	3046	1/1	0.96	0.07	34,34,34,34	0
56	MG	2A	3786	1/1	0.96	0.10	49,49,49,49	0
56	MG	1a	1815	1/1	0.96	0.11	58,58,58,58	0
56	MG	1A	3769	1/1	0.96	0.05	36,36,36,36	0
56	MG	2a	1667	1/1	0.96	0.06	56,56,56,56	0
56	MG	16	103	1/1	0.96	0.14	32,32,32,32	0
56	MG	1A	3138	1/1	0.96	0.23	28,28,28,28	0
56	MG	1A	4150	1/1	0.96	0.09	38,38,38,38	0
56	MG	1A	3110	1/1	0.96	0.19	29,29,29,29	0
56	MG	1A	3772	1/1	0.96	0.08	17,17,17,17	0
56	MG	1A	3876	1/1	0.96	0.14	21,21,21,21	0
56	MG	2A	3796	1/1	0.96	0.08	69,69,69,69	0
56	MG	2A	3288	1/1	0.96	0.13	47,47,47,47	0
56	MG	1A	3773	1/1	0.96	0.05	58,58,58,58	0
56	MG	1A	3292	1/1	0.96	0.08	50,50,50,50	0
56	MG	2A	3142	1/1	0.96	0.21	32,32,32,32	0
56	MG	2A	3292	1/1	0.96	0.26	47,47,47,47	0
56	MG	1A	3501	1/1	0.96	0.16	39,39,39,39	0
56	MG	1A	3393	1/1	0.96	0.24	59,59,59,59	0
56	MG	2a	1684	1/1	0.96	0.10	52,52,52,52	0
56	MG	1a	1611	1/1	0.96	0.11	23,23,23,23	0
56	MG	2A	3633	1/1	0.96	0.06	63,63,63,63	0
56	MG	1A	4014	1/1	0.96	0.09	60,60,60,60	0
56	MG	2A	3810	1/1	0.96	0.05	51,51,51,51	0
56	MG	2a	1689	1/1	0.96	0.11	52,52,52,52	0
56	MG	1A	4015	1/1	0.96	0.07	72,72,72,72	0
56	MG	1A	3343	1/1	0.96	0.21	38,38,38,38	0
56	MG	2A	3813	1/1	0.96	0.07	56,56,56,56	0
56	MG	2A	3148	1/1	0.96	0.14	50,50,50,50	0
56	MG	2a	1694	1/1	0.96	0.21	51,51,51,51	0
56	MG	2A	3638	1/1	0.96	0.06	25,25,25,25	0
56	MG	1A	3213	1/1	0.96	0.13	40,40,40,40	0
56	MG	1a	1843	1/1	0.96	0.08	52,52,52,52	0
56	MG	2A	3150	1/1	0.96	0.05	40,40,40,40	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3641	1/1	0.96	0.06	51,51,51,51	0
56	MG	1A	3657	1/1	0.96	0.07	44,44,44,44	0
56	MG	2A	3013	1/1	0.96	0.16	37,37,37,37	0
56	MG	1A	3089	1/1	0.96	0.07	47,47,47,47	0
56	MG	2A	3827	1/1	0.96	0.08	51,51,51,51	0
56	MG	1A	3042	1/1	0.96	0.12	28,28,28,28	0
56	MG	1A	3297	1/1	0.96	0.23	32,32,32,32	0
56	MG	1A	3891	1/1	0.96	0.06	38,38,38,38	0
56	MG	1A	3667	1/1	0.96	0.04	18,18,18,18	0
56	MG	1A	3033	1/1	0.96	0.16	29,29,29,29	0
56	MG	1A	3578	1/1	0.96	0.21	28,28,28,28	0
56	MG	2A	3840	1/1	0.96	0.06	72,72,72,72	0
56	MG	1A	4030	1/1	0.96	0.10	53,53,53,53	0
56	MG	2A	3464	1/1	0.96	0.16	31,31,31,31	0
56	MG	1A	3579	1/1	0.96	0.08	59,59,59,59	0
56	MG	1A	3093	1/1	0.96	0.14	58,58,58,58	0
56	MG	2A	3467	1/1	0.96	0.23	29,29,29,29	0
56	MG	2A	3848	1/1	0.96	0.12	29,29,29,29	0
56	MG	2A	3314	1/1	0.96	0.05	51,51,51,51	0
56	MG	2A	3658	1/1	0.96	0.13	51,51,51,51	0
56	MG	1A	3301	1/1	0.96	0.21	40,40,40,40	0
56	MG	1a	1647	1/1	0.96	0.06	35,35,35,35	0
56	MG	1A	3512	1/1	0.96	0.08	52,52,52,52	0
56	MG	1A	3218	1/1	0.96	0.25	57,57,57,57	0
56	MG	1A	3584	1/1	0.96	0.14	50,50,50,50	0
56	MG	2A	3856	1/1	0.96	0.22	37,37,37,37	0
56	MG	1A	3117	1/1	0.96	0.32	41,41,41,41	0
56	MG	1A	3220	1/1	0.96	0.09	48,48,48,48	0
56	MG	1A	3065	1/1	0.96	0.09	35,35,35,35	0
56	MG	1A	3096	1/1	0.96	0.16	54,54,54,54	0
56	MG	1A	4042	1/1	0.96	0.05	41,41,41,41	0
56	MG	1A	3908	1/1	0.96	0.07	46,46,46,46	0
56	MG	1A	3262	1/1	0.96	0.16	43,43,43,43	0
56	MG	1y	101	1/1	0.96	0.15	34,34,34,34	0
56	MG	1A	3411	1/1	0.96	0.14	44,44,44,44	0
56	MG	2a	1734	1/1	0.96	0.07	57,57,57,57	0
56	MG	2A	3038	1/1	0.96	0.26	41,41,41,41	0
56	MG	2A	3672	1/1	0.96	0.05	46,46,46,46	0
56	MG	2a	1738	1/1	0.96	0.07	65,65,65,65	0
56	MG	1A	3120	1/1	0.96	0.10	47,47,47,47	0
