



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 3, 2020 – 11:35 am BST

PDB ID : 6ND6  
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with erythromycin and bound to mRNA and A-, P-, and E-site tRNAs at 2.85Å resolution  
Authors : Svetlov, M.S.; Plessa, E.; Chen, C.-W.; Bougas, A.; Krokidis, M.G.; Dinos, G.P.; Polikanov, Y.S.  
Deposited on : 2018-12-13  
Resolution : 2.85 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](mailto: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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

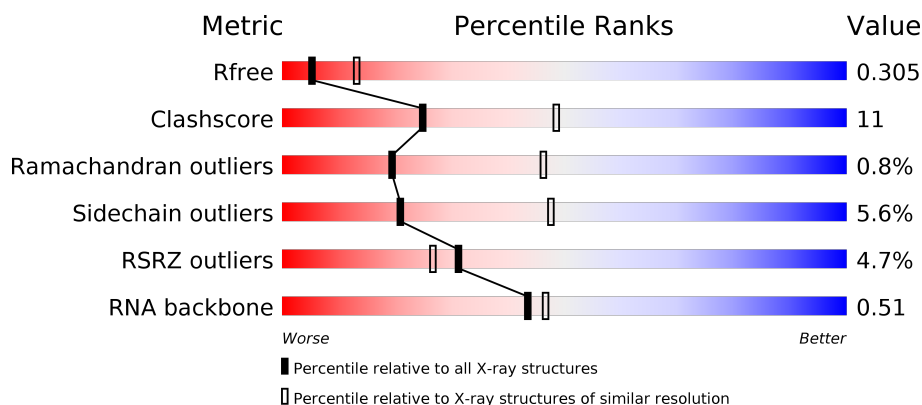
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 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.
















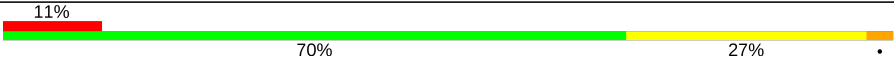

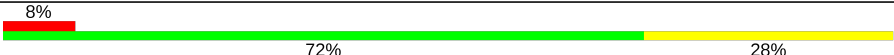


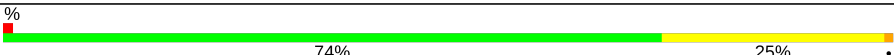
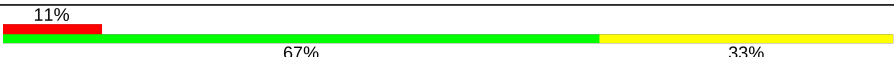
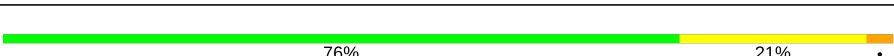


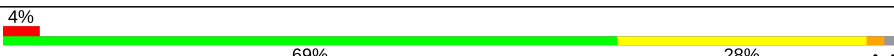
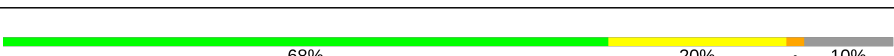
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)
RNA backbone	3102	1088 (3.12-2.60)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	
1	2A	2915	
2	1B	121	
2	2B	121	

*Continued on next page...*

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	6MZ	2y	37	-	-	-	X
56	MG	1A	3348	-	-	-	X
56	MG	1A	4073	-	-	-	X
56	MG	1F	314	-	-	-	X
56	MG	2A	3316	-	-	-	X
56	MG	2A	3359	-	-	-	X
56	MG	2A	3773	-	-	-	X
56	MG	2A	3774	-	-	-	X
56	MG	2A	3801	-	-	-	X
56	MG	2T	202	-	-	-	X

## 2 Entry composition [i](#)

There are 60 unique types of molecules in this entry. The entry contains 300104 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

*Continued on next page...*

*Continued from previous page...*

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

*Continued on next page...*

*Continued from previous page...*

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

*Continued on next page...*

*Continued from previous page...*

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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1v	13	Total	C	N	O	P	0	0	0
			276	124	48	91	13			
53	2v	13	Total	C	N	O	P	0	0	0
			276	124	48	91	13			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
54	1w	73	Total 1568	C 700	N 282	O 512	P 73	S 1	0	0	0
54	1y	74	Total 1591	C 710	N 287	O 519	P 74	S 1	0	0	0
54	2w	73	Total 1568	C 700	N 282	O 512	P 73	S 1	0	0	0
54	2y	73	Total 1568	C 700	N 282	O 512	P 73	S 1	0	0	0

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

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

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2r	1	Total	Mg	0	0
			1	1		
56	1T	2	Total	Mg	0	0
			2	2		
56	20	2	Total	Mg	0	0
			2	2		
56	1Y	1	Total	Mg	0	0
			1	1		
56	2F	7	Total	Mg	0	0
			7	7		
56	1n	1	Total	Mg	0	0
			1	1		
56	2w	1	Total	Mg	0	0
			1	1		
56	1S	2	Total	Mg	0	0
			2	2		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	25	3	Total 3	Mg 3	0	0
56	1D	13	Total 13	Mg 13	0	0
56	1I	1	Total 1	Mg 1	0	0
56	2X	2	Total 2	Mg 2	0	0
56	1w	6	Total 6	Mg 6	0	0
56	1x	13	Total 13	Mg 13	0	0
56	1m	1	Total 1	Mg 1	0	0
56	2t	1	Total 1	Mg 1	0	0
56	2g	1	Total 1	Mg 1	0	0
56	2R	3	Total 3	Mg 3	0	0
56	14	1	Total 1	Mg 1	0	0
56	1r	1	Total 1	Mg 1	0	0
56	19	3	Total 3	Mg 3	0	0
56	2y	4	Total 4	Mg 4	0	0
56	2d	1	Total 1	Mg 1	0	0
56	1N	4	Total 4	Mg 4	0	0
56	2W	1	Total 1	Mg 1	0	0
56	13	6	Total 6	Mg 6	0	0
56	2B	21	Total 21	Mg 21	0	0
56	1b	1	Total 1	Mg 1	0	0
56	1W	8	Total 8	Mg 8	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2I	1	Total 1	Mg 1	0	0
56	1X	5	Total 5	Mg 5	0	0
56	2i	2	Total 2	Mg 2	0	0
56	2T	3	Total 3	Mg 3	0	0
56	2G	1	Total 1	Mg 1	0	0
56	1a	229	Total 229	Mg 229	0	0
56	2p	1	Total 1	Mg 1	0	0
56	1R	2	Total 2	Mg 2	0	0
56	26	2	Total 2	Mg 2	0	0
56	1G	3	Total 3	Mg 3	0	0
56	1v	1	Total 1	Mg 1	0	0
56	2D	7	Total 7	Mg 7	0	0
56	1l	3	Total 3	Mg 3	0	0
56	1Q	8	Total 8	Mg 8	0	0
56	1B	35	Total 35	Mg 35	0	0
56	17	5	Total 5	Mg 5	0	0
56	18	2	Total 2	Mg 2	0	0
56	1f	1	Total 1	Mg 1	0	0
56	28	1	Total 1	Mg 1	0	0
56	2e	1	Total 1	Mg 1	0	0
56	1A	1073	Total 1073	Mg 1073	0	0

*Continued on next page...*

*Continued from previous page...*

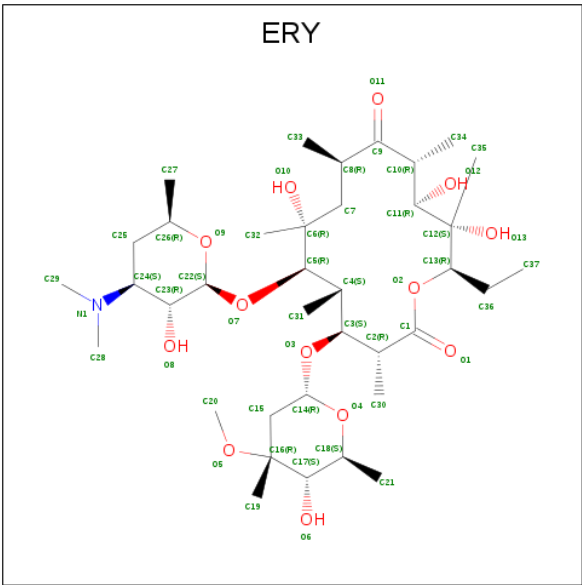
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2P	2	Total 2	Mg 2	0	0
56	12	2	Total 2	Mg 2	0	0
56	1p	1	Total 1	Mg 1	0	0
56	2N	1	Total 1	Mg 1	0	0
56	1e	2	Total 2	Mg 2	0	0
56	1V	8	Total 8	Mg 8	0	0
56	22	1	Total 1	Mg 1	0	0
56	2j	2	Total 2	Mg 2	0	0
56	2U	3	Total 3	Mg 3	0	0
56	11	1	Total 1	Mg 1	0	0
56	2q	3	Total 3	Mg 3	0	0
56	1U	10	Total 10	Mg 10	0	0
56	27	2	Total 2	Mg 2	0	0
56	1F	14	Total 14	Mg 14	0	0
56	2Z	1	Total 1	Mg 1	0	0
56	2E	8	Total 8	Mg 8	0	0
56	2v	2	Total 2	Mg 2	0	0
56	1P	8	Total 8	Mg 8	0	0
56	2a	233	Total 233	Mg 233	0	0
56	1E	15	Total 15	Mg 15	0	0
56	2l	5	Total 5	Mg 5	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	16	4	Total 4	Mg 4	0	0
56	1t	1	Total 1	Mg 1	0	0
56	1y	5	Total 5	Mg 5	0	0
56	2f	2	Total 2	Mg 2	0	0
56	2Q	5	Total 5	Mg 5	0	0
56	15	7	Total 7	Mg 7	0	0
56	1s	1	Total 1	Mg 1	0	0
56	2O	1	Total 1	Mg 1	0	0
56	1d	1	Total 1	Mg 1	0	0
56	23	3	Total 3	Mg 3	0	0
56	2x	5	Total 5	Mg 5	0	0
56	1Z	3	Total 3	Mg 3	0	0
56	2k	1	Total 1	Mg 1	0	0
56	1O	2	Total 2	Mg 2	0	0
56	2V	1	Total 1	Mg 1	0	0
56	10	7	Total 7	Mg 7	0	0
56	2A	874	Total 874	Mg 874	0	0

- Molecule 57 is ERYTHROMYCIN A (three-letter code: ERY) (formula: C<sub>37</sub>H<sub>67</sub>NO<sub>13</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
57	1A	1	Total	C	N	O	0	0
			51	37	1	13		
57	2A	1	Total	C	N	O	0	0
			51	37	1	13		

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

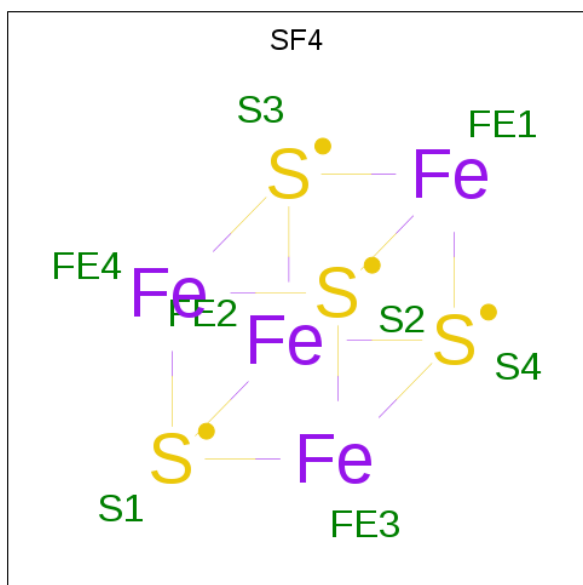
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1Y	1	Total	Zn	0	0
			1	1		
58	14	1	Total	Zn	0	0
			1	1		
58	1n	1	Total	Zn	0	0
			1	1		
58	15	1	Total	Zn	0	0
			1	1		
58	29	1	Total	Zn	0	0
			1	1		
58	19	1	Total	Zn	0	0
			1	1		
58	26	1	Total	Zn	0	0
			1	1		
58	25	1	Total	Zn	0	0
			1	1		
58	24	1	Total	Zn	0	0
			1	1		
58	2n	1	Total	Zn	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	2Y	1	Total	Zn	0	0
			1	1		
58	16	1	Total	Zn	0	0
			1	1		

- Molecule 59 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
59	1d	1	Total	Fe	S	0	0
			8	4	4		
59	2d	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 60 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	3	Total	O	0	0
			3	3		
60	1A	1	Total	O	0	0
			1	1		
60	1A	5	Total	O	0	0
			5	5		
60	1A	5	Total	O	0	0
			5	5		
60	1A	2	Total	O	0	0
			2	2		

Continued on next page...



*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	4	Total 4	O 4	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	4	Total 4	O 4	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	5	Total 5	O 5	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	1	Total 1	O 1	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	1	Total 1	O 1	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	4	Total 4	O 4	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	5	Total 5	O 5	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	3	Total 3	O 3	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	3	Total 3	O 3	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	2	Total 2	O 2	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	2	Total 2	O 2	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	3	Total 3	O 3	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	2	Total 2	O 2	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	4	Total 4	O 4	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	2	Total 2	O 2	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	2	Total 2	O 2	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	1	Total 1	O 1	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	2	Total 2	O 2	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	1	Total 1	O 1	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	1	Total 1	O 1	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	2	Total 2	O 2	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	1	Total 1	O 1	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	2	Total 2	O 2	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	1	Total 1	O 1	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	3	Total 3	O 3	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	3	Total 3	O 3	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	6	Total 6	O 6	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	5	Total 5	O 5	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	3	Total 3	O 3	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	3	Total 3	O 3	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	5	Total 5	O 5	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	5	Total 5	O 5	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	3	Total 3	O 3	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	2	Total 2	O 2	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	6	Total 6	O 6	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	6	Total 6	O 6	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	3	Total 3	O 3	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	3	Total 3	O 3	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	2	Total 2	O 2	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	3	Total 3	O 3	0	0
60	1A	5	Total 5	O 5	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	4	Total 4	O 4	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	2	Total 2	O 2	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	6	Total 6	O 6	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	2	Total 2	O 2	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	2	Total 2	O 2	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	2	Total 2	O 2	0	0
60	1A	1	Total 1	O 1	0	0
60	1A	6	Total 6	O 6	0	0
60	1A	384	Total 384	O 384	0	0
60	1B	1	Total 1	O 1	0	0
60	1B	5	Total 5	O 5	0	0
60	1B	3	Total 3	O 3	0	0
60	1B	3	Total 3	O 3	0	0
60	1B	1	Total 1	O 1	0	0
60	1B	1	Total 1	O 1	0	0
60	1B	1	Total 1	O 1	0	0
60	1B	1	Total 1	O 1	0	0
60	1B	1	Total 1	O 1	0	0
60	1B	2	Total 2	O 2	0	0
60	1B	2	Total 2	O 2	0	0
60	1B	2	Total 2	O 2	0	0
60	1B	1	Total 1	O 1	0	0
60	1B	4	Total 4	O 4	0	0
60	1B	1	Total 1	O 1	0	0
60	1B	1	Total 1	O 1	0	0
60	1B	1	Total 1	O 1	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1B	2	Total 2	O 2	0	0
60	1B	1	Total 1	O 1	0	0
60	1B	1	Total 1	O 1	0	0
60	1B	2	Total 2	O 2	0	0
60	1B	1	Total 1	O 1	0	0
60	1B	5	Total 5	O 5	0	0
60	1B	1	Total 1	O 1	0	0
60	1B	15	Total 15	O 15	0	0
60	1D	4	Total 4	O 4	0	0
60	1D	1	Total 1	O 1	0	0
60	1D	1	Total 1	O 1	0	0
60	1D	10	Total 10	O 10	0	0
60	1E	2	Total 2	O 2	0	0
60	1E	5	Total 5	O 5	0	0
60	1E	1	Total 1	O 1	0	0
60	1E	5	Total 5	O 5	0	0
60	1E	8	Total 8	O 8	0	0
60	1F	1	Total 1	O 1	0	0
60	1F	6	Total 6	O 6	0	0
60	1G	2	Total 2	O 2	0	0
60	1G	2	Total 2	O 2	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1H	1	Total 1	O 1	0	0
60	1I	2	Total 2	O 2	0	0
60	1N	5	Total 5	O 5	0	0
60	1O	1	Total 1	O 1	0	0
60	1O	1	Total 1	O 1	0	0
60	1O	5	Total 5	O 5	0	0
60	1P	4	Total 4	O 4	0	0
60	1P	1	Total 1	O 1	0	0
60	1P	2	Total 2	O 2	0	0
60	1P	4	Total 4	O 4	0	0
60	1Q	4	Total 4	O 4	0	0
60	1Q	1	Total 1	O 1	0	0
60	1Q	5	Total 5	O 5	0	0
60	1R	1	Total 1	O 1	0	0
60	1R	7	Total 7	O 7	0	0
60	1S	1	Total 1	O 1	0	0
60	1S	4	Total 4	O 4	0	0
60	1T	1	Total 1	O 1	0	0
60	1T	1	Total 1	O 1	0	0
60	1U	6	Total 6	O 6	0	0
60	1V	1	Total 1	O 1	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1V	9	Total 9	O 9	0	0
60	1W	8	Total 8	O 8	0	0
60	1X	2	Total 2	O 2	0	0
60	1X	4	Total 4	O 4	0	0
60	1X	2	Total 2	O 2	0	0
60	1Y	4	Total 4	O 4	0	0
60	1Z	1	Total 1	O 1	0	0
60	10	3	Total 3	O 3	0	0
60	10	2	Total 2	O 2	0	0
60	10	4	Total 4	O 4	0	0
60	11	1	Total 1	O 1	0	0
60	11	9	Total 9	O 9	0	0
60	12	3	Total 3	O 3	0	0
60	13	1	Total 1	O 1	0	0
60	13	1	Total 1	O 1	0	0
60	14	2	Total 2	O 2	0	0
60	15	3	Total 3	O 3	0	0
60	16	1	Total 1	O 1	0	0
60	16	2	Total 2	O 2	0	0
60	17	2	Total 2	O 2	0	0
60	17	7	Total 7	O 7	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	18	2	Total 2	O 2	0	0
60	18	3	Total 3	O 3	0	0
60	19	2	Total 2	O 2	0	0
60	1a	2	Total 2	O 2	0	0
60	1a	3	Total 3	O 3	0	0
60	1a	4	Total 4	O 4	0	0
60	1a	1	Total 1	O 1	0	0
60	1a	2	Total 2	O 2	0	0
60	1a	2	Total 2	O 2	0	0
60	1a	1	Total 1	O 1	0	0
60	1a	5	Total 5	O 5	0	0
60	1a	4	Total 4	O 4	0	0
60	1a	4	Total 4	O 4	0	0
60	1a	5	Total 5	O 5	0	0
60	1a	2	Total 2	O 2	0	0
60	1a	4	Total 4	O 4	0	0
60	1a	1	Total 1	O 1	0	0
60	1a	2	Total 2	O 2	0	0
60	1a	1	Total 1	O 1	0	0
60	1a	1	Total 1	O 1	0	0
60	1a	2	Total 2	O 2	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1a	2	Total 2	O 2	0	0
60	1a	5	Total 5	O 5	0	0
60	1a	6	Total 6	O 6	0	0
60	1a	1	Total 1	O 1	0	0
60	1a	3	Total 3	O 3	0	0
60	1a	3	Total 3	O 3	0	0
60	1a	5	Total 5	O 5	0	0
60	1a	5	Total 5	O 5	0	0
60	1a	4	Total 4	O 4	0	0
60	1a	1	Total 1	O 1	0	0
60	1a	1	Total 1	O 1	0	0
60	1a	5	Total 5	O 5	0	0
60	1a	2	Total 2	O 2	0	0
60	1a	4	Total 4	O 4	0	0
60	1a	1	Total 1	O 1	0	0
60	1a	6	Total 6	O 6	0	0
60	1a	5	Total 5	O 5	0	0
60	1a	4	Total 4	O 4	0	0
60	1a	4	Total 4	O 4	0	0
60	1a	3	Total 3	O 3	0	0
60	1a	1	Total 1	O 1	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1a	1	Total 1	O 1	0	0
60	1a	1	Total 1	O 1	0	0
60	1a	6	Total 6	O 6	0	0
60	1a	3	Total 3	O 3	0	0
60	1a	3	Total 3	O 3	0	0
60	1a	1	Total 1	O 1	0	0
60	1a	3	Total 3	O 3	0	0
60	1a	4	Total 4	O 4	0	0
60	1a	2	Total 2	O 2	0	0
60	1a	4	Total 4	O 4	0	0
60	1a	5	Total 5	O 5	0	0
60	1a	5	Total 5	O 5	0	0
60	1a	6	Total 6	O 6	0	0
60	1a	4	Total 4	O 4	0	0
60	1a	5	Total 5	O 5	0	0
60	1a	4	Total 4	O 4	0	0
60	1a	3	Total 3	O 3	0	0
60	1a	3	Total 3	O 3	0	0
60	1a	6	Total 6	O 6	0	0
60	1a	3	Total 3	O 3	0	0
60	1a	3	Total 3	O 3	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1a	4	Total 4	O 4	0	0
60	1a	6	Total 6	O 6	0	0
60	1a	6	Total 6	O 6	0	0
60	1a	6	Total 6	O 6	0	0
60	1a	6	Total 6	O 6	0	0
60	1a	5	Total 5	O 5	0	0
60	1a	4	Total 4	O 4	0	0
60	1a	5	Total 5	O 5	0	0
60	1a	6	Total 6	O 6	0	0
60	1a	6	Total 6	O 6	0	0
60	1a	6	Total 6	O 6	0	0
60	1a	6	Total 6	O 6	0	0
60	1a	6	Total 6	O 6	0	0
60	1a	2	Total 2	O 2	0	0
60	1a	4	Total 4	O 4	0	0
60	1a	5	Total 5	O 5	0	0
60	1a	6	Total 6	O 6	0	0
60	1a	6	Total 6	O 6	0	0
60	1a	3	Total 3	O 3	0	0
60	1a	6	Total 6	O 6	0	0
60	1a	5	Total 5	O 5	0	0
60	1a	6	Total 6	O 6	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1a	1	Total 1	O 1	0	0
60	1a	1	Total 1	O 1	0	0
60	1a	2	Total 2	O 2	0	0
60	1a	1	Total 1	O 1	0	0
60	1a	2	Total 2	O 2	0	0
60	1a	2	Total 2	O 2	0	0
60	1a	71	Total 71	O 71	0	0
60	1b	1	Total 1	O 1	0	0
60	1g	1	Total 1	O 1	0	0
60	1k	1	Total 1	O 1	0	0
60	1l	2	Total 2	O 2	0	0
60	1q	4	Total 4	O 4	0	0
60	1v	1	Total 1	O 1	0	0
60	1w	2	Total 2	O 2	0	0
60	1x	1	Total 1	O 1	0	0
60	1x	1	Total 1	O 1	0	0
60	1x	1	Total 1	O 1	0	0
60	1x	2	Total 2	O 2	0	0
60	1x	2	Total 2	O 2	0	0
60	1x	1	Total 1	O 1	0	0
60	1x	1	Total 1	O 1	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1x	1	Total 1	O 1	0	0
60	1x	5	Total 5	O 5	0	0
60	1y	2	Total 2	O 2	0	0
60	2A	6	Total 6	O 6	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	6	Total 6	O 6	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	6	Total 6	O 6	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	3	Total 3	O 3	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	1	Total 1	O 1	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	5	Total 5	O 5	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2A	5	Total 5	O 5	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2A	1	Total 1	O 1	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	6	Total 6	O 6	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	6	Total 6	O 6	0	0
60	2A	6	Total 6	O 6	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	4	Total 4	O 4	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2A	2	Total 2	O 2	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	6	Total 6	O 6	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	1	Total 1	O 1	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2A	5	Total 5	O 5	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	4	Total 4	O 4	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2A	1	Total 1	O 1	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	2A	2	Total O 2 2	0	0
60	2A	2	Total O 2 2	0	0
60	2A	1	Total O 1 1	0	0
60	2A	1	Total O 1 1	0	0
60	2A	3	Total O 3 3	0	0
60	2A	1	Total O 1 1	0	0
60	2A	2	Total O 2 2	0	0
60	2A	2	Total O 2 2	0	0
60	2A	1	Total O 1 1	0	0
60	2A	1	Total O 1 1	0	0
60	2A	1	Total O 1 1	0	0
60	2A	2	Total O 2 2	0	0
60	2A	4	Total O 4 4	0	0
60	2A	3	Total O 3 3	0	0
60	2A	2	Total O 2 2	0	0
60	2A	2	Total O 2 2	0	0
60	2A	2	Total O 2 2	0	0
60	2A	1	Total O 1 1	0	0
60	2A	5	Total O 5 5	0	0
60	2A	1	Total O 1 1	0	0
60	2A	4	Total O 4 4	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2A	2	Total 2	O 2	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	6	Total 6	O 6	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	2	Total 2	O 2	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2A	1	Total 1	O 1	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	6	Total 6	O 6	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	6	Total 6	O 6	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	6	Total 6	O 6	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2A	2	Total 2	O 2	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	6	Total 6	O 6	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	1	Total 1	O 1	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2A	2	Total 2	O 2	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	5	Total 5	O 5	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2A	4	Total 4	O 4	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	6	Total 6	O 6	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	6	Total 6	O 6	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	6	Total 6	O 6	0	0
60	2A	6	Total 6	O 6	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	6	Total 6	O 6	0	0
60	2A	6	Total 6	O 6	0	0
60	2A	3	Total 3	O 3	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2A	4	Total 4	O 4	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	6	Total 6	O 6	0	0
60	2A	6	Total 6	O 6	0	0
60	2A	6	Total 6	O 6	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	6	Total 6	O 6	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	6	Total 6	O 6	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	3	Total 3	O 3	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2A	4	Total 4	O 4	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	6	Total 6	O 6	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	3	Total 3	O 3	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	6	Total 6	O 6	0	0
60	2A	6	Total 6	O 6	0	0
60	2A	6	Total 6	O 6	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	6	Total 6	O 6	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	6	Total 6	O 6	0	0
60	2A	5	Total 5	O 5	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	4	Total 4	O 4	0	0
60	2A	6	Total 6	O 6	0	0
60	2A	5	Total 5	O 5	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2A	5	Total	O	0	0
			5	5		
60	2A	5	Total	O	0	0
			5	5		
60	2A	4	Total	O	0	0
			4	4		
60	2A	5	Total	O	0	0
			5	5		
60	2A	5	Total	O	0	0
			5	5		
60	2A	4	Total	O	0	0
			4	4		
60	2A	6	Total	O	0	0
			6	6		
60	2A	4	Total	O	0	0
			4	4		
60	2A	4	Total	O	0	0
			4	4		
60	2A	6	Total	O	0	0
			6	6		
60	2A	5	Total	O	0	0
			5	5		
60	2A	5	Total	O	0	0
			5	5		
60	2A	6	Total	O	0	0
			6	6		
60	2A	6	Total	O	0	0
			6	6		
60	2A	6	Total	O	0	0
			6	6		
60	2A	4	Total	O	0	0
			4	4		
60	2A	6	Total	O	0	0
			6	6		
60	2A	5	Total	O	0	0
			5	5		
60	2A	4	Total	O	0	0
			4	4		
60	2A	3	Total	O	0	0
			3	3		
60	2A	5	Total	O	0	0
			5	5		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2A	5	Total	O	0	0
			5	5		
60	2A	5	Total	O	0	0
			5	5		
60	2A	4	Total	O	0	0
			4	4		
60	2A	6	Total	O	0	0
			6	6		
60	2A	6	Total	O	0	0
			6	6		
60	2A	6	Total	O	0	0
			6	6		
60	2A	6	Total	O	0	0
			6	6		
60	2A	5	Total	O	0	0
			5	5		
60	2A	5	Total	O	0	0
			5	5		
60	2A	5	Total	O	0	0
			5	5		
60	2A	6	Total	O	0	0
			6	6		
60	2A	5	Total	O	0	0
			5	5		
60	2A	3	Total	O	0	0
			3	3		
60	2A	6	Total	O	0	0
			6	6		
60	2A	6	Total	O	0	0
			6	6		
60	2A	4	Total	O	0	0
			4	4		
60	2A	2	Total	O	0	0
			2	2		
60	2A	1	Total	O	0	0
			1	1		
60	2A	1	Total	O	0	0
			1	1		
60	2A	4	Total	O	0	0
			4	4		
60	2A	2	Total	O	0	0
			2	2		

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2A	3	Total 3	O 3	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	2	Total 2	O 2	0	0
60	2A	1	Total 1	O 1	0	0
60	2A	6	Total 6	O 6	0	0
60	2A	214	Total 214	O 214	0	0
60	2B	2	Total 2	O 2	0	0
60	2B	3	Total 3	O 3	0	0
60	2B	3	Total 3	O 3	0	0
60	2B	1	Total 1	O 1	0	0
60	2B	2	Total 2	O 2	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2B	2	Total 2	O 2	0	0
60	2B	1	Total 1	O 1	0	0
60	2B	12	Total 12	O 12	0	0
60	2D	1	Total 1	O 1	0	0
60	2D	5	Total 5	O 5	0	0
60	2D	8	Total 8	O 8	0	0
60	2E	4	Total 4	O 4	0	0
60	2E	2	Total 2	O 2	0	0
60	2E	3	Total 3	O 3	0	0
60	2F	8	Total 8	O 8	0	0
60	2I	4	Total 4	O 4	0	0
60	2N	1	Total 1	O 1	0	0
60	2O	1	Total 1	O 1	0	0
60	2P	2	Total 2	O 2	0	0
60	2P	3	Total 3	O 3	0	0
60	2Q	1	Total 1	O 1	0	0
60	2Q	1	Total 1	O 1	0	0
60	2R	1	Total 1	O 1	0	0
60	2R	1	Total 1	O 1	0	0
60	2T	4	Total 4	O 4	0	0
60	2U	2	Total 2	O 2	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2W	4	Total 4	O 4	0	0
60	2X	4	Total 4	O 4	0	0
60	2Z	1	Total 1	O 1	0	0
60	20	6	Total 6	O 6	0	0
60	20	2	Total 2	O 2	0	0
60	20	1	Total 1	O 1	0	0
60	21	8	Total 8	O 8	0	0
60	22	1	Total 1	O 1	0	0
60	22	1	Total 1	O 1	0	0
60	23	1	Total 1	O 1	0	0
60	25	4	Total 4	O 4	0	0
60	27	1	Total 1	O 1	0	0
60	27	2	Total 2	O 2	0	0
60	28	4	Total 4	O 4	0	0
60	29	1	Total 1	O 1	0	0
60	2a	6	Total 6	O 6	0	0
60	2a	4	Total 4	O 4	0	0
60	2a	5	Total 5	O 5	0	0
60	2a	3	Total 3	O 3	0	0
60	2a	2	Total 2	O 2	0	0
60	2a	6	Total 6	O 6	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2a	6	Total 6	O 6	0	0
60	2a	3	Total 3	O 3	0	0
60	2a	5	Total 5	O 5	0	0
60	2a	3	Total 3	O 3	0	0
60	2a	3	Total 3	O 3	0	0
60	2a	5	Total 5	O 5	0	0
60	2a	6	Total 6	O 6	0	0
60	2a	2	Total 2	O 2	0	0
60	2a	2	Total 2	O 2	0	0
60	2a	2	Total 2	O 2	0	0
60	2a	2	Total 2	O 2	0	0
60	2a	5	Total 5	O 5	0	0
60	2a	2	Total 2	O 2	0	0
60	2a	5	Total 5	O 5	0	0
60	2a	2	Total 2	O 2	0	0
60	2a	6	Total 6	O 6	0	0
60	2a	5	Total 5	O 5	0	0
60	2a	4	Total 4	O 4	0	0
60	2a	2	Total 2	O 2	0	0
60	2a	4	Total 4	O 4	0	0
60	2a	6	Total 6	O 6	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2a	6	Total 6	O 6	0	0
60	2a	5	Total 5	O 5	0	0
60	2a	5	Total 5	O 5	0	0
60	2a	2	Total 2	O 2	0	0
60	2a	4	Total 4	O 4	0	0
60	2a	4	Total 4	O 4	0	0
60	2a	4	Total 4	O 4	0	0
60	2a	5	Total 5	O 5	0	0
60	2a	4	Total 4	O 4	0	0
60	2a	2	Total 2	O 2	0	0
60	2a	2	Total 2	O 2	0	0
60	2a	3	Total 3	O 3	0	0
60	2a	6	Total 6	O 6	0	0
60	2a	3	Total 3	O 3	0	0
60	2a	6	Total 6	O 6	0	0
60	2a	2	Total 2	O 2	0	0
60	2a	3	Total 3	O 3	0	0
60	2a	2	Total 2	O 2	0	0
60	2a	2	Total 2	O 2	0	0
60	2a	4	Total 4	O 4	0	0
60	2a	2	Total 2	O 2	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2a	2	Total 2	O 2	0	0
60	2a	1	Total 1	O 1	0	0
60	2a	2	Total 2	O 2	0	0
60	2a	1	Total 1	O 1	0	0
60	2a	5	Total 5	O 5	0	0
60	2a	1	Total 1	O 1	0	0
60	2a	3	Total 3	O 3	0	0
60	2a	1	Total 1	O 1	0	0
60	2a	2	Total 2	O 2	0	0
60	2a	1	Total 1	O 1	0	0
60	2a	2	Total 2	O 2	0	0
60	2a	2	Total 2	O 2	0	0
60	2a	1	Total 1	O 1	0	0
60	2a	1	Total 1	O 1	0	0
60	2a	3	Total 3	O 3	0	0
60	2a	1	Total 1	O 1	0	0
60	2a	3	Total 3	O 3	0	0
60	2a	1	Total 1	O 1	0	0
60	2a	3	Total 3	O 3	0	0
60	2a	3	Total 3	O 3	0	0
60	2a	1	Total 1	O 1	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2a	1	Total 1	O 1	0	0
60	2a	4	Total 4	O 4	0	0
60	2a	4	Total 4	O 4	0	0
60	2a	2	Total 2	O 2	0	0
60	2a	2	Total 2	O 2	0	0
60	2a	2	Total 2	O 2	0	0
60	2a	1	Total 1	O 1	0	0
60	2a	1	Total 1	O 1	0	0
60	2a	1	Total 1	O 1	0	0
60	2a	1	Total 1	O 1	0	0
60	2a	1	Total 1	O 1	0	0
60	2a	1	Total 1	O 1	0	0
60	2a	1	Total 1	O 1	0	0
60	2a	1	Total 1	O 1	0	0
60	2a	2	Total 2	O 2	0	0
60	2a	2	Total 2	O 2	0	0
60	2a	2	Total 2	O 2	0	0
60	2a	2	Total 2	O 2	0	0
60	2a	1	Total 1	O 1	0	0
60	2a	2	Total 2	O 2	0	0
60	2a	2	Total 2	O 2	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2a	1	Total 1	O 1	0	0
60	2a	1	Total 1	O 1	0	0
60	2a	2	Total 2	O 2	0	0
60	2a	1	Total 1	O 1	0	0
60	2a	1	Total 1	O 1	0	0
60	2a	1	Total 1	O 1	0	0
60	2a	1	Total 1	O 1	0	0
60	2a	39	Total 39	O 39	0	0
60	2d	1	Total 1	O 1	0	0
60	2g	1	Total 1	O 1	0	0
60	2g	1	Total 1	O 1	0	0
60	2h	1	Total 1	O 1	0	0
60	2i	1	Total 1	O 1	0	0
60	2i	1	Total 1	O 1	0	0
60	2i	1	Total 1	O 1	0	0
60	2j	2	Total 2	O 2	0	0
60	2j	1	Total 1	O 1	0	0
60	2j	1	Total 1	O 1	0	0
60	2l	1	Total 1	O 1	0	0
60	2l	3	Total 3	O 3	0	0

*Continued on next page...*



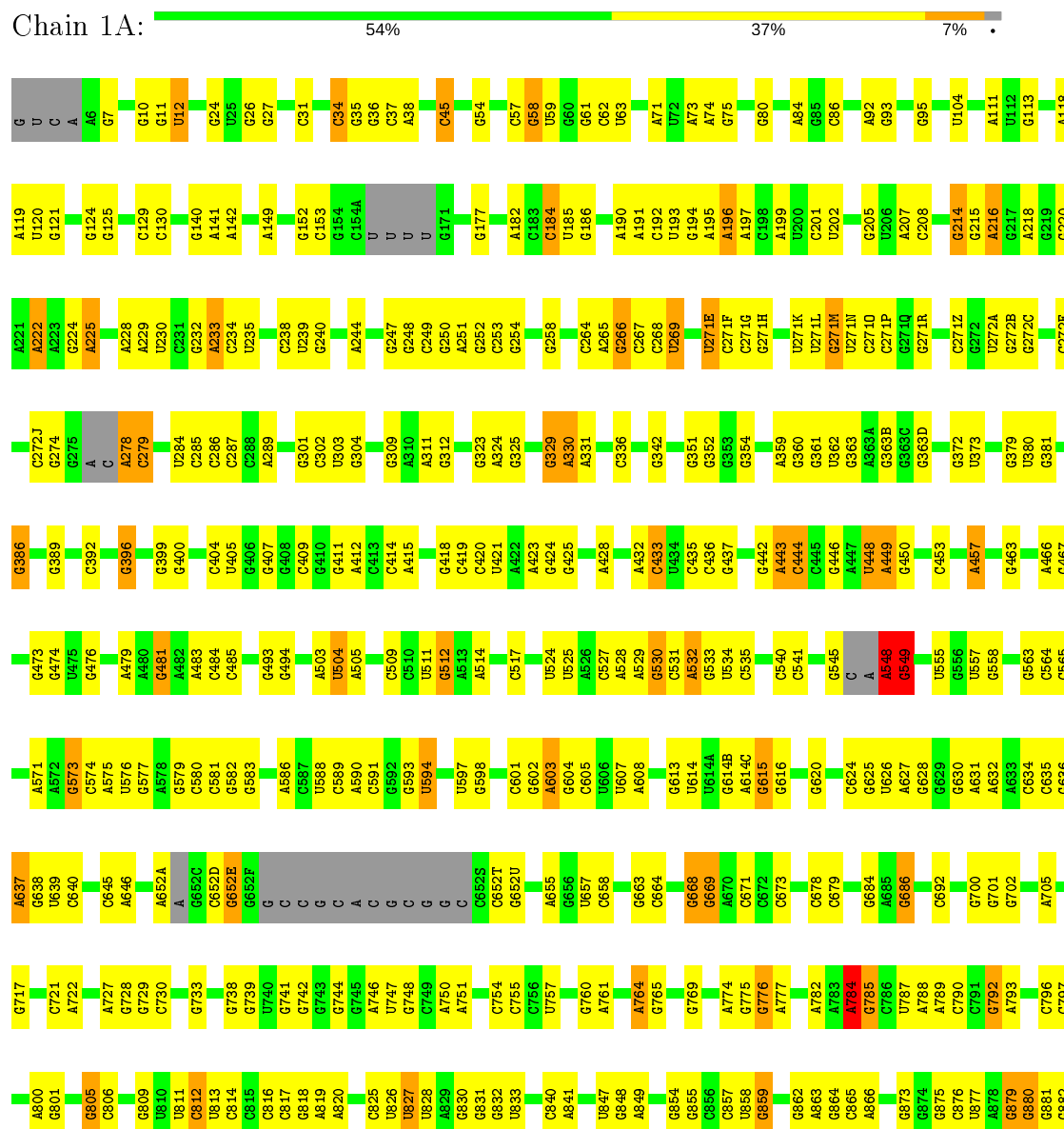
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2p	1	Total 1	O 1	0	0
60	2r	1	Total 1	O 1	0	0
60	2t	2	Total 2	O 2	0	0
60	2v	1	Total 1	O 1	0	0
60	2x	2	Total 2	O 2	0	0
60	2x	2	Total 2	O 2	0	0
60	2x	4	Total 4	O 4	0	0
60	2y	1	Total 1	O 1	0	0
60	2y	10	Total 10	O 10	0	0

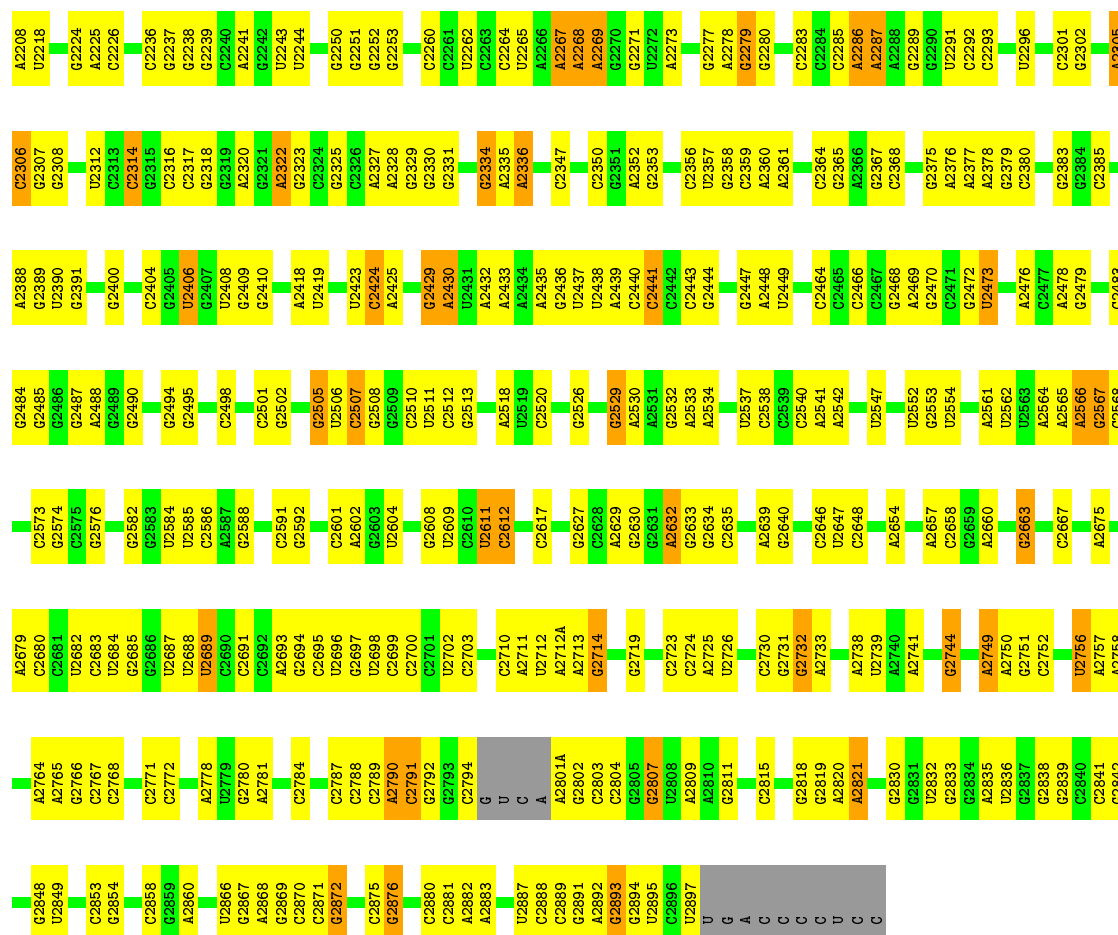
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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

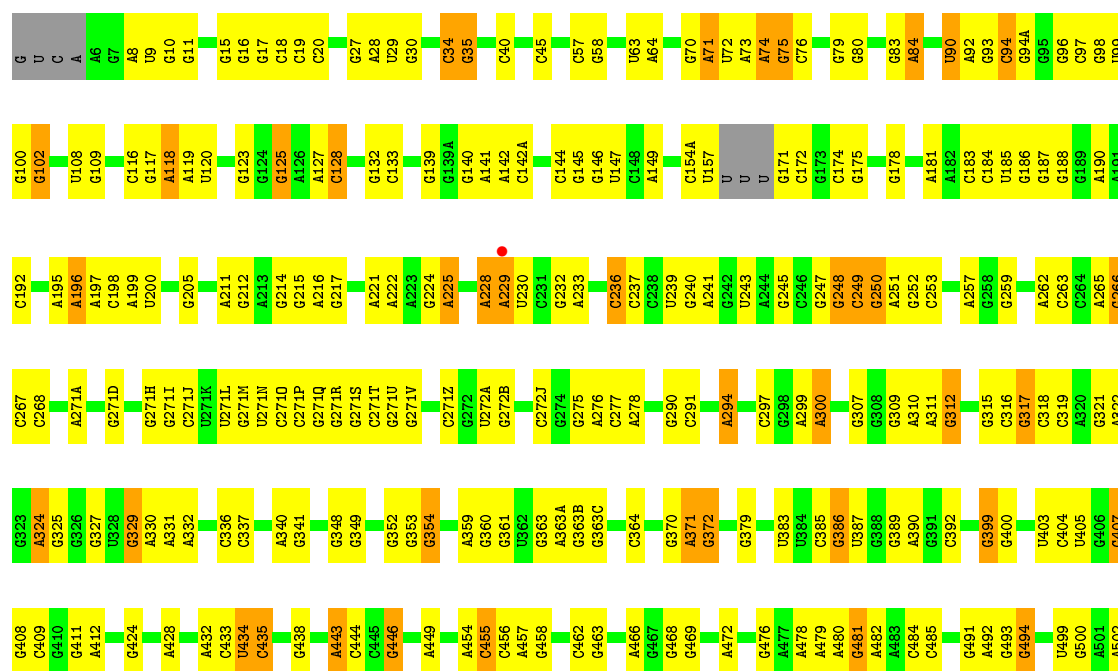


G2141	G2142	G2143	G2144	G2145	G2146	G2147	G2148	G2149	G2150	G2151	G2152	G2153	G2154	G2155	G2156	G2157	G2158	G2159	G2160	G2161	G2162	G2163	G2164	G2165	G2166	G2167	G2168	A2171	U2172	A2173	C2174	C2175	A2176	C2177	C2178	C2179	U2180	G2181	G2182	G2183	G2184	G2185	G2186	G2187	G2188	G2189	G2190	G2193	G2194	A2198	C2202	U2203	G2205	G2206	G2207	
A2060	G2061	A2062		C2065	C2066	G2067	U2068	G2069	G2070	A2071	G2072	G2073	G2074	G2075	G2076	G2077	G2078	U2079	G2080	C2081	U2086	G2087	U2092	C2095	G2096	G2097	U2098	G2100	G2101	U2102	G2103	G2104	C2107	C2108	U2109	G2112	U2113	A2117	G2120	G2124	G2125	A2126	G2127	C2128	C2129	U2130	G2131	U2132	G2133	A2134	A2135	C2136	G2137	C2138	G2139	G2140
U1955	A1956	C1958	U1963	G1964	C1967	A1970	A1971	A1972	G1973	U1991	G1992	U1993	C1994	G1997	G1998	A1999	G2000	A2001	G2002	U2011	G2012	A2013	A2014	G2018	A2019	A2020	C2021	U2022	G2023	G2029	A2030	A2031	G2032	A2033	G2037	U2041	C2042	C2043	G2046	G2053	A2054	C2055	G2056	A2057	G2058	A2198	C2202	U2203	G2205	G2206	G2207					
G1850	A1853	A1854	G1858	A1859	G1860	U1861	U1864	G1865	G1866	A1877	G1878	C1879	G1883	A1889	A1890	G1891	C1892	U1898	G1899	A1900	G1906	A1913	G1914	U1915	A1918	A1919	G1920	G1921	G1922	U1923	C1924	G1925	U1926	A1927	A1928	G1929	U1930	U1931	A1932	G1933	C1934	G1935	A1936	A1937	A1938	U1939	C1942	U1943								
G1750	G1753	G1754	A1755	G1756	A1762	G1763	G1764	G1769	A1773	U1778	U1779	A1780	C1781	A1782	A1783	A1784	A1785	A1786	A1789	C1790	A1791	G1792	U1796	C1797	U1798	G1799	C1800	G1801	C1804	A1810	G1811	A1812	A1815	G1817	A1825	G1826	C1827	C1830	G1843	C1844	A1847	A1848	G1849													
G1641	G1642	C1646	U1647	C1648	G1649	G1650	G1651	G1652	G1653	A1654	C1658	U1659	A1665	G1666	G1667	A1668	A1669	G1674	A1675	A1676	C1684	C1685	C1686	G1687	U1688	A1689	A1690	C1691	U1692	U1693	C1694	G1695	A1700	G1703	C1710	C1711	C1712	U1720	G1721	A1722	U1739	G1740	A1741	G1742	G1746	G1747	G1748									
G1525	C1532	G1533	U1534	A1535	C1537	G1541	A1542	C1546	A1554	G1555	A1558	G1559	A1566	A1567	G1568	A1569	A1570	A1571	U1578	A1579	A1580	C1584	A1586	A1587	C1588	C1589	G1593	G1594	G1595	A1603	A1608	A1609	A1610	C1611	C1612	G1613	A1614	C1615	G1622	G1628	U1629	A1634														
G1422	G1423	G1426	A1427	C1428	G1429	C1430	U1438	G1441	G1442	A1445	G1448	A1449	G1450	U1453	G1455	G1459	A1460	G1461	G1466	C1467	A1471	G1478	G1482	A1486	G1487	A1490	C1493	A1494	A1495	A1496	U1497	C1504	C1505	C1506	A1507	A1508	C1509	A1509A	A1509B	U1514	U1518	G1519														
U1329	G1337	G1338	G1339	A1342	G1343	G1344	U1352	G1358	A1359	A1360	G1361	C1362	C1363	G1364	A1365	A1366	G1371	U1372	A1373	G1374	C1376	A1379	G1380	A1384	G1385	A1386	U1390	U1391	A1392	A1393	A1394	A1395	U1396	U1397	C1398	U1405	U1406	C1407	C1408	C1409	G1410	C1411	G1416	G1417	G1418	A1419	A1420	G1421								
U1188	A1189	C1200	C1201	C1202	G1206	A1210	U1211	G1212	C1218	G1223	A1226	C1230	G1231	G1236	G1239	U1240	A1241	G1252	A1253	G1256	G1266	U1267	A1268	A1269	C1270	G1271	A1272	U1273	A1286	U1292	C1293	C1297	U1300	A1301	A1302	G1310	U1313	C1314	C1315	G1318																
G1112	U1113	G1114	G1115	C1116	G1117	C1118	C1119	C1123	A1126	G1127	G1128	A1129	C1136	G1137	G1138	G1144	C1145	C1146	C1147	G1151	C1152	C1153	G1154	A1155	A1156	U1159	G1160	C1161	G1164	U1165	U1167	G1168	G1169	G1170	G1171	A1173	U1174	U1175	G1176	A1177	C1178	C1179	C1180	G1183	G1184	G1185	G1186	G1187								
G983	C984	C985	C986	A987	C988	C989	A990	C992	C993	U994	G995	A996	A1000	A1001	G1002	G1003	C1006	C1007	A1008	A1009	A1010	G1011	U1012	C1013	U1014	G1015	A1016	G1017	C1018	A1021	G1024	G1025	U1026	A1027	G1030	G1031	A1032	U1033	G1034	G1035	G1036	A1039	C1040	A1041	G1042	G1043	G1044	A1045	A1046	G1047	A1048	G1049				



