



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 01:15 PM UTC

PDB ID : 5VP2 / pdb_00005vp2
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with madumycin II and bound to mRNA and A-, P- and E-site tRNAs at 2.8Å resolution
Authors : Osterman, I.A.; Khabibullina, N.F.; Komarova, E.S.; Kasatsky, P.; Kartsev, V.G.; Bogdanov, A.A.; Dontsova, O.A.; Konevega, A.L.; Sergiev, P.V.; Polikanov, Y.S.
Deposited on : 2017-05-04
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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)

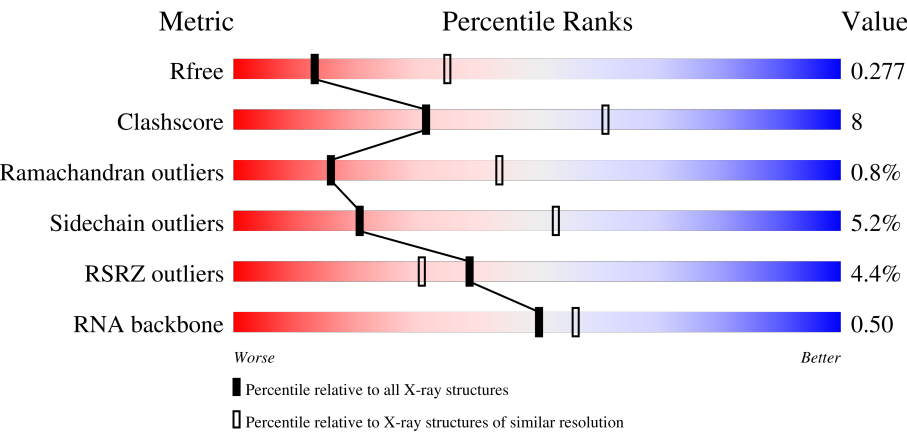
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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% 63%29%6%
1	2A	2915	3% 56%33%7%

Continued on next page...

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

Validation Pipeline (wwPDB-VP) : 2.49

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
52	1u	27	
52	2u	27	
53	1v	24	
53	2v	24	
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	2A	3084	-	-	-	X
56	MG	2A	3204	-	-	-	X
60	SF4	1d	501	-	-	X	-
60	SF4	2d	302	-	-	X	-

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 300935 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 53 is a RNA chain called mRNA.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	1w	72	Total	C	N	O	P	S	0	0
			1550	694	277	505	72	2		
54	1y	74	Total	C	N	O	P	S	0	0
			1585	707	285	518	74	1		
54	2w	69	Total	C	N	O	P	S	0	0
			1482	662	267	482	69	2		
54	2y	73	Total	C	N	O	P	S	0	0
			1565	698	283	510	73	1		

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	1x	76	Total	C	N	O	P	S	0	0
			1625	725	294	529	76	1		
55	2x	76	Total	C	N	O	P	S	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	1143	Total	Mg	0	0
			1143	1143		
56	1B	36	Total	Mg	0	0
			36	36		
56	1D	14	Total	Mg	0	0
			14	14		
56	1E	12	Total	Mg	0	0
			12	12		
56	1F	8	Total	Mg	0	0
			8	8		
56	1G	5	Total	Mg	0	0
			5	5		
56	1I	1	Total	Mg	0	0
			1	1		
56	1N	6	Total	Mg	0	0
			6	6		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1O	5	Total 5	Mg 5	0	0
56	1P	3	Total 3	Mg 3	0	0
56	1Q	5	Total 5	Mg 5	0	0
56	1R	4	Total 4	Mg 4	0	0
56	1S	3	Total 3	Mg 3	0	0
56	1T	3	Total 3	Mg 3	0	0
56	1U	7	Total 7	Mg 7	0	0
56	1V	2	Total 2	Mg 2	0	0
56	1W	7	Total 7	Mg 7	0	0
56	1X	5	Total 5	Mg 5	0	0
56	1Y	3	Total 3	Mg 3	0	0
56	1Z	4	Total 4	Mg 4	0	0
56	10	8	Total 8	Mg 8	0	0
56	11	4	Total 4	Mg 4	0	0
56	12	2	Total 2	Mg 2	0	0
56	13	1	Total 1	Mg 1	0	0
56	15	3	Total 3	Mg 3	0	0
56	16	2	Total 2	Mg 2	0	0
56	17	3	Total 3	Mg 3	0	0
56	18	4	Total 4	Mg 4	0	0
56	19	2	Total 2	Mg 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1a	235	Total 235	Mg 235	0	0
56	1b	2	Total 2	Mg 2	0	0
56	1d	1	Total 1	Mg 1	0	0
56	1e	1	Total 1	Mg 1	0	0
56	1f	2	Total 2	Mg 2	0	0
56	1l	3	Total 3	Mg 3	0	0
56	1m	1	Total 1	Mg 1	0	0
56	1n	2	Total 2	Mg 2	0	0
56	1p	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	11	Total 11	Mg 11	0	0
56	1x	15	Total 15	Mg 15	0	0
56	1y	5	Total 5	Mg 5	0	0
56	2A	876	Total 876	Mg 876	0	0
56	2B	21	Total 21	Mg 21	0	0
56	2D	7	Total 7	Mg 7	0	0
56	2E	7	Total 7	Mg 7	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	1	Total 1	Mg 1	0	0
56	2Q	4	Total 4	Mg 4	0	0
56	2R	2	Total 2	Mg 2	0	0
56	2T	3	Total 3	Mg 3	0	0
56	2U	6	Total 6	Mg 6	0	0
56	2V	1	Total 1	Mg 1	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	23	1	Total 1	Mg 1	0	0
56	25	4	Total 4	Mg 4	0	0
56	26	1	Total 1	Mg 1	0	0
56	27	1	Total 1	Mg 1	0	0
56	28	1	Total 1	Mg 1	0	0
56	2a	230	Total 230	Mg 230	0	0
56	2d	2	Total 2	Mg 2	0	0
56	2e	1	Total 1	Mg 1	0	0
56	2f	1	Total 1	Mg 1	0	0
56	2g	1	Total 1	Mg 1	0	0
56	2j	2	Total 2	Mg 2	0	0

Continued on next page...

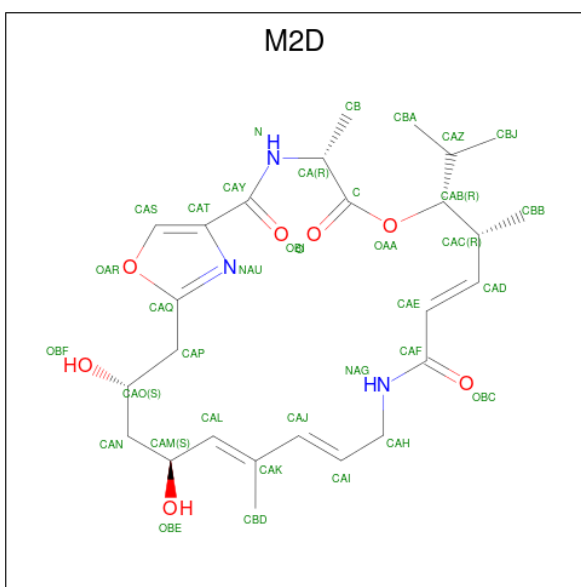
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
56	2l	2	Total Mg 2 2	0	0
56	2p	1	Total Mg 1 1	0	0
56	2q	3	Total Mg 3 3	0	0
56	2r	2	Total Mg 2 2	0	0
56	2t	1	Total Mg 1 1	0	0
56	2v	3	Total Mg 3 3	0	0
56	2w	7	Total Mg 7 7	0	0
56	2x	6	Total Mg 6 6	0	0
56	2y	6	Total Mg 6 6	0	0

- Molecule 57 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	1A	1	Total K 1 1	0	0
57	2A	1	Total K 1 1	0	0

- Molecule 58 is Madumycin II (CCD ID: M2D) (formula: C₂₆H₃₇N₃O₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
58	1A	1	Total 36	C 26	N 3	O 7	0	0
58	2A	1	Total 36	C 26	N 3	O 7	0	0

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

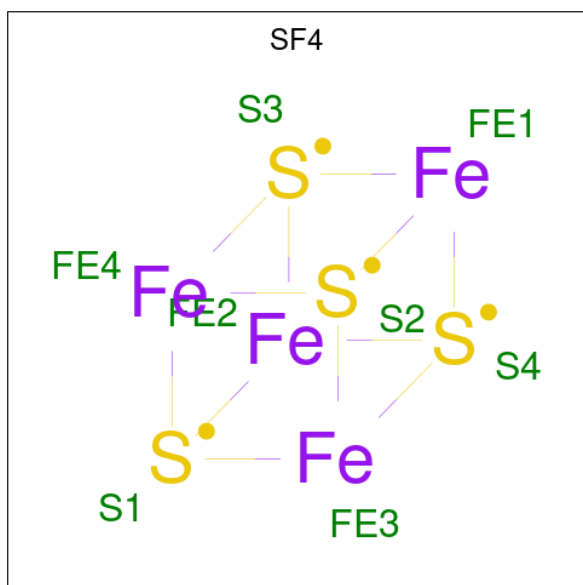
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	1Y	1	Total Zn 1 1	0	0
59	14	1	Total Zn 1 1	0	0
59	15	1	Total Zn 1 1	0	0
59	16	1	Total Zn 1 1	0	0
59	19	1	Total Zn 1 1	0	0
59	1n	1	Total Zn 1 1	0	0
59	2Y	1	Total Zn 1 1	0	0
59	24	1	Total Zn 1 1	0	0
59	25	1	Total Zn 1 1	0	0
59	26	1	Total Zn 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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: Fe_4S_4).



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	2255	Total	O	0	0
			2255	2255		
61	1B	68	Total	O	0	0
			68	68		
61	1D	30	Total	O	0	0
			30	30		
61	1E	28	Total	O	0	0
			28	28		
61	1F	21	Total	O	0	0
			21	21		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1G	5	Total 5	O 5	0	0
61	1H	1	Total 1	O 1	0	0
61	1I	2	Total 2	O 2	0	0
61	1N	8	Total 8	O 8	0	0
61	1O	11	Total 11	O 11	0	0
61	1P	25	Total 25	O 25	0	0
61	1Q	13	Total 13	O 13	0	0
61	1R	15	Total 15	O 15	0	0
61	1S	4	Total 4	O 4	0	0
61	1T	5	Total 5	O 5	0	0
61	1U	13	Total 13	O 13	0	0
61	1V	10	Total 10	O 10	0	0
61	1W	9	Total 9	O 9	0	0
61	1X	6	Total 6	O 6	0	0
61	1Y	5	Total 5	O 5	0	0
61	1Z	1	Total 1	O 1	0	0
61	10	8	Total 8	O 8	0	0
61	11	14	Total 14	O 14	0	0
61	12	4	Total 4	O 4	0	0
61	13	4	Total 4	O 4	0	0
61	14	1	Total 1	O 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	15	7	Total 7	O 7	0	0
61	16	4	Total 4	O 4	0	0
61	17	7	Total 7	O 7	0	0
61	18	13	Total 13	O 13	0	0
61	19	3	Total 3	O 3	0	0
61	1a	454	Total 454	O 454	0	0
61	1b	1	Total 1	O 1	0	0
61	1f	1	Total 1	O 1	0	0
61	1l	7	Total 7	O 7	0	0
61	1m	2	Total 2	O 2	0	0
61	1o	1	Total 1	O 1	0	0
61	1q	3	Total 3	O 3	0	0
61	1r	1	Total 1	O 1	0	0
61	1u	1	Total 1	O 1	0	0
61	1v	6	Total 6	O 6	0	0
61	1w	18	Total 18	O 18	0	0
61	1x	16	Total 16	O 16	0	0
61	1y	3	Total 3	O 3	0	0
61	2A	1418	Total 1418	O 1418	0	0
61	2B	26	Total 26	O 26	0	0
61	2D	29	Total 29	O 29	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2E	14	Total 14	O 14	0	0
61	2F	15	Total 15	O 15	0	0
61	2I	4	Total 4	O 4	0	0
61	2N	2	Total 2	O 2	0	0
61	2O	1	Total 1	O 1	0	0
61	2P	13	Total 13	O 13	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	2	Total 2	O 2	0	0
61	2V	1	Total 1	O 1	0	0
61	2W	3	Total 3	O 3	0	0
61	2X	5	Total 5	O 5	0	0
61	2Y	1	Total 1	O 1	0	0
61	2Z	2	Total 2	O 2	0	0
61	20	5	Total 5	O 5	0	0
61	21	14	Total 14	O 14	0	0
61	22	1	Total 1	O 1	0	0
61	23	2	Total 2	O 2	0	0
61	25	5	Total 5	O 5	0	0
61	26	1	Total 1	O 1	0	0

Continued on next page...

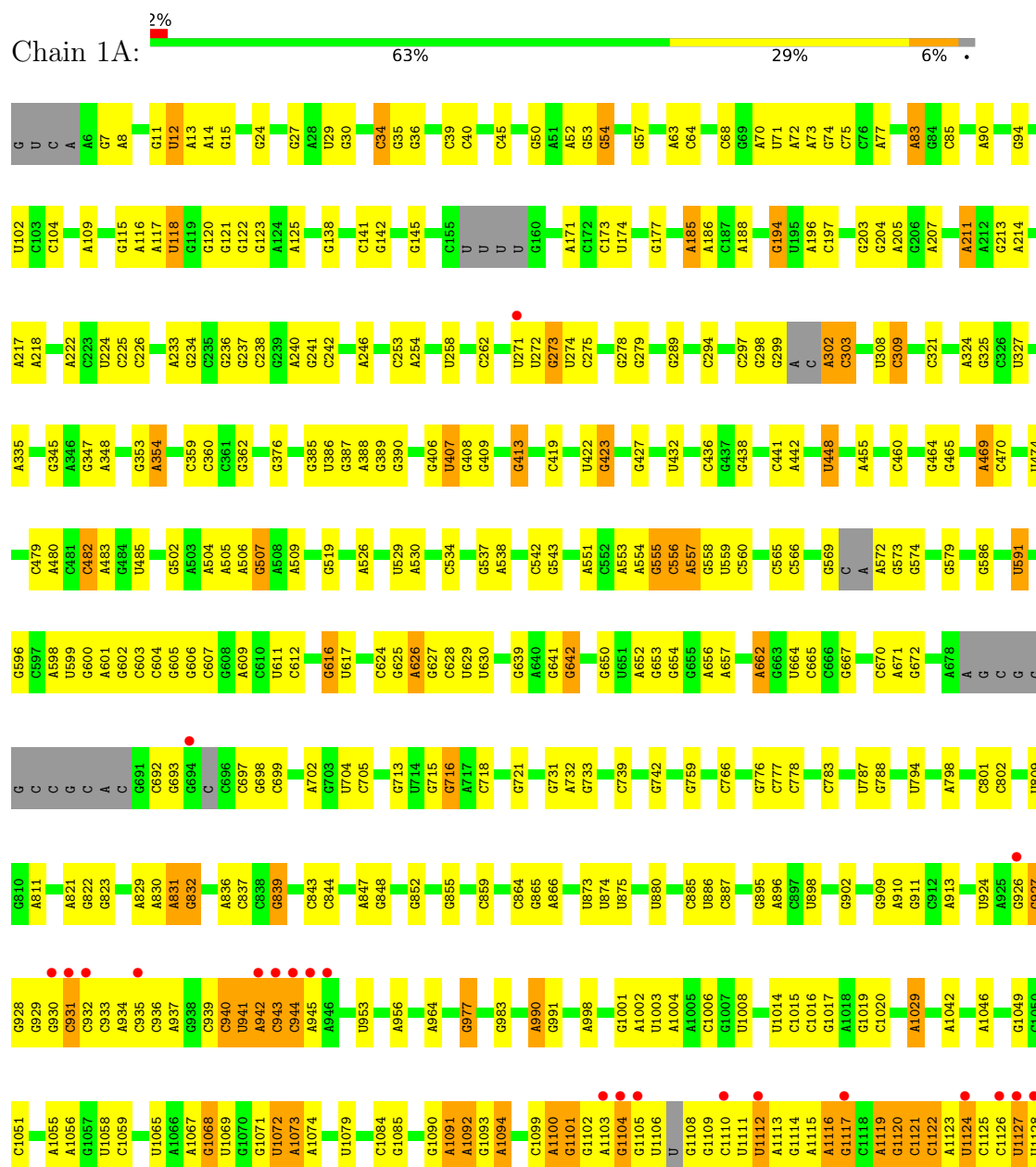
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	27	3	Total 3	O 3	0	0
61	28	5	Total 5	O 5	0	0
61	29	1	Total 1	O 1	0	0
61	2a	392	Total 392	O 392	0	0
61	2c	2	Total 2	O 2	0	0
61	2d	4	Total 4	O 4	0	0
61	2e	2	Total 2	O 2	0	0
61	2g	1	Total 1	O 1	0	0
61	2j	4	Total 4	O 4	0	0
61	2k	1	Total 1	O 1	0	0
61	2l	6	Total 6	O 6	0	0
61	2o	4	Total 4	O 4	0	0
61	2p	2	Total 2	O 2	0	0
61	2q	1	Total 1	O 1	0	0
61	2r	1	Total 1	O 1	0	0
61	2t	3	Total 3	O 3	0	0
61	2u	1	Total 1	O 1	0	0
61	2v	4	Total 4	O 4	0	0
61	2w	1	Total 1	O 1	0	0
61	2x	6	Total 6	O 6	0	0
61	2y	19	Total 19	O 19	0	0

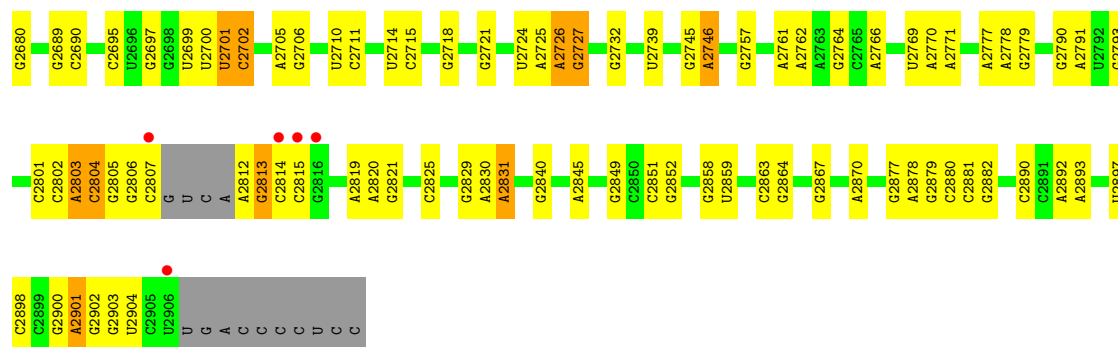
3 Residue-property plots [i](#)

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

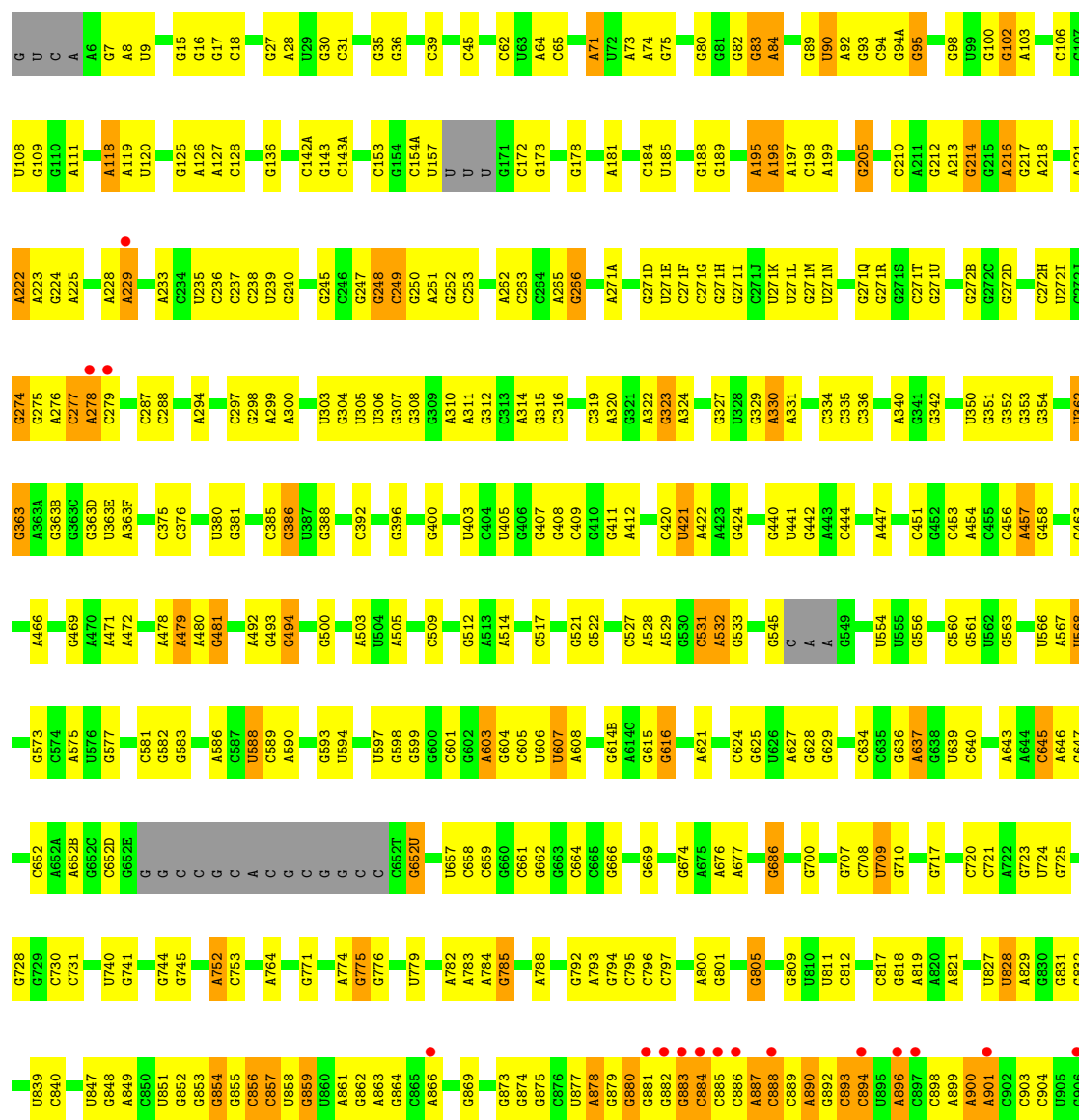
• Molecule 1: 23S Ribosomal RNA



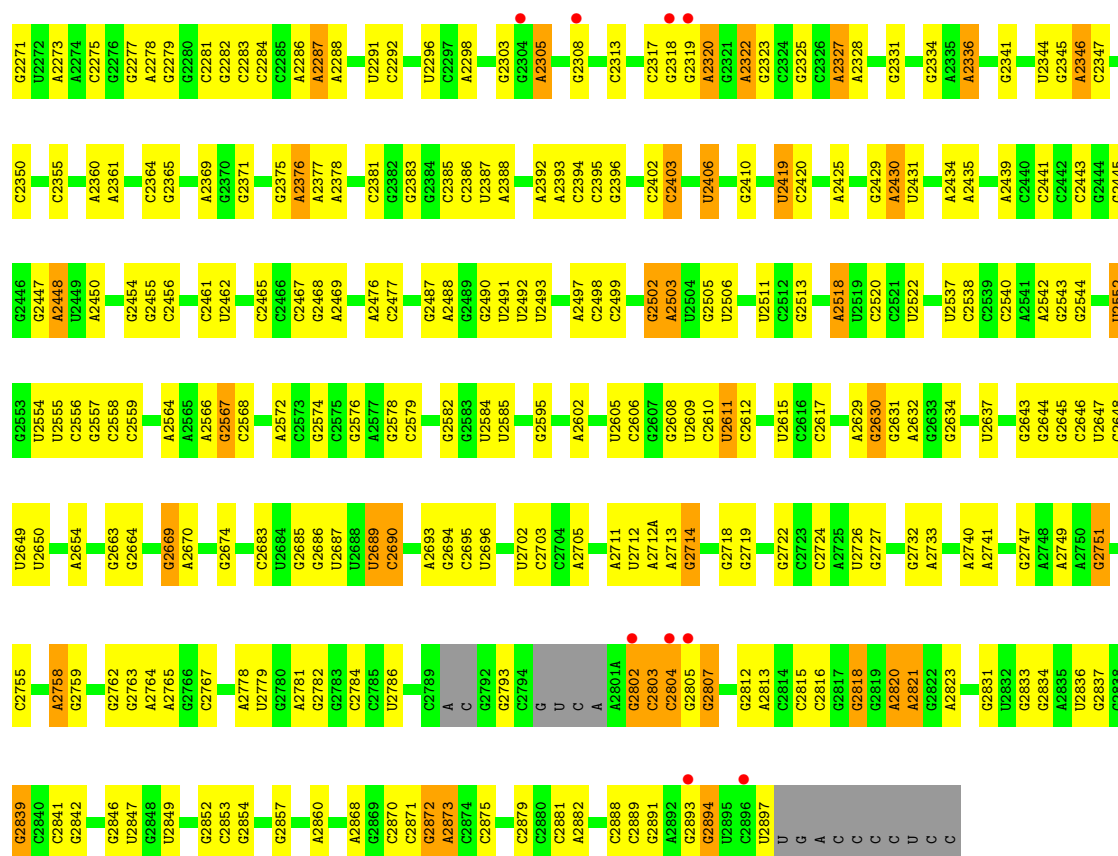
U2549	A2430	C2328	A2229	C2158	G2077	A1974	G1842	A1715	C1604	U1442	A1333	C1223	A1131
C2550	U2431	C2329	G2235	C2159	G2078	A1975	G1847	A1716	A1605	U1451	U1334	C1224	A1132
G2556	A2434	G2330	G2236	C2160	A2079	G1976	G1848	C1717	G1606	U1452	U1338	C1225	G1133
G2561	U2435	G2331	A2237	C2162	A2081	G1977	A1860	G1721	A1613	C1453	C1339	G1228	G1135
U2564	C2436	A2332	G2240	G2163	A2082	A1982	G1870	G1730	A1616	G1462	G1342	G1230	U1136
U2566	A2437	G2337	U2245	C2165	G2083	C1983	G1874	C1731	G1619	G1463	C1343	G1231	G1139
U2567	G2440	G2338	G2246	U2166	A2084	C1984	C1874	G1732	G1625	U1465	U1346	G1232	U1140
A2576	A2441	A2339	G2250	C2168	G2091	U1985	A1878	G1733	U1626	A1466	A1347	U1233	A1141
A2577	G2442	G2341	G2251	G2170	G2094	U1989	U1740	G1734	A1627	G1467	A1348	G1236	A1142
A2578	A2446	G2342	G2255	G2171	G2095	G1990	U1743	U1740	G1628	G1472	G1349	C1241	U1143
G2579	A2451	G2346	U2256	G2172	G2096	A1991	G1743	G1743	C1631	A1473	G1356	C1246	U1147
C2580	C2452	A2347	U2257	G2173	U2097	A1992	A1747	C1747	A1632	C1474	U1362	C1246	C1148
G2585	C2453	A2348	G2262	G2174	U2101	A1993	G1750	C1750	A1633	G1475	A1363	C1255	A1149
G2588	G2457	C2355	G2263	G2176	G2105	A2008	G1750	G1750	C1634	C1476	U1256	G1257	C1150
A2589	G2458	C2356	C2272	G2177	C2106	U2013	A1897	A1767	C1635	A1491	C1366	G1257	U1151
G2590	U2459	G2359	C2273	G2179	G2112	G2014	A1898	U1768	C1636	G1497	G1370	C1263	G1152
G2595	A2460	G2362	U2274	A2180	U2113	U2015	A1899	U1768	C1637	G1502	G1371	C1263	G1153
G2600	G2470	G2363	A2280	G2181	G2114	C2018	C1901	G1776	G1638	C1502	G1371	C1264	C1155
A2601	G2470	A2364	A2281	G2182	G2115	G2019	C1902	G1776	G1639	C1502	G1371	A1265	A1156
A2602	C2473	G2365	A2282	G2183	G2122	A2023	C1903	G1781	C1644	C1514	G1384	G1273	A1157
C2613	U2474	G2366	G2283	G2184	U2124	G2024	C1904	C1785	A1649	G1529	G1385	G1276	G1158
C2614	A2481	C2367	U2284	C2185	U2124	A2025	A1912	A1786	A1649	G1530	U1387	C1276	G1159
G2615	G2482	G2368	A2285	C2186	G2128	A2036	A1912	G1787	A1654	C1536	C1391	G1277	G1160
G2616	G2482	U2369	A2286	G2187	G2129	A2037	G1913	A1804	A1654	A1536	U1398	G1282	C1162
U2617	G2488	G2370	G2291	U2188	G2130	U2038	U1933	A1793	A1681	C1539	U1398	G1282	C1165
G2620	A2489	C2371	G2292	G2190	U2131	G2039	A1934	G1794	A1682	A1540	U1403	G1285	G1171
U2621	A2490	A2372	G2293	U2194	U2132	A2040	A1935	G1795	A1683	A1541	G1404	U1286	A1174
G2622	G2496	G2376	C2295	A2195	G2133	A2041	A1936	G1795	C1682	A1542	A1405	G1291	A1175
U2623	G2496	G2377	C2296	C2196	G2134	U2042	U1937	A1814	A1683	U1543	A1406	G1294	U1176
C2624	C2510	G2385	C2297	C2197	U2135	A2043	A1938	A1817	C1683	A1553	C1409	U1295	C1180
U2627	G2514	G2386	A2298	A2198	A2136	C2044	A1940	A1811	A1684	C1554	G1410	G1296	G1181
C2628	A2515	G2387	A2299	C2199	G2137	U2045	A1941	C1812	A1688	C1555	A1411	G1296	G1181
G2629	G2516	G2396	G2301	C2199	U2138	G2046	U1937	C1813	A1688	A1556	G1417	A1299	G1195
C2640	U2517	C2397	G2302	G2203	U2139	A2047	A1938	A1814	G1690	A1557	U1418	G1302	C1199
A2641	U2518	C2397	C2303	C2204	U2140	G2051	U1939	A1817	C1691	U1566	A1419	G1302	C1199
G2642	G2521	U2402	C2304	C2205	G2142	A2052	A1940	A1817	C1691	U1567	G1419	G1310	G1200
G2643	G2521	G2408	C2305	G2206	G2143	G2053	A1941	C1821	G1694	G1579	C1422	A1310	A1201
A2644	G2530	G2411	C2306	G2209	U2144	A2055	C1942	A1822	C1695	G1579	C1422	G1312	G1210
C2647	G2537	G2412	A2310	U2210	G2145	G2060	G1951	U1825	A1699	G1579	C1422	U1313	U1211
G2658	G2541	C2416	G2311	U2211	G2147	C2061	G1952	C1826	G1700	G1579	C1422	A1314	C1212
U2659	A2542	G2417	G2316	G2214	A2148	C2062	G1952	U1827	A1701	G1579	C1422	A1314	C1212
G2666	G2543	U2418	G2317	U2215	G2149	U2063	A1959	U1828	A1702	G1584	A1430	G1317	G1214
G2666	G2544	G2419	C2318	A2220	C2150	A2064	A1960	U1829	C1703	G1584	G1431	G1317	G1214
A2669	U2420	G2421	G2319	U2225	U2152	C2065	U1961	G1831	C1704	G1585	C1432	U1319	G1214
G2679	G2422	G2422	G2320	C2226	G2154	G2071	C1964	G1832	C1710	U1587	U1436	A1320	G1217
			A2321	G2227	G2155	G2074	A1834	A1833	A1711	G1588	A1439	A1321	G1218
			U2324	G2228	A2157	G2074	U1968	A1834	G1712	A1589	U1440	A1322	A1219
				G2228			C1969	A1841	G1714	G1599	A1441	G1327	U1220
													A1222



• Molecule 1: 23S Ribosomal RNA

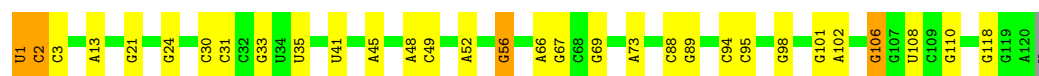






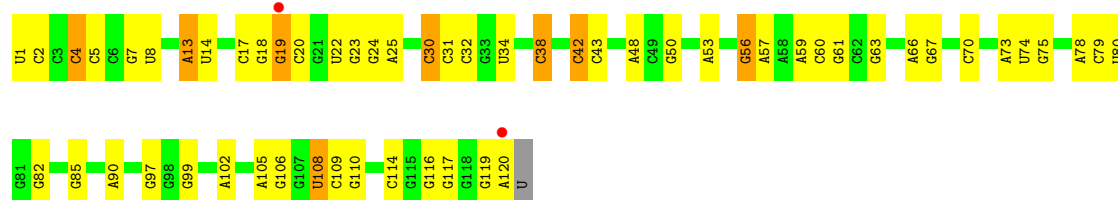
• Molecule 2: 5S ribosomal RNA

Chain 1B: 74% 22%



• Molecule 2: 5S ribosomal RNA

Chain 2B: 52% 40% 7%



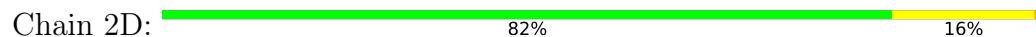
• Molecule 3: 50S ribosomal protein L2

Chain 1D: 81% 17%

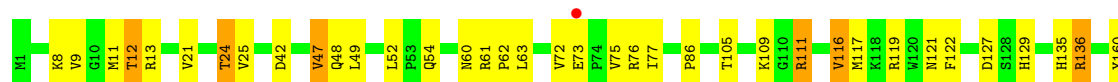
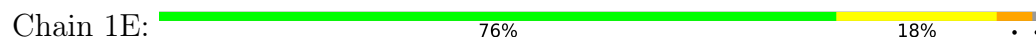




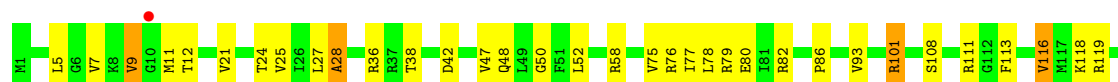
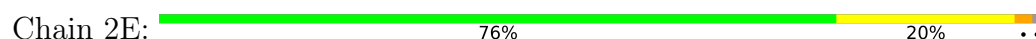
- Molecule 3: 50S ribosomal protein L2



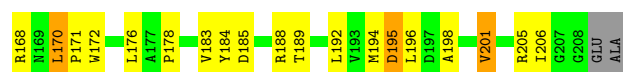
- Molecule 4: 50S ribosomal protein L3



- Molecule 4: 50S ribosomal protein L3

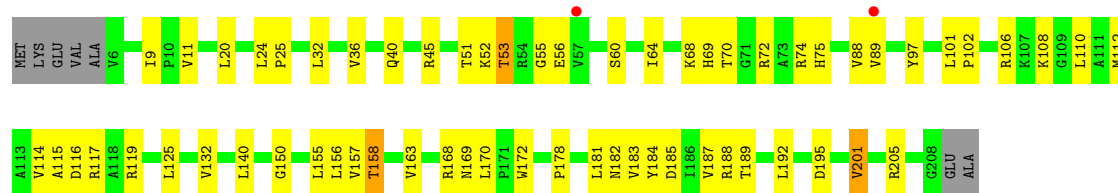


- Molecule 5: 50S ribosomal protein L4

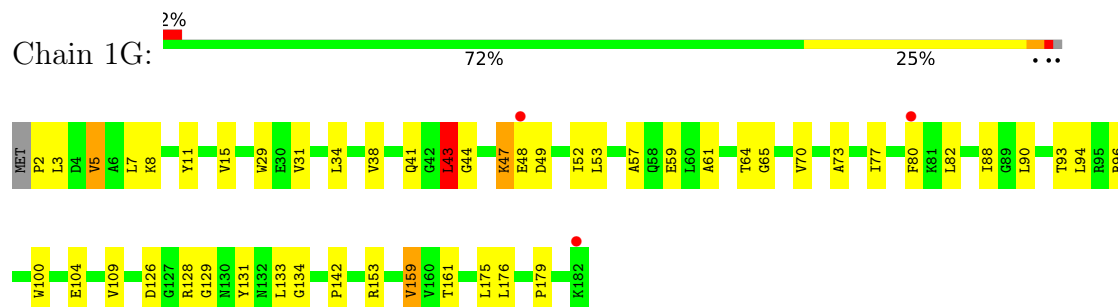


- Molecule 5: 50S ribosomal protein L4

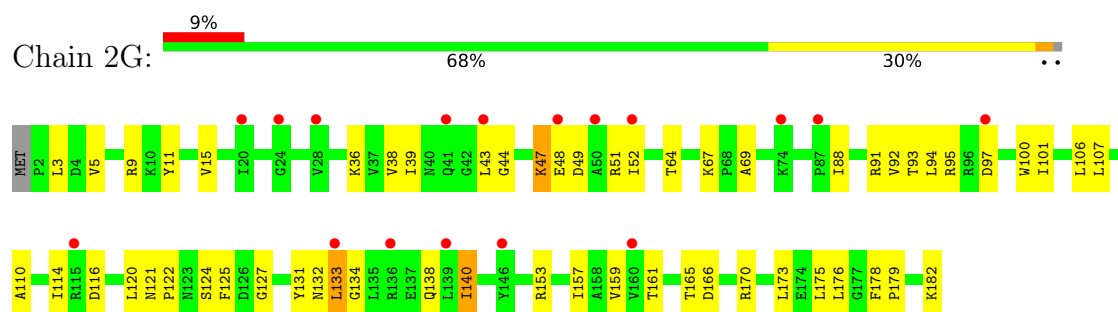




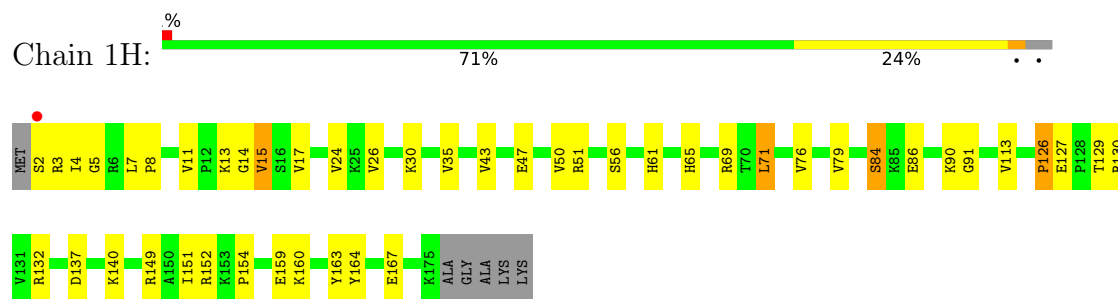
• Molecule 6: 50S ribosomal protein L5



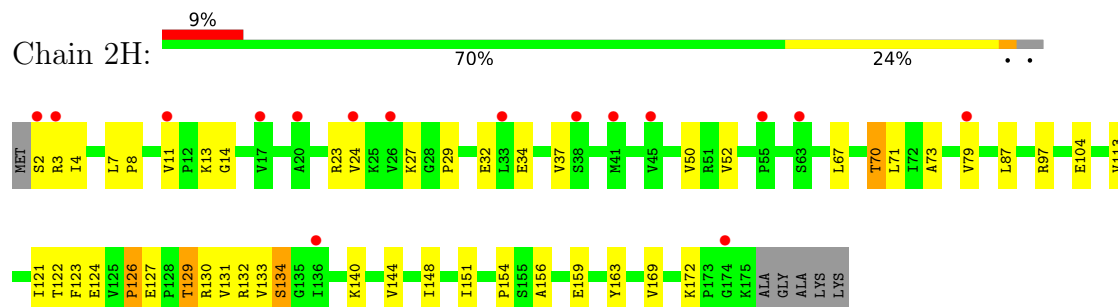
• Molecule 6: 50S ribosomal protein L5



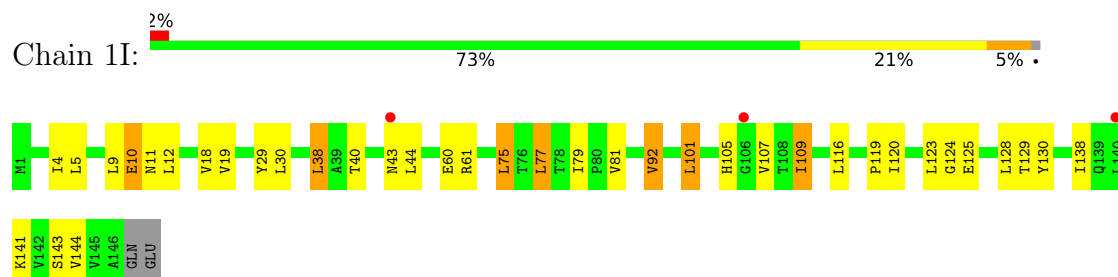
• Molecule 7: 50S ribosomal protein L6



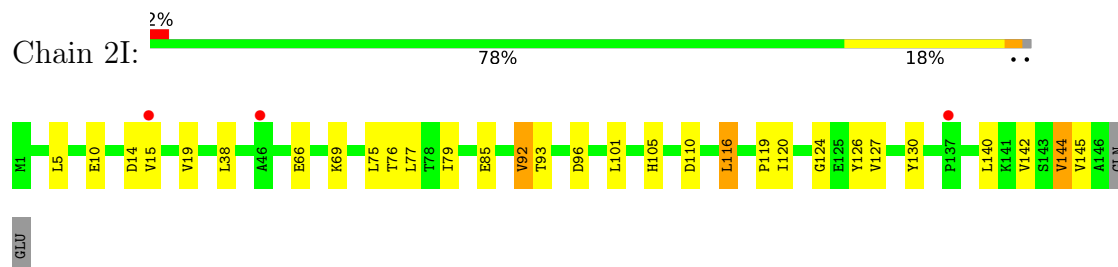
• Molecule 7: 50S ribosomal protein L6



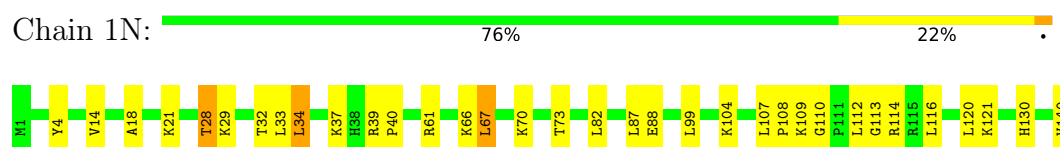
- Molecule 8: 50S ribosomal protein L9



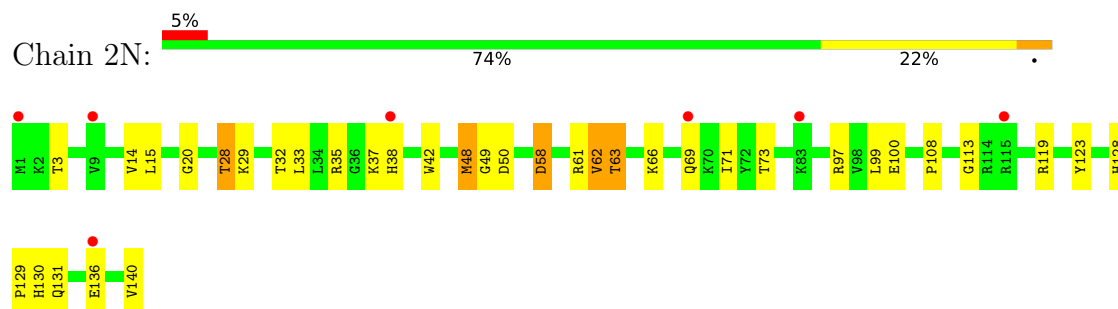
- Molecule 8: 50S ribosomal protein L9



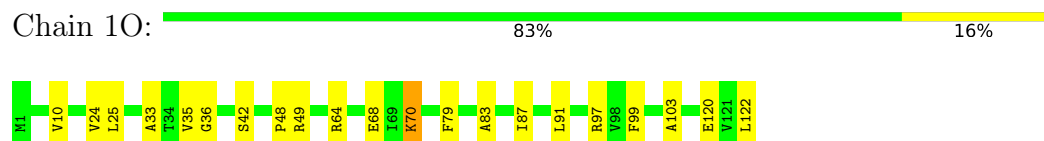
- Molecule 9: 50S ribosomal protein L13



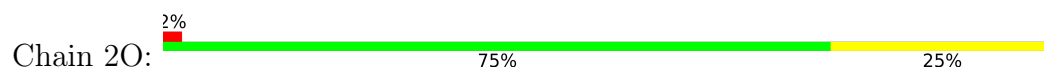
- Molecule 9: 50S ribosomal protein L13

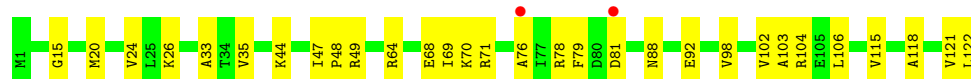


- Molecule 10: 50S ribosomal protein L14

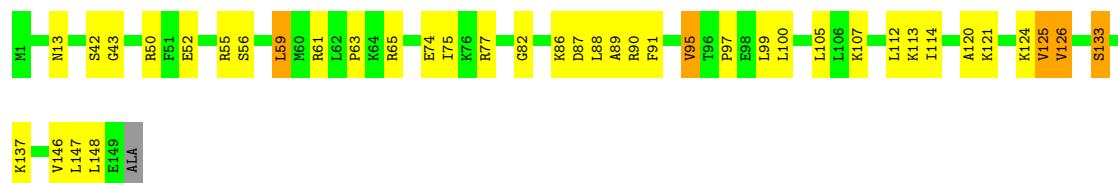


- Molecule 10: 50S ribosomal protein L14

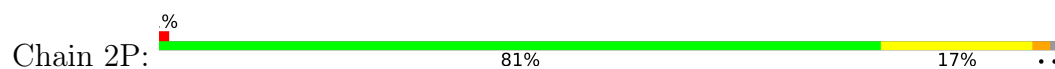




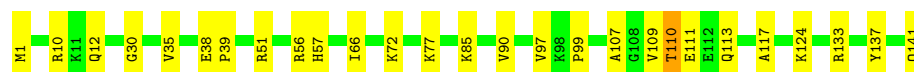
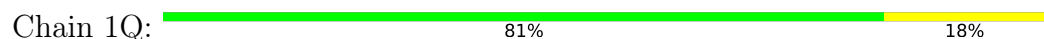
- Molecule 11: 50S ribosomal protein L15



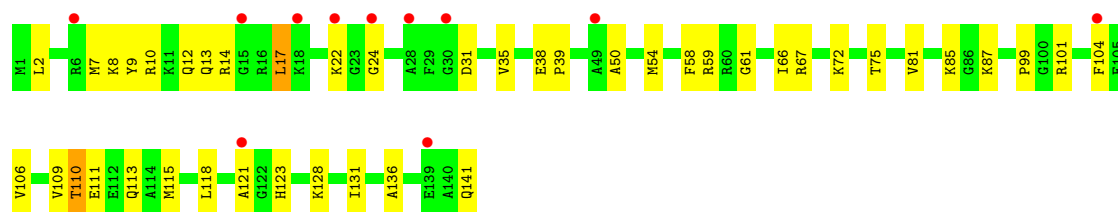
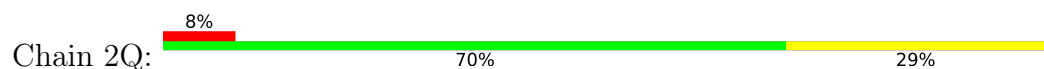
- Molecule 11: 50S ribosomal protein L15



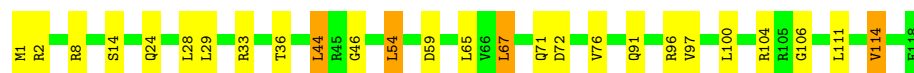
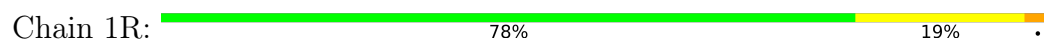
- Molecule 12: 50S ribosomal protein L16



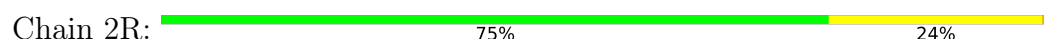
- Molecule 12: 50S ribosomal protein L16



- Molecule 13: 50S ribosomal protein L17



- Molecule 13: 50S ribosomal protein L17





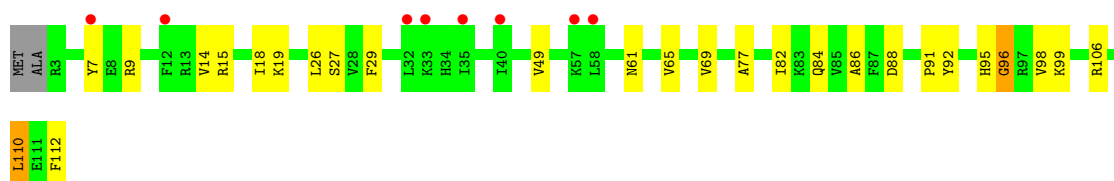
- Molecule 14: 50S ribosomal protein L18

Chain 1S: 79% 16% . .



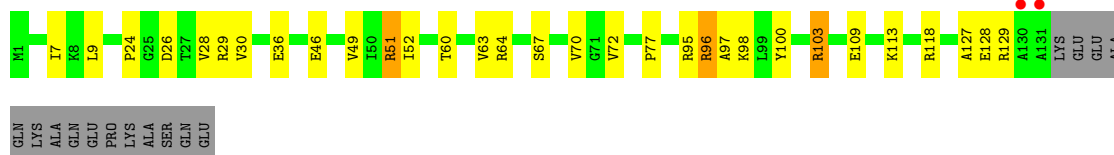
- Molecule 14: 50S ribosomal protein L18

Chain 2S: 74% 22% . .



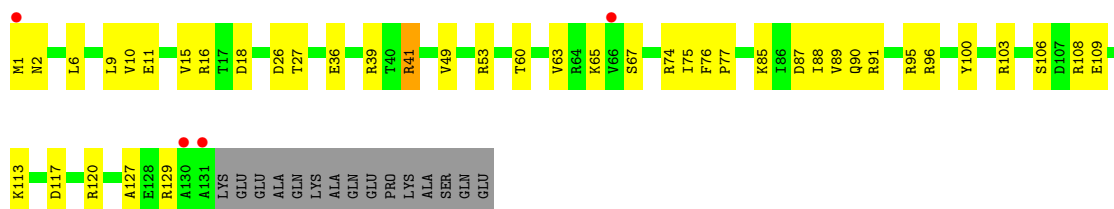
- Molecule 15: 50S ribosomal protein L19

Chain 1T: 68% 19% . 10%



- Molecule 15: 50S ribosomal protein L19

Chain 2T: 61% 28% . 10%

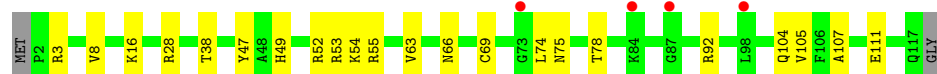
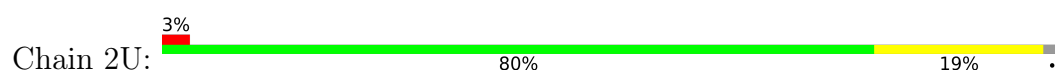


- Molecule 16: 50S ribosomal protein L20

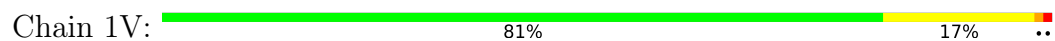
Chain 1U: 85% 14% .



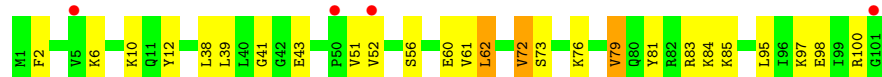
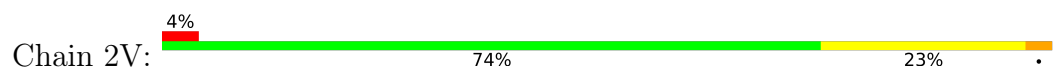
- Molecule 16: 50S ribosomal protein L20



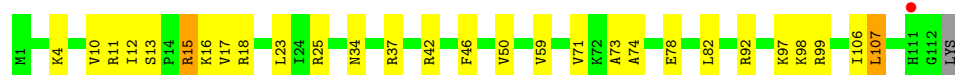
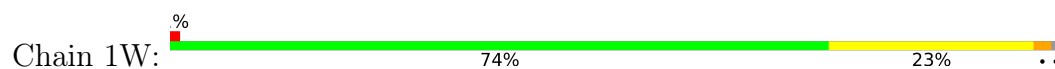
- Molecule 17: 50S ribosomal protein L21



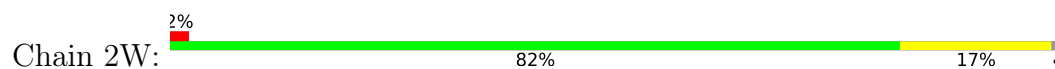
- Molecule 17: 50S ribosomal protein L21



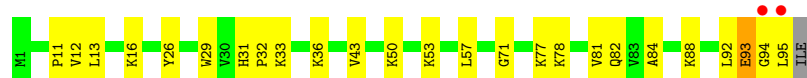
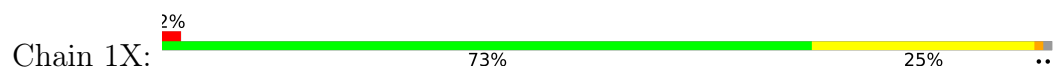
- Molecule 18: 50S ribosomal protein L22



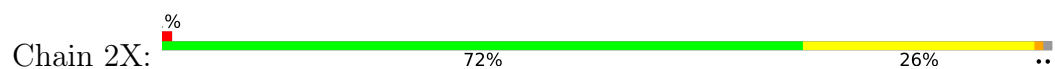
- Molecule 18: 50S ribosomal protein L22



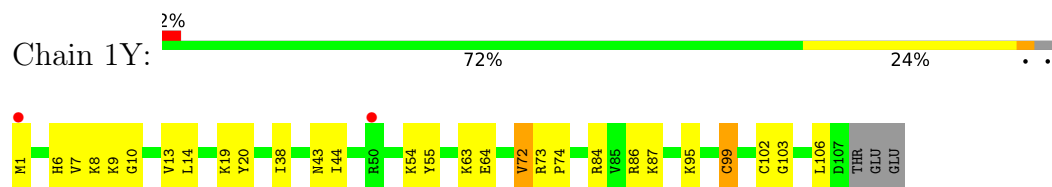
- Molecule 19: 50S ribosomal protein L23



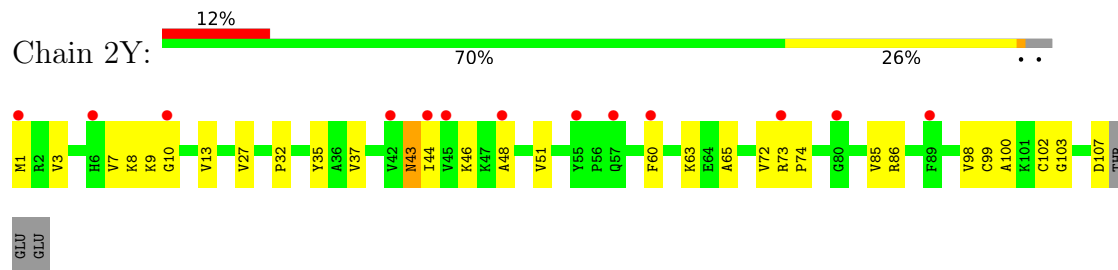
- Molecule 19: 50S ribosomal protein L23



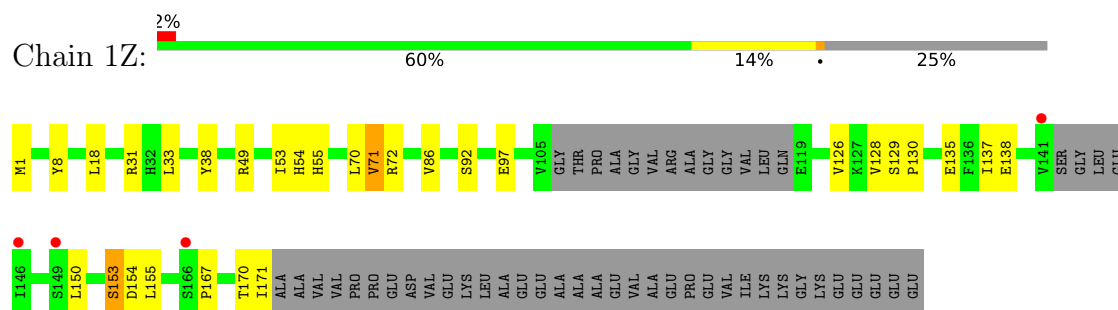
- Molecule 20: 50S ribosomal protein L24



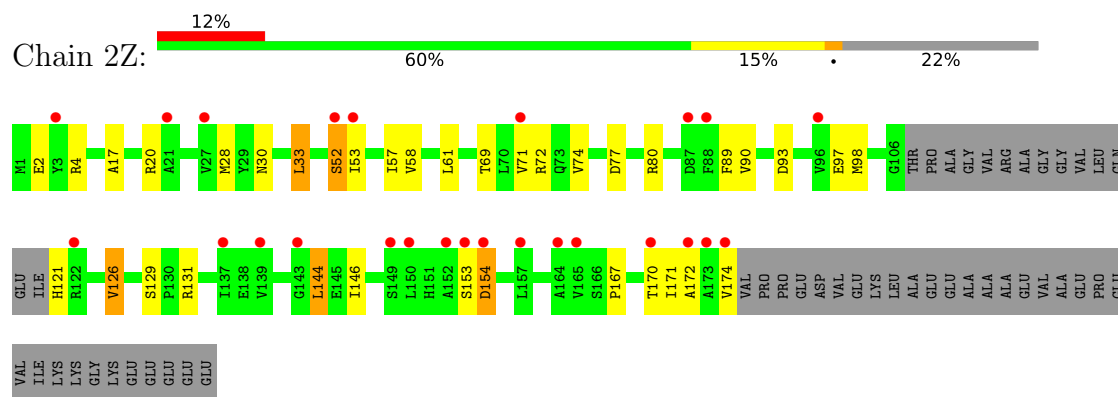
- Molecule 20: 50S ribosomal protein L24



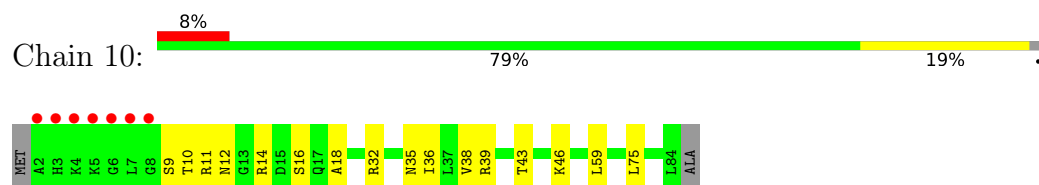
- Molecule 21: 50S ribosomal protein L25



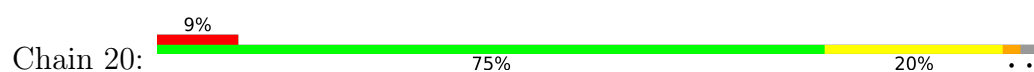
- Molecule 21: 50S ribosomal protein L25



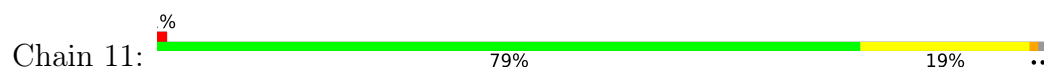
- Molecule 22: 50S ribosomal protein L27



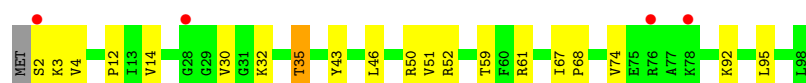
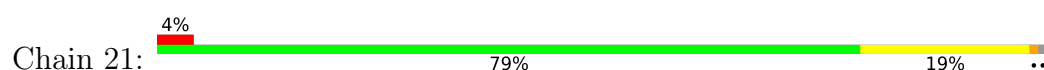
- Molecule 22: 50S ribosomal protein L27



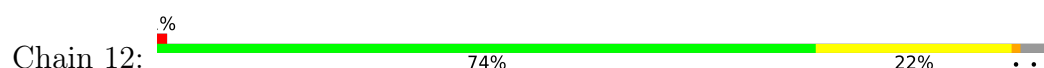
- Molecule 23: 50S ribosomal protein L28



- Molecule 23: 50S ribosomal protein L28



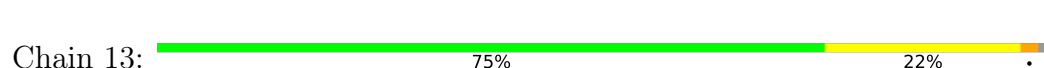
- Molecule 24: 50S ribosomal protein L29



- Molecule 24: 50S ribosomal protein L29



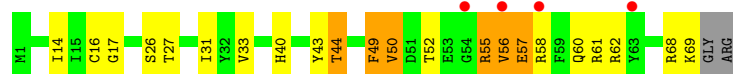
- Molecule 25: 50S ribosomal protein L30



- Molecule 25: 50S ribosomal protein L30



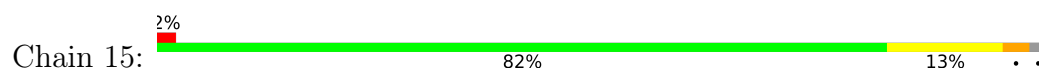
- Molecule 26: 50S ribosomal protein L31



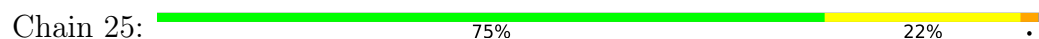
- Molecule 26: 50S ribosomal protein L31



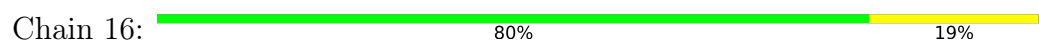
- Molecule 27: 50S ribosomal protein L32



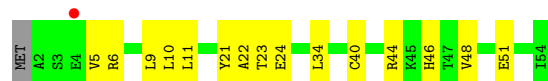
- Molecule 27: 50S ribosomal protein L32



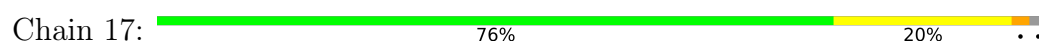
- Molecule 28: 50S ribosomal protein L33



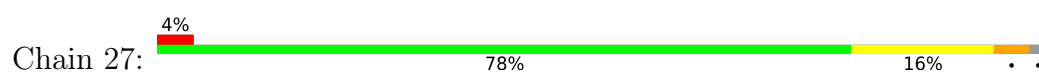
- Molecule 28: 50S ribosomal protein L33



- Molecule 29: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L34



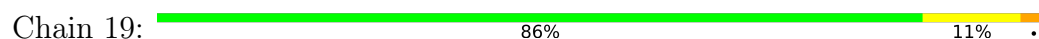
- Molecule 30: 50S ribosomal protein L35



- Molecule 30: 50S ribosomal protein L35



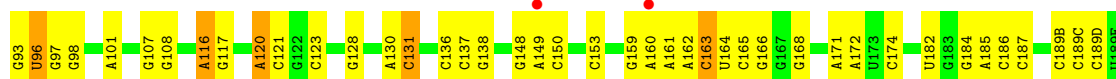
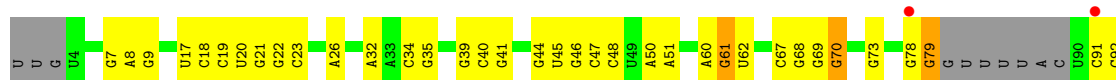
- Molecule 31: 50S ribosomal protein L36

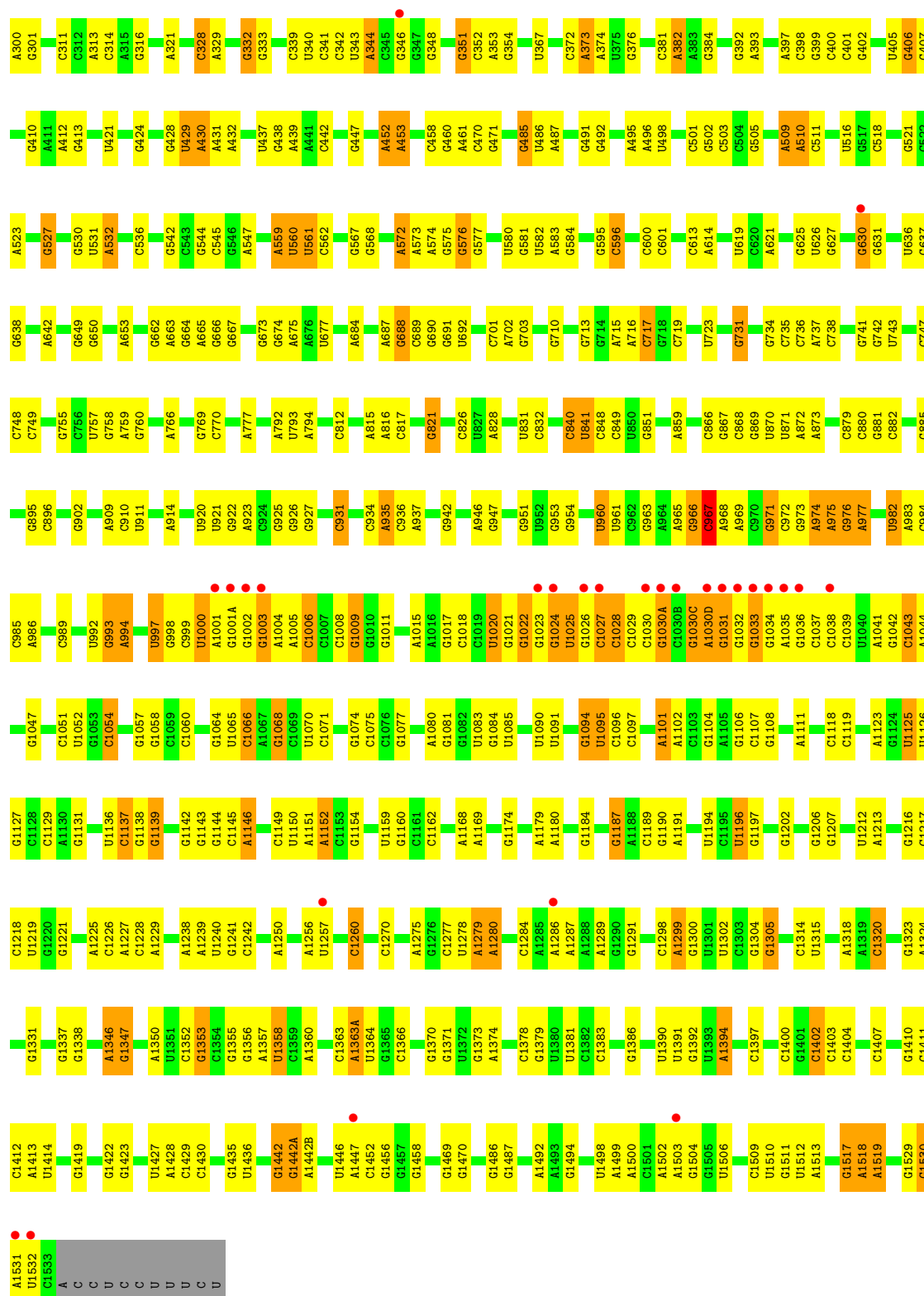


- Molecule 31: 50S ribosomal protein L36



- Molecule 32: 16S ribosomal RNA

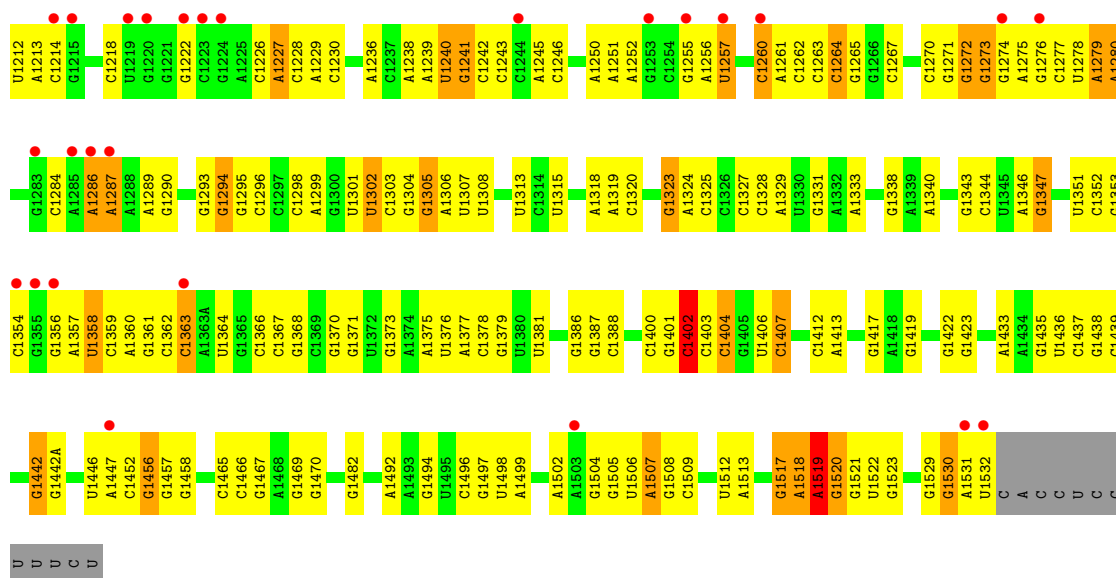




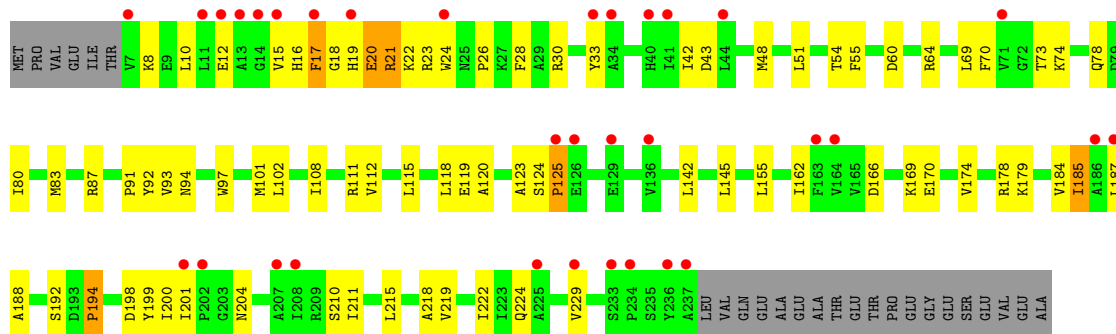
• Molecule 32: 16S ribosomal RNA



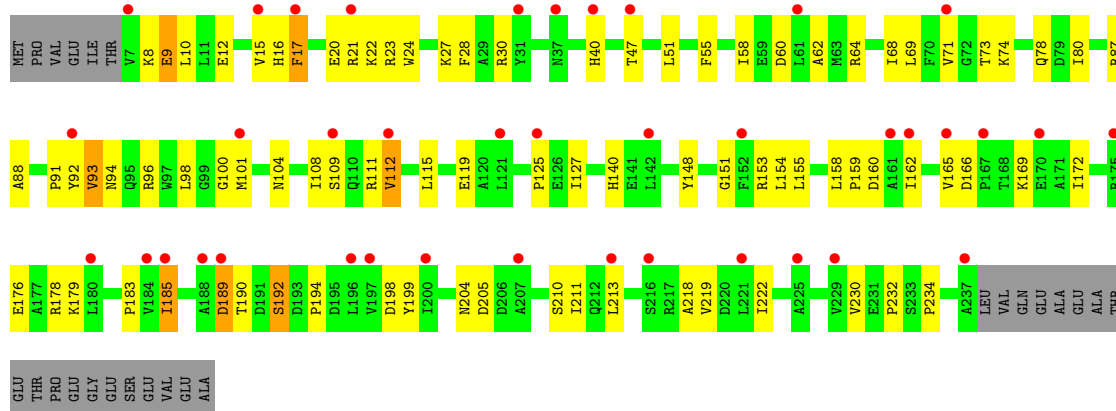
A1146	G1084	G1021	A958	U863	G755	C656	G558	G475	A373	A274	U164	G78	U
C1147	U1086	G1022	A959	A864	C756	G660	A859	C476	A374	G275	U164	G79	U
U1148	U1086	G1023	U960	A865	U757	G660	U860	A477	G376	G276	A172	G80	G
C1149	U1086	G1024	U961	C966	G758	G661	U861	C479	G377	G281	C174	U	U4
U1150	U1089	U1025	C962	C967	A759	G662	C562	U480	C381	G289	C175	U	U5
A1151	U1089	G1026	C968	C968	G760	A663	A563	C484	G384	G289	U162	U84	G6
A1152	A1092	C1027	A965	G664	G765	A665	C564	G485	G384	G289	U162	U84	G7
G1153	A1093	G1028	G966	C967	G765	A665	U866	G485	G384	G289	U162	U84	A8
G1154	G1094	C1029	C967	A873	G765	A665	U866	G485	G384	G289	U162	U84	A9
A1157	U1096	C1030	A968	C974	A768	G671	G567	C488	C390	G297	C187	U90	A10
C1158	U1096	G1030A	A969	C975	A768	G672	G568	C489	C391	C299	C188	C91	G11
U1159	C1097	G1030B	C970	G876	U772	G673	U871	C490	G396	A300	U189E	C92	U12
U1159	C1098	G1030C	G971	G876	U772	G674	A572	C491	G397	G309	U189F	C93	U13
G1160	A1030D	G1031	C972	G881	G773	A675	A573	C492	C398	G311	U189K	U96	U14
C1161	G1032	G1032	G973	G885	A777	A684	A574	A496	C401	G311	U189K	G97	G15
C1162	A1101	G1033	A974	C985	G778	A684	A574	U498	C402	G318	G189L	A101	U17
C1163	G1103	G1034	A975	G890	C779	G688	G575	C501	G403	A321	A196	G102	C18
G1166	G1104	A1035	A977	G890	A780	C689	G577	C502	U494	G326	A196	G102	C19
A1168	A1106	G1036	A978	A901	A782	A695	C578	C503	U405	G326	A196	G102	U20
A1169	G1107	C1037	U882	G902	A782	A695	C578	C504	U406	G326	A196	G102	G21
C1172	U1108	C1038	A983	G906	U793	C701	U582	C505	G407	G326	A196	G102	G22
G1173	C1039	G1039	A984	A907	A794	A702	G584	C505	G407	G326	A196	G102	G23
G1174	A1110	U1040	C985	A908	A794	A702	G584	C505	G407	G326	A196	G102	A26
G1175	A1111	G1042	A986	A909	C811	G703	G588	A509	A411	G326	A196	G102	A32
A1176	C1112	C1043	G987	A909	C812	G703	C589	A510	A412	G326	A196	G102	A33
G1177	C1113	A1044	G988	A914	C812	G703	C590	C511	A413	G326	A196	G102	A34
A1179	C1114	C1045	C989	A914	C812	G703	C591	C512	C417	G326	A196	G102	G35
G1180	C1115	A1046	U992	A918	A815	A712	G595	U516	U421	G326	A196	G102	G39
A1181	G1116	G1047	G993	A919	C917	G713	C596	U517	U422	G326	A196	G102	C40
G1182	C1117	U1049	A994	U920	G918	G714	C597	C518	G423	G326	A196	G102	G41
A1183	C1119	G1050	C995	U921	G922	A716	U598	C521	G424	G326	A196	G102	G42
G1184	G1120	U1051	A996	G922	G821	A716	C599	C522	G425	G326	A196	G102	U45
G1186	U1121	A1055	U997	G926	C826	C719	C600	C523	G426	G326	A196	G102	U46
A1187	U1122	U1056	G998	G927	U827	C720	C601	A524	U429	G326	A196	G102	C47
A1188	A1123	G1057	C999	G927	A828	G721	A607	C525	A430	G326	A196	G102	C48
C1189	G1124	U1058	U1000	C930	G829	A722	C526	C527	C436	G326	A196	G102	U49
G1190	U1125	C1059	A1001	C931	G830	U723	C527	C527	C437	G326	A196	G102	A50
A1191	U1126	G1060	G1001A	C932	U831	G724	C515	C530	U437	G326	A196	G102	A51
C1192	G1127	G1061	G1002	G933	C832	G724	C515	C530	U437	G326	A196	G102	C54
G1193	C1128	U1062	G1003	C934	U833	A728	A621	C530	U437	G326	A196	G102	A55
U1194	C1129	C1063	A1004	A935	C934	A729	A621	C530	U437	G326	A196	G102	U56
C1195	A1130	G1064	A1005	C936	U835	G730	G628	C530	U437	G326	A196	G102	G57
U1196	G1132	U1065	C1006	A937	U835	G731	G628	C530	U437	G326	A196	G102	C58
G1197	C1133	C1066	C1007	G939	G838	C736	G630	C530	U437	G326	A196	G102	A59
C1200	G1134	G1068	G1008	G939	C839	C736	G630	C530	U437	G326	A196	G102	G64
A1201	U1135	C1069	C1009	A946	U841	A737	G630	C530	U437	G326	A196	G102	U65
G1202	U1136	U1073	G1010	G947	C948	G741	C643	C530	U437	G326	A196	G102	G66
C1203	C1137	G1074	U1012	U950	G853	G742	G644	C530	U437	G326	A196	G102	C67
A1204	G1138	G1074	A1013	G951	G853	U743	C645	C530	U437	G326	A196	G102	G68
G1207	G1139	U1077	A1014	G951	G853	C744	U646	C530	U437	G326	A196	G102	G69
C1208	C1141	U1078	A1015	U952	C857	C745	A648	C530	U437	G326	A196	G102	G73
C1209	C1142	G1079	A1016	G953	A858	C745	A648	C530	U437	G326	A196	G102	C76
G1210	G1143	A1080	G1017	G954	A859	C745	A648	C530	U437	G326	A196	G102	G77
U1211	C1144	G1081	C1018	U955	A860	C749	A653	C530	U437	G326	A196	G102	
	G1145		U1020	U957	C862	G750	A653	C530	U437	G326	A196	G102	



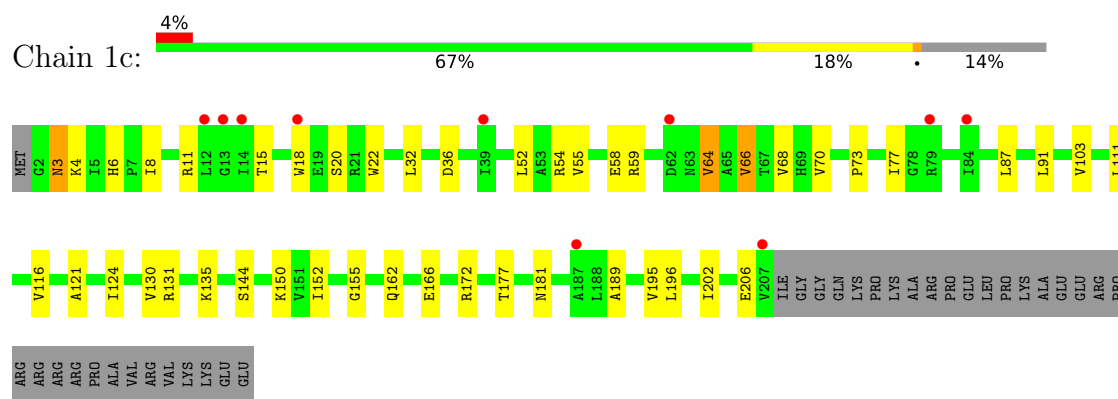
• Molecule 33: 30S ribosomal protein S2



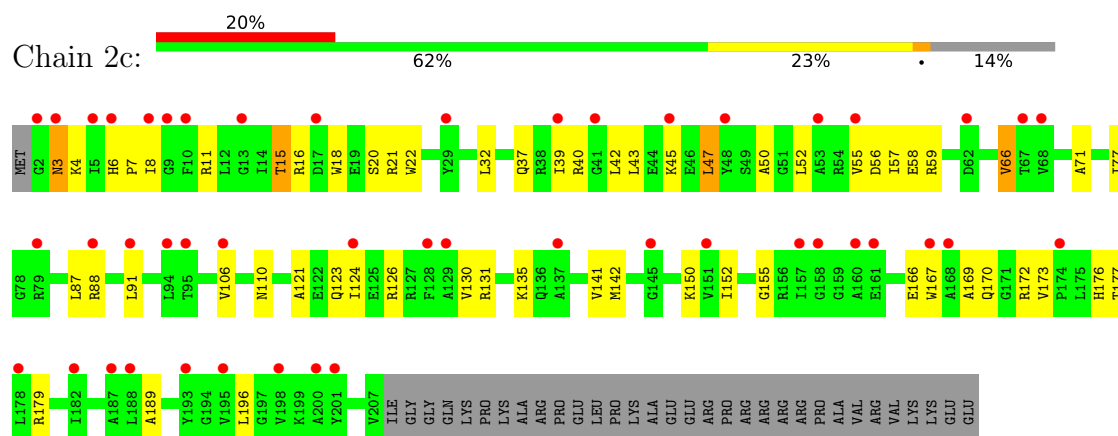
• Molecule 33: 30S ribosomal protein S2



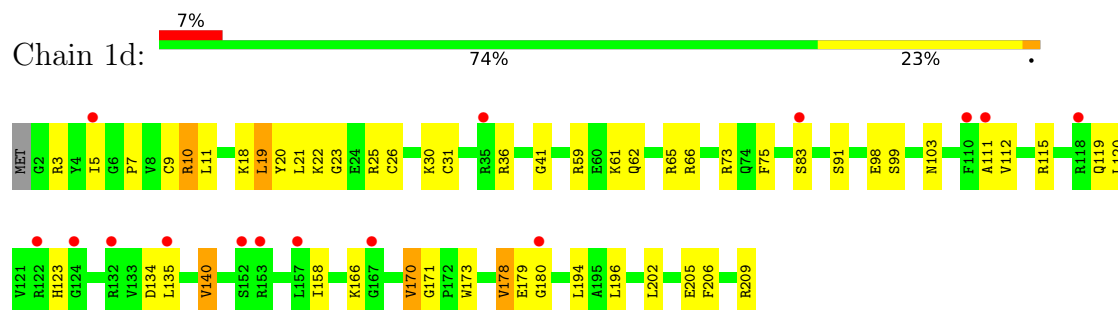
• Molecule 34: 30S ribosomal protein S3



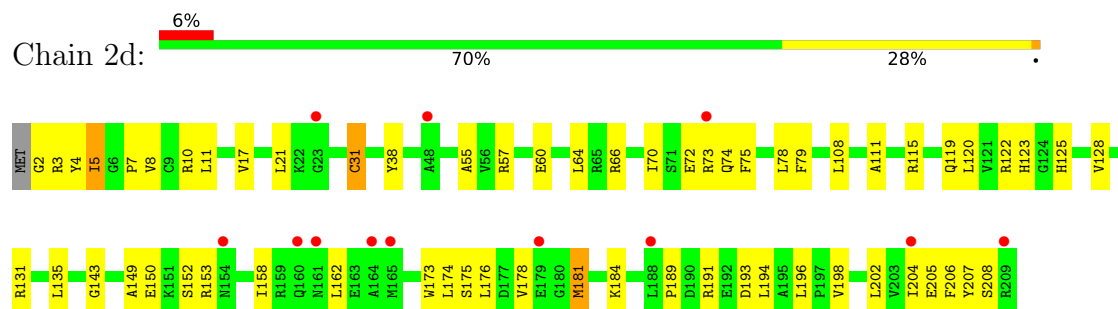
• Molecule 34: 30S ribosomal protein S3



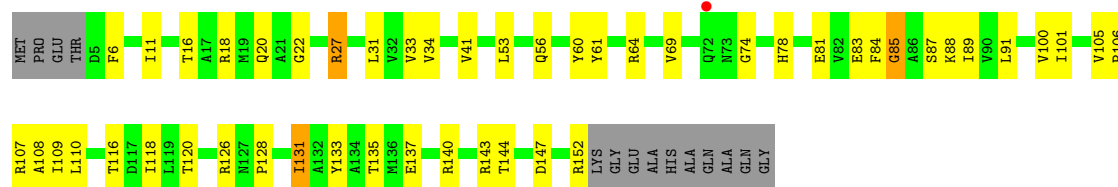
• Molecule 35: 30S ribosomal protein S4



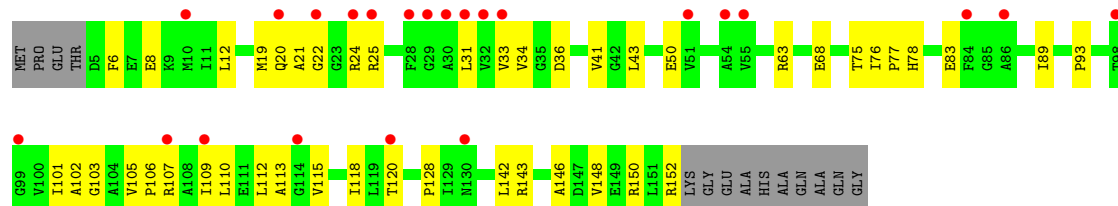
• Molecule 35: 30S ribosomal protein S4



• Molecule 36: 30S ribosomal protein S5



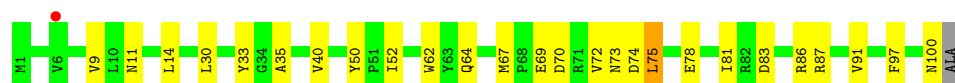
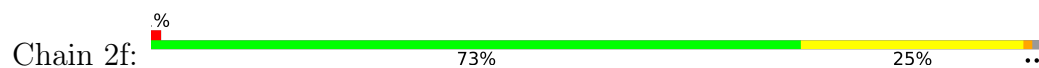
- Molecule 36: 30S ribosomal protein S5



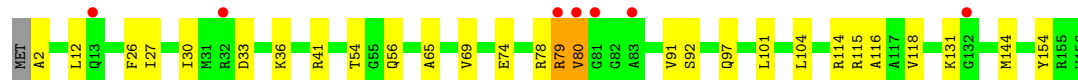
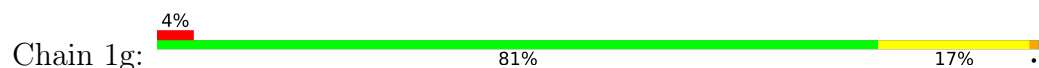
- Molecule 37: 30S ribosomal protein S6



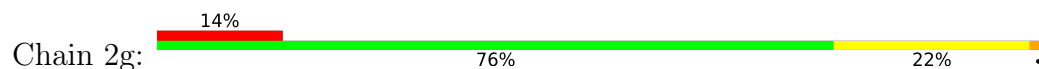
- Molecule 37: 30S ribosomal protein S6



- Molecule 38: 30S ribosomal protein S7

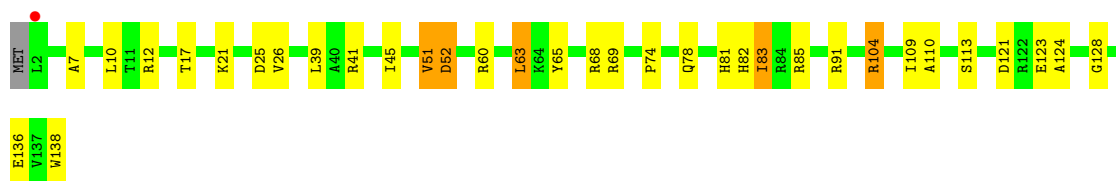
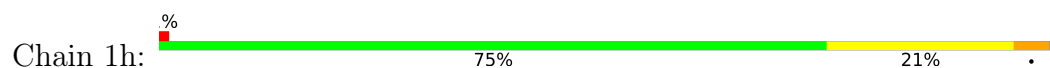


- Molecule 38: 30S ribosomal protein S7

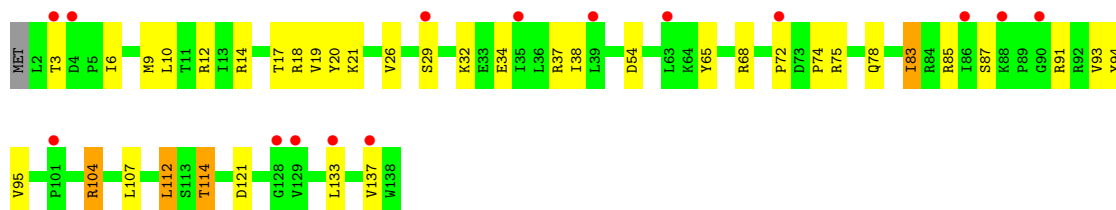




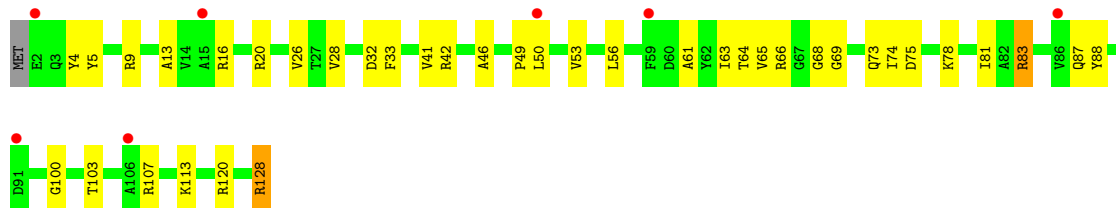
- Molecule 39: 30S ribosomal protein S8



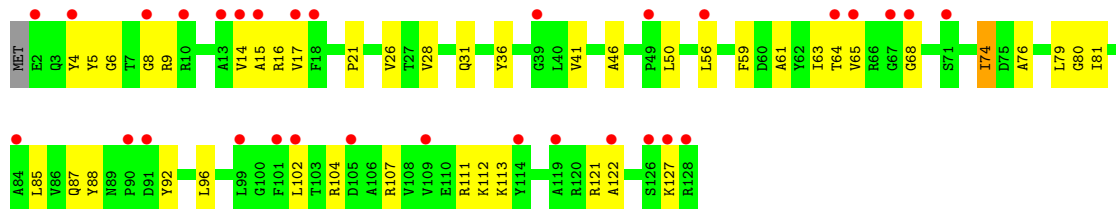
- Molecule 39: 30S ribosomal protein S8



- Molecule 40: 30S ribosomal protein S9

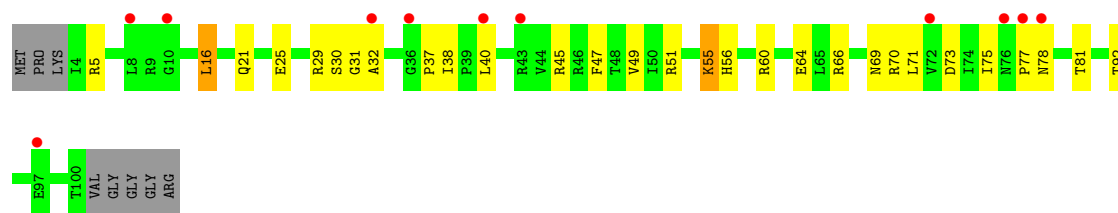


- Molecule 40: 30S ribosomal protein S9

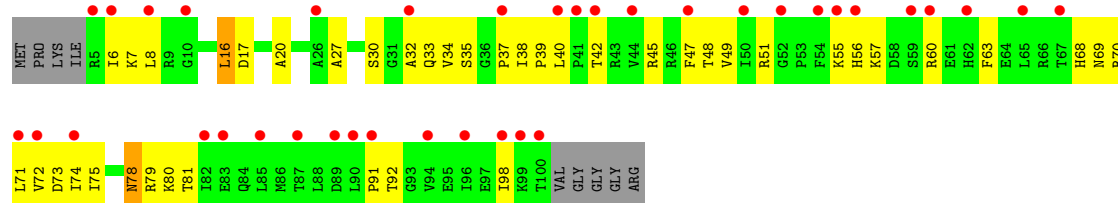


- Molecule 41: 30S ribosomal protein S10

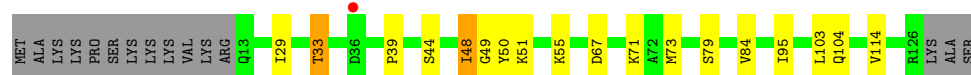
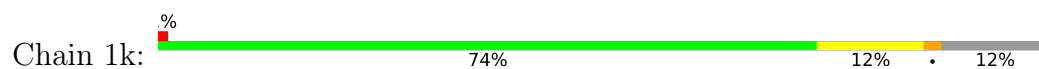




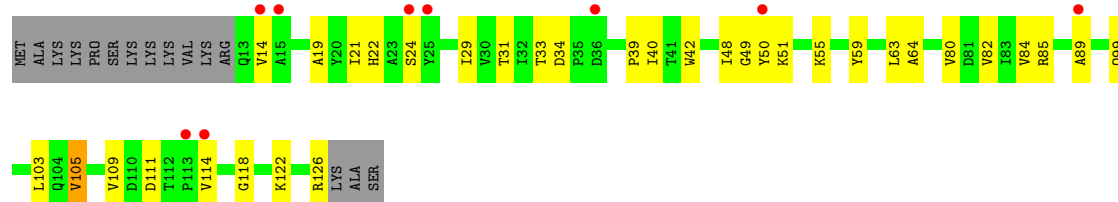
- Molecule 41: 30S ribosomal protein S10



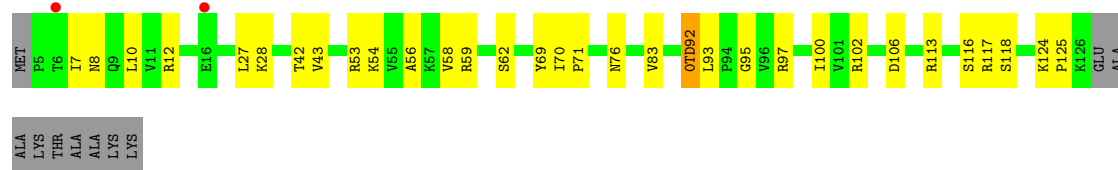
- Molecule 42: 30S ribosomal protein S11



- Molecule 42: 30S ribosomal protein S11

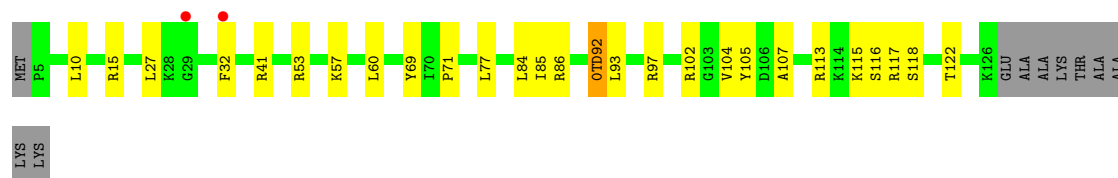


- Molecule 43: 30S ribosomal protein S12

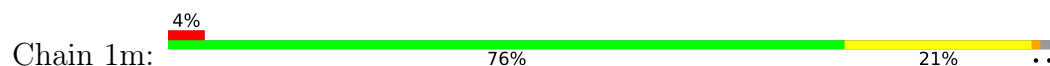


- Molecule 43: 30S ribosomal protein S12

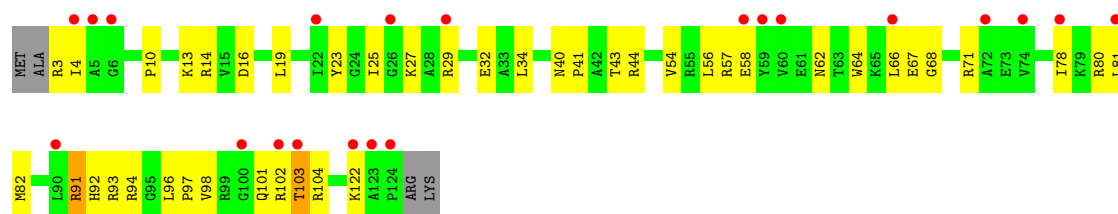




- Molecule 44: 30S ribosomal protein S13



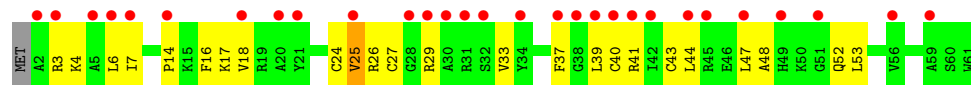
- Molecule 44: 30S ribosomal protein S13



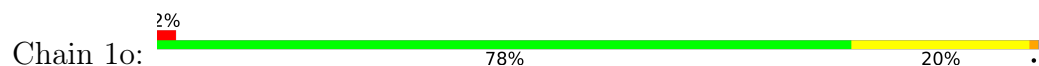
- Molecule 45: 30S ribosomal protein S14 type Z



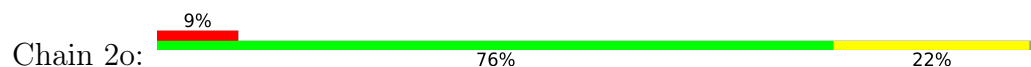
- Molecule 45: 30S ribosomal protein S14 type Z



- Molecule 46: 30S ribosomal protein S15

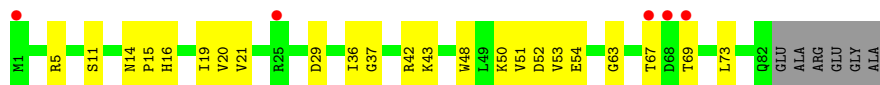


- Molecule 46: 30S ribosomal protein S15





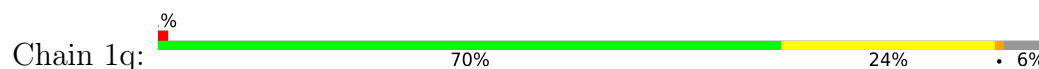
- Molecule 47: 30S ribosomal protein S16



- Molecule 47: 30S ribosomal protein S16



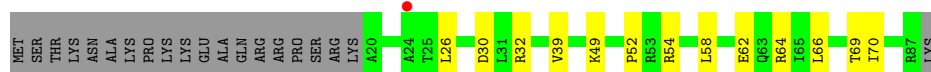
- Molecule 48: 30S ribosomal protein S17



- Molecule 48: 30S ribosomal protein S17



- Molecule 49: 30S ribosomal protein S18

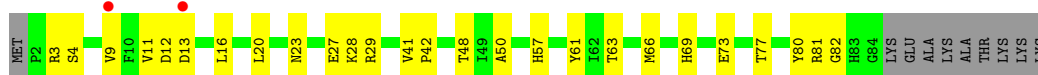


- Molecule 49: 30S ribosomal protein S18

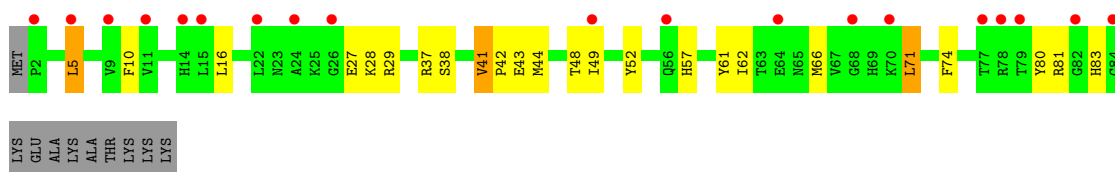




- Molecule 50: 30S ribosomal protein S19



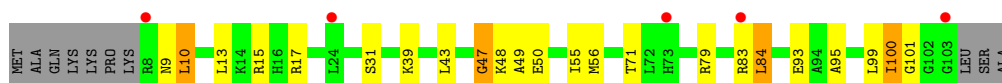
- Molecule 50: 30S ribosomal protein S19



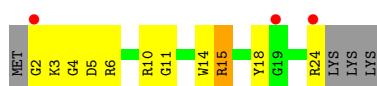
- Molecule 51: 30S ribosomal protein S20



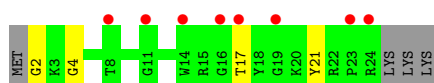
- Molecule 51: 30S ribosomal protein S20



- Molecule 52: 30S ribosomal protein Thx



- Molecule 52: 30S ribosomal protein Thx



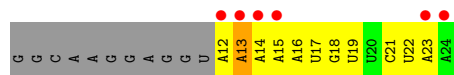
- Molecule 53: mRNA

Chain 1v: 



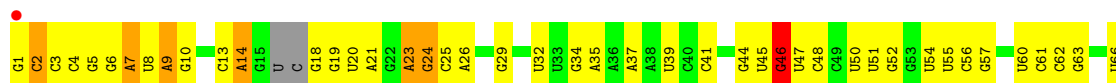
- Molecule 53: mRNA

Chain 2v: 



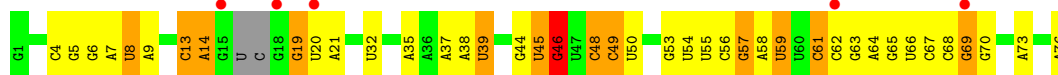
- Molecule 54: A-site and E-site tRNAs

Chain 1w: 



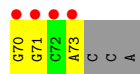
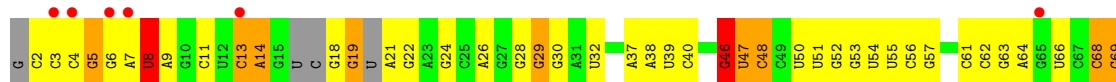
- Molecule 54: A-site and E-site tRNAs

Chain 1y: 



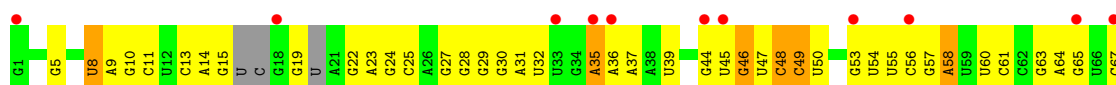
- Molecule 54: A-site and E-site tRNAs

Chain 2w: 



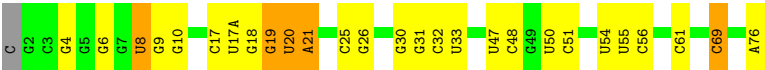
- Molecule 54: A-site and E-site tRNAs

Chain 2y: 

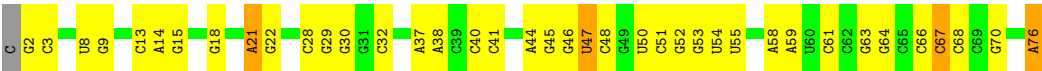




● Molecule 55: P-site tRNA



● 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	209.94Å 451.23Å 622.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	155.61 – 2.80 155.61 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.6 (155.61-2.80) 96.6 (155.61-2.80)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 2.82Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, R_{free}	0.229 , 0.278 0.230 , 0.277	Depositor DCC
R_{free} test set	69403 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	53.5	Xtriage
Anisotropy	0.220	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 69.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	300935	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.66% 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: ZN, 4OC, 2MU, M2G, 2MA, MIA, M2D, SF4, 2MG, 5MC, PSU, MA6, 7MG, 4SU, 0TD, OMG, MG, K, UR3, 5MU

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	0.17	0/69009	0.35	0/107712
1	2A	0.14	0/67293	0.32	0/105034
2	1B	0.14	0/2882	0.31	0/4494
2	2B	0.13	0/2879	0.30	0/4487
3	1D	0.17	0/2186	0.43	0/2944
3	2D	0.15	0/2186	0.40	0/2944
4	1E	0.17	0/1592	0.41	0/2149
4	2E	0.14	0/1592	0.38	0/2149
5	1F	0.17	0/1619	0.39	0/2193
5	2F	0.14	0/1615	0.37	0/2188
6	1G	0.15	0/1448	0.40	0/1957
6	2G	0.14	0/1453	0.37	0/1963
7	1H	0.15	0/1356	0.34	0/1834
7	2H	0.15	0/1356	0.33	0/1834
8	1I	0.13	0/1112	0.37	0/1514
8	2I	0.13	0/1079	0.34	0/1475
9	1N	0.18	0/1144	0.37	0/1543
9	2N	0.13	0/1144	0.35	0/1543
10	1O	0.16	0/943	0.36	0/1269
10	2O	0.14	0/943	0.33	0/1269
11	1P	0.20	0/1152	0.39	0/1533
11	2P	0.17	0/1152	0.41	0/1533
12	1Q	0.16	0/1143	0.38	0/1527
12	2Q	0.13	0/1143	0.34	0/1527
13	1R	0.18	0/982	0.42	0/1312
13	2R	0.15	0/982	0.40	0/1312
14	1S	0.14	0/883	0.39	0/1176
14	2S	0.13	0/880	0.37	0/1172
15	1T	0.16	0/1105	0.43	0/1477
15	2T	0.14	0/1097	0.37	0/1468
16	1U	0.18	0/977	0.39	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	2U	0.14	0/977	0.35	0/1301
17	1V	0.24	0/782	0.37	0/1049
17	2V	0.16	0/782	0.35	0/1049
18	1W	0.18	0/897	0.38	0/1205
18	2W	0.14	0/897	0.35	0/1205
19	1X	0.18	0/764	0.44	0/1025
19	2X	0.13	0/764	0.34	0/1025
20	1Y	0.16	0/819	0.43	0/1095
20	2Y	0.13	0/819	0.36	0/1095
21	1Z	0.18	0/1267	0.39	0/1717
21	2Z	0.15	0/1299	0.42	0/1763
22	10	0.18	0/662	0.44	0/881
22	20	0.14	0/662	0.39	0/881
23	11	0.21	0/762	0.39	0/1014
23	21	0.14	0/762	0.36	0/1014
24	12	0.16	0/590	0.37	0/781
24	22	0.14	0/590	0.33	0/781
25	13	0.17	0/474	0.41	0/635
25	23	0.13	0/469	0.36	0/630
26	14	0.25	0/565	0.57	1/761 (0.1%)
26	24	0.18	0/545	0.51	0/737
27	15	0.18	0/469	0.45	0/635
27	25	0.15	0/469	0.37	0/635
28	16	0.19	0/460	0.41	0/613
28	26	0.16	0/456	0.43	0/608
29	17	0.19	0/426	0.45	0/561
29	27	0.17	0/426	0.47	0/561
30	18	0.17	0/525	0.41	0/691
30	28	0.13	0/525	0.33	0/691
31	19	0.17	0/310	0.40	0/407
31	29	0.15	0/310	0.43	0/407
32	1a	0.14	0/35795	0.32	0/55864
32	2a	0.14	0/35886	0.32	0/56005
33	1b	0.16	0/1881	0.44	0/2542
33	2b	0.17	0/1860	0.44	0/2518
34	1c	0.14	0/1572	0.34	0/2126
34	2c	0.15	0/1566	0.38	0/2119
35	1d	0.14	0/1685	0.38	0/2262
35	2d	0.14	0/1704	0.41	0/2284
36	1e	0.15	0/1145	0.42	0/1543
36	2e	0.16	0/1149	0.42	0/1548
37	1f	0.13	0/823	0.34	0/1115
37	2f	0.13	0/829	0.35	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	1g	0.13	0/1250	0.36	0/1679
38	2g	0.16	0/1254	0.36	0/1683
39	1h	0.14	0/1108	0.37	0/1494
39	2h	0.13	0/1108	0.36	0/1494
40	1i	0.15	0/1002	0.41	0/1346
40	2i	0.15	0/997	0.44	1/1343 (0.1%)
41	1j	0.14	0/722	0.37	0/982
41	2j	0.18	0/727	0.45	0/988
42	1k	0.12	0/844	0.31	0/1145
42	2k	0.14	0/848	0.33	0/1149
43	1l	0.15	0/937	0.39	0/1260
43	2l	0.17	0/937	0.37	0/1260
44	1m	0.15	0/969	0.40	0/1302
44	2m	0.18	0/961	0.39	0/1291
45	1n	0.16	0/501	0.35	0/664
45	2n	0.14	0/501	0.37	0/664
46	1o	0.13	0/739	0.33	0/985
46	2o	0.13	0/739	0.33	0/985
47	1p	0.12	0/697	0.37	0/939
47	2p	0.13	0/693	0.38	0/935
48	1q	0.14	0/836	0.35	0/1117
48	2q	0.14	0/836	0.38	0/1117
49	1r	0.15	0/560	0.36	0/746
49	2r	0.12	0/560	0.33	0/746
50	1s	0.17	0/667	0.46	0/900
50	2s	0.17	0/661	0.42	0/893
51	1t	0.15	0/730	0.48	1/965 (0.1%)
51	2t	0.15	0/729	0.45	0/965
52	1u	0.13	0/203	0.39	0/266
52	2u	0.17	0/203	0.44	0/266
53	1v	0.13	0/310	0.26	0/480
53	2v	0.16	0/310	0.30	0/480
54	1w	0.21	1/1559 (0.1%)	0.36	0/2424
54	1y	0.20	1/1606 (0.1%)	0.34	0/2497
54	2w	0.21	0/1487	0.33	0/2311
54	2y	0.19	0/1583	0.32	0/2459
55	1x	0.20	0/1725	0.33	0/2689
55	2x	0.19	0/1725	0.33	0/2689
All	All	0.15	2/316570 (0.0%)	0.35	3/473933 (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	24	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1y	8	4SU	O3'-P	5.20	1.61	1.56
54	1w	8	4SU	O3'-P	5.07	1.61	1.56