56	MG	1A	3076	1/1	0.96	0.09	33,33,33,33	0
56	MG	1A	4053	1/1	0.96	0.11	41,41,41,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3100	1/1	0.96	0.11	52,52,52,52	0
56	MG	1B	212	1/1	0.96	0.14	51,51,51,51	0
56	MG	1A	3524	1/1	0.96	0.18	37,37,37,37	0
56	MG	1A	3597	1/1	0.96	0.07	52,52,52,52	0
56	MG	2A	3185	1/1	0.96	0.08	43,43,43,43	0
56	MG	2A	3186	1/1	0.96	0.09	56,56,56,56	0
56	MG	1A	4057	1/1	0.96	0.11	51,51,51,51	0
56	MG	1A	4058	1/1	0.96	0.11	48,48,48,48	0
56	MG	2A	3341	1/1	0.96	0.09	73,73,73,73	0
56	MG	2a	1754	1/1	0.96	0.06	57,57,57,57	0
56	MG	1A	4059	1/1	0.96	0.13	48,48,48,48	0
56	MG	2A	3190	1/1	0.96	0.22	43,43,43,43	0
56	MG	1A	3229	1/1	0.96	0.08	51,51,51,51	0
56	MG	1A	3699	1/1	0.96	0.09	33,33,33,33	0
56	MG	1A	3077	1/1	0.96	0.18	39,39,39,39	0
56	MG	1A	3814	1/1	0.96	0.10	58,58,58,58	0
56	MG	1A	4064	1/1	0.96	0.07	48,48,48,48	0
56	MG	1A	3124	1/1	0.96	0.10	35,35,35,35	0
56	MG	1A	3315	1/1	0.96	0.09	36,36,36,36	0
56	MG	1A	3924	1/1	0.96	0.06	57,57,57,57	0
56	MG	1A	3603	1/1	0.96	0.07	31,31,31,31	0
56	MG	2A	3200	1/1	0.96	0.20	47,47,47,47	0
56	MG	1A	3189	1/1	0.96	0.36	44,44,44,44	0
56	MG	2A	3060	1/1	0.96	0.12	38,38,38,38	0
56	MG	1A	3473	1/1	0.96	0.12	34,34,34,34	0
56	MG	1A	3931	1/1	0.96	0.09	44,44,44,44	0
56	MG	1A	3474	1/1	0.96	0.06	41,41,41,41	0
56	MG	2a	1775	1/1	0.96	0.06	49,49,49,49	0
56	MG	2a	1776	1/1	0.96	0.17	49,49,49,49	0
56	MG	1D	304	1/1	0.96	0.11	36,36,36,36	0
56	MG	1A	3710	1/1	0.96	0.07	54,54,54,54	0
56	MG	1A	4076	1/1	0.96	0.07	44,44,44,44	0
56	MG	2A	3211	1/1	0.96	0.15	32,32,32,32	0
56	MG	2a	1781	1/1	0.96	0.19	55,55,55,55	0
56	MG	1A	3935	1/1	0.96	0.08	45,45,45,45	0
56	MG	2a	1783	1/1	0.96	0.23	58,58,58,58	0
56	MG	1A	3318	1/1	0.96	0.17	32,32,32,32	0
56	MG	1A	3003	1/1	0.96	0.11	20,20,20,20	0
56	MG	2G	201	1/1	0.96	0.11	62,62,62,62	0
56	MG	1A	3234	1/1	0.96	0.26	35,35,35,35	0
56	MG	1A	3942	1/1	0.96	0.10	43,43,43,43	0
56	MG	2A	3218	1/1	0.96	0.07	57,57,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3715	1/1	0.96	0.09	35,35,35,35	0
56	MG	1A	3611	1/1	0.96	0.06	21,21,21,21	0
56	MG	1a	1707	1/1	0.96	0.18	42,42,42,42	0
56	MG	1A	3235	1/1	0.96	0.18	26,26,26,26	0
56	MG	1A	3946	1/1	0.96	0.07	47,47,47,47	0
56	MG	1A	3948	1/1	0.96	0.05	32,32,32,32	0
56	MG	1F	307	1/1	0.96	0.14	34,34,34,34	0
56	MG	1A	3538	1/1	0.96	0.06	39,39,39,39	0
56	MG	2A	3375	1/1	0.96	0.08	47,47,47,47	0
56	MG	1A	3615	1/1	0.96	0.13	30,30,30,30	0
56	MG	1A	4090	1/1	0.96	0.24	61,61,61,61	0
56	MG	2A	3081	1/1	0.96	0.06	41,41,41,41	0
56	MG	1A	3724	1/1	0.96	0.07	76,76,76,76	0
56	MG	1A	3479	1/1	0.96	0.15	45,45,45,45	0
56	MG	2A	3085	1/1	0.96	0.05	34,34,34,34	0
56	MG	1A	3191	1/1	0.96	0.23	34,34,34,34	0
56	MG	2A	3088	1/1	0.96	0.11	48,48,48,48	0
56	MG	1A	3323	1/1	0.96	0.17	42,42,42,42	0
56	MG	2A	3548	1/1	0.96	0.08	42,42,42,42	0
56	MG	1a	1725	1/1	0.96	0.13	46,46,46,46	0
56	MG	1A	3729	1/1	0.96	0.08	44,44,44,44	0
56	MG	1A	3619	1/1	0.96	0.09	31,31,31,31	0
56	MG	1a	1729	1/1	0.96	0.11	48,48,48,48	0
56	MG	2A	3092	1/1	0.96	0.07	35,35,35,35	0
56	MG	2A	3238	1/1	0.96	0.10	28,28,28,28	0
56	MG	1a	1732	1/1	0.96	0.06	50,50,50,50	0
56	MG	1a	1733	1/1	0.96	0.08	52,52,52,52	0
56	MG	1A	3128	1/1	0.96	0.20	30,30,30,30	0
56	MG	1O	204	1/1	0.96	0.07	51,51,51,51	0
56	MG	1a	1736	1/1	0.96	0.09	34,34,34,34	0