• Molecule 1: 23S Ribosomal RNA

Chain 2A:  47% 40% 8% •



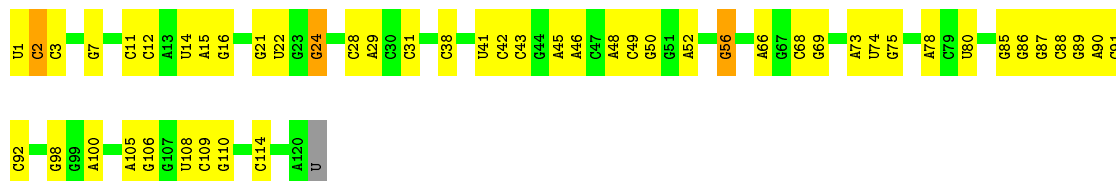
C1557	A1469	G1206	C1135	G1011	A941	A861	G785	A706	G652	C581	A503
A1558	G1470	A1210	G1156	U1012	G942	G862	A788	G707	A652A	G582	U504
A1566	A1471	G1211	G1137	C1013	G943	A863	A789	U709	A652B	A586	A505
G1567	G1400	G1212	G1138	U1014	A945	G864	G790	G708	G652C	G587	G506
A1569	G1401	A1213	C1139	G1015	G946	C865	G791	G710	C652D	U588	C509
A1570	U1405	A1214	G1140	G1016	G947	A866	G792	G711	G652E	C589	C510
A1571	U1406	U1141	U1142	G1017	G948	G869	A793	G715	G	U511	U512
U1578	C1407	C1218	A1142A	U1019	A953	G874	G796	A716	G	G592	G513
A1579	C1408	G1223	A1143	G1022	G954	G875	C797	G717	C	C595	A514
A1580	C1409	G1224	A1144	U1023	C955	G876	A800	C720	G	G596	A515
G1581	G1411	G1225	G1149	G1024	G956	U877	G801	C721	A	U597	C517
C1584	C1416	A1226	C1150	G1025	A957	A878	A802	A722	C	G599	G521
A1586	G1417	G1229	G1151	U1026	U958	G879	G805	C723	G	G602	U524
U1590	C1417	G1230	C1152	A1027	A959	G880	G806	U724	G	A603	U525
G1591	U1420	G1231	G1153	U1028	G960	G881	G807	G726	G	G604	A526
G1592	G1421	G1232	A1155	A1029	C961	G882	U807	G729	C	C605	C527
G1593	G1422	G1236	C1158	G1030	G966	G883	U811	C731	G	U606	A528
A1594	G1423	G1239	G1159	G1031	C967	C885	C812	C732	G	A608	A529
G1595	G1424	G1241	U1165	U1032	G970	C886	G817	C733	A	G530	C531
A1596	A1427	A1242	C1166	U1033	C971	A887	A819	A734	C	C612	A532
C1599	C1428	G1243	U1167	G1034	G972	C888	G818	U740	G	U614A	U534
A1603	G1429	G1244	C1168	U1035	A973	G889	A820	G741	G	G614B	C535
C1604	C1430	G1245	G1169	G1036	C975	A890	A821	G742	G	A614C	A536
A1608	U1431	G1246	G1170	U1037	G977	U895	G823	G746	G	G615	G545
A1609	A1434	A1247	G1171	C1038	G978	A896	U827	U747	G	G619	C
A1610	C1437	G1248	G	U1041	A980	C897	U828	U750	A	G620	A
C1611	G1442	A1253	A	G1042	A989	A899	A829	A751	G	A621	G549
A1614	G1443	G1256	U	C1043	A983	A900	G832	A752	C	C624	G551
C1615	G1444	C1257	C1178	U1044	C985	A901	U833	C753	G	U627	U554
G1630	C1445A	G1258	C1179	G1045	C986	C903	C834	C754	G	G628	U555
A1632	G1446	G1259	C1180	G	G987	C904	A835	C755	G	G629	G556
G1633	G1447	G1260	G1183	A	A988	U907	G836	G760	G	G630	G561
A1634	G1448	U1263	G1184	C	C992	U839	U839	G763	A	A631	U562
G1635	A1449	G1264	C1185	U1112	G993	A910	C840	A764	G	A632	G563
C1636	G1450	A1265	G1186	G1115	C994	C914	A841	G765	G	G634	U566
A1637	C1450A	G1266	G1187	C1116	C995	C915	G845	C766	G	A637	A567
U1647	C1451	G1271	U1188	G1117	A996	G916	U847	G771	G	U638	U568
C1648	U1453	A1272	A1189	U	C998	A917	G848	G774	G	C640	G569
A1651	G1455	U1273	G1190	C1121	U999	A918	A849	G775	G	G641	G570
A1652	G1456	A1274	G1192	G	A1000	G919	C850	G776	G	G642	A571
G1653	C1457	G1277	C1193	C1122	A1001	U922	U851	A777	G	A643	A572
A1654	A1458	A1278	G1194	C1123	G1002	C923	G854	G778	G	A644	C574
C1655	A1459	G1286	U1195	C1124	U1003	C924	G855	U779	G	G645	U576
G1656	A1460	A1287	U1199	A1127	C1005	G856	C857	G780	G	G646	A577
C1662	C1461	U1288	C1202	A1129	G1006	G928	U858	A781	G	G648	G577
C1663	G1462	G1297	G1203	U1130	C1007	G932	A782	A783	G	G649	A578
	C1463		U1205	G1131	A1008	G938	U860	A784	G	G650	C580
	G1464				A1010						
	G1465										
	G1466										
	G1467										
	C1468										

C2768	C2699	A2459	A2378	G2308	G2223	C2141	U2068	U1991	C1890	A1780	A1664
C2769	U2702	U2460	G2379	A2309	G2224	C2142	G2069	U1992	A1890	C1781	A1668
A	C2703	C2461	C2380	U2312	C2226	U2144	A2071	U1993	C1893	C1782	
C2792	A2711	C2465	G2382	C2317	A2227	C2146	C2072	C1996	C1894	A1785	U1671
C2793	U2712	C2466	G2383	G2318	G2230	C2147	C2073	C1997	C1895	A1786	C1672
C2794	A2712A	U2468	G2384	G2319	G2233	C2148	U2074	G1998	C1896	U1673	
G	U2713	A2469	C2385	A2320	G2234	G2149	U2075	U1999	C1897	G1674	
U	G2714	A2470	G2388	A2321	G2235	G2150			C1898	C1683	
C	C2715	C2471	G2389	A2322	G2236	G2151	U2079	A2001	G1899	A1791	
A	C2716	C2472	G2390	G2323	G2238	G2152	U2089	G2002	C1684	C1792	
A2801A	U2717	U2473	A2392	C2324	G2239	G2153			C1685	C1793	
C2802	G2717	C2474	A2393	G2325	C2240	G2154	U2092	G2010	C1686	U1794	
C2803	U2718	C2475	A2396	G2326	G2241	G2155	G2093	G2011	C1687	C1795	
C2804	G2719	A2476	G2397	C2327	G2242	G2156	U2094	A2012	U1796	U1796	
C2805	U2720	C2477	C2403	A2328	G2243	G2157	C2095	A2013	C1797	U1688	
C2806	A2721	C2478	U2406	G2329	U2245	G2158	U2096	A2014	U1798	U1689	
U2808	G2722	C2479	U2406	G2330	G2246	G2159	U2099	U2017	G1799	U1693	
C2809	C2723	C2480	U2406	G2331	G2247	G2160	U2099	G2018	C1800		
A2810	C2724	U2481	U2406	G2332	G2248	G2161	G2100	A2019	G1801		
G2811	A2725	C2482	G2410	G2334	U2249	G2162	G2101	A2020	A1802		
	U2726	C2483	U2418	G2335	G2250	G2163	U2102	C2021	A1803		
C2815	G2727	C2484	U2419	A2336	G2251	G2164	C2103	U2022	U1808		
C2816		U2485	U2420	A2337	G2252	G2165	C2104	G2023	A1809		
C2817	G2732	C2486	U2425	G2338		G2166	U2099	G2024	A1810		
C2818	A2733	U2487	A2426	C2342	C2261	U2167	G2106	C2025	A1927		
C2819	G2734	C2488	A2427	G2343	U2262	G2168	C2107	A2026	A1928		
A2820	A2735	C2489	G2428	G2344	C2263	A2169	C2108	G2027	U1709		
A2821	C2736	U2490	G2429	G2345	G2264	A2170	U2109	U2028	C1710		
C2822		C2491	A2430	U2346	U2271	A2171	G2110	G2029	G1816		
A2823	U2739	C2492	U2431	G2347	U2272	U2172	C2111	A2030	G1817		
	A2740	U2493	G2432	U2348	A2273	U2173	G2112	A2031	U1818		
A2835	G2744	C2494	G2433	G2349	C2274	C2174	U2113	A2032	G1824		
U2836	C2745	U2495	A2434	G2350	U2275	A2175	U2114	A2033	A1825		
C2837	G2746	C2496	A2435	G2351	C2276	G2176	G2115	U2034	G1826		
C2838		U2497	A2439	G2352	G2277	C2177	G2116	G2035	C1827		
C2839	A2748	C2498	U2440	U2357	U2278	C2178		G2036	G1740		
C2840	U2751	U2504	C2441	G2358	G2281	C2179	A2119	G2037			
C2841	C2752	C2505	C2442	G2359	G2282	C2185	G2120	U1943	G1839		
G2842		U2506	C2443	U2357	C2283	G2186	G2121	A1953	G1746		
	G2759	C2512	G2444	G2358	A2286	G2187	U2122	G1954	G1753		
G2845	U2764	G2513	C2445	G2359	A2287	G2188	G2123	U1955	C1754		
G2846	A2765	C2514	C2446	A2361	U2290	U2189	G2124	A1960	A1756		
U2847	G2766	U2515	G2447	G2364	U2291	G2190	A2126	G2049	U1757		
G2848	C2767	C2516	G2448	G2365	C2292	G2191	G2127	C2050	G1857		
U2849	U2768	U2517	G2449	G2366	G2293	G2192	C2128	A2051	G1858		
A2851	C2769	C2518	G2450	G2367	C2294	G2193	C2129	G1965	A1859		
	G2770	U2519	G2451	G2368	C2295	G2194	U2130	A1966	G1860		
G2857		U2520	G2452	U2368	U2296	G2198	G2131	G2056	G1764		
C2858	A2778	C2521	G2453	A2369	U2297	A2199	G2132	A2059	U1864		
G2859	U2779	U2522	G2454	G2370	C2297	A2199	U2133	A2060	A1877		
A2860	C2780	C2523	G2455	G2371	A2298	C2200	G2134	G2061	A1772		
	A2781	U2524	G2456	G2372	G2302	G2206	A2135	A2062	C1879		
G2867	G2782	C2525	G2457	G2373	G2303	G2207	C2136		G1776		
C2868		U2526	G2458	C2374	G2304	A2208	C2137	G2065	G1883		
	C2785	C2527	G2459	A2375	A2305	U2218	C2138	C2066	U1777		
G2870	U2786	U2528	U2457	A2376			C2139	C1982	A1884		
C2871		G2529	U2457	A2377			C2140	G1984	U1778		
G2872	G2787	U2530	G2458	A2377					U1779		



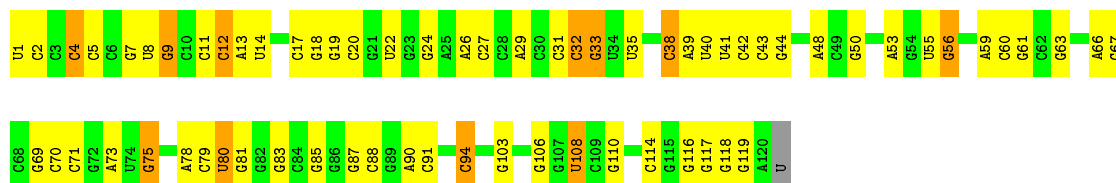
• Molecule 2: 5S Ribosomal RNA

Chain 1B: 58% 39%



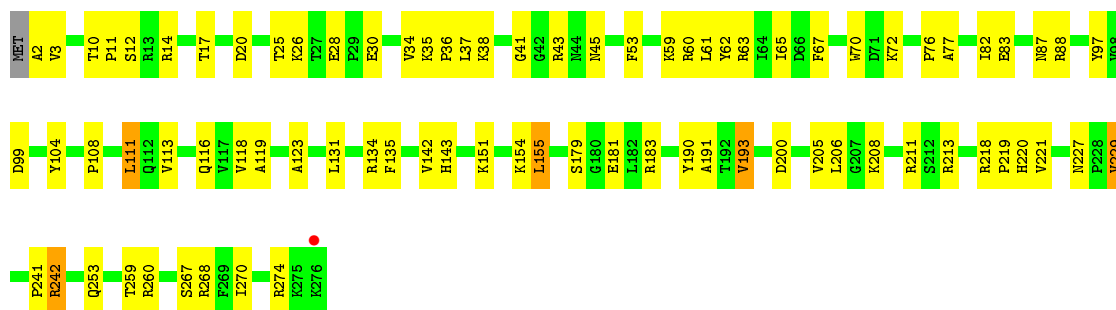
• Molecule 2: 5S Ribosomal RNA

Chain 2B: 44% 46% 9%



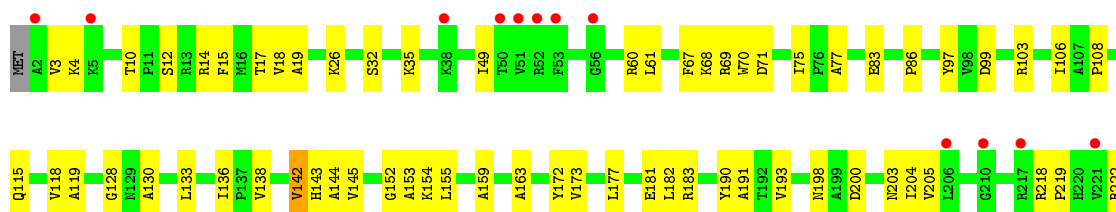
• Molecule 3: 50S ribosomal protein L2

Chain 1D: 70% 28%



• Molecule 3: 50S ribosomal protein L2

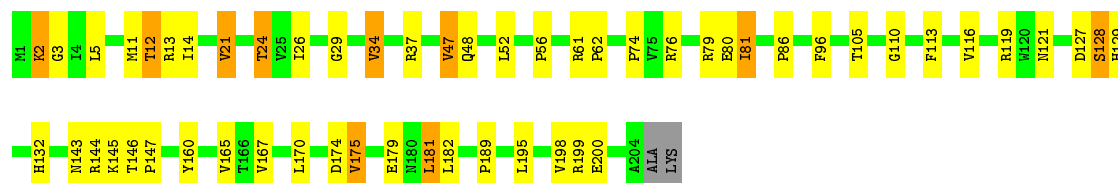
Chain 2D: 5% 72% 27%





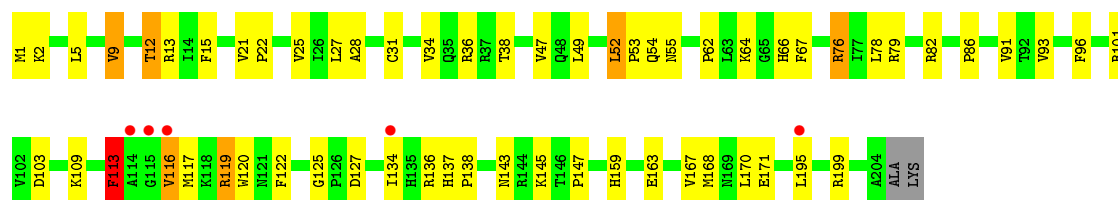
• Molecule 4: 50S ribosomal protein L3

Chain 1E: 72% 22% 5%



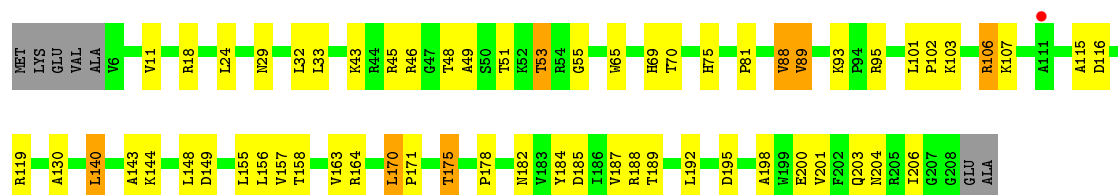
• Molecule 4: 50S ribosomal protein L3

Chain 2E: 2% 70% 26%



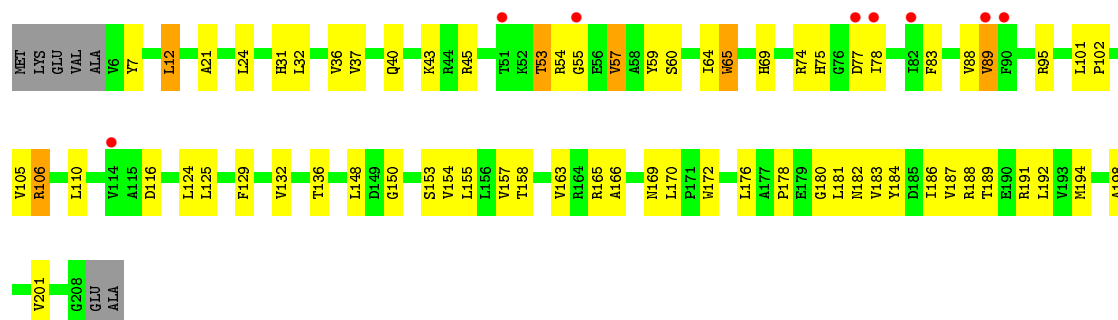
• Molecule 5: 50S ribosomal protein L4

Chain 1F: 68% 26%



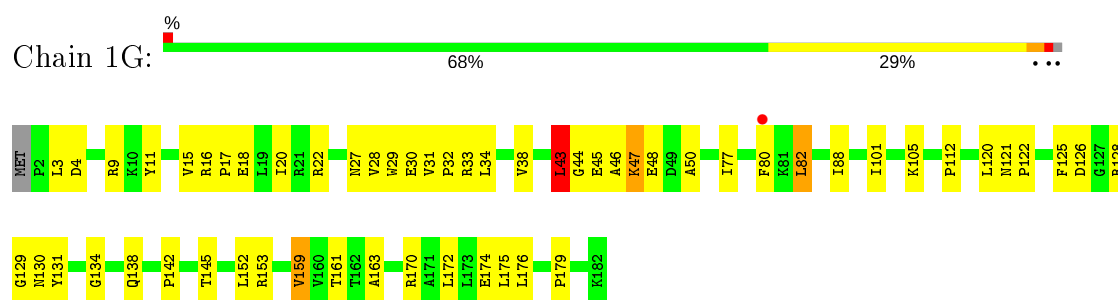
• Molecule 5: 50S ribosomal protein L4

Chain 2F: 4% 64% 30%

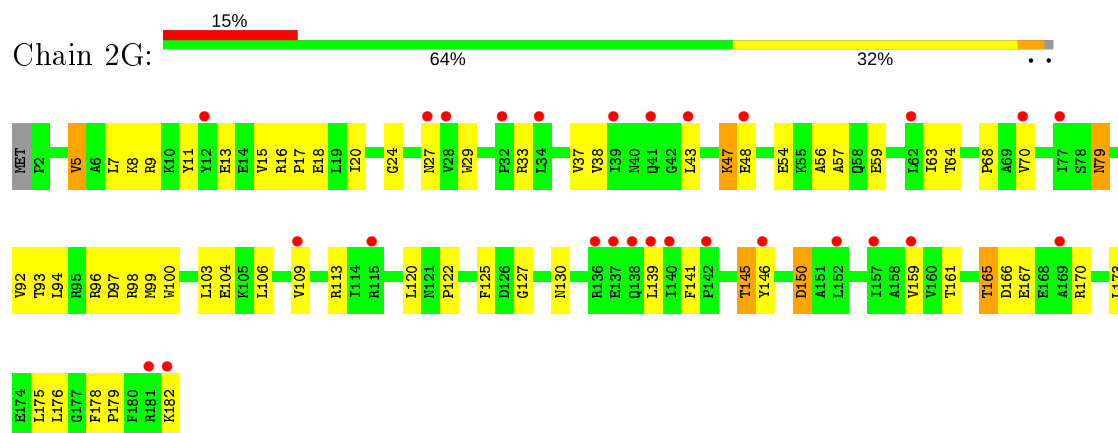


• Molecule 6: 50S ribosomal protein L5

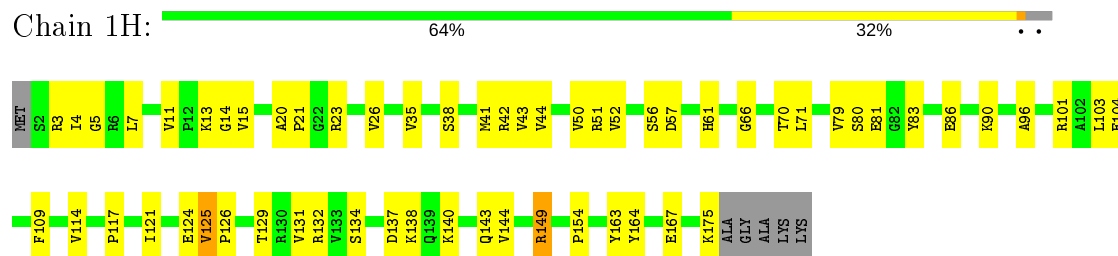




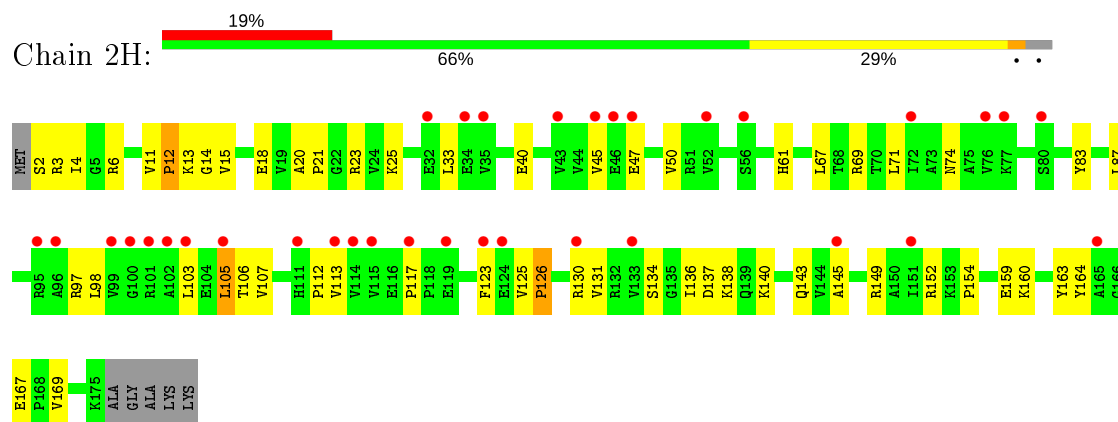
• Molecule 6: 50S ribosomal protein L5



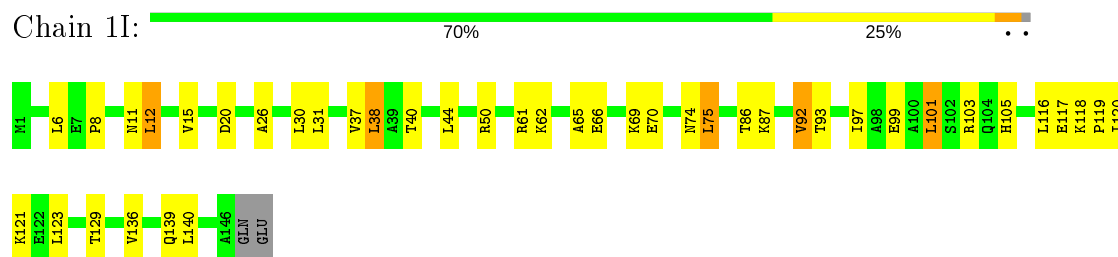
• Molecule 7: 50S ribosomal protein L6



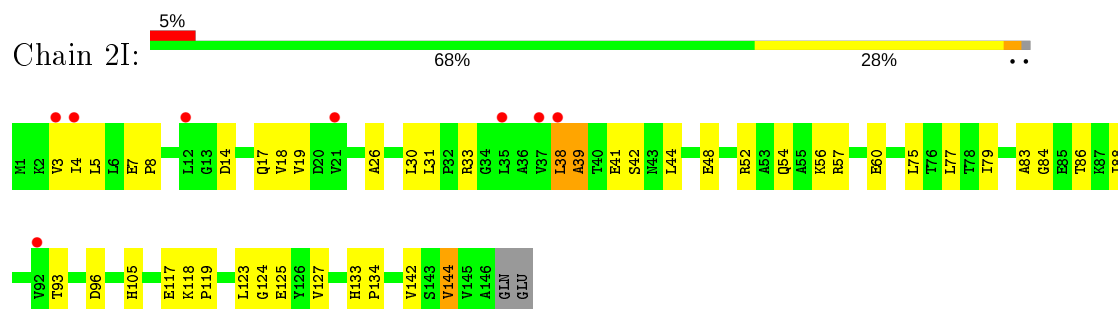
• Molecule 7: 50S ribosomal protein L6



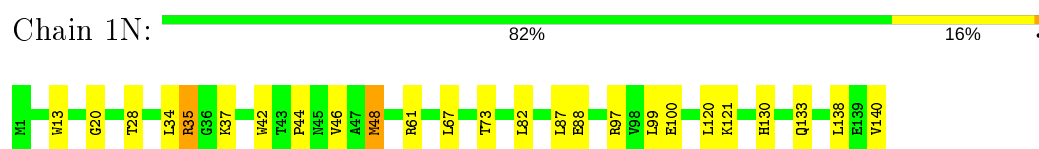
• Molecule 8: 50S ribosomal protein L9



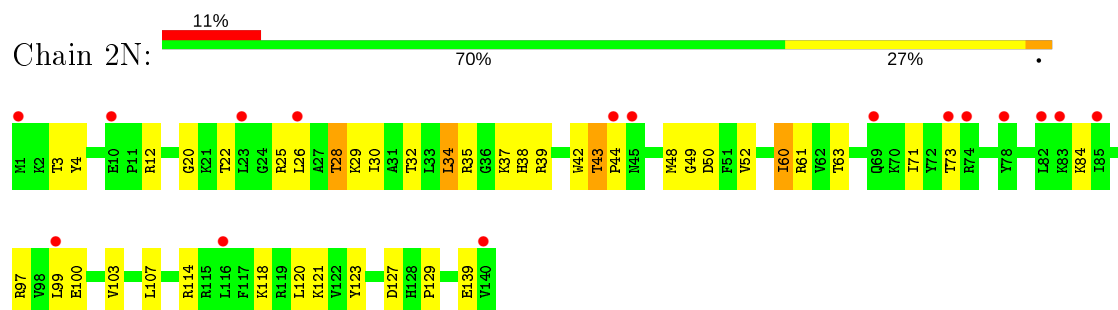
- Molecule 8: 50S ribosomal protein L9



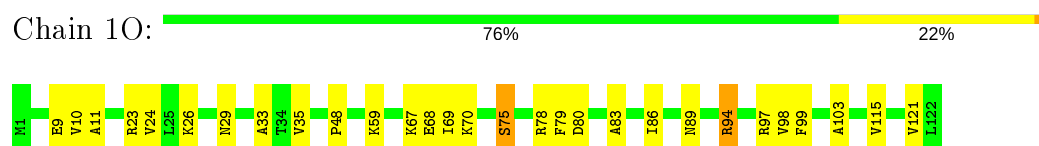
- Molecule 9: 50S ribosomal protein L13



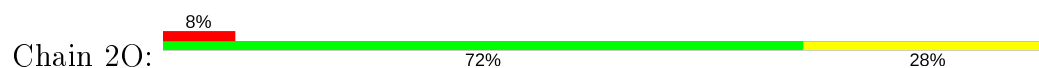
- Molecule 9: 50S ribosomal protein L13

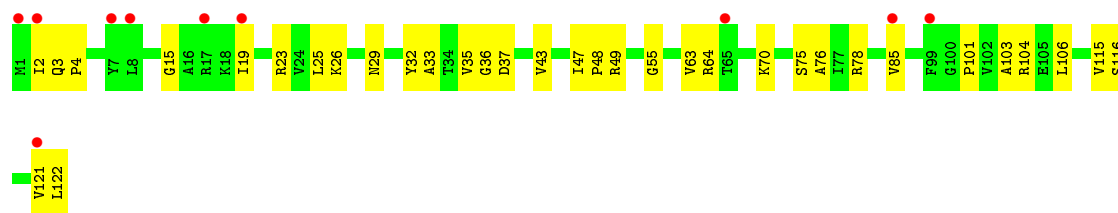


- Molecule 10: 50S ribosomal protein L14

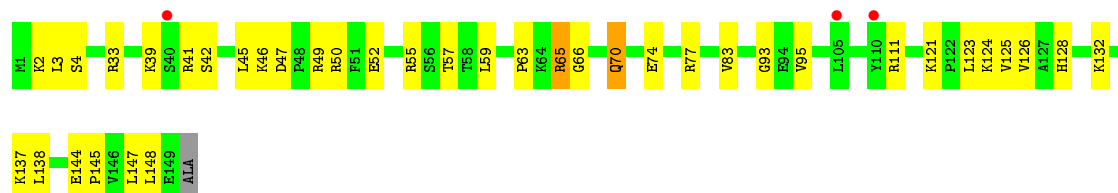
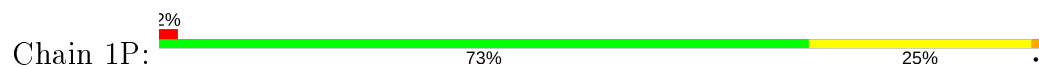


- Molecule 10: 50S ribosomal protein L14

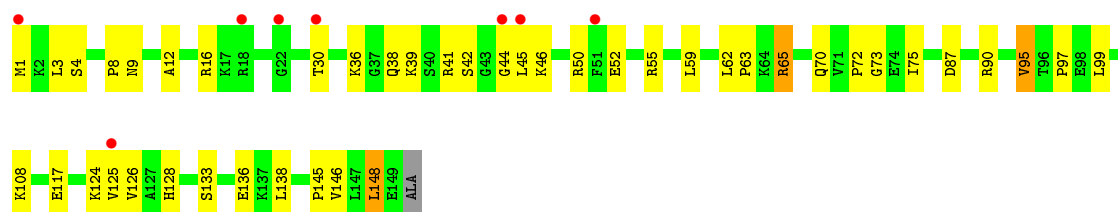




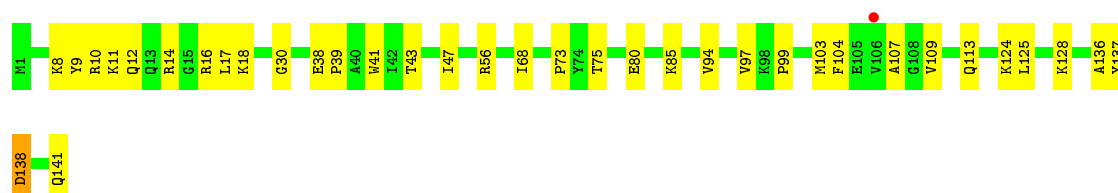
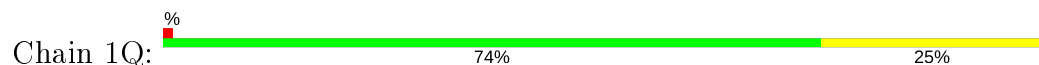
• Molecule 11: 50S ribosomal protein L15



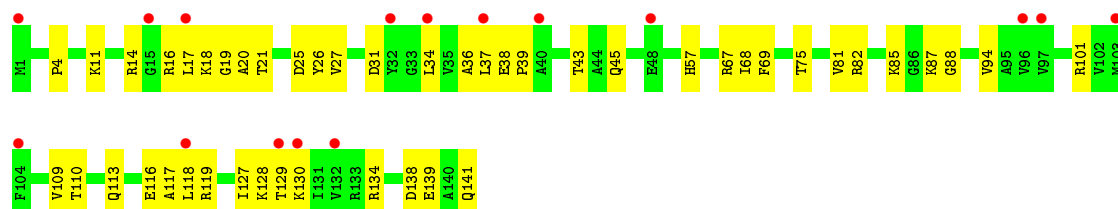
• Molecule 11: 50S ribosomal protein L15




• Molecule 12: 50S ribosomal protein L16

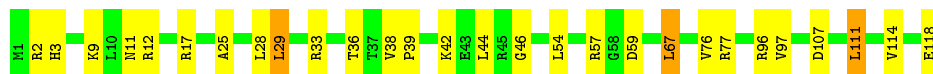


• Molecule 12: 50S ribosomal protein L16



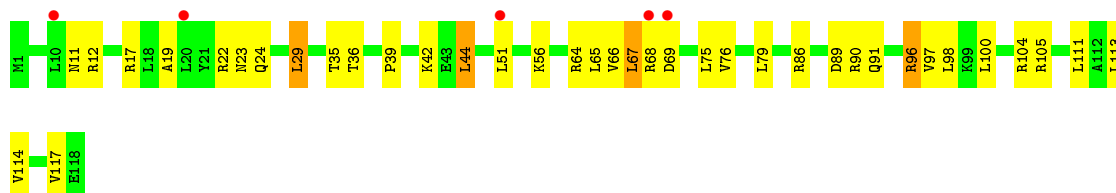
- Molecule 13: 50S ribosomal protein L17

Chain 1R:  76% 21% .



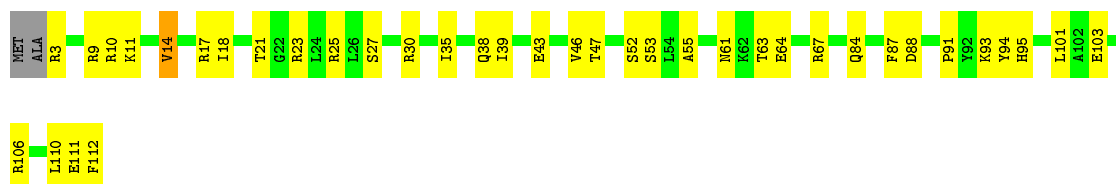
- Molecule 13: 50S ribosomal protein L17

Chain 2R:  4% 68% 29% .



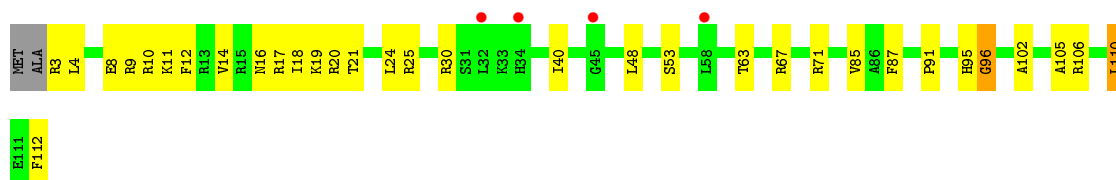
- Molecule 14: 50S ribosomal protein L18

Chain 1S:  64% 33% ..



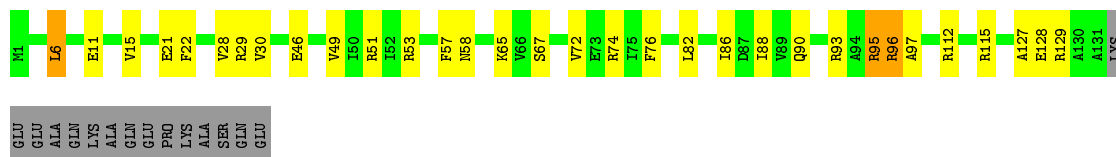
- Molecule 14: 50S ribosomal protein L18

Chain 2S:  4% 69% 28% ..



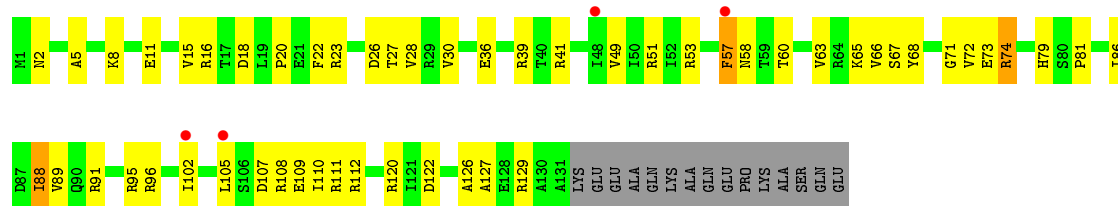
- Molecule 15: 50S ribosomal protein L19

Chain 1T:  68% 20% 10% .

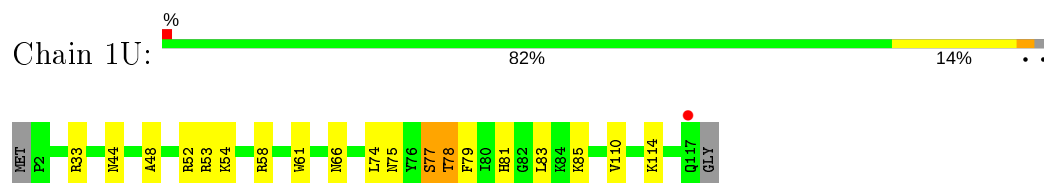


- Molecule 15: 50S ribosomal protein L19

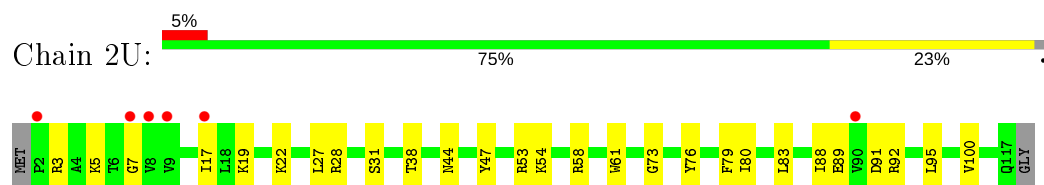
Chain 2T:  3% 53% 34% 10% .



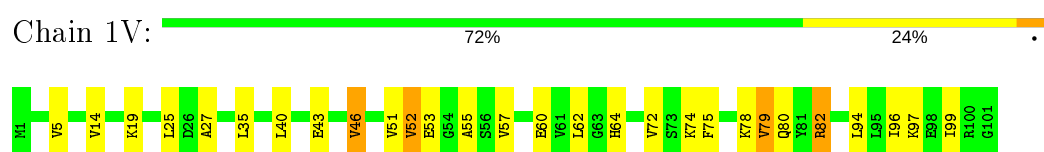
• Molecule 16: 50S ribosomal protein L20



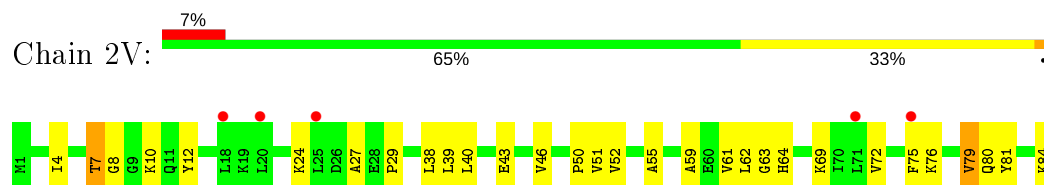
• Molecule 17: 50S ribosomal protein L21



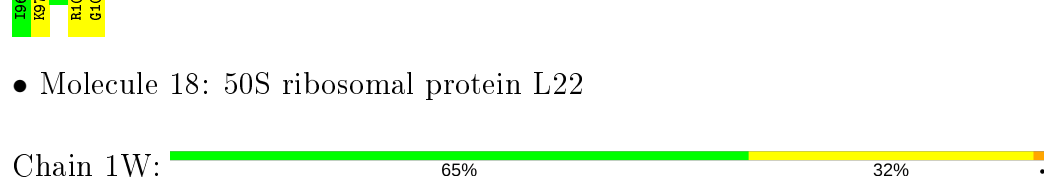
• Molecule 18: 50S ribosomal protein L22



• Molecule 19: 50S ribosomal protein L23



• Molecule 20: 50S ribosomal protein L24

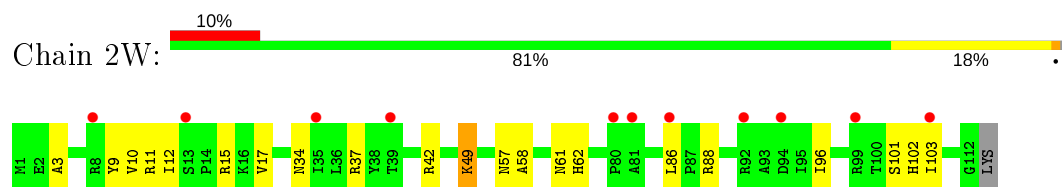


• Molecule 21: 50S ribosomal protein L25

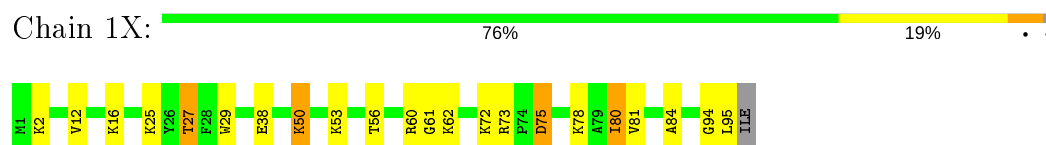


• Molecule 22: 50S ribosomal protein L26

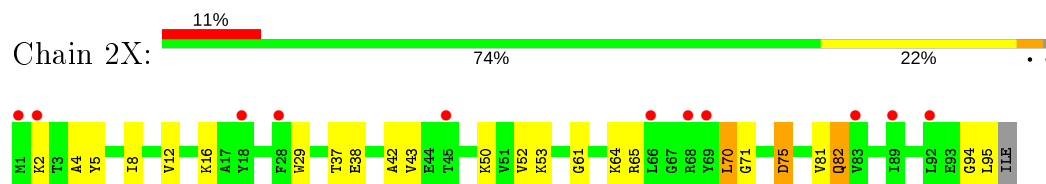
- Molecule 18: 50S ribosomal protein L22



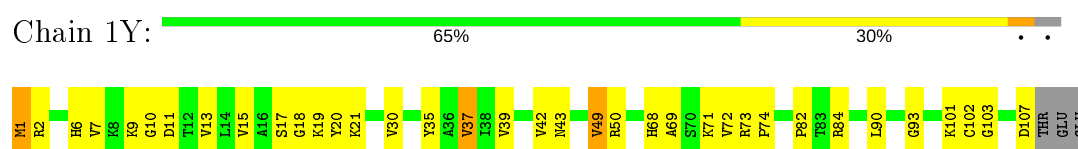
- Molecule 19: 50S ribosomal protein L23



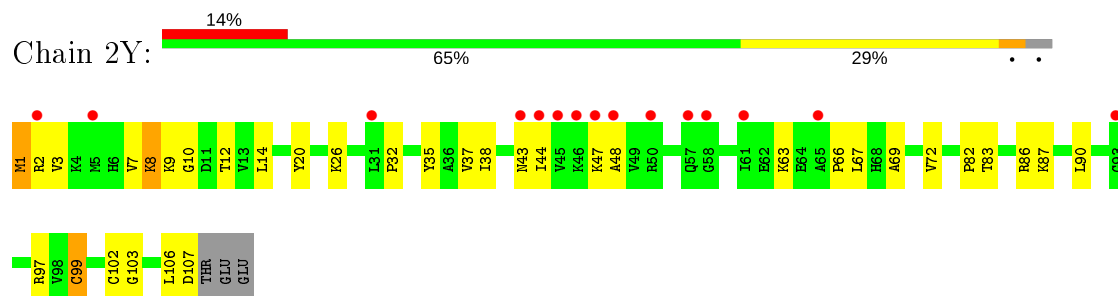
- Molecule 19: 50S ribosomal protein L23



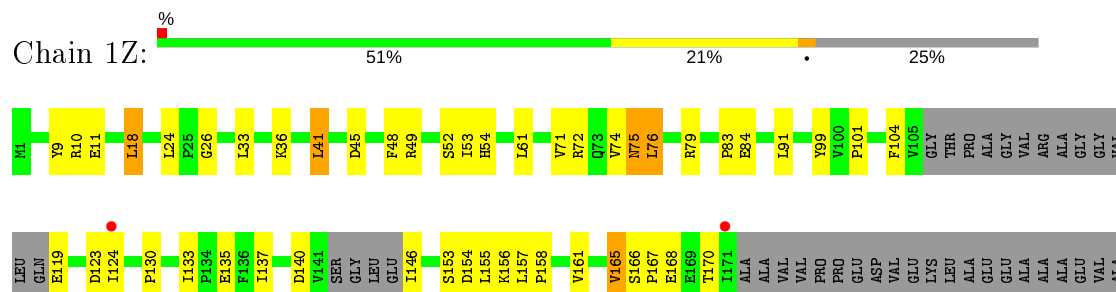
- Molecule 20: 50S ribosomal protein L24



- Molecule 20: 50S ribosomal protein L24

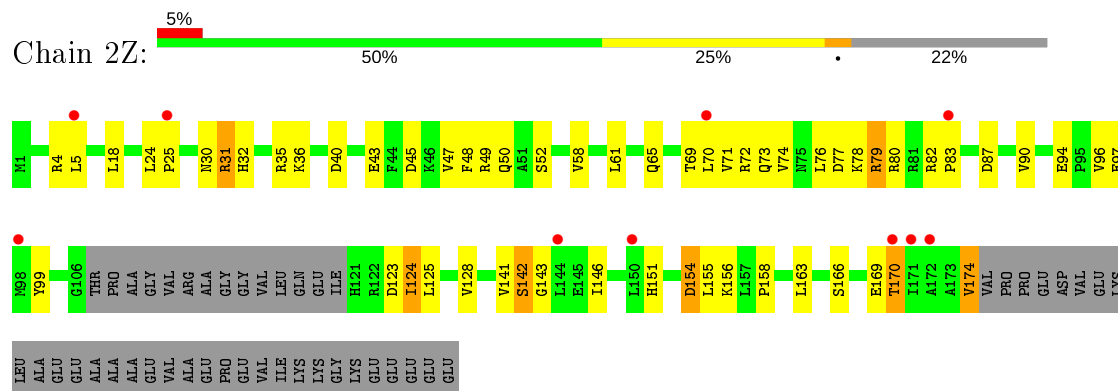


- Molecule 21: 50S ribosomal protein L25

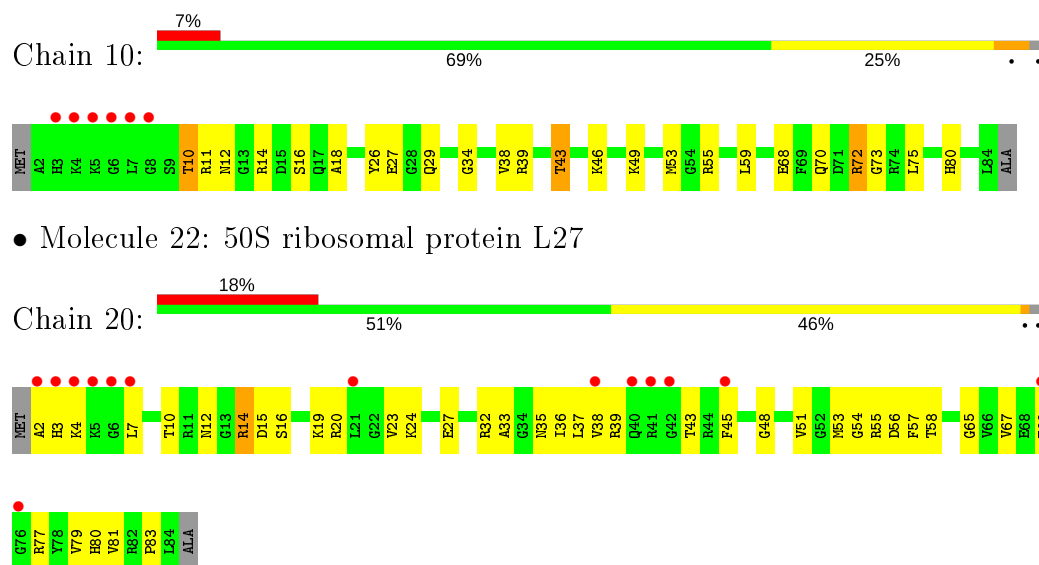


GLU  
PRO  
GLU  
VAL  
ILE  
LYS  
LYS  
GLY  
LYS  
GLU  
GLU  
GLU  
GLU

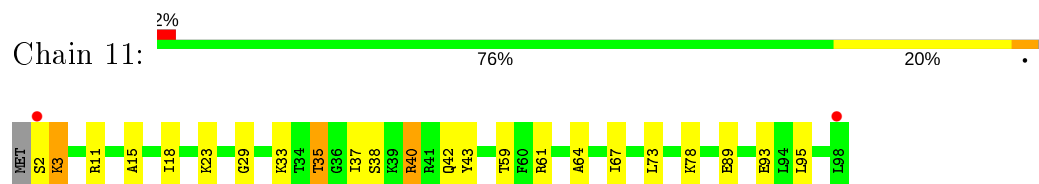
- Molecule 21: 50S ribosomal protein L25