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	1t	99	LEU	CB-CA-C	-6.55	109.03	116.63
40	2i	96	LEU	N-CA-C	-5.79	108.02	114.62
26	14	62	ARG	CB-CA-C	-5.57	110.14	116.54

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	24	56	VAL	Peptide
26	24	63	TYR	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	31191	599	0
1	2A	60322	0	30426	696	0
2	1B	2577	0	1305	20	0
2	2B	2575	0	1303	33	0
3	1D	2136	0	2218	41	0
3	2D	2136	0	2218	32	0
4	1E	1559	0	1618	33	0
4	2E	1559	0	1618	27	0
5	1F	1584	0	1625	35	0
5	2F	1580	0	1619	40	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	1G	1423	0	1436	31	0
6	2G	1428	0	1438	36	0
7	1H	1330	0	1407	31	0
7	2H	1330	0	1407	28	0
8	1I	1097	0	1140	22	0
8	2I	1064	0	1082	15	0
9	1N	1117	0	1184	20	0
9	2N	1117	0	1184	19	0
10	1O	933	0	996	15	0
10	2O	933	0	996	22	0
11	1P	1135	0	1212	33	0
11	2P	1135	0	1212	22	0
12	1Q	1122	0	1179	17	0
12	2Q	1122	0	1179	32	0
13	1R	968	0	1033	17	0
13	2R	968	0	1033	19	0
14	1S	873	0	927	14	0
14	2S	870	0	923	17	0
15	1T	1091	0	1151	20	0
15	2T	1083	0	1136	25	0
16	1U	959	0	1019	8	0
16	2U	959	0	1019	16	0
17	1V	771	0	830	11	0
17	2V	771	0	830	13	0
18	1W	886	0	940	15	0
18	2W	886	0	940	13	0
19	1X	750	0	814	16	0
19	2X	750	0	814	19	0
20	1Y	806	0	881	19	0
20	2Y	806	0	881	17	0
21	1Z	1240	0	1240	10	0
21	2Z	1271	0	1273	23	0
22	10	653	0	674	11	0
22	20	653	0	674	12	0
23	11	755	0	826	13	0
23	21	755	0	826	15	0
24	12	588	0	643	11	0
24	22	588	0	643	11	0
25	13	469	0	518	8	0
25	23	464	0	514	12	0
26	14	552	0	533	16	0
26	24	532	0	503	18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	15	455	0	465	8	0
27	25	455	0	465	10	0
28	16	453	0	473	7	0
28	26	449	0	469	9	0
29	17	418	0	467	6	0
29	27	418	0	467	7	0
30	18	517	0	582	19	0
30	28	517	0	582	19	0
31	19	307	0	335	4	0
31	29	307	0	335	9	0
32	1a	32246	0	16295	411	0
32	2a	32327	0	16339	535	0
33	1b	1846	0	1867	53	0
33	2b	1825	0	1828	57	0
34	1c	1548	0	1535	29	0
34	2c	1542	0	1517	41	0
35	1d	1655	0	1672	40	0
35	2d	1674	0	1714	45	0
36	1e	1129	0	1185	30	0
36	2e	1133	0	1191	32	0
37	1f	810	0	804	14	0
37	2f	816	0	808	18	0
38	1g	1231	0	1238	19	0
38	2g	1235	0	1249	26	0
39	1h	1088	0	1126	25	0
39	2h	1088	0	1126	32	0
40	1i	983	0	986	27	0
40	2i	978	0	966	25	0
41	1j	709	0	650	18	0
41	2j	714	0	672	33	0
42	1k	829	0	825	8	0
42	2k	833	0	836	18	0
43	1l	932	0	981	18	0
43	2l	932	0	981	19	0
44	1m	958	0	1002	19	0
44	2m	950	0	988	34	0
45	1n	492	0	529	9	0
45	2n	492	0	529	18	0
46	1o	728	0	760	10	0
46	2o	728	0	760	13	0
47	1p	681	0	697	14	0
47	2p	677	0	686	14	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	1q	823	0	891	18	0
48	2q	823	0	891	25	0
49	1r	555	0	618	8	0
49	2r	555	0	618	14	0
50	1s	652	0	662	18	0
50	2s	646	0	644	17	0
51	1t	728	0	798	17	0
51	2t	727	0	796	17	0
52	1u	199	0	208	11	0
52	2u	199	0	208	4	0
53	1v	277	0	140	2	0
53	2v	277	0	140	8	0
54	1w	1550	0	797	25	0
54	1y	1585	0	804	17	0
54	2w	1482	0	755	28	0
54	2y	1565	0	795	17	0
55	1x	1625	0	829	9	0
55	2x	1625	0	829	24	0
56	10	8	0	0	0	0
56	11	4	0	0	0	0
56	12	2	0	0	0	0
56	13	1	0	0	0	0
56	15	3	0	0	0	0
56	16	2	0	0	0	0
56	17	3	0	0	0	0
56	18	4	0	0	0	0
56	19	2	0	0	0	0
56	1A	1143	0	0	0	0
56	1B	36	0	0	0	0
56	1D	14	0	0	0	0
56	1E	12	0	0	0	0
56	1F	8	0	0	0	0
56	1G	5	0	0	0	0
56	1I	1	0	0	0	0
56	1N	6	0	0	0	0
56	1O	5	0	0	0	0
56	1P	3	0	0	0	0
56	1Q	5	0	0	0	0
56	1R	4	0	0	0	0
56	1S	3	0	0	0	0
56	1T	3	0	0	0	0
56	1U	7	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	1V	2	0	0	0	0
56	1W	7	0	0	0	0
56	1X	5	0	0	0	0
56	1Y	3	0	0	0	0
56	1Z	4	0	0	0	0
56	1a	235	0	0	0	0
56	1b	2	0	0	0	0
56	1d	1	0	0	0	0
56	1e	1	0	0	0	0
56	1f	2	0	0	0	0
56	1l	3	0	0	0	0
56	1m	1	0	0	0	0
56	1n	2	0	0	0	0
56	1p	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	11	0	0	0	0
56	1x	15	0	0	0	0
56	1y	5	0	0	0	0
56	20	2	0	0	0	0
56	23	1	0	0	0	0
56	25	4	0	0	0	0
56	26	1	0	0	0	0
56	27	1	0	0	0	0
56	28	1	0	0	0	0
56	2A	876	0	0	0	0
56	2B	21	0	0	0	0
56	2D	7	0	0	0	0
56	2E	7	0	0	0	0
56	2F	4	0	0	0	0
56	2G	1	0	0	0	0
56	2O	1	0	0	0	0
56	2Q	4	0	0	0	0
56	2R	2	0	0	0	0
56	2T	3	0	0	0	0
56	2U	6	0	0	0	0
56	2V	1	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	230	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	2d	2	0	0	0	0
56	2e	1	0	0	0	0
56	2f	1	0	0	0	0
56	2g	1	0	0	0	0
56	2j	2	0	0	0	0
56	2l	2	0	0	0	0
56	2p	1	0	0	0	0
56	2q	3	0	0	0	0
56	2r	2	0	0	0	0
56	2t	1	0	0	0	0
56	2v	3	0	0	0	0
56	2w	7	0	0	0	0
56	2x	6	0	0	0	0
56	2y	6	0	0	0	0
57	1A	1	0	0	0	0
57	2A	1	0	0	0	0
58	1A	36	0	0	0	0
58	2A	36	0	0	0	0
59	14	1	0	0	0	0
59	15	1	0	0	0	0
59	16	1	0	0	0	0
59	19	1	0	0	0	0
59	1Y	1	0	0	0	0
59	1n	1	0	0	0	0
59	24	1	0	0	0	0
59	25	1	0	0	0	0
59	26	1	0	0	0	0
59	29	1	0	0	0	0
59	2Y	1	0	0	0	0
59	2n	1	0	0	0	0
60	1d	8	0	0	2	0
60	2d	8	0	0	2	0
61	10	8	0	0	1	0
61	11	14	0	0	2	0
61	12	4	0	0	1	0
61	13	4	0	0	0	0
61	14	1	0	0	0	0
61	15	7	0	0	0	0
61	16	4	0	0	0	0
61	17	7	0	0	0	0
61	18	13	0	0	0	0
61	19	3	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	1A	2255	0	0	63	0
61	1B	68	0	0	1	0
61	1D	30	0	0	3	0
61	1E	28	0	0	5	0
61	1F	21	0	0	1	0
61	1G	5	0	0	0	0
61	1H	1	0	0	0	0
61	1I	2	0	0	0	0
61	1N	8	0	0	1	0
61	1O	11	0	0	1	0
61	1P	25	0	0	2	0
61	1Q	13	0	0	0	0
61	1R	15	0	0	1	0
61	1S	4	0	0	1	0
61	1T	5	0	0	0	0
61	1U	13	0	0	0	0
61	1V	10	0	0	1	0
61	1W	9	0	0	0	0
61	1X	6	0	0	0	0
61	1Y	5	0	0	0	0
61	1Z	1	0	0	0	0
61	1a	454	0	0	17	0
61	1b	1	0	0	0	0
61	1f	1	0	0	0	0
61	1l	7	0	0	0	0
61	1m	2	0	0	1	0
61	1o	1	0	0	0	0
61	1q	3	0	0	0	0
61	1r	1	0	0	0	0
61	1u	1	0	0	1	0
61	1v	6	0	0	0	0
61	1w	18	0	0	0	0
61	1x	16	0	0	0	0
61	1y	3	0	0	0	0
61	20	5	0	0	0	0
61	21	14	0	0	0	0
61	22	1	0	0	0	0
61	23	2	0	0	0	0
61	25	5	0	0	0	0
61	26	1	0	0	0	0
61	27	3	0	0	1	0
61	28	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	29	1	0	0	0	0
61	2A	1418	0	0	60	0
61	2B	26	0	0	2	0
61	2D	29	0	0	1	0
61	2E	14	0	0	2	0
61	2F	15	0	0	0	0
61	2I	4	0	0	0	0
61	2N	2	0	0	0	0
61	2O	1	0	0	0	0
61	2P	13	0	0	1	0
61	2Q	2	0	0	0	0
61	2R	2	0	0	0	0
61	2T	4	0	0	0	0
61	2U	2	0	0	0	0
61	2V	1	0	0	0	0
61	2W	3	0	0	0	0
61	2X	5	0	0	0	0
61	2Y	1	0	0	0	0
61	2Z	2	0	0	0	0
61	2a	392	0	0	15	0
61	2c	2	0	0	0	0
61	2d	4	0	0	0	0
61	2e	2	0	0	0	0
61	2g	1	0	0	0	0
61	2j	4	0	0	0	0
61	2k	1	0	0	0	0
61	2l	6	0	0	1	0
61	2o	4	0	0	0	0
61	2p	2	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	2u	1	0	0	1	0
61	2v	4	0	0	0	0
61	2w	1	0	0	0	0
61	2x	6	0	0	0	0
61	2y	19	0	0	1	0
All	All	300935	0	196636	3823	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (3823) 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:1128:U:H3	1:1A:1132:A:N6	1.38	1.22
1:1A:1128:U:O4	1:1A:1132:A:N1	1.87	1.04
1:2A:2121:G:H1	1:2A:2177:C:H42	1.05	1.00
1:2A:2129:C:N4	1:2A:2159:G:H1	1.59	1.00
32:2a:997:U:H3	32:2a:1044:A:N6	1.59	0.99
32:2a:1002:G:H1	32:2a:1038:C:N4	1.61	0.99
1:1A:2146:G:H1	1:1A:2196:C:N4	1.61	0.98
55:2x:3:C:H42	55:2x:70:G:H1	1.09	0.97
32:1a:998:G:H1	32:1a:1043:C:N4	1.63	0.95
1:2A:2138:C:H42	1:2A:2153:G:H1	1.06	0.95
32:2a:1133:G:H1	32:2a:1141:C:H42	1.08	0.95
32:1a:998:G:H1	32:1a:1043:C:H42	0.98	0.94
32:2a:1264:C:H42	32:2a:1271:G:H1	1.14	0.94
1:1A:2149:G:H1	1:1A:2183:C:N4	1.66	0.93
32:1a:931:C:H42	32:1a:1386:G:H1	1.13	0.92
1:1A:1104:G:H1	1:1A:1126:C:H42	1.11	0.90
32:1a:559:A:H4'	32:1a:560:U:H3'	1.51	0.90
41:2j:32:ALA:HB1	41:2j:33:GLN:HA	1.54	0.90
1:1A:2158:C:N3	1:1A:2177:G:N2	2.21	0.89
32:1a:1162:C:H42	32:1a:1174:G:H1	1.20	0.89
32:2a:1089:G:H1	32:2a:1096:C:H42	1.17	0.89
1:1A:2146:G:H1	1:1A:2196:C:H42	0.88	0.88
1:2A:2104:G:H1	1:2A:2185:C:H42	1.22	0.88
32:2a:1002:G:H1	32:2a:1038:C:H42	0.91	0.88
1:1A:2149:G:H1	1:1A:2183:C:H42	1.17	0.87
1:2A:2127:G:C6	1:2A:2161:C:N4	2.44	0.86
54:2w:4:C:N3	54:2w:69:G:N2	2.23	0.85
1:1A:2158:C:N4	1:1A:2177:G:N1	2.24	0.85
14:1S:61:ASN:HD22	14:1S:64:GLU:H	1.23	0.84
19:1X:57:LEU:HD11	19:1X:78:LYS:HE2	1.57	0.84
31:29:25:VAL:HB	31:29:34:GLN:HB2	1.59	0.84
1:2A:2127:G:N1	1:2A:2161:C:C4	2.44	0.84
1:2A:2345:G:H4'	1:2A:2346:A:H5''	1.59	0.84
1:1A:1085:G:H1	1:1A:1162:C:H42	1.25	0.84
32:1a:664:G:H22	32:1a:741:G:H1	1.21	0.84
1:1A:2122:G:H1	1:1A:2211:U:H3	1.21	0.84
1:1A:1110:C:N3	1:1A:1120:G:O6	2.11	0.84
1:1A:1104:G:H1	1:1A:1126:C:N4	1.75	0.84
21:2Z:153:SER:HB3	21:2Z:167:PRO:HB3	1.58	0.83
47:2p:51:VAL:HG12	47:2p:53:VAL:H	1.43	0.83
12:2Q:85:LYS:HG2	22:20:7:LEU:HB3	1.59	0.83
32:1a:1027:C:C2	32:1a:1034:G:N2	2.47	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:1s:27:GLU:HB2	50:1s:28:LYS:HA	1.62	0.82
1:1A:1111:U:O2	1:1A:1119:A:N6	2.12	0.82
1:2A:2121:G:H1	1:2A:2177:C:N4	1.77	0.82
1:2A:2129:C:H42	1:2A:2159:G:H1	0.85	0.81
1:2A:2136:C:N4	1:2A:2155:G:H1	1.76	0.81
50:2s:27:GLU:HB2	50:2s:28:LYS:HA	1.62	0.81
32:2a:1133:G:H1	32:2a:1141:C:N4	1.77	0.81
32:2a:1271:G:N2	32:2a:1272:G:N7	2.29	0.81
10:1O:35:VAL:HG11	10:1O:103:ALA:HB3	1.63	0.81
1:2A:1204:A:H2	1:2A:1241:A:H62	1.28	0.81
1:2A:2138:C:N4	1:2A:2153:G:H1	1.77	0.81
11:1P:100:LEU:HD12	11:1P:112:LEU:HD11	1.63	0.80
1:2A:2136:C:N3	1:2A:2155:G:N2	2.29	0.80
10:2O:35:VAL:HG11	10:2O:103:ALA:HB3	1.62	0.80
27:25:16:ARG:NH1	27:25:17:ASP:OD1	2.14	0.80
54:2w:4:C:N4	54:2w:69:G:N1	2.30	0.80
32:1a:998:G:N2	32:1a:1043:C:N3	2.29	0.80
32:1a:1009:G:O6	32:1a:1020:U:O2	1.99	0.80
1:2A:2127:G:C2	1:2A:2161:C:N3	2.50	0.80
1:1A:294:C:H42	1:1A:390:G:H1	1.30	0.79
11:1P:50:ARG:HD3	30:18:7:HIS:CD2	2.17	0.79
1:1A:1436:U:O2	1:1A:1441:A:N6	2.15	0.79
55:2x:3:C:N4	55:2x:70:G:H1	1.81	0.79
11:1P:126:VAL:HG12	11:1P:148:LEU:HD23	1.65	0.79
32:1a:1162:C:N4	32:1a:1174:G:H1	1.80	0.79
1:2A:424:G:N7	61:2A:3972:HOH:O	2.16	0.78
1:2A:1798:U:H5'	3:2D:259:THR:HG22	1.65	0.78
1:1A:927:G:H2'	1:1A:928:G:H8	1.48	0.78
5:2F:40:GLN:HE22	5:2F:182:ASN:HB2	1.47	0.78
55:2x:51:C:H42	55:2x:63:G:H1	1.29	0.78
32:2a:1264:C:N4	32:2a:1271:G:H1	1.79	0.78
1:2A:2127:G:N2	1:2A:2161:C:C2	2.51	0.78
32:2a:1119:C:H2'	32:2a:1120:G:H8	1.46	0.78
1:1A:1100:A:H61	1:1A:1151:U:H3	1.30	0.78
42:2k:51:LYS:HA	42:2k:55:LYS:HE3	1.65	0.78
21:1Z:1:MET:N	21:1Z:135:GLU:OE2	2.17	0.77
22:10:10:THR:HG22	22:10:12:ASN:H	1.48	0.77
1:2A:2099:U:H3	1:2A:2190:G:H1	1.26	0.77
1:2A:1031:G:H5''	31:29:8:LYS:HE3	1.67	0.77
1:2A:2136:C:N4	1:2A:2155:G:N1	2.33	0.77
1:1A:2140:U:O4	1:1A:2170:G:N2	2.18	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:997:U:H3	32:2a:1044:A:H61	0.82	0.77
1:1A:1848:G:OP1	3:1D:88:ARG:NH2	2.18	0.77
24:12:9:GLN:HE22	24:12:56:GLN:HB3	1.50	0.77
32:1a:931:C:N4	32:1a:1386:G:H1	1.81	0.77
1:2A:1530:C:O2'	1:2A:1531:C:O5'	2.02	0.77
1:2A:2127:G:C2	1:2A:2161:C:C4	2.73	0.77
10:2O:68:GLU:HB3	10:2O:78:ARG:HG3	1.65	0.77
32:2a:1055:A:N7	32:2a:1200:C:N4	2.33	0.77
1:1A:542:C:OP1	27:15:16:ARG:NH2	2.18	0.77
1:2A:1153:C:OP1	16:2U:92:ARG:NH2	2.17	0.76
32:2a:1026:G:O6	32:2a:1036:G:N2	2.18	0.76
54:2w:30:G:H1	54:2w:40:C:H42	1.32	0.76
54:2y:15:G:H22	54:2y:48:C:H42	1.32	0.76
32:1a:1008:C:N3	32:1a:1021:G:O6	2.18	0.76
32:2a:1086:U:H3	32:2a:1099:G:H22	1.34	0.76
54:1w:7:A:H61	54:1w:66:U:H3	1.31	0.76
33:1b:10:LEU:H	33:1b:48:MET:HE1	1.49	0.76
41:1j:30:SER:HG	41:1j:81:THR:HG1	1.31	0.76
41:1j:40:LEU:HB2	41:1j:69:ASN:HB2	1.68	0.76
52:1u:5:ASP:OD2	61:1u:101:HOH:O	2.03	0.76
11:2P:42:SER:O	61:2P:201:HOH:O	2.03	0.76
33:2b:69:LEU:HB3	33:2b:162:ILE:HG22	1.66	0.76
32:2a:953:G:H5'	32:2a:965:A:H61	1.51	0.76
32:2a:1025:U:H3	32:2a:1036:G:H1	1.31	0.76
1:2A:2815:C:H5'	27:25:29:THR:HG21	1.66	0.76
32:2a:1002:G:N2	32:2a:1038:C:N3	2.32	0.75
32:2a:1381:U:H1'	38:2g:79:ARG:HD3	1.68	0.75
1:1A:2158:C:N4	1:1A:2177:G:H1	1.84	0.75
32:1a:1025:U:O2	32:1a:1036:G:O6	2.03	0.75
8:2I:124:GLY:H	8:2I:144:VAL:HG23	1.51	0.75
32:1a:1119:C:OP1	40:1i:83:ARG:NH2	2.19	0.75
1:2A:335:C:H4'	20:2Y:73:ARG:HD3	1.69	0.74
1:1A:64:C:O2	1:1A:482:C:N4	2.18	0.74
4:1E:127:ASP:OD2	61:1E:401:HOH:O	2.04	0.74
1:2A:2129:C:N3	1:2A:2159:G:N2	2.33	0.74
1:2A:994:C:OP1	16:2U:53:ARG:NH2	2.20	0.74
1:1A:427:G:N7	61:1A:4294:HOH:O	2.19	0.74
30:18:62:LEU:HB3	30:18:65:GLU:HG2	1.70	0.74
32:1a:1002:G:H3'	32:1a:1003:G:H4'	1.68	0.74
4:2E:119:ARG:HD2	4:2E:160:TYR:HB2	1.68	0.74
1:1A:929:G:H1	1:1A:940:C:H42	1.36	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1060:C:H5''	41:1j:51:ARG:HG2	1.68	0.74
36:1e:78:HIS:HE1	36:1e:143:ARG:H	1.33	0.74
1:1A:1055:A:OP2	9:1N:37:LYS:NZ	2.15	0.73
32:1a:78:G:C6	32:1a:91:C:N4	2.56	0.73
23:21:51:VAL:HG11	23:21:74:VAL:HG21	1.70	0.73
54:2y:57:G:N2	61:2y:201:HOH:O	2.21	0.73
1:1A:2185:C:OP1	1:1A:2187:G:N2	2.22	0.73
1:2A:2630:G:H2'	1:2A:2631:G:C8	2.23	0.73
1:2A:2630:G:H2'	1:2A:2631:G:H8	1.53	0.73
35:2d:57:ARG:HD3	35:2d:205:GLU:HB3	1.70	0.73
1:1A:1649:A:OP1	61:1A:4235:HOH:O	2.06	0.73
40:2i:46:ALA:HB2	40:2i:74:ILE:HG23	1.71	0.73
43:2l:86:ARG:NH1	61:2l:301:HOH:O	2.21	0.73
32:1a:972:C:O2'	41:1j:55:LYS:O	2.07	0.73
32:1a:1270:C:OP2	52:1u:24:ARG:NH2	2.22	0.73
32:2a:974:A:OP2	45:2n:29:ARG:NH2	2.23	0.72
4:1E:135:HIS:NE2	61:1E:404:HOH:O	2.21	0.72
32:2a:266:G:H5''	32:2a:268:C:H41	1.55	0.72
1:2A:775:G:N3	61:2A:4003:HOH:O	2.23	0.72
32:1a:975:A:H4'	32:1a:976:G:H5''	1.70	0.72
47:1p:51:VAL:HG12	47:1p:53:VAL:H	1.53	0.72
32:2a:1029:C:C4	32:2a:1032:G:N1	2.58	0.72
32:1a:26:A:H1'	35:1d:209:ARG:HH21	1.55	0.72
1:1A:2641:A:O2'	1:1A:2642:G:OP2	2.07	0.72
17:1V:40:LEU:HB2	17:1V:46:VAL:HG13	1.72	0.72
1:1A:1104:G:N2	1:1A:1126:C:N3	2.35	0.72
1:2A:2126:A:N6	1:2A:2162:G:O2'	2.21	0.72
1:1A:1814:A:N7	61:1A:4316:HOH:O	2.24	0.71
1:2A:1689:A:H62	1:2A:1698:A:H2	1.38	0.71
11:2P:59:LEU:HD11	30:28:10:ALA:HB2	1.72	0.71
1:1A:39:C:O2	5:1F:46:ARG:NH2	2.23	0.71
1:2A:1015:G:H2'	1:2A:1016:G:H8	1.56	0.71
1:1A:625:G:O2'	1:1A:702:A:N6	2.23	0.71
1:2A:1652:A:OP1	13:2R:8:ARG:NH1	2.24	0.71
1:2A:2683:C:O2	10:2O:70:LYS:NZ	2.23	0.71
54:2w:4:C:N4	54:2w:69:G:H1	1.87	0.71
1:2A:2646:C:OP2	1:2A:2732:G:O2'	2.09	0.71
1:2A:1762:A:N1	61:2A:4009:HOH:O	2.23	0.71
32:2a:1296:C:H5''	44:2m:44:ARG:HH22	1.54	0.71
32:2a:1404:5MC:O2	32:2a:1519:MA6:O2'	2.09	0.71
32:1a:200:G:H1	32:1a:217:C:H42	1.38	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:1q:66:SER:O	48:1q:70:ARG:NH1	2.24	0.71
5:2F:70:THR:HG23	5:2F:72:ARG:H	1.54	0.71
32:2a:1274:G:N2	32:2a:1275:A:N7	2.38	0.70
40:2i:31:GLN:HE21	40:2i:36:TYR:HD1	1.38	0.70
32:1a:812:C:N3	61:1a:3329:HOH:O	2.23	0.70
54:2w:8:4SU:S4	54:2w:13:C:O2'	2.47	0.70
54:1w:1:G:O6	54:1w:72:C:N3	2.24	0.70
25:23:8:LEU:HB2	25:23:28:LEU:HD13	1.73	0.70
32:2a:8:A:H5'	36:2e:101:ILE:HG22	1.73	0.70
43:2l:117:ARG:HG2	43:2l:122:THR:HB	1.72	0.70
1:2A:880:G:N2	1:2A:898:C:O2	2.20	0.70
1:1A:1140:U:H1'	1:1A:1143:U:H5	1.57	0.70
23:11:50:ARG:HG2	23:11:59:THR:HG22	1.73	0.70
33:1b:21:ARG:O	33:1b:23:ARG:N	2.24	0.70
34:2c:52:LEU:HD21	34:2c:55:VAL:HG23	1.72	0.70
1:2A:643:A:N1	1:2A:2369:A:O2'	2.24	0.69
1:1A:1230:C:OP2	61:1A:4271:HOH:O	2.10	0.69
42:2k:22:HIS:HB3	42:2k:29:ILE:HB	1.74	0.69
3:2D:108:PRO:HG2	3:2D:111:LEU:HB2	1.73	0.69
1:2A:1245:G:OP1	11:2P:13:ASN:ND2	2.25	0.69
1:2A:2287:A:H62	1:2A:2344:U:H3	1.39	0.69
1:1A:2146:G:N2	1:1A:2196:C:N3	2.35	0.69
1:1A:436:C:OP1	61:1A:4272:HOH:O	2.10	0.69
2:1B:106:G:H5'	21:1Z:31:ARG:HG2	1.73	0.69
32:1a:1021:G:O2'	32:1a:1022:G:O5'	2.06	0.69
32:2a:391:G:N7	61:2a:3333:HOH:O	2.26	0.69
32:2a:818:G:N2	32:2a:873:A:OP1	2.24	0.69
32:2a:1347:G:H22	32:2a:1373:G:H2'	1.57	0.69
5:1F:53:THR:HG23	5:1F:55:GLY:H	1.58	0.69
54:1w:51:U:H2'	54:1w:52:G:C8	2.28	0.69
1:2A:223:A:O2'	1:2A:420:C:O2	2.11	0.69
1:2A:854:G:H2'	1:2A:855:G:H8	1.57	0.69
1:2A:2104:G:H1	1:2A:2185:C:N4	1.91	0.69
1:2A:2502:G:N7	61:2A:4019:HOH:O	2.25	0.69
1:2A:2448:A:N6	61:2A:4027:HOH:O	2.26	0.69
15:2T:39:ARG:NH2	32:2a:345:C:OP2	2.25	0.69
1:1A:1069:U:OP2	61:1A:4273:HOH:O	2.11	0.69
7:1H:84:SER:OG	7:1H:132:ARG:NH1	2.26	0.69
32:1a:567:G:N3	61:1a:3342:HOH:O	2.26	0.69
1:1A:1101:G:H1	1:1A:1150:C:H42	1.41	0.68
1:1A:207:A:N7	61:1A:4318:HOH:O	2.24	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:1j:49:VAL:HG23	45:1n:41:ARG:HB2	1.75	0.68
1:2A:2162:G:H4'	1:2A:2172:U:H2'	1.74	0.68
52:1u:6:ARG:HG2	52:1u:15:ARG:HD2	1.75	0.68
33:1b:33:TYR:HB2	33:1b:43:ASP:HB2	1.75	0.68
32:2a:1119:C:H2'	32:2a:1120:G:C8	2.27	0.68
33:2b:189:ASP:N	33:2b:189:ASP:OD1	2.26	0.68
40:1i:50:LEU:HD13	40:1i:56:LEU:HA	1.76	0.68
32:2a:1089:G:H1	32:2a:1096:C:N4	1.89	0.68
44:2m:58:GLU:O	44:2m:62:ASN:ND2	2.25	0.68
1:1A:2766:A:O2'	31:19:15:LYS:NZ	2.27	0.68
1:2A:1532:C:H42	1:2A:1537:G:H1	1.42	0.68
47:2p:52:ASP:O	47:2p:54:GLU:N	2.27	0.68
4:2E:36:ARG:HG2	4:2E:47:VAL:HG12	1.75	0.68
1:2A:2690:C:OP1	13:2R:17:ARG:NH2	2.26	0.68
3:2D:26:LYS:NZ	3:2D:30:GLU:OE1	2.27	0.68
32:2a:426:G:OP1	35:2d:38:TYR:OH	2.10	0.68
44:2m:82:MET:O	44:2m:93:ARG:NH2	2.26	0.68
32:1a:953:G:H5'	32:1a:965:A:H61	1.59	0.68
30:18:6:THR:HG22	30:18:63:PRO:HD2	1.75	0.67
32:1a:117:G:OP2	61:1a:3320:HOH:O	2.11	0.67
32:1a:1029:C:N3	32:1a:1032:G:O6	2.27	0.67
1:2A:987:G:O2'	1:2A:1000:A:N3	2.26	0.67
1:1A:2762:A:OP1	7:1H:3:ARG:NH1	2.26	0.67
1:2A:1448:G:N7	61:2A:4016:HOH:O	2.25	0.67
32:2a:1112:C:O2	34:2c:179:ARG:N	2.26	0.67
1:1A:1699:A:OP1	13:1R:8:ARG:NH1	2.25	0.67
1:2A:111:A:O2'	24:22:65:ASN:ND2	2.27	0.67
6:2G:38:VAL:HG22	6:2G:93:THR:HG23	1.76	0.67
35:2d:60:GLU:HG3	35:2d:202:LEU:HD12	1.75	0.67
1:1A:1123:A:H2'	1:1A:1124:U:H4'	1.75	0.67
1:2A:794:G:OP1	61:2A:3960:HOH:O	2.12	0.67
32:2a:1347:G:N2	32:2a:1373:G:H2'	2.09	0.67
2:1B:21:G:N7	61:1B:3103:HOH:O	2.27	0.67
32:1a:410:G:OP1	35:1d:30:LYS:NZ	2.23	0.67
46:1o:54:ARG:HG2	46:1o:58:MET:HE2	1.77	0.67
32:1a:1030:C:N3	32:1a:1031:G:C2	2.63	0.67
55:2x:51:C:N4	55:2x:63:G:H1	1.93	0.67
1:1A:2457:G:OP1	5:1F:74:ARG:NH2	2.28	0.67
12:1Q:10:ARG:HH12	12:1Q:90:VAL:H	1.42	0.67
1:1A:2177:G:H3'	1:1A:2178:G:H8	1.59	0.67
1:1A:2317:A:H5''	6:1G:134:GLY:HA3	1.77	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1027:C:C4	32:1a:1034:G:C2	2.82	0.67
39:1h:82:HIS:NE2	39:1h:136:GLU:OE2	2.28	0.67
44:2m:23:TYR:HB3	44:2m:67:GLU:HA	1.76	0.67
54:2w:18:G:O2'	54:2w:57:G:N2	2.24	0.67
1:2A:400:G:N7	61:2A:4030:HOH:O	2.27	0.67
1:2A:2114:A:N6	1:2A:2119:A:N7	2.42	0.67
1:1A:1310:G:OP1	27:15:19:ARG:NH2	2.25	0.67
32:1a:984:C:H42	32:1a:1221:G:H1	1.41	0.67
1:2A:677:A:OP1	61:2A:3962:HOH:O	2.13	0.67
1:2A:1773:A:OP2	61:2A:3963:HOH:O	2.13	0.67
38:2g:113:GLU:HB2	38:2g:119:ARG:HG2	1.76	0.67
32:1a:1346:A:OP1	40:1i:120:ARG:NH1	2.21	0.66
1:2A:2846:G:N7	61:2A:4040:HOH:O	2.28	0.66
33:2b:74:LYS:NZ	33:2b:205:ASP:O	2.25	0.66
33:2b:178:ARG:NH1	33:2b:198:ASP:OD1	2.27	0.66
36:2e:20:GLN:NE2	36:2e:21:ALA:O	2.29	0.66
1:1A:1370:G:N7	61:1A:4334:HOH:O	2.26	0.66
1:2A:1960:A:N7	61:2A:4041:HOH:O	2.28	0.66
41:2j:40:LEU:HB2	41:2j:69:ASN:HB3	1.76	0.66
10:2O:49:ARG:NH1	32:2a:1422:G:O3'	2.29	0.66
1:1A:2015:U:OP2	61:1A:4274:HOH:O	2.13	0.66
32:1a:1029:C:H41	32:1a:1030(A):G:H21	1.40	0.66
1:2A:700:G:O2'	1:2A:1632:A:N3	2.28	0.66
1:2A:2060:A:N3	61:2A:4039:HOH:O	2.28	0.66
32:2a:56:U:H2'	32:2a:57:G:H8	1.61	0.66
1:2A:918:A:O2'	2:2B:97:G:N2	2.29	0.66
1:2A:1817:G:OP1	3:2D:88:ARG:NH2	2.28	0.66
32:2a:148:G:H2'	32:2a:149:A:H8	1.61	0.66
32:2a:324:G:N7	61:2a:3337:HOH:O	2.27	0.66
32:2a:712:A:N6	61:2a:3338:HOH:O	2.27	0.66
32:2a:1204:A:OP1	45:2n:3:ARG:NH2	2.29	0.66
1:2A:1266:G:O5'	18:2W:15:ARG:NH2	2.29	0.66
7:2H:27:LYS:HZ2	7:2H:32:GLU:HB2	1.61	0.66
19:2X:8:ILE:O	24:22:36:ARG:NH2	2.29	0.66
23:21:3:LYS:HB2	23:21:61:ARG:HH12	1.61	0.66
1:1A:2227:G:H3'	1:1A:2228:G:C8	2.31	0.66
1:1A:2718:G:N7	61:1A:4346:HOH:O	2.28	0.66
38:1g:78:ARG:NH1	38:1g:154:TYR:O	2.29	0.66
5:2F:53:THR:HG23	5:2F:55:GLY:H	1.60	0.66
54:2y:15:G:N2	54:2y:48:C:H42	1.94	0.66
32:1a:559:A:OP1	36:1e:126:ARG:NH2	2.29	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:1b:69:LEU:HB3	33:1b:162:ILE:HG22	1.76	0.66
38:1g:79:ARG:HD2	38:1g:80:VAL:H	1.60	0.66
48:1q:9:VAL:HG12	48:1q:56:VAL:HG22	1.76	0.66
39:1h:10:LEU:HD22	39:1h:83:ILE:HD11	1.78	0.66
1:2A:307:G:N1	1:2A:310:A:OP2	2.28	0.66
3:2D:108:PRO:HB3	3:2D:143:HIS:HE1	1.59	0.66
4:2E:48:GLN:HE21	4:2E:78:LEU:HB3	1.61	0.66
23:21:50:ARG:HG2	23:21:59:THR:HG22	1.78	0.66
8:1I:38:LEU:HD12	8:1I:38:LEU:H	1.60	0.65
10:1O:48:PRO:HB3	32:1a:1422:G:H5''	1.77	0.65
50:1s:11:VAL:HG11	50:1s:16:LEU:HB2	1.77	0.65
32:2a:1010:G:N2	32:2a:1020:U:O2'	2.29	0.65
32:1a:120:A:OP1	61:1a:3322:HOH:O	2.14	0.65
1:2A:2296:U:OP2	14:2S:9:ARG:NH2	2.29	0.65
1:2A:2849:U:OP2	15:2T:95:ARG:NH1	2.29	0.65
3:1D:71:ASP:HB3	3:1D:103:ARG:HH12	1.61	0.65
1:2A:2218:U:H1'	23:21:52:ARG:HH12	1.61	0.65
32:2a:986:A:N3	50:2s:52:TYR:OH	2.25	0.65
1:1A:1001:G:O6	61:1A:4270:HOH:O	2.09	0.65
32:1a:1470:G:N7	61:1a:3351:HOH:O	2.30	0.65
40:1i:46:ALA:HB2	40:1i:74:ILE:HG23	1.79	0.65
12:2Q:136:ALA:HB1	21:2Z:52:SER:HB2	1.77	0.65
39:2h:37:ARG:HH21	39:2h:38:ILE:HD11	1.62	0.65
1:1A:2459:G:OP2	61:1A:4275:HOH:O	2.14	0.65
10:1O:36:GLY:O	61:1O:3101:HOH:O	2.14	0.65
32:1a:1077:G:N2	32:1a:1080:A:OP2	2.26	0.65
54:1w:1:G:N1	54:1w:72:C:O2	2.27	0.65
1:2A:731:C:OP2	61:2A:3964:HOH:O	2.14	0.65
43:2l:71:PRO:O	43:2l:102:ARG:NH1	2.30	0.65
32:1a:78:G:C2	32:1a:91:C:N3	2.64	0.65
32:2a:1077:G:N1	32:2a:1080:A:OP2	2.26	0.65
32:1a:1033:G:H2'	32:1a:1034:G:H8	1.61	0.65
37:2f:67:MET:HE1	37:2f:75:LEU:HD22	1.78	0.65
32:1a:1366:C:O2'	41:1j:60:ARG:NH1	2.30	0.65
35:2d:153:ARG:HH11	35:2d:181:MET:HE3	1.62	0.65
37:2f:97:PHE:HD2	49:2r:31:LEU:HD11	1.62	0.65
1:1A:359:C:H4'	20:1Y:73:ARG:HD3	1.79	0.65
1:2A:900:A:O2'	1:2A:901:A:OP1	2.13	0.65
1:2A:1920:4OC:HM22	1:2A:1921:G:H5'	1.77	0.65
41:2j:49:VAL:HG23	45:2n:41:ARG:HB2	1.78	0.65
1:1A:2658:C:OP2	1:1A:2745:G:O2'	2.15	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1T:51:ARG:HB2	15:1T:98:LYS:HD3	1.79	0.64
36:1e:110:LEU:HD13	36:1e:118:ILE:HG21	1.79	0.64
50:1s:50:ALA:HB1	50:1s:57:HIS:HB3	1.78	0.64
7:2H:159:GLU:HG3	7:2H:169:VAL:HG11	1.80	0.64
48:2q:66:SER:O	48:2q:70:ARG:NH1	2.30	0.64
1:1A:1700:G:H3'	13:1R:2:ARG:HD3	1.79	0.64
1:1A:2600:G:OP1	61:1A:4279:HOH:O	2.15	0.64
32:2a:1004:A:H5''	32:2a:1024:G:H22	1.60	0.64
1:1A:303:C:H42	1:1A:385:G:H1	1.45	0.64
1:1A:408:G:N7	61:1A:4360:HOH:O	2.30	0.64
34:1c:131:ARG:HH11	34:1c:166:GLU:HG3	1.62	0.64
4:2E:28:ALA:HB3	4:2E:93:VAL:HG12	1.79	0.64
17:2V:43:GLU:OE1	17:2V:43:GLU:N	2.29	0.64
32:2a:959:A:O2'	32:2a:984:C:O2'	2.14	0.64
49:2r:52:PRO:HB2	49:2r:54:ARG:HG2	1.79	0.64
32:1a:1373:G:H5''	38:1g:36:LYS:HE2	1.80	0.64
37:1f:36:ARG:NH2	37:1f:66:GLU:OE1	2.30	0.64
1:2A:2025:C:OP2	61:2A:3966:HOH:O	2.15	0.64
32:2a:984:C:H2'	32:2a:985:C:H6	1.63	0.64
1:1A:1219:A:H4'	1:1A:1220:U:OP1	1.97	0.64
1:1A:2149:G:N2	1:1A:2183:C:N3	2.35	0.64
37:1f:8:ILE:HD11	37:1f:79:LEU:HD13	1.80	0.64
46:1o:39:LEU:HD22	46:1o:56:LEU:HD13	1.78	0.64
24:22:32:LEU:HD11	24:22:54:LYS:HG2	1.78	0.64
33:2b:185:ILE:HG22	33:2b:199:TYR:HB2	1.79	0.64
43:2l:32:PHE:HB3	43:2l:84:LEU:HD11	1.78	0.64
44:2m:78:ILE:HA	44:2m:81:LEU:HD12	1.78	0.64
1:1A:2155:G:O2'	1:1A:2178:G:N2	2.29	0.64
10:1O:122:LEU:HD13	15:1T:72:VAL:HG11	1.78	0.64
22:10:9:SER:O	61:10:201:HOH:O	2.14	0.64
32:1a:642:A:N3	39:1h:113:SER:OG	2.27	0.64
6:2G:39:ILE:HG12	6:2G:157:ILE:HG12	1.78	0.64
1:1A:902:G:N7	61:1A:4359:HOH:O	2.30	0.64
17:1V:5:VAL:HG21	17:1V:35:LEU:HD23	1.79	0.64
25:13:7:LYS:HB2	25:13:34:GLU:HG3	1.79	0.64
21:2Z:77:ASP:OD2	21:2Z:80:ARG:NH1	2.31	0.64
32:2a:157:G:H1	32:2a:164:U:H3	1.45	0.64
1:1A:855:G:OP1	61:1A:4280:HOH:O	2.15	0.64
1:2A:1779:U:OP2	61:2A:3967:HOH:O	2.15	0.64
1:1A:1100:A:N6	1:1A:1151:U:H3	1.93	0.64
4:1E:122:PHE:O	61:1E:402:HOH:O	2.15	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1I:101:LEU:HD22	8:1I:107:VAL:HB	1.80	0.64
12:1Q:111:GLU:OE2	12:1Q:133:ARG:NH2	2.29	0.64
1:2A:271(H):G:H2'	1:2A:271(I):G:H8	1.62	0.64
1:2A:1443:G:N7	61:2A:4050:HOH:O	2.30	0.64
32:2a:1003:G:N2	32:2a:1025:U:O4	2.30	0.64
32:2a:1263:C:N4	32:2a:1271:G:O6	2.30	0.64
47:2p:18:ARG:HD3	47:2p:35:LYS:HD2	1.78	0.64
32:1a:150:C:H42	32:1a:171:A:H62	1.45	0.63
35:1d:7:PRO:HB2	35:1d:10:ARG:HD2	1.80	0.63
32:2a:157:G:H2'	32:2a:158:G:H8	1.63	0.63
41:2j:47:PHE:N	41:2j:63:PHE:O	2.29	0.63
28:26:34:LEU:HB2	28:26:51:GLU:HB3	1.80	0.63
35:2d:119:GLN:HG3	35:2d:123:HIS:HD2	1.63	0.63
1:1A:325:G:OP2	20:1Y:84:ARG:NH2	2.31	0.63
1:1A:809:U:OP1	61:1A:4278:HOH:O	2.15	0.63
8:1I:92:VAL:HG13	8:1I:120:ILE:HB	1.81	0.63
12:1Q:30:GLY:HA2	12:1Q:107:ALA:HB2	1.79	0.63
36:1e:78:HIS:CE1	36:1e:143:ARG:H	2.15	0.63
40:2i:28:VAL:HG22	40:2i:63:ILE:HB	1.81	0.63
9:1N:70:LYS:HD3	9:1N:87:LEU:HD12	1.80	0.63
35:1d:194:LEU:HB3	35:1d:196:LEU:HD13	1.80	0.63
12:2Q:141:GLN:NE2	21:2Z:74:VAL:O	2.31	0.63
1:1A:2521:G:N3	61:1A:4366:HOH:O	2.30	0.63
1:2A:752:A:H3'	29:27:1:MET:HE1	1.78	0.63
32:2a:861:G:O2'	32:2a:874:G:O2'	2.16	0.63
1:1A:1959:A:H1'	1:1A:1961:5MU:H72	1.81	0.63
3:1D:237:GLU:OE2	61:1D:401:HOH:O	2.16	0.63
1:2A:1780:A:N7	61:2A:4064:HOH:O	2.31	0.63
1:2A:2375:G:N2	1:2A:2378:A:OP2	2.31	0.63
32:2a:442:C:H42	32:2a:492:G:H1	1.44	0.63
32:2a:1412:C:H2'	32:2a:1413:A:C8	2.34	0.63
3:1D:17:THR:O	3:1D:211:ARG:NH2	2.32	0.63
39:1h:17:THR:O	39:1h:78:GLN:NE2	2.30	0.63
8:2I:116:LEU:HD11	8:2I:120:ILE:HG13	1.81	0.63
9:2N:97:ARG:HA	9:2N:100:GLU:HB2	1.80	0.63
32:2a:953:G:N7	44:2m:104:ARG:NH2	2.45	0.63
32:2a:1190:G:H5'	34:2c:176:HIS:HE1	1.63	0.63
1:1A:2160:C:H42	1:1A:2175:G:H1	1.47	0.63
33:1b:118:LEU:HB3	33:1b:142:LEU:HD12	1.79	0.63
21:2Z:72:ARG:NH2	21:2Z:97:GLU:O	2.31	0.63
32:2a:1133:G:N2	32:2a:1141:C:N3	2.45	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:2h:21:LYS:O	39:2h:65:TYR:OH	2.15	0.63
54:2w:7:A:H5'	54:2w:8:4SU:H5	1.81	0.63
26:24:64:GLY:O	26:24:66:SER:N	2.29	0.63
32:2a:976:G:H5'	32:2a:1358:U:O2'	1.99	0.63
32:2a:1000:U:H3	32:2a:1041:A:H61	1.46	0.63
33:2b:100:GLY:N	33:2b:176:GLU:OE2	2.29	0.63
40:2i:85:LEU:HB3	40:2i:92:TYR:HD2	1.64	0.63
32:1a:1518:MA6:N6	32:1a:1519:MA6:H103	2.14	0.62
39:1h:21:LYS:O	39:1h:65:TYR:OH	2.16	0.62
41:1j:38:ILE:HD11	41:1j:71:LEU:HD23	1.81	0.62
1:2A:2125:G:H1'	1:2A:2173:A:H61	1.64	0.62
4:2E:47:VAL:HG11	4:2E:86:PRO:HD2	1.80	0.62
5:2F:40:GLN:NE2	5:2F:182:ASN:HB2	2.13	0.62
13:2R:51:LEU:HD22	13:2R:66:VAL:HG13	1.80	0.62
17:2V:98:GLU:OE2	17:2V:100:ARG:NH1	2.32	0.62
34:2c:18:TRP:O	34:2c:21:ARG:NH2	2.32	0.62
50:2s:38:SER:HB2	50:2s:71:LEU:HD22	1.81	0.62
7:1H:86:GLU:OE2	7:1H:132:ARG:NH2	2.32	0.62
32:2a:1134:G:H1	32:2a:1140:C:H42	1.47	0.62
22:10:11:ARG:O	22:10:14:ARG:NH2	2.32	0.62
33:1b:16:HIS:HB3	33:1b:210:SER:HB2	1.81	0.62
51:1t:57:ARG:HH12	51:1t:100:ILE:HD12	1.64	0.62
54:1y:13:C:H2'	54:1y:14:A:H5''	1.81	0.62
1:2A:2066:C:OP1	61:2A:3969:HOH:O	2.16	0.62
34:2c:20:SER:HB3	34:2c:22:TRP:HE1	1.64	0.62
26:14:61:ARG:HH21	50:1s:42:PRO:HD3	1.64	0.62
34:1c:3:ASN:OD1	34:1c:3:ASN:N	2.31	0.62
40:1i:50:LEU:HA	40:1i:53:VAL:HG22	1.81	0.62
32:2a:959:A:HO2'	32:2a:984:C:HO2'	1.47	0.62
1:2A:568:U:H5'	1:2A:945:A:N1	2.14	0.62
1:1A:1613:A:OP1	3:1D:211:ARG:NH1	2.33	0.62
1:1A:2084:A:OP1	61:1A:4282:HOH:O	2.16	0.62
24:12:55:ARG:NH2	61:12:3101:HOH:O	2.32	0.62
32:1a:649:G:H2'	32:1a:650:G:H8	1.64	0.62
6:2G:15:VAL:HG22	6:2G:175:LEU:HB3	1.82	0.62
13:2R:24:GLN:HE22	13:2R:36:THR:HG21	1.65	0.62
55:2x:47:U:N3	55:2x:50:U:OP1	2.32	0.62
15:1T:109:GLU:O	15:1T:113:LYS:HG2	2.00	0.62
1:2A:1021:A:H62	1:2A:1141:U:H3	1.45	0.62
32:2a:263:A:OP1	51:2t:79:ARG:NH1	2.31	0.62
1:1A:238:C:O2	30:18:12:LYS:NZ	2.29	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:2Q:10:ARG:HH22	55:2x:64:G:H4'	1.65	0.62
32:2a:274:A:N7	61:2a:3343:HOH:O	2.31	0.62
34:2c:20:SER:OG	34:2c:40:ARG:NH2	2.33	0.62
32:1a:1031:G:H2'	32:1a:1032:G:C8	2.35	0.62
34:1c:87:LEU:O	34:1c:91:LEU:N	2.30	0.62
54:1w:7:A:N6	54:1w:66:U:H3	1.97	0.62
1:2A:2143:C:H42	1:2A:2148:G:H1	1.46	0.62
2:2B:32:C:H42	2:2B:50:G:H1	1.48	0.62
32:2a:1255:G:OP1	41:2j:45:ARG:NH2	2.32	0.62
32:2a:1376:U:H2'	32:2a:1377:A:C8	2.35	0.62
34:2c:42:LEU:HA	34:2c:45:LYS:HE2	1.81	0.62
1:1A:419:C:OP1	61:1A:4272:HOH:O	2.16	0.62
1:1A:2008:A:OP1	61:1A:4281:HOH:O	2.16	0.62
1:1A:2807:C:H42	1:1A:2813:G:H22	1.48	0.62
8:1I:75:LEU:HD22	8:1I:105:HIS:CD2	2.35	0.62
32:1a:1002:G:H3'	32:1a:1003:G:C4'	2.30	0.62
1:2A:854:G:H2'	1:2A:855:G:C8	2.34	0.62
1:2A:2805:G:H2'	1:2A:2807:G:C8	2.35	0.62
15:2T:65:LYS:HE3	15:2T:67:SER:HB2	1.80	0.62
33:2b:88:ALA:HB2	33:2b:219:VAL:HG13	1.81	0.62
1:2A:392:C:H5''	1:2A:409:C:H5''	1.82	0.61
1:1A:718:C:N4	61:1A:4379:HOH:O	2.32	0.61
1:1A:739:C:O2'	3:1D:38:LYS:NZ	2.29	0.61
1:1A:2790:G:O6	61:1A:4276:HOH:O	2.14	0.61
33:1b:16:HIS:HD2	33:1b:204:ASN:H	1.46	0.61
1:2A:2313:C:H5''	6:2G:91:ARG:HD3	1.81	0.61
32:2a:446:G:H1	32:2a:488:C:H42	1.48	0.61
32:2a:1347:G:HO2'	32:2a:1373:G:H1	1.47	0.61
32:2a:1402:4OC:HM22	32:2a:1403:C:H5'	1.81	0.61
52:2u:2:GLY:N	61:2u:101:HOH:O	2.32	0.61
1:1A:2849:G:N2	13:1R:91:GLN:O	2.28	0.61
1:2A:992:C:OP1	16:2U:47:TYR:OH	2.15	0.61
3:2D:148:GLU:HB2	3:2D:151:LYS:HD2	1.83	0.61
5:2F:185:ASP:OD1	5:2F:188:ARG:NH1	2.33	0.61
32:2a:107:G:N7	51:2t:15:ARG:NH2	2.47	0.61
32:2a:1007:C:N3	32:2a:1022:G:O6	2.33	0.61
12:1Q:51:ARG:HD3	12:1Q:66:ILE:HD11	1.82	0.61
1:2A:1446:C:H42	1:2A:1465:G:H1	1.48	0.61
5:2F:110:LEU:HD21	5:2F:181:LEU:HD23	1.82	0.61
32:2a:137:C:H2'	32:2a:138:G:H8	1.65	0.61
32:2a:1147:C:O2	40:2i:16:ARG:NH1	2.34	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1187:G:H5'	40:2i:113:LYS:HE3	1.83	0.61
39:2h:9:MET:HG3	39:2h:26:VAL:HG11	1.82	0.61
32:1a:159:G:N2	32:1a:162:A:OP2	2.34	0.61
1:2A:84:A:H5''	20:2Y:8:LYS:HE3	1.82	0.61
1:2A:2143:C:H2'	1:2A:2144:U:O4'	2.00	0.61
32:2a:188:C:H42	32:2a:189(L):G:H1	1.47	0.61
32:2a:201:C:H42	32:2a:216:G:H1	1.48	0.61
47:2p:22:THR:HA	47:2p:33:ILE:HG13	1.83	0.61
7:1H:7:LEU:HD12	7:1H:8:PRO:HD2	1.82	0.61
32:1a:715:A:H2'	32:1a:716:A:C8	2.35	0.61
1:2A:1693:U:H1'	3:2D:14:ARG:NH2	2.16	0.61
1:2A:2511:U:O2'	4:2E:138:PRO:O	2.16	0.61
1:2A:2513:G:N2	4:2E:143:ASN:OD1	2.34	0.61
32:2a:975:A:H4'	32:2a:976:G:H5''	1.82	0.61
54:2y:15:G:H22	54:2y:48:C:N4	1.99	0.61
1:1A:927:G:H2'	1:1A:928:G:C8	2.34	0.61
4:2E:116:VAL:HG13	4:2E:122:PHE:HB2	1.83	0.61
32:2a:523:A:H61	43:2l:92:0TD:CG	2.14	0.61
32:2a:1114:C:H42	32:2a:1186:G:H1	1.48	0.61
32:2a:1032:G:H2'	32:2a:1033:G:C8	2.35	0.61
32:2a:1128:C:O2'	32:2a:1147:C:N3	2.30	0.61
11:1P:59:LEU:HD11	30:18:10:ALA:HB2	1.82	0.61
32:1a:946:A:H2'	32:1a:947:G:C8	2.36	0.61
32:1a:1194:U:H4'	36:1e:22:GLY:HA2	1.82	0.61
5:2F:140:LEU:HD11	5:2F:170:LEU:HD11	1.83	0.61
11:2P:63:PRO:HG2	30:28:25:MET:HB2	1.83	0.61
21:2Z:4:ARG:HG2	21:2Z:58:VAL:HB	1.81	0.61
32:2a:1005:A:H5''	32:2a:1006:C:C5	2.35	0.61
1:1A:1151:U:H2'	1:1A:1152:G:H8	1.64	0.61
1:1A:2695:C:O2	10:1O:70:LYS:NZ	2.34	0.61
6:1G:43:LEU:HD11	6:1G:153:ARG:HD2	1.82	0.61
46:1o:11:VAL:HG21	46:1o:34:LEU:HD22	1.82	0.61
1:2A:908:C:OP2	12:2Q:22:LYS:NZ	2.33	0.61
1:2A:958:U:O2	2:2B:90:A:O2'	2.15	0.61
1:2A:1141:U:OP2	9:2N:63:THR:OG1	2.16	0.61
32:2a:1011:G:H1	32:2a:1018:C:H42	1.48	0.61
34:2c:37:GLN:NE2	45:2n:52:GLN:OE1	2.24	0.61
1:1A:2157:A:H5'	1:1A:2182:G:H4'	1.82	0.60
13:1R:67:LEU:HD13	13:1R:76:VAL:HG21	1.83	0.60
32:1a:1030(A):G:H1'	32:1a:1031:G:H1	1.66	0.60
1:2A:2689:U:H4'	1:2A:2690:C:H5'	1.81	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:15:G:H4'	36:2e:24:ARG:HE	1.65	0.60
1:1A:2481:A:O2'	12:1Q:56:ARG:NH1	2.34	0.60
32:2a:489:C:H2'	32:2a:490:G:H8	1.65	0.60
32:2a:660:G:H1	32:2a:745:C:H42	1.49	0.60
32:2a:1240:U:N3	38:2g:30:ILE:O	2.31	0.60
1:1A:1228:G:O2'	25:13:29:ARG:NH1	2.33	0.60
5:1F:185:ASP:HA	5:1F:188:ARG:HD3	1.82	0.60
7:1H:154:PRO:HB3	7:1H:163:TYR:CZ	2.36	0.60
32:1a:1015:A:N3	32:1a:1218:C:O2'	2.35	0.60
38:1g:78:ARG:HG2	38:1g:79:ARG:H	1.66	0.60
39:2h:10:LEU:HD22	39:2h:83:ILE:HD11	1.83	0.60
1:1A:847:A:H8	1:1A:847:A:OP1	1.84	0.60
39:1h:110:ALA:HB3	39:1h:121:ASP:HB3	1.84	0.60
44:1m:17:VAL:O	44:1m:20:THR:OG1	2.20	0.60
2:2B:24:G:N7	2:2B:56:G:H2'	2.17	0.60
32:2a:1242:C:H42	32:2a:1295:G:H1	1.49	0.60
33:2b:115:LEU:O	33:2b:119:GLU:N	2.32	0.60
34:2c:58:GLU:HB3	41:2j:92:THR:HG21	1.82	0.60
46:2o:4:THR:OG1	46:2o:7:GLU:OE1	2.20	0.60
1:1A:1599:G:N7	61:1A:4363:HOH:O	2.30	0.60
1:2A:624:C:OP1	61:2A:3968:HOH:O	2.15	0.60
32:2a:953:G:H5'	32:2a:965:A:N6	2.15	0.60
33:2b:74:LYS:HD2	33:2b:166:ASP:HB2	1.82	0.60
51:2t:43:LEU:O	51:2t:47:GLY:N	2.31	0.60
1:1A:2482:G:H5'	12:1Q:56:ARG:HH22	1.66	0.60
4:1E:47:VAL:HG11	4:1E:86:PRO:HD2	1.83	0.60
11:1P:59:LEU:HD21	30:18:10:ALA:HA	1.84	0.60
21:1Z:153:SER:HB3	21:1Z:167:PRO:HB3	1.83	0.60
1:2A:1225:G:H4'	17:2V:84:LYS:HG2	1.83	0.60
32:2a:1132:C:H42	32:2a:1142:G:H1	1.50	0.60
1:1A:2442:A:H2'	1:1A:2442:A:N3	2.17	0.60
3:1D:12:SER:HB3	3:1D:208:LYS:HB3	1.84	0.60
21:2Z:144:LEU:HD23	21:2Z:174:VAL:HG12	1.83	0.60
35:2d:191:ARG:NH1	35:2d:194:LEU:O	2.34	0.60
1:1A:345:G:N3	5:1F:165:ARG:HD2	2.17	0.60
1:1A:409:G:N7	61:1A:4374:HOH:O	2.32	0.60
3:1D:83:GLU:OE1	3:1D:104:TYR:OH	2.13	0.60
32:1a:677:U:H3	32:1a:713:G:H22	1.48	0.60
1:2A:142(A):C:OP1	61:2A:3973:HOH:O	2.17	0.60
6:2G:47:LYS:HG3	6:2G:48:GLU:H	1.66	0.60
34:2c:43:LEU:HD21	34:2c:91:LEU:HD13	1.82	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:1O:64:ARG:HG2	10:1O:83:ALA:HB3	1.83	0.60
24:12:51:ARG:HD3	24:12:55:ARG:HH11	1.67	0.60
1:1A:1291:G:OP1	11:1P:13:ASN:ND2	2.28	0.59
32:1a:1097:C:O2'	32:1a:1169:A:N3	2.35	0.59
1:2A:89:G:H3'	1:2A:90:U:H5''	1.84	0.59
1:2A:2875:C:O2'	15:2T:2:ASN:OD1	2.18	0.59
6:2G:64:THR:HB	6:2G:94:LEU:HD21	1.83	0.59
19:2X:53:LYS:HB3	19:2X:82:GLN:HB3	1.84	0.59
1:1A:2801:C:OP1	4:1E:61:ARG:NH2	2.36	0.59
34:1c:150:LYS:HE3	34:1c:152:ILE:HD11	1.83	0.59
42:1k:79:SER:HA	42:1k:104:GLN:HB3	1.84	0.59
1:2A:1627:G:OP1	61:2A:3971:HOH:O	2.16	0.59
54:2w:30:G:H1	54:2w:40:C:N4	2.01	0.59
1:1A:64:C:O2'	1:1A:482:C:N3	2.35	0.59
1:2A:2048:G:N7	61:2A:4068:HOH:O	2.31	0.59
26:24:24:THR:OG1	26:24:25:TYR:N	2.28	0.59
32:2a:401:C:O2'	32:2a:621:A:N3	2.28	0.59
32:2a:909:A:N3	32:2a:1413:A:O2'	2.30	0.59
32:2a:1304:G:O2'	32:2a:1333:A:N6	2.35	0.59
32:2a:1406:U:H3'	32:2a:1407:5MC:HM53	1.85	0.59
51:2t:49:ALA:HB3	51:2t:99:LEU:HD13	1.84	0.59
33:1b:30:ARG:HH21	33:1b:194:PRO:HB2	1.67	0.59
10:2O:88:ASN:HD21	10:2O:92:GLU:HB2	1.67	0.59
32:2a:1030(A):G:N2	32:2a:1030(D):A:OP2	2.31	0.59
1:1A:1263:C:H42	1:1A:1277:G:H1	1.51	0.59
33:1b:16:HIS:CG	33:1b:17:PHE:N	2.71	0.59
1:2A:583:G:O6	61:2A:3965:HOH:O	2.15	0.59
1:2A:586:A:H5'	5:2F:89:VAL:HG21	1.85	0.59
1:2A:2305:A:H5''	6:2G:134:GLY:HA3	1.84	0.59
32:2a:1000:U:H3	32:2a:1041:A:N6	2.01	0.59
35:2d:64:LEU:HB2	35:2d:198:VAL:HG11	1.85	0.59
1:1A:692:C:H42	1:1A:698:G:H1	1.50	0.59
1:1A:1094:A:OP2	1:1A:1155:C:N4	2.35	0.59
7:1H:113:VAL:HG11	7:1H:151:ILE:HG21	1.84	0.59
44:1m:80:ARG:HH21	50:1s:69:HIS:HE1	1.50	0.59
1:2A:2058:A:N7	61:2A:4058:HOH:O	2.30	0.59
8:2I:110:ASP:H	8:2I:130:TYR:HH	1.51	0.59
9:2N:123:TYR:OH	9:2N:130:HIS:NE2	2.30	0.59
48:2q:45:HIS:HB2	48:2q:65:ILE:HD13	1.84	0.59
1:1A:2133:C:N4	1:1A:2166:U:O2'	2.34	0.59
1:1A:2434:A:O4'	54:1y:76:A:N6	2.35	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1074:G:O2'	32:1a:1101:A:N1	2.33	0.59
36:1e:137:GLU:OE1	36:1e:140:ARG:NH1	2.31	0.59
1:2A:882:G:H2'	1:2A:883:G:H8	1.67	0.59
1:2A:1155:A:H5''	16:2U:55:ARG:HH11	1.65	0.59
32:2a:396:G:O2'	32:2a:398:C:OP1	2.17	0.59
40:2i:9:ARG:HG2	40:2i:14:VAL:HG12	1.83	0.59
54:2w:28:G:H2'	54:2w:29:G:O4'	2.03	0.59
1:1A:2034:G:OP2	18:1W:16:LYS:NZ	2.36	0.59
3:2D:145:VAL:HG13	3:2D:191:ALA:HB2	1.84	0.59
6:2G:44:GLY:N	6:2G:88:ILE:O	2.35	0.59
34:2c:11:ARG:HB3	34:2c:15:THR:HB	1.84	0.59
40:2i:8:GLY:HA2	40:2i:79:LEU:HD23	1.84	0.59
51:2t:9:ASN:O	51:2t:10:LEU:HB2	2.02	0.59
1:1A:1553:A:O2'	1:1A:1556:A:N6	2.35	0.59
32:1a:1006:C:H42	32:1a:1023:G:H1	1.49	0.59
47:2p:52:ASP:HB3	47:2p:55:ARG:HB2	1.83	0.59
37:1f:37:VAL:HA	37:1f:65:VAL:HG12	1.84	0.59
1:2A:1796:U:H2'	1:2A:1797:C:C6	2.38	0.59
1:2A:2705:A:O2'	1:2A:2852:G:OP1	2.19	0.59
4:2E:7:VAL:HG12	4:2E:27:LEU:HB3	1.85	0.59
32:2a:1011:G:H1	32:2a:1018:C:N4	2.01	0.59
35:2d:196:LEU:H	35:2d:196:LEU:HD12	1.68	0.59
40:2i:26:VAL:HG22	40:2i:61:ALA:HB3	1.83	0.59
3:1D:242:ARG:O	61:1D:402:HOH:O	2.17	0.58
1:2A:2141:G:O6	1:2A:2150:U:O2	2.21	0.58
7:2H:23:ARG:NH1	7:2H:34:GLU:OE1	2.36	0.58
32:2a:407:G:OP1	35:2d:115:ARG:HD3	2.02	0.58
32:2a:1029:C:N3	32:2a:1032:G:N2	2.51	0.58
32:2a:1190:G:H5'	34:2c:176:HIS:CE1	2.38	0.58
1:1A:194:G:O6	23:11:39:LYS:NZ	2.36	0.58
7:1H:15:VAL:HG21	7:1H:76:VAL:HG13	1.85	0.58
1:2A:143:G:H2'	1:2A:143(A):C:C6	2.37	0.58
1:2A:2206:G:H3'	1:2A:2207:G:C8	2.37	0.58
1:2A:2317:C:N4	1:2A:2318:G:O6	2.37	0.58
32:2a:736:C:H2'	32:2a:737:A:C8	2.38	0.58
34:2c:32:LEU:HD23	34:2c:59:ARG:HD3	1.84	0.58
11:1P:50:ARG:HD3	30:18:7:HIS:HD2	1.66	0.58
32:1a:1004:A:H5'	32:1a:1024:G:H1	1.68	0.58
32:1a:1064:G:O2'	32:1a:1190:G:N2	2.36	0.58
1:2A:2131:G:N7	1:2A:2133:G:N2	2.51	0.58
18:1W:78:GLU:OE2	18:1W:99:ARG:NH1	2.30	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:1s:27:GLU:OE1	50:1s:27:GLU:N	2.33	0.58
1:2A:597:U:H2'	1:2A:598:G:C8	2.39	0.58
1:2A:861:A:N3	2:2B:79:C:O2'	2.36	0.58
1:2A:2537:U:H2'	1:2A:2538:C:C6	2.38	0.58
1:1A:2556:G:H1'	1:1A:2658:C:H4'	1.85	0.58
1:1A:2803:A:H5'	1:1A:2902:G:H21	1.69	0.58
33:1b:16:HIS:CD2	33:1b:204:ASN:H	2.22	0.58
11:2P:100:LEU:HD12	11:2P:112:LEU:HD11	1.85	0.58
1:1A:1110:C:O2	1:1A:1120:G:N1	2.21	0.58
8:1I:109:ILE:HG13	8:1I:130:TYR:CZ	2.39	0.58
32:1a:407:G:H5''	35:1d:115:ARG:HG2	1.85	0.58
37:1f:11:ASN:HB3	37:1f:14:LEU:HG	1.84	0.58
1:2A:577:G:O2'	1:2A:1254:A:OP1	2.22	0.58
32:2a:11:G:H1	32:2a:23:C:H42	1.50	0.58
32:2a:748:C:H4'	32:2a:749:C:O5'	2.04	0.58
34:2c:11:ARG:NH2	34:2c:177:THR:O	2.36	0.58
40:2i:50:LEU:HD13	40:2i:56:LEU:HA	1.84	0.58
1:1A:1346:U:H4'	1:1A:1347:A:H5''	1.83	0.58
1:1A:1712:A:OP2	61:1A:4225:HOH:O	2.16	0.58
32:1a:976:G:H5'	32:1a:1358:U:O2'	2.03	0.58
54:1y:50:U:O4	54:1y:64:A:N1	2.37	0.58
1:2A:307:G:H21	1:2A:330:A:H62	1.52	0.58
3:2D:71:ASP:HB3	3:2D:103:ARG:HH12	1.68	0.58
32:1a:1027:C:N4	32:1a:1034:G:C6	2.71	0.58
43:1l:70:ILE:HG12	43:1l:100:ILE:HD12	1.85	0.58
1:2A:2012:G:OP1	18:2W:11:ARG:NH2	2.35	0.58
32:2a:35:G:O2'	43:2l:118:SER:O	2.19	0.58
32:2a:1106:G:H5''	34:2c:172:ARG:HG3	1.85	0.58
48:2q:58:GLU:O	48:2q:74:LEU:N	2.36	0.58
1:1A:1139:G:H3'	1:1A:1140:U:H5''	1.84	0.58
1:1A:1466:U:O2'	1:1A:1467:G:OP1	2.21	0.58
5:1F:195:ASP:HB3	5:1F:198:ALA:H	1.68	0.58
32:1a:619:U:N3	35:1d:134:ASP:OD1	2.35	0.58
32:1a:997:U:H3	32:1a:1044:A:H61	1.51	0.58
1:2A:2818:G:OP2	13:2R:42:LYS:NZ	2.36	0.58
20:2Y:13:VAL:HG12	20:2Y:74:PRO:HA	1.85	0.58
1:1A:599:U:O4	61:1A:4284:HOH:O	2.17	0.58
1:1A:2175:G:H2'	1:1A:2176:G:C8	2.39	0.58
32:1a:1029:C:H41	32:1a:1030(A):G:N2	2.02	0.58
1:2A:1264:G:OP1	27:25:19:ARG:NH2	2.20	0.58
1:2A:2136:C:O2'	1:2A:2137:C:O5'	2.21	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:2Q:111:GLU:O	12:2Q:115:MET:HG2	2.04	0.58
19:2X:43:VAL:HG21	19:2X:81:VAL:HG11	1.86	0.58
32:2a:1301:U:O2'	32:2a:1302:U:H5'	2.04	0.58
32:2a:1315:U:O2'	32:2a:1360:A:N3	2.27	0.58
35:2d:11:LEU:HD23	35:2d:66:ARG:HB3	1.86	0.58
1:1A:704:U:H2'	1:1A:705:C:C6	2.39	0.57
1:1A:1121:C:H2'	1:1A:1122:C:H5'	1.86	0.57
1:1A:1817:A:H1'	1:1A:1960:A:N6	2.18	0.57
32:1a:701:C:OP1	32:1a:702:A:O2'	2.18	0.57
17:2V:76:LYS:HB2	17:2V:81:TYR:HB3	1.85	0.57
20:2Y:102:CYS:SG	20:2Y:103:GLY:N	2.77	0.57
32:2a:148:G:H2'	32:2a:149:A:C8	2.39	0.57
1:1A:1108:G:H1	1:1A:1123:A:H61	1.51	0.57
32:1a:532:A:N6	32:1a:1206:G:O2'	2.37	0.57
32:1a:1083:U:OP1	61:1a:3324:HOH:O	2.17	0.57
32:1a:1350:A:O2'	38:1g:33:ASP:OD1	2.21	0.57
1:2A:616:G:H5'	5:2F:205:ARG:HD3	1.86	0.57
11:2P:126:VAL:HG12	11:2P:148:LEU:HD23	1.86	0.57
32:2a:34:C:H2'	32:2a:35:G:C8	2.40	0.57
32:2a:123:C:OP1	32:2a:311:C:O2'	2.19	0.57
32:2a:1183:A:O2'	32:2a:1184:G:OP1	2.22	0.57
32:2a:1356:G:H2'	32:2a:1357:A:C8	2.39	0.57
44:2m:54:VAL:HA	44:2m:57:ARG:HB3	1.86	0.57
1:1A:1589:A:O2'	61:1A:4224:HOH:O	2.14	0.57
11:1P:52:GLU:OE1	11:1P:55:ARG:NH1	2.37	0.57
32:1a:184:G:H2'	32:1a:185:A:H8	1.70	0.57
32:1a:1075:C:OP1	33:1b:179:LYS:NZ	2.29	0.57
34:1c:15:THR:HG21	34:1c:181:ASN:HA	1.85	0.57
35:1d:62:GLN:HE21	35:1d:66:ARG:HH21	1.52	0.57
1:2A:947:G:H2'	1:2A:948:G:C8	2.39	0.57
1:2A:947:G:H2'	1:2A:948:G:H8	1.69	0.57
1:2A:1356:G:O6	61:2A:3961:HOH:O	2.13	0.57
1:2A:1507:A:O2'	1:2A:1508:A:O5'	2.22	0.57
32:2a:309:G:O2'	32:2a:607:A:N1	2.37	0.57
32:2a:489:C:H2'	32:2a:490:G:C8	2.39	0.57
32:2a:578:C:OP1	61:2a:3320:HOH:O	2.17	0.57
32:1a:674:G:H2'	32:1a:675:A:H8	1.70	0.57
32:1a:1225:A:N6	61:1a:3366:HOH:O	2.37	0.57
11:2P:52:GLU:OE1	11:2P:55:ARG:NH1	2.26	0.57
32:2a:362:G:N2	32:2a:365:U:OP2	2.37	0.57
1:2A:514:A:N3	1:2A:581:C:O2'	2.35	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:974:G:OP1	1:2A:1187:G:O2'	2.18	0.57
9:2N:128:HIS:O	9:2N:131:GLN:NE2	2.38	0.57
1:1A:2166:U:H3	1:1A:2169:G:H22	1.52	0.57
18:1W:13:SER:HB3	18:1W:16:LYS:HD2	1.85	0.57
32:1a:45:U:H2'	32:1a:46:G:C8	2.40	0.57
32:1a:376:G:O3'	47:1p:5:ARG:NH1	2.30	0.57
35:1d:98:GLU:OE1	35:1d:103:ASN:ND2	2.37	0.57
39:1h:51:VAL:HG12	39:1h:52:ASP:H	1.69	0.57
44:1m:27:LYS:NZ	61:1m:5001:HOH:O	2.36	0.57
1:2A:840:C:OP2	1:2A:932:G:N2	2.31	0.57
1:2A:857:C:OP2	22:20:77:ARG:NH2	2.38	0.57
5:2F:9:ILE:HG21	5:2F:125:LEU:HD13	1.87	0.57
5:2F:187:VAL:HG12	11:2P:3:LEU:HD12	1.87	0.57
32:2a:1226:C:H4'	50:2s:80:TYR:CZ	2.39	0.57
46:2o:54:ARG:HG2	46:2o:58:MET:HE2	1.86	0.57
1:1A:1362:U:H2'	1:1A:1363:A:C8	2.40	0.57
14:1S:11:LYS:HG3	14:1S:91:PRO:HD3	1.86	0.57
32:1a:401:C:H2'	32:1a:402:G:C8	2.40	0.57
32:1a:911:U:OP2	43:1l:97:ARG:NH2	2.35	0.57
33:1b:73:THR:OG1	33:1b:170:GLU:OE2	2.20	0.57
1:2A:796:C:H2'	1:2A:797:C:C6	2.40	0.57
1:2A:2741:A:H5''	31:29:22:ARG:HH22	1.68	0.57
10:2O:115:VAL:HG13	10:2O:121:VAL:HG21	1.86	0.57
32:2a:839:U:H3'	32:2a:840:C:H6	1.68	0.57
26:14:55:ARG:H	26:14:56:VAL:HA	1.70	0.57
40:1i:42:ARG:NH2	40:1i:75:ASP:OD1	2.38	0.57
1:2A:2683:C:OP1	15:2T:53:ARG:NH2	2.33	0.57
25:23:11:SER:HA	25:23:31:LEU:HD21	1.86	0.57
32:2a:253:U:H2'	32:2a:254:G:H8	1.70	0.57
32:2a:952:U:H2'	32:2a:953:G:H8	1.69	0.57
32:2a:987:G:H1	32:2a:1218:C:H42	1.53	0.57
32:2a:1264:C:N3	32:2a:1271:G:N2	2.45	0.57
4:1E:119:ARG:HD2	4:1E:160:TYR:HB2	1.87	0.57
32:1a:255:G:OP1	48:1q:69:LYS:NZ	2.38	0.57
1:2A:300:A:OP1	20:2Y:86:ARG:NH2	2.38	0.57
1:2A:907:U:O2'	12:2Q:101:ARG:NH2	2.38	0.57
21:2Z:52:SER:OG	21:2Z:53:ILE:N	2.29	0.57
42:2k:48:ILE:O	42:2k:50:TYR:N	2.37	0.57
1:1A:1241:C:HO2'	1:1A:1273:G:HO2'	1.51	0.56
1:1A:2318:C:O2	61:1A:4285:HOH:O	2.17	0.56
32:1a:1191:A:OP1	34:1c:4:LYS:NZ	2.28	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1d:170:VAL:HG12	35:1d:171:GLY:H	1.68	0.56
1:2A:247:G:H4'	1:2A:386:G:C5	2.40	0.56
1:2A:800:A:H8	1:2A:800:A:OP1	1.87	0.56
3:2D:45:ASN:OD1	3:2D:45:ASN:N	2.38	0.56
32:2a:1376:U:H2'	32:2a:1377:A:H8	1.70	0.56
33:2b:178:ARG:HH12	39:2h:68:ARG:HH22	1.52	0.56
34:2c:150:LYS:HG3	34:2c:169:ALA:HB2	1.86	0.56
1:1A:2364:A:N6	1:1A:2377:G:O2'	2.38	0.56
4:1E:77:ILE:HD13	4:1E:195:LEU:HD13	1.88	0.56
32:1a:1315:U:O2'	32:1a:1360:A:O2'	2.23	0.56
1:2A:1593:G:H2'	1:2A:1594:G:C8	2.39	0.56
10:2O:64:ARG:NH1	10:2O:81:ASP:OD2	2.37	0.56
30:28:6:THR:HG22	30:28:63:PRO:HD2	1.86	0.56
32:2a:1138:G:C6	32:2a:1140:C:H1'	2.40	0.56
33:2b:98:LEU:HB2	33:2b:101:MET:HG3	1.86	0.56
1:1A:1714:G:O2'	1:1A:2013:U:O4	2.20	0.56
1:1A:2124:U:H3	1:1A:2209:G:H1	1.52	0.56
3:1D:146:GLU:HB2	3:1D:189:CYS:HB3	1.87	0.56
32:1a:951:G:OP1	61:1a:3323:HOH:O	2.17	0.56
32:1a:1391:U:H2'	32:1a:1392:G:C8	2.40	0.56
40:1i:65:VAL:HG11	40:1i:73:GLN:HB3	1.87	0.56
5:2F:24:LEU:HD23	5:2F:115:ALA:HA	1.87	0.56
11:2P:50:ARG:HD3	30:28:7:HIS:CD2	2.40	0.56
12:2Q:81:VAL:HG12	22:20:5:LYS:HD3	1.87	0.56
32:2a:34:C:H2'	32:2a:35:G:H8	1.70	0.56
32:2a:952:U:H2'	32:2a:953:G:C8	2.40	0.56
1:1A:2820:A:N6	1:1A:2900:G:O2'	2.37	0.56
2:1B:33:G:H5'	6:1G:2:PRO:HD3	1.88	0.56
7:1H:56:SER:HB3	7:1H:61:HIS:ND1	2.21	0.56
32:1a:530:G:N3	54:1w:35:A:O2'	2.34	0.56
34:1c:52:LEU:HD21	34:1c:55:VAL:HG23	1.88	0.56
4:2E:174:ASP:OD1	4:2E:175:VAL:N	2.38	0.56
13:2R:97:VAL:HG22	13:2R:114:VAL:HG22	1.87	0.56
32:2a:297:G:N2	32:2a:300:A:OP2	2.39	0.56
32:2a:1187:G:H4'	40:2i:111:ARG:HH11	1.70	0.56
32:2a:1403:C:H2'	32:2a:1404:5MC:HM53	1.87	0.56
1:1A:1151:U:H2'	1:1A:1152:G:C8	2.39	0.56
32:1a:1027:C:C4	32:1a:1034:G:N1	2.74	0.56
39:1h:124:ALA:O	39:1h:128:GLY:N	2.39	0.56
1:2A:2291:U:H2'	1:2A:2292:C:C6	2.40	0.56
1:2A:2759:G:OP2	61:2A:3976:HOH:O	2.18	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:828:A:N6	32:2a:858:G:O2'	2.36	0.56
32:2a:1226:C:OP2	44:2m:91:ARG:NH2	2.36	0.56
28:16:34:LEU:H	28:16:51:GLU:HG2	1.71	0.56
1:2A:2498:C:OP2	61:2A:3915:HOH:O	2.17	0.56
32:2a:985:C:H2'	32:2a:986:A:C8	2.40	0.56
32:2a:1305:G:N2	32:2a:1331:G:H1'	2.20	0.56
33:2b:40:HIS:HB3	33:2b:190:THR:HG21	1.86	0.56
1:1A:1338:U:H2'	1:1A:1339:C:C6	2.41	0.56
32:1a:78:G:N1	32:1a:91:C:N4	2.53	0.56
36:1e:101:ILE:O	36:1e:120:THR:OG1	2.23	0.56
1:2A:2355:C:H1'	22:20:39:ARG:HH21	1.71	0.56
32:2a:54:C:N4	32:2a:353:A:OP2	2.39	0.56
32:2a:1189:C:O2'	34:2c:176:HIS:ND1	2.36	0.56
32:2a:1251:A:H2'	32:2a:1252:A:C8	2.40	0.56
32:2a:1318:A:O2'	50:2s:37:ARG:HB2	2.06	0.56
1:1A:2175:G:H2'	1:1A:2176:G:H8	1.70	0.56
32:1a:1027:C:N3	32:1a:1034:G:N2	2.54	0.56
1:2A:1434:A:H61	1:2A:1558:A:H62	1.54	0.56
1:2A:1796:U:H2'	1:2A:1797:C:H6	1.71	0.56
4:2E:76:ARG:NH1	61:2E:403:HOH:O	2.37	0.56
17:2V:72:VAL:HG13	17:2V:85:LYS:HB3	1.88	0.56
26:24:33:VAL:HG12	26:24:34:GLU:H	1.71	0.56
1:1A:2669:A:O3'	7:1H:160:LYS:NZ	2.39	0.56
1:2A:500:G:N1	1:2A:503:A:OP2	2.39	0.56
1:2A:839:U:H2'	1:2A:840:C:C6	2.41	0.56
21:2Z:154:ASP:OD1	21:2Z:154:ASP:N	2.26	0.56
32:2a:684:A:N6	61:2a:3357:HOH:O	2.39	0.56
34:2c:155:GLY:HA3	34:2c:196:LEU:HD22	1.88	0.56
37:2f:9:VAL:HB	37:2f:87:ARG:HB2	1.86	0.56
1:1A:605:G:H2'	1:1A:606:G:C8	2.41	0.56
1:1A:880:U:O2	11:1P:55:ARG:NH2	2.38	0.56
1:1A:2549:U:H2'	1:1A:2550:C:C6	2.41	0.56
7:1H:90:LYS:HD2	7:1H:159:GLU:HG2	1.88	0.56
32:1a:17:U:H2'	32:1a:18:C:C6	2.41	0.56
32:1a:78:G:N2	32:1a:91:C:N3	2.54	0.56
33:1b:178:ARG:HH22	39:1h:74:PRO:HB3	1.70	0.56
1:2A:793:A:OP2	1:2A:2071:A:O2'	2.24	0.56
1:2A:882:G:H2'	1:2A:883:G:C8	2.42	0.56
1:2A:973:A:H8	1:2A:973:A:OP1	1.88	0.56
2:2B:42:C:N4	6:2G:91:ARG:HH12	2.04	0.56
1:1A:2160:C:N4	1:1A:2175:G:H1	2.04	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1T:60:THR:HG22	15:1T:77:PRO:HA	1.88	0.55
32:1a:429:U:OP2	35:1d:36:ARG:NH2	2.38	0.55
42:1k:84:VAL:HG21	42:1k:95:ILE:HD11	1.88	0.55
1:2A:2151:G:H2'	1:2A:2152:G:H8	1.72	0.55
32:2a:64:G:H4'	32:2a:65:U:H3'	1.88	0.55
32:2a:139:G:H2'	32:2a:140:A:H8	1.70	0.55
32:2a:973:G:H3'	32:2a:974:A:H5''	1.86	0.55
34:2c:87:LEU:O	34:2c:91:LEU:N	2.37	0.55
1:1A:1814:A:H5'	1:1A:2620:G:H4'	1.89	0.55
11:1P:42:SER:O	61:1P:301:HOH:O	2.18	0.55
32:1a:974:A:OP2	45:1n:29:ARG:NH2	2.39	0.55
34:1c:11:ARG:HB3	34:1c:15:THR:HB	1.87	0.55
1:2A:1449:A:O2'	1:2A:1529:G:N2	2.39	0.55
1:2A:2327:A:H2'	1:2A:2328:A:C8	2.41	0.55
1:2A:2552:2MU:H6	1:2A:2552:2MU:O5'	2.06	0.55
25:23:6:VAL:HG12	25:23:28:LEU:HD11	1.87	0.55
32:2a:576:G:OP1	61:2a:3321:HOH:O	2.17	0.55
33:2b:28:PHE:HD1	33:2b:194:PRO:HG3	1.71	0.55
44:2m:19:LEU:HD21	44:2m:56:LEU:HD21	1.88	0.55
1:1A:2274:U:H5	22:10:16:SER:HB3	1.71	0.55
10:1O:64:ARG:HB2	10:1O:79:PHE:CG	2.41	0.55
46:1o:4:THR:OG1	46:1o:7:GLU:OE1	2.25	0.55
1:2A:106:C:H1'	20:2Y:1:MET:HE2	1.87	0.55
1:2A:658:C:H2'	1:2A:659:C:C6	2.41	0.55
3:2D:108:PRO:HD2	3:2D:111:LEU:HD22	1.88	0.55
5:2F:108:LYS:HG2	5:2F:112:MET:HE2	1.89	0.55
15:2T:127:ALA:C	15:2T:129:ARG:H	2.14	0.55
19:2X:4:ALA:HB1	19:2X:42:ALA:HA	1.88	0.55
28:26:10:LEU:HD23	28:26:22:ALA:HB2	1.87	0.55
34:2c:3:ASN:N	34:2c:3:ASN:OD1	2.40	0.55
1:1A:1221:G:N2	1:1A:1223:C:OP2	2.39	0.55
6:1G:34:LEU:HD23	6:1G:161:THR:HG22	1.88	0.55
16:1U:49:HIS:HA	16:1U:52:ARG:HB2	1.89	0.55
32:1a:649:G:H2'	32:1a:650:G:C8	2.40	0.55
44:1m:84:ILE:HB	50:1s:66:MET:HE2	1.87	0.55
1:2A:1530:C:HO2'	1:2A:1531:C:P	2.29	0.55
1:2A:1816:G:O6	3:2D:35:LYS:NZ	2.26	0.55
1:2A:2117:A:O2'	1:2A:2118:U:H5''	2.07	0.55
1:2A:2518:A:OP2	61:2A:3975:HOH:O	2.18	0.55
1:2A:2595:G:N7	61:2A:4084:HOH:O	2.33	0.55
32:2a:76:C:H42	32:2a:93:G:H1	1.52	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:939:G:O2'	32:2a:1375:A:N3	2.31	0.55
42:2k:48:ILE:HG12	42:2k:63:LEU:HB3	1.89	0.55
1:1A:1827:U:H2'	1:1A:1828:C:C6	2.40	0.55
1:1A:2128:G:H1	1:1A:2205:C:H42	1.54	0.55
32:1a:67:C:H2'	32:1a:68:G:C8	2.42	0.55
55:1x:19:G:H4'	55:1x:20:U:OP2	2.06	0.55
1:2A:1889:A:H2'	1:2A:1890:A:C8	2.41	0.55
34:2c:15:THR:HG22	34:2c:16:ARG:HG2	1.89	0.55
35:2d:175:SER:HB3	35:2d:184:LYS:HB3	1.89	0.55
34:1c:6:HIS:HD2	34:1c:8:ILE:H	1.53	0.55
1:2A:964:C:O2'	1:2A:2273:A:N3	2.31	0.55
1:2A:1557:C:OP2	1:2A:1558:A:O2'	2.20	0.55
32:2a:54:C:O2	32:2a:357:G:N2	2.35	0.55
32:2a:922:G:H4'	36:2e:20:GLN:HA	1.89	0.55
35:2d:3:ARG:HG3	35:2d:5:ILE:HG23	1.89	0.55
1:1A:2324:U:H5'	6:1G:88:ILE:HD11	1.89	0.55
32:1a:742:G:OP2	46:1o:35:ARG:NH2	2.39	0.55
32:1a:1027:C:N4	32:1a:1034:G:N1	2.55	0.55
1:2A:911:A:OP1	61:2A:3979:HOH:O	2.18	0.55
4:2E:101:ARG:HB3	4:2E:201:THR:HG21	1.87	0.55
19:2X:12:VAL:HG22	19:2X:29:TRP:CE2	2.42	0.55
32:2a:67:C:H2'	32:2a:68:G:C8	2.42	0.55
32:1a:130:A:O2'	32:1a:131:C:O5'	2.22	0.55
32:1a:1025:U:C2	32:1a:1036:G:O6	2.58	0.55
32:1a:1435:G:H2'	32:1a:1436:U:C6	2.41	0.55
33:1b:16:HIS:HB2	33:1b:204:ASN:HB2	1.89	0.55
52:1u:3:LYS:HB3	52:1u:14:TRP:CD1	2.41	0.55
1:2A:775:G:O3'	61:2A:3974:HOH:O	2.17	0.55
1:2A:852:G:H2'	1:2A:853:G:C8	2.41	0.55
1:2A:2171:A:N3	1:2A:2172:U:N3	2.55	0.55
6:2G:114:ILE:HG12	6:2G:140:ILE:HG13	1.87	0.55
12:2Q:17:LEU:HB3	12:2Q:39:PRO:HB2	1.88	0.55
18:2W:34:ASN:OD1	18:2W:37:ARG:NH2	2.40	0.55
21:2Z:171:ILE:HG13	21:2Z:172:ALA:H	1.72	0.55
32:2a:554:C:H2'	32:2a:555:C:C6	2.42	0.55
32:2a:1239:A:H62	32:2a:1299:A:N6	2.05	0.55
54:2y:58:A:O2'	54:2y:60:U:OP2	2.18	0.55
1:1A:186:A:N6	1:1A:2442:A:O2'	2.39	0.55
1:1A:1781:G:O2'	1:1A:2870:A:N1	2.36	0.55
1:1A:2130:C:H2'	1:1A:2131:U:H6	1.72	0.55
2:1B:13:A:N1	2:1B:69:G:O2'	2.35	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1029:C:O2	32:1a:1032:G:N1	2.30	0.55
33:1b:74:LYS:HD2	33:1b:166:ASP:HB2	1.88	0.55
1:2A:1259:G:N7	61:2A:4088:HOH:O	2.33	0.55
1:2A:1616:A:O2'	61:2A:3977:HOH:O	2.18	0.55
8:2I:110:ASP:N	8:2I:130:TYR:OH	2.32	0.55
11:2P:95:VAL:HG13	11:2P:125:VAL:HA	1.88	0.55
33:2b:12:GLU:O	33:2b:15:VAL:HG22	2.06	0.55
34:2c:123:GLN:HA	34:2c:126:ARG:HD2	1.89	0.55
1:1A:928:G:H3'	1:1A:929:G:H8	1.71	0.55
1:1A:2761:A:H5'	7:1H:4:ILE:HD12	1.87	0.55
5:1F:61:GLY:O	61:1F:401:HOH:O	2.18	0.55
6:1G:179:PRO:HG3	26:14:43:TYR:OH	2.06	0.55
34:1c:73:PRO:HB3	34:1c:103:VAL:HG11	1.89	0.55
47:1p:52:ASP:O	47:1p:54:GLU:N	2.40	0.55
1:2A:212:G:H2'	1:2A:213:A:O4'	2.07	0.55
6:2G:97:ASP:HA	6:2G:100:TRP:HD1	1.72	0.55
39:2h:121:ASP:N	39:2h:121:ASP:OD1	2.40	0.55
7:1H:17:VAL:HG22	7:1H:26:VAL:HG22	1.90	0.54
19:1X:32:PRO:HA	19:1X:77:LYS:HB2	1.89	0.54
8:2I:93:THR:H	8:2I:96:ASP:HB2	1.72	0.54
32:2a:189(K):U:H2'	32:2a:189(L):G:C8	2.42	0.54
32:2a:1128:C:H1'	32:2a:1147:C:H42	1.72	0.54
32:2a:1271:G:C2	32:2a:1272:G:N7	2.75	0.54
34:2c:131:ARG:HH21	36:2e:50:GLU:HG3	1.72	0.54
1:1A:1128:U:C4	1:1A:1132:A:N1	2.73	0.54
4:1E:121:ASN:ND2	61:1E:408:HOH:O	2.38	0.54
21:1Z:1:MET:HA	21:1Z:55:HIS:HB3	1.89	0.54
34:1c:58:GLU:HB3	41:1j:92:THR:HG21	1.89	0.54
39:1h:51:VAL:HG21	39:1h:60:ARG:HG3	1.89	0.54
7:2H:127:GLU:OE1	7:2H:130:ARG:NE	2.39	0.54
32:2a:1264:C:N4	32:2a:1265:G:O6	2.40	0.54
35:2d:143:GLY:HA2	35:2d:184:LYS:HE2	1.89	0.54
54:2w:9:A:OP2	54:2w:13:C:N4	2.33	0.54
54:2w:14:A:H61	54:2w:21:A:H2	1.56	0.54
1:1A:242:C:OP2	30:18:5:LYS:NZ	2.29	0.54
1:1A:2297:C:OP2	28:16:6:ARG:HD3	2.08	0.54
32:1a:1412:C:H2'	32:1a:1413:A:C8	2.42	0.54
36:1e:78:HIS:HD2	39:1h:104:ARG:HD2	1.72	0.54
37:1f:6:VAL:HG22	37:1f:90:VAL:HG22	1.89	0.54
1:2A:65:C:O2'	1:2A:456:C:N3	2.36	0.54
1:2A:586:A:N1	1:2A:809:G:O2'	2.35	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2138:C:N3	1:2A:2153:G:N2	2.49	0.54
32:2a:995:C:O2	45:2n:4:LYS:NZ	2.37	0.54
1:1A:173:C:H2'	1:1A:174:U:C6	2.42	0.54
3:1D:168:ARG:HG2	3:1D:173:VAL:HG12	1.90	0.54
6:1G:38:VAL:HG22	6:1G:93:THR:HG23	1.87	0.54
32:1a:1442:G:H2'	32:1a:1442:G:N3	2.21	0.54
35:1d:173:TRP:CD1	35:1d:173:TRP:H	2.22	0.54
1:2A:994:C:O2'	1:2A:996:A:OP1	2.21	0.54
1:2A:1592:C:H2'	1:2A:1593:G:C8	2.42	0.54
1:2A:2031:A:N3	1:2A:2455:G:O2'	2.34	0.54
1:2A:2032:G:OP2	1:2A:2454:G:O2'	2.22	0.54
1:2A:2693:A:H2'	1:2A:2694:G:H8	1.72	0.54
1:2A:2820:A:O2'	1:2A:2821:A:OP1	2.26	0.54
17:2V:62:LEU:HD21	17:2V:95:LEU:HB2	1.89	0.54
32:2a:174:C:H2'	32:2a:175:C:H6	1.73	0.54
33:2b:8:LYS:HG3	33:2b:9:GLU:HG2	1.90	0.54
1:1A:715:G:H5'	1:1A:716:G:OP2	2.08	0.54
1:1A:1211:U:H2'	1:1A:1212:C:C6	2.43	0.54
32:1a:954:G:O6	44:1m:104:ARG:NH1	2.39	0.54
44:1m:20:THR:C	44:1m:22:ILE:H	2.16	0.54
1:2A:303:U:H2'	1:2A:304:G:C8	2.43	0.54
1:2A:852:G:H2'	1:2A:853:G:H8	1.72	0.54
9:2N:32:THR:HG23	9:2N:37:LYS:HB2	1.90	0.54
15:2T:16:ARG:NH2	15:2T:18:ASP:OD2	2.39	0.54
32:2a:996:A:H3'	32:2a:997:U:H5''	1.88	0.54
32:2a:1174:G:N7	61:2a:3324:HOH:O	2.33	0.54
32:2a:1367:C:OP2	40:2i:112:LYS:NZ	2.40	0.54
33:2b:73:THR:O	33:2b:78:GLN:NE2	2.40	0.54
1:1A:2346:G:H5'	14:1S:9:ARG:HG2	1.90	0.54
9:1N:73:THR:OG1	9:1N:82:LEU:HD11	2.08	0.54
32:1a:138:G:H1	32:1a:225:C:H42	1.54	0.54
32:1a:848:C:H2'	32:1a:849:C:H6	1.72	0.54
32:1a:985:C:H2'	32:1a:986:A:C8	2.42	0.54
32:1a:989:C:H42	32:1a:1216:G:H1	1.56	0.54
1:2A:674:G:H1'	5:2F:74:ARG:HD3	1.88	0.54
9:2N:58:ASP:OD1	9:2N:58:ASP:N	2.31	0.54
32:2a:756:C:N4	61:2a:3359:HOH:O	2.40	0.54
54:2w:53:G:H1	54:2w:61:C:H42	1.54	0.54
1:1A:1740:U:H1'	3:1D:14:ARG:NH2	2.23	0.54
32:1a:92:C:H2'	32:1a:93:G:H8	1.72	0.54
32:1a:636:U:H2'	32:1a:637:G:H8	1.73	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:1b:93:VAL:HG21	33:1b:97:TRP:HD1	1.73	0.54
1:2A:1607:C:N4	1:2A:1622:G:OP2	2.30	0.54
2:2B:66:A:N6	2:2B:108:U:H3'	2.22	0.54
19:2X:60:ARG:HH22	29:27:47:ARG:HH12	1.54	0.54
35:2d:11:LEU:HG	35:2d:66:ARG:HD3	1.89	0.54
1:1A:642:G:H5'	5:1F:205:ARG:HD3	1.89	0.54
1:1A:2152:U:H2'	1:1A:2180:A:H61	1.72	0.54
1:1A:2262:G:OP1	12:1Q:85:LYS:NZ	2.35	0.54
6:1G:142:PRO:HB2	26:14:31:ILE:HG21	1.90	0.54
11:1P:89:ALA:O	11:1P:121:LYS:NZ	2.40	0.54
17:1V:78:LYS:O	61:1V:301:HOH:O	2.18	0.54
33:1b:18:GLY:HA3	33:1b:42:ILE:HG13	1.90	0.54
34:1c:32:LEU:O	34:1c:36:ASP:HB2	2.08	0.54
18:2W:11:ARG:NH1	18:2W:99:ARG:O	2.41	0.54
32:2a:56:U:H2'	32:2a:57:G:C8	2.41	0.54
32:2a:984:C:H2'	32:2a:985:C:C6	2.42	0.54
32:2a:1060:C:H5''	41:2j:51:ARG:HG2	1.90	0.54
39:2h:87:SER:HB2	39:2h:93:VAL:HB	1.89	0.54
48:2q:9:VAL:HG12	48:2q:56:VAL:HG22	1.89	0.54
33:1b:80:ILE:HD13	33:1b:211:ILE:HG22	1.90	0.54
41:1j:5:ARG:NH2	41:1j:73:ASP:OD2	2.32	0.54
1:2A:479:A:N3	1:2A:481:G:H5''	2.23	0.54
1:2A:661:C:H2'	1:2A:662:G:C8	2.42	0.54
1:2A:1671:U:OP2	61:2A:3926:HOH:O	2.18	0.54
1:2A:2371:G:O2'	28:26:46:HIS:ND1	2.33	0.54
2:2B:22:U:H3	2:2B:61:G:H22	1.55	0.54
11:2P:91:PHE:O	11:2P:121:LYS:NZ	2.29	0.54
32:2a:656:C:O2	46:2o:28:GLN:NE2	2.41	0.54
32:2a:1029:C:N4	32:2a:1032:G:N1	2.55	0.54
39:2h:29:SER:HB3	39:2h:32:LYS:HG3	1.90	0.54
41:2j:6:ILE:HB	41:2j:72:VAL:HG23	1.90	0.54
1:1A:1001:G:H5''	12:1Q:77:LYS:HD2	1.90	0.54
1:1A:1342:G:OP1	1:1A:2721:G:O2'	2.18	0.54
1:1A:2227:G:H5''	1:1A:2228:G:N7	2.23	0.54
1:1A:2328:C:H2'	1:1A:2329:C:H6	1.72	0.54
7:1H:3:ARG:NH1	7:1H:4:ILE:H	2.06	0.54
32:1a:976:G:OP2	32:1a:1358:U:O2'	2.21	0.54
32:1a:1530:G:H2'	32:1a:1531:A:C8	2.43	0.54
35:1d:178:VAL:HG12	35:1d:179:GLU:H	1.72	0.54
1:2A:463:G:N2	1:2A:466:A:OP2	2.29	0.54
1:2A:666:G:H1'	30:28:4:MET:HE3	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2148:G:H2'	1:2A:2149:G:C8	2.42	0.54
9:2N:20:GLY:HA2	9:2N:61:ARG:HG3	1.89	0.54
10:2O:48:PRO:HB3	32:2a:1422:G:H5''	1.89	0.54
32:2a:1005:A:OP1	32:2a:1006:C:N4	2.41	0.54
33:2b:55:PHE:HE1	33:2b:218:ALA:HA	1.73	0.54
37:2f:50:TYR:CE2	49:2r:77:GLY:HA2	2.43	0.54
41:2j:51:ARG:H	41:2j:60:ARG:HA	1.73	0.54
1:1A:122:G:OP1	1:1A:1422:C:O2'	2.21	0.53
1:1A:2328:C:O2'	6:1G:128:ARG:NH2	2.34	0.53
2:1B:45:A:OP2	6:1G:96:ARG:NH2	2.33	0.53
6:1G:64:THR:HB	6:1G:94:LEU:HD21	1.90	0.53
35:1d:11:LEU:HD23	35:1d:66:ARG:HB3	1.90	0.53
1:2A:728:G:H5''	3:2D:13:ARG:HH21	1.73	0.53
1:2A:1015:G:H2'	1:2A:1016:G:C8	2.41	0.53
1:2A:1794:U:H2'	1:2A:1795:C:C6	2.43	0.53
9:2N:62:VAL:HG22	9:2N:66:LYS:HD2	1.89	0.53
1:1A:1362:U:H2'	1:1A:1363:A:H8	1.73	0.53
18:1W:25:ARG:NH2	18:1W:74:ALA:O	2.33	0.53
32:1a:925:G:H1'	32:1a:1502:A:C4	2.42	0.53
35:1d:26:CYS:HB3	60:1d:501:SF4:S1	2.47	0.53
1:2A:143:G:H4'	19:2X:35:THR:HG21	1.90	0.53
1:2A:521:G:H2'	1:2A:522:G:H8	1.72	0.53
1:2A:862:G:O2'	2:2B:78:A:N3	2.41	0.53
1:2A:1340:U:OP2	19:2X:78:LYS:NZ	2.41	0.53
1:2A:1647:G:H3'	1:2A:1647:G:OP2	2.09	0.53
32:2a:1062:U:H2'	32:2a:1063:C:C6	2.43	0.53
32:2a:1305:G:O2'	32:2a:1331:G:N2	2.41	0.53
48:2q:53:LEU:HD23	48:2q:82:MET:HE1	1.91	0.53
1:1A:848:G:O6	5:1F:53:THR:OG1	2.27	0.53
2:1B:41:U:H5	6:1G:70:VAL:H	1.57	0.53
3:1D:183:ARG:NH2	61:1D:407:HOH:O	2.42	0.53
11:1P:63:PRO:HG2	30:18:25:MET:HB2	1.90	0.53
13:1R:71:GLN:NE2	61:1R:304:HOH:O	2.41	0.53
32:1a:392:G:H2'	32:1a:393:A:H8	1.73	0.53
1:2A:1243:G:O2'	11:2P:4:SER:O	2.23	0.53
12:2Q:110:THR:HG23	12:2Q:113:GLN:HB2	1.91	0.53
30:28:36:LYS:HB2	30:28:41:ILE:HD11	1.89	0.53
32:2a:17:U:H2'	32:2a:18:C:C6	2.43	0.53
32:2a:598:U:H2'	32:2a:599:C:H6	1.72	0.53
32:2a:1027:C:O2'	32:2a:1034:G:N2	2.41	0.53
1:1A:236:G:H4'	1:1A:413:G:C5	2.43	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2080:A:OP1	61:1A:4289:HOH:O	2.19	0.53
1:1A:2156:A:N3	1:1A:2181:G:O2'	2.35	0.53
9:1N:18:ALA:HA	9:1N:21:LYS:HD2	1.89	0.53
15:1T:127:ALA:C	15:1T:129:ARG:H	2.16	0.53
19:1X:11:PRO:HG2	19:1X:13:LEU:HD21	1.90	0.53
32:1a:576:G:O6	32:1a:880:C:O2'	2.24	0.53
32:1a:1379:G:O6	38:1g:2:ALA:N	2.42	0.53
39:1h:41:ARG:NH2	39:1h:123:GLU:OE2	2.41	0.53
1:2A:82:G:N1	1:2A:103:A:OP2	2.33	0.53
1:2A:878:A:H61	1:2A:899:A:H1'	1.72	0.53
32:2a:1239:A:H4'	32:2a:1240:U:H5'	1.89	0.53
33:2b:115:LEU:HD23	33:2b:153:ARG:HD3	1.90	0.53
35:2d:173:TRP:CD2	35:2d:189:PRO:HG3	2.42	0.53
1:1A:778:C:OP1	61:1A:4287:HOH:O	2.18	0.53
23:11:59:THR:O	23:11:91:LYS:NZ	2.40	0.53
32:1a:78:G:N1	32:1a:91:C:C4	2.76	0.53
32:1a:299:G:O6	61:1a:3321:HOH:O	2.13	0.53
55:1x:8:4SU:O2	55:1x:21:A:H2	1.92	0.53
1:2A:1169:G:H1	1:2A:1180:C:H42	1.55	0.53
1:2A:2857:G:N2	1:2A:2860:A:OP2	2.40	0.53
14:2S:14:VAL:O	14:2S:18:ILE:HG12	2.08	0.53
32:2a:1105:A:H2'	32:2a:1106:G:H8	1.73	0.53
32:2a:1518:MA6:N6	32:2a:1519:MA6:H103	2.24	0.53
33:2b:219:VAL:HA	33:2b:222:ILE:HB	1.91	0.53
40:2i:17:VAL:HG11	40:2i:81:ILE:HA	1.91	0.53
1:1A:1001:G:H2'	1:1A:1002:A:H2'	1.90	0.53
1:1A:1233:U:H4'	17:1V:79:VAL:HG22	1.90	0.53
13:1R:33:ARG:NH2	27:15:57:VAL:O	2.39	0.53
28:16:13:CYS:SG	28:16:47:THR:HG21	2.48	0.53
1:2A:581:C:H2'	1:2A:582:G:C8	2.44	0.53
1:2A:2303:G:O2'	6:2G:132:ASN:ND2	2.40	0.53
3:2D:206:LEU:O	3:2D:211:ARG:HD3	2.07	0.53
14:2S:77:ALA:HB1	14:2S:82:ILE:HB	1.91	0.53
14:2S:92:TYR:HB3	14:2S:98:VAL:HG21	1.91	0.53
16:2U:28:ARG:NH1	16:2U:38:THR:OG1	2.41	0.53
32:2a:475:G:H2'	32:2a:476:G:H8	1.74	0.53
1:1A:1347:A:OP1	61:1A:4291:HOH:O	2.19	0.53
1:1A:2148:A:N1	1:1A:2184:G:O2'	2.39	0.53
10:1O:49:ARG:HH12	32:1a:1423:G:P	2.32	0.53
54:1w:9:A:O2'	54:1w:10:G:N7	2.41	0.53
1:2A:1147:C:H2'	1:2A:1148:A:H8	1.74	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2456:C:N4	61:2A:4131:HOH:O	2.41	0.53
4:2E:5:LEU:HD21	4:2E:79:ARG:HB2	1.90	0.53
13:2R:42:LYS:HB3	13:2R:45:ARG:HH21	1.73	0.53
32:2a:521:G:N7	43:2l:53:ARG:NH2	2.56	0.53
32:2a:715:A:H2'	32:2a:716:A:C8	2.43	0.53
33:2b:16:HIS:HB2	33:2b:204:ASN:HB3	1.90	0.53
1:1A:1431:G:O2'	1:1A:1442:U:O2	2.21	0.53
7:1H:3:ARG:HH21	7:1H:65:HIS:HB3	1.73	0.53
32:1a:21:G:H2'	32:1a:22:G:C8	2.44	0.53
32:1a:171:A:H2'	32:1a:172:A:C8	2.44	0.53
32:1a:405:U:OP2	35:1d:3:ARG:NH1	2.39	0.53
32:1a:985:C:H2'	32:1a:986:A:H8	1.74	0.53
32:1a:1009:G:O6	32:1a:1020:U:C2	2.62	0.53
33:1b:28:PHE:HD1	33:1b:194:PRO:HG3	1.73	0.53
54:1y:38:A:H2'	54:1y:39:PSU:O4'	2.09	0.53
1:2A:2839:G:N2	13:2R:91:GLN:O	2.41	0.53
2:2B:78:A:H62	2:2B:99:G:H21	1.57	0.53
32:2a:644:G:OP1	61:2a:3322:HOH:O	2.18	0.53
1:1A:406:G:N2	23:11:42:GLN:OE1	2.34	0.53
1:1A:2177:G:H3'	1:1A:2178:G:C8	2.40	0.53
10:1O:24:VAL:HG12	10:1O:33:ALA:HB2	1.91	0.53
11:1P:95:VAL:HA	11:1P:99:LEU:HD12	1.91	0.53
23:11:21:ARG:NH2	61:11:5001:HOH:O	2.42	0.53
23:11:65:SER:HA	61:11:5006:HOH:O	2.09	0.53
32:1a:503:C:OP2	43:1l:116:SER:OG	2.17	0.53
1:2A:271(H):G:H2'	1:2A:271(I):G:C8	2.43	0.53
1:2A:1423:G:OP1	1:2A:1492:G:O2'	2.27	0.53
1:2A:2284:C:P	28:26:6:ARG:HG3	2.49	0.53
1:2A:2836:U:H2'	1:2A:2837:G:C8	2.44	0.53
1:1A:599:U:H2'	1:1A:600:G:C8	2.44	0.53
1:1A:2143:G:H1	1:1A:2199:C:H42	1.57	0.53
5:1F:155:LEU:HB2	5:1F:189:THR:HG21	1.90	0.53
19:1X:53:LYS:HB3	19:1X:82:GLN:HB3	1.90	0.53
32:1a:1006:C:N3	32:1a:1023:G:N2	2.56	0.53
37:1f:82:ARG:HB2	37:1f:85:VAL:HG23	1.91	0.53
1:2A:1412:A:H2'	1:2A:1413:G:C8	2.43	0.53
1:2A:2646:C:H2'	1:2A:2647:U:O4'	2.09	0.53
32:2a:811:C:O2'	32:2a:901:A:N1	2.41	0.53
33:2b:230:VAL:HG22	33:2b:232:PRO:HD2	1.91	0.53
47:2p:15:PRO:HD2	47:2p:42:ARG:HD2	1.91	0.53
48:2q:80:GLY:O	48:2q:82:MET:N	2.37	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1D:108:PRO:HB3	3:1D:143:HIS:CE1	2.43	0.52
7:1H:24:VAL:HG22	7:1H:35:VAL:HB	1.90	0.52
17:1V:59:ALA:HB1	17:1V:94:LEU:HB3	1.91	0.52
1:2A:492:A:H2'	1:2A:493:G:O4'	2.08	0.52
1:2A:723:G:H2'	1:2A:724:U:O4'	2.09	0.52
1:2A:1336:A:H2'	1:2A:1337:G:C8	2.44	0.52
1:2A:1752:C:H2'	1:2A:1753:G:C8	2.44	0.52
1:2A:2154:G:H2'	1:2A:2155:G:H5'	1.91	0.52
6:2G:127:GLY:H	6:2G:166:ASP:CG	2.17	0.52
31:29:7:VAL:HG12	31:29:34:GLN:HB3	1.91	0.52
33:2b:16:HIS:HB3	33:2b:210:SER:HB2	1.90	0.52
1:1A:555:G:N1	1:1A:2045:G:OP1	2.33	0.52
5:1F:53:THR:HG22	5:1F:56:GLU:HG3	1.92	0.52
6:1G:47:LYS:HG3	6:1G:48:GLU:H	1.74	0.52
8:1I:92:VAL:HG11	8:1I:144:VAL:HG11	1.92	0.52
54:1w:60:U:H5''	54:1w:61:C:H5	1.74	0.52
1:2A:1592:C:H2'	1:2A:1593:G:H8	1.74	0.52
32:2a:376:G:H5''	47:2p:5:ARG:HB2	1.90	0.52
32:2a:559:A:H4'	32:2a:560:U:H3'	1.91	0.52
32:2a:646:U:H2'	32:2a:647:C:C6	2.45	0.52
36:2e:8:GLU:OE2	36:2e:63:ARG:NH2	2.42	0.52
40:2i:5:TYR:H	40:2i:87:GLN:NE2	2.06	0.52
44:2m:91:ARG:HG3	44:2m:96:LEU:HB2	1.91	0.52
1:1A:485:U:OP2	29:17:39:ARG:NH1	2.43	0.52
5:1F:127:GLU:HA	5:1F:196:LEU:HD12	1.91	0.52
17:1V:52:VAL:HG23	17:1V:55:ALA:HB3	1.91	0.52
32:1a:1125:U:H4'	41:1j:5:ARG:NH2	2.24	0.52
1:2A:2151:G:H2'	1:2A:2152:G:C8	2.44	0.52
32:2a:80:G:H1	32:2a:89:C:H42	1.57	0.52
32:2a:921:U:O2	36:2e:19:MET:HB2	2.08	0.52
36:2e:78:HIS:HE1	36:2e:143:ARG:H	1.56	0.52
41:2j:6:ILE:HG12	41:2j:98:ILE:HG13	1.91	0.52
49:2r:32:ARG:HA	49:2r:69:THR:HG21	1.91	0.52
1:1A:2045:G:H5'	1:1A:2629:C:H4'	1.91	0.52
1:1A:2094:G:N2	61:1A:4478:HOH:O	2.42	0.52
1:1A:2564:2MU:O5'	1:1A:2564:2MU:H6	2.10	0.52
32:1a:92:C:H2'	32:1a:93:G:C8	2.44	0.52
32:1a:1510:U:H2'	32:1a:1511:G:C8	2.44	0.52
34:1c:155:GLY:HA3	34:1c:196:LEU:HD22	1.89	0.52
44:1m:16:ASP:OD1	44:1m:16:ASP:N	2.43	0.52
1:2A:1834:U:H4'	1:2A:1969:A:C6	2.44	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2S:95:HIS:O	14:2S:99:LYS:HB3	2.09	0.52
16:2U:52:ARG:HA	16:2U:55:ARG:HE	1.74	0.52
32:2a:1020:U:H2'	32:2a:1021:G:H8	1.73	0.52
54:2w:51:U:H3	54:2w:63:G:H1	1.57	0.52
55:2x:40:C:H2'	55:2x:41:C:H6	1.74	0.52
1:1A:2859:U:H4'	1:1A:2878:A:C2	2.45	0.52
32:1a:935:A:O2'	32:1a:1383:C:N3	2.40	0.52
33:1b:224:GLN:HG2	33:1b:229:VAL:HG22	1.91	0.52
30:28:28:GLY:O	30:28:36:LYS:NZ	2.42	0.52
8:1I:38:LEU:HB2	8:1I:40:THR:HG23	1.91	0.52
12:1Q:12:GLN:HE21	12:1Q:72:LYS:HG3	1.74	0.52
32:1a:1189:C:OP1	41:1j:51:ARG:NH2	2.36	0.52
39:1h:81:HIS:N	39:1h:138:TRP:O	2.41	0.52
1:2A:458:G:O2'	1:2A:469:G:O6	2.19	0.52
1:2A:597:U:H2'	1:2A:598:G:H8	1.75	0.52
1:2A:2010:G:H5''	18:2W:42:ARG:HB2	1.92	0.52
6:2G:131:TYR:HE2	6:2G:133:LEU:HD23	1.74	0.52
6:2G:179:PRO:HB2	26:24:42:PHE:HE2	1.74	0.52
14:2S:15:ARG:HB3	14:2S:19:LYS:HE3	1.90	0.52
32:2a:91:C:H2'	32:2a:92:C:C6	2.45	0.52
32:2a:1228:C:H2'	32:2a:1229:A:H8	1.75	0.52
35:2d:173:TRP:CE3	35:2d:189:PRO:HG3	2.45	0.52
1:1A:83:A:H5''	20:1Y:8:LYS:HE3	1.92	0.52
1:1A:909:G:H2'	1:1A:910:A:O4'	2.09	0.52
1:1A:2892:A:OP1	13:1R:96:ARG:NH1	2.41	0.52
24:12:32:LEU:HD11	24:12:54:LYS:HG2	1.90	0.52
32:1a:523:A:H61	43:1l:92:0TD:CG	2.22	0.52
32:1a:1025:U:O2	32:1a:1036:G:C6	2.62	0.52
32:1a:1218:C:H2'	32:1a:1219:U:C6	2.45	0.52
32:2a:1192:C:OP2	34:2c:4:LYS:NZ	2.34	0.52
44:2m:92:HIS:CE1	44:2m:98:VAL:HG21	2.45	0.52
1:1A:2158:C:N3	1:1A:2177:G:C2	2.77	0.52
1:1A:2859:U:OP2	15:1T:95:ARG:NH1	2.43	0.52
33:1b:97:TRP:HZ2	33:1b:102:LEU:HD13	1.74	0.52
34:1c:116:VAL:HG21	34:1c:202:ILE:HD11	1.90	0.52
44:1m:9:ILE:HB	44:1m:18:ALA:HB1	1.91	0.52
48:1q:6:LEU:HD23	48:1q:23:VAL:HG11	1.91	0.52
1:2A:1170:G:O6	1:2A:1180:C:N4	2.43	0.52
1:2A:2125:G:H1'	1:2A:2173:A:N6	2.25	0.52
1:2A:2540:C:O2'	1:2A:2740:A:N3	2.37	0.52
6:2G:11:TYR:HA	6:2G:15:VAL:HB	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1132:C:H2'	32:2a:1133:G:C8	2.44	0.52
33:2b:28:PHE:CD1	33:2b:194:PRO:HG3	2.45	0.52
33:2b:91:PRO:HG3	33:2b:154:LEU:HB3	1.90	0.52
38:2g:32:ARG:HH21	38:2g:109:ASN:ND2	2.08	0.52
44:2m:25:ILE:HD11	44:2m:66:LEU:HD13	1.92	0.52
1:1A:1104:G:N2	1:1A:1127:U:O2	2.43	0.52
1:1A:2416:C:O3'	11:1P:77:ARG:NH2	2.43	0.52
25:13:6:VAL:HG12	25:13:28:LEU:HD11	1.92	0.52
32:1a:1054:C:C4	54:1w:34:G:H1'	2.44	0.52
32:1a:1145:C:H4'	32:1a:1146:A:H5'	1.90	0.52
32:1a:1305:G:N2	32:1a:1331:G:H1'	2.25	0.52
38:1g:74:GLU:HG2	38:1g:91:VAL:HG22	1.92	0.52
51:1t:25:ARG:HG2	51:1t:29:LYS:HE2	1.92	0.52
1:2A:18:C:O2'	1:2A:554:U:OP1	2.28	0.52
1:2A:1388:G:H2'	1:2A:1389:G:H8	1.75	0.52
30:28:26:LYS:HB2	30:28:44:LYS:O	2.10	0.52
32:2a:840:C:H4'	32:2a:841:U:OP1	2.10	0.52
41:2j:38:ILE:HG12	41:2j:71:LEU:HB3	1.91	0.52
51:2t:39:LYS:HD2	51:2t:55:ILE:HG21	1.90	0.52
51:2t:100:ILE:HG13	51:2t:101:GLY:H	1.75	0.52
1:1A:1785:C:OP1	15:1T:96:ARG:NH1	2.43	0.52
1:1A:2647:C:H4'	4:1E:48:GLN:HE21	1.74	0.52
4:1E:116:VAL:HG13	4:1E:122:PHE:HB2	1.91	0.52
32:1a:673:G:H2'	32:1a:674:G:C8	2.45	0.52
35:1d:119:GLN:HG2	35:1d:123:HIS:CD2	2.45	0.52
36:1e:74:GLY:HA3	36:1e:116:THR:HG22	1.90	0.52
1:2A:271(T):C:H2'	1:2A:271(U):G:H8	1.73	0.52
1:2A:848:G:H2'	1:2A:849:A:C8	2.44	0.52
1:2A:1024:G:HO2'	1:2A:1144:G:HO2'	1.58	0.52
32:2a:460:G:N2	32:2a:471:G:N7	2.58	0.52
35:2d:31:CYS:CB	60:2d:302:SF4:S3	2.98	0.52
41:2j:16:LEU:HD23	41:2j:70:ARG:HG2	1.91	0.52
44:2m:10:PRO:HB2	44:2m:13:LYS:HD2	1.92	0.52
1:1A:1071:G:C4	1:1A:1180:C:H1'	2.45	0.51
1:1A:1898:A:H2'	1:1A:1899:A:C8	2.45	0.51
1:1A:2272:C:H2'	1:1A:2273:C:H6	1.75	0.51
1:1A:2831:A:OP2	61:1A:4218:HOH:O	2.19	0.51
3:1D:26:LYS:HB3	3:1D:83:GLU:HG2	1.92	0.51
43:1l:53:ARG:HG3	43:1l:93:LEU:HD21	1.92	0.51
54:1y:63:G:H2'	54:1y:64:A:O4'	2.10	0.51
1:2A:1113:U:H2'	1:2A:1114:G:C8	2.45	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2079:U:O3'	23:21:35:THR:OG1	2.29	0.51
12:2Q:118:LEU:HD12	12:2Q:131:ILE:HG23	1.91	0.51
26:24:16:CYS:SG	26:24:17:GLY:N	2.83	0.51
32:2a:1442:G:H2'	32:2a:1442:G:N3	2.25	0.51
1:1A:742:G:OP1	1:1A:1426:G:O2'	2.28	0.51
2:1B:1:U:O2'	2:1B:2:C:OP1	2.25	0.51
4:1E:8:LYS:NZ	4:1E:188:VAL:O	2.44	0.51
1:2A:2271:G:OP1	22:20:18:ALA:HB1	2.10	0.51
32:2a:1063:C:H3'	32:2a:1064:G:H2'	1.90	0.51
1:1A:1099:C:H42	1:1A:1152:G:H1	1.58	0.51
1:1A:1106:U:N3	1:1A:1108:G:O2'	2.44	0.51
1:1A:1681:A:H5''	61:1A:5529:HOH:O	2.11	0.51
24:12:10:LEU:HD21	24:12:59:ARG:HD3	1.91	0.51
28:16:6:ARG:NH2	28:16:24:GLU:OE1	2.36	0.51
32:1a:452:A:O2'	32:1a:453:A:OP2	2.27	0.51
32:1a:1036:G:H3'	32:1a:1037:C:C6	2.45	0.51
43:1l:124:LYS:HD2	43:1l:125:PRO:HD2	1.90	0.51
1:2A:1902:C:OP2	61:2A:3981:HOH:O	2.19	0.51
32:2a:259:G:OP2	51:2t:83:ARG:NH1	2.43	0.51
32:2a:662:G:H2'	32:2a:663:A:C8	2.45	0.51
32:2a:1298:C:OP2	38:2g:114:ARG:NH2	2.43	0.51
53:2v:13:A:H8	53:2v:13:A:OP2	1.93	0.51
1:1A:85:C:H4'	1:1A:102:U:H1'	1.92	0.51
1:1A:1536:A:O2'	3:1D:99:ASP:OD1	2.28	0.51
1:1A:2032:G:H5''	18:1W:42:ARG:HB2	1.91	0.51
18:1W:10:VAL:HG12	18:1W:12:ILE:HG22	1.93	0.51
19:1X:88:LYS:HE2	19:1X:93:GLU:HG3	1.91	0.51
40:1i:49:PRO:HD3	40:1i:78:LYS:HG3	1.91	0.51
1:2A:1843:C:H5'	3:2D:253:GLN:OE1	2.11	0.51
1:2A:2393:A:O2'	30:28:13:ARG:NH2	2.42	0.51
19:2X:2:LYS:NZ	19:2X:38:GLU:OE2	2.38	0.51
32:2a:1137:C:H5''	32:2a:1138:G:OP1	2.10	0.51
32:2a:1176:A:H2'	32:2a:1177:G:C8	2.46	0.51
32:2a:1327:C:H2'	32:2a:1328:C:H6	1.75	0.51
39:2h:10:LEU:HD12	39:2h:85:ARG:HG2	1.92	0.51
41:2j:27:ALA:HB1	41:2j:74:ILE:HD12	1.93	0.51
1:1A:611:U:H2'	1:1A:612:C:C6	2.45	0.51
32:1a:431:A:H2'	32:1a:432:A:O4'	2.11	0.51
32:1a:1030:C:N3	32:1a:1031:G:N2	2.59	0.51
33:1b:185:ILE:HG22	33:1b:199:TYR:HB2	1.91	0.51
43:1l:56:ALA:HB2	43:1l:70:ILE:HD11	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:1t:87:LYS:O	51:1t:91:LEU:HG	2.10	0.51
1:2A:774:A:H2'	1:2A:774:A:N3	2.25	0.51
2:2B:42:C:C6	6:2G:69:ALA:HB2	2.45	0.51
5:2F:101:LEU:O	5:2F:106:ARG:NH1	2.43	0.51
32:2a:1134:G:H1	32:2a:1140:C:N4	2.09	0.51
33:2b:166:ASP:HB3	33:2b:169:LYS:HB3	1.93	0.51
1:1A:1111:U:H5''	1:1A:1112:U:OP2	2.10	0.51
7:1H:4:ILE:O	7:1H:69:ARG:HD2	2.11	0.51
7:1H:11:VAL:HG13	7:1H:15:VAL:HG22	1.93	0.51
32:1a:662:G:H2'	32:1a:663:A:C8	2.46	0.51
32:1a:848:C:H2'	32:1a:849:C:C6	2.45	0.51
32:1a:1337:G:N7	61:1a:3362:HOH:O	2.34	0.51
33:1b:91:PRO:HG2	33:1b:155:LEU:HD13	1.92	0.51
1:2A:253:C:OP2	30:28:5:LYS:NZ	2.37	0.51
1:2A:353:G:H2'	1:2A:354:G:C8	2.46	0.51
1:2A:785:G:OP2	61:2A:3980:HOH:O	2.19	0.51
1:2A:2134:A:O2'	1:2A:2159:G:N2	2.43	0.51
32:2a:1104:G:H4'	33:2b:111:ARG:NH2	2.25	0.51
32:2a:1250:A:H4'	40:2i:68:GLY:N	2.26	0.51
46:2o:39:LEU:HD22	46:2o:56:LEU:HD13	1.91	0.51
1:1A:591:U:H5'	1:1A:990:A:N6	2.26	0.51
1:1A:873:U:H4'	11:1P:55:ARG:HB3	1.92	0.51
1:1A:2377:G:N7	30:18:39:LYS:NZ	2.57	0.51
4:1E:162:ALA:O	61:1E:403:HOH:O	2.19	0.51
31:19:25:VAL:HB	31:19:34:GLN:HB2	1.93	0.51
32:1a:40:C:H2'	32:1a:41:G:H8	1.76	0.51
32:1a:447:G:O6	32:1a:485:G:O2'	2.22	0.51
32:1a:1070:U:H2'	32:1a:1071:C:C6	2.46	0.51
32:1a:1228:C:OP1	44:1m:115:LYS:NZ	2.40	0.51
33:1b:10:LEU:N	33:1b:48:MET:HE1	2.21	0.51
36:1e:6:PHE:HB3	36:1e:34:VAL:HG22	1.92	0.51
40:1i:50:LEU:HD23	40:1i:81:ILE:HD11	1.92	0.51
41:1j:16:LEU:HD21	41:1j:70:ARG:HG2	1.92	0.51
41:1j:55:LYS:HG2	41:1j:56:HIS:N	2.26	0.51
1:2A:108:U:H2'	1:2A:109:G:H8	1.75	0.51
1:2A:1426:G:OP2	1:2A:1427:A:O2'	2.23	0.51
1:2A:1514:U:H2'	1:2A:1515:G:H8	1.76	0.51
1:2A:2049:G:O6	61:2A:3970:HOH:O	2.16	0.51
22:20:48:GLY:HA3	22:20:80:HIS:ND1	2.26	0.51
24:22:29:LYS:HG2	24:22:57:ILE:HD13	1.92	0.51
32:2a:1507:A:OP2	53:2v:13:A:N6	2.44	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:2w:4:C:C2	54:2w:69:G:N2	2.79	0.51
1:1A:1387:U:O4'	19:1X:57:LEU:HD23	2.11	0.51
1:1A:2143:G:O6	1:1A:2198:A:N6	2.43	0.51
2:1B:2:C:H2'	2:1B:3:C:C6	2.45	0.51
35:1d:23:GLY:HA3	35:1d:112:VAL:HG12	1.93	0.51
44:1m:19:LEU:HD21	44:1m:56:LEU:HD21	1.92	0.51
1:2A:189:G:O6	1:2A:205:G:O2'	2.25	0.51
1:2A:880:G:H2'	1:2A:881:G:H8	1.76	0.51
1:2A:956:G:OP2	12:2Q:14:ARG:NH1	2.39	0.51
32:2a:978:A:N6	32:2a:1318:A:N7	2.58	0.51
32:2a:1239:A:H62	32:2a:1299:A:H62	1.57	0.51
34:2c:142:MET:HG3	34:2c:170:GLN:HB3	1.92	0.51
1:1A:1232:G:H5''	17:1V:81:TYR:CE1	2.45	0.51
1:1A:2804:C:H2'	1:1A:2805:G:C8	2.46	0.51
7:1H:164:TYR:HB2	7:1H:167:GLU:HB2	1.93	0.51
15:1T:26:ASP:O	15:1T:49:VAL:HG22	2.11	0.51
32:1a:1127:G:H5'	32:1a:1280:A:O2'	2.11	0.51
1:2A:1116:C:H2'	1:2A:1117:G:C8	2.46	0.51
1:2A:1485:G:H1	1:2A:1504:C:H42	1.59	0.51
32:2a:340:U:H2'	32:2a:341:C:C6	2.46	0.51
1:1A:63:A:O3'	19:1X:71:GLY:HA3	2.11	0.51
5:1F:155:LEU:HD11	5:1F:176:LEU:HD12	1.93	0.51
5:1F:185:ASP:OD1	5:1F:188:ARG:NH1	2.43	0.51
10:1O:87:ILE:HD12	10:1O:91:LEU:HA	1.93	0.51
29:17:20:ALA:HA	29:17:23:ARG:HH21	1.76	0.51
32:1a:392:G:H2'	32:1a:393:A:C8	2.46	0.51
44:1m:3:ARG:HB2	44:1m:57:ARG:HH21	1.76	0.51
50:1s:11:VAL:HG12	50:1s:13:ASP:H	1.75	0.51
1:2A:108:U:H2'	1:2A:109:G:C8	2.46	0.51
1:2A:1406:U:H2'	1:2A:1407:C:C6	2.46	0.51
1:2A:1656:C:H5''	4:2E:136:ARG:HB2	1.93	0.51
10:2O:64:ARG:HB2	10:2O:79:PHE:CG	2.45	0.51
32:2a:41:G:H2'	32:2a:42:G:H8	1.76	0.51
32:2a:1242:C:H2'	32:2a:1243:C:O4'	2.12	0.51
1:1A:1116:A:N6	1:1A:1142:A:N3	2.59	0.50
1:1A:2291:G:O6	22:10:14:ARG:HG3	2.10	0.50
32:1a:108:G:N1	51:1t:15:ARG:HG2	2.26	0.50
32:1a:953:G:N7	44:1m:104:ARG:NH2	2.59	0.50
1:2A:994:C:H3'	16:2U:54:LYS:HE3	1.93	0.50
1:2A:1300:U:H4'	1:2A:1301:A:H5''	1.92	0.50
1:2A:2751:G:H5'	7:2H:2:SER:HA	1.91	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:2E:9:VAL:HG22	4:2E:25:VAL:HB	1.92	0.50
5:2F:156:LEU:HD21	5:2F:163:VAL:HG12	1.92	0.50
16:2U:69:CYS:HB3	16:2U:74:LEU:HD12	1.93	0.50
32:2a:276:G:OP1	48:2q:12:SER:OG	2.15	0.50
32:2a:1029:C:C2	32:2a:1032:G:N2	2.77	0.50
32:2a:1161:C:H2'	32:2a:1162:C:C6	2.45	0.50
32:2a:1287:A:H2	32:2a:1353:G:H1'	1.75	0.50
32:2a:1366:C:H2'	32:2a:1367:C:C6	2.46	0.50
35:2d:72:GLU:OE2	35:2d:207:TYR:OH	2.29	0.50
41:2j:35:SER:HB3	41:2j:73:ASP:HB2	1.93	0.50
51:1t:60:GLU:HG3	51:1t:81:LYS:HD2	1.93	0.50
1:2A:566:U:H5''	11:2P:29:LYS:HE3	1.94	0.50
1:2A:2320:A:N3	1:2A:2320:A:H2'	2.25	0.50
1:2A:2543:G:H2'	1:2A:2544:G:C8	2.46	0.50
3:2D:72:LYS:NZ	3:2D:99:ASP:OD2	2.43	0.50
32:2a:8:A:N7	35:2d:208:SER:OG	2.45	0.50
32:2a:1366:C:HO2'	41:2j:60:ARG:HH12	1.59	0.50
35:2d:119:GLN:HG3	35:2d:123:HIS:CD2	2.44	0.50
44:2m:3:ARG:HG3	44:2m:4:ILE:H	1.76	0.50
1:1A:1165:C:N4	61:1A:4492:HOH:O	2.45	0.50
1:1A:2812:A:H5''	1:1A:2813:G:C8	2.46	0.50
32:1a:501:C:H2'	32:1a:502:G:H8	1.76	0.50
32:1a:984:C:N4	32:1a:1221:G:H1	2.06	0.50
32:1a:1000:U:O4	32:1a:1041:A:N1	2.44	0.50
33:1b:24:TRP:CD1	33:1b:24:TRP:H	2.29	0.50
1:2A:832:G:OP1	61:2A:3982:HOH:O	2.19	0.50
1:2A:1379:A:H4'	1:2A:1380:G:OP2	2.11	0.50
2:2B:42:C:O2'	6:2G:67:LYS:O	2.19	0.50
32:2a:673:G:H2'	32:2a:674:G:C8	2.46	0.50
32:2a:716:A:N3	42:2k:118:GLY:HA2	2.26	0.50
32:2a:1074:G:O2'	32:2a:1101:A:N1	2.43	0.50
35:2d:31:CYS:HB2	60:2d:302:SF4:S3	2.51	0.50
48:2q:45:HIS:CD2	48:2q:47:PRO:HD3	2.46	0.50
54:2w:19:G:H1	54:2w:56:C:H42	1.58	0.50
1:1A:2255:U:H2'	1:1A:2256:U:C6	2.46	0.50
4:1E:111:ARG:HG3	4:1E:160:TYR:CD2	2.47	0.50
32:1a:216:G:H2'	32:1a:217:C:C6	2.46	0.50
32:1a:769:G:H4'	32:1a:1513:A:H4'	1.93	0.50
40:1i:28:VAL:HG22	40:1i:63:ILE:HB	1.93	0.50
50:1s:80:TYR:CZ	50:1s:82:GLY:HA2	2.47	0.50
1:2A:848:G:N3	1:2A:933:A:H1'	2.27	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2105:C:H2'	1:2A:2106:G:H8	1.76	0.50
1:2A:2727:G:O2'	10:2O:70:LYS:NZ	2.40	0.50
28:26:23:THR:OG1	28:26:24:GLU:N	2.41	0.50
32:2a:236:G:O2'	48:2q:4:LYS:NZ	2.44	0.50
32:2a:373:A:H61	32:2a:391:G:H1'	1.77	0.50
32:2a:919:A:O2'	32:2a:1080:A:N1	2.38	0.50
32:2a:1327:C:H2'	32:2a:1328:C:C6	2.47	0.50
1:1A:2180:A:N3	1:1A:2181:G:H1'	2.26	0.50
1:1A:2732:G:OP2	61:1A:4290:HOH:O	2.19	0.50
22:10:32:ARG:H	22:10:35:ASN:ND2	2.10	0.50
32:1a:572:A:OP1	61:1a:3326:HOH:O	2.20	0.50
32:1a:710:G:H5''	37:1f:54:LYS:HE2	1.93	0.50
46:1o:55:GLY:HA2	46:1o:58:MET:HE3	1.92	0.50
1:2A:303:U:H2'	1:2A:304:G:H8	1.76	0.50
1:2A:731:C:OP1	61:2A:3985:HOH:O	2.20	0.50
1:2A:828:U:H4'	1:2A:831:G:N1	2.27	0.50
1:2A:1019:U:H3	1:2A:1142(A):A:H62	1.59	0.50
32:2a:1245:A:H2'	32:2a:1246:C:O4'	2.11	0.50
36:2e:12:LEU:HB3	36:2e:31:LEU:HB2	1.93	0.50
43:2l:10:LEU:HB3	48:2q:32:TYR:CE2	2.47	0.50
32:1a:613:C:H2'	32:1a:614:A:H8	1.77	0.50
32:1a:674:G:N2	32:1a:717:C:O2	2.45	0.50
33:1b:80:ILE:HG12	33:1b:215:LEU:HD23	1.92	0.50
40:1i:26:VAL:HG13	40:1i:61:ALA:HB3	1.92	0.50
51:1t:47:GLY:HA2	51:1t:48:LYS:C	2.37	0.50
1:2A:271(D):G:H2'	1:2A:271(E):U:C6	2.46	0.50
1:2A:2121:G:N2	1:2A:2177:C:N3	2.47	0.50
1:2A:2152:G:C2	1:2A:2153:G:H1'	2.46	0.50
32:2a:9:G:H2'	32:2a:10:A:C8	2.46	0.50
32:2a:26:A:N6	32:2a:558:G:O2'	2.43	0.50
32:2a:103:C:O2'	32:2a:172:A:N1	2.41	0.50
32:2a:137:C:H2'	32:2a:138:G:C8	2.45	0.50
35:2d:79:PHE:HE1	35:2d:204:ILE:HD13	1.76	0.50
37:2f:33:TYR:CE2	37:2f:78:GLU:HG3	2.45	0.50
40:2i:6:GLY:HA3	40:2i:80:GLY:O	2.11	0.50
1:1A:348:A:N6	1:1A:362:G:O2'	2.45	0.50
1:1A:650:G:N7	11:1P:107:LYS:NZ	2.58	0.50
1:1A:821:A:H2'	1:1A:821:A:N3	2.26	0.50
1:1A:2044:U:O2'	1:1A:2629:C:H5'	2.12	0.50
7:1H:91:GLY:HA2	7:1H:160:LYS:HG2	1.93	0.50
19:1X:50:LYS:HB3	19:1X:84:ALA:HB2	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:148:G:H2'	32:1a:149:A:C8	2.46	0.50
32:1a:983:A:H5'	32:1a:984:C:OP2	2.11	0.50
32:1a:1030:C:N4	32:1a:1031:G:N1	2.54	0.50
36:1e:105:VAL:HB	36:1e:106:PRO:HD3	1.94	0.50
48:1q:3:LYS:HD2	48:1q:60:ILE:HD11	1.92	0.50
1:2A:1411:C:H42	1:2A:1591:G:H1	1.59	0.50
1:2A:2261:C:H1'	1:2A:2388:A:N3	2.26	0.50
5:2F:116:ASP:OD1	5:2F:119:ARG:NH2	2.45	0.50
24:22:37:PHE:O	24:22:40:SER:OG	2.23	0.50
30:28:58:ILE:HA	30:28:61:LEU:HD12	1.93	0.50
32:2a:598:U:H4'	39:2h:94:TYR:CG	2.47	0.50
32:2a:834:C:H2'	32:2a:835:U:H6	1.76	0.50
32:2a:1040:U:H2'	32:2a:1041:A:H8	1.76	0.50
33:2b:178:ARG:NH2	39:2h:74:PRO:HB3	2.25	0.50
44:2m:16:ASP:HB2	44:2m:27:LYS:HE3	1.93	0.50
54:2w:4:C:N3	54:2w:69:G:C2	2.79	0.50
6:1G:7:LEU:HD12	6:1G:104:GLU:HA	1.94	0.50
6:1G:11:TYR:HA	6:1G:15:VAL:HB	1.93	0.50
20:1Y:6:HIS:H	20:1Y:6:HIS:CD2	2.30	0.50
30:18:63:PRO:HG2	30:18:64:TYR:CE2	2.46	0.50
37:1f:35:ALA:HA	37:1f:67:MET:HB3	1.94	0.50
40:1i:128:ARG:NH2	55:1x:33:U:OP2	2.45	0.50
54:1y:50:U:H3	54:1y:64:A:H2	1.57	0.50
1:2A:8:A:H2'	1:2A:9:U:H6	1.76	0.50
1:2A:2849:U:H4'	1:2A:2868:A:C2	2.47	0.50
5:2F:185:ASP:HA	5:2F:188:ARG:HD3	1.93	0.50
10:2O:76:ALA:HB3	15:2T:75:ILE:HB	1.92	0.50
32:2a:950:U:H2'	32:2a:951:G:H8	1.77	0.50
34:2c:121:ALA:HB1	34:2c:189:ALA:HB2	1.93	0.50
39:2h:20:TYR:HE2	39:2h:75:ARG:HD2	1.75	0.50
50:2s:66:MET:HB2	50:2s:74:PHE:CZ	2.47	0.50
55:2x:3:C:N3	55:2x:70:G:N2	2.52	0.50
55:2x:66:C:H2'	55:2x:67:C:O4'	2.12	0.50
1:1A:713:G:H1'	30:18:4:MET:HE3	1.93	0.50
1:1A:1068:G:N7	9:1N:66:LYS:HE3	2.27	0.50
1:1A:1683:C:H2'	1:1A:1684:A:C8	2.47	0.50
8:1I:130:TYR:HB3	8:1I:138:ILE:HB	1.94	0.50
12:1Q:10:ARG:NH1	12:1Q:90:VAL:H	2.09	0.50
17:1V:76:LYS:HB2	17:1V:81:TYR:HB3	1.92	0.50
18:1W:97:LYS:HE2	18:1W:99:ARG:NH2	2.27	0.50
33:1b:74:LYS:O	33:1b:78:GLN:HG2	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1c:172:ARG:NH2	34:1c:206:GLU:OE2	2.45	0.50
1:2A:1590:U:H2'	1:2A:1591:G:C8	2.47	0.50
4:2E:179:GLU:HG3	15:2T:9:LEU:HD21	1.94	0.50
32:2a:643:C:H2'	32:2a:644:G:H8	1.77	0.50
32:2a:1149:C:O2'	32:2a:1280:A:N1	2.36	0.50
32:2a:1353:G:H2'	32:2a:1354:C:C6	2.47	0.50
36:2e:102:ALA:O	36:2e:107:ARG:NH2	2.44	0.50
1:1A:886:U:H2'	1:1A:887:C:C6	2.47	0.49
1:1A:1072:U:OP1	61:1A:4273:HOH:O	2.20	0.49
1:1A:2579:G:H2'	1:1A:2580:C:C6	2.47	0.49
32:1a:1356:G:H2'	32:1a:1357:A:C8	2.47	0.49
33:1b:60:ASP:O	33:1b:64:ARG:HG2	2.12	0.49
39:1h:7:ALA:HB2	39:1h:85:ARG:HG3	1.93	0.49
1:2A:221:A:N1	1:2A:265:A:O2'	2.44	0.49
1:2A:322:A:OP2	5:2F:169:ASN:HB2	2.12	0.49
1:2A:1022:G:H22	1:2A:1142(A):A:H2	1.60	0.49
1:2A:2394:C:N3	54:2y:76:A:O2'	2.40	0.49
32:2a:475:G:H2'	32:2a:476:G:C8	2.46	0.49
32:2a:728:A:H2'	32:2a:729:A:C8	2.47	0.49
32:2a:997:U:O2	32:2a:1044:A:N1	2.45	0.49
32:2a:1499:A:H1'	32:2a:1520:G:H5'	1.94	0.49
38:2g:93:PRO:HA	38:2g:96:GLN:HB2	1.92	0.49
45:2n:25:VAL:HG23	45:2n:39:LEU:HD23	1.94	0.49
1:1A:1831:C:P	3:1D:183:ARG:HH12	2.35	0.49
32:1a:1136:U:H5''	32:1a:1137:C:C4	2.47	0.49
1:2A:821:A:N1	61:2A:4091:HOH:O	2.34	0.49
1:2A:1213:A:N3	1:2A:1238:G:O2'	2.40	0.49
1:2A:1264:G:H2'	1:2A:2014:A:N6	2.27	0.49
1:2A:2112:G:C2	1:2A:2113:U:H1'	2.47	0.49
21:2Z:98:MET:O	21:2Z:126:VAL:N	2.45	0.49
32:2a:109:A:C6	32:2a:326:G:C6	3.00	0.49
44:2m:40:ASN:HB3	44:2m:43:THR:HG23	1.94	0.49
49:2r:61:LYS:O	49:2r:65:ILE:HG12	2.11	0.49
1:1A:27:G:N2	1:1A:537:G:H1'	2.27	0.49
1:1A:656:A:OP1	11:1P:65:ARG:NE	2.36	0.49
18:1W:34:ASN:OD1	18:1W:37:ARG:NH2	2.45	0.49
32:1a:595:G:N3	32:1a:596:C:N4	2.60	0.49
1:2A:1030:G:OP2	12:2Q:128:LYS:NZ	2.45	0.49
3:2D:125:ILE:HB	37:2f:81:ILE:HD11	1.94	0.49
20:2Y:86:ARG:HD2	20:2Y:100:ALA:HA	1.93	0.49
32:2a:1497:G:H1'	32:2a:1518:MA6:H2	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:2e:148:VAL:HG21	39:2h:107:LEU:HD22	1.94	0.49
37:2f:100:ASN:ND2	49:2r:23:LYS:HE2	2.27	0.49
1:1A:321:C:H5''	20:1Y:87:LYS:HG3	1.94	0.49
1:1A:1913:G:O6	61:1A:4295:HOH:O	2.20	0.49
1:1A:1958:A:OP1	1:1A:1959:A:H5'	2.12	0.49
1:1A:2071:G:N7	61:1A:4390:HOH:O	2.34	0.49
15:1T:24:PRO:HA	15:1T:49:VAL:HG23	1.93	0.49
32:1a:332:G:H2'	32:1a:333:G:H8	1.77	0.49
38:1g:69:VAL:HG21	38:1g:104:LEU:HD11	1.94	0.49
38:1g:79:ARG:CD	38:1g:80:VAL:H	2.23	0.49
1:2A:1495:A:H2'	1:2A:1496:A:C8	2.48	0.49
6:2G:48:GLU:O	6:2G:51:ARG:NH1	2.44	0.49
8:2I:75:LEU:HD22	8:2I:105:HIS:CD2	2.48	0.49
15:2T:85:LYS:NZ	15:2T:87:ASP:OD2	2.46	0.49
21:2Z:93:ASP:HB2	21:2Z:131:ARG:HH12	1.78	0.49
55:2x:58:A:H4'	55:2x:59:A:OP1	2.12	0.49
1:1A:1201:A:OP1	16:1U:55:ARG:HD3	2.13	0.49
32:1a:204:U:H4'	32:1a:216:G:O5'	2.11	0.49
32:1a:1144:G:H21	32:1a:1146:A:H62	1.60	0.49
49:1r:52:PRO:HB2	49:1r:54:ARG:HG2	1.93	0.49
1:2A:27:G:N2	1:2A:512:G:H1'	2.28	0.49
1:2A:249:C:O2	30:28:12:LYS:NZ	2.39	0.49
1:2A:1218:C:H42	1:2A:1231:G:H1	1.60	0.49
7:2H:154:PRO:HB3	7:2H:163:TYR:CE1	2.47	0.49
20:2Y:44:ILE:HA	20:2Y:63:LYS:O	2.12	0.49
32:2a:21:G:H2'	32:2a:22:G:C8	2.47	0.49
32:2a:139:G:H2'	32:2a:140:A:C8	2.47	0.49
32:2a:983:A:N1	32:2a:1222:G:N2	2.61	0.49
50:2s:48:THR:HG22	50:2s:61:TYR:HA	1.93	0.49
1:1A:1634:C:H2'	1:1A:1635:C:H6	1.76	0.49
1:1A:2430:A:H2'	1:1A:2431:U:C6	2.48	0.49
5:1F:178:PRO:HB2	5:1F:201:VAL:HG21	1.93	0.49
5:1F:184:TYR:CE2	5:1F:188:ARG:HD2	2.47	0.49
19:1X:94:GLY:H	19:1X:95:LEU:HB2	1.78	0.49
32:1a:684:A:N6	61:1a:3375:HOH:O	2.43	0.49
49:1r:32:ARG:HA	49:1r:69:THR:HG21	1.95	0.49
1:2A:380:U:H2'	1:2A:381:G:H8	1.78	0.49
1:2A:831:G:O2'	11:2P:38:GLN:OE1	2.29	0.49
1:2A:1027:A:C2	1:2A:2488:A:H5'	2.48	0.49
1:2A:1769:G:O2'	1:2A:1958:C:OP1	2.23	0.49
1:2A:2206:G:H5''	1:2A:2207:G:N7	2.28	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2360:A:H2'	1:2A:2361:A:O4'	2.11	0.49
1:2A:2758:A:C2	1:2A:2759:G:H1'	2.48	0.49
9:2N:49:GLY:O	9:2N:119:ARG:NH1	2.45	0.49
32:2a:1207:2MG:H2'	32:2a:1208:C:C6	2.48	0.49
33:2b:16:HIS:CG	33:2b:17:PHE:N	2.80	0.49
54:2w:11:C:H42	54:2w:24:G:H1	1.61	0.49
55:2x:44:A:H2'	55:2x:45:G:C8	2.47	0.49
1:1A:273:G:O2'	1:1A:274:U:H5''	2.12	0.49
1:1A:944:C:N4	1:1A:945:A:H62	2.11	0.49
1:1A:1417:G:H2'	1:1A:1418:U:H5	1.77	0.49
6:1G:41:GLN:HB3	6:1G:43:LEU:HD13	1.94	0.49
9:1N:121:LYS:HD3	9:1N:130:HIS:CE1	2.48	0.49
32:1a:328:C:H4'	32:1a:329:A:H5'	1.94	0.49
32:1a:1047:G:H5''	45:1n:4:LYS:HD3	1.94	0.49
32:1a:1162:C:N3	32:1a:1174:G:N2	2.50	0.49
32:1a:1499:A:OP2	61:1a:3302:HOH:O	2.20	0.49
1:2A:2001:A:H2'	1:2A:2002:G:C8	2.48	0.49
1:2A:2127:G:C5	1:2A:2161:C:N4	2.80	0.49
1:2A:2542:A:H4'	1:2A:2543:G:C8	2.48	0.49
36:2e:102:ALA:HB3	36:2e:107:ARG:HB2	1.94	0.49
41:2j:55:LYS:HE2	41:2j:56:HIS:CE1	2.48	0.49
1:1A:943:C:H2'	1:1A:944:C:C6	2.48	0.49
1:1A:2150:C:H42	1:1A:2182:G:H1	1.59	0.49
1:1A:2441:G:N7	11:1P:56:SER:OG	2.37	0.49
1:1A:2614:A:OP1	61:1A:4293:HOH:O	2.19	0.49
9:1N:29:LYS:HD2	9:1N:140:VAL:HB	1.94	0.49
32:1a:67:C:H2'	32:1a:68:G:H8	1.78	0.49
32:1a:78:G:N2	32:1a:91:C:C2	2.81	0.49
32:1a:189(K):U:H2'	32:1a:189(L):G:C8	2.48	0.49
54:1y:5:G:H1'	54:1y:69:G:N2	2.28	0.49
1:2A:300:A:N3	1:2A:319:C:H1'	2.27	0.49
1:2A:861:A:N6	1:2A:916:G:O2'	2.46	0.49
1:2A:1568:G:H5'	3:2D:60:ARG:HA	1.94	0.49
1:2A:2030:A:H4'	1:2A:2031:A:C8	2.48	0.49
1:2A:2127:G:C6	1:2A:2161:C:C4	2.95	0.49
12:2Q:66:ILE:HG12	12:2Q:104:PHE:HD1	1.77	0.49
21:2Z:33:LEU:HD21	21:2Z:90:VAL:HG21	1.95	0.49
32:2a:328:C:H4'	32:2a:329:A:H5'	1.94	0.49
32:2a:950:U:H2'	32:2a:951:G:C8	2.47	0.49
32:2a:1356:G:N2	32:2a:1367:C:O2	2.46	0.49
32:2a:1375:A:O2'	38:2g:29:LYS:NZ	2.46	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:2q:54:GLY:O	48:2q:81:ARG:N	2.45	0.49
50:2s:41:VAL:HG12	50:2s:44:MET:HG3	1.95	0.49
6:1G:5:VAL:HG21	6:1G:100:TRP:HB3	1.95	0.49
20:1Y:99:CYS:HB2	20:1Y:106:LEU:HD21	1.94	0.49
32:1a:1036:G:H5'	32:1a:1037:C:C5	2.48	0.49
32:1a:1458:G:H5'	51:1t:32:ALA:HB2	1.95	0.49
34:1c:68:VAL:HG12	34:1c:70:VAL:HG23	1.95	0.49
7:2H:29:PRO:HD2	7:2H:79:VAL:O	2.13	0.49
21:2Z:121:HIS:N	21:2Z:171:ILE:O	2.45	0.49
25:23:10:LYS:HB3	25:23:53:LEU:HA	1.95	0.49
32:2a:46:G:H2'	32:2a:366:C:C5	2.48	0.49
32:2a:841:U:C5	32:2a:848:C:H1'	2.48	0.49
1:1A:698:G:H2'	1:1A:699:C:C6	2.48	0.49
1:1A:1108:G:P	1:1A:1116:A:H1'	2.53	0.49
1:1A:1210:G:H2'	1:1A:1211:U:C6	2.48	0.49
1:1A:1273:G:OP1	16:1U:13:LYS:NZ	2.45	0.49
1:1A:1704:C:OP2	4:1E:136:ARG:HG3	2.12	0.49
4:1E:178:GLU:OE1	4:1E:178:GLU:N	2.45	0.49
25:13:8:LEU:HB2	25:13:28:LEU:HD13	1.95	0.49
31:19:16:VAL:HG22	31:19:25:VAL:HG22	1.95	0.49
32:1a:381:C:H2'	32:1a:382:A:O4'	2.11	0.49
32:1a:1469:G:H2'	32:1a:1470:G:C8	2.47	0.49
35:1d:26:CYS:CB	60:1d:501:SF4:S1	2.92	0.49
1:2A:2022:U:O2'	1:2A:2617:C:H5'	2.13	0.49
1:2A:2722:G:H5'	13:2R:4:LEU:HD12	1.94	0.49
32:2a:671:G:H2'	32:2a:672:U:O4'	2.13	0.49
32:2a:867:G:O2'	32:2a:873:A:N6	2.46	0.49
32:2a:1029:C:N4	32:2a:1032:G:C6	2.81	0.49
32:2a:1517:G:H3'	32:2a:1518:MA6:H8	1.94	0.49
33:2b:30:ARG:HH21	33:2b:194:PRO:HB2	1.78	0.49
33:2b:87:ARG:HD2	33:2b:234:PRO:HD2	1.95	0.49
1:1A:1074:A:N6	1:1A:1171:G:H2'	2.28	0.48
9:1N:21:LYS:HE3	9:1N:140:VAL:OXT	2.13	0.48
13:1R:97:VAL:HG22	13:1R:114:VAL:HG13	1.94	0.48
32:1a:545:C:OP1	35:1d:61:LYS:NZ	2.40	0.48
32:1a:871:U:OP1	61:1a:3325:HOH:O	2.19	0.48
32:1a:1402:4OC:HM22	32:1a:1403:C:H5'	1.95	0.48
32:1a:1469:G:H2'	32:1a:1470:G:H8	1.77	0.48
41:1j:21:GLN:NE2	41:1j:25:GLU:OE2	2.39	0.48
47:1p:19:ILE:HG22	47:1p:36:ILE:HG13	1.95	0.48
1:2A:839:U:H2'	1:2A:840:C:H6	1.77	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1239:G:H2'	1:2A:1240:U:O4'	2.13	0.48
1:2A:1636:C:H2'	1:2A:1637:A:C8	2.48	0.48
1:2A:1777:U:H2'	1:2A:1778:U:H6	1.77	0.48
1:2A:2376:A:H3'	1:2A:2377:A:H8	1.77	0.48
11:2P:48:PRO:O	30:28:57:ARG:NH2	2.38	0.48
13:2R:100:LEU:HD11	13:2R:113:LEU:HD23	1.95	0.48
32:2a:501:C:H2'	32:2a:502:G:C8	2.48	0.48
32:2a:649:G:N7	61:2a:3354:HOH:O	2.35	0.48
32:2a:957:U:H2'	32:2a:959:A:OP2	2.13	0.48
35:2d:150:GLU:HA	35:2d:153:ARG:HG2	1.95	0.48
46:2o:55:GLY:HA2	46:2o:58:MET:HE3	1.95	0.48
1:1A:324:A:OP1	20:1Y:86:ARG:NH2	2.46	0.48
1:1A:1101:G:H1	1:1A:1150:C:N4	2.08	0.48
1:1A:1717:C:O2	4:1E:129:HIS:NE2	2.45	0.48
1:1A:2303:U:H2'	1:1A:2304:C:C6	2.48	0.48
1:1A:2331:G:N1	14:1S:3:ARG:HA	2.28	0.48
26:14:40:HIS:HB3	26:14:43:TYR:HD2	1.76	0.48
32:1a:69:G:H2'	32:1a:70:G:C8	2.48	0.48
32:1a:96:U:H2'	32:1a:97:G:H8	1.78	0.48
33:1b:120:ALA:HA	33:1b:123:ALA:HB3	1.94	0.48
33:1b:166:ASP:HB3	33:1b:169:LYS:HB3	1.94	0.48
1:2A:71:A:H5''	1:2A:73:A:C8	2.48	0.48
3:2D:18:VAL:HG12	3:2D:211:ARG:HH12	1.78	0.48
3:2D:211:ARG:O	3:2D:215:LEU:HG	2.13	0.48
13:2R:12:ARG:HB3	13:2R:16:HIS:HB3	1.95	0.48
29:27:2:LYS:NZ	61:27:201:HOH:O	2.29	0.48
32:2a:1152:A:OP1	41:2j:70:ARG:NH2	2.32	0.48
35:2d:202:LEU:HA	35:2d:205:GLU:HB2	1.95	0.48
38:2g:69:VAL:HG22	38:2g:135:VAL:HG22	1.94	0.48
38:2g:126:ASP:O	38:2g:131:LYS:N	2.33	0.48
39:2h:95:VAL:HG11	39:2h:133:LEU:HD12	1.95	0.48
43:2l:113:ARG:NH2	43:2l:115:LYS:O	2.45	0.48
2:1B:48:A:H4'	14:1S:95:HIS:HD2	1.77	0.48
32:1a:60:A:H4'	32:1a:61:G:H5'	1.94	0.48
38:1g:97:GLN:O	38:1g:101:LEU:HG	2.13	0.48
1:2A:1688:U:O2	1:2A:1700:A:H5'	2.13	0.48
1:2A:2882:A:OP1	13:2R:96:ARG:NH1	2.46	0.48
13:2R:96:ARG:NH2	13:2R:117:VAL:HG13	2.27	0.48
15:2T:74:ARG:HG2	15:2T:76:PHE:CZ	2.48	0.48
18:2W:88:ARG:NH1	18:2W:94:ASP:OD2	2.47	0.48
21:2Z:28:MET:HE1	21:2Z:61:LEU:HD21	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:614:A:H2'	32:2a:615:C:C6	2.48	0.48
32:2a:1502:A:C8	32:2a:1505:G:N2	2.81	0.48
36:2e:101:ILE:O	36:2e:120:THR:OG1	2.30	0.48
1:1A:1462:G:O2'	1:1A:1463:C:OP2	2.22	0.48
4:1E:174:ASP:HB3	4:1E:183:LEU:HD22	1.94	0.48
5:1F:101:LEU:O	5:1F:106:ARG:NH1	2.43	0.48
6:1G:129:GLY:O	6:1G:161:THR:OG1	2.31	0.48
11:1P:63:PRO:HD3	30:18:27:THR:HG22	1.95	0.48
32:1a:1068:G:H8	32:1a:1068:G:OP2	1.97	0.48
54:1w:2:C:N3	54:1w:71:G:N2	2.61	0.48
1:2A:93:G:H2'	1:2A:94:C:C6	2.48	0.48
1:2A:1005:C:H2'	1:2A:1006:C:C6	2.49	0.48
2:2B:66:A:H61	2:2B:108:U:H3'	1.78	0.48
32:2a:972:C:H4'	41:2j:57:LYS:HB2	1.95	0.48
1:1A:1312:G:O2'	1:1A:2034:G:O6	2.30	0.48
1:1A:1787:G:O6	61:1A:4288:HOH:O	2.19	0.48
1:1A:2147:G:N1	1:1A:2194:U:OP1	2.24	0.48
1:1A:2613:C:H2'	1:1A:2615:G:C8	2.48	0.48
17:1V:46:VAL:HG22	17:1V:52:VAL:HG11	1.96	0.48
32:1a:997:U:H3	32:1a:1044:A:N6	2.12	0.48
1:2A:83:G:O2'	1:2A:102:G:N2	2.46	0.48
1:2A:686:G:N2	1:2A:788:A:H61	2.11	0.48
1:2A:1779:U:OP2	1:2A:1784:A:N6	2.36	0.48
1:2A:1991:U:H2'	1:2A:1992:G:H5''	1.95	0.48
32:2a:1260:C:O5'	32:2a:1284:C:H4'	2.13	0.48
44:2m:101:GLN:OE1	44:2m:101:GLN:N	2.47	0.48
1:1A:109:A:O3'	24:12:65:ASN:ND2	2.46	0.48
1:1A:721:G:OP2	61:1A:4296:HOH:O	2.20	0.48
18:1W:82:LEU:HB2	18:1W:98:LYS:HB2	1.95	0.48
24:12:1:MET:HB2	24:12:52:ASP:OD2	2.14	0.48
32:1a:544:G:OP1	35:1d:59:ARG:NH2	2.42	0.48
32:1a:931:C:N3	32:1a:1386:G:N2	2.51	0.48
32:1a:1179:A:H2'	32:1a:1180:A:O4'	2.13	0.48
33:1b:24:TRP:CZ3	33:1b:26:PRO:HA	2.48	0.48
1:2A:1011:G:OP2	16:2U:66:ASN:ND2	2.45	0.48
10:2O:49:ARG:HH12	32:2a:1423:G:P	2.35	0.48
11:2P:120:ALA:HB2	11:2P:137:LYS:HB3	1.95	0.48
32:2a:1366:C:O2'	41:2j:60:ARG:NH1	2.43	0.48
45:2n:27:CYS:SG	45:2n:29:ARG:HG3	2.54	0.48
1:1A:211:A:H5''	1:1A:448:U:OP1	2.14	0.48
1:1A:939:C:H2'	1:1A:940:C:C6	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1I:60:GLU:HG3	8:1I:61:ARG:NH1	2.28	0.48
20:1Y:9:LYS:HA	20:1Y:10:GLY:HA2	1.59	0.48
32:1a:107:G:N7	51:1t:15:ARG:NH2	2.62	0.48
32:1a:757:U:O2'	32:1a:879:C:O2	2.28	0.48
46:1o:82:ILE:O	46:1o:86:GLY:N	2.47	0.48
1:2A:601:C:O2	1:2A:605:C:H4'	2.14	0.48
1:2A:603:A:N1	1:2A:625:G:O2'	2.46	0.48
7:2H:113:VAL:HG11	7:2H:151:ILE:HD13	1.94	0.48
16:2U:107:ALA:O	16:2U:111:GLU:HG2	2.14	0.48
32:2a:22:G:H4'	32:2a:885:G:C8	2.49	0.48
32:2a:1114:C:N4	32:2a:1186:G:H1	2.12	0.48
35:2d:74:GLN:O	35:2d:78:LEU:HG	2.13	0.48
44:2m:34:LEU:HD13	44:2m:41:PRO:HB3	1.94	0.48
1:1A:831:A:N6	3:1D:229:VAL:HG11	2.29	0.48
9:1N:34:LEU:HD21	9:1N:120:LEU:HB2	1.96	0.48
15:1T:24:PRO:HD3	15:1T:52:ILE:HD12	1.96	0.48
25:13:5:LYS:NZ	25:13:34:GLU:OE2	2.31	0.48
32:1a:159:G:HO2'	32:1a:161:A:H62	1.61	0.48
32:1a:1512:U:H2'	32:1a:1513:A:C8	2.48	0.48
33:1b:101:MET:HG2	33:1b:108:ILE:HG21	1.95	0.48
1:2A:94(A):G:H2'	1:2A:95:G:O4'	2.14	0.48
1:2A:127:A:H5''	1:2A:128:C:C6	2.48	0.48
1:2A:995:C:O2	9:2N:3:THR:OG1	2.28	0.48
1:2A:1274:A:N3	1:2A:1297:C:H1'	2.28	0.48
1:2A:1458:C:H4'	1:2A:1459:G:O4'	2.14	0.48
1:2A:2841:C:H2'	1:2A:2842:G:C8	2.49	0.48
28:26:6:ARG:HH21	28:26:24:GLU:CD	2.22	0.48
32:2a:542:G:OP1	35:2d:10:ARG:NH2	2.35	0.48
32:2a:920:U:H2'	32:2a:921:U:C6	2.49	0.48
32:2a:1136:U:OP2	32:2a:1137:C:N4	2.47	0.48
32:2a:1226:C:H2'	44:2m:103:THR:HB	1.96	0.48
44:2m:23:TYR:CE2	44:2m:71:ARG:HG3	2.48	0.48
50:2s:27:GLU:HB2	50:2s:28:LYS:HD3	1.94	0.48
1:1A:441:C:H2'	1:1A:442:A:C8	2.49	0.48
1:1A:2366:G:H21	22:10:36:ILE:HD11	1.79	0.48
4:1E:60:ASN:HD22	4:1E:62:PRO:HD2	1.78	0.48
4:1E:174:ASP:OD1	4:1E:175:VAL:N	2.47	0.48
5:1F:95:ARG:HD3	5:1F:97:TYR:CZ	2.49	0.48
32:1a:343:U:O2'	32:1a:346:G:O6	2.30	0.48
42:1k:51:LYS:HA	42:1k:55:LYS:HE2	1.95	0.48
1:2A:224:G:H2'	1:2A:225:A:O4'	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:320:A:H1'	5:2F:169:ASN:HD22	1.78	0.48
1:2A:1702:G:H2'	1:2A:1703:G:O4'	2.14	0.48
8:2I:66:GLU:HA	8:2I:69:LYS:HB3	1.94	0.48
12:2Q:12:GLN:HE21	12:2Q:72:LYS:HG3	1.79	0.48
32:2a:707:C:H2'	32:2a:708:C:C6	2.49	0.48
41:2j:57:LYS:HG3	41:2j:60:ARG:HH21	1.79	0.48
54:2y:10:G:H1	54:2y:25:C:H42	1.61	0.48
1:1A:196:A:H2'	1:1A:197:C:O4'	2.14	0.48
1:1A:213:G:H2'	1:1A:214:A:O4'	2.14	0.48
1:1A:626:A:O4'	1:1A:702:A:N6	2.46	0.48
1:1A:1715:A:H4'	1:1A:1716:A:O5'	2.14	0.48
1:1A:2163:G:C4	1:1A:2164:C:H1'	2.49	0.48
7:1H:30:LYS:HB2	7:1H:79:VAL:HA	1.95	0.48
32:1a:613:C:H2'	32:1a:614:A:C8	2.49	0.48
32:1a:1118:C:H1'	32:1a:1179:A:C4	2.49	0.48
1:2A:407:G:H2'	1:2A:408:G:C8	2.49	0.48
1:2A:2142:C:N3	1:2A:2149:G:O6	2.47	0.48
7:2H:129:THR:O	7:2H:129:THR:OG1	2.30	0.48
13:2R:88:ARG:NH2	13:2R:89:ASP:OD1	2.47	0.48
32:2a:1033:G:H2'	32:2a:1034:G:H8	1.78	0.48
33:2b:178:ARG:NH1	39:2h:68:ARG:HH22	2.12	0.48
41:2j:30:SER:O	41:2j:81:THR:OG1	2.31	0.48
44:2m:91:ARG:HD3	44:2m:97:PRO:O	2.14	0.48
48:2q:6:LEU:HB3	48:2q:23:VAL:HG11	1.96	0.48
1:1A:225:C:H2'	1:1A:226:C:H6	1.79	0.47
1:1A:1073:A:N3	61:1A:4405:HOH:O	2.35	0.47
1:1A:1085:G:H1	1:1A:1162:C:N4	2.03	0.47
1:1A:2123:G:H2'	1:1A:2124:U:C6	2.49	0.47