56	MG	1A	3160	1/1	0.96	0.21	32,32,32,32	0
56	MG	1A	3239	1/1	0.96	0.26	29,29,29,29	0
56	MG	1A	3080	1/1	0.96	0.09	55,55,55,55	0
56	MG	1P	203	1/1	0.96	0.20	29,29,29,29	0
56	MG	2A	3559	1/1	0.96	0.05	32,32,32,32	0
56	MG	2A	3243	1/1	0.96	0.13	50,50,50,50	0
56	MG	1A	3628	1/1	0.96	0.04	25,25,25,25	0
56	MG	2A	3562	1/1	0.96	0.06	43,43,43,43	0
56	MG	1A	4106	1/1	0.96	0.07	52,52,52,52	0
56	MG	1a	1750	1/1	0.96	0.07	53,53,53,53	0
56	MG	1A	3738	1/1	0.96	0.09	26,26,26,26	0
56	MG	1a	1752	1/1	0.96	0.13	43,43,43,43	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	4109	1/1	0.96	0.10	37,37,37,37	0
56	MG	1A	3739	1/1	0.96	0.11	35,35,35,35	0
56	MG	1A	3968	1/1	0.96	0.12	52,52,52,52	0
56	MG	1S	202	1/1	0.96	0.09	45,45,45,45	0
56	MG	2A	3401	1/1	0.96	0.18	46,46,46,46	0
56	MG	2A	3572	1/1	0.96	0.07	36,36,36,36	0
56	MG	2I	201	1/1	0.96	0.09	65,65,65,65	0
56	MG	1A	4113	1/1	0.96	0.13	49,49,49,49	0
56	MG	1U	201	1/1	0.96	0.17	37,37,37,37	0
56	MG	1a	1763	1/1	0.96	0.11	38,38,38,38	0
56	MG	1A	3067	1/1	0.96	0.08	29,29,29,29	0
56	MG	1A	3630	1/1	0.96	0.10	33,33,33,33	0
56	MG	2A	3576	1/1	0.96	0.07	49,49,49,49	0
56	MG	1A	3632	1/1	0.96	0.06	44,44,44,44	0
56	MG	1A	3032	1/1	0.96	0.34	32,32,32,32	0
56	MG	1A	3748	1/1	0.96	0.07	20,20,20,20	0
56	MG	1A	3976	1/1	0.96	0.07	66,66,66,66	0
56	MG	1A	4123	1/1	0.96	0.13	36,36,36,36	0
56	MG	2A	3586	1/1	0.96	0.06	32,32,32,32	0
56	MG	1A	3977	1/1	0.96	0.16	38,38,38,38	0
56	MG	1A	3069	1/1	0.96	0.14	27,27,27,27	0
56	MG	1A	3202	1/1	0.96	0.09	25,25,25,25	0
56	MG	1X	103	1/1	0.96	0.06	40,40,40,40	0
56	MG	2A	3115	1/1	0.96	0.10	40,40,40,40	0
56	MG	2A	3591	1/1	0.96	0.09	34,34,34,34	0
56	MG	1A	3439	1/1	0.96	0.09	42,42,42,42	0
56	MG	1A	3857	1/1	0.96	0.13	54,54,54,54	0
56	MG	1A	3491	1/1	0.96	0.33	34,34,34,34	0
56	MG	2A	3596	1/1	0.96	0.12	46,46,46,46	0
56	MG	1A	3061	1/1	0.96	0.05	35,35,35,35	0
56	MG	1A	4132	1/1	0.96	0.14	34,34,34,34	0
56	MG	1A	3860	1/1	0.96	0.05	29,29,29,29	0
56	MG	1A	3556	1/1	0.96	0.22	37,37,37,37	0
56	MG	1A	3134	1/1	0.96	0.13	46,46,46,46	0
59	ZN	2n	501	1/1	0.96	0.07	97,97,97,97	0
56	MG	1B	206	1/1	0.97	0.06	44,44,44,44	0
56	MG	1A	3022	1/1	0.97	0.06	34,34,34,34	0
56	MG	1a	1635	1/1	0.97	0.10	36,36,36,36	0
56	MG	1A	3839	1/1	0.97	0.12	45,45,45,45	0
56	MG	2a	1672	1/1	0.97	0.15	40,40,40,40	0
56	MG	1A	3417	1/1	0.97	0.12	58,58,58,58	0
56	MG	2A	3412	1/1	0.97	0.08	57,57,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3554	1/1	0.97	0.08	46,46,46,46	0
56	MG	1A	3024	1/1	0.97	0.16	33,33,33,33	0
56	MG	1A	3056	1/1	0.97	0.13	34,34,34,34	0
56	MG	2A	3161	1/1	0.97	0.05	42,42,42,42	0
56	MG	1A	3126	1/1	0.97	0.19	32,32,32,32	0
56	MG	1A	3655	1/1	0.97	0.07	14,14,14,14	0
56	MG	1A	4074	1/1	0.97	0.07	49,49,49,49	0
56	MG	1A	3845	1/1	0.97	0.10	28,28,28,28	0
56	MG	2A	3047	1/1	0.97	0.20	31,31,31,31	0
56	MG	2A	3564	1/1	0.97	0.07	57,57,57,57	0
56	MG	1A	3153	1/1	0.97	0.11	42,42,42,42	0
56	MG	1A	3753	1/1	0.97	0.07	26,26,26,26	0
56	MG	1A	3330	1/1	0.97	0.15	46,46,46,46	0
56	MG	1A	3331	1/1	0.97	0.11	43,43,43,43	0
56	MG	1A	3590	1/1	0.97	0.24	34,34,34,34	0
56	MG	1A	3961	1/1	0.97	0.04	64,64,64,64	0
56	MG	1A	3851	1/1	0.97	0.08	51,51,51,51	0
56	MG	1A	3662	1/1	0.97	0.08	21,21,21,21	0
56	MG	2A	3723	1/1	0.97	0.06	26,26,26,26	0