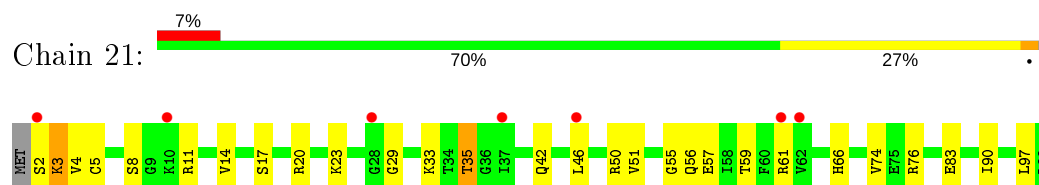
- Molecule 22: 50S ribosomal protein L27



- Molecule 23: 50S ribosomal protein L28

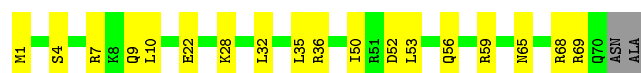


- Molecule 23: 50S ribosomal protein L28




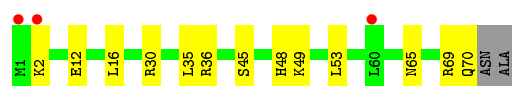
- Molecule 24: 50S ribosomal protein L29

Chain 12:  72% 25%



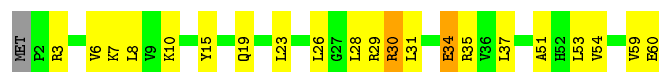
- Molecule 24: 50S ribosomal protein L29

Chain 22:  4% 79% 18%



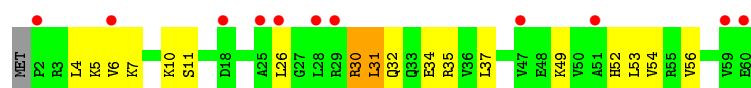
- Molecule 25: 50S ribosomal protein L30

Chain 13:  63% 32%



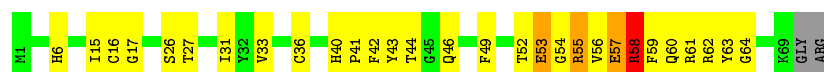
- Molecule 25: 50S ribosomal protein L30

Chain 23:  18% 68% 27%



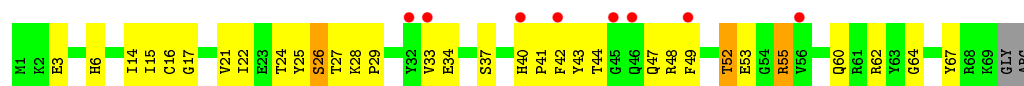
- Molecule 26: 50S ribosomal protein L31

Chain 14:  56% 35%



- Molecule 26: 50S ribosomal protein L31

Chain 24:  11% 52% 41%



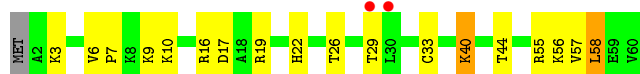
- Molecule 27: 50S ribosomal protein L32

Chain 15:  80% 13% 5%



- Molecule 27: 50S ribosomal protein L32





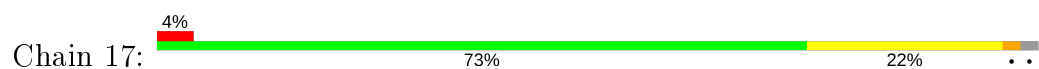
- Molecule 28: 50S ribosomal protein L33



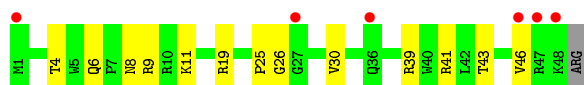
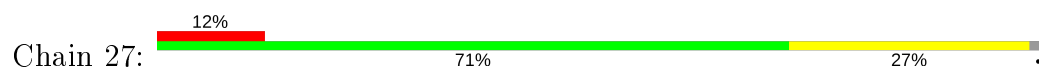
- Molecule 28: 50S ribosomal protein L33



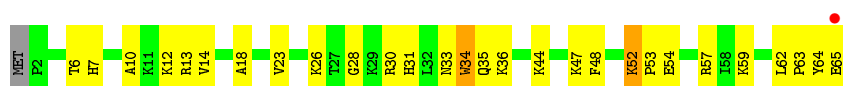
- Molecule 29: 50S ribosomal protein L34



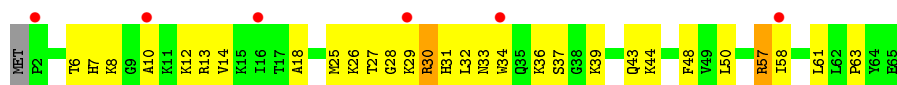
- Molecule 29: 50S ribosomal protein L34



- Molecule 30: 50S ribosomal protein L35

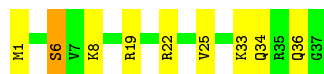


- Molecule 30: 50S ribosomal protein L35



- Molecule 31: 50S ribosomal protein L36

Chain 19:  76% 22%




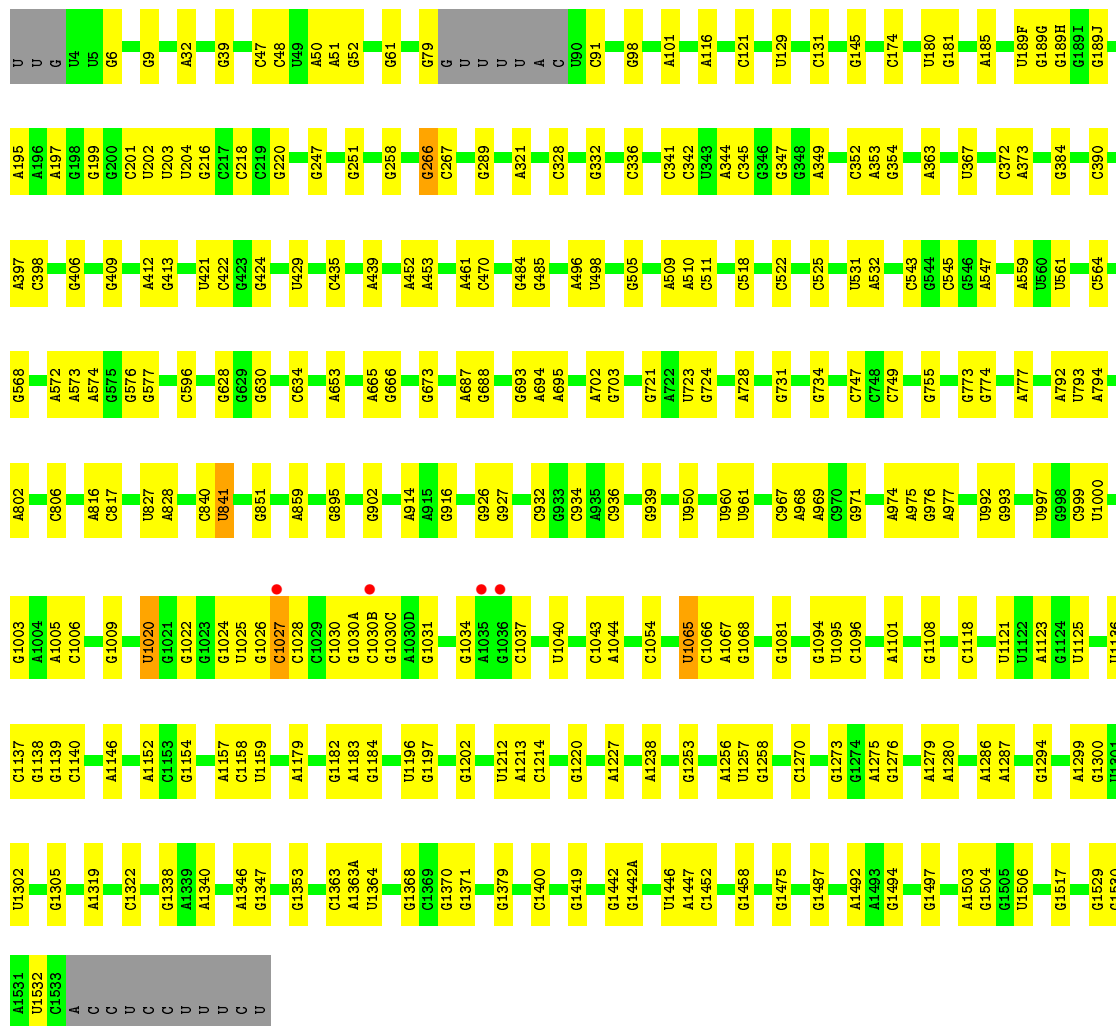
- Molecule 31: 50S ribosomal protein L36

Chain 29:  32% 62% 38%

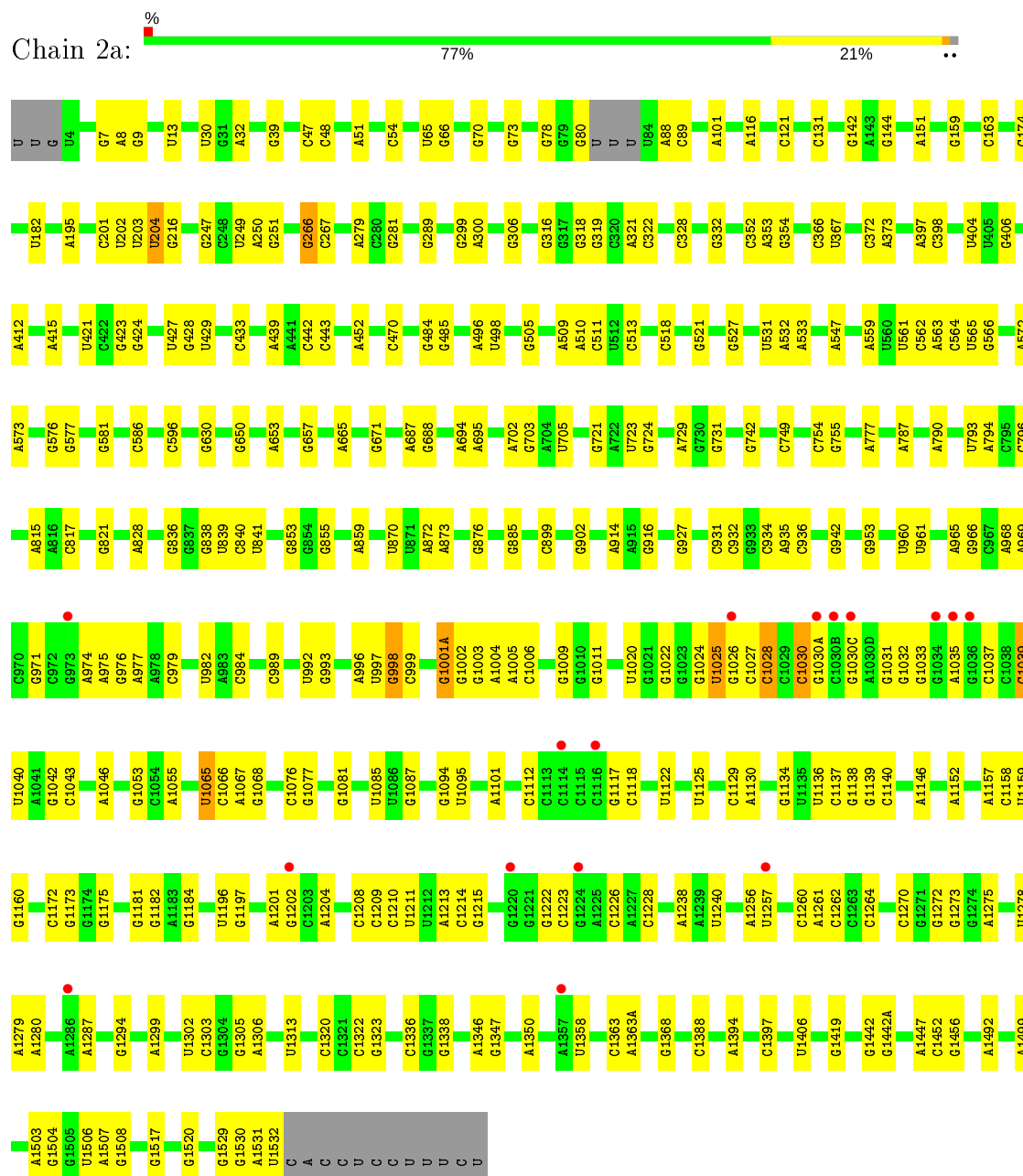


- Molecule 32: 16S Ribosomal RNA

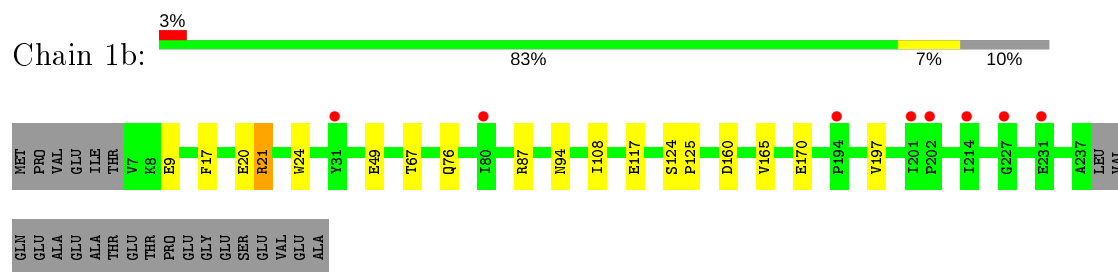
Chain 1a:  80% 18%



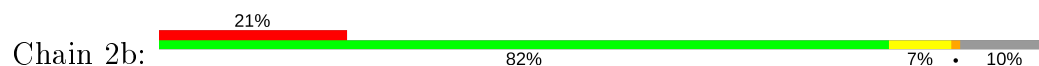
- Molecule 32: 16S Ribosomal RNA

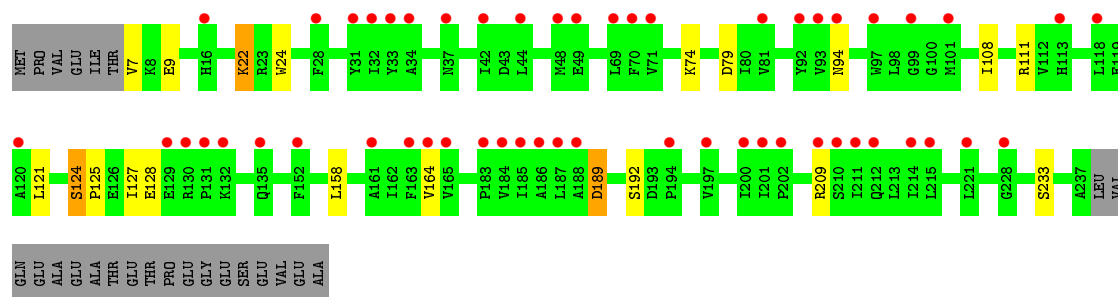


• Molecule 33: 30S ribosomal protein S2

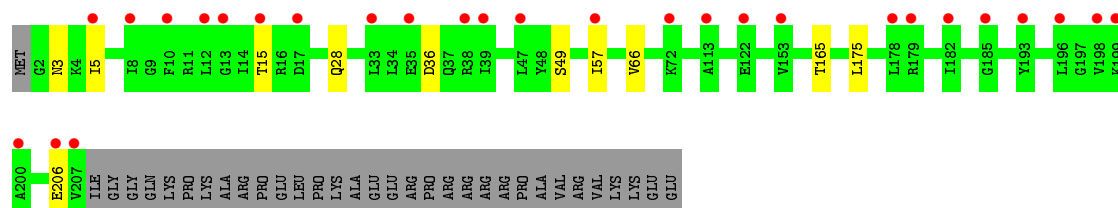
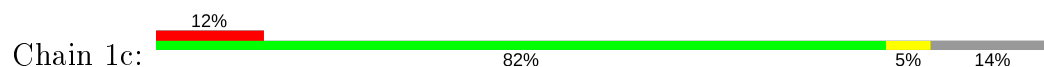


• Molecule 33: 30S ribosomal protein S2

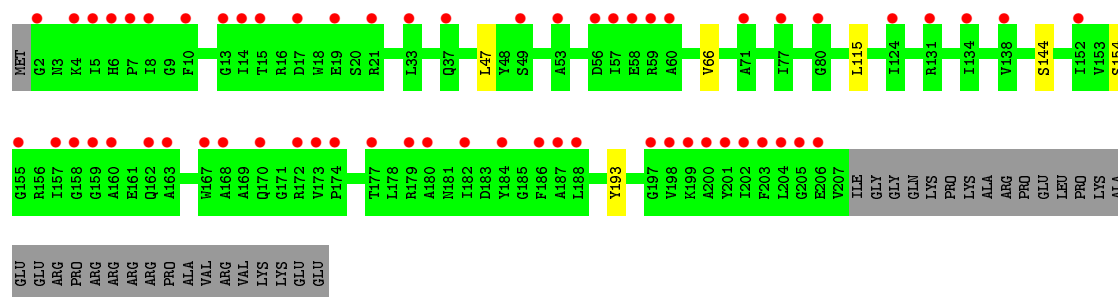
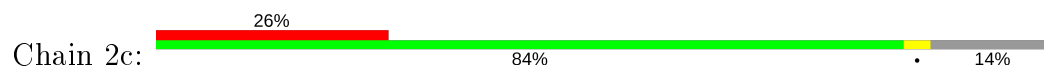




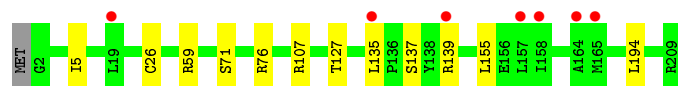
- Molecule 34: 30S ribosomal protein S3



- Molecule 34: 30S ribosomal protein S3



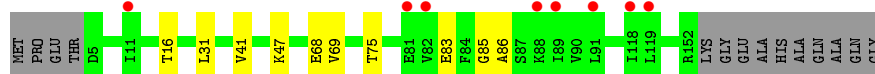
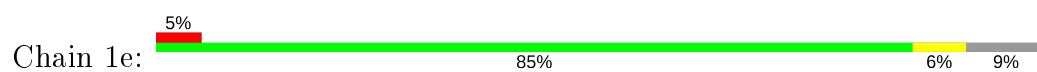
- Molecule 35: 30S ribosomal protein S4



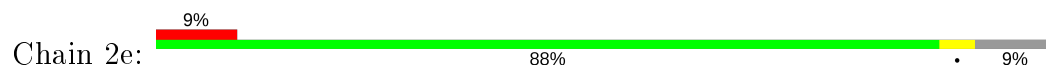
- Molecule 35: 30S ribosomal protein S4



- Molecule 36: 30S ribosomal protein S5



- Molecule 36: 30S ribosomal protein S5



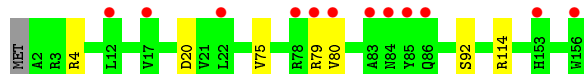
- Molecule 37: 30S ribosomal protein S6



- Molecule 37: 30S ribosomal protein S6



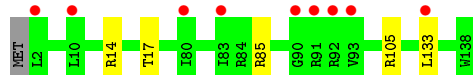
- Molecule 38: 30S ribosomal protein S7



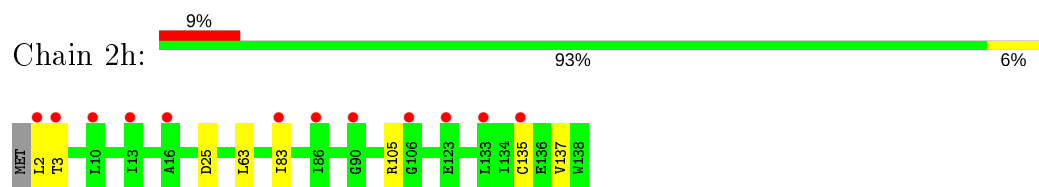
- Molecule 38: 30S ribosomal protein S7



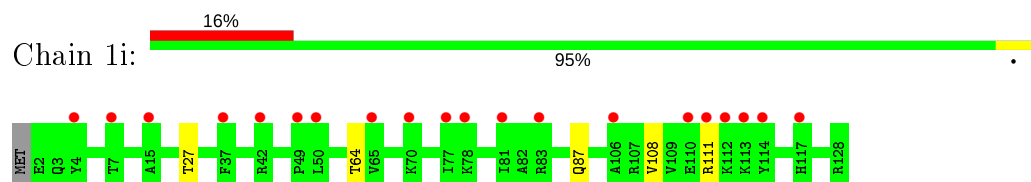
- Molecule 39: 30S ribosomal protein S8



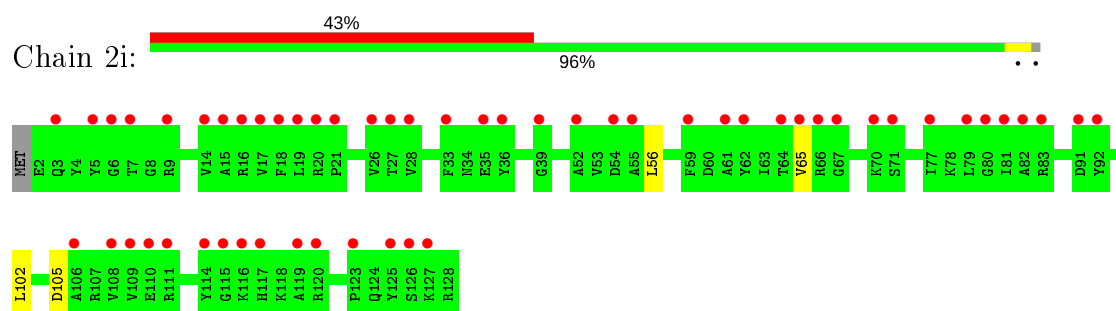
- Molecule 39: 30S ribosomal protein S8



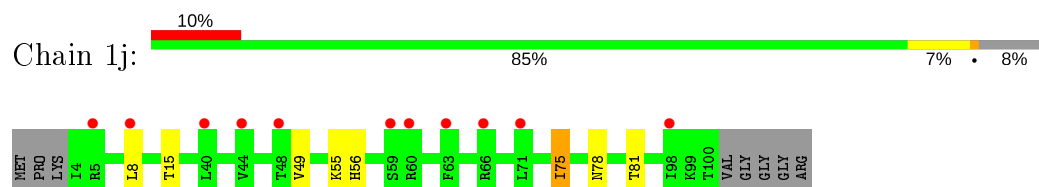
- Molecule 40: 30S ribosomal protein S9



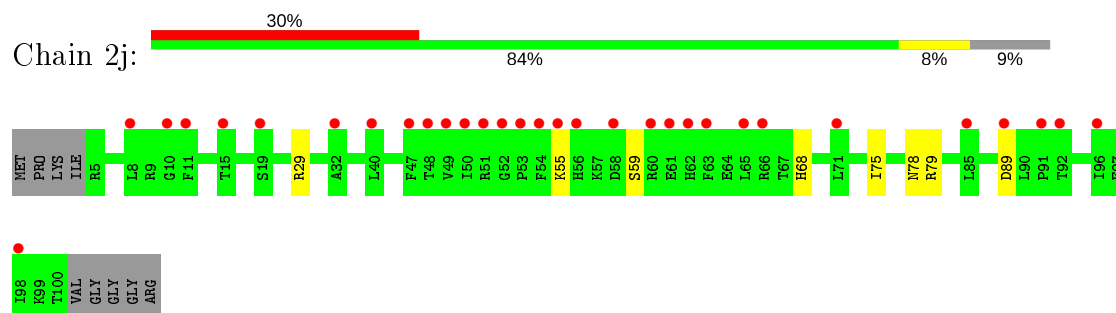
- Molecule 40: 30S ribosomal protein S9



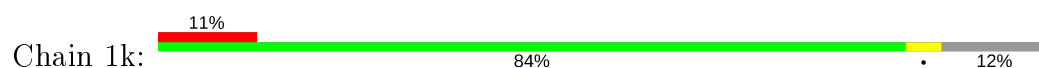
- Molecule 41: 30S ribosomal protein S10

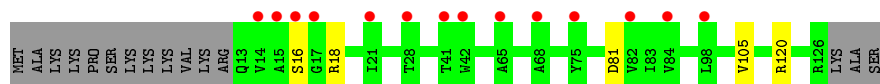


- Molecule 41: 30S ribosomal protein S10

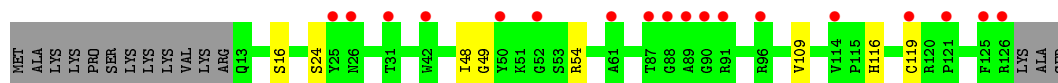
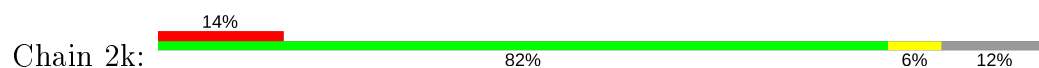


- Molecule 42: 30S ribosomal protein S11

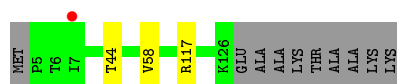




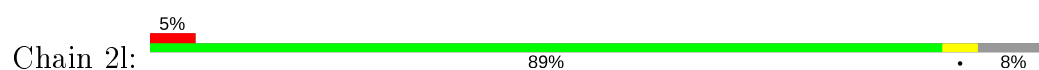
- Molecule 42: 30S ribosomal protein S11



- Molecule 43: 30S ribosomal protein S12



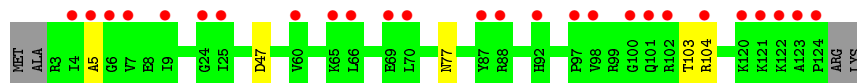
- Molecule 43: 30S ribosomal protein S12



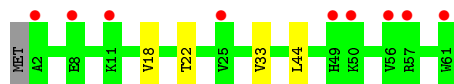
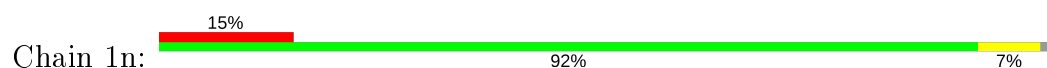
- Molecule 44: 30S ribosomal protein S13



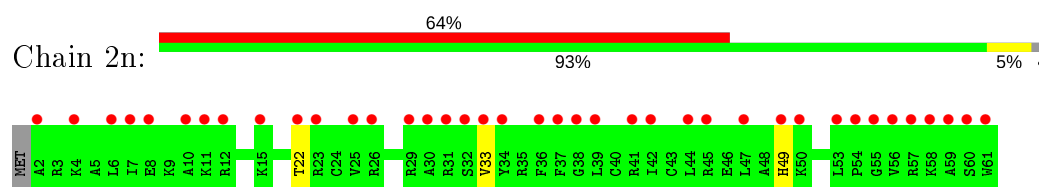
- Molecule 44: 30S ribosomal protein S13



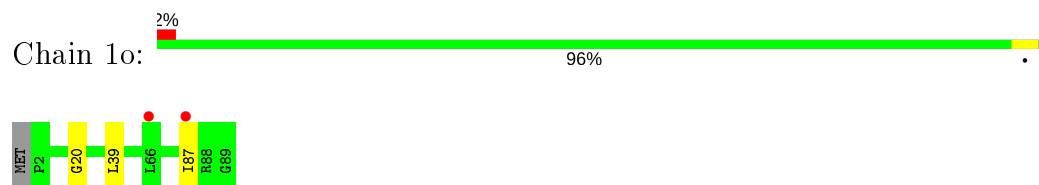
- Molecule 45: 30S ribosomal protein S14 type Z



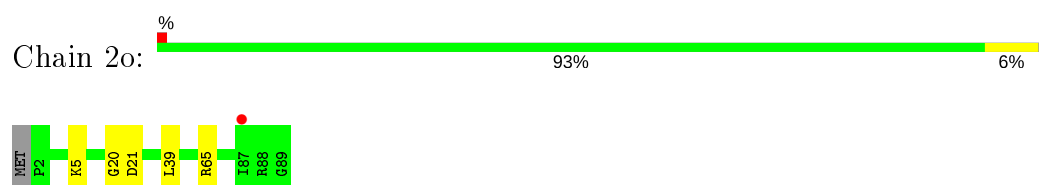
- Molecule 45: 30S ribosomal protein S14 type Z



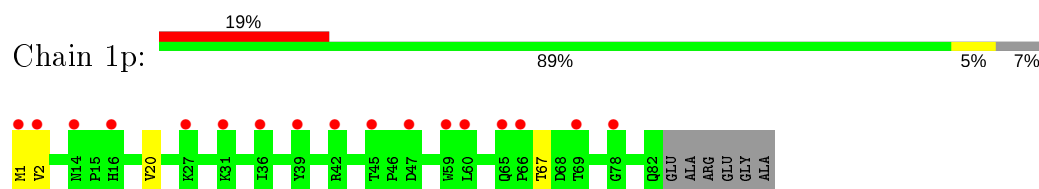
- Molecule 46: 30S ribosomal protein S15



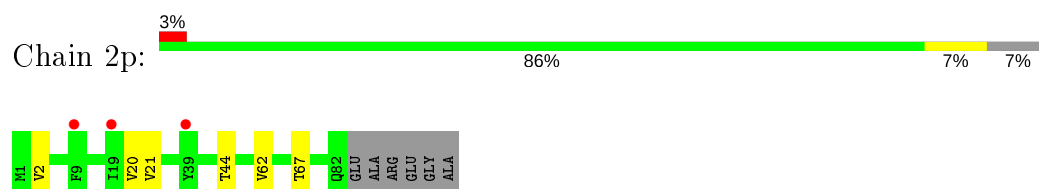
- Molecule 46: 30S ribosomal protein S15



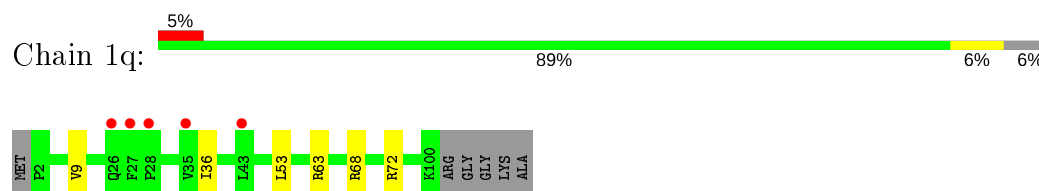
- Molecule 47: 30S ribosomal protein S16



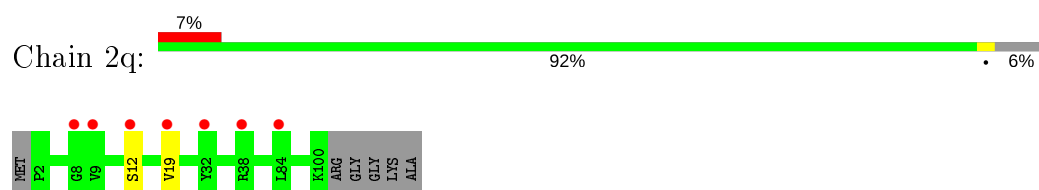
- Molecule 47: 30S ribosomal protein S16



- Molecule 48: 30S ribosomal protein S17

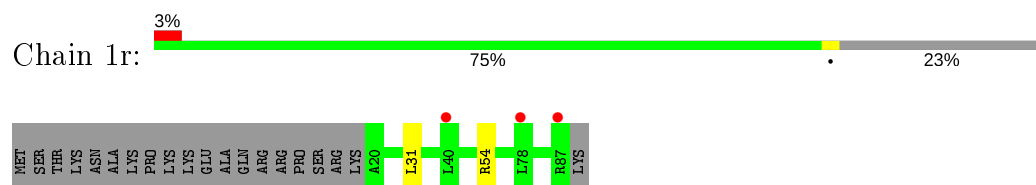


- Molecule 48: 30S ribosomal protein S17

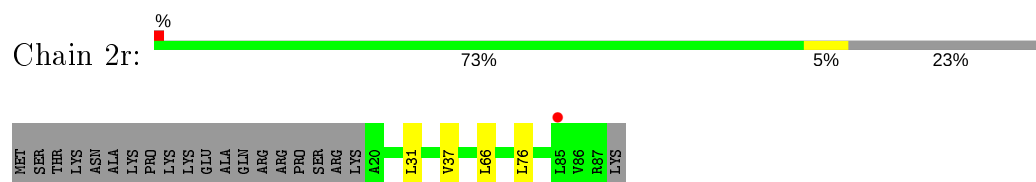




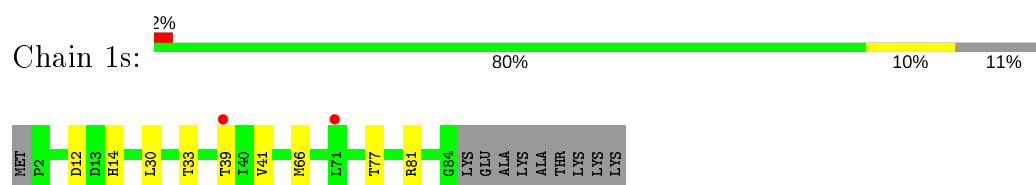
- Molecule 49: 30S ribosomal protein S18



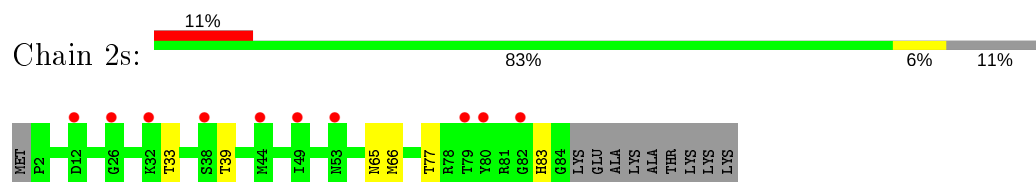
- Molecule 49: 30S ribosomal protein S18



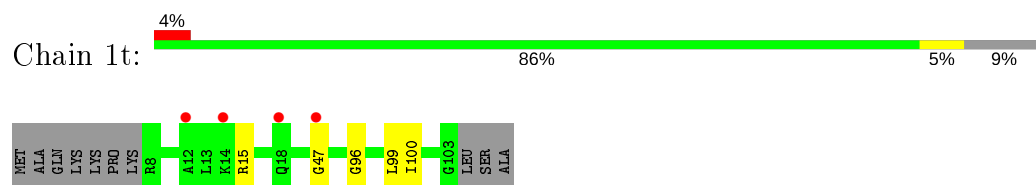
- Molecule 50: 30S ribosomal protein S19



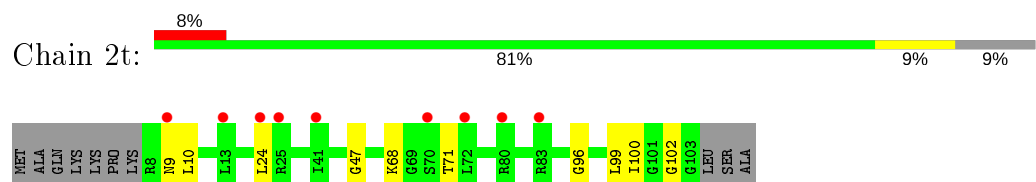
- Molecule 50: 30S ribosomal protein S19



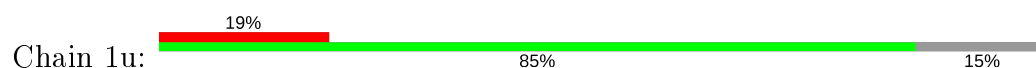
- Molecule 51: 30S ribosomal protein S20



- Molecule 51: 30S ribosomal protein S20

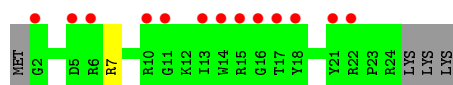
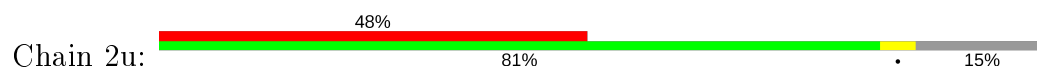


- Molecule 52: 30S ribosomal protein Thx

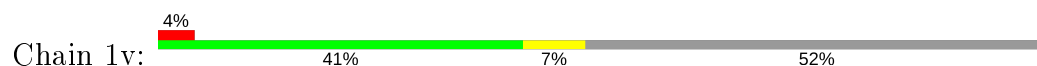




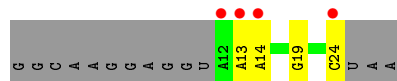
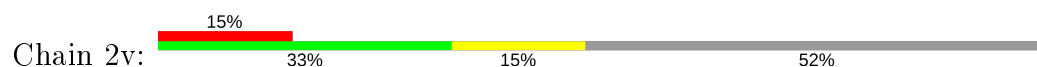
- Molecule 52: 30S ribosomal protein Thx



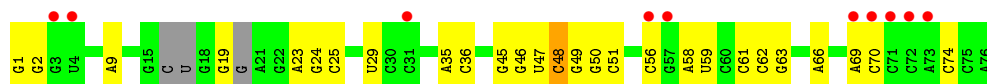
- Molecule 53: mRNA



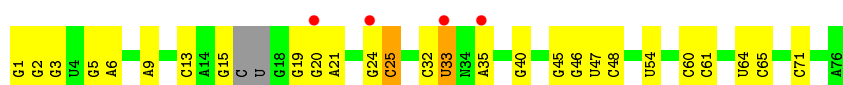
- Molecule 53: mRNA



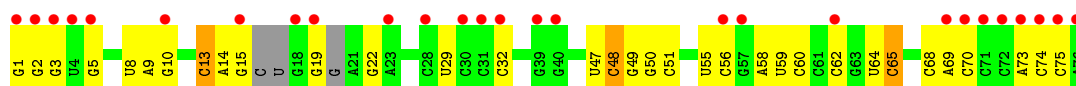
- Molecule 54: A-site and E-site tRNAs



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

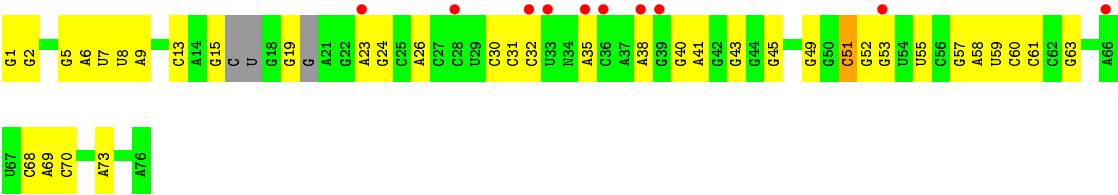


- Molecule 54: A-site and E-site tRNAs

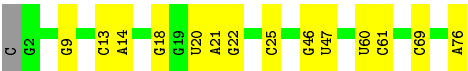
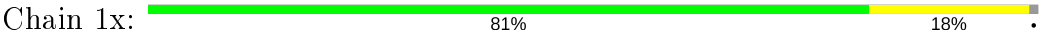


- Molecule 54: A-site and E-site tRNAs

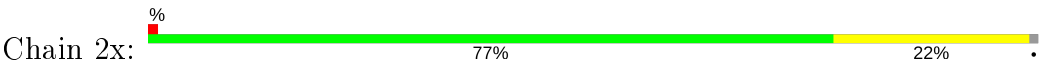




• Molecule 55: P-site tRNA



• Molecule 55: P-site tRNA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.05Å 448.09Å 621.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	224.04 – 2.85 224.04 – 2.85	Depositor EDS
% Data completeness (in resolution range)	98.7 (224.04-2.85) 98.7 (224.04-2.85)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.19 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, $R_{free}$	0.249 , 0.305 0.250 , 0.305	Depositor DCC
$R_{free}$ test set	66731 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.2	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 59.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.34$ , $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	300104	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.61% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 5MU, PSU, ZN, M2G, OMG, 2MU, SF4, 0TD, MG, ERY, 2MA, 6MZ, 2MG, 5MC, UR3, MA6, 4OC, 4SU, 7MG, CM0

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	0.33	0/69009	0.82	26/107712 (0.0%)
1	2A	0.26	0/67293	0.80	19/105034 (0.0%)
2	1B	0.33	1/2882 (0.0%)	0.78	0/4494
2	2B	0.31	1/2879 (0.0%)	0.80	1/4487 (0.0%)
3	1D	0.31	0/2186	0.49	0/2944
3	2D	0.29	0/2186	0.48	0/2944
4	1E	0.29	0/1592	0.49	0/2149
4	2E	0.27	0/1592	0.47	0/2149
5	1F	0.28	0/1619	0.47	0/2193
5	2F	0.27	0/1615	0.44	0/2188
6	1G	0.26	0/1448	0.44	0/1957
6	2G	0.26	0/1453	0.44	0/1963
7	1H	0.27	0/1356	0.46	0/1834
7	2H	0.26	0/1356	0.44	0/1834
8	1I	0.26	0/1112	0.45	0/1514
8	2I	0.25	0/1079	0.46	0/1475
9	1N	0.28	0/1144	0.45	0/1543
9	2N	0.26	0/1144	0.45	0/1543
10	1O	0.29	0/943	0.49	0/1269
10	2O	0.28	0/943	0.48	0/1269
11	1P	0.28	0/1152	0.53	1/1533 (0.1%)
11	2P	0.28	0/1152	0.47	0/1533
12	1Q	0.29	0/1143	0.46	0/1527
12	2Q	0.26	0/1143	0.46	0/1527
13	1R	0.27	0/982	0.48	0/1312
13	2R	0.24	0/982	0.45	0/1312
14	1S	0.26	0/883	0.45	0/1176
14	2S	0.25	0/880	0.44	0/1172
15	1T	0.27	0/1105	0.46	0/1477
15	2T	0.26	0/1097	0.44	0/1468
16	1U	0.28	0/977	0.43	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	2U	0.26	0/977	0.39	0/1301
17	1V	0.30	0/782	0.53	0/1049
17	2V	0.28	0/782	0.50	0/1049
18	1W	0.29	0/897	0.48	0/1205
18	2W	0.26	0/897	0.45	0/1205
19	1X	0.28	0/764	0.48	0/1025
19	2X	0.27	0/764	0.45	0/1025
20	1Y	0.28	0/819	0.48	0/1095
20	2Y	0.27	0/819	0.47	0/1095
21	1Z	0.27	0/1267	0.48	0/1717
21	2Z	0.28	0/1299	0.50	0/1763
22	10	0.30	0/662	0.47	0/881
22	20	0.28	0/662	0.47	0/881
23	11	0.28	0/762	0.46	0/1014
23	21	0.28	0/762	0.44	0/1014
24	12	0.26	0/590	0.41	0/781
24	22	0.24	0/590	0.38	0/781
25	13	0.27	0/474	0.44	0/635
25	23	0.24	0/469	0.42	0/630
26	14	0.28	0/565	0.56	0/761
26	24	0.27	0/545	0.53	0/737
27	15	0.29	0/469	0.47	0/635
27	25	0.27	0/469	0.45	0/635
28	16	0.29	0/460	0.47	0/613
28	26	0.27	0/456	0.46	0/608
29	17	0.26	0/426	0.45	0/561
29	27	0.25	0/426	0.46	0/561
30	18	0.28	0/525	0.47	0/691
30	28	0.25	0/525	0.46	0/691
31	19	0.30	0/310	0.46	0/407
31	29	0.26	0/310	0.49	0/407
32	1a	0.26	0/35795	0.82	25/55864 (0.0%)
32	2a	0.26	0/35886	0.84	46/56005 (0.1%)
33	1b	0.26	0/1881	0.45	0/2542
33	2b	0.25	0/1860	0.45	0/2518
34	1c	0.26	0/1572	0.45	0/2126
34	2c	0.25	0/1566	0.44	0/2119
35	1d	0.26	0/1685	0.45	0/2262
35	2d	0.31	1/1704 (0.1%)	0.44	0/2284
36	1e	0.26	0/1145	0.46	0/1543
36	2e	0.27	0/1149	0.48	0/1548
37	1f	0.26	0/823	0.46	0/1115
37	2f	0.27	0/829	0.46	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	1g	0.26	0/1250	0.41	0/1679
38	2g	0.25	0/1254	0.40	0/1683
39	1h	0.24	0/1108	0.44	0/1494
39	2h	0.25	0/1108	0.45	0/1494
40	1i	0.27	0/1002	0.45	0/1346
40	2i	0.27	0/997	0.51	0/1343
41	1j	0.24	0/722	0.48	1/982 (0.1%)
41	2j	0.24	0/727	0.47	0/988
42	1k	0.25	0/844	0.44	0/1145
42	2k	0.25	0/848	0.45	0/1149
43	1l	0.27	0/937	0.48	0/1260
43	2l	0.27	0/937	0.46	0/1260
44	1m	0.26	0/969	0.49	0/1302
44	2m	0.25	0/961	0.46	0/1291
45	1n	0.25	0/501	0.40	0/664
45	2n	0.25	0/501	0.42	0/664
46	1o	0.23	0/739	0.40	0/985
46	2o	0.25	0/739	0.44	0/985
47	1p	0.25	0/697	0.45	0/939
47	2p	0.25	0/693	0.45	0/935
48	1q	0.26	0/836	0.45	0/1117
48	2q	0.26	0/836	0.47	0/1117
49	1r	0.25	0/560	0.43	0/746
49	2r	0.24	0/560	0.42	0/746
50	1s	0.25	0/667	0.49	0/900
50	2s	0.27	0/661	0.52	0/893
51	1t	0.25	0/730	0.42	0/965
51	2t	0.24	0/729	0.46	0/965
52	1u	0.25	0/203	0.50	0/266
52	2u	0.25	0/203	0.48	0/266
53	1v	0.29	0/308	0.82	0/477
53	2v	0.30	0/308	0.83	0/477
54	1w	0.45	1/1600 (0.1%)	1.05	5/2482 (0.2%)
54	1y	0.43	1/1627 (0.1%)	1.01	3/2527 (0.1%)
54	2w	0.46	1/1600 (0.1%)	1.16	10/2482 (0.4%)
54	2y	0.47	1/1600 (0.1%)	1.11	6/2482 (0.2%)
55	1x	0.38	0/1725	0.98	7/2689 (0.3%)
55	2x	0.35	0/1725	1.02	2/2689 (0.1%)
All	All	0.29	7/316758 (0.0%)	0.75	152/474209 (0.0%)

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
26	14	0	1
26	24	0	2
33	1b	0	1
33	2b	0	1
51	1t	0	1
All	All	0	6

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2w	1	G	OP3-P	-10.58	1.48	1.61
2	2B	1	U	OP3-P	-10.49	1.48	1.61
54	1y	1	G	OP3-P	-10.45	1.48	1.61
54	1w	1	G	OP3-P	-10.42	1.48	1.61
54	2y	1	G	OP3-P	-10.40	1.48	1.61
2	1B	1	U	OP3-P	-10.37	1.48	1.61
35	2d	196	LEU	C-N	5.52	1.44	1.34

All (152) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2136	C	N1-C2-O2	11.11	125.56	118.90
32	1a	1027	C	N3-C4-C5	-9.53	118.09	121.90
32	1a	1030(B)	C	C2-N1-C1'	9.04	128.74	118.80
2	2B	80	U	O4'-C1'-N1	8.80	115.24	108.20
1	2A	2155	G	N3-C2-N2	8.55	125.88	119.90
32	2a	1158	C	N1-C2-O2	8.43	123.96	118.90
32	2a	1158	C	C2-N1-C1'	8.35	127.99	118.80
32	2a	1001(A)	G	N3-C4-N9	8.32	130.99	126.00
32	1a	1030(B)	C	N1-C2-O2	8.30	123.88	118.90
32	2a	754	C	C2-N1-C1'	8.29	127.92	118.80
1	1A	1075	C	N1-C2-O2	8.03	123.72	118.90
32	1a	1027	C	C5-C4-N4	7.96	125.77	120.20
1	1A	2167	U	N1-C2-O2	7.85	128.29	122.80
55	1x	14	A	C4-C5-C6	7.77	120.89	117.00
1	1A	2167	U	C2-N1-C1'	7.74	126.99	117.70
32	2a	754	C	N1-C2-O2	7.63	123.48	118.90
54	1w	23	A	N1-C6-N6	7.63	123.18	118.60
1	1A	2167	U	N3-C2-O2	-7.57	116.90	122.20
32	2a	1028	C	C2-N3-C4	7.56	123.68	119.90
54	2w	50	G	C5-C6-O6	-7.40	124.16	128.60