1:1A:2576:A:C2	1:1A:2659:U:H4'	2.49	0.47
22:10:46:LYS:NZ	22:10:75:LEU:O	2.38	0.47
24:12:32:LEU:HD22	24:12:36:ARG:HH11	1.79	0.47
32:1a:376:G:H5''	47:1p:5:ARG:HD2	1.96	0.47
32:1a:584:G:H5'	48:1q:91:ARG:HH22	1.79	0.47
32:1a:1314:C:OP2	50:1s:4:SER:OG	2.20	0.47
33:1b:174:VAL:HG13	33:1b:184:VAL:HG11	1.96	0.47
36:1e:33:VAL:HG21	36:1e:109:ILE:HA	1.96	0.47
42:1k:33:THR:HA	42:1k:39:PRO:HA	1.94	0.47
48:1q:62:SER:OG	48:1q:72:ARG:HG2	2.13	0.47
1:2A:2143:C:N4	1:2A:2148:G:H1	2.11	0.47
6:2G:101:ILE:HD13	26:24:25:TYR:HB2	1.96	0.47
6:2G:173:LEU:HB3	6:2G:178:PHE:CD2	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:936:C:H2'	32:2a:937:A:O4'	2.14	0.47
32:2a:997:U:H2'	32:2a:998:G:C8	2.48	0.47
1:1A:602:G:H2'	1:1A:603:C:C6	2.49	0.47
1:1A:2339:A:H2'	1:1A:2340:A:C8	2.49	0.47
1:1A:2801:C:O2'	1:1A:2819:A:N3	2.37	0.47
32:1a:1033:G:C4	32:1a:1034:G:C8	3.02	0.47
32:1a:1129:C:OP1	40:1i:66:ARG:NH1	2.47	0.47
40:1i:69:GLY:O	40:1i:73:GLN:HG3	2.14	0.47
47:1p:19:ILE:N	47:1p:37:GLY:O	2.48	0.47
1:2A:315:G:H2'	1:2A:316:C:C6	2.49	0.47
1:2A:451:C:H4'	5:2F:52:LYS:HE2	1.96	0.47
1:2A:884:C:H3'	1:2A:885:C:C6	2.50	0.47
1:2A:1541:G:OP2	1:2A:1542:A:O2'	2.31	0.47
1:2A:2061:G:H5''	1:2A:2503:2MA:C2	2.43	0.47
32:2a:46:G:O2'	32:2a:365:U:H1'	2.13	0.47
32:2a:565:U:OP2	32:2a:566:G:O2'	2.27	0.47
32:2a:918:A:H2'	32:2a:919:A:O4'	2.14	0.47
32:2a:1323:G:H4'	32:2a:1363:C:N3	2.29	0.47
1:1A:1103:A:N6	1:1A:1133:G:OP2	2.46	0.47
1:1A:1452:U:H2'	1:1A:1453:C:C6	2.50	0.47
1:1A:1475:G:H2'	1:1A:1476:C:C6	2.48	0.47
5:1F:172:TRP:CD1	5:1F:172:TRP:H	2.32	0.47
18:1W:71:VAL:HA	18:1W:107:LEU:HD12	1.97	0.47
32:1a:1429:C:H2'	32:1a:1430:C:C6	2.49	0.47
36:1e:85:GLY:C	36:1e:87:SER:H	2.23	0.47
1:2A:478:A:N1	1:2A:500:G:H4'	2.29	0.47
1:2A:2637:U:H5''	4:2E:82:ARG:NH1	2.29	0.47
9:2N:108:PRO:O	9:2N:113:GLY:HA3	2.15	0.47
32:2a:148:G:H1	32:2a:174:C:H42	1.61	0.47
32:2a:266:G:H2'	32:2a:266:G:N3	2.28	0.47
32:2a:405:U:O4	35:2d:2:GLY:N	2.47	0.47
35:2d:8:VAL:HG22	35:2d:21:LEU:HD13	1.95	0.47
39:2h:18:ARG:HA	39:2h:78:GLN:HE22	1.79	0.47
45:2n:4:LYS:HA	45:2n:7:ILE:HG22	1.96	0.47
50:2s:41:VAL:HG13	50:2s:43:GLU:H	1.79	0.47
53:2v:12:A:N3	53:2v:12:A:H2'	2.29	0.47
1:1A:783:C:OP1	61:1A:4292:HOH:O	2.19	0.47
1:1A:941:U:O2'	1:1A:942:A:OP1	2.23	0.47
1:1A:2153:G:H5''	1:1A:2154:U:H3'	1.97	0.47
1:1A:2544:G:O2'	1:1A:2669:A:N1	2.44	0.47
1:1A:2867:G:N2	1:1A:2870:A:OP2	2.38	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1I:116:LEU:HD21	8:1I:119:PRO:HA	1.96	0.47
32:1a:34:C:H2'	32:1a:35:G:C8	2.49	0.47
32:1a:1126:U:O2	32:1a:1280:A:H2'	2.14	0.47
44:1m:86:CYS:HB2	50:1s:73:GLU:HB3	1.96	0.47
1:2A:989:G:OP2	25:23:11:SER:OG	2.25	0.47
1:2A:2556:C:H2'	1:2A:2557:G:O4'	2.15	0.47
3:2D:274:ARG:O	3:2D:275:LYS:HD2	2.14	0.47
5:2F:155:LEU:HB2	5:2F:189:THR:HG21	1.97	0.47
32:2a:937:A:H1'	32:2a:1379:G:N2	2.30	0.47
33:2b:92:TYR:CE2	33:2b:151:GLY:HA3	2.49	0.47
33:2b:162:ILE:O	33:2b:185:ILE:HG12	2.14	0.47
34:2c:20:SER:HB3	34:2c:22:TRP:NE1	2.30	0.47
36:2e:33:VAL:HG21	36:2e:109:ILE:HA	1.97	0.47
49:2r:47:THR:O	49:2r:47:THR:OG1	2.32	0.47
1:1A:246:A:OP2	61:1A:4300:HOH:O	2.20	0.47
7:1H:149:ARG:HH12	7:1H:167:GLU:CD	2.22	0.47
32:1a:299:G:C6	32:1a:300:A:C6	3.03	0.47
32:1a:719:C:O2'	49:1r:49:LYS:HB3	2.14	0.47
32:1a:1068:G:N7	32:1a:1094:G:H2'	2.30	0.47
32:1a:1104:G:H4'	33:1b:111:ARG:NH2	2.30	0.47
35:1d:111:ALA:HB2	35:1d:120:LEU:HD12	1.96	0.47
43:1l:76:ASN:ND2	43:1l:106:ASP:O	2.46	0.47
50:1s:27:GLU:CB	50:1s:28:LYS:HA	2.38	0.47
55:1x:4:G:H1	55:1x:69:C:H42	1.61	0.47
1:2A:1292:U:H2'	1:2A:1293:C:C6	2.49	0.47
1:2A:1528:A:H2'	1:2A:1528(A):A:C8	2.50	0.47
1:2A:2144:U:H1'	1:2A:2148:G:N2	2.30	0.47
2:2B:43:C:OP1	26:24:6:HIS:NE2	2.46	0.47
14:2S:95:HIS:CG	14:2S:96:GLY:H	2.32	0.47
19:2X:35:THR:HG22	19:2X:38:GLU:H	1.79	0.47
32:2a:1013:G:H2'	32:2a:1015:A:OP2	2.14	0.47
34:2c:124:ILE:HG21	34:2c:130:VAL:HG13	1.96	0.47
35:2d:4:TYR:C	35:2d:5:ILE:HG13	2.39	0.47
1:1A:479:C:O2	1:1A:483:A:O2'	2.33	0.47
1:1A:2018:C:H4'	1:1A:2019:G:OP1	2.13	0.47
3:1D:37:LEU:HD22	3:1D:87:ASN:HD21	1.79	0.47
14:1S:92:TYR:OH	61:1S:3101:HOH:O	2.18	0.47
32:1a:261:U:OP2	51:1t:79:ARG:NH2	2.47	0.47
32:1a:600:C:H2'	32:1a:601:C:C6	2.49	0.47
32:1a:999:C:H42	32:1a:1042:G:H1	1.63	0.47
32:1a:1346:A:N1	32:1a:1374:A:H5''	2.29	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1429:C:H2'	32:1a:1430:C:H6	1.80	0.47
40:1i:4:TYR:CE1	40:1i:88:TYR:HA	2.49	0.47
54:1y:19:G:N2	54:1y:56:C:N3	2.63	0.47
1:2A:299:A:H5''	20:2Y:86:ARG:HH21	1.79	0.47
2:2B:82:G:N7	61:2B:5003:HOH:O	2.36	0.47
2:2B:105:A:OP1	21:2Z:72:ARG:NH1	2.48	0.47
32:2a:501:C:H2'	32:2a:502:G:H8	1.80	0.47
32:2a:1049:U:H4'	32:2a:1050:G:H5''	1.95	0.47
33:2b:58:ILE:O	33:2b:62:ALA:N	2.44	0.47
53:2v:22:U:H2'	53:2v:23:A:H8	1.80	0.47
54:2y:67:C:H2'	54:2y:68:C:C6	2.49	0.47
1:1A:1263:C:N4	1:1A:1277:G:H1	2.13	0.47
1:1A:1556:A:H3'	1:1A:1557:A:H8	1.79	0.47
1:1A:1961:5MU:OP1	1:1A:2616:U:O2'	2.32	0.47
1:1A:2051:G:H2'	1:1A:2053:A:OP1	2.14	0.47
1:1A:2642:G:H21	1:1A:2901:A:H1'	1.78	0.47
8:1I:40:THR:O	8:1I:44:LEU:HB2	2.15	0.47
14:1S:10:ARG:O	14:1S:14:VAL:HG13	2.15	0.47
15:1T:29:ARG:HG3	15:1T:46:GLU:HB2	1.96	0.47
15:1T:49:VAL:HG12	15:1T:63:VAL:HG22	1.97	0.47
20:1Y:13:VAL:HG12	20:1Y:74:PRO:HA	1.96	0.47
32:1a:1090:U:H2'	32:1a:1091:U:C6	2.49	0.47
32:1a:1123:A:O2'	41:1j:37:PRO:O	2.32	0.47
32:1a:1196:U:H3	34:1c:162:GLN:HE22	1.62	0.47
32:1a:1239:A:H62	32:1a:1299:A:N6	2.12	0.47
39:1h:104:ARG:HD3	39:1h:104:ARG:HA	1.72	0.47
44:1m:16:ASP:HB2	44:1m:27:LYS:HE3	1.97	0.47
48:1q:61:GLU:HA	48:1q:71:PHE:CD1	2.50	0.47
1:2A:27:G:O2'	1:2A:28:A:OP2	2.29	0.47
1:2A:652(D):C:H42	1:2A:652(U):G:H1	1.62	0.47
1:2A:887:A:H4'	1:2A:888:C:C5	2.50	0.47
1:2A:1839:G:C8	1:2A:1927:A:H1'	2.50	0.47
1:2A:2467:C:H4'	12:2Q:123:HIS:CD2	2.50	0.47
8:2I:38:LEU:H	8:2I:38:LEU:HD12	1.79	0.47
17:2V:2:PHE:CZ	17:2V:41:GLY:HA3	2.49	0.47
22:20:23:VAL:HG13	22:20:38:VAL:HG22	1.95	0.47
24:22:35:LEU:HD12	24:22:53:LEU:HD12	1.97	0.47
32:2a:130:A:N3	32:2a:263:A:O2'	2.47	0.47
32:2a:324:G:O2'	32:2a:326:G:N7	2.38	0.47
32:2a:447:G:O6	32:2a:485:G:O2'	2.22	0.47
32:2a:750:G:N3	46:2o:23:GLY:HA3	2.30	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:985:C:H2'	32:2a:986:A:H8	1.79	0.47
32:2a:1227:A:C8	50:2s:83:HIS:HB3	2.49	0.47
32:2a:1318:A:H4'	50:2s:10:PHE:CE2	2.50	0.47
33:2b:80:ILE:HD13	33:2b:211:ILE:HG22	1.96	0.47
51:2t:56:MET:HG3	51:2t:84:LEU:HD21	1.96	0.47
55:2x:28:C:H2'	55:2x:29:G:H8	1.79	0.47
55:2x:37:A:H2'	55:2x:38:A:O4'	2.15	0.47
54:2y:67:C:H2'	54:2y:68:C:H6	1.78	0.47
1:1A:2240:G:H22	23:11:47:GLN:HE22	1.62	0.47
3:1D:61:LEU:O	3:1D:63:ARG:NH1	2.48	0.47
10:1O:97:ARG:NH1	32:1a:339:C:OP2	2.38	0.47
18:1W:46:PHE:O	18:1W:50:VAL:HG23	2.14	0.47
32:1a:194:C:H2'	32:1a:195:A:H5''	1.96	0.47
32:1a:936:C:H2'	32:1a:937:A:O4'	2.13	0.47
32:1a:974:A:H8	32:1a:974:A:OP1	1.98	0.47
1:2A:661:C:H2'	1:2A:662:G:H8	1.79	0.47
1:2A:1300:U:OP1	61:2A:3988:HOH:O	2.20	0.47
15:2T:6:LEU:O	15:2T:10:VAL:HG23	2.15	0.47
32:2a:674:G:OP1	37:2f:87:ARG:NH2	2.47	0.47
32:2a:1118:C:H1'	32:2a:1179:A:C5	2.49	0.47
32:2a:1438:G:H2'	32:2a:1439:C:C6	2.49	0.47
47:2p:23:ASP:OD1	47:2p:25:ARG:NH1	2.48	0.47
1:1A:27:G:C2	1:1A:537:G:N3	2.83	0.47
1:1A:1159:U:H2'	1:1A:1160:G:C8	2.49	0.47
8:1I:4:ILE:HG12	8:1I:18:VAL:HG22	1.97	0.47
32:1a:313:A:H2'	32:1a:314:C:C6	2.50	0.47
36:1e:60:TYR:OH	36:1e:64:ARG:NH2	2.40	0.47
54:1y:7:A:O2'	54:1y:49:C:H5'	2.15	0.47
1:2A:1434:A:H2'	1:2A:1435:G:C8	2.50	0.47
1:2A:1803:A:O2'	3:2D:259:THR:HG21	2.15	0.47
1:2A:2749:A:OP1	7:2H:3:ARG:NH1	2.47	0.47
12:2Q:24:GLY:HA2	12:2Q:67:ARG:NH2	2.30	0.47
12:2Q:39:PRO:HD3	12:2Q:99:PRO:HG3	1.97	0.47
32:2a:41:G:H2'	32:2a:42:G:C8	2.50	0.47
32:2a:187:C:H2'	32:2a:188:C:C6	2.49	0.47
32:2a:335:C:O2'	32:2a:1433:A:N3	2.40	0.47
32:2a:448:A:OP2	32:2a:485:G:N1	2.45	0.47
32:2a:757:U:H2'	32:2a:758:G:O4'	2.14	0.47
32:2a:841:U:OP1	32:2a:841:U:H6	1.98	0.47
32:2a:954:G:H2'	32:2a:955:U:O4'	2.15	0.47
32:2a:1192:C:P	34:2c:4:LYS:HZ1	2.37	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:2j:17:ASP:OD1	41:2j:70:ARG:NE	2.47	0.47
45:2n:24:CYS:HB2	45:2n:40:CYS:HB3	1.97	0.47
51:2t:93:GLU:C	51:2t:95:ALA:H	2.23	0.47
1:1A:624:C:O2'	1:1A:628:C:OP1	2.31	0.47
1:1A:1218:G:O2'	1:1A:1219:A:O4'	2.32	0.47
1:1A:1384:G:O2'	1:1A:1439:A:N1	2.48	0.47
1:1A:1634:C:H2'	1:1A:1635:C:C6	2.50	0.47
1:1A:2849:G:H5'	13:1R:46:GLY:HA2	1.96	0.47
21:1Z:92:SER:O	21:1Z:130:PRO:HG2	2.15	0.47
26:14:57:GLU:HB3	26:14:58:ARG:HD2	1.97	0.47
27:15:16:ARG:HG3	27:15:17:ASP:N	2.30	0.47
32:1a:1008:C:O2	32:1a:1021:G:N1	2.32	0.47
1:2A:1364:G:OP2	23:21:3:LYS:HG3	2.15	0.47
8:2I:79:ILE:O	8:2I:144:VAL:HA	2.15	0.47
26:24:58:ARG:HD3	44:2m:80:ARG:NH1	2.30	0.47
32:2a:946:A:H2'	32:2a:947:G:C8	2.50	0.47
32:2a:1132:C:H2'	32:2a:1133:G:H8	1.80	0.47
32:2a:1436:U:H2'	32:2a:1437:C:O4'	2.15	0.47
43:2l:77:LEU:HD21	43:2l:107:ALA:HB2	1.96	0.47
1:1A:207:A:C2	1:1A:224:U:H4'	2.50	0.46
1:1A:794:U:O2	1:1A:2036:A:H1'	2.16	0.46
6:1G:53:LEU:O	6:1G:57:ALA:N	2.43	0.46
9:1N:4:TYR:CD2	16:1U:100:VAL:HG11	2.50	0.46
19:1X:31:HIS:CD2	19:1X:33:LYS:H	2.33	0.46
30:18:23:VAL:CG1	30:18:47:LYS:HB3	2.45	0.46
32:1a:78:G:O2'	32:1a:79:G:H5'	2.15	0.46
32:1a:339:C:H2'	32:1a:340:U:H6	1.80	0.46
1:2A:607:U:OP1	5:2F:102:PRO:HA	2.15	0.46
1:2A:1428:C:N4	1:2A:1570:A:OP2	2.43	0.46
1:2A:1518:U:H2'	1:2A:1519:G:O4'	2.16	0.46
1:2A:2564:A:OP1	1:2A:2648:C:H4'	2.14	0.46
14:2S:27:SER:HA	14:2S:88:ASP:HB3	1.97	0.46
18:2W:18:ARG:HG2	18:2W:76:VAL:HB	1.96	0.46
19:2X:94:GLY:N	19:2X:95:LEU:HA	2.30	0.46
28:26:11:LEU:N	28:26:21:TYR:O	2.46	0.46
32:2a:524:G:H2'	32:2a:525:C:C6	2.50	0.46
32:2a:582:U:OP1	46:2o:64:ARG:NH1	2.48	0.46
32:2a:1201:A:H1'	32:2a:1202:G:OP2	2.15	0.46
43:2l:53:ARG:HB3	43:2l:69:TYR:HE1	1.80	0.46
50:2s:49:ILE:HG13	50:2s:62:ILE:HD11	1.97	0.46
1:1A:662:A:OP1	11:1P:133:SER:OG	2.22	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1140:U:O2'	1:1A:1141:A:N7	2.45	0.46
1:1A:1334:U:O4	13:1R:106:GLY:HA3	2.15	0.46
1:1A:2549:U:H2'	1:1A:2550:C:H6	1.80	0.46
2:1B:66:A:H61	2:1B:108:U:H2'	1.80	0.46
8:1I:120:ILE:HD11	8:1I:128:LEU:HD11	1.97	0.46
26:14:26:SER:OG	26:14:27:THR:N	2.48	0.46
28:16:8:LYS:HD3	30:18:34:TRP:CD2	2.50	0.46
32:1a:1291:G:OP1	38:1g:41:ARG:NH2	2.49	0.46
33:1b:19:HIS:CD2	33:1b:20:GLU:HG3	2.50	0.46
47:1p:14:ASN:HA	47:1p:42:ARG:NH1	2.30	0.46
2:2B:4:C:H42	2:2B:117:G:H1	1.63	0.46
12:2Q:8:LYS:HD2	12:2Q:9:TYR:CE2	2.50	0.46
32:2a:627:G:H2'	32:2a:628:G:H8	1.79	0.46
32:2a:737:A:H1'	37:2f:73:ASN:HD21	1.79	0.46
45:2n:48:ALA:HB2	45:2n:53:LEU:HD12	1.97	0.46
1:1A:505:A:N3	1:1A:507:G:H5''	2.29	0.46
1:1A:664:U:H2'	1:1A:665:C:C6	2.51	0.46
1:1A:667:G:OP1	61:1A:4297:HOH:O	2.20	0.46
1:1A:1154:U:H2'	1:1A:1155:C:O4'	2.15	0.46
1:1A:2096:U:H2'	1:1A:2097:U:C6	2.50	0.46
1:1A:2193:A:O2'	1:1A:2194:U:H5''	2.16	0.46
11:1P:91:PHE:O	11:1P:121:LYS:NZ	2.43	0.46
37:1f:76:ALA:O	37:1f:80:ARG:HG3	2.16	0.46
54:1w:23:A:H3'	54:1w:24:G:H8	1.80	0.46
1:2A:184:C:H2'	1:2A:185:U:C6	2.51	0.46
1:2A:322:A:OP1	5:2F:168:ARG:HD2	2.16	0.46
1:2A:1996:C:H4'	1:2A:1997:G:OP1	2.15	0.46
1:2A:2572:A:OP1	1:2A:2574:G:O2'	2.33	0.46
1:2A:2781:A:H5''	1:2A:2782:G:H5'	1.97	0.46
3:2D:108:PRO:HB3	3:2D:143:HIS:CE1	2.46	0.46
15:2T:36:GLU:CD	15:2T:41:ARG:HH21	2.24	0.46
17:2V:73:SER:HA	17:2V:83:ARG:O	2.15	0.46
32:2a:522:C:H41	43:2l:53:ARG:NH1	2.13	0.46
32:2a:815:A:N7	32:2a:1509:C:O2'	2.41	0.46
32:2a:975:A:N1	41:2j:48:THR:HB	2.29	0.46
32:2a:1299:A:H2'	32:2a:1299:A:N3	2.30	0.46
36:2e:146:ALA:O	36:2e:150:ARG:HG2	2.14	0.46
1:1A:233:A:H4'	11:1P:74:GLU:HB2	1.97	0.46
1:1A:551:A:O2'	1:1A:2065:C:O2	2.32	0.46
1:1A:1110:C:N3	1:1A:1120:G:C6	2.82	0.46
1:1A:1810:U:H2'	61:1A:4316:HOH:O	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1893:G:H2'	1:1A:1894:G:H8	1.80	0.46
1:1A:1921:G:N3	1:1A:1921:G:H2'	2.30	0.46
1:1A:2023:A:H2'	1:1A:2024:G:C8	2.50	0.46
1:1A:2158:C:N4	1:1A:2177:G:C6	2.77	0.46
11:1P:97:PRO:HD3	11:1P:126:VAL:O	2.15	0.46
32:1a:1131:G:OP1	40:1i:20:ARG:NH2	2.40	0.46
34:1c:20:SER:OG	34:1c:36:ASP:OD2	2.27	0.46
50:1s:63:THR:OG1	50:1s:66:MET:HE3	2.16	0.46
1:2A:2102:U:H2'	1:2A:2103:C:C6	2.51	0.46
1:2A:2281:C:N4	61:2A:4167:HOH:O	2.45	0.46
3:2D:158:ALA:O	3:2D:161:THR:OG1	2.32	0.46
5:2F:25:PRO:HD2	5:2F:115:ALA:HB2	1.97	0.46
9:2N:42:TRP:HA	9:2N:48:MET:SD	2.55	0.46
14:2S:7:TYR:CZ	14:2S:91:PRO:HG3	2.50	0.46
15:2T:88:ILE:HG21	15:2T:91:ARG:CZ	2.45	0.46
18:2W:77:ASP:HB2	18:2W:102:HIS:HB2	1.96	0.46
26:24:57:GLU:CB	26:24:58:ARG:HD2	2.46	0.46
29:27:12:ARG:NH2	29:27:44:PRO:HB3	2.30	0.46
32:2a:77:G:H1	32:2a:92:C:H42	1.62	0.46
32:2a:967:5MC:H2'	32:2a:968:A:C8	2.51	0.46
32:2a:1020:U:H2'	32:2a:1021:G:C8	2.50	0.46
33:2b:155:LEU:HD21	33:2b:159:PRO:HD3	1.98	0.46
38:2g:47:CYS:O	38:2g:50:ILE:HG22	2.14	0.46
1:1A:2038:U:O2'	27:15:7:PRO:O	2.27	0.46
1:1A:2644:A:O2'	1:1A:2821:G:O2'	2.27	0.46
1:1A:2705:A:H2'	1:1A:2706:G:H8	1.81	0.46
10:1O:64:ARG:NH2	10:1O:99:PHE:O	2.45	0.46
32:1a:757:U:H2'	32:1a:758:G:O4'	2.16	0.46
46:1o:74:ASP:OD2	46:1o:77:ARG:HD3	2.15	0.46
1:2A:385:C:O2'	1:2A:388:G:N2	2.49	0.46
1:2A:851:U:H5'	25:23:49:LYS:HD2	1.97	0.46
1:2A:910:A:N1	1:2A:2277:G:H1'	2.30	0.46
1:2A:1514:U:H2'	1:2A:1515:G:C8	2.51	0.46
1:2A:2331:G:O2'	1:2A:2336:A:N1	2.43	0.46
8:2I:93:THR:HG22	8:2I:119:PRO:HB3	1.98	0.46
32:2a:390:C:H2'	32:2a:391:G:C8	2.50	0.46
32:2a:1030(A):G:N2	32:2a:1030(C):G:H8	2.13	0.46
32:2a:1142:G:H2'	32:2a:1143:G:O4'	2.16	0.46
39:2h:91:ARG:HD3	48:2q:33:GLY:HA3	1.97	0.46
42:2k:48:ILE:C	42:2k:50:TYR:H	2.23	0.46
46:2o:21:ASP:OD2	46:2o:24:SER:OG	2.28	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1821:C:H2'	1:1A:1822:A:C5	2.50	0.46
16:1U:69:CYS:HB3	16:1U:74:LEU:HD12	1.98	0.46
33:1b:218:ALA:O	33:1b:222:ILE:HG13	2.16	0.46
1:2A:239:U:H2'	1:2A:240:G:O4'	2.15	0.46
1:2A:858:U:O2	1:2A:2268:A:H2'	2.16	0.46
1:2A:1359:A:H2'	1:2A:1360:A:H5'	1.98	0.46
1:2A:2133:G:O2'	1:2A:2157:G:N2	2.48	0.46
1:2A:2674:G:H5''	10:2O:26:LYS:HE3	1.97	0.46
13:2R:17:ARG:HG2	13:2R:21:TYR:CE2	2.50	0.46
21:2Z:72:ARG:HD3	21:2Z:72:ARG:HA	1.67	0.46
31:29:18:ARG:HG3	31:29:22:ARG:O	2.16	0.46
32:2a:6:G:H4'	32:2a:298:A:H4'	1.97	0.46
32:2a:582:U:OP2	32:2a:758:G:N1	2.41	0.46
32:2a:1226:C:N4	44:2m:104:ARG:HG3	2.31	0.46
36:2e:110:LEU:HD13	36:2e:118:ILE:HG21	1.98	0.46
39:2h:83:ILE:HG13	39:2h:137:VAL:HG22	1.97	0.46
1:1A:1829:U:H5'	3:1D:259:THR:HG22	1.98	0.46
1:1A:2376:C:H2'	1:1A:2377:G:O4'	2.16	0.46
3:1D:37:LEU:HD22	3:1D:87:ASN:ND2	2.30	0.46
8:1I:125:GLU:HG2	8:1I:143:SER:HA	1.98	0.46
23:11:64:ALA:HA	23:11:67:ILE:HG13	1.97	0.46
32:1a:413:G:N2	32:1a:428:G:H1'	2.31	0.46
32:1a:1034:G:N2	32:1a:1035:A:N3	2.64	0.46
32:1a:1289:A:N1	32:1a:1371:G:O2'	2.44	0.46
35:1d:178:VAL:O	35:1d:180:GLY:N	2.44	0.46
48:1q:66:SER:OG	48:1q:69:LYS:HB2	2.16	0.46
54:1w:4:C:N3	54:1w:69:G:O6	2.49	0.46
1:2A:305:U:H2'	1:2A:306:U:C6	2.51	0.46
1:2A:312:G:H4'	1:2A:331:A:N3	2.31	0.46
7:2H:97:ARG:NE	7:2H:104:GLU:OE1	2.46	0.46
30:28:23:VAL:HG11	30:28:47:LYS:HD3	1.98	0.46
32:2a:9:G:H2'	32:2a:10:A:H8	1.79	0.46
32:2a:1073:U:O2'	33:2b:104:ASN:OD1	2.33	0.46
32:2a:1242:C:N4	32:2a:1295:G:H1	2.14	0.46
32:2a:1263:C:N3	32:2a:1272:G:O6	2.49	0.46
33:2b:101:MET:HG2	33:2b:108:ILE:HG21	1.97	0.46
35:2d:175:SER:OG	35:2d:176:LEU:N	2.48	0.46
44:2m:29:ARG:HA	44:2m:32:GLU:HB2	1.97	0.46
1:1A:39:C:H2'	1:1A:40:C:C6	2.50	0.46
1:1A:556:C:H4'	1:1A:557:A:H5''	1.97	0.46
1:1A:1941:A:O2'	32:1a:1517:G:N3	2.44	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2156:A:OP2	1:1A:2178:G:N2	2.48	0.46
1:1A:2219:U:H1'	1:1A:2220:A:C8	2.51	0.46
1:1A:2545:A:H2'	1:1A:2546:A:O4'	2.16	0.46
1:1A:2858:G:H1'	1:1A:2877:G:N2	2.31	0.46
14:1S:6:ALA:O	14:1S:10:ARG:HG3	2.16	0.46
32:1a:8:A:N6	35:1d:205:GLU:O	2.48	0.46
32:1a:501:C:H2'	32:1a:502:G:C8	2.50	0.46
32:1a:1030(D):A:H2'	32:1a:1031:G:H4'	1.96	0.46
36:1e:84:PHE:CE2	36:1e:133:TYR:HD2	2.33	0.46
38:1g:115:ARG:HH11	38:1g:118:VAL:HG21	1.80	0.46
40:1i:5:TYR:H	40:1i:87:GLN:NE2	2.13	0.46
1:2A:322:A:H5'	1:2A:340:A:H1'	1.97	0.46
1:2A:839:U:H1'	1:2A:1191:G:H1'	1.97	0.46
1:2A:1149:G:H2'	1:2A:1150:C:C6	2.51	0.46
1:2A:2191:G:H2'	1:2A:2192:G:O4'	2.15	0.46
1:2A:2695:C:H2'	1:2A:2696:U:C6	2.51	0.46
6:2G:179:PRO:HG3	26:24:43:TYR:OH	2.15	0.46
11:2P:50:ARG:O	11:2P:52:GLU:HG3	2.16	0.46
12:2Q:39:PRO:HB3	12:2Q:99:PRO:HD3	1.98	0.46
32:2a:537:G:H5''	43:2l:113:ARG:NH1	2.31	0.46
44:2m:14:ARG:HG3	44:2m:44:ARG:NH1	2.30	0.46
54:2w:51:U:H2'	54:2w:52:G:C8	2.50	0.46
1:1A:809:U:H5''	61:1A:5117:HOH:O	2.15	0.46
1:1A:1136:U:C2	1:1A:1148:C:H1'	2.51	0.46
1:1A:1874:C:H5'	3:1D:253:GLN:OE1	2.16	0.46
1:1A:1903:C:H2'	1:1A:1904:C:H6	1.80	0.46
1:1A:2348:A:H61	22:10:43:THR:CG2	2.29	0.46
1:1A:2897:U:H2'	1:1A:2898:C:C6	2.50	0.46
8:1I:5:LEU:HD11	8:1I:19:VAL:HG22	1.97	0.46
13:1R:54:LEU:HD12	13:1R:54:LEU:HA	1.80	0.46
14:1S:27:SER:HA	14:1S:88:ASP:HB3	1.96	0.46
22:10:38:VAL:HB	22:10:59:LEU:HB2	1.98	0.46
32:1a:977:A:H1'	32:1a:982:U:O4	2.16	0.46
32:1a:1512:U:H2'	32:1a:1513:A:H8	1.79	0.46
35:1d:65:ARG:HG2	35:1d:75:PHE:CD1	2.51	0.46
1:2A:2558:C:H2'	1:2A:2559:C:O4'	2.16	0.46
4:2E:127:ASP:OD2	61:2E:401:HOH:O	2.20	0.46
5:2F:184:TYR:CE2	5:2F:188:ARG:HD2	2.51	0.46
15:2T:60:THR:HG22	15:2T:77:PRO:HA	1.98	0.46
18:2W:78:GLU:OE2	18:2W:99:ARG:NH1	2.35	0.46
22:20:8:GLY:HA2	55:2x:2:G:H5''	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:451:A:N6	32:2a:480:U:H2'	2.30	0.46
32:2a:600:C:H2'	32:2a:601:C:C6	2.50	0.46
32:2a:1328:C:H2'	32:2a:1329:A:O4'	2.16	0.46
32:2a:1386:G:H2'	32:2a:1387:G:H8	1.81	0.46
1:1A:1121:C:C2'	1:1A:1122:C:H5'	2.45	0.46
1:1A:1834:A:O2'	3:1D:259:THR:HG21	2.16	0.46
1:1A:1911:A:H2'	1:1A:1912:A:C8	2.50	0.46
2:1B:1:U:HO2'	2:1B:2:C:P	2.37	0.46
32:1a:160:A:H1'	32:1a:344:A:C5	2.50	0.46
32:1a:1030(A):G:O2'	32:1a:1031:G:N2	2.49	0.46
36:1e:78:HIS:CD2	39:1h:104:ARG:HD2	2.51	0.46
1:2A:645:C:H5''	1:2A:646:A:OP2	2.16	0.46
1:2A:740:U:H2'	1:2A:741:G:C8	2.51	0.46
1:2A:1405:U:H2'	1:2A:1406:U:C6	2.51	0.46
1:2A:1507:A:O2'	1:2A:1508:A:O4'	2.29	0.46
1:2A:2893:G:H5''	1:2A:2894:G:O4'	2.16	0.46
12:2Q:31:ASP:N	12:2Q:106:VAL:O	2.48	0.46
19:2X:5:TYR:CE2	24:22:30:ARG:HB2	2.50	0.46
26:24:15:ILE:O	26:24:33:VAL:N	2.47	0.46
26:24:26:SER:OG	26:24:27:THR:N	2.47	0.46
32:2a:674:G:H2'	32:2a:675:A:C8	2.52	0.46
32:2a:939:G:H5'	38:2g:102:ARG:NH1	2.31	0.46
40:2i:8:GLY:HA3	40:2i:76:ALA:O	2.16	0.46
43:2l:53:ARG:HG3	43:2l:93:LEU:HD21	1.99	0.46
54:2y:35:A:H3'	54:2y:36:A:C8	2.51	0.46
1:1A:611:U:H1'	5:1F:90:PHE:CG	2.51	0.45
1:1A:1320:A:N3	1:1A:1343:C:H1'	2.31	0.45
1:1A:1715:A:O2'	1:1A:1721:G:N7	2.40	0.45
1:1A:2418:U:H2'	1:1A:2418:U:OP2	2.15	0.45
1:1A:2710:U:H2'	1:1A:2711:C:C6	2.51	0.45
26:14:55:ARG:N	26:14:56:VAL:HA	2.30	0.45
32:1a:184:G:H2'	32:1a:185:A:C8	2.50	0.45
32:1a:625:G:H4'	47:1p:16:HIS:CD2	2.51	0.45
33:1b:12:GLU:O	33:1b:15:VAL:HG22	2.16	0.45
42:1k:48:ILE:O	42:1k:50:TYR:N	2.38	0.45
47:1p:19:ILE:HD12	47:1p:51:VAL:HG22	1.99	0.45
4:2E:50:GLY:HA2	4:2E:77:ILE:O	2.16	0.45
5:2F:117:ARG:NH2	5:2F:189:THR:O	2.49	0.45
32:2a:596:C:OP2	61:2a:3301:HOH:O	2.20	0.45
32:2a:833:U:H2'	32:2a:834:C:C6	2.50	0.45
33:2b:60:ASP:O	33:2b:64:ARG:HG2	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:2j:20:ALA:HB1	41:2j:37:PRO:HB3	1.98	0.45
41:2j:32:ALA:CB	41:2j:33:GLN:HA	2.34	0.45
1:1A:1159:U:H2'	1:1A:1160:G:H8	1.81	0.45
1:1A:2402:U:P	30:18:35:GLN:HE22	2.40	0.45
13:1R:72:ASP:O	13:1R:76:VAL:HG23	2.17	0.45
32:1a:1101:A:H4'	32:1a:1102:A:O5'	2.16	0.45
32:1a:1131:G:P	40:1i:20:ARG:HH22	2.38	0.45
1:2A:910:A:N6	1:2A:2277:G:O2'	2.47	0.45
1:2A:1579:A:H2'	1:2A:1580:A:C8	2.51	0.45
1:2A:2167:U:O2'	1:2A:2168:G:O4'	2.33	0.45
1:2A:2663:G:H3'	1:2A:2664:G:H8	1.80	0.45
1:2A:2712:U:OP1	1:2A:2714:G:H4'	2.17	0.45
2:2B:24:G:H4'	2:2B:25:A:C8	2.51	0.45
7:2H:13:LYS:HA	7:2H:14:GLY:HA2	1.57	0.45
7:2H:122:THR:HB	7:2H:134:SER:HB2	1.98	0.45
7:2H:123:PHE:HE1	7:2H:133:VAL:HG13	1.82	0.45
19:2X:57:LEU:HD11	19:2X:78:LYS:HE2	1.97	0.45
32:2a:865:A:N3	32:2a:918:A:O2'	2.43	0.45
32:2a:1128:C:O2'	32:2a:1129:C:OP1	2.34	0.45
39:2h:17:THR:HA	39:2h:65:TYR:HE1	1.81	0.45
42:2k:21:ILE:HD12	42:2k:84:VAL:HG22	1.97	0.45
44:2m:94:ARG:NH2	50:2s:81:ARG:HA	2.32	0.45
1:1A:1541:A:H2'	1:1A:1542:A:C8	2.51	0.45
1:1A:1935:A:H4'	1:1A:1936:C:H5''	1.98	0.45
1:1A:2724:U:OP1	1:1A:2727:G:H4'	2.17	0.45
8:1I:12:LEU:HD23	8:1I:12:LEU:HA	1.78	0.45
19:1X:26:TYR:HB3	19:1X:92:LEU:HD22	1.98	0.45
32:1a:128:G:O2'	48:1q:3:LYS:NZ	2.49	0.45
44:1m:3:ARG:HG3	44:1m:4:ILE:H	1.82	0.45
1:2A:884:C:H3'	1:2A:885:C:H6	1.81	0.45
1:2A:998:C:H2'	1:2A:999:U:O4'	2.17	0.45
1:2A:1899:G:H2'	1:2A:1899:G:N3	2.31	0.45
5:2F:53:THR:HG22	5:2F:56:GLU:HG3	1.97	0.45
32:2a:688:G:H2'	32:2a:689:C:H6	1.81	0.45
32:2a:1113:C:H2'	32:2a:1114:C:H6	1.81	0.45
1:1A:52:A:H2'	1:1A:53:G:O4'	2.16	0.45
1:1A:555:G:H4'	1:1A:556:C:OP1	2.16	0.45
1:1A:1834:A:H4'	3:1D:259:THR:HG23	1.98	0.45
1:1A:1952:G:O2'	1:1A:1990:G:O6	2.27	0.45
1:1A:2149:G:N1	1:1A:2183:C:N4	2.42	0.45
5:1F:140:LEU:HD11	5:1F:170:LEU:HD11	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:1P:86:LYS:NZ	11:1P:87:ASP:OD1	2.49	0.45
32:1a:236:G:H5''	48:1q:42:TYR:OH	2.16	0.45
32:1a:509:A:O2'	32:1a:510:A:OP1	2.32	0.45
32:1a:826:C:H4'	39:1h:12:ARG:HG2	1.97	0.45
32:1a:1226:C:O2'	44:1m:111:LYS:NZ	2.26	0.45
32:1a:1277:C:O2'	32:1a:1279:A:H1'	2.17	0.45
34:1c:22:TRP:CZ2	45:1n:54:PRO:HG2	2.52	0.45
51:1t:43:LEU:HD13	51:1t:51:GLU:HB3	1.98	0.45
54:1w:18:G:H4'	54:1w:60:U:C6	2.52	0.45
1:2A:30:G:H2'	1:2A:31:C:C6	2.51	0.45
1:2A:2870:C:H2'	1:2A:2871:C:O4'	2.17	0.45
27:25:51:TYR:CZ	27:25:56:LYS:HD2	2.51	0.45
32:2a:862:C:H1'	32:2a:874:G:H5''	1.99	0.45
42:2k:48:ILE:HD11	42:2k:64:ALA:HA	1.99	0.45
54:2w:46:7MG:O2'	54:2w:47:U:H4'	2.16	0.45
1:1A:831:A:H5'	1:1A:832:G:OP1	2.16	0.45
3:1D:169:GLU:O	3:1D:169:GLU:HG3	2.16	0.45
21:1Z:53:ILE:HG22	21:1Z:71:VAL:HG12	1.98	0.45
29:17:12:ARG:HH21	29:17:44:PRO:HB3	1.82	0.45
32:1a:271:C:H2'	32:1a:272:C:H6	1.82	0.45
32:1a:401:C:O2'	32:1a:621:A:N3	2.44	0.45
32:1a:922:G:H4'	36:1e:20:GLN:HA	1.98	0.45
51:1t:10:LEU:HD23	51:1t:12:ALA:HB2	1.99	0.45
1:2A:196:A:O2'	1:2A:805:G:O6	2.27	0.45
1:2A:276:A:H5''	1:2A:277:C:H5'	1.98	0.45
1:2A:287:C:H2'	1:2A:288:C:C6	2.52	0.45
1:2A:375:C:H2'	1:2A:376:C:C6	2.51	0.45
1:2A:453:C:O2	1:2A:457:A:O2'	2.34	0.45
1:2A:887:A:H4'	1:2A:888:C:H5	1.81	0.45
1:2A:1777:U:H2'	1:2A:1778:U:C6	2.51	0.45
26:24:64:GLY:C	26:24:66:SER:H	2.23	0.45
30:28:63:PRO:HG2	30:28:64:TYR:CE2	2.51	0.45
32:2a:562:C:H1'	43:2l:15:ARG:HD2	1.99	0.45
32:2a:772:U:H2'	32:2a:773:G:O4'	2.16	0.45
32:2a:868:C:H2'	32:2a:869:G:O4'	2.16	0.45
32:2a:876:G:O5'	39:2h:14:ARG:NH1	2.50	0.45
36:2e:8:GLU:HG2	36:2e:34:VAL:HG23	1.98	0.45
1:1A:469:A:N7	5:1F:45:ARG:HG2	2.31	0.45
1:1A:831:A:C5	3:1D:229:VAL:HG21	2.51	0.45
1:1A:2193:A:HO2'	1:1A:2194:U:H6	1.65	0.45
8:1I:77:LEU:HD21	8:1I:79:ILE:HD11	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1T:64:ARG:CZ	15:1T:103:ARG:HB3	2.46	0.45
32:1a:116:A:H61	32:1a:313:A:H1'	1.81	0.45
45:1n:45:ARG:O	45:1n:49:HIS:HD2	1.99	0.45
51:1t:30:LYS:HB3	51:1t:34:LYS:NZ	2.32	0.45
1:2A:531:C:OP1	1:2A:561:G:N1	2.43	0.45
1:2A:817:C:H2'	1:2A:818:G:O4'	2.17	0.45
1:2A:2028:U:O4	61:2A:3984:HOH:O	2.20	0.45
1:2A:2104:G:N2	1:2A:2185:C:N3	2.57	0.45
1:2A:2110:G:H3'	1:2A:2111:C:H5'	1.99	0.45
1:2A:2567:G:H2'	1:2A:2568:C:C6	2.52	0.45
1:2A:2784:C:O2'	4:2E:42:ASP:OD1	2.34	0.45
2:2B:22:U:H3	2:2B:61:G:H1	1.65	0.45
7:2H:11:VAL:HG21	7:2H:50:VAL:HG23	1.99	0.45
7:2H:70:THR:HA	7:2H:73:ALA:HB3	1.97	0.45
12:2Q:54:MET:HE1	12:2Q:104:PHE:HB3	1.99	0.45
32:2a:189(F):U:H3	48:2q:72:ARG:HH22	1.64	0.45
32:2a:299:G:H8	32:2a:299:G:O5'	2.00	0.45
32:2a:719:C:N4	49:2r:71:LYS:HE2	2.31	0.45
32:2a:1359:C:O2'	32:2a:1361:G:N7	2.49	0.45
33:2b:101:MET:HA	33:2b:108:ILE:HG21	1.99	0.45
55:2x:76:A:C8	55:2x:76:A:H5'	2.51	0.45
1:1A:75:C:H5'	61:1A:4422:HOH:O	2.16	0.45
1:1A:385:G:N1	1:1A:386:U:O4	2.50	0.45
1:1A:1589:A:H8	1:1A:1589:A:OP1	1.99	0.45
1:1A:1825:U:H2'	1:1A:1826:C:C6	2.52	0.45
1:1A:2285:A:H2'	1:1A:2286:A:C8	2.51	0.45
1:1A:2880:C:H2'	1:1A:2881:C:O4'	2.17	0.45
4:1E:11:MET:HG2	4:1E:24:THR:HB	1.99	0.45
20:1Y:19:LYS:HE2	20:1Y:20:TYR:CE2	2.52	0.45
32:1a:137:C:H2'	32:1a:138:G:C8	2.52	0.45
32:1a:229:U:H2'	32:1a:230:G:C8	2.51	0.45
32:1a:831:U:H2'	32:1a:832:C:H6	1.81	0.45
32:1a:963:G:H4'	61:1a:3560:HOH:O	2.16	0.45
33:1b:16:HIS:HB2	33:1b:204:ASN:CB	2.47	0.45
43:1l:42:THR:HA	43:1l:53:ARG:O	2.17	0.45
51:1t:10:LEU:HD12	51:1t:10:LEU:HA	1.76	0.45
55:1x:25:C:H2'	55:1x:26:G:O4'	2.17	0.45
1:2A:817:C:O2'	1:2A:839:U:H5''	2.17	0.45
1:2A:1126:A:H4'	1:2A:1127:A:H5''	1.98	0.45
1:2A:1345:C:OP2	61:2A:3987:HOH:O	2.20	0.45
1:2A:1790:C:H5''	1:2A:1791:A:OP1	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2477:C:O2	31:29:4:ARG:NH2	2.42	0.45
1:2A:2853:C:H2'	1:2A:2854:G:H8	1.81	0.45
32:2a:674:G:H2'	32:2a:675:A:H8	1.80	0.45
32:2a:743:U:H2'	32:2a:744:C:C6	2.52	0.45
32:2a:1084:G:C5	32:2a:1085:U:C4	3.05	0.45
32:2a:1306:A:H2'	32:2a:1307:U:O4'	2.16	0.45
33:2b:24:TRP:CD1	33:2b:24:TRP:H	2.34	0.45
1:1A:327:U:O4	61:1A:4299:HOH:O	2.20	0.45
1:1A:653:G:H2'	1:1A:654:G:C8	2.51	0.45
1:1A:964:A:H5''	2:1B:98:G:O2'	2.16	0.45
1:1A:1117:G:H1'	1:1A:1135:G:H2'	1.99	0.45
1:1A:1385:G:H5''	19:1X:16:LYS:HD3	1.99	0.45
1:1A:1688:A:H2'	1:1A:1689:G:O4'	2.16	0.45
1:1A:2420:U:H2'	1:1A:2421:G:C8	2.52	0.45
5:1F:53:THR:CG2	5:1F:55:GLY:H	2.27	0.45
9:1N:104:LYS:HA	9:1N:107:LEU:HD12	1.99	0.45
20:1Y:7:VAL:HG21	20:1Y:72:VAL:HG12	1.99	0.45
26:14:58:ARG:O	26:14:61:ARG:HB3	2.17	0.45
33:1b:83:MET:O	33:1b:87:ARG:HG3	2.16	0.45
33:1b:162:ILE:O	33:1b:185:ILE:HG12	2.16	0.45
37:1f:33:TYR:CE1	37:1f:74:ASP:HB3	2.51	0.45
41:1j:64:GLU:CD	41:1j:66:ARG:HE	2.25	0.45
48:1q:58:GLU:O	48:1q:74:LEU:N	2.46	0.45
1:2A:1364:G:P	23:21:3:LYS:HG3	2.56	0.45
1:2A:2137:C:O2'	1:2A:2138:C:OP2	2.35	0.45
1:2A:2185:C:H2'	1:2A:2186:G:O4'	2.17	0.45
1:2A:2206:G:H3'	1:2A:2207:G:H8	1.79	0.45
32:2a:1036:G:H5''	32:2a:1037:C:OP2	2.17	0.45
32:2a:1458:G:H5''	51:2t:31:SER:HB3	1.99	0.45
54:2w:56:C:H2'	54:2w:57:G:O4'	2.17	0.45
54:2y:9:A:H8	54:2y:11:C:H41	1.63	0.45
1:1A:574:G:O2'	1:1A:1265:A:N3	2.39	0.45
1:1A:1566:U:H2'	1:1A:1567:G:O4'	2.17	0.45
1:1A:1990:G:OP1	61:1A:4303:HOH:O	2.21	0.45
1:1A:2614:A:H4'	1:1A:2615:G:C5'	2.47	0.45
1:1A:2640:C:H5''	1:1A:2641:A:O5'	2.17	0.45
21:1Z:54:HIS:HB2	21:1Z:55:HIS:CD2	2.52	0.45
32:1a:1021:G:HO2'	32:1a:1022:G:P	2.38	0.45
33:1b:51:LEU:HD22	33:1b:55:PHE:HE2	1.82	0.45
33:1b:124:SER:HA	33:1b:125:PRO:HA	1.71	0.45
39:1h:25:ASP:OD1	39:1h:60:ARG:HG2	2.15	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:1q:5:VAL:HA	48:1q:59:ILE:O	2.17	0.45
1:2A:582:G:H2'	1:2A:583:G:C8	2.52	0.45
1:2A:1607:C:H5''	1:2A:1608:A:H5'	1.99	0.45
1:2A:1924:C:H4'	55:2x:13:C:O2'	2.17	0.45
1:2A:2145:C:O2'	1:2A:2147:G:N7	2.47	0.45
1:2A:2889:C:H2'	1:2A:2891:G:O4'	2.16	0.45
5:2F:32:LEU:O	5:2F:36:VAL:HG23	2.16	0.45
32:2a:155:C:H2'	32:2a:156:G:O4'	2.17	0.45
32:2a:359:U:H2'	32:2a:360:A:C8	2.52	0.45
32:2a:1057:G:H2'	32:2a:1058:G:O4'	2.17	0.45
33:2b:92:TYR:N	33:2b:151:GLY:O	2.36	0.45
33:2b:179:LYS:HA	39:2h:72:PRO:HG3	1.98	0.45
54:2w:8:4SU:H1'	54:2w:48:C:H1'	1.98	0.45
1:1A:1105:G:OP2	1:1A:1106:U:H3'	2.17	0.45
1:1A:2062:C:H2'	1:1A:2063:U:O4'	2.17	0.45
11:1P:90:ARG:NH1	11:1P:105:LEU:HD11	2.32	0.45
14:1S:14:VAL:O	14:1S:18:ILE:HG12	2.17	0.45
25:13:26:LEU:O	25:13:35:ARG:NE	2.50	0.45
32:1a:575:G:O2'	32:1a:821:G:H5'	2.17	0.45
32:1a:737:A:H2'	32:1a:738:C:C6	2.51	0.45
32:1a:881:G:H2'	32:1a:882:C:O4'	2.17	0.45
36:1e:78:HIS:CD2	39:1h:104:ARG:HH11	2.35	0.45
51:1t:54:LYS:HG3	51:1t:57:ARG:NH2	2.32	0.45
54:1y:19:G:C4'	54:1y:57:G:H22	2.30	0.45
1:2A:2031:A:C6	1:2A:2498:C:H1'	2.52	0.45
1:2A:2165:G:H2'	1:2A:2166:G:H5''	1.99	0.45
1:2A:2238:G:H2'	1:2A:2238:G:N3	2.31	0.45
1:2A:2447:G:N2	1:2A:2450:A:OP2	2.50	0.45
1:2A:2881:C:H2'	1:2A:2882:A:O4'	2.17	0.45
2:2B:48:A:H4'	14:2S:95:HIS:HD2	1.82	0.45
10:2O:24:VAL:HG12	10:2O:33:ALA:HB2	1.99	0.45
32:2a:253:U:H2'	32:2a:254:G:C8	2.50	0.45
32:2a:530:G:O6	53:2v:21:C:H1'	2.16	0.45
32:2a:890:G:O2'	32:2a:906:G:O6	2.18	0.45
32:2a:1040:U:C2	32:2a:1041:A:C8	3.05	0.45
38:2g:49:ILE:H	38:2g:49:ILE:HG13	1.57	0.45
1:1A:302:A:H2'	1:1A:303:C:C6	2.52	0.44
1:1A:759:G:H1	1:1A:766:C:H42	1.65	0.44
1:1A:1105:G:H1	1:1A:1125:C:H42	1.65	0.44
1:1A:1653:C:H5''	1:1A:1654:A:H5'	1.98	0.44
1:1A:2658:C:H2'	1:1A:2659:U:O4'	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1F:33:LEU:HD13	5:1F:112:MET:HE3	1.98	0.44
23:11:56:GLN:HB3	23:11:87:PRO:HG3	1.99	0.44
32:1a:40:C:H2'	32:1a:41:G:C8	2.51	0.44
32:1a:625:G:H2'	32:1a:626:U:C6	2.52	0.44
1:2A:238:C:O2'	1:2A:608:A:N3	2.50	0.44
1:2A:527:C:C4	1:2A:2779:U:H2'	2.52	0.44
1:2A:849:A:C2	25:23:24:LYS:HD2	2.52	0.44
1:2A:1037:G:H2'	1:2A:1038:C:O4'	2.17	0.44
1:2A:1662:C:O2'	1:2A:2687:U:OP1	2.32	0.44
31:29:15:LYS:HD2	31:29:26:ILE:HD11	1.99	0.44
32:2a:503:C:H2'	32:2a:504:C:C6	2.51	0.44
32:2a:509:A:H5'	35:2d:55:ALA:HB2	1.99	0.44
32:2a:1109:C:H2'	32:2a:1110:A:O4'	2.17	0.44
42:2k:31:THR:HG22	42:2k:42:TRP:HB2	1.99	0.44
44:2m:122:LYS:HA	44:2m:122:LYS:HD2	1.78	0.44
1:1A:731:G:OP1	29:17:16:HIS:ND1	2.45	0.44
1:1A:843:C:H2'	1:1A:844:C:C6	2.51	0.44
1:1A:2112:G:N2	23:11:45:ASN:OD1	2.45	0.44
24:12:52:ASP:O	24:12:56:GLN:HG3	2.17	0.44
32:1a:636:U:H2'	32:1a:637:G:C8	2.52	0.44
32:1a:1118:C:OP1	40:1i:9:ARG:NH1	2.50	0.44
39:1h:17:THR:HG22	39:1h:63:LEU:HG	1.99	0.44
39:1h:91:ARG:HD3	48:1q:32:TYR:O	2.16	0.44
1:2A:118:A:N3	1:2A:178:G:H1'	2.32	0.44
1:2A:262:A:H2'	1:2A:263:C:O4'	2.17	0.44
1:2A:1131:G:O6	1:2A:2040:C:H1'	2.17	0.44
1:2A:1926:U:O2'	1:2A:1928:A:N7	2.39	0.44
1:2A:2160:G:H2'	1:2A:2161:C:H5''	1.98	0.44
5:2F:150:GLY:HA2	5:2F:172:TRP:CD2	2.53	0.44
32:2a:1347:G:H5''	40:2i:107:ARG:HB3	1.99	0.44
35:2d:108:LEU:HD12	35:2d:174:LEU:HD13	1.99	0.44
45:2n:37:PHE:HB3	45:2n:39:LEU:HD12	1.99	0.44
49:2r:53:ARG:HG2	49:2r:63:GLN:HE21	1.82	0.44
1:1A:1822:A:H8	1:1A:1822:A:OP2	2.00	0.44
1:1A:2362:C:OP2	61:1A:4302:HOH:O	2.21	0.44
4:1E:12:THR:HG22	4:1E:13:ARG:H	1.81	0.44
12:1Q:38:GLU:HA	12:1Q:99:PRO:HG3	1.98	0.44
32:1a:993:G:O2'	32:1a:994:A:N7	2.51	0.44
1:2A:764:A:H5'	3:2D:210:GLY:HA2	1.99	0.44
1:2A:2105:C:H2'	1:2A:2106:G:C8	2.51	0.44
1:2A:2386:C:H2'	1:2A:2387:U:C6	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:2H:87:LEU:N	7:2H:131:VAL:O	2.45	0.44
20:2Y:9:LYS:HA	20:2Y:10:GLY:HA2	1.56	0.44
32:2a:437:U:O2	35:2d:119:GLN:NE2	2.50	0.44
32:2a:523:A:N1	43:2l:92:OTD:H6	2.33	0.44
32:2a:1279:A:OP1	41:2j:7:LYS:NZ	2.45	0.44
51:2t:13:LEU:O	51:2t:17:ARG:HG3	2.18	0.44
1:1A:502:G:N1	1:1A:505:A:OP2	2.47	0.44
1:1A:654:G:N3	1:1A:664:U:O2'	2.51	0.44
1:1A:787:U:H2'	1:1A:788:G:C8	2.52	0.44
1:1A:1276:C:H2'	1:1A:1277:G:C8	2.51	0.44
1:1A:1690:G:H2'	1:1A:1691:C:O4'	2.16	0.44
32:1a:966:M2G:HM13	32:1a:967:5MC:H1'	1.98	0.44
35:1d:18:LYS:HD2	35:1d:20:TYR:CZ	2.53	0.44
38:1g:65:ALA:O	38:1g:69:VAL:HG23	2.18	0.44
54:1w:29:G:H1	54:1w:41:C:H42	1.66	0.44
1:2A:62:C:H42	1:2A:93:G:H1	1.66	0.44
1:2A:265:A:C8	1:2A:266:G:H1'	2.52	0.44
1:2A:744:G:H2'	1:2A:745:G:O4'	2.17	0.44
1:2A:890:A:H2'	1:2A:892:G:H8	1.83	0.44
1:2A:2718:G:O2'	1:2A:2847:U:OP1	2.34	0.44
5:2F:178:PRO:HB2	5:2F:201:VAL:HG21	1.98	0.44
5:2F:184:TYR:CZ	5:2F:188:ARG:HD2	2.52	0.44
6:2G:11:TYR:HB2	6:2G:176:LEU:HD21	1.99	0.44
21:2Z:146:ILE:HG13	21:2Z:174:VAL:HG13	2.00	0.44
32:2a:130:A:H1'	32:2a:263:A:O2'	2.18	0.44
32:2a:769:G:H4'	32:2a:1513:A:H4'	1.98	0.44
32:2a:1135:U:H2'	32:2a:1137:C:C2	2.52	0.44
32:2a:1241:G:H2'	32:2a:1242:C:C6	2.52	0.44
38:2g:16:LEU:HD22	40:2i:41:VAL:O	2.17	0.44
1:1A:234:G:O6	30:18:8:LYS:NZ	2.44	0.44
1:1A:2340:A:H2'	1:1A:2341:G:C8	2.52	0.44
2:1B:101:G:H2'	2:1B:102:A:O4'	2.18	0.44
4:1E:179:GLU:HG3	15:1T:9:LEU:HD21	1.99	0.44
7:1H:11:VAL:HG21	7:1H:50:VAL:HG23	2.00	0.44
32:1a:542:G:H5'	35:1d:41:GLY:HA3	2.00	0.44
32:1a:637:G:H2'	32:1a:638:G:C8	2.53	0.44
32:1a:909:A:H2'	32:1a:910:C:O4'	2.18	0.44
33:1b:155:LEU:HD12	33:1b:155:LEU:HA	1.88	0.44
52:1u:18:TYR:CG	52:1u:24:ARG:HD3	2.53	0.44
1:2A:214:G:H1'	1:2A:216:A:O2'	2.17	0.44
1:2A:218:A:C2	1:2A:235:U:H4'	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1027:A:C6	1:2A:1126:A:C4	3.05	0.44
1:2A:1568:G:N7	61:2A:4102:HOH:O	2.36	0.44
1:2A:2056:G:N2	27:25:5:PRO:HA	2.33	0.44
7:2H:121:ILE:HD11	7:2H:140:LYS:HG2	1.99	0.44
8:2I:5:LEU:HD11	8:2I:19:VAL:HG22	1.98	0.44
32:2a:59:A:N6	61:2a:3366:HOH:O	2.43	0.44
32:2a:765:G:N1	32:2a:812:C:O2'	2.38	0.44
32:2a:1257:U:O4	45:2n:17:LYS:NZ	2.50	0.44
32:2a:1387:G:H2'	32:2a:1388:C:C6	2.53	0.44
32:2a:1435:G:H2'	32:2a:1436:U:C6	2.53	0.44
34:2c:110:ASN:O	34:2c:141:VAL:HG22	2.17	0.44
54:2w:2:C:N3	54:2w:71:G:O6	2.50	0.44
1:1A:601:A:OP2	61:1A:4304:HOH:O	2.21	0.44
1:1A:1464:G:N7	61:1A:4417:HOH:O	2.37	0.44
1:1A:1900:G:H2'	1:1A:1901:C:C6	2.53	0.44
1:1A:2205:C:O2'	1:1A:2206:G:OP1	2.35	0.44
1:1A:2496:G:H1'	12:1Q:124:LYS:HD2	1.99	0.44
2:1B:2:C:H2'	2:1B:3:C:H6	1.82	0.44
4:1E:105:THR:OG1	4:1E:199:ARG:NH2	2.50	0.44
6:1G:131:TYR:HB3	6:1G:159:VAL:HG13	2.00	0.44
20:1Y:20:TYR:CE2	20:1Y:43:ASN:HA	2.53	0.44
32:1a:438:G:H4'	35:1d:123:HIS:ND1	2.32	0.44
32:1a:1168:A:H8	32:1a:1168:A:OP1	2.00	0.44
40:1i:13:ALA:HB2	40:1i:68:GLY:HA3	2.00	0.44
1:2A:7:G:H2'	1:2A:8:A:O4'	2.17	0.44
1:2A:90:U:H1'	1:2A:92:A:C8	2.53	0.44
1:2A:320:A:H4'	1:2A:322:A:N7	2.33	0.44
1:2A:336:C:O2'	20:2Y:35:TYR:OH	2.34	0.44
1:2A:2298:A:H62	1:2A:2318:G:H8	1.65	0.44
1:2A:2542:A:H4'	1:2A:2543:G:H8	1.82	0.44
25:23:41:PRO:HA	25:23:44:ARG:HB2	2.00	0.44
32:2a:540:G:H2'	32:2a:541:G:O4'	2.16	0.44
32:2a:627:G:H2'	32:2a:628:G:C8	2.52	0.44
32:2a:1084:G:H5'	32:2a:1102:A:OP2	2.18	0.44
32:2a:1139:G:N2	32:2a:1142:G:O6	2.46	0.44
32:2a:1338:G:H21	55:2x:41:C:H1'	1.81	0.44
33:2b:178:ARG:HH22	39:2h:74:PRO:HB3	1.82	0.44
38:2g:94:ARG:O	38:2g:98:SER:OG	2.35	0.44
44:2m:92:HIS:NE2	44:2m:98:VAL:HG21	2.32	0.44
1:1A:1046:A:H62	1:1A:1200:G:H2'	1.82	0.44
1:1A:1110:C:H2'	1:1A:1111:U:O4'	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2164:C:H2'	1:1A:2165:C:C6	2.53	0.44
1:1A:2190:G:N1	1:1A:2193:A:C8	2.86	0.44
1:1A:2417:G:H5'	11:1P:75:ILE:HD13	2.00	0.44
2:1B:31:C:H4'	6:1G:29:TRP:CH2	2.52	0.44
3:1D:26:LYS:HD3	3:1D:83:GLU:OE2	2.18	0.44
32:1a:96:U:H2'	32:1a:97:G:C8	2.53	0.44
32:1a:491:G:H2'	32:1a:492:G:O4'	2.18	0.44
32:1a:1149:C:H2'	32:1a:1150:U:C6	2.53	0.44
33:1b:70:PHE:O	33:1b:92:TYR:HA	2.16	0.44
36:1e:144:THR:H	36:1e:147:ASP:HB2	1.83	0.44
1:2A:272(H):C:H2'	1:2A:272(I):U:C6	2.53	0.44
1:2A:593:G:H1	1:2A:664:C:H42	1.64	0.44
1:2A:639:U:H2'	1:2A:640:C:C6	2.52	0.44
1:2A:646:A:H2'	1:2A:647:G:O4'	2.18	0.44
1:2A:829:A:N7	1:2A:2248:C:H5'	2.33	0.44
1:2A:2184:G:H2'	1:2A:2185:C:C6	2.52	0.44
1:2A:2695:C:H2'	1:2A:2696:U:H6	1.83	0.44
2:2B:30:C:H2'	2:2B:31:C:H5'	2.00	0.44
15:2T:26:ASP:O	15:2T:49:VAL:HG22	2.17	0.44
32:2a:114:U:H2'	32:2a:115:G:C8	2.53	0.44
32:2a:228:A:H2'	32:2a:229:U:O4'	2.17	0.44
32:2a:406:G:H21	35:2d:119:GLN:NE2	2.14	0.44
32:2a:1129:C:O2'	32:2a:1130:A:N7	2.44	0.44
32:2a:1193:G:O2'	36:2e:25:ARG:NH2	2.50	0.44
32:2a:1496:C:H2'	32:2a:1497:G:C8	2.53	0.44
36:2e:31:LEU:HD22	36:2e:43:LEU:HD11	1.99	0.44
38:2g:26:PHE:O	38:2g:30:ILE:HD12	2.17	0.44
1:1A:910:A:H2'	1:1A:911:G:C8	2.51	0.44
1:1A:1105:G:H2'	1:1A:1106:U:C5	2.53	0.44
1:1A:1410:G:O5'	23:11:3:LYS:HG3	2.17	0.44
1:1A:2367:C:H5'	61:1A:4322:HOH:O	2.17	0.44
8:1I:124:GLY:H	8:1I:144:VAL:HG23	1.82	0.44
26:14:49:PHE:HB3	26:14:50:VAL:H	1.47	0.44
32:1a:536:C:OP1	61:1a:3327:HOH:O	2.21	0.44
32:1a:920:U:H2'	32:1a:921:U:C6	2.53	0.44
34:1c:18:TRP:O	34:1c:54:ARG:NH2	2.50	0.44
34:1c:124:ILE:HG22	34:1c:130:VAL:HG22	2.00	0.44
48:1q:59:ILE:HD12	48:1q:71:PHE:HD2	1.82	0.44
50:1s:20:LEU:HD23	50:1s:23:ASN:HD22	1.82	0.44
1:2A:80:G:H1	1:2A:106:C:H42	1.65	0.44
1:2A:271(A):A:N1	1:2A:272(D):G:O2'	2.49	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2522:U:O2'	1:2A:2647:U:OP1	2.35	0.44
1:2A:2632:A:H61	1:2A:2786:U:H3	1.65	0.44
1:2A:2782:G:OP2	61:2A:3992:HOH:O	2.21	0.44
8:2I:14:ASP:OD1	8:2I:15:VAL:N	2.45	0.44
15:2T:26:ASP:OD1	15:2T:120:ARG:NH2	2.48	0.44
21:2Z:69:THR:HG22	21:2Z:90:VAL:HA	1.99	0.44
22:20:10:THR:HG22	22:20:12:ASN:HB2	1.99	0.44
32:2a:174:C:H2'	32:2a:175:C:C6	2.52	0.44
32:2a:583:A:H2'	32:2a:584:G:O4'	2.18	0.44
32:2a:1456:G:O2'	51:2t:39:LYS:HE3	2.18	0.44
1:1A:104:C:H1'	20:1Y:1:MET:HE2	2.00	0.44
1:1A:240:A:C5	1:1A:241:G:H1'	2.53	0.44
1:1A:609:A:H5'	5:1F:89:VAL:HG21	2.00	0.44
1:1A:1464:G:O5'	1:1A:1464:G:H8	2.01	0.44
1:1A:1938:A:H2'	1:1A:1939:PSU:O4'	2.18	0.44
9:1N:112:LEU:O	9:1N:116:LEU:HG	2.18	0.44
32:1a:742:G:H2'	32:1a:743:U:O4'	2.18	0.44
32:1a:831:U:H2'	32:1a:832:C:C6	2.52	0.44
32:1a:1057:G:H2'	32:1a:1058:G:O4'	2.18	0.44
32:1a:1305:G:H5''	52:1u:4:GLY:HA3	1.99	0.44
32:1a:1352:C:OP1	52:1u:3:LYS:NZ	2.34	0.44
32:1a:1427:U:H2'	32:1a:1428:A:C8	2.53	0.44
54:1w:26:A:H61	54:1w:44:G:H1	1.64	0.44
54:1y:58:A:O2'	54:1y:59:U:OP1	2.35	0.44
1:2A:71:A:H5''	1:2A:73:A:N9	2.33	0.44
1:2A:903:C:H2'	1:2A:904:C:C6	2.52	0.44
1:2A:1012:U:OP1	16:2U:75:ASN:ND2	2.43	0.44
3:2D:231:HIS:CD2	3:2D:249:PRO:HG3	2.53	0.44
7:2H:144:VAL:O	7:2H:148:ILE:HG13	2.18	0.44
32:2a:108:G:N1	51:2t:15:ARG:HG2	2.33	0.44
32:2a:397:A:H3'	32:2a:397:A:N3	2.32	0.44
33:2b:16:HIS:HB2	33:2b:204:ASN:CB	2.47	0.44
37:2f:11:ASN:HB3	37:2f:14:LEU:HG	1.98	0.44
37:2f:69:GLU:CD	37:2f:69:GLU:H	2.25	0.44
40:2i:21:PRO:HA	40:2i:59:PHE:HA	2.00	0.44
54:2y:23:A:H2'	54:2y:24:G:C8	2.53	0.44
1:1A:225:C:H2'	1:1A:226:C:C6	2.52	0.43
1:1A:308:U:H2'	1:1A:309:C:C6	2.53	0.43
1:1A:553:A:O2'	1:1A:554:A:H5'	2.18	0.43
1:1A:865:G:H4'	1:1A:885:C:O3'	2.18	0.43
1:1A:1974:A:C6	1:1A:1975:A:N1	2.86	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2184:G:H1'	1:1A:2195:A:H1'	2.00	0.43
1:1A:2602:A:O3'	3:1D:239:ARG:NH2	2.51	0.43
1:1A:2814:C:H2'	1:1A:2815:C:C6	2.53	0.43
11:1P:43:GLY:HA3	61:1P:301:HOH:O	2.17	0.43
26:14:40:HIS:HB3	26:14:43:TYR:CD2	2.53	0.43
32:1a:458:C:H2'	32:1a:460:G:O4'	2.17	0.43
32:1a:664:G:P	49:1r:64:ARG:HH21	2.41	0.43
32:1a:960:U:H2'	32:1a:1225:A:H62	1.83	0.43
52:1u:15:ARG:H	52:1u:15:ARG:HG2	1.51	0.43
54:1y:9:A:O3'	54:1y:45:U:O2'	2.33	0.43
1:2A:16:G:H2'	1:2A:17:G:H8	1.83	0.43
1:2A:1248:G:C5	16:2U:3:ARG:HB2	2.53	0.43
1:2A:1709:U:H2'	1:2A:1710:C:C6	2.53	0.43
1:2A:1853:A:H2'	1:2A:1854:A:C8	2.53	0.43
1:2A:1916:A:H2'	1:2A:1917:PSU:O4'	2.18	0.43
1:2A:1999:C:O2	1:2A:2687:U:O2'	2.33	0.43
1:2A:2498:C:H3'	61:2A:3915:HOH:O	2.15	0.43
2:2B:38:C:O4'	14:2S:95:HIS:NE2	2.47	0.43
6:2G:170:ARG:NH2	6:2G:182:LYS:O	2.49	0.43
9:2N:15:LEU:N	9:2N:136:GLU:O	2.51	0.43
11:2P:95:VAL:HA	11:2P:99:LEU:HD12	1.99	0.43
15:2T:100:TYR:O	15:2T:103:ARG:HG2	2.18	0.43
18:2W:88:ARG:HB2	18:2W:92:ARG:HG3	1.99	0.43
23:21:35:THR:OG1	23:21:35:THR:O	2.33	0.43
24:22:64:LEU:O	24:22:68:ARG:HG3	2.17	0.43
32:2a:512:U:H2'	32:2a:513:C:H6	1.81	0.43
32:2a:539:A:H2'	32:2a:540:G:C8	2.53	0.43
35:2d:111:ALA:HB2	35:2d:120:LEU:HD12	1.99	0.43
40:2i:121:ARG:NH1	40:2i:122:ALA:O	2.50	0.43
41:2j:78:ASN:O	41:2j:80:LYS:N	2.51	0.43
1:1A:347:G:C8	5:1F:171:PRO:HG3	2.53	0.43
1:1A:1255:A:H5''	1:1A:1257:G:O4'	2.18	0.43
1:1A:1639:G:H2'	1:1A:1640:G:C8	2.52	0.43
1:1A:1733:C:H2'	1:1A:1734:G:O4'	2.18	0.43
1:1A:2151:C:H42	1:1A:2181:G:H1	1.64	0.43
1:1A:2624:C:OP2	27:15:2:ALA:N	2.52	0.43
3:1D:246:PRO:O	3:1D:254:THR:HG22	2.18	0.43
5:1F:60:SER:OG	5:1F:61:GLY:N	2.50	0.43
5:1F:165:ARG:HG3	5:1F:168:ARG:NH2	2.33	0.43
24:12:31:GLU:O	24:12:35:LEU:HG	2.18	0.43
32:1a:189(C):C:H2'	32:1a:189(D):C:O4'	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:1003:G:N3	32:1a:1004:A:H2	2.17	0.43
32:1a:1004:A:C5'	32:1a:1024:G:H1	2.30	0.43
32:1a:1221:G:OP1	32:1a:1320:C:N4	2.50	0.43
54:1y:46:7MG:H81	54:1y:46:7MG:H2'	1.74	0.43
1:2A:271(G):C:H42	1:2A:271(Q):G:H1	1.66	0.43
1:2A:521:G:H2'	1:2A:522:G:C8	2.51	0.43
1:2A:709:U:H2'	1:2A:710:G:C8	2.53	0.43
1:2A:2584:U:H2'	1:2A:2585:U:C6	2.52	0.43
3:2D:4:LYS:HB3	3:2D:18:VAL:HG23	2.00	0.43
9:2N:69:GLN:O	9:2N:71:ILE:HG13	2.18	0.43
12:2Q:12:GLN:NE2	12:2Q:72:LYS:HG3	2.32	0.43
14:2S:61:ASN:O	14:2S:65:VAL:HG23	2.18	0.43
32:2a:336:C:H2'	32:2a:337:C:C6	2.53	0.43
32:2a:598:U:H2'	32:2a:599:C:C6	2.53	0.43
32:2a:1261:A:H5'	32:2a:1284:C:OP1	2.17	0.43
32:2a:1304:G:C6	32:2a:1305:G:N1	2.86	0.43
32:2a:1517:G:N7	32:2a:1518:MA6:H103	2.32	0.43
33:2b:21:ARG:O	33:2b:23:ARG:N	2.52	0.43
33:2b:27:LYS:HB2	33:2b:194:PRO:HD2	2.00	0.43
33:2b:96:ARG:HB2	33:2b:148:TYR:CD1	2.53	0.43
33:2b:160:ASP:O	33:2b:183:PRO:HD2	2.18	0.43
36:2e:103:GLY:O	36:2e:106:PRO:HD2	2.18	0.43
38:2g:78:ARG:HH21	38:2g:79:ARG:NH1	2.16	0.43
1:1A:1356:G:OP2	29:17:9:ARG:NE	2.49	0.43
1:1A:1633:A:H2'	1:1A:1634:C:C6	2.53	0.43
1:1A:2702:C:OP2	13:1R:14:SER:HB2	2.19	0.43
1:1A:2858:G:C8	15:1T:97:ALA:HB2	2.54	0.43
2:1B:88:C:H2'	2:1B:89:G:O4'	2.19	0.43
6:1G:59:GLU:CD	6:1G:153:ARG:HH21	2.26	0.43
25:13:18:ASP:OD1	25:13:18:ASP:N	2.45	0.43
30:18:6:THR:HG23	30:18:64:TYR:HD2	1.82	0.43
32:1a:731:G:H5'	32:1a:766:A:H4'	2.00	0.43
32:1a:1144:G:N2	32:1a:1146:A:H62	2.16	0.43
32:1a:1353:G:OP1	52:1u:10:ARG:NH1	2.52	0.43
32:1a:1381:U:H1'	38:1g:79:ARG:HG2	1.99	0.43
32:1a:1530:G:H4'	32:1a:1530:G:OP1	2.19	0.43
1:2A:531:C:H4'	1:2A:532:A:H5''	1.99	0.43
1:2A:2284:C:OP2	28:26:6:ARG:HG3	2.18	0.43
2:2B:17:C:H2'	2:2B:18:G:O4'	2.18	0.43
3:2D:237:GLU:OE2	61:2D:401:HOH:O	2.21	0.43
6:2G:120:LEU:N	6:2G:179:PRO:O	2.38	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:2e:105:VAL:HB	36:2e:106:PRO:HD3	1.99	0.43
55:2x:15:G:N2	55:2x:21:A:N3	2.67	0.43
1:1A:2627:U:OP2	61:1A:4301:HOH:O	2.21	0.43
2:1B:3:C:H42	2:1B:118:G:H1	1.65	0.43
32:1a:35:G:O2'	43:1l:118:SER:O	2.30	0.43
32:1a:1095:U:P	32:1a:1108:G:H1	2.41	0.43
1:2A:64:A:O3'	19:2X:71:GLY:HA3	2.19	0.43
1:2A:621:A:OP2	11:2P:108:LYS:NZ	2.42	0.43
1:2A:896:A:H1'	54:2w:56:C:H5'	2.00	0.43
1:2A:1668:A:O2'	1:2A:1674:G:N7	2.43	0.43
1:2A:2376:A:N3	14:2S:106:ARG:NH2	2.64	0.43
1:2A:2611:U:OP1	61:2A:3989:HOH:O	2.21	0.43
10:2O:88:ASN:ND2	10:2O:92:GLU:HB2	2.33	0.43
27:25:16:ARG:HG3	27:25:17:ASP:N	2.34	0.43
28:26:40:CYS:O	28:26:44:ARG:N	2.52	0.43
32:2a:1272:G:N2	32:2a:1273:G:N9	2.66	0.43
37:2f:33:TYR:CE1	37:2f:74:ASP:HB3	2.53	0.43
38:2g:144:MET:HE3	38:2g:144:MET:HB3	1.84	0.43
1:1A:1120:G:N1	1:1A:1121:C:H1'	2.33	0.43
1:1A:2105:G:H2'	1:1A:2106:C:C6	2.53	0.43
21:1Z:126:VAL:HG12	21:1Z:128:VAL:HB	2.00	0.43
32:1a:430:A:OP1	35:1d:9:CYS:HB2	2.18	0.43
32:1a:637:G:H2'	32:1a:638:G:H8	1.84	0.43
49:1r:58:LEU:HD13	49:1r:62:GLU:HB3	2.01	0.43
1:2A:251:A:C5	1:2A:252:G:H1'	2.53	0.43
1:2A:362:U:O2'	1:2A:363:G:H5''	2.19	0.43
1:2A:527:C:N4	1:2A:2779:U:OP2	2.51	0.43
6:2G:5:VAL:HG12	26:24:25:TYR:CE2	2.54	0.43
6:2G:106:LEU:HA	6:2G:110:ALA:HB3	2.00	0.43
27:25:8:LYS:O	27:25:9:LYS:HD2	2.18	0.43
32:2a:97:G:H2'	32:2a:98:G:O4'	2.19	0.43
32:2a:448:A:P	32:2a:485:G:H22	2.41	0.43
32:2a:1002:G:N3	32:2a:1003:G:H1'	2.34	0.43
32:2a:1026:G:N3	32:2a:1026:G:H2'	2.34	0.43
33:2b:109:SER:O	33:2b:112:VAL:HG22	2.18	0.43
39:2h:104:ARG:HD3	39:2h:104:ARG:HA	1.73	0.43
47:2p:3:LYS:O	47:2p:21:VAL:HA	2.18	0.43
51:2t:99:LEU:HB3	51:2t:100:ILE:H	1.65	0.43
1:1A:1091:A:H4'	1:1A:1091:A:OP1	2.19	0.43
1:1A:2881:C:N3	61:1A:4411:HOH:O	2.36	0.43
13:1R:28:LEU:HD22	13:1R:44:LEU:HD13	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1Y:102:CYS:SG	20:1Y:103:GLY:N	2.91	0.43
32:1a:61:G:H2'	32:1a:62:U:O4'	2.19	0.43
32:1a:406:G:N2	32:1a:437:U:O2	2.52	0.43
32:1a:1151:A:HO2'	32:1a:1152:A:H8	1.61	0.43
32:1a:1217:C:H2'	32:1a:1218:C:O4'	2.18	0.43
32:1a:1355:G:H2'	32:1a:1356:G:C8	2.54	0.43
36:1e:61:TYR:HA	36:1e:64:ARG:HD2	2.01	0.43
50:1s:63:THR:O	50:1s:66:MET:HG2	2.18	0.43
54:1w:46:7MG:H81	54:1w:46:7MG:H2'	1.78	0.43
1:2A:1283:G:O2'	1:2A:1285:G:N7	2.40	0.43
1:2A:1477:A:H2'	1:2A:1478:G:O4'	2.19	0.43
1:2A:1791:A:H3'	1:2A:1792:G:H8	1.83	0.43
1:2A:2112:G:H2'	1:2A:2113:U:O4'	2.18	0.43
1:2A:2823:A:OP1	4:2E:113:PHE:HB2	2.18	0.43
32:2a:254:G:OP1	48:2q:66:SER:OG	2.36	0.43
32:2a:834:C:H2'	32:2a:835:U:C6	2.54	0.43
32:2a:857:C:H2'	32:2a:858:G:O4'	2.18	0.43
32:2a:1004:A:N6	32:2a:1037:C:H1'	2.34	0.43
32:2a:1179:A:H2'	32:2a:1180:A:O4'	2.18	0.43
32:2a:1194:U:H4'	36:2e:22:GLY:HA2	2.01	0.43
33:2b:27:LYS:O	33:2b:194:PRO:HG2	2.18	0.43
35:2d:57:ARG:HB3	35:2d:206:PHE:HB2	1.99	0.43
36:2e:78:HIS:CD2	39:2h:104:ARG:HH11	2.37	0.43
39:2h:6:ILE:O	39:2h:10:LEU:HG	2.18	0.43
1:1A:24:G:O2'	18:1W:78:GLU:O	2.28	0.43
1:1A:354:A:N7	1:1A:1255:A:O2'	2.36	0.43
1:1A:1002:A:N1	1:1A:2470:G:H4'	2.34	0.43
1:1A:1472:G:O2'	1:1A:1619:A:N6	2.49	0.43
1:1A:1896:G:H5''	61:1A:4498:HOH:O	2.19	0.43
1:1A:1899:A:H5''	1:1A:1900:G:OP2	2.19	0.43
1:1A:2421:G:N7	61:1A:4420:HOH:O	2.37	0.43
6:1G:43:LEU:HB3	6:1G:44:GLY:H	1.57	0.43
6:1G:77:ILE:HG22	6:1G:80:PHE:H	1.84	0.43
6:1G:109:VAL:HG11	26:14:14:ILE:HG21	2.01	0.43
32:1a:22:G:H4'	32:1a:885:G:C8	2.53	0.43
32:1a:1129:C:O2'	32:1a:1139:G:N7	2.43	0.43
32:1a:1142:G:H2'	32:1a:1143:G:O4'	2.19	0.43
32:1a:1229:A:O2'	55:1x:30:G:OP1	2.36	0.43
32:1a:1305:G:OP2	52:1u:2:GLY:HA3	2.18	0.43
32:1a:1394:A:N1	32:1a:1500:A:O2'	2.49	0.43
41:1j:31:GLY:HA3	41:1j:32:ALA:HA	1.67	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:1l:113:ARG:HB3	43:1l:117:ARG:HG2	2.01	0.43
55:1x:17:C:H5'	55:1x:61:C:OP1	2.19	0.43
1:2A:589:C:H2'	1:2A:590:A:C8	2.54	0.43
1:2A:864:G:H4'	2:2B:102:A:H4'	2.00	0.43
1:2A:1584:C:O2'	1:2A:1586:A:O5'	2.29	0.43
1:2A:1915:5MU:H2'	1:2A:1916:A:O4'	2.17	0.43
1:2A:2134:A:H2'	1:2A:2134:A:N3	2.33	0.43
1:2A:2578:G:OP1	61:2A:3995:HOH:O	2.21	0.43
4:2E:48:GLN:HA	4:2E:80:GLU:HA	2.01	0.43
5:2F:24:LEU:HD21	5:2F:114:VAL:HG12	2.00	0.43
9:2N:28:THR:HG22	9:2N:29:LYS:N	2.34	0.43
21:2Z:98:MET:HE3	21:2Z:98:MET:HB2	1.93	0.43
32:2a:571:U:O4	32:2a:864:A:N6	2.52	0.43
32:2a:646:U:H2'	32:2a:647:C:H6	1.84	0.43
32:2a:999:C:H42	32:2a:1042:G:H1	1.67	0.43
32:2a:1157:A:H4'	32:2a:1158:C:O5'	2.18	0.43
38:2g:150:ALA:HA	42:2k:59:TYR:HB3	2.00	0.43
40:2i:4:TYR:CE1	40:2i:88:TYR:HA	2.54	0.43
40:2i:85:LEU:HB3	40:2i:92:TYR:CD2	2.50	0.43
54:2y:49:C:H2'	54:2y:50:U:C6	2.53	0.43
1:1A:34:C:H5''	1:1A:35:G:OP2	2.19	0.43
1:1A:945:A:H2'	1:1A:945:A:N3	2.32	0.43
1:1A:1091:A:OP1	1:1A:1092:A:H3'	2.18	0.43
1:1A:1140:U:H1'	1:1A:1143:U:C5	2.46	0.43
1:1A:1451:U:H2'	1:1A:1452:U:C6	2.54	0.43
1:1A:2641:A:HO2'	1:1A:2642:G:P	2.40	0.43
5:1F:106:ARG:H	5:1F:106:ARG:HG2	1.47	0.43
9:1N:67:LEU:HG	9:1N:87:LEU:HD22	2.01	0.43
11:1P:88:LEU:HD11	11:1P:114:ILE:HD12	2.00	0.43
11:1P:95:VAL:HG13	11:1P:125:VAL:HB	2.00	0.43
16:1U:46:ALA:O	16:1U:50:ARG:HG2	2.18	0.43
32:1a:23:C:OP2	32:1a:561:U:N3	2.31	0.43
32:1a:406:G:O2'	35:1d:3:ARG:NH2	2.51	0.43
32:1a:1065:U:O2'	32:1a:1066:C:OP2	2.31	0.43
35:1d:99:SER:O	35:1d:140:VAL:N	2.46	0.43
38:1g:54:THR:O	38:1g:56:GLN:N	2.49	0.43
1:2A:1187:G:H5'	17:2V:81:TYR:CE1	2.53	0.43
1:2A:2127:G:N1	1:2A:2161:C:C5	2.87	0.43
1:2A:2137:C:N3	1:2A:2155:G:C6	2.86	0.43
1:2A:2141:G:H2'	1:2A:2142:C:O4'	2.18	0.43
1:2A:2643:G:H2'	1:2A:2644:G:O4'	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2802:G:H2'	1:2A:2803:C:O4'	2.19	0.43
4:2E:108:SER:HB3	4:2E:165:VAL:HG21	2.01	0.43
14:2S:110:LEU:HD12	14:2S:110:LEU:HA	1.87	0.43
19:2X:32:PRO:HA	19:2X:77:LYS:HD2	2.00	0.43
21:2Z:30:ASN:HA	21:2Z:89:PHE:HE1	1.84	0.43
32:2a:160:A:H61	32:2a:347:G:H1'	1.84	0.43
32:2a:173:U:H5''	32:2a:197:A:O4'	2.18	0.43
32:2a:403:C:O2'	35:2d:122:ARG:NH2	2.51	0.43
32:2a:411:A:H2'	32:2a:412:A:H4'	2.00	0.43
32:2a:1121:U:O2'	32:2a:1122:U:H5'	2.18	0.43
32:2a:1401:G:OP1	53:2v:18:G:O2'	2.28	0.43
32:2a:1522:U:H2'	32:2a:1523:G:H8	1.84	0.43
34:2c:47:LEU:HD22	34:2c:50:ALA:HB3	2.01	0.43
34:2c:152:ILE:HG12	34:2c:167:TRP:HB3	2.00	0.43
35:2d:70:ILE:HG23	35:2d:75:PHE:HB2	2.01	0.43
36:2e:76:ILE:O	36:2e:93:PRO:HB3	2.18	0.43
39:2h:12:ARG:HD3	39:2h:26:VAL:HG12	2.01	0.43
43:2l:104:VAL:HG12	43:2l:105:TYR:CD2	2.53	0.43
54:2w:4:C:C4	54:2w:69:G:N1	2.87	0.43
1:1A:895:G:H2'	1:1A:896:A:C8	2.54	0.43
1:1A:2342:G:H2'	1:1A:2343:G:O4'	2.19	0.43
11:1P:124:LYS:HE2	11:1P:146:VAL:HG21	2.01	0.43
19:1X:43:VAL:HG21	19:1X:81:VAL:HG11	1.99	0.43
32:1a:582:U:H2'	32:1a:583:A:H8	1.83	0.43
32:1a:626:U:H2'	32:1a:627:G:C8	2.54	0.43
32:1a:1106:G:H2'	32:1a:1107:C:C6	2.54	0.43
32:1a:1187:G:H5'	40:1i:113:LYS:HE2	1.99	0.43
32:1a:1414:U:H3	32:1a:1486:G:H1	1.66	0.43
36:1e:89:ILE:HG21	36:1e:135:THR:HA	2.01	0.43
38:1g:144:MET:HE2	38:1g:144:MET:HB3	1.86	0.43
43:1l:53:ARG:HB3	43:1l:69:TYR:HE1	1.84	0.43
1:2A:588:U:H2'	1:2A:589:C:C6	2.53	0.43
1:2A:1864:U:OP1	1:2A:2410:G:O2'	2.33	0.43
1:2A:1932:A:H2'	1:2A:1933:G:O4'	2.18	0.43
1:2A:2747:G:O6	1:2A:2755:C:H5''	2.18	0.43
2:2B:7:G:H5'	14:2S:29:PHE:CZ	2.54	0.43
5:2F:36:VAL:O	5:2F:40:GLN:HG3	2.18	0.43
15:2T:1:MET:HE3	15:2T:1:MET:HB2	1.86	0.43
16:2U:104:GLN:NE2	16:2U:105:VAL:HG23	2.33	0.43
32:2a:93:G:C6	32:2a:96:U:C4	3.07	0.43
32:2a:115:G:H4'	32:2a:116:A:O5'	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1122:U:H2'	32:2a:1123:A:H8	1.83	0.43
32:2a:1183:A:O2'	32:2a:1185:G:OP2	2.36	0.43
32:2a:1207:2MG:H2'	32:2a:1208:C:H6	1.84	0.43
32:2a:1343:G:H2'	32:2a:1344:C:C6	2.54	0.43
1:1A:1051:C:O2'	9:1N:28:THR:HG21	2.19	0.43
1:1A:1604:C:H5''	1:1A:1605:A:OP2	2.18	0.43
1:1A:2171:G:N1	1:1A:2172:U:O2	2.52	0.43
1:1A:2272:C:H2'	1:1A:2273:C:C6	2.53	0.43
1:1A:2411:G:H2'	1:1A:2412:G:O4'	2.19	0.43
5:1F:150:GLY:HA2	5:1F:172:TRP:CE3	2.54	0.43
8:1I:75:LEU:O	8:1I:141:LYS:NZ	2.35	0.43
32:1a:911:U:OP1	43:1l:95:GLY:HA2	2.19	0.43
32:1a:1037:C:O5'	32:1a:1037:C:H6	2.02	0.43
32:1a:1318:A:H5''	50:1s:3:ARG:NH1	2.34	0.43
52:1u:5:ASP:O	52:1u:11:GLY:HA3	2.19	0.43
1:2A:39:C:H42	1:2A:440:G:H1	1.66	0.43
1:2A:84:A:N1	1:2A:98:G:O2'	2.42	0.43
1:2A:900:A:HO2'	1:2A:901:A:P	2.37	0.43
1:2A:1812:A:OP2	61:2A:3993:HOH:O	2.21	0.43
5:2F:158:THR:HB	5:2F:195:ASP:HB2	2.00	0.43
6:2G:133:LEU:HD12	6:2G:157:ILE:HB	2.01	0.43
13:2R:100:LEU:HD12	13:2R:100:LEU:HA	1.91	0.43
23:21:2:SER:HB3	23:21:46:LEU:HD12	2.00	0.43
32:2a:590:C:H2'	32:2a:591:U:C6	2.54	0.43
32:2a:1009:G:H22	32:2a:1021:G:H1'	1.84	0.43
32:2a:1145:C:H4'	32:2a:1146:A:H5'	2.01	0.43
32:2a:1325:C:H5''	52:2u:17:THR:HG21	2.01	0.43
32:2a:1417:G:C6	32:2a:1482:G:C6	3.07	0.43
1:1A:118:U:H5''	1:1A:120:G:OP2	2.18	0.42
1:1A:253:C:O2'	1:1A:254:A:H2'	2.19	0.42
1:1A:930:G:H2'	1:1A:931:C:H5	1.83	0.42
1:1A:2150:C:H2'	1:1A:2151:C:O4'	2.19	0.42
1:1A:2745:G:H3'	1:1A:2746:A:O4'	2.19	0.42
26:14:68:ARG:HD3	26:14:69:LYS:H	1.84	0.42
32:1a:691:G:H2'	32:1a:692:U:C6	2.54	0.42
32:1a:1009:G:C6	32:1a:1020:U:O2	2.70	0.42
32:1a:1241:G:H2'	32:1a:1242:C:C6	2.53	0.42
36:1e:11:ILE:HD11	36:1e:108:ALA:HB3	2.01	0.42
54:1w:13:C:H2'	54:1w:14:A:H5''	2.01	0.42
1:2A:323:G:H1'	1:2A:1205:U:O2	2.19	0.42
1:2A:380:U:H2'	1:2A:381:G:C8	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:636:G:OP1	11:2P:132:LYS:NZ	2.49	0.42
1:2A:848:G:C2	1:2A:933:A:H1'	2.54	0.42
1:2A:946:G:H2'	1:2A:947:G:C8	2.54	0.42
1:2A:2693:A:H2'	1:2A:2694:G:C8	2.51	0.42
1:2A:2846:G:H2'	1:2A:2847:U:O4'	2.19	0.42
2:2B:59:A:H2'	2:2B:60:C:O4'	2.18	0.42
7:2H:113:VAL:HG11	7:2H:151:ILE:HG21	2.01	0.42
20:2Y:86:ARG:HB2	20:2Y:98:VAL:HG23	2.01	0.42
24:22:35:LEU:HD23	24:22:35:LEU:HA	1.83	0.42
25:23:46:ASN:O	25:23:50:VAL:HG22	2.18	0.42
32:2a:1328:C:OP1	52:2u:21:TYR:OH	2.35	0.42
33:2b:15:VAL:HG11	33:2b:213:LEU:HD12	2.01	0.42
37:2f:30:LEU:O	37:2f:35:ALA:HB3	2.19	0.42
42:2k:122:LYS:O	42:2k:126:ARG:HG3	2.19	0.42
50:2s:52:TYR:HB2	50:2s:57:HIS:CE1	2.54	0.42
1:1A:29:U:H2'	1:1A:30:G:C8	2.55	0.42
1:1A:141:C:H2'	1:1A:142:G:O4'	2.19	0.42
1:1A:464:G:H2'	1:1A:465:G:C8	2.54	0.42
1:1A:629:U:OP1	5:1F:104:LYS:HD2	2.19	0.42
1:1A:801:C:H2'	1:1A:802:C:C6	2.54	0.42
1:1A:2324:U:OP1	6:1G:73:ALA:HA	2.19	0.42
1:1A:2764:G:C4	7:1H:2:SER:HA	2.54	0.42
1:1A:2879:G:H2'	1:1A:2880:C:O4'	2.18	0.42
7:1H:13:LYS:HA	7:1H:14:GLY:HA2	1.55	0.42
11:1P:120:ALA:HB2	11:1P:137:LYS:HB3	2.00	0.42
12:1Q:1:MET:HE3	12:1Q:1:MET:HB2	1.90	0.42
20:1Y:44:ILE:HD11	20:1Y:64:GLU:HG3	2.00	0.42
32:1a:240:C:H2'	32:1a:241:C:H6	1.83	0.42
32:1a:316:G:OP2	32:1a:351:G:O2'	2.37	0.42
33:1b:16:HIS:CG	33:1b:17:PHE:H	2.36	0.42
42:1k:29:ILE:HG23	42:1k:44:SER:HB3	2.01	0.42
47:1p:43:LYS:HG2	47:1p:48:TRP:CD2	2.54	0.42
54:1w:2:C:N4	54:1w:71:G:N1	2.67	0.42
1:2A:954:G:H5''	12:2Q:13:GLN:HB3	2.02	0.42
1:2A:2184:G:O2'	1:2A:2185:C:H5'	2.19	0.42
1:2A:2615:U:C2	27:25:7:PRO:HA	2.54	0.42
5:2F:64:ILE:HD11	5:2F:75:HIS:HB2	2.00	0.42
6:2G:116:ASP:OD2	44:2m:68:GLY:HA3	2.18	0.42
7:2H:7:LEU:HD12	7:2H:8:PRO:HD2	2.00	0.42
7:2H:127:GLU:C	7:2H:129:THR:H	2.26	0.42
8:2I:92:VAL:HG13	8:2I:120:ILE:HB	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:20:69:PHE:CD1	22:20:79:VAL:HG22	2.54	0.42
26:24:14:ILE:HB	26:24:22:ILE:HB	2.00	0.42
32:2a:107:G:H2'	32:2a:108:G:O4'	2.19	0.42
32:2a:375:U:OP1	47:2p:69:THR:HG21	2.19	0.42
32:2a:448:A:O5'	32:2a:485:G:N2	2.52	0.42
32:2a:1126:U:O2	41:2j:40:LEU:HD21	2.19	0.42
32:2a:1202:G:O4'	45:2n:29:ARG:NH1	2.51	0.42
33:2b:74:LYS:O	33:2b:78:GLN:HG2	2.19	0.42
41:2j:47:PHE:CZ	45:2n:37:PHE:HE2	2.37	0.42
47:2p:3:LYS:HE3	47:2p:3:LYS:HB3	1.90	0.42
48:2q:40:LYS:HD3	48:2q:42:TYR:OH	2.20	0.42
54:2w:4:C:N4	54:2w:69:G:C6	2.83	0.42
1:1A:831:A:C6	3:1D:229:VAL:HG11	2.54	0.42
1:1A:886:U:H1'	1:1A:1236:G:H1'	1.99	0.42
1:1A:1016:C:H2'	1:1A:1017:G:O4'	2.19	0.42
1:1A:2225:U:H4'	3:1D:151:LYS:HG2	2.01	0.42
1:1A:2679:C:H2'	1:1A:2680:G:O4'	2.19	0.42
5:1F:157:VAL:HB	5:1F:194:MET:HG2	2.01	0.42
9:1N:61:ARG:HD3	9:1N:61:ARG:HA	1.82	0.42
13:1R:59:ASP:OD1	13:1R:59:ASP:N	2.50	0.42
14:1S:61:ASN:ND2	14:1S:64:GLU:H	2.03	0.42
32:1a:8:A:H5'	36:1e:101:ILE:HG22	2.00	0.42
32:1a:148:G:H2'	32:1a:149:A:H8	1.84	0.42
32:1a:165:C:H2'	32:1a:166:G:C8	2.54	0.42
32:1a:262:A:H2'	32:1a:263:A:C8	2.54	0.42
32:1a:690:G:C6	32:1a:691:G:C6	3.07	0.42
32:1a:1347:G:H5''	40:1i:107:ARG:HB3	2.00	0.42
32:1a:1456:G:O6	51:1t:54:LYS:NZ	2.26	0.42
33:1b:219:VAL:HA	33:1b:222:ILE:HD12	2.01	0.42
34:1c:111:LEU:HD21	34:1c:144:SER:O	2.20	0.42
36:1e:105:VAL:HG21	36:1e:128:PRO:HB3	2.00	0.42
51:1t:10:LEU:HB3	51:1t:12:ALA:H	1.84	0.42
1:2A:248:G:C2	1:2A:2431:U:H4'	2.54	0.42
1:2A:676:A:H1'	1:2A:2443:C:H1'	2.01	0.42
1:2A:1357:U:H2'	1:2A:1358:G:O4'	2.19	0.42
1:2A:1508:A:H4'	1:2A:1509(A):A:C8	2.54	0.42
3:2D:77:ALA:HB2	3:2D:97:TYR:CD1	2.54	0.42
11:2P:47:ASP:OD2	11:2P:49:ARG:NH2	2.47	0.42
12:2Q:58:PHE:CE1	12:2Q:109:VAL:HG21	2.54	0.42
23:21:67:ILE:N	23:21:68:PRO:HD2	2.34	0.42
32:2a:147:G:H2'	32:2a:148:G:C8	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:663:A:O3'	49:2r:64:ARG:NH2	2.51	0.42
32:2a:921:U:H2'	32:2a:922:G:O4'	2.18	0.42
32:2a:1507:A:C2	32:2a:1530:G:H1'	2.54	0.42
33:2b:47:THR:O	33:2b:51:LEU:HG	2.20	0.42
34:2c:88:ARG:HA	34:2c:91:LEU:HB3	2.01	0.42
38:2g:69:VAL:HG11	38:2g:134:ALA:HB1	2.01	0.42
49:2r:33:ASP:OD2	49:2r:36:ASN:HB2	2.19	0.42
1:1A:7:G:H2'	1:1A:8:A:C8	2.55	0.42
1:1A:83:A:H5'	20:1Y:8:LYS:HG2	2.01	0.42
1:1A:171:A:N3	1:1A:460:C:O2'	2.40	0.42
1:1A:2101:U:O3'	23:11:35:THR:OG1	2.35	0.42
1:1A:2245:U:H2'	1:1A:2246:G:C8	2.55	0.42
1:1A:2371:C:H2'	1:1A:2372:A:O4'	2.20	0.42
32:1a:19:C:H2'	32:1a:20:U:C6	2.53	0.42
32:1a:584:G:H5'	48:1q:91:ARG:NH2	2.35	0.42
32:1a:1051:C:H2'	32:1a:1052:U:C6	2.55	0.42
36:1e:18:ARG:HH11	36:1e:27:ARG:HH12	1.66	0.42
55:1x:50:U:H2'	55:1x:51:C:C6	2.53	0.42
1:2A:184:C:H1'	1:2A:217:G:H1'	2.02	0.42
1:2A:271(Q):G:H2'	1:2A:271(R):G:C8	2.55	0.42
1:2A:471:A:H2'	1:2A:472:A:O4'	2.19	0.42
1:2A:601:C:O2'	1:2A:605:C:H5''	2.19	0.42
1:2A:848:G:C4	1:2A:933:A:H8	2.38	0.42
1:2A:956:G:H2'	1:2A:957:A:H2'	2.01	0.42
1:2A:1012:U:C5	9:2N:28:THR:HG21	2.55	0.42
1:2A:1127:A:H2'	1:2A:1128:A:H5''	2.01	0.42
1:2A:1384:A:N3	1:2A:1405:U:H1'	2.35	0.42
1:2A:1603:A:OP1	61:2A:3986:HOH:O	2.20	0.42
1:2A:2176:A:H2'	1:2A:2177:C:C6	2.55	0.42
3:2D:71:ASP:CG	3:2D:103:ARG:HH22	2.28	0.42
9:2N:38:HIS:NE2	9:2N:50:ASP:OD2	2.52	0.42
10:2O:102:VAL:HB	10:2O:106:LEU:HD12	2.01	0.42
12:2Q:10:ARG:HH12	55:2x:64:G:H4'	1.84	0.42
32:2a:76:C:N4	32:2a:93:G:H1	2.17	0.42
32:2a:163:C:H2'	32:2a:164:U:C6	2.55	0.42
32:2a:222:U:H2'	32:2a:223:U:C6	2.54	0.42
32:2a:554:C:H2'	32:2a:555:C:H6	1.83	0.42
32:2a:1151:A:O2'	32:2a:1152:A:H8	2.03	0.42
32:2a:1406:U:O2	32:2a:1517:G:N2	2.52	0.42
32:2a:1466:C:H2'	32:2a:1467:G:O4'	2.19	0.42
34:2c:71:ALA:HA	34:2c:106:VAL:HB	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:2w:5:G:H2'	54:2w:6:G:H8	1.84	0.42
54:2w:50:U:H2'	54:2w:51:U:C6	2.54	0.42
1:1A:798:A:C6	1:1A:836:A:C5	3.07	0.42
1:1A:865:G:H5'	1:1A:886:U:OP1	2.20	0.42
1:1A:1841:A:H2'	1:1A:1842:G:O4'	2.18	0.42
1:1A:2541:G:H5''	1:1A:2542:A:H5''	2.01	0.42
1:1A:2705:A:H2'	1:1A:2706:G:C8	2.55	0.42
3:1D:140:THR:HG22	3:1D:141:VAL:O	2.20	0.42
6:1G:5:VAL:HG22	6:1G:8:LYS:HB2	2.00	0.42
32:1a:44:G:C2	32:1a:45:U:H1'	2.54	0.42
32:1a:193:C:H2'	32:1a:194:C:C6	2.54	0.42
34:1c:64:VAL:HG22	34:1c:66:VAL:HG23	2.00	0.42
51:1t:48:LYS:HD2	51:1t:51:GLU:HG3	2.01	0.42
1:2A:197:A:N6	1:2A:2430:A:H2'	2.34	0.42
1:2A:956:G:O6	61:2A:3990:HOH:O	2.21	0.42
1:2A:1614:A:P	1:2A:1614:A:H8	2.41	0.42
1:2A:1660:C:H2'	1:2A:1661:G:H8	1.84	0.42
1:2A:1676:A:H2'	1:2A:1677:A:O4'	2.20	0.42
7:2H:126:PRO:HB2	7:2H:127:GLU:H	1.65	0.42
15:2T:109:GLU:O	15:2T:113:LYS:HG2	2.19	0.42
20:2Y:7:VAL:CG1	20:2Y:27:VAL:HG21	2.49	0.42
31:29:2:LYS:HB2	31:29:34:GLN:HG2	2.01	0.42
31:29:14:CYS:HA	31:29:27:CYS:HB2	2.01	0.42
32:2a:224:C:H2'	32:2a:225:C:C6	2.55	0.42
32:2a:768:A:N3	32:2a:1512:U:O2'	2.50	0.42
32:2a:782:A:OP1	32:2a:1521:G:N2	2.52	0.42
32:2a:830:G:H2'	32:2a:831:U:O4'	2.19	0.42
32:2a:966:M2G:HM23	32:2a:967:5MC:H1'	2.01	0.42
33:2b:189:ASP:O	33:2b:192:SER:OG	2.38	0.42
42:2k:48:ILE:H	42:2k:48:ILE:HD12	1.83	0.42
46:2o:4:THR:C	46:2o:6:GLU:H	2.28	0.42
1:1A:1333:A:O4'	13:1R:104:ARG:HD3	2.20	0.42
1:1A:1529:G:H2'	1:1A:1530:G:C8	2.55	0.42
1:1A:2060:G:H2'	1:1A:2061:C:O4'	2.20	0.42
1:1A:2158:C:C2	1:1A:2177:G:N2	2.88	0.42
1:1A:2701:U:H4'	1:1A:2702:C:O5'	2.19	0.42
6:1G:126:ASP:HB3	6:1G:128:ARG:H	1.84	0.42
32:1a:186:C:H2'	32:1a:187:C:C6	2.54	0.42
32:1a:262:A:C6	32:1a:263:A:C6	3.08	0.42
32:1a:407:G:H5''	35:1d:115:ARG:CG	2.48	0.42
32:1a:1001(A):G:C2	32:1a:1002:G:H1'	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:1b:51:LEU:HD21	33:1b:201:ILE:HG23	2.01	0.42
39:1h:17:THR:C	39:1h:78:GLN:HE22	2.26	0.42
44:1m:108:ARG:HD3	44:1m:108:ARG:HA	1.82	0.42
45:1n:24:CYS:SG	45:1n:40:CYS:N	2.91	0.42
1:2A:918:A:C2	2:2B:80:U:H4'	2.54	0.42
1:2A:1038:C:H42	1:2A:1117:G:H1	1.65	0.42
1:2A:1186:G:H2'	1:2A:1187:G:O4'	2.20	0.42
1:2A:2023:G:H1	1:2A:2040:C:H42	1.68	0.42
1:2A:2220:G:H2'	1:2A:2221:G:H8	1.84	0.42
1:2A:2286:A:H4'	1:2A:2287:A:O4'	2.20	0.42
1:2A:2499:C:O2	61:2A:3994:HOH:O	2.21	0.42
10:2O:64:ARG:HB2	10:2O:79:PHE:CD2	2.53	0.42
24:22:51:ARG:O	24:22:55:ARG:HG3	2.19	0.42
32:2a:65:U:H1'	32:2a:66:G:OP2	2.19	0.42
32:2a:254:G:O2'	48:2q:16:GLN:O	2.37	0.42
32:2a:598:U:H4'	39:2h:94:TYR:CD2	2.55	0.42
32:2a:713:G:H2'	32:2a:714:G:C8	2.55	0.42
32:2a:865:A:H2	32:2a:918:A:H4'	1.83	0.42
32:2a:951:G:OP2	44:2m:102:ARG:NH1	2.53	0.42
32:2a:1271:G:H2'	32:2a:1272:G:H5''	2.01	0.42
32:2a:1328:C:O2'	44:2m:29:ARG:NH2	2.51	0.42
36:2e:31:LEU:HD23	36:2e:31:LEU:HA	1.93	0.42
39:2h:34:GLU:O	39:2h:38:ILE:HG12	2.20	0.42
48:2q:66:SER:OG	48:2q:69:LYS:HB2	2.19	0.42
1:1A:704:U:H2'	1:1A:705:C:H6	1.80	0.42
1:1A:1115:A:H2'	1:1A:1119:A:N7	2.35	0.42
1:1A:1529:G:H2'	1:1A:1530:G:H8	1.85	0.42
1:1A:1644:C:H5''	19:1X:36:LYS:HB2	2.02	0.42
1:1A:2198:A:H2'	1:1A:2199:C:C6	2.54	0.42
1:1A:2250:G:N3	1:1A:2250:G:H2'	2.33	0.42
1:1A:2310:A:H2'	1:1A:2311:G:O4'	2.19	0.42
7:1H:126:PRO:HB2	7:1H:127:GLU:H	1.66	0.42
9:1N:108:PRO:O	9:1N:113:GLY:HA3	2.19	0.42
19:1X:12:VAL:HG22	19:1X:29:TRP:CE2	2.54	0.42
30:18:26:LYS:HB2	30:18:44:LYS:O	2.20	0.42
32:1a:162:A:N7	32:1a:163:C:H1'	2.34	0.42
32:1a:339:C:H2'	32:1a:340:U:C6	2.54	0.42
32:1a:580:U:H2'	32:1a:581:G:O4'	2.19	0.42
32:1a:973:G:H3'	32:1a:974:A:H5''	2.01	0.42
42:1k:67:ASP:OD1	42:1k:71:LYS:HE3	2.20	0.42
47:1p:43:LYS:HG2	47:1p:48:TRP:CE2	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:229:A:H2'	1:2A:229:A:N3	2.35	0.42
1:2A:236:C:H2'	1:2A:237:C:H6	1.84	0.42
1:2A:271(F):C:H42	1:2A:271(R):G:H1	1.66	0.42
1:2A:657:U:H2'	1:2A:658:C:C6	2.55	0.42
1:2A:783:A:OP2	61:2A:3912:HOH:O	2.22	0.42
1:2A:2168:G:C8	1:2A:2170:A:N7	2.88	0.42
1:2A:2564:A:C2	1:2A:2647:U:H4'	2.55	0.42
4:2E:111:ARG:HD2	4:2E:160:TYR:CE2	2.55	0.42
32:2a:20:U:H2'	32:2a:21:G:O4'	2.20	0.42
32:2a:134:A:H61	47:2p:25:ARG:NH1	2.18	0.42
32:2a:401:C:P	35:2d:73:ARG:HH21	2.42	0.42
32:2a:1089:G:N2	32:2a:1096:C:N3	2.58	0.42
32:2a:1360:A:H2'	32:2a:1361:G:O4'	2.19	0.42
48:2q:78:GLU:OE1	48:2q:81:ARG:NH1	2.44	0.42
1:1A:776:G:C6	3:1D:208:LYS:HB2	2.55	0.42
1:1A:1224:C:H2'	1:1A:1225:C:H6	1.85	0.42
1:1A:1473:A:H4'	1:1A:1474:C:O4'	2.20	0.42
1:1A:2171:G:C6	1:1A:2172:U:C2	3.08	0.42
1:1A:2190:G:C6	1:1A:2193:A:C8	3.07	0.42
1:1A:2235:G:OP1	3:1D:172:TYR:OH	2.25	0.42
2:1B:24:G:N7	2:1B:56:G:H2'	2.35	0.42
6:1G:61:ALA:O	6:1G:65:GLY:N	2.50	0.42
7:1H:3:ARG:CZ	7:1H:5:GLY:H	2.33	0.42
17:1V:43:GLU:OE1	17:1V:43:GLU:N	2.50	0.42
21:1Z:8:TYR:HB2	21:1Z:38:TYR:CE2	2.54	0.42
37:1f:96:PRO:HB3	49:1r:30:ASP:CG	2.45	0.42
43:1l:8:ASN:O	43:1l:12:ARG:HG3	2.20	0.42
1:2A:245:G:O6	30:28:8:LYS:HE3	2.20	0.42
1:2A:441:U:H2'	1:2A:442:G:C8	2.55	0.42
1:2A:724:U:H2'	1:2A:725:G:O4'	2.19	0.42
1:2A:1469:A:H2'	1:2A:1470:G:O4'	2.20	0.42
1:2A:1882:C:H2'	1:2A:1883:G:O4'	2.19	0.42
1:2A:2364:C:H2'	1:2A:2365:G:O4'	2.20	0.42
1:2A:2803:C:H2'	1:2A:2804:C:C6	2.55	0.42
7:2H:156:ALA:O	7:2H:172:LYS:HG2	2.19	0.42
10:2O:98:VAL:HG23	10:2O:118:ALA:HA	2.01	0.42
18:2W:46:PHE:O	18:2W:50:VAL:HG23	2.19	0.42
18:2W:65:LEU:O	18:2W:69:LEU:HG	2.20	0.42
32:2a:1069:C:O2'	32:2a:1192:C:H1'	2.19	0.42
32:2a:1097:C:H2'	32:2a:1098:C:C6	2.55	0.42
32:2a:1263:C:C4	32:2a:1272:G:O6	2.73	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1275:A:H2'	32:2a:1276:G:O4'	2.19	0.42
36:2e:89:ILE:HD12	36:2e:89:ILE:HA	1.88	0.42
36:2e:105:VAL:HG21	36:2e:128:PRO:HB3	2.01	0.42
38:2g:97:GLN:O	38:2g:101:LEU:HG	2.20	0.42
1:1A:616:G:C6	1:1A:617:U:C4	3.08	0.42
1:1A:672:G:N3	1:1A:2362:C:O2'	2.53	0.42
1:1A:2210:C:H2'	1:1A:2211:U:O4'	2.19	0.42
1:1A:2829:G:OP1	61:1A:4306:HOH:O	2.22	0.42
2:1B:48:A:H2'	2:1B:49:C:C6	2.55	0.42
4:1E:60:ASN:HD21	4:1E:63:LEU:HG	1.85	0.42
34:1c:59:ARG:HG2	34:1c:64:VAL:HB	2.02	0.42
48:1q:50:LYS:HE2	48:1q:51:TYR:CZ	2.55	0.42
1:2A:250:G:C6	1:2A:251:A:C6	3.07	0.42
1:2A:856:C:H2'	1:2A:857:C:C6	2.54	0.42
1:2A:1022:G:N7	9:2N:66:LYS:HE2	2.35	0.42
1:2A:1794:U:H2'	1:2A:1795:C:H6	1.82	0.42
1:2A:2140:C:H2'	1:2A:2141:G:H5'	2.02	0.42
1:2A:2649:U:H2'	1:2A:2650:U:C6	2.54	0.42
1:2A:2815:C:H2'	1:2A:2816:C:C6	2.54	0.42
8:2I:77:LEU:HD23	8:2I:142:VAL:HG12	2.02	0.42
10:2O:20:MET:HE3	10:2O:44:LYS:HE2	2.01	0.42
32:2a:237:C:H5''	48:2q:25:ARG:CZ	2.50	0.42
32:2a:765:G:H1	32:2a:812:C:HO2'	1.61	0.42
32:2a:1006:C:H2'	32:2a:1007:C:C6	2.55	0.42
32:2a:1101:A:H4'	32:2a:1102:A:O5'	2.19	0.42
41:2j:8:LEU:N	41:2j:70:ARG:O	2.51	0.42
1:1A:422:U:O2'	1:1A:423:G:N7	2.46	0.42
1:1A:469:A:H1'	1:1A:1246:C:O4'	2.20	0.42
1:1A:559:U:H2'	1:1A:560:C:C6	2.54	0.42
1:1A:1102:G:H4'	1:1A:1132:A:H8	1.85	0.42
1:1A:1371:G:OP1	1:1A:1694:G:O2'	2.30	0.42
1:1A:1403:U:H2'	1:1A:1404:G:O4'	2.20	0.42
1:1A:1730:C:H2'	1:1A:1731:C:C6	2.54	0.42
1:1A:1825:U:H2'	1:1A:1826:C:H6	1.85	0.42
1:1A:2053:A:C6	1:1A:2510:C:H1'	2.55	0.42
1:1A:2473:C:H2'	1:1A:2474:U:H6	1.85	0.42
1:1A:2702:C:N4	1:1A:2726:A:H1'	2.35	0.42
4:1E:111:ARG:H	4:1E:111:ARG:HG2	1.73	0.42
14:1S:65:VAL:O	14:1S:69:VAL:HG12	2.19	0.42
15:1T:118:ARG:HG2	32:1a:1442(A):G:C8	2.55	0.42
15:1T:127:ALA:C	15:1T:129:ARG:N	2.78	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1T:127:ALA:O	15:1T:128:GLU:HG2	2.20	0.42
32:1a:190:U:H2'	32:1a:191:G:H8	1.84	0.42
32:1a:407:G:OP1	35:1d:115:ARG:HD3	2.20	0.42
36:1e:100:VAL:O	36:1e:107:ARG:NH1	2.52	0.42
39:1h:39:LEU:O	39:1h:45:ILE:HG12	2.20	0.42
42:1k:73:MET:HG2	42:1k:103:LEU:HD21	2.02	0.42
44:1m:117:VAL:HG22	44:1m:118:ALA:H	1.85	0.42
48:1q:45:HIS:O	48:1q:73:VAL:HG23	2.20	0.42
55:1x:10:G:N2	55:1x:26:G:H1'	2.35	0.42
54:1y:48:C:C2	54:1y:59:U:H1'	2.55	0.42
1:2A:637:A:C6	1:2A:652:C:H4'	2.55	0.42
1:2A:955:C:OP1	12:2Q:87:LYS:NZ	2.51	0.42
1:2A:1582:C:H2'	1:2A:1583:A:H8	1.85	0.42
1:2A:2402:C:O2	1:2A:2403:C:N4	2.47	0.42
1:2A:2645:G:N2	1:2A:2767:C:OP2	2.53	0.42
2:2B:19:G:H2'	2:2B:20:C:O4'	2.20	0.42
5:2F:11:VAL:HG21	5:2F:20:LEU:HB2	2.02	0.42
10:2O:104:ARG:N	10:2O:122:LEU:O	2.51	0.42
24:22:7:ARG:HA	24:22:10:LEU:HD12	2.02	0.42
25:23:45:GLY:O	25:23:49:LYS:N	2.48	0.42
32:2a:736:C:H2'	32:2a:737:A:H8	1.83	0.42
32:2a:1107:C:OP1	34:2c:172:ARG:HG2	2.20	0.42
34:2c:131:ARG:NE	34:2c:135:LYS:HE3	2.35	0.42
36:2e:33:VAL:HG22	36:2e:112:LEU:HD12	2.01	0.42
51:2t:50:GLU:HB2	51:2t:99:LEU:HD22	2.01	0.42
1:1A:565:C:H2'	1:1A:566:C:C6	2.55	0.41
1:1A:1199:C:H2'	1:1A:1200:G:O4'	2.19	0.41
11:1P:82:GLY:HA2	11:1P:113:LYS:O	2.19	0.41
12:1Q:57:HIS:CD2	12:1Q:117:ALA:HB2	2.55	0.41
13:1R:1:MET:HE3	13:1R:1:MET:HB2	1.92	0.41
16:1U:76:TYR:CZ	16:1U:80:ILE:HG13	2.55	0.41
32:1a:123:C:OP1	32:1a:311:C:O2'	2.31	0.41
32:1a:219:C:H2'	32:1a:220:G:O4'	2.20	0.41
32:1a:438:G:N1	32:1a:495:A:OP2	2.52	0.41
32:1a:922:G:C6	32:1a:923:A:C6	3.08	0.41
32:1a:1030(C):G:C2'	32:1a:1030(D):A:H5'	2.50	0.41
33:1b:54:THR:HG21	33:1b:201:ILE:HD11	2.02	0.41
33:1b:178:ARG:NH1	33:1b:198:ASP:OD1	2.53	0.41
33:1b:188:ALA:HB1	33:1b:192:SER:OG	2.19	0.41
34:1c:162:GLN:NE2	53:1v:24:A:O2'	2.52	0.41
35:1d:22:LYS:HB2	35:1d:26:CYS:SG	2.60	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1d:202:LEU:O	35:1d:206:PHE:N	2.51	0.41
54:1w:56:C:H2'	54:1w:57:G:O4'	2.20	0.41
54:1y:4:C:H2'	54:1y:5:G:O4'	2.20	0.41
54:1y:61:C:H2'	54:1y:62:C:C6	2.55	0.41
1:2A:628:G:H2'	1:2A:629:G:C8	2.55	0.41
1:2A:893:C:H2'	1:2A:894:C:C5	2.55	0.41
1:2A:898:C:H2'	1:2A:899:A:H5'	2.02	0.41
1:2A:1637:A:H4'	1:2A:2711:A:O2'	2.20	0.41
1:2A:1913:A:H4'	1:2A:1914:C:O5'	2.19	0.41
5:2F:45:ARG:HB2	5:2F:97:TYR:HB2	2.02	0.41
8:2I:126:TYR:HB2	8:2I:142:VAL:HG23	2.02	0.41
32:2a:582:U:H5''	46:2o:64:ARG:HH12	1.85	0.41
35:2d:4:TYR:O	35:2d:5:ILE:HG13	2.19	0.41
37:2f:30:LEU:HD23	37:2f:75:LEU:HD11	2.02	0.41
50:2s:5:LEU:H	50:2s:5:LEU:HG	1.69	0.41
1:1A:1539:C:N4	1:1A:2227:G:O2'	2.53	0.41
3:1D:70:TRP:HB3	3:1D:190:TYR:CE2	2.55	0.41
8:1I:10:GLU:HG3	8:1I:11:ASN:H	1.85	0.41
8:1I:79:ILE:HG22	8:1I:81:VAL:HG13	2.02	0.41
32:1a:67:C:H1'	32:1a:171:A:H2	1.84	0.41
32:1a:667:G:H4'	46:1o:51:HIS:ND1	2.35	0.41
32:1a:867:G:O2'	32:1a:873:A:N1	2.50	0.41
34:1c:131:ARG:HH21	34:1c:135:LYS:HE3	1.85	0.41
36:1e:83:GLU:HG2	36:1e:88:LYS:HB2	2.01	0.41
38:1g:26:PHE:CE2	38:1g:30:ILE:HD11	2.55	0.41
41:1j:45:ARG:HG2	41:1j:47:PHE:CZ	2.55	0.41
1:2A:350:U:H2'	1:2A:351:G:O4'	2.20	0.41
1:2A:984:A:H5''	1:2A:985:C:H5	1.85	0.41
1:2A:1019:U:H2'	1:2A:1020:A:H8	1.85	0.41
1:2A:1161:C:H2'	1:2A:1162:G:C8	2.54	0.41
1:2A:1987:G:H2'	1:2A:1988:C:C6	2.55	0.41
1:2A:2164:C:H3'	1:2A:2165:G:O4'	2.19	0.41
1:2A:2322:A:H2'	1:2A:2323:G:O4'	2.20	0.41
6:2G:138:GLN:HB3	6:2G:153:ARG:O	2.20	0.41
12:2Q:66:ILE:HG12	12:2Q:104:PHE:CD1	2.54	0.41
15:2T:106:SER:OG	15:2T:109:GLU:OE1	2.31	0.41
19:2X:11:PRO:HB3	19:2X:92:LEU:HD11	2.01	0.41
22:20:63:VAL:HG21	22:20:83:PRO:HG3	2.02	0.41
26:24:50:VAL:HG11	44:2m:64:TRP:C	2.45	0.41
32:2a:437:U:O2'	35:2d:125:HIS:HE1	2.03	0.41
32:2a:660:G:H1	32:2a:745:C:N4	2.18	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:927:G:O2'	61:2a:3326:HOH:O	2.22	0.41
32:2a:1273:G:H3'	32:2a:1274:G:H8	1.84	0.41
32:2a:1293:G:H2'	32:2a:1294:G:C8	2.54	0.41
1:1A:1139:G:H3'	1:1A:1140:U:C5'	2.50	0.41
1:1A:2163:G:C6	1:1A:2164:C:C2	3.08	0.41
1:1A:2283:G:OP1	22:10:18:ALA:HB1	2.20	0.41
1:1A:2840:G:O2'	1:1A:2893:A:N1	2.51	0.41
3:1D:77:ALA:HA	3:1D:97:TYR:HA	2.02	0.41
10:1O:64:ARG:HB2	10:1O:79:PHE:CD2	2.55	0.41
17:1V:85:LYS:HE3	17:1V:85:LYS:HB2	1.87	0.41
32:1a:438:G:H4'	35:1d:123:HIS:CE1	2.55	0.41
32:1a:748:C:O5'	32:1a:748:C:H6	2.03	0.41
37:1f:67:MET:SD	37:1f:72:VAL:HG12	2.60	0.41
38:1g:79:ARG:HD2	38:1g:80:VAL:N	2.32	0.41
45:1n:39:LEU:HD11	45:1n:47:LEU:HD12	2.01	0.41
54:1y:67:C:H2'	54:1y:68:C:C6	2.56	0.41
1:2A:517:C:OP1	27:25:16:ARG:NH2	2.53	0.41
1:2A:927:G:H2'	1:2A:928:G:O4'	2.21	0.41
1:2A:1720:U:H3	1:2A:1742:G:H1	1.67	0.41
1:2A:1969:A:O2'	1:2A:1972:A:N3	2.49	0.41
1:2A:1983:C:H4'	1:2A:2606:C:H4'	2.01	0.41
1:2A:2669:G:H2'	1:2A:2670:A:H8	1.84	0.41
1:2A:2724:C:OP1	4:2E:118:LYS:NZ	2.51	0.41
1:2A:2758:A:C4	7:2H:67:LEU:HD21	2.55	0.41
2:2B:14:U:OP2	2:2B:70:C:O2'	2.32	0.41
7:2H:3:ARG:NH1	7:2H:4:ILE:H	2.18	0.41
10:2O:15:GLY:O	10:2O:47:ILE:HG12	2.21	0.41
12:2Q:59:ARG:C	12:2Q:61:GLY:H	2.28	0.41
20:2Y:48:ALA:HA	20:2Y:60:PHE:HA	2.03	0.41
32:2a:589:C:OP1	39:2h:32:LYS:NZ	2.53	0.41
35:2d:128:VAL:N	35:2d:131:ARG:O	2.52	0.41
1:1A:605:G:H2'	1:1A:606:G:H8	1.84	0.41
1:1A:1636:U:H2'	1:1A:1637:G:C8	2.55	0.41
1:1A:2164:C:N3	1:1A:2171:G:O6	2.53	0.41
1:1A:2595:G:OP2	61:1A:4305:HOH:O	2.21	0.41
1:1A:2812:A:N3	1:1A:2904:U:H1'	2.35	0.41
7:1H:137:ASP:HB3	7:1H:140:LYS:HB3	2.01	0.41
10:1O:48:PRO:CB	32:1a:1422:G:H5''	2.47	0.41
21:1Z:72:ARG:NH2	21:1Z:97:GLU:O	2.53	0.41
26:14:61:ARG:HH12	50:1s:9:VAL:HG11	1.85	0.41
32:1a:674:G:H2'	32:1a:675:A:C8	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:840:C:H4'	32:1a:841:U:OP1	2.19	0.41
32:1a:1129:C:H5''	40:1i:16:ARG:HH12	1.86	0.41
32:1a:1304:G:C6	32:1a:1305:G:N1	2.88	0.41
35:1d:73:ARG:HD2	35:1d:73:ARG:HA	1.91	0.41
46:1o:25:THR:HG21	46:1o:70:LEU:HB2	2.01	0.41
1:2A:801:G:O6	5:2F:53:THR:OG1	2.38	0.41
1:2A:863:A:H2'	1:2A:864:G:C8	2.56	0.41
1:2A:1028:A:N6	1:2A:1125:G:H2'	2.36	0.41
1:2A:2841:C:H2'	1:2A:2842:G:H8	1.85	0.41
12:2Q:7:MET:HE2	12:2Q:7:MET:HB3	1.99	0.41
32:2a:417:C:H42	32:2a:426:G:H1	1.69	0.41
32:2a:939:G:H5'	38:2g:102:ARG:CZ	2.50	0.41
32:2a:1189:C:OP1	41:2j:51:ARG:NH2	2.48	0.41
32:2a:1286:A:H3'	32:2a:1286:A:H8	1.86	0.41
32:2a:1307:U:H2'	32:2a:1308:U:C6	2.55	0.41
45:2n:26:ARG:HD3	45:2n:43:CYS:HB3	2.01	0.41
46:2o:11:VAL:HG21	46:2o:34:LEU:HD22	2.02	0.41
48:2q:45:HIS:HB3	48:2q:72:ARG:HB2	2.02	0.41
54:2y:63:G:H2'	54:2y:64:A:O4'	2.21	0.41
1:1A:185:A:H2'	1:1A:185:A:N3	2.34	0.41
1:1A:294:C:N4	1:1A:390:G:H1	2.09	0.41
1:1A:2332:A:H2'	1:1A:2332:A:N3	2.36	0.41
1:1A:2825:C:H5'	27:15:29:THR:HG21	2.03	0.41
3:1D:20:ASP:OD2	3:1D:22:SER:OG	2.38	0.41
4:1E:9:VAL:HG22	4:1E:25:VAL:O	2.20	0.41
4:1E:54:GLN:NE2	4:1E:76:ARG:HG2	2.35	0.41
19:1X:31:HIS:CD2	19:1X:33:LYS:HB2	2.56	0.41
20:1Y:13:VAL:HB	20:1Y:72:VAL:HG13	2.02	0.41
29:17:24:THR:O	29:17:28:ARG:HG3	2.20	0.41
32:1a:1029:C:C4	32:1a:1030:C:N4	2.88	0.41
32:1a:1323:G:H2'	32:1a:1324:A:C8	2.54	0.41
32:1a:1509:C:H2'	32:1a:1510:U:O4'	2.21	0.41
50:1s:48:THR:HG22	50:1s:61:TYR:CD1	2.55	0.41
54:1w:66:U:H2'	54:1w:67:C:C6	2.56	0.41
1:2A:153:C:OP1	23:21:92:LYS:HD3	2.19	0.41
1:2A:480:A:O2'	20:2Y:46:LYS:O	2.38	0.41
1:2A:493:G:H2'	1:2A:494:G:O4'	2.21	0.41
1:2A:928:G:H8	1:2A:928:G:O5'	2.04	0.41
1:2A:2685:G:O6	61:2A:3978:HOH:O	2.18	0.41
2:2B:13:A:O2'	2:2B:14:U:H3'	2.20	0.41
10:2O:71:ARG:HH22	10:2O:122:LEU:C	2.29	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:2Q:50:ALA:HB1	12:2Q:121:ALA:HB1	2.02	0.41
17:2V:10:LYS:HE2	17:2V:12:TYR:OH	2.21	0.41
21:2Z:57:ILE:HD12	21:2Z:71:VAL:HG23	2.02	0.41
25:23:12:PRO:HB2	25:23:20:LYS:HG2	2.02	0.41
30:28:3:LYS:H	30:28:3:LYS:HG2	1.57	0.41
32:2a:198:G:H1	32:2a:219:C:H42	1.68	0.41
32:2a:1289:A:O2'	38:2g:35:LYS:NZ	2.52	0.41
33:2b:71:VAL:HA	33:2b:93:VAL:HG23	2.01	0.41
39:2h:112:LEU:HD12	39:2h:114:THR:HG22	2.02	0.41
41:2j:34:VAL:HA	41:2j:74:ILE:HA	2.02	0.41
49:2r:70:ILE:HG22	49:2r:74:ARG:HD2	2.03	0.41
53:2v:16:A:H2'	53:2v:17:U:O4'	2.21	0.41
1:1A:54:G:O2'	1:1A:125:A:N1	2.47	0.41
1:1A:801:C:H2'	1:1A:802:C:H6	1.85	0.41
1:1A:1100:A:N6	1:1A:1101:G:C6	2.88	0.41
1:1A:1149:A:H8	1:1A:1149:A:O5'	2.04	0.41
3:1D:148:GLU:HB2	3:1D:151:LYS:HD2	2.02	0.41
4:1E:72:VAL:HG12	4:1E:73:GLU:O	2.21	0.41
14:1S:51:ALA:HB3	14:1S:73:LEU:HB2	2.03	0.41
18:1W:73:ALA:HB3	18:1W:106:ILE:HB	2.03	0.41
32:1a:866:C:C4	32:1a:867:G:H1'	2.55	0.41
34:1c:121:ALA:HB1	34:1c:189:ALA:HB2	2.02	0.41
44:1m:40:ASN:C	44:1m:42:ALA:H	2.28	0.41
54:1w:5:G:H2'	54:1w:6:G:H8	1.85	0.41
54:1w:5:G:H2'	54:1w:6:G:C8	2.55	0.41
1:2A:188:G:H5'	23:21:14:VAL:HG21	2.02	0.41
1:2A:314:A:H2'	1:2A:315:G:H8	1.85	0.41
1:2A:889:C:O2'	1:2A:890:A:O4'	2.24	0.41
1:2A:990:A:N6	1:2A:1186:G:H1'	2.36	0.41
1:2A:1224:C:O2'	17:2V:85:LYS:HA	2.21	0.41
1:2A:1509(B):A:H2'	1:2A:1510:G:C8	2.56	0.41
1:2A:2149:G:C6	1:2A:2150:U:C2	3.09	0.41
6:2G:36:LYS:HD3	6:2G:95:ARG:NH1	2.36	0.41
6:2G:124:SER:HB2	6:2G:131:TYR:CE1	2.56	0.41
7:2H:24:VAL:HG13	7:2H:37:VAL:HG21	2.02	0.41
15:2T:108:ARG:HH22	32:2a:1465:C:P	2.42	0.41
29:27:1:MET:HE3	29:27:3:ARG:NH2	2.35	0.41
34:2c:6:HIS:HA	34:2c:7:PRO:HD3	1.91	0.41
35:2d:158:ILE:O	35:2d:162:LEU:N	2.53	0.41
39:2h:20:TYR:HA	39:2h:65:TYR:CE1	2.56	0.41
42:2k:80:VAL:HG22	42:2k:103:LEU:HB3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:2n:3:ARG:HG3	45:2n:4:LYS:N	2.35	0.41
45:2n:14:PRO:HG2	45:2n:16:PHE:O	2.21	0.41
53:2v:14:A:N3	53:2v:14:A:H2'	2.35	0.41
54:2y:30:G:H2'	54:2y:31:A:H8	1.86	0.41
1:1A:68:C:O2	1:1A:72:A:O2'	2.27	0.41
1:1A:2851:C:H2'	1:1A:2852:G:H8	1.85	0.41
3:1D:65:ILE:HG13	3:1D:88:ARG:CZ	2.50	0.41
4:1E:109:LYS:O	4:1E:111:ARG:NH1	2.54	0.41
9:1N:109:LYS:HE2	61:1N:3105:HOH:O	2.21	0.41
32:1a:67:C:H1'	32:1a:171:A:C2	2.55	0.41
32:1a:1028:C:H2'	32:1a:1029:C:O4'	2.20	0.41
32:1a:1070:U:H2'	32:1a:1071:C:H6	1.85	0.41
34:1c:11:ARG:NH2	34:1c:177:THR:O	2.45	0.41
43:1l:113:ARG:HA	43:1l:113:ARG:HD2	1.70	0.41
1:2A:274:G:H2'	1:2A:275:G:C8	2.56	0.41
1:2A:1450(A):C:N4	1:2A:1451:C:H41	2.19	0.41
1:2A:1791:A:H3'	1:2A:1792:G:C8	2.56	0.41
1:2A:1919:A:O2'	32:2a:1517:G:N3	2.47	0.41
1:2A:2287:A:N6	1:2A:2344:U:H3	2.14	0.41
16:2U:16:LYS:HB3	16:2U:16:LYS:HE2	1.80	0.41
32:2a:595:G:H21	32:2a:596:C:N4	2.19	0.41
32:2a:1022:G:H2'	32:2a:1023:G:O4'	2.21	0.41
32:2a:1030(A):G:N2	32:2a:1030(C):G:H3'	2.36	0.41
32:2a:1118:C:OP1	40:2i:104:ARG:NH1	2.45	0.41
32:2a:1121:U:H2'	32:2a:1122:U:C6	2.56	0.41
32:2a:1351:U:H3	32:2a:1371:G:H1	1.68	0.41
32:2a:1402:4OC:H2'	32:2a:1403:C:O4'	2.21	0.41
34:2c:6:HIS:HD2	34:2c:8:ILE:H	1.68	0.41
37:2f:62:TRP:CH2	37:2f:64:GLN:HB2	2.55	0.41
37:2f:70:ASP:OD1	37:2f:70:ASP:N	2.52	0.41
38:2g:20:ASP:OD2	38:2g:22:LEU:HB3	2.20	0.41
38:2g:126:ASP:O	38:2g:130:GLY:N	2.53	0.41
39:2h:19:VAL:HG23	39:2h:21:LYS:HG3	2.02	0.41
44:2m:29:ARG:HD3	44:2m:64:TRP:CE2	2.56	0.41
52:2u:2:GLY:C	52:2u:4:GLY:H	2.29	0.41
1:1A:11:G:H2'	1:1A:12:U:H5''	2.02	0.41
1:1A:543:G:H4'	18:1W:18:ARG:NE	2.36	0.41
1:1A:1152:G:H2'	1:1A:1153:G:O4'	2.20	0.41
1:1A:2183:C:O2'	1:1A:2184:G:H8	2.04	0.41
1:1A:2489:C:O2	31:19:4:ARG:NH2	2.52	0.41
4:1E:117:MET:HE2	4:1E:117:MET:HB3	1.95	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1F:14:PRO:HD2	5:1F:127:GLU:OE1	2.20	0.41
7:1H:24:VAL:HG11	7:1H:43:VAL:HG11	2.02	0.41
20:1Y:6:HIS:HE1	20:1Y:72:VAL:O	2.04	0.41
32:1a:136:C:H42	32:1a:227:G:H1	1.69	0.41
32:1a:153:C:H42	32:1a:168:G:H1	1.69	0.41
32:1a:1084:G:C5	32:1a:1085:U:C4	3.09	0.41
32:1a:1240:U:OP2	38:1g:116:ALA:N	2.53	0.41
40:1i:26:VAL:HG22	40:1i:61:ALA:HB3	2.03	0.41
40:1i:100:GLY:O	40:1i:103:THR:HG22	2.21	0.41
49:1r:26:LEU:HD21	49:1r:39:VAL:HG13	2.02	0.41
1:2A:236:C:H2'	1:2A:237:C:C6	2.55	0.41
1:2A:1155:A:OP1	16:2U:55:ARG:HD2	2.21	0.41
1:2A:1783:A:H5'	1:2A:2608:G:H4'	2.03	0.41
1:2A:2030:A:H4'	1:2A:2031:A:H8	1.85	0.41
1:2A:2140:C:H42	1:2A:2151:G:H1	1.69	0.41
1:2A:2168:G:H8	1:2A:2170:A:N7	2.18	0.41
1:2A:2762:G:H2'	1:2A:2763:G:O4'	2.21	0.41
1:2A:2888:C:H2'	1:2A:2889:C:C6	2.55	0.41
5:2F:68:LYS:HB2	5:2F:69:HIS:ND1	2.35	0.41
7:2H:124:GLU:OE2	7:2H:132:ARG:HD2	2.20	0.41
17:2V:60:GLU:HB2	17:2V:97:LYS:HE2	2.03	0.41
21:2Z:17:ALA:HA	21:2Z:20:ARG:HE	1.85	0.41
32:2a:406:G:H1	32:2a:436:C:H42	1.68	0.41
32:2a:1352:C:H2'	32:2a:1353:G:C8	2.56	0.41
42:2k:85:ARG:HG2	42:2k:111:ASP:C	2.45	0.41
47:2p:55:ARG:HD2	47:2p:55:ARG:HA	1.87	0.41
1:1A:604:C:H2'	1:1A:605:G:C8	2.56	0.41
1:1A:1016:C:O2'	1:1A:1029:A:N3	2.50	0.41
1:1A:1425:A:H4'	1:1A:1426:G:OP2	2.20	0.41
1:1A:2203:G:O2'	1:1A:2204:G:OP1	2.36	0.41
1:1A:2368:C:H2'	1:1A:2369:U:O4'	2.20	0.41
1:1A:2697:G:H5'	10:1O:68:GLU:OE2	2.20	0.41
1:1A:2863:C:H2'	1:1A:2864:G:C8	2.56	0.41
3:1D:232:PRO:HB3	3:1D:244:ARG:CZ	2.51	0.41
4:1E:181:LEU:HA	4:1E:181:LEU:HD12	1.81	0.41
5:1F:102:PRO:O	5:1F:106:ARG:HG2	2.21	0.41
6:1G:82:LEU:HD23	6:1G:82:LEU:HA	1.83	0.41
7:1H:152:ARG:HA	7:1H:152:ARG:HD3	1.78	0.41
8:1I:29:TYR:HD2	8:1I:30:LEU:HD23	1.85	0.41
9:1N:39:ARG:HA	9:1N:40:PRO:HD3	1.95	0.41
12:1Q:110:THR:HG23	12:1Q:113:GLN:HG3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:12:2:LYS:O	24:12:6:VAL:HG23	2.20	0.41
26:14:16:CYS:SG	26:14:17:GLY:N	2.94	0.41
28:16:34:LEU:N	28:16:51:GLU:HG2	2.33	0.41
32:1a:256:U:H2'	32:1a:257:G:O4'	2.20	0.41
32:1a:266:G:N3	32:1a:266:G:H2'	2.35	0.41
32:1a:688:G:H2'	32:1a:689:C:H6	1.86	0.41
32:1a:1017:G:H2'	32:1a:1018:C:C6	2.56	0.41
32:1a:1037:C:H2'	32:1a:1038:C:C6	2.56	0.41
32:1a:1410:G:H2'	32:1a:1411:C:C6	2.55	0.41
35:1d:166:LYS:NZ	35:1d:179:GLU:OE2	2.53	0.41
36:1e:85:GLY:O	36:1e:87:SER:N	2.38	0.41
36:1e:131:ILE:HD13	36:1e:131:ILE:HA	1.88	0.41
39:1h:63:LEU:HD12	39:1h:63:LEU:HA	1.83	0.41
47:1p:15:PRO:O	47:1p:16:HIS:ND1	2.54	0.41
1:2A:210:C:OP1	29:27:29:LYS:HD2	2.21	0.41
1:2A:277:C:H4'	1:2A:278:A:C8	2.56	0.41
1:2A:300:A:H2'	1:2A:334:C:H1'	2.02	0.41
1:2A:560:C:O2	16:2U:49:HIS:NE2	2.54	0.41
1:2A:918:A:N3	2:2B:80:U:O2'	2.47	0.41
1:2A:945:A:C4	1:2A:2448:A:C2	3.09	0.41
1:2A:1115:G:H2'	1:2A:1116:C:O4'	2.21	0.41
1:2A:2719:G:OP2	61:2A:3991:HOH:O	2.21	0.41
2:2B:1:U:OP3	61:2B:5001:HOH:O	2.22	0.41
3:2D:142:VAL:N	3:2D:163:ALA:O	2.43	0.41
12:2Q:10:ARG:NH2	55:2x:64:G:H4'	2.35	0.41
14:2S:106:ARG:HG3	14:2S:112:PHE:CZ	2.55	0.41
15:2T:27:THR:N	15:2T:90:GLN:O	2.34	0.41
19:2X:12:VAL:HG21	19:2X:27:THR:HG22	2.03	0.41
19:2X:35:THR:CG2	19:2X:38:GLU:H	2.33	0.41
19:2X:64:LYS:HA	19:2X:64:LYS:HD3	1.82	0.41
20:2Y:3:VAL:HB	20:2Y:32:PRO:HB3	2.02	0.41
23:21:32:LYS:HE3	23:21:32:LYS:HB3	1.93	0.41
32:2a:7:G:H5'	32:2a:298:A:O4'	2.20	0.41
32:2a:554:C:O2'	61:2a:3319:HOH:O	2.15	0.41
32:2a:701:C:OP1	32:2a:702:A:O2'	2.27	0.41
32:2a:1166:G:N2	32:2a:1169:A:O5'	2.54	0.41
32:2a:1184:G:H2'	32:2a:1185:G:H8	1.86	0.41
32:2a:1230:C:H5'	55:2x:30:G:H5''	2.02	0.41
33:2b:87:ARG:HB2	33:2b:219:VAL:HG11	2.03	0.41
34:2c:131:ARG:NH2	36:2e:50:GLU:HG3	2.34	0.41
35:2d:149:ALA:HB3	35:2d:152:SER:HB2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:2f:52:ILE:HG22	37:2f:86:ARG:HD3	2.02	0.41
42:2k:33:THR:HA	42:2k:39:PRO:HA	2.03	0.41
44:2m:25:ILE:HG23	44:2m:29:ARG:HB2	2.02	0.41
48:2q:55:ASP:HA	48:2q:79:SER:HA	2.03	0.41
55:2x:21:A:H62	55:2x:46:G:H2'	1.85	0.41
1:1A:297:C:H2'	1:1A:298:G:H8	1.85	0.41
1:1A:1418:U:H2'	1:1A:1419:A:O4'	2.20	0.41
1:1A:1968:U:H2'	1:1A:1969:C:C6	2.56	0.41
1:1A:2372:A:O2'	11:1P:61:ARG:NH1	2.53	0.41
6:1G:15:VAL:HG21	6:1G:176:LEU:HD23	2.03	0.41
14:1S:110:LEU:HD12	14:1S:110:LEU:HA	1.80	0.41
32:1a:19:C:O2'	32:1a:572:A:N1	2.48	0.41
32:1a:373:A:H2'	32:1a:374:A:H8	1.85	0.41
32:1a:486:U:H2'	32:1a:487:A:C8	2.56	0.41
32:1a:993:G:H2'	32:1a:993:G:N3	2.36	0.41
32:1a:1060:C:OP1	45:1n:45:ARG:NH2	2.48	0.41
40:1i:32:ASP:OD1	40:1i:33:PHE:N	2.53	0.41
47:1p:69:THR:O	47:1p:73:LEU:HG	2.20	0.41
49:1r:66:LEU:O	49:1r:70:ILE:HG13	2.21	0.41
54:1w:24:G:C6	54:1w:25:C:C4	3.09	0.41
1:2A:274:G:H2'	1:2A:275:G:H8	1.86	0.41
1:2A:1418:G:H8	1:2A:1418:G:O5'	2.04	0.41
1:2A:1957:C:H2'	1:2A:1958:C:C6	2.56	0.41
3:2D:144:ALA:O	3:2D:191:ALA:HA	2.21	0.41
6:2G:64:THR:HG21	6:2G:92:VAL:HG11	2.01	0.41
6:2G:125:PHE:HB3	6:2G:166:ASP:CG	2.46	0.41
9:2N:123:TYR:CZ	9:2N:129:PRO:HD2	2.56	0.41
17:2V:6:LYS:HB2	17:2V:38:LEU:HD11	2.02	0.41
23:21:12:PRO:HB3	23:21:43:TYR:HD1	1.86	0.41
26:24:33:VAL:HG12	26:24:34:GLU:N	2.35	0.41
32:2a:503:C:H2'	32:2a:504:C:H6	1.85	0.41
32:2a:908:A:H2'	32:2a:909:A:C8	2.55	0.41
32:2a:1113:C:H2'	32:2a:1114:C:C6	2.56	0.41
32:2a:1324:A:H4'	32:2a:1362:C:O3'	2.20	0.41
38:2g:65:ALA:O	38:2g:69:VAL:HG23	2.20	0.41
42:2k:34:ASP:HB3	42:2k:40:ILE:HD11	2.03	0.41
42:2k:99:GLN:HA	42:2k:105:VAL:HG21	2.02	0.41
48:2q:3:LYS:HB3	48:2q:61:GLU:HB3	2.02	0.41
1:1A:653:G:H2'	1:1A:654:G:H8	1.84	0.40
1:1A:864:C:H4'	1:1A:977:G:C5	2.56	0.40
1:1A:898:U:O2'	25:13:42:ALA:O	2.29	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1120:G:C2	1:1A:1121:C:H1'	2.56	0.40
1:1A:1314:A:C2	1:1A:2035:A:C4	3.09	0.40
1:1A:2284:U:H5''	1:1A:2285:A:OP1	2.20	0.40
1:1A:2315:G:O6	61:1A:4298:HOH:O	2.20	0.40
1:1A:2589:A:OP2	27:15:3:LYS:NZ	2.48	0.40
1:1A:2701:U:H5'	1:1A:2701:U:O2	2.21	0.40
12:1Q:39:PRO:HA	12:1Q:97:VAL:O	2.22	0.40
26:14:40:HIS:O	26:14:43:TYR:N	2.54	0.40
32:1a:44:G:C6	32:1a:45:U:C2	3.10	0.40
32:1a:401:C:P	35:1d:73:ARG:HH21	2.44	0.40
32:1a:770:C:H5''	61:1a:3393:HOH:O	2.21	0.40
33:1b:115:LEU:O	33:1b:119:GLU:N	2.52	0.40
33:1b:178:ARG:HH12	39:1h:68:ARG:HH22	1.68	0.40
54:1w:4:C:H2'	54:1w:5:G:C8	2.56	0.40
1:2A:265:A:H1'	1:2A:266:G:O4'	2.21	0.40
1:2A:707:G:H2'	1:2A:708:C:O4'	2.21	0.40
1:2A:720:C:H2'	1:2A:721:C:C6	2.56	0.40
1:2A:795:C:OP2	61:2A:3996:HOH:O	2.22	0.40
1:2A:859:G:O2'	1:2A:916:G:O6	2.28	0.40
1:2A:878:A:N6	1:2A:899:A:O2'	2.54	0.40
6:2G:107:LEU:HD21	6:2G:178:PHE:CE1	2.56	0.40
13:2R:33:ARG:NH2	27:25:57:VAL:O	2.49	0.40
15:2T:11:GLU:O	15:2T:15:VAL:HG23	2.20	0.40
25:23:28:LEU:HD23	25:23:28:LEU:HA	1.90	0.40
32:2a:582:U:C2	32:2a:760:G:C6	3.09	0.40
36:2e:113:ALA:HB3	36:2e:115:VAL:HG23	2.03	0.40
37:2f:91:VAL:HG11	49:2r:72:ARG:NH1	2.36	0.40
38:2g:131:LYS:HB3	38:2g:131:LYS:HE2	1.73	0.40
51:2t:47:GLY:HA2	51:2t:48:LYS:C	2.46	0.40
1:1A:504:A:C6	1:1A:506:A:C6	3.09	0.40
1:1A:656:A:H2'	1:1A:657:A:O4'	2.21	0.40
1:1A:831:A:C8	1:1A:839:G:C5	3.09	0.40
1:1A:1014:U:H2'	1:1A:1015:C:C6	2.56	0.40
1:1A:1703:C:H5''	4:1E:136:ARG:HB2	2.03	0.40
4:1E:9:VAL:HG23	15:1T:7:ILE:HD11	2.01	0.40
9:1N:67:LEU:O	9:1N:88:GLU:HG3	2.21	0.40
9:1N:110:GLY:O	9:1N:114:ARG:HG3	2.21	0.40
12:1Q:137:TYR:O	12:1Q:141:GLN:HG2	2.21	0.40
15:1T:100:TYR:O	15:1T:103:ARG:HG3	2.22	0.40
32:1a:410:G:OP2	35:1d:25:ARG:NH1	2.53	0.40
32:1a:530:G:O6	53:1v:21:C:H1'	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1a:735:C:H2'	32:1a:736:C:C6	2.56	0.40
32:1a:1111:A:N1	34:1c:177:THR:OG1	2.43	0.40
32:1a:1260:C:O5'	32:1a:1284:C:H4'	2.21	0.40
33:1b:118:LEU:HD12	33:1b:145:LEU:HD12	2.04	0.40
43:1l:7:ILE:HD13	43:1l:10:LEU:HD12	2.03	0.40
43:1l:71:PRO:O	43:1l:102:ARG:NH1	2.47	0.40
54:1w:2:C:N4	54:1w:71:G:H1	2.19	0.40
1:2A:252:G:P	11:2P:50:ARG:HH22	2.45	0.40
1:2A:857:C:H1'	22:20:26:TYR:HE1	1.86	0.40
1:2A:1147:C:H2'	1:2A:1148:A:C8	2.53	0.40
1:2A:2164:C:H5''	1:2A:2165:G:OP2	2.21	0.40
1:2A:2461:C:H2'	1:2A:2462:U:C6	2.56	0.40
1:2A:2812:G:H2'	1:2A:2813:A:C8	2.56	0.40
4:2E:11:MET:HG2	4:2E:24:THR:HB	2.02	0.40
15:2T:117:ASP:OD2	15:2T:120:ARG:NE	2.36	0.40
29:27:34:ARG:HH21	29:27:39:ARG:HG2	1.86	0.40
32:2a:200:G:H2'	32:2a:201:C:O4'	2.20	0.40
32:2a:553:A:H2'	32:2a:554:C:C6	2.56	0.40
32:2a:977:A:H2'	32:2a:978:A:H5''	2.02	0.40
32:2a:1163:C:H42	32:2a:1173:G:H1	1.69	0.40
32:2a:1323:G:H4'	32:2a:1363:C:C2	2.57	0.40
36:2e:6:PHE:CD1	36:2e:36:ASP:HB3	2.56	0.40
43:2l:60:LEU:HD21	43:2l:85:ILE:HD11	2.01	0.40
46:2o:39:LEU:HD23	46:2o:43:LEU:HG	2.03	0.40
1:1A:560:C:O3'	16:1U:53:ARG:NH1	2.49	0.40
1:1A:1466:U:HO2'	1:1A:1467:G:P	2.42	0.40
1:1A:1830:G:H4'	1:1A:1831:C:H5''	2.03	0.40
1:1A:2355:C:O3'	1:1A:2385:G:H4'	2.21	0.40
1:1A:2689:G:H2'	1:1A:2690:C:C6	2.56	0.40
2:1B:94:C:H2'	2:1B:95:C:H6	1.87	0.40
20:1Y:95:LYS:HE2	20:1Y:95:LYS:HB3	1.84	0.40
28:16:11:LEU:HD23	28:16:11:LEU:HA	1.90	0.40
32:1a:240:C:H2'	32:1a:241:C:C6	2.57	0.40
32:1a:895:G:H2'	32:1a:896:C:C6	2.57	0.40
32:1a:1239:A:C4	32:1a:1298:C:N4	2.89	0.40
35:1d:19:LEU:O	35:1d:21:LEU:HG	2.20	0.40
36:1e:91:LEU:HG	36:1e:118:ILE:HD11	2.04	0.40
37:1f:69:GLU:CD	37:1f:69:GLU:H	2.30	0.40
43:1l:28:LYS:HD3	43:1l:62:SER:HB2	2.03	0.40
45:1n:48:ALA:HB2	45:1n:53:LEU:HD12	2.03	0.40
1:2A:297:C:H2'	1:2A:298:G:O4'	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:593:G:H2'	1:2A:594:U:C6	2.57	0.40
1:2A:946:G:H2'	1:2A:947:G:H8	1.85	0.40
1:2A:2169:A:H1'	54:2y:56:C:C6	2.56	0.40
1:2A:2345:G:N3	1:2A:2381:C:H2'	2.36	0.40
1:2A:2419:U:H2'	1:2A:2420:C:C6	2.57	0.40
1:2A:2872:G:O2'	1:2A:2873:A:H5'	2.22	0.40
4:2E:101:ARG:HB3	4:2E:201:THR:CG2	2.50	0.40
6:2G:121:ASN:HA	6:2G:122:PRO:HD3	1.96	0.40
13:2R:28:LEU:HD23	13:2R:48:VAL:HG21	2.03	0.40
14:2S:26:LEU:N	14:2S:86:ALA:O	2.54	0.40
32:2a:264:U:O2	48:2q:64:PRO:HG2	2.21	0.40
32:2a:430:A:H4'	35:2d:7:PRO:HG3	2.04	0.40
32:2a:719:C:O2'	49:2r:49:LYS:HB3	2.20	0.40
32:2a:741:G:H2'	32:2a:742:G:O4'	2.20	0.40
32:2a:779:C:H2'	32:2a:780:A:O4'	2.21	0.40
32:2a:1469:G:H2'	32:2a:1470:G:C8	2.56	0.40
34:2c:39:ILE:O	34:2c:43:LEU:HG	2.20	0.40
41:2j:42:THR:HG23	41:2j:68:HIS:HA	2.03	0.40
42:2k:19:ALA:HB3	42:2k:82:VAL:HG22	2.03	0.40
46:2o:48:LYS:HD3	46:2o:48:LYS:HA	1.93	0.40
54:2w:5:G:H1	54:2w:68:C:H42	1.70	0.40
1:1A:407:U:H5''	23:11:18:ILE:HD12	2.03	0.40
1:1A:1123:A:C5	1:1A:1124:U:H1'	2.56	0.40
1:1A:1133:G:H2'	1:1A:1135:G:C8	2.57	0.40
1:1A:1285:G:H2'	1:1A:1286:U:O4'	2.21	0.40
1:1A:1409:C:H2'	1:1A:1410:G:H8	1.87	0.40
1:1A:1893:G:C2	1:1A:1903:C:C2	3.10	0.40
1:1A:2517:G:O6	1:1A:2588:G:H2'	2.22	0.40
32:1a:93:G:H2'	32:1a:96:U:O4'	2.21	0.40
32:1a:165:C:H2'	32:1a:166:G:H8	1.86	0.40
32:1a:630:G:H2'	32:1a:631:G:H8	1.85	0.40
32:1a:1511:G:H2'	32:1a:1512:U:O4'	2.22	0.40
37:1f:75:LEU:O	37:1f:79:LEU:HG	2.21	0.40
40:1i:63:ILE:HG22	40:1i:65:VAL:HG23	2.03	0.40
47:1p:50:LYS:HD2	47:1p:50:LYS:HA	1.78	0.40
1:2A:195:A:H2'	1:2A:198:C:N4	2.37	0.40
1:2A:1405:U:H2'	1:2A:1406:U:H6	1.84	0.40
1:2A:2025:C:H2'	1:2A:2026:C:C6	2.57	0.40
1:2A:2392:A:OP2	30:28:31:HIS:NE2	2.35	0.40
1:2A:2406:U:H6	1:2A:2406:U:H2'	1.73	0.40
32:2a:80:G:H1	32:2a:89:C:N4	2.19	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:337:C:H2'	32:2a:338:A:C8	2.57	0.40
32:2a:826:C:H2'	32:2a:827:U:C6	2.56	0.40
34:2c:56:ASP:O	34:2c:66:VAL:HA	2.22	0.40
48:2q:83:ASP:OD1	48:2q:84:LEU:N	2.54	0.40
50:2s:41:VAL:HG22	50:2s:42:PRO:HD2	2.02	0.40
1:1A:941:U:HO2'	1:1A:942:A:P	2.40	0.40
1:1A:1049:G:O2'	1:1A:1056:A:N1	2.38	0.40
1:1A:1312:G:O5'	18:1W:15:ARG:NH2	2.55	0.40
1:1A:1895:U:OP1	1:1A:2422:G:O2'	2.33	0.40
1:1A:1903:C:H2'	1:1A:1904:C:C6	2.56	0.40
1:1A:2699:U:H2'	1:1A:2700:U:O4'	2.22	0.40
5:1F:111:ALA:HB2	5:1F:206:ILE:HG21	2.02	0.40
7:1H:71:LEU:HD12	7:1H:71:LEU:HA	1.94	0.40
7:1H:127:GLU:OE1	7:1H:130:ARG:NE	2.54	0.40
32:1a:163:C:H2'	32:1a:164:U:C6	2.57	0.40
32:1a:399:G:H2'	32:1a:400:C:C6	2.57	0.40
32:1a:509:A:H2'	32:1a:510:A:C8	2.56	0.40
32:1a:868:C:H2'	32:1a:869:G:O4'	2.22	0.40
32:1a:971:G:N1	32:1a:1363(A):A:OP2	2.29	0.40
1:2A:222:A:H5''	1:2A:421:U:OP1	2.22	0.40
1:2A:862:G:H2'	1:2A:863:A:O4'	2.21	0.40
1:2A:1268:A:H2'	1:2A:1269:A:O4'	2.22	0.40
1:2A:1301:A:O2'	1:2A:1302:A:H3'	2.21	0.40
1:2A:1593:G:H2'	1:2A:1594:G:H8	1.84	0.40
1:2A:1599:C:OP1	61:2A:3997:HOH:O	2.22	0.40
1:2A:1786:A:H1'	1:2A:1938:A:N6	2.37	0.40
1:2A:1803:A:N1	1:2A:1822:G:O2'	2.48	0.40
1:2A:2176:A:H2'	1:2A:2177:C:H6	1.87	0.40
1:2A:2395:C:O2'	23:21:30:VAL:HG13	2.22	0.40
1:2A:2492:U:H2'	1:2A:2493:U:C6	2.56	0.40
1:2A:2831:G:OP1	1:2A:2834:G:H4'	2.21	0.40
2:2B:42:C:C4	2:2B:43:C:C4	3.10	0.40
13:2R:104:ARG:HB2	13:2R:107:ASP:OD1	2.21	0.40
18:2W:9:TYR:H	18:2W:102:HIS:CE1	2.39	0.40
20:2Y:43:ASN:CG	20:2Y:65:ALA:HB3	2.47	0.40
26:24:48:ARG:HA	26:24:48:ARG:HD3	1.77	0.40
30:28:21:LYS:HD3	30:28:49:VAL:HG11	2.04	0.40
32:2a:45:U:H2'	32:2a:46:G:C8	2.56	0.40
32:2a:472:A:H4'	47:2p:80:PHE:O	2.22	0.40
32:2a:539:A:H2'	32:2a:540:G:H8	1.86	0.40
32:2a:1007:C:N3	32:2a:1022:G:C6	2.89	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:2a:1073:U:H2'	32:2a:1074:G:H8	1.85	0.40
32:2a:1127:G:H1	32:2a:1145:C:H42	1.69	0.40
36:2e:77:PRO:HD2	36:2e:142:LEU:HD13	2.04	0.40
40:2i:8:GLY:O	40:2i:15:ALA:N	2.52	0.40
43:2l:41:ARG:HH12	43:2l:57:LYS:NZ	2.20	0.40
45:2n:26:ARG:HD2	45:2n:47:LEU:HD11	2.03	0.40
55:2x:14:A:N6	55:2x:21:A:C2	2.88	0.40
55:2x:28:C:H2'	55:2x:29:G:C8	2.55	0.40
54:2y:28:G:H2'	54:2y:29:G:H8	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	258 (94%)	15 (6%)	0	100	100
3	2D	273/276 (99%)	260 (95%)	13 (5%)	0	100	100
4	1E	202/206 (98%)	192 (95%)	9 (4%)	1 (0%)	24	55
4	2E	202/206 (98%)	192 (95%)	8 (4%)	2 (1%)	12	38
5	1F	201/210 (96%)	195 (97%)	5 (2%)	1 (0%)	24	55
5	2F	201/210 (96%)	192 (96%)	9 (4%)	0	100	100
6	1G	179/182 (98%)	163 (91%)	12 (7%)	4 (2%)	5	19
6	2G	179/182 (98%)	164 (92%)	12 (7%)	3 (2%)	7	25
7	1H	172/180 (96%)	160 (93%)	10 (6%)	2 (1%)	10	34
7	2H	172/180 (96%)	154 (90%)	17 (10%)	1 (1%)	21	51
8	1I	144/148 (97%)	129 (90%)	14 (10%)	1 (1%)	18	47
8	2I	144/148 (97%)	124 (86%)	17 (12%)	3 (2%)	5	20
9	1N	138/140 (99%)	134 (97%)	4 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	2N	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
10	1O	120/122 (98%)	111 (92%)	8 (7%)	1 (1%)	16	44
10	2O	120/122 (98%)	109 (91%)	11 (9%)	0	100	100
11	1P	147/150 (98%)	139 (95%)	8 (5%)	0	100	100
11	2P	147/150 (98%)	136 (92%)	11 (8%)	0	100	100
12	1Q	139/141 (99%)	128 (92%)	11 (8%)	0	100	100
12	2Q	139/141 (99%)	129 (93%)	9 (6%)	1 (1%)	18	47
13	1R	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
13	2R	116/118 (98%)	109 (94%)	7 (6%)	0	100	100
14	1S	108/112 (96%)	104 (96%)	4 (4%)	0	100	100
14	2S	108/112 (96%)	103 (95%)	4 (4%)	1 (1%)	14	41
15	1T	129/146 (88%)	122 (95%)	7 (5%)	0	100	100
15	2T	129/146 (88%)	119 (92%)	10 (8%)	0	100	100
16	1U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
16	2U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
17	1V	99/101 (98%)	92 (93%)	6 (6%)	1 (1%)	12	38
17	2V	99/101 (98%)	91 (92%)	7 (7%)	1 (1%)	12	38
18	1W	110/113 (97%)	110 (100%)	0	0	100	100
18	2W	110/113 (97%)	107 (97%)	3 (3%)	0	100	100
19	1X	93/96 (97%)	89 (96%)	3 (3%)	1 (1%)	11	36
19	2X	93/96 (97%)	91 (98%)	2 (2%)	0	100	100
20	1Y	105/110 (96%)	97 (92%)	6 (6%)	2 (2%)	6	22
20	2Y	105/110 (96%)	97 (92%)	6 (6%)	2 (2%)	6	22
21	1Z	148/206 (72%)	134 (90%)	14 (10%)	0	100	100
21	2Z	156/206 (76%)	132 (85%)	23 (15%)	1 (1%)	21	51
22	10	81/85 (95%)	79 (98%)	2 (2%)	0	100	100
22	20	81/85 (95%)	78 (96%)	3 (4%)	0	100	100
23	11	95/98 (97%)	94 (99%)	1 (1%)	0	100	100
23	21	95/98 (97%)	92 (97%)	3 (3%)	0	100	100
24	12	68/72 (94%)	68 (100%)	0	0	100	100
24	22	68/72 (94%)	64 (94%)	4 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	13	57/60 (95%)	56 (98%)	1 (2%)	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%)	57 (85%)	9 (13%)	1 (2%)	8	28
27	15	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
27	25	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
28	16	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
28	26	51/54 (94%)	49 (96%)	2 (4%)	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%)	61 (98%)	0	1 (2%)	7	27
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%)	193 (84%)	29 (13%)	7 (3%)	3	12
33	2b	229/256 (90%)	202 (88%)	20 (9%)	7 (3%)	3	12
34	1c	204/239 (85%)	185 (91%)	18 (9%)	1 (0%)	24	55
34	2c	204/239 (85%)	184 (90%)	17 (8%)	3 (2%)	8	28
35	1d	206/209 (99%)	196 (95%)	10 (5%)	0	100	100
35	2d	206/209 (99%)	189 (92%)	17 (8%)	0	100	100
36	1e	146/162 (90%)	131 (90%)	12 (8%)	3 (2%)	5	20
36	2e	146/162 (90%)	135 (92%)	11 (8%)	0	100	100
37	1f	98/101 (97%)	93 (95%)	4 (4%)	1 (1%)	12	38
37	2f	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
38	1g	153/156 (98%)	141 (92%)	10 (6%)	2 (1%)	9	31
38	2g	153/156 (98%)	140 (92%)	11 (7%)	2 (1%)	9	31
39	1h	135/138 (98%)	130 (96%)	5 (4%)	0	100	100
39	2h	135/138 (98%)	130 (96%)	5 (4%)	0	100	100
40	1i	125/128 (98%)	110 (88%)	15 (12%)	0	100	100
40	2i	125/128 (98%)	109 (87%)	16 (13%)	0	100	100
41	1j	95/105 (90%)	81 (85%)	10 (10%)	4 (4%)	2	7