56	MG	1A	3758	1/1	0.97	0.08	34,34,34,34	0
56	MG	1A	3154	1/1	0.97	0.15	44,44,44,44	0
56	MG	1A	3184	1/1	0.97	0.08	40,40,40,40	0
56	MG	2A	3059	1/1	0.97	0.06	48,48,48,48	0
56	MG	2A	3179	1/1	0.97	0.22	46,46,46,46	0
56	MG	1D	302	1/1	0.97	0.06	33,33,33,33	0
56	MG	1A	3761	1/1	0.97	0.05	43,43,43,43	0
56	MG	1A	3593	1/1	0.97	0.08	34,34,34,34	0
56	MG	2A	3585	1/1	0.97	0.06	45,45,45,45	0
56	MG	1D	306	1/1	0.97	0.12	23,23,23,23	0
56	MG	1w	107	1/1	0.97	0.08	38,38,38,38	0
56	MG	1A	3669	1/1	0.97	0.07	20,20,20,20	0
56	MG	1D	308	1/1	0.97	0.23	31,31,31,31	0
56	MG	1A	3973	1/1	0.97	0.11	20,20,20,20	0
56	MG	1A	3127	1/1	0.97	0.22	35,35,35,35	0
56	MG	1A	3377	1/1	0.97	0.10	44,44,44,44	0
56	MG	1E	301	1/1	0.97	0.10	35,35,35,35	0
56	MG	1A	3767	1/1	0.97	0.05	21,21,21,21	0
56	MG	1E	303	1/1	0.97	0.11	36,36,36,36	0
56	MG	1A	3768	1/1	0.97	0.05	20,20,20,20	0
56	MG	1A	3221	1/1	0.97	0.13	39,39,39,39	0
56	MG	1A	3379	1/1	0.97	0.07	20,20,20,20	0
56	MG	1A	3085	1/1	0.97	0.14	36,36,36,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1F	301	1/1	0.97	0.04	31,31,31,31	0
56	MG	1a	1682	1/1	0.97	0.23	36,36,36,36	0
56	MG	1A	4101	1/1	0.97	0.05	47,47,47,47	0
56	MG	1F	303	1/1	0.97	0.26	36,36,36,36	0
56	MG	1a	1685	1/1	0.97	0.16	44,44,44,44	0
56	MG	1A	4102	1/1	0.97	0.32	41,41,41,41	0
56	MG	2A	3598	1/1	0.97	0.09	29,29,29,29	0
56	MG	1A	3677	1/1	0.97	0.05	22,22,22,22	0
56	MG	1A	3037	1/1	0.97	0.13	22,22,22,22	0
56	MG	2A	3075	1/1	0.97	0.07	40,40,40,40	0
56	MG	2A	3602	1/1	0.97	0.04	35,35,35,35	0
56	MG	2A	3603	1/1	0.97	0.08	49,49,49,49	0
56	MG	1A	4105	1/1	0.97	0.10	30,30,30,30	0
56	MG	1A	3038	1/1	0.97	0.50	36,36,36,36	0
56	MG	1A	3601	1/1	0.97	0.07	38,38,38,38	0
56	MG	1A	3435	1/1	0.97	0.32	50,50,50,50	0
56	MG	2A	3080	1/1	0.97	0.07	39,39,39,39	0
56	MG	1A	3871	1/1	0.97	0.06	46,46,46,46	0
56	MG	1N	201	1/1	0.97	0.07	48,48,48,48	0
56	MG	1A	3778	1/1	0.97	0.08	16,16,16,16	0
56	MG	1a	1701	1/1	0.97	0.22	46,46,46,46	0
56	MG	2A	3203	1/1	0.97	0.16	35,35,35,35	0
56	MG	1N	204	1/1	0.97	0.07	46,46,46,46	0
56	MG	2A	3083	1/1	0.97	0.08	36,36,36,36	0
56	MG	1A	3683	1/1	0.97	0.06	13,13,13,13	0
56	MG	1A	3992	1/1	0.97	0.05	70,70,70,70	0
56	MG	2D	301	1/1	0.97	0.07	34,34,34,34	0
56	MG	1A	3874	1/1	0.97	0.05	18,18,18,18	0
56	MG	2a	1747	1/1	0.97	0.14	51,51,51,51	0
56	MG	2a	1748	1/1	0.97	0.05	56,56,56,56	0
56	MG	1A	3383	1/1	0.97	0.08	43,43,43,43	0
56	MG	1A	3015	1/1	0.97	0.07	37,37,37,37	0
56	MG	1O	203	1/1	0.97	0.07	51,51,51,51	0
56	MG	2A	3336	1/1	0.97	0.18	50,50,50,50	0
56	MG	2A	3338	1/1	0.97	0.09	47,47,47,47	0
56	MG	2A	3212	1/1	0.97	0.12	35,35,35,35	0
56	MG	1A	3385	1/1	0.97	0.15	32,32,32,32	0
56	MG	1A	4121	1/1	0.97	0.10	27,27,27,27	0
56	MG	1A	3783	1/1	0.97	0.09	18,18,18,18	0
56	MG	1A	4000	1/1	0.97	0.04	36,36,36,36	0
56	MG	2A	3628	1/1	0.97	0.11	55,55,55,55	0
56	MG	1A	3882	1/1	0.97	0.07	20,20,20,20	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	4002	1/1	0.97	0.05	32,32,32,32	0
56	MG	1A	3687	1/1	0.97	0.07	35,35,35,35	0
56	MG	1A	3299	1/1	0.97	0.06	32,32,32,32	0
56	MG	1A	4005	1/1	0.97	0.05	53,53,53,53	0
56	MG	1a	1724	1/1	0.97	0.08	23,23,23,23	0
56	MG	1A	3226	1/1	0.97	0.16	39,39,39,39	0
56	MG	2P	203	1/1	0.97	0.28	49,49,49,49	0
56	MG	2A	3779	1/1	0.97	0.06	36,36,36,36	0