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1272	G	C8-N9-C1'	-7.38	117.41	127.00
32	2a	1039	C	C5-C4-N4	-7.36	115.05	120.20
32	2a	1272	G	C4-N9-C1'	7.35	136.06	126.50
1	1A	1063	G	C5-C6-O6	7.34	133.00	128.60
1	2A	1142	U	C2-N1-C1'	7.15	126.28	117.70
32	2a	1272	G	N3-C2-N2	7.12	124.89	119.90
32	2a	1272	G	N3-C4-N9	7.11	130.27	126.00
1	2A	2136	C	N3-C2-O2	-7.09	116.94	121.90
1	1A	847	U	C2-N1-C1'	7.09	126.20	117.70
1	2A	2155	G	C6-N1-C2	7.07	129.34	125.10
32	2a	1001(A)	G	C6-C5-N7	-6.95	126.23	130.40
54	2w	65	C	N1-C2-O2	6.93	123.06	118.90
1	2A	2473	U	C2-N1-C1'	6.87	125.94	117.70
32	1a	1030(B)	C	C6-N1-C2	-6.82	117.57	120.30
32	2a	1264	C	N1-C2-O2	6.79	122.98	118.90
32	2a	1158	C	N3-C2-O2	-6.73	117.19	121.90
1	2A	1313	U	C2-N1-C1'	6.73	125.77	117.70
1	1A	1313	U	C2-N1-C1'	6.72	125.77	117.70
1	1A	1075	C	C2-N3-C4	6.70	123.25	119.90
32	1a	1030(B)	C	N3-C2-O2	-6.68	117.22	121.90
32	1a	1027	C	C2-N3-C4	6.66	123.23	119.90
32	1a	1027	C	C6-N1-C1'	6.62	128.74	120.80
32	1a	1020	U	C2-N1-C1'	6.56	125.57	117.70
32	1a	841	U	C2-N1-C1'	6.44	125.43	117.70
32	2a	754	C	C6-N1-C1'	-6.43	113.08	120.80
54	2w	15	G	N3-C2-N2	6.41	124.39	119.90
32	2a	1272	G	N1-C2-N2	-6.39	110.45	116.20
54	2y	23	A	N1-C6-N6	6.39	122.43	118.60
54	2w	48	C	N1-C2-O2	-6.32	115.11	118.90
32	2a	1033	G	C6-N1-C2	6.30	128.88	125.10
32	1a	1034	G	N3-C2-N2	6.30	124.31	119.90
32	2a	1039	C	C2-N1-C1'	6.28	125.71	118.80
1	1A	1176	G	OP1-P-O3'	6.22	118.88	105.20
32	2a	1025	U	C2-N1-C1'	6.17	125.10	117.70
32	2a	1272	G	C5-C6-O6	6.11	132.27	128.60
32	2a	1039	C	C5-C6-N1	6.11	124.06	121.00
32	1a	266	G	P-O3'-C3'	6.10	127.02	119.70
54	1y	15	G	N3-C2-N2	6.08	124.16	119.90
54	2y	60	C	C6-N1-C2	-6.06	117.88	120.30
32	2a	1001(A)	G	C4-C5-N7	6.04	113.22	110.80
32	1a	1030(B)	C	C6-N1-C1'	-6.02	113.57	120.80
1	1A	1063	G	C6-N1-C2	6.01	128.71	125.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	549	G	O5'-P-OP1	-6.00	100.30	105.70
1	1A	12	U	C2-N1-C1'	5.99	124.89	117.70
1	1A	2473	U	C2-N1-C1'	5.94	124.83	117.70
54	2y	51	C	C5-C4-N4	5.93	124.35	120.20
55	1x	22	G	N1-C6-O6	-5.92	116.35	119.90
32	2a	563	A	O4'-C1'-N9	5.88	112.90	108.20
32	1a	1020	U	N1-C2-O2	5.88	126.91	122.80
11	1P	33	ARG	C-N-CA	-5.87	109.97	122.30
54	1w	23	A	C5-C6-N6	-5.87	119.00	123.70
32	2a	1039	C	N3-C4-N4	5.85	122.10	118.00
32	2a	1001(A)	G	C4-N9-C1'	5.84	134.09	126.50
32	1a	1020	U	N3-C2-O2	-5.83	118.12	122.20
1	1A	548	A	P-O3'-C3'	5.82	126.68	119.70
1	1A	512	G	O4'-C1'-N9	5.81	112.85	108.20
41	1j	75	ILE	C-N-CA	-5.80	107.21	121.70
54	2w	13	C	OP1-P-O3'	5.80	117.95	105.20
32	1a	1034	G	C6-N1-C2	5.79	128.57	125.10
1	1A	847	U	N1-C2-O2	5.73	126.81	122.80
32	2a	1158	C	C6-N1-C2	-5.73	118.01	120.30
54	1y	25	C	C2-N1-C1'	5.72	125.09	118.80
32	2a	998	G	C5-C6-O6	5.71	132.03	128.60
32	1a	1027	C	C2-N1-C1'	-5.70	112.53	118.80
54	1w	23	A	C6-C5-N7	-5.69	128.32	132.30
54	2w	13	C	P-O3'-C3'	5.68	126.52	119.70
32	2a	1001(A)	G	C5-C6-O6	-5.67	125.20	128.60
1	2A	847	U	C2-N1-C1'	5.67	124.51	117.70
32	2a	1158	C	C6-N1-C1'	-5.66	114.00	120.80
32	2a	266	G	P-O3'-C3'	5.65	126.47	119.70
32	2a	1001(A)	G	N3-C4-C5	-5.63	125.78	128.60
1	1A	1075	C	C5-C4-N4	5.62	124.14	120.20
1	1A	1313	U	N3-C2-O2	-5.62	118.27	122.20
55	1x	14	A	C5-C6-N1	-5.58	114.91	117.70
1	1A	614	U	C2-N1-C1'	5.58	124.40	117.70
32	2a	1025	U	N1-C2-O2	5.57	126.69	122.80
1	2A	2155	G	C5-C6-O6	5.55	131.93	128.60
55	2x	46	G	C6-N1-C2	-5.53	121.78	125.10
32	1a	1030(B)	C	C5-C6-N1	5.52	123.76	121.00
1	2A	2149	G	N3-C4-N9	5.52	129.31	126.00
54	2w	50	G	N3-C4-N9	5.50	129.30	126.00
54	1w	48	C	N1-C2-O2	5.50	122.20	118.90
54	2w	64	U	N1-C2-O2	5.50	126.65	122.80
54	2y	68	C	N1-C2-O2	5.50	122.20	118.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1174	A	OP1-P-O3'	5.48	117.26	105.20
32	2a	754	C	N3-C2-O2	-5.48	118.06	121.90
32	2a	1067	A	P-O3'-C3'	5.48	126.28	119.70
32	2a	1001(A)	G	N9-C4-C5	-5.43	103.23	105.40
55	1x	14	A	C5-N7-C8	5.42	106.61	103.90
1	1A	1313	U	N1-C2-O2	5.41	126.59	122.80
32	2a	1272	G	N3-C4-C5	-5.40	125.90	128.60
54	2w	64	U	C2-N3-C4	5.40	130.24	127.00
32	1a	1065	U	P-O3'-C3'	5.39	126.17	119.70
1	1A	1063	G	N3-C2-N2	5.38	123.67	119.90
1	1A	2473	U	N1-C2-O2	5.38	126.56	122.80
1	2A	784	A	O4'-C1'-N9	5.35	112.48	108.20
55	1x	14	A	C4-N9-C1'	5.34	135.91	126.30
32	2a	1025	U	C6-N1-C1'	-5.31	113.76	121.20
32	1a	1158	C	C2-N1-C1'	5.30	124.63	118.80
32	2a	1030	C	N1-C2-O2	5.30	122.08	118.90
32	1a	1067	A	P-O3'-C3'	5.29	126.05	119.70
55	1x	14	A	C8-N9-C1'	-5.29	118.17	127.70
54	2y	51	C	N3-C4-N4	-5.29	114.30	118.00
32	1a	1034	G	C5-C6-O6	5.29	131.77	128.60
1	2A	1313	U	N1-C2-O2	5.27	126.49	122.80
54	2w	65	C	C2-N3-C4	5.26	122.53	119.90
1	2A	2129	C	N1-C2-O2	5.25	122.05	118.90
32	2a	953	G	N3-C4-N9	5.23	129.14	126.00
32	1a	841	U	C5-C6-N1	5.23	125.31	122.70
32	2a	204	U	C2-N1-C1'	5.22	123.96	117.70
1	2A	645	C	C2-N1-C1'	5.18	124.50	118.80
55	2x	22	G	N1-C6-O6	-5.16	116.80	119.90
54	1y	33	U	C2-N1-C1'	5.15	123.88	117.70
1	2A	528	A	OP1-P-O3'	5.13	116.48	105.20
54	1w	23	A	N9-C4-C5	-5.12	103.75	105.80
32	2a	1001(A)	G	C8-N9-C1'	-5.12	120.34	127.00
32	2a	1028	C	C5-C6-N1	5.11	123.55	121.00
1	1A	784	A	O4'-C1'-N9	5.10	112.28	108.20
1	2A	2140	C	N1-C2-O2	5.08	121.95	118.90
32	2a	1033	G	C5-C6-O6	5.08	131.65	128.60
32	2a	1043	C	C2-N3-C4	5.08	122.44	119.90
55	1x	46	G	C6-N1-C2	-5.07	122.06	125.10
32	1a	1027	C	N3-C2-O2	-5.05	118.36	121.90
32	2a	1065	U	P-O3'-C3'	5.04	125.75	119.70
32	1a	1034	G	N9-C4-C5	-5.03	103.39	105.40
54	2y	63	G	C6-N1-C2	5.03	128.12	125.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2096	U	N1-C2-O2	5.02	126.31	122.80
1	2A	1142	U	C6-N1-C1'	-5.02	114.17	121.20
1	2A	2321	G	C4-N9-C1'	5.01	133.02	126.50
1	1A	1086	A	N1-C6-N6	-5.01	115.59	118.60
1	2A	1313	U	N3-C2-O2	-5.01	118.69	122.20
32	2a	65	U	P-O3'-C3'	5.00	125.71	119.70

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	14	57	GLU	Peptide
33	1b	124	SER	Peptide
51	1t	99	LEU	Peptide
26	24	53	GLU	Peptide
26	24	55	ARG	Peptide
33	2b	22	LYS	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	819	0
1	2A	60322	0	30418	967	0
2	1B	2577	0	1305	33	0
2	2B	2575	0	1303	41	0
3	1D	2136	0	2218	66	0
3	2D	2136	0	2218	54	0
4	1E	1559	0	1617	37	0
4	2E	1559	0	1618	41	0
5	1F	1584	0	1625	38	0
5	2F	1580	0	1618	44	0
6	1G	1423	0	1436	42	0
6	2G	1428	0	1438	45	0
7	1H	1330	0	1407	32	0
7	2H	1330	0	1407	38	0
8	1I	1097	0	1140	22	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	2I	1064	0	1082	23	0
9	1N	1117	0	1184	13	0
9	2N	1117	0	1184	25	0
10	1O	933	0	996	21	0
10	2O	933	0	996	27	0
11	1P	1135	0	1212	33	0
11	2P	1135	0	1212	38	0
12	1Q	1122	0	1179	27	0
12	2Q	1122	0	1179	34	0
13	1R	968	0	1033	17	0
13	2R	968	0	1033	24	0
14	1S	873	0	927	26	0
14	2S	870	0	923	26	0
15	1T	1091	0	1151	21	0
15	2T	1083	0	1136	40	0
16	1U	959	0	1019	15	0
16	2U	959	0	1018	20	0
17	1V	771	0	830	17	0
17	2V	771	0	830	23	0
18	1W	886	0	939	24	0
18	2W	886	0	940	15	0
19	1X	750	0	814	14	0
19	2X	750	0	814	15	0
20	1Y	806	0	881	22	0
20	2Y	806	0	881	18	0
21	1Z	1240	0	1240	28	0
21	2Z	1271	0	1273	42	0
22	10	653	0	674	18	0
22	20	653	0	674	33	0
23	11	755	0	826	18	0
23	21	755	0	826	22	0
24	12	588	0	643	13	0
24	22	588	0	643	11	0
25	13	469	0	518	14	0
25	23	464	0	514	11	0
26	14	552	0	533	26	0
26	24	532	0	503	17	0
27	15	455	0	465	9	0
27	25	455	0	465	15	0
28	16	453	0	472	9	0
28	26	449	0	469	8	0
29	17	418	0	467	8	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	27	418	0	467	8	0
30	18	517	0	582	22	0
30	28	517	0	582	25	0
31	19	307	0	335	10	0
31	29	307	0	335	11	0
32	1a	32246	0	16294	0	0
32	2a	32327	0	16338	0	0
33	1b	1846	0	1867	0	0
33	2b	1825	0	1828	0	0
34	1c	1548	0	1535	0	0
34	2c	1542	0	1517	0	0
35	1d	1655	0	1672	0	0
35	2d	1674	0	1714	0	0
36	1e	1129	0	1185	0	0
36	2e	1133	0	1191	0	0
37	1f	810	0	804	0	0
37	2f	816	0	808	0	0
38	1g	1231	0	1238	0	0
38	2g	1235	0	1249	0	0
39	1h	1088	0	1126	0	0
39	2h	1088	0	1126	0	0
40	1i	983	0	986	0	0
40	2i	978	0	966	0	0
41	1j	709	0	650	0	0
41	2j	714	0	672	0	0
42	1k	829	0	825	0	0
42	2k	833	0	836	0	0
43	1l	932	0	981	0	0
43	2l	932	0	981	0	0
44	1m	958	0	1002	0	0
44	2m	950	0	988	0	0
45	1n	492	0	529	0	0
45	2n	492	0	529	0	0
46	1o	728	0	760	0	0
46	2o	728	0	760	0	0
47	1p	681	0	697	0	0
47	2p	677	0	686	0	0
48	1q	823	0	891	0	0
48	2q	823	0	891	0	0
49	1r	555	0	618	0	0
49	2r	555	0	618	0	0
50	1s	652	0	662	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	2s	646	0	644	0	0
51	1t	728	0	798	0	0
51	2t	727	0	796	0	0
52	1u	199	0	208	0	0
52	2u	199	0	208	0	0
53	1v	276	0	139	0	0
53	2v	276	0	139	0	0
54	1w	1568	0	801	0	0
54	1y	1591	0	812	0	0
54	2w	1568	0	802	0	0
54	2y	1568	0	802	0	0
55	1x	1625	0	829	0	0
55	2x	1625	0	829	0	0
56	10	7	0	0	0	0
56	11	1	0	0	0	0
56	12	2	0	0	0	0
56	13	6	0	0	0	0
56	14	1	0	0	0	0
56	15	7	0	0	0	0
56	16	4	0	0	0	0
56	17	5	0	0	0	0
56	18	2	0	0	0	0
56	19	3	0	0	0	0
56	1A	1073	0	0	0	0
56	1B	35	0	0	0	0
56	1D	13	0	0	0	0
56	1E	15	0	0	0	0
56	1F	14	0	0	0	0
56	1G	3	0	0	0	0
56	1I	1	0	0	0	0
56	1N	4	0	0	0	0
56	1O	2	0	0	0	0
56	1P	8	0	0	0	0
56	1Q	8	0	0	0	0
56	1R	2	0	0	0	0
56	1S	2	0	0	0	0
56	1T	2	0	0	0	0
56	1U	10	0	0	0	0
56	1V	8	0	0	0	0
56	1W	8	0	0	0	0
56	1X	5	0	0	0	0
56	1Y	1	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	1Z	3	0	0	0	0
56	1a	229	0	0	0	0
56	1b	1	0	0	0	0
56	1d	1	0	0	0	0
56	1e	2	0	0	0	0
56	1f	1	0	0	0	0
56	1l	3	0	0	0	0
56	1m	1	0	0	0	0
56	1n	1	0	0	0	0
56	1p	1	0	0	0	0
56	1r	1	0	0	0	0
56	1s	1	0	0	0	0
56	1t	1	0	0	0	0
56	1v	1	0	0	0	0
56	1w	6	0	0	0	0
56	1x	13	0	0	0	0
56	1y	5	0	0	0	0
56	20	2	0	0	0	0
56	21	1	0	0	0	0
56	22	1	0	0	0	0
56	23	3	0	0	0	0
56	25	3	0	0	0	0
56	26	2	0	0	0	0
56	27	2	0	0	0	0
56	28	1	0	0	0	0
56	2A	874	0	0	0	0
56	2B	21	0	0	0	0
56	2D	7	0	0	0	0
56	2E	8	0	0	0	0
56	2F	7	0	0	0	0
56	2G	1	0	0	0	0
56	2N	1	0	0	0	0
56	2O	1	0	0	0	0
56	2P	2	0	0	0	0
56	2Q	5	0	0	0	0
56	2R	3	0	0	0	0
56	2T	3	0	0	0	0
56	2U	3	0	0	0	0
56	2V	1	0	0	0	0
56	2W	1	0	0	0	0
56	2X	2	0	0	0	0
56	2Z	1	0	0	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	2a	233	0	0	0	0
56	2d	1	0	0	0	0
56	2e	1	0	0	0	0
56	2f	2	0	0	0	0
56	2g	1	0	0	0	0
56	2i	2	0	0	0	0
56	2j	2	0	0	0	0
56	2k	1	0	0	0	0
56	2l	5	0	0	0	0
56	2p	1	0	0	0	0
56	2q	3	0	0	0	0
56	2r	1	0	0	0	0
56	2t	1	0	0	0	0
56	2v	2	0	0	0	0
56	2w	1	0	0	0	0
56	2x	5	0	0	0	0
56	2y	4	0	0	0	0
57	1A	51	0	67	3	0
57	2A	51	0	67	3	0
58	14	1	0	0	0	0
58	15	1	0	0	0	0
58	16	1	0	0	0	0
58	19	1	0	0	0	0
58	1Y	1	0	0	0	0
58	1n	1	0	0	0	0
58	24	1	0	0	0	0
58	25	1	0	0	0	0
58	26	1	0	0	0	0
58	29	1	0	0	0	0
58	2Y	1	0	0	0	0
58	2n	1	0	0	0	0
59	1d	8	0	0	0	0
59	2d	8	0	0	0	0
60	10	9	0	0	0	0
60	11	10	0	0	0	0
60	12	3	0	0	0	0
60	13	2	0	0	0	0
60	14	2	0	0	0	0
60	15	3	0	0	0	0
60	16	3	0	0	0	0
60	17	9	0	0	0	0
60	18	5	0	0	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	19	2	0	0	0	0
60	1A	1719	0	0	66	0
60	1B	59	0	0	0	0
60	1D	16	0	0	1	0
60	1E	21	0	0	3	0
60	1F	7	0	0	0	0
60	1G	4	0	0	3	0
60	1H	1	0	0	0	0
60	1I	2	0	0	0	0
60	1N	5	0	0	0	0
60	1O	7	0	0	0	0
60	1P	11	0	0	1	0
60	1Q	10	0	0	0	0
60	1R	8	0	0	0	0
60	1S	5	0	0	0	0
60	1T	2	0	0	0	0
60	1U	6	0	0	0	0
60	1V	10	0	0	0	0
60	1W	8	0	0	0	0
60	1X	8	0	0	0	0
60	1Y	4	0	0	0	0
60	1Z	1	0	0	0	0
60	1a	381	0	0	0	0
60	1b	1	0	0	0	0
60	1g	1	0	0	0	0
60	1k	1	0	0	0	0
60	1l	2	0	0	0	0
60	1q	4	0	0	0	0
60	1v	1	0	0	0	0
60	1w	2	0	0	0	0
60	1x	15	0	0	0	0
60	1y	2	0	0	0	0
60	20	9	0	0	2	0
60	21	8	0	0	0	0
60	22	2	0	0	0	0
60	23	1	0	0	0	0
60	25	4	0	0	0	0
60	27	3	0	0	0	0
60	28	4	0	0	2	0
60	29	1	0	0	0	0
60	2A	1401	0	0	84	0
60	2B	26	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	2D	14	0	0	1	0
60	2E	9	0	0	0	0
60	2F	8	0	0	0	0
60	2I	4	0	0	0	0
60	2N	1	0	0	0	0
60	2O	1	0	0	0	0
60	2P	5	0	0	0	0
60	2Q	2	0	0	0	0
60	2R	2	0	0	0	0
60	2T	4	0	0	0	0
60	2U	2	0	0	1	0
60	2W	4	0	0	0	0
60	2X	4	0	0	0	0
60	2Z	1	0	0	0	0
60	2a	306	0	0	0	0
60	2d	1	0	0	0	0
60	2g	2	0	0	0	0
60	2h	1	0	0	0	0
60	2i	3	0	0	0	0
60	2j	4	0	0	0	0
60	2l	4	0	0	0	0
60	2p	1	0	0	0	0
60	2r	1	0	0	0	0
60	2t	2	0	0	0	0
60	2v	1	0	0	0	0
60	2x	8	0	0	0	0
60	2y	11	0	0	0	0
All	All	300104	0	196819	2823	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 11.

All (2823) 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:2136:C:N4	1:1A:2155:G:H1	1.44	1.15
1:2A:1002:G:H1	1:2A:1038:C:N4	42.20	1.11
1:1A:1082:U:O4	1:1A:1086:A:N1	1.95	1.00
1:1A:1054:A:H61	1:1A:1105:U:H3	1.07	0.99
1:2A:2138:C:H42	1:2A:2153:G:H1	1.02	0.98
1:1A:2138:C:N4	1:1A:2153:G:H1	1.65	0.94

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2104:G:H1	1:2A:2185:C:N4	1.64	0.94
1:2A:2121:G:H1	1:2A:2177:C:H42	1.10	0.94
1:2A:2138:C:N4	1:2A:2153:G:H1	1.65	0.93
1:1A:1054:A:N6	1:1A:1105:U:H3	1.66	0.92
1:1A:2138:C:H42	1:1A:2153:G:H1	1.07	0.92
1:1A:765:G:H1	1:1A:812:C:HO2'	84.70	0.92
1:2A:2143:C:H42	1:2A:2148:G:H1	1.06	0.92
1:2A:2140:C:H42	1:2A:2151:G:H1	1.07	0.91
1:2A:1024:G:HO2'	1:2A:1144:G:HO2'	1.15	0.91
1:2A:2140:C:N4	1:2A:2151:G:H1	1.69	0.90
1:2A:2137:C:N4	1:2A:2154:G:H1	1.71	0.89
1:1A:1082:U:H3	1:1A:1086:A:N6	1.69	0.89
1:2A:2104:G:H1	1:2A:2185:C:H42	0.90	0.88
1:1A:517:C:OP1	27:15:16:ARG:NH2	2.08	0.87
1:2A:455:C:H42	1:2A:476:G:H1	22.11	0.87
1:2A:1002:G:N2	1:2A:1038:C:N3	41.54	0.86
1:1A:2099:U:H3	1:1A:2190:G:H1	1.21	0.85
22:10:11:ARG:O	22:10:14:ARG:NH2	2.09	0.85
1:1A:2136:C:N3	1:1A:2155:G:N2	2.23	0.85
1:2A:2143:C:N4	1:2A:2148:G:H1	1.75	0.84
1:1A:2103:C:H42	1:1A:2186:G:H1	1.25	0.84
1:2A:2121:G:H1	1:2A:2177:C:N4	1.75	0.84
1:2A:2138:C:N3	1:2A:2153:G:N2	2.25	0.84
1:2A:1032:A:H61	1:2A:1122:G:H1	1.23	0.83
1:1A:530:G:N1	1:1A:2023:G:OP1	2.11	0.83
1:1A:279:C:H42	1:1A:361:G:H1	1.25	0.83
1:2A:2345:G:H4'	1:2A:2346:A:H5''	1.62	0.82
1:2A:2807:G:N1	1:2A:2893:G:O6	2.11	0.82
1:1A:2790:A:H5''	1:1A:2893:G:H21	1.45	0.82
1:2A:2096:U:H3	1:2A:2193:G:H1	1.28	0.82
1:1A:1082:U:H3	1:1A:1086:A:H61	0.86	0.82
1:2A:2113:U:H3	1:2A:2170:A:H61	1.27	0.82
1:2A:125:G:H5''	29:27:19:ARG:HD3	1.62	0.81
1:1A:1992:G:N7	60:1A:5061:HOH:O	2.14	0.81
1:1A:2807:G:N1	1:1A:2893:G:O6	2.13	0.81
1:1A:1060:U:H3	1:1A:1088:A:H8	1.29	0.80
27:25:16:ARG:NH1	27:25:17:ASP:OD1	2.15	0.80
1:1A:993:G:H2'	1:1A:995:C:H41	14.66	0.80
11:1P:52:GLU:OE1	11:1P:55:ARG:NH1	2.14	0.80
23:11:3:LYS:HB2	23:11:61:ARG:HH12	1.45	0.80
1:1A:2103:C:N4	1:1A:2186:G:H1	1.80	0.79

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2206:G:OP1	3:2D:68:LYS:NZ	2.16	0.79
1:2A:1153:C:OP1	16:2U:92:ARG:NH2	2.16	0.79
1:1A:1817:G:OP1	3:1D:88:ARG:NH2	2.16	0.78
20:2Y:83:THR:HG21	20:2Y:99:CYS:HB2	1.65	0.78
1:1A:532:A:N6	1:1A:1206:G:O2'	62.22	0.78
1:1A:875:G:H1	1:1A:902:C:H42	1.28	0.78
10:1O:35:VAL:HG11	10:1O:103:ALA:HB3	1.64	0.77
1:1A:1390:U:O2	1:1A:1395:A:N6	2.17	0.77
1:1A:1086:A:O2'	1:1A:1087:G:N7	2.16	0.77
1:1A:833:U:O2	11:1P:55:ARG:NH2	2.18	0.77
24:12:10:LEU:HD21	24:12:59:ARG:HD2	1.64	0.77
1:2A:874:G:H21	21:2Z:170:THR:HG21	1.49	0.77
1:2A:2845:G:H2'	1:2A:2846:G:H8	1.50	0.77
5:2F:53:THR:HG23	5:2F:55:GLY:H	1.51	0.77
1:1A:631:A:OP1	11:1P:65:ARG:NH1	2.17	0.76
31:29:25:VAL:HB	31:29:34:GLN:HG2	1.68	0.76
1:2A:2103:C:H42	1:2A:2186:G:H1	1.34	0.75
1:2A:2145:C:O2'	1:2A:2147:G:N7	2.19	0.75
1:2A:1801:G:OP2	3:2D:154:LYS:NZ	2.19	0.75
1:2A:2073:C:HO2'	1:2A:2598:A:HO2'	1.25	0.75
26:14:53:GLU:HB2	26:14:55:ARG:H	1.50	0.75
2:2B:22:U:H3	2:2B:61:G:H1	1.35	0.75
1:2A:2528:U:H5''	31:29:31:LYS:HE2	1.67	0.75
18:1W:78:GLU:OE2	18:1W:99:ARG:NH1	2.18	0.74
1:1A:2685:G:N2	1:1A:2724:C:O2	2.20	0.74
1:1A:692:C:O2'	3:1D:38:LYS:NZ	2.20	0.74
8:2I:26:ALA:HA	8:2I:30:LEU:HB2	1.70	0.74
1:2A:2099:U:H3	1:2A:2190:G:H1	0.81	0.74
1:1A:882:G:H1	1:1A:894:C:H42	1.35	0.74
1:1A:1007:C:OP1	9:1N:37:LYS:NZ	2.17	0.73
1:1A:2683:C:O2	10:1O:70:LYS:NZ	2.17	0.73
1:1A:2183:C:H2'	1:1A:2184:G:H8	1.53	0.73
1:1A:192:C:OP1	60:1A:4536:HOH:O	2.06	0.73
23:21:50:ARG:HG2	23:21:59:THR:HG22	1.70	0.73
1:2A:1218:C:H42	1:2A:1231:G:H1	1.36	0.73
18:2W:12:ILE:O	18:2W:101:SER:OG	2.07	0.73
1:2A:307:G:N1	1:2A:310:A:OP2	2.21	0.73
15:2T:26:ASP:OD1	15:2T:120:ARG:NH2	2.18	0.73
1:1A:2660:A:N7	7:1H:175:LYS:NZ	2.36	0.73
27:25:40:LYS:NZ	27:25:44:THR:O	2.22	0.73
1:1A:2466:C:H5''	31:19:6:SER:HB3	1.71	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1264:G:OP1	27:25:19:ARG:NH1	2.19	0.73
1:2A:2129:C:N4	1:2A:2159:G:H1	1.86	0.72
1:2A:2133:G:O2'	1:2A:2157:G:N2	2.21	0.72
11:1P:42:SER:O	60:1P:308:HOH:O	2.06	0.72
1:1A:1568:G:H5''	3:1D:61:LEU:HD13	1.72	0.72
1:1A:613:G:N2	1:1A:614(C):A:O2'	2.22	0.72
1:1A:994:C:OP1	16:1U:53:ARG:NH2	2.22	0.72
19:2X:8:ILE:O	24:22:36:ARG:NH2	2.23	0.72
1:2A:309:G:N3	1:2A:329:G:O2'	2.23	0.72
25:13:10:LYS:NZ	25:13:15:TYR:OH	2.21	0.72
26:14:16:CYS:SG	26:14:17:GLY:N	2.62	0.72
1:2A:1920:4OC:HM22	1:2A:1921:G:H5'	1.72	0.72
1:2A:765:G:H1	1:2A:812:C:HO2'	84.40	0.72
1:1A:1159:U:O2	1:1A:1161:C:N4	8.05	0.72
1:1A:2267:A:H5''	1:1A:2268:A:H5'	1.71	0.72
1:2A:642:G:N2	1:2A:645:C:OP2	2.23	0.72
1:2A:1119:C:H2'	1:2A:1120:G:C8	3.57	0.71
1:2A:1859:A:N6	1:2A:1883:G:O2'	2.23	0.71
2:2B:71:C:O2	2:2B:106:G:N2	2.21	0.71
31:29:22:ARG:HH11	31:29:35:ARG:HD2	1.54	0.71
1:2A:615:G:OP2	5:2F:43:LYS:NZ	2.22	0.71
1:2A:1771:C:OP1	60:2A:6246:HOH:O	2.08	0.71
1:1A:1900:A:OP2	60:1A:6567:HOH:O	2.08	0.71
1:2A:2365:G:O6	30:28:43:GLN:NE2	2.23	0.71
1:1A:34:C:H2'	1:1A:35:G:H8	4.74	0.71
1:1A:2612:C:OP2	27:15:2:ALA:N	2.24	0.71
1:2A:2592:G:N7	60:2A:4506:HOH:O	2.24	0.71
26:24:16:CYS:SG	26:24:17:GLY:N	2.64	0.71
1:1A:2409:G:N7	60:1A:4861:HOH:O	2.24	0.70
1:1A:1997:G:OP2	60:1A:6076:HOH:O	2.09	0.70
6:1G:43:LEU:HD11	6:1G:153:ARG:HD2	1.73	0.70
1:1A:2296:U:OP2	14:1S:9:ARG:NH2	2.24	0.70
1:2A:481:G:N7	60:2A:3916:HOH:O	2.24	0.70
1:1A:2138:C:N3	1:1A:2153:G:N2	2.37	0.70
1:1A:2067:G:O6	1:1A:2443:C:N4	2.20	0.70
1:2A:1568:G:H5''	3:2D:61:LEU:HD13	1.73	0.70
10:2O:35:VAL:HG11	10:2O:103:ALA:HB3	1.73	0.70
1:1A:2124:G:H1	1:1A:2174:C:H42	1.38	0.70
4:1E:11:MET:HG2	4:1E:24:THR:HB	1.73	0.70
6:1G:142:PRO:HB2	26:14:31:ILE:HG21	1.71	0.70
1:1A:218:A:N7	60:1A:6409:HOH:O	2.23	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2G:18:GLU:HG2	6:2G:175:LEU:HD21	1.74	0.70
1:2A:907:U:O2'	12:2Q:101:ARG:NH2	2.24	0.70
1:2A:2150:U:H2'	1:2A:2151:G:H8	1.55	0.70
1:1A:1918:A:N6	60:1A:6381:HOH:O	2.24	0.70
1:1A:197:A:N6	1:1A:2430:A:O2'	2.25	0.70
11:1P:47:ASP:OD2	11:1P:49:ARG:NH2	2.24	0.70
1:2A:1385:G:O2'	1:2A:1396:U:O2	2.10	0.70
1:2A:2677:G:N3	60:2A:3915:HOH:O	2.24	0.70
1:1A:1993:U:OP2	60:1E:419:HOH:O	2.10	0.70
1:2A:1356:G:O6	60:2A:6213:HOH:O	2.09	0.70
1:2A:2296:U:OP2	14:2S:9:ARG:NH2	2.24	0.70
10:1O:75:SER:OG	15:1T:74:ARG:NH1	2.25	0.69
19:1X:27:THR:HG23	19:1X:80:ILE:HG12	1.74	0.69
1:2A:1376:C:OP2	60:2A:4188:HOH:O	2.10	0.69
1:2A:2198:A:OP1	8:2I:33:ARG:NH2	2.25	0.69
1:2A:2736:G:N2	1:2A:2768:C:O2	2.15	0.69
13:2R:67:LEU:HD13	13:2R:76:VAL:HG21	1.74	0.69
1:1A:2125:G:N1	1:1A:2172:U:OP1	2.25	0.69
1:2A:1015:G:H2'	1:2A:1016:G:H8	1.57	0.69
25:13:8:LEU:HG	25:13:31:LEU:HD23	1.75	0.69
60:2A:4476:HOH:O	3:2D:237:GLU:OE1	2.11	0.69
1:2A:855:G:O2'	22:20:27:GLU:OE1	2.09	0.69
1:2A:271(Z):C:OP2	60:2A:5971:HOH:O	2.11	0.69
1:1A:987:G:O2'	1:1A:1000:A:N3	2.25	0.69
4:1E:119:ARG:HD2	4:1E:160:TYR:HB2	1.75	0.69
21:2Z:5:LEU:HB2	21:2Z:47:VAL:HG21	1.75	0.69
1:1A:1058:G:N2	1:1A:1080:C:N3	2.40	0.69
1:1A:769:G:N7	60:1A:6615:HOH:O	2.24	0.69
1:2A:760:G:OP1	60:2A:6024:HOH:O	2.10	0.69
1:2A:2129:C:H42	1:2A:2159:G:H1	1.40	0.69
2:2B:38:C:H2'	2:2B:39:A:H8	1.56	0.69
1:1A:1514:U:O2'	1:1A:1558:A:OP2	2.10	0.69
1:1A:80:G:N7	60:1A:5405:HOH:O	2.25	0.69
1:1A:968:G:N7	60:1A:4113:HOH:O	2.26	0.69
1:2A:2137:C:H42	1:2A:2154:G:H1	1.38	0.69
1:1A:1971:A:OP2	3:1D:242:ARG:NH2	2.26	0.69
1:2A:1816:G:O6	3:2D:35:LYS:NZ	2.23	0.69
1:2A:392:C:H5''	1:2A:409:C:H5''	1.75	0.69
5:2F:64:ILE:HG21	5:2F:78:ILE:HG23	1.75	0.68
4:2E:34:VAL:HG21	4:2E:78:LEU:HD23	1.75	0.68
1:2A:2171:A:N3	1:2A:2172:U:N3	2.41	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2261:C:OP1	22:20:19:LYS:NZ	2.24	0.68
1:2A:1568:G:H5'	3:2D:60:ARG:HA	1.76	0.68
4:1E:5:LEU:HD21	4:1E:79:ARG:HB2	1.74	0.68
6:1G:122:PRO:HB3	6:1G:170:ARG:HH12	1.57	0.68
1:1A:1338:G:O6	19:1X:62:LYS:NZ	2.26	0.68
21:1Z:156:LYS:HE3	21:1Z:158:PRO:HD3	1.75	0.68
1:1A:1859:A:N6	1:1A:1883:G:O2'	2.27	0.68
1:2A:2349:G:H1	1:2A:2368:C:H42	1.39	0.68
1:2A:361:G:N7	60:2A:5854:HOH:O	2.27	0.68
1:2A:807:U:OP2	11:2P:41:ARG:NH2	2.27	0.68
1:2A:612:C:H42	1:2A:628:G:H1	45.70	0.68
2:1B:92:C:OP1	21:1Z:79:ARG:NH1	2.26	0.68
21:1Z:157:LEU:HB3	21:1Z:161:VAL:HG11	1.75	0.68
1:2A:2114:A:N6	1:2A:2119:A:N7	2.41	0.68
1:2A:266:G:H5''	1:2A:268:C:H41	11.66	0.68
1:1A:2011:U:OP1	18:1W:42:ARG:NH1	2.27	0.68
12:1Q:138:ASP:OD1	12:1Q:138:ASP:N	2.25	0.68
1:1A:1082:U:C4	1:1A:1086:A:N1	2.62	0.67
1:1A:1568:G:H4'	3:1D:59:LYS:HG3	1.77	0.67
3:1D:26:LYS:NZ	3:1D:30:GLU:OE1	2.27	0.67
17:1V:40:LEU:HB2	17:1V:46:VAL:HG23	1.75	0.67
20:1Y:102:CYS:SG	20:1Y:103:GLY:N	2.67	0.67
10:2O:78:ARG:NH2	15:2T:73:GLU:OE1	2.25	0.67
1:2A:641:C:H42	1:2A:647:G:H1	1.42	0.67
1:2A:631:A:OP1	11:2P:65:ARG:NH1	2.26	0.67
1:1A:1453:U:OP1	13:1R:77:ARG:NH1	2.25	0.67
1:2A:1449:A:O2'	1:2A:1529:G:N2	2.27	0.67
1:1A:601:C:O2'	1:1A:605:C:OP1	2.09	0.67
1:1A:586:A:H5'	5:1F:89:VAL:HG21	1.76	0.67
1:2A:2104:G:N2	1:2A:2185:C:N3	2.34	0.67
21:2Z:156:LYS:HE3	21:2Z:158:PRO:HD3	1.76	0.67
1:1A:2285:C:OP2	28:16:6:ARG:NH1	2.27	0.67
8:1I:92:VAL:HG13	8:1I:120:ILE:HB	1.76	0.67
1:2A:2055:C:N3	60:2A:5736:HOH:O	2.28	0.67
1:2A:2682:U:OP2	60:2A:4295:HOH:O	2.12	0.67
1:2A:72:U:OP1	60:2A:5997:HOH:O	2.12	0.67
1:2A:1783:A:OP1	60:2A:3903:HOH:O	2.13	0.67
1:2A:1857:G:O2'	1:2A:1885:A:N6	2.28	0.67
1:2A:2079:U:O3'	23:21:35:THR:OG1	2.12	0.67
1:2A:307:G:H21	1:2A:330:A:H62	1.43	0.67
7:2H:20:ALA:HB3	7:2H:23:ARG:HG3	1.77	0.67