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	2j	94/105 (90%)	79 (84%)	10 (11%)	5 (5%)	1	5
42	1k	112/129 (87%)	104 (93%)	7 (6%)	1 (1%)	14	41
42	2k	112/129 (87%)	99 (88%)	10 (9%)	3 (3%)	4	15
43	1l	119/132 (90%)	112 (94%)	7 (6%)	0	100	100
43	2l	119/132 (90%)	108 (91%)	11 (9%)	0	100	100
44	1m	121/126 (96%)	104 (86%)	15 (12%)	2 (2%)	7	25
44	2m	120/126 (95%)	108 (90%)	12 (10%)	0	100	100
45	1n	58/61 (95%)	54 (93%)	4 (7%)	0	100	100
45	2n	58/61 (95%)	53 (91%)	5 (9%)	0	100	100
46	1o	86/89 (97%)	81 (94%)	4 (5%)	1 (1%)	10	34
46	2o	86/89 (97%)	77 (90%)	9 (10%)	0	100	100
47	1p	80/88 (91%)	72 (90%)	7 (9%)	1 (1%)	9	31
47	2p	80/88 (91%)	69 (86%)	10 (12%)	1 (1%)	9	31
48	1q	97/105 (92%)	89 (92%)	8 (8%)	0	100	100
48	2q	97/105 (92%)	87 (90%)	6 (6%)	4 (4%)	2	8
49	1r	66/88 (75%)	60 (91%)	6 (9%)	0	100	100
49	2r	66/88 (75%)	61 (92%)	5 (8%)	0	100	100
50	1s	81/93 (87%)	68 (84%)	11 (14%)	2 (2%)	4	16
50	2s	81/93 (87%)	71 (88%)	9 (11%)	1 (1%)	10	34
51	1t	94/106 (89%)	89 (95%)	3 (3%)	2 (2%)	5	20
51	2t	94/106 (89%)	83 (88%)	8 (8%)	3 (3%)	3	11
52	1u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
52	2u	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
All	All	11370/12128 (94%)	10535 (93%)	745 (7%)	90 (1%)	16	44