56	MG	2a	1771	1/1	0.97	0.08	54,54,54,54	0
56	MG	2Q	202	1/1	0.97	0.23	41,41,41,41	0
56	MG	1a	1727	1/1	0.97	0.14	30,30,30,30	0
56	MG	2a	1774	1/1	0.97	0.06	63,63,63,63	0
56	MG	1A	4007	1/1	0.97	0.06	54,54,54,54	0
56	MG	1A	3109	1/1	0.97	0.41	35,35,35,35	0
56	MG	1A	3547	1/1	0.97	0.28	38,38,38,38	0
56	MG	2A	3783	1/1	0.97	0.07	48,48,48,48	0
56	MG	1A	4134	1/1	0.97	0.24	29,29,29,29	0
56	MG	2A	3104	1/1	0.97	0.25	51,51,51,51	0
56	MG	1A	3048	1/1	0.97	0.09	23,23,23,23	0
56	MG	2U	203	1/1	0.97	0.25	58,58,58,58	0
56	MG	2A	3787	1/1	0.97	0.04	55,55,55,55	0
56	MG	1A	3693	1/1	0.97	0.08	24,24,24,24	0
56	MG	1A	3049	1/1	0.97	0.09	38,38,38,38	0
56	MG	1A	3697	1/1	0.97	0.07	18,18,18,18	0
56	MG	1A	3075	1/1	0.97	0.07	28,28,28,28	0
56	MG	1A	3796	1/1	0.97	0.27	30,30,30,30	0
56	MG	2a	1789	1/1	0.97	0.10	45,45,45,45	0
56	MG	2a	1790	1/1	0.97	0.10	58,58,58,58	0
56	MG	1W	202	1/1	0.97	0.14	35,35,35,35	0
56	MG	1A	3392	1/1	0.97	0.05	51,51,51,51	0
56	MG	1a	1745	1/1	0.97	0.06	35,35,35,35	0
56	MG	1W	204	1/1	0.97	0.24	39,39,39,39	0
56	MG	2A	3491	1/1	0.97	0.10	51,51,51,51	0
56	MG	1a	1748	1/1	0.97	0.11	62,62,62,62	0
56	MG	2A	3797	1/1	0.97	0.08	32,32,32,32	0
56	MG	1X	102	1/1	0.97	0.20	39,39,39,39	0
56	MG	1A	3195	1/1	0.97	0.05	39,39,39,39	0
56	MG	27	101	1/1	0.97	0.13	50,50,50,50	0
56	MG	1X	104	1/1	0.97	0.21	43,43,43,43	0
56	MG	1A	3114	1/1	0.97	0.07	39,39,39,39	0
56	MG	1A	3800	1/1	0.97	0.07	43,43,43,43	0
56	MG	1A	3702	1/1	0.97	0.05	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3555	1/1	0.97	0.09	41,41,41,41	0
56	MG	1A	3094	1/1	0.97	0.13	17,17,17,17	0
56	MG	1a	1759	1/1	0.97	0.06	39,39,39,39	0
56	MG	2A	3804	1/1	0.97	0.11	70,70,70,70	0
56	MG	1A	3050	1/1	0.97	0.13	42,42,42,42	0
56	MG	10	101	1/1	0.97	0.08	38,38,38,38	0
56	MG	1A	3707	1/1	0.97	0.03	16,16,16,16	0
56	MG	1A	3560	1/1	0.97	0.27	42,42,42,42	0
56	MG	2A	3809	1/1	0.97	0.10	57,57,57,57	0
56	MG	2A	3371	1/1	0.97	0.11	55,55,55,55	0
56	MG	1A	3623	1/1	0.97	0.07	26,26,26,26	0
56	MG	1A	3398	1/1	0.97	0.13	40,40,40,40	0
56	MG	1a	1769	1/1	0.97	0.06	74,74,74,74	0
56	MG	1A	3626	1/1	0.97	0.06	19,19,19,19	0
56	MG	1A	3399	1/1	0.97	0.05	51,51,51,51	0
56	MG	11	104	1/1	0.97	0.06	44,44,44,44	0
56	MG	1A	3031	1/1	0.97	0.19	32,32,32,32	0
56	MG	1A	3168	1/1	0.97	0.28	34,34,34,34	0
56	MG	2A	3818	1/1	0.97	0.10	42,42,42,42	0
56	MG	1A	3097	1/1	0.97	0.14	34,34,34,34	0
56	MG	1A	3631	1/1	0.97	0.05	20,20,20,20	0
56	MG	15	101	1/1	0.97	0.05	41,41,41,41	0
56	MG	1A	3010	1/1	0.97	0.12	38,38,38,38	0
56	MG	2a	1828	1/1	0.97	0.14	41,41,41,41	0
56	MG	2A	3511	1/1	0.97	0.27	42,42,42,42	0
56	MG	1A	4039	1/1	0.97	0.07	19,19,19,19	0
56	MG	2A	3255	1/1	0.97	0.15	55,55,55,55	0
56	MG	2A	3828	1/1	0.97	0.04	43,43,43,43	0
56	MG	1A	3567	1/1	0.97	0.27	35,35,35,35	0
56	MG	1A	3205	1/1	0.97	0.08	46,46,46,46	0
56	MG	1A	3144	1/1	0.97	0.14	36,36,36,36	0
56	MG	18	101	1/1	0.97	0.09	45,45,45,45	0
56	MG	2A	3834	1/1	0.97	0.08	34,34,34,34	0
56	MG	2A	3835	1/1	0.97	0.05	73,73,73,73	0
56	MG	1a	1793	1/1	0.97	0.05	51,51,51,51	0
56	MG	1A	3726	1/1	0.97	0.06	65,65,65,65	0
56	MG	2A	3837	1/1	0.97	0.07	61,61,61,61	0
56	MG	1a	1796	1/1	0.97	0.06	42,42,42,42	0
56	MG	2A	3520	1/1	0.97	0.12	40,40,40,40	0
56	MG	2A	3521	1/1	0.97	0.09	53,53,53,53	0
56	MG	2A	3017	1/1	0.97	0.07	53,53,53,53	0