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1599:C:OP1	60:2A:3902:HOH:O	2.12	0.67
1:2A:18:C:OP2	60:2A:3901:HOH:O	2.11	0.67
1:2A:1890:A:OP2	60:2A:5311:HOH:O	2.13	0.67
1:2A:987:G:O2'	1:2A:1000:A:N3	2.26	0.67
1:1A:1174:A:H4'	1:1A:1175:U:OP1	1.93	0.66
16:2U:89:GLU:HB3	17:2V:38:LEU:HD21	1.76	0.66
1:1A:942:G:O2'	1:1A:1189:A:N3	2.27	0.66
1:2A:34:C:H2'	1:2A:35:G:H8	3.97	0.66
1:1A:2140:C:N3	1:1A:2151:G:O6	2.29	0.66
13:1R:67:LEU:HD13	13:1R:76:VAL:HG21	1.77	0.66
1:2A:2547:U:O2	10:2O:23:ARG:NH2	2.28	0.66
16:1U:75:ASN:OD1	16:1U:78:THR:OG1	2.12	0.66
1:2A:821:A:N1	60:2A:4680:HOH:O	2.28	0.66
11:1P:63:PRO:HB2	30:18:30:ARG:HH21	1.59	0.66
1:1A:2444:G:N7	60:1A:4665:HOH:O	2.28	0.66
16:2U:73:GLY:O	60:2U:301:HOH:O	2.14	0.66
1:1A:1253:A:OP1	60:1A:6970:HOH:O	2.14	0.66
1:1A:881:G:N2	1:1A:897:C:N3	2.43	0.66
1:1A:1398:C:OP1	19:1X:53:LYS:NZ	2.29	0.66
20:1Y:15:VAL:HG21	20:1Y:42:VAL:HG11	1.76	0.66
1:2A:248:G:OP1	60:2A:6306:HOH:O	2.13	0.66
1:1A:2469:A:O3'	12:1Q:56:ARG:NH2	2.28	0.66
17:2V:27:ALA:O	17:2V:64:HIS:NE2	2.28	0.66
3:1D:41:GLY:O	3:1D:43:ARG:NH1	2.28	0.66
12:1Q:109:VAL:HG13	12:1Q:113:GLN:HB3	1.78	0.66
60:1A:6687:HOH:O	19:1X:56:THR:O	2.14	0.66
1:1A:1010:A:OP2	60:1A:5436:HOH:O	2.13	0.66
1:1A:449:A:N7	60:1A:6875:HOH:O	2.28	0.65
1:2A:2351:G:HO2'	1:2A:2352:A:H8	1.43	0.65
21:2Z:4:ARG:HG2	21:2Z:58:VAL:HB	1.77	0.65
1:2A:2448:A:OP2	60:2A:5622:HOH:O	2.13	0.65
1:2A:2526:G:N3	31:29:1:MET:N	2.45	0.65
1:2A:424:G:N7	60:2A:6265:HOH:O	2.29	0.65
4:2E:116:VAL:HG21	4:2E:138:PRO:HB3	1.77	0.65
24:12:1:MET:SD	24:12:56:GLN:NE2	2.70	0.65
1:1A:1541:G:OP2	60:1A:6220:HOH:O	2.12	0.65
1:1A:764:A:OP1	3:1D:208:LYS:NZ	2.29	0.65
1:2A:615:G:OP1	5:2F:40:GLN:NE2	2.27	0.65
1:2A:2690:C:OP2	13:2R:17:ARG:NH2	2.30	0.65
1:2A:1753:G:H5''	15:2T:95:ARG:HD2	1.77	0.65
1:1A:1466:G:HO2'	1:1A:1546:C:HO2'	1.39	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2328:A:H2'	1:1A:2329:G:C8	2.31	0.65
1:2A:1223:G:N2	1:2A:1226:A:OP2	2.22	0.65
1:1A:2206:G:H3'	1:1A:2207:G:C8	2.32	0.65
1:1A:944:G:N7	60:1A:4117:HOH:O	2.29	0.65
1:2A:1443:G:N7	60:2A:5809:HOH:O	2.29	0.65
1:2A:2027:G:N7	60:2A:4453:HOH:O	2.30	0.65
1:2A:2587:A:OP1	60:2A:4475:HOH:O	2.14	0.65
1:2A:995:C:O2	9:2N:3:THR:OG1	2.12	0.65
1:2A:2010:G:H5''	18:2W:42:ARG:HB2	1.79	0.65
1:1A:576:U:H2'	1:1A:577:G:C8	2.32	0.65
1:1A:859:G:O2'	1:1A:916:G:O6	2.15	0.65
1:2A:1568:G:N7	60:2A:5771:HOH:O	2.29	0.65
3:2D:242:ARG:HD3	3:2D:246:PRO:HG3	1.79	0.65
1:1A:2278:A:OP2	22:10:12:ASN:ND2	2.30	0.65
1:1A:2791:C:H2'	1:1A:2792:G:H8	1.60	0.65
4:1E:144:ARG:O	4:1E:146:THR:N	2.27	0.65
19:1X:2:LYS:NZ	19:1X:38:GLU:OE2	2.28	0.65
1:2A:2721:A:OP1	60:2A:4295:HOH:O	2.14	0.65
1:2A:975:C:OP1	60:2A:5954:HOH:O	2.15	0.65
1:1A:548:A:H61	17:1V:19:LYS:H	1.44	0.65
1:2A:605:C:O2	1:2A:657:U:O2'	2.14	0.65
4:2E:36:ARG:HG2	4:2E:47:VAL:HG12	1.79	0.65
1:1A:1094:U:N3	1:1A:1097:U:OP2	2.30	0.64
1:1A:652(D):C:H42	1:1A:652(U):G:H1	1.44	0.64
1:1A:2553:G:N7	60:1A:6516:HOH:O	2.29	0.64
1:2A:2017:U:OP2	60:2A:4283:HOH:O	2.15	0.64
1:2A:2666:C:N3	7:2H:152:ARG:NH2	2.45	0.64
1:2A:195:A:OP1	11:2P:46:LYS:NZ	2.30	0.64
13:2R:29:LEU:HB3	13:2R:75:LEU:HD11	1.79	0.64
1:2A:570:G:O6	60:2A:5975:HOH:O	2.14	0.64
7:1H:164:TYR:HB2	7:1H:167:GLU:HB2	1.79	0.64
9:1N:34:LEU:HD21	9:1N:120:LEU:HB2	1.77	0.64
1:2A:827:U:OP1	60:2A:4985:HOH:O	2.14	0.64
1:1A:1720:U:H3	1:1A:1742:G:H1	1.44	0.64
6:1G:18:GLU:HG3	6:1G:22:ARG:HD2	1.79	0.64
1:2A:801:G:O6	5:2F:53:THR:OG1	2.16	0.64
11:1P:59:LEU:HD11	30:18:10:ALA:HB2	1.78	0.64
1:1A:1058:G:N1	1:1A:1080:C:N4	2.46	0.64
1:1A:34:C:H2'	1:1A:35:G:C8	5.56	0.64
11:1P:121:LYS:HE2	11:1P:123:LEU:HD11	1.79	0.64
1:2A:2674:G:H5'	10:2O:26:LYS:HE2	1.80	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2685:G:OP2	15:1T:51:ARG:NH2	2.31	0.64
1:1A:880:G:H2'	1:1A:881:G:H8	1.63	0.64
1:1A:975:C:O2	60:1A:5969:HOH:O	2.14	0.64
6:1G:125:PHE:O	60:1G:304:HOH:O	2.15	0.64
7:1H:137:ASP:HB3	7:1H:140:LYS:HB3	1.80	0.64
1:2A:1827:C:OP2	3:2D:222:ARG:NH1	2.29	0.64
1:2A:2037:G:N7	60:2A:4814:HOH:O	2.29	0.64
1:2A:854:G:H2'	1:2A:855:G:H8	1.63	0.64
1:1A:1850:G:H1	1:1A:1892:C:H42	1.47	0.64
1:1A:2484:G:H1'	12:1Q:124:LYS:HG3	1.79	0.64
4:2E:28:ALA:HB3	4:2E:93:VAL:HG12	1.80	0.64
3:2D:106:ILE:HD11	3:2D:144:ALA:HB2	1.80	0.63
1:2A:746:A:O2'	1:2A:2611:U:O2'	2.16	0.63
1:2A:1422:G:H5''	10:2O:48:PRO:HB3	98.38	0.63
1:1A:191:A:N1	60:1A:5471:HOH:O	2.30	0.63
1:1A:2821:A:OP1	4:1E:110:GLY:N	2.26	0.63
1:2A:2163:C:OP1	1:2A:2165:G:N2	2.31	0.63
1:2A:2327:A:H2'	1:2A:2328:A:C8	2.33	0.63
6:2G:127:GLY:N	6:2G:166:ASP:OD2	2.31	0.63
1:1A:272(F):C:H42	1:1A:363(D):G:H1	1.46	0.63
12:2Q:109:VAL:HG13	12:2Q:113:GLN:HB3	1.80	0.63
1:2A:2805:G:H2'	1:2A:2807:G:C8	2.34	0.63
2:2B:43:C:OP1	26:24:6:HIS:NE2	2.28	0.63
19:1X:72:LYS:NZ	19:1X:75:ASP:OD1	2.31	0.63
4:2E:1:MET:HE3	4:2E:199:ARG:HB3	1.80	0.63
1:1A:2163:C:OP1	1:1A:2165:G:N2	2.31	0.63
15:1T:112:ARG:HG3	15:1T:115:ARG:HH21	1.63	0.63
1:2A:2280:G:N7	60:20:205:HOH:O	2.30	0.63
1:1A:1366:A:OP1	23:11:3:LYS:NZ	2.31	0.63
1:1A:140:G:N3	1:1A:142:A:N6	2.44	0.63
1:2A:2143:C:N3	1:2A:2148:G:N2	2.40	0.63
12:1Q:141:GLN:NE2	21:1Z:74:VAL:O	2.30	0.63
1:2A:1546:C:H5'	1:2A:1547:C:H5'	1.81	0.63
1:2A:40:C:H42	1:2A:438:G:H1	1.47	0.63
1:2A:848:G:OP2	1:2A:928:G:N2	2.29	0.63
24:12:22:GLU:OE2	24:12:68:ARG:NH2	2.32	0.62
6:1G:101:ILE:HG22	6:1G:105:LYS:HE2	1.81	0.62
1:2A:1502:C:H2'	1:2A:1503:U:H6	1.64	0.62
1:2A:271(H):G:H2'	1:2A:271(I):G:H8	1.64	0.62
9:2N:26:LEU:HD23	9:2N:60:ILE:HD11	1.80	0.62
1:1A:1315:C:O2'	1:1A:1392:A:N3	2.30	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:396:G:H1'	23:11:42:GLN:HB3	1.80	0.62
3:2D:242:ARG:H	3:2D:242:ARG:HH11	1.47	0.62
7:2H:125:VAL:HG12	7:2H:131:VAL:HG22	1.80	0.62
12:2Q:11:LYS:HD3	12:2Q:87:LYS:HG2	1.79	0.62
1:1A:58:G:O2'	1:1A:73:A:N1	2.31	0.62
1:2A:1446:C:O2	1:2A:1545:A:O2'	2.17	0.62
1:1A:1509(A):A:H3'	1:1A:1509(B):A:H8	1.65	0.62
12:1Q:43:THR:HG22	12:1Q:94:VAL:HG12	1.82	0.62
1:2A:1007:C:N3	1:2A:1022:G:O6	16.82	0.62
1:1A:1173:G:N2	1:1A:1177:A:OP2	2.33	0.62
8:1I:129:THR:HG22	8:1I:139:GLN:HE22	1.65	0.62
1:2A:1420:U:O2'	1:2A:1421:G:OP1	2.13	0.62
16:2U:79:PHE:HE2	16:2U:95:LEU:HD21	1.65	0.62
1:1A:1053:C:H42	1:1A:1106:G:H1	1.46	0.62
1:1A:2141:G:O6	1:1A:2150:U:O2	2.16	0.62
6:1G:112:PRO:HG3	26:14:43:TYR:HE2	1.64	0.62
6:2G:64:THR:HB	6:2G:94:LEU:HD21	1.80	0.62
1:1A:1048:A:OP2	1:1A:1109:C:N4	2.33	0.62
1:2A:2126:A:N6	1:2A:2162:G:O2'	2.31	0.62
1:2A:463:G:N2	1:2A:466:A:OP2	2.31	0.62
1:1A:602:G:O2'	1:1A:655:A:N6	2.33	0.62
26:24:24:THR:OG1	26:24:25:TYR:N	2.33	0.62
1:1A:2095:C:H42	1:1A:2194:G:H1	1.45	0.62
1:2A:2818:G:OP2	13:2R:42:LYS:NZ	2.31	0.62
1:1A:1267:U:OP1	60:1A:5943:HOH:O	2.16	0.62
1:2A:2630:G:H2'	1:2A:2631:G:C8	2.35	0.62
2:2B:4:C:H42	2:2B:117:G:H1	1.48	0.62
1:1A:463:G:N2	1:1A:466:A:OP2	2.32	0.61
1:1A:785:G:N2	1:1A:797:C:O2	28.02	0.61
1:2A:597:U:H2'	1:2A:598:G:C8	2.34	0.61
5:2F:101:LEU:O	5:2F:106:ARG:NH1	2.32	0.61
1:2A:2655:G:O2'	1:2A:2664:G:O6	2.18	0.61
1:2A:662:G:O2'	1:2A:836:G:OP1	26.36	0.61
12:2Q:85:LYS:HG2	22:20:7:LEU:HB3	1.82	0.61
17:2V:40:LEU:HB2	17:2V:46:VAL:HG22	1.82	0.61
25:23:7:LYS:NZ	25:23:32:GLN:O	2.32	0.61
8:2I:77:LEU:HB3	8:2I:142:VAL:HG22	1.80	0.61
25:23:7:LYS:HB2	25:23:34:GLU:HG3	1.81	0.61
1:2A:30:G:O2'	1:2A:1214:A:N3	2.33	0.61
1:2A:682:G:N2	1:2A:708:C:O2	69.58	0.61
5:2F:12:LEU:HB2	5:2F:124:LEU:HD11	1.81	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:2I:3:VAL:HG12	8:2I:38:LEU:HA	1.81	0.61
30:18:62:LEU:HB3	30:18:65:GLU:HG3	1.83	0.61
1:1A:1176:G:H1'	1:1A:1177:A:H5''	1.82	0.61
1:1A:2146:C:H5''	1:1A:2147:G:C5	2.35	0.61
1:2A:1121:C:N4	60:2A:6111:HOH:O	2.28	0.61
1:2A:942:G:O2'	1:2A:1189:A:N3	2.34	0.61
1:2A:184:C:H2'	1:2A:185:U:C6	2.35	0.61
30:18:6:THR:HG22	30:18:63:PRO:HD2	1.81	0.61
60:1A:6075:HOH:O	4:1E:127:ASP:OD2	2.16	0.61
1:1A:1300:U:H4'	1:1A:1301:A:H5''	1.82	0.61
1:1A:2250:G:OP1	12:1Q:85:LYS:NZ	2.27	0.61
1:1A:787:U:OP1	60:1A:4900:HOH:O	2.16	0.61
1:2A:468:G:O6	29:27:39:ARG:NH1	2.31	0.61
1:2A:1689:A:OP2	1:2A:1698:A:N6	2.34	0.61
1:2A:2121:G:N2	1:2A:2177:C:N3	2.44	0.61
1:2A:245:G:O6	30:28:8:LYS:NZ	2.33	0.61
1:2A:2572:A:OP1	1:2A:2574:G:O2'	2.17	0.61
1:2A:297:C:OP1	20:2Y:87:LYS:NZ	2.30	0.61
1:1A:1815:A:OP1	60:1A:4102:HOH:O	2.16	0.61
1:1A:2131:G:H5''	1:1A:2132:U:H3'	1.83	0.61
1:1A:2327:A:H2'	1:1A:2328:A:C8	2.35	0.61
1:2A:500:G:N1	1:2A:503:A:OP2	2.32	0.61
11:2P:62:LEU:O	30:28:13:ARG:NH1	2.34	0.61
1:1A:2291:U:OP1	1:1A:2380:C:O2'	2.18	0.61
6:1G:131:TYR:HB3	6:1G:159:VAL:HG23	1.82	0.61
1:2A:1253:A:N7	60:2A:4393:HOH:O	2.31	0.61
31:19:1:MET:HE2	31:19:33:LYS:HD2	1.82	0.60
1:2A:597:U:H2'	1:2A:598:G:H8	1.65	0.60
1:1A:218:A:C2	1:1A:235:U:H4'	2.36	0.60
1:1A:744:G:OP1	4:1E:132:HIS:ND1	2.34	0.60
5:1F:24:LEU:HD23	5:1F:115:ALA:HA	1.83	0.60
1:2A:1859:A:N6	1:2A:1883:G:HO2'	1.98	0.60
15:2T:102:ILE:HA	15:2T:105:LEU:HD12	1.83	0.60
1:1A:2830:G:OP1	4:1E:76:ARG:NH1	2.34	0.60
1:1A:467:G:N7	29:17:39:ARG:NH2	2.49	0.60
1:2A:2162:G:H4'	1:2A:2172:U:H2'	1.83	0.60
1:2A:517:C:OP1	27:25:16:ARG:NH2	2.34	0.60
6:2G:11:TYR:OH	6:2G:16:ARG:NH1	2.34	0.60
22:10:10:THR:HG23	22:10:12:ASN:H	1.65	0.60
1:1A:729:G:C6	3:1D:208:LYS:HB2	2.36	0.60
1:2A:200:U:O2	1:2A:386:G:N2	2.34	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2161:C:H2'	1:2A:2162:G:O4'	2.01	0.60
1:2A:2123:G:H1	1:2A:2175:C:H42	1.50	0.60
17:2V:8:GLY:O	17:2V:10:LYS:NZ	2.32	0.60
1:1A:1093:G:H3'	1:1A:1094:U:H5''	1.84	0.60
1:1A:2127:G:N2	1:1A:2161:C:N3	2.50	0.60
1:1A:811:U:OP1	60:1A:6683:HOH:O	2.16	0.60
20:2Y:102:CYS:SG	20:2Y:103:GLY:N	2.75	0.60
26:24:40:HIS:HB3	26:24:43:TYR:HD2	1.67	0.60
1:2A:1032:A:N6	1:2A:1122:G:H1	1.97	0.60
1:2A:783:A:OP2	60:2A:6227:HOH:O	2.16	0.60
1:2A:1012:U:H5	9:2N:28:THR:HG21	1.66	0.60
1:1A:2107:C:H42	1:1A:2182:G:H1	1.50	0.60
13:1R:33:ARG:NH2	27:15:57:VAL:O	2.34	0.60
1:2A:2532:G:O2'	1:2A:2657:A:N6	2.31	0.60
1:2A:988:A:N7	60:2A:4370:HOH:O	2.32	0.60
2:2B:14:U:OP2	2:2B:70:C:O2'	2.18	0.60
21:2Z:141:VAL:HG13	21:2Z:142:SER:H	1.67	0.60
5:1F:185:ASP:OD1	5:1F:188:ARG:NH1	2.32	0.60
13:1R:12:ARG:O	13:1R:17:ARG:NH1	2.35	0.60
3:2D:152:GLY:O	60:2D:401:HOH:O	2.16	0.60
1:1A:2658:C:O2	1:1A:2663:G:N2	2.34	0.60
5:1F:158:THR:O	5:1F:164:ARG:NH1	2.35	0.60
24:22:35:LEU:HD12	24:22:53:LEU:HD12	1.82	0.60
15:2T:16:ARG:NH2	15:2T:18:ASP:OD2	2.35	0.60
1:1A:2693:A:H2'	1:1A:2694:G:C8	2.37	0.59
21:1Z:24:LEU:HB2	21:1Z:41:LEU:HD12	1.84	0.59
21:1Z:91:LEU:HD23	21:1Z:130:PRO:HB3	1.84	0.59
1:2A:785:G:OP2	60:2A:6123:HOH:O	2.15	0.59
1:1A:1053:C:N4	1:1A:1106:G:H1	1.98	0.59
1:1A:1508:A:O2'	1:1A:1509:C:OP1	2.18	0.59
5:1F:185:ASP:HA	5:1F:188:ARG:HD3	1.83	0.59
6:1G:34:LEU:HD23	6:1G:161:THR:HG22	1.84	0.59
1:2A:1116:C:H2'	1:2A:1117:G:H8	1.67	0.59
1:2A:628:G:H2'	1:2A:629:G:C8	2.37	0.59
6:2G:56:ALA:HA	6:2G:59:GLU:HG2	1.83	0.59
11:2P:124:LYS:HE3	11:2P:146:VAL:HG21	1.83	0.59
1:1A:2226:C:OP2	60:1A:6236:HOH:O	2.15	0.59
1:1A:220:G:O2'	1:1A:233:A:N3	2.31	0.59
5:1F:155:LEU:HB2	5:1F:189:THR:HG21	1.84	0.59
18:1W:18:ARG:HG3	18:1W:76:VAL:HB	1.84	0.59
1:2A:1446:C:H42	1:2A:1465:G:H1	1.50	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2683:C:O2	10:2O:70:LYS:NZ	2.21	0.59
1:2A:819:A:OP2	1:2A:1187:G:N2	2.25	0.59
13:2R:19:ALA:O	13:2R:23:ASN:ND2	2.35	0.59
17:2V:29:PRO:HG3	17:2V:63:GLY:HA2	1.82	0.59
1:1A:2693:A:H2'	1:1A:2694:G:H8	1.67	0.59
9:1N:97:ARG:HA	9:1N:100:GLU:HB2	1.84	0.59
13:1R:38:VAL:HG12	13:1R:42:LYS:HE3	1.83	0.59
1:2A:2137:C:N4	1:2A:2154:G:N1	2.47	0.59
1:2A:1530:C:O2'	1:2A:1531:C:O5'	2.19	0.59
6:2G:15:VAL:HG22	6:2G:175:LEU:HB3	1.85	0.59
1:1A:784:A:O4'	3:1D:227:ASN:ND2	2.35	0.59
4:1E:128:SER:OG	4:1E:129:HIS:N	2.35	0.59
1:2A:1422:G:O3'	10:2O:49:ARG:NH1	99.20	0.59
1:2A:2693:A:H2'	1:2A:2694:G:H8	1.68	0.59
1:2A:271(R):G:H2'	1:2A:271(S):G:C8	2.37	0.59
5:2F:110:LEU:HD11	5:2F:181:LEU:HG	1.84	0.59
1:2A:1187:G:H5'	17:2V:81:TYR:CE1	2.37	0.59
1:1A:2741:A:OP1	31:19:22:ARG:NH2	2.36	0.59
1:1A:1593:G:H2'	1:1A:1594:G:C8	2.37	0.59
1:1A:2635:C:O2'	4:1E:80:GLU:OE2	2.19	0.59
1:2A:2787:C:H1'	4:2E:62:PRO:HG3	1.84	0.59
17:2V:43:GLU:OE1	17:2V:43:GLU:N	2.35	0.59
26:14:58:ARG:HD2	26:14:58:ARG:H	1.68	0.59
1:1A:2791:C:H2'	1:1A:2792:G:C8	2.38	0.59
8:1I:31:LEU:HD21	8:1I:38:LEU:HD23	1.85	0.59
12:1Q:16:ARG:HG3	12:1Q:18:LYS:HG3	1.84	0.59
22:20:10:THR:HG22	22:20:12:ASN:H	1.67	0.59
28:26:11:LEU:N	28:26:21:TYR:O	2.36	0.59
1:2A:1711:C:H2'	1:2A:1712:C:H6	1.67	0.59
1:2A:2199:A:N1	1:2A:2226:C:N4	2.51	0.59
11:2P:126:VAL:HG12	11:2P:148:LEU:HD22	1.85	0.59
1:1A:636:G:OP1	11:1P:132:LYS:NZ	2.32	0.59
1:2A:1324:G:O2'	1:2A:1326:U:OP2	2.18	0.59
1:2A:1475:G:OP1	1:2A:1700:A:N6	72.16	0.59
1:2A:2532:G:HO2'	1:2A:2657:A:H61	1.51	0.59
1:2A:637:A:OP1	11:2P:133:SER:OG	2.21	0.59
3:2D:75:ILE:HG21	3:2D:99:ASP:HB2	1.85	0.59
1:2A:1266:G:O5'	18:2W:15:ARG:NH2	2.35	0.59
1:1A:1506:C:H2'	1:1A:1507:A:H8	1.67	0.59
1:2A:857:C:OP2	22:20:77:ARG:NH2	2.35	0.59
1:2A:2857:G:N2	1:2A:2860:A:OP2	2.36	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:959:A:N3	1:2A:2457:U:O2'	2.35	0.59
1:2A:2744:G:N2	7:2H:143:GLN:OE1	2.34	0.59
1:1A:1568:G:H5'	3:1D:60:ARG:HA	1.84	0.58
6:2G:37:VAL:HG22	6:2G:159:VAL:HG12	1.85	0.58
8:2I:5:LEU:HD11	8:2I:19:VAL:HG22	1.85	0.58
30:18:33:ASN:HA	30:18:36:LYS:HD2	1.85	0.58
1:1A:686:G:O5'	29:17:11:LYS:NZ	2.36	0.58
6:1G:45:GLU:OE2	60:1G:301:HOH:O	2.17	0.58
1:2A:1671:U:HO2'	1:2A:1673:U:H5	1.49	0.58
1:2A:1777:U:H2'	1:2A:1778:U:H6	1.68	0.58
16:2U:27:LEU:HD22	16:2U:31:SER:HB2	1.85	0.58
1:1A:2140:C:H42	1:1A:2150:U:H3	1.49	0.58
1:1A:2547:U:O2	10:1O:23:ARG:NH2	2.36	0.58
1:1A:54:G:O6	60:1A:4623:HOH:O	2.16	0.58
1:2A:1226:A:OP1	17:2V:84:LYS:NZ	2.21	0.58
1:2A:2151:G:H2'	1:2A:2152:G:H8	1.67	0.58
15:2T:30:VAL:HG22	15:2T:86:ILE:HG12	1.84	0.58
1:1A:61:G:H5'	24:12:50:ILE:HG21	1.84	0.58
1:1A:2756:U:H5''	31:19:19:ARG:HG2	1.86	0.58
19:1X:50:LYS:HG2	19:1X:84:ALA:HB2	1.85	0.58
1:2A:108:U:H2'	1:2A:109:G:C8	2.39	0.58
1:2A:1141:U:OP2	9:2N:63:THR:OG1	2.22	0.58
1:1A:1173:G:O2'	1:1A:1174:A:O4'	2.22	0.58
1:2A:1002:G:H1	1:2A:1038:C:H42	42.46	0.58
1:2A:535:C:H2'	1:2A:536:A:C8	2.38	0.58
1:2A:740:U:OP2	60:2A:3903:HOH:O	2.16	0.58
7:2H:11:VAL:HG21	7:2H:50:VAL:HG23	1.84	0.58
1:1A:27:G:N2	1:1A:512:G:H1'	2.18	0.58
7:1H:20:ALA:HB3	7:1H:23:ARG:HG3	1.85	0.58
1:2A:1202:C:H42	1:2A:1243:G:H1	1.52	0.58
1:1A:2364:C:OP1	22:10:55:ARG:NH1	2.36	0.58
1:2A:2160:G:H2'	1:2A:2161:C:H5''	1.86	0.58
1:2A:2524:G:O6	60:2A:6317:HOH:O	2.15	0.58
1:1A:1218:C:H42	1:1A:1231:G:H1	1.52	0.58
1:1A:615:G:OP2	5:1F:43:LYS:NZ	2.30	0.58
21:1Z:10:ARG:NH2	21:1Z:26:GLY:O	2.36	0.58
1:2A:1864:U:OP1	1:2A:2410:G:O2'	2.22	0.58
1:2A:2176:A:H2'	1:2A:2177:C:C6	2.39	0.58
2:2B:24:G:N7	2:2B:56:G:H2'	2.19	0.58
1:2A:660:G:N2	11:2P:12:ALA:O	2.36	0.58
22:10:26:TYR:H	22:10:29:GLN:NE2	2.02	0.58

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2526:G:N3	31:19:1:MET:N	2.52	0.58
8:2I:4:ILE:HG12	8:2I:18:VAL:HG22	1.86	0.58
1:1A:1266:G:N2	1:1A:1269:A:OP2	13.45	0.57
1:1A:214:G:H21	1:1A:216:A:H1'	1.68	0.57
18:2W:10:VAL:HG12	18:2W:12:ILE:HG22	1.85	0.57
1:1A:1913:A:H4'	1:1A:1914:C:H5''	1.85	0.57
15:1T:127:ALA:C	15:1T:129:ARG:H	2.06	0.57
1:2A:1342:A:OP2	60:2A:6126:HOH:O	2.18	0.57
1:2A:586:A:H5'	5:2F:89:VAL:HG21	1.86	0.57
19:2X:2:LYS:NZ	19:2X:38:GLU:OE2	2.35	0.57
4:1E:56:PRO:HG3	4:1E:74:PRO:HG2	1.86	0.57
6:1G:47:LYS:HG3	6:1G:48:GLU:H	1.69	0.57
21:1Z:153:SER:HA	21:1Z:167:PRO:HB3	1.86	0.57
1:2A:2001:A:H2'	1:2A:2002:G:C8	2.39	0.57
1:2A:2140:C:N3	1:2A:2151:G:N2	2.43	0.57
1:2A:2110:G:H3'	1:2A:2111:C:H5'	1.85	0.57
1:2A:2691:C:HO2'	1:2A:2871:C:HO2'	1.52	0.57
3:2D:3:VAL:HG21	3:2D:203:ASN:HB2	1.86	0.57
1:1A:2000:G:O6	60:1A:6307:HOH:O	2.16	0.57
1:2A:2263:C:N4	22:20:15:ASP:OD1	2.37	0.57
11:2P:63:PRO:HG2	30:28:25:MET:HB2	1.86	0.57
1:2A:805:G:H5''	11:2P:38:GLN:HG3	1.86	0.57
5:1F:156:LEU:HD21	5:1F:163:VAL:HG12	1.86	0.57
1:2A:2238:G:OP2	60:2A:3905:HOH:O	2.18	0.57
1:1A:1422:G:H5''	10:1O:48:PRO:HB3	99.43	0.57
6:1G:11:TYR:HA	6:1G:15:VAL:HB	1.86	0.57
9:1N:121:LYS:HD3	9:1N:130:HIS:CE1	2.40	0.57
1:2A:1434:A:H61	1:2A:1558:A:H62	1.52	0.57
1:2A:2129:C:N3	1:2A:2159:G:N2	2.44	0.57
1:2A:970:C:O2'	1:2A:984:A:O2'	2.21	0.57
4:2E:116:VAL:HG13	4:2E:122:PHE:HB2	1.85	0.57
6:2G:11:TYR:HB2	6:2G:176:LEU:HD21	1.86	0.57
60:1A:7030:HOH:O	27:15:17:ASP:OD2	2.18	0.57
1:2A:2336:A:H61	22:20:43:THR:HG22	1.69	0.57
1:2A:1652:A:N6	13:2R:11:ASN:OD1	2.30	0.57
1:1A:2533:A:H2'	1:1A:2534:A:O4'	2.05	0.57
6:1G:138:GLN:HE22	6:1G:152:LEU:HA	1.70	0.57
3:2D:26:LYS:HB3	3:2D:83:GLU:HG2	1.87	0.57
1:1A:624:C:O2'	1:1A:657:U:OP1	2.21	0.57
2:1B:50:G:OP1	14:1S:63:THR:OG1	2.20	0.57
1:2A:2365:G:N7	30:28:39:LYS:NZ	2.51	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1F:182:ASN:ND2	5:1F:185:ASP:OD2	2.30	0.56
16:1U:44:ASN:HD21	17:1V:75:PHE:HB3	1.70	0.56
1:2A:1826:G:H4'	3:2D:242:ARG:NH2	2.20	0.56
7:2H:164:TYR:HB2	7:2H:167:GLU:HB2	1.87	0.56
10:2O:75:SER:OG	15:2T:74:ARG:NH1	2.38	0.56
1:1A:1853:A:H2'	1:1A:1854:A:C8	2.40	0.56
3:1D:142:VAL:HG22	3:1D:193:VAL:HA	1.86	0.56
4:1E:105:THR:OG1	4:1E:199:ARG:NH2	2.38	0.56
28:26:9:LEU:HA	28:26:54:ILE:HB	1.87	0.56
1:2A:1786:A:H1'	1:2A:1938:A:N6	2.20	0.56
1:2A:817:C:O2'	1:2A:839:U:OP1	2.21	0.56
1:1A:2314:C:H5''	6:1G:38:VAL:HG21	1.88	0.56
9:1N:73:THR:HG23	9:1N:82:LEU:HD11	1.87	0.56
12:2Q:81:VAL:HB	22:20:7:LEU:HD21	1.86	0.56
60:2A:4338:HOH:O	23:21:17:SER:OG	2.18	0.56
1:2A:117:G:OP2	1:2A:119:A:O2'	2.22	0.56
1:1A:2183:C:H2'	1:1A:2184:G:C8	2.38	0.56
1:2A:1309:G:O2'	1:2A:1611:C:O2'	2.21	0.56
1:2A:2111:C:N4	1:2A:2144:U:O2'	2.35	0.56
1:2A:1247:A:OP1	5:2F:95:ARG:NH2	2.39	0.56
9:2N:20:GLY:HA2	9:2N:61:ARG:HG3	1.87	0.56
1:1A:266:G:H2'	1:1A:266:G:N3	3.11	0.56
1:2A:1171:G:H22	1:2A:1178:C:H42	1.53	0.56
1:2A:2689:U:H4'	1:2A:2690:C:H5'	1.87	0.56
1:2A:271(R):G:H2'	1:2A:271(S):G:H8	1.69	0.56
1:1A:1769:G:O2'	1:1A:1958:C:OP1	2.20	0.56
1:2A:1165:U:H3	1:2A:1184:G:H1	1.52	0.56
1:2A:1754:C:H5	15:2T:96:ARG:HH22	1.53	0.56
1:2A:386:G:O2'	60:2A:6309:HOH:O	2.17	0.56
2:2B:41:U:H5	6:2G:70:VAL:H	1.53	0.56
6:2G:37:VAL:O	6:2G:94:LEU:N	2.38	0.56
12:2Q:116:GLU:OE2	12:2Q:119:ARG:NH2	2.37	0.56
1:1A:527:C:OP1	60:1A:5440:HOH:O	2.18	0.56
1:1A:801:G:OP2	60:1A:4612:HOH:O	2.17	0.56
7:1H:86:GLU:OE2	7:1H:132:ARG:NH2	2.38	0.56
1:1A:2484:G:O2'	12:1Q:124:LYS:O	2.23	0.56
6:2G:179:PRO:HB2	26:24:42:PHE:HE2	1.69	0.56
1:2A:568:U:OP1	1:2A:945:A:N6	2.35	0.56
4:2E:167:VAL:HG22	4:2E:170:LEU:HD11	1.88	0.56
14:2S:11:LYS:HG3	14:2S:91:PRO:HD3	1.86	0.56
19:2X:94:GLY:N	19:2X:95:LEU:HA	2.21	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1359:A:H2'	1:2A:1360:A:H5'	1.88	0.56
1:2A:1656:C:H5''	4:2E:136:ARG:HB2	1.88	0.56
1:2A:2317:C:N4	1:2A:2318:G:O6	2.39	0.56
1:2A:900:A:H2'	1:2A:901:A:H8	1.70	0.56
1:1A:2136:C:H42	1:1A:2155:G:H1	0.69	0.56
1:1A:2494:G:H2'	1:1A:2495:G:H8	1.71	0.56
1:1A:289:A:N6	1:1A:351:G:O2'	2.39	0.56
8:1I:93:THR:HG22	8:1I:119:PRO:HB3	1.88	0.56
9:1N:20:GLY:HA2	9:1N:61:ARG:HG2	1.88	0.56
22:20:14:ARG:NH2	60:20:207:HOH:O	2.39	0.56
1:2A:1003:G:O2'	1:2A:1010:A:N1	2.37	0.56
1:2A:2498:C:OP2	60:2A:5622:HOH:O	2.18	0.56
1:2A:253:C:O2'	60:2A:5005:HOH:O	2.18	0.56
1:2A:2802:G:H2'	1:2A:2803:C:O4'	2.05	0.56
1:2A:643:A:N1	1:2A:2369:A:O2'	2.37	0.56
15:2T:127:ALA:C	15:2T:129:ARG:H	2.09	0.56
1:1A:2723:C:OP1	13:1R:3:HIS:ND1	2.32	0.56
2:1B:14:U:O3'	2:1B:108:U:O2'	2.22	0.56
20:1Y:11:ASP:N	20:1Y:11:ASP:OD1	2.38	0.56
1:2A:1405:U:H2'	1:2A:1406:U:C6	2.41	0.56
1:2A:140:G:H1'	1:2A:141:A:H2	1.69	0.56
5:2F:132:VAL:HG21	5:2F:163:VAL:HG22	1.87	0.56
1:1A:1385:G:O2'	1:1A:1396:U:O2	2.23	0.56
1:1A:1800:C:OP2	3:1D:183:ARG:NH1	2.35	0.56
60:2A:4807:HOH:O	11:2P:44:GLY:O	2.18	0.56
23:11:23:LYS:HB3	23:11:29:GLY:HA3	1.88	0.55
1:1A:2022:U:O2'	1:1A:2617:C:H5'	2.05	0.55
1:2A:171:G:H2'	1:2A:172:C:C6	2.40	0.55
1:2A:27:G:O2'	1:2A:28:A:OP2	2.23	0.55
1:1A:1065:U:H1'	1:1A:1074:G:C2	2.41	0.55
1:1A:184:C:H2'	1:1A:185:U:C6	2.41	0.55
1:1A:2632:A:HO2'	1:1A:2811:G:HO2'	1.50	0.55
17:1V:60:GLU:HB2	17:1V:97:LYS:HD3	1.88	0.55
29:27:8:ASN:HB3	29:27:11:LYS:HB3	1.88	0.55
1:2A:1355:G:H2'	1:2A:1356:G:C8	3.10	0.55
1:2A:1921:G:H2'	1:2A:1922:G:H8	1.70	0.55
1:1A:1090:U:C2	1:1A:1102:C:H1'	2.40	0.55
1:1A:414:C:O2	1:1A:1864:U:O2'	2.24	0.55
3:1D:37:LEU:HD13	3:1D:62:TYR:HB2	1.87	0.55
7:1H:56:SER:OG	7:1H:57:ASP:N	2.39	0.55
14:1S:52:SER:HB2	14:1S:55:ALA:H	1.70	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1300:U:H4'	1:2A:1301:A:H5'	1.86	0.55
1:2A:259:G:O6	1:2A:267:C:N4	25.79	0.55
1:2A:723:G:H2'	1:2A:724:U:O4'	2.05	0.55
1:1A:389:G:N1	11:1P:70:GLN:HG3	2.21	0.55
1:1A:2682:U:O2'	15:1T:58:ASN:ND2	2.40	0.55
1:2A:2836:U:H2'	1:2A:2837:G:C8	2.41	0.55
1:2A:80:G:O2'	1:2A:294:A:N1	2.30	0.55
1:2A:476:G:OP1	60:2A:5363:HOH:O	2.18	0.55
1:2A:862:G:O6	1:2A:916:G:N2	2.39	0.55
1:2A:923:C:H2'	1:2A:924:C:H6	1.72	0.55
12:2Q:141:GLN:NE2	21:2Z:74:VAL:O	2.39	0.55
1:1A:1634:A:OP2	60:1A:4797:HOH:O	2.18	0.55
1:1A:2156:G:H2'	1:1A:2157:G:C2	2.41	0.55
14:1S:14:VAL:O	14:1S:18:ILE:HG12	2.07	0.55
1:2A:1029:A:N1	1:2A:2465:C:O2'	2.37	0.55
1:2A:2103:C:N4	1:2A:2186:G:H1	2.03	0.55
1:2A:2870:C:H5''	13:2R:65:LEU:HD21	1.89	0.55
1:2A:970:C:HO2'	1:2A:984:A:HO2'	1.51	0.55
1:1A:1364:G:N7	23:11:3:LYS:HD2	2.21	0.55
1:1A:1796:U:H2'	1:1A:1797:C:C6	2.42	0.55
1:1A:2712:U:OP1	1:1A:2714:G:H4'	2.06	0.55
1:1A:400:G:N7	60:1A:5807:HOH:O	2.33	0.55
1:1A:880:G:H2'	1:1A:881:G:C8	2.40	0.55
23:21:83:GLU:OE1	23:21:83:GLU:N	2.39	0.55
1:2A:1410:G:H2'	1:2A:1411:C:C6	2.41	0.55
1:2A:1579:A:H2'	1:2A:1580:A:C8	2.41	0.55
1:2A:1777:U:H2'	1:2A:1778:U:C6	2.42	0.55
4:2E:143:ASN:HD22	4:2E:147:PRO:HD3	1.72	0.55
4:2E:2:LYS:HG3	4:2E:96:PHE:HE1	1.71	0.55
6:1G:112:PRO:HG3	26:14:43:TYR:CE2	2.41	0.55
1:1A:2150:U:N3	1:1A:2151:G:O6	2.38	0.55
1:1A:2404:C:O3'	11:1P:77:ARG:NH2	2.40	0.55
11:2P:50:ARG:HD3	30:28:7:HIS:CD2	2.42	0.55
1:2A:2447:G:N2	1:2A:2450:A:OP2	2.40	0.55
1:2A:854:G:H2'	1:2A:855:G:C8	2.41	0.55
2:2B:66:A:H61	2:2B:108:U:H3'	1.71	0.55
19:2X:43:VAL:HG11	19:2X:81:VAL:HG11	1.89	0.55
4:1E:47:VAL:HG11	4:1E:86:PRO:HD2	1.88	0.55
1:2A:1671:U:N3	1:2A:1674:G:OP2	2.31	0.55
1:2A:2375:G:N2	1:2A:2378:A:OP2	2.33	0.55
1:2A:1012:U:C5	9:2N:28:THR:HG21	2.41	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1493:C:N4	1:1A:2206:G:O2'	2.39	0.55
7:1H:3:ARG:NH1	7:1H:5:GLY:H	2.04	0.55
1:1A:271(M):G:N2	8:1I:50:ARG:HH12	2.04	0.55
11:1P:111:ARG:HH11	11:1P:128:HIS:CD2	2.24	0.55
1:2A:2137:C:O2'	1:2A:2138:C:OP2	2.23	0.55
1:2A:2342:C:O2'	1:2A:2374:C:OP1	2.25	0.55
1:2A:864:G:H1'	1:2A:914:C:N4	2.21	0.55
1:1A:1747(A):G:H2'	1:1A:1748:G:C8	2.42	0.55
1:1A:586:A:N1	1:1A:809:G:O2'	2.37	0.55
1:1A:787:U:H5''	1:1A:788:A:H5'	1.88	0.55
3:1D:274:ARG:NH1	60:1D:402:HOH:O	2.39	0.55
1:2A:2815:C:H5'	27:25:29:THR:HG21	1.89	0.55
21:2Z:97:GLU:HB3	21:2Z:125:LEU:HD11	1.89	0.55
1:1A:1095:A:H2'	1:1A:1096:A:H8	1.72	0.54
1:2A:1358:G:O2'	1:2A:1373:A:N6	2.39	0.54
1:2A:2012:G:OP1	18:2W:11:ARG:NH2	2.39	0.54
1:2A:776:G:N7	1:2A:793:A:O2'	2.38	0.54
2:2B:38:C:H2'	2:2B:39:A:C8	2.40	0.54
1:1A:1062:G:H1	1:1A:1077:A:H61	1.54	0.54
10:1O:68:GLU:OE1	10:1O:78:ARG:NH1	2.37	0.54
11:1P:39:LYS:HG3	11:1P:45:LEU:HD11	1.90	0.54
1:2A:1158:C:N4	60:2A:5040:HOH:O	2.40	0.54
1:2A:1636:C:H2'	1:2A:1637:A:C8	2.42	0.54
1:2A:2735:G:H2'	1:2A:2736:G:H8	1.73	0.54
1:2A:900:A:O2'	1:2A:901:A:OP1	2.24	0.54
1:2A:918:A:N3	2:2B:80:U:O2'	2.38	0.54
10:2O:63:VAL:HG23	10:2O:64:ARG:HG3	1.89	0.54
14:2S:12:PHE:O	14:2S:16:ASN:ND2	2.41	0.54
26:14:26:SER:OG	26:14:27:THR:N	2.41	0.54
1:2A:1309:G:HO2'	1:2A:1611:C:HO2'	1.54	0.54
1:2A:2030:A:H4'	1:2A:2031:A:C8	2.43	0.54
1:2A:2294:C:H42	1:2A:2338:G:H1	1.54	0.54
19:2X:12:VAL:HG22	19:2X:29:TRP:CE2	2.42	0.54
23:11:64:ALA:HA	23:11:67:ILE:HG13	1.89	0.54
1:1A:1364:G:OP1	23:11:2:SER:N	2.41	0.54
1:1A:185:U:H2'	1:1A:186:G:H8	1.73	0.54
1:1A:2124:G:H1	1:1A:2174:C:N4	2.05	0.54
1:1A:278:A:H2'	1:1A:279:C:C6	2.43	0.54
7:1H:121:ILE:HG13	7:1H:144:VAL:HG21	1.90	0.54
1:2A:2035:G:O6	60:2A:4280:HOH:O	2.16	0.54
1:2A:2845:G:H2'	1:2A:2846:G:C8	2.37	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1541:G:H3'	1:1A:1542:A:H2'	1.90	0.54
5:1F:107:LYS:HG3	5:1F:206:ILE:HA	1.90	0.54
7:1H:104:GLU:HG3	7:1H:114:VAL:HG22	1.89	0.54
27:25:56:LYS:NZ	27:25:58:LEU:O	2.36	0.54
1:2A:1204:A:H2	1:2A:1241:A:H62	1.55	0.54
1:2A:514:A:N3	1:2A:581:C:O2'	2.36	0.54
1:2A:731:C:OP1	60:2A:6025:HOH:O	2.19	0.54
7:2H:45:VAL:HG12	7:2H:50:VAL:HG22	1.90	0.54
11:2P:52:GLU:OE1	11:2P:55:ARG:NH1	2.40	0.54
12:2Q:20:ALA:HB2	21:2Z:79:ARG:HG2	1.89	0.54
1:1A:1358:G:OP2	60:1A:6801:HOH:O	2.19	0.54
1:1A:1843:C:H5'	3:1D:253:GLN:OE1	2.06	0.54
1:2A:198:C:OP2	60:2A:4967:HOH:O	2.18	0.54
1:2A:2444:G:OP2	60:2A:4289:HOH:O	2.19	0.54
1:2A:2820:A:O2'	1:2A:2821:A:OP1	2.24	0.54
4:1E:181:LEU:HD21	15:1T:6:LEU:HD12	1.90	0.54
1:2A:2033:A:O2'	1:2A:2035:G:OP2	2.26	0.54
1:2A:251:A:C5	1:2A:252:G:H1'	2.43	0.54
13:2R:104:ARG:HG3	13:2R:111:LEU:HD11	1.90	0.54
1:1A:2134:A:OP1	1:1A:2156:G:N2	2.40	0.54
1:1A:582:G:H2'	1:1A:583:G:C8	2.43	0.54
3:1D:17:THR:HG1	3:1D:205:VAL:H	1.55	0.54
1:1A:323:G:C8	5:1F:171:PRO:HG3	2.42	0.54
1:1A:684:G:OP1	29:17:16:HIS:ND1	2.38	0.54
16:1U:81:HIS:CE1	16:1U:85:LYS:HE2	2.43	0.54
1:2A:1030:G:OP2	12:2Q:128:LYS:NZ	2.40	0.54
1:2A:1913:A:H4'	1:2A:1914:C:O5'	2.07	0.54
1:2A:2538:C:H2'	1:2A:2539:C:C6	2.43	0.54
1:2A:2637:U:OP1	4:2E:82:ARG:NH1	2.40	0.54
1:2A:271(D):G:H1	1:2A:271(T):C:H42	1.55	0.54
1:2A:733:G:OP2	60:2A:4164:HOH:O	2.18	0.54
8:2I:31:LEU:HD21	8:2I:38:LEU:HD23	1.88	0.54
15:2T:23:ARG:N	15:2T:26:ASP:OD2	2.38	0.54
1:1A:2134:A:O2'	1:1A:2135:A:OP1	2.21	0.54
3:1D:12:SER:HB3	3:1D:208:LYS:HB3	1.90	0.54
1:2A:2223:G:OP1	3:2D:172:TYR:OH	2.23	0.54
1:2A:359:A:H2'	1:2A:360:G:O4'	2.08	0.54
1:2A:577:G:O6	60:2A:4919:HOH:O	2.18	0.54
19:2X:4:ALA:HB1	19:2X:42:ALA:HA	1.89	0.54
1:1A:882:G:H1	1:1A:894:C:N4	2.06	0.53
1:2A:1782:C:O2	1:2A:2608:G:O2'	2.20	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2S:67:ARG:HG2	14:2S:71:ARG:HE	1.73	0.53
26:14:40:HIS:HB3	26:14:43:TYR:HD2	1.73	0.53
1:1A:1164:G:H1	1:1A:1185:C:H42	1.55	0.53
1:1A:1747(A):G:H2'	1:1A:1748:G:H8	1.73	0.53
1:1A:911:A:H2'	12:1Q:9:TYR:OH	2.08	0.53
60:2A:5441:HOH:O	22:20:2:ALA:N	2.41	0.53
1:2A:2137:C:N3	1:2A:2154:G:N2	2.44	0.53
6:2G:11:TYR:O	6:2G:16:ARG:N	2.41	0.53
11:2P:95:VAL:HG13	11:2P:125:VAL:HA	1.90	0.53
1:2A:994:C:OP1	16:2U:53:ARG:NH2	2.41	0.53
1:1A:380:U:H2'	1:1A:381:G:H8	1.71	0.53
1:1A:86:C:H4'	1:1A:104:U:H1'	1.90	0.53
1:2A:2218:U:N3	23:21:55:GLY:O	2.31	0.53
31:29:16:VAL:HG22	31:29:25:VAL:HG22	1.90	0.53
1:2A:1272:A:H3'	1:2A:1273:U:H5''	1.91	0.53
1:2A:2025:C:H2'	1:2A:2026:C:C6	2.44	0.53
6:2G:165:THR:OG1	6:2G:167:GLU:OE1	2.21	0.53
1:1A:1025:G:C4	1:1A:1135:C:H1'	2.44	0.53
1:1A:1105:U:H2'	1:1A:1106:G:H8	1.74	0.53
1:1A:1165:U:H2'	1:1A:1166:C:C6	2.44	0.53
2:1B:87:G:N2	2:1B:90:A:OP2	2.36	0.53
8:1I:87:LYS:HE2	8:1I:121:LYS:HE3	1.89	0.53
1:2A:1662:C:O2'	1:2A:2687:U:OP1	2.22	0.53
3:2D:108:PRO:HB3	3:2D:143:HIS:CE1	2.43	0.53
1:1A:548:A:N6	17:1V:19:LYS:H	2.06	0.53
5:1F:101:LEU:O	5:1F:106:ARG:NH1	2.41	0.53
1:2A:2105:C:H2'	1:2A:2106:G:H8	1.73	0.53
1:2A:363:G:H2'	1:2A:363(A):A:H8	1.74	0.53
7:2H:159:GLU:HG3	7:2H:169:VAL:HG11	1.90	0.53
22:10:46:LYS:NZ	22:10:75:LEU:O	2.42	0.53
5:1F:116:ASP:OD1	5:1F:119:ARG:NH2	2.42	0.53
12:1Q:38:GLU:HA	12:1Q:99:PRO:HG3	1.90	0.53
1:2A:1782:C:OP1	60:2A:6383:HOH:O	2.18	0.53
1:2A:659:C:H2'	1:2A:660:G:H8	1.72	0.53
1:2A:973:A:H8	1:2A:973:A:OP1	1.91	0.53
1:1A:1058:G:H1	1:1A:1080:C:N4	2.06	0.53
1:1A:26:G:O2'	1:1A:514:A:N6	2.39	0.53
1:1A:31:C:OP1	60:1A:5563:HOH:O	2.19	0.53
4:1E:3:GLY:HA3	4:1E:81:ILE:HG21	1.90	0.53
18:1W:17:VAL:O	18:1W:20:VAL:N	2.41	0.53
1:2A:2206:G:H3'	1:2A:2207:G:C8	2.44	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:228:A:O2'	1:2A:229:A:O4'	2.27	0.53
1:2A:2261:C:H1'	1:2A:2388:A:N3	2.23	0.53
1:2A:2848:G:H1'	1:2A:2867:G:N2	2.24	0.53
2:2B:103:G:N2	21:2Z:73:GLN:OE1	2.37	0.53
1:1A:1068:G:OP2	1:1A:1068:G:H8	2.96	0.53
1:1A:1587:A:H2'	1:1A:1588:C:C6	2.44	0.53
15:1T:65:LYS:HE2	15:1T:67:SER:HB2	1.91	0.53
17:1V:5:VAL:HG21	17:1V:35:LEU:HD23	1.91	0.53
1:2A:2105:C:H2'	1:2A:2106:G:C8	2.44	0.53
1:2A:27:G:N2	1:2A:512:G:H1'	2.23	0.53
1:2A:535:C:H2'	1:2A:536:A:H8	1.72	0.53
21:2Z:76:LEU:HA	21:2Z:83:PRO:HA	1.91	0.53
1:1A:2436:G:O2'	60:1A:4103:HOH:O	2.18	0.53
1:1A:2591:C:H2'	1:1A:2592:G:C8	2.43	0.53
3:1D:3:VAL:HG12	3:1D:17:THR:HB	1.91	0.53
1:1A:442:G:H4'	5:1F:46:ARG:HG3	1.91	0.53
15:1T:74:ARG:HG2	15:1T:76:PHE:CZ	2.44	0.53
1:2A:144:C:H2'	1:2A:145:G:H8	1.74	0.53
1:2A:2242:G:OP1	60:2A:3906:HOH:O	2.19	0.53
1:2A:236:C:H2'	1:2A:237:C:C6	2.44	0.53
1:2A:2671:A:H2'	1:2A:2672:G:O4'	2.09	0.53
1:2A:524:U:H2'	1:2A:525:U:C6	2.44	0.53
6:2G:11:TYR:HA	6:2G:15:VAL:HB	1.91	0.53
8:2I:93:THR:H	8:2I:96:ASP:HB2	1.73	0.53
1:1A:1053:C:N3	1:1A:1106:G:N2	2.52	0.53
1:1A:2853:C:H2'	1:1A:2854:G:H8	1.74	0.53
1:1A:483:A:O2'	20:1Y:49:VAL:O	2.22	0.53
22:20:65:GLY:HA3	22:20:83:PRO:HA	1.91	0.53
1:2A:1246:A:O2'	5:2F:45:ARG:NH1	2.36	0.53
1:2A:2152:G:C2	1:2A:2153:G:H1'	2.44	0.53
1:2A:2886:G:H2'	1:2A:2887:U:H6	1.72	0.53
1:2A:658:C:H2'	1:2A:659:C:C6	2.44	0.53
1:2A:1818:U:O2'	3:2D:154:LYS:O	2.13	0.53
1:1A:1094:U:H2'	1:1A:1095:A:C8	2.44	0.52
1:1A:2224:G:H4'	1:1A:2226:C:C2	2.45	0.52
1:1A:2751:G:H4'	7:1H:4:ILE:HD11	1.91	0.52
1:1A:1750:G:O2'	1:1A:2860:A:N1	2.38	0.52
1:1A:534:U:H2'	1:1A:535:C:C6	2.44	0.52
1:1A:956:G:H2'	1:1A:957:A:H2'	1.91	0.52
1:2A:2291:U:H2'	1:2A:2292:C:C6	2.44	0.52
1:2A:2841:C:H2'	1:2A:2842:G:C8	2.44	0.52