All (90) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
6	1G	47	LYS
6	1G	49	ASP
7	1H	126	PRO
8	1I	10	GLU
17	1V	79	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	1Y	55	TYR
33	1b	17	PHE
33	1b	22	LYS
51	1t	100	ILE
6	2G	49	ASP
7	2H	126	PRO
8	2I	10	GLU
14	2S	96	GLY
33	2b	125	PRO
41	2j	75	ILE
47	2p	53	VAL
33	1b	20	GLU
41	1j	29	ARG
41	1j	75	ILE
44	1m	67	GLU
50	1s	29	ARG
50	1s	81	ARG
51	1t	47	GLY
26	24	65	ASP
33	2b	9	GLU
33	2b	10	LEU
33	2b	17	PHE
33	2b	22	LYS
42	2k	49	GLY
51	2t	47	GLY
51	2t	100	ILE
7	1H	47	GLU
10	1O	25	LEU
19	1X	93	GLU
33	1b	21	ARG
36	1e	27	ARG
37	1f	38	GLU
38	1g	114	ARG
46	1o	17	ARG
17	2V	79	VAL
21	2Z	2	GLU
38	2g	4	ARG
41	2j	78	ASN
42	2k	89	ALA
48	2q	68	ARG
48	2q	81	ARG
50	2s	29	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	2t	10	LEU
4	1E	52	LEU
6	1G	43	LEU
20	1Y	54	LYS
26	14	44	THR
26	14	57	GLU
38	1g	80	VAL
41	1j	77	PRO
41	1j	78	ASN
4	2E	28	ALA
4	2E	52	LEU
6	2G	47	LYS
8	2I	85	GLU
33	2b	20	GLU
34	2c	3	ASN
26	14	55	ARG
30	18	37	SER
44	1m	21	TYR
38	2g	80	VAL
41	2j	79	ARG
48	2q	74	LEU
33	1b	8	LYS
33	1b	194	PRO
12	2Q	17	LEU
20	2Y	43	ASN
34	2c	47	LEU
34	2c	66	VAL
41	2j	91	PRO
34	1c	66	VAL
42	1k	49	GLY
47	1p	63	GLY
6	2G	52	ILE
41	2j	39	PRO
36	1e	69	VAL
36	1e	85	GLY
8	2I	145	VAL
20	2Y	51	VAL
6	1G	52	ILE
33	2b	165	VAL
42	2k	105	VAL
48	2q	77	VAL
33	1b	125	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%)	206 (96%)	9 (4%)	26	61
3	2D	215/218 (99%)	204 (95%)	11 (5%)	21	54
4	1E	164/166 (99%)	151 (92%)	13 (8%)	11	35
4	2E	164/166 (99%)	153 (93%)	11 (7%)	15	42
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%)	135 (94%)	8 (6%)	19	50
6	2G	143/156 (92%)	135 (94%)	8 (6%)	19	50
7	1H	144/148 (97%)	139 (96%)	5 (4%)	32	67
7	2H	144/148 (97%)	139 (96%)	5 (4%)	32	67
8	1I	113/124 (91%)	103 (91%)	10 (9%)	9	29
8	2I	105/124 (85%)	98 (93%)	7 (7%)	15	42
9	1N	118/119 (99%)	111 (94%)	7 (6%)	18	48
9	2N	118/119 (99%)	107 (91%)	11 (9%)	8	27
10	1O	100/100 (100%)	96 (96%)	4 (4%)	28	63
10	2O	100/100 (100%)	99 (99%)	1 (1%)	68	88
11	1P	115/116 (99%)	109 (95%)	6 (5%)	21	53
11	2P	115/116 (99%)	111 (96%)	4 (4%)	32	67
12	1Q	111/111 (100%)	108 (97%)	3 (3%)	39	74
12	2Q	111/111 (100%)	106 (96%)	5 (4%)	24	58
13	1R	101/101 (100%)	91 (90%)	10 (10%)	7	24
13	2R	101/101 (100%)	95 (94%)	6 (6%)	18	48
14	1S	86/88 (98%)	81 (94%)	5 (6%)	18	49
14	2S	85/88 (97%)	81 (95%)	4 (5%)	23	57
15	1T	115/127 (91%)	107 (93%)	8 (7%)	14	40
15	2T	113/127 (89%)	109 (96%)	4 (4%)	32	67

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	1U	93/94 (99%)	89 (96%)	4 (4%)	26	60
16	2U	93/94 (99%)	90 (97%)	3 (3%)	34	70
17	1V	80/82 (98%)	73 (91%)	7 (9%)	9	29
17	2V	80/82 (98%)	72 (90%)	8 (10%)	7	24
18	1W	90/92 (98%)	82 (91%)	8 (9%)	9	29
18	2W	90/92 (98%)	90 (100%)	0	100	100
19	1X	77/78 (99%)	77 (100%)	0	100	100
19	2X	77/78 (99%)	75 (97%)	2 (3%)	40	75
20	1Y	85/91 (93%)	80 (94%)	5 (6%)	18	48
20	2Y	85/91 (93%)	80 (94%)	5 (6%)	18	48
21	1Z	135/179 (75%)	120 (89%)	15 (11%)	6	20
21	2Z	137/179 (76%)	130 (95%)	7 (5%)	21	54
22	10	65/67 (97%)	64 (98%)	1 (2%)	57	84
22	20	65/67 (97%)	61 (94%)	4 (6%)	16	45
23	11	80/83 (96%)	75 (94%)	5 (6%)	16	45
23	21	80/83 (96%)	77 (96%)	3 (4%)	29	64
24	12	65/67 (97%)	63 (97%)	2 (3%)	35	70
24	22	65/67 (97%)	62 (95%)	3 (5%)	24	58
25	13	51/52 (98%)	47 (92%)	4 (8%)	11	35
25	23	50/52 (96%)	48 (96%)	2 (4%)	28	63
26	14	59/63 (94%)	52 (88%)	7 (12%)	5	17
26	24	53/63 (84%)	48 (91%)	5 (9%)	8	27
27	15	50/52 (96%)	46 (92%)	4 (8%)	11	34
27	25	50/52 (96%)	46 (92%)	4 (8%)	11	34
28	16	51/52 (98%)	49 (96%)	2 (4%)	28	64
28	26	50/52 (96%)	47 (94%)	3 (6%)	17	47
29	17	41/42 (98%)	38 (93%)	3 (7%)	13	38
29	27	41/42 (98%)	38 (93%)	3 (7%)	13	38
30	18	54/55 (98%)	52 (96%)	2 (4%)	30	65
30	28	54/55 (98%)	50 (93%)	4 (7%)	13	37
31	19	34/34 (100%)	33 (97%)	1 (3%)	37	73

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	29	34/34 (100%)	33 (97%)	1 (3%)	37	73
33	1b	192/220 (87%)	187 (97%)	5 (3%)	40	75
33	2b	187/220 (85%)	176 (94%)	11 (6%)	18	48
34	1c	142/188 (76%)	138 (97%)	4 (3%)	38	73
34	2c	140/188 (74%)	135 (96%)	5 (4%)	31	66
35	1d	169/181 (93%)	158 (94%)	11 (6%)	15	43
35	2d	173/181 (96%)	166 (96%)	7 (4%)	28	63
36	1e	113/123 (92%)	105 (93%)	8 (7%)	13	39
36	2e	114/123 (93%)	109 (96%)	5 (4%)	25	59
37	1f	84/90 (93%)	81 (96%)	3 (4%)	31	66
37	2f	85/90 (94%)	81 (95%)	4 (5%)	23	57
38	1g	119/127 (94%)	114 (96%)	5 (4%)	26	61
38	2g	120/127 (94%)	115 (96%)	5 (4%)	26	61
39	1h	114/119 (96%)	106 (93%)	8 (7%)	14	40
39	2h	114/119 (96%)	108 (95%)	6 (5%)	20	52
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%)	64 (97%)	2 (3%)	36	72
41	2j	69/92 (75%)	68 (99%)	1 (1%)	59	85
42	1k	82/99 (83%)	79 (96%)	3 (4%)	30	65
42	2k	83/99 (84%)	79 (95%)	4 (5%)	23	56
43	1l	96/108 (89%)	90 (94%)	6 (6%)	16	45
43	2l	96/108 (89%)	93 (97%)	3 (3%)	35	70
44	1m	93/101 (92%)	90 (97%)	3 (3%)	34	70
44	2m	92/101 (91%)	90 (98%)	2 (2%)	45	78
45	1n	49/50 (98%)	43 (88%)	6 (12%)	5	16
45	2n	49/50 (98%)	44 (90%)	5 (10%)	7	23
46	1o	78/80 (98%)	76 (97%)	2 (3%)	40	75
46	2o	78/80 (98%)	75 (96%)	3 (4%)	29	64
47	1p	69/74 (93%)	64 (93%)	5 (7%)	13	39
47	2p	68/74 (92%)	60 (88%)	8 (12%)	5	17

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	1q	94/97 (97%)	91 (97%)	3 (3%)	34	70
48	2q	94/97 (97%)	92 (98%)	2 (2%)	47	79
49	1r	59/77 (77%)	59 (100%)	0	100	100
49	2r	59/77 (77%)	55 (93%)	4 (7%)	14	42
50	1s	69/80 (86%)	66 (96%)	3 (4%)	26	60
50	2s	67/80 (84%)	63 (94%)	4 (6%)	17	47
51	1t	70/82 (85%)	69 (99%)	1 (1%)	59	85
51	2t	70/82 (85%)	68 (97%)	2 (3%)	37	73
52	1u	18/22 (82%)	17 (94%)	1 (6%)	19	50
52	2u	18/22 (82%)	18 (100%)	0	100	100
All	All	9303/10064 (92%)	8819 (95%)	484 (5%)	21	53

All (484) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	22	SER
3	1D	61	LEU
3	1D	142	VAL
3	1D	155	LEU
3	1D	211	ARG
3	1D	217	ARG
3	1D	221	VAL
3	1D	229	VAL
3	1D	242	ARG
4	1E	12	THR
4	1E	21	VAL
4	1E	24	THR
4	1E	42	ASP
4	1E	47	VAL
4	1E	49	LEU
4	1E	75	VAL
4	1E	111	ARG
4	1E	116	VAL
4	1E	136	ARG
4	1E	175	VAL
4	1E	181	LEU
4	1E	195	LEU
5	1F	28	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	1F	33	LEU
5	1F	53	THR
5	1F	57	VAL
5	1F	74	ARG
5	1F	88	VAL
5	1F	106	ARG
5	1F	110	LEU
5	1F	170	LEU
5	1F	183	VAL
5	1F	192	LEU
5	1F	195	ASP
5	1F	201	VAL
6	1G	3	LEU
6	1G	5	VAL
6	1G	31	VAL
6	1G	43	LEU
6	1G	90	LEU
6	1G	133	LEU
6	1G	159	VAL
6	1G	175	LEU
7	1H	15	VAL
7	1H	51	ARG
7	1H	71	LEU
7	1H	84	SER
7	1H	129	THR
8	1I	9	LEU
8	1I	38	LEU
8	1I	43	ASN
8	1I	75	LEU
8	1I	77	LEU
8	1I	92	VAL
8	1I	101	LEU
8	1I	109	ILE
8	1I	123	LEU
8	1I	129	THR
9	1N	14	VAL
9	1N	28	THR
9	1N	32	THR
9	1N	33	LEU
9	1N	34	LEU
9	1N	67	LEU
9	1N	99	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	1O	10	VAL
10	1O	42	SER
10	1O	70	LYS
10	1O	120	GLU
11	1P	59	LEU
11	1P	95	VAL
11	1P	125	VAL
11	1P	126	VAL
11	1P	133	SER
11	1P	147	LEU
12	1Q	35	VAL
12	1Q	109	VAL
12	1Q	110	THR
13	1R	24	GLN
13	1R	29	LEU
13	1R	36	THR
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	14	VAL
14	1S	36	TYR
14	1S	69	VAL
14	1S	85	VAL
14	1S	110	LEU
15	1T	28	VAL
15	1T	30	VAL
15	1T	36	GLU
15	1T	51	ARG
15	1T	67	SER
15	1T	70	VAL
15	1T	96	ARG
15	1T	103	ARG
16	1U	17	ILE
16	1U	77	SER
16	1U	83	LEU
16	1U	95	LEU
17	1V	46	VAL
17	1V	51	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	1V	61	VAL
17	1V	62	LEU
17	1V	72	VAL
17	1V	73	SER
17	1V	79	VAL
18	1W	4	LYS
18	1W	11	ARG
18	1W	15	ARG
18	1W	17	VAL
18	1W	23	LEU
18	1W	59	VAL
18	1W	92	ARG
18	1W	107	LEU
20	1Y	14	LEU
20	1Y	38	ILE
20	1Y	63	LYS
20	1Y	72	VAL
20	1Y	99	CYS
21	1Z	18	LEU
21	1Z	33	LEU
21	1Z	49	ARG
21	1Z	70	LEU
21	1Z	71	VAL
21	1Z	86	VAL
21	1Z	129	SER
21	1Z	137	ILE
21	1Z	138	GLU
21	1Z	150	LEU
21	1Z	153	SER
21	1Z	154	ASP
21	1Z	155	LEU
21	1Z	170	THR
21	1Z	171	ILE
22	10	39	ARG
23	11	3	LYS
23	11	11	ARG
23	11	30	VAL
23	11	33	LYS
23	11	95	LEU
24	12	40	SER
24	12	52	ASP
25	13	23	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	13	34	GLU
25	13	54	VAL
25	13	56	VAL
26	14	33	VAL
26	14	44	THR
26	14	49	PHE
26	14	50	VAL
26	14	52	THR
26	14	56	VAL
26	14	60	GLN
27	15	6	VAL
27	15	16	ARG
27	15	26	THR
27	15	29	THR
28	16	9	LEU
28	16	48	VAL
29	17	35	ARG
29	17	39	ARG
29	17	43	THR
30	18	30	ARG
30	18	32	LEU
31	19	4	ARG
33	1b	94	ASN
33	1b	112	VAL
33	1b	185	ILE
33	1b	187	LEU
33	1b	200	ILE
34	1c	3	ASN
34	1c	64	VAL
34	1c	77	ILE
34	1c	195	VAL
35	1d	5	ILE
35	1d	10	ARG
35	1d	19	LEU
35	1d	31	CYS
35	1d	83	SER
35	1d	91	SER
35	1d	135	LEU
35	1d	140	VAL
35	1d	158	ILE
35	1d	170	VAL
35	1d	178	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	1e	16	THR
36	1e	31	LEU
36	1e	41	VAL
36	1e	53	LEU
36	1e	56	GLN
36	1e	81	GLU
36	1e	131	ILE
36	1e	152	ARG
37	1f	40	VAL
37	1f	45	LEU
37	1f	72	VAL
38	1g	12	LEU
38	1g	27	ILE
38	1g	79	ARG
38	1g	92	SER
38	1g	131	LYS
39	1h	26	VAL
39	1h	51	VAL
39	1h	52	ASP
39	1h	63	LEU
39	1h	69	ARG
39	1h	83	ILE
39	1h	104	ARG
39	1h	109	ILE
40	1i	41	VAL
40	1i	64	THR
40	1i	83	ARG
40	1i	128	ARG
41	1j	16	LEU
41	1j	55	LYS
42	1k	33	THR
42	1k	48	ILE
42	1k	114	VAL
43	1l	27	LEU
43	1l	43	VAL
43	1l	54	LYS
43	1l	58	VAL
43	1l	59	ARG
43	1l	83	VAL
44	1m	15	VAL
44	1m	19	LEU
44	1m	91	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
45	1n	6	LEU
45	1n	18	VAL
45	1n	23	ARG
45	1n	29	ARG
45	1n	33	VAL
45	1n	56	VAL
46	1o	7	GLU
46	1o	87	ILE
47	1p	11	SER
47	1p	20	VAL
47	1p	21	VAL
47	1p	29	ASP
47	1p	67	THR
48	1q	35	VAL
48	1q	60	ILE
48	1q	68	ARG
50	1s	12	ASP
50	1s	41	VAL
50	1s	77	THR
51	1t	90	GLN
52	1u	15	ARG
3	2D	3	VAL
3	2D	38	LYS
3	2D	61	LEU
3	2D	68	LYS
3	2D	138	VAL
3	2D	142	VAL
3	2D	145	VAL
3	2D	169	GLU
3	2D	221	VAL
3	2D	242	ARG
3	2D	259	THR
4	2E	9	VAL
4	2E	12	THR
4	2E	21	VAL
4	2E	38	THR
4	2E	58	ARG
4	2E	75	VAL
4	2E	101	ARG
4	2E	116	VAL
4	2E	170	LEU
4	2E	175	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	2E	181	LEU
5	2F	51	THR
5	2F	53	THR
5	2F	60	SER
5	2F	88	VAL
5	2F	132	VAL
5	2F	157	VAL
5	2F	158	THR
5	2F	183	VAL
5	2F	192	LEU
5	2F	201	VAL
6	2G	3	LEU
6	2G	9	ARG
6	2G	43	LEU
6	2G	133	LEU
6	2G	140	ILE
6	2G	159	VAL
6	2G	161	THR
6	2G	165	THR
7	2H	52	VAL
7	2H	70	THR
7	2H	71	LEU
7	2H	129	THR
7	2H	134	SER
8	2I	76	THR
8	2I	92	VAL
8	2I	101	LEU
8	2I	116	LEU
8	2I	127	VAL
8	2I	140	LEU
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	58	ASP
9	2N	62	VAL
9	2N	63	THR
9	2N	73	THR
9	2N	99	LEU
9	2N	140	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	2O	69	ILE
11	2P	95	VAL
11	2P	105	LEU
11	2P	112	LEU
11	2P	126	VAL
12	2Q	2	LEU
12	2Q	35	VAL
12	2Q	38	GLU
12	2Q	75	THR
12	2Q	110	THR
13	2R	24	GLN
13	2R	29	LEU
13	2R	44	LEU
13	2R	65	LEU
13	2R	100	LEU
13	2R	111	LEU
14	2S	49	VAL
14	2S	69	VAL
14	2S	84	GLN
14	2S	110	LEU
15	2T	41	ARG
15	2T	63	VAL
15	2T	89	VAL
15	2T	96	ARG
16	2U	8	VAL
16	2U	63	VAL
16	2U	78	THR
17	2V	39	LEU
17	2V	51	VAL
17	2V	52	VAL
17	2V	56	SER
17	2V	61	VAL
17	2V	62	LEU
17	2V	72	VAL
17	2V	79	VAL
19	2X	35	THR
19	2X	52	VAL
20	2Y	37	VAL
20	2Y	72	VAL
20	2Y	85	VAL
20	2Y	99	CYS
20	2Y	107	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	2Z	33	LEU
21	2Z	52	SER
21	2Z	126	VAL
21	2Z	129	SER
21	2Z	144	LEU
21	2Z	154	ASP
21	2Z	170	THR
22	20	10	THR
22	20	63	VAL
22	20	67	VAL
22	20	74	ARG
23	21	4	VAL
23	21	35	THR
23	21	95	LEU
24	22	19	VAL
24	22	53	LEU
24	22	59	ARG
25	23	30	ARG
25	23	31	LEU
26	24	26	SER
26	24	34	GLU
26	24	44	THR
26	24	49	PHE
26	24	50	VAL
27	25	6	VAL
27	25	29	THR
27	25	33	CYS
27	25	58	LEU
28	26	5	VAL
28	26	9	LEU
28	26	48	VAL
29	27	1	MET
29	27	35	ARG
29	27	39	ARG
30	28	14	VAL
30	28	30	ARG
30	28	32	LEU
30	28	41	ILE
31	29	7	VAL
33	2b	68	ILE
33	2b	93	VAL
33	2b	94	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	2b	112	VAL
33	2b	127	ILE
33	2b	140	HIS
33	2b	158	LEU
33	2b	172	ILE
33	2b	185	ILE
33	2b	189	ASP
33	2b	192	SER
34	2c	15	THR
34	2c	57	ILE
34	2c	77	ILE
34	2c	166	GLU
34	2c	173	VAL
35	2d	5	ILE
35	2d	17	VAL
35	2d	31	CYS
35	2d	135	LEU
35	2d	178	VAL
35	2d	181	MET
35	2d	193	ASP
36	2e	41	VAL
36	2e	68	GLU
36	2e	75	THR
36	2e	83	GLU
36	2e	152	ARG
37	2f	40	VAL
37	2f	72	VAL
37	2f	75	LEU
37	2f	83	ASP
38	2g	30	ILE
38	2g	52	GLU
38	2g	79	ARG
38	2g	98	SER
38	2g	111	ARG
39	2h	3	THR
39	2h	54	ASP
39	2h	83	ILE
39	2h	104	ARG
39	2h	112	LEU
39	2h	114	THR
40	2i	64	THR
40	2i	65	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	2i	74	ILE
40	2i	102	LEU
40	2i	127	LYS
41	2j	16	LEU
42	2k	14	VAL
42	2k	24	SER
42	2k	109	VAL
42	2k	114	VAL
43	2l	27	LEU
43	2l	97	ARG
43	2l	116	SER
44	2m	91	ARG
44	2m	103	THR
45	2n	6	LEU
45	2n	18	VAL
45	2n	25	VAL
45	2n	33	VAL
45	2n	44	LEU
46	2o	37	ASN
46	2o	72	ARG
46	2o	87	ILE
47	2p	2	VAL
47	2p	20	VAL
47	2p	21	VAL
47	2p	44	THR
47	2p	53	VAL
47	2p	62	VAL
47	2p	67	THR
47	2p	69	THR
48	2q	5	VAL
48	2q	36	ILE
49	2r	31	LEU
49	2r	37	VAL
49	2r	47	THR
49	2r	76	LEU
50	2s	5	LEU
50	2s	16	LEU
50	2s	41	VAL
50	2s	71	LEU
51	2t	71	THR
51	2t	84	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (114)

such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	87	ASN
4	1E	60	ASN
4	1E	192	ASN
5	1F	8	GLN
5	1F	203	GLN
6	1G	26	GLN
6	1G	58	GLN
6	1G	79	ASN
8	1I	105	HIS
9	1N	94	HIS
12	1Q	12	GLN
12	1Q	89	ASN
13	1R	71	GLN
14	1S	61	ASN
15	1T	43	GLN
15	1T	58	ASN
16	1U	72	HIS
19	1X	31	HIS
19	1X	82	GLN
20	1Y	6	HIS
21	1Z	65	GLN
22	10	12	ASN
22	10	50	ASN
23	11	47	GLN
23	11	56	GLN
24	12	9	GLN
28	16	20	ASN
30	18	35	GLN
31	19	34	GLN
33	1b	40	HIS
34	1c	6	HIS
34	1c	162	GLN
34	1c	176	HIS
35	1d	77	ASN
36	1e	78	HIS
37	1f	32	ASN
37	1f	57	GLN
37	1f	73	ASN
38	1g	28	ASN
38	1g	148	ASN
40	1i	3	GLN
40	1i	87	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	1i	124	GLN
41	1j	62	HIS
43	1l	99	HIS
44	1m	92	HIS
46	1o	50	HIS
46	1o	62	GLN
47	1p	13	HIS
47	1p	14	ASN
50	1s	23	ASN
50	1s	47	HIS
50	1s	69	HIS
51	1t	42	GLN
51	1t	45	GLN
51	1t	73	HIS
3	2D	87	ASN
3	2D	143	HIS
4	2E	48	GLN
5	2F	69	HIS
5	2F	75	HIS
5	2F	133	ASN
7	2H	139	GLN
8	2I	139	GLN
9	2N	94	HIS
10	2O	5	GLN
12	2Q	12	GLN
12	2Q	123	HIS
13	2R	13	HIS
13	2R	24	GLN
13	2R	50	HIS
13	2R	71	GLN
14	2S	16	ASN
16	2U	81	HIS
18	2W	60	ASN
18	2W	62	HIS
19	2X	31	HIS
21	2Z	32	HIS
21	2Z	55	HIS
24	22	65	ASN
27	25	4	HIS
28	26	20	ASN
31	29	20	HIS
33	2b	78	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	2b	110	GLN
34	2c	108	ASN
34	2c	162	GLN
34	2c	170	GLN
34	2c	181	ASN
35	2d	77	ASN
35	2d	119	GLN
35	2d	123	HIS
35	2d	125	HIS
36	2e	78	HIS
36	2e	141	GLN
37	2f	100	ASN
38	2g	28	ASN
38	2g	109	ASN
38	2g	148	ASN
39	2h	78	GLN
40	2i	31	GLN
40	2i	87	GLN
40	2i	124	GLN
41	2j	56	HIS
42	2k	22	HIS
42	2k	93	GLN
42	2k	104	GLN
44	2m	77	ASN
45	2n	49	HIS
47	2p	16	HIS
49	2r	63	GLN
50	2s	23	ASN
50	2s	57	HIS
50	2s	69	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2864/2915 (98%)	450 (15%)	29 (1%)
1	2A	2791/2915 (95%)	473 (16%)	20 (0%)
2	1B	120/121 (99%)	9 (7%)	1 (0%)
2	2B	118/121 (97%)	28 (23%)	0
32	1a	1497/1521 (98%)	242 (16%)	0
32	2a	1501/1521 (98%)	290 (19%)	0
53	1v	12/24 (50%)	2 (16%)	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
53	2v	12/24 (50%)	3 (25%)	0
54	1w	70/76 (92%)	22 (31%)	0
54	1y	72/76 (94%)	22 (30%)	0
54	2w	66/76 (86%)	20 (30%)	0
54	2y	70/76 (92%)	21 (30%)	0
55	1x	75/77 (97%)	13 (17%)	0
55	2x	75/77 (97%)	12 (16%)	0
All	All	9343/9620 (97%)	1607 (17%)	50 (0%)

All (1607) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	13	A
1	1A	14	A
1	1A	15	G
1	1A	34	C
1	1A	36	G
1	1A	45	C
1	1A	50	G
1	1A	54	G
1	1A	57	G
1	1A	70	A
1	1A	71	U
1	1A	73	A
1	1A	74	G
1	1A	77	A
1	1A	83	A
1	1A	90	A
1	1A	94	G
1	1A	116	A
1	1A	117	A
1	1A	118	U
1	1A	121	G
1	1A	123	G
1	1A	138	G
1	1A	145	G
1	1A	177	G
1	1A	185	A
1	1A	188	A
1	1A	194	G
1	1A	203	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	204	G
1	1A	205	A
1	1A	211	A
1	1A	217	A
1	1A	218	A
1	1A	222	A
1	1A	237	G
1	1A	258	U
1	1A	262	C
1	1A	272	U
1	1A	273	G
1	1A	275	C
1	1A	278	G
1	1A	279	G
1	1A	289	G
1	1A	299	G
1	1A	303	C
1	1A	309	C
1	1A	335	A
1	1A	353	G
1	1A	354	A
1	1A	360	C
1	1A	376	G
1	1A	387	G
1	1A	388	A
1	1A	389	G
1	1A	407	U
1	1A	413	G
1	1A	423	G
1	1A	432	U
1	1A	438	G
1	1A	448	U
1	1A	455	A
1	1A	469	A
1	1A	470	C
1	1A	474	U
1	1A	480	A
1	1A	482	C
1	1A	507	G
1	1A	519	G
1	1A	526	A
1	1A	529	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	530	A
1	1A	534	C
1	1A	538	A
1	1A	555	G
1	1A	556	C
1	1A	557	A
1	1A	558	G
1	1A	569	G
1	1A	573	G
1	1A	579	G
1	1A	586	G
1	1A	591	U
1	1A	596	G
1	1A	598	A
1	1A	607	C
1	1A	616	G
1	1A	626	A
1	1A	627	G
1	1A	630	U
1	1A	639	G
1	1A	641	G
1	1A	642	G
1	1A	652	A
1	1A	662	A
1	1A	670	C
1	1A	671	A
1	1A	693	G
1	1A	697	C
1	1A	716	G
1	1A	732	A
1	1A	733	G
1	1A	777	C
1	1A	811	A
1	1A	822	G
1	1A	823	G
1	1A	829	A
1	1A	830	A
1	1A	831	A
1	1A	832	G
1	1A	837	C
1	1A	839	G
1	1A	852	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	859	C
1	1A	866	A
1	1A	874	U
1	1A	875	U
1	1A	913	A
1	1A	924	U
1	1A	926	G
1	1A	927	G
1	1A	931	C
1	1A	932	C
1	1A	933	C
1	1A	934	A
1	1A	935	C
1	1A	936	C
1	1A	937	A
1	1A	940	C
1	1A	941	U
1	1A	942	A
1	1A	943	C
1	1A	944	C
1	1A	953	U
1	1A	956	A
1	1A	977	G
1	1A	983	G
1	1A	990	A
1	1A	991	G
1	1A	998	A
1	1A	1003	U
1	1A	1004	A
1	1A	1006	C
1	1A	1008	U
1	1A	1019	G
1	1A	1020	C
1	1A	1029	A
1	1A	1042	A
1	1A	1058	U
1	1A	1059	C
1	1A	1068	G
1	1A	1072	U
1	1A	1073	A
1	1A	1079	U
1	1A	1084	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1090	G
1	1A	1091	A
1	1A	1092	A
1	1A	1093	G
1	1A	1094	A
1	1A	1100	A
1	1A	1101	G
1	1A	1104	G
1	1A	1109	G
1	1A	1112	U
1	1A	1113	A
1	1A	1114	G
1	1A	1116	A
1	1A	1117	G
1	1A	1119	A
1	1A	1120	G
1	1A	1121	C
1	1A	1122	C
1	1A	1124	U
1	1A	1127	U
1	1A	1131	A
1	1A	1134	A
1	1A	1135	G
1	1A	1136	U
1	1A	1140	U
1	1A	1142	A
1	1A	1147	U
1	1A	1154	U
1	1A	1157	A
1	1A	1158	G
1	1A	1161	G
1	1A	1162	C
1	1A	1174	A
1	1A	1176	U
1	1A	1180	C
1	1A	1181	G
1	1A	1195	G
1	1A	1214	G
1	1A	1217	G
1	1A	1218	G
1	1A	1219	A
1	1A	1220	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1221	G
1	1A	1222	A
1	1A	1223	C
1	1A	1256	U
1	1A	1263	C
1	1A	1282	G
1	1A	1294	G
1	1A	1296	G
1	1A	1299	A
1	1A	1302	G
1	1A	1317	G
1	1A	1318	A
1	1A	1322	A
1	1A	1327	G
1	1A	1346	U
1	1A	1347	A
1	1A	1349	G
1	1A	1366	C
1	1A	1391	C
1	1A	1398	U
1	1A	1405	A
1	1A	1406	A
1	1A	1411	A
1	1A	1430	A
1	1A	1431	G
1	1A	1432	C
1	1A	1441	A
1	1A	1442	U
1	1A	1462	G
1	1A	1463	C
1	1A	1466	U
1	1A	1467	G
1	1A	1474	C
1	1A	1491	A
1	1A	1497	G
1	1A	1502	G
1	1A	1514	C
1	1A	1529	G
1	1A	1539	C
1	1A	1543	U
1	1A	1554	A
1	1A	1555	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1556	A
1	1A	1586	G
1	1A	1587	U
1	1A	1605	A
1	1A	1613	A
1	1A	1616	A
1	1A	1625	U
1	1A	1627	A
1	1A	1628	G
1	1A	1631	C
1	1A	1632	A
1	1A	1654	A
1	1A	1655	A
1	1A	1656	A
1	1A	1695	C
1	1A	1701	A
1	1A	1711	A
1	1A	1721	G
1	1A	1743	G
1	1A	1747	A
1	1A	1750	G
1	1A	1767	A
1	1A	1768	U
1	1A	1776	G
1	1A	1787	G
1	1A	1793	A
1	1A	1794	G
1	1A	1795	G
1	1A	1804	A
1	1A	1811	A
1	1A	1813	C
1	1A	1817	A
1	1A	1822	A
1	1A	1831	C
1	1A	1832	G
1	1A	1847	G
1	1A	1860	A
1	1A	1870	G
1	1A	1878	A
1	1A	1889	G
1	1A	1899	A
1	1A	1911	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1922	A
1	1A	1928	G
1	1A	1936	C
1	1A	1951	G
1	1A	1952	G
1	1A	1959	A
1	1A	1960	A
1	1A	1977	U
1	1A	1982	A
1	1A	1985	U
1	1A	1989	C
1	1A	1992	A
1	1A	1993	A
1	1A	1994	A
1	1A	2014	G
1	1A	2015	U
1	1A	2019	G
1	1A	2042	A
1	1A	2045	G
1	1A	2053	A
1	1A	2055	A
1	1A	2065	C
1	1A	2074	G
1	1A	2077	C
1	1A	2078	G
1	1A	2082	A
1	1A	2083	G
1	1A	2084	A
1	1A	2091	G
1	1A	2114	U
1	1A	2115	G
1	1A	2124	U
1	1A	2132	G
1	1A	2133	C
1	1A	2134	G
1	1A	2135	U
1	1A	2136	A
1	1A	2138	G
1	1A	2142	G
1	1A	2143	G
1	1A	2144	U
1	1A	2148	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2149	G
1	1A	2151	C
1	1A	2152	U
1	1A	2153	G
1	1A	2154	U
1	1A	2155	G
1	1A	2156	A
1	1A	2157	A
1	1A	2158	C
1	1A	2162	C
1	1A	2163	G
1	1A	2164	C
1	1A	2165	C
1	1A	2166	U
1	1A	2168	C
1	1A	2170	G
1	1A	2172	U
1	1A	2173	G
1	1A	2178	G
1	1A	2179	G
1	1A	2180	A
1	1A	2181	G
1	1A	2182	G
1	1A	2184	G
1	1A	2188	G
1	1A	2189	U
1	1A	2193	A
1	1A	2194	U
1	1A	2195	A
1	1A	2204	G
1	1A	2206	G
1	1A	2211	U
1	1A	2214	G
1	1A	2220	A
1	1A	2227	G
1	1A	2228	G
1	1A	2229	A
1	1A	2237	A
1	1A	2250	G
1	1A	2251	G
1	1A	2280	A
1	1A	2281	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2285	A
1	1A	2291	G
1	1A	2292	G
1	1A	2295	C
1	1A	2299	A
1	1A	2301	G
1	1A	2306	C
1	1A	2317	A
1	1A	2319	G
1	1A	2320	G
1	1A	2321	A
1	1A	2332	A
1	1A	2337	G
1	1A	2346	G
1	1A	2348	A
1	1A	2359	C
1	1A	2362	C
1	1A	2373	A
1	1A	2395	G
1	1A	2397	C
1	1A	2408	G
1	1A	2412	G
1	1A	2418	U
1	1A	2436	C
1	1A	2437	A
1	1A	2440	G
1	1A	2441	G
1	1A	2442	A
1	1A	2446	A
1	1A	2447	A
1	1A	2451	A
1	1A	2453	C
1	1A	2460	A
1	1A	2488	A
1	1A	2490	A
1	1A	2514	G
1	1A	2517	G
1	1A	2518	U
1	1A	2530	A
1	1A	2537	G
1	1A	2541	G
1	1A	2547	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	2561	G
1	1A	2566	U
1	1A	2578	A
1	1A	2579	G
1	1A	2585	C
1	1A	2614	A
1	1A	2621	U
1	1A	2623	U
1	1A	2624	C
1	1A	2640	C
1	1A	2641	A
1	1A	2642	G
1	1A	2666	A
1	1A	2701	U
1	1A	2702	C
1	1A	2714	U
1	1A	2715	C
1	1A	2725	A
1	1A	2726	A
1	1A	2727	G
1	1A	2739	U
1	1A	2746	A
1	1A	2757	G
1	1A	2770	A
1	1A	2771	A
1	1A	2777	A
1	1A	2778	A
1	1A	2779	G
1	1A	2791	A
1	1A	2793	G
1	1A	2802	C
1	1A	2803	A
1	1A	2804	C
1	1A	2806	G
1	1A	2813	G
1	1A	2830	A
1	1A	2831	A
1	1A	2845	A
1	1A	2882	G
1	1A	2890	C
1	1A	2901	A
1	1A	2903	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	1B	2	C
2	1B	30	C
2	1B	35	U
2	1B	52	A
2	1B	56	G
2	1B	67	G
2	1B	73	A
2	1B	106	G
2	1B	110	G
32	1a	7	G
32	1a	9	G
32	1a	32	A
32	1a	39	G
32	1a	47	C
32	1a	48	C
32	1a	50	A
32	1a	51	A
32	1a	61	G
32	1a	70	G
32	1a	73	G
32	1a	79	G
32	1a	96	U
32	1a	98	G
32	1a	101	A
32	1a	116	A
32	1a	120	A
32	1a	121	C
32	1a	131	C
32	1a	163	C
32	1a	174	C
32	1a	182	U
32	1a	189(B)	C
32	1a	189(F)	U
32	1a	189(G)	G
32	1a	189(J)	G
32	1a	195	A
32	1a	197	A
32	1a	202	U
32	1a	203	U
32	1a	204	U
32	1a	216	G
32	1a	217	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	220	G
32	1a	247	G
32	1a	251	G
32	1a	258	G
32	1a	266	G
32	1a	267	C
32	1a	289	G
32	1a	301	G
32	1a	321	A
32	1a	328	C
32	1a	332	G
32	1a	341	C
32	1a	342	C
32	1a	344	A
32	1a	348	G
32	1a	351	G
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	382	A
32	1a	384	G
32	1a	397	A
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	421	U
32	1a	424	G
32	1a	429	U
32	1a	430	A
32	1a	439	A
32	1a	442	C
32	1a	452	A
32	1a	453	A
32	1a	461	A
32	1a	470	C
32	1a	471	G
32	1a	485	G
32	1a	496	A
32	1a	498	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	505	G
32	1a	509	A
32	1a	510	A
32	1a	511	C
32	1a	518	C
32	1a	521	G
32	1a	527	7MG
32	1a	531	U
32	1a	532	A
32	1a	547	A
32	1a	559	A
32	1a	560	U
32	1a	561	U
32	1a	562	C
32	1a	568	G
32	1a	572	A
32	1a	573	A
32	1a	574	A
32	1a	576	G
32	1a	577	G
32	1a	596	C
32	1a	630	G
32	1a	653	A
32	1a	665	A
32	1a	666	G
32	1a	687	A
32	1a	688	G
32	1a	703	G
32	1a	717	C
32	1a	723	U
32	1a	731	G
32	1a	734	G
32	1a	747	C
32	1a	749	C
32	1a	755	G
32	1a	759	A
32	1a	760	G
32	1a	777	A
32	1a	792	A
32	1a	793	U
32	1a	794	A
32	1a	815	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	872	A
32	1a	902	G
32	1a	914	A
32	1a	926	G
32	1a	927	G
32	1a	931	C
32	1a	934	C
32	1a	935	A
32	1a	942	G
32	1a	960	U
32	1a	961	U
32	1a	967	5MC
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	982	U
32	1a	992	U
32	1a	993	G
32	1a	994	A
32	1a	997	U
32	1a	1000	U
32	1a	1001	A
32	1a	1003	G
32	1a	1005	A
32	1a	1006	C
32	1a	1009	G
32	1a	1011	G
32	1a	1020	U
32	1a	1022	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	1024	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C
32	1a	1028	C
32	1a	1030(A)	G
32	1a	1030(C)	G
32	1a	1030(D)	A
32	1a	1031	G
32	1a	1033	G
32	1a	1039	C
32	1a	1043	C
32	1a	1054	C
32	1a	1066	C
32	1a	1068	G
32	1a	1081	G
32	1a	1094	G
32	1a	1095	U
32	1a	1096	C
32	1a	1101	A
32	1a	1125	U
32	1a	1137	C
32	1a	1138	G
32	1a	1139	G
32	1a	1146	A
32	1a	1152	A
32	1a	1154	G
32	1a	1159	U
32	1a	1160	G
32	1a	1184	G
32	1a	1187	G
32	1a	1196	U
32	1a	1197	G
32	1a	1202	G
32	1a	1212	U
32	1a	1213	A
32	1a	1227	A
32	1a	1238	A
32	1a	1250	A
32	1a	1256	A
32	1a	1257	U
32	1a	1260	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	1a	1275	A
32	1a	1278	U
32	1a	1279	A
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1305	G
32	1a	1320	C
32	1a	1338	G
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1358	U
32	1a	1363	C
32	1a	1363(A)	A
32	1a	1364	U
32	1a	1370	G
32	1a	1378	C
32	1a	1390	U
32	1a	1394	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	1487	G
32	1a	1492	A
32	1a	1494	G
32	1a	1503	A
32	1a	1504	G
32	1a	1506	U
32	1a	1517	G
32	1a	1529	G
32	1a	1530	G
32	1a	1532	U
53	1v	13	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	1v	24	A
54	1w	2	C
54	1w	3	C
54	1w	7	A
54	1w	9	A
54	1w	14	A
54	1w	19	G
54	1w	20	U
54	1w	21	A
54	1w	23	A
54	1w	24	G
54	1w	45	U
54	1w	46	7MG
54	1w	47	U
54	1w	48	C
54	1w	50	U
54	1w	62	C
54	1w	63	G
54	1w	68	C
54	1w	69	G
54	1w	70	G
54	1w	73	A
54	1w	74	C
55	1x	6	G
55	1x	9	G
55	1x	17(A)	U
55	1x	18	G
55	1x	19	G
55	1x	20	U
55	1x	21	A
55	1x	31	G
55	1x	47	U
55	1x	48	C
55	1x	56	C
55	1x	69	C
55	1x	76	A
54	1y	6	G
54	1y	8	4SU
54	1y	13	C
54	1y	14	A
54	1y	19	G
54	1y	20	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	1y	21	A
54	1y	35	A
54	1y	44	G
54	1y	45	U
54	1y	46	7MG
54	1y	48	C
54	1y	49	C
54	1y	53	G
54	1y	57	G
54	1y	59	U
54	1y	61	C
54	1y	65	G
54	1y	66	U
54	1y	69	G
54	1y	70	G
54	1y	73	A
1	2A	15	G
1	2A	35	G
1	2A	36	G
1	2A	45	C
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	83	G
1	2A	84	A
1	2A	90	U
1	2A	95	G
1	2A	100	G
1	2A	102	G
1	2A	118	A
1	2A	119	A
1	2A	120	U
1	2A	125	G
1	2A	126	A
1	2A	136	G
1	2A	154(A)	C
1	2A	157	U
1	2A	172	C
1	2A	173	G
1	2A	181	A
1	2A	196	A
1	2A	199	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	205	G
1	2A	214	G
1	2A	216	A
1	2A	222	A
1	2A	228	A
1	2A	229	A
1	2A	233	A
1	2A	248	G
1	2A	249	C
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	272(B)	G
1	2A	274	G
1	2A	277	C
1	2A	278	A
1	2A	279	C
1	2A	294	A
1	2A	308	G
1	2A	311	A
1	2A	323	G
1	2A	324	A
1	2A	327	G
1	2A	329	G
1	2A	330	A
1	2A	342	G
1	2A	352	G
1	2A	362	U
1	2A	363	G
1	2A	363(B)	G
1	2A	363(D)	G
1	2A	363(E)	U
1	2A	363(F)	A
1	2A	386	G
1	2A	396	G
1	2A	403	U
1	2A	405	U
1	2A	411	G
1	2A	412	A
1	2A	421	U
1	2A	422	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	444	C
1	2A	447	A
1	2A	454	A
1	2A	457	A
1	2A	479	A
1	2A	481	G
1	2A	494	G
1	2A	505	A
1	2A	509	C
1	2A	529	A
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	545	G
1	2A	556	G
1	2A	563	G
1	2A	567	A
1	2A	568	U
1	2A	573	G
1	2A	575	A
1	2A	588	U
1	2A	599	G
1	2A	603	A
1	2A	604	G
1	2A	606	U
1	2A	607	U
1	2A	614(B)	G
1	2A	615	G
1	2A	616	G
1	2A	627	A
1	2A	634	C
1	2A	637	A
1	2A	645	C
1	2A	652(B)	A
1	2A	652(U)	G
1	2A	669	G
1	2A	686	G
1	2A	709	U
1	2A	717	G
1	2A	730	C
1	2A	753	C
1	2A	771	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	775	G
1	2A	776	G
1	2A	779	U
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	792	G
1	2A	805	G
1	2A	811	U
1	2A	812	C
1	2A	819	A
1	2A	827	U
1	2A	828	U
1	2A	847	U
1	2A	854	G
1	2A	857	C
1	2A	859	G
1	2A	866	A
1	2A	869	G
1	2A	873	G
1	2A	874	G
1	2A	875	G
1	2A	877	U
1	2A	878	A
1	2A	879	G
1	2A	880	G
1	2A	883	G
1	2A	884	C
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	890	A
1	2A	893	C
1	2A	894	C
1	2A	896	A
1	2A	900	A
1	2A	901	A
1	2A	910	A
1	2A	914	C
1	2A	915	C
1	2A	917	A
1	2A	932	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	953	A
1	2A	957	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	997	G
1	2A	1006	C
1	2A	1012	U
1	2A	1013	C
1	2A	1017	G
1	2A	1022	G
1	2A	1025	G
1	2A	1026	U
1	2A	1033	U
1	2A	1036	G
1	2A	1038	C
1	2A	1039	G
1	2A	1041	C
1	2A	1043	C
1	2A	1116	C
1	2A	1122	G
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1139	G
1	2A	1142(A)	A
1	2A	1144	G
1	2A	1166	C
1	2A	1171	G
1	2A	1180	C
1	2A	1206	G
1	2A	1211	U
1	2A	1220	A
1	2A	1237	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1244	G
1	2A	1250	G
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1273	U
1	2A	1284	A
1	2A	1300	U
1	2A	1301	A
1	2A	1308	A
1	2A	1314	C
1	2A	1320	C
1	2A	1345	C
1	2A	1352	U
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1368	G
1	2A	1370	C
1	2A	1380	G
1	2A	1384	A
1	2A	1385	G
1	2A	1386	C
1	2A	1398	C
1	2A	1411	C
1	2A	1416	G
1	2A	1417	C
1	2A	1420	U
1	2A	1421	G
1	2A	1427	A
1	2A	1428	C
1	2A	1437	C
1	2A	1445	A
1	2A	1449	A
1	2A	1450	G
1	2A	1455	G
1	2A	1460	A
1	2A	1463	C
1	2A	1467	C
1	2A	1471	A
1	2A	1482	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1490	A
1	2A	1493	C
1	2A	1497	U
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1531	C
1	2A	1532	C
1	2A	1542	A
1	2A	1545	A
1	2A	1558	A
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1579	A
1	2A	1580	A
1	2A	1583	A
1	2A	1584	C
1	2A	1586	A
1	2A	1608	A
1	2A	1609	A
1	2A	1610	A
1	2A	1640	C
1	2A	1648	C
1	2A	1654	A
1	2A	1674	G
1	2A	1675	C
1	2A	1696	G
1	2A	1700	A
1	2A	1701	A
1	2A	1703	G
1	2A	1721	G
1	2A	1722	A
1	2A	1739	U
1	2A	1740	G
1	2A	1746	G
1	2A	1747	G
1	2A	1750	G
1	2A	1756	G
1	2A	1758	G
1	2A	1762	A
1	2A	1763	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	1764	G
1	2A	1773	A
1	2A	1780	A
1	2A	1782	C
1	2A	1786	A
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1811	G
1	2A	1812	A
1	2A	1816	G
1	2A	1829	A
1	2A	1835	G
1	2A	1847	A
1	2A	1848	A
1	2A	1857	G
1	2A	1877	A
1	2A	1878	G
1	2A	1889	A
1	2A	1896	G
1	2A	1900	A
1	2A	1906	G
1	2A	1914	C
1	2A	1929	G
1	2A	1930	G
1	2A	1936	A
1	2A	1937	A
1	2A	1938	A
1	2A	1955	U
1	2A	1963	U
1	2A	1964	G
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1993	U
1	2A	1997	G
1	2A	2023	G
1	2A	2027	G
1	2A	2031	A
1	2A	2033	A
1	2A	2043	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2062	A
1	2A	2069	G
1	2A	2093	G
1	2A	2105	C
1	2A	2108	C
1	2A	2111	C
1	2A	2112	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	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	2142	C
1	2A	2146	C
1	2A	2147	G
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	2161	C
1	2A	2165	G
1	2A	2166	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2167	U
1	2A	2168	G
1	2A	2172	U
1	2A	2174	C
1	2A	2178	C
1	2A	2185	C
1	2A	2189	U
1	2A	2192	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2218	U
1	2A	2225	A
1	2A	2239	G
1	2A	2275	C
1	2A	2278	A
1	2A	2279	G
1	2A	2282	G
1	2A	2283	C
1	2A	2287	A
1	2A	2288	A
1	2A	2305	A
1	2A	2308	G
1	2A	2319	G
1	2A	2320	A
1	2A	2322	A
1	2A	2325	G
1	2A	2327	A
1	2A	2334	G
1	2A	2336	A
1	2A	2341	G
1	2A	2346	A
1	2A	2347	C
1	2A	2350	C
1	2A	2376	A
1	2A	2383	G
1	2A	2385	C
1	2A	2396	G
1	2A	2403	C
1	2A	2406	U
1	2A	2419	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2425	A
1	2A	2429	G
1	2A	2430	A
1	2A	2434	A
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2445	G
1	2A	2448	A
1	2A	2465	C
1	2A	2468	G
1	2A	2469	A
1	2A	2476	A
1	2A	2487	G
1	2A	2490	G
1	2A	2491	U
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	2554	U
1	2A	2555	U
1	2A	2566	A
1	2A	2567	G
1	2A	2576	G
1	2A	2579	C
1	2A	2582	G
1	2A	2602	A
1	2A	2609	U
1	2A	2610	C
1	2A	2611	U
1	2A	2612	C
1	2A	2629	A
1	2A	2630	G
1	2A	2634	G
1	2A	2654	A
1	2A	2669	G
1	2A	2686	G
1	2A	2689	U
1	2A	2690	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	2A	2702	U
1	2A	2703	C
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2726	U
1	2A	2733	A
1	2A	2751	G
1	2A	2758	A
1	2A	2764	A
1	2A	2765	A
1	2A	2778	A
1	2A	2793	G
1	2A	2802	G
1	2A	2803	C
1	2A	2804	C
1	2A	2807	G
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2833	G
1	2A	2839	G
1	2A	2872	G
1	2A	2873	A
1	2A	2879	C
1	2A	2894	G
1	2A	2897	U
2	2B	2	C
2	2B	4	C
2	2B	5	C
2	2B	8	U
2	2B	13	A
2	2B	19	G
2	2B	23	G
2	2B	30	C
2	2B	34	U
2	2B	38	C
2	2B	42	C
2	2B	53	A
2	2B	56	G
2	2B	57	A
2	2B	63	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2B	67	G
2	2B	73	A
2	2B	74	U
2	2B	75	G
2	2B	85	G
2	2B	106	G
2	2B	108	U
2	2B	109	C
2	2B	110	G
2	2B	114	C
2	2B	116	G
2	2B	119	G
2	2B	120	A
32	2a	6	G
32	2a	9	G
32	2a	13	U
32	2a	15	G
32	2a	32	A
32	2a	39	G
32	2a	47	C
32	2a	48	C
32	2a	50	A
32	2a	51	A
32	2a	66	G
32	2a	73	G
32	2a	79	G
32	2a	80	G
32	2a	89	C
32	2a	98	G
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	152	A
32	2a	156	G
32	2a	163	C
32	2a	174	C
32	2a	182	U
32	2a	189(E)	U
32	2a	189(F)	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	195	A
32	2a	196	A
32	2a	197	A
32	2a	201	C
32	2a	202	U
32	2a	203	U
32	2a	204	U
32	2a	216	G
32	2a	247	G
32	2a	251	G
32	2a	258	G
32	2a	266	G
32	2a	267	C
32	2a	281	G
32	2a	289	G
32	2a	318	G
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	350	G
32	2a	351	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	365	U
32	2a	367	U
32	2a	372	C
32	2a	373	A
32	2a	381	C
32	2a	384	G
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	412	A
32	2a	413	G
32	2a	421	U
32	2a	423	G
32	2a	424	G
32	2a	429	U
32	2a	441	A
32	2a	442	C
32	2a	443	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	452	A
32	2a	461	A
32	2a	470	C
32	2a	477	A
32	2a	484	G
32	2a	485	G
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	510	A
32	2a	511	C
32	2a	518	C
32	2a	524	G
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	564	C
32	2a	568	G
32	2a	572	A
32	2a	573	A
32	2a	575	G
32	2a	576	G
32	2a	577	G
32	2a	588	G
32	2a	596	C
32	2a	630	G
32	2a	653	A
32	2a	656	C
32	2a	665	A
32	2a	672	U
32	2a	688	G
32	2a	695	A
32	2a	702	A
32	2a	703	G
32	2a	721	G
32	2a	723	U
32	2a	724	G
32	2a	731	G
32	2a	749	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	755	G
32	2a	777	A
32	2a	793	U
32	2a	794	A
32	2a	816	A
32	2a	817	C
32	2a	821	G
32	2a	828	A
32	2a	833	U
32	2a	838	G
32	2a	840	C
32	2a	841	U
32	2a	853	G
32	2a	859	A
32	2a	873	A
32	2a	881	G
32	2a	885	G
32	2a	902	G
32	2a	914	A
32	2a	926	G
32	2a	927	G
32	2a	930	C
32	2a	931	C
32	2a	932	C
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	984	C
32	2a	989	C
32	2a	992	U
32	2a	993	G
32	2a	997	U
32	2a	999	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1001	A
32	2a	1001(A)	G
32	2a	1002	G
32	2a	1003	G
32	2a	1005	A
32	2a	1006	C
32	2a	1009	G
32	2a	1016	A
32	2a	1020	U
32	2a	1021	G
32	2a	1022	G
32	2a	1023	G
32	2a	1025	U
32	2a	1026	G
32	2a	1027	C
32	2a	1029	C
32	2a	1030(A)	G
32	2a	1031	G
32	2a	1032	G
32	2a	1033	G
32	2a	1034	G
32	2a	1036	G
32	2a	1037	C
32	2a	1038	C
32	2a	1039	C
32	2a	1040	U
32	2a	1045	C
32	2a	1055	A
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1077	G
32	2a	1079	G
32	2a	1081	G
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A
32	2a	1108	G
32	2a	1113	C
32	2a	1115	C
32	2a	1117	G
32	2a	1121	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1122	U
32	2a	1125	U
32	2a	1129	C
32	2a	1130	A
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1146	A
32	2a	1147	C
32	2a	1152	A
32	2a	1154	G
32	2a	1157	A
32	2a	1158	C
32	2a	1159	U
32	2a	1160	G
32	2a	1161	C
32	2a	1163	C
32	2a	1172	C
32	2a	1182	G
32	2a	1183	A
32	2a	1184	G
32	2a	1191	A
32	2a	1192	C
32	2a	1196	U
32	2a	1197	G
32	2a	1202	G
32	2a	1204	A
32	2a	1209	C
32	2a	1211	U
32	2a	1212	U
32	2a	1213	A
32	2a	1214	C
32	2a	1227	A
32	2a	1236	A
32	2a	1238	A
32	2a	1240	U
32	2a	1241	G
32	2a	1256	A
32	2a	1257	U
32	2a	1260	C
32	2a	1262	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1264	C
32	2a	1267	C
32	2a	1270	C
32	2a	1272	G
32	2a	1273	G
32	2a	1277	C
32	2a	1278	U
32	2a	1279	A
32	2a	1280	A
32	2a	1286	A
32	2a	1287	A
32	2a	1290	G
32	2a	1294	G
32	2a	1302	U
32	2a	1303	C
32	2a	1305	G
32	2a	1313	U
32	2a	1319	A
32	2a	1320	C
32	2a	1323	G
32	2a	1340	A
32	2a	1346	A
32	2a	1347	G
32	2a	1358	U
32	2a	1363	C
32	2a	1364	U
32	2a	1368	G
32	2a	1370	G
32	2a	1378	C
32	2a	1402	4OC
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	1457	G
32	2a	1492	A
32	2a	1494	G
32	2a	1504	G
32	2a	1506	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2a	1507	A
32	2a	1508	G
32	2a	1517	G
32	2a	1519	MA6
32	2a	1520	G
32	2a	1529	G
32	2a	1530	G
32	2a	1531	A
32	2a	1532	U
53	2v	13	A
53	2v	15	A
53	2v	19	U
54	2w	3	C
54	2w	5	G
54	2w	8	4SU
54	2w	13	C
54	2w	14	A
54	2w	19	G
54	2w	22	G
54	2w	26	A
54	2w	29	G
54	2w	38	A
54	2w	46	7MG
54	2w	47	U
54	2w	48	C
54	2w	62	C
54	2w	64	A
54	2w	66	U
54	2w	68	C
54	2w	69	G
54	2w	70	G
54	2w	73	A
55	2x	9	G
55	2x	18	G
55	2x	21	A
55	2x	22	G
55	2x	47	U
55	2x	48	C
55	2x	52	G
55	2x	53	G
55	2x	61	C
55	2x	67	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
55	2x	68	C
55	2x	76	A
54	2y	5	G
54	2y	8	4SU
54	2y	13	C
54	2y	14	A
54	2y	19	G
54	2y	22	G
54	2y	27	G
54	2y	35	A
54	2y	44	G
54	2y	45	U
54	2y	46	7MG
54	2y	47	U
54	2y	48	C
54	2y	49	C
54	2y	53	G
54	2y	58	A
54	2y	61	C
54	2y	65	G
54	2y	69	G
54	2y	70	G
54	2y	73	A

All (50) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	115	G
1	1A	271	U
1	1A	302	A
1	1A	509	A
1	1A	572	A
1	1A	913	A
1	1A	941	U
1	1A	1065	U
1	1A	1067	A
1	1A	1093	G
1	1A	1201	A
1	1A	1219	A
1	1A	1220	U
1	1A	1221	G
1	1A	1255	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1A	1321	A
1	1A	1466	U
1	1A	1554	A
1	1A	1654	A
1	1A	1700	G
1	1A	1710	C
1	1A	2014	G
1	1A	2156	A
1	1A	2203	G
1	1A	2205	C
1	1A	2418	U
1	1A	2641	A
1	1A	2701	U
1	1A	2769	U
2	1B	1	U
1	2A	195	A
1	2A	228	A
1	2A	266	G
1	2A	271(K)	U
1	2A	271(M)	G
1	2A	277	C
1	2A	528	A
1	2A	752	A
1	2A	827	U
1	2A	856	C
1	2A	900	A
1	2A	1210	A
1	2A	1379	A
1	2A	1420	U
1	2A	1442	G
1	2A	1530	C
1	2A	1653	G
1	2A	1913	A
1	2A	1992	G
1	2A	2689	U

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	5MU	2x	54	55	19,22,23	1.41	5 (26%)	27,32,35	2.19	6 (22%)
32	PSU	1a	516	56,32	18,21,22	1.38	2 (11%)	21,30,33	2.05	5 (23%)
1	5MC	2A	1942	1	19,22,23	1.67	3 (15%)	26,32,35	1.13	2 (7%)
54	5MU	2y	54	54	19,22,23	1.46	5 (26%)	27,32,35	1.75	8 (29%)
32	UR3	1a	1498	32	19,22,23	0.99	1 (5%)	26,32,35	1.67	2 (7%)
54	PSU	1w	55	54	18,21,22	1.39	2 (11%)	21,30,33	2.05	3 (14%)
32	MA6	2a	1519	32	23,26,27	1.57	4 (17%)	33,38,41	2.29	11 (33%)
54	PSU	2w	55	54	18,21,22	1.39	2 (11%)	21,30,33	2.02	3 (14%)
32	5MC	2a	1404	32	19,22,23	1.69	3 (15%)	26,32,35	1.21	3 (11%)
32	2MG	1a	1207	32	23,26,27	1.26	4 (17%)	33,38,41	2.11	5 (15%)
1	PSU	2A	1917	1	18,21,22	1.35	2 (11%)	21,30,33	2.02	4 (19%)
32	5MC	2a	967	32	19,22,23	1.72	3 (15%)	26,32,35	1.11	2 (7%)
54	PSU	1w	32	54	18,21,22	1.37	2 (11%)	21,30,33	1.93	3 (14%)
32	4OC	1a	1402	32	20,23,24	0.74	0	25,32,35	0.92	1 (4%)
55	5MC	1x	32	55	19,22,23	1.72	3 (15%)	26,32,35	1.15	2 (7%)
32	5MC	2a	1407	32	19,22,23	1.55	3 (15%)	26,32,35	1.15	3 (11%)
54	7MG	1y	46	54	23,26,27	1.35	3 (13%)	27,39,42	2.73	6 (22%)
54	PSU	2w	39	54	18,21,22	1.37	2 (11%)	21,30,33	1.89	3 (14%)
1	2MU	2A	2552	56,1	19,22,24	1.29	4 (21%)	25,31,36	1.79	5 (20%)
32	2MG	2a	1207	32	23,26,27	1.25	3 (13%)	33,38,41	2.20	7 (21%)
1	PSU	1A	2617	56,1	18,21,22	1.36	2 (11%)	21,30,33	1.96	3 (14%)
54	MIA	1w	37	54	28,31,32	2.34	6 (21%)	38,44,47	2.77	13 (34%)
32	5MC	1a	1400	32	19,22,23	1.67	3 (15%)	26,32,35	1.16	3 (11%)
54	4SU	1w	8	54	18,21,22	1.88	5 (27%)	25,30,33	2.01	5 (20%)
54	4SU	2y	8	56,54	18,21,22	1.86	5 (27%)	25,30,33	2.16	4 (16%)
54	5MU	1w	54	54	19,22,23	1.40	5 (26%)	27,32,35	2.01	6 (22%)
54	7MG	2w	46	54	23,26,27	1.34	4 (17%)	27,39,42	2.63	7 (25%)
54	7MG	1w	46	54	23,26,27	1.41	3 (13%)	27,39,42	2.60	7 (25%)
1	5MC	1A	1984	1	19,22,23	1.66	3 (15%)	26,32,35	1.10	2 (7%)
1	4OC	1A	1942	1	19,22,24	0.79	0	25,31,35	0.98	1 (4%)
54	PSU	2w	32	54	18,21,22	1.34	2 (11%)	21,30,33	2.00	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	2MA	1A	2515	56,1	22,25,26	1.42	5 (22%)	32,37,40	2.30	9 (28%)
54	PSU	1y	39	54	18,21,22	1.35	2 (11%)	21,30,33	2.11	3 (14%)
54	5MU	1y	54	54	19,22,23	1.44	6 (31%)	27,32,35	2.06	7 (25%)
54	MIA	1y	37	54	21,24,32	1.60	4 (19%)	30,35,47	2.00	8 (26%)
1	PSU	1A	1933	1	18,21,22	1.37	2 (11%)	21,30,33	2.01	3 (14%)
1	OMG	1A	2263	56,1,55	23,26,27	1.21	3 (13%)	32,38,41	2.05	6 (18%)
55	5MU	1x	54	56,55	19,22,23	1.38	5 (26%)	27,32,35	1.97	7 (25%)
54	7MG	2y	46	54	23,26,27	1.34	3 (13%)	27,39,42	2.79	7 (25%)
1	PSU	2A	2605	1	18,21,22	1.36	3 (16%)	21,30,33	2.02	4 (19%)
32	5MC	1a	1404	32	19,22,23	1.71	3 (15%)	26,32,35	1.13	2 (7%)
54	PSU	2y	32	54	18,21,22	1.38	2 (11%)	21,30,33	1.97	3 (14%)
1	OMG	2A	2251	56,1,55	23,26,27	1.21	3 (13%)	32,38,41	1.99	5 (15%)
54	MIA	2y	37	54	21,24,32	1.58	4 (19%)	30,35,47	2.04	8 (26%)
54	5MU	2w	54	54	19,22,23	1.36	5 (26%)	27,32,35	2.00	7 (25%)
43	0TD	2l	92	43	8,9,10	4.62	1 (12%)	6,11,13	5.22	3 (50%)
32	MA6	1a	1519	32	23,26,27	1.57	4 (17%)	33,38,41	2.32	11 (33%)
32	UR3	2a	1498	32	19,22,23	1.03	1 (5%)	26,32,35	1.83	2 (7%)
32	MA6	1a	1518	32	23,26,27	1.52	5 (21%)	33,38,41	2.31	14 (42%)
1	2MA	2A	2503	56,1	22,25,26	1.49	4 (18%)	32,37,40	2.26	9 (28%)
1	5MU	2A	1939	56,1	19,22,23	1.41	6 (31%)	27,32,35	2.14	6 (22%)
32	MA6	2a	1518	32	23,26,27	1.58	4 (17%)	33,38,41	2.29	13 (39%)
1	5MU	2A	1915	1	19,22,23	1.47	6 (31%)	27,32,35	2.09	6 (22%)
54	PSU	1w	39	54	18,21,22	1.33	2 (11%)	21,30,33	2.07	3 (14%)
55	PSU	2x	55	56,55	18,21,22	1.37	2 (11%)	21,30,33	2.03	3 (14%)
55	4SU	2x	8	55	18,21,22	2.02	6 (33%)	25,30,33	1.74	6 (24%)
54	PSU	2y	55	54	18,21,22	1.36	2 (11%)	21,30,33	2.06	4 (19%)
54	4SU	1y	8	54	18,21,22	1.77	4 (22%)	25,30,33	2.21	4 (16%)
1	2MU	1A	2564	56,1	19,22,24	1.31	3 (15%)	25,31,36	1.85	6 (24%)
55	5MC	2x	32	55	19,22,23	1.67	3 (15%)	26,32,35	1.21	3 (11%)
1	5MU	1A	1937	1	19,22,23	1.43	6 (31%)	27,32,35	2.05	6 (22%)
1	PSU	1A	1939	1	18,21,22	1.36	2 (11%)	21,30,33	2.05	4 (19%)
55	4SU	1x	8	55	18,21,22	2.10	5 (27%)	25,30,33	1.66	5 (20%)
1	PSU	2A	1911	1	18,21,22	1.34	2 (11%)	21,30,33	1.99	3 (14%)
32	PSU	2a	516	32	18,21,22	1.35	2 (11%)	21,30,33	1.99	4 (19%)
1	5MU	1A	1961	56,1	19,22,23	1.42	6 (31%)	27,32,35	2.21	6 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	5MC	1a	1407	32	19,22,23	1.61	3 (15%)	26,32,35	1.14	2 (7%)
32	M2G	1a	966	32	24,27,28	1.32	4 (16%)	33,40,43	1.89	6 (18%)
1	4OC	2A	1920	1	19,22,24	0.78	0	25,31,35	0.87	0
43	0TD	1l	92	43	8,9,10	4.51	1 (12%)	6,11,13	4.77	2 (33%)
54	4SU	2w	8	54	18,21,22	1.80	4 (22%)	25,30,33	2.40	5 (20%)
32	7MG	1a	527	56,32	23,26,27	1.33	3 (13%)	27,39,42	2.59	7 (25%)
54	MIA	2w	37	54	24,27,32	2.05	5 (20%)	32,39,47	2.36	10 (31%)
54	PSU	1y	32	54	18,21,22	1.37	2 (11%)	21,30,33	1.98	3 (14%)
1	5MC	2A	1962	56,1	19,22,23	1.64	3 (15%)	26,32,35	1.08	2 (7%)
54	PSU	2y	39	54	18,21,22	1.28	2 (11%)	21,30,33	2.19	4 (19%)
32	7MG	2a	527	56,32	23,26,27	1.33	3 (13%)	27,39,42	2.63	7 (25%)
1	5MC	1A	1964	56,1	19,22,23	1.49	3 (15%)	26,32,35	1.11	2 (7%)
32	M2G	2a	966	32	24,27,28	1.29	4 (16%)	33,40,43	1.88	6 (18%)
32	5MC	1a	967	32	19,22,23	1.64	3 (15%)	26,32,35	1.19	4 (15%)
32	5MC	2a	1400	32	19,22,23	1.63	3 (15%)	26,32,35	1.15	2 (7%)
54	PSU	1y	55	54	18,21,22	1.39	2 (11%)	21,30,33	2.07	3 (14%)
55	PSU	1x	55	55	18,21,22	1.38	2 (11%)	21,30,33	2.05	3 (14%)
32	4OC	2a	1402	32	20,23,24	0.79	0	25,32,35	1.06	2 (8%)

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
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	56,32	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
54	5MU	2y	54	54	-	0/7/25/26	0/2/2/2
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
32	MA6	2a	1519	32	-	5/11/29/30	0/3/3/3
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	1/9/27/28	0/3/3/3
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	1/7/25/26	0/2/2/2
54	PSU	1w	32	54	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	4OC	1a	1402	32	-	1/9/29/30	0/2/2/2
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
54	7MG	1y	46	54	-	2/7/37/38	0/3/3/3
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
1	2MU	2A	2552	56,1	-	0/9/27/28	0/2/2/2
32	2MG	2a	1207	32	-	2/9/27/28	0/3/3/3
1	PSU	1A	2617	56,1	-	0/7/25/26	0/2/2/2
54	MIA	1w	37	54	-	1/15/33/34	0/3/3/3
32	5MC	1a	1400	32	-	0/7/25/26	0/2/2/2
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
54	4SU	2y	8	56,54	-	2/7/25/26	0/2/2/2
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
54	7MG	2w	46	54	-	4/7/37/38	0/3/3/3
54	7MG	1w	46	54	-	3/7/37/38	0/3/3/3
1	5MC	1A	1984	1	-	0/7/25/26	0/2/2/2
1	4OC	1A	1942	1	-	1/9/27/30	0/2/2/2
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
1	2MA	1A	2515	56,1	-	1/7/25/26	0/3/3/3
54	PSU	1y	39	54	-	0/7/25/26	0/2/2/2
54	5MU	1y	54	54	-	0/7/25/26	0/2/2/2
54	MIA	1y	37	54	-	2/7/25/34	0/3/3/3
1	PSU	1A	1933	1	-	0/7/25/26	0/2/2/2
1	OMG	1A	2263	56,1,55	-	0/9/27/28	0/3/3/3
55	5MU	1x	54	56,55	-	0/7/25/26	0/2/2/2
54	7MG	2y	46	54	-	3/7/37/38	0/3/3/3
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
54	PSU	2y	32	54	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	56,1,55	-	1/9/27/28	0/3/3/3
54	MIA	2y	37	54	-	2/7/25/34	0/3/3/3
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	2/7/12/14	-
32	MA6	1a	1519	32	-	3/11/29/30	0/3/3/3
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
32	MA6	1a	1518	32	-	2/11/29/30	0/3/3/3
1	2MA	2A	2503	56,1	-	2/7/25/26	0/3/3/3
1	5MU	2A	1939	56,1	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	2/11/29/30	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
54	PSU	1w	39	54	-	0/7/25/26	0/2/2/2
55	PSU	2x	55	56,55	-	0/7/25/26	0/2/2/2
55	4SU	2x	8	55	-	1/7/25/26	0/2/2/2
54	PSU	2y	55	54	-	2/7/25/26	0/2/2/2
54	4SU	1y	8	54	-	3/7/25/26	0/2/2/2
1	2MU	1A	2564	56,1	-	0/9/27/28	0/2/2/2
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
1	5MU	1A	1937	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	1939	1	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
1	5MU	1A	1961	56,1	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/11/29/30	0/3/3/3
1	4OC	2A	1920	1	-	2/9/27/30	0/2/2/2
43	0TD	1l	92	43	-	3/7/12/14	-
54	4SU	2w	8	54	-	1/7/25/26	0/2/2/2
32	7MG	1a	527	56,32	-	2/7/37/38	0/3/3/3
54	MIA	2w	37	54	-	2/11/29/34	0/3/3/3
54	PSU	1y	32	54	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	56,1	-	0/7/25/26	0/2/2/2
54	PSU	2y	39	54	-	0/7/25/26	0/2/2/2
32	7MG	2a	527	56,32	-	2/7/37/38	0/3/3/3
1	5MC	1A	1964	56,1	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/11/29/30	0/3/3/3
32	5MC	1a	967	32	-	2/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
54	PSU	1y	55	54	-	2/7/25/26	0/2/2/2
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32	-	2/9/29/30	0/2/2/2

All (267) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-12.73	1.69	1.82
43	1l	92	0TD	CB-SB	-12.32	1.69	1.82
54	1w	37	MIA	C2-S10	-7.04	1.69	1.75
54	1w	37	MIA	C13-C14	6.84	1.52	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2w	37	MIA	C2-S10	-6.73	1.70	1.75
32	2a	967	5MC	C5-C4	6.32	1.48	1.44
55	1x	32	5MC	C5-C4	6.29	1.48	1.44
32	1a	1404	5MC	C5-C4	6.29	1.48	1.44
32	2a	1404	5MC	C5-C4	6.15	1.48	1.44
1	2A	1942	5MC	C5-C4	6.09	1.48	1.44
32	1a	1400	5MC	C5-C4	6.03	1.48	1.44
1	1A	1984	5MC	C5-C4	6.00	1.48	1.44
55	2x	32	5MC	C5-C4	5.94	1.48	1.44
32	1a	1407	5MC	C5-C4	5.93	1.48	1.44
32	1a	967	5MC	C5-C4	5.89	1.48	1.44
32	2a	1400	5MC	C5-C4	5.88	1.48	1.44
1	2A	1962	5MC	C5-C4	5.87	1.48	1.44
32	2a	1407	5MC	C5-C4	5.45	1.48	1.44
1	1A	1964	5MC	C5-C4	5.22	1.48	1.44
54	2y	8	4SU	C4-S4	-5.06	1.59	1.68
32	2a	1518	MA6	C5-C4	5.02	1.48	1.39
54	1w	8	4SU	C4-S4	-4.96	1.59	1.68
32	2a	1519	MA6	C5-C4	4.94	1.47	1.39
54	2y	37	MIA	C5-C4	4.92	1.47	1.39
54	2w	8	4SU	C4-S4	-4.92	1.60	1.68
55	1x	8	4SU	C4-S4	-4.90	1.60	1.68
55	2x	8	4SU	C4-S4	-4.90	1.60	1.68
32	1a	1519	MA6	C5-C4	4.90	1.47	1.39
54	1y	37	MIA	C5-C4	4.89	1.47	1.39
54	1w	37	MIA	C5-C4	4.88	1.47	1.39
54	1y	8	4SU	C4-S4	-4.77	1.60	1.68
54	2w	37	MIA	C5-C4	4.76	1.47	1.39
32	1a	1518	MA6	C5-C4	4.64	1.47	1.39
1	2A	2503	2MA	C5-C4	4.48	1.47	1.39
55	1x	8	4SU	C4-N3	-4.43	1.33	1.37
1	1A	2515	2MA	C5-C4	4.22	1.46	1.39
55	2x	8	4SU	C4-N3	-4.11	1.33	1.37
54	2w	55	PSU	C6-C5	3.85	1.39	1.35
54	1w	55	PSU	C6-C5	3.84	1.39	1.35
54	1y	32	PSU	C6-C5	3.76	1.39	1.35
54	2y	32	PSU	C6-C5	3.68	1.39	1.35
54	2y	55	PSU	C6-C5	3.66	1.39	1.35
54	1y	55	PSU	C6-C5	3.64	1.39	1.35
54	2y	46	7MG	C5-C4	3.61	1.48	1.37
55	1x	55	PSU	C6-C5	3.59	1.39	1.35
54	2w	39	PSU	C6-C5	3.59	1.39	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1y	46	7MG	C5-C4	3.56	1.48	1.37
54	1y	39	PSU	C6-C5	3.54	1.39	1.35
55	2x	55	PSU	C6-C5	3.54	1.39	1.35
1	1A	1939	PSU	C6-C5	3.53	1.39	1.35
32	2a	516	PSU	C6-C5	3.49	1.39	1.35
54	2w	32	PSU	C6-C5	3.47	1.39	1.35
1	1A	1933	PSU	C6-C5	3.45	1.39	1.35
1	2A	1911	PSU	C6-C5	3.43	1.39	1.35
1	2A	1917	PSU	C6-C5	3.43	1.39	1.35
54	1w	46	7MG	C5-C4	3.42	1.48	1.37
54	1w	39	PSU	C6-C5	3.42	1.39	1.35
32	1a	527	7MG	C5-C4	3.41	1.48	1.37
54	1w	32	PSU	C6-C5	3.41	1.39	1.35
32	1a	516	PSU	C6-C5	3.40	1.39	1.35
54	1w	8	4SU	C4-N3	-3.39	1.34	1.37
55	1x	8	4SU	C5-C4	-3.34	1.38	1.42
54	2w	46	7MG	C5-C4	3.32	1.47	1.37
1	1A	2263	OMG	C5-C4	3.31	1.47	1.38
1	2A	2605	PSU	C6-C5	3.30	1.38	1.35
55	1x	8	4SU	C2-N3	-3.30	1.32	1.38
54	2y	39	PSU	C6-C5	3.30	1.38	1.35
54	1w	46	7MG	C4-N9	-3.29	1.33	1.37
32	2a	527	7MG	C5-C4	3.27	1.47	1.37
55	2x	8	4SU	C5-C4	-3.25	1.38	1.42
1	2A	2251	OMG	C5-C4	3.25	1.47	1.38
54	2y	8	4SU	C4-N3	-3.23	1.34	1.37
54	1y	8	4SU	C4-N3	-3.21	1.34	1.37
32	2a	966	M2G	C5-C4	3.21	1.47	1.38
32	2a	1207	2MG	C5-C4	3.20	1.47	1.38
1	1A	2617	PSU	C6-C5	3.16	1.38	1.35
32	2a	1518	MA6	C5-C6	3.15	1.49	1.41
32	1a	1207	2MG	C5-C4	3.13	1.47	1.38
32	1a	966	M2G	C5-C4	3.11	1.47	1.38
1	2A	1915	5MU	C6-C5	3.09	1.39	1.34
32	2a	1519	MA6	C5-C6	3.05	1.49	1.41
1	1A	2564	2MU	C4-N3	-3.04	1.33	1.38
32	1a	1519	MA6	C5-C6	2.99	1.49	1.41
32	1a	1518	MA6	C5-C6	2.97	1.49	1.41
32	1a	966	M2G	C2-N2	2.96	1.40	1.35
32	2a	527	7MG	C4-N9	-2.95	1.34	1.37
54	2w	46	7MG	C4-N9	-2.94	1.34	1.37
54	2y	37	MIA	C5-C6	2.94	1.49	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2a	1404	5MC	C6-C5	2.93	1.39	1.34
55	2x	32	5MC	C6-C5	2.91	1.39	1.34
55	1x	32	5MC	C6-C5	2.91	1.39	1.34
54	1y	54	5MU	C6-C5	2.91	1.39	1.34
54	1y	37	MIA	C5-C6	2.90	1.49	1.41
54	2w	8	4SU	C4-N3	-2.88	1.34	1.37
54	2y	8	4SU	C5-C4	-2.86	1.39	1.42
1	1A	1937	5MU	C6-C5	2.86	1.39	1.34
1	1A	1961	5MU	C4-N3	-2.85	1.33	1.38
55	2x	54	5MU	C6-C5	2.84	1.39	1.34
32	1a	1404	5MC	C6-C5	2.83	1.39	1.34
1	1A	1961	5MU	C6-C5	2.82	1.39	1.34
32	1a	1400	5MC	C6-C5	2.82	1.39	1.34
54	1w	8	4SU	C5-C4	-2.81	1.39	1.42
54	1w	54	5MU	C6-C5	2.80	1.39	1.34
32	2a	967	5MC	C6-C5	2.80	1.39	1.34
54	1w	37	MIA	C5-C6	2.80	1.48	1.41
54	2w	8	4SU	C5-C4	-2.78	1.39	1.42
1	2A	2552	2MU	C4-N3	-2.77	1.33	1.38
1	1A	1984	5MC	C6-C5	2.77	1.39	1.34
54	2y	54	5MU	C6-C5	2.77	1.39	1.34
1	2A	1962	5MC	C6-C5	2.76	1.39	1.34
1	2A	2605	PSU	C4-N3	-2.76	1.33	1.38
1	2A	1942	5MC	C6-C5	2.75	1.39	1.34
54	2w	54	5MU	C6-C5	2.74	1.39	1.34
54	2w	37	MIA	C5-C6	2.74	1.48	1.41
1	2A	1939	5MU	C6-C5	2.74	1.39	1.34
32	1a	967	5MC	C6-C5	2.72	1.39	1.34
32	1a	527	7MG	C4-N9	-2.72	1.34	1.37
1	1A	2617	PSU	C4-N3	-2.71	1.33	1.38
54	2y	54	5MU	C2-N1	2.71	1.42	1.38
32	2a	966	M2G	C2-N2	2.71	1.40	1.35
32	2a	1400	5MC	C6-C5	2.70	1.39	1.34
1	2A	1939	5MU	C4-N3	-2.68	1.33	1.38
1	2A	2503	2MA	C5-C6	2.67	1.48	1.41
1	2A	1915	5MU	C4-N3	-2.66	1.33	1.38
1	1A	1964	5MC	C6-C5	2.65	1.38	1.34
54	2y	54	5MU	C4-N3	-2.65	1.33	1.38
54	1y	54	5MU	C4-N3	-2.64	1.33	1.38
1	2A	1915	5MU	C4-C5	2.63	1.49	1.44
55	1x	54	5MU	C6-C5	2.62	1.38	1.34
32	2a	1407	5MC	C6-C5	2.60	1.38	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1a	516	PSU	C4-N3	-2.60	1.34	1.38
1	1A	1937	5MU	C4-N3	-2.60	1.34	1.38
54	1w	54	5MU	C4-N3	-2.58	1.34	1.38
1	1A	1933	PSU	C4-N3	-2.58	1.34	1.38
54	2w	8	4SU	C2-N1	2.57	1.42	1.38
1	1A	1939	PSU	C4-N3	-2.56	1.34	1.38
32	1a	966	M2G	C6-N1	-2.56	1.34	1.38
55	1x	54	5MU	C4-N3	-2.56	1.34	1.38
54	1w	46	7MG	C6-N1	-2.56	1.34	1.38
32	1a	1207	2MG	C6-N1	-2.55	1.34	1.38
54	1w	32	PSU	C4-N3	-2.54	1.34	1.38
54	2y	55	PSU	C4-N3	-2.53	1.34	1.38
54	2w	39	PSU	C4-N3	-2.53	1.34	1.38
54	1y	55	PSU	C4-N3	-2.53	1.34	1.38
55	2x	8	4SU	C2-N3	-2.52	1.33	1.38
1	2A	1917	PSU	C4-N3	-2.52	1.34	1.38
54	1y	54	5MU	C4-C5	2.52	1.48	1.44
1	2A	2503	2MA	C8-N7	2.52	1.36	1.31
32	1a	1407	5MC	C6-C5	2.51	1.38	1.34
55	2x	54	5MU	C4-N3	-2.51	1.34	1.38
54	1y	39	PSU	C4-N3	-2.50	1.34	1.38
1	1A	1937	5MU	C2-N1	2.50	1.42	1.38
1	2A	2251	OMG	C6-N1	-2.49	1.34	1.38
1	2A	1911	PSU	C4-N3	-2.49	1.34	1.38
1	1A	2515	2MA	C5-C6	2.48	1.47	1.41
55	2x	55	PSU	C4-N3	-2.48	1.34	1.38
54	2w	55	PSU	C4-N3	-2.46	1.34	1.38
54	2y	37	MIA	C8-N7	2.45	1.36	1.31
54	1y	8	4SU	C5-C4	-2.45	1.39	1.42
55	2x	54	5MU	C4-C5	2.44	1.48	1.44
54	2w	32	PSU	C4-N3	-2.44	1.34	1.38
32	2a	966	M2G	C6-N1	-2.43	1.34	1.38
54	1y	32	PSU	C4-N3	-2.42	1.34	1.38
54	1y	37	MIA	C8-N7	2.42	1.36	1.31
54	1w	39	PSU	C4-N3	-2.41	1.34	1.38
54	1w	54	5MU	C4-C5	2.41	1.48	1.44
32	2a	516	PSU	C4-N3	-2.41	1.34	1.38
54	2w	54	5MU	C4-N3	-2.41	1.34	1.38
54	2w	54	5MU	C4-C5	2.40	1.48	1.44
1	1A	1961	5MU	C2-N3	-2.40	1.33	1.38
54	1y	46	7MG	C6-N1	-2.39	1.34	1.38
55	1x	55	PSU	C4-N3	-2.39	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1937	5MU	C4-C5	2.39	1.48	1.44
55	2x	8	4SU	C2-N1	2.39	1.42	1.38
54	2y	32	PSU	C4-N3	-2.39	1.34	1.38
54	2w	37	MIA	C8-N7	2.39	1.36	1.31
54	2y	46	7MG	C6-N1	-2.38	1.34	1.38
1	2A	2552	2MU	C5-C4	2.38	1.48	1.43
1	1A	2564	2MU	C2-N3	-2.38	1.33	1.38
1	2A	1915	5MU	C2-N1	2.38	1.42	1.38
1	2A	2503	2MA	C5-N7	-2.35	1.34	1.39
1	1A	2263	OMG	C6-N1	-2.34	1.34	1.38
55	2x	54	5MU	C2-N1	2.33	1.42	1.38
1	2A	1939	5MU	C4-C5	2.33	1.48	1.44
54	1w	55	PSU	C4-N3	-2.32	1.34	1.38
1	1A	1984	5MC	C6-N1	-2.30	1.34	1.38
1	2A	1939	5MU	C6-N1	-2.30	1.34	1.38
1	1A	2564	2MU	C5-C4	2.30	1.48	1.43
32	2a	1207	2MG	C6-N1	-2.30	1.34	1.38
55	1x	54	5MU	C2-N1	2.30	1.42	1.38
54	2y	54	5MU	C4-C5	2.30	1.48	1.44
32	2a	527	7MG	C6-N1	-2.29	1.34	1.38
32	2a	1518	MA6	C8-N7	2.29	1.36	1.31
32	1a	1519	MA6	C5-N7	-2.28	1.34	1.39
55	1x	54	5MU	C4-C5	2.28	1.48	1.44
32	1a	1519	MA6	C8-N7	2.27	1.36	1.31
32	2a	1400	5MC	C6-N1	-2.27	1.34	1.38
54	1w	8	4SU	C2-N1	2.25	1.42	1.38
54	2y	8	4SU	C2-N1	2.25	1.42	1.38
54	1y	54	5MU	C2-N1	2.25	1.42	1.38
54	2w	37	MIA	C5-N7	-2.25	1.35	1.39
54	1y	8	4SU	C2-N1	2.24	1.42	1.38
54	1w	37	MIA	C8-N7	2.24	1.36	1.31
32	1a	527	7MG	C6-N1	-2.23	1.34	1.38
54	1w	37	MIA	C5-N7	-2.23	1.35	1.39
1	1A	2515	2MA	C5-N7	-2.23	1.35	1.39
32	2a	1498	UR3	C2-N1	2.23	1.41	1.38
32	2a	1519	MA6	C8-N7	2.23	1.36	1.31
32	1a	967	5MC	C6-N1	-2.22	1.34	1.38
32	1a	1407	5MC	C6-N1	-2.22	1.34	1.38
32	1a	1518	MA6	C8-N7	2.22	1.35	1.31
54	2y	39	PSU	C4-N3	-2.21	1.34	1.38
1	2A	1962	5MC	C6-N1	-2.21	1.34	1.38
32	2a	1407	5MC	C6-N1	-2.21	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2a	1207	2MG	C2-N3	2.20	1.36	1.32
1	1A	1961	5MU	C6-N1	-2.20	1.34	1.38
54	1y	37	MIA	C5-N7	-2.19	1.35	1.39
1	1A	1961	5MU	C4-C5	2.19	1.48	1.44
1	1A	1964	5MC	C6-N1	-2.19	1.34	1.38
55	1x	32	5MC	C6-N1	-2.19	1.34	1.38
54	2w	46	7MG	C8-N9	2.18	1.47	1.45
1	1A	2515	2MA	C4-N9	-2.18	1.33	1.37
1	2A	1942	5MC	C6-N1	-2.18	1.34	1.38
54	1w	8	4SU	C2-N3	-2.18	1.34	1.38
1	2A	1939	5MU	C2-N1	2.16	1.41	1.38
55	2x	54	5MU	C6-N1	-2.16	1.34	1.38
54	1w	54	5MU	C2-N1	2.16	1.41	1.38
32	1a	1404	5MC	C6-N1	-2.15	1.34	1.38
54	1y	46	7MG	C8-N9	2.15	1.47	1.45
1	1A	2263	OMG	C5-N7	-2.15	1.34	1.39
32	2a	1404	5MC	C6-N1	-2.15	1.34	1.38
54	1y	54	5MU	C6-N1	-2.15	1.34	1.38
32	1a	1400	5MC	C6-N1	-2.13	1.34	1.38
32	1a	966	M2G	C5-N7	-2.13	1.34	1.39
32	2a	1519	MA6	C5-N7	-2.13	1.35	1.39
1	2A	2251	OMG	C5-N7	-2.12	1.34	1.39
1	2A	1939	5MU	C2-N3	-2.12	1.34	1.38
55	2x	8	4SU	O2-C2	2.12	1.26	1.23
55	1x	54	5MU	C6-N1	-2.11	1.34	1.38
54	2y	46	7MG	C8-N9	2.11	1.47	1.45
1	2A	1915	5MU	C6-N1	-2.10	1.34	1.38
32	1a	1518	MA6	C5-N7	-2.10	1.35	1.39
54	1y	54	5MU	C2-N3	-2.10	1.34	1.38
1	2A	1915	5MU	C2-N3	-2.10	1.34	1.38
55	1x	8	4SU	C2-N1	2.09	1.41	1.38
1	1A	1961	5MU	C2-N1	2.09	1.41	1.38
54	2w	54	5MU	C6-N1	-2.08	1.34	1.38
54	2y	54	5MU	C2-N3	-2.07	1.34	1.38
32	1a	1207	2MG	C2-N3	2.07	1.35	1.32
54	1w	54	5MU	C6-N1	-2.06	1.34	1.38
54	2y	8	4SU	C2-N3	-2.06	1.34	1.38
32	2a	967	5MC	C6-N1	-2.05	1.34	1.38
1	1A	1937	5MU	C6-N1	-2.05	1.34	1.38
1	2A	2605	PSU	C2-N3	-2.05	1.34	1.37
54	2w	54	5MU	C2-N1	2.04	1.41	1.38
32	1a	1498	UR3	C6-C5	2.04	1.39	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1a	1518	MA6	C4-N9	-2.04	1.33	1.37
54	2w	46	7MG	C6-N1	-2.03	1.35	1.38
1	2A	2552	2MU	C2-N1	2.03	1.41	1.38
1	1A	2515	2MA	C8-N7	2.02	1.35	1.31
54	2y	37	MIA	C5-N7	-2.02	1.35	1.39
32	2a	966	M2G	C5-N7	-2.02	1.35	1.39
55	2x	32	5MC	C6-N1	-2.02	1.34	1.38
32	2a	1518	MA6	C5-N7	-2.02	1.35	1.39
1	1A	1937	5MU	C2-N3	-2.01	1.34	1.38
1	2A	2552	2MU	C2-N3	-2.01	1.34	1.38
32	1a	1207	2MG	C5-N7	-2.00	1.35	1.39