56	MG	1A	3099	1/1	0.97	0.11	23,23,23,23	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3317	1/1	0.97	0.08	47,47,47,47	0
56	MG	1A	3278	1/1	0.97	0.25	27,27,27,27	0
56	MG	1a	1807	1/1	0.97	0.08	67,67,67,67	0
56	MG	1A	4050	1/1	0.97	0.10	37,37,37,37	0
56	MG	1A	3824	1/1	0.97	0.06	24,24,24,24	0
56	MG	1A	3513	1/1	0.97	0.07	49,49,49,49	0
56	MG	1A	3732	1/1	0.97	0.05	23,23,23,23	0
56	MG	2A	3531	1/1	0.97	0.07	40,40,40,40	0
56	MG	1A	3360	1/1	0.97	0.11	38,38,38,38	0
56	MG	2A	3533	1/1	0.97	0.05	59,59,59,59	0
56	MG	1A	3575	1/1	0.97	0.14	40,40,40,40	0
56	MG	1A	3208	1/1	0.97	0.07	35,35,35,35	0
56	MG	1A	3936	1/1	0.97	0.06	62,62,62,62	0
56	MG	1A	3079	1/1	0.97	0.10	27,27,27,27	0
56	MG	1A	3210	1/1	0.97	0.28	32,32,32,32	0
56	MG	2A	3541	1/1	0.97	0.05	54,54,54,54	0
56	MG	1A	3833	1/1	0.97	0.06	46,46,46,46	0
56	MG	1A	3941	1/1	0.97	0.07	49,49,49,49	0
56	MG	1A	3009	1/1	0.97	0.04	17,17,17,17	0
56	MG	1A	3176	1/1	0.97	0.12	26,26,26,26	0
56	MG	1A	3284	1/1	0.97	0.12	45,45,45,45	0
59	ZN	2Y	201	1/1	0.97	0.05	106,106,106,106	0
56	MG	2A	3279	1/1	0.97	0.18	54,54,54,54	0
56	MG	1A	3744	1/1	0.97	0.04	25,25,25,25	0
56	MG	1A	4025	1/1	0.98	0.05	42,42,42,42	0
56	MG	1D	309	1/1	0.98	0.12	27,27,27,27	0
56	MG	1A	3008	1/1	0.98	0.05	23,23,23,23	0
56	MG	2A	3337	1/1	0.98	0.06	37,37,37,37	0
56	MG	1A	3177	1/1	0.98	0.10	25,25,25,25	0
56	MG	1D	313	1/1	0.98	0.22	39,39,39,39	0
56	MG	1A	3610	1/1	0.98	0.04	29,29,29,29	0
56	MG	1A	3305	1/1	0.98	0.09	40,40,40,40	0
56	MG	1A	3552	1/1	0.98	0.04	33,33,33,33	0
56	MG	1A	3963	1/1	0.98	0.06	59,59,59,59	0
56	MG	1A	3647	1/1	0.98	0.06	28,28,28,28	0
56	MG	2a	1753	1/1	0.98	0.05	67,67,67,67	0
56	MG	1A	3965	1/1	0.98	0.07	52,52,52,52	0
56	MG	1A	3152	1/1	0.98	0.07	35,35,35,35	0
56	MG	1E	308	1/1	0.98	0.08	43,43,43,43	0
56	MG	1A	4107	1/1	0.98	0.13	22,22,22,22	0
56	MG	2A	3807	1/1	0.98	0.07	65,65,65,65	0
56	MG	1A	3141	1/1	0.98	0.19	17,17,17,17	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1a	1617	1/1	0.98	0.05	58,58,58,58	0
56	MG	2A	3430	1/1	0.98	0.03	40,40,40,40	0
56	MG	1A	3430	1/1	0.98	0.19	41,41,41,41	0
56	MG	1a	1620	1/1	0.98	0.05	44,44,44,44	0
56	MG	2a	1764	1/1	0.98	0.05	65,65,65,65	0
56	MG	1w	106	1/1	0.98	0.06	77,77,77,77	0
56	MG	2A	3613	1/1	0.98	0.05	34,34,34,34	0
56	MG	2A	3517	1/1	0.98	0.09	17,17,17,17	0
56	MG	2A	3432	1/1	0.98	0.06	33,33,33,33	0
56	MG	1A	3092	1/1	0.98	0.16	43,43,43,43	0
56	MG	1A	3694	1/1	0.98	0.07	15,15,15,15	0
56	MG	2A	3816	1/1	0.98	0.05	28,28,28,28	0
56	MG	1a	1744	1/1	0.98	0.05	36,36,36,36	0
56	MG	2A	3619	1/1	0.98	0.05	35,35,35,35	0
56	MG	1A	3971	1/1	0.98	0.07	28,28,28,28	0
56	MG	1A	3695	1/1	0.98	0.06	16,16,16,16	0
56	MG	1a	1630	1/1	0.98	0.05	36,36,36,36	0
56	MG	1A	3012	1/1	0.98	0.07	23,23,23,23	0
56	MG	2A	3821	1/1	0.98	0.05	28,28,28,28	0
56	MG	1A	3559	1/1	0.98	0.19	34,34,34,34	0
56	MG	1A	4117	1/1	0.98	0.18	29,29,29,29	0
56	MG	1A	3750	1/1	0.98	0.06	38,38,38,38	0
56	MG	1A	3530	1/1	0.98	0.05	33,33,33,33	0
56	MG	2A	3528	1/1	0.98	0.06	70,70,70,70	0
56	MG	1A	4045	1/1	0.98	0.06	37,37,37,37	0
56	MG	1A	4046	1/1	0.98	0.04	31,31,31,31	0
56	MG	2A	3831	1/1	0.98	0.08	29,29,29,29	0
56	MG	2A	3832	1/1	0.98	0.04	53,53,53,53	0
56	MG	1A	4047	1/1	0.98	0.05	41,41,41,41	0
56	MG	1A	3621	1/1	0.98	0.06	47,47,47,47	0