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:708:C:H42	1:2A:723:G:H1	1.56	0.52
1:2A:698:C:O2'	1:2A:734:A:N6	2.42	0.52
1:2A:947:G:H2'	1:2A:948:G:C8	2.44	0.52
60:1A:4987:HOH:O	30:18:30:ARG:NH1	2.41	0.52
1:1A:832:G:OP1	60:1A:5587:HOH:O	2.19	0.52
2:1B:41:U:OP1	2:1B:43:C:N4	2.41	0.52
7:1H:3:ARG:NH1	7:1H:4:ILE:H	2.07	0.52
1:2A:2114:A:H2	1:2A:2171:A:H61	1.56	0.52
1:2A:2781:A:H5''	1:2A:2782:G:H5'	1.90	0.52
1:2A:8:A:H2'	1:2A:9:U:H6	1.74	0.52
6:2G:16:ARG:HB3	6:2G:17:PRO:HD3	1.91	0.52
13:2R:56:LYS:NZ	13:2R:90:ARG:O	2.42	0.52
1:1A:1174:A:H1'	1:1A:1175:U:H5''	1.89	0.52
1:1A:222:A:H5''	1:1A:421:U:OP1	2.09	0.52
22:20:38:VAL:HG11	22:20:45:PHE:HD2	1.73	0.52
1:2A:2150:U:H2'	1:2A:2151:G:C8	2.42	0.52
1:2A:2470:G:O6	1:2A:2481:G:N2	2.42	0.52
1:2A:2611:U:C5	57:2A:3875:ERY:H312	2.44	0.52
15:2T:39:ARG:HH12	15:2T:41:ARG:HD3	1.74	0.52
21:2Z:18:LEU:HD23	21:2Z:25:PRO:HG3	1.90	0.52
1:1A:2646:C:H2'	1:1A:2647:U:O4'	2.10	0.52
1:1A:620:G:H5'	1:1A:620:G:N3	2.25	0.52
21:1Z:45:ASP:OD1	21:1Z:49:ARG:NE	2.40	0.52
1:2A:188:G:H5'	23:21:14:VAL:HG21	1.91	0.52
23:21:5:CYS:SG	23:21:8:SER:OG	2.61	0.52
1:2A:1231:G:H2'	1:2A:1232:G:C8	2.44	0.52
1:2A:184:C:H1'	1:2A:217:G:H1'	1.90	0.52
1:2A:2693:A:H2'	1:2A:2694:G:C8	2.44	0.52
1:1A:2125:G:H1'	1:1A:2173:A:H61	1.75	0.52
1:1A:250:G:OP2	30:18:13:ARG:NH2	2.39	0.52
12:1Q:68:ILE:HD13	12:1Q:103:MET:HE3	1.91	0.52
1:2A:1451:C:H4'	1:2A:1452:A:C8	2.44	0.52
3:2D:71:ASP:HB3	3:2D:103:ARG:HH12	1.74	0.52
4:2E:125:GLY:HA3	4:2E:134:ILE:HD12	1.91	0.52
6:2G:113:ARG:NH2	6:2G:139:LEU:O	2.39	0.52
9:2N:38:HIS:CD2	9:2N:39:ARG:HG3	2.44	0.52
28:16:6:ARG:NH1	28:16:26:ASN:HB2	2.25	0.52
1:1A:603:A:N1	1:1A:625:G:O2'	2.42	0.52
2:1B:88:C:H2'	2:1B:89:G:O4'	2.09	0.52
1:2A:2355:C:H1'	22:20:39:ARG:HH21	1.74	0.52
1:2A:1379:A:H4'	1:2A:1380:G:OP2	2.09	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:70:G:H1	1:2A:99:U:H3	37.60	0.52
26:14:58:ARG:N	26:14:58:ARG:HD2	2.25	0.52
2:1B:86:G:H1	2:1B:91:C:H42	1.57	0.52
3:1D:25:THR:HG21	3:1D:113:VAL:HG11	1.91	0.52
1:2A:1116:C:H2'	1:2A:1117:G:C8	2.45	0.52
24:12:28:LYS:HD2	24:12:53:LEU:HD21	1.92	0.52
1:1A:1009:A:OP2	9:1N:37:LYS:NZ	2.38	0.52
1:1A:1151:G:H5''	16:1U:81:HIS:CD2	2.44	0.52
1:1A:1266:G:O5'	18:1W:15:ARG:NH2	2.42	0.52
1:1A:2206:G:H5''	1:1A:2207:G:C5	2.44	0.52
3:1D:108:PRO:HB3	3:1D:143:HIS:CE1	2.45	0.52
26:24:41:PRO:HG3	26:24:49:PHE:CZ	2.45	0.52
1:2A:1449:A:H2	1:2A:1529:G:H1'	1.74	0.52
5:2F:148:LEU:HD13	5:2F:154:VAL:HG21	1.91	0.52
12:2Q:68:ILE:HG22	12:2Q:101:ARG:HE	1.74	0.52
2:2B:91:C:H5'	12:2Q:18:LYS:HA	1.91	0.52
17:2V:76:LYS:HB2	17:2V:81:TYR:HB3	1.91	0.52
1:1A:2552:2MU:O5'	1:1A:2552:2MU:H6	2.10	0.52
5:1F:184:TYR:CE2	5:1F:188:ARG:HD2	2.45	0.52
7:1H:96:ALA:HB1	7:1H:103:LEU:HD11	1.91	0.52
1:2A:1593:G:H2'	1:2A:1594:G:C8	2.45	0.52
1:2A:2290:G:N2	1:2A:2373:G:O2'	2.42	0.52
1:2A:2630:G:H1	1:2A:2788:C:H42	1.57	0.52
6:2G:150:ASP:OD1	6:2G:150:ASP:N	2.43	0.52
6:2G:9:ARG:NE	6:2G:13:GLU:OE2	2.42	0.52
17:2V:7:THR:HG23	17:2V:12:TYR:HE2	1.75	0.52
1:1A:1441:G:O2'	1:1A:1442:G:N2	9.65	0.52
1:1A:234:C:H2'	1:1A:235:U:H6	1.74	0.52
1:1A:2488:A:N6	60:1A:4131:HOH:O	2.39	0.52
1:1A:881:G:H1	1:1A:897:C:H42	1.57	0.52
1:2A:2624:G:N7	60:2A:6325:HOH:O	2.34	0.52
1:2A:2870:C:H2'	1:2A:2871:C:O4'	2.09	0.52
5:2F:116:ASP:OD2	11:2P:1:MET:N	2.26	0.52
6:2G:15:VAL:HA	6:2G:175:LEU:HD23	1.92	0.52
25:13:7:LYS:HB2	25:13:34:GLU:HG3	1.93	0.51
1:1A:2306:C:O2	60:1G:301:HOH:O	2.18	0.51
1:1A:2710:C:H2'	1:1A:2711:A:C8	2.45	0.51
1:1A:27:G:H22	1:1A:512:G:H1'	1.75	0.51
18:1W:13:SER:HB3	18:1W:16:LYS:HD2	1.92	0.51
1:2A:2623:G:H2'	1:2A:2624:G:C8	2.44	0.51
2:2B:55:U:O3'	6:2G:27:ASN:ND2	2.36	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:322:A:OP2	5:2F:169:ASN:HB2	2.09	0.51
8:2I:93:THR:HG22	8:2I:119:PRO:HB3	1.91	0.51
21:2Z:69:THR:HG22	21:2Z:90:VAL:HA	1.92	0.51
24:12:9:GLN:HE22	24:12:56:GLN:HB3	1.76	0.51
1:1A:1779:U:OP2	60:1A:6070:HOH:O	2.19	0.51
1:1A:1667:G:O2'	1:1A:1991:U:O4	2.23	0.51
1:1A:234:C:H2'	1:1A:235:U:C6	2.45	0.51
1:1A:625:G:H2'	1:1A:626:U:C6	3.26	0.51
1:1A:671:C:N4	60:1A:5643:HOH:O	2.43	0.51
8:1I:40:THR:O	8:1I:44:LEU:HB2	2.11	0.51
1:2A:1711:C:H2'	1:2A:1712:C:C6	2.45	0.51
1:2A:861:A:N3	2:2B:79:C:O2'	2.42	0.51
1:1A:1272:A:O2'	60:1A:4101:HOH:O	2.13	0.51
1:1A:271(H):G:H1	1:1A:271(P):C:H42	1.57	0.51
3:1D:206:LEU:O	3:1D:211:ARG:HD3	2.10	0.51
14:1S:35:ILE:HD13	14:1S:101:LEU:HD12	1.93	0.51
1:2A:2152:G:C4	1:2A:2153:G:H1'	2.46	0.51
1:2A:2689:U:P	1:2A:2719:G:H22	2.33	0.51
18:2W:58:ALA:HA	18:2W:62:HIS:HB2	1.91	0.51
21:2Z:48:PHE:HE1	21:2Z:71:VAL:HG11	1.75	0.51
1:1A:1442:G:H2'	1:1A:1442:G:N3	3.08	0.51
1:2A:1037:G:H2'	1:2A:1038:C:O4'	2.10	0.51
1:2A:839:U:H2'	1:2A:840:C:C6	2.46	0.51
21:2Z:99:TYR:HA	21:2Z:124:ILE:O	2.11	0.51
21:2Z:151:HIS:ND1	21:2Z:169:GLU:O	2.43	0.51
1:1A:2153:G:H2'	1:1A:2154:G:C8	2.45	0.51
1:1A:247:G:H4'	1:1A:386:G:C5	2.46	0.51
18:1W:46:PHE:O	18:1W:50:VAL:HG23	2.11	0.51
30:28:6:THR:HG22	30:28:63:PRO:HD2	1.92	0.51
1:2A:1423:G:H2'	1:2A:1424:G:H8	1.76	0.51
2:2B:66:A:N6	2:2B:108:U:H3'	2.23	0.51
1:2A:599:G:H5'	11:2P:9:ASN:HD22	1.75	0.51
1:2A:2378:A:H2'	14:2S:21:THR:HG21	1.91	0.51
1:1A:1095:A:H2'	1:1A:1096:A:C8	2.46	0.51
1:1A:2375:G:O2'	1:1A:2377:A:N7	2.36	0.51
1:1A:2464:C:OP2	60:1A:4104:HOH:O	2.19	0.51
1:1A:1490:A:O2'	3:1D:99:ASP:OD1	2.28	0.51
1:2A:1773:A:OP2	60:2A:4856:HOH:O	2.19	0.51
1:2A:90:U:H1'	1:2A:92:A:C8	2.46	0.51
2:2B:55:U:H2'	2:2B:56:G:O4'	2.10	0.51
1:2A:2785:C:H1'	4:2E:66:HIS:CE1	2.46	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2F:150:GLY:HA2	5:2F:172:TRP:CD2	2.45	0.51
1:1A:432:A:N6	60:1A:4756:HOH:O	2.38	0.51
1:1A:484:C:H2'	1:1A:485:C:C6	2.45	0.51
1:1A:1799:G:N7	3:1D:179:SER:OG	2.43	0.51
1:1A:1789:A:H5''	3:1D:220:HIS:O	2.10	0.51
5:1F:51:THR:HB	5:1F:88:VAL:HG11	1.92	0.51
7:1H:20:ALA:HB1	7:1H:21:PRO:HD2	1.93	0.51
21:1Z:11:GLU:O	21:1Z:36:LYS:NZ	2.30	0.51
1:2A:1913:A:H4'	1:2A:1914:C:C5'	2.41	0.51
1:2A:2070:G:H2'	1:2A:2071:A:C8	2.45	0.51
1:2A:2652:C:H2'	1:2A:2653:U:O4'	2.11	0.51
3:2D:69:ARG:NH1	3:2D:128:GLY:O	2.37	0.51
3:2D:133:LEU:HA	3:2D:136:ILE:HD12	1.93	0.51
1:2A:662:G:H5''	11:2P:16:ARG:HG2	1.91	0.51
21:2Z:50:GLN:OE1	21:2Z:50:GLN:N	2.44	0.51
1:1A:1686:C:H2'	1:1A:1687:G:O4'	2.11	0.51
1:1A:862:G:H2'	1:1A:863:A:O4'	2.11	0.51
7:2H:154:PRO:HB3	7:2H:163:TYR:CZ	2.46	0.51
3:1D:260:ARG:NH1	3:1D:267:SER:OG	2.39	0.51
22:20:51:VAL:HG22	22:20:81:VAL:HG23	1.92	0.51
23:21:3:LYS:HB2	23:21:61:ARG:HH12	1.74	0.51
1:2A:1007:C:O2	1:2A:1022:G:N1	18.93	0.51
1:2A:1170:G:O6	1:2A:1180:C:N4	2.44	0.51
1:2A:2227:A:OP1	3:2D:263:ARG:NH1	2.39	0.51
1:2A:840:C:OP2	1:2A:932:G:N2	2.40	0.51
6:1G:179:PRO:HB2	26:14:42:PHE:HE2	1.76	0.51
1:1A:1689:A:H2'	1:1A:1690:A:C8	2.46	0.51
1:1A:1971:A:C4	3:1D:241:PRO:HD3	2.46	0.51
1:1A:1972:A:H2'	1:1A:1973:G:H8	1.76	0.51
14:1S:38:GLN:HE21	14:1S:47:THR:HG21	1.76	0.51
1:2A:2140:C:H2'	1:2A:2141:G:H5'	1.93	0.51
1:2A:2322:A:H3'	1:2A:2323:G:H8	1.76	0.51
1:2A:2023:G:H5'	1:2A:2617:C:H4'	1.93	0.51
1:2A:403:U:H4'	1:2A:404:C:H5'	1.92	0.51
4:2E:47:VAL:HG11	4:2E:86:PRO:HD2	1.93	0.51
7:2H:87:LEU:HD21	7:2H:145:ALA:HB1	1.92	0.51
15:2T:2:ASN:OD1	15:2T:5:ALA:N	2.39	0.51
1:1A:1826:G:H4'	3:1D:242:ARG:CZ	2.40	0.50
1:1A:548:A:H1'	1:1A:549:G:OP1	2.10	0.50
3:1D:11:PRO:O	3:1D:14:ARG:HG3	2.12	0.50
10:1O:59:LYS:NZ	10:1O:89:ASN:OD1	2.44	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1794:U:H2'	1:2A:1795:C:C6	2.47	0.50
7:2H:105:LEU:O	7:2H:113:VAL:N	2.41	0.50
1:1A:1420:U:O2'	1:1A:1421:G:OP1	2.28	0.50
1:1A:2183:C:O2'	1:1A:2184:G:OP1	2.27	0.50
1:1A:2364:C:H2'	1:1A:2365:G:O4'	2.12	0.50
1:1A:2430:A:N3	1:1A:2430:A:H2'	2.25	0.50
1:2A:1512:U:H2'	1:2A:1513:C:C6	2.47	0.50
1:2A:171:G:H2'	1:2A:172:C:H6	1.76	0.50
1:2A:1878:G:H2'	1:2A:1879:C:C6	2.46	0.50
1:2A:2143:C:H2'	1:2A:2144:U:O4'	2.10	0.50
18:2W:17:VAL:HG11	18:2W:103:ILE:HD11	1.93	0.50
1:1A:1939:5MU:OP1	1:1A:2604:U:O2'	2.26	0.50
1:1A:286:C:H2'	1:1A:287:C:C6	2.47	0.50
1:1A:668:G:H5'	1:1A:669:G:OP2	2.11	0.50
12:1Q:12:GLN:H	12:1Q:73:PRO:HG2	1.75	0.50
24:22:35:LEU:HD11	24:22:49:LYS:HB2	1.92	0.50
26:24:26:SER:OG	26:24:27:THR:N	2.44	0.50
1:2A:1335:U:OP1	19:2X:65:ARG:NH1	2.43	0.50
1:2A:2126:A:N6	1:2A:2162:G:HO2'	2.08	0.50
1:2A:2089:U:H3	1:2A:2230:G:H1	1.59	0.50
2:2B:83:G:H1	2:2B:94:C:H42	1.58	0.50
5:2F:155:LEU:HB2	5:2F:189:THR:HG21	1.93	0.50
7:2H:154:PRO:HA	7:2H:160:LYS:O	2.10	0.50
15:2T:91:ARG:HH11	15:2T:120:ARG:HH12	1.60	0.50
1:1A:2286:A:H4'	1:1A:2287:A:O4'	2.11	0.50
1:1A:2788:C:O2'	1:1A:2809:A:N3	2.40	0.50
1:1A:2815:C:H5'	27:15:29:THR:HG21	1.92	0.50
1:1A:2841:C:H2'	1:1A:2842:G:H8	1.77	0.50
1:1A:579:G:H2'	1:1A:580:C:C6	2.47	0.50
1:1A:686:G:N2	1:1A:788:A:H61	2.09	0.50
8:1I:116:LEU:HD21	8:1I:119:PRO:HA	1.93	0.50
17:1V:27:ALA:O	17:1V:64:HIS:NE2	2.42	0.50
1:2A:1580:A:H3'	1:2A:1581:G:H8	1.76	0.50
1:2A:247:G:H4'	1:2A:386:G:C5	2.47	0.50
1:2A:2849:U:H4'	1:2A:2868:A:C2	2.46	0.50
1:2A:661:C:H2'	1:2A:662:G:C8	2.46	0.50
60:2A:6365:HOH:O	4:2E:127:ASP:OD2	2.18	0.50
1:1A:380:U:H2'	1:1A:381:G:C8	2.46	0.50
15:1T:11:GLU:OE1	15:1T:57:PHE:HB3	2.11	0.50
1:2A:1993:U:OP2	60:2A:6365:HOH:O	2.20	0.50
1:2A:2291:U:O2'	1:2A:2374:C:O2	2.28	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2F:186:ILE:HG23	5:2F:192:LEU:HD12	1.93	0.50
1:1A:1015:G:H1	1:1A:1147:C:H42	1.59	0.50
1:1A:2107:C:N4	1:1A:2182:G:H1	2.09	0.50
25:23:10:LYS:HB3	25:23:53:LEU:HA	1.93	0.50
1:2A:2319:G:H22	14:2S:3:ARG:HD2	1.77	0.50
1:2A:492:A:H2'	1:2A:493:G:O4'	2.11	0.50
4:2E:101:ARG:CZ	4:2E:171:GLU:HB2	2.41	0.50
9:2N:42:TRP:HA	9:2N:48:MET:SD	2.51	0.50
10:2O:104:ARG:NH2	15:2T:36:GLU:OE2	2.43	0.50
1:1A:1653:G:N2	60:1A:4641:HOH:O	2.45	0.50
1:1A:2117:A:H61	1:1A:2172:U:H3	1.58	0.50
1:1A:252:G:OP1	11:1P:50:ARG:NH1	2.35	0.50
1:1A:2682:U:OP2	60:1A:4677:HOH:O	2.19	0.50
1:1A:278:A:O2'	1:1A:279:C:OP1	2.25	0.50
1:1A:597:U:H2'	1:1A:598:G:C8	2.46	0.50
2:1B:2:C:H2'	2:1B:3:C:C6	2.46	0.50
1:1A:2053:G:H5'	4:1E:145:LYS:H	1.76	0.50
8:1I:117:GLU:HG3	8:1I:118:LYS:H	1.76	0.50
9:1N:42:TRP:CH2	9:1N:44:PRO:HB3	2.46	0.50
1:2A:2032:G:N7	60:2A:5735:HOH:O	2.35	0.50
1:2A:602:G:O2'	1:2A:655:A:N6	2.45	0.50
8:2I:117:GLU:HG3	8:2I:118:LYS:H	1.76	0.50
16:2U:83:LEU:HG	16:2U:88:ILE:HB	1.93	0.50
17:2V:62:LEU:HD11	17:2V:95:LEU:HB2	1.93	0.50
1:1A:1999:C:OP1	1:1A:2723:C:O2'	2.26	0.50
1:1A:919:G:N2	1:1A:2269:A:OP2	2.44	0.50
1:2A:183:C:O2'	1:2A:432:A:N3	2.40	0.50
1:2A:646:A:H2'	1:2A:647:G:O4'	2.12	0.50
19:2X:53:LYS:HB3	19:2X:82:GLN:HB3	1.92	0.50
20:2Y:44:ILE:HA	20:2Y:63:LYS:O	2.12	0.50
1:1A:2432:A:C5	23:11:33:LYS:HG2	2.47	0.50
1:1A:2154:G:C2	1:1A:2155:G:H1'	2.47	0.50
1:1A:2181:G:O2'	1:1A:2182:G:OP1	2.28	0.50
1:1A:805:G:OP2	11:1P:41:ARG:HD2	2.11	0.50
22:20:32:ARG:H	22:20:35:ASN:ND2	2.10	0.50
1:2A:2823:A:OP1	4:2E:113:PHE:HB2	2.11	0.50
26:14:56:VAL:HB	26:14:60:GLN:HG3	1.93	0.49
1:1A:858:U:O2	1:1A:2268:A:H2'	2.11	0.49
1:1A:2316:C:O2'	6:1G:128:ARG:NH2	2.45	0.49
2:1B:48:A:OP2	14:1S:30:ARG:NH2	2.44	0.49
1:2A:1183:G:H5''	25:23:30:ARG:HH22	1.76	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1351:C:O3'	1:2A:1571:A:O2'	2.29	0.49
1:2A:1791:A:H3'	1:2A:1792:G:H8	1.77	0.49
1:2A:2113:U:H3	1:2A:2170:A:N6	2.04	0.49
1:2A:2126:A:H61	1:2A:2162:G:HO2'	1.56	0.49
1:2A:2193:G:H2'	1:2A:2194:G:C8	2.47	0.49
1:2A:266:G:H2'	1:2A:266:G:N3	3.02	0.49
1:2A:511:U:O4	1:2A:512:G:N1	2.45	0.49
1:2A:882:G:H2'	1:2A:883:G:H8	1.77	0.49
1:2A:889:C:O2'	1:2A:890:A:O4'	2.20	0.49
3:2D:69:ARG:HD3	3:2D:130:ALA:HB2	1.93	0.49
1:1A:2101:G:H1	1:1A:2188:C:H42	1.58	0.49
1:1A:826:U:H4'	11:1P:55:ARG:HB3	1.95	0.49
1:2A:1557:C:OP2	1:2A:1558:A:O2'	2.29	0.49
1:2A:2125:G:H22	1:2A:2172:U:P	2.34	0.49
1:2A:2604:U:H2'	1:2A:2605:PSU:H6	1.77	0.49
4:2E:103:ASP:HB3	4:2E:168:MET:HG2	1.93	0.49
25:13:6:VAL:HG13	25:13:54:VAL:HG21	1.94	0.49
1:1A:2390:U:P	30:18:35:GLN:HE22	2.35	0.49
1:1A:1108:U:H2'	1:1A:1109:C:O4'	2.13	0.49
1:1A:373:U:O2'	1:1A:423:A:N3	2.34	0.49
1:2A:531:C:OP1	1:2A:561:G:N2	2.41	0.49
15:2T:105:LEU:HB2	15:2T:110:ILE:HG13	1.93	0.49
1:1A:1017:G:H2'	1:1A:1018:C:C6	3.07	0.49
1:1A:639:U:H2'	1:1A:640:C:C6	2.47	0.49
1:1A:895:U:H4'	1:1A:896:A:OP1	2.11	0.49
7:1H:149:ARG:NH2	7:1H:167:GLU:OE2	2.45	0.49
1:1A:1266:G:O4'	18:1W:15:ARG:NH2	2.44	0.49
20:1Y:6:HIS:CD2	20:1Y:6:HIS:H	2.30	0.49
1:2A:1614:A:P	1:2A:1614:A:H8	2.35	0.49
1:2A:1792:G:H5'	3:2D:205:VAL:HG13	1.94	0.49
1:2A:2059:A:O3'	5:2F:69:HIS:HA	2.12	0.49
8:2I:75:LEU:HD22	8:2I:105:HIS:CD2	2.48	0.49
9:2N:97:ARG:HA	9:2N:100:GLU:HB2	1.93	0.49
1:1A:1379:A:H4'	1:1A:1380:G:OP2	2.11	0.49
1:1A:185:U:H2'	1:1A:186:G:C8	2.47	0.49
1:1A:2108:C:H2'	1:1A:2109:U:H6	1.77	0.49
1:1A:2127:G:N1	1:1A:2161:C:N4	2.60	0.49
1:1A:2127:G:H1	1:1A:2161:C:N4	2.11	0.49
1:2A:2446:G:N2	1:2A:2449:U:O2	2.45	0.49
1:2A:902:C:H2'	1:2A:903:C:C6	2.47	0.49
1:1A:224:G:H2'	1:1A:225:A:O4'	2.12	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:251:A:C5	1:1A:252:G:H1'	2.47	0.49
1:1A:746:A:O2'	1:1A:2611:U:O2'	2.21	0.49
3:1D:87:ASN:HB2	3:1D:88:ARG:NH1	2.27	0.49
7:1H:38:SER:HB3	7:1H:41:MET:HG2	1.93	0.49
8:1I:70:GLU:O	8:1I:74:ASN:HB2	2.12	0.49
30:28:30:ARG:NH1	60:28:103:HOH:O	2.31	0.49
1:2A:108:U:H2'	1:2A:109:G:H8	1.78	0.49
1:2A:2748:A:H5'	7:2H:4:ILE:HD12	1.94	0.49
1:2A:300:A:N3	1:2A:319:C:H1'	2.27	0.49
1:2A:955:C:OP2	12:2Q:14:ARG:HG3	2.11	0.49
1:1A:2095:C:N4	1:1A:2194:G:H1	2.11	0.49
1:1A:2376:A:H2'	1:1A:2377:A:O4'	2.12	0.49
1:1A:2379:G:O2'	14:1S:17:ARG:NH1	2.43	0.49
1:1A:2635:C:H4'	4:1E:48:GLN:HE21	1.78	0.49
1:1A:761:A:N7	60:1A:4528:HOH:O	2.35	0.49
3:1D:34:VAL:HG12	3:1D:63:ARG:HG3	1.93	0.49
15:1T:30:VAL:HG13	15:1T:86:ILE:HG12	1.93	0.49
1:2A:385:C:O2'	1:2A:390:A:N1	2.41	0.49
1:2A:856:C:H2'	1:2A:857:C:C6	2.48	0.49
2:2B:24:G:N3	2:2B:26:A:N6	2.60	0.49
8:2I:3:VAL:HA	8:2I:39:ALA:H	1.77	0.49
1:1A:2176:A:H2'	1:1A:2177:C:C6	2.48	0.49
1:1A:249:C:O2	30:18:12:LYS:NZ	2.34	0.49
1:1A:557:U:H2'	1:1A:558:G:C8	2.48	0.49
4:1E:2:LYS:HG3	4:1E:200:GLU:HB2	1.93	0.49
1:2A:2632:A:O2'	1:2A:2811:G:O2'	2.10	0.49
1:2A:783:A:O2'	1:2A:785:G:OP1	2.23	0.49
1:2A:851:U:H5'	25:23:49:LYS:HD2	1.95	0.49
19:2X:65:ARG:HG3	19:2X:70:LEU:HD23	1.93	0.49
1:1A:881:G:H1	1:1A:897:C:N4	2.09	0.49
5:1F:103:LYS:HA	5:1F:106:ARG:HG3	1.94	0.49
8:1I:99:GLU:HB3	8:1I:103:ARG:HH22	1.77	0.49
1:2A:1632:A:O5'	1:2A:1632:A:H8	1.96	0.49
1:2A:1668:A:O2'	1:2A:1674:G:N7	2.32	0.49
1:2A:118:A:N3	1:2A:178:G:H1'	2.28	0.49
1:2A:893:C:H2'	1:2A:894:C:C5	2.47	0.49
1:2A:995:C:OP2	16:2U:54:LYS:NZ	2.44	0.49
17:2V:55:ALA:HA	17:2V:101:GLY:HA2	1.95	0.49
1:1A:2001:A:H2'	1:1A:2002:G:C8	2.47	0.49
1:1A:2080:G:H2'	1:1A:2081:C:C6	2.48	0.49
1:1A:1783:A:H5'	1:1A:2608:G:H4'	1.94	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2870:C:OP1	13:1R:57:ARG:NH2	2.46	0.49
3:1D:242:ARG:HD3	3:1D:242:ARG:N	2.28	0.49
8:1I:75:LEU:HD22	8:1I:105:HIS:CD2	2.48	0.49
9:1N:35:ARG:HG2	9:1N:37:LYS:HG3	1.95	0.49
18:1W:73:ALA:HB3	18:1W:106:ILE:HD12	1.95	0.49
1:2A:1325:G:OP1	1:2A:1647:G:O2'	2.27	0.49
1:2A:1824:G:N3	3:2D:254:THR:OG1	2.46	0.49
1:2A:2127:G:C6	1:2A:2161:C:C4	3.01	0.49
1:1A:2353:G:N2	22:10:34:GLY:O	2.22	0.48
1:1A:806:C:O2	1:1A:2444:G:O2'	2.30	0.48
1:1A:2472:G:O2'	1:1A:2478:A:N6	2.40	0.48
1:1A:614(C):A:H4'	1:1A:615:G:OP1	2.13	0.48
3:1D:70:TRP:HB3	3:1D:190:TYR:CE2	2.48	0.48
19:1X:12:VAL:HB	19:1X:27:THR:HB	1.95	0.48
21:1Z:48:PHE:HE1	21:1Z:71:VAL:HG11	1.76	0.48
1:2A:1966:A:H2	1:2A:2592:G:N3	2.12	0.48
1:2A:312:G:H4'	1:2A:331:A:N3	2.28	0.48
22:10:53:MET:HG3	22:10:59:LEU:HD23	1.94	0.48
1:1A:1588:C:H2'	1:1A:1589:C:H6	1.78	0.48
1:1A:2166:G:N7	1:1A:2168:G:N2	2.61	0.48
1:1A:918:A:N3	2:1B:80:U:O2'	2.40	0.48
1:1A:764:A:N3	3:1D:213:ARG:NH1	2.60	0.48
60:1A:4277:HOH:O	17:1V:82:ARG:HB2	2.12	0.48
24:22:65:ASN:ND2	24:22:69:ARG:HH12	2.11	0.48
1:2A:1360:A:OP2	9:2N:35:ARG:NH2	117.18	0.48
1:2A:324:A:H2'	1:2A:325:G:O4'	2.13	0.48
5:2F:157:VAL:HB	5:2F:194:MET:HG2	1.96	0.48
21:2Z:141:VAL:C	21:2Z:143:GLY:H	2.17	0.48
26:14:57:GLU:O	26:14:60:GLN:N	2.38	0.48
1:1A:1041:C:H42	1:1A:1114:G:H1	1.59	0.48
1:1A:854:G:H1	1:1A:923:C:H42	1.61	0.48
6:1G:46:ALA:HB1	6:1G:50:ALA:O	2.13	0.48
1:2A:387:U:OP2	23:21:20:ARG:NH1	2.45	0.48
23:21:51:VAL:HG11	23:21:74:VAL:HG21	1.96	0.48
23:21:76:ARG:NH2	23:21:97:LEU:HB3	2.28	0.48
1:2A:1286:A:C8	1:2A:1287:A:H4'	8.19	0.48
1:2A:1883:G:HO2'	1:2A:1884:A:H8	1.60	0.48
1:2A:1996:C:H4'	1:2A:1997:G:OP1	2.13	0.48
1:2A:2494:G:H2'	1:2A:2495:G:H8	1.78	0.48
1:2A:705:A:H2'	1:2A:706:A:O4'	2.13	0.48
1:1A:2688:U:OP1	60:1A:4105:HOH:O	2.19	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:910:A:N1	1:1A:2277:G:H1'	2.28	0.48
6:1G:32:PRO:HB3	6:1G:163:ALA:HB2	1.96	0.48
18:1W:48:ALA:O	18:1W:52:GLU:HG2	2.13	0.48
1:2A:2099:U:N3	1:2A:2190:G:N1	2.29	0.48
1:2A:2291:U:OP1	1:2A:2380:C:O2'	2.31	0.48
1:2A:572:A:H61	1:2A:2029:G:H21	1.60	0.48
1:2A:796:C:H2'	1:2A:797:C:C6	2.49	0.48
1:2A:848:G:H2'	1:2A:849:A:C8	2.48	0.48
3:2D:77:ALA:HB2	3:2D:97:TYR:CD1	2.47	0.48
60:2A:4937:HOH:O	11:2P:36:LYS:O	2.20	0.48
21:2Z:154:ASP:N	21:2Z:154:ASP:OD1	2.46	0.48
1:1A:2432:A:C4	23:11:33:LYS:HG2	2.47	0.48
1:1A:2352:A:N6	1:1A:2365:G:O2'	2.46	0.48
1:1A:579:G:N7	60:1A:6554:HOH:O	2.35	0.48
3:1D:118:VAL:HG22	3:1D:119:ALA:H	1.78	0.48
3:1D:72:LYS:NZ	3:1D:99:ASP:OD2	2.34	0.48
6:1G:129:GLY:O	6:1G:161:THR:OG1	2.31	0.48
1:2A:652(B):A:H61	1:2A:655:A:H1'	1.78	0.48
7:2H:83:TYR:CZ	7:2H:138:LYS:HD2	2.48	0.48
11:2P:138:LEU:HD23	11:2P:145:PRO:HB3	1.96	0.48
1:1A:1069:A:H2'	1:1A:1073:A:N7	2.29	0.48
1:1A:1441:G:H21	1:1A:1460:A:H62	25.00	0.48
1:1A:792:G:O2'	1:1A:2440:C:N3	2.39	0.48
7:1H:35:VAL:HG11	7:1H:71:LEU:HB3	1.95	0.48
8:1I:6:LEU:HD11	8:1I:37:VAL:HG23	1.95	0.48
18:1W:57:ASN:HA	18:1W:61:ASN:HD22	1.79	0.48
1:2A:1507:A:O2'	1:2A:1508:A:O5'	2.21	0.48
1:2A:1953:A:H1'	1:2A:2560:C:H1'	1.95	0.48
15:2T:109:GLU:HG2	15:2T:112:ARG:NH2	2.29	0.48
4:1E:167:VAL:HG22	4:1E:170:LEU:HD11	1.96	0.48
1:1A:2784:C:H1'	4:1E:37:ARG:HH12	1.79	0.48
1:1A:2744:G:N2	7:1H:143:GLN:OE1	2.46	0.48
1:1A:7:G:H5"	9:1N:121:LYS:HE3	1.95	0.48
7:2H:137:ASP:OD1	7:2H:138:LYS:N	2.46	0.48
20:2Y:47:LYS:NZ	20:2Y:48:ALA:O	2.44	0.48
21:2Z:77:ASP:OD2	21:2Z:80:ARG:NH1	2.36	0.48
22:10:70:GLN:OE1	22:10:80:HIS:NE2	2.46	0.48
24:12:65:ASN:O	24:12:69:ARG:NH1	2.47	0.48
1:1A:1754:C:OP1	15:1T:96:ARG:NH1	2.47	0.48
1:1A:2103:C:N3	1:1A:2186:G:N2	2.52	0.48
1:1A:2378:A:H4'	14:1S:23:ARG:NH1	2.29	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:1P:2:LYS:HG2	11:1P:4:SER:H	1.79	0.48
20:1Y:1:MET:HB3	20:1Y:2:ARG:H	1.51	0.48
1:2A:1243:G:O2'	11:2P:4:SER:O	2.31	0.48
1:2A:1487:G:H2'	1:2A:1488:G:H8	1.78	0.48
1:2A:2162:G:H2'	1:2A:2163:C:O4'	2.13	0.48
1:2A:2564:A:OP1	1:2A:2648:C:H4'	2.14	0.48
9:2N:4:TYR:CD2	16:2U:100:VAL:HG11	2.48	0.48
20:2Y:37:VAL:N	20:2Y:67:LEU:O	2.42	0.48
1:1A:1426:G:O2'	1:1A:1572:A:N6	2.47	0.48
1:1A:2367:G:H2'	1:1A:2368:C:C6	2.49	0.48
1:1A:266:G:O2'	1:1A:267:C:OP2	4.96	0.48
1:1A:826:U:C4'	11:1P:55:ARG:HB3	2.44	0.48
3:1D:76:PRO:HB2	3:1D:116:GLN:NE2	2.29	0.48
3:1D:77:ALA:HA	3:1D:97:TYR:HA	1.95	0.48
24:22:69:ARG:O	24:22:70:GLN:HG2	2.14	0.48
26:24:48:ARG:HG2	26:24:52:THR:HG23	1.95	0.48
1:2A:1190:G:OP1	11:2P:30:THR:OG1	2.29	0.48
1:2A:1514:U:H2'	1:2A:1515:G:C8	2.49	0.48
1:2A:2099:U:O2	1:2A:2190:G:N2	2.32	0.48
1:2A:2240:C:OP2	60:2A:6141:HOH:O	2.20	0.48
1:2A:2645:G:H4'	1:2A:2732:G:O3'	2.13	0.48
1:2A:2651:C:H42	1:2A:2669:G:H1	1.59	0.48
1:2A:974:G:O2'	1:2A:975:C:OP1	2.26	0.48
3:2D:145:VAL:HG13	3:2D:191:ALA:HB2	1.96	0.48
6:2G:29:TRP:O	6:2G:33:ARG:NH1	2.39	0.48
12:2Q:34:LEU:HB2	12:2Q:118:LEU:HD22	1.95	0.48
30:18:54:GLU:OE2	60:18:201:HOH:O	2.20	0.48
1:1A:2058:A:H2	57:1A:4074:ERY:H311	1.79	0.48
1:1A:865:C:N3	1:1A:908:C:N4	2.62	0.48
2:1B:66:A:H61	2:1B:109:C:H5''	1.78	0.48
10:1O:86:ILE:HG22	10:1O:94:ARG:HD3	1.96	0.48
11:1P:59:LEU:HD23	30:18:13:ARG:HD2	1.95	0.48
18:1W:58:ALA:HB1	18:1W:64:MET:HB2	1.95	0.48
31:29:2:LYS:NZ	31:29:31:LYS:O	2.40	0.48
1:2A:1009:A:OP2	9:2N:37:LYS:NZ	2.42	0.48
1:2A:146:G:H2'	1:2A:147:U:C6	2.49	0.48
1:2A:2319:G:N2	14:2S:3:ARG:HD2	2.29	0.48
1:2A:2349:G:H1	1:2A:2368:C:N4	2.11	0.48
1:2A:484:C:H2'	1:2A:485:C:H6	1.78	0.48
1:2A:817:C:O2'	1:2A:839:U:H5''	2.14	0.48
2:2B:75:G:N2	21:2Z:87:ASP:OD1	2.46	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:10:38:VAL:HB	22:10:59:LEU:HB2	1.96	0.47
1:1A:1086:A:H3'	1:1A:1086:A:N3	2.29	0.47
1:1A:1518:U:H2'	1:1A:1519:G:O4'	2.14	0.47
1:1A:1935:G:H1'	1:1A:1964:G:N2	2.29	0.47
1:1A:873:G:H1	1:1A:904:C:H42	1.62	0.47
1:1A:1693:U:H1'	3:1D:14:ARG:NH2	2.29	0.47
11:1P:52:GLU:HG2	30:18:57:ARG:HH22	1.80	0.47
1:2A:1202:C:N3	1:2A:1243:G:N2	2.59	0.47
1:2A:140:G:N2	1:2A:1596:A:H4'	2.29	0.47
1:2A:1710:C:H5'	1:2A:2859:G:H1'	1.96	0.47
2:2B:32:C:H2'	2:2B:33:G:O4'	2.13	0.47
4:2E:12:THR:HG22	15:2T:58:ASN:HD21	1.79	0.47
4:2E:49:LEU:HD21	4:2E:91:VAL:HG21	1.96	0.47
15:2T:49:VAL:HG12	15:2T:63:VAL:HG22	1.96	0.47
18:2W:34:ASN:OD1	18:2W:37:ARG:NH2	2.47	0.47
25:13:19:GLN:O	25:13:23:LEU:HD12	2.12	0.47
1:1A:2096:U:H3	1:1A:2193:G:H1	1.63	0.47
1:1A:264:C:O2'	1:1A:265:A:H2'	2.13	0.47
5:1F:157:VAL:HG12	5:1F:198:ALA:HB1	1.96	0.47
16:1U:48:ALA:O	16:1U:52:ARG:HG3	2.14	0.47
1:1A:1152:C:H1'	16:1U:77:SER:HB3	1.96	0.47
26:24:15:ILE:HD12	26:24:21:VAL:HG22	1.94	0.47
1:2A:2615:U:C2	27:25:7:PRO:HA	2.50	0.47
1:2A:700:G:O2'	1:2A:1632:A:N3	2.36	0.47
1:2A:2151:G:H2'	1:2A:2152:G:C8	2.48	0.47
1:2A:631:A:H2'	1:2A:632:A:O4'	2.13	0.47
1:2A:97:C:OP1	24:22:2:LYS:NZ	2.47	0.47
2:2B:11:C:H3'	2:2B:12:C:H6	1.78	0.47
4:2E:9:VAL:HG22	4:2E:25:VAL:HB	1.95	0.47
1:1A:379:G:N2	23:11:42:GLN:OE1	2.38	0.47
1:1A:1030:G:OP2	12:1Q:128:LYS:NZ	2.47	0.47
1:1A:121:G:H4'	1:1A:149:A:H5'	1.96	0.47
1:1A:1740:G:H2'	1:1A:1741:A:C8	2.49	0.47
1:1A:266:G:H4'	1:1A:267:C:C5	8.18	0.47
1:1A:2749:A:OP1	7:1H:3:ARG:NH1	2.48	0.47
25:23:6:VAL:HG13	25:23:56:VAL:HG22	1.96	0.47
1:2A:1603:A:OP1	60:2A:5399:HOH:O	2.19	0.47
1:2A:2106:G:H2'	1:2A:2107:C:O4'	2.13	0.47
1:2A:2532:G:HO2'	1:2A:2657:A:N6	2.11	0.47
1:2A:1983:C:H4'	1:2A:2606:C:H4'	1.95	0.47
1:2A:271(U):G:H2'	1:2A:271(V):G:C8	2.49	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2G:122:PRO:HB3	6:2G:170:ARG:NH1	2.29	0.47
30:18:23:VAL:CG2	30:18:47:LYS:HB3	2.43	0.47
1:1A:2875:C:H2'	1:1A:2876:G:O4'	2.13	0.47
1:1A:479:A:N3	1:1A:481:G:H5''	2.29	0.47
6:1G:120:LEU:N	6:1G:179:PRO:O	2.45	0.47
22:20:54:GLY:O	22:20:57:PHE:N	2.47	0.47
30:28:26:LYS:HB2	30:28:44:LYS:O	2.15	0.47
1:2A:1313:U:H5''	60:2A:4383:HOH:O	2.13	0.47
1:2A:16:G:H2'	1:2A:17:G:H8	1.80	0.47
1:2A:240:G:O2'	1:2A:257:A:N6	2.38	0.47
1:2A:2439:A:H8	1:2A:2439:A:H5'	1.79	0.47
1:2A:196:A:O2'	1:2A:805:G:O6	2.28	0.47
3:2D:218:ARG:HB3	3:2D:219:PRO:HD2	1.97	0.47
2:2B:31:C:H4'	6:2G:29:TRP:CH2	2.50	0.47
6:2G:54:GLU:HA	6:2G:57:ALA:HB3	1.95	0.47
2:1B:12:C:H2'	22:10:73:GLY:HA3	1.96	0.47
26:14:56:VAL:HG23	26:14:57:GLU:H	1.79	0.47
1:1A:1486:A:H2'	1:1A:1487:G:C8	2.50	0.47
1:1A:634:C:H2'	1:1A:635:C:C6	2.49	0.47
4:1E:14:ILE:HG13	4:1E:21:VAL:HG13	1.95	0.47
1:2A:1409:C:H5'	1:2A:1916:A:N1	128.57	0.47
1:2A:1785:A:N6	60:2A:3953:HOH:O	2.47	0.47
1:2A:2712:U:OP1	1:2A:2714:G:H4'	2.14	0.47
1:2A:529:A:H62	1:2A:2041:U:H3	1.62	0.47
1:2A:686:G:N2	1:2A:788:A:H61	2.13	0.47
1:2A:1803:A:O2'	3:2D:259:THR:HG21	2.14	0.47
5:2F:32:LEU:O	5:2F:36:VAL:HG23	2.13	0.47
12:2Q:17:LEU:HB3	12:2Q:39:PRO:HB2	1.95	0.47
15:2T:27:THR:HB	15:2T:89:VAL:HG23	1.95	0.47
27:15:55:ARG:HE	27:15:57:VAL:HG13	1.79	0.47
1:1A:1614:A:H8	1:1A:1614:A:P	2.38	0.47
1:1A:793:A:OP2	1:1A:2071:A:O2'	2.32	0.47
1:1A:2301:C:H2'	1:1A:2302:G:H8	1.80	0.47
1:1A:2584:U:H2'	1:1A:2585:U:H2'	1.95	0.47
8:1I:61:ARG:HA	8:1I:61:ARG:HD3	1.65	0.47
11:1P:124:LYS:HA	11:1P:144:GLU:HB3	1.97	0.47
1:2A:196:A:H2'	1:2A:196:A:N3	2.30	0.47
3:2D:118:VAL:HG22	3:2D:119:ALA:H	1.79	0.47
10:2O:29:ASN:OD1	10:2O:29:ASN:N	2.47	0.47
26:14:16:CYS:HB2	26:14:36:CYS:HB3	1.95	0.47
1:1A:1039:G:H1	1:1A:1116:C:H42	1.61	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1441:G:N3	1:1A:1460:A:N6	26.12	0.47
1:1A:1692:U:H2'	1:1A:1694:C:C5	2.50	0.47
1:1A:191:A:H2'	1:1A:192:C:C6	2.50	0.47
1:1A:2564:A:C2	1:1A:2647:U:H4'	2.50	0.47
1:1A:589:C:O3'	5:1F:95:ARG:NE	2.40	0.47
14:1S:10:ARG:O	14:1S:14:VAL:HG13	2.15	0.47
30:28:28:GLY:O	30:28:36:LYS:NZ	2.48	0.47
1:2A:1179:C:H2'	1:2A:1180:C:C6	2.49	0.47
1:2A:2735:G:H2'	1:2A:2736:G:C8	2.50	0.47
1:2A:690:G:O5'	1:2A:690:G:H8	2.47	0.47
1:2A:948:G:N1	1:2A:970:C:O2	2.48	0.47
5:2F:37:VAL:HG22	5:2F:183:VAL:HG23	1.96	0.47
1:2A:245:G:O5'	11:2P:73:GLY:HA2	2.15	0.47
15:2T:65:LYS:O	15:2T:72:VAL:N	2.40	0.47
21:2Z:61:LEU:HD22	21:2Z:65:GLN:HB2	1.97	0.47
18:1W:25:ARG:NH2	18:1W:74:ALA:O	2.40	0.47
1:2A:2420:C:P	30:28:33:ASN:H	2.37	0.47
1:2A:1223:G:N2	1:2A:1225:G:H3'	2.29	0.47
1:2A:2364:C:H4'	22:20:56:ASP:OD1	2.14	0.47
1:2A:372:G:N2	1:2A:400:G:H2'	2.30	0.47
1:2A:93:G:H2'	1:2A:94:C:C6	2.49	0.47
12:2Q:57:HIS:HD2	12:2Q:117:ALA:HB2	1.80	0.47
12:2Q:27:VAL:O	12:2Q:138:ASP:HB3	2.15	0.47
15:2T:16:ARG:HH11	15:2T:81:PRO:HA	1.80	0.47
25:13:51:ALA:HA	25:13:54:VAL:HG12	1.97	0.47
1:1A:2080:G:H2'	1:1A:2081:C:H6	1.80	0.47
1:1A:2129:C:H42	1:1A:2159:G:H1	1.60	0.47
1:1A:2683:C:OP1	15:1T:53:ARG:NH2	2.44	0.47
1:1A:57:C:H2'	1:1A:58:G:O4'	2.14	0.47
7:1H:125:VAL:HG13	7:1H:131:VAL:HG22	1.97	0.47
8:1I:65:ALA:O	8:1I:69:LYS:N	2.42	0.47
14:1S:67:ARG:NH2	14:1S:103:GLU:OE1	2.31	0.47
14:1S:110:LEU:HA	14:1S:110:LEU:HD12	1.80	0.47
18:1W:69:LEU:HD13	18:1W:107:LEU:HD23	1.97	0.47
1:2A:1149:G:H2'	1:2A:1150:C:C6	2.50	0.47
1:2A:2191:G:H2'	1:2A:2192:G:O4'	2.15	0.47
1:2A:34:C:H2'	1:2A:35:G:C8	4.80	0.47
1:2A:531:C:H4'	1:2A:532:A:H5''	1.96	0.47
1:2A:8:A:H2'	1:2A:9:U:C6	2.49	0.47
23:11:2:SER:HB2	23:11:43:TYR:CD1	2.49	0.47
1:1A:1075:C:C2'	1:1A:1076:C:H5'	2.44	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1508:A:HO2'	1:1A:1509:C:P	2.37	0.47
1:1A:2012:G:OP1	18:1W:11:ARG:NH2	2.46	0.47
1:1A:2126:A:N7	1:1A:2163:C:H1'	2.30	0.47
1:1A:493:G:H2'	1:1A:494:G:O4'	2.15	0.47
1:2A:580:C:H42	1:2A:1260:G:H1	1.63	0.47
1:2A:1713:U:H2'	1:2A:1714:G:H8	1.79	0.47
1:2A:2431:U:O4	60:2A:5180:HOH:O	2.18	0.47
1:2A:2472:G:H2'	1:2A:2475:C:H42	1.80	0.47
1:2A:595:C:H42	1:2A:662:G:H1	1.63	0.47
1:2A:832:G:OP1	60:2A:4941:HOH:O	2.21	0.47
6:2G:96:ARG:O	6:2G:99:MET:HB3	2.14	0.47
12:2Q:31:ASP:OD1	12:2Q:134:ARG:NH1	2.35	0.47
18:2W:9:TYR:H	18:2W:102:HIS:CE1	2.33	0.47
20:2Y:9:LYS:HA	20:2Y:10:GLY:HA2	1.52	0.47
1:1A:1035:U:H2'	1:1A:1036:G:C8	2.50	0.47
1:1A:2322:A:H2'	1:1A:2323:G:O4'	2.15	0.47
1:1A:1799:G:O2'	3:1D:181:GLU:OE2	2.28	0.47
5:1F:187:VAL:HG12	11:1P:3:LEU:HD12	1.97	0.47
21:1Z:76:LEU:HD12	21:1Z:83:PRO:HA	1.96	0.47
25:23:26:LEU:O	25:23:35:ARG:HD3	2.15	0.47
1:2A:1263:U:H1'	27:25:10:LYS:HG3	1.97	0.47
1:2A:116:C:H2'	1:2A:117:G:O4'	2.15	0.47
1:2A:2126:A:O2'	1:2A:2162:G:N2	2.48	0.47
1:2A:2600:A:N6	60:2A:4507:HOH:O	2.44	0.47
1:2A:271(H):G:H2'	1:2A:271(I):G:C8	2.49	0.47
1:2A:336:C:H2'	1:2A:337:C:C6	2.52	0.47
3:2D:177:LEU:HD12	3:2D:181:GLU:HB3	1.97	0.47
11:2P:128:HIS:NE2	11:2P:148:LEU:HD11	2.29	0.47
5:2F:187:VAL:HG12	11:2P:3:LEU:HD12	1.96	0.47
12:2Q:38:GLU:HG3	12:2Q:127:ILE:HG22	1.96	0.47
21:2Z:35:ARG:HA	21:2Z:35:ARG:HD2	1.73	0.47
1:1A:1183:G:O2'	25:13:29:ARG:NH1	2.47	0.46
1:1A:1066:U:N3	1:1A:1069:A:OP2	2.47	0.46
1:1A:1406:U:H2'	1:1A:1407:C:C6	2.50	0.46
1:1A:1417:C:H2'	1:1A:1418:G:O4'	2.15	0.46
1:1A:193:U:OP2	60:1A:4535:HOH:O	2.20	0.46
1:1A:751:A:H5'	18:1W:90:ARG:HA	1.97	0.46
1:1A:857:C:N4	1:1A:858:U:O4	2.48	0.46
10:1O:68:GLU:H	10:1O:68:GLU:CD	2.18	0.46
1:2A:127:A:H5''	1:2A:128:C:O5'	2.15	0.46
1:2A:1502:C:H2'	1:2A:1503:U:C6	2.48	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2110:G:H1	1:2A:2179:C:H42	1.61	0.46