All (408) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	2l	92	0TD	CSB-SB-CB	-11.95	80.88	102.36
43	1l	92	0TD	CSB-SB-CB	-11.02	82.56	102.36
54	2y	46	7MG	N9-C4-N3	10.12	140.30	125.46
54	1y	46	7MG	N9-C4-N3	9.77	139.78	125.46
54	1w	46	7MG	N9-C4-N3	9.10	138.79	125.46
32	1a	527	7MG	N9-C4-N3	8.90	138.51	125.46
32	2a	527	7MG	N9-C4-N3	8.87	138.45	125.46
54	2w	46	7MG	N9-C4-N3	8.84	138.41	125.46
54	1w	37	MIA	C12-C13-C14	-8.71	111.38	127.01
54	1w	37	MIA	C5-C4-N3	-8.27	118.47	127.18
54	2w	37	MIA	C5-C4-N3	-7.97	118.78	127.18
1	2A	2503	2MA	C5-C4-N3	-7.95	118.81	127.18
32	2a	1498	UR3	C4-N3-C2	-7.44	118.59	124.58
1	1A	2515	2MA	C5-C4-N3	-7.43	119.35	127.18
54	2w	8	4SU	C4-N3-C2	-7.09	120.52	127.31
32	2a	1207	2MG	C2-N3-C4	7.09	120.86	112.00
32	1a	1207	2MG	C2-N3-C4	6.89	120.61	112.00
54	1y	8	4SU	C4-N3-C2	-6.78	120.81	127.31
54	2y	39	PSU	N1-C2-N3	6.64	122.17	115.17
54	1w	37	MIA	N3-C4-N9	6.62	135.40	126.99
32	1a	1498	UR3	C4-N3-C2	-6.61	119.26	124.58
54	1y	55	PSU	N1-C2-N3	6.52	122.05	115.17
54	1y	39	PSU	N1-C2-N3	6.46	121.99	115.17
54	2y	55	PSU	N1-C2-N3	6.46	121.98	115.17
1	1A	2263	OMG	C5-C4-N3	-6.45	118.12	128.39
55	1x	55	PSU	N1-C2-N3	6.44	121.96	115.17
32	1a	516	PSU	N1-C2-N3	6.44	121.96	115.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2251	OMG	C5-C4-N3	-6.40	118.21	128.39
55	2x	55	PSU	N1-C2-N3	6.37	121.89	115.17
54	1w	39	PSU	N1-C2-N3	6.36	121.87	115.17
1	1A	2515	2MA	N3-C4-N9	6.32	135.00	126.99
1	2A	1917	PSU	N1-C2-N3	6.30	121.81	115.17
54	1w	55	PSU	N1-C2-N3	6.27	121.78	115.17
1	1A	1939	PSU	N1-C2-N3	6.25	121.76	115.17
32	1a	966	M2G	C5-C4-N3	-6.25	118.45	128.39
54	2w	55	PSU	N1-C2-N3	6.24	121.75	115.17
54	2y	8	4SU	C4-N3-C2	-6.23	121.34	127.31
54	2w	32	PSU	N1-C2-N3	6.23	121.73	115.17
32	2a	516	PSU	N1-C2-N3	6.21	121.72	115.17
54	1y	32	PSU	N1-C2-N3	6.20	121.70	115.17
54	2y	32	PSU	N1-C2-N3	6.19	121.70	115.17
54	2w	37	MIA	N3-C4-N9	6.17	134.83	126.99
1	1A	1933	PSU	N1-C2-N3	6.17	121.68	115.17
1	2A	1911	PSU	N1-C2-N3	6.14	121.65	115.17
54	1w	32	PSU	N1-C2-N3	6.12	121.62	115.17
1	2A	2605	PSU	N1-C2-N3	6.10	121.61	115.17
32	2a	966	M2G	C5-C4-N3	-6.09	118.69	128.39
32	2a	1207	2MG	C5-C4-N3	-6.02	118.80	128.39
54	2y	46	7MG	C5-C4-N3	-5.99	116.88	128.13
1	1A	2617	PSU	N1-C2-N3	5.98	121.47	115.17
1	2A	2503	2MA	N3-C4-N9	5.94	134.53	126.99
54	1y	46	7MG	C5-C4-N3	-5.93	117.00	128.13
32	1a	1519	MA6	C5-C4-N3	-5.90	118.59	126.72
32	1a	1207	2MG	C5-C4-N3	-5.82	119.13	128.39
54	2y	8	4SU	C5-C4-N3	5.80	120.15	114.75
54	1y	37	MIA	C5-C4-N3	-5.79	118.74	126.72
54	2w	39	PSU	N1-C2-N3	5.79	121.27	115.17
54	2w	8	4SU	C5-C4-N3	5.77	120.12	114.75
54	2y	37	MIA	C5-C4-N3	-5.76	118.78	126.72
54	1w	8	4SU	C4-N3-C2	-5.62	121.93	127.31
32	2a	1519	MA6	C5-C4-N3	-5.59	119.02	126.72
54	1w	8	4SU	C5-C4-N3	5.58	119.94	114.75
32	1a	527	7MG	C5-C4-N3	-5.49	117.83	128.13
1	1A	1961	5MU	C4-N3-C2	-5.49	120.15	127.34
54	1y	8	4SU	C5-C4-N3	5.44	119.81	114.75
32	2a	527	7MG	N9-C8-N7	-5.43	95.68	103.37
55	2x	54	5MU	C4-N3-C2	-5.41	120.25	127.34
54	2w	46	7MG	C5-C4-N3	-5.38	118.03	128.13
1	2A	1915	5MU	N3-C2-N1	5.35	121.85	114.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	527	7MG	C5-C4-N3	-5.31	118.16	128.13
32	1a	1518	MA6	C5-C4-N3	-5.31	119.41	126.72
32	2a	1518	MA6	C5-C4-N3	-5.30	119.42	126.72
1	1A	1961	5MU	N3-C2-N1	5.28	121.77	114.89
54	2w	46	7MG	N9-C8-N7	-5.28	95.89	103.37
1	2A	1939	5MU	C4-N3-C2	-5.28	120.42	127.34
54	1w	46	7MG	N9-C8-N7	-5.28	95.90	103.37
55	2x	54	5MU	N3-C2-N1	5.27	121.76	114.89
1	2A	1915	5MU	C4-N3-C2	-5.21	120.50	127.34
1	1A	2564	2MU	N3-C2-N1	5.17	121.63	114.89
1	1A	2263	OMG	C2-N3-C4	5.17	121.20	112.30
54	1y	54	5MU	N3-C2-N1	5.07	121.50	114.89
1	2A	2251	OMG	C2-N3-C4	5.04	120.99	112.30
32	1a	527	7MG	N9-C8-N7	-5.02	96.26	103.37
54	1y	54	5MU	C4-N3-C2	-5.01	120.77	127.34
1	1A	1937	5MU	N3-C2-N1	5.01	121.41	114.89
1	2A	2552	2MU	N3-C2-N1	5.00	121.40	114.89
1	1A	1937	5MU	C4-N3-C2	-4.98	120.82	127.34
1	2A	1939	5MU	N3-C2-N1	4.96	121.35	114.89
54	1w	54	5MU	N3-C2-N1	4.95	121.33	114.89
1	1A	1961	5MU	C5-C4-N3	4.90	119.58	115.32
54	1w	54	5MU	C4-N3-C2	-4.87	120.95	127.34
54	1w	46	7MG	C5-C4-N3	-4.81	119.10	128.13
32	2a	1518	MA6	C9-N6-C6	-4.78	108.36	120.52
1	1A	2263	OMG	N9-C4-N3	4.75	135.45	125.95
54	2w	54	5MU	C4-N3-C2	-4.75	121.11	127.34
1	2A	2251	OMG	N9-C4-N3	4.74	135.43	125.95
54	2w	54	5MU	N3-C2-N1	4.73	121.05	114.89
54	1y	46	7MG	N9-C8-N7	-4.73	96.68	103.37
55	1x	54	5MU	N3-C2-N1	4.72	121.03	114.89
1	2A	1939	5MU	C5-C4-N3	4.70	119.41	115.32
54	2y	46	7MG	N9-C8-N7	-4.70	96.72	103.37
54	2y	46	7MG	C2-N3-C4	4.68	120.37	112.30
54	2y	39	PSU	C4-N3-C2	-4.67	119.94	126.37
54	1y	46	7MG	C2-N3-C4	4.65	120.30	112.30
32	1a	966	M2G	N9-C4-N3	4.62	135.20	125.95
32	2a	966	M2G	N9-C4-N3	4.62	135.19	125.95
55	1x	54	5MU	C4-N3-C2	-4.62	121.29	127.34
55	2x	8	4SU	C5-C4-N3	4.61	119.04	114.75
32	1a	966	M2G	C2-N3-C4	4.59	120.99	112.51
1	1A	2564	2MU	C4-N3-C2	-4.57	120.94	126.61
54	2w	46	7MG	C2-N3-C4	4.55	120.14	112.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2552	2MU	C4-N3-C2	-4.54	120.97	126.61
55	2x	54	5MU	C5-C4-N3	4.51	119.24	115.32
32	2a	1518	MA6	C2-N1-C6	4.50	122.82	111.83
54	2y	37	MIA	N3-C4-N9	4.49	134.81	127.17
32	2a	1519	MA6	C9-N6-C6	-4.45	109.19	120.52
32	2a	527	7MG	C2-N3-C4	4.45	119.97	112.30
32	2a	966	M2G	C2-N3-C4	4.45	120.73	112.51
54	1y	37	MIA	N3-C4-N9	4.44	134.73	127.17
32	1a	527	7MG	C2-N3-C4	4.43	119.93	112.30
32	1a	1519	MA6	N3-C4-N9	4.42	134.68	127.17
55	1x	8	4SU	C5-C4-N3	4.42	118.86	114.75
32	1a	1518	MA6	C2-N1-C6	4.41	122.61	111.83
32	2a	1518	MA6	C4-C5-N7	-4.41	105.54	110.58
1	1A	1937	5MU	C5-C4-N3	4.41	119.16	115.32
54	2w	8	4SU	C5-C4-S4	-4.37	119.32	124.31
54	1y	39	PSU	C4-N3-C2	-4.33	120.40	126.37
32	1a	1518	MA6	C9-N6-C6	-4.33	109.52	120.52
32	2a	1519	MA6	C2-N1-C6	4.32	122.39	111.83
54	1y	8	4SU	N3-C2-N1	4.32	120.52	114.89
1	2A	1915	5MU	C5-C4-N3	4.29	119.05	115.32
1	2A	2605	PSU	C4-N3-C2	-4.29	120.46	126.37
32	2a	1519	MA6	N3-C4-N9	4.28	134.45	127.17
54	1y	54	5MU	C5-C4-N3	4.25	119.02	115.32
54	2y	39	PSU	O2-C2-N1	-4.24	118.42	122.79
32	2a	1207	2MG	N9-C4-N3	4.23	134.42	125.95
54	2w	8	4SU	N3-C2-N1	4.23	120.40	114.89
32	1a	1519	MA6	C2-N1-C6	4.22	122.14	111.83
1	1A	1961	5MU	O4-C4-C5	-4.22	120.09	124.92
54	1w	39	PSU	C4-N3-C2	-4.21	120.57	126.37
1	1A	1939	PSU	C4-N3-C2	-4.20	120.58	126.37
54	1w	54	5MU	C5-C4-N3	4.20	118.97	115.32
54	2w	54	5MU	C5-C4-N3	4.18	118.96	115.32
32	1a	1207	2MG	N9-C4-N3	4.16	134.27	125.95
55	2x	54	5MU	O4-C4-C5	-4.15	120.16	124.92
1	1A	1961	5MU	C5-C6-N1	-4.15	118.80	123.31
32	1a	1519	MA6	C9-N6-C6	-4.14	109.98	120.52
54	2y	55	PSU	C4-N3-C2	-4.14	120.67	126.37
54	2y	8	4SU	C5-C4-S4	-4.13	119.59	124.31
55	2x	8	4SU	C1'-N1-C2	4.12	124.99	117.59
32	1a	516	PSU	C4-N3-C2	-4.10	120.73	126.37
1	2A	1939	5MU	O4-C4-C5	-4.09	120.24	124.92
54	2w	54	5MU	O4-C4-C5	-4.08	120.25	124.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1518	MA6	C4-C5-N7	-4.08	105.92	110.58
54	2w	32	PSU	C4-N3-C2	-4.06	120.77	126.37
54	1w	55	PSU	O2-C2-N1	-4.06	118.60	122.79
54	1y	55	PSU	O2-C2-N1	-4.06	118.60	122.79
32	1a	1518	MA6	N3-C4-N9	4.05	134.05	127.17
54	1w	37	MIA	C15-C14-C13	-4.05	110.51	122.66
32	2a	1519	MA6	C4-C5-N7	-4.04	105.96	110.58
1	2A	1917	PSU	C4-N3-C2	-4.03	120.82	126.37
32	1a	1519	MA6	C4-C5-N7	-4.00	106.01	110.58
1	1A	1933	PSU	C4-N3-C2	-4.00	120.87	126.37
55	2x	55	PSU	C4-N3-C2	-3.99	120.87	126.37
1	2A	1911	PSU	C4-N3-C2	-3.98	120.89	126.37
55	1x	54	5MU	C5-C4-N3	3.97	118.77	115.32
32	2a	516	PSU	C4-N3-C2	-3.97	120.91	126.37
54	1w	39	PSU	O2-C2-N1	-3.96	118.70	122.79
54	1y	55	PSU	C4-N3-C2	-3.94	120.95	126.37
55	1x	55	PSU	C4-N3-C2	-3.93	120.95	126.37
54	1w	46	7MG	C2-N3-C4	3.92	119.05	112.30
54	2w	55	PSU	C4-N3-C2	-3.91	120.99	126.37
55	1x	55	PSU	O2-C2-N1	-3.90	118.77	122.79
54	1y	39	PSU	O2-C2-N1	-3.89	118.78	122.79
1	1A	2617	PSU	C4-N3-C2	-3.88	121.02	126.37
54	2y	54	5MU	C5-C4-N3	3.87	118.68	115.32
54	2y	32	PSU	C4-N3-C2	-3.85	121.06	126.37
54	1w	55	PSU	C4-N3-C2	-3.85	121.07	126.37
1	2A	1915	5MU	C5-C6-N1	-3.85	119.14	123.31
54	1w	54	5MU	O4-C4-C5	-3.83	120.54	124.92
32	2a	1518	MA6	N3-C4-N9	3.81	133.65	127.17
1	1A	1937	5MU	O4-C4-C5	-3.81	120.56	124.92
54	1y	32	PSU	C4-N3-C2	-3.81	121.12	126.37
1	2A	1939	5MU	C5-C6-N1	-3.80	119.18	123.31
54	1w	37	MIA	C16-C14-C13	-3.77	111.35	122.66
54	1y	8	4SU	C5-C4-S4	-3.75	120.02	124.31
1	2A	1911	PSU	O2-C2-N1	-3.75	118.92	122.79
54	2w	55	PSU	O2-C2-N1	-3.74	118.93	122.79
55	2x	55	PSU	O2-C2-N1	-3.74	118.93	122.79
1	1A	1933	PSU	O2-C2-N1	-3.74	118.94	122.79
54	1w	32	PSU	C4-N3-C2	-3.73	121.24	126.37
54	2y	37	MIA	C2-N3-C4	3.72	120.93	111.83
55	1x	54	5MU	O4-C4-C5	-3.71	120.67	124.92
54	2w	39	PSU	C4-N3-C2	-3.71	121.26	126.37
54	1y	37	MIA	C2-N3-C4	3.69	120.85	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2y	8	4SU	N3-C2-N1	3.68	119.68	114.89
54	2y	37	MIA	C4-C5-N7	-3.68	106.38	110.58
1	1A	2515	2MA	N6-C6-N1	3.66	121.97	117.03
1	2A	1917	PSU	O2-C2-N1	-3.66	119.01	122.79
32	2a	1519	MA6	C2-N3-C4	3.66	120.76	111.83
32	1a	1519	MA6	C2-N3-C4	3.65	120.75	111.83
54	1y	32	PSU	O2-C2-N1	-3.65	119.03	122.79
1	2A	2503	2MA	C4-C5-N7	-3.64	106.42	110.58
54	2y	54	5MU	N3-C2-N1	3.63	119.61	114.89
54	1y	37	MIA	C4-C5-N7	-3.62	106.45	110.58
1	1A	2617	PSU	O2-C2-N1	-3.61	119.06	122.79
32	2a	1400	5MC	C5-C6-N1	-3.60	119.40	123.31
32	1a	1518	MA6	C2-N3-C4	3.60	120.62	111.83
54	2y	54	5MU	C4-N3-C2	-3.59	122.63	127.34
1	1A	1939	PSU	O2-C2-N1	-3.59	119.08	122.79
54	2y	55	PSU	O2-C2-N1	-3.59	119.09	122.79
54	1y	54	5MU	C5-C6-N1	-3.58	119.42	123.31
54	2w	32	PSU	O2-C2-N1	-3.58	119.10	122.79
55	2x	54	5MU	C5-C6-N1	-3.57	119.44	123.31
54	1y	54	5MU	O4-C4-C5	-3.56	120.84	124.92
54	1w	8	4SU	C5-C4-S4	-3.55	120.25	124.31
32	2a	1498	UR3	C5-C4-N3	3.55	119.71	115.04
32	2a	1518	MA6	C2-N3-C4	3.52	120.44	111.83
54	2y	37	MIA	N3-C2-N1	-3.52	123.25	128.58
54	2y	32	PSU	O2-C2-N1	-3.52	119.16	122.79
1	1A	2515	2MA	C4-N9-C8	3.51	109.42	105.74
54	2y	54	5MU	O4-C4-C5	-3.48	120.94	124.92
54	1y	37	MIA	N3-C2-N1	-3.47	123.33	128.58
54	2w	37	MIA	C2-N3-C4	3.47	121.37	112.29
32	1a	1207	2MG	C6-C5-N7	3.46	136.59	130.29
32	1a	1404	5MC	C5-C6-N1	-3.45	119.56	123.31
32	2a	1207	2MG	C6-C5-N7	3.45	136.57	130.29
55	1x	32	5MC	C5-C6-N1	-3.44	119.57	123.31
43	2l	92	0TD	OD2-CG-CB	3.43	120.56	113.15
1	2A	1915	5MU	O4-C4-C5	-3.42	121.00	124.92
32	2a	516	PSU	O2-C2-N1	-3.42	119.26	122.79
32	1a	1518	MA6	N1-C2-N3	-3.42	123.41	128.58
32	1a	516	PSU	O2-C2-N1	-3.41	119.27	122.79
32	1a	1400	5MC	C5-C6-N1	-3.41	119.61	123.31
54	1w	37	MIA	C2-N3-C4	3.38	121.15	112.29
55	1x	8	4SU	C1'-N1-C2	3.37	123.65	117.59
54	2w	37	MIA	C4-C5-N7	-3.36	106.73	110.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1w	32	PSU	O2-C2-N1	-3.35	119.33	122.79
1	1A	1984	5MC	C5-C6-N1	-3.34	119.69	123.31
54	1w	37	MIA	C4-C5-N7	-3.32	106.78	110.58
54	1w	8	4SU	N3-C2-N1	3.32	119.22	114.89
54	1w	46	7MG	C5-C4-N9	-3.31	102.09	106.33
32	2a	1404	5MC	C5-C6-N1	-3.30	119.73	123.31
32	2a	967	5MC	C5-C6-N1	-3.29	119.74	123.31
54	2w	8	4SU	C1'-N1-C2	3.29	123.51	117.59
1	2A	1962	5MC	C5-C6-N1	-3.29	119.74	123.31
32	2a	1518	MA6	N1-C2-N3	-3.29	123.61	128.58
32	2a	1519	MA6	N1-C2-N3	-3.28	123.62	128.58
1	1A	1937	5MU	C5-C6-N1	-3.23	119.81	123.31
54	1w	54	5MU	C5-C6-N1	-3.23	119.81	123.31
32	1a	966	M2G	C6-C5-N7	3.17	136.07	130.29
32	2a	966	M2G	C6-C5-N7	3.17	136.06	130.29
1	1A	2564	2MU	O2-C2-N1	-3.16	118.68	122.80
1	2A	2605	PSU	O2-C2-N1	-3.16	119.53	122.79
32	1a	1519	MA6	N1-C2-N3	-3.14	123.82	128.58
54	2w	37	MIA	C6-C5-N7	3.13	135.85	132.43
1	1A	2263	OMG	C6-C5-N7	3.12	135.98	130.29
1	2A	1942	5MC	C5-C6-N1	-3.12	119.92	123.31
1	1A	1964	5MC	C5-C6-N1	-3.10	119.95	123.31
32	1a	1407	5MC	C5-C6-N1	-3.10	119.95	123.31
1	2A	2552	2MU	C5-C4-N3	3.05	119.06	114.80
1	2A	2251	OMG	C6-C5-N7	3.04	135.83	130.29
55	1x	32	5MC	C5-C4-N3	-3.04	118.64	121.75
54	2w	37	MIA	C12-N6-C6	-3.04	120.03	122.85
32	1a	1498	UR3	C5-C4-N3	3.03	119.04	115.04
1	1A	2515	2MA	C4-C5-N7	-3.03	107.11	110.58
54	2w	39	PSU	O2-C2-N1	-3.00	119.69	122.79
32	1a	1518	MA6	C4-N9-C8	3.00	108.89	105.74
32	2a	1518	MA6	C5-N7-C8	2.99	108.16	103.45
54	1w	37	MIA	C6-C5-N7	2.99	135.69	132.43
1	1A	2564	2MU	C5-C4-N3	2.99	118.98	114.80
55	2x	32	5MC	C5-C6-N1	-2.96	120.10	123.31
55	1x	54	5MU	C5-C6-N1	-2.95	120.11	123.31
32	1a	1518	MA6	C5-N7-C8	2.93	108.05	103.45
54	2w	54	5MU	C5-C6-N1	-2.93	120.14	123.31
32	2a	1404	5MC	C5-C4-N3	-2.92	118.76	121.75
55	1x	8	4SU	C6-C5-C4	-2.92	117.43	119.95
32	2a	1407	5MC	C5-C6-N1	-2.90	120.16	123.31
32	2a	527	7MG	C5-C6-N1	2.88	116.01	110.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1407	5MC	C5-C4-N3	-2.87	118.81	121.75
32	1a	1407	5MC	C5-C4-N3	-2.87	118.81	121.75
32	1a	967	5MC	C5-C6-N1	-2.86	120.21	123.31
43	1l	92	0TD	OD2-CG-CB	2.85	119.32	113.15
1	1A	2515	2MA	C2-N1-C6	2.85	122.49	118.10
32	2a	1519	MA6	C5-N7-C8	2.83	107.90	103.45
32	1a	1518	MA6	C10-N6-C6	-2.82	113.33	120.52
1	1A	1964	5MC	C5-C4-N3	-2.82	118.87	121.75
1	2A	1942	5MC	C5-C4-N3	-2.81	118.88	121.75
54	2w	46	7MG	C5-C6-N1	2.80	115.86	110.94
1	2A	2503	2MA	N6-C6-N1	2.79	120.80	117.03
32	1a	967	5MC	C5-C4-N3	-2.79	118.90	121.75
32	1a	1519	MA6	C5-N7-C8	2.78	107.83	103.45
32	2a	1207	2MG	C4-C5-N7	-2.78	106.26	110.67
1	1A	1984	5MC	C5-C4-N3	-2.78	118.90	121.75
55	2x	32	5MC	C5-C4-N3	-2.78	118.91	121.75
55	2x	32	5MC	O2-C2-N3	-2.76	117.98	122.33
55	2x	54	5MU	O2-C2-N1	-2.76	119.21	122.80
54	2y	46	7MG	C5-C4-N9	-2.75	102.81	106.33
32	1a	1207	2MG	C4-C5-N7	-2.75	106.32	110.67
32	1a	1404	5MC	C5-C4-N3	-2.74	118.95	121.75
55	1x	8	4SU	O2-C2-N1	2.72	126.34	122.80
32	2a	967	5MC	C5-C4-N3	-2.72	118.97	121.75
1	1A	2263	OMG	C4-C5-N7	-2.71	106.38	110.67
1	2A	2552	2MU	O2-C2-N1	-2.71	119.28	122.80
55	2x	8	4SU	C5-C4-S4	-2.70	121.22	124.31
32	1a	527	7MG	C5-C6-N1	2.70	115.70	110.94
32	1a	1400	5MC	C5-C4-N3	-2.69	119.00	121.75
54	2y	37	MIA	C5-N7-C8	2.68	107.66	103.45
54	2y	54	5MU	C5-C6-N1	-2.66	120.42	123.31
32	1a	1519	MA6	N1-C6-N6	2.65	120.09	116.86
1	2A	2503	2MA	C2-N1-C6	2.65	122.17	118.10
32	2a	1519	MA6	C10-N6-C6	-2.63	113.82	120.52
32	2a	1519	MA6	C4-N9-C8	2.63	108.50	105.74
54	1w	54	5MU	O2-C2-N1	-2.63	119.38	122.80
1	2A	1962	5MC	C5-C4-N3	-2.62	119.07	121.75
1	2A	2503	2MA	C4-N9-C8	2.60	108.47	105.74
54	2y	46	7MG	C5-C6-N1	2.60	115.51	110.94
32	1a	966	M2G	C4-C5-N7	-2.60	106.55	110.67
1	2A	2251	OMG	C4-C5-N7	-2.59	106.56	110.67
54	2w	54	5MU	O2-C2-N1	-2.59	119.43	122.80
32	1a	1519	MA6	C10-N6-C6	-2.59	113.94	120.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2503	2MA	C5-N7-C8	2.58	107.51	103.45
54	1y	54	5MU	O2-C2-N1	-2.58	119.44	122.80
54	1y	37	MIA	C5-N7-C8	2.57	107.49	103.45
1	2A	1915	5MU	O2-C2-N1	-2.54	119.49	122.80
54	1y	46	7MG	C5-C6-N1	2.54	115.41	110.94
32	2a	1518	MA6	C4-N9-C8	2.54	108.40	105.74
54	2y	37	MIA	C4-N9-C8	2.53	108.39	105.74
32	2a	1518	MA6	C6-C5-N7	2.53	137.47	133.43
1	2A	2552	2MU	O4-C4-C5	-2.52	120.81	125.16
54	1w	37	MIA	C11-S10-C2	-2.52	100.36	102.25
32	2a	1404	5MC	O2-C2-N3	-2.52	118.36	122.33
32	2a	1518	MA6	C10-N6-C9	-2.51	108.12	116.18
32	2a	966	M2G	C4-C5-N7	-2.51	106.70	110.67
1	1A	2564	2MU	C2'-C1'-N1	-2.50	109.49	114.24
1	1A	2515	2MA	C5-N7-C8	2.49	107.37	103.45
32	2a	1400	5MC	C5-C4-N3	-2.48	119.21	121.75
1	2A	1939	5MU	O2-C2-N1	-2.48	119.57	122.80
54	2w	37	MIA	N3-C2-N1	-2.47	122.49	127.00
43	2l	92	0TD	OD1-CG-CB	-2.47	117.27	122.44
1	1A	2515	2MA	N9-C8-N7	-2.45	110.46	113.94
55	2x	8	4SU	C4-N3-C2	-2.45	124.97	127.31
32	1a	1402	4OC	C6-C5-C4	2.44	119.94	117.00
54	2w	37	MIA	C5-N7-C8	2.44	107.28	103.45
54	1y	46	7MG	C5-C4-N9	-2.43	103.22	106.33
55	1x	8	4SU	O2-C2-N3	-2.43	117.00	121.49
1	1A	1961	5MU	O2-C2-N1	-2.42	119.64	122.80
54	1w	37	MIA	C5-N7-C8	2.42	107.25	103.45
54	1w	37	MIA	C2-N1-C6	2.42	122.13	117.54
54	1w	37	MIA	C4-N9-C8	2.40	108.26	105.74
54	2y	54	5MU	C1'-N1-C2	2.38	121.88	117.59
55	2x	8	4SU	C6-C5-C4	-2.38	117.89	119.95
1	1A	1937	5MU	O2-C2-N1	-2.38	119.70	122.80
54	2w	37	MIA	C4-N9-C8	2.37	108.23	105.74
32	1a	1518	MA6	N9-C8-N7	-2.35	110.60	113.94
32	1a	1400	5MC	O2-C2-N3	-2.34	118.64	122.33
55	1x	54	5MU	O2-C2-N1	-2.34	119.75	122.80
54	1y	37	MIA	C4-N9-C8	2.33	108.18	105.74
54	2w	37	MIA	C2-N1-C6	2.32	121.95	117.54
54	1w	37	MIA	N3-C2-N1	-2.32	122.77	127.00
32	1a	1519	MA6	C4-N9-C8	2.32	108.17	105.74
32	2a	1402	4OC	C6-C5-C4	2.32	119.79	117.00
1	2A	2503	2MA	C6-C5-N7	2.32	136.55	132.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2y	54	5MU	C1'-N1-C6	-2.31	117.35	121.15
32	2a	527	7MG	C5-C4-N9	-2.31	103.38	106.33
32	1a	1518	MA6	C6-C5-N7	2.30	137.10	133.43
55	2x	8	4SU	C1'-N1-C6	-2.29	115.88	120.78
1	1A	1942	4OC	O2-C2-N3	-2.29	118.72	122.33
54	2w	46	7MG	O6-C6-C5	-2.29	122.00	127.62
1	2A	2605	PSU	C5-C6-N1	-2.28	118.98	122.14
55	1x	54	5MU	C5M-C5-C4	2.26	121.19	118.78
1	1A	2564	2MU	O4-C4-C5	-2.24	121.30	125.16
54	2y	39	PSU	C5-C6-N1	-2.24	119.03	122.14
32	2a	1407	5MC	O2-C2-N3	-2.24	118.81	122.33
32	1a	967	5MC	C1'-N1-C6	-2.24	117.47	121.15
32	1a	1518	MA6	C10-N6-C9	-2.22	109.04	116.18
32	2a	1402	4OC	O2-C2-N3	-2.22	118.83	122.33
32	2a	1519	MA6	C6-C5-N7	2.21	136.96	133.43
32	1a	516	PSU	O4'-C1'-C2'	2.21	108.21	105.15
54	1w	46	7MG	C4-C5-N7	2.21	107.98	105.38
32	2a	1207	2MG	N1-C2-N2	2.18	118.78	116.56
32	2a	527	7MG	O6-C6-C5	-2.17	122.29	127.62
1	1A	2263	OMG	O6-C6-C5	-2.17	120.81	126.53
54	2w	46	7MG	C5-C4-N9	-2.17	103.56	106.33
32	2a	1518	MA6	C10-N6-C6	-2.16	115.02	120.52
1	1A	1939	PSU	C5-C6-N1	-2.15	119.16	122.14
54	1w	46	7MG	C5-C6-N1	2.12	114.67	110.94
1	2A	2503	2MA	N9-C8-N7	-2.12	110.94	113.94
54	2y	46	7MG	O6-C6-C5	-2.11	122.43	127.62
32	2a	966	M2G	O6-C6-C5	-2.10	120.98	126.53
54	2y	37	MIA	C6-C5-N7	2.09	136.13	132.09
32	2a	1518	MA6	N9-C8-N7	-2.09	110.97	113.94
32	1a	527	7MG	C5-C4-N9	-2.09	103.66	106.33
1	1A	2515	2MA	C6-C5-N7	2.08	136.10	132.09
54	2w	54	5MU	C5M-C5-C4	2.07	120.99	118.78
54	2y	55	PSU	C5-C6-N1	-2.07	119.27	122.14
32	1a	516	PSU	C5-C6-N1	-2.06	119.29	122.14
32	2a	516	PSU	O4'-C1'-C2'	2.05	107.99	105.15
1	2A	1917	PSU	C5-C6-N1	-2.05	119.30	122.14
32	1a	1518	MA6	N1-C6-N6	2.05	119.35	116.86
32	1a	966	M2G	O6-C6-C5	-2.04	121.14	126.53
54	2y	54	5MU	C5M-C5-C4	2.03	120.95	118.78
32	1a	967	5MC	O2-C2-N3	-2.03	119.13	122.33
54	1y	37	MIA	C6-C5-N7	2.03	136.00	132.09
32	2a	1207	2MG	O6-C6-C5	-2.02	121.20	126.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	527	7MG	O6-C6-C5	-2.02	122.67	127.62
54	1w	8	4SU	C1'-N1-C2	2.01	121.21	117.59
54	1y	54	5MU	C5M-C5-C4	2.00	120.92	118.78

There are no chirality outliers.

All (67) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	967	5MC	O4'-C4'-C5'-O5'
32	1a	1207	2MG	N3-C2-N2-CM2
43	1l	92	0TD	O-C-CA-CB
32	2a	1402	4OC	O4'-C4'-C5'-O5'
32	2a	1518	MA6	C5-C6-N6-C9
32	2a	1519	MA6	O4'-C4'-C5'-O5'
43	2l	92	0TD	O-C-CA-CB
54	1y	8	4SU	O4'-C4'-C5'-O5'
54	1w	37	MIA	C12-C13-C14-C16
54	2w	37	MIA	C5-C6-N6-C12
54	2w	37	MIA	N1-C6-N6-C12
32	1a	527	7MG	C3'-C4'-C5'-O5'
32	1a	967	5MC	C3'-C4'-C5'-O5'
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
54	1y	8	4SU	C3'-C4'-C5'-O5'
54	2y	8	4SU	O4'-C4'-C5'-O5'
54	2y	8	4SU	C3'-C4'-C5'-O5'
54	1w	46	7MG	C4'-C5'-O5'-P
32	2a	1518	MA6	N1-C6-N6-C9
32	2a	1402	4OC	C3'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
54	1y	37	MIA	C3'-C4'-C5'-O5'
54	2y	37	MIA	C3'-C4'-C5'-O5'
32	1a	527	7MG	O4'-C4'-C5'-O5'
32	2a	1207	2MG	O4'-C4'-C5'-O5'
32	1a	1518	MA6	C5-C6-N6-C10
32	2a	1519	MA6	C5-C6-N6-C9
32	2a	1519	MA6	C5-C6-N6-C10
54	2w	46	7MG	C2'-C1'-N9-C8
54	1w	46	7MG	C3'-C4'-C5'-O5'
32	1a	1402	4OC	O4'-C4'-C5'-O5'
54	2y	37	MIA	O4'-C4'-C5'-O5'
54	1w	46	7MG	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
54	1y	37	MIA	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C5-C6-N6-C10
54	2y	46	7MG	C2'-C1'-N9-C8
54	2w	46	7MG	O4'-C4'-C5'-O5'
43	2l	92	0TD	CG-CB-SB-CSB
32	2a	1519	MA6	C4'-C5'-O5'-P
54	1y	46	7MG	C4'-C5'-O5'-P
54	2y	46	7MG	C4'-C5'-O5'-P
54	1y	55	PSU	O4'-C1'-C5-C4
54	2y	55	PSU	O4'-C1'-C5-C4
32	2a	527	7MG	C3'-C4'-C5'-O5'
32	1a	1518	MA6	C5-C6-N6-C9
32	2a	527	7MG	C4'-C5'-O5'-P
32	2a	967	5MC	O4'-C4'-C5'-O5'
43	1l	92	0TD	SB-CB-CG-OD2
1	2A	1920	4OC	C1'-C2'-O2'-CM2
1	2A	2251	OMG	C4'-C5'-O5'-P
1	2A	2503	2MA	C4'-C5'-O5'-P
54	1y	55	PSU	O4'-C1'-C5-C6
54	2y	55	PSU	O4'-C1'-C5-C6
1	2A	1920	4OC	C3'-C2'-O2'-CM2
32	2a	1207	2MG	C3'-C4'-C5'-O5'
54	2w	46	7MG	O4'-C1'-N9-C8
54	1y	46	7MG	C2'-C1'-N9-C8
54	2y	46	7MG	O4'-C1'-N9-C8
43	1l	92	0TD	CG-CB-SB-CSB
54	2w	46	7MG	C3'-C4'-C5'-O5'
1	1A	2515	2MA	C4'-C5'-O5'-P
1	1A	1942	4OC	C2'-C1'-N1-C2
54	2w	8	4SU	C2'-C1'-N1-C2
1	2A	2503	2MA	O4'-C4'-C5'-O5'
54	1y	8	4SU	C4'-C5'-O5'-P
55	2x	8	4SU	C2'-C1'-N1-C2

There are no ring outliers.

29 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	2a	1519	MA6	2	0
32	2a	1404	5MC	2	0
1	2A	1917	PSU	1	0
32	2a	967	5MC	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	1a	1402	4OC	1	0
32	2a	1407	5MC	1	0
54	1y	46	7MG	1	0
1	2A	2552	2MU	1	0
32	2a	1207	2MG	2	0
54	2w	46	7MG	1	0
54	1w	46	7MG	1	0
54	1y	39	PSU	1	0
43	2l	92	0TD	2	0
32	1a	1519	MA6	1	0
32	1a	1518	MA6	1	0
1	2A	2503	2MA	1	0
32	2a	1518	MA6	4	0
1	2A	1915	5MU	1	0
1	1A	2564	2MU	1	0
1	1A	1939	PSU	1	0
55	1x	8	4SU	1	0
1	1A	1961	5MU	2	0
32	1a	966	M2G	1	0
1	2A	1920	4OC	1	0
43	1l	92	0TD	1	0
54	2w	8	4SU	3	0
32	2a	966	M2G	1	0
32	1a	967	5MC	1	0
32	2a	1402	4OC	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2821 ligands modelled in this entry, 2817 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
60	SF4	2d	302	35	0,12,12	-	-	-		
58	M2D	2A	3864	-	36,37,37	3.09	16 (44%)	42,50,50	2.03	11 (26%)
60	SF4	1d	501	35	0,12,12	-	-	-		
58	M2D	1A	4118	-	36,37,37	3.02	16 (44%)	42,50,50	2.08	8 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	SF4	2d	302	35	-	-	0/6/5/5
58	M2D	2A	3864	-	-	6/48/48/48	0/1/2/2
60	SF4	1d	501	35	-	-	0/6/5/5
58	M2D	1A	4118	-	-	5/48/48/48	0/1/2/2

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	2A	3864	M2D	CAT-CAY	-8.31	1.33	1.48
58	2A	3864	M2D	CAM-CAL	-8.19	1.40	1.50
58	1A	4118	M2D	CAT-CAY	-8.17	1.33	1.48
58	1A	4118	M2D	CAM-CAL	-7.38	1.41	1.50
58	2A	3864	M2D	CAP-CAQ	-6.07	1.39	1.49
58	1A	4118	M2D	CAP-CAQ	-5.66	1.39	1.49
58	1A	4118	M2D	CBD-CAK	-5.54	1.39	1.50
58	2A	3864	M2D	CBD-CAK	-5.37	1.40	1.50
58	1A	4118	M2D	CAC-CAD	-4.72	1.40	1.51
58	2A	3864	M2D	CAC-CAD	-4.54	1.40	1.51
58	2A	3864	M2D	CAE-CAF	-4.20	1.39	1.48
58	1A	4118	M2D	CAE-CAF	-4.09	1.39	1.48
58	1A	4118	M2D	CAF-NAG	3.97	1.42	1.34
58	2A	3864	M2D	CAF-NAG	3.82	1.42	1.34
58	1A	4118	M2D	CAQ-NAU	3.51	1.33	1.29
58	1A	4118	M2D	CA-C	-3.50	1.39	1.51
58	2A	3864	M2D	CAQ-NAU	3.48	1.33	1.29
58	2A	3864	M2D	CA-C	-3.43	1.39	1.51
58	1A	4118	M2D	CAJ-CAI	3.32	1.41	1.32
58	2A	3864	M2D	CAJ-CAI	3.26	1.41	1.32
58	2A	3864	M2D	CAE-CAD	3.25	1.39	1.32
58	1A	4118	M2D	CAE-CAD	3.25	1.39	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	2A	3864	M2D	CAY-N	2.80	1.40	1.34
58	2A	3864	M2D	CAH-CAI	-2.67	1.40	1.49
58	1A	4118	M2D	CAH-CAI	-2.62	1.40	1.49
58	1A	4118	M2D	CAL-CAK	2.52	1.41	1.34
58	1A	4118	M2D	CAY-N	2.46	1.39	1.34
58	1A	4118	M2D	CAT-NAU	-2.46	1.33	1.38
58	2A	3864	M2D	CAJ-CAK	-2.45	1.40	1.46
58	2A	3864	M2D	CAT-NAU	-2.43	1.33	1.38
58	1A	4118	M2D	CAJ-CAK	-2.39	1.40	1.46
58	2A	3864	M2D	CAL-CAK	2.32	1.40	1.34

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	1A	4118	M2D	CAI-CAJ-CAK	7.81	137.69	125.89
58	2A	3864	M2D	CAI-CAJ-CAK	6.59	135.85	125.89
58	1A	4118	M2D	OAR-CAQ-NAU	-6.42	107.15	114.09
58	2A	3864	M2D	OAR-CAQ-NAU	-5.82	107.80	114.09
58	2A	3864	M2D	CAN-CAM-CAL	3.84	116.91	111.28
58	2A	3864	M2D	CBD-CAK-CAJ	3.58	123.56	118.09
58	1A	4118	M2D	CBD-CAK-CAJ	3.34	123.19	118.09
58	2A	3864	M2D	CAS-CAT-CAY	2.95	133.23	127.81
58	1A	4118	M2D	CAS-CAT-CAY	2.92	133.16	127.81
58	1A	4118	M2D	CAH-NAG-CAF	2.71	126.56	122.17
58	2A	3864	M2D	CAB-OAA-C	-2.62	113.42	117.76
58	1A	4118	M2D	CAN-CAM-CAL	2.58	115.06	111.28
58	2A	3864	M2D	CAH-NAG-CAF	2.53	126.28	122.17
58	2A	3864	M2D	CAC-CAB-CAZ	-2.44	109.97	115.98
58	1A	4118	M2D	CAT-CAY-N	2.19	118.34	115.22
58	2A	3864	M2D	OAA-C-CA	2.17	114.46	110.83
58	2A	3864	M2D	CAT-CAY-N	2.15	118.28	115.22
58	1A	4118	M2D	CAN-CAO-CAP	-2.11	108.66	112.96
58	2A	3864	M2D	CAC-CAD-CAE	-2.10	120.75	126.30

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	1A	4118	M2D	CAM-CAN-CAO-CAP
58	1A	4118	M2D	CAM-CAN-CAO-OBF
58	2A	3864	M2D	CAM-CAN-CAO-OBF
58	2A	3864	M2D	CAI-CAH-NAG-CAF

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
58	2A	3864	M2D	CBB-CAC-CAD-CAE
58	1A	4118	M2D	CAI-CAH-NAG-CAF
58	1A	4118	M2D	CBB-CAC-CAD-CAE
58	1A	4118	M2D	CAB-CAC-CAD-CAE
58	2A	3864	M2D	CAB-CAC-CAD-CAE
58	2A	3864	M2D	O-C-CA-CB
58	2A	3864	M2D	OAA-C-CA-CB

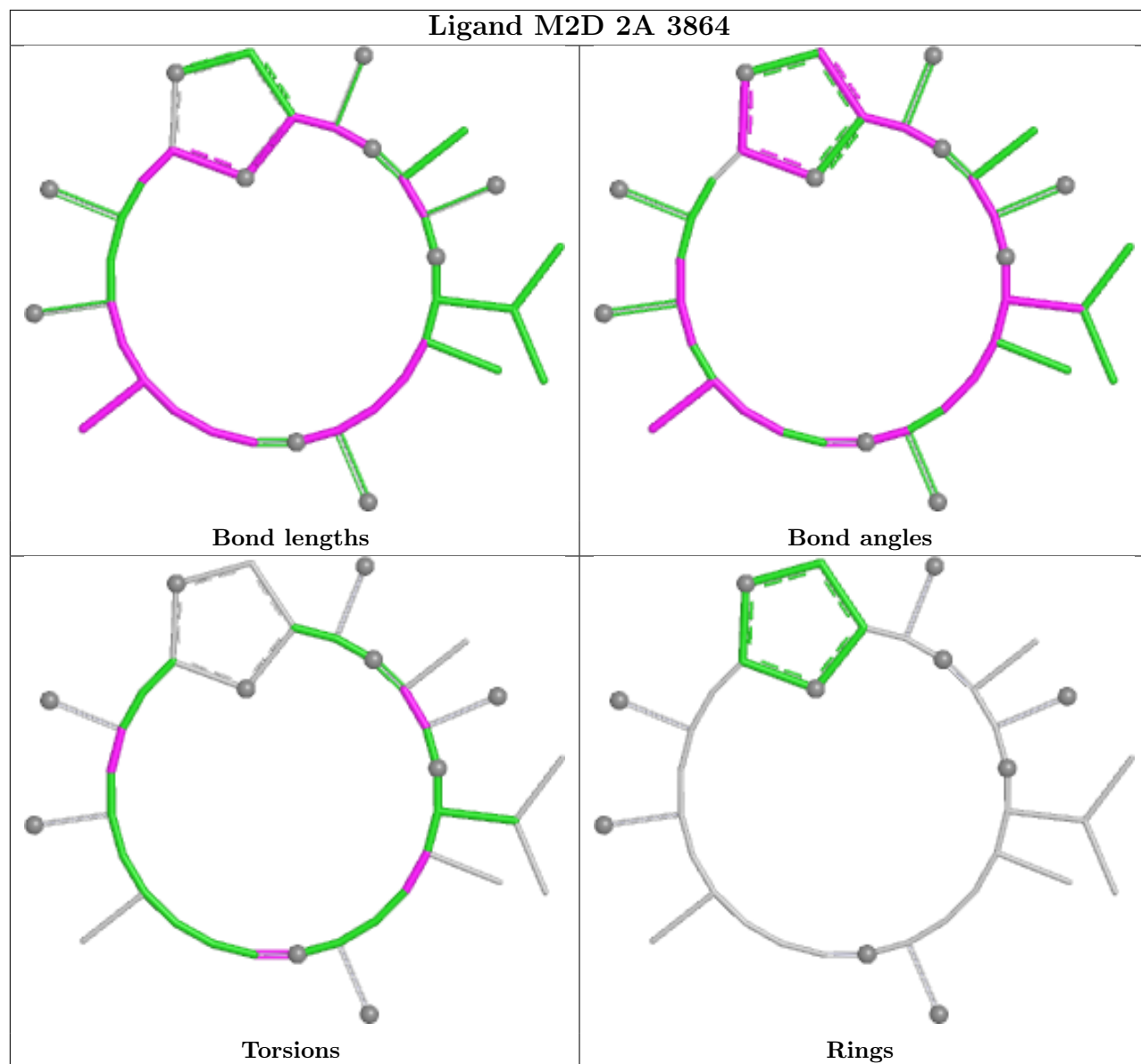
There are no ring outliers.

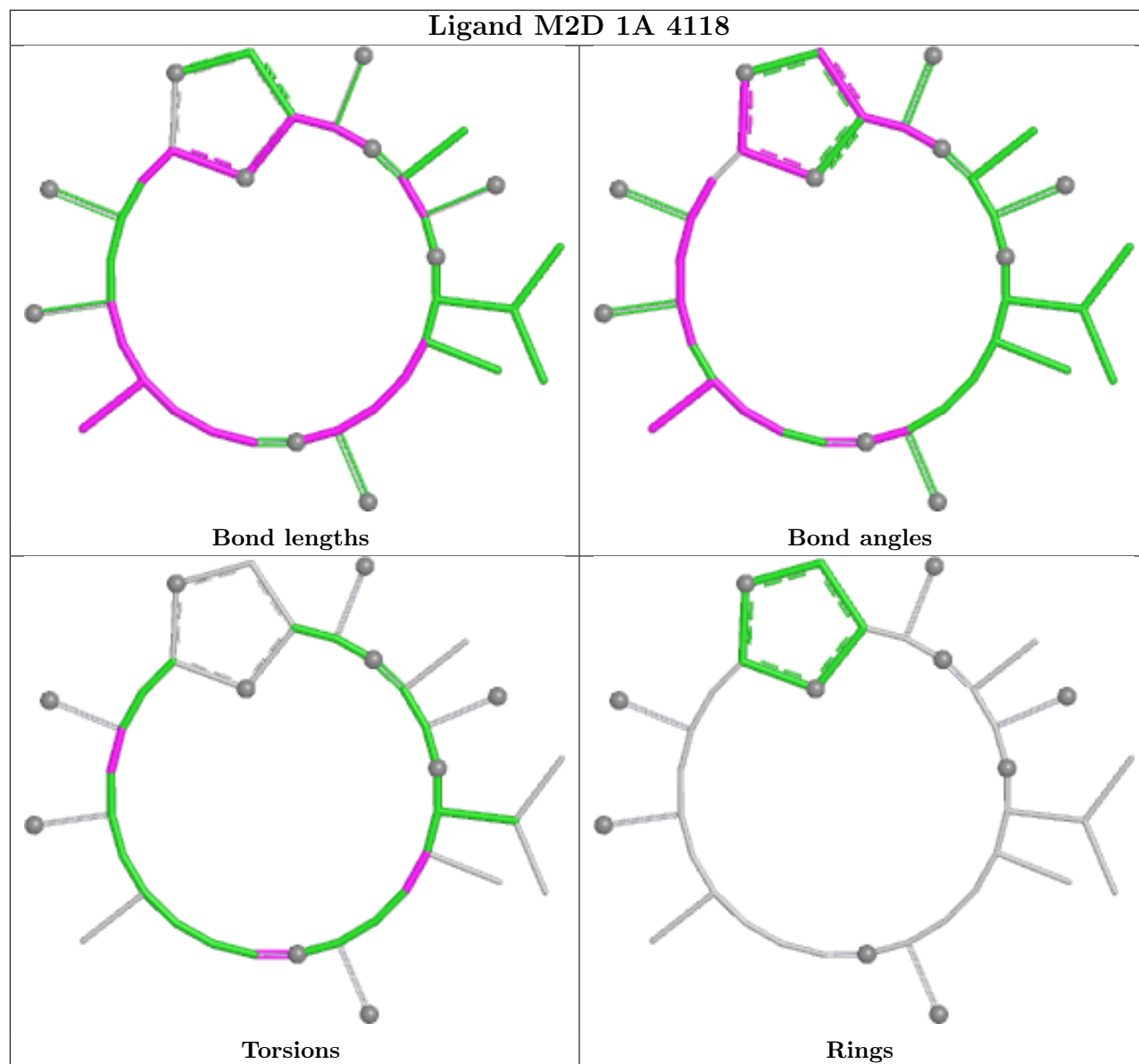
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	2d	302	SF4	2	0
60	1d	501	SF4	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 M2D 2A 3864





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%)	-0.45	50 (1%) 69 60	10, 26, 82, 97	0
1	2A	2789/2915 (95%)	0.09	73 (2%) 57 47	25, 51, 82, 96	0
2	1B	120/121 (99%)	-0.42	0 100 100	19, 38, 50, 74	0
2	2B	120/121 (99%)	0.75	2 (1%) 69 60	55, 70, 76, 82	0
3	1D	275/276 (99%)	-0.19	1 (0%) 88 84	12, 29, 43, 62	0
3	2D	275/276 (99%)	0.29	1 (0%) 88 84	25, 43, 56, 69	0
4	1E	204/206 (99%)	-0.25	1 (0%) 87 82	11, 29, 48, 68	0
4	2E	204/206 (99%)	0.17	1 (0%) 87 82	29, 51, 62, 71	0
5	1F	203/210 (96%)	-0.16	0 100 100	12, 32, 62, 75	0
5	2F	203/210 (96%)	0.52	2 (0%) 79 72	28, 58, 70, 80	0
6	1G	181/182 (99%)	0.26	3 (1%) 69 60	28, 46, 61, 72	0
6	2G	181/182 (99%)	1.05	17 (9%) 14 10	59, 69, 78, 88	0
7	1H	174/180 (96%)	0.09	1 (0%) 85 80	24, 42, 54, 60	0
7	2H	174/180 (96%)	1.06	16 (9%) 14 10	55, 72, 81, 84	0
8	1I	146/148 (98%)	0.56	3 (2%) 63 54	35, 63, 72, 78	0
8	2I	146/148 (98%)	0.69	3 (2%) 63 54	44, 62, 72, 76	0
9	1N	140/140 (100%)	-0.23	0 100 100	15, 27, 46, 57	0
9	2N	140/140 (100%)	0.68	7 (5%) 34 26	40, 57, 67, 74	0
10	1O	122/122 (100%)	-0.22	0 100 100	20, 30, 45, 55	0
10	2O	122/122 (100%)	0.44	2 (1%) 70 61	38, 53, 63, 68	0
11	1P	149/150 (99%)	-0.07	0 100 100	12, 36, 59, 70	0
11	2P	149/150 (99%)	0.48	2 (1%) 75 66	31, 59, 71, 79	0
12	1Q	141/141 (100%)	-0.19	0 100 100	19, 32, 44, 66	0
12	2Q	141/141 (100%)	0.74	11 (7%) 19 14	44, 60, 73, 77	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%)	-0.37	0 100 100	14, 24, 36, 43	0
13	2R	118/118 (100%)	0.12	0 100 100	33, 44, 55, 64	0
14	1S	110/112 (98%)	-0.05	0 100 100	27, 38, 50, 59	0
14	2S	110/112 (98%)	1.00	8 (7%) 21 15	55, 65, 71, 75	0
15	1T	131/146 (89%)	-0.01	2 (1%) 72 63	23, 33, 55, 64	0
15	2T	131/146 (89%)	0.51	4 (3%) 51 41	41, 55, 68, 81	0
16	1U	116/118 (98%)	-0.42	1 (0%) 81 74	12, 19, 37, 59	0
16	2U	116/118 (98%)	0.55	4 (3%) 48 39	38, 53, 68, 76	0
17	1V	101/101 (100%)	-0.45	0 100 100	12, 27, 43, 51	0
17	2V	101/101 (100%)	0.64	4 (3%) 42 33	39, 60, 69, 78	0
18	1W	112/113 (99%)	-0.41	1 (0%) 81 74	15, 21, 44, 69	0
18	2W	112/113 (99%)	0.30	2 (1%) 67 58	30, 41, 55, 81	0
19	1X	95/96 (98%)	-0.15	2 (2%) 63 54	17, 29, 46, 63	0
19	2X	95/96 (98%)	0.53	1 (1%) 78 70	37, 53, 62, 68	0
20	1Y	107/110 (97%)	0.20	2 (1%) 66 57	26, 40, 55, 72	0
20	2Y	107/110 (97%)	1.01	13 (12%) 8 6	51, 61, 69, 75	0
21	1Z	154/206 (74%)	0.39	4 (2%) 57 47	30, 50, 75, 82	0
21	2Z	160/206 (77%)	1.35	25 (15%) 5 4	61, 73, 81, 84	0
22	10	83/85 (97%)	0.28	7 (8%) 17 12	19, 28, 59, 80	0
22	20	83/85 (97%)	0.76	8 (9%) 13 10	46, 57, 69, 78	0
23	11	97/98 (98%)	0.20	1 (1%) 79 72	15, 35, 58, 63	0
23	21	97/98 (98%)	0.48	4 (4%) 41 33	32, 49, 67, 71	0
24	12	70/72 (97%)	0.10	1 (1%) 73 64	25, 39, 50, 69	0
24	22	70/72 (97%)	0.46	1 (1%) 73 64	49, 60, 69, 73	0
25	13	59/60 (98%)	-0.25	0 100 100	15, 26, 46, 64	0
25	23	59/60 (98%)	0.48	0 100 100	46, 56, 70, 78	0
26	14	69/71 (97%)	0.50	4 (5%) 29 22	40, 59, 76, 82	0
26	24	69/71 (97%)	1.33	11 (15%) 5 4	64, 75, 83, 84	0
27	15	59/60 (98%)	-0.39	1 (1%) 69 60	11, 22, 41, 58	0
27	25	59/60 (98%)	0.12	0 100 100	31, 44, 54, 65	0
28	16	53/54 (98%)	-0.38	0 100 100	22, 32, 46, 48	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%)	0.67	1 (1%) 66 57	43, 53, 61, 66	0
29	17	48/49 (97%)	-0.24	0 100 100	13, 19, 51, 54	0
29	27	48/49 (97%)	0.11	2 (4%) 40 32	26, 33, 54, 65	0
30	18	64/65 (98%)	-0.14	0 100 100	17, 24, 32, 43	0
30	28	64/65 (98%)	0.36	0 100 100	39, 47, 55, 57	0
31	19	37/37 (100%)	-0.25	0 100 100	18, 30, 46, 50	0
31	29	37/37 (100%)	1.06	2 (5%) 31 24	51, 63, 68, 70	0
32	1a	1488/1521 (97%)	0.28	33 (2%) 62 52	28, 57, 81, 96	0
32	2a	1491/1521 (98%)	0.70	82 (5%) 30 23	48, 69, 85, 95	0
33	1b	231/256 (90%)	0.99	33 (14%) 6 5	55, 68, 79, 83	0
33	2b	231/256 (90%)	1.37	39 (16%) 4 3	65, 77, 83, 86	0
34	1c	206/239 (86%)	0.63	10 (4%) 35 27	50, 63, 74, 80	0
34	2c	206/239 (86%)	1.38	47 (22%) 2 1	65, 75, 82, 88	0
35	1d	208/209 (99%)	0.90	15 (7%) 21 16	47, 62, 71, 82	0
35	2d	208/209 (99%)	0.88	12 (5%) 29 22	52, 63, 72, 73	0
36	1e	148/162 (91%)	0.45	1 (0%) 84 77	44, 56, 62, 69	0
36	2e	148/162 (91%)	1.18	23 (15%) 5 4	58, 69, 77, 80	0
37	1f	100/101 (99%)	0.60	0 100 100	46, 59, 68, 71	0
37	2f	100/101 (99%)	0.50	1 (1%) 79 72	52, 63, 70, 72	0
38	1g	155/156 (99%)	0.65	7 (4%) 38 30	48, 59, 70, 81	0
38	2g	155/156 (99%)	1.16	22 (14%) 6 5	60, 69, 78, 90	0
39	1h	137/138 (99%)	0.60	1 (0%) 84 77	47, 58, 66, 72	0
39	2h	137/138 (99%)	1.17	15 (10%) 10 8	59, 69, 75, 78	0
40	1i	127/128 (99%)	1.08	7 (5%) 30 23	42, 66, 74, 76	0
40	2i	127/128 (99%)	1.41	31 (24%) 2 1	65, 75, 82, 85	0
41	1j	97/105 (92%)	1.06	11 (11%) 10 7	50, 68, 77, 80	0
41	2j	96/105 (91%)	1.73	37 (38%) 1 0	67, 76, 84, 94	0
42	1k	114/129 (88%)	0.61	1 (0%) 81 74	36, 54, 65, 69	0
42	2k	114/129 (88%)	1.04	9 (7%) 18 13	44, 65, 72, 75	0
43	1l	121/132 (91%)	0.32	2 (1%) 69 60	38, 46, 58, 65	0
43	2l	121/132 (91%)	0.65	2 (1%) 69 60	49, 61, 69, 74	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%)	0.50	5 (4%) 41 33	44, 57, 67, 72	0
44	2m	122/126 (96%)	1.41	21 (17%) 4 3	60, 72, 77, 82	0
45	1n	60/61 (98%)	0.82	3 (5%) 34 26	52, 58, 65, 71	0
45	2n	60/61 (98%)	1.97	29 (48%) 0 0	69, 75, 81, 84	0
46	1o	88/89 (98%)	0.43	2 (2%) 61 51	41, 55, 65, 69	0
46	2o	88/89 (98%)	0.86	8 (9%) 15 11	50, 64, 71, 77	0
47	1p	82/88 (93%)	0.90	5 (6%) 27 20	49, 60, 68, 73	0
47	2p	82/88 (93%)	0.94	2 (2%) 59 49	48, 60, 68, 70	0
48	1q	99/105 (94%)	0.65	1 (1%) 79 72	44, 56, 66, 70	0
48	2q	99/105 (94%)	0.84	3 (3%) 52 42	56, 64, 71, 74	0
49	1r	68/88 (77%)	0.52	1 (1%) 72 63	45, 56, 68, 74	0
49	2r	68/88 (77%)	0.59	0 100 100	55, 63, 70, 77	0
50	1s	83/93 (89%)	0.57	2 (2%) 59 49	48, 60, 68, 73	0
50	2s	83/93 (89%)	1.56	19 (22%) 2 1	67, 76, 81, 84	0
51	1t	96/106 (90%)	0.76	4 (4%) 40 32	47, 59, 70, 75	0
51	2t	96/106 (90%)	0.70	5 (5%) 33 25	50, 61, 71, 75	0
52	1u	23/27 (85%)	0.94	3 (13%) 7 6	50, 55, 61, 62	0
52	2u	23/27 (85%)	1.70	8 (34%) 1 0	64, 69, 74, 76	0
53	1v	13/24 (54%)	0.36	0 100 100	39, 52, 75, 87	0
53	2v	13/24 (54%)	1.92	6 (46%) 0 0	60, 75, 88, 90	0
54	1w	65/76 (85%)	0.72	6 (9%) 14 10	48, 76, 89, 95	0
54	1y	67/76 (88%)	0.93	5 (7%) 20 15	25, 79, 88, 91	0
54	2w	62/76 (81%)	1.26	10 (16%) 4 4	71, 83, 91, 97	0
54	2y	66/76 (86%)	1.35	11 (16%) 4 3	45, 86, 91, 92	0
55	1x	72/77 (93%)	0.13	0 100 100	35, 52, 70, 80	0
55	2x	72/77 (93%)	0.61	0 100 100	55, 70, 80, 83	0
All	All	20870/21748 (95%)	0.34	912 (4%) 39 31	10, 55, 80, 97	0