56	MG	1A	3112	1/1	0.98	0.19	37,37,37,37	0
56	MG	1A	3806	1/1	0.98	0.17	25,25,25,25	0
56	MG	1A	3532	1/1	0.98	0.29	40,40,40,40	0
56	MG	2A	3205	1/1	0.98	0.07	47,47,47,47	0
56	MG	2A	3206	1/1	0.98	0.11	41,41,41,41	0
56	MG	2A	3538	1/1	0.98	0.05	29,29,29,29	0
56	MG	1A	3658	1/1	0.98	0.06	35,35,35,35	0
56	MG	1A	3624	1/1	0.98	0.04	38,38,38,38	0
56	MG	1A	3983	1/1	0.98	0.06	37,37,37,37	0
56	MG	2A	3543	1/1	0.98	0.05	35,35,35,35	0
56	MG	1A	3704	1/1	0.98	0.11	51,51,51,51	0
56	MG	1A	3506	1/1	0.98	0.17	26,26,26,26	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3661	1/1	0.98	0.06	17,17,17,17	0
56	MG	2a	1674	1/1	0.98	0.04	59,59,59,59	0
56	MG	1A	3227	1/1	0.98	0.06	34,34,34,34	0
56	MG	1A	3276	1/1	0.98	0.07	47,47,47,47	0
56	MG	1A	3664	1/1	0.98	0.04	39,39,39,39	0
56	MG	2A	3853	1/1	0.98	0.13	53,53,53,53	0
56	MG	1a	1780	1/1	0.98	0.04	64,64,64,64	0
56	MG	1A	3991	1/1	0.98	0.04	68,68,68,68	0
56	MG	1A	3763	1/1	0.98	0.06	16,16,16,16	0
56	MG	1A	4140	1/1	0.98	0.28	31,31,31,31	0
56	MG	1A	3929	1/1	0.98	0.05	37,37,37,37	0
56	MG	2A	3652	1/1	0.98	0.08	26,26,26,26	0
56	MG	1a	1787	1/1	0.98	0.04	64,64,64,64	0
56	MG	1A	3930	1/1	0.98	0.05	47,47,47,47	0
56	MG	2A	3381	1/1	0.98	0.14	43,43,43,43	0
56	MG	2A	3861	1/1	0.98	0.07	45,45,45,45	0
56	MG	2A	3556	1/1	0.98	0.05	33,33,33,33	0
56	MG	2A	3221	1/1	0.98	0.13	36,36,36,36	0
56	MG	2A	3301	1/1	0.98	0.16	54,54,54,54	0
56	MG	1A	3995	1/1	0.98	0.08	18,18,18,18	0
56	MG	1A	3665	1/1	0.98	0.08	22,22,22,22	0
56	MG	1A	3666	1/1	0.98	0.05	22,22,22,22	0
56	MG	1A	3294	1/1	0.98	0.05	28,28,28,28	0
56	MG	1a	1798	1/1	0.98	0.04	66,66,66,66	0
56	MG	1a	1676	1/1	0.98	0.14	35,35,35,35	0
56	MG	1W	206	1/1	0.98	0.12	31,31,31,31	0
56	MG	1a	1803	1/1	0.98	0.06	70,70,70,70	0
56	MG	1A	3999	1/1	0.98	0.03	30,30,30,30	0
56	MG	1A	3713	1/1	0.98	0.04	20,20,20,20	0
56	MG	1A	3437	1/1	0.98	0.16	54,54,54,54	0
56	MG	1A	3021	1/1	0.98	0.05	21,21,21,21	0
56	MG	1A	3013	1/1	0.98	0.27	26,26,26,26	0
56	MG	1A	4075	1/1	0.98	0.12	36,36,36,36	0
56	MG	1a	1810	1/1	0.98	0.04	59,59,59,59	0
56	MG	2A	3569	1/1	0.98	0.08	47,47,47,47	0
56	MG	1B	215	1/1	0.98	0.03	52,52,52,52	0
56	MG	1B	216	1/1	0.98	0.09	38,38,38,38	0
56	MG	2A	3153	1/1	0.98	0.04	49,49,49,49	0
56	MG	2A	3571	1/1	0.98	0.06	36,36,36,36	0
56	MG	1A	3395	1/1	0.98	0.05	33,33,33,33	0
56	MG	1A	3718	1/1	0.98	0.04	39,39,39,39	0
56	MG	2X	101	1/1	0.98	0.09	47,47,47,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3199	1/1	0.98	0.07	35,35,35,35	0
56	MG	1A	3720	1/1	0.98	0.05	32,32,32,32	0
56	MG	1A	3828	1/1	0.98	0.10	56,56,56,56	0
56	MG	1A	3673	1/1	0.98	0.04	51,51,51,51	0
56	MG	1A	3200	1/1	0.98	0.07	37,37,37,37	0
56	MG	1a	1824	1/1	0.98	0.18	51,51,51,51	0
56	MG	1l	101	1/1	0.98	0.05	27,27,27,27	0
56	MG	2A	3580	1/1	0.98	0.09	37,37,37,37	0
56	MG	1A	3947	1/1	0.98	0.04	53,53,53,53	0
56	MG	1A	3023	1/1	0.98	0.04	18,18,18,18	0
56	MG	2A	3087	1/1	0.98	0.06	29,29,29,29	0
56	MG	2A	3584	1/1	0.98	0.10	33,33,33,33	0
56	MG	1A	3886	1/1	0.98	0.04	49,49,49,49	0
56	MG	1A	3036	1/1	0.98	0.06	27,27,27,27	0
56	MG	1A	3637	1/1	0.98	0.07	12,12,12,12	0
56	MG	1A	3421	1/1	0.98	0.10	40,40,40,40	0
56	MG	1A	4089	1/1	0.98	0.05	30,30,30,30	0
56	MG	1A	3953	1/1	0.98	0.05	34,34,34,34	0
56	MG	1A	3014	1/1	0.98	0.06	29,29,29,29	0