1:2A:2431:U:O2'	1:2A:2433:A:N7	2.42	0.46
1:2A:2461:C:H2'	1:2A:2462:U:C6	2.50	0.46
1:2A:2711:A:OP2	60:2A:4577:HOH:O	2.21	0.46
1:2A:271(P):C:H2'	1:2A:271(Q):G:C8	2.50	0.46
1:2A:724:U:H2'	1:2A:725:G:O4'	2.15	0.46
1:2A:774:A:N3	1:2A:774:A:H2'	2.30	0.46
9:2N:30:ILE:HG23	9:2N:52:VAL:HG11	1.98	0.46
1:2A:2377:A:O2'	14:2S:112:PHE:O	2.21	0.46
15:2T:122:ASP:O	15:2T:126:ALA:N	2.46	0.46
1:1A:2375:G:N2	1:1A:2378:A:OP2	2.40	0.46
1:1A:2406:U:OP2	1:1A:2406:U:H2'	2.16	0.46
1:1A:784:A:C6	3:1D:229:VAL:HG11	2.50	0.46
23:21:3:LYS:HB3	23:21:4:VAL:H	1.49	0.46
1:2A:1520:G:H3'	1:2A:1523:U:H6	1.80	0.46
2:2B:78:A:H2'	2:2B:79:C:O4'	2.15	0.46
9:2N:103:VAL:HG11	9:2N:120:LEU:HD22	1.97	0.46
1:1A:1471:A:OP2	1:1A:1519:G:N1	2.35	0.46
1:1A:1628:G:H2'	1:1A:1629:U:C6	2.50	0.46
1:1A:196:A:N3	1:1A:196:A:H2'	2.30	0.46
1:1A:272(J):C:H2'	1:1A:274:G:H8	1.81	0.46
1:1A:2849:U:H4'	1:1A:2868:A:C2	2.51	0.46
1:1A:958:U:O2	2:1B:90:A:O2'	2.18	0.46
3:1D:2:ALA:O	3:1D:20:ASP:HB3	2.15	0.46
5:1F:65:TRP:CZ2	5:1F:75:HIS:HD2	2.33	0.46
15:1T:22:PHE:HB3	15:1T:88:ILE:HD11	1.97	0.46
21:1Z:99:TYR:HA	21:1Z:124:ILE:O	2.15	0.46
25:23:11:SER:HA	25:23:31:LEU:HD21	1.98	0.46
1:2A:1915:5MU:H73	1:2A:1916:A:N6	2.30	0.46
1:2A:2156:G:H2'	1:2A:2157:G:C4	2.49	0.46
1:2A:731:C:H5''	60:2A:6025:HOH:O	2.15	0.46
3:2D:67:PHE:HB3	3:2D:153:ALA:H	1.81	0.46
8:2I:83:ALA:HB2	8:2I:88:ILE:HG12	1.98	0.46
16:2U:76:TYR:CZ	16:2U:80:ILE:HG13	2.50	0.46
1:1A:1359:A:H2'	1:1A:1360:A:H5'	1.96	0.46
1:1A:195:A:OP1	11:1P:46:LYS:NZ	2.43	0.46
1:1A:2537:U:H2'	1:1A:2538:C:C6	2.51	0.46
1:1A:2698:U:H2'	1:1A:2699:C:C6	2.51	0.46
1:1A:284:U:H2'	1:1A:285:C:H6	1.80	0.46
1:1A:450:G:OP2	60:1A:6867:HOH:O	2.21	0.46
6:1G:16:ARG:NH2	6:1G:28:VAL:O	2.48	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:252:G:P	11:1P:50:ARG:HH12	2.37	0.46
14:1S:27:SER:HA	14:1S:88:ASP:HB3	1.97	0.46
1:1A:1188:U:H4'	17:1V:79:VAL:HG22	1.96	0.46
25:23:5:LYS:O	25:23:56:VAL:HA	2.16	0.46
1:2A:1196:C:H2'	1:2A:1197:G:H8	1.80	0.46
1:2A:1471:A:OP2	1:2A:1519:G:N2	2.49	0.46
1:2A:2320:A:H2'	1:2A:2320:A:N3	2.31	0.46
1:2A:239:U:H2'	1:2A:240:G:O4'	2.15	0.46
1:2A:2432:A:C8	23:21:33:LYS:HD3	2.51	0.46
1:2A:340:A:H2'	1:2A:341:G:O4'	2.15	0.46
1:2A:493:G:H2'	1:2A:494:G:O4'	2.14	0.46
15:2T:28:VAL:HG13	15:2T:86:ILE:HG23	1.97	0.46
17:2V:4:ILE:HD12	17:2V:39:LEU:HB3	1.97	0.46
1:1A:1137:G:H2'	1:1A:1138:G:C8	2.50	0.46
1:1A:2689:U:OP2	1:1A:2719:G:N2	2.41	0.46
1:1A:2887:U:H2'	1:1A:2888:C:C6	2.51	0.46
6:1G:27:ASN:HB3	6:1G:30:GLU:HG3	1.98	0.46
8:1I:93:THR:O	8:1I:97:ILE:HG13	2.15	0.46
10:1O:29:ASN:OD1	10:1O:29:ASN:N	2.47	0.46
14:1S:43:GLU:OE2	22:10:49:LYS:HE3	2.15	0.46
14:1S:93:LYS:O	14:1S:95:HIS:N	2.49	0.46
22:20:69:PHE:CE1	22:20:79:VAL:HG22	2.51	0.46
23:21:2:SER:HB3	23:21:46:LEU:HD12	1.98	0.46
28:26:10:LEU:HD13	28:26:19:ARG:HD3	1.98	0.46
1:2A:1022:G:N2	1:2A:1023:U:O4	2.48	0.46
1:2A:1199:U:O2'	60:2A:4243:HOH:O	2.20	0.46
1:2A:2065:C:H4'	1:2A:2251:OMG:HM22	1.97	0.46
1:2A:2166:G:H5'	1:2A:2167:U:OP2	2.16	0.46
1:2A:2615:U:N1	27:25:7:PRO:HA	2.29	0.46
1:2A:2635:C:H5''	4:2E:78:LEU:O	2.15	0.46
1:2A:330:A:H2	1:2A:1210:A:HO2'	1.62	0.46
3:2D:133:LEU:HB3	3:2D:173:VAL:HG21	1.97	0.46
16:2U:76:TYR:OH	16:2U:92:ARG:NE	2.39	0.46
25:13:26:LEU:O	25:13:35:ARG:HD3	2.15	0.46
1:1A:1405:U:H2'	1:1A:1406:U:C6	2.51	0.46
1:1A:1721:G:H2'	1:1A:1722:A:H2'	1.98	0.46
1:1A:453:C:O2	1:1A:457:A:O2'	2.32	0.46
2:1B:7:G:H1	2:1B:114:C:H42	1.64	0.46
6:1G:131:TYR:HB3	6:1G:159:VAL:CG2	2.46	0.46
19:1X:61:GLY:HA3	19:1X:73:ARG:O	2.15	0.46
21:1Z:166:SER:O	21:1Z:168:GLU:N	2.49	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2384:G:OP2	22:20:55:ARG:NH2	2.48	0.46
1:2A:1116:C:H2'	1:2A:1117:G:O4'	3.29	0.46
1:2A:1754:C:N3	1:2A:2716:U:O2'	2.46	0.46
1:2A:954:G:O2'	1:2A:2274:A:N1	2.26	0.46
1:2A:833:U:H2'	1:2A:834:C:C6	2.85	0.46
3:2D:4:LYS:HB3	3:2D:18:VAL:HG23	1.97	0.46
6:2G:17:PRO:HA	6:2G:20:ILE:HD12	1.98	0.46
7:2H:40:GLU:OE1	7:2H:61:HIS:NE2	2.47	0.46
21:2Z:146:ILE:HA	21:2Z:174:VAL:HG13	1.97	0.46
1:1A:2059:A:O2'	5:1F:69:HIS:HD2	1.99	0.46
1:1A:309:G:H1'	1:1A:608:A:C2	64.26	0.46
1:1A:359:A:H2'	1:1A:360:G:O4'	2.16	0.46
1:1A:894:C:H2'	1:1A:895:U:O4'	2.16	0.46
1:2A:1368:G:OP1	29:27:25:PRO:HG3	2.15	0.46
1:2A:1005:C:H2'	1:2A:1006:C:C6	2.51	0.46
1:2A:1991:U:H2'	1:2A:1992:G:H5''	1.96	0.46
1:2A:2262:U:H2'	1:2A:2263:C:C6	2.50	0.46
1:2A:2291:U:H5''	1:2A:2380:C:O2'	2.15	0.46
1:2A:648:G:H2'	1:2A:649:G:C8	2.51	0.46
1:2A:928:G:H8	1:2A:928:G:O5'	1.97	0.46
3:2D:274:ARG:O	3:2D:275:LYS:HD2	2.16	0.46
13:2R:98:LEU:O	13:2R:113:LEU:HG	2.16	0.46
13:2R:51:LEU:HD22	13:2R:66:VAL:HG13	1.98	0.46
15:2T:66:VAL:HA	15:2T:71:GLY:HA2	1.98	0.46
1:1A:1021:A:O2'	1:1A:1123:C:OP1	2.21	0.46
1:1A:747:U:O2	1:1A:2014:A:H1'	2.15	0.46
1:1A:2145:C:H3'	1:1A:2146:C:H5'	1.97	0.46
1:1A:2801(A):A:H1'	1:1A:2895:U:H1'	1.98	0.46
1:1A:448:U:H5'	60:1A:6875:HOH:O	2.15	0.46
1:1A:774:A:N3	1:1A:774:A:H2'	2.31	0.46
3:1D:26:LYS:HB3	3:1D:83:GLU:HG2	1.98	0.46
1:1A:2305:A:H5''	6:1G:134:GLY:HA3	1.97	0.46
12:1Q:14:ARG:HG2	12:1Q:41:TRP:HH2	1.81	0.46
14:1S:11:LYS:HG3	14:1S:91:PRO:HD3	1.96	0.46
1:2A:1025:G:C4	1:2A:1135:C:H1'	2.51	0.46
1:2A:1857:G:C6	1:2A:1858:G:N1	2.84	0.46
1:2A:195:A:OP2	60:2A:4968:HOH:O	2.20	0.46
1:2A:2250:G:C8	1:2A:2496:C:H5''	2.51	0.46
1:2A:2538:C:H2'	1:2A:2539:C:H6	1.79	0.46
1:2A:903:C:H2'	1:2A:904:C:C6	2.51	0.46
6:2G:100:TRP:O	6:2G:104:GLU:HB2	2.15	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2B:43:C:H4'	6:2G:98:ARG:HH21	1.80	0.46
8:2I:56:LYS:O	8:2I:60:GLU:N	2.48	0.46
9:2N:22:THR:HB	9:2N:25:ARG:HB2	1.97	0.46
18:2W:86:LEU:HD22	18:2W:96:ILE:HD11	1.98	0.46
21:2Z:79:ARG:HD2	21:2Z:80:ARG:HH12	1.81	0.46
1:1A:1210:A:H5''	1:1A:1212:G:O4'	2.15	0.46
1:1A:1711:C:H2'	1:1A:1712:C:H6	1.80	0.46
1:1A:2567:G:H2'	1:1A:2568:C:C6	2.51	0.46
1:1A:312:G:H4'	1:1A:331:A:C2	2.51	0.46
31:29:7:VAL:HA	31:29:34:GLN:HE21	1.81	0.46
1:2A:1263:U:C4	1:2A:1264:G:C6	3.04	0.46
1:2A:1442:G:N3	1:2A:1442:G:H2'	2.88	0.46
1:2A:1464:C:H2'	1:2A:1465:G:C8	2.51	0.46
1:2A:1796:U:H2'	1:2A:1797:C:C6	2.51	0.46
1:2A:1847:A:H3'	1:2A:1848:A:H5'	1.97	0.46
1:2A:249:C:O2	30:28:12:LYS:NZ	2.46	0.46
1:2A:579:G:H2'	1:2A:580:C:C6	2.50	0.46
1:2A:699:A:H2'	1:2A:700:G:O4'	2.16	0.46
1:2A:722:A:H2'	1:2A:723:G:C8	2.51	0.46
1:2A:84:A:N1	1:2A:98:G:O2'	2.42	0.46
1:2A:918:A:C5	1:2A:919:G:H1'	2.51	0.46
5:2F:136:THR:HA	5:2F:166:ALA:HB1	1.98	0.46
1:2A:2685:G:OP2	15:2T:51:ARG:NH2	2.48	0.46
16:2U:19:LYS:HA	16:2U:22:LYS:HG3	1.97	0.46
1:1A:1114:G:H2'	1:1A:1115:G:C8	2.51	0.46
1:1A:1422:G:H2'	1:1A:1423:G:C8	3.41	0.46
1:1A:2680:C:H5'	4:1E:189:PRO:HA	1.98	0.46
1:1A:748:G:C8	18:1W:89:ALA:HB1	2.51	0.46
1:1A:800:A:H8	1:1A:800:A:OP1	1.99	0.46
18:1W:10:VAL:HG12	18:1W:12:ILE:HG22	1.98	0.46
1:2A:829:A:N7	1:2A:2248:C:H5'	2.31	0.46
1:2A:2330:G:H2'	1:2A:2331:G:O4'	2.15	0.46
1:2A:2881:C:H2'	1:2A:2882:A:O4'	2.15	0.46
1:2A:478:A:N1	1:2A:500:G:H4'	2.31	0.46
3:2D:60:ARG:NH1	3:2D:86:PRO:O	2.49	0.46
9:2N:114:ARG:O	9:2N:118:LYS:HG3	2.16	0.46
10:2O:75:SER:OG	10:2O:76:ALA:N	2.49	0.46
15:2T:39:ARG:NH1	15:2T:41:ARG:HB3	2.31	0.46
20:2Y:35:TYR:CE2	20:2Y:69:ALA:HB3	2.51	0.46
28:16:26:ASN:HB3	28:16:29:ASN:HB2	1.98	0.45
30:18:63:PRO:HG2	30:18:64:TYR:CE2	2.51	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1588:C:H2'	1:1A:1589:C:C6	2.51	0.45
1:1A:1753:G:H5''	15:1T:95:ARG:HD3	1.98	0.45
4:1E:174:ASP:OD1	4:1E:175:VAL:N	2.49	0.45
7:1H:83:TYR:CE2	7:1H:138:LYS:HB2	2.51	0.45
15:1T:11:GLU:O	15:1T:15:VAL:HG23	2.16	0.45
17:1V:14:VAL:HB	17:1V:96:ILE:HG13	1.97	0.45
21:1Z:52:SER:OG	21:1Z:53:ILE:N	2.48	0.45
1:2A:1410:G:H2'	1:2A:1411:C:H6	1.79	0.45
1:2A:2155:G:N7	1:2A:2156:G:H1'	2.31	0.45
1:2A:2375:G:O2'	1:2A:2377:A:N7	2.39	0.45
1:2A:621:A:OP2	11:2P:108:LYS:NZ	2.42	0.45
1:1A:1899:G:N3	1:1A:1899:G:H2'	2.31	0.45
1:1A:2377:A:H2'	1:1A:2378:A:C8	2.51	0.45
1:1A:828:U:H4'	1:1A:831:G:N1	2.31	0.45
16:1U:79:PHE:HE1	16:1U:110:VAL:HA	1.82	0.45
20:1Y:13:VAL:HG12	20:1Y:74:PRO:HA	1.97	0.45
1:2A:2355:C:H4'	22:20:24:LYS:HG3	1.98	0.45
1:2A:1127:A:H2'	1:2A:1128:A:H5''	1.97	0.45
1:2A:1218:C:N4	1:2A:1231:G:H1	2.08	0.45
1:2A:1444:G:N2	1:2A:1445(A):C:O2	2.49	0.45
1:2A:1514:U:H2'	1:2A:1515:G:H8	1.82	0.45
1:2A:2356:C:H2'	1:2A:2357:U:O4'	2.15	0.45
1:2A:2809:A:N6	1:2A:2891:G:H2'	2.30	0.45
1:2A:2819:G:H2'	1:2A:2821:A:N7	2.31	0.45
1:2A:882:G:H1	1:2A:894:C:H42	1.63	0.45
10:2O:115:VAL:HG13	10:2O:121:VAL:HG21	1.98	0.45
12:2Q:110:THR:HG23	12:2Q:113:GLN:OE1	2.16	0.45
26:14:40:HIS:CD2	26:14:41:PRO:HD2	2.52	0.45
1:1A:1042:G:N2	1:1A:1113:U:O2	2.41	0.45
1:1A:1153:C:H2'	1:1A:1154:G:O4'	2.15	0.45
1:1A:1429:G:H2'	1:1A:1430:C:C6	2.51	0.45
1:1A:2889:C:H2'	1:1A:2891:G:O4'	2.16	0.45
1:1A:875:G:N2	1:1A:902:C:N3	2.47	0.45
1:2A:651:G:H4'	30:28:18:ALA:HB3	1.99	0.45
1:2A:1138:G:C6	1:2A:1140:C:H1'	6.70	0.45
1:2A:2070:G:H2'	1:2A:2071:A:H8	1.80	0.45
1:2A:2593:U:H2'	1:2A:2594:C:C6	2.50	0.45
1:2A:27:G:H22	1:2A:512:G:H1'	1.81	0.45
1:1A:111:A:O3'	24:12:65:ASN:ND2	2.49	0.45
1:1A:2031:A:C6	1:1A:2498:C:H1'	2.51	0.45
1:1A:2053:G:C5'	4:1E:145:LYS:H	2.29	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2161:C:O2'	1:1A:2162:G:OP2	2.26	0.45
1:1A:473:G:H2'	1:1A:474:G:H8	2.79	0.45
1:1A:503:A:H4'	1:1A:504:U:H5''	1.98	0.45
4:1E:26:ILE:O	4:1E:182:LEU:N	2.46	0.45
1:1A:244:A:H4'	11:1P:74:GLU:HB2	1.99	0.45
25:23:4:LEU:N	25:23:37:LEU:O	2.46	0.45
1:2A:1015:G:H2'	1:2A:1016:G:C8	2.44	0.45
1:2A:1590:U:H2'	1:2A:1591:G:C8	2.52	0.45
1:2A:1630:G:N2	1:2A:1636:C:O2	2.40	0.45
1:2A:174:C:H2'	1:2A:175:G:H8	1.82	0.45
1:2A:2537:U:H2'	1:2A:2538:C:C6	2.52	0.45
6:2G:7:LEU:HB2	6:2G:104:GLU:HG3	1.99	0.45
8:2I:48:GLU:HB3	8:2I:52:ARG:HH22	1.81	0.45
10:2O:36:GLY:HA2	10:2O:106:LEU:HD23	1.99	0.45
16:2U:28:ARG:NH1	16:2U:38:THR:OG1	2.45	0.45
17:2V:72:VAL:HG13	17:2V:85:LYS:HB3	1.98	0.45
20:2Y:12:THR:HA	20:2Y:26:LYS:HA	1.98	0.45
1:1A:141:A:N3	1:1A:1408:C:O2'	2.42	0.45
1:1A:2292:C:H2'	1:1A:2293:C:C6	2.51	0.45
1:1A:2627:G:O2'	1:1A:2781:A:N1	2.32	0.45
1:1A:2832:U:O4	1:1A:2883:A:H5''	2.16	0.45
5:1F:143:ALA:HB1	5:1F:148:LEU:HB2	1.99	0.45
1:2A:1278:A:OP1	13:2R:36:THR:HG22	2.16	0.45
1:2A:1266:G:O2'	1:2A:2012:G:O6	2.24	0.45
1:2A:2361:A:H5'	30:28:27:THR:OG1	2.17	0.45
57:2A:3875:ERY:H71	57:2A:3875:ERY:H4	1.92	0.45
1:2A:581:C:H2'	1:2A:582:G:C8	2.51	0.45
1:2A:984:A:H5''	1:2A:985:C:H5	1.82	0.45
2:2B:50:G:OP1	14:2S:63:THR:OG1	2.23	0.45
1:2A:1257:C:H4'	5:2F:83:PHE:CD1	2.52	0.45
12:2Q:21:THR:O	21:2Z:78:LYS:HD2	2.17	0.45
13:2R:44:LEU:HD11	13:2R:79:LEU:HD13	10.37	0.45
1:1A:1024:G:C6	1:1A:1025:G:C6	3.05	0.45
1:1A:1684:C:H2'	1:1A:1685:C:C6	2.52	0.45
1:1A:2532:G:O2'	1:1A:2657:A:N1	2.45	0.45
1:1A:271(E):U:H2'	1:1A:271(F):C:C6	2.51	0.45
1:1A:673:C:H5''	5:1F:81:PRO:HD2	1.99	0.45
1:1A:863:A:H2'	1:1A:864:G:C8	2.51	0.45
1:1A:947:G:H2'	1:1A:948:G:C8	2.52	0.45
4:1E:143:ASN:HD22	4:1E:147:PRO:HD3	1.80	0.45
6:1G:32:PRO:HB2	6:1G:172:LEU:HD22	1.97	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:1O:35:VAL:HG21	10:1O:69:ILE:HD13	1.97	0.45
12:1Q:30:GLY:HA2	12:1Q:107:ALA:HB2	1.98	0.45
21:1Z:41:LEU:HD11	21:1Z:83:PRO:HG2	1.99	0.45
22:20:51:VAL:HG21	22:20:79:VAL:O	2.16	0.45
27:25:57:VAL:HG12	27:25:58:LEU:HD13	1.97	0.45
29:27:26:GLY:O	29:27:30:VAL:HG23	2.16	0.45
31:29:10:ILE:HD12	31:29:32:HIS:HA	1.98	0.45
1:2A:1013:C:H2'	1:2A:1014:U:C6	2.52	0.45
1:2A:1429:G:H2'	1:2A:1430:C:C6	2.51	0.45
1:2A:1509:C:O2	1:2A:1526:G:N2	44.98	0.45
1:2A:2207:G:H3'	1:2A:2208:A:H5''	1.98	0.45
1:2A:2369:A:H2'	1:2A:2370:G:C8	2.51	0.45
1:2A:479:A:N3	1:2A:481:G:H5''	2.32	0.45
14:2S:67:ARG:HD2	14:2S:71:ARG:HH21	1.82	0.45
28:16:18:ARG:HD2	28:16:42:TRP:CD1	2.51	0.45
1:1A:2494:G:O2'	12:1Q:80:GLU:HA	2.17	0.45
1:1A:796:C:H2'	1:1A:797:C:C6	2.51	0.45
1:1A:918:A:H5''	2:1B:98:G:O2'	2.17	0.45
1:2A:2093:G:H2'	1:2A:2094:G:H8	1.82	0.45
1:2A:923:C:H2'	1:2A:924:C:C6	2.50	0.45
2:2B:59:A:H2'	2:2B:60:C:O4'	2.17	0.45
3:2D:71:ASP:CG	3:2D:103:ARG:HH22	2.20	0.45
7:2H:3:ARG:HG2	7:2H:6:ARG:HG2	1.99	0.45
1:1A:1270:C:H2'	1:1A:1271:G:H8	5.79	0.45
1:1A:2029:G:N1	1:1A:2033:A:OP1	2.47	0.45
1:1A:2473:U:H2'	1:1A:2473:U:O2	2.16	0.45
1:1A:2684:U:H3	1:1A:2725:A:H61	1.63	0.45
1:1A:2869:G:H2'	1:1A:2870:C:O4'	2.16	0.45
1:1A:303:U:H2'	1:1A:304:G:H8	1.82	0.45
1:1A:407:G:O6	1:1A:435:C:N4	52.27	0.45
1:1A:424:G:H2'	1:1A:425:G:H8	2.44	0.45
1:1A:1812:A:O2'	3:1D:45:ASN:N	2.48	0.45
5:1F:11:VAL:HB	5:1F:18:ARG:HB3	1.98	0.45
7:1H:101:ARG:NH1	7:1H:117:PRO:HG2	2.31	0.45
7:1H:44:VAL:N	7:1H:51:ARG:O	2.36	0.45
28:26:5:VAL:O	28:26:27:LYS:HG2	2.17	0.45
1:2A:1327:C:O2'	13:2R:105:ARG:NH1	2.48	0.45
1:2A:1507:A:O2'	1:2A:1508:A:O4'	2.34	0.45
1:2A:1686:C:H2'	1:2A:1687:G:O4'	2.17	0.45
1:2A:2252:G:O6	22:20:4:LYS:NZ	2.39	0.45
1:2A:2365:G:O6	30:28:39:LYS:HD2	2.16	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2430:A:H5'	1:2A:2431:U:OP2	2.17	0.45
1:2A:370:G:H4'	1:2A:371:A:OP2	2.14	0.45
1:2A:832:G:H5'	11:2P:45:LEU:HD22	1.98	0.45
1:2A:882:G:H1	1:2A:894:C:N4	2.14	0.45
1:2A:2638:G:OP1	4:2E:82:ARG:NH2	2.49	0.45
8:2I:14:ASP:O	8:2I:17:GLN:HG2	2.17	0.45
13:2R:97:VAL:HG22	13:2R:114:VAL:HG13	1.99	0.45
19:2X:5:TYR:CE2	24:22:30:ARG:HB2	2.52	0.45
21:2Z:30:ASN:O	21:2Z:32:HIS:N	2.50	0.45
28:16:8:LYS:HD3	30:18:34:TRP:CE3	2.52	0.45
1:1A:1593:G:H2'	1:1A:1594:G:H8	1.82	0.45
1:1A:1992:G:H5'	1:1A:1994:C:H41	1.81	0.45
1:1A:2135:A:N6	1:1A:2156:G:O2'	2.50	0.45
1:1A:776:G:N2	1:1A:2241:A:OP1	2.50	0.45
1:1A:250:G:C6	1:1A:251:A:C6	3.05	0.45
1:1A:329:G:O6	20:1Y:19:LYS:N	2.46	0.45
5:1F:200:GLU:HG3	5:1F:204:ASN:HD21	1.81	0.45
6:1G:43:LEU:HD12	6:1G:43:LEU:HA	1.81	0.45
7:1H:3:ARG:HH11	7:1H:4:ILE:H	1.62	0.45
10:1O:115:VAL:HG13	10:1O:121:VAL:HG21	1.99	0.45
1:1A:565:C:H5''	17:1V:80:GLN:HE22	1.80	0.45
20:1Y:17:SER:OG	20:1Y:71:LYS:NZ	2.36	0.45
1:2A:1896:G:H2'	1:2A:1897:G:H8	1.82	0.45
1:2A:2123:G:H1	1:2A:2175:C:N4	2.15	0.45
1:2A:330:A:H2	1:2A:1210:A:H2'	1.81	0.45
3:2D:142:VAL:N	3:2D:163:ALA:O	2.43	0.45
9:2N:28:THR:HG22	9:2N:29:LYS:HG3	1.99	0.45
15:2T:11:GLU:O	15:2T:15:VAL:HG23	2.17	0.45
23:11:89:GLU:O	23:11:93:GLU:HG2	2.17	0.45
1:1A:1179:C:H2'	1:1A:1180:C:C6	2.52	0.45
1:1A:190:A:N3	1:1A:679:C:O2'	2.41	0.45
1:1A:1926:U:O2'	1:1A:1928:A:N7	2.28	0.45
1:1A:2018:G:H2'	1:1A:2019:A:C8	2.51	0.45
1:1A:2079:U:O3'	23:11:35:THR:OG1	2.33	0.45
1:1A:232:G:N2	1:1A:420:C:OP1	2.43	0.45
1:1A:573:G:O2'	1:1A:574:C:H3'	2.16	0.45
1:1A:657:U:H2'	1:1A:658:C:C6	2.52	0.45
1:1A:817:C:H2'	1:1A:818:G:O4'	2.16	0.45
4:1E:29:GLY:HA3	60:1E:401:HOH:O	2.16	0.45
23:21:76:ARG:HH22	23:21:97:LEU:HB3	1.80	0.45
1:2A:2134:A:N3	1:2A:2134:A:H2'	2.32	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2137:C:C2	1:2A:2154:G:N2	2.79	0.45
1:2A:2167:U:O2'	1:2A:2168:G:N3	2.40	0.45
1:2A:2602:A:N6	60:2A:3929:HOH:O	2.29	0.45
1:2A:2698:U:H2'	1:2A:2699:C:C6	2.52	0.45
1:2A:2540:C:O2'	1:2A:2740:A:N3	2.47	0.45
1:2A:291:C:O2	1:2A:309:G:N2	48.91	0.45
5:2F:7:TYR:O	5:2F:21:ALA:HA	2.17	0.45
1:2A:1248:G:C2	16:2U:3:ARG:HD2	2.52	0.45
23:11:35:THR:OG1	23:11:35:THR:O	2.35	0.44
30:18:52:LYS:HE2	30:18:52:LYS:HB3	1.76	0.44
1:1A:1292:U:H2'	1:1A:1293:C:C6	2.52	0.44
1:1A:1362:C:HO2'	1:1A:1810:A:HO2'	1.61	0.44
1:1A:2142:C:H2'	1:1A:2143:C:C6	2.52	0.44
7:1H:154:PRO:HB3	7:1H:163:TYR:CZ	2.52	0.44
9:1N:67:LEU:O	9:1N:88:GLU:HG3	2.17	0.44
24:22:35:LEU:HA	24:22:35:LEU:HD23	1.81	0.44
1:2A:1508:A:H4'	1:2A:1509(A):A:C8	2.52	0.44
1:2A:1526:G:C6	1:2A:1527:G:C2	3.05	0.44
1:2A:2823:A:OP1	4:2E:159:HIS:NE2	2.48	0.44
1:2A:606:U:H4'	1:2A:658:C:H4'	1.98	0.44
1:2A:619:G:H3'	1:2A:620:G:N2	2.32	0.44
1:2A:624:C:OP1	60:2A:4313:HOH:O	2.20	0.44
1:2A:729:G:OP1	3:2D:12:SER:HB2	2.17	0.44
4:2E:54:GLN:NE2	4:2E:76:ARG:HD3	2.32	0.44
8:2I:41:GLU:HA	8:2I:44:LEU:HB3	1.99	0.44
9:2N:71:ILE:HG21	9:2N:84:LYS:HB3	1.99	0.44
11:2P:87:ASP:O	11:2P:90:ARG:NH1	2.51	0.44
12:2Q:19:GLY:HA2	21:2Z:79:ARG:HH12	1.82	0.44
21:2Z:141:VAL:O	21:2Z:143:GLY:N	2.50	0.44
23:11:73:LEU:HD23	23:11:73:LEU:HA	1.86	0.44
25:13:15:TYR:CZ	25:13:53:LEU:HD21	2.52	0.44
1:1A:2061:G:H2'	1:1A:2501:C:O2'	2.17	0.44
1:1A:399:G:OP2	60:1A:5806:HOH:O	2.21	0.44
1:1A:721:C:H2'	1:1A:722:A:C8	2.52	0.44
12:1Q:104:PHE:HE2	12:1Q:125:LEU:HD11	1.82	0.44
1:2A:1798:U:H5'	3:2D:259:THR:HG22	1.99	0.44
1:2A:299:A:N1	1:2A:322:A:O2'	2.40	0.44
1:2A:598:G:H2'	1:2A:599:G:O4'	2.16	0.44
2:2B:17:C:H2'	2:2B:18:G:O4'	2.17	0.44
2:2B:26:A:H2'	2:2B:27:C:C6	2.52	0.44
6:2G:179:PRO:HB2	26:24:42:PHE:CE2	2.52	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2S:24:LEU:HB2	14:2S:85:VAL:HG23	2.00	0.44
26:14:54:GLY:O	26:14:56:VAL:HA	2.17	0.44
60:1A:4397:HOH:O	29:17:29:LYS:HD3	2.17	0.44
1:1A:1594:G:H2'	1:1A:1595:G:O4'	2.17	0.44
1:1A:1936:A:OP1	1:1A:1937:A:H5'	2.16	0.44
1:1A:529:A:H62	1:1A:2041:U:H3	1.63	0.44
1:1A:2839:G:H5'	13:1R:46:GLY:HA2	1.98	0.44
1:1A:113:G:H1'	1:1A:354:G:H5'	46.04	0.44
1:1A:483:A:O3'	20:1Y:50:ARG:HA	2.18	0.44
1:1A:848:G:O6	1:1A:928:G:H2'	2.17	0.44
7:1H:56:SER:HB3	7:1H:61:HIS:ND1	2.33	0.44
1:2A:379:G:N2	23:21:42:GLN:OE1	2.42	0.44
2:2B:83:G:H4'	25:23:52:HIS:CG	2.52	0.44
30:28:26:LYS:HD2	30:28:48:PHE:CD2	2.53	0.44
1:2A:1485:G:H2'	1:2A:1486:A:C8	2.53	0.44
1:2A:1899:G:N3	1:2A:1899:G:H2'	2.33	0.44
1:2A:195:A:H61	1:2A:198:C:H3'	1.82	0.44
1:2A:1998:G:H4'	1:2A:2724:C:O2'	2.17	0.44
1:2A:807:U:O2'	1:2A:2060:A:N1	2.43	0.44
1:2A:2101:G:H1	1:2A:2188:C:H42	1.65	0.44
1:2A:224:G:H2'	1:2A:225:A:O4'	2.18	0.44
1:2A:76:C:H42	1:2A:93:G:H1	26.94	0.44
1:2A:839:U:H2'	1:2A:840:C:H6	1.81	0.44
8:2I:7:GLU:HG3	8:2I:8:PRO:HD2	1.98	0.44
9:2N:103:VAL:O	9:2N:107:LEU:HG	2.18	0.44
1:2A:2318:G:H21	14:2S:3:ARG:HG3	1.83	0.44
21:2Z:40:ASP:OD2	21:2Z:43:GLU:N	2.26	0.44
57:1A:4074:ERY:H8	57:1A:4074:ERY:H321	1.66	0.44
4:1E:121:ASN:ND2	60:1E:410:HOH:O	2.45	0.44
14:1S:87:PHE:HB2	14:1S:112:PHE:CD1	2.53	0.44
1:2A:1028:A:N6	1:2A:1125:G:H2'	2.32	0.44
1:2A:1188:U:H4'	17:2V:79:VAL:HG22	1.99	0.44
1:2A:1463:C:H2'	1:2A:1464:C:C6	2.53	0.44
1:2A:2129:C:N4	1:2A:2159:G:N1	2.49	0.44
1:2A:2166:G:H3'	1:2A:2167:U:H5''	2.00	0.44
1:2A:652(T):C:H2'	1:2A:652(U):G:C8	2.53	0.44
5:2F:65:TRP:CZ2	5:2F:75:HIS:HD2	2.35	0.44
1:1A:1060:U:C2	1:1A:1062:G:H1'	2.52	0.44
1:1A:1087:G:H2'	1:1A:1089:G:C8	2.53	0.44
1:1A:1373:A:H2'	1:1A:1374:G:O4'	2.17	0.44
1:1A:1460:A:H2'	1:1A:1461:G:O4'	6.29	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1878:G:C2	1:1A:1879:C:C2	3.05	0.44
1:1A:2058:A:N7	60:1A:4833:HOH:O	2.36	0.44
1:1A:2130:U:H2'	1:1A:2158:A:N1	2.32	0.44
1:1A:2305:A:H2'	1:1A:2306:C:O4'	2.17	0.44
1:1A:2330:G:H2'	1:1A:2331:G:O4'	2.17	0.44
1:1A:2853:C:H2'	1:1A:2854:G:C8	2.52	0.44
1:1A:483:A:H5''	20:1Y:50:ARG:HG2	2.00	0.44
1:2A:2141:G:N2	1:2A:2151:G:H1'	2.33	0.44
1:2A:2245:U:H5''	1:2A:2246:G:H5'	1.98	0.44
1:2A:2364:C:H2'	1:2A:2365:G:O4'	2.18	0.44
1:2A:2646:C:H2'	1:2A:2647:U:O4'	2.18	0.44
1:2A:750:A:OP1	1:2A:1615:C:N4	2.44	0.44
4:2E:31:CYS:HB2	4:2E:91:VAL:HB	2.00	0.44
5:2F:129:PHE:HB2	5:2F:132:VAL:HG22	1.99	0.44
5:2F:148:LEU:HB3	5:2F:172:TRP:HZ3	1.81	0.44
6:2G:125:PHE:HB3	6:2G:166:ASP:OD2	2.18	0.44
9:2N:123:TYR:CE2	9:2N:129:PRO:HD2	2.52	0.44
14:2S:105:ALA:O	14:2S:110:LEU:HB2	2.18	0.44
16:2U:91:ASP:O	16:2U:95:LEU:HB2	2.17	0.44
17:2V:52:VAL:HG13	17:2V:55:ALA:HB3	1.98	0.44
1:2A:491:G:O6	18:2W:49:LYS:NZ	2.50	0.44
21:2Z:70:LEU:HA	21:2Z:70:LEU:HD23	1.86	0.44
1:1A:1239:G:H2'	1:1A:1240:U:O4'	2.18	0.44
1:1A:1801:G:OP2	3:1D:154:LYS:NZ	2.47	0.44
1:1A:225:A:N6	1:1A:419:C:O2'	2.51	0.44
1:1A:2787:C:H2'	1:1A:2788:C:H6	1.82	0.44
6:1G:179:PRO:HG3	26:14:43:TYR:OH	2.17	0.44
7:1H:80:SER:OG	7:1H:81:GLU:N	2.50	0.44
13:1R:97:VAL:HG22	13:1R:114:VAL:HG13	2.00	0.44
14:1S:64:GLU:HB3	26:14:59:PHE:CD2	86.11	0.44
1:2A:2019:A:N7	27:25:9:LYS:HE2	2.33	0.44
1:2A:1541:G:OP2	1:2A:1542:A:O2'	2.31	0.44
1:2A:1798:U:H5'	3:2D:259:THR:CG2	2.47	0.44
1:2A:2026:C:H42	1:2A:2037:G:H1	1.66	0.44
1:2A:2392:A:OP2	1:2A:2422:A:N6	2.51	0.44
1:2A:29:U:H2'	1:2A:30:G:C8	2.53	0.44
1:2A:407:G:H2'	1:2A:408:G:C8	2.52	0.44
1:2A:652(A):A:N3	1:2A:652(A):A:H2'	2.31	0.44
6:2G:103:LEU:HA	6:2G:106:LEU:HB3	2.00	0.44
6:2G:79:ASN:N	6:2G:79:ASN:OD1	2.50	0.44
7:2H:87:LEU:N	7:2H:131:VAL:O	2.50	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2B:9:G:OP1	14:2S:25:ARG:NH1	2.51	0.44
18:2W:3:ALA:HB2	18:2W:62:HIS:HD2	1.83	0.44
21:2Z:31:ARG:NH1	21:2Z:94:GLU:OE2	2.50	0.44
28:16:9:LEU:HA	28:16:54:ILE:HB	2.00	0.44
1:1A:1371:G:H2'	1:1A:1372:U:H5	1.82	0.44
1:1A:1740:G:H2'	1:1A:1741:A:H8	1.82	0.44
1:1A:2367:G:H2'	1:1A:2368:C:H6	1.82	0.44
1:1A:2588:G:OP1	60:1A:5392:HOH:O	2.21	0.44
1:1A:2667:C:H1'	7:1H:109:PHE:CD1	2.53	0.44
1:1A:2695:C:H2'	1:1A:2696:U:C6	2.52	0.44
3:1D:35:LYS:HB2	3:1D:36:PRO:HD2	1.99	0.44
1:1A:1649:G:O2'	13:1R:107:ASP:OD2	2.26	0.44
21:1Z:137:ILE:HA	21:1Z:156:LYS:HE2	1.99	0.44
26:24:33:VAL:HG12	26:24:34:GLU:H	1.83	0.44
1:2A:1023:U:O2'	1:2A:1122:G:H5'	2.17	0.44
1:2A:1265:A:H61	1:2A:2013:A:H5''	1.83	0.44
1:2A:710:G:H2'	1:2A:711:G:C8	2.62	0.44
1:2A:882:G:H2'	1:2A:883:G:C8	2.53	0.44
6:2G:47:LYS:HG3	6:2G:48:GLU:H	1.82	0.44
7:2H:20:ALA:HB1	7:2H:21:PRO:HD2	2.00	0.44
1:2A:2495:G:H5''	12:2Q:82:ARG:HG2	2.00	0.44
1:2A:1223:G:O6	17:2V:69:LYS:NZ	2.51	0.44
24:12:4:SER:HA	24:12:7:ARG:CZ	2.48	0.44
1:1A:1064:C:N3	1:1A:1074:G:O6	2.50	0.44
1:1A:2236:C:H2'	1:1A:2237:G:O4'	2.17	0.44
1:1A:238:C:H2'	1:1A:239:U:O4'	2.17	0.44
1:1A:571:A:O2'	17:1V:78:LYS:HE2	2.18	0.44
6:1G:77:ILE:HG22	6:1G:80:PHE:H	1.83	0.44
60:1A:6766:HOH:O	13:1R:11:ASN:ND2	2.51	0.44
1:2A:1604:C:O2'	1:2A:1610:A:N1	2.41	0.44
1:2A:570:G:H2'	1:2A:2030:A:C5	2.52	0.44
1:2A:211:A:H2'	1:2A:212:G:O4'	2.17	0.44
1:2A:2516:G:C6	1:2A:2517:C:C4	3.06	0.44
1:2A:2542:A:H4'	1:2A:2543:G:C8	2.52	0.44
1:2A:875:G:H2'	1:2A:876:C:O4'	2.18	0.44
1:2A:892:G:C5	1:2A:893:C:H1'	2.52	0.44
7:2H:137:ASP:HB3	7:2H:140:LYS:HB2	2.00	0.44
14:2S:16:ASN:HA	14:2S:19:LYS:HD2	1.99	0.44
20:2Y:37:VAL:O	20:2Y:67:LEU:N	2.39	0.44
11:1P:50:ARG:HH21	30:18:7:HIS:HD2	1.66	0.44
1:1A:1002:G:H2'	1:1A:1003:G: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:827:U:O2'	1:1A:2068:U:C2	2.64	0.44
1:1A:2803:C:H2'	1:1A:2804:C:C6	2.53	0.44
1:1A:303:U:H2'	1:1A:304:G:C8	2.53	0.44
1:1A:750:A:OP1	1:1A:1615:C:N4	2.46	0.44
4:1E:12:THR:HG22	4:1E:13:ARG:H	1.82	0.44
4:1E:96:PHE:O	4:1E:175:VAL:HG11	2.18	0.44
10:1O:24:VAL:HG13	10:1O:33:ALA:HB2	1.98	0.44
16:1U:74:LEU:HD23	16:1U:114:LYS:HE3	1.99	0.44
18:1W:14:PRO:HB3	18:1W:76:VAL:HG12	2.00	0.44
1:2A:1274:A:N3	1:2A:1297:C:H1'	2.33	0.44
1:2A:1683:C:O2'	60:2A:3910:HOH:O	2.21	0.44
1:2A:186:G:H2'	1:2A:187:G:H8	1.82	0.44
1:2A:2154:G:C2	1:2A:2155:G:C5	3.06	0.44
1:2A:2345:G:N3	1:2A:2381:C:H2'	2.33	0.44
1:2A:2441:C:OP2	1:2A:2586:C:O2'	2.25	0.44
1:2A:2552:2MU:O5'	1:2A:2552:2MU:H6	2.18	0.44
1:2A:2751:G:O2'	1:2A:2752:C:O4'	2.34	0.44
1:2A:317:G:C2	1:2A:318:C:C2	3.06	0.44
1:2A:568:U:H5'	1:2A:945:A:C6	2.53	0.44
1:2A:96:G:H4'	24:22:48:HIS:CD2	2.53	0.44
7:2H:106:THR:HG22	7:2H:112:PRO:HB3	1.99	0.44
15:2T:107:ASP:OD2	15:2T:111:ARG:NH1	2.40	0.44
1:1A:686:G:H21	1:1A:788:A:H61	1.65	0.43
14:1S:25:ARG:O	14:1S:39:ILE:HA	2.18	0.43
21:1Z:104:PHE:CE2	21:1Z:119:GLU:HG2	2.53	0.43
30:28:50:LEU:HA	30:28:50:LEU:HD23	1.83	0.43
1:2A:1914:C:H2'	1:2A:1915:5MU:C6	2.53	0.43
1:2A:2298:A:N6	1:2A:2318:G:C8	2.86	0.43
1:2A:2425:A:H4'	1:2A:2426:A:H5''	2.00	0.43
1:2A:2847:U:O4	1:2A:2848:G:N1	2.51	0.43
1:2A:822:U:H2'	1:2A:823:G:H8	1.83	0.43
1:2A:948:G:H21	1:2A:985:C:P	2.40	0.43
3:2D:3:VAL:HG12	3:2D:17:THR:HB	2.00	0.43
7:2H:117:PRO:HD3	7:2H:123:PHE:CD2	2.53	0.43
1:2A:637:A:H2'	11:2P:117:GLU:OE1	2.18	0.43
15:2T:63:VAL:O	15:2T:73:GLU:HA	2.18	0.43
21:2Z:124:ILE:HD13	21:2Z:163:LEU:HD11	2.00	0.43
1:1A:239:U:H2'	1:1A:240:G:O4'	2.19	0.43
1:1A:2699:C:H2'	1:1A:2700:C:O4'	2.19	0.43
6:1G:121:ASN:O	6:1G:131:TYR:OH	2.23	0.43
1:2A:2262:U:H5	22:20:16:SER:HB3	1.83	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:24:60:GLN:HA	26:24:62:ARG:HH12	1.84	0.43
1:2A:1131:G:O6	1:2A:2040:C:H1'	2.18	0.43
1:2A:2136:C:O2'	1:2A:2137:C:O5'	2.36	0.43
1:2A:2809:A:H62	1:2A:2891:G:H2'	1.82	0.43
5:2F:40:GLN:OE1	5:2F:183:VAL:HG22	2.18	0.43
14:2S:14:VAL:O	14:2S:18:ILE:HG12	2.18	0.43
17:2V:59:ALA:HA	17:2V:97:LYS:HG2	1.99	0.43
21:2Z:72:ARG:HD3	21:2Z:72:ARG:HA	1.79	0.43
1:1A:2271:G:OP1	22:10:18:ALA:HB1	2.19	0.43
23:11:15:ALA:HB3	23:11:40:ARG:HD3	2.00	0.43
1:1A:1031:G:H21	31:19:36:GLN:HE22	1.66	0.43
1:1A:1342:A:O2'	1:1A:1344:G:OP2	2.32	0.43
1:1A:2086:U:H2'	1:1A:2087:G:C8	2.53	0.43
1:1A:2317:C:H2'	1:1A:2318:G:O4'	2.18	0.43
1:1A:2788:C:OP1	4:1E:61:ARG:NH2	2.49	0.43
1:1A:2881:C:H2'	1:1A:2882:A:C8	2.54	0.43
1:1A:2893:G:H8	1:1A:2893:G:OP2	2.00	0.43
1:1A:301:G:OP2	20:1Y:84:ARG:NH2	2.48	0.43
1:1A:879:G:O5'	1:1A:879:G:H8	2.01	0.43
2:1B:28:C:H2'	2:1B:29:A:O4'	2.18	0.43
1:1A:389:G:C6	11:1P:70:GLN:HG3	2.53	0.43
13:1R:25:ALA:O	13:1R:29:LEU:HB2	2.19	0.43
26:24:48:ARG:HA	26:24:48:ARG:HD3	1.68	0.43
1:2A:1430:C:H2'	1:2A:1431:U:C6	2.53	0.43
1:2A:1851:U:H2'	1:2A:1852:C:O4'	2.19	0.43
1:2A:1877:A:H5'	1:2A:1878:G:OP2	2.18	0.43
1:2A:1981:A:OP1	60:2A:4182:HOH:O	2.21	0.43
1:2A:664:C:H2'	1:2A:665:C:H6	1.83	0.43
1:2A:855:G:H2'	1:2A:856:C:C6	2.53	0.43
2:2B:39:A:O2'	2:2B:40:U:H5'	2.18	0.43
12:2Q:36:ALA:HA	12:2Q:129:THR:HG22	2.01	0.43
20:2Y:7:VAL:HG21	20:2Y:72:VAL:HG12	2.00	0.43
24:12:35:LEU:HD12	24:12:53:LEU:HD12	2.00	0.43
1:1A:1339:G:H5''	19:1X:16:LYS:HD3	2.01	0.43
1:1A:1923:U:H2'	1:1A:1924:C:C6	2.53	0.43
1:1A:2540:C:H2'	1:1A:2541:A:O4'	2.18	0.43
1:1A:2787:C:H1'	4:1E:62:PRO:HG3	2.01	0.43
1:1A:392:C:H5''	1:1A:409:C:H5''	1.99	0.43
1:1A:628:G:H5''	30:18:18:ALA:HB2	1.99	0.43
3:1D:26:LYS:HE2	3:1D:28:GLU:O	2.18	0.43
5:1F:53:THR:HG23	5:1F:55:GLY:H	1.84	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1524:G:N2	1:2A:1525:G:H1'	2.34	0.43
1:2A:2049:G:N7	60:2A:6073:HOH:O	2.36	0.43
1:2A:2051:A:OP1	4:2E:137:HIS:ND1	2.41	0.43
1:2A:2152:G:N3	1:2A:2153:G:H1'	2.33	0.43
1:2A:2127:G:C2	1:2A:2161:C:C2	3.07	0.43
1:2A:2526:G:C2'	31:29:1:MET:H1	2.32	0.43
9:2N:34:LEU:HD21	9:2N:120:LEU:HB2	2.01	0.43
21:2Z:155:LEU:HB3	21:2Z:156:LYS:H	1.50	0.43
1:1A:1126:A:H4'	1:1A:1127:A:O5'	2.17	0.43
1:1A:124:G:OP1	1:1A:1376:C:O2'	2.17	0.43
1:1A:1495:A:H2'	1:1A:1496:A:C8	2.53	0.43
1:1A:152:G:H2'	1:1A:153:C:C6	2.53	0.43
1:1A:2359:C:H2'	1:1A:2360:A:O4'	2.18	0.43
1:1A:2698:U:O4	60:1A:4684:HOH:O	2.19	0.43
1:1A:2848:G:C8	15:1T:97:ALA:HB2	2.53	0.43
1:1A:24:G:O2'	18:1W:78:GLU:O	2.27	0.43
22:20:36:ILE:HD13	22:20:58:THR:HG21	2.01	0.43
1:2A:2687:U:H2'	1:2A:2688:U:O4'	2.18	0.43
1:2A:644:A:H4'	1:2A:645:C:C5	2.54	0.43
1:2A:861:A:N6	1:2A:916:G:O2'	2.51	0.43
1:2A:942:G:OP2	11:2P:39:LYS:NZ	2.31	0.43
7:2H:98:LEU:HA	7:2H:103:LEU:HA	2.01	0.43
10:2O:15:GLY:O	10:2O:47:ILE:HG12	2.18	0.43
1:2A:389:G:O6	11:2P:70:GLN:HB2	2.18	0.43
14:2S:87:PHE:CZ	14:2S:102:ALA:HB2	2.53	0.43
21:2Z:48:PHE:CE1	21:2Z:71:VAL:HG11	2.53	0.43
1:1A:1118:C:H2'	1:1A:1119:C:C6	2.75	0.43
1:1A:2078:C:C4	1:1A:2079:U:C4	3.06	0.43
1:1A:414:C:H2'	1:1A:415:A:C8	2.53	0.43
2:1B:74:U:H2'	2:1B:75:G:O4'	2.18	0.43
7:1H:3:ARG:HH22	7:1H:66:GLY:N	2.17	0.43
11:1P:111:ARG:HH11	11:1P:128:HIS:HD2	1.65	0.43
15:1T:127:ALA:C	15:1T:129:ARG:N	2.71	0.43
20:1Y:30:VAL:HG22	20:1Y:37:VAL:HG12	2.00	0.43
21:1Z:155:LEU:HD12	21:1Z:155:LEU:HA	1.76	0.43
1:2A:1791:A:H5'	1:2A:1792:G:OP2	2.18	0.43
1:2A:195:A:H5''	11:2P:46:LYS:HZ1	1.82	0.43
1:2A:2379:G:O2'	14:2S:17:ARG:NH1	2.26	0.43
1:2A:784:A:OP2	60:2A:6227:HOH:O	2.21	0.43
1:2A:902:C:H2'	1:2A:903:C:H6	1.83	0.43
2:2B:33:G:C2	2:2B:50:G:C2	3.07	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2F:178:PRO:HB3	5:2F:198:ALA:HA	2.00	0.43