All (912) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	10	6	GLY	8.8
45	1n	2	ALA	7.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
38	2g	80	VAL	7.0
38	1g	80	VAL	5.5
32	1a	1002	G	5.4
44	2m	102	ARG	5.4
1	2A	883	G	5.3
22	10	4	LYS	5.1
1	1A	942	A	5.0
38	2g	84	ASN	5.0
22	10	3	HIS	4.9
33	1b	237	ALA	4.8
38	2g	82	GLY	4.8
44	2m	6	GLY	4.8
7	1H	2	SER	4.7
22	10	5	LYS	4.7
40	2i	109	VAL	4.7
45	2n	7	ILE	4.7
44	2m	60	VAL	4.7
53	2v	14	A	4.6
44	2m	124	PRO	4.5
34	2c	2	GLY	4.5
45	2n	39	LEU	4.5
32	1a	1001(A)	G	4.4
21	2Z	21	ALA	4.3
1	1A	1555	C	4.3
44	1m	124	PRO	4.3
1	2A	2133	G	4.3
38	2g	81	GLY	4.2
32	2a	1033	G	4.2
34	2c	129	ALA	4.2
41	2j	59	SER	4.1
32	2a	1030(B)	C	4.1
34	2c	198	VAL	4.0
32	2a	1532	U	4.0
40	2i	14	VAL	4.0
7	2H	2	SER	4.0
44	2m	5	ALA	4.0
22	10	7	LEU	3.9
21	2Z	172	ALA	3.9
45	2n	37	PHE	3.9
41	2j	50	ILE	3.9
22	10	2	ALA	3.9
41	2j	65	LEU	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	2E	10	GLY	3.8
52	2u	16	GLY	3.8
22	20	6	GLY	3.8
32	1a	1003	G	3.7
44	2m	123	ALA	3.7
45	2n	38	GLY	3.7
1	1A	932	C	3.6
6	2G	50	ALA	3.6
26	24	59	PHE	3.6
7	2H	136	ILE	3.6
32	2a	1030(A)	G	3.6
33	2b	165	VAL	3.6
33	2b	152	PHE	3.6
1	2A	1536	C	3.6
42	2k	14	VAL	3.6
1	2A	2896	C	3.5
41	2j	42	THR	3.5
21	2Z	173	ALA	3.5
32	1a	204	U	3.5
41	1j	72	VAL	3.5
50	2s	9	VAL	3.5
33	1b	12	GLU	3.5
21	1Z	146	ILE	3.4
6	2G	28	VAL	3.4
1	1A	1103	A	3.4
45	2n	2	ALA	3.4
36	2e	22	GLY	3.4
40	1i	2	GLU	3.4
54	2w	3	C	3.4
41	2j	47	PHE	3.4
45	2n	34	TYR	3.4
54	1w	1	G	3.3
40	2i	10	ARG	3.3
46	2o	64	ARG	3.3
1	1A	1126	C	3.3
41	2j	74	ILE	3.3
47	1p	68	ASP	3.3
1	2A	2175	C	3.3
34	2c	182	ILE	3.3
32	2a	1356	G	3.3
41	1j	76	ASN	3.3
1	2A	2176	A	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
36	2e	31	LEU	3.3
33	1b	136	VAL	3.3
32	1a	1034	G	3.3
52	2u	14	TRP	3.3
6	2G	20	ILE	3.2
41	2j	54	PHE	3.2
53	2v	12	A	3.2
33	2b	112	VAL	3.2
1	1A	943	C	3.2
48	2q	99	SER	3.2
33	2b	161	ALA	3.2
33	1b	15	VAL	3.2
43	1l	16	GLU	3.2
23	1l	2	SER	3.2
32	2a	1030	C	3.2
32	1a	1033	G	3.2
26	24	56	VAL	3.2
44	1m	122	LYS	3.2
51	1t	69	GLY	3.2
53	2v	13	A	3.2
33	2b	237	ALA	3.2
32	1a	1447	A	3.1
54	2w	73	A	3.1
29	27	47	ARG	3.1
34	2c	188	LEU	3.1
22	20	3	HIS	3.1
33	2b	184	VAL	3.1
34	2c	68	VAL	3.1
41	1j	77	PRO	3.1
38	2g	4	ARG	3.1
32	2a	1183	A	3.1
1	2A	886	C	3.1
44	2m	4	ILE	3.1
50	2s	77	THR	3.1
21	1Z	141	VAL	3.1
45	2n	44	LEU	3.1
38	2g	152	ALA	3.1
34	2c	48	TYR	3.1
1	1A	1133	G	3.1
32	1a	1001	A	3.1
32	2a	1061	G	3.1
21	2Z	122	ARG	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
21	2Z	170	THR	3.1
32	2a	1060	C	3.1
45	1n	59	ALA	3.0
16	2U	87	GLY	3.0
20	2Y	44	ILE	3.0
41	2j	91	PRO	3.0
1	2A	2802	G	3.0
54	1w	70	G	3.0
1	1A	2136	A	3.0
34	2c	195	VAL	3.0
45	2n	18	VAL	3.0
1	2A	2149	G	3.0
6	2G	146	TYR	3.0
9	2N	83	LYS	3.0
36	2e	20	GLN	3.0
1	2A	2117	A	3.0
32	2a	1092	A	3.0
14	2S	58	LEU	3.0
1	2A	2155	G	3.0
32	2a	89	C	3.0
31	29	25	VAL	3.0
6	2G	139	LEU	2.9
43	2l	29	GLY	2.9
45	2n	47	LEU	2.9
23	2l	2	SER	2.9
1	2A	884	C	2.9
33	1b	163	PHE	2.9
45	2n	25	VAL	2.9
29	27	48	LYS	2.9
17	2V	50	PRO	2.9
45	1n	8	GLU	2.9
26	24	65	ASP	2.9
32	2a	962	C	2.9
41	2j	60	ARG	2.9
22	20	7	LEU	2.9
38	2g	16	LEU	2.9
41	2j	52	GLY	2.9
35	2d	179	GLU	2.9
32	1a	1531	A	2.9
54	1w	73	A	2.9
54	2y	36	A	2.9
33	2b	200	ILE	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	2c	157	ILE	2.9
50	2s	5	LEU	2.9
1	2A	279	C	2.9
22	10	8	GLY	2.9
32	2a	1182	G	2.9
54	1w	71	G	2.9
15	1T	131	ALA	2.9
20	2Y	48	ALA	2.9
33	2b	229	VAL	2.9
50	2s	24	ALA	2.9
21	2Z	149	SER	2.9
34	2c	128	PHE	2.9
53	2v	24	A	2.9
26	14	54	GLY	2.8
50	2s	68	GLY	2.8
1	1A	1110	C	2.8
1	1A	1140	U	2.8
32	2a	1027	C	2.8
33	1b	236	TYR	2.8
7	2H	24	VAL	2.8
12	2Q	121	ALA	2.8
33	1b	186	ALA	2.8
35	1d	111	ALA	2.8
40	2i	15	ALA	2.8
40	2i	17	VAL	2.8
44	1m	123	ALA	2.8
45	2n	3	ARG	2.8
1	2A	901	A	2.8
50	2s	84	GLY	2.8
3	2D	38	LYS	2.8
1	2A	2132	U	2.8
32	1a	1257	U	2.8
1	2A	885	C	2.8
1	2A	2146	C	2.8
26	14	56	VAL	2.8
34	2c	137	ALA	2.8
35	1d	122	ARG	2.8
40	2i	84	ALA	2.8
34	2c	39	ILE	2.8
1	2A	2159	G	2.8
32	1a	1023	G	2.8
32	2a	1031	G	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	2a	1224	G	2.8
1	1A	945	A	2.8
26	24	17	GLY	2.8
36	2e	99	GLY	2.8
41	1j	10	GLY	2.8
41	2j	55	LYS	2.8
38	1g	13	GLN	2.8
51	2t	8	ARG	2.8
41	2j	56	HIS	2.8
34	2c	17	ASP	2.8
50	2s	26	GLY	2.8
1	1A	930	G	2.8
1	2A	2160	G	2.8
20	2Y	57	GLN	2.8
32	2a	1503	A	2.8
33	1b	126	GLU	2.8
52	2u	24	ARG	2.8
50	2s	11	VAL	2.8
33	2b	92	TYR	2.8
43	2l	32	PHE	2.8
1	1A	2135	U	2.8
21	1Z	166	SER	2.8
32	2a	1223	C	2.8
32	2a	1260	C	2.8
54	2w	72	C	2.8
36	2e	114	GLY	2.8
50	2s	2	PRO	2.8
1	1A	1141	A	2.7
1	2A	881	G	2.7
33	2b	196	LEU	2.7
40	1i	50	LEU	2.7
44	2m	78	ILE	2.7
32	2a	1257	U	2.7
16	2U	84	LYS	2.7
21	2Z	154	ASP	2.7
34	2c	41	GLY	2.7
34	2c	174	PRO	2.7
32	1a	1027	C	2.7
21	2Z	139	VAL	2.7
33	2b	71	VAL	2.7
33	1b	201	ILE	2.7
1	2A	906	G	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	2156	G	2.7
32	2a	1034	G	2.7
32	2a	1184	G	2.7
35	2d	154	ASN	2.7
7	2H	55	PRO	2.7
33	2b	167	PRO	2.7
1	1A	2807	C	2.7
19	2X	92	LEU	2.7
33	1b	207	ALA	2.7
1	2A	896	A	2.7
1	2A	2169	A	2.7
32	2a	1286	A	2.7
1	1A	1124	U	2.7
18	2W	112	GLY	2.7
36	2e	29	GLY	2.7
41	2j	100	THR	2.7
44	2m	100	GLY	2.7
54	1y	20	U	2.7
1	2A	882	G	2.7
1	2A	2112	G	2.7
54	2w	71	G	2.7
54	2y	44	G	2.7
21	2Z	52	SER	2.7
50	2s	64	GLU	2.7
34	2c	91	LEU	2.7
41	2j	8	LEU	2.7
1	1A	2814	C	2.7
40	2i	114	TYR	2.7
35	1d	180	GLY	2.7
39	2h	3	THR	2.7
1	1A	1127	U	2.7
32	2a	88	A	2.7
6	2G	48	GLU	2.7
33	2b	213	LEU	2.7
21	2Z	164	ALA	2.6
45	2n	5	ALA	2.6
1	2A	2319	G	2.6
38	2g	85	TYR	2.6
54	1w	74	C	2.6
12	2Q	30	GLY	2.6
31	29	37	GLY	2.6
34	1c	13	GLY	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
34	2c	161	GLU	2.6
41	1j	40	LEU	2.6
44	2m	90	LEU	2.6
32	2a	1531	A	2.6
34	2c	160	ALA	2.6
45	2n	20	ALA	2.6
1	1A	1221	G	2.6
1	1A	2181	G	2.6
1	2A	2805	G	2.6
39	2h	90	GLY	2.6
52	1u	2	GLY	2.6
44	2m	103	THR	2.6
1	2A	2145	C	2.6
35	1d	135	LEU	2.6
35	2d	161	ASN	2.6
51	2t	24	LEU	2.6
9	2N	69	GLN	2.6
24	22	66	GLU	2.6
27	15	60	VAL	2.6
33	2b	185	ILE	2.6
44	2m	22	ILE	2.6
32	2a	994	A	2.6
33	2b	40	HIS	2.6
1	1A	2816	G	2.6
1	2A	2168	G	2.6
7	2H	33	LEU	2.6
32	2a	630	G	2.6
32	2a	1036	G	2.6
32	2a	1222	G	2.6
54	2w	6	G	2.6
16	1U	117	GLN	2.6
47	1p	1	MET	2.6
40	1i	106	ALA	2.6
41	2j	32	ALA	2.6
42	2k	89	ALA	2.6
1	1A	935	C	2.6
1	2A	2128	C	2.6
1	2A	2174	C	2.6
1	1A	1128	U	2.6
5	2F	57	VAL	2.6
33	2b	15	VAL	2.6
33	2b	197	VAL	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
12	2Q	28	ALA	2.6
20	2Y	60	PHE	2.6
40	2i	122	ALA	2.6
1	2A	2147	G	2.5
32	2a	973	G	2.5
32	2a	1117	G	2.5
54	2w	70	G	2.5
45	2n	31	ARG	2.5
32	2a	1116	C	2.5
1	2A	2119	A	2.5
1	2A	2170	A	2.5
32	2a	1287	A	2.5
12	2Q	24	GLY	2.5
21	2Z	150	LEU	2.5
33	1b	44	LEU	2.5
34	1c	39	ILE	2.5
24	12	70	GLN	2.5
28	26	4	GLU	2.5
20	2Y	89	PHE	2.5
38	2g	3	ARG	2.5
45	2n	45	ARG	2.5
1	1A	1220	U	2.5
1	1A	1104	G	2.5
1	2A	2115	G	2.5
1	2A	2154	G	2.5
32	2a	1283	G	2.5
54	1y	15	G	2.5
1	2A	897	C	2.5
32	2a	1114	C	2.5
39	2h	72	PRO	2.5
33	1b	14	GLY	2.5
45	2n	28	GLY	2.5
34	2c	5	ILE	2.5
32	2a	996	A	2.5
32	2a	1030(D)	A	2.5
33	1b	17	PHE	2.5
45	2n	59	ALA	2.5
20	2Y	73	ARG	2.5
1	2A	1026	U	2.5
21	1Z	149	SER	2.5
35	1d	83	SER	2.5
16	2U	98	LEU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	1b	11	LEU	2.5
34	2c	178	LEU	2.5
8	1I	106	GLY	2.5
23	2I	28	GLY	2.5
33	2b	162	ILE	2.5
34	2c	124	ILE	2.5
5	2F	89	VAL	2.5
41	2j	94	VAL	2.5
32	2a	1028	C	2.5
32	2a	1038	C	2.5
32	2a	1354	C	2.5
40	2i	101	PHE	2.5
33	2b	207	ALA	2.5
51	1t	59	ALA	2.5
36	2e	25	ARG	2.5
34	2c	94	LEU	2.5
39	2h	39	LEU	2.5
41	2j	90	LEU	2.5
8	2I	137	PRO	2.5
33	1b	233	SER	2.5
33	2b	216	SER	2.5
39	2h	101	PRO	2.5
1	2A	2109	U	2.5
50	2s	82	GLY	2.5
51	1t	103	GLY	2.5
54	2y	45	U	2.5
7	2H	79	VAL	2.5
17	2V	5	VAL	2.5
33	2b	188	ALA	2.5
34	2c	88	ARG	2.5
44	1m	2	ALA	2.5
45	2n	41	ARG	2.5
49	1r	24	ALA	2.5
51	2t	83	ARG	2.5
1	1A	2815	C	2.5
36	2e	98	THR	2.5
32	2a	1131	G	2.5
32	1a	1035	A	2.5
42	2k	36	ASP	2.4
50	2s	15	LEU	2.4
41	2j	82	ILE	2.4
52	2u	23	PRO	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
21	2Z	71	VAL	2.4
26	24	66	SER	2.4
34	2c	55	VAL	2.4
39	2h	137	VAL	2.4
7	2H	3	ARG	2.4
35	2d	73	ARG	2.4
33	1b	225	ALA	2.4
34	2c	168	ALA	2.4
41	1j	32	ALA	2.4
38	2g	24	THR	2.4
50	2s	79	THR	2.4
50	2s	14	HIS	2.4
1	2A	1509	C	2.4
8	1I	140	LEU	2.4
22	20	84	LEU	2.4
1	2A	2131	G	2.4
1	2A	2157	G	2.4
33	1b	234	PRO	2.4
36	2e	109	ILE	2.4
41	2j	6	ILE	2.4
45	2n	14	PRO	2.4
7	2H	45	VAL	2.4
11	2P	109	GLY	2.4
36	2e	33	VAL	2.4
46	2o	60	VAL	2.4
46	2o	89	GLY	2.4
47	1p	25	ARG	2.4
32	1a	1532	U	2.4
41	2j	83	GLU	2.4
34	1c	187	ALA	2.4
33	2b	31	TYR	2.4
42	2k	50	TYR	2.4
44	2m	59	TYR	2.4
40	2i	64	THR	2.4
14	2S	32	LEU	2.4
33	2b	61	LEU	2.4
34	1c	12	LEU	2.4
39	2h	63	LEU	2.4
40	2i	56	LEU	2.4
21	2Z	53	ILE	2.4
41	2j	96	ILE	2.4
1	2A	2138	C	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	2H	17	VAL	2.4
8	2I	15	VAL	2.4
33	2b	7	VAL	2.4
34	2c	145	GLY	2.4
40	2i	65	VAL	2.4
1	1A	1132	A	2.4
1	1A	2141	A	2.4
32	1a	1286	A	2.4
34	2c	79	ARG	2.4
38	1g	79	ARG	2.4
12	2Q	104	PHE	2.4
32	1a	1036	G	2.4
40	1i	15	ALA	2.4
32	2a	1219	U	2.4
34	2c	201	TYR	2.4
52	2u	17	THR	2.4
50	2s	49	ILE	2.4
33	2b	37	ASN	2.4
9	2N	9	VAL	2.4
21	2Z	165	VAL	2.4
47	2p	2	VAL	2.4
26	24	51	ASP	2.4
36	2e	107	ARG	2.4
40	2i	127	LYS	2.4
1	1A	2160	C	2.4
1	2A	888	C	2.4
1	2A	2137	C	2.4
32	2a	1149	C	2.4
54	2y	56	C	2.4
35	2d	164	ALA	2.4
36	2e	86	ALA	2.4
44	2m	72	ALA	2.4
7	2H	63	SER	2.4
38	2g	86	GLN	2.4
45	2n	32	SER	2.4
32	2a	1253	G	2.4
21	2Z	137	ILE	2.4
40	2i	90	PRO	2.4
33	1b	71	VAL	2.3
36	2e	32	VAL	2.3
40	1i	86	VAL	2.3
19	1X	94	GLY	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
40	1i	91	ASP	2.3
41	2j	89	ASP	2.3
15	1T	130	ALA	2.3
33	1b	34	ALA	2.3
1	1A	931	C	2.3
1	2A	894	C	2.3
32	2a	1363	C	2.3
20	1Y	1	MET	2.3
32	1a	1030(D)	A	2.3
32	2a	965	A	2.3
35	1d	152	SER	2.3
34	2c	67	THR	2.3
45	2n	6	LEU	2.3
34	2c	45	LYS	2.3
41	2j	37	PRO	2.3
1	2A	2151	G	2.3
32	1a	1031	G	2.3
32	2a	1190	G	2.3
34	2c	151	VAL	2.3
39	2h	129	VAL	2.3
52	1u	24	ARG	2.3
54	1y	18	G	2.3
20	2Y	10	GLY	2.3
38	1g	81	GLY	2.3
14	2S	12	PHE	2.3
35	1d	110	PHE	2.3
40	2i	2	GLU	2.3
21	2Z	153	SER	2.3
21	2Z	157	LEU	2.3
33	2b	109	SER	2.3
41	2j	40	LEU	2.3
32	1a	91	C	2.3
1	1A	1142	A	2.3
34	1c	14	ILE	2.3
40	2i	4	TYR	2.3
40	2i	49	PRO	2.3
46	2o	68	ARG	2.3
21	2Z	96	VAL	2.3
26	24	50	VAL	2.3
38	2g	66	VAL	2.3
45	2n	56	VAL	2.3
45	2n	51	GLY	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1A	2137	G	2.3
1	2A	1533	G	2.3
1	2A	2153	G	2.3
6	1G	48	GLU	2.3
44	2m	58	GLU	2.3
19	1X	95	LEU	2.3
33	2b	221	LEU	2.3
6	1G	182	LYS	2.3
47	1p	69	THR	2.3
6	2G	136	ARG	2.3
38	1g	32	ARG	2.3
40	2i	128	ARG	2.3
41	2j	41	PRO	2.3
1	2A	2111	C	2.3
32	2a	999	C	2.3
32	2a	1059	C	2.3
41	2j	44	VAL	2.3
54	2y	33	U	2.3
39	2h	128	GLY	2.3
34	2c	3	ASN	2.3
36	2e	130	ASN	2.3
7	2H	20	ALA	2.3
20	2Y	1	MET	2.3
22	20	2	ALA	2.3
33	1b	129	GLU	2.3
33	2b	101	MET	2.3
36	2e	54	ALA	2.3
39	1h	2	LEU	2.3
40	2i	99	LEU	2.3
14	2S	33	LYS	2.3
41	2j	99	LYS	2.3
9	2N	38	HIS	2.3
32	1a	1032	G	2.3
32	2a	987	G	2.3
32	2a	1042	G	2.3
32	2a	1058	G	2.3
41	2j	62	HIS	2.3
43	1l	6	THR	2.3
21	2Z	27	VAL	2.3
33	1b	164	VAL	2.3
36	2e	55	VAL	2.3
12	2Q	15	GLY	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
21	2Z	143	GLY	2.3
40	2i	39	GLY	2.3
51	2t	103	GLY	2.3
52	2u	11	GLY	2.3
1	1A	944	C	2.2
32	1a	1030	C	2.2
54	2w	7	A	2.2
54	2y	67	C	2.2
8	1I	43	ASN	2.2
8	2I	46	ALA	2.2
18	2W	89	ALA	2.2
34	2c	187	ALA	2.2
36	2e	30	ALA	2.2
40	2i	102	LEU	2.2
41	2j	85	LEU	2.2
23	2l	78	LYS	2.2
50	2s	56	GLN	2.2
34	1c	62	ASP	2.2
38	2g	27	ILE	2.2
39	2h	35	ILE	2.2
20	2Y	6	HIS	2.2
35	1d	153	ARG	2.2
38	2g	76	ARG	2.2
36	2e	120	THR	2.2
21	2Z	174	VAL	2.2
33	1b	7	VAL	2.2
33	1b	202	PRO	2.2
34	2c	193	TYR	2.2
42	2k	25	TYR	2.2
1	1A	926	G	2.2
1	1A	2187	G	2.2
32	1a	1026	G	2.2
32	2a	1024	G	2.2
32	2a	1032	G	2.2
54	2y	53	G	2.2
34	2c	13	GLY	2.2
21	2Z	88	PHE	2.2
1	1A	2906	U	2.2
33	2b	170	GLU	2.2
34	2c	200	ALA	2.2
45	2n	30	ALA	2.2
39	2h	133	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	2139	C	2.2
32	2a	977	A	2.2
32	2a	1004	A	2.2
32	2a	1285	A	2.2
33	1b	187	LEU	2.2
6	2G	52	ILE	2.2
26	14	58	ARG	2.2
34	2c	6	HIS	2.2
34	2c	62	ASP	2.2
6	2G	160	VAL	2.2
34	2c	95	THR	2.2
47	1p	67	THR	2.2
7	2H	38	SER	2.2
20	2Y	55	TYR	2.2
34	2c	158	GLY	2.2
35	1d	167	GLY	2.2
40	2i	67	GLY	2.2
34	2c	10	PHE	2.2
1	2A	2308	G	2.2
10	2O	76	ALA	2.2
14	2S	57	LYS	2.2
1	1A	2173	G	2.2
32	2a	1215	G	2.2
32	2a	1276	G	2.2
34	2c	53	ALA	2.2
38	2g	2	ALA	2.2
44	1m	27	LYS	2.2
44	2m	122	LYS	2.2
48	2q	98	LEU	2.2
50	2s	70	LYS	2.2
54	2y	65	G	2.2
9	2N	115	ARG	2.2
33	1b	208	ILE	2.2
35	1d	35	ARG	2.2
36	2e	24	ARG	2.2
41	2j	98	ILE	2.2
46	2o	65	ARG	2.2
32	2a	1035	A	2.2
32	2a	1029	C	2.2
32	2a	1210	C	2.2
45	2n	49	HIS	2.2
54	1w	72	C	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
6	2G	97	ASP	2.2
6	2G	87	PRO	2.2
38	2g	88	PRO	2.2
42	2k	114	VAL	2.2
41	2j	87	THR	2.2
9	2N	1	MET	2.2
20	2Y	80	GLY	2.2
21	2Z	3	TYR	2.2
40	2i	68	GLY	2.2
40	2i	71	SER	2.2
40	2i	126	SER	2.2
33	2b	17	PHE	2.2
40	2i	18	PHE	2.2
50	2s	22	LEU	2.2
38	2g	83	ALA	2.2
42	2k	15	ALA	2.2
34	2c	8	ILE	2.2
1	1A	1143	U	2.2
1	2A	2113	U	2.2
41	2j	5	ARG	2.2
50	2s	78	ARG	2.2
6	2G	41	GLN	2.2
1	1A	694	G	2.2
1	2A	2110	G	2.2
32	2a	1274	G	2.2
33	1b	19	HIS	2.2
1	2A	866	A	2.2
1	2A	2134	A	2.2
7	2H	11	VAL	2.2
17	2V	52	VAL	2.2
21	2Z	87	ASP	2.2
32	1a	1503	A	2.2
34	2c	106	VAL	2.2
37	2f	6	VAL	2.2
39	2h	4	ASP	2.2
42	2k	113	PRO	2.2
46	2o	27	VAL	2.2
15	2T	1	MET	2.2
32	2a	1244	C	2.2
36	2e	10	MET	2.2
54	2w	4	C	2.2
17	2V	101	GLY	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
39	2h	88	LYS	2.2
41	2j	10	GLY	2.2
44	2m	26	GLY	2.2
52	2u	19	GLY	2.2
45	2n	21	TYR	2.2
38	2g	5	ARG	2.1
38	2g	110	GLN	2.1
48	1q	93	GLN	2.1
1	1A	271	U	2.1
33	2b	125	PRO	2.1
41	2j	72	VAL	2.1
40	2i	105	ASP	2.1
1	1A	2146	G	2.1
1	2A	2127	G	2.1
1	2A	2162	G	2.1
32	1a	78	G	2.1
32	2a	1030(C)	G	2.1
32	2a	1047	G	2.1
32	2a	1160	G	2.1
33	2b	47	THR	2.1
38	1g	132	GLY	2.1
53	2v	15	A	2.1
54	1y	69	G	2.1
54	2w	65	G	2.1
1	1A	2167	C	2.1
6	1G	80	PHE	2.1
6	2G	133	LEU	2.1
32	2a	1043	C	2.1
33	2b	121	LEU	2.1
46	1o	69	TYR	2.1
21	2Z	152	ALA	2.1
33	2b	225	ALA	2.1
39	2h	29	SER	2.1
40	2i	119	ALA	2.1
42	2k	24	SER	2.1
33	2b	175	ARG	2.1
34	1c	79	ARG	2.1
33	1b	41	ILE	2.1
39	2h	86	ILE	2.1
45	2n	42	ILE	2.1
18	1W	111	HIS	2.1
20	2Y	45	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
32	1a	203	U	2.1
32	2a	90	U	2.1
50	1s	9	VAL	2.1
35	2d	165	MET	2.1
6	2G	74	LYS	2.1
12	2Q	22	LYS	2.1
11	2P	26	GLY	2.1
40	2i	8	GLY	2.1
52	2u	8	THR	2.1
35	2d	188	LEU	2.1
40	1i	59	PHE	2.1
44	2m	81	LEU	2.1
46	2o	18	PHE	2.1
1	2A	2171	A	2.1
2	2B	120	A	2.1
32	2a	975	A	2.1
33	2b	21	ARG	2.1
35	1d	118	ARG	2.1
38	2g	79	ARG	2.1
40	2i	13	ALA	2.1
41	2j	26	ALA	2.1
45	2n	29	ARG	2.1
53	2v	23	A	2.1
1	2A	2893	G	2.1
14	2S	40	ILE	2.1
32	2a	1017	G	2.1
32	2a	1255	G	2.1
32	2a	1355	G	2.1
1	2A	2804	C	2.1
32	1a	1038	C	2.1
54	2w	13	C	2.1
35	2d	160	GLN	2.1
36	1e	72	GLN	2.1
3	1D	275	LYS	2.1
22	20	4	LYS	2.1
41	1j	78	ASN	2.1
32	2a	997	U	2.1
6	2G	43	LEU	2.1
7	2H	174	GLY	2.1
35	1d	124	GLY	2.1
33	1b	24	TRP	2.1
35	1d	132	ARG	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
41	1j	43	ARG	2.1
14	2S	7	TYR	2.1
34	1c	84	ILE	2.1
41	1j	97	GLU	2.1
1	2A	2135	A	2.1
32	1a	149	A	2.1
32	2a	1447	A	2.1
51	2t	73	HIS	2.1
1	1A	1105	G	2.1
1	1A	1117	G	2.1
1	1A	2228	G	2.1
1	2A	2100	G	2.1
1	2A	2304	G	2.1
54	1y	62	C	2.1
20	2Y	42	VAL	2.1
22	20	5	LYS	2.1
32	1a	346	G	2.1
32	1a	1024	G	2.1
32	1a	1030(A)	G	2.1
32	2a	1202	G	2.1
36	2e	51	VAL	2.1
26	24	29	PRO	2.1
41	2j	71	LEU	2.1
47	2p	74	LEU	2.1
48	2q	31	LEU	2.1
6	2G	24	GLY	2.1
26	24	54	GLY	2.1
34	2c	9	GLY	2.1
36	2e	28	PHE	2.1
6	2G	115	ARG	2.1
33	1b	13	ALA	2.1
35	1d	5	ILE	2.1
35	2d	204	ILE	2.1
34	2c	29	TYR	2.1
38	2g	154	TYR	2.1
7	2H	41	MET	2.0
33	1b	40	HIS	2.0
1	1A	946	A	2.0
32	1a	160	A	2.0
32	2a	1179	A	2.0
34	1c	207	VAL	2.0
1	1A	2168	C	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2A	2108	C	2.0
32	2a	1214	C	2.0
41	1j	8	LEU	2.0
1	1A	2163	G	2.0
1	2A	2116	G	2.0
2	2B	19	G	2.0
12	2Q	6	ARG	2.0
16	2U	73	GLY	2.0
23	2I	76	ARG	2.0
32	1a	630	G	2.0
32	2a	1001(A)	G	2.0
35	2d	23	GLY	2.0
35	2d	209	ARG	2.0
36	2e	84	PHE	2.0
44	2m	29	ARG	2.0
46	2o	88	ARG	2.0
52	1u	19	GLY	2.0
54	2y	1	G	2.0
54	2y	18	G	2.0
14	2S	35	ILE	2.0
51	1t	94	ALA	2.0
12	2Q	139	GLU	2.0
34	1c	18	TRP	2.0
12	2Q	18	LYS	2.0
33	1b	33	TYR	2.0
15	2T	66	VAL	2.0
33	1b	229	VAL	2.0
33	1b	125	PRO	2.0
45	2n	40	CYS	2.0
1	2A	229	A	2.0
1	2A	278	A	2.0
33	2b	142	LEU	2.0
33	2b	180	LEU	2.0
35	1d	157	LEU	2.0
44	2m	66	LEU	2.0
54	2y	35	A	2.0
20	1Y	50	ARG	2.0
22	20	11	ARG	2.0
26	24	49	PHE	2.0
41	1j	36	GLY	2.0
46	1o	89	GLY	2.0
32	1a	1030(B)	C	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
12	2Q	49	ALA	2.0
15	2T	130	ALA	2.0
15	2T	131	ALA	2.0
35	2d	48	ALA	2.0
38	1g	83	ALA	2.0
38	2g	150	ALA	2.0
41	2j	67	THR	2.0
1	1A	1112	U	2.0
1	2A	2118	U	2.0
1	2A	2150	U	2.0
9	2N	136	GLU	2.0
10	2O	81	ASP	2.0
32	2a	1062	U	2.0
33	2b	189	ASP	2.0
40	2i	91	ASP	2.0
42	1k	36	ASP	2.0
50	1s	13	ASP	2.0
1	1A	1584	G	2.0
1	2A	2106	G	2.0
1	2A	2318	G	2.0
4	1E	73	GLU	2.0
32	2a	1021	G	2.0
32	2a	1220	G	2.0
34	2c	167	TRP	2.0
26	14	63	TYR	2.0
26	24	63	TYR	2.0
7	2H	26	VAL	2.0
44	2m	74	VAL	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	2y	55	20/21	0.57	0.20	79,93,100,105	0
54	7MG	2y	46	24/25	0.59	0.20	84,90,96,114	0
54	7MG	1w	46	24/25	0.59	0.15	67,77,94,110	0
54	7MG	1y	46	24/25	0.63	0.17	73,85,99,104	0
54	7MG	2w	46	24/25	0.64	0.16	71,87,94,109	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
54	5MU	2y	54	21/22	0.65	0.17	76,85,92,102	0
54	PSU	1y	55	20/21	0.66	0.15	78,86,93,105	0
54	MIA	2y	37	22/30	0.66	0.17	64,78,97,111	0
54	4SU	2w	8	20/21	0.70	0.15	78,86,91,102	0
54	MIA	1y	37	22/30	0.75	0.15	62,72,77,85	0
54	5MU	1y	54	21/22	0.76	0.14	78,82,88,97	0
43	0TD	2l	92	10/11	0.78	0.16	52,60,64,75	0
54	4SU	2y	8	20/21	0.79	0.13	79,88,94,100	0
54	PSU	2y	32	20/21	0.80	0.19	65,77,84,86	0
32	2MG	2a	1207	24/25	0.82	0.14	68,74,82,88	0
54	PSU	1y	32	20/21	0.83	0.17	64,71,75,82	0
54	PSU	2w	55	20/21	0.83	0.12	64,79,86,88	0
54	4SU	1y	8	20/21	0.83	0.12	77,82,89,92	0
54	PSU	2y	39	20/21	0.84	0.15	72,77,89,97	0
54	5MU	2w	54	21/22	0.84	0.10	66,71,77,82	0
54	PSU	2w	32	20/21	0.85	0.12	70,78,89,93	0
1	5MU	2A	1915	21/22	0.86	0.13	63,70,76,88	0
43	0TD	1l	92	10/11	0.86	0.16	38,44,52,72	0
55	5MU	2x	54	21/22	0.86	0.11	65,73,79,82	0
55	PSU	2x	55	20/21	0.86	0.11	66,75,77,78	0
55	5MC	2x	32	21/22	0.87	0.15	57,66,73,74	0
32	M2G	2a	966	25/26	0.88	0.14	48,59,69,78	0
1	PSU	2A	1911	20/21	0.88	0.12	54,62,67,68	0
55	4SU	2x	8	20/21	0.88	0.12	64,75,77,77	0
54	PSU	1w	55	20/21	0.89	0.11	54,67,73,75	0
54	PSU	1y	39	20/21	0.89	0.12	61,69,75,82	0
32	5MC	2a	1400	21/22	0.89	0.18	63,66,71,75	0
1	4OC	2A	1920	21/23	0.89	0.13	53,60,63,65	0
32	PSU	2a	516	20/21	0.90	0.10	61,68,74,74	0
54	MIA	2w	37	25/30	0.90	0.12	63,70,76,85	0
32	7MG	2a	527	24/25	0.90	0.13	51,57,66,74	0
1	PSU	2A	1917	20/21	0.90	0.10	52,61,72,74	0
54	4SU	1w	8	20/21	0.91	0.09	65,70,76,79	0
32	4OC	2a	1402	22/23	0.91	0.12	52,62,65,65	0
54	5MU	1w	54	21/22	0.91	0.10	46,56,65,71	0
54	PSU	2w	39	20/21	0.91	0.10	63,71,75,79	0
32	5MC	2a	1407	21/22	0.91	0.12	45,53,58,61	0
32	5MC	2a	967	21/22	0.91	0.12	56,62,70,74	0
54	PSU	1w	32	20/21	0.91	0.12	54,60,77,78	0
32	UR3	2a	1498	21/22	0.92	0.13	44,57,63,66	0
55	5MU	1x	54	21/22	0.92	0.09	50,57,63,68	0
55	5MC	1x	32	21/22	0.93	0.12	43,50,54,58	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	5MC	2a	1404	21/22	0.93	0.12	50,56,61,66	0
32	MA6	2a	1518	24/25	0.93	0.11	46,64,67,69	0
55	4SU	1x	8	20/21	0.93	0.11	46,54,68,74	0
55	PSU	1x	55	20/21	0.93	0.09	41,51,60,65	0
1	5MU	1A	1937	21/22	0.93	0.10	38,48,53,61	0
1	5MU	2A	1939	21/22	0.94	0.10	30,38,42,42	0
1	PSU	1A	1939	20/21	0.94	0.10	38,45,50,52	0
32	PSU	1a	516	20/21	0.94	0.09	39,50,55,56	0
32	7MG	1a	527	24/25	0.94	0.10	39,45,48,52	0
32	M2G	1a	966	25/26	0.94	0.11	33,45,55,56	0
32	2MG	1a	1207	24/25	0.94	0.10	50,59,63,65	0
32	MA6	2a	1519	24/25	0.94	0.12	46,57,63,65	0
54	PSU	1w	39	20/21	0.95	0.10	44,55,60,63	0
32	5MC	1a	967	21/22	0.95	0.10	38,49,53,55	0
32	5MC	1a	1404	21/22	0.95	0.10	30,36,40,44	0
1	5MC	2A	1962	21/22	0.95	0.09	39,48,55,58	0
1	5MC	1A	1964	21/22	0.96	0.09	24,30,36,39	0
32	5MC	1a	1407	21/22	0.96	0.08	29,34,39,42	0
54	MIA	1w	37	29/30	0.96	0.10	35,48,55,63	0
1	5MU	1A	1961	21/22	0.96	0.09	15,21,26,34	0
1	5MC	2A	1942	21/22	0.96	0.10	44,52,59,61	0
32	5MC	1a	1400	21/22	0.96	0.09	33,44,49,57	0
1	OMG	2A	2251	24/25	0.96	0.09	34,40,45,47	0
1	2MA	2A	2503	23/24	0.96	0.09	26,29,33,34	0
1	PSU	2A	2605	20/21	0.96	0.08	26,37,41,42	0
32	4OC	1a	1402	22/23	0.96	0.09	37,41,51,56	0
32	UR3	1a	1498	21/22	0.97	0.07	28,35,39,40	0
32	MA6	1a	1518	24/25	0.97	0.10	25,33,39,39	0
32	MA6	1a	1519	24/25	0.97	0.08	29,35,39,41	0
1	2MU	2A	2552	21/23	0.97	0.09	32,38,45,57	0
1	2MU	1A	2564	21/23	0.97	0.07	14,20,26,28	0
1	4OC	1A	1942	21/23	0.97	0.09	27,36,42,43	0
1	PSU	1A	1933	20/21	0.98	0.07	33,40,47,48	0
1	PSU	1A	2617	20/21	0.98	0.06	15,18,23,23	0
1	5MC	1A	1984	21/22	0.98	0.07	20,27,30,40	0
1	OMG	1A	2263	24/25	0.98	0.07	13,19,21,24	0
1	2MA	1A	2515	23/24	0.98	0.07	7,11,15,21	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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
56	MG	2a	3208	1/1	0.42	0.26	69,69,69,69	0
56	MG	2A	3675	1/1	0.54	0.29	63,63,63,63	0
56	MG	1A	3975	1/1	0.55	0.23	21,21,21,21	0
56	MG	1w	110	1/1	0.55	0.17	79,79,79,79	0
56	MG	2y	104	1/1	0.55	0.19	85,85,85,85	0
56	MG	2j	8001	1/1	0.57	0.16	77,77,77,77	0
56	MG	1a	3109	1/1	0.57	0.24	70,70,70,70	0
56	MG	2a	3194	1/1	0.58	0.22	71,71,71,71	0
56	MG	2a	3113	1/1	0.58	0.19	72,72,72,72	0
56	MG	2A	3723	1/1	0.60	0.18	65,65,65,65	0
56	MG	1A	3891	1/1	0.60	0.23	74,74,74,74	0
56	MG	2A	3850	1/1	0.62	0.22	67,67,67,67	0
56	MG	2A	3290	1/1	0.65	0.21	77,77,77,77	0
56	MG	2A	3575	1/1	0.65	0.19	38,38,38,38	0
56	MG	2U	202	1/1	0.65	0.15	63,63,63,63	0
56	MG	1a	3145	1/1	0.65	0.25	78,78,78,78	0
56	MG	2A	3542	1/1	0.66	0.17	52,52,52,52	0
56	MG	2A	3741	1/1	0.67	0.25	76,76,76,76	0
56	MG	1A	4023	1/1	0.67	0.15	31,31,31,31	0
56	MG	1A	3916	1/1	0.67	0.15	26,26,26,26	0
56	MG	1A	3770	1/1	0.67	0.16	43,43,43,43	0
56	MG	2a	3198	1/1	0.68	0.20	59,59,59,59	0
56	MG	2A	3650	1/1	0.68	0.24	53,53,53,53	0
56	MG	2A	3671	1/1	0.68	0.14	47,47,47,47	0
56	MG	1a	3194	1/1	0.68	0.19	55,55,55,55	0
56	MG	2B	3009	1/1	0.69	0.16	60,60,60,60	0
56	MG	2R	202	1/1	0.69	0.17	51,51,51,51	0
56	MG	2A	3669	1/1	0.69	0.15	64,64,64,64	0
56	MG	1A	3244	1/1	0.70	0.14	65,65,65,65	0
56	MG	1a	3187	1/1	0.70	0.17	77,77,77,77	0
56	MG	2v	102	1/1	0.70	0.18	62,62,62,62	0
56	MG	2y	101	1/1	0.70	0.20	59,59,59,59	0
56	MG	2A	3651	1/1	0.70	0.13	56,56,56,56	0
56	MG	2A	3627	1/1	0.71	0.14	60,60,60,60	0
56	MG	2A	3338	1/1	0.71	0.20	66,66,66,66	0
56	MG	2A	3224	1/1	0.71	0.23	58,58,58,58	0
56	MG	2A	3204	1/1	0.71	0.43	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	2A	3743	1/1	0.71	0.18	47,47,47,47	0
56	MG	2A	3766	1/1	0.71	0.17	85,85,85,85	0
56	MG	2A	3022	1/1	0.72	0.10	51,51,51,51	0
56	MG	2A	3247	1/1	0.72	0.30	64,64,64,64	0
56	MG	2A	3584	1/1	0.72	0.14	52,52,52,52	0
56	MG	2A	3089	1/1	0.72	0.24	56,56,56,56	0
56	MG	1A	4078	1/1	0.72	0.13	37,37,37,37	0
56	MG	1A	4019	1/1	0.73	0.14	29,29,29,29	0
56	MG	2A	3863	1/1	0.73	0.15	70,70,70,70	0
56	MG	1a	3169	1/1	0.73	0.22	57,57,57,57	0
56	MG	2B	3017	1/1	0.73	0.12	58,58,58,58	0
56	MG	2j	8002	1/1	0.73	0.16	77,77,77,77	0
56	MG	2A	3207	1/1	0.73	0.09	48,48,48,48	0
56	MG	2A	3757	1/1	0.73	0.15	50,50,50,50	0
56	MG	1A	3968	1/1	0.73	0.14	53,53,53,53	0
56	MG	2a	3195	1/1	0.74	0.13	69,69,69,69	0
56	MG	2A	3115	1/1	0.74	0.20	64,64,64,64	0
56	MG	2A	3170	1/1	0.74	0.23	66,66,66,66	0
56	MG	28	101	1/1	0.74	0.19	60,60,60,60	0
56	MG	2A	3686	1/1	0.74	0.20	52,52,52,52	0
56	MG	2a	3178	1/1	0.74	0.30	70,70,70,70	0
56	MG	2a	3180	1/1	0.74	0.18	65,65,65,65	0
56	MG	1A	4009	1/1	0.74	0.14	56,56,56,56	0
56	MG	2A	3006	1/1	0.75	0.13	51,51,51,51	0
56	MG	2F	301	1/1	0.75	0.16	58,58,58,58	0
56	MG	2G	3001	1/1	0.75	0.20	62,62,62,62	0
56	MG	2A	3659	1/1	0.75	0.12	64,64,64,64	0
56	MG	2A	3244	1/1	0.75	0.17	65,65,65,65	0
56	MG	20	3001	1/1	0.75	0.14	57,57,57,57	0
56	MG	1A	3458	1/1	0.75	0.12	49,49,49,49	0
56	MG	2A	3285	1/1	0.75	0.14	68,68,68,68	0
56	MG	2A	3084	1/1	0.75	0.43	71,71,71,71	0
56	MG	2A	3690	1/1	0.75	0.19	68,68,68,68	0
56	MG	1A	4033	1/1	0.75	0.20	55,55,55,55	0
56	MG	2A	3473	1/1	0.75	0.12	71,71,71,71	0
56	MG	1A	3591	1/1	0.75	0.27	38,38,38,38	0
56	MG	2A	3165	1/1	0.75	0.14	53,53,53,53	0
56	MG	15	104	1/1	0.75	0.16	40,40,40,40	0
56	MG	2A	3810	1/1	0.75	0.12	44,44,44,44	0
56	MG	2A	3587	1/1	0.75	0.23	68,68,68,68	0
56	MG	1A	3187	1/1	0.75	0.14	51,51,51,51	0
56	MG	1y	105	1/1	0.75	0.10	81,81,81,81	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	3221	1/1	0.76	0.22	61,61,61,61	0
56	MG	2A	3695	1/1	0.76	0.12	55,55,55,55	0
56	MG	1v	3001	1/1	0.76	0.16	67,67,67,67	0
56	MG	1w	104	1/1	0.76	0.22	54,54,54,54	0
56	MG	2A	3154	1/1	0.76	0.14	56,56,56,56	0
56	MG	1B	3027	1/1	0.76	0.12	59,59,59,59	0
56	MG	1A	3837	1/1	0.76	0.14	22,22,22,22	0
56	MG	19	101	1/1	0.76	0.25	33,33,33,33	0
56	MG	1B	3007	1/1	0.76	0.20	56,56,56,56	0
56	MG	2A	3075	1/1	0.76	0.17	62,62,62,62	0
56	MG	2Q	204	1/1	0.77	0.14	49,49,49,49	0
56	MG	2A	3682	1/1	0.77	0.18	37,37,37,37	0
56	MG	2A	3425	1/1	0.77	0.15	56,56,56,56	0
56	MG	2A	3168	1/1	0.77	0.16	71,71,71,71	0
56	MG	2A	3481	1/1	0.77	0.15	47,47,47,47	0
56	MG	2a	3033	1/1	0.77	0.23	61,61,61,61	0
56	MG	1B	3023	1/1	0.77	0.12	65,65,65,65	0
56	MG	2A	3021	1/1	0.77	0.21	64,64,64,64	0
56	MG	1A	3777	1/1	0.77	0.14	37,37,37,37	0
56	MG	1A	3924	1/1	0.77	0.15	40,40,40,40	0
56	MG	2A	3607	1/1	0.77	0.14	56,56,56,56	0
56	MG	2A	3225	1/1	0.77	0.17	69,69,69,69	0
56	MG	2a	3200	1/1	0.77	0.22	64,64,64,64	0
56	MG	1A	3676	1/1	0.77	0.19	32,32,32,32	0
56	MG	1a	3028	1/1	0.77	0.17	53,53,53,53	0
56	MG	1a	3097	1/1	0.77	0.17	59,59,59,59	0
56	MG	1A	3845	1/1	0.77	0.18	41,41,41,41	0
56	MG	2w	3002	1/1	0.77	0.11	46,46,46,46	0
56	MG	2A	3323	1/1	0.77	0.22	54,54,54,54	0
56	MG	1A	3611	1/1	0.77	0.09	63,63,63,63	0
56	MG	2A	3443	1/1	0.78	0.11	50,50,50,50	0
56	MG	2A	3143	1/1	0.78	0.15	51,51,51,51	0
56	MG	2a	3149	1/1	0.78	0.18	62,62,62,62	0
56	MG	2a	3172	1/1	0.78	0.24	67,67,67,67	0
56	MG	2A	3837	1/1	0.78	0.14	62,62,62,62	0
56	MG	1A	4058	1/1	0.78	0.13	71,71,71,71	0
56	MG	1a	3001	1/1	0.78	0.29	65,65,65,65	0
56	MG	1a	3235	1/1	0.78	0.12	68,68,68,68	0
56	MG	2B	3015	1/1	0.78	0.14	54,54,54,54	0
56	MG	2a	3199	1/1	0.78	0.22	57,57,57,57	0
56	MG	1a	3016	1/1	0.78	0.12	51,51,51,51	0
56	MG	1a	3149	1/1	0.78	0.24	67,67,67,67	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	3603	1/1	0.78	0.12	44,44,44,44	0
56	MG	1A	3939	1/1	0.78	0.11	32,32,32,32	0
56	MG	2A	3343	1/1	0.78	0.16	65,65,65,65	0
56	MG	2v	103	1/1	0.78	0.20	60,60,60,60	0
56	MG	1a	3055	1/1	0.78	0.20	68,68,68,68	0
56	MG	2A	3745	1/1	0.78	0.12	56,56,56,56	0
56	MG	2A	3432	1/1	0.78	0.13	65,65,65,65	0
56	MG	1V	202	1/1	0.79	0.11	52,52,52,52	0
56	MG	2A	3830	1/1	0.79	0.19	51,51,51,51	0
56	MG	1A	4034	1/1	0.79	0.14	53,53,53,53	0
56	MG	2A	3838	1/1	0.79	0.12	61,61,61,61	0
56	MG	2A	3510	1/1	0.79	0.13	37,37,37,37	0
56	MG	1A	3282	1/1	0.79	0.14	48,48,48,48	0
56	MG	2A	3563	1/1	0.79	0.11	46,46,46,46	0
56	MG	1A	3253	1/1	0.79	0.12	43,43,43,43	0
56	MG	1a	3167	1/1	0.79	0.13	51,51,51,51	0
56	MG	2A	3346	1/1	0.79	0.11	70,70,70,70	0
56	MG	2A	3588	1/1	0.79	0.27	70,70,70,70	0
56	MG	2a	3224	1/1	0.79	0.10	51,51,51,51	0
56	MG	2A	3377	1/1	0.79	0.16	56,56,56,56	0
56	MG	2A	3396	1/1	0.79	0.10	58,58,58,58	0
56	MG	1A	3803	1/1	0.79	0.11	24,24,24,24	0
56	MG	1A	3495	1/1	0.79	0.10	61,61,61,61	0
56	MG	1A	3681	1/1	0.79	0.24	49,49,49,49	0
56	MG	2w	3005	1/1	0.79	0.10	66,66,66,66	0
56	MG	2x	3002	1/1	0.79	0.17	69,69,69,69	0
56	MG	2A	3767	1/1	0.79	0.12	39,39,39,39	0
56	MG	2a	3105	1/1	0.79	0.24	55,55,55,55	0
56	MG	2a	3170	1/1	0.80	0.21	55,55,55,55	0
56	MG	2a	3171	1/1	0.80	0.10	53,53,53,53	0
56	MG	2A	3742	1/1	0.80	0.16	69,69,69,69	0
56	MG	1A	3502	1/1	0.80	0.11	62,62,62,62	0
56	MG	1A	3884	1/1	0.80	0.20	35,35,35,35	0
56	MG	2A	3261	1/1	0.80	0.16	57,57,57,57	0
56	MG	2A	3192	1/1	0.80	0.22	67,67,67,67	0
56	MG	1A	3940	1/1	0.80	0.18	36,36,36,36	0
56	MG	1A	3825	1/1	0.80	0.10	28,28,28,28	0
56	MG	1A	3713	1/1	0.80	0.11	66,66,66,66	0
56	MG	2a	3201	1/1	0.80	0.18	70,70,70,70	0
56	MG	2A	3339	1/1	0.80	0.10	68,68,68,68	0
56	MG	2a	3211	1/1	0.80	0.17	62,62,62,62	0
56	MG	2A	3608	1/1	0.80	0.23	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	3008	1/1	0.80	0.17	54,54,54,54	0
56	MG	2a	3025	1/1	0.80	0.16	58,58,58,58	0
56	MG	2A	3841	1/1	0.80	0.14	62,62,62,62	0
56	MG	2a	3050	1/1	0.80	0.12	57,57,57,57	0
56	MG	2a	3076	1/1	0.80	0.31	64,64,64,64	0
56	MG	2A	3493	1/1	0.80	0.19	46,46,46,46	0
56	MG	2x	3001	1/1	0.80	0.19	60,60,60,60	0
56	MG	2A	3856	1/1	0.80	0.18	35,35,35,35	0
56	MG	2a	3141	1/1	0.80	0.10	71,71,71,71	0
56	MG	1A	4039	1/1	0.80	0.12	54,54,54,54	0
56	MG	2A	3549	1/1	0.81	0.12	34,34,34,34	0
56	MG	1A	3161	1/1	0.81	0.18	49,49,49,49	0
56	MG	1a	3183	1/1	0.81	0.18	64,64,64,64	0
56	MG	2a	3024	1/1	0.81	0.10	58,58,58,58	0
56	MG	1A	3810	1/1	0.81	0.12	27,27,27,27	0
56	MG	2A	3036	1/1	0.81	0.17	66,66,66,66	0
56	MG	1A	4036	1/1	0.81	0.11	37,37,37,37	0
56	MG	2a	3055	1/1	0.81	0.19	70,70,70,70	0
56	MG	1a	3069	1/1	0.81	0.12	53,53,53,53	0
56	MG	2A	3873	1/1	0.81	0.26	41,41,41,41	0
56	MG	1A	3932	1/1	0.81	0.11	25,25,25,25	0
56	MG	1A	3821	1/1	0.81	0.16	49,49,49,49	0
56	MG	2A	3625	1/1	0.81	0.14	53,53,53,53	0
56	MG	2A	3139	1/1	0.81	0.20	69,69,69,69	0
56	MG	1A	3765	1/1	0.81	0.14	18,18,18,18	0
56	MG	1A	4080	1/1	0.81	0.11	39,39,39,39	0
56	MG	1x	102	1/1	0.81	0.20	50,50,50,50	0
56	MG	2x	3004	1/1	0.81	0.17	59,59,59,59	0
56	MG	1a	3013	1/1	0.81	0.21	48,48,48,48	0
56	MG	2a	3189	1/1	0.81	0.14	73,73,73,73	0
56	MG	1B	3034	1/1	0.82	0.15	59,59,59,59	0
56	MG	2a	3125	1/1	0.82	0.10	78,78,78,78	0
56	MG	1O	3001	1/1	0.82	0.12	60,60,60,60	0
56	MG	1A	3997	1/1	0.82	0.14	52,52,52,52	0
56	MG	2A	3455	1/1	0.82	0.17	61,61,61,61	0
56	MG	1Z	303	1/1	0.82	0.07	56,56,56,56	0
56	MG	2A	3478	1/1	0.82	0.15	40,40,40,40	0
56	MG	1A	3392	1/1	0.82	0.12	33,33,33,33	0
56	MG	2A	3672	1/1	0.82	0.12	67,67,67,67	0
56	MG	2B	3014	1/1	0.82	0.12	58,58,58,58	0
56	MG	1A	3258	1/1	0.82	0.14	47,47,47,47	0
56	MG	2A	3291	1/1	0.82	0.16	67,67,67,67	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	2B	3021	1/1	0.82	0.22	69,69,69,69	0
56	MG	2A	3292	1/1	0.82	0.19	51,51,51,51	0
56	MG	2A	3299	1/1	0.82	0.09	46,46,46,46	0
56	MG	1x	110	1/1	0.82	0.17	63,63,63,63	0
56	MG	2A	3703	1/1	0.82	0.16	41,41,41,41	0
56	MG	1A	3793	1/1	0.82	0.12	25,25,25,25	0
56	MG	2A	3736	1/1	0.82	0.21	72,72,72,72	0
56	MG	2A	3579	1/1	0.82	0.17	65,65,65,65	0
56	MG	1a	3002	1/1	0.82	0.18	50,50,50,50	0
56	MG	2a	3011	1/1	0.82	0.21	62,62,62,62	0
56	MG	1a	3173	1/1	0.82	0.10	55,55,55,55	0
56	MG	1A	3610	1/1	0.82	0.15	51,51,51,51	0
56	MG	2A	3596	1/1	0.82	0.18	63,63,63,63	0
56	MG	2a	3034	1/1	0.82	0.25	51,51,51,51	0
56	MG	1A	3155	1/1	0.82	0.18	56,56,56,56	0
56	MG	2A	3378	1/1	0.82	0.19	57,57,57,57	0
56	MG	1A	3768	1/1	0.82	0.11	47,47,47,47	0
56	MG	2A	3622	1/1	0.82	0.11	56,56,56,56	0
56	MG	2A	3382	1/1	0.83	0.13	62,62,62,62	0
56	MG	2A	3388	1/1	0.83	0.20	45,45,45,45	0
56	MG	1y	104	1/1	0.83	0.33	63,63,63,63	0
56	MG	2A	3404	1/1	0.83	0.28	65,65,65,65	0
56	MG	2A	3411	1/1	0.83	0.16	71,71,71,71	0
56	MG	2a	3014	1/1	0.83	0.23	60,60,60,60	0
56	MG	1A	3281	1/1	0.83	0.16	40,40,40,40	0
56	MG	2A	3678	1/1	0.83	0.11	60,60,60,60	0
56	MG	2A	3680	1/1	0.83	0.10	52,52,52,52	0
56	MG	1A	3461	1/1	0.83	0.15	40,40,40,40	0
56	MG	1A	3635	1/1	0.83	0.09	18,18,18,18	0
56	MG	2A	3444	1/1	0.83	0.12	35,35,35,35	0
56	MG	1A	3055	1/1	0.83	0.18	63,63,63,63	0
56	MG	2A	3226	1/1	0.83	0.10	47,47,47,47	0
56	MG	2a	3110	1/1	0.83	0.26	60,60,60,60	0
56	MG	2A	3234	1/1	0.83	0.26	53,53,53,53	0
56	MG	2A	3734	1/1	0.83	0.13	65,65,65,65	0
56	MG	1A	4018	1/1	0.83	0.12	52,52,52,52	0
56	MG	2A	3056	1/1	0.83	0.14	56,56,56,56	0
56	MG	2a	3163	1/1	0.83	0.24	65,65,65,65	0
56	MG	2A	3497	1/1	0.83	0.14	46,46,46,46	0
56	MG	2A	3248	1/1	0.83	0.27	51,51,51,51	0
56	MG	2A	3255	1/1	0.83	0.15	63,63,63,63	0
56	MG	1A	3089	1/1	0.83	0.18	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	2A	3554	1/1	0.83	0.18	51,51,51,51	0
56	MG	2A	3262	1/1	0.83	0.25	59,59,59,59	0
56	MG	2A	3806	1/1	0.83	0.20	55,55,55,55	0
56	MG	1A	3712	1/1	0.83	0.10	10,10,10,10	0
56	MG	1A	3446	1/1	0.83	0.20	54,54,54,54	0
56	MG	2A	3583	1/1	0.83	0.12	27,27,27,27	0
56	MG	1N	3006	1/1	0.83	0.28	46,46,46,46	0
56	MG	2A	3839	1/1	0.83	0.18	55,55,55,55	0
56	MG	1a	3060	1/1	0.83	0.34	59,59,59,59	0
56	MG	1a	3068	1/1	0.83	0.09	54,54,54,54	0
56	MG	2a	3218	1/1	0.83	0.18	60,60,60,60	0
56	MG	2a	3220	1/1	0.83	0.17	57,57,57,57	0
56	MG	1A	3738	1/1	0.83	0.15	23,23,23,23	0
56	MG	2A	3597	1/1	0.83	0.21	50,50,50,50	0
56	MG	2A	3160	1/1	0.83	0.11	33,33,33,33	0
56	MG	1a	3092	1/1	0.83	0.32	62,62,62,62	0
56	MG	1R	203	1/1	0.83	0.14	30,30,30,30	0
56	MG	2A	3169	1/1	0.83	0.17	61,61,61,61	0
56	MG	2A	3624	1/1	0.83	0.11	50,50,50,50	0
56	MG	2A	3352	1/1	0.83	0.14	57,57,57,57	0
56	MG	1A	3756	1/1	0.83	0.12	37,37,37,37	0
56	MG	2A	3636	1/1	0.83	0.11	62,62,62,62	0
56	MG	2A	3643	1/1	0.83	0.12	57,57,57,57	0
56	MG	2A	3176	1/1	0.83	0.25	62,62,62,62	0
56	MG	1A	3883	1/1	0.84	0.09	13,13,13,13	0
56	MG	1A	3096	1/1	0.84	0.27	54,54,54,54	0
56	MG	1A	4105	1/1	0.84	0.18	44,44,44,44	0
56	MG	1A	3160	1/1	0.84	0.17	66,66,66,66	0
56	MG	2A	3712	1/1	0.84	0.08	59,59,59,59	0
56	MG	2A	3286	1/1	0.84	0.23	46,46,46,46	0
56	MG	2A	3726	1/1	0.84	0.10	61,61,61,61	0
56	MG	1a	3175	1/1	0.84	0.10	70,70,70,70	0
56	MG	2A	3545	1/1	0.84	0.10	56,56,56,56	0
56	MG	1A	3393	1/1	0.84	0.16	44,44,44,44	0
56	MG	2a	3080	1/1	0.84	0.30	56,56,56,56	0
56	MG	2a	3084	1/1	0.84	0.19	60,60,60,60	0
56	MG	1a	3026	1/1	0.84	0.19	48,48,48,48	0
56	MG	1A	4020	1/1	0.84	0.18	44,44,44,44	0
56	MG	2A	3320	1/1	0.84	0.20	62,62,62,62	0
56	MG	1a	3052	1/1	0.84	0.19	45,45,45,45	0
56	MG	2A	3324	1/1	0.84	0.17	58,58,58,58	0
56	MG	1A	3606	1/1	0.84	0.15	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	3794	1/1	0.84	0.15	67,67,67,67	0
56	MG	2A	3797	1/1	0.84	0.10	57,57,57,57	0
56	MG	2A	3798	1/1	0.84	0.16	51,51,51,51	0
56	MG	1b	3002	1/1	0.84	0.19	54,54,54,54	0
56	MG	2A	3342	1/1	0.84	0.20	57,57,57,57	0
56	MG	1E	307	1/1	0.84	0.10	55,55,55,55	0
56	MG	1w	102	1/1	0.84	0.12	54,54,54,54	0
56	MG	1w	103	1/1	0.84	0.11	55,55,55,55	0
56	MG	2A	3356	1/1	0.84	0.18	51,51,51,51	0
56	MG	1a	3062	1/1	0.84	0.19	65,65,65,65	0
56	MG	1A	3608	1/1	0.84	0.10	15,15,15,15	0
56	MG	2A	3205	1/1	0.84	0.08	44,44,44,44	0
56	MG	1A	3776	1/1	0.84	0.17	46,46,46,46	0
56	MG	1A	3475	1/1	0.84	0.24	67,67,67,67	0
56	MG	2a	3210	1/1	0.84	0.15	56,56,56,56	0
56	MG	1A	3874	1/1	0.84	0.08	35,35,35,35	0
56	MG	2a	3212	1/1	0.84	0.18	54,54,54,54	0
56	MG	1a	3107	1/1	0.84	0.13	55,55,55,55	0
56	MG	2A	3415	1/1	0.84	0.16	56,56,56,56	0
56	MG	2B	3016	1/1	0.84	0.17	63,63,63,63	0
56	MG	2A	3418	1/1	0.84	0.31	65,65,65,65	0
56	MG	2B	3018	1/1	0.84	0.14	74,74,74,74	0
56	MG	1A	3876	1/1	0.84	0.12	30,30,30,30	0
56	MG	2A	3429	1/1	0.84	0.16	60,60,60,60	0
56	MG	2A	3235	1/1	0.84	0.12	47,47,47,47	0
56	MG	2w	3004	1/1	0.84	0.17	60,60,60,60	0
56	MG	1a	3111	1/1	0.84	0.15	54,54,54,54	0
56	MG	2w	3006	1/1	0.84	0.14	78,78,78,78	0
56	MG	1a	3137	1/1	0.84	0.12	46,46,46,46	0
56	MG	2T	3001	1/1	0.84	0.13	57,57,57,57	0
56	MG	1A	4065	1/1	0.84	0.11	41,41,41,41	0
56	MG	2A	3472	1/1	0.84	0.14	50,50,50,50	0
56	MG	2A	3251	1/1	0.84	0.12	52,52,52,52	0
56	MG	2a	3039	1/1	0.85	0.21	61,61,61,61	0
56	MG	2a	3048	1/1	0.85	0.11	61,61,61,61	0
56	MG	2A	3762	1/1	0.85	0.11	51,51,51,51	0
56	MG	1w	108	1/1	0.85	0.18	80,80,80,80	0
56	MG	2a	3068	1/1	0.85	0.23	70,70,70,70	0
56	MG	1A	3617	1/1	0.85	0.09	36,36,36,36	0
56	MG	1A	3842	1/1	0.85	0.19	28,28,28,28	0
56	MG	1A	4092	1/1	0.85	0.14	10,10,10,10	0
56	MG	1A	3457	1/1	0.85	0.18	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	1A	3858	1/1	0.85	0.12	21,21,21,21	0
56	MG	1a	3077	1/1	0.85	0.10	58,58,58,58	0
56	MG	2A	3821	1/1	0.85	0.12	47,47,47,47	0
56	MG	2A	3198	1/1	0.85	0.19	58,58,58,58	0
56	MG	2A	3454	1/1	0.85	0.17	52,52,52,52	0
56	MG	2a	3155	1/1	0.85	0.11	75,75,75,75	0
56	MG	2A	3203	1/1	0.85	0.25	53,53,53,53	0
56	MG	2A	3647	1/1	0.85	0.12	39,39,39,39	0
56	MG	2A	3465	1/1	0.85	0.09	54,54,54,54	0
56	MG	1A	3034	1/1	0.85	0.12	56,56,56,56	0
56	MG	1a	3188	1/1	0.85	0.13	55,55,55,55	0
56	MG	2A	3663	1/1	0.85	0.18	55,55,55,55	0
56	MG	2A	3666	1/1	0.85	0.18	58,58,58,58	0
56	MG	2A	3326	1/1	0.85	0.18	50,50,50,50	0
56	MG	1A	3947	1/1	0.85	0.09	23,23,23,23	0
56	MG	2A	3483	1/1	0.85	0.12	35,35,35,35	0
56	MG	2A	3211	1/1	0.85	0.17	58,58,58,58	0
56	MG	1a	3106	1/1	0.85	0.20	55,55,55,55	0
56	MG	2A	3508	1/1	0.85	0.10	30,30,30,30	0
56	MG	2B	3019	1/1	0.85	0.10	75,75,75,75	0
56	MG	2A	3509	1/1	0.85	0.12	51,51,51,51	0
56	MG	2E	301	1/1	0.85	0.12	53,53,53,53	0
56	MG	1a	3228	1/1	0.85	0.18	58,58,58,58	0
56	MG	1A	3806	1/1	0.85	0.20	41,41,41,41	0
56	MG	2A	3229	1/1	0.85	0.07	44,44,44,44	0
56	MG	2a	3223	1/1	0.85	0.09	54,54,54,54	0
56	MG	1A	3498	1/1	0.85	0.14	43,43,43,43	0
56	MG	2A	3358	1/1	0.85	0.14	35,35,35,35	0
56	MG	2A	3560	1/1	0.85	0.11	40,40,40,40	0
56	MG	2r	101	1/1	0.85	0.10	75,75,75,75	0
56	MG	2A	3375	1/1	0.85	0.30	47,47,47,47	0
56	MG	1F	308	1/1	0.85	0.21	44,44,44,44	0
56	MG	2a	3002	1/1	0.85	0.18	50,50,50,50	0
56	MG	2A	3138	1/1	0.85	0.14	40,40,40,40	0
56	MG	2A	3737	1/1	0.85	0.21	47,47,47,47	0
56	MG	2a	3012	1/1	0.85	0.14	59,59,59,59	0
56	MG	1a	3121	1/1	0.85	0.20	59,59,59,59	0
56	MG	2A	3142	1/1	0.85	0.12	41,41,41,41	0
56	MG	1A	3143	1/1	0.85	0.18	30,30,30,30	0
56	MG	2A	3403	1/1	0.85	0.17	52,52,52,52	0
56	MG	2y	103	1/1	0.85	0.12	51,51,51,51	0
56	MG	1A	3543	1/1	0.85	0.21	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	3688	1/1	0.86	0.12	50,50,50,50	0
56	MG	2A	3103	1/1	0.86	0.15	59,59,59,59	0
56	MG	2a	3019	1/1	0.86	0.10	50,50,50,50	0
56	MG	2A	3482	1/1	0.86	0.13	54,54,54,54	0
56	MG	2A	3109	1/1	0.86	0.11	52,52,52,52	0
56	MG	1a	3180	1/1	0.86	0.09	55,55,55,55	0
56	MG	1a	3037	1/1	0.86	0.21	44,44,44,44	0
56	MG	2A	3503	1/1	0.86	0.11	25,25,25,25	0
56	MG	2A	3732	1/1	0.86	0.12	43,43,43,43	0
56	MG	2A	3295	1/1	0.86	0.23	62,62,62,62	0
56	MG	2a	3054	1/1	0.86	0.22	65,65,65,65	0
56	MG	1a	3046	1/1	0.86	0.18	55,55,55,55	0
56	MG	1A	3994	1/1	0.86	0.16	48,48,48,48	0
56	MG	2A	3539	1/1	0.86	0.27	46,46,46,46	0
56	MG	1A	3426	1/1	0.86	0.15	48,48,48,48	0
56	MG	1a	3197	1/1	0.86	0.12	46,46,46,46	0
56	MG	2a	3098	1/1	0.86	0.15	58,58,58,58	0
56	MG	1A	3861	1/1	0.86	0.11	15,15,15,15	0
56	MG	1a	3224	1/1	0.86	0.19	49,49,49,49	0
56	MG	1A	3328	1/1	0.86	0.18	44,44,44,44	0
56	MG	1A	3204	1/1	0.86	0.11	41,41,41,41	0
56	MG	1A	3536	1/1	0.86	0.14	33,33,33,33	0
56	MG	1m	3001	1/1	0.86	0.22	48,48,48,48	0
56	MG	2A	3188	1/1	0.86	0.48	41,41,41,41	0
56	MG	1a	3074	1/1	0.86	0.17	49,49,49,49	0
56	MG	2a	3165	1/1	0.86	0.19	52,52,52,52	0
56	MG	1A	3200	1/1	0.86	0.18	47,47,47,47	0
56	MG	2A	3372	1/1	0.86	0.28	51,51,51,51	0
56	MG	2A	3595	1/1	0.86	0.12	73,73,73,73	0
56	MG	1a	3087	1/1	0.86	0.26	63,63,63,63	0
56	MG	1A	3709	1/1	0.86	0.10	12,12,12,12	0
56	MG	2A	3599	1/1	0.86	0.14	52,52,52,52	0
56	MG	1A	3900	1/1	0.86	0.12	42,42,42,42	0
56	MG	1A	3915	1/1	0.86	0.13	8,8,8,8	0
56	MG	12	3001	1/1	0.86	0.10	45,45,45,45	0
56	MG	2A	3621	1/1	0.86	0.18	62,62,62,62	0
56	MG	2A	3389	1/1	0.86	0.26	49,49,49,49	0
56	MG	2A	3220	1/1	0.86	0.23	60,60,60,60	0
56	MG	2a	3207	1/1	0.86	0.14	57,57,57,57	0
56	MG	2B	3007	1/1	0.86	0.11	53,53,53,53	0
56	MG	2A	3401	1/1	0.86	0.30	52,52,52,52	0
56	MG	2A	3626	1/1	0.86	0.12	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	3564	1/1	0.86	0.10	51,51,51,51	0
56	MG	2a	3216	1/1	0.86	0.19	51,51,51,51	0
56	MG	1x	115	1/1	0.86	0.15	62,62,62,62	0
56	MG	1A	3420	1/1	0.86	0.15	62,62,62,62	0
56	MG	1A	3421	1/1	0.86	0.15	46,46,46,46	0
56	MG	2A	3416	1/1	0.86	0.23	52,52,52,52	0
56	MG	2a	3229	1/1	0.86	0.13	72,72,72,72	0
56	MG	1A	3752	1/1	0.86	0.08	58,58,58,58	0
56	MG	1a	3006	1/1	0.86	0.10	49,49,49,49	0
56	MG	1A	3829	1/1	0.86	0.15	52,52,52,52	0
56	MG	2A	3665	1/1	0.86	0.10	47,47,47,47	0
56	MG	1a	3155	1/1	0.86	0.18	50,50,50,50	0
56	MG	2A	3047	1/1	0.86	0.10	46,46,46,46	0
56	MG	1A	3479	1/1	0.86	0.12	38,38,38,38	0
56	MG	2A	3072	1/1	0.86	0.25	61,61,61,61	0
56	MG	1a	3022	1/1	0.86	0.13	52,52,52,52	0
56	MG	25	105	1/1	0.86	0.10	55,55,55,55	0
56	MG	1A	3485	1/1	0.86	0.20	33,33,33,33	0
56	MG	2x	3003	1/1	0.86	0.24	66,66,66,66	0
56	MG	2A	3268	1/1	0.86	0.17	59,59,59,59	0
56	MG	2A	3276	1/1	0.86	0.07	46,46,46,46	0
56	MG	2a	3010	1/1	0.86	0.21	56,56,56,56	0
56	MG	1A	3766	1/1	0.86	0.12	44,44,44,44	0
56	MG	2V	201	1/1	0.87	0.13	58,58,58,58	0
56	MG	2A	3649	1/1	0.87	0.11	54,54,54,54	0
56	MG	25	102	1/1	0.87	0.20	60,60,60,60	0
56	MG	1A	3248	1/1	0.87	0.10	35,35,35,35	0
56	MG	2A	3408	1/1	0.87	0.12	48,48,48,48	0
56	MG	2A	3655	1/1	0.87	0.09	55,55,55,55	0
56	MG	2a	3004	1/1	0.87	0.18	58,58,58,58	0
56	MG	1A	3332	1/1	0.87	0.08	46,46,46,46	0
56	MG	2A	3661	1/1	0.87	0.11	53,53,53,53	0
56	MG	1A	3380	1/1	0.87	0.10	37,37,37,37	0
56	MG	1a	3066	1/1	0.87	0.19	49,49,49,49	0
56	MG	1A	4113	1/1	0.87	0.09	44,44,44,44	0
56	MG	2a	3017	1/1	0.87	0.14	65,65,65,65	0
56	MG	2A	3668	1/1	0.87	0.13	57,57,57,57	0
56	MG	2A	3423	1/1	0.87	0.12	48,48,48,48	0
56	MG	1A	4127	1/1	0.87	0.14	23,23,23,23	0
56	MG	1a	3070	1/1	0.87	0.19	44,44,44,44	0
56	MG	1A	3481	1/1	0.87	0.20	66,66,66,66	0
56	MG	1x	112	1/1	0.87	0.20	67,67,67,67	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	3679	1/1	0.87	0.14	54,54,54,54	0
56	MG	2A	3243	1/1	0.87	0.17	62,62,62,62	0
56	MG	1A	3800	1/1	0.87	0.10	35,35,35,35	0
56	MG	2A	3685	1/1	0.87	0.11	47,47,47,47	0
56	MG	1A	3631	1/1	0.87	0.11	45,45,45,45	0
56	MG	2a	3069	1/1	0.87	0.13	55,55,55,55	0
56	MG	2a	3073	1/1	0.87	0.13	73,73,73,73	0
56	MG	1B	3028	1/1	0.87	0.09	38,38,38,38	0
56	MG	2a	3077	1/1	0.87	0.14	44,44,44,44	0
56	MG	2A	3466	1/1	0.87	0.17	48,48,48,48	0
56	MG	2A	3468	1/1	0.87	0.09	53,53,53,53	0
56	MG	2a	3086	1/1	0.87	0.25	57,57,57,57	0
56	MG	2A	3250	1/1	0.87	0.08	46,46,46,46	0
56	MG	1A	3388	1/1	0.87	0.10	39,39,39,39	0
56	MG	2a	3106	1/1	0.87	0.15	43,43,43,43	0
56	MG	2A	3722	1/1	0.87	0.11	57,57,57,57	0
56	MG	1D	313	1/1	0.87	0.27	35,35,35,35	0
56	MG	1A	3955	1/1	0.87	0.10	48,48,48,48	0
56	MG	2a	3126	1/1	0.87	0.12	70,70,70,70	0
56	MG	1A	3654	1/1	0.87	0.17	51,51,51,51	0
56	MG	1A	3673	1/1	0.87	0.13	24,24,24,24	0
56	MG	2A	3490	1/1	0.87	0.18	65,65,65,65	0
56	MG	1A	3492	1/1	0.87	0.19	71,71,71,71	0
56	MG	1A	3252	1/1	0.87	0.27	53,53,53,53	0
56	MG	2a	3166	1/1	0.87	0.10	66,66,66,66	0
56	MG	1a	3140	1/1	0.87	0.10	37,37,37,37	0
56	MG	2A	3079	1/1	0.87	0.07	50,50,50,50	0
56	MG	1A	3708	1/1	0.87	0.16	27,27,27,27	0
56	MG	2a	3173	1/1	0.87	0.11	62,62,62,62	0
56	MG	1A	3123	1/1	0.87	0.17	62,62,62,62	0
56	MG	2A	3516	1/1	0.87	0.17	74,74,74,74	0
56	MG	2A	3523	1/1	0.87	0.15	58,58,58,58	0
56	MG	2A	3293	1/1	0.87	0.21	67,67,67,67	0
56	MG	1A	3125	1/1	0.87	0.05	17,17,17,17	0
56	MG	2A	3296	1/1	0.87	0.07	63,63,63,63	0
56	MG	1A	3847	1/1	0.87	0.14	26,26,26,26	0
56	MG	17	102	1/1	0.87	0.09	36,36,36,36	0
56	MG	2A	3120	1/1	0.87	0.20	56,56,56,56	0
56	MG	2A	3123	1/1	0.87	0.12	50,50,50,50	0
56	MG	18	101	1/1	0.87	0.16	59,59,59,59	0
56	MG	1A	3277	1/1	0.87	0.13	49,49,49,49	0
56	MG	1A	4026	1/1	0.87	0.36	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	3715	1/1	0.87	0.09	48,48,48,48	0
56	MG	2A	3146	1/1	0.87	0.16	51,51,51,51	0
56	MG	1A	3280	1/1	0.87	0.06	25,25,25,25	0
56	MG	1A	3545	1/1	0.87	0.21	60,60,60,60	0
56	MG	1a	3189	1/1	0.87	0.12	56,56,56,56	0
56	MG	1A	3061	1/1	0.87	0.08	22,22,22,22	0
56	MG	2A	3369	1/1	0.87	0.35	58,58,58,58	0
56	MG	2A	3600	1/1	0.87	0.10	53,53,53,53	0
56	MG	2A	3371	1/1	0.87	0.21	49,49,49,49	0
56	MG	2q	203	1/1	0.87	0.18	55,55,55,55	0
56	MG	1A	4041	1/1	0.87	0.16	45,45,45,45	0
56	MG	2r	102	1/1	0.87	0.07	75,75,75,75	0
56	MG	1A	4053	1/1	0.87	0.10	45,45,45,45	0
56	MG	2A	3612	1/1	0.87	0.22	60,60,60,60	0
56	MG	2A	3614	1/1	0.87	0.15	68,68,68,68	0
56	MG	2w	3003	1/1	0.87	0.10	51,51,51,51	0
56	MG	1a	3222	1/1	0.87	0.16	60,60,60,60	0
56	MG	1A	3180	1/1	0.87	0.09	38,38,38,38	0
56	MG	2A	3191	1/1	0.87	0.15	43,43,43,43	0
56	MG	2E	307	1/1	0.87	0.13	49,49,49,49	0
56	MG	1A	4061	1/1	0.87	0.13	27,27,27,27	0
56	MG	1a	3230	1/1	0.87	0.12	49,49,49,49	0
56	MG	2A	3390	1/1	0.87	0.23	57,57,57,57	0
56	MG	1a	3038	1/1	0.87	0.17	50,50,50,50	0
56	MG	1A	3593	1/1	0.87	0.14	41,41,41,41	0
56	MG	1A	3308	1/1	0.87	0.12	29,29,29,29	0
56	MG	1A	3494	1/1	0.88	0.08	41,41,41,41	0
56	MG	1A	3929	1/1	0.88	0.11	28,28,28,28	0
56	MG	16	103	1/1	0.88	0.17	33,33,33,33	0
56	MG	2A	3181	1/1	0.88	0.17	49,49,49,49	0
56	MG	2a	3031	1/1	0.88	0.33	62,62,62,62	0
56	MG	2A	3331	1/1	0.88	0.22	51,51,51,51	0
56	MG	2A	3710	1/1	0.88	0.10	71,71,71,71	0
56	MG	2a	3036	1/1	0.88	0.13	50,50,50,50	0
56	MG	2A	3337	1/1	0.88	0.22	44,44,44,44	0
56	MG	2A	3183	1/1	0.88	0.13	54,54,54,54	0
56	MG	1A	3251	1/1	0.88	0.18	49,49,49,49	0
56	MG	1A	3835	1/1	0.88	0.12	26,26,26,26	0
56	MG	1A	3760	1/1	0.88	0.12	40,40,40,40	0
56	MG	2a	3064	1/1	0.88	0.23	51,51,51,51	0
56	MG	2A	3345	1/1	0.88	0.07	54,54,54,54	0
56	MG	2A	3735	1/1	0.88	0.13	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	3838	1/1	0.88	0.09	35,35,35,35	0
56	MG	2A	3348	1/1	0.88	0.13	50,50,50,50	0
56	MG	2A	3200	1/1	0.88	0.19	51,51,51,51	0
56	MG	1A	3159	1/1	0.88	0.13	26,26,26,26	0
56	MG	2A	3576	1/1	0.88	0.13	35,35,35,35	0
56	MG	2A	3577	1/1	0.88	0.11	49,49,49,49	0
56	MG	2a	3087	1/1	0.88	0.22	53,53,53,53	0
56	MG	2A	3750	1/1	0.88	0.11	48,48,48,48	0
56	MG	2a	3102	1/1	0.88	0.16	60,60,60,60	0
56	MG	2a	3104	1/1	0.88	0.13	34,34,34,34	0
56	MG	1a	3146	1/1	0.88	0.14	44,44,44,44	0
56	MG	1A	3391	1/1	0.88	0.21	47,47,47,47	0
56	MG	1A	3692	1/1	0.88	0.10	56,56,56,56	0
56	MG	2a	3112	1/1	0.88	0.09	61,61,61,61	0
56	MG	1A	3700	1/1	0.88	0.12	49,49,49,49	0
56	MG	2a	3120	1/1	0.88	0.10	75,75,75,75	0
56	MG	2A	3769	1/1	0.88	0.08	46,46,46,46	0
56	MG	2A	3779	1/1	0.88	0.11	27,27,27,27	0
56	MG	2a	3137	1/1	0.88	0.10	48,48,48,48	0
56	MG	2A	3789	1/1	0.88	0.16	62,62,62,62	0
56	MG	2a	3142	1/1	0.88	0.12	56,56,56,56	0
56	MG	2A	3213	1/1	0.88	0.09	61,61,61,61	0
56	MG	2a	3153	1/1	0.88	0.10	68,68,68,68	0
56	MG	2A	3594	1/1	0.88	0.09	38,38,38,38	0
56	MG	2a	3161	1/1	0.88	0.14	70,70,70,70	0
56	MG	1A	3297	1/1	0.88	0.12	42,42,42,42	0
56	MG	2A	3802	1/1	0.88	0.16	60,60,60,60	0
56	MG	1B	3020	1/1	0.88	0.09	28,28,28,28	0
56	MG	1B	3022	1/1	0.88	0.16	48,48,48,48	0
56	MG	2A	3062	1/1	0.88	0.08	56,56,56,56	0
56	MG	2A	3826	1/1	0.88	0.11	62,62,62,62	0
56	MG	1a	3176	1/1	0.88	0.17	63,63,63,63	0
56	MG	2A	3074	1/1	0.88	0.09	47,47,47,47	0
56	MG	1A	3862	1/1	0.88	0.12	15,15,15,15	0
56	MG	2a	3182	1/1	0.88	0.21	56,56,56,56	0
56	MG	2a	3185	1/1	0.88	0.15	47,47,47,47	0
56	MG	2a	3187	1/1	0.88	0.08	54,54,54,54	0
56	MG	1A	4016	1/1	0.88	0.12	32,32,32,32	0
56	MG	2a	3192	1/1	0.88	0.14	64,64,64,64	0
56	MG	2A	3609	1/1	0.88	0.19	35,35,35,35	0
56	MG	1a	3041	1/1	0.88	0.10	59,59,59,59	0
56	MG	1A	3484	1/1	0.88	0.20	33,33,33,33	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	3033	1/1	0.88	0.10	53,53,53,53	0
56	MG	2A	3108	1/1	0.88	0.07	43,43,43,43	0
56	MG	2B	3002	1/1	0.88	0.09	50,50,50,50	0
56	MG	2A	3623	1/1	0.88	0.16	57,57,57,57	0
56	MG	1A	3789	1/1	0.88	0.11	26,26,26,26	0
56	MG	2A	3253	1/1	0.88	0.07	58,58,58,58	0
56	MG	1A	3877	1/1	0.88	0.14	31,31,31,31	0
56	MG	1A	3356	1/1	0.88	0.16	47,47,47,47	0
56	MG	1A	3401	1/1	0.88	0.09	29,29,29,29	0
56	MG	2a	3217	1/1	0.88	0.20	62,62,62,62	0
56	MG	2A	3640	1/1	0.88	0.09	34,34,34,34	0
56	MG	2A	3266	1/1	0.88	0.10	53,53,53,53	0
56	MG	2a	3221	1/1	0.88	0.17	57,57,57,57	0
56	MG	2A	3125	1/1	0.88	0.14	51,51,51,51	0
56	MG	2D	304	1/1	0.88	0.15	59,59,59,59	0
56	MG	2a	3227	1/1	0.88	0.27	49,49,49,49	0
56	MG	2A	3440	1/1	0.88	0.09	40,40,40,40	0
56	MG	2A	3274	1/1	0.88	0.13	47,47,47,47	0
56	MG	1A	3588	1/1	0.88	0.12	24,24,24,24	0
56	MG	2A	3445	1/1	0.88	0.16	50,50,50,50	0
56	MG	2A	3450	1/1	0.88	0.19	46,46,46,46	0
56	MG	2A	3453	1/1	0.88	0.20	52,52,52,52	0
56	MG	1A	3898	1/1	0.88	0.11	23,23,23,23	0
56	MG	1A	3733	1/1	0.88	0.12	15,15,15,15	0
56	MG	2A	3287	1/1	0.88	0.10	45,45,45,45	0
56	MG	1T	3003	1/1	0.88	0.10	34,34,34,34	0
56	MG	1A	3647	1/1	0.88	0.13	27,27,27,27	0
56	MG	1X	104	1/1	0.88	0.21	30,30,30,30	0
56	MG	1Y	503	1/1	0.88	0.10	58,58,58,58	0
56	MG	2A	3163	1/1	0.88	0.11	53,53,53,53	0
56	MG	1A	3748	1/1	0.88	0.11	29,29,29,29	0
56	MG	1a	3098	1/1	0.88	0.23	60,60,60,60	0
56	MG	2A	3311	1/1	0.88	0.10	38,38,38,38	0
56	MG	2A	3312	1/1	0.88	0.18	51,51,51,51	0
56	MG	2A	3683	1/1	0.88	0.22	51,51,51,51	0
56	MG	2A	3318	1/1	0.88	0.11	52,52,52,52	0
56	MG	1a	3031	1/1	0.89	0.16	48,48,48,48	0
56	MG	2a	3001	1/1	0.89	0.10	56,56,56,56	0
56	MG	1A	3584	1/1	0.89	0.12	7,7,7,7	0
56	MG	1A	3088	1/1	0.89	0.22	43,43,43,43	0
56	MG	1A	3802	1/1	0.89	0.11	20,20,20,20	0
56	MG	1B	3003	1/1	0.89	0.18	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	1n	502	1/1	0.89	0.25	57,57,57,57	0
56	MG	1t	3001	1/1	0.89	0.18	53,53,53,53	0
56	MG	1a	3048	1/1	0.89	0.24	52,52,52,52	0
56	MG	2a	3015	1/1	0.89	0.16	46,46,46,46	0
56	MG	2a	3016	1/1	0.89	0.08	47,47,47,47	0
56	MG	1A	3346	1/1	0.89	0.12	45,45,45,45	0
56	MG	1B	3008	1/1	0.89	0.20	53,53,53,53	0
56	MG	2a	3022	1/1	0.89	0.22	53,53,53,53	0
56	MG	1a	3058	1/1	0.89	0.08	53,53,53,53	0
56	MG	1w	107	1/1	0.89	0.07	48,48,48,48	0
56	MG	2a	3030	1/1	0.89	0.25	51,51,51,51	0
56	MG	1A	3235	1/1	0.89	0.23	46,46,46,46	0
56	MG	2A	3673	1/1	0.89	0.12	38,38,38,38	0
56	MG	1A	3376	1/1	0.89	0.16	39,39,39,39	0
56	MG	2A	3434	1/1	0.89	0.11	38,38,38,38	0
56	MG	1A	3813	1/1	0.89	0.13	51,51,51,51	0
56	MG	2a	3044	1/1	0.89	0.13	68,68,68,68	0
56	MG	2a	3046	1/1	0.89	0.16	52,52,52,52	0
56	MG	1x	108	1/1	0.89	0.15	47,47,47,47	0
56	MG	1A	3241	1/1	0.89	0.12	46,46,46,46	0
56	MG	1A	3961	1/1	0.89	0.09	19,19,19,19	0
56	MG	1A	3718	1/1	0.89	0.10	42,42,42,42	0
56	MG	2a	3056	1/1	0.89	0.21	46,46,46,46	0
56	MG	2a	3059	1/1	0.89	0.08	52,52,52,52	0
56	MG	1A	3973	1/1	0.89	0.11	23,23,23,23	0
56	MG	1A	3729	1/1	0.89	0.15	10,10,10,10	0
56	MG	2A	3239	1/1	0.89	0.12	46,46,46,46	0
56	MG	1a	3086	1/1	0.89	0.17	46,46,46,46	0
56	MG	2a	3075	1/1	0.89	0.25	54,54,54,54	0
56	MG	2A	3699	1/1	0.89	0.12	60,60,60,60	0
56	MG	2A	3013	1/1	0.89	0.18	52,52,52,52	0
56	MG	2a	3078	1/1	0.89	0.21	60,60,60,60	0
56	MG	2A	3706	1/1	0.89	0.08	58,58,58,58	0
56	MG	2A	3467	1/1	0.89	0.11	32,32,32,32	0
56	MG	2A	3246	1/1	0.89	0.18	55,55,55,55	0
56	MG	2A	3017	1/1	0.89	0.20	37,37,37,37	0
56	MG	2a	3091	1/1	0.89	0.10	60,60,60,60	0
56	MG	1A	3983	1/1	0.89	0.09	14,14,14,14	0
56	MG	2a	3101	1/1	0.89	0.13	66,66,66,66	0
56	MG	1E	309	1/1	0.89	0.09	45,45,45,45	0
56	MG	2a	3103	1/1	0.89	0.25	68,68,68,68	0
56	MG	2A	3480	1/1	0.89	0.10	33,33,33,33	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	3030	1/1	0.89	0.15	56,56,56,56	0
56	MG	1F	305	1/1	0.89	0.08	36,36,36,36	0
56	MG	2A	3038	1/1	0.89	0.14	46,46,46,46	0
56	MG	2A	3043	1/1	0.89	0.13	53,53,53,53	0
56	MG	2A	3740	1/1	0.89	0.11	55,55,55,55	0
56	MG	1A	3991	1/1	0.89	0.20	41,41,41,41	0
56	MG	2A	3049	1/1	0.89	0.09	30,30,30,30	0
56	MG	1A	3834	1/1	0.89	0.14	57,57,57,57	0
56	MG	2a	3128	1/1	0.89	0.12	57,57,57,57	0
56	MG	2a	3131	1/1	0.89	0.07	87,87,87,87	0
56	MG	2A	3272	1/1	0.89	0.13	43,43,43,43	0
56	MG	1A	3456	1/1	0.89	0.10	41,41,41,41	0
56	MG	2A	3064	1/1	0.89	0.15	59,59,59,59	0
56	MG	2A	3068	1/1	0.89	0.22	54,54,54,54	0
56	MG	1a	3108	1/1	0.89	0.16	60,60,60,60	0
56	MG	2A	3536	1/1	0.89	0.08	32,32,32,32	0
56	MG	2a	3156	1/1	0.89	0.09	56,56,56,56	0
56	MG	1A	4006	1/1	0.89	0.07	53,53,53,53	0
56	MG	2A	3541	1/1	0.89	0.12	50,50,50,50	0
56	MG	1A	3735	1/1	0.89	0.08	25,25,25,25	0
56	MG	2A	3076	1/1	0.89	0.13	53,53,53,53	0
56	MG	1A	3387	1/1	0.89	0.06	42,42,42,42	0
56	MG	1A	3021	1/1	0.89	0.14	20,20,20,20	0
56	MG	2A	3799	1/1	0.89	0.15	59,59,59,59	0
56	MG	2A	3294	1/1	0.89	0.22	61,61,61,61	0
56	MG	2A	3805	1/1	0.89	0.14	42,42,42,42	0
56	MG	2a	3179	1/1	0.89	0.12	53,53,53,53	0
56	MG	2A	3562	1/1	0.89	0.10	32,32,32,32	0
56	MG	2A	3085	1/1	0.89	0.19	49,49,49,49	0
56	MG	2A	3570	1/1	0.89	0.13	33,33,33,33	0
56	MG	1A	3618	1/1	0.89	0.11	34,34,34,34	0
56	MG	2A	3827	1/1	0.89	0.17	64,64,64,64	0
56	MG	2A	3090	1/1	0.89	0.16	38,38,38,38	0
56	MG	2A	3308	1/1	0.89	0.14	50,50,50,50	0
56	MG	2A	3098	1/1	0.89	0.07	32,32,32,32	0
56	MG	2a	3196	1/1	0.89	0.22	53,53,53,53	0
56	MG	1Z	301	1/1	0.89	0.16	35,35,35,35	0
56	MG	1A	3509	1/1	0.89	0.25	47,47,47,47	0
56	MG	2A	3845	1/1	0.89	0.15	44,44,44,44	0
56	MG	2A	3846	1/1	0.89	0.13	41,41,41,41	0
56	MG	10	108	1/1	0.89	0.07	45,45,45,45	0
56	MG	1A	3263	1/1	0.89	0.16	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	2a	3209	1/1	0.89	0.14	55,55,55,55	0
56	MG	2A	3117	1/1	0.89	0.17	36,36,36,36	0
56	MG	2A	3869	1/1	0.89	0.13	55,55,55,55	0
56	MG	2A	3118	1/1	0.89	0.13	35,35,35,35	0
56	MG	1A	3473	1/1	0.89	0.08	23,23,23,23	0
56	MG	2B	3004	1/1	0.89	0.17	53,53,53,53	0
56	MG	1A	3324	1/1	0.89	0.09	42,42,42,42	0
56	MG	2A	3124	1/1	0.89	0.24	52,52,52,52	0
56	MG	2B	3012	1/1	0.89	0.11	63,63,63,63	0
56	MG	1A	3865	1/1	0.89	0.17	14,14,14,14	0
56	MG	2A	3127	1/1	0.89	0.31	61,61,61,61	0
56	MG	2A	3131	1/1	0.89	0.13	51,51,51,51	0
56	MG	1A	3662	1/1	0.89	0.10	26,26,26,26	0
56	MG	1A	3546	1/1	0.89	0.21	57,57,57,57	0
56	MG	1A	3172	1/1	0.89	0.16	22,22,22,22	0
56	MG	1A	3572	1/1	0.89	0.12	34,34,34,34	0
56	MG	2D	301	1/1	0.89	0.10	36,36,36,36	0
56	MG	2A	3617	1/1	0.89	0.10	48,48,48,48	0
56	MG	2t	3001	1/1	0.89	0.16	48,48,48,48	0
56	MG	2A	3620	1/1	0.89	0.25	50,50,50,50	0
56	MG	2E	304	1/1	0.89	0.15	58,58,58,58	0
56	MG	1a	3003	1/1	0.89	0.18	49,49,49,49	0
56	MG	2A	3149	1/1	0.89	0.30	56,56,56,56	0
56	MG	1A	3784	1/1	0.89	0.11	42,42,42,42	0
56	MG	2A	3158	1/1	0.89	0.11	47,47,47,47	0
56	MG	1A	3787	1/1	0.89	0.13	40,40,40,40	0
56	MG	2w	3007	1/1	0.89	0.12	60,60,60,60	0
56	MG	1A	3788	1/1	0.89	0.07	15,15,15,15	0
56	MG	2A	3164	1/1	0.89	0.06	18,18,18,18	0
56	MG	2U	205	1/1	0.89	0.09	46,46,46,46	0
56	MG	1A	3573	1/1	0.89	0.12	22,22,22,22	0
56	MG	1A	3905	1/1	0.89	0.12	43,43,43,43	0
56	MG	1A	3791	1/1	0.89	0.16	32,32,32,32	0
56	MG	1a	3029	1/1	0.89	0.21	63,63,63,63	0
56	MG	1A	3104	1/1	0.90	0.08	29,29,29,29	0
56	MG	2A	3231	1/1	0.90	0.29	52,52,52,52	0
56	MG	1A	3447	1/1	0.90	0.12	32,32,32,32	0
56	MG	2a	3032	1/1	0.90	0.23	59,59,59,59	0
56	MG	2A	3448	1/1	0.90	0.14	23,23,23,23	0
56	MG	1a	3110	1/1	0.90	0.18	50,50,50,50	0
56	MG	2A	3236	1/1	0.90	0.08	50,50,50,50	0
56	MG	2A	3691	1/1	0.90	0.18	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3868	1/1	0.90	0.10	43,43,43,43	0
56	MG	2A	3048	1/1	0.90	0.08	43,43,43,43	0
56	MG	2A	3457	1/1	0.90	0.11	51,51,51,51	0
56	MG	1a	3112	1/1	0.90	0.16	48,48,48,48	0
56	MG	2A	3245	1/1	0.90	0.09	58,58,58,58	0
56	MG	1A	3453	1/1	0.90	0.11	44,44,44,44	0
56	MG	1A	3515	1/1	0.90	0.09	49,49,49,49	0
56	MG	2a	3058	1/1	0.90	0.09	50,50,50,50	0
56	MG	2A	3469	1/1	0.90	0.16	50,50,50,50	0
56	MG	1A	3524	1/1	0.90	0.20	30,30,30,30	0
56	MG	1a	3144	1/1	0.90	0.15	43,43,43,43	0
56	MG	1A	3242	1/1	0.90	0.21	33,33,33,33	0
56	MG	1A	4040	1/1	0.90	0.10	52,52,52,52	0
56	MG	1A	3663	1/1	0.90	0.07	32,32,32,32	0
56	MG	2A	3257	1/1	0.90	0.17	43,43,43,43	0
56	MG	2A	3738	1/1	0.90	0.11	46,46,46,46	0
56	MG	2A	3260	1/1	0.90	0.09	48,48,48,48	0
56	MG	2a	3079	1/1	0.90	0.18	53,53,53,53	0
56	MG	1A	4044	1/1	0.90	0.06	17,17,17,17	0
56	MG	2A	3077	1/1	0.90	0.09	44,44,44,44	0
56	MG	2A	3494	1/1	0.90	0.10	46,46,46,46	0
56	MG	2A	3744	1/1	0.90	0.08	76,76,76,76	0
56	MG	2A	3263	1/1	0.90	0.29	68,68,68,68	0
56	MG	2a	3092	1/1	0.90	0.32	59,59,59,59	0
56	MG	2a	3093	1/1	0.90	0.16	60,60,60,60	0
56	MG	2a	3096	1/1	0.90	0.11	62,62,62,62	0
56	MG	2a	3097	1/1	0.90	0.12	54,54,54,54	0
56	MG	1a	3157	1/1	0.90	0.10	46,46,46,46	0
56	MG	1a	3160	1/1	0.90	0.12	62,62,62,62	0
56	MG	2A	3269	1/1	0.90	0.10	54,54,54,54	0
56	MG	1A	3261	1/1	0.90	0.16	23,23,23,23	0
56	MG	1A	4055	1/1	0.90	0.13	56,56,56,56	0
56	MG	1A	3674	1/1	0.90	0.14	38,38,38,38	0
56	MG	1A	3899	1/1	0.90	0.07	28,28,28,28	0
56	MG	2a	3108	1/1	0.90	0.15	48,48,48,48	0
56	MG	1a	3005	1/1	0.90	0.12	52,52,52,52	0
56	MG	2A	3105	1/1	0.90	0.21	51,51,51,51	0
56	MG	1A	3094	1/1	0.90	0.15	43,43,43,43	0
56	MG	1a	3007	1/1	0.90	0.26	56,56,56,56	0
56	MG	2a	3123	1/1	0.90	0.10	75,75,75,75	0
56	MG	2A	3548	1/1	0.90	0.11	25,25,25,25	0
56	MG	1A	3678	1/1	0.90	0.17	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	2A	3550	1/1	0.90	0.12	43,43,43,43	0
56	MG	2A	3552	1/1	0.90	0.12	40,40,40,40	0
56	MG	2a	3134	1/1	0.90	0.12	60,60,60,60	0
56	MG	2a	3135	1/1	0.90	0.14	55,55,55,55	0
56	MG	1A	3910	1/1	0.90	0.10	45,45,45,45	0
56	MG	2A	3813	1/1	0.90	0.22	51,51,51,51	0
56	MG	2A	3815	1/1	0.90	0.25	59,59,59,59	0
56	MG	1A	3264	1/1	0.90	0.09	48,48,48,48	0
56	MG	1a	3023	1/1	0.90	0.07	47,47,47,47	0
56	MG	1a	3196	1/1	0.90	0.10	51,51,51,51	0
56	MG	2A	3564	1/1	0.90	0.14	34,34,34,34	0
56	MG	2a	3160	1/1	0.90	0.09	66,66,66,66	0
56	MG	2A	3298	1/1	0.90	0.10	47,47,47,47	0
56	MG	1A	4096	1/1	0.90	0.15	39,39,39,39	0
56	MG	1a	3211	1/1	0.90	0.09	65,65,65,65	0
56	MG	2A	3840	1/1	0.90	0.08	68,68,68,68	0
56	MG	1A	3682	1/1	0.90	0.09	12,12,12,12	0
56	MG	1A	3922	1/1	0.90	0.10	63,63,63,63	0
56	MG	2A	3136	1/1	0.90	0.10	54,54,54,54	0
56	MG	1A	3796	1/1	0.90	0.18	41,41,41,41	0
56	MG	2a	3177	1/1	0.90	0.10	58,58,58,58	0
56	MG	1a	3226	1/1	0.90	0.11	55,55,55,55	0
56	MG	2A	3140	1/1	0.90	0.15	44,44,44,44	0
56	MG	2A	3141	1/1	0.90	0.13	53,53,53,53	0
56	MG	1A	3548	1/1	0.90	0.17	45,45,45,45	0
56	MG	1A	3562	1/1	0.90	0.35	26,26,26,26	0
56	MG	1A	3934	1/1	0.90	0.07	14,14,14,14	0
56	MG	1A	3464	1/1	0.90	0.14	29,29,29,29	0
56	MG	2A	3150	1/1	0.90	0.22	53,53,53,53	0
56	MG	1f	3002	1/1	0.90	0.22	60,60,60,60	0
56	MG	1B	3021	1/1	0.90	0.11	50,50,50,50	0
56	MG	1A	3176	1/1	0.90	0.10	52,52,52,52	0
56	MG	1A	3334	1/1	0.90	0.10	46,46,46,46	0
56	MG	2A	3349	1/1	0.90	0.19	45,45,45,45	0
56	MG	1a	3056	1/1	0.90	0.19	56,56,56,56	0
56	MG	1A	3579	1/1	0.90	0.11	27,27,27,27	0
56	MG	2a	3205	1/1	0.90	0.16	66,66,66,66	0
56	MG	2A	3619	1/1	0.90	0.11	50,50,50,50	0
56	MG	1A	3476	1/1	0.90	0.12	44,44,44,44	0
56	MG	1B	3031	1/1	0.90	0.17	59,59,59,59	0
56	MG	1a	3063	1/1	0.90	0.12	41,41,41,41	0
56	MG	2A	3171	1/1	0.90	0.13	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	2E	306	1/1	0.90	0.11	45,45,45,45	0
56	MG	2a	3214	1/1	0.90	0.07	51,51,51,51	0
56	MG	1A	3717	1/1	0.90	0.09	23,23,23,23	0
56	MG	2A	3376	1/1	0.90	0.16	47,47,47,47	0
56	MG	2A	3178	1/1	0.90	0.10	41,41,41,41	0
56	MG	2a	3219	1/1	0.90	0.24	53,53,53,53	0
56	MG	1a	3067	1/1	0.90	0.15	44,44,44,44	0
56	MG	1A	3399	1/1	0.90	0.12	42,42,42,42	0
56	MG	2A	3185	1/1	0.90	0.09	46,46,46,46	0
56	MG	2A	3186	1/1	0.90	0.11	43,43,43,43	0
56	MG	1A	3726	1/1	0.90	0.10	12,12,12,12	0
56	MG	1A	3223	1/1	0.90	0.16	47,47,47,47	0
56	MG	2a	3230	1/1	0.90	0.18	61,61,61,61	0
56	MG	2A	3397	1/1	0.90	0.08	59,59,59,59	0
56	MG	1A	3347	1/1	0.90	0.14	34,34,34,34	0
56	MG	2l	202	1/1	0.90	0.16	62,62,62,62	0
56	MG	1A	3348	1/1	0.90	0.13	46,46,46,46	0
56	MG	1y	103	1/1	0.90	0.17	80,80,80,80	0
56	MG	2A	3660	1/1	0.90	0.12	31,31,31,31	0
56	MG	1A	3144	1/1	0.90	0.22	39,39,39,39	0
56	MG	1A	3430	1/1	0.90	0.11	32,32,32,32	0
56	MG	2a	3006	1/1	0.90	0.16	53,53,53,53	0
56	MG	1a	3090	1/1	0.90	0.18	27,27,27,27	0
56	MG	2a	3009	1/1	0.90	0.17	58,58,58,58	0
56	MG	1A	3440	1/1	0.90	0.10	54,54,54,54	0
56	MG	2A	3016	1/1	0.90	0.24	58,58,58,58	0
56	MG	1O	3004	1/1	0.90	0.15	41,41,41,41	0
56	MG	1A	3754	1/1	0.90	0.08	21,21,21,21	0
56	MG	2A	3222	1/1	0.90	0.18	53,53,53,53	0
56	MG	1A	3859	1/1	0.90	0.09	27,27,27,27	0
56	MG	1A	3497	1/1	0.90	0.12	34,34,34,34	0
56	MG	2A	3438	1/1	0.90	0.21	47,47,47,47	0
56	MG	2x	3006	1/1	0.90	0.20	58,58,58,58	0
56	MG	2a	3021	1/1	0.90	0.24	64,64,64,64	0
56	MG	2A	3439	1/1	0.90	0.11	51,51,51,51	0
56	MG	2A	3031	1/1	0.90	0.13	55,55,55,55	0
56	MG	2Q	202	1/1	0.91	0.12	31,31,31,31	0
56	MG	2A	3572	1/1	0.91	0.09	25,25,25,25	0
56	MG	1A	3414	1/1	0.91	0.10	27,27,27,27	0
56	MG	1A	3153	1/1	0.91	0.30	23,23,23,23	0
56	MG	2T	3003	1/1	0.91	0.07	59,59,59,59	0
56	MG	1D	301	1/1	0.91	0.18	29,29,29,29	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	3578	1/1	0.91	0.10	31,31,31,31	0
56	MG	2A	3271	1/1	0.91	0.08	50,50,50,50	0
56	MG	2Z	8001	1/1	0.91	0.15	47,47,47,47	0
56	MG	2A	3582	1/1	0.91	0.12	57,57,57,57	0
56	MG	1a	3096	1/1	0.91	0.26	45,45,45,45	0
56	MG	2A	3273	1/1	0.91	0.15	51,51,51,51	0
56	MG	1A	3751	1/1	0.91	0.09	14,14,14,14	0
56	MG	2A	3275	1/1	0.91	0.09	47,47,47,47	0
56	MG	1E	306	1/1	0.91	0.11	32,32,32,32	0
56	MG	1a	3101	1/1	0.91	0.17	48,48,48,48	0
56	MG	1a	3102	1/1	0.91	0.27	59,59,59,59	0
56	MG	2A	3071	1/1	0.91	0.21	53,53,53,53	0
56	MG	1A	3988	1/1	0.91	0.08	28,28,28,28	0
56	MG	1A	3989	1/1	0.91	0.08	21,21,21,21	0
56	MG	1E	310	1/1	0.91	0.16	28,28,28,28	0
56	MG	1A	3057	1/1	0.91	0.08	36,36,36,36	0
56	MG	1A	3852	1/1	0.91	0.10	17,17,17,17	0
56	MG	1A	3855	1/1	0.91	0.12	32,32,32,32	0
56	MG	2A	3080	1/1	0.91	0.17	59,59,59,59	0
56	MG	2A	3297	1/1	0.91	0.08	52,52,52,52	0
56	MG	2A	3615	1/1	0.91	0.12	54,54,54,54	0
56	MG	2A	3082	1/1	0.91	0.08	52,52,52,52	0
56	MG	2A	3618	1/1	0.91	0.07	35,35,35,35	0
56	MG	2A	3083	1/1	0.91	0.13	51,51,51,51	0
56	MG	2A	3303	1/1	0.91	0.07	35,35,35,35	0
56	MG	1A	3998	1/1	0.91	0.09	51,51,51,51	0
56	MG	1a	3115	1/1	0.91	0.20	38,38,38,38	0
56	MG	2A	3087	1/1	0.91	0.10	61,61,61,61	0
56	MG	1O	3002	1/1	0.91	0.24	40,40,40,40	0
56	MG	1a	3128	1/1	0.91	0.08	36,36,36,36	0
56	MG	2A	3091	1/1	0.91	0.18	50,50,50,50	0
56	MG	2a	3037	1/1	0.91	0.10	53,53,53,53	0
56	MG	1a	3130	1/1	0.91	0.10	53,53,53,53	0
56	MG	2A	3632	1/1	0.91	0.10	42,42,42,42	0
56	MG	2a	3045	1/1	0.91	0.15	55,55,55,55	0
56	MG	1A	3628	1/1	0.91	0.08	17,17,17,17	0
56	MG	2a	3047	1/1	0.91	0.14	56,56,56,56	0
56	MG	2A	3637	1/1	0.91	0.10	53,53,53,53	0
56	MG	2a	3049	1/1	0.91	0.16	79,79,79,79	0
56	MG	2A	3328	1/1	0.91	0.08	45,45,45,45	0
56	MG	2a	3053	1/1	0.91	0.09	57,57,57,57	0
56	MG	1A	3227	1/1	0.91	0.14	28,28,28,28	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	3106	1/1	0.91	0.23	37,37,37,37	0
56	MG	1a	3142	1/1	0.91	0.13	63,63,63,63	0
56	MG	1A	3342	1/1	0.91	0.24	31,31,31,31	0
56	MG	2A	3341	1/1	0.91	0.20	43,43,43,43	0
56	MG	2A	3110	1/1	0.91	0.13	49,49,49,49	0
56	MG	2A	3658	1/1	0.91	0.10	31,31,31,31	0
56	MG	2A	3112	1/1	0.91	0.13	34,34,34,34	0
56	MG	2a	3071	1/1	0.91	0.07	55,55,55,55	0
56	MG	1U	203	1/1	0.91	0.13	22,22,22,22	0
56	MG	1V	201	1/1	0.91	0.07	25,25,25,25	0
56	MG	1A	3005	1/1	0.91	0.08	32,32,32,32	0
56	MG	1a	3153	1/1	0.91	0.12	43,43,43,43	0
56	MG	1A	3864	1/1	0.91	0.11	23,23,23,23	0
56	MG	1A	3441	1/1	0.91	0.09	40,40,40,40	0
56	MG	1A	3523	1/1	0.91	0.34	31,31,31,31	0
56	MG	2a	3082	1/1	0.91	0.20	50,50,50,50	0
56	MG	2A	3363	1/1	0.91	0.14	52,52,52,52	0
56	MG	2A	3367	1/1	0.91	0.16	35,35,35,35	0
56	MG	2A	3368	1/1	0.91	0.27	49,49,49,49	0
56	MG	1a	3165	1/1	0.91	0.22	45,45,45,45	0
56	MG	2A	3676	1/1	0.91	0.09	48,48,48,48	0
56	MG	2A	3128	1/1	0.91	0.16	50,50,50,50	0
56	MG	1A	3077	1/1	0.91	0.22	21,21,21,21	0
56	MG	10	105	1/1	0.91	0.18	30,30,30,30	0
56	MG	1A	3671	1/1	0.91	0.07	40,40,40,40	0
56	MG	11	104	1/1	0.91	0.10	53,53,53,53	0
56	MG	1A	3113	1/1	0.91	0.15	40,40,40,40	0
56	MG	1A	4035	1/1	0.91	0.07	13,13,13,13	0
56	MG	2A	3384	1/1	0.91	0.11	42,42,42,42	0
56	MG	1A	3448	1/1	0.91	0.10	28,28,28,28	0
56	MG	1A	3355	1/1	0.91	0.14	43,43,43,43	0
56	MG	2A	3692	1/1	0.91	0.09	43,43,43,43	0
56	MG	2A	3693	1/1	0.91	0.07	54,54,54,54	0
56	MG	1A	3885	1/1	0.91	0.08	18,18,18,18	0
56	MG	2A	3698	1/1	0.91	0.15	51,51,51,51	0
56	MG	1A	3887	1/1	0.91	0.20	50,50,50,50	0
56	MG	1A	4042	1/1	0.91	0.12	64,64,64,64	0
56	MG	2A	3704	1/1	0.91	0.20	58,58,58,58	0
56	MG	1A	3085	1/1	0.91	0.29	37,37,37,37	0
56	MG	2A	3156	1/1	0.91	0.23	52,52,52,52	0
56	MG	1A	4049	1/1	0.91	0.14	36,36,36,36	0
56	MG	1a	3198	1/1	0.91	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	3359	1/1	0.91	0.06	33,33,33,33	0
56	MG	1a	3219	1/1	0.91	0.08	53,53,53,53	0
56	MG	1A	3367	1/1	0.91	0.24	14,14,14,14	0
56	MG	1A	3036	1/1	0.91	0.30	25,25,25,25	0
56	MG	1a	3012	1/1	0.91	0.11	50,50,50,50	0
56	MG	1a	3225	1/1	0.91	0.24	62,62,62,62	0
56	MG	2A	3428	1/1	0.91	0.07	41,41,41,41	0
56	MG	1A	3571	1/1	0.91	0.11	28,28,28,28	0
56	MG	2A	3174	1/1	0.91	0.08	43,43,43,43	0
56	MG	1A	3126	1/1	0.91	0.12	35,35,35,35	0
56	MG	1A	4076	1/1	0.91	0.10	34,34,34,34	0
56	MG	1A	3801	1/1	0.91	0.14	56,56,56,56	0
56	MG	1A	3472	1/1	0.91	0.08	52,52,52,52	0
56	MG	2a	3169	1/1	0.91	0.15	59,59,59,59	0
56	MG	1a	3027	1/1	0.91	0.23	42,42,42,42	0
56	MG	1l	203	1/1	0.91	0.13	55,55,55,55	0
56	MG	1A	3306	1/1	0.91	0.11	43,43,43,43	0
56	MG	1A	3923	1/1	0.91	0.09	56,56,56,56	0
56	MG	2a	3176	1/1	0.91	0.14	55,55,55,55	0
56	MG	2A	3765	1/1	0.91	0.10	39,39,39,39	0
56	MG	1p	101	1/1	0.91	0.15	46,46,46,46	0
56	MG	1A	4102	1/1	0.91	0.09	11,11,11,11	0
56	MG	1A	3004	1/1	0.91	0.06	23,23,23,23	0
56	MG	2A	3770	1/1	0.91	0.09	40,40,40,40	0
56	MG	2A	3778	1/1	0.91	0.10	57,57,57,57	0
56	MG	2A	3202	1/1	0.91	0.34	51,51,51,51	0
56	MG	1A	4108	1/1	0.91	0.12	28,28,28,28	0
56	MG	2a	3191	1/1	0.91	0.17	61,61,61,61	0
56	MG	2A	3464	1/1	0.91	0.08	29,29,29,29	0
56	MG	1a	3039	1/1	0.91	0.23	59,59,59,59	0
56	MG	1A	3926	1/1	0.91	0.09	31,31,31,31	0
56	MG	1w	105	1/1	0.91	0.15	48,48,48,48	0
56	MG	2a	3197	1/1	0.91	0.18	54,54,54,54	0
56	MG	1A	4121	1/1	0.91	0.27	23,23,23,23	0
56	MG	2A	3804	1/1	0.91	0.21	40,40,40,40	0
56	MG	1A	4125	1/1	0.91	0.12	27,27,27,27	0
56	MG	2A	3215	1/1	0.91	0.14	49,49,49,49	0
56	MG	2a	3202	1/1	0.91	0.18	57,57,57,57	0
56	MG	2A	3217	1/1	0.91	0.12	40,40,40,40	0
56	MG	2A	3475	1/1	0.91	0.08	28,28,28,28	0
56	MG	2A	3218	1/1	0.91	0.12	49,49,49,49	0
56	MG	1a	3051	1/1	0.91	0.13	65,65,65,65	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	3714	1/1	0.91	0.09	59,59,59,59	0
56	MG	1A	4132	1/1	0.91	0.11	29,29,29,29	0
56	MG	2A	3828	1/1	0.91	0.10	40,40,40,40	0
56	MG	1x	109	1/1	0.91	0.12	68,68,68,68	0
56	MG	1A	4133	1/1	0.91	0.18	29,29,29,29	0
56	MG	1A	3314	1/1	0.91	0.07	44,44,44,44	0
56	MG	1A	3316	1/1	0.91	0.26	49,49,49,49	0
56	MG	2A	3232	1/1	0.91	0.06	42,42,42,42	0
56	MG	1A	3323	1/1	0.91	0.12	41,41,41,41	0
56	MG	1A	3827	1/1	0.91	0.20	22,22,22,22	0
56	MG	1a	3064	1/1	0.91	0.10	57,57,57,57	0
56	MG	1A	3605	1/1	0.91	0.07	32,32,32,32	0
56	MG	2a	3225	1/1	0.91	0.12	72,72,72,72	0
56	MG	1A	3091	1/1	0.91	0.09	35,35,35,35	0
56	MG	2A	3517	1/1	0.91	0.08	32,32,32,32	0
56	MG	2A	3520	1/1	0.91	0.17	62,62,62,62	0
56	MG	2d	303	1/1	0.91	0.11	65,65,65,65	0
56	MG	1A	3956	1/1	0.91	0.12	58,58,58,58	0
56	MG	2A	3533	1/1	0.91	0.07	54,54,54,54	0
56	MG	1A	3325	1/1	0.91	0.18	44,44,44,44	0
56	MG	2q	201	1/1	0.91	0.15	46,46,46,46	0
56	MG	2B	3006	1/1	0.91	0.16	60,60,60,60	0
56	MG	2A	3018	1/1	0.91	0.15	36,36,36,36	0
56	MG	2A	3540	1/1	0.91	0.12	32,32,32,32	0
56	MG	2B	3010	1/1	0.91	0.13	64,64,64,64	0
56	MG	1A	3402	1/1	0.91	0.14	27,27,27,27	0
56	MG	1B	3030	1/1	0.91	0.08	44,44,44,44	0
56	MG	2A	3026	1/1	0.91	0.11	47,47,47,47	0
56	MG	2A	3547	1/1	0.91	0.09	48,48,48,48	0
56	MG	2A	3028	1/1	0.91	0.13	30,30,30,30	0
56	MG	2A	3252	1/1	0.91	0.06	35,35,35,35	0
56	MG	2A	3029	1/1	0.91	0.17	52,52,52,52	0
56	MG	1a	3075	1/1	0.91	0.28	58,58,58,58	0
56	MG	1A	3970	1/1	0.91	0.10	25,25,25,25	0
56	MG	2A	3556	1/1	0.91	0.11	52,52,52,52	0
56	MG	1a	3084	1/1	0.91	0.11	42,42,42,42	0
56	MG	2A	3037	1/1	0.91	0.23	44,44,44,44	0
56	MG	1B	3032	1/1	0.91	0.07	35,35,35,35	0
56	MG	2A	3042	1/1	0.91	0.21	52,52,52,52	0
56	MG	2A	3565	1/1	0.91	0.08	51,51,51,51	0
56	MG	2A	3264	1/1	0.91	0.11	47,47,47,47	0
56	MG	1a	3134	1/1	0.92	0.10	38,38,38,38	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	3039	1/1	0.92	0.12	54,54,54,54	0
56	MG	16	102	1/1	0.92	0.09	46,46,46,46	0
56	MG	1a	3138	1/1	0.92	0.07	30,30,30,30	0
56	MG	2A	3045	1/1	0.92	0.19	52,52,52,52	0
56	MG	2a	3026	1/1	0.92	0.08	43,43,43,43	0
56	MG	2A	3046	1/1	0.92	0.09	56,56,56,56	0
56	MG	1A	4081	1/1	0.92	0.07	40,40,40,40	0
56	MG	1A	4083	1/1	0.92	0.15	41,41,41,41	0
56	MG	2A	3233	1/1	0.92	0.06	41,41,41,41	0
56	MG	1A	3173	1/1	0.92	0.09	30,30,30,30	0
56	MG	1A	3839	1/1	0.92	0.17	30,30,30,30	0
56	MG	2A	3061	1/1	0.92	0.08	38,38,38,38	0
56	MG	1A	3948	1/1	0.92	0.06	42,42,42,42	0
56	MG	2a	3041	1/1	0.92	0.09	43,43,43,43	0
56	MG	2a	3043	1/1	0.92	0.08	51,51,51,51	0
56	MG	1A	3840	1/1	0.92	0.10	29,29,29,29	0
56	MG	2A	3689	1/1	0.92	0.12	56,56,56,56	0
56	MG	1A	3525	1/1	0.92	0.24	51,51,51,51	0
56	MG	1A	4109	1/1	0.92	0.39	32,32,32,32	0
56	MG	1A	3059	1/1	0.92	0.14	42,42,42,42	0
56	MG	2A	3459	1/1	0.92	0.16	64,64,64,64	0
56	MG	1A	3962	1/1	0.92	0.09	15,15,15,15	0
56	MG	2a	3052	1/1	0.92	0.21	55,55,55,55	0
56	MG	2A	3696	1/1	0.92	0.10	42,42,42,42	0
56	MG	1a	3161	1/1	0.92	0.10	45,45,45,45	0
56	MG	1a	3164	1/1	0.92	0.12	41,41,41,41	0
56	MG	1A	3650	1/1	0.92	0.25	43,43,43,43	0
56	MG	1A	3537	1/1	0.92	0.19	38,38,38,38	0
56	MG	1A	4131	1/1	0.92	0.13	16,16,16,16	0
56	MG	1a	3171	1/1	0.92	0.09	55,55,55,55	0
56	MG	2a	3067	1/1	0.92	0.16	45,45,45,45	0
56	MG	1A	3658	1/1	0.92	0.13	15,15,15,15	0
56	MG	2A	3474	1/1	0.92	0.12	40,40,40,40	0
56	MG	1A	3660	1/1	0.92	0.10	8,8,8,8	0
56	MG	2a	3072	1/1	0.92	0.12	44,44,44,44	0
56	MG	1A	3540	1/1	0.92	0.13	29,29,29,29	0
56	MG	2a	3074	1/1	0.92	0.24	43,43,43,43	0
56	MG	2A	3729	1/1	0.92	0.10	66,66,66,66	0
56	MG	1A	3769	1/1	0.92	0.08	37,37,37,37	0
56	MG	2A	3733	1/1	0.92	0.10	70,70,70,70	0
56	MG	1A	3459	1/1	0.92	0.13	41,41,41,41	0
56	MG	1A	3052	1/1	0.92	0.12	29,29,29,29	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	3030	1/1	0.92	0.22	46,46,46,46	0
56	MG	2A	3092	1/1	0.92	0.12	41,41,41,41	0
56	MG	1A	3184	1/1	0.92	0.10	37,37,37,37	0
56	MG	2A	3739	1/1	0.92	0.11	69,69,69,69	0
56	MG	1a	3192	1/1	0.92	0.07	53,53,53,53	0
56	MG	2a	3088	1/1	0.92	0.17	67,67,67,67	0
56	MG	2a	3089	1/1	0.92	0.16	56,56,56,56	0
56	MG	1a	3033	1/1	0.92	0.33	56,56,56,56	0
56	MG	1a	3036	1/1	0.92	0.22	40,40,40,40	0
56	MG	1A	3781	1/1	0.92	0.14	42,42,42,42	0
56	MG	1A	3062	1/1	0.92	0.16	36,36,36,36	0
56	MG	1A	4004	1/1	0.92	0.08	62,62,62,62	0
56	MG	1a	3212	1/1	0.92	0.14	54,54,54,54	0
56	MG	2a	3099	1/1	0.92	0.22	51,51,51,51	0
56	MG	2a	3100	1/1	0.92	0.11	51,51,51,51	0
56	MG	2A	3114	1/1	0.92	0.24	52,52,52,52	0
56	MG	2A	3518	1/1	0.92	0.19	49,49,49,49	0
56	MG	1a	3218	1/1	0.92	0.07	55,55,55,55	0
56	MG	2A	3289	1/1	0.92	0.07	58,58,58,58	0
56	MG	2A	3526	1/1	0.92	0.07	57,57,57,57	0
56	MG	1A	3247	1/1	0.92	0.13	31,31,31,31	0
56	MG	2A	3534	1/1	0.92	0.15	52,52,52,52	0
56	MG	2A	3535	1/1	0.92	0.16	48,48,48,48	0
56	MG	2a	3111	1/1	0.92	0.20	46,46,46,46	0
56	MG	1A	3017	1/1	0.92	0.09	17,17,17,17	0
56	MG	2A	3783	1/1	0.92	0.09	40,40,40,40	0
56	MG	2A	3788	1/1	0.92	0.08	57,57,57,57	0
56	MG	1A	3084	1/1	0.92	0.20	50,50,50,50	0
56	MG	1a	3223	1/1	0.92	0.19	48,48,48,48	0
56	MG	1a	3050	1/1	0.92	0.11	51,51,51,51	0
56	MG	1A	4017	1/1	0.92	0.15	57,57,57,57	0
56	MG	2A	3126	1/1	0.92	0.13	39,39,39,39	0
56	MG	1A	3209	1/1	0.92	0.08	45,45,45,45	0
56	MG	1a	3227	1/1	0.92	0.20	46,46,46,46	0
56	MG	1A	3212	1/1	0.92	0.13	36,36,36,36	0
56	MG	2A	3132	1/1	0.92	0.27	57,57,57,57	0
56	MG	2A	3135	1/1	0.92	0.10	53,53,53,53	0
56	MG	2a	3144	1/1	0.92	0.09	76,76,76,76	0
56	MG	2A	3309	1/1	0.92	0.08	55,55,55,55	0
56	MG	2a	3152	1/1	0.92	0.10	67,67,67,67	0
56	MG	2A	3555	1/1	0.92	0.22	55,55,55,55	0
56	MG	2A	3817	1/1	0.92	0.12	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	3820	1/1	0.92	0.14	41,41,41,41	0
56	MG	2A	3310	1/1	0.92	0.21	59,59,59,59	0
56	MG	1A	3794	1/1	0.92	0.14	37,37,37,37	0
56	MG	1D	302	1/1	0.92	0.31	29,29,29,29	0
56	MG	2A	3315	1/1	0.92	0.08	40,40,40,40	0
56	MG	2A	3316	1/1	0.92	0.16	52,52,52,52	0
56	MG	2A	3831	1/1	0.92	0.14	56,56,56,56	0
56	MG	1A	3890	1/1	0.92	0.08	51,51,51,51	0
56	MG	1D	314	1/1	0.92	0.25	34,34,34,34	0
56	MG	2A	3571	1/1	0.92	0.17	38,38,38,38	0
56	MG	1E	304	1/1	0.92	0.14	44,44,44,44	0
56	MG	1A	4025	1/1	0.92	0.11	18,18,18,18	0
56	MG	1A	3213	1/1	0.92	0.27	27,27,27,27	0
56	MG	1A	4030	1/1	0.92	0.08	32,32,32,32	0
56	MG	1A	3317	1/1	0.92	0.08	36,36,36,36	0
56	MG	2A	3336	1/1	0.92	0.11	45,45,45,45	0
56	MG	1A	3429	1/1	0.92	0.07	39,39,39,39	0
56	MG	2a	3184	1/1	0.92	0.09	46,46,46,46	0
56	MG	2A	3866	1/1	0.92	0.08	31,31,31,31	0
56	MG	1A	3493	1/1	0.92	0.11	63,63,63,63	0
56	MG	1A	3319	1/1	0.92	0.14	38,38,38,38	0
56	MG	2A	3157	1/1	0.92	0.25	58,58,58,58	0
56	MG	1A	3601	1/1	0.92	0.16	55,55,55,55	0
56	MG	2A	3593	1/1	0.92	0.24	58,58,58,58	0
56	MG	1A	3911	1/1	0.92	0.06	34,34,34,34	0
56	MG	2B	3008	1/1	0.92	0.12	49,49,49,49	0
56	MG	2A	3344	1/1	0.92	0.06	48,48,48,48	0
56	MG	2A	3162	1/1	0.92	0.06	42,42,42,42	0
56	MG	1a	3083	1/1	0.92	0.13	53,53,53,53	0
56	MG	1A	3912	1/1	0.92	0.07	43,43,43,43	0
56	MG	1P	201	1/1	0.92	0.12	20,20,20,20	0
56	MG	1Q	3003	1/1	0.92	0.07	40,40,40,40	0
56	MG	2A	3606	1/1	0.92	0.09	35,35,35,35	0
56	MG	2A	3353	1/1	0.92	0.18	44,44,44,44	0
56	MG	1x	106	1/1	0.92	0.20	52,52,52,52	0
56	MG	1A	3368	1/1	0.92	0.07	42,42,42,42	0
56	MG	2A	3611	1/1	0.92	0.07	61,61,61,61	0
56	MG	2A	3359	1/1	0.92	0.21	43,43,43,43	0
56	MG	1A	3370	1/1	0.92	0.07	29,29,29,29	0
56	MG	1a	3093	1/1	0.92	0.23	35,35,35,35	0
56	MG	1x	111	1/1	0.92	0.12	52,52,52,52	0
56	MG	1U	201	1/1	0.92	0.17	22,22,22,22	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	3320	1/1	0.92	0.14	28,28,28,28	0