56	MG	1A	4019	1/1	0.98	0.04	44,44,44,44	0
56	MG	1A	3730	1/1	0.98	0.07	47,47,47,47	0
56	MG	2a	1736	1/1	0.98	0.04	84,84,84,84	0
56	MG	2A	3022	1/1	0.98	0.14	47,47,47,47	0
56	MG	1A	3081	1/1	0.98	0.13	39,39,39,39	0
59	ZN	14	501	1/1	0.98	0.05	94,94,94,94	0
56	MG	2A	3793	1/1	0.98	0.08	63,63,63,63	0
56	MG	17	103	1/1	0.98	0.07	41,41,41,41	0
56	MG	1A	3341	1/1	0.98	0.13	47,47,47,47	0
60	SF4	2d	303	8/8	0.98	0.04	62,72,82,88	0
56	MG	1A	3989	1/1	0.99	0.03	34,34,34,34	0
56	MG	1A	3879	1/1	0.99	0.08	40,40,40,40	0
56	MG	1a	1758	1/1	0.99	0.08	49,49,49,49	0
56	MG	1a	1801	1/1	0.99	0.04	53,53,53,53	0
56	MG	1A	3173	1/1	0.99	0.29	34,34,34,34	0
56	MG	1A	3895	1/1	0.99	0.06	42,42,42,42	0
56	MG	1A	3932	1/1	0.99	0.04	38,38,38,38	0
56	MG	2A	3737	1/1	0.99	0.03	41,41,41,41	0
56	MG	1A	3140	1/1	0.99	0.12	34,34,34,34	0
56	MG	1A	3086	1/1	0.99	0.11	34,34,34,34	0
56	MG	2A	3618	1/1	0.99	0.04	30,30,30,30	0
56	MG	1A	3557	1/1	0.99	0.04	19,19,19,19	0
56	MG	2A	3842	1/1	0.99	0.06	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	4111	1/1	0.99	0.15	32,32,32,32	0
56	MG	1A	3192	1/1	0.99	0.21	23,23,23,23	0
56	MG	2A	3592	1/1	0.99	0.04	33,33,33,33	0
56	MG	1A	3681	1/1	0.99	0.05	31,31,31,31	0
56	MG	1A	3938	1/1	0.99	0.03	49,49,49,49	0
56	MG	1A	3901	1/1	0.99	0.03	19,19,19,19	0
56	MG	2A	3540	1/1	0.99	0.13	23,23,23,23	0
56	MG	1A	4023	1/1	0.99	0.04	39,39,39,39	0
56	MG	1a	1819	1/1	0.99	0.04	37,37,37,37	0
56	MG	1B	227	1/1	0.99	0.06	45,45,45,45	0
56	MG	1a	1737	1/1	0.99	0.09	33,33,33,33	0
56	MG	1A	3919	1/1	0.99	0.04	44,44,44,44	0
56	MG	1A	4118	1/1	0.99	0.14	35,35,35,35	0
56	MG	1A	3795	1/1	0.99	0.07	27,27,27,27	0
56	MG	1A	3921	1/1	0.99	0.04	47,47,47,47	0
56	MG	1A	3742	1/1	0.99	0.04	40,40,40,40	0
56	MG	1a	1783	1/1	0.99	0.03	38,38,38,38	0
56	MG	1A	3722	1/1	0.99	0.06	21,21,21,21	0
56	MG	1A	3875	1/1	0.99	0.02	28,28,28,28	0
56	MG	1A	4052	1/1	0.99	0.08	22,22,22,22	0
56	MG	1A	3058	1/1	0.99	0.03	27,27,27,27	0
56	MG	2A	3791	1/1	0.99	0.03	67,67,67,67	0
56	MG	2A	3825	1/1	0.99	0.04	33,33,33,33	0
56	MG	2A	3826	1/1	0.99	0.05	32,32,32,32	0
56	MG	1A	3675	1/1	0.99	0.10	22,22,22,22	0
59	ZN	1Y	204	1/1	0.99	0.08	84,84,84,84	0
56	MG	2A	3579	1/1	0.99	0.08	32,32,32,32	0
59	ZN	15	106	1/1	0.99	0.03	42,42,42,42	0
56	MG	2A	3729	1/1	0.99	0.06	26,26,26,26	0
56	MG	1A	3878	1/1	0.99	0.04	35,35,35,35	0
59	ZN	25	105	1/1	0.99	0.05	66,66,66,66	0
59	ZN	26	501	1/1	0.99	0.04	58,58,58,58	0
59	ZN	29	501	1/1	0.99	0.03	65,65,65,65	0
56	MG	1A	4128	1/1	0.99	0.09	30,30,30,30	0
60	SF4	1d	3102	8/8	0.99	0.04	47,58,62,63	0
56	MG	1B	207	1/1	0.99	0.13	41,41,41,41	0
56	MG	1A	3743	1/1	1.00	0.06	23,23,23,23	0
56	MG	1A	3902	1/1	1.00	0.02	26,26,26,26	0
59	ZN	16	102	1/1	1.00	0.02	38,38,38,38	0
59	ZN	19	501	1/1	1.00	0.08	57,57,57,57	0
59	ZN	1n	101	1/1	1.00	0.01	49,49,49,49	0
56	MG	1A	3614	1/1	1.00	0.04	31,31,31,31	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3925	1/1	1.00	0.05	23,23,23,23	0
56	MG	1A	4022	1/1	1.00	0.03	17,17,17,17	0
56	MG	1a	1799	1/1	1.00	0.02	36,36,36,36	0
56	MG	1A	3741	1/1	1.00	0.06	38,38,38,38	0
56	MG	1A	3784	1/1	1.00	0.06	16,16,16,16	0
56	MG	1A	3774	1/1	1.00	0.05	34,34,34,34	0
56	MG	1A	3723	1/1	1.00	0.07	14,14,14,14	0

6.5 Other polymers [i](#)

There are no such residues in this entry.