1:2A:468:G:H5''	5:2F:60:SER:HB3	2.00	0.43
1:2A:674:G:H1'	5:2F:74:ARG:NE	2.33	0.43
16:2U:58:ARG:HA	16:2U:61:TRP:CE3	2.53	0.43
1:1A:1047:G:H2'	1:1A:1110:G:H1	1.84	0.43
1:1A:1337:G:H2'	1:1A:1338:G:O4'	2.18	0.43
1:1A:1843:C:H2'	1:1A:1844:C:C6	2.54	0.43
1:1A:2224:G:OP1	3:1D:268:ARG:NE	2.51	0.43
1:1A:2379:G:O2'	14:1S:17:ARG:NH2	2.50	0.43
1:1A:2838:G:OP1	60:1A:6351:HOH:O	2.22	0.43
1:1A:432:A:H3'	1:1A:433:C:C6	3.49	0.43
1:1A:733:G:N7	60:1A:4528:HOH:O	2.37	0.43
1:1A:741:G:H2'	1:1A:742:G:H8	2.46	0.43
1:1A:1993:U:H4'	4:1E:128:SER:HB3	2.01	0.43
20:1Y:39:VAL:HB	20:1Y:42:VAL:HB	2.01	0.43
1:2A:2286:A:OP1	28:26:29:ASN:ND2	2.52	0.43
1:2A:2513:G:N2	4:2E:143:ASN:OD1	2.52	0.43
1:2A:629:G:H2'	1:2A:630:G:O4'	2.73	0.43
1:2A:710:G:H2'	1:2A:711:G:H8	2.08	0.43
1:2A:971:C:H2'	1:2A:972:G:O4'	2.19	0.43
1:2A:1693:U:O2'	3:2D:14:ARG:NH2	2.52	0.43
13:2R:22:ARG:NE	13:2R:69:ASP:OD1	2.52	0.43
13:2R:96:ARG:NH2	13:2R:117:VAL:HG13	2.34	0.43
15:2T:96:ARG:HA	15:2T:96:ARG:HD3	1.64	0.43
1:2A:2012:G:P	18:2W:11:ARG:HH22	2.42	0.43
1:1A:1372:U:H2'	1:1A:1373:A:O4'	2.19	0.43
1:1A:2356:C:H2'	1:1A:2357:U:O4'	2.19	0.43
1:1A:2406:U:OP1	60:1A:4860:HOH:O	2.21	0.43
1:1A:2532:G:N2	1:1A:2663:G:O2'	2.52	0.43
1:1A:424:G:H2'	1:1A:425:G:C8	3.14	0.43
1:1A:593:G:C6	1:1A:594:U:C4	3.07	0.43
1:1A:721:C:H2'	1:1A:722:A:H8	1.83	0.43
1:1A:880:G:H8	1:1A:880:G:OP2	2.01	0.43
2:1B:41:U:P	2:1B:43:C:H41	2.42	0.43
10:1O:97:ARG:NE	10:1O:99:PHE:HE1	2.17	0.43
17:1V:25:LEU:HD11	17:1V:94:LEU:HD11	2.01	0.43
22:20:19:LYS:HD3	22:20:19:LYS:HA	1.91	0.43
1:2A:2494:G:OP1	22:20:3:HIS:N	2.44	0.43
6:2G:173:LEU:HB3	6:2G:178:PHE:CD2	2.53	0.43
6:2G:68:PRO:HA	6:2G:92:VAL:HB	2.00	0.43
13:2R:64:ARG:O	13:2R:68:ARG:HG3	2.18	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:2Y:8:LYS:HD2	20:2Y:97:ARG:NH1	2.34	0.43
25:13:30:ARG:HD3	25:13:30:ARG:H	1.84	0.43
26:14:15:ILE:O	26:14:33:VAL:N	2.36	0.43
26:14:57:GLU:HB3	26:14:58:ARG:H	1.55	0.43
1:1A:1804:C:OP1	3:1D:259:THR:OG1	2.36	0.43
1:1A:2390:U:O2'	1:1A:2391:G:H5'	2.19	0.43
1:1A:2771:C:H2'	1:1A:2772:C:C6	2.54	0.43
1:1A:191:A:O2'	1:1A:678:C:O2	2.36	0.43
2:1B:48:A:H2'	2:1B:49:C:C6	2.54	0.43
1:1A:1799:G:C2	3:1D:155:LEU:HD12	2.54	0.43
5:1F:102:PRO:O	5:1F:106:ARG:HG2	2.19	0.43
6:1G:15:VAL:HG13	6:1G:175:LEU:HB3	2.01	0.43
8:1I:62:LYS:O	8:1I:66:GLU:HG2	2.19	0.43
12:1Q:136:ALA:HB1	21:1Z:52:SER:HB2	2.01	0.43
1:1A:1753:G:H5''	15:1T:95:ARG:CD	2.48	0.43
1:1A:581:C:OP1	16:1U:33:ARG:HG3	2.19	0.43
23:21:50:ARG:NH1	23:21:57:GLU:OE2	2.52	0.43
1:2A:1191:G:H2'	1:2A:1192:G:H8	1.84	0.43
1:2A:1259:G:H2'	1:2A:1260:G:C8	2.53	0.43
1:2A:2032:G:OP2	1:2A:2454:G:O2'	2.28	0.43
1:2A:2271:G:H2'	1:2A:2272:U:C6	2.53	0.43
1:2A:2418:A:H2'	1:2A:2419:U:C6	2.54	0.43
1:2A:2512:C:H42	1:2A:2574:G:H1	1.67	0.43
6:2G:145:THR:OG1	6:2G:146:TYR:N	2.50	0.43
8:2I:124:GLY:H	8:2I:144:VAL:HG23	1.84	0.43
9:2N:34:LEU:O	9:2N:49:GLY:HA3	2.18	0.43
10:2O:26:LYS:HD2	10:2O:37:ASP:CG	2.39	0.43
12:2Q:16:ARG:HG3	12:2Q:18:LYS:HG3	2.00	0.43
14:2S:95:HIS:CG	14:2S:96:GLY:H	2.37	0.43
1:1A:2336:A:H61	22:10:43:THR:CG2	2.31	0.43
24:12:32:LEU:O	24:12:36:ARG:HG3	2.19	0.43
18:1W:19:LEU:HB3	27:15:25:LEU:HD11	2.01	0.43
31:19:25:VAL:HB	31:19:34:GLN:HG2	2.01	0.43
1:1A:1174:A:H1'	1:1A:1175:U:C5'	2.48	0.43
1:1A:1570:A:H2'	1:1A:1571:A:C8	2.53	0.43
1:1A:876:C:H2'	1:1A:877:U:O4'	2.18	0.43
6:1G:170:ARG:NE	6:1G:174:GLU:OE2	2.52	0.43
6:1G:20:ILE:HG13	6:1G:20:ILE:H	1.62	0.43
7:1H:43:VAL:HA	7:1H:52:VAL:HG22	2.01	0.43
14:1S:61:ASN:HD22	14:1S:64:GLU:HG3	1.84	0.43
18:1W:20:VAL:HG11	18:1W:44:ALA:HA	2.01	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:20:48:GLY:HA3	22:20:80:HIS:ND1	2.34	0.43
1:2A:1458:C:H4'	1:2A:1459:G:O4'	2.19	0.43
1:2A:1707:G:H2'	1:2A:1708:C:C6	2.54	0.43
1:2A:275:G:H2'	1:2A:276:A:O4'	2.18	0.43
1:2A:399:G:H5''	1:2A:400:G:OP2	2.19	0.43
1:2A:715:G:H2'	1:2A:716:A:C8	2.53	0.43
5:2F:102:PRO:HB2	5:2F:105:VAL:HG23	2.00	0.43
10:2O:63:VAL:HG11	10:2O:85:VAL:HG23	1.99	0.43
12:2Q:45:GLN:N	12:2Q:45:GLN:OE1	2.49	0.43
15:2T:20:PRO:HG2	15:2T:88:ILE:HD11	2.00	0.43
1:2A:566:U:P	17:2V:80:GLN:HE21	2.42	0.43
20:2Y:1:MET:HB2	20:2Y:2:ARG:H	1.55	0.43
20:2Y:38:ILE:HG12	20:2Y:66:PRO:HA	2.00	0.43
21:2Z:77:ASP:N	21:2Z:82:ARG:O	2.47	0.43
28:16:33:LYS:HD3	28:16:51:GLU:OE2	2.19	0.42
1:1A:1754:C:H2'	1:1A:1755:A:O4'	2.19	0.42
1:1A:2037:G:N7	60:1A:5453:HOH:O	2.36	0.42
1:1A:2147:G:H2'	1:1A:2148:G:O4'	2.18	0.42
1:1A:2466:C:C2	1:1A:2485:G:C2	3.07	0.42
1:1A:2696:U:H2'	1:1A:2697:G:C8	2.54	0.42
3:1D:62:TYR:HA	3:1D:87:ASN:OD1	2.19	0.42
7:1H:11:VAL:HG21	7:1H:50:VAL:HG23	2.01	0.42
8:1I:97:ILE:O	8:1I:101:LEU:HB2	2.19	0.42
11:1P:138:LEU:HD23	11:1P:145:PRO:HB3	2.00	0.42
12:1Q:137:TYR:O	12:1Q:141:GLN:HG2	2.19	0.42
12:1Q:17:LEU:HB3	12:1Q:39:PRO:HB2	2.01	0.42
1:2A:139:G:H2'	1:2A:140:G:N7	2.33	0.42
1:2A:1683:C:H2'	1:2A:1684:C:C6	2.54	0.42
1:2A:2540:C:H2'	1:2A:2541:A:O4'	2.19	0.42
1:2A:2544:G:H2'	1:2A:2545:G:H8	1.84	0.42
1:2A:2649:U:H3	1:2A:2671:A:H61	1.67	0.42
1:2A:2792:G:H2'	1:2A:2792:G:N3	2.34	0.42
1:2A:2815:C:H2'	1:2A:2816:C:C6	2.53	0.42
1:2A:353:G:H2'	1:2A:354:G:C8	2.54	0.42
18:2W:88:ARG:HA	18:2W:88:ARG:HD2	1.64	0.42
23:11:18:ILE:HG12	23:11:37:ILE:HG12	2.01	0.42
28:16:39:TYR:HB2	28:16:46:HIS:CE1	2.54	0.42
1:1A:2871:C:N4	60:1A:6156:HOH:O	2.52	0.42
1:1A:652(D):C:H2'	1:1A:652(E):G:O4'	2.19	0.42
2:1B:105:A:OP1	21:1Z:72:ARG:NH1	2.51	0.42
3:1D:87:ASN:HB2	3:1D:88:ARG:HH12	1.84	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1F:53:THR:CG2	5:1F:55:GLY:H	2.32	0.42
18:1W:32:ALA:HA	18:1W:35:ILE:HD12	2.01	0.42
1:2A:1265:A:OP1	60:2A:6163:HOH:O	2.22	0.42
1:2A:1311:G:N2	1:2A:1312:U:O4	2.43	0.42
1:2A:2452:C:H5''	60:2A:5443:HOH:O	2.19	0.42
1:2A:966:G:H2'	1:2A:967:C:C6	2.55	0.42
2:2B:11:C:H3'	2:2B:12:C:C6	2.54	0.42
2:2B:87:G:N2	2:2B:90:A:OP2	2.51	0.42
2:2B:48:A:OP2	14:2S:30:ARG:NH2	2.52	0.42
14:2S:3:ARG:HD2	14:2S:3:ARG:HA	1.81	0.42
1:1A:1051:G:H2'	1:1A:1052:C:O4'	2.19	0.42
1:1A:1653:G:C6	13:1R:9:LYS:HB2	2.55	0.42
1:1A:2202:C:O2	3:1D:151:LYS:NZ	2.46	0.42
1:1A:2285:C:H2'	1:1A:2286:A:H5''	2.01	0.42
1:1A:2633:G:H2'	1:1A:2634:G:O4'	2.19	0.42
1:1A:741:G:H2'	1:1A:742:G:C8	2.99	0.42
5:1F:65:TRP:HZ2	5:1F:75:HIS:HD2	1.67	0.42
8:1I:12:LEU:HD23	8:1I:12:LEU:HA	1.76	0.42
1:2A:1528(A):A:H2'	1:2A:1529:G:O4'	2.20	0.42
1:2A:1651:G:H2'	1:2A:1652:A:O4'	2.19	0.42
1:2A:329:G:H8	1:2A:329:G:OP1	2.02	0.42
1:2A:900:A:HO2'	1:2A:901:A:P	2.40	0.42
1:2A:922:U:H2'	1:2A:923:C:C6	2.54	0.42
3:2D:19:ALA:HB2	3:2D:204:ILE:HD11	2.00	0.42
7:2H:149:ARG:NH2	7:2H:154:PRO:HG2	2.34	0.42
11:2P:70:GLN:O	11:2P:73:GLY:N	2.44	0.42
28:16:47:THR:O	28:16:49:HIS:ND1	2.47	0.42
1:1A:1651:G:H4'	13:1R:39:PRO:HG2	2.02	0.42
1:1A:1721:G:O5'	1:1A:1721:G:H8	2.03	0.42
1:1A:1992:G:H2'	1:1A:1992:G:H8	1.73	0.42
1:1A:2206:G:H4'	1:1A:2206:G:OP2	2.20	0.42
1:1A:2647:U:H2'	1:1A:2648:C:C6	2.54	0.42
1:1A:2719:G:N2	1:1A:2872:G:H1	2.17	0.42
1:1A:62:C:O2	1:1A:93:G:N2	2.40	0.42
1:1A:760:G:H2'	1:1A:761:A:O4'	2.20	0.42
2:1B:11:C:P	22:10:72:ARG:HH21	2.43	0.42
3:1D:218:ARG:HB3	3:1D:219:PRO:HD2	1.99	0.42
6:1G:43:LEU:HB3	6:1G:44:GLY:H	1.51	0.42
20:1Y:35:TYR:CE2	20:1Y:69:ALA:HB3	2.54	0.42
26:24:40:HIS:O	26:24:44:THR:HG22	2.19	0.42
28:26:43:CYS:HB3	28:26:45:LYS:HG2	2.01	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1002:G:H2'	1:2A:1003:G:O4'	2.68	0.42
1:2A:1400:G:H2'	1:2A:1401:G:C8	2.54	0.42
1:2A:271(U):G:H2'	1:2A:271(V):G:H8	1.84	0.42
1:2A:478:A:N6	1:2A:480:A:N1	2.68	0.42
1:2A:741:G:H4'	10:2O:55:GLY:HA3	35.91	0.42
1:2A:817:C:H2'	1:2A:818:G:O4'	2.19	0.42
2:2B:90:A:C5	2:2B:91:C:H1'	2.55	0.42
5:2F:176:LEU:HD23	5:2F:176:LEU:HA	1.84	0.42
6:2G:47:LYS:H	6:2G:47:LYS:HG2	1.68	0.42
8:2I:54:GLN:HA	8:2I:57:ARG:NH2	2.34	0.42
21:2Z:48:PHE:CE1	21:2Z:52:SER:HA	2.55	0.42
1:1A:2406:U:H2'	1:1A:2406:U:H6	1.67	0.42
1:1A:2408:U:H2'	1:1A:2409:G:C8	2.55	0.42
1:1A:1710:C:O2'	1:1A:2858:C:N3	2.45	0.42
1:1A:620:G:N2	1:1A:620:G:OP2	2.37	0.42
5:1F:158:THR:OG1	5:1F:195:ASP:OD2	2.30	0.42
1:2A:1202:C:N4	1:2A:1243:G:H1	2.18	0.42
1:2A:1448:G:H4'	1:2A:1542:A:OP1	2.19	0.42
1:2A:2273:A:H2'	1:2A:2274:A:H8	1.85	0.42
1:2A:240:G:H3'	1:2A:241:A:H2'	2.01	0.42
1:2A:2611:U:C4	27:25:3:LYS:HG2	2.54	0.42
1:2A:2022:U:O2'	1:2A:2617:C:H5'	2.20	0.42
1:2A:2723:C:P	4:2E:109:LYS:HZ3	2.42	0.42
1:2A:2837:G:N7	60:2A:4783:HOH:O	2.50	0.42
1:2A:434:U:H2'	1:2A:435:C:C6	6.53	0.42
1:2A:500:G:N2	1:2A:502:A:H3'	2.35	0.42
5:2F:150:GLY:HA2	5:2F:172:TRP:CE3	2.54	0.42
6:2G:8:LYS:HE2	6:2G:8:LYS:HB3	1.91	0.42
8:2I:79:ILE:O	8:2I:144:VAL:HA	2.19	0.42
21:2Z:166:SER:O	21:2Z:169:GLU:HB2	2.19	0.42
1:1A:2262:U:H5	22:10:16:SER:HB3	1.84	0.42
26:14:63:TYR:CD1	26:14:63:TYR:N	2.88	0.42
30:18:26:LYS:HD3	30:18:48:PHE:HB3	2.02	0.42
1:1A:1438:U:O2	1:1A:1555:G:N2	2.52	0.42
1:1A:1810:A:H2'	1:1A:1811:G:O4'	2.20	0.42
1:1A:2437:U:H2'	1:1A:2438:U:C6	2.55	0.42
1:1A:2483:C:O2	12:1Q:124:LYS:HE3	2.19	0.42
1:1A:2679:A:H4'	4:1E:165:VAL:HG11	2.01	0.42
1:1A:269:U:H1'	1:1A:424:G:N2	2.35	0.42
1:1A:705:A:C2	1:1A:727:A:H1'	2.55	0.42
7:1H:13:LYS:HA	7:1H:14:GLY:HA2	1.66	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1Y:9:LYS:HA	20:1Y:10:GLY:HA2	1.69	0.42
21:1Z:9:TYR:OH	21:1Z:61:LEU:HD23	2.19	0.42
23:21:56:GLN:HG3	23:21:90:ILE:HD12	2.02	0.42
6:2G:179:PRO:HG3	26:24:43:TYR:OH	2.19	0.42
1:2A:1310:G:OP2	29:27:9:ARG:NE	2.30	0.42
1:2A:455:C:N3	1:2A:472:A:H2'	2.34	0.42
4:2E:52:LEU:HB2	4:2E:76:ARG:HB2	2.01	0.42
10:2O:2:ILE:HB	10:2O:33:ALA:HB3	2.02	0.42
11:2P:8:PRO:HB2	11:2P:12:ALA:HB3	2.02	0.42
19:2X:61:GLY:N	19:2X:75:ASP:OD1	2.49	0.42
20:2Y:14:LEU:HD22	20:2Y:82:PRO:HG3	2.01	0.42
25:13:3:ARG:HD3	25:13:60:GLU:OE2	2.20	0.42
1:1A:1223:G:N2	1:1A:1226:A:OP2	2.35	0.42
1:1A:2065:C:H2'	1:1A:2066:C:C6	2.55	0.42
1:1A:414:C:H4'	1:1A:1879:C:O2	2.18	0.42
1:1A:27:G:C2	1:1A:512:G:N3	2.88	0.42
1:1A:700:G:H2'	1:1A:701:G:O4'	2.20	0.42
3:1D:53:PHE:C	3:1D:218:ARG:HB2	2.39	0.42
2:1B:91:C:H5'	12:1Q:18:LYS:HA	2.01	0.42
15:1T:93:ARG:NH2	15:1T:95:ARG:HH21	2.18	0.42
1:1A:994:C:P	16:1U:54:LYS:HZ1	2.42	0.42
18:1W:68:ARG:HH11	18:1W:111:HIS:HA	1.85	0.42
20:1Y:82:PRO:O	20:1Y:101:LYS:HE2	2.19	0.42
1:2A:1791:A:H3'	1:2A:1792:G:C8	2.53	0.42
1:2A:2552:2MU:H2'	1:2A:2554:U:H5''	2.02	0.42
1:2A:2745:C:O2'	7:2H:143:GLN:N	2.53	0.42
1:2A:315:G:H2'	1:2A:316:C:C6	2.55	0.42
1:2A:845:G:N2	1:2A:845:G:OP2	2.30	0.42
4:2E:5:LEU:HD21	4:2E:79:ARG:HB2	2.02	0.42
5:2F:57:VAL:HG13	5:2F:59:TYR:H	1.83	0.42
6:2G:38:VAL:HG22	6:2G:93:THR:HG23	2.01	0.42
9:2N:99:LEU:O	9:2N:103:VAL:HG23	2.20	0.42
1:1A:1297:C:O2'	1:1A:1302:A:N1	2.40	0.42
1:1A:1999:C:H5''	1:1A:2723:C:O2'	2.19	0.42
1:1A:2819:G:N7	60:1A:6720:HOH:O	2.37	0.42
1:1A:2848:G:H1'	1:1A:2867:G:N2	2.34	0.42
1:1A:324:A:H2'	1:1A:325:G:O4'	2.20	0.42
1:1A:443:A:H5''	1:1A:444:C:OP1	2.19	0.42
1:1A:840:C:H2'	1:1A:841:A:C8	2.55	0.42
1:1A:887:A:H1'	1:1A:889:C:OP2	2.20	0.42
14:1S:39:ILE:HD11	14:1S:110:LEU:HD21	2.02	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1T:29:ARG:HG3	15:1T:46:GLU:HB2	2.02	0.42
20:1Y:18:GLY:O	20:1Y:21:LYS:NZ	2.43	0.42
20:1Y:20:TYR:CE2	20:1Y:43:ASN:HA	2.54	0.42
30:28:30:ARG:O	60:28:105:HOH:O	2.22	0.42
1:2A:1206:G:O5'	1:2A:1206:G:H8	2.02	0.42
1:2A:1316:U:H2'	1:2A:1317:A:C8	2.55	0.42
1:2A:2494:G:C4	1:2A:2495:G:C8	3.08	0.42
1:2A:676:A:H1'	1:2A:2443:C:H1'	2.01	0.42
1:2A:977:G:C6	1:2A:987:G:C6	3.08	0.42
5:2F:184:TYR:CE2	5:2F:188:ARG:HD2	2.54	0.42
7:2H:12:PRO:HD2	7:2H:15:VAL:HG11	2.01	0.42
11:2P:59:LEU:HD11	30:28:10:ALA:HA	2.02	0.42
12:2Q:37:LEU:HD21	12:2Q:130:LYS:HG2	2.01	0.42
12:2Q:57:HIS:NE2	12:2Q:116:GLU:HB3	2.35	0.42
15:2T:22:PHE:CE1	15:2T:49:VAL:HG11	2.55	0.42
1:2A:64:A:O3'	19:2X:71:GLY:HA3	2.20	0.42
26:14:62:ARG:HD3	26:14:62:ARG:HA	1.88	0.42
1:1A:1031:G:N2	31:19:36:GLN:HE22	2.16	0.42
1:1A:1144:G:C6	1:1A:1145:C:C4	3.08	0.42
1:1A:1394:U:H4'	1:1A:1603:A:H4'	2.02	0.42
1:1A:1798:U:H5'	3:1D:259:THR:CG2	2.50	0.42
1:1A:1816:G:O6	3:1D:35:LYS:NZ	2.46	0.42
1:1A:2134:A:OP2	1:1A:2157:G:N2	2.48	0.42
1:1A:35:G:H2'	1:1A:36:G:O4'	2.20	0.42
1:1A:922:U:H2'	1:1A:923:C:C6	2.55	0.42
4:1E:182:LEU:HD21	4:1E:198:VAL:HG11	2.02	0.42
7:1H:26:VAL:O	7:1H:79:VAL:HG11	2.20	0.42
9:1N:42:TRP:HA	9:1N:48:MET:SD	2.60	0.42
13:1R:111:LEU:HD12	13:1R:111:LEU:HA	1.91	0.42
10:1O:79:PHE:CD1	15:1T:72:VAL:HG22	2.54	0.42
19:1X:29:TRP:CE3	19:1X:78:LYS:HB3	2.55	0.42
19:1X:94:GLY:HA2	19:1X:95:LEU:C	2.40	0.42
13:2R:96:ARG:NE	27:25:55:ARG:HH22	2.17	0.42
31:29:11:CYS:N	31:29:14:CYS:SG	2.90	0.42
1:2A:1183:G:H2'	1:2A:1184:G:H8	1.85	0.42
1:2A:1231:G:H2'	1:2A:1232:G:H8	1.82	0.42
1:2A:1451:C:H42	1:2A:1459:G:H1	1.67	0.42
1:2A:1363:C:O2'	1:2A:1809:A:N3	2.47	0.42
1:2A:2014:A:N1	60:2A:3935:HOH:O	2.36	0.42
1:2A:700:G:H2'	1:2A:701:G:O4'	2.19	0.42
1:2A:992:C:OP1	16:2U:47:TYR:OH	2.26	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2D:155:LEU:HA	3:2D:155:LEU:HD23	4.46	0.42
4:2E:119:ARG:HG2	4:2E:120:TRP:CD1	2.55	0.42
4:2E:52:LEU:HA	4:2E:53:PRO:HD3	1.95	0.42
7:2H:97:ARG:O	7:2H:103:LEU:HD12	2.20	0.42
20:2Y:20:TYR:CE2	20:2Y:43:ASN:HA	2.55	0.42
24:12:35:LEU:HB3	24:12:50:ILE:HD13	2.02	0.42
1:1A:11:G:H2'	1:1A:12:U:O4'	2.20	0.42
1:1A:1286:A:C6	1:1A:1329:U:C2	3.08	0.42
1:1A:253:C:H2'	1:1A:254:G:O4'	2.19	0.42
1:1A:2767:C:H2'	1:1A:2768:C:H6	1.85	0.42
1:1A:784:A:N6	3:1D:229:VAL:HG11	2.35	0.42
5:1F:203:GLN:H	5:1F:203:GLN:HG2	1.61	0.42
8:1I:75:LEU:HD13	8:1I:105:HIS:CE1	2.55	0.42
24:22:12:GLU:O	24:22:16:LEU:HG	2.20	0.42
30:28:29:LYS:HE3	30:28:29:LYS:HB2	1.87	0.42
1:2A:833:U:O3'	30:28:57:ARG:NH1	2.53	0.42
1:2A:1287:A:C5	1:2A:1288:U:C4	3.08	0.42
1:2A:1364:G:H4'	1:2A:1808:U:H3	1.85	0.42
1:2A:1390:U:H2'	1:2A:1391:U:C6	3.32	0.42
1:2A:1516:C:H2'	1:2A:1517:G:C8	2.55	0.42
1:2A:1689:A:H62	1:2A:1698:A:H2	1.67	0.42
1:2A:1916:A:H2'	1:2A:1917:PSU:O4'	2.19	0.42
1:2A:2406:U:C4	11:2P:72:PRO:HD2	2.55	0.42
1:2A:2563:U:H1'	1:2A:2566:A:N6	2.35	0.42
1:2A:2712(A):A:H5''	1:2A:2713:A:OP2	2.19	0.42
1:2A:83:G:H1	1:2A:102:G:HO2'	1.65	0.42
1:2A:994:C:O2'	1:2A:996:A:OP1	2.26	0.42
1:2A:599:G:H4'	5:2F:31:HIS:HD2	1.85	0.42
6:2G:170:ARG:NH2	6:2G:182:LYS:O	2.52	0.42
7:2H:103:LEU:HD21	7:2H:105:LEU:HD21	2.02	0.42
7:2H:126:PRO:HG2	7:2H:130:ARG:NH1	2.35	0.42
1:2A:2851:A:O2'	13:2R:64:ARG:NH2	2.53	0.42
16:2U:76:TYR:HH	16:2U:92:ARG:HE	1.64	0.42
17:2V:38:LEU:HD23	17:2V:50:PRO:O	2.20	0.42
21:2Z:96:VAL:HG12	21:2Z:128:VAL:O	2.20	0.42
22:10:27:GLU:HG3	22:10:68:GLU:HA	2.01	0.41
27:15:42:PRO:HB2	27:15:43:HIS:ND1	2.34	0.41
1:1A:1059:G:H2'	1:1A:1060:U:C5	2.54	0.41
1:1A:1062:G:P	1:1A:1070:A:HO2'	2.43	0.41
1:1A:1827:C:O2'	1:1A:1970:A:N3	2.46	0.41
1:1A:2147:G:H3'	1:1A:2147:G:N3	2.35	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2157:G:H4'	1:1A:2158:A:OP1	2.20	0.41
1:1A:2756:U:OP2	31:19:19:ARG:HD3	2.19	0.41
1:1A:741:G:H2'	1:1A:742:G:O4'	2.40	0.41
1:1A:776:G:HO2'	1:1A:777:A:H8	5.85	0.41
2:1B:31:C:H4'	6:1G:29:TRP:CH2	2.54	0.41
2:1B:86:G:H1	2:1B:91:C:N4	2.17	0.41
11:1P:93:GLY:H	11:1P:123:LEU:HD22	1.85	0.41
1:1A:994:C:C5	16:1U:54:LYS:HE3	2.55	0.41
21:1Z:18:LEU:HD12	21:1Z:18:LEU:HA	1.88	0.41
21:1Z:75:ASN:O	21:1Z:84:GLU:N	2.38	0.41
23:21:8:SER:HB3	23:21:66:HIS:CD2	2.55	0.41
1:2A:1007:C:N3	1:2A:1022:G:C6	17.18	0.41
1:2A:1422:G:H5''	10:2O:48:PRO:CB	99.21	0.41
1:2A:2875:C:H2'	1:2A:2876:G:O4'	2.19	0.41
1:2A:741:G:H2'	1:2A:742:G:O4'	2.57	0.41
1:2A:192:C:O2'	1:2A:802:A:N3	2.45	0.41
3:2D:70:TRP:HB3	3:2D:190:TYR:CE2	2.54	0.41
3:2D:258:LYS:HE2	3:2D:273:ARG:CZ	2.50	0.41
7:2H:13:LYS:HA	7:2H:14:GLY:HA2	1.77	0.41
8:2I:133:HIS:ND1	8:2I:134:PRO:O	2.52	0.41
11:2P:97:PRO:HD3	11:2P:126:VAL:O	2.20	0.41
1:2A:2379:G:HO2'	14:2S:17:ARG:HH12	1.60	0.41
18:2W:57:ASN:HA	18:2W:61:ASN:HD22	1.85	0.41
21:2Z:45:ASP:O	21:2Z:49:ARG:HG3	2.19	0.41
1:1A:1047:G:H2'	1:1A:1110:G:H22	1.85	0.41
1:1A:1168:G:H2'	1:1A:1169:G:H8	1.85	0.41
1:1A:1504:C:H2'	1:1A:1505:C:C6	2.55	0.41
1:1A:2202:C:H2'	1:1A:2203:U:O4'	2.20	0.41
1:1A:590:A:H2'	1:1A:591:C:O4'	2.20	0.41
2:1B:16:G:C6	2:1B:69:G:C2	3.08	0.41
3:1D:183:ARG:HG3	3:1D:270:ILE:HG12	2.01	0.41
3:1D:142:VAL:CG1	3:1D:191:ALA:HB1	2.51	0.41
10:1O:70:LYS:HE2	10:1O:70:LYS:HB3	1.76	0.41
1:2A:262:A:H2'	1:2A:263:C:O4'	2.20	0.41
1:2A:720:C:H2'	1:2A:721:C:C6	2.55	0.41
1:2A:740:U:H2'	1:2A:741:G:C8	2.55	0.41
1:2A:918:A:C2	2:2B:81:G:H5'	2.54	0.41
1:2A:993:G:H2'	1:2A:993:G:N3	2.83	0.41
2:2B:26:A:H2'	2:2B:27:C:H6	1.85	0.41
6:2G:120:LEU:HD12	6:2G:178:PHE:HB3	2.02	0.41
6:2G:5:VAL:HG22	6:2G:8:LYS:HB2	2.01	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:300:A:P	20:2Y:86:ARG:HH21	2.43	0.41
1:1A:129:C:H2'	1:1A:130:C:C6	2.55	0.41
1:1A:1448:G:H5''	1:1A:1542:A:OP1	2.20	0.41
1:1A:1942:5MC:OP2	1:1A:1943:U:O2'	2.30	0.41
1:1A:185:U:H4'	1:1A:218:A:H4'	2.02	0.41
1:1A:2312:U:H5'	6:1G:88:ILE:HD11	2.01	0.41
1:1A:813:U:H2'	1:1A:814:C:C6	2.55	0.41
2:1B:38:C:O2'	14:1S:93:LYS:NZ	2.49	0.41
3:1D:134:ARG:HG3	3:1D:135:PHE:CD2	2.55	0.41
11:1P:137:LYS:HE3	11:1P:137:LYS:HB2	1.85	0.41
20:1Y:90:LEU:O	20:1Y:93:GLY:N	2.47	0.41
26:24:14:ILE:HB	26:24:22:ILE:HB	2.02	0.41
1:2A:1028:A:H2'	1:2A:1029:A:C8	2.55	0.41
1:2A:1167:U:O2	1:2A:1183:G:N2	2.53	0.41
1:2A:1406:U:H2'	1:2A:1407:C:C6	2.55	0.41
1:2A:2164:C:H5''	1:2A:2165:G:OP2	2.19	0.41
1:2A:2432:A:C6	1:2A:2433:A:C6	3.08	0.41
1:2A:628:G:H5''	30:28:18:ALA:HB2	2.02	0.41
3:2D:204:ILE:H	3:2D:204:ILE:HG12	3.39	0.41
5:2F:180:GLY:O	5:2F:182:ASN:ND2	2.51	0.41
17:2V:29:PRO:HA	17:2V:61:VAL:HG13	2.01	0.41
26:14:40:HIS:HB3	26:14:43:TYR:CD2	2.55	0.41
19:1X:60:ARG:HH22	29:17:47:ARG:NH1	2.18	0.41
1:1A:1071:G:H2'	1:1A:1072:C:C6	2.55	0.41
1:1A:1466:G:O2'	1:1A:1546:C:O2'	2.15	0.41
1:1A:218:A:H2	1:1A:235:U:H4'	1.80	0.41
1:1A:2507:C:H2'	1:1A:2508:G:O4'	2.20	0.41
1:1A:2510:C:H2'	1:1A:2511:U:O4'	2.20	0.41
1:1A:258:G:H1	1:1A:268:C:H42	33.20	0.41
1:1A:45:C:OP2	1:1A:215:G:H5''	2.19	0.41
6:1G:16:ARG:HB3	6:1G:17:PRO:HD3	2.02	0.41
13:1R:118:GLU:H	13:1R:118:GLU:CD	2.23	0.41
1:2A:251:A:P	30:28:7:HIS:HE2	2.39	0.41
1:2A:1394:U:O2	19:2X:16:LYS:NZ	2.52	0.41
1:2A:2133:G:C4	1:2A:2157:G:C2	3.08	0.41
1:2A:2199:A:H3'	1:2A:2200:C:C6	2.55	0.41
1:2A:2727:G:O2'	10:2O:70:LYS:NZ	2.53	0.41
1:2A:57:C:H2'	1:2A:58:G:O4'	2.20	0.41
1:2A:652(U):G:H2'	1:2A:652(V):C:O4'	2.20	0.41
1:2A:659:C:H2'	1:2A:660:G:C8	2.53	0.41
9:2N:43:THR:HG22	9:2N:44:PRO:HD2	2.03	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:2Q:85:LYS:HG2	22:20:7:LEU:CB	2.48	0.41
1:2A:2875:C:O2'	15:2T:2:ASN:ND2	2.53	0.41
20:2Y:3:VAL:HB	20:2Y:32:PRO:HB3	2.02	0.41
25:13:59:VAL:O	25:13:60:GLU:HG2	2.20	0.41
30:18:63:PRO:HG2	30:18:64:TYR:CD2	2.56	0.41
1:1A:1200:C:H2'	1:1A:1201:C:C6	2.54	0.41
1:1A:2375:G:N2	1:1A:2377:A:H3'	2.36	0.41
2:1B:24:G:N7	2:1B:56:G:H2'	2.36	0.41
3:1D:123:ALA:HB3	3:1D:131:LEU:HG	2.01	0.41
5:1F:140:LEU:HD11	5:1F:170:LEU:HD11	2.02	0.41
6:1G:80:PHE:HB2	6:1G:82:LEU:HB2	2.01	0.41
2:2B:12:C:H2'	22:20:73:GLY:HA3	2.03	0.41
1:2A:94(A):G:O3'	24:22:45:SER:OG	2.39	0.41
13:2R:96:ARG:CZ	27:25:55:ARG:HH22	2.32	0.41
1:2A:686:G:C2	29:27:11:LYS:HE3	2.55	0.41
1:2A:1035:U:H2'	1:2A:1036:G:C8	2.56	0.41
1:2A:1286:A:H8	1:2A:1287:A:H4'	8.14	0.41
1:2A:132:G:H2'	1:2A:133:C:C6	2.56	0.41
1:2A:1361:G:H2'	1:2A:1362:C:C6	2.56	0.41
1:2A:1423:G:H2'	1:2A:1424:G:C8	2.54	0.41
1:2A:2169:A:H2'	1:2A:2170:A:C8	2.55	0.41
1:2A:2556:C:H2'	1:2A:2557:G:O4'	2.21	0.41
1:2A:2734:A:H62	1:2A:2770:G:H21	1.67	0.41
1:2A:321:G:H4'	5:2F:165:ARG:O	2.19	0.41
1:2A:668:G:H5'	1:2A:669:G:OP2	2.20	0.41
10:2O:19:ILE:HG22	10:2O:43:VAL:HA	2.01	0.41
1:2A:1651:G:H5'	13:2R:39:PRO:HG2	2.01	0.41
15:2T:57:PHE:HA	15:2T:79:HIS:CD2	2.56	0.41
16:2U:44:ASN:HD21	17:2V:75:PHE:H	1.69	0.41
26:14:40:HIS:O	26:14:44:THR:HG22	2.20	0.41
31:19:8:LYS:O	31:19:34:GLN:NE2	2.54	0.41
1:1A:1062:G:C5	1:1A:1088:A:H2'	2.56	0.41
1:1A:1083:U:H2'	1:1A:1085:A:OP2	2.21	0.41
1:1A:564:C:O2'	1:1A:1253:A:N1	2.35	0.41
1:1A:1641:A:H2'	1:1A:1642:G:O4'	2.20	0.41
1:1A:1826:G:H2'	1:1A:1827:C:O4'	2.20	0.41
1:1A:1866:C:H2'	1:1A:1876:A:O4'	2.20	0.41
1:1A:2243:U:H2'	1:1A:2244:U:C6	2.56	0.41
1:1A:2432:A:H2'	1:1A:2433:A:C8	2.55	0.41
1:1A:820:A:H1'	1:1A:943:U:H1'	2.01	0.41
1:1A:848:G:H2'	1:1A:849:A:C8	2.56	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:444:C:H4'	5:1F:49:ALA:HB2	2.02	0.41
6:1G:11:TYR:HB2	6:1G:176:LEU:HD21	2.03	0.41
1:1A:2675:A:H5'	10:1O:29:ASN:O	2.21	0.41
1:2A:686:G:H8	29:27:6:GLN:O	2.03	0.41
1:2A:144:C:H2'	1:2A:145:G:C8	2.55	0.41
1:2A:197:A:H62	1:2A:2430:A:H2'	1.85	0.41
1:2A:1996:C:N4	10:2O:32:TYR:OH	2.54	0.41
1:2A:2502:G:H5''	1:2A:2503:2MA:H5''	2.01	0.41
1:2A:250:G:C6	1:2A:251:A:C6	3.09	0.41
1:2A:2851:A:O3'	13:2R:64:ARG:NH2	2.52	0.41
1:2A:443:A:C5	5:2F:45:ARG:HD2	2.55	0.41
1:2A:779:U:OP1	3:2D:49:ILE:HG13	2.21	0.41
7:2H:4:ILE:O	7:2H:69:ARG:HD2	2.21	0.41
14:2S:20:ARG:HD2	14:2S:20:ARG:HA	1.85	0.41
25:13:35:ARG:HG2	25:13:37:LEU:HD21	2.03	0.41
25:13:6:VAL:HG12	25:13:28:LEU:HD11	2.02	0.41
30:18:28:GLY:HA3	30:18:44:LYS:HZ3	1.85	0.41
1:1A:1114:G:H2'	1:1A:1115:G:H8	1.85	0.41
1:1A:1658:C:H2'	1:1A:1659:U:C6	2.55	0.41
1:1A:1694:C:H4'	1:1A:1695:G:O5'	2.21	0.41
1:1A:1792:G:O2'	1:1A:1830:C:OP1	2.38	0.41
1:1A:1268:A:C2	1:1A:2013:A:C4	3.08	0.41
1:1A:2155:G:H3'	1:1A:2156:G:C8	2.55	0.41
1:1A:2389:G:H5''	1:1A:2390:U:O4'	2.21	0.41
1:1A:2730:C:H2'	1:1A:2731:G:H8	1.86	0.41
1:1A:302:C:P	20:1Y:73:ARG:HH22	2.44	0.41
1:1A:511:U:O4	1:1A:512:G:N1	2.54	0.41
1:1A:557:U:H2'	1:1A:558:G:H8	1.84	0.41
1:1A:630:G:N2	1:1A:632:A:H3'	2.36	0.41
1:1A:995:C:OP2	16:1U:54:LYS:NZ	2.48	0.41
13:1R:57:ARG:HG2	13:1R:59:ASP:OD1	2.21	0.41
21:1Z:130:PRO:HA	21:1Z:133:ILE:HG13	2.03	0.41
23:21:35:THR:OG1	23:21:35:THR:O	2.37	0.41
28:26:26:ASN:HB3	28:26:29:ASN:HB2	2.02	0.41
28:26:8:LYS:HD3	30:28:34:TRP:CD2	2.55	0.41
1:2A:1469:A:H2'	1:2A:1470:G:O4'	2.20	0.41
1:2A:1794:U:H2'	1:2A:1795:C:H6	1.84	0.41
1:2A:190:A:N3	1:2A:679:C:O2'	2.47	0.41
1:2A:2149:G:C6	1:2A:2150:U:C2	3.08	0.41
1:2A:2370:G:C6	1:2A:2371:G:C6	3.09	0.41
1:2A:2674:G:H2'	1:2A:2675:A:C8	2.55	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2751:G:H8	7:2H:2:SER:HA	1.85	0.41
57:2A:3875:ERY:H353	57:2A:3875:ERY:H10	1.82	0.41
2:2B:40:U:O2'	2:2B:43:C:OP2	2.28	0.41
6:2G:63:ILE:HD13	6:2G:141:PHE:CD2	2.55	0.41
7:2H:140:LYS:HB2	7:2H:140:LYS:HE3	1.90	0.41
7:2H:74:ASN:ND2	7:2H:138:LYS:HD3	2.36	0.41
10:2O:25:LEU:HD23	10:2O:25:LEU:HA	1.68	0.41
15:2T:39:ARG:HH12	15:2T:41:ARG:HB3	1.86	0.41
15:2T:53:ARG:HH11	15:2T:60:THR:HG23	1.84	0.41
29:17:12:ARG:NH2	29:17:44:PRO:HB3	2.36	0.41
1:1A:686:G:H8	29:17:6:GLN:O	2.03	0.41
1:1A:1153:C:OP2	60:1A:5427:HOH:O	2.22	0.41
1:1A:2291:U:H2'	1:1A:2292:C:C6	2.56	0.41
1:1A:436:C:H2'	1:1A:437:G:H8	1.85	0.41
1:1A:524:U:H2'	1:1A:525:U:C6	2.56	0.41
1:1A:637:A:H4'	1:1A:638:G:O5'	2.21	0.41
3:1D:82:ILE:HD11	3:1D:111:LEU:HD23	2.02	0.41
3:1D:83:GLU:OE1	3:1D:104:TYR:OH	2.24	0.41
10:1O:9:GLU:O	10:1O:83:ALA:HA	2.20	0.41
1:1A:631:A:H1'	11:1P:66:GLY:HA2	2.02	0.41
12:1Q:47:ILE:HG12	12:1Q:68:ILE:HD11	2.02	0.41
19:1X:25:LYS:HA	19:1X:81:VAL:O	2.20	0.41
1:2A:1123:C:H1'	31:29:18:ARG:HH21	1.86	0.41
1:2A:1027:A:C6	1:2A:1126:A:C4	3.08	0.41
1:2A:1309:G:H2'	1:2A:1310:G:O4'	2.71	0.41
1:2A:1361:G:H2'	1:2A:1362:C:H6	1.84	0.41
1:2A:174:C:H2'	1:2A:175:G:C8	2.56	0.41
1:2A:2103:C:O2	1:2A:2187:G:N2	2.53	0.41
1:2A:2188:C:H5'	1:2A:2189:U:OP2	2.21	0.41
1:2A:265:A:H1'	1:2A:266:G:O4'	2.21	0.41
1:2A:2872:G:O2'	1:2A:2873:A:H5'	2.21	0.41
1:2A:656:G:H2'	1:2A:657:U:O4'	2.21	0.41
1:2A:754:C:H2'	1:2A:755:C:C6	2.55	0.41
10:2O:104:ARG:N	10:2O:122:LEU:O	2.52	0.41
12:2Q:4:PRO:HG3	12:2Q:69:PHE:HE2	1.86	0.41
12:2Q:25:ASP:HB3	21:2Z:78:LYS:HD3	2.02	0.41
26:14:61:ARG:HG3	26:14:62:ARG:N	2.36	0.41
1:1A:1889:A:H2'	1:1A:1890:A:O4'	2.21	0.41
1:1A:2334:G:H5'	14:1S:9:ARG:HG2	2.02	0.41
1:1A:2646:C:OP2	1:1A:2732:G:O2'	2.25	0.41
1:1A:271(Z):C:H1'	1:1A:272(C):G:H1'	2.02	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:330:A:HO2'	1:1A:331:A:H8	1.67	0.41
1:1A:443:A:C5	5:1F:45:ARG:HD2	2.55	0.41
12:1Q:10:ARG:HG2	12:1Q:11:LYS:HG3	2.03	0.41
17:1V:52:VAL:HG13	17:1V:55:ALA:HB3	2.03	0.41
21:1Z:75:ASN:N	21:1Z:75:ASN:OD1	2.53	0.41
22:20:23:VAL:HG22	22:20:38:VAL:HG22	2.02	0.41
1:2A:1664:A:OP2	1:2A:1664:A:C8	2.73	0.41
1:2A:2282:G:H4'	1:2A:2389:G:O2'	2.21	0.41
1:2A:336:C:H2'	1:2A:337:C:H6	1.88	0.41
1:2A:446:G:H5''	1:2A:449:A:H1'	2.03	0.41
1:2A:493:G:H8	1:2A:493:G:O5'	2.17	0.41
1:2A:690:G:O2'	1:2A:780:G:OP1	2.38	0.41
1:2A:822:U:H2'	1:2A:823:G:C8	2.56	0.41
3:2D:182:LEU:HD23	3:2D:182:LEU:HA	1.90	0.41
4:2E:64:LYS:HA	4:2E:67:PHE:HD2	1.86	0.41
14:2S:106:ARG:HG3	14:2S:112:PHE:CZ	2.56	0.41
24:12:52:ASP:O	24:12:56:GLN:HG3	2.21	0.41
1:1A:2251:OMG:HM23	1:1A:2251:OMG:H1'	1.85	0.41
1:1A:2260:C:HO2'	1:1A:2388:A:HO2'	1.65	0.41
1:1A:2424:C:C2	1:1A:2429:G:H1'	2.56	0.41
1:1A:2478:A:H2'	1:1A:2479:G:O4'	2.21	0.41
57:1A:4074:ERY:H312	57:1A:4074:ERY:H2	1.75	0.41
1:1A:663:G:H2'	1:1A:664:C:O4'	2.20	0.41
1:1A:754:C:H2'	1:1A:755:C:H6	1.85	0.41
1:1A:992:C:OP1	17:1V:74:LYS:NZ	2.41	0.41
2:1B:2:C:H2'	2:1B:3:C:H6	1.84	0.41
2:1B:68:C:H2'	2:1B:69:G:O4'	2.21	0.41
10:1O:11:ALA:HB1	10:1O:99:PHE:O	2.21	0.41
16:1U:58:ARG:HA	16:1U:61:TRP:CE3	2.56	0.41
22:20:56:ASP:OD2	22:20:58:THR:OG1	2.35	0.41
1:2A:1159:U:O2'	1:2A:1160:G:OP2	4.82	0.41
1:2A:1800:C:OP2	3:2D:183:ARG:NH2	2.51	0.41
1:2A:2233:U:H2'	1:2A:2234:G:C8	2.56	0.41
1:2A:432:A:H3'	1:2A:433:C:H6	2.99	0.41
1:2A:482:A:N6	1:2A:506:G:O2'	2.54	0.41
1:2A:599:G:H5'	11:2P:9:ASN:ND2	2.36	0.41
1:2A:840:C:H2'	1:2A:841:A:H8	1.85	0.41
1:2A:978:G:H1	1:2A:985:C:N4	2.18	0.41
4:2E:119:ARG:HG2	4:2E:120:TRP:NE1	2.35	0.41
7:2H:154:PRO:HB3	7:2H:163:TYR:CE1	2.56	0.41
9:2N:12:ARG:NH2	9:2N:50:ASP:OD2	2.54	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:2Q:26:TYR:O	12:2Q:67:ARG:NH1	2.49	0.41
19:2X:64:LYS:HD3	19:2X:64:LYS:HA	1.69	0.41
1:1A:1011:G:OP2	16:1U:66:ASN:ND2	2.38	0.41
1:1A:1674:G:H1'	1:1A:1676:A:N6	2.35	0.41
1:1A:1791:A:OP2	1:1A:1791:A:H8	2.04	0.41
1:1A:207:A:H2'	1:1A:208:C:O4'	2.20	0.41
1:1A:2252:G:H2'	1:1A:2253:G:O4'	2.21	0.41
1:1A:1027:A:C2	1:1A:2488:A:H5'	2.56	0.41
1:1A:2811:G:N2	1:1A:2891:G:H1'	2.36	0.41
1:1A:588:U:H2'	1:1A:589:C:C6	2.56	0.41
1:1A:742:G:H4'	1:1A:1676:A:H5'	2.03	0.41
8:1I:26:ALA:HA	8:1I:30:LEU:HB2	2.01	0.41
10:1O:26:LYS:HB3	10:1O:26:LYS:HE2	1.94	0.41
12:1Q:39:PRO:HA	12:1Q:97:VAL:O	2.20	0.41
14:1S:106:ARG:NE	14:1S:112:PHE:OXT	2.41	0.41
1:2A:1430:C:H2'	1:2A:1431:U:H6	1.84	0.41
1:2A:1860:G:O6	1:2A:1883:G:N2	2.54	0.41
1:2A:1913:A:H4'	1:2A:1914:C:H5''	2.02	0.41
1:2A:2448:A:OP1	60:2A:5975:HOH:O	2.22	0.41
1:2A:2528:U:H2'	1:2A:2530:A:H5''	2.02	0.41
1:2A:2883:A:H5''	1:2A:2884:U:H5'	2.02	0.41
1:2A:2886:G:H2'	1:2A:2887:U:C6	2.54	0.41
1:2A:458:G:O2'	1:2A:469:G:O6	2.25	0.41
3:2D:159:ALA:HB1	3:2D:198:ASN:O	2.21	0.41
8:2I:84:GLY:C	8:2I:86:THR:H	2.24	0.41
10:2O:3:GLN:HG3	10:2O:4:PRO:O	2.21	0.41
1:2A:2393:A:O3'	11:2P:63:PRO:HA	2.21	0.41
12:2Q:87:LYS:HG3	12:2Q:88:GLY:N	2.36	0.41
15:2T:108:ARG:HH12	15:2T:112:ARG:NH1	2.19	0.41
1:1A:1364:G:C8	23:11:3:LYS:HD2	2.57	0.40
1:1A:1230:C:H2'	1:1A:1231:G:C8	2.56	0.40
1:1A:1405:U:H2'	1:1A:1406:U:H6	1.86	0.40
1:1A:2505:G:O6	1:1A:2576:G:H2'	2.21	0.40
1:1A:2512:C:H2'	1:1A:2513:G:O4'	2.21	0.40
1:1A:2529:G:H5''	1:1A:2530:A:H5''	2.03	0.40
1:1A:2687:U:H2'	1:1A:2688:U:O4'	2.22	0.40
1:1A:37:C:H2'	1:1A:38:A:C8	2.55	0.40
1:1A:540:C:H2'	1:1A:541:C:C6	2.56	0.40
1:1A:875:G:H1	1:1A:902:C:N4	2.06	0.40
2:1B:21:G:H2'	2:1B:22:U:O4'	2.21	0.40
4:1E:179:GLU:HB2	4:1E:181:LEU:HD22	2.03	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1F:164:ARG:HD2	5:1F:175:THR:HG23	2.03	0.40
6:1G:29:TRP:O	6:1G:33:ARG:NH1	2.52	0.40
11:1P:126:VAL:HG