56	MG	1U	205	1/1	0.92	0.12	35,35,35,35	0
56	MG	2O	8001	1/1	0.92	0.08	54,54,54,54	0
56	MG	2A	3373	1/1	0.92	0.24	47,47,47,47	0
56	MG	2Q	203	1/1	0.92	0.07	47,47,47,47	0
56	MG	1A	3822	1/1	0.92	0.07	47,47,47,47	0
56	MG	1A	3377	1/1	0.92	0.09	25,25,25,25	0
56	MG	1a	3103	1/1	0.92	0.09	57,57,57,57	0
56	MG	2A	3011	1/1	0.92	0.14	42,42,42,42	0
56	MG	1a	3104	1/1	0.92	0.11	49,49,49,49	0
56	MG	2U	204	1/1	0.92	0.09	57,57,57,57	0
56	MG	1A	3379	1/1	0.92	0.07	39,39,39,39	0
56	MG	1A	4059	1/1	0.92	0.12	34,34,34,34	0
56	MG	2W	202	1/1	0.92	0.08	38,38,38,38	0
56	MG	2p	3001	1/1	0.92	0.11	45,45,45,45	0
56	MG	1A	3615	1/1	0.92	0.07	22,22,22,22	0
56	MG	2q	202	1/1	0.92	0.10	64,64,64,64	0
56	MG	1A	3931	1/1	0.92	0.06	36,36,36,36	0
56	MG	10	102	1/1	0.92	0.10	49,49,49,49	0
56	MG	1A	4068	1/1	0.92	0.07	42,42,42,42	0
56	MG	26	502	1/1	0.92	0.24	62,62,62,62	0
56	MG	2A	3399	1/1	0.92	0.24	53,53,53,53	0
56	MG	2A	3648	1/1	0.92	0.10	33,33,33,33	0
56	MG	2A	3400	1/1	0.92	0.19	51,51,51,51	0
56	MG	2a	3003	1/1	0.92	0.10	53,53,53,53	0
56	MG	2A	3206	1/1	0.92	0.07	57,57,57,57	0
56	MG	10	107	1/1	0.92	0.12	53,53,53,53	0
56	MG	2A	3208	1/1	0.92	0.05	29,29,29,29	0
56	MG	2A	3406	1/1	0.92	0.29	59,59,59,59	0
56	MG	1A	4069	1/1	0.92	0.11	26,26,26,26	0
56	MG	1a	3117	1/1	0.92	0.15	31,31,31,31	0
56	MG	1A	3513	1/1	0.92	0.06	34,34,34,34	0
56	MG	2A	3216	1/1	0.92	0.34	53,53,53,53	0
56	MG	1A	3045	1/1	0.92	0.08	22,22,22,22	0
56	MG	2A	3421	1/1	0.92	0.33	54,54,54,54	0
56	MG	1A	3382	1/1	0.92	0.11	41,41,41,41	0
56	MG	2a	3018	1/1	0.92	0.15	50,50,50,50	0
56	MG	1A	3050	1/1	0.93	0.21	39,39,39,39	0
56	MG	10	104	1/1	0.93	0.06	30,30,30,30	0
56	MG	1A	3592	1/1	0.93	0.10	46,46,46,46	0
56	MG	2A	3305	1/1	0.93	0.12	53,53,53,53	0
56	MG	2A	3585	1/1	0.93	0.17	45,45,45,45	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	3586	1/1	0.93	0.23	41,41,41,41	0
56	MG	2A	3306	1/1	0.93	0.06	45,45,45,45	0
56	MG	1A	3878	1/1	0.93	0.10	30,30,30,30	0
56	MG	2A	3592	1/1	0.93	0.09	48,48,48,48	0
56	MG	1A	3002	1/1	0.93	0.13	40,40,40,40	0
56	MG	1A	4052	1/1	0.93	0.10	49,49,49,49	0
56	MG	1A	3285	1/1	0.93	0.23	32,32,32,32	0
56	MG	1A	4054	1/1	0.93	0.10	37,37,37,37	0
56	MG	1A	3468	1/1	0.93	0.12	26,26,26,26	0
56	MG	2A	3113	1/1	0.93	0.13	47,47,47,47	0
56	MG	1A	3761	1/1	0.93	0.10	47,47,47,47	0
56	MG	2A	3319	1/1	0.93	0.10	51,51,51,51	0
56	MG	2A	3605	1/1	0.93	0.08	46,46,46,46	0
56	MG	1a	3172	1/1	0.93	0.11	65,65,65,65	0
56	MG	1A	3764	1/1	0.93	0.14	16,16,16,16	0
56	MG	1A	3375	1/1	0.93	0.06	25,25,25,25	0
56	MG	2A	3325	1/1	0.93	0.06	33,33,33,33	0
56	MG	1A	3894	1/1	0.93	0.07	36,36,36,36	0
56	MG	1A	3292	1/1	0.93	0.07	22,22,22,22	0
56	MG	1a	3182	1/1	0.93	0.10	56,56,56,56	0
56	MG	2A	3332	1/1	0.93	0.09	43,43,43,43	0
56	MG	2A	3334	1/1	0.93	0.13	63,63,63,63	0
56	MG	2A	3335	1/1	0.93	0.09	48,48,48,48	0
56	MG	2a	3013	1/1	0.93	0.17	44,44,44,44	0
56	MG	1A	3224	1/1	0.93	0.07	41,41,41,41	0
56	MG	1A	4070	1/1	0.93	0.10	49,49,49,49	0
56	MG	1A	3299	1/1	0.93	0.08	27,27,27,27	0
56	MG	1A	3612	1/1	0.93	0.15	16,16,16,16	0
56	MG	1A	3772	1/1	0.93	0.09	14,14,14,14	0
56	MG	1a	3010	1/1	0.93	0.10	53,53,53,53	0
56	MG	2A	3133	1/1	0.93	0.09	44,44,44,44	0
56	MG	1A	3301	1/1	0.93	0.19	54,54,54,54	0
56	MG	1A	4082	1/1	0.93	0.08	29,29,29,29	0
56	MG	2A	3137	1/1	0.93	0.12	35,35,35,35	0
56	MG	2A	3633	1/1	0.93	0.07	59,59,59,59	0
56	MG	2a	3028	1/1	0.93	0.32	58,58,58,58	0
56	MG	2a	3029	1/1	0.93	0.26	43,43,43,43	0
56	MG	2A	3347	1/1	0.93	0.08	58,58,58,58	0
56	MG	1a	3015	1/1	0.93	0.11	60,60,60,60	0
56	MG	1A	3225	1/1	0.93	0.14	42,42,42,42	0
56	MG	1A	4089	1/1	0.93	0.11	34,34,34,34	0
56	MG	2A	3644	1/1	0.93	0.08	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	2a	3035	1/1	0.93	0.23	53,53,53,53	0
56	MG	1A	3011	1/1	0.93	0.07	26,26,26,26	0
56	MG	1A	4093	1/1	0.93	0.17	25,25,25,25	0
56	MG	1A	3231	1/1	0.93	0.08	25,25,25,25	0
56	MG	1A	4097	1/1	0.93	0.17	40,40,40,40	0
56	MG	2a	3042	1/1	0.93	0.05	63,63,63,63	0
56	MG	1A	3390	1/1	0.93	0.09	32,32,32,32	0
56	MG	1A	3634	1/1	0.93	0.11	12,12,12,12	0
56	MG	2A	3151	1/1	0.93	0.10	46,46,46,46	0
56	MG	2A	3153	1/1	0.93	0.12	47,47,47,47	0
56	MG	1A	3233	1/1	0.93	0.23	24,24,24,24	0
56	MG	1A	3041	1/1	0.93	0.06	16,16,16,16	0
56	MG	2A	3662	1/1	0.93	0.07	34,34,34,34	0
56	MG	1a	3035	1/1	0.93	0.13	43,43,43,43	0
56	MG	2a	3051	1/1	0.93	0.09	52,52,52,52	0
56	MG	1A	3928	1/1	0.93	0.07	42,42,42,42	0
56	MG	1A	4115	1/1	0.93	0.08	32,32,32,32	0
56	MG	1A	3792	1/1	0.93	0.08	22,22,22,22	0
56	MG	1A	3163	1/1	0.93	0.09	32,32,32,32	0
56	MG	2A	3670	1/1	0.93	0.12	50,50,50,50	0
56	MG	1e	201	1/1	0.93	0.06	63,63,63,63	0
56	MG	1A	3044	1/1	0.93	0.10	14,14,14,14	0
56	MG	2A	3386	1/1	0.93	0.22	51,51,51,51	0
56	MG	2A	3674	1/1	0.93	0.07	62,62,62,62	0
56	MG	1A	3322	1/1	0.93	0.12	31,31,31,31	0
56	MG	1a	3047	1/1	0.93	0.19	52,52,52,52	0
56	MG	2a	3070	1/1	0.93	0.21	46,46,46,46	0
56	MG	1A	3128	1/1	0.93	0.10	38,38,38,38	0
56	MG	2A	3393	1/1	0.93	0.09	30,30,30,30	0
56	MG	1A	3403	1/1	0.93	0.05	29,29,29,29	0
56	MG	1A	3405	1/1	0.93	0.10	30,30,30,30	0
56	MG	2A	3175	1/1	0.93	0.17	45,45,45,45	0
56	MG	1A	3665	1/1	0.93	0.07	14,14,14,14	0
56	MG	1A	3950	1/1	0.93	0.16	46,46,46,46	0
56	MG	2A	3402	1/1	0.93	0.09	39,39,39,39	0
56	MG	2A	3179	1/1	0.93	0.10	56,56,56,56	0
56	MG	1B	3010	1/1	0.93	0.16	32,32,32,32	0
56	MG	1A	3174	1/1	0.93	0.12	48,48,48,48	0
56	MG	2a	3083	1/1	0.93	0.16	42,42,42,42	0
56	MG	1A	3807	1/1	0.93	0.08	42,42,42,42	0
56	MG	1a	3061	1/1	0.93	0.09	50,50,50,50	0
56	MG	2A	3414	1/1	0.93	0.21	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	3958	1/1	0.93	0.09	8,8,8,8	0
56	MG	2A	3697	1/1	0.93	0.12	51,51,51,51	0
56	MG	1A	3129	1/1	0.93	0.25	20,20,20,20	0
56	MG	1A	3177	1/1	0.93	0.09	26,26,26,26	0
56	MG	2A	3702	1/1	0.93	0.07	37,37,37,37	0
56	MG	2A	3420	1/1	0.93	0.06	40,40,40,40	0
56	MG	2A	3194	1/1	0.93	0.14	30,30,30,30	0
56	MG	2A	3195	1/1	0.93	0.07	41,41,41,41	0
56	MG	2A	3707	1/1	0.93	0.15	65,65,65,65	0
56	MG	1x	105	1/1	0.93	0.23	66,66,66,66	0
56	MG	2A	3427	1/1	0.93	0.12	58,58,58,58	0
56	MG	2A	3714	1/1	0.93	0.10	44,44,44,44	0
56	MG	2A	3718	1/1	0.93	0.22	56,56,56,56	0
56	MG	2A	3720	1/1	0.93	0.10	54,54,54,54	0
56	MG	1A	3815	1/1	0.93	0.06	48,48,48,48	0
56	MG	2A	3201	1/1	0.93	0.19	52,52,52,52	0
56	MG	1x	107	1/1	0.93	0.12	53,53,53,53	0
56	MG	2A	3433	1/1	0.93	0.23	51,51,51,51	0
56	MG	1A	3424	1/1	0.93	0.07	31,31,31,31	0
56	MG	1A	3531	1/1	0.93	0.09	35,35,35,35	0
56	MG	1A	3823	1/1	0.93	0.11	17,17,17,17	0
56	MG	2a	3114	1/1	0.93	0.19	47,47,47,47	0
56	MG	1A	3976	1/1	0.93	0.08	17,17,17,17	0
56	MG	1a	3071	1/1	0.93	0.08	41,41,41,41	0
56	MG	1A	3978	1/1	0.93	0.12	57,57,57,57	0
56	MG	1y	102	1/1	0.93	0.06	40,40,40,40	0
56	MG	1A	3679	1/1	0.93	0.11	43,43,43,43	0
56	MG	2a	3129	1/1	0.93	0.07	64,64,64,64	0
56	MG	1A	3826	1/1	0.93	0.10	41,41,41,41	0
56	MG	1a	3082	1/1	0.93	0.17	45,45,45,45	0
56	MG	2A	3002	1/1	0.93	0.16	49,49,49,49	0
56	MG	1D	312	1/1	0.93	0.20	20,20,20,20	0
56	MG	1A	3131	1/1	0.93	0.08	29,29,29,29	0
56	MG	2A	3012	1/1	0.93	0.07	24,24,24,24	0
56	MG	2A	3461	1/1	0.93	0.07	30,30,30,30	0
56	MG	2a	3146	1/1	0.93	0.07	76,76,76,76	0
56	MG	1a	3085	1/1	0.93	0.21	53,53,53,53	0
56	MG	2a	3150	1/1	0.93	0.09	68,68,68,68	0
56	MG	2A	3015	1/1	0.93	0.15	35,35,35,35	0
56	MG	1A	3132	1/1	0.93	0.24	32,32,32,32	0
56	MG	2a	3154	1/1	0.93	0.10	66,66,66,66	0
56	MG	2A	3228	1/1	0.93	0.07	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	3339	1/1	0.93	0.07	44,44,44,44	0
56	MG	2a	3158	1/1	0.93	0.11	66,66,66,66	0
56	MG	1a	3088	1/1	0.93	0.06	52,52,52,52	0
56	MG	2A	3019	1/1	0.93	0.21	45,45,45,45	0
56	MG	2a	3162	1/1	0.93	0.15	57,57,57,57	0
56	MG	2A	3776	1/1	0.93	0.08	48,48,48,48	0
56	MG	2a	3164	1/1	0.93	0.08	49,49,49,49	0
56	MG	1A	3431	1/1	0.93	0.10	40,40,40,40	0
56	MG	1A	3435	1/1	0.93	0.10	51,51,51,51	0
56	MG	2A	3023	1/1	0.93	0.07	34,34,34,34	0
56	MG	2A	3476	1/1	0.93	0.09	52,52,52,52	0
56	MG	1A	4000	1/1	0.93	0.12	34,34,34,34	0
56	MG	1a	3094	1/1	0.93	0.17	39,39,39,39	0
56	MG	2A	3240	1/1	0.93	0.09	43,43,43,43	0
56	MG	2A	3242	1/1	0.93	0.07	47,47,47,47	0
56	MG	1A	3029	1/1	0.93	0.16	28,28,28,28	0
56	MG	2A	3487	1/1	0.93	0.07	27,27,27,27	0
56	MG	2A	3803	1/1	0.93	0.09	52,52,52,52	0
56	MG	1F	302	1/1	0.93	0.06	31,31,31,31	0
56	MG	2A	3491	1/1	0.93	0.10	35,35,35,35	0
56	MG	1A	3711	1/1	0.93	0.06	28,28,28,28	0
56	MG	1a	3099	1/1	0.93	0.12	51,51,51,51	0
56	MG	1A	3344	1/1	0.93	0.06	29,29,29,29	0
56	MG	2a	3188	1/1	0.93	0.12	72,72,72,72	0
56	MG	1G	3001	1/1	0.93	0.13	28,28,28,28	0
56	MG	2A	3507	1/1	0.93	0.09	52,52,52,52	0
56	MG	1G	3002	1/1	0.93	0.07	38,38,38,38	0
56	MG	1G	3004	1/1	0.93	0.07	39,39,39,39	0
56	MG	1I	3001	1/1	0.93	0.06	50,50,50,50	0
56	MG	2A	3511	1/1	0.93	0.10	38,38,38,38	0
56	MG	1A	4010	1/1	0.93	0.13	54,54,54,54	0
56	MG	2A	3829	1/1	0.93	0.08	40,40,40,40	0
56	MG	2A	3254	1/1	0.93	0.09	53,53,53,53	0
56	MG	1A	3443	1/1	0.93	0.07	46,46,46,46	0
56	MG	2A	3833	1/1	0.93	0.06	42,42,42,42	0
56	MG	2A	3834	1/1	0.93	0.07	47,47,47,47	0
56	MG	2a	3203	1/1	0.93	0.15	64,64,64,64	0
56	MG	1A	3843	1/1	0.93	0.20	23,23,23,23	0
56	MG	2A	3258	1/1	0.93	0.15	40,40,40,40	0
56	MG	2A	3525	1/1	0.93	0.06	38,38,38,38	0
56	MG	2A	3259	1/1	0.93	0.07	46,46,46,46	0
56	MG	1A	3260	1/1	0.93	0.11	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	1O	3005	1/1	0.93	0.07	62,62,62,62	0
56	MG	2A	3050	1/1	0.93	0.12	38,38,38,38	0
56	MG	2a	3213	1/1	0.93	0.14	56,56,56,56	0
56	MG	1A	3568	1/1	0.93	0.12	51,51,51,51	0
56	MG	2A	3851	1/1	0.93	0.08	43,43,43,43	0
56	MG	2A	3852	1/1	0.93	0.06	43,43,43,43	0
56	MG	2A	3538	1/1	0.93	0.16	47,47,47,47	0
56	MG	1P	203	1/1	0.93	0.14	34,34,34,34	0
56	MG	2A	3865	1/1	0.93	0.23	39,39,39,39	0
56	MG	1A	3849	1/1	0.93	0.10	28,28,28,28	0
56	MG	2a	3222	1/1	0.93	0.10	51,51,51,51	0
56	MG	2A	3867	1/1	0.93	0.09	36,36,36,36	0
56	MG	2A	3267	1/1	0.93	0.11	49,49,49,49	0
56	MG	2A	3871	1/1	0.93	0.15	36,36,36,36	0
56	MG	2a	3226	1/1	0.93	0.16	55,55,55,55	0
56	MG	1a	3119	1/1	0.93	0.06	28,28,28,28	0
56	MG	2A	3875	1/1	0.93	0.17	32,32,32,32	0
56	MG	2A	3876	1/1	0.93	0.11	43,43,43,43	0
56	MG	2d	301	1/1	0.93	0.26	58,58,58,58	0
56	MG	1a	3120	1/1	0.93	0.17	46,46,46,46	0
56	MG	2A	3270	1/1	0.93	0.06	41,41,41,41	0
56	MG	2B	3005	1/1	0.93	0.10	55,55,55,55	0
56	MG	1A	4021	1/1	0.93	0.07	45,45,45,45	0
56	MG	1a	3124	1/1	0.93	0.13	40,40,40,40	0
56	MG	1a	3127	1/1	0.93	0.14	33,33,33,33	0
56	MG	1A	3197	1/1	0.93	0.09	44,44,44,44	0
56	MG	2A	3553	1/1	0.93	0.08	39,39,39,39	0
56	MG	1A	3047	1/1	0.93	0.26	47,47,47,47	0
56	MG	1A	3147	1/1	0.93	0.14	36,36,36,36	0
56	MG	2A	3279	1/1	0.93	0.13	51,51,51,51	0
56	MG	2A	3557	1/1	0.93	0.21	41,41,41,41	0
56	MG	2A	3078	1/1	0.93	0.17	31,31,31,31	0
56	MG	1A	3577	1/1	0.93	0.07	16,16,16,16	0
56	MG	1U	207	1/1	0.93	0.17	22,22,22,22	0
56	MG	1A	3150	1/1	0.93	0.09	39,39,39,39	0
56	MG	1a	3141	1/1	0.93	0.18	53,53,53,53	0
56	MG	1A	3734	1/1	0.93	0.09	14,14,14,14	0
56	MG	1a	3143	1/1	0.93	0.15	52,52,52,52	0
56	MG	2E	302	1/1	0.93	0.07	28,28,28,28	0
56	MG	1A	3583	1/1	0.93	0.10	31,31,31,31	0
56	MG	2E	305	1/1	0.93	0.15	39,39,39,39	0
56	MG	2A	3088	1/1	0.93	0.19	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	3736	1/1	0.93	0.12	16,16,16,16	0
56	MG	1A	3063	1/1	0.93	0.13	14,14,14,14	0
56	MG	2F	303	1/1	0.93	0.09	38,38,38,38	0
56	MG	1A	3362	1/1	0.93	0.26	41,41,41,41	0
58	M2D	2A	3864	36/36	0.93	0.12	32,41,50,52	0
56	MG	1A	3723	1/1	0.94	0.13	46,46,46,46	0
56	MG	1A	4038	1/1	0.94	0.08	39,39,39,39	0
56	MG	1A	3575	1/1	0.94	0.10	21,21,21,21	0
56	MG	1A	3162	1/1	0.94	0.27	32,32,32,32	0
56	MG	1A	3731	1/1	0.94	0.07	20,20,20,20	0
56	MG	1a	3168	1/1	0.94	0.06	44,44,44,44	0
56	MG	1A	3578	1/1	0.94	0.10	47,47,47,47	0
56	MG	1A	4043	1/1	0.94	0.05	30,30,30,30	0
56	MG	1A	3249	1/1	0.94	0.09	49,49,49,49	0
56	MG	1A	3081	1/1	0.94	0.14	23,23,23,23	0
56	MG	1a	3174	1/1	0.94	0.09	76,76,76,76	0
56	MG	1A	4050	1/1	0.94	0.08	34,34,34,34	0
56	MG	1A	3009	1/1	0.94	0.08	16,16,16,16	0
56	MG	2A	3130	1/1	0.94	0.13	49,49,49,49	0
56	MG	2A	3610	1/1	0.94	0.06	42,42,42,42	0
56	MG	2X	3001	1/1	0.94	0.09	52,52,52,52	0
56	MG	1A	3109	1/1	0.94	0.09	28,28,28,28	0
56	MG	1A	3740	1/1	0.94	0.07	44,44,44,44	0
56	MG	20	3002	1/1	0.94	0.07	40,40,40,40	0
56	MG	1A	3880	1/1	0.94	0.19	16,16,16,16	0
56	MG	2A	3134	1/1	0.94	0.15	42,42,42,42	0
56	MG	1A	3881	1/1	0.94	0.07	18,18,18,18	0
56	MG	1A	3742	1/1	0.94	0.08	15,15,15,15	0
56	MG	1A	4060	1/1	0.94	0.07	25,25,25,25	0
56	MG	1A	3467	1/1	0.94	0.19	31,31,31,31	0
56	MG	1a	3193	1/1	0.94	0.08	37,37,37,37	0
56	MG	1A	3255	1/1	0.94	0.09	38,38,38,38	0
56	MG	2A	3351	1/1	0.94	0.11	59,59,59,59	0
56	MG	2a	3007	1/1	0.94	0.10	38,38,38,38	0
56	MG	1A	3886	1/1	0.94	0.11	34,34,34,34	0
56	MG	1A	3470	1/1	0.94	0.12	33,33,33,33	0
56	MG	2A	3355	1/1	0.94	0.15	29,29,29,29	0
56	MG	1A	3471	1/1	0.94	0.12	41,41,41,41	0
56	MG	2A	3628	1/1	0.94	0.07	34,34,34,34	0
56	MG	2A	3629	1/1	0.94	0.10	56,56,56,56	0
56	MG	2A	3357	1/1	0.94	0.18	37,37,37,37	0
56	MG	1A	4072	1/1	0.94	0.07	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	3148	1/1	0.94	0.10	35,35,35,35	0
56	MG	2A	3362	1/1	0.94	0.20	26,26,26,26	0
56	MG	2A	3639	1/1	0.94	0.10	62,62,62,62	0
56	MG	1A	4073	1/1	0.94	0.07	39,39,39,39	0
56	MG	2A	3641	1/1	0.94	0.08	56,56,56,56	0
56	MG	1a	3217	1/1	0.94	0.09	35,35,35,35	0
56	MG	2a	3023	1/1	0.94	0.17	49,49,49,49	0
56	MG	1A	3602	1/1	0.94	0.10	24,24,24,24	0
56	MG	1A	3757	1/1	0.94	0.12	8,8,8,8	0
56	MG	1A	3897	1/1	0.94	0.10	40,40,40,40	0
56	MG	1a	3024	1/1	0.94	0.19	37,37,37,37	0
56	MG	1A	3758	1/1	0.94	0.10	59,59,59,59	0
56	MG	2A	3374	1/1	0.94	0.19	39,39,39,39	0
56	MG	2A	3653	1/1	0.94	0.14	51,51,51,51	0
56	MG	1A	3214	1/1	0.94	0.10	46,46,46,46	0
56	MG	2A	3656	1/1	0.94	0.08	44,44,44,44	0
56	MG	1A	3389	1/1	0.94	0.17	36,36,36,36	0
56	MG	2A	3161	1/1	0.94	0.07	36,36,36,36	0
56	MG	1A	4088	1/1	0.94	0.07	49,49,49,49	0
56	MG	2A	3381	1/1	0.94	0.15	43,43,43,43	0
56	MG	1A	3901	1/1	0.94	0.13	37,37,37,37	0
56	MG	1A	3902	1/1	0.94	0.08	34,34,34,34	0
56	MG	2A	3664	1/1	0.94	0.09	50,50,50,50	0
56	MG	2A	3385	1/1	0.94	0.10	36,36,36,36	0
56	MG	1a	3032	1/1	0.94	0.17	20,20,20,20	0
56	MG	2A	3387	1/1	0.94	0.13	39,39,39,39	0
56	MG	1a	3232	1/1	0.94	0.13	54,54,54,54	0
56	MG	1A	3762	1/1	0.94	0.07	13,13,13,13	0
56	MG	1a	3034	1/1	0.94	0.18	49,49,49,49	0
56	MG	1A	3218	1/1	0.94	0.19	33,33,33,33	0
56	MG	2A	3394	1/1	0.94	0.08	48,48,48,48	0
56	MG	2A	3395	1/1	0.94	0.20	45,45,45,45	0
56	MG	1A	3609	1/1	0.94	0.19	6,6,6,6	0
56	MG	1A	3221	1/1	0.94	0.06	34,34,34,34	0
56	MG	1A	3018	1/1	0.94	0.08	28,28,28,28	0
56	MG	1A	3115	1/1	0.94	0.12	19,19,19,19	0
56	MG	1A	3394	1/1	0.94	0.09	39,39,39,39	0
56	MG	1a	3042	1/1	0.94	0.08	55,55,55,55	0
56	MG	2A	3182	1/1	0.94	0.18	51,51,51,51	0
56	MG	2a	3060	1/1	0.94	0.09	49,49,49,49	0
56	MG	2a	3061	1/1	0.94	0.17	40,40,40,40	0
56	MG	2a	3062	1/1	0.94	0.21	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	2a	3063	1/1	0.94	0.09	46,46,46,46	0
56	MG	1A	3398	1/1	0.94	0.12	48,48,48,48	0
56	MG	1A	3487	1/1	0.94	0.10	25,25,25,25	0
56	MG	2A	3687	1/1	0.94	0.21	37,37,37,37	0
56	MG	2A	3407	1/1	0.94	0.25	45,45,45,45	0
56	MG	1A	3622	1/1	0.94	0.09	37,37,37,37	0
56	MG	2A	3409	1/1	0.94	0.30	65,65,65,65	0
56	MG	1A	3624	1/1	0.94	0.07	39,39,39,39	0
56	MG	1A	3782	1/1	0.94	0.14	35,35,35,35	0
56	MG	1A	3783	1/1	0.94	0.07	24,24,24,24	0
56	MG	2A	3694	1/1	0.94	0.07	44,44,44,44	0
56	MG	2A	3193	1/1	0.94	0.18	40,40,40,40	0
56	MG	1A	3268	1/1	0.94	0.15	15,15,15,15	0
56	MG	1w	109	1/1	0.94	0.11	51,51,51,51	0
56	MG	2A	3197	1/1	0.94	0.06	46,46,46,46	0
56	MG	2A	3422	1/1	0.94	0.17	31,31,31,31	0
56	MG	2A	3700	1/1	0.94	0.08	36,36,36,36	0
56	MG	2A	3701	1/1	0.94	0.07	32,32,32,32	0
56	MG	1A	3400	1/1	0.94	0.14	50,50,50,50	0
56	MG	1x	101	1/1	0.94	0.10	43,43,43,43	0
56	MG	1A	4144	1/1	0.94	0.13	27,27,27,27	0
56	MG	2A	3705	1/1	0.94	0.16	51,51,51,51	0
56	MG	1a	3059	1/1	0.94	0.16	40,40,40,40	0
56	MG	1B	3001	1/1	0.94	0.17	27,27,27,27	0
56	MG	1A	3335	1/1	0.94	0.06	28,28,28,28	0
56	MG	2A	3711	1/1	0.94	0.14	61,61,61,61	0
56	MG	2a	3095	1/1	0.94	0.11	59,59,59,59	0
56	MG	1A	3119	1/1	0.94	0.32	24,24,24,24	0
56	MG	1A	3944	1/1	0.94	0.11	53,53,53,53	0
56	MG	2A	3717	1/1	0.94	0.06	39,39,39,39	0
56	MG	1A	3790	1/1	0.94	0.07	19,19,19,19	0
56	MG	1B	3011	1/1	0.94	0.14	29,29,29,29	0
56	MG	2A	3210	1/1	0.94	0.09	42,42,42,42	0
56	MG	1B	3015	1/1	0.94	0.06	29,29,29,29	0
56	MG	2A	3724	1/1	0.94	0.08	55,55,55,55	0
56	MG	2A	3725	1/1	0.94	0.10	67,67,67,67	0
56	MG	2A	3212	1/1	0.94	0.12	54,54,54,54	0
56	MG	2A	3727	1/1	0.94	0.07	45,45,45,45	0
56	MG	1x	114	1/1	0.94	0.05	54,54,54,54	0
56	MG	2A	3214	1/1	0.94	0.06	38,38,38,38	0
56	MG	1A	3638	1/1	0.94	0.07	27,27,27,27	0
56	MG	1A	3646	1/1	0.94	0.08	15,15,15,15	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	3951	1/1	0.94	0.12	56,56,56,56	0
56	MG	1A	3087	1/1	0.94	0.13	8,8,8,8	0
56	MG	2a	3116	1/1	0.94	0.09	73,73,73,73	0
56	MG	2A	3219	1/1	0.94	0.16	42,42,42,42	0
56	MG	1A	3343	1/1	0.94	0.12	32,32,32,32	0
56	MG	2A	3460	1/1	0.94	0.10	35,35,35,35	0
56	MG	2A	3221	1/1	0.94	0.17	46,46,46,46	0
56	MG	2a	3127	1/1	0.94	0.10	66,66,66,66	0
56	MG	1A	3006	1/1	0.94	0.10	44,44,44,44	0
56	MG	2A	3003	1/1	0.94	0.07	44,44,44,44	0
56	MG	2a	3130	1/1	0.94	0.10	67,67,67,67	0
56	MG	1B	3029	1/1	0.94	0.13	59,59,59,59	0
56	MG	2A	3009	1/1	0.94	0.12	36,36,36,36	0
56	MG	1A	3345	1/1	0.94	0.08	34,34,34,34	0
56	MG	2A	3746	1/1	0.94	0.08	58,58,58,58	0
56	MG	2a	3138	1/1	0.94	0.20	48,48,48,48	0
56	MG	2A	3749	1/1	0.94	0.11	66,66,66,66	0
56	MG	1A	3186	1/1	0.94	0.37	31,31,31,31	0
56	MG	2A	3755	1/1	0.94	0.06	53,53,53,53	0
56	MG	1A	3423	1/1	0.94	0.12	53,53,53,53	0
56	MG	1A	3518	1/1	0.94	0.08	48,48,48,48	0
56	MG	1A	3664	1/1	0.94	0.06	13,13,13,13	0
56	MG	1A	3028	1/1	0.94	0.31	22,22,22,22	0
56	MG	1A	3667	1/1	0.94	0.05	35,35,35,35	0
56	MG	2A	3768	1/1	0.94	0.09	24,24,24,24	0
56	MG	2A	3477	1/1	0.94	0.08	44,44,44,44	0
56	MG	1D	304	1/1	0.94	0.18	48,48,48,48	0
56	MG	2A	3773	1/1	0.94	0.06	57,57,57,57	0
56	MG	1a	3091	1/1	0.94	0.29	38,38,38,38	0
56	MG	1D	311	1/1	0.94	0.07	29,29,29,29	0
56	MG	1A	3811	1/1	0.94	0.08	41,41,41,41	0
56	MG	2A	3782	1/1	0.94	0.08	44,44,44,44	0
56	MG	2A	3025	1/1	0.94	0.09	28,28,28,28	0
56	MG	2A	3785	1/1	0.94	0.07	63,63,63,63	0
56	MG	2A	3485	1/1	0.94	0.07	33,33,33,33	0
56	MG	1A	3979	1/1	0.94	0.07	63,63,63,63	0
56	MG	2A	3488	1/1	0.94	0.12	30,30,30,30	0
56	MG	1A	3980	1/1	0.94	0.07	61,61,61,61	0
56	MG	1A	3668	1/1	0.94	0.11	21,21,21,21	0
56	MG	2A	3492	1/1	0.94	0.06	27,27,27,27	0
56	MG	2a	3175	1/1	0.94	0.07	51,51,51,51	0
56	MG	1A	3984	1/1	0.94	0.07	21,21,21,21	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	3985	1/1	0.94	0.07	20,20,20,20	0
56	MG	1A	3237	1/1	0.94	0.10	28,28,28,28	0
56	MG	2A	3499	1/1	0.94	0.09	33,33,33,33	0
56	MG	1A	3819	1/1	0.94	0.08	10,10,10,10	0
56	MG	2A	3809	1/1	0.94	0.06	27,27,27,27	0
56	MG	2a	3183	1/1	0.94	0.08	59,59,59,59	0
56	MG	1F	301	1/1	0.94	0.23	26,26,26,26	0
56	MG	2A	3812	1/1	0.94	0.14	52,52,52,52	0
56	MG	1A	3428	1/1	0.94	0.10	26,26,26,26	0
56	MG	2A	3041	1/1	0.94	0.16	46,46,46,46	0
56	MG	1A	3526	1/1	0.94	0.12	18,18,18,18	0
56	MG	2a	3190	1/1	0.94	0.08	61,61,61,61	0
56	MG	2A	3818	1/1	0.94	0.08	38,38,38,38	0
56	MG	2A	3256	1/1	0.94	0.09	35,35,35,35	0
56	MG	2a	3193	1/1	0.94	0.13	54,54,54,54	0
56	MG	2A	3513	1/1	0.94	0.12	36,36,36,36	0
56	MG	2A	3822	1/1	0.94	0.20	48,48,48,48	0
56	MG	1A	3995	1/1	0.94	0.07	52,52,52,52	0
56	MG	1A	3529	1/1	0.94	0.13	32,32,32,32	0
56	MG	1A	3677	1/1	0.94	0.10	44,44,44,44	0
56	MG	1A	3351	1/1	0.94	0.09	27,27,27,27	0
56	MG	1A	3535	1/1	0.94	0.23	38,38,38,38	0
56	MG	1A	4005	1/1	0.94	0.06	34,34,34,34	0
56	MG	2A	3832	1/1	0.94	0.10	41,41,41,41	0
56	MG	1A	3296	1/1	0.94	0.08	34,34,34,34	0
56	MG	2A	3051	1/1	0.94	0.05	40,40,40,40	0
56	MG	2a	3206	1/1	0.94	0.11	58,58,58,58	0
56	MG	2A	3054	1/1	0.94	0.08	39,39,39,39	0
56	MG	1a	3116	1/1	0.94	0.14	35,35,35,35	0
56	MG	1A	3188	1/1	0.94	0.07	24,24,24,24	0
56	MG	1a	3118	1/1	0.94	0.15	37,37,37,37	0
56	MG	2A	3063	1/1	0.94	0.06	33,33,33,33	0
56	MG	1A	3298	1/1	0.94	0.09	45,45,45,45	0
56	MG	2A	3066	1/1	0.94	0.12	43,43,43,43	0
56	MG	2A	3067	1/1	0.94	0.10	35,35,35,35	0
56	MG	2a	3215	1/1	0.94	0.08	68,68,68,68	0
56	MG	1A	4011	1/1	0.94	0.08	35,35,35,35	0
56	MG	1A	3693	1/1	0.94	0.09	45,45,45,45	0
56	MG	1A	3439	1/1	0.94	0.07	35,35,35,35	0
56	MG	2A	3858	1/1	0.94	0.18	57,57,57,57	0
56	MG	1a	3126	1/1	0.94	0.15	45,45,45,45	0
56	MG	2A	3283	1/1	0.94	0.07	38,38,38,38	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	3706	1/1	0.94	0.06	48,48,48,48	0
56	MG	1Q	3004	1/1	0.94	0.05	36,36,36,36	0
56	MG	1R	201	1/1	0.94	0.16	23,23,23,23	0
56	MG	2A	3870	1/1	0.94	0.11	40,40,40,40	0
56	MG	1a	3131	1/1	0.94	0.12	46,46,46,46	0
56	MG	1a	3132	1/1	0.94	0.12	51,51,51,51	0
56	MG	1a	3133	1/1	0.94	0.18	48,48,48,48	0
56	MG	1A	3042	1/1	0.94	0.11	15,15,15,15	0
56	MG	2B	3001	1/1	0.94	0.15	54,54,54,54	0
56	MG	2A	3561	1/1	0.94	0.10	46,46,46,46	0
56	MG	2e	3001	1/1	0.94	0.12	58,58,58,58	0
56	MG	1R	204	1/1	0.94	0.16	34,34,34,34	0
56	MG	1A	3043	1/1	0.94	0.11	28,28,28,28	0
56	MG	1A	3304	1/1	0.94	0.07	49,49,49,49	0
56	MG	1A	3245	1/1	0.94	0.11	19,19,19,19	0
56	MG	1A	3372	1/1	0.94	0.20	25,25,25,25	0
56	MG	1A	3848	1/1	0.94	0.14	48,48,48,48	0
56	MG	1A	3373	1/1	0.94	0.08	30,30,30,30	0
56	MG	2B	3011	1/1	0.94	0.21	48,48,48,48	0
56	MG	2A	3574	1/1	0.94	0.09	49,49,49,49	0
56	MG	2B	3013	1/1	0.94	0.12	57,57,57,57	0
56	MG	1A	4032	1/1	0.94	0.07	19,19,19,19	0
56	MG	2A	3304	1/1	0.94	0.06	44,44,44,44	0
56	MG	1W	201	1/1	0.94	0.13	28,28,28,28	0
56	MG	2A	3093	1/1	0.94	0.06	55,55,55,55	0
56	MG	1W	203	1/1	0.94	0.12	35,35,35,35	0
56	MG	2A	3580	1/1	0.94	0.08	45,45,45,45	0
56	MG	2A	3100	1/1	0.94	0.16	43,43,43,43	0
56	MG	1a	3150	1/1	0.94	0.12	56,56,56,56	0
56	MG	1a	3151	1/1	0.94	0.12	45,45,45,45	0
56	MG	2D	306	1/1	0.94	0.23	34,34,34,34	0
56	MG	1A	3449	1/1	0.94	0.14	49,49,49,49	0
56	MG	1A	3374	1/1	0.94	0.08	27,27,27,27	0
56	MG	2x	3005	1/1	0.94	0.07	59,59,59,59	0
56	MG	2E	303	1/1	0.94	0.17	55,55,55,55	0
56	MG	1A	3203	1/1	0.94	0.19	25,25,25,25	0
56	MG	1a	3159	1/1	0.94	0.09	52,52,52,52	0
56	MG	2A	3589	1/1	0.94	0.10	38,38,38,38	0
56	MG	2y	106	1/1	0.94	0.15	64,64,64,64	0
57	K	2A	3398	1/1	0.94	0.15	70,70,70,70	0
56	MG	2A	3591	1/1	0.94	0.11	54,54,54,54	0
56	MG	1A	3844	1/1	0.95	0.18	21,21,21,21	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	101	1/1	0.95	0.06	22,22,22,22	0
56	MG	1A	3071	1/1	0.95	0.25	26,26,26,26	0
56	MG	1A	3504	1/1	0.95	0.12	39,39,39,39	0
56	MG	1A	3507	1/1	0.95	0.13	36,36,36,36	0
56	MG	1A	3675	1/1	0.95	0.17	32,32,32,32	0
56	MG	1A	3118	1/1	0.95	0.12	29,29,29,29	0
56	MG	1A	3511	1/1	0.95	0.09	15,15,15,15	0
56	MG	1A	3046	1/1	0.95	0.07	40,40,40,40	0
56	MG	1A	4066	1/1	0.95	0.12	32,32,32,32	0
56	MG	1A	4067	1/1	0.95	0.12	40,40,40,40	0
56	MG	1A	3078	1/1	0.95	0.06	20,20,20,20	0
56	MG	2B	3020	1/1	0.95	0.19	66,66,66,66	0
56	MG	1A	3680	1/1	0.95	0.09	46,46,46,46	0
56	MG	2A	3566	1/1	0.95	0.08	35,35,35,35	0
56	MG	2D	303	1/1	0.95	0.22	40,40,40,40	0
56	MG	1A	3001	1/1	0.95	0.13	22,22,22,22	0
56	MG	2A	3265	1/1	0.95	0.25	39,39,39,39	0
56	MG	2D	307	1/1	0.95	0.31	43,43,43,43	0
56	MG	1a	3043	1/1	0.95	0.12	49,49,49,49	0
56	MG	2A	3573	1/1	0.95	0.09	44,44,44,44	0
56	MG	1A	3521	1/1	0.95	0.10	17,17,17,17	0
56	MG	1A	3683	1/1	0.95	0.11	39,39,39,39	0
56	MG	1A	3866	1/1	0.95	0.07	35,35,35,35	0
56	MG	1a	3049	1/1	0.95	0.08	35,35,35,35	0
56	MG	1A	4077	1/1	0.95	0.08	53,53,53,53	0
56	MG	1A	3685	1/1	0.95	0.07	37,37,37,37	0
56	MG	2A	3024	1/1	0.95	0.09	45,45,45,45	0
56	MG	1A	3871	1/1	0.95	0.10	18,18,18,18	0
56	MG	1a	3053	1/1	0.95	0.15	46,46,46,46	0
56	MG	1a	3054	1/1	0.95	0.16	57,57,57,57	0
56	MG	1A	3873	1/1	0.95	0.10	40,40,40,40	0
56	MG	2A	3280	1/1	0.95	0.14	43,43,43,43	0
56	MG	2R	201	1/1	0.95	0.09	39,39,39,39	0
56	MG	2A	3281	1/1	0.95	0.08	60,60,60,60	0
56	MG	2A	3282	1/1	0.95	0.07	41,41,41,41	0
56	MG	1A	3690	1/1	0.95	0.07	40,40,40,40	0
56	MG	2A	3284	1/1	0.95	0.07	41,41,41,41	0
56	MG	1A	3048	1/1	0.95	0.10	26,26,26,26	0
56	MG	1A	4086	1/1	0.95	0.16	31,31,31,31	0
56	MG	1A	3037	1/1	0.95	0.26	28,28,28,28	0
56	MG	2W	201	1/1	0.95	0.14	42,42,42,42	0
56	MG	1A	3326	1/1	0.95	0.17	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	1A	4091	1/1	0.95	0.08	28,28,28,28	0
56	MG	1A	3702	1/1	0.95	0.05	31,31,31,31	0
56	MG	1A	3705	1/1	0.95	0.10	39,39,39,39	0
56	MG	1A	3250	1/1	0.95	0.11	56,56,56,56	0
56	MG	23	3001	1/1	0.95	0.05	46,46,46,46	0
56	MG	2A	3601	1/1	0.95	0.07	45,45,45,45	0
56	MG	25	103	1/1	0.95	0.14	47,47,47,47	0
56	MG	2A	3044	1/1	0.95	0.12	36,36,36,36	0
56	MG	1A	3528	1/1	0.95	0.23	45,45,45,45	0
56	MG	1A	4099	1/1	0.95	0.07	43,43,43,43	0
56	MG	1A	4101	1/1	0.95	0.09	23,23,23,23	0
56	MG	1A	3412	1/1	0.95	0.08	41,41,41,41	0
56	MG	1A	3530	1/1	0.95	0.21	42,42,42,42	0
56	MG	2A	3302	1/1	0.95	0.07	50,50,50,50	0
56	MG	2a	3005	1/1	0.95	0.14	42,42,42,42	0
56	MG	1A	4106	1/1	0.95	0.09	17,17,17,17	0
56	MG	1A	3330	1/1	0.95	0.13	20,20,20,20	0
56	MG	2A	3613	1/1	0.95	0.06	38,38,38,38	0
56	MG	1A	3533	1/1	0.95	0.29	39,39,39,39	0
56	MG	1a	3080	1/1	0.95	0.13	40,40,40,40	0
56	MG	2A	3058	1/1	0.95	0.21	47,47,47,47	0
56	MG	1A	4112	1/1	0.95	0.25	31,31,31,31	0
56	MG	1A	3417	1/1	0.95	0.10	19,19,19,19	0
56	MG	1A	3892	1/1	0.95	0.07	30,30,30,30	0
56	MG	1A	3086	1/1	0.95	0.16	40,40,40,40	0
56	MG	2A	3313	1/1	0.95	0.09	46,46,46,46	0
56	MG	1A	3039	1/1	0.95	0.05	23,23,23,23	0
56	MG	1A	3422	1/1	0.95	0.06	24,24,24,24	0
56	MG	1A	3194	1/1	0.95	0.07	35,35,35,35	0
56	MG	2A	3069	1/1	0.95	0.06	43,43,43,43	0
56	MG	2A	3070	1/1	0.95	0.09	34,34,34,34	0
56	MG	2A	3321	1/1	0.95	0.14	50,50,50,50	0
56	MG	1A	3724	1/1	0.95	0.11	34,34,34,34	0
56	MG	2A	3631	1/1	0.95	0.06	44,44,44,44	0
56	MG	1A	3336	1/1	0.95	0.06	27,27,27,27	0
56	MG	1A	4137	1/1	0.95	0.12	20,20,20,20	0
56	MG	2A	3635	1/1	0.95	0.08	50,50,50,50	0
56	MG	1A	4143	1/1	0.95	0.18	26,26,26,26	0
56	MG	1A	3338	1/1	0.95	0.13	37,37,37,37	0
56	MG	2A	3329	1/1	0.95	0.15	29,29,29,29	0
56	MG	2A	3330	1/1	0.95	0.25	47,47,47,47	0
56	MG	1A	3730	1/1	0.95	0.07	21,21,21,21	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	3547	1/1	0.95	0.08	39,39,39,39	0
56	MG	1B	3006	1/1	0.95	0.07	29,29,29,29	0
56	MG	2A	3645	1/1	0.95	0.10	42,42,42,42	0
56	MG	1A	3427	1/1	0.95	0.05	35,35,35,35	0
56	MG	1a	3100	1/1	0.95	0.18	41,41,41,41	0
56	MG	1A	3550	1/1	0.95	0.06	26,26,26,26	0
56	MG	1A	3552	1/1	0.95	0.30	44,44,44,44	0
56	MG	1A	3558	1/1	0.95	0.12	42,42,42,42	0
56	MG	1B	3012	1/1	0.95	0.05	39,39,39,39	0
56	MG	1A	3918	1/1	0.95	0.08	51,51,51,51	0
56	MG	1B	3016	1/1	0.95	0.07	22,22,22,22	0
56	MG	1B	3018	1/1	0.95	0.09	51,51,51,51	0
56	MG	1A	3559	1/1	0.95	0.26	30,30,30,30	0
56	MG	1A	3739	1/1	0.95	0.08	21,21,21,21	0
56	MG	1A	3040	1/1	0.95	0.12	35,35,35,35	0
56	MG	2A	3094	1/1	0.95	0.07	43,43,43,43	0
56	MG	1A	3925	1/1	0.95	0.08	39,39,39,39	0
56	MG	2A	3350	1/1	0.95	0.17	60,60,60,60	0
56	MG	2A	3099	1/1	0.95	0.06	43,43,43,43	0
56	MG	1a	3113	1/1	0.95	0.12	37,37,37,37	0
56	MG	2a	3057	1/1	0.95	0.05	53,53,53,53	0
56	MG	1A	3340	1/1	0.95	0.12	44,44,44,44	0
56	MG	1A	3744	1/1	0.95	0.07	55,55,55,55	0
56	MG	1A	3746	1/1	0.95	0.06	15,15,15,15	0
56	MG	1A	3198	1/1	0.95	0.11	26,26,26,26	0
56	MG	1A	3569	1/1	0.95	0.09	23,23,23,23	0
56	MG	1A	3199	1/1	0.95	0.11	37,37,37,37	0
56	MG	2A	3111	1/1	0.95	0.19	29,29,29,29	0
56	MG	2a	3066	1/1	0.95	0.09	49,49,49,49	0
56	MG	1A	3935	1/1	0.95	0.14	41,41,41,41	0
56	MG	2A	3364	1/1	0.95	0.24	34,34,34,34	0
56	MG	2A	3677	1/1	0.95	0.28	43,43,43,43	0
56	MG	1A	3936	1/1	0.95	0.06	40,40,40,40	0
56	MG	1B	3036	1/1	0.95	0.07	27,27,27,27	0
56	MG	1A	3136	1/1	0.95	0.11	48,48,48,48	0
56	MG	2A	3116	1/1	0.95	0.07	41,41,41,41	0
56	MG	1A	3139	1/1	0.95	0.05	28,28,28,28	0
56	MG	2A	3684	1/1	0.95	0.05	46,46,46,46	0
56	MG	1a	3129	1/1	0.95	0.06	46,46,46,46	0
56	MG	1A	3941	1/1	0.95	0.10	40,40,40,40	0
56	MG	2A	3121	1/1	0.95	0.10	49,49,49,49	0
56	MG	1D	310	1/1	0.95	0.06	34,34,34,34	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	3942	1/1	0.95	0.06	31,31,31,31	0
56	MG	1A	3142	1/1	0.95	0.15	16,16,16,16	0
56	MG	2A	3379	1/1	0.95	0.19	36,36,36,36	0
56	MG	1A	3945	1/1	0.95	0.08	39,39,39,39	0
56	MG	1A	3022	1/1	0.95	0.16	38,38,38,38	0
56	MG	1A	3269	1/1	0.95	0.14	20,20,20,20	0
56	MG	1A	3949	1/1	0.95	0.07	58,58,58,58	0
56	MG	1A	3444	1/1	0.95	0.07	37,37,37,37	0
56	MG	1A	3270	1/1	0.95	0.22	18,18,18,18	0
56	MG	1A	3353	1/1	0.95	0.16	23,23,23,23	0
56	MG	1A	3587	1/1	0.95	0.06	39,39,39,39	0
56	MG	1A	3354	1/1	0.95	0.07	36,36,36,36	0
56	MG	2A	3392	1/1	0.95	0.18	35,35,35,35	0
56	MG	1F	303	1/1	0.95	0.11	14,14,14,14	0
56	MG	1A	3767	1/1	0.95	0.08	25,25,25,25	0
56	MG	1F	307	1/1	0.95	0.09	34,34,34,34	0
56	MG	1A	3271	1/1	0.95	0.20	25,25,25,25	0
56	MG	1A	3964	1/1	0.95	0.06	73,73,73,73	0
56	MG	1A	3965	1/1	0.95	0.08	65,65,65,65	0
56	MG	2A	3708	1/1	0.95	0.06	48,48,48,48	0
56	MG	2A	3709	1/1	0.95	0.08	43,43,43,43	0
56	MG	1G	3003	1/1	0.95	0.06	47,47,47,47	0
56	MG	1A	3450	1/1	0.95	0.06	22,22,22,22	0
56	MG	2A	3145	1/1	0.95	0.07	33,33,33,33	0
56	MG	1G	3005	1/1	0.95	0.08	50,50,50,50	0
56	MG	2A	3716	1/1	0.95	0.12	63,63,63,63	0
56	MG	1A	3452	1/1	0.95	0.06	40,40,40,40	0
56	MG	1a	3163	1/1	0.95	0.07	47,47,47,47	0
56	MG	2A	3719	1/1	0.95	0.10	64,64,64,64	0
56	MG	2a	3115	1/1	0.95	0.06	56,56,56,56	0
56	MG	1N	3005	1/1	0.95	0.05	18,18,18,18	0
56	MG	2A	3721	1/1	0.95	0.06	49,49,49,49	0
56	MG	1A	3594	1/1	0.95	0.07	18,18,18,18	0
56	MG	2a	3124	1/1	0.95	0.07	56,56,56,56	0
56	MG	2A	3152	1/1	0.95	0.06	37,37,37,37	0
56	MG	1A	3773	1/1	0.95	0.07	26,26,26,26	0
56	MG	2A	3412	1/1	0.95	0.08	37,37,37,37	0
56	MG	1A	3596	1/1	0.95	0.06	20,20,20,20	0
56	MG	1O	3003	1/1	0.95	0.05	42,42,42,42	0
56	MG	2A	3728	1/1	0.95	0.07	55,55,55,55	0
56	MG	1A	3597	1/1	0.95	0.06	25,25,25,25	0
56	MG	2A	3730	1/1	0.95	0.05	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	1A	3030	1/1	0.95	0.05	27,27,27,27	0
56	MG	2A	3159	1/1	0.95	0.08	28,28,28,28	0
56	MG	1A	3455	1/1	0.95	0.12	23,23,23,23	0
56	MG	1A	3981	1/1	0.95	0.05	49,49,49,49	0
56	MG	1A	3604	1/1	0.95	0.08	29,29,29,29	0
56	MG	1A	3357	1/1	0.95	0.09	12,12,12,12	0
56	MG	1a	3177	1/1	0.95	0.08	46,46,46,46	0
56	MG	1A	3146	1/1	0.95	0.14	38,38,38,38	0
56	MG	1A	3986	1/1	0.95	0.06	13,13,13,13	0
56	MG	2a	3151	1/1	0.95	0.07	53,53,53,53	0
56	MG	2A	3431	1/1	0.95	0.22	47,47,47,47	0
56	MG	1A	3360	1/1	0.95	0.10	27,27,27,27	0
56	MG	1S	3003	1/1	0.95	0.08	69,69,69,69	0
56	MG	1T	3001	1/1	0.95	0.20	50,50,50,50	0
56	MG	1T	3002	1/1	0.95	0.05	33,33,33,33	0
56	MG	1a	3191	1/1	0.95	0.10	64,64,64,64	0
56	MG	2A	3748	1/1	0.95	0.15	48,48,48,48	0
56	MG	1A	3093	1/1	0.95	0.11	41,41,41,41	0
56	MG	1A	3363	1/1	0.95	0.18	29,29,29,29	0
56	MG	2A	3751	1/1	0.95	0.07	68,68,68,68	0
56	MG	2A	3752	1/1	0.95	0.06	47,47,47,47	0
56	MG	1A	3217	1/1	0.95	0.08	33,33,33,33	0
56	MG	2A	3756	1/1	0.95	0.08	45,45,45,45	0
56	MG	2A	3180	1/1	0.95	0.17	45,45,45,45	0
56	MG	2A	3759	1/1	0.95	0.07	74,74,74,74	0
56	MG	2A	3760	1/1	0.95	0.10	34,34,34,34	0
56	MG	2A	3447	1/1	0.95	0.08	44,44,44,44	0
56	MG	2A	3763	1/1	0.95	0.07	29,29,29,29	0
56	MG	1A	3031	1/1	0.95	0.07	21,21,21,21	0
56	MG	1A	3290	1/1	0.95	0.12	37,37,37,37	0
56	MG	1A	3095	1/1	0.95	0.06	29,29,29,29	0
56	MG	2A	3184	1/1	0.95	0.13	36,36,36,36	0
56	MG	1a	3202	1/1	0.95	0.09	53,53,53,53	0
56	MG	1A	3795	1/1	0.95	0.07	32,32,32,32	0
56	MG	2a	3181	1/1	0.95	0.17	52,52,52,52	0
56	MG	2A	3771	1/1	0.95	0.06	30,30,30,30	0
56	MG	2A	3187	1/1	0.95	0.33	43,43,43,43	0
56	MG	1A	4001	1/1	0.95	0.07	59,59,59,59	0
56	MG	2A	3190	1/1	0.95	0.06	30,30,30,30	0
56	MG	2A	3463	1/1	0.95	0.06	40,40,40,40	0
56	MG	2A	3780	1/1	0.95	0.09	37,37,37,37	0
56	MG	1A	4002	1/1	0.95	0.08	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	1A	3222	1/1	0.95	0.23	28,28,28,28	0
56	MG	1A	3025	1/1	0.95	0.19	12,12,12,12	0
56	MG	2A	3786	1/1	0.95	0.08	57,57,57,57	0
56	MG	1A	3156	1/1	0.95	0.14	28,28,28,28	0
56	MG	1A	3097	1/1	0.95	0.08	15,15,15,15	0
56	MG	1Z	304	1/1	0.95	0.11	40,40,40,40	0
56	MG	2A	3796	1/1	0.95	0.08	25,25,25,25	0
56	MG	2A	3470	1/1	0.95	0.05	32,32,32,32	0
56	MG	10	101	1/1	0.95	0.08	43,43,43,43	0
56	MG	1A	3300	1/1	0.95	0.07	40,40,40,40	0
56	MG	1A	3804	1/1	0.95	0.07	30,30,30,30	0
56	MG	1A	4014	1/1	0.95	0.17	35,35,35,35	0
56	MG	1A	3632	1/1	0.95	0.06	27,27,27,27	0
56	MG	1A	3098	1/1	0.95	0.17	25,25,25,25	0
56	MG	2a	3204	1/1	0.95	0.05	66,66,66,66	0
56	MG	1a	3231	1/1	0.95	0.16	41,41,41,41	0
56	MG	2A	3808	1/1	0.95	0.08	46,46,46,46	0
56	MG	11	101	1/1	0.95	0.10	39,39,39,39	0
56	MG	1a	3234	1/1	0.95	0.05	38,38,38,38	0
56	MG	11	102	1/1	0.95	0.09	47,47,47,47	0
56	MG	1b	3001	1/1	0.95	0.06	69,69,69,69	0
56	MG	1A	3303	1/1	0.95	0.32	25,25,25,25	0
56	MG	1d	502	1/1	0.95	0.20	41,41,41,41	0
56	MG	1A	3637	1/1	0.95	0.08	14,14,14,14	0
56	MG	15	102	1/1	0.95	0.24	28,28,28,28	0
56	MG	1A	3100	1/1	0.95	0.10	15,15,15,15	0
56	MG	1A	3642	1/1	0.95	0.06	15,15,15,15	0
56	MG	1A	4022	1/1	0.95	0.06	29,29,29,29	0
56	MG	1A	3383	1/1	0.95	0.09	28,28,28,28	0
56	MG	2A	3496	1/1	0.95	0.12	42,42,42,42	0
56	MG	1s	3001	1/1	0.95	0.12	42,42,42,42	0
56	MG	1A	4024	1/1	0.95	0.08	14,14,14,14	0
56	MG	1A	3486	1/1	0.95	0.23	26,26,26,26	0
56	MG	2A	3506	1/1	0.95	0.10	50,50,50,50	0
56	MG	1A	3386	1/1	0.95	0.05	34,34,34,34	0
56	MG	2A	3223	1/1	0.95	0.12	55,55,55,55	0
56	MG	2A	3835	1/1	0.95	0.13	53,53,53,53	0
56	MG	1A	3652	1/1	0.95	0.05	41,41,41,41	0
56	MG	2a	3228	1/1	0.95	0.15	53,53,53,53	0
56	MG	1A	3489	1/1	0.95	0.09	47,47,47,47	0
56	MG	1A	3656	1/1	0.95	0.08	12,12,12,12	0
56	MG	2A	3227	1/1	0.95	0.19	69,69,69,69	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	3514	1/1	0.95	0.10	42,42,42,42	0
56	MG	2A	3844	1/1	0.95	0.08	34,34,34,34	0
56	MG	2f	3001	1/1	0.95	0.12	42,42,42,42	0
56	MG	1w	106	1/1	0.95	0.14	50,50,50,50	0
56	MG	1A	3035	1/1	0.95	0.07	27,27,27,27	0
56	MG	2l	201	1/1	0.95	0.06	53,53,53,53	0
56	MG	2A	3847	1/1	0.95	0.10	54,54,54,54	0
56	MG	2A	3849	1/1	0.95	0.11	24,24,24,24	0
56	MG	2A	3230	1/1	0.95	0.06	40,40,40,40	0
56	MG	1A	3659	1/1	0.95	0.09	6,6,6,6	0
56	MG	1A	3831	1/1	0.95	0.06	40,40,40,40	0
56	MG	2A	3854	1/1	0.95	0.09	50,50,50,50	0
56	MG	2A	3855	1/1	0.95	0.10	48,48,48,48	0
56	MG	1A	3832	1/1	0.95	0.08	34,34,34,34	0
56	MG	2v	101	1/1	0.95	0.29	48,48,48,48	0
56	MG	1w	111	1/1	0.95	0.05	37,37,37,37	0
56	MG	2A	3530	1/1	0.95	0.06	45,45,45,45	0
56	MG	2A	3532	1/1	0.95	0.11	42,42,42,42	0
56	MG	1A	3833	1/1	0.95	0.08	46,46,46,46	0
56	MG	1A	3068	1/1	0.95	0.28	50,50,50,50	0
56	MG	2A	3238	1/1	0.95	0.07	30,30,30,30	0
56	MG	1x	103	1/1	0.95	0.07	38,38,38,38	0
56	MG	1A	3311	1/1	0.95	0.21	40,40,40,40	0
56	MG	2A	3872	1/1	0.95	0.24	37,37,37,37	0
56	MG	1a	3017	1/1	0.95	0.08	37,37,37,37	0
56	MG	2A	3874	1/1	0.95	0.09	37,37,37,37	0
56	MG	1A	3312	1/1	0.95	0.20	41,41,41,41	0
56	MG	1A	3496	1/1	0.95	0.40	40,40,40,40	0
56	MG	2A	3877	1/1	0.95	0.10	57,57,57,57	0
56	MG	1A	3069	1/1	0.95	0.03	16,16,16,16	0
56	MG	2y	102	1/1	0.95	0.07	59,59,59,59	0
56	MG	1a	3025	1/1	0.95	0.14	42,42,42,42	0
56	MG	2A	3546	1/1	0.95	0.09	57,57,57,57	0
56	MG	1A	3666	1/1	0.95	0.06	33,33,33,33	0
56	MG	1A	3240	1/1	0.95	0.05	31,31,31,31	0
56	MG	1A	3501	1/1	0.95	0.13	22,22,22,22	0
56	MG	2A	3322	1/1	0.96	0.04	32,32,32,32	0
56	MG	1E	311	1/1	0.96	0.08	41,41,41,41	0
56	MG	1A	3818	1/1	0.96	0.14	28,28,28,28	0
56	MG	1A	3278	1/1	0.96	0.09	37,37,37,37	0
56	MG	1A	3992	1/1	0.96	0.07	28,28,28,28	0
56	MG	2A	3616	1/1	0.96	0.09	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	3125	1/1	0.96	0.17	37,37,37,37	0
56	MG	1A	3108	1/1	0.96	0.05	23,23,23,23	0
56	MG	1F	306	1/1	0.96	0.10	34,34,34,34	0
56	MG	1A	3138	1/1	0.96	0.20	16,16,16,16	0
56	MG	2A	3095	1/1	0.96	0.12	39,39,39,39	0
56	MG	2A	3097	1/1	0.96	0.14	38,38,38,38	0
56	MG	1A	3038	1/1	0.96	0.12	26,26,26,26	0
56	MG	2U	203	1/1	0.96	0.12	47,47,47,47	0
56	MG	1A	3349	1/1	0.96	0.10	47,47,47,47	0
56	MG	1A	3534	1/1	0.96	0.24	40,40,40,40	0
56	MG	1A	3283	1/1	0.96	0.14	46,46,46,46	0
56	MG	1A	3828	1/1	0.96	0.10	21,21,21,21	0
56	MG	1A	3175	1/1	0.96	0.08	35,35,35,35	0
56	MG	2A	3107	1/1	0.96	0.18	30,30,30,30	0
56	MG	2X	3002	1/1	0.96	0.09	40,40,40,40	0
56	MG	1a	3136	1/1	0.96	0.06	52,52,52,52	0
56	MG	1A	3830	1/1	0.96	0.13	40,40,40,40	0
56	MG	1N	3001	1/1	0.96	0.30	34,34,34,34	0
56	MG	1A	3438	1/1	0.96	0.06	30,30,30,30	0
56	MG	1A	4007	1/1	0.96	0.13	45,45,45,45	0
56	MG	1A	3538	1/1	0.96	0.13	45,45,45,45	0
56	MG	25	104	1/1	0.96	0.09	45,45,45,45	0
56	MG	1A	3287	1/1	0.96	0.07	25,25,25,25	0
56	MG	1A	3542	1/1	0.96	0.11	29,29,29,29	0
56	MG	1A	3140	1/1	0.96	0.10	32,32,32,32	0
56	MG	1A	4015	1/1	0.96	0.06	40,40,40,40	0
56	MG	1a	3147	1/1	0.96	0.05	32,32,32,32	0
56	MG	2A	3119	1/1	0.96	0.08	30,30,30,30	0
56	MG	1A	3226	1/1	0.96	0.12	42,42,42,42	0
56	MG	1A	3686	1/1	0.96	0.08	34,34,34,34	0
56	MG	2A	3122	1/1	0.96	0.10	41,41,41,41	0
56	MG	1A	3442	1/1	0.96	0.13	40,40,40,40	0
56	MG	2A	3360	1/1	0.96	0.19	30,30,30,30	0
56	MG	2A	3361	1/1	0.96	0.20	36,36,36,36	0
56	MG	2A	3654	1/1	0.96	0.05	46,46,46,46	0
56	MG	1A	3293	1/1	0.96	0.13	41,41,41,41	0
56	MG	1a	3154	1/1	0.96	0.09	38,38,38,38	0
56	MG	1A	3841	1/1	0.96	0.13	12,12,12,12	0
56	MG	2A	3366	1/1	0.96	0.12	31,31,31,31	0
56	MG	1a	3156	1/1	0.96	0.18	30,30,30,30	0
56	MG	1A	3294	1/1	0.96	0.11	30,30,30,30	0
56	MG	1a	3158	1/1	0.96	0.08	43,43,43,43	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
56	MG	1A	3694	1/1	0.96	0.10	49,49,49,49	0
56	MG	1S	3002	1/1	0.96	0.09	37,37,37,37	0
56	MG	2a	3020	1/1	0.96	0.09	32,32,32,32	0
56	MG	1A	3699	1/1	0.96	0.07	55,55,55,55	0
56	MG	1A	3141	1/1	0.96	0.21	21,21,21,21	0
56	MG	2A	3667	1/1	0.96	0.06	33,33,33,33	0
56	MG	1A	3846	1/1	0.96	0.12	18,18,18,18	0
56	MG	1A	3701	1/1	0.96	0.06	42,42,42,42	0
56	MG	1a	3166	1/1	0.96	0.10	55,55,55,55	0
56	MG	2a	3027	1/1	0.96	0.20	45,45,45,45	0
56	MG	1A	4029	1/1	0.96	0.07	35,35,35,35	0
56	MG	1A	3178	1/1	0.96	0.09	42,42,42,42	0
56	MG	1U	204	1/1	0.96	0.19	22,22,22,22	0
56	MG	1a	3170	1/1	0.96	0.12	49,49,49,49	0
56	MG	2A	3383	1/1	0.96	0.15	43,43,43,43	0
56	MG	1A	4031	1/1	0.96	0.12	37,37,37,37	0
56	MG	1A	3703	1/1	0.96	0.12	24,24,24,24	0
56	MG	1A	3851	1/1	0.96	0.07	28,28,28,28	0
56	MG	1A	3556	1/1	0.96	0.08	9,9,9,9	0
56	MG	2A	3147	1/1	0.96	0.12	37,37,37,37	0
56	MG	2A	3681	1/1	0.96	0.10	52,52,52,52	0
56	MG	2a	3040	1/1	0.96	0.12	47,47,47,47	0
56	MG	1A	3853	1/1	0.96	0.07	7,7,7,7	0
56	MG	1A	3016	1/1	0.96	0.14	33,33,33,33	0
56	MG	1A	3856	1/1	0.96	0.11	40,40,40,40	0
56	MG	1a	3178	1/1	0.96	0.05	41,41,41,41	0
56	MG	1a	3179	1/1	0.96	0.09	64,64,64,64	0
56	MG	1X	105	1/1	0.96	0.08	36,36,36,36	0
56	MG	1Y	502	1/1	0.96	0.13	37,37,37,37	0
56	MG	2A	3155	1/1	0.96	0.13	37,37,37,37	0
56	MG	1A	3181	1/1	0.96	0.16	24,24,24,24	0
56	MG	1a	3184	1/1	0.96	0.08	63,63,63,63	0
56	MG	1a	3185	1/1	0.96	0.08	60,60,60,60	0
56	MG	1A	3182	1/1	0.96	0.14	25,25,25,25	0
56	MG	1Z	302	1/1	0.96	0.05	26,26,26,26	0
56	MG	1A	3860	1/1	0.96	0.07	14,14,14,14	0
56	MG	1A	3710	1/1	0.96	0.13	22,22,22,22	0
56	MG	1A	3239	1/1	0.96	0.10	49,49,49,49	0
56	MG	1A	3863	1/1	0.96	0.10	46,46,46,46	0
56	MG	10	103	1/1	0.96	0.17	24,24,24,24	0
56	MG	2A	3166	1/1	0.96	0.10	36,36,36,36	0
56	MG	1A	4047	1/1	0.96	0.07	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	1A	3566	1/1	0.96	0.06	25,25,25,25	0
56	MG	10	106	1/1	0.96	0.08	48,48,48,48	0
56	MG	1a	3201	1/1	0.96	0.06	51,51,51,51	0
56	MG	1A	3302	1/1	0.96	0.10	23,23,23,23	0
56	MG	2a	3065	1/1	0.96	0.10	36,36,36,36	0
56	MG	1A	3114	1/1	0.96	0.05	18,18,18,18	0
56	MG	1A	3080	1/1	0.96	0.27	28,28,28,28	0
56	MG	1A	3869	1/1	0.96	0.06	39,39,39,39	0
56	MG	11	103	1/1	0.96	0.05	27,27,27,27	0
56	MG	1A	3116	1/1	0.96	0.05	28,28,28,28	0
56	MG	1A	3872	1/1	0.96	0.16	12,12,12,12	0
56	MG	12	3002	1/1	0.96	0.14	41,41,41,41	0
56	MG	13	101	1/1	0.96	0.07	31,31,31,31	0
56	MG	2A	3430	1/1	0.96	0.16	61,61,61,61	0
56	MG	1A	3010	1/1	0.96	0.08	22,22,22,22	0
56	MG	1A	3722	1/1	0.96	0.05	28,28,28,28	0
56	MG	1A	3193	1/1	0.96	0.06	24,24,24,24	0
56	MG	1A	3576	1/1	0.96	0.07	39,39,39,39	0
56	MG	2A	3436	1/1	0.96	0.06	40,40,40,40	0
56	MG	1A	3148	1/1	0.96	0.09	23,23,23,23	0
56	MG	2a	3081	1/1	0.96	0.09	70,70,70,70	0
56	MG	1A	3879	1/1	0.96	0.16	20,20,20,20	0
56	MG	18	103	1/1	0.96	0.09	29,29,29,29	0
56	MG	1A	3727	1/1	0.96	0.16	32,32,32,32	0
56	MG	2a	3085	1/1	0.96	0.20	41,41,41,41	0
56	MG	1A	3462	1/1	0.96	0.06	38,38,38,38	0
56	MG	1A	3463	1/1	0.96	0.12	49,49,49,49	0
56	MG	1A	3313	1/1	0.96	0.10	23,23,23,23	0
56	MG	1a	3004	1/1	0.96	0.17	43,43,43,43	0
56	MG	2a	3090	1/1	0.96	0.21	64,64,64,64	0
56	MG	1A	3466	1/1	0.96	0.13	19,19,19,19	0
56	MG	2A	3452	1/1	0.96	0.15	42,42,42,42	0
56	MG	1A	4074	1/1	0.96	0.09	36,36,36,36	0
56	MG	2a	3094	1/1	0.96	0.07	64,64,64,64	0
56	MG	1A	3195	1/1	0.96	0.06	8,8,8,8	0
56	MG	1A	3083	1/1	0.96	0.05	41,41,41,41	0
56	MG	2A	3456	1/1	0.96	0.10	31,31,31,31	0
56	MG	1A	3385	1/1	0.96	0.09	35,35,35,35	0
56	MG	2A	3458	1/1	0.96	0.10	40,40,40,40	0
56	MG	1A	3737	1/1	0.96	0.07	17,17,17,17	0
56	MG	1A	3121	1/1	0.96	0.16	32,32,32,32	0
56	MG	1A	3154	1/1	0.96	0.21	34,34,34,34	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	0.96	0.09	60,60,60,60	0
56	MG	1a	3018	1/1	0.96	0.16	44,44,44,44	0
56	MG	2A	3209	1/1	0.96	0.15	55,55,55,55	0
56	MG	1a	3019	1/1	0.96	0.07	49,49,49,49	0
56	MG	1A	4084	1/1	0.96	0.10	24,24,24,24	0
56	MG	1A	4085	1/1	0.96	0.08	25,25,25,25	0
56	MG	1A	3054	1/1	0.96	0.07	37,37,37,37	0
56	MG	1A	3741	1/1	0.96	0.05	11,11,11,11	0
56	MG	2A	3471	1/1	0.96	0.09	34,34,34,34	0
56	MG	1A	3201	1/1	0.96	0.09	26,26,26,26	0
56	MG	2A	3753	1/1	0.96	0.09	36,36,36,36	0
56	MG	1A	4090	1/1	0.96	0.07	32,32,32,32	0
56	MG	2a	3118	1/1	0.96	0.06	68,68,68,68	0
56	MG	1A	3202	1/1	0.96	0.09	22,22,22,22	0
56	MG	1A	3600	1/1	0.96	0.09	14,14,14,14	0
56	MG	1A	3477	1/1	0.96	0.19	30,30,30,30	0
56	MG	1A	3065	1/1	0.96	0.13	20,20,20,20	0
56	MG	2A	3761	1/1	0.96	0.09	42,42,42,42	0
56	MG	1A	3480	1/1	0.96	0.05	34,34,34,34	0
56	MG	1A	3259	1/1	0.96	0.15	37,37,37,37	0
56	MG	1A	4100	1/1	0.96	0.27	18,18,18,18	0
56	MG	1A	3755	1/1	0.96	0.04	34,34,34,34	0
56	MG	1A	3913	1/1	0.96	0.08	34,34,34,34	0
56	MG	2A	3484	1/1	0.96	0.06	32,32,32,32	0
56	MG	1A	4104	1/1	0.96	0.09	47,47,47,47	0
56	MG	2A	3486	1/1	0.96	0.10	46,46,46,46	0
56	MG	1A	3482	1/1	0.96	0.08	18,18,18,18	0
56	MG	2a	3140	1/1	0.96	0.06	52,52,52,52	0
56	MG	1A	3607	1/1	0.96	0.11	40,40,40,40	0
56	MG	2A	3489	1/1	0.96	0.11	38,38,38,38	0
56	MG	2a	3143	1/1	0.96	0.06	51,51,51,51	0
56	MG	1a	3040	1/1	0.96	0.21	39,39,39,39	0
56	MG	1A	3483	1/1	0.96	0.13	23,23,23,23	0
56	MG	1A	3013	1/1	0.96	0.15	9,9,9,9	0
56	MG	1A	4110	1/1	0.96	0.17	31,31,31,31	0
56	MG	1a	3044	1/1	0.96	0.09	50,50,50,50	0
56	MG	2A	3495	1/1	0.96	0.09	22,22,22,22	0
56	MG	1a	3045	1/1	0.96	0.10	38,38,38,38	0
56	MG	1A	3327	1/1	0.96	0.13	40,40,40,40	0
56	MG	1A	3205	1/1	0.96	0.17	47,47,47,47	0
56	MG	2A	3792	1/1	0.96	0.06	37,37,37,37	0
56	MG	2A	3501	1/1	0.96	0.06	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	3099	1/1	0.96	0.07	24,24,24,24	0
56	MG	2A	3505	1/1	0.96	0.07	34,34,34,34	0
56	MG	2A	3001	1/1	0.96	0.24	41,41,41,41	0
56	MG	1A	4116	1/1	0.96	0.15	38,38,38,38	0
56	MG	2A	3801	1/1	0.96	0.10	47,47,47,47	0
56	MG	2A	3241	1/1	0.96	0.10	66,66,66,66	0
56	MG	1A	4117	1/1	0.96	0.11	52,52,52,52	0
56	MG	2a	3167	1/1	0.96	0.12	37,37,37,37	0
56	MG	2A	3005	1/1	0.96	0.12	38,38,38,38	0
56	MG	1A	4120	1/1	0.96	0.09	23,23,23,23	0
56	MG	2A	3512	1/1	0.96	0.05	29,29,29,29	0
56	MG	2A	3807	1/1	0.96	0.06	42,42,42,42	0
56	MG	2A	3007	1/1	0.96	0.06	29,29,29,29	0
56	MG	1A	3613	1/1	0.96	0.06	18,18,18,18	0
56	MG	2A	3515	1/1	0.96	0.08	42,42,42,42	0
56	MG	2A	3811	1/1	0.96	0.04	54,54,54,54	0
56	MG	1A	4122	1/1	0.96	0.09	35,35,35,35	0
56	MG	1A	4123	1/1	0.96	0.17	18,18,18,18	0
56	MG	1A	3927	1/1	0.96	0.07	33,33,33,33	0
56	MG	2A	3519	1/1	0.96	0.07	39,39,39,39	0
56	MG	2A	3014	1/1	0.96	0.07	28,28,28,28	0
56	MG	2A	3819	1/1	0.96	0.07	48,48,48,48	0
56	MG	2A	3522	1/1	0.96	0.08	30,30,30,30	0
56	MG	1A	4126	1/1	0.96	0.13	34,34,34,34	0
56	MG	1A	3331	1/1	0.96	0.29	14,14,14,14	0
56	MG	2A	3823	1/1	0.96	0.07	48,48,48,48	0
56	MG	2A	3825	1/1	0.96	0.11	58,58,58,58	0
56	MG	1A	3616	1/1	0.96	0.04	23,23,23,23	0
56	MG	1A	3490	1/1	0.96	0.19	31,31,31,31	0
56	MG	1A	3491	1/1	0.96	0.05	40,40,40,40	0
56	MG	1A	3619	1/1	0.96	0.05	18,18,18,18	0
56	MG	1A	3056	1/1	0.96	0.07	33,33,33,33	0
56	MG	1A	3333	1/1	0.96	0.12	37,37,37,37	0
56	MG	1A	4145	1/1	0.96	0.19	28,28,28,28	0
56	MG	2A	3537	1/1	0.96	0.14	54,54,54,54	0
56	MG	1A	3266	1/1	0.96	0.08	32,32,32,32	0
56	MG	1A	3630	1/1	0.96	0.07	12,12,12,12	0
56	MG	2A	3836	1/1	0.96	0.08	44,44,44,44	0
56	MG	1B	3004	1/1	0.96	0.11	43,43,43,43	0
56	MG	1A	3404	1/1	0.96	0.13	21,21,21,21	0
56	MG	1A	3027	1/1	0.96	0.14	16,16,16,16	0
56	MG	1A	3407	1/1	0.96	0.11	29,29,29,29	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	3032	1/1	0.96	0.08	56,56,56,56	0
56	MG	2A	3842	1/1	0.96	0.15	41,41,41,41	0
56	MG	2A	3843	1/1	0.96	0.06	32,32,32,32	0
56	MG	2A	3035	1/1	0.96	0.14	19,19,19,19	0
56	MG	1B	3009	1/1	0.96	0.14	34,34,34,34	0
56	MG	1a	3076	1/1	0.96	0.07	46,46,46,46	0
56	MG	1A	3408	1/1	0.96	0.09	39,39,39,39	0
56	MG	1a	3078	1/1	0.96	0.16	47,47,47,47	0
56	MG	1A	3946	1/1	0.96	0.13	30,30,30,30	0
56	MG	1A	3409	1/1	0.96	0.16	52,52,52,52	0
56	MG	1A	3411	1/1	0.96	0.16	22,22,22,22	0
56	MG	2A	3853	1/1	0.96	0.07	37,37,37,37	0
56	MG	1A	3106	1/1	0.96	0.10	28,28,28,28	0
56	MG	2A	3277	1/1	0.96	0.10	46,46,46,46	0
56	MG	2A	3559	1/1	0.96	0.07	23,23,23,23	0
56	MG	2A	3278	1/1	0.96	0.05	35,35,35,35	0
56	MG	2A	3862	1/1	0.96	0.06	35,35,35,35	0
56	MG	1A	3505	1/1	0.96	0.14	25,25,25,25	0
56	MG	1A	3413	1/1	0.96	0.12	32,32,32,32	0
56	MG	1A	3337	1/1	0.96	0.10	38,38,38,38	0
56	MG	1A	3651	1/1	0.96	0.09	12,12,12,12	0
56	MG	1a	3089	1/1	0.96	0.23	37,37,37,37	0
56	MG	1A	3510	1/1	0.96	0.17	29,29,29,29	0
56	MG	1A	3959	1/1	0.96	0.05	26,26,26,26	0
56	MG	1A	3415	1/1	0.96	0.21	23,23,23,23	0
56	MG	1A	3655	1/1	0.96	0.06	17,17,17,17	0
56	MG	2A	3288	1/1	0.96	0.14	48,48,48,48	0
56	MG	2A	3057	1/1	0.96	0.06	42,42,42,42	0
56	MG	1A	3963	1/1	0.96	0.06	16,16,16,16	0
56	MG	2A	3060	1/1	0.96	0.09	47,47,47,47	0
56	MG	2g	8001	1/1	0.96	0.10	70,70,70,70	0
56	MG	1a	3095	1/1	0.96	0.23	42,42,42,42	0
56	MG	1A	3797	1/1	0.96	0.13	25,25,25,25	0
56	MG	2B	3003	1/1	0.96	0.15	44,44,44,44	0
56	MG	1A	3416	1/1	0.96	0.25	27,27,27,27	0
56	MG	1A	3966	1/1	0.96	0.12	41,41,41,41	0
56	MG	2A	3581	1/1	0.96	0.08	42,42,42,42	0
56	MG	1A	3967	1/1	0.96	0.15	56,56,56,56	0
56	MG	1A	3514	1/1	0.96	0.12	33,33,33,33	0
56	MG	1A	3165	1/1	0.96	0.13	29,29,29,29	0
56	MG	1A	3418	1/1	0.96	0.06	36,36,36,36	0
56	MG	2A	3300	1/1	0.96	0.11	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	3301	1/1	0.96	0.06	39,39,39,39	0
56	MG	1A	3661	1/1	0.96	0.07	48,48,48,48	0
56	MG	1D	305	1/1	0.96	0.20	24,24,24,24	0
56	MG	2A	3590	1/1	0.96	0.12	41,41,41,41	0
56	MG	1A	3805	1/1	0.96	0.09	40,40,40,40	0
56	MG	2A	3073	1/1	0.96	0.08	25,25,25,25	0
56	MG	1A	3519	1/1	0.96	0.05	43,43,43,43	0
56	MG	2A	3307	1/1	0.96	0.05	41,41,41,41	0
56	MG	1A	3168	1/1	0.96	0.11	20,20,20,20	0
56	MG	1A	3809	1/1	0.96	0.08	32,32,32,32	0
56	MG	1A	3272	1/1	0.96	0.07	30,30,30,30	0
56	MG	1E	301	1/1	0.96	0.17	18,18,18,18	0
56	MG	1A	3274	1/1	0.96	0.09	28,28,28,28	0
56	MG	2D	305	1/1	0.96	0.10	27,27,27,27	0
56	MG	1A	3276	1/1	0.96	0.14	33,33,33,33	0
56	MG	2A	3314	1/1	0.96	0.07	40,40,40,40	0
56	MG	2A	3081	1/1	0.96	0.13	38,38,38,38	0
56	MG	1A	3220	1/1	0.96	0.10	17,17,17,17	0
56	MG	1E	308	1/1	0.96	0.13	14,14,14,14	0
56	MG	1A	3816	1/1	0.96	0.11	36,36,36,36	0
57	K	1A	3527	1/1	0.96	0.18	57,57,57,57	0
56	MG	1A	3817	1/1	0.96	0.06	28,28,28,28	0
58	M2D	1A	4118	36/36	0.96	0.10	13,19,23,24	0
56	MG	2A	3086	1/1	0.96	0.14	39,39,39,39	0
59	ZN	24	501	1/1	0.96	0.05	86,86,86,86	0
59	ZN	29	501	1/1	0.96	0.06	77,77,77,77	0
59	ZN	2n	501	1/1	0.96	0.07	93,93,93,93	0
56	MG	1B	3024	1/1	0.97	0.07	49,49,49,49	0
56	MG	1B	3026	1/1	0.97	0.06	27,27,27,27	0
56	MG	2A	3435	1/1	0.97	0.06	62,62,62,62	0
56	MG	1a	3057	1/1	0.97	0.09	47,47,47,47	0
56	MG	1A	3238	1/1	0.97	0.13	25,25,25,25	0
56	MG	1A	3544	1/1	0.97	0.14	32,32,32,32	0
56	MG	1A	3451	1/1	0.97	0.07	35,35,35,35	0
56	MG	1A	3092	1/1	0.97	0.12	11,11,11,11	0
56	MG	1A	3117	1/1	0.97	0.06	24,24,24,24	0
56	MG	1x	113	1/1	0.97	0.09	46,46,46,46	0
56	MG	1A	3454	1/1	0.97	0.07	29,29,29,29	0
56	MG	1A	3549	1/1	0.97	0.14	45,45,45,45	0
56	MG	1a	3065	1/1	0.97	0.12	54,54,54,54	0
56	MG	1A	3060	1/1	0.97	0.15	32,32,32,32	0
56	MG	1A	3551	1/1	0.97	0.10	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	3149	1/1	0.97	0.07	18,18,18,18	0
56	MG	1A	3554	1/1	0.97	0.05	36,36,36,36	0
56	MG	1A	3555	1/1	0.97	0.09	11,11,11,11	0
56	MG	1A	3691	1/1	0.97	0.10	34,34,34,34	0
56	MG	1a	3073	1/1	0.97	0.10	34,34,34,34	0
56	MG	2A	3004	1/1	0.97	0.11	40,40,40,40	0
56	MG	1D	307	1/1	0.97	0.10	41,41,41,41	0
56	MG	1D	308	1/1	0.97	0.20	26,26,26,26	0
56	MG	1D	309	1/1	0.97	0.13	23,23,23,23	0
56	MG	2A	3008	1/1	0.97	0.11	39,39,39,39	0
56	MG	1A	3189	1/1	0.97	0.19	29,29,29,29	0
56	MG	2A	3715	1/1	0.97	0.07	56,56,56,56	0
56	MG	2A	3010	1/1	0.97	0.05	31,31,31,31	0
56	MG	1A	3836	1/1	0.97	0.07	39,39,39,39	0
56	MG	1a	3079	1/1	0.97	0.13	30,30,30,30	0
56	MG	1A	3305	1/1	0.97	0.14	23,23,23,23	0
56	MG	1a	3081	1/1	0.97	0.15	47,47,47,47	0
56	MG	1A	3190	1/1	0.97	0.04	31,31,31,31	0
56	MG	2a	3038	1/1	0.97	0.04	37,37,37,37	0
56	MG	1A	3696	1/1	0.97	0.05	31,31,31,31	0
56	MG	1A	3246	1/1	0.97	0.08	28,28,28,28	0
56	MG	1A	3563	1/1	0.97	0.16	19,19,19,19	0
56	MG	1E	305	1/1	0.97	0.08	26,26,26,26	0
56	MG	1A	3381	1/1	0.97	0.07	25,25,25,25	0
56	MG	1A	3565	1/1	0.97	0.05	25,25,25,25	0
56	MG	1A	3020	1/1	0.97	0.04	18,18,18,18	0
56	MG	1A	3704	1/1	0.97	0.04	37,37,37,37	0
56	MG	1A	3567	1/1	0.97	0.05	41,41,41,41	0
56	MG	2A	3731	1/1	0.97	0.05	64,64,64,64	0
56	MG	1A	3151	1/1	0.97	0.10	14,14,14,14	0
56	MG	1A	3152	1/1	0.97	0.14	20,20,20,20	0
56	MG	1A	3120	1/1	0.97	0.14	16,16,16,16	0
56	MG	1A	3315	1/1	0.97	0.16	31,31,31,31	0
56	MG	2A	3249	1/1	0.97	0.12	48,48,48,48	0
56	MG	1A	3469	1/1	0.97	0.05	36,36,36,36	0
56	MG	1A	3574	1/1	0.97	0.08	27,27,27,27	0
56	MG	2A	3033	1/1	0.97	0.16	44,44,44,44	0
56	MG	2A	3034	1/1	0.97	0.12	43,43,43,43	0
56	MG	1A	3079	1/1	0.97	0.16	25,25,25,25	0
56	MG	1A	3026	1/1	0.97	0.18	14,14,14,14	0
56	MG	1A	3857	1/1	0.97	0.04	22,22,22,22	0
56	MG	1A	3318	1/1	0.97	0.04	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	3023	1/1	0.97	0.16	18,18,18,18	0
56	MG	1A	3474	1/1	0.97	0.18	21,21,21,21	0
56	MG	2A	3747	1/1	0.97	0.05	59,59,59,59	0
56	MG	1A	3719	1/1	0.97	0.04	37,37,37,37	0
56	MG	1a	3105	1/1	0.97	0.05	35,35,35,35	0
56	MG	2A	3500	1/1	0.97	0.12	60,60,60,60	0
56	MG	1A	3580	1/1	0.97	0.10	33,33,33,33	0
56	MG	1A	3581	1/1	0.97	0.04	30,30,30,30	0
56	MG	1N	3003	1/1	0.97	0.08	32,32,32,32	0
56	MG	2A	3754	1/1	0.97	0.05	42,42,42,42	0
56	MG	1A	3254	1/1	0.97	0.05	32,32,32,32	0
56	MG	1A	3725	1/1	0.97	0.06	29,29,29,29	0
56	MG	1A	3157	1/1	0.97	0.16	17,17,17,17	0
56	MG	2A	3758	1/1	0.97	0.06	42,42,42,42	0
56	MG	1A	3586	1/1	0.97	0.10	16,16,16,16	0
56	MG	1A	3256	1/1	0.97	0.06	20,20,20,20	0
56	MG	2A	3053	1/1	0.97	0.12	30,30,30,30	0
56	MG	1a	3114	1/1	0.97	0.09	26,26,26,26	0
56	MG	1A	3478	1/1	0.97	0.07	38,38,38,38	0
56	MG	1A	3590	1/1	0.97	0.05	21,21,21,21	0
56	MG	1A	3158	1/1	0.97	0.05	12,12,12,12	0
56	MG	2A	3059	1/1	0.97	0.10	29,29,29,29	0
56	MG	1P	202	1/1	0.97	0.25	16,16,16,16	0
56	MG	1A	3082	1/1	0.97	0.23	34,34,34,34	0
56	MG	1Q	3001	1/1	0.97	0.04	26,26,26,26	0
56	MG	1A	3127	1/1	0.97	0.08	19,19,19,19	0
56	MG	2A	3521	1/1	0.97	0.13	50,50,50,50	0
56	MG	2A	3775	1/1	0.97	0.06	51,51,51,51	0
56	MG	1a	3122	1/1	0.97	0.25	46,46,46,46	0
56	MG	2A	3777	1/1	0.97	0.07	55,55,55,55	0
56	MG	2A	3065	1/1	0.97	0.14	37,37,37,37	0
56	MG	1a	3123	1/1	0.97	0.17	40,40,40,40	0
56	MG	1A	4046	1/1	0.97	0.05	38,38,38,38	0
56	MG	1A	3032	1/1	0.97	0.11	8,8,8,8	0
56	MG	1R	202	1/1	0.97	0.29	25,25,25,25	0
56	MG	1A	3262	1/1	0.97	0.23	36,36,36,36	0
56	MG	1A	3206	1/1	0.97	0.10	34,34,34,34	0
56	MG	1S	3001	1/1	0.97	0.07	30,30,30,30	0
56	MG	1A	4051	1/1	0.97	0.06	44,44,44,44	0
56	MG	2A	3790	1/1	0.97	0.05	32,32,32,32	0
56	MG	2A	3791	1/1	0.97	0.05	45,45,45,45	0
56	MG	1A	3598	1/1	0.97	0.05	7,7,7,7	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	3066	1/1	0.97	0.09	21,21,21,21	0
56	MG	1A	3211	1/1	0.97	0.09	33,33,33,33	0
56	MG	1A	3067	1/1	0.97	0.05	8,8,8,8	0
56	MG	2a	3107	1/1	0.97	0.21	38,38,38,38	0
56	MG	1a	3135	1/1	0.97	0.05	46,46,46,46	0
56	MG	1A	4056	1/1	0.97	0.07	45,45,45,45	0
56	MG	2A	3800	1/1	0.97	0.06	26,26,26,26	0
56	MG	1A	3603	1/1	0.97	0.07	15,15,15,15	0
56	MG	1A	3488	1/1	0.97	0.06	42,42,42,42	0
56	MG	1A	3164	1/1	0.97	0.05	31,31,31,31	0
56	MG	1A	3888	1/1	0.97	0.06	23,23,23,23	0
56	MG	1A	4063	1/1	0.97	0.10	17,17,17,17	0
56	MG	2a	3117	1/1	0.97	0.07	51,51,51,51	0
56	MG	1A	4064	1/1	0.97	0.07	48,48,48,48	0
56	MG	1A	3749	1/1	0.97	0.08	38,38,38,38	0
56	MG	2a	3121	1/1	0.97	0.07	62,62,62,62	0
56	MG	1W	202	1/1	0.97	0.17	31,31,31,31	0
56	MG	1A	3105	1/1	0.97	0.19	25,25,25,25	0
56	MG	1W	207	1/1	0.97	0.10	9,9,9,9	0
56	MG	1X	103	1/1	0.97	0.05	22,22,22,22	0
56	MG	1A	3410	1/1	0.97	0.08	20,20,20,20	0
56	MG	2A	3558	1/1	0.97	0.05	29,29,29,29	0
56	MG	2A	3814	1/1	0.97	0.07	45,45,45,45	0
56	MG	1A	3753	1/1	0.97	0.04	31,31,31,31	0
56	MG	2A	3816	1/1	0.97	0.07	55,55,55,55	0
56	MG	2a	3132	1/1	0.97	0.12	67,67,67,67	0
56	MG	1a	3152	1/1	0.97	0.05	55,55,55,55	0
56	MG	1A	3215	1/1	0.97	0.06	29,29,29,29	0
56	MG	1A	3216	1/1	0.97	0.09	42,42,42,42	0
56	MG	1A	3273	1/1	0.97	0.09	46,46,46,46	0
56	MG	1A	3166	1/1	0.97	0.27	22,22,22,22	0
56	MG	1A	3133	1/1	0.97	0.06	17,17,17,17	0
56	MG	1A	3759	1/1	0.97	0.12	35,35,35,35	0
56	MG	2A	3824	1/1	0.97	0.10	43,43,43,43	0
56	MG	2A	3568	1/1	0.97	0.07	42,42,42,42	0
56	MG	2A	3569	1/1	0.97	0.07	31,31,31,31	0
56	MG	2A	3101	1/1	0.97	0.14	34,34,34,34	0
56	MG	2A	3317	1/1	0.97	0.04	55,55,55,55	0
56	MG	2A	3102	1/1	0.97	0.15	33,33,33,33	0
56	MG	1A	3341	1/1	0.97	0.10	29,29,29,29	0
56	MG	2A	3104	1/1	0.97	0.09	30,30,30,30	0
56	MG	1A	3903	1/1	0.97	0.05	34,34,34,34	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	3219	1/1	0.97	0.09	24,24,24,24	0
56	MG	1A	3908	1/1	0.97	0.04	18,18,18,18	0
56	MG	1A	3499	1/1	0.97	0.09	21,21,21,21	0
56	MG	2a	3159	1/1	0.97	0.05	58,58,58,58	0
56	MG	1A	3500	1/1	0.97	0.17	27,27,27,27	0
56	MG	1A	3170	1/1	0.97	0.05	13,13,13,13	0
56	MG	1A	3419	1/1	0.97	0.12	23,23,23,23	0
56	MG	1A	3620	1/1	0.97	0.10	26,26,26,26	0
56	MG	1A	3503	1/1	0.97	0.14	30,30,30,30	0
56	MG	1A	3917	1/1	0.97	0.14	52,52,52,52	0
56	MG	1A	3279	1/1	0.97	0.13	12,12,12,12	0
56	MG	1A	3919	1/1	0.97	0.05	35,35,35,35	0
56	MG	2a	3168	1/1	0.97	0.09	61,61,61,61	0
56	MG	1A	3626	1/1	0.97	0.08	19,19,19,19	0
56	MG	1A	3771	1/1	0.97	0.04	13,13,13,13	0
56	MG	1A	3627	1/1	0.97	0.06	15,15,15,15	0
56	MG	15	103	1/1	0.97	0.10	17,17,17,17	0
56	MG	2A	3848	1/1	0.97	0.09	33,33,33,33	0
56	MG	2a	3174	1/1	0.97	0.20	47,47,47,47	0
56	MG	1A	3171	1/1	0.97	0.05	21,21,21,21	0
56	MG	2A	3340	1/1	0.97	0.04	48,48,48,48	0
56	MG	1A	3775	1/1	0.97	0.28	19,19,19,19	0
56	MG	1A	3629	1/1	0.97	0.06	13,13,13,13	0
56	MG	17	101	1/1	0.97	0.07	15,15,15,15	0
56	MG	1A	3135	1/1	0.97	0.07	42,42,42,42	0
56	MG	1A	3024	1/1	0.97	0.04	26,26,26,26	0
56	MG	18	102	1/1	0.97	0.11	19,19,19,19	0
56	MG	1A	3058	1/1	0.97	0.11	36,36,36,36	0
56	MG	2A	3860	1/1	0.97	0.12	38,38,38,38	0
56	MG	2A	3129	1/1	0.97	0.11	31,31,31,31	0
56	MG	1A	3425	1/1	0.97	0.07	21,21,21,21	0
56	MG	19	103	1/1	0.97	0.06	26,26,26,26	0
56	MG	1A	3933	1/1	0.97	0.05	46,46,46,46	0
56	MG	1A	3512	1/1	0.97	0.15	30,30,30,30	0
56	MG	2A	3868	1/1	0.97	0.07	35,35,35,35	0
56	MG	1A	3785	1/1	0.97	0.27	21,21,21,21	0
56	MG	2A	3354	1/1	0.97	0.07	43,43,43,43	0
56	MG	1A	3070	1/1	0.97	0.04	23,23,23,23	0
56	MG	1A	3350	1/1	0.97	0.08	34,34,34,34	0
56	MG	1a	3195	1/1	0.97	0.07	51,51,51,51	0
56	MG	1A	3286	1/1	0.97	0.20	38,38,38,38	0
56	MG	1A	3643	1/1	0.97	0.08	15,15,15,15	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	3008	1/1	0.97	0.10	37,37,37,37	0
56	MG	1a	3199	1/1	0.97	0.08	61,61,61,61	0
56	MG	1a	3009	1/1	0.97	0.24	44,44,44,44	0
56	MG	1A	3517	1/1	0.97	0.05	37,37,37,37	0
56	MG	2A	3144	1/1	0.97	0.08	42,42,42,42	0
56	MG	1a	3210	1/1	0.97	0.05	57,57,57,57	0
56	MG	1A	3943	1/1	0.97	0.05	52,52,52,52	0
56	MG	1A	3352	1/1	0.97	0.05	34,34,34,34	0
56	MG	1a	3216	1/1	0.97	0.05	62,62,62,62	0
56	MG	1a	3014	1/1	0.97	0.06	36,36,36,36	0
56	MG	1A	3110	1/1	0.97	0.17	22,22,22,22	0
56	MG	1A	3289	1/1	0.97	0.12	33,33,33,33	0
56	MG	1A	3522	1/1	0.97	0.05	26,26,26,26	0
56	MG	1A	3653	1/1	0.97	0.06	9,9,9,9	0
56	MG	1A	3432	1/1	0.97	0.04	25,25,25,25	0
56	MG	2A	3630	1/1	0.97	0.06	49,49,49,49	0
56	MG	1a	3020	1/1	0.97	0.10	33,33,33,33	0
56	MG	1a	3021	1/1	0.97	0.06	43,43,43,43	0
56	MG	1A	3799	1/1	0.97	0.09	32,32,32,32	0
56	MG	1A	3433	1/1	0.97	0.05	12,12,12,12	0
56	MG	1A	3953	1/1	0.97	0.09	36,36,36,36	0
56	MG	1A	3111	1/1	0.97	0.16	15,15,15,15	0
56	MG	1A	4134	1/1	0.97	0.15	31,31,31,31	0
56	MG	1A	4136	1/1	0.97	0.27	28,28,28,28	0
56	MG	1a	3233	1/1	0.97	0.17	32,32,32,32	0
56	MG	2A	3642	1/1	0.97	0.09	37,37,37,37	0
56	MG	1A	3657	1/1	0.97	0.06	17,17,17,17	0
56	MG	1A	4140	1/1	0.97	0.19	21,21,21,21	0
56	MG	1A	4141	1/1	0.97	0.08	27,27,27,27	0
56	MG	1A	3436	1/1	0.97	0.17	24,24,24,24	0
56	MG	2A	3391	1/1	0.97	0.22	36,36,36,36	0
56	MG	1A	3291	1/1	0.97	0.10	36,36,36,36	0
56	MG	1A	3228	1/1	0.97	0.12	18,18,18,18	0
56	MG	1f	3001	1/1	0.97	0.12	34,34,34,34	0
56	MG	2A	3652	1/1	0.97	0.08	50,50,50,50	0
56	MG	2A	3173	1/1	0.97	0.10	39,39,39,39	0
56	MG	1A	3358	1/1	0.97	0.17	21,21,21,21	0
56	MG	2F	302	1/1	0.97	0.08	39,39,39,39	0
56	MG	1l	201	1/1	0.97	0.16	29,29,29,29	0
56	MG	1l	202	1/1	0.97	0.05	61,61,61,61	0
56	MG	2A	3657	1/1	0.97	0.06	45,45,45,45	0
56	MG	2A	3177	1/1	0.97	0.11	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	3051	1/1	0.97	0.06	25,25,25,25	0
56	MG	1A	3808	1/1	0.97	0.06	29,29,29,29	0
56	MG	1B	3005	1/1	0.97	0.23	50,50,50,50	0
56	MG	1n	503	1/1	0.97	0.08	43,43,43,43	0
56	MG	2A	3405	1/1	0.97	0.03	34,34,34,34	0
56	MG	2T	3002	1/1	0.97	0.06	38,38,38,38	0
56	MG	1A	3090	1/1	0.97	0.12	22,22,22,22	0
56	MG	2U	201	1/1	0.97	0.18	39,39,39,39	0
56	MG	1A	3295	1/1	0.97	0.07	42,42,42,42	0
56	MG	1A	3073	1/1	0.97	0.05	19,19,19,19	0
56	MG	1A	3812	1/1	0.97	0.05	38,38,38,38	0
56	MG	1w	101	1/1	0.97	0.08	67,67,67,67	0
56	MG	2U	206	1/1	0.97	0.04	32,32,32,32	0
56	MG	1A	3445	1/1	0.97	0.07	33,33,33,33	0
56	MG	2A	3413	1/1	0.97	0.16	50,50,50,50	0
56	MG	1A	3971	1/1	0.97	0.06	43,43,43,43	0
56	MG	1A	3814	1/1	0.97	0.07	38,38,38,38	0
56	MG	1B	3013	1/1	0.97	0.04	31,31,31,31	0
56	MG	1A	3365	1/1	0.97	0.11	17,17,17,17	0
56	MG	2A	3419	1/1	0.97	0.18	28,28,28,28	0
56	MG	1A	3236	1/1	0.97	0.23	23,23,23,23	0
56	MG	1B	3017	1/1	0.97	0.03	19,19,19,19	0
56	MG	1A	3539	1/1	0.97	0.04	27,27,27,27	0
56	MG	2A	3196	1/1	0.97	0.08	38,38,38,38	0
56	MG	2A	3424	1/1	0.97	0.07	35,35,35,35	0
56	MG	1B	3019	1/1	0.97	0.07	34,34,34,34	0
56	MG	1A	3145	1/1	0.97	0.05	18,18,18,18	0
56	MG	27	101	1/1	0.97	0.13	32,32,32,32	0
56	MG	2A	3199	1/1	0.97	0.11	44,44,44,44	0
56	MG	1A	3369	1/1	0.97	0.14	44,44,44,44	0
56	MG	1A	3820	1/1	0.97	0.10	27,27,27,27	0
56	MG	1A	3982	1/1	0.97	0.06	31,31,31,31	0
56	MG	1x	104	1/1	0.97	0.13	51,51,51,51	0
56	MG	1A	3122	1/1	0.98	0.08	24,24,24,24	0
56	MG	1A	3508	1/1	0.98	0.10	13,13,13,13	0
56	MG	1A	3560	1/1	0.98	0.08	21,21,21,21	0
56	MG	1A	4057	1/1	0.98	0.08	50,50,50,50	0
56	MG	1B	3035	1/1	0.98	0.07	21,21,21,21	0
56	MG	1A	3561	1/1	0.98	0.08	16,16,16,16	0
56	MG	1a	3139	1/1	0.98	0.09	31,31,31,31	0
56	MG	1A	3695	1/1	0.98	0.04	24,24,24,24	0
56	MG	1A	3621	1/1	0.98	0.07	34,34,34,34	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	303	1/1	0.98	0.04	23,23,23,23	0
56	MG	2A	3479	1/1	0.98	0.04	37,37,37,37	0
56	MG	1A	3778	1/1	0.98	0.04	22,22,22,22	0
56	MG	1A	4062	1/1	0.98	0.07	23,23,23,23	0
56	MG	1D	306	1/1	0.98	0.06	14,14,14,14	0
56	MG	1A	3780	1/1	0.98	0.07	41,41,41,41	0
56	MG	1A	3954	1/1	0.98	0.07	50,50,50,50	0
56	MG	1a	3148	1/1	0.98	0.06	31,31,31,31	0
56	MG	1A	3465	1/1	0.98	0.12	22,22,22,22	0
56	MG	1A	3234	1/1	0.98	0.04	25,25,25,25	0
56	MG	2A	3167	1/1	0.98	0.08	44,44,44,44	0
56	MG	1A	3957	1/1	0.98	0.07	37,37,37,37	0
56	MG	1A	3191	1/1	0.98	0.16	14,14,14,14	0
56	MG	2A	3857	1/1	0.98	0.05	51,51,51,51	0
56	MG	2A	3020	1/1	0.98	0.11	26,26,26,26	0
56	MG	2A	3859	1/1	0.98	0.23	38,38,38,38	0
56	MG	1A	3192	1/1	0.98	0.07	20,20,20,20	0
56	MG	2A	3861	1/1	0.98	0.06	51,51,51,51	0
56	MG	2A	3172	1/1	0.98	0.18	44,44,44,44	0
56	MG	1A	3960	1/1	0.98	0.05	25,25,25,25	0
56	MG	1A	4071	1/1	0.98	0.06	34,34,34,34	0
56	MG	2A	3327	1/1	0.98	0.12	40,40,40,40	0
56	MG	1E	302	1/1	0.98	0.06	16,16,16,16	0
56	MG	1E	303	1/1	0.98	0.05	23,23,23,23	0
56	MG	1A	3384	1/1	0.98	0.06	33,33,33,33	0
56	MG	2a	3109	1/1	0.98	0.12	43,43,43,43	0
56	MG	2A	3027	1/1	0.98	0.07	30,30,30,30	0
56	MG	2A	3502	1/1	0.98	0.08	35,35,35,35	0
56	MG	1A	3786	1/1	0.98	0.05	42,42,42,42	0
56	MG	2A	3333	1/1	0.98	0.09	33,33,33,33	0
56	MG	1A	3288	1/1	0.98	0.06	17,17,17,17	0
56	MG	1A	4075	1/1	0.98	0.05	39,39,39,39	0
56	MG	1A	3867	1/1	0.98	0.06	18,18,18,18	0
56	MG	1A	3049	1/1	0.98	0.06	24,24,24,24	0
56	MG	1A	3516	1/1	0.98	0.13	37,37,37,37	0
56	MG	2a	3119	1/1	0.98	0.04	59,59,59,59	0
56	MG	1A	3870	1/1	0.98	0.04	25,25,25,25	0
56	MG	1A	3570	1/1	0.98	0.07	16,16,16,16	0
56	MG	1A	3969	1/1	0.98	0.12	33,33,33,33	0
56	MG	1A	3064	1/1	0.98	0.14	6,6,6,6	0
56	MG	2A	3189	1/1	0.98	0.04	38,38,38,38	0
56	MG	1F	304	1/1	0.98	0.22	28,28,28,28	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	3074	1/1	0.98	0.05	37,37,37,37	0
56	MG	2A	3040	1/1	0.98	0.04	38,38,38,38	0
56	MG	1A	3321	1/1	0.98	0.04	16,16,16,16	0
56	MG	1A	3520	1/1	0.98	0.16	55,55,55,55	0
56	MG	1A	3640	1/1	0.98	0.06	12,12,12,12	0
56	MG	1A	3641	1/1	0.98	0.10	9,9,9,9	0
56	MG	2a	3133	1/1	0.98	0.04	69,69,69,69	0
56	MG	1A	3196	1/1	0.98	0.07	21,21,21,21	0
56	MG	2A	3524	1/1	0.98	0.04	44,44,44,44	0
56	MG	2a	3136	1/1	0.98	0.05	60,60,60,60	0
56	MG	1A	3112	1/1	0.98	0.14	29,29,29,29	0
56	MG	1A	3645	1/1	0.98	0.06	14,14,14,14	0
56	MG	2a	3139	1/1	0.98	0.04	41,41,41,41	0
56	MG	2A	3527	1/1	0.98	0.15	41,41,41,41	0
56	MG	1A	3882	1/1	0.98	0.04	25,25,25,25	0
56	MG	2A	3531	1/1	0.98	0.12	51,51,51,51	0
56	MG	1A	4095	1/1	0.98	0.04	19,19,19,19	0
56	MG	1a	3181	1/1	0.98	0.10	68,68,68,68	0
56	MG	2D	302	1/1	0.98	0.09	38,38,38,38	0
56	MG	2a	3147	1/1	0.98	0.10	45,45,45,45	0
56	MG	1A	3267	1/1	0.98	0.12	16,16,16,16	0
56	MG	2A	3713	1/1	0.98	0.04	55,55,55,55	0
56	MG	1N	3002	1/1	0.98	0.03	25,25,25,25	0
56	MG	1A	3720	1/1	0.98	0.05	19,19,19,19	0
56	MG	2A	3055	1/1	0.98	0.10	24,24,24,24	0
56	MG	1N	3004	1/1	0.98	0.10	27,27,27,27	0
56	MG	1A	3075	1/1	0.98	0.15	14,14,14,14	0
56	MG	1A	3648	1/1	0.98	0.10	38,38,38,38	0
56	MG	2a	3157	1/1	0.98	0.05	73,73,73,73	0
56	MG	1A	3649	1/1	0.98	0.04	13,13,13,13	0
56	MG	1a	3190	1/1	0.98	0.05	44,44,44,44	0
56	MG	2A	3543	1/1	0.98	0.04	51,51,51,51	0
56	MG	1A	3243	1/1	0.98	0.06	38,38,38,38	0
56	MG	1A	4103	1/1	0.98	0.08	16,16,16,16	0
56	MG	1A	3990	1/1	0.98	0.04	19,19,19,19	0
56	MG	2A	3370	1/1	0.98	0.18	43,43,43,43	0
56	MG	2F	304	1/1	0.98	0.09	46,46,46,46	0
56	MG	1A	3889	1/1	0.98	0.04	57,57,57,57	0
56	MG	1A	3395	1/1	0.98	0.11	35,35,35,35	0
56	MG	2Q	201	1/1	0.98	0.04	43,43,43,43	0
56	MG	2A	3551	1/1	0.98	0.07	29,29,29,29	0
56	MG	1A	4107	1/1	0.98	0.17	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	3396	1/1	0.98	0.04	29,29,29,29	0
56	MG	1A	3397	1/1	0.98	0.04	27,27,27,27	0
56	MG	1Q	3002	1/1	0.98	0.08	21,21,21,21	0
56	MG	1a	3200	1/1	0.98	0.05	42,42,42,42	0
56	MG	1A	3076	1/1	0.98	0.13	26,26,26,26	0
56	MG	1A	4111	1/1	0.98	0.07	20,20,20,20	0
56	MG	2A	3380	1/1	0.98	0.16	36,36,36,36	0
56	MG	1a	3204	1/1	0.98	0.06	27,27,27,27	0
56	MG	1a	3205	1/1	0.98	0.11	55,55,55,55	0
56	MG	1a	3206	1/1	0.98	0.04	54,54,54,54	0
56	MG	1a	3208	1/1	0.98	0.05	62,62,62,62	0
56	MG	1Q	3005	1/1	0.98	0.04	25,25,25,25	0
56	MG	1A	3895	1/1	0.98	0.05	61,61,61,61	0
56	MG	1A	3999	1/1	0.98	0.05	35,35,35,35	0
56	MG	2A	3567	1/1	0.98	0.06	45,45,45,45	0
56	MG	1a	3213	1/1	0.98	0.05	44,44,44,44	0
56	MG	1a	3215	1/1	0.98	0.04	49,49,49,49	0
56	MG	1A	4114	1/1	0.98	0.12	25,25,25,25	0
56	MG	1A	3130	1/1	0.98	0.29	30,30,30,30	0
56	MG	1A	3732	1/1	0.98	0.07	16,16,16,16	0
56	MG	1a	3072	1/1	0.98	0.06	36,36,36,36	0
56	MG	2A	3237	1/1	0.98	0.16	31,31,31,31	0
56	MG	1a	3220	1/1	0.98	0.04	42,42,42,42	0
56	MG	1A	3532	1/1	0.98	0.19	29,29,29,29	0
56	MG	1A	4119	1/1	0.98	0.26	27,27,27,27	0
56	MG	1A	3329	1/1	0.98	0.17	22,22,22,22	0
56	MG	1A	3361	1/1	0.98	0.05	25,25,25,25	0
56	MG	1A	3007	1/1	0.98	0.04	27,27,27,27	0
56	MG	1A	3008	1/1	0.98	0.04	9,9,9,9	0
56	MG	1A	4124	1/1	0.98	0.08	17,17,17,17	0
56	MG	1A	3364	1/1	0.98	0.24	23,23,23,23	0
56	MG	1a	3229	1/1	0.98	0.12	42,42,42,42	0
56	MG	2A	3096	1/1	0.98	0.06	33,33,33,33	0
56	MG	2A	3764	1/1	0.98	0.04	23,23,23,23	0
56	MG	1A	3904	1/1	0.98	0.06	6,6,6,6	0
56	MG	1U	206	1/1	0.98	0.16	24,24,24,24	0
56	MG	1A	3003	1/1	0.98	0.08	13,13,13,13	0
56	MG	2A	3410	1/1	0.98	0.04	22,22,22,22	0
56	MG	1A	4128	1/1	0.98	0.05	22,22,22,22	0
56	MG	1A	4130	1/1	0.98	0.10	20,20,20,20	0
56	MG	1A	3906	1/1	0.98	0.04	43,43,43,43	0
56	MG	2A	3772	1/1	0.98	0.04	30,30,30,30	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	3366	1/1	0.98	0.31	24,24,24,24	0
56	MG	1A	3275	1/1	0.98	0.05	30,30,30,30	0
56	MG	1W	205	1/1	0.98	0.08	24,24,24,24	0
56	MG	2A	3417	1/1	0.98	0.13	22,22,22,22	0
56	MG	1W	206	1/1	0.98	0.09	17,17,17,17	0
56	MG	2A	3598	1/1	0.98	0.06	27,27,27,27	0
56	MG	1A	3541	1/1	0.98	0.12	29,29,29,29	0
56	MG	2A	3781	1/1	0.98	0.05	33,33,33,33	0
56	MG	1X	101	1/1	0.98	0.07	25,25,25,25	0
56	MG	1X	102	1/1	0.98	0.09	20,20,20,20	0
56	MG	1A	4135	1/1	0.98	0.11	20,20,20,20	0
56	MG	2A	3604	1/1	0.98	0.09	35,35,35,35	0
56	MG	2A	3787	1/1	0.98	0.04	48,48,48,48	0
56	MG	1A	3743	1/1	0.98	0.06	17,17,17,17	0
56	MG	1A	3824	1/1	0.98	0.10	10,10,10,10	0
56	MG	1A	4139	1/1	0.98	0.07	23,23,23,23	0
56	MG	2A	3426	1/1	0.98	0.04	39,39,39,39	0
56	MG	1A	3599	1/1	0.98	0.07	16,16,16,16	0
56	MG	2A	3793	1/1	0.98	0.03	19,19,19,19	0
56	MG	1Y	504	1/1	0.98	0.14	45,45,45,45	0
56	MG	2A	3795	1/1	0.98	0.05	34,34,34,34	0
56	MG	1A	3053	1/1	0.98	0.10	38,38,38,38	0
56	MG	1A	3747	1/1	0.98	0.05	18,18,18,18	0
56	MG	1A	3015	1/1	0.98	0.08	20,20,20,20	0
56	MG	1A	3669	1/1	0.98	0.05	15,15,15,15	0
56	MG	1A	3920	1/1	0.98	0.04	41,41,41,41	0
56	MG	1B	3002	1/1	0.98	0.12	27,27,27,27	0
56	MG	1A	3750	1/1	0.98	0.19	41,41,41,41	0
56	MG	1A	4028	1/1	0.98	0.05	24,24,24,24	0
56	MG	2A	3437	1/1	0.98	0.05	43,43,43,43	0
56	MG	1A	3107	1/1	0.98	0.06	25,25,25,25	0
56	MG	1A	3672	1/1	0.98	0.06	9,9,9,9	0
56	MG	1A	3371	1/1	0.98	0.18	32,32,32,32	0
56	MG	2A	3442	1/1	0.98	0.06	41,41,41,41	0
56	MG	1A	3208	1/1	0.98	0.09	24,24,24,24	0
56	MG	1A	3307	1/1	0.98	0.13	32,32,32,32	0
56	MG	2w	3001	1/1	0.98	0.15	34,34,34,34	0
56	MG	1A	3230	1/1	0.98	0.20	19,19,19,19	0
56	MG	2A	3446	1/1	0.98	0.04	30,30,30,30	0
56	MG	1A	3309	1/1	0.98	0.07	37,37,37,37	0
56	MG	1A	3930	1/1	0.98	0.06	40,40,40,40	0
56	MG	1A	4037	1/1	0.98	0.07	45,45,45,45	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	3451	1/1	0.98	0.06	29,29,29,29	0
56	MG	1A	3310	1/1	0.98	0.21	43,43,43,43	0
56	MG	1A	3460	1/1	0.98	0.07	20,20,20,20	0
56	MG	2A	3634	1/1	0.98	0.06	54,54,54,54	0
56	MG	1A	3033	1/1	0.98	0.18	23,23,23,23	0
56	MG	1A	3553	1/1	0.98	0.07	32,32,32,32	0
56	MG	1A	3378	1/1	0.98	0.04	25,25,25,25	0
56	MG	2A	3638	1/1	0.98	0.06	48,48,48,48	0
56	MG	1A	3232	1/1	0.98	0.13	15,15,15,15	0
56	MG	1A	3937	1/1	0.98	0.10	33,33,33,33	0
56	MG	1A	4045	1/1	0.98	0.05	30,30,30,30	0
56	MG	2y	105	1/1	0.98	0.04	65,65,65,65	0
56	MG	1A	3938	1/1	0.98	0.05	32,32,32,32	0
56	MG	17	103	1/1	0.98	0.05	36,36,36,36	0
56	MG	1A	3684	1/1	0.98	0.05	24,24,24,24	0
56	MG	1A	3614	1/1	0.98	0.04	22,22,22,22	0
56	MG	1A	3506	1/1	0.98	0.16	18,18,18,18	0
59	ZN	14	501	1/1	0.98	0.04	71,71,71,71	0
56	MG	1A	3687	1/1	0.98	0.04	30,30,30,30	0
59	ZN	25	101	1/1	0.98	0.03	44,44,44,44	0
56	MG	1A	3688	1/1	0.98	0.10	20,20,20,20	0
56	MG	1A	3557	1/1	0.98	0.09	19,19,19,19	0
60	SF4	1d	501	8/8	0.98	0.06	51,59,62,71	0
60	SF4	2d	302	8/8	0.98	0.05	53,66,72,75	0
56	MG	1A	3972	1/1	0.99	0.05	35,35,35,35	0
56	MG	1A	3639	1/1	0.99	0.03	19,19,19,19	0
56	MG	1A	3974	1/1	0.99	0.07	8,8,8,8	0
56	MG	2A	3441	1/1	0.99	0.09	47,47,47,47	0
56	MG	1A	3210	1/1	0.99	0.19	37,37,37,37	0
56	MG	1A	3265	1/1	0.99	0.14	25,25,25,25	0
56	MG	2A	3365	1/1	0.99	0.07	23,23,23,23	0
56	MG	1A	4094	1/1	0.99	0.09	22,22,22,22	0
56	MG	2A	3878	1/1	0.99	0.08	36,36,36,36	0
56	MG	2A	3528	1/1	0.99	0.05	28,28,28,28	0
56	MG	2A	3529	1/1	0.99	0.06	31,31,31,31	0
56	MG	1B	3014	1/1	0.99	0.08	31,31,31,31	0
56	MG	1A	3977	1/1	0.99	0.03	17,17,17,17	0
56	MG	1A	3582	1/1	0.99	0.09	13,13,13,13	0
56	MG	2A	3449	1/1	0.99	0.09	53,53,53,53	0
56	MG	1A	3437	1/1	0.99	0.11	27,27,27,27	0
56	MG	1A	3716	1/1	0.99	0.04	25,25,25,25	0
56	MG	1A	3798	1/1	0.99	0.09	39,39,39,39	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	3644	1/1	0.99	0.04	12,12,12,12	0
56	MG	1A	3179	1/1	0.99	0.10	24,24,24,24	0
56	MG	1A	3229	1/1	0.99	0.14	32,32,32,32	0
56	MG	1A	3167	1/1	0.99	0.16	20,20,20,20	0
56	MG	1a	3203	1/1	0.99	0.04	56,56,56,56	0
56	MG	1A	3137	1/1	0.99	0.11	24,24,24,24	0
56	MG	1B	3025	1/1	0.99	0.06	21,21,21,21	0
56	MG	2A	3544	1/1	0.99	0.09	40,40,40,40	0
56	MG	2a	3122	1/1	0.99	0.04	73,73,73,73	0
56	MG	1A	3987	1/1	0.99	0.03	21,21,21,21	0
56	MG	1a	3207	1/1	0.99	0.06	33,33,33,33	0
56	MG	2A	3462	1/1	0.99	0.05	20,20,20,20	0
56	MG	1A	3589	1/1	0.99	0.09	19,19,19,19	0
56	MG	1a	3209	1/1	0.99	0.04	44,44,44,44	0
56	MG	18	104	1/1	0.99	0.07	19,19,19,19	0
56	MG	1A	3169	1/1	0.99	0.07	18,18,18,18	0
56	MG	1A	4048	1/1	0.99	0.03	17,17,17,17	0
56	MG	1A	3183	1/1	0.99	0.14	24,24,24,24	0
56	MG	1a	3214	1/1	0.99	0.06	70,70,70,70	0
56	MG	1A	3012	1/1	0.99	0.05	14,14,14,14	0
56	MG	1A	3893	1/1	0.99	0.07	21,21,21,21	0
56	MG	1A	3993	1/1	0.99	0.04	30,30,30,30	0
56	MG	1A	3185	1/1	0.99	0.14	22,22,22,22	0
56	MG	1A	3850	1/1	0.99	0.05	33,33,33,33	0
56	MG	2A	3646	1/1	0.99	0.04	23,23,23,23	0
56	MG	1A	3996	1/1	0.99	0.02	50,50,50,50	0
56	MG	1A	3072	1/1	0.99	0.27	23,23,23,23	0
56	MG	1A	3595	1/1	0.99	0.03	32,32,32,32	0
56	MG	1A	3623	1/1	0.99	0.07	17,17,17,17	0
56	MG	1a	3011	1/1	0.99	0.10	19,19,19,19	0
56	MG	1A	3101	1/1	0.99	0.11	24,24,24,24	0
56	MG	2a	3145	1/1	0.99	0.05	64,64,64,64	0
56	MG	1A	3625	1/1	0.99	0.04	23,23,23,23	0
56	MG	1U	202	1/1	0.99	0.08	19,19,19,19	0
56	MG	2a	3148	1/1	0.99	0.04	65,65,65,65	0
56	MG	1A	3102	1/1	0.99	0.12	23,23,23,23	0
56	MG	1A	4003	1/1	0.99	0.05	33,33,33,33	0
56	MG	1A	3774	1/1	0.99	0.03	25,25,25,25	0
56	MG	1A	3257	1/1	0.99	0.04	18,18,18,18	0
56	MG	1A	3952	1/1	0.99	0.03	52,52,52,52	0
56	MG	1A	3124	1/1	0.99	0.16	17,17,17,17	0
56	MG	1A	4129	1/1	0.99	0.04	16,16,16,16	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	3697	1/1	0.99	0.03	8,8,8,8	0
56	MG	1A	3103	1/1	0.99	0.12	18,18,18,18	0
56	MG	1a	3162	1/1	0.99	0.08	42,42,42,42	0
56	MG	1A	3779	1/1	0.99	0.08	25,25,25,25	0
56	MG	1W	204	1/1	0.99	0.03	21,21,21,21	0
56	MG	1A	4013	1/1	0.99	0.02	26,26,26,26	0
56	MG	1A	3909	1/1	0.99	0.02	23,23,23,23	0
56	MG	1A	3406	1/1	0.99	0.14	24,24,24,24	0
56	MG	2A	3498	1/1	0.99	0.04	39,39,39,39	0
56	MG	1A	3134	1/1	0.99	0.06	8,8,8,8	0
56	MG	1A	3207	1/1	0.99	0.14	25,25,25,25	0
56	MG	1A	4138	1/1	0.99	0.16	29,29,29,29	0
56	MG	1A	3633	1/1	0.99	0.06	24,24,24,24	0
56	MG	1A	3014	1/1	0.99	0.06	15,15,15,15	0
56	MG	2A	3504	1/1	0.99	0.03	41,41,41,41	0
56	MG	1A	3019	1/1	0.99	0.06	8,8,8,8	0
56	MG	1A	4142	1/1	0.99	0.04	16,16,16,16	0
56	MG	1E	312	1/1	0.99	0.05	20,20,20,20	0
56	MG	1A	3745	1/1	0.99	0.03	28,28,28,28	0
56	MG	1A	4079	1/1	0.99	0.04	29,29,29,29	0
56	MG	1A	3636	1/1	0.99	0.07	6,6,6,6	0
56	MG	1A	3707	1/1	0.99	0.06	40,40,40,40	0
56	MG	1A	3670	1/1	0.99	0.06	8,8,8,8	0
56	MG	1A	3921	1/1	0.99	0.04	45,45,45,45	0
56	MG	1A	3284	1/1	0.99	0.03	27,27,27,27	0
59	ZN	1Y	501	1/1	0.99	0.03	49,49,49,49	0
56	MG	1A	4027	1/1	0.99	0.08	59,59,59,59	0
59	ZN	15	101	1/1	0.99	0.04	37,37,37,37	0
59	ZN	16	101	1/1	0.99	0.04	33,33,33,33	0
59	ZN	1n	501	1/1	0.99	0.03	55,55,55,55	0
59	ZN	2Y	501	1/1	0.99	0.05	75,75,75,75	0
56	MG	2A	3052	1/1	0.99	0.06	37,37,37,37	0
56	MG	2A	3602	1/1	0.99	0.04	37,37,37,37	0
59	ZN	26	501	1/1	0.99	0.03	55,55,55,55	0
56	MG	1A	3875	1/1	0.99	0.03	22,22,22,22	0
56	MG	1A	3434	1/1	0.99	0.03	24,24,24,24	0
56	MG	2a	3186	1/1	0.99	0.10	37,37,37,37	0
56	MG	1a	3186	1/1	0.99	0.05	57,57,57,57	0
56	MG	1A	3689	1/1	1.00	0.06	12,12,12,12	0
56	MG	1A	4008	1/1	1.00	0.03	22,22,22,22	0
56	MG	1A	4098	1/1	1.00	0.05	14,14,14,14	0
56	MG	1A	3698	1/1	1.00	0.03	8,8,8,8	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	3774	1/1	1.00	0.02	27,27,27,27	0
56	MG	1A	4087	1/1	1.00	0.03	14,14,14,14	0
59	ZN	19	102	1/1	1.00	0.02	31,31,31,31	0
56	MG	1A	3763	1/1	1.00	0.08	7,7,7,7	0
56	MG	1A	3854	1/1	1.00	0.04	18,18,18,18	0
56	MG	1A	4012	1/1	1.00	0.02	17,17,17,17	0
56	MG	1A	3728	1/1	1.00	0.06	27,27,27,27	0
56	MG	1A	3585	1/1	1.00	0.06	15,15,15,15	0
56	MG	1A	3914	1/1	1.00	0.02	26,26,26,26	0
56	MG	1A	3721	1/1	1.00	0.05	16,16,16,16	0
56	MG	1A	3907	1/1	1.00	0.08	11,11,11,11	0
56	MG	2A	3784	1/1	1.00	0.02	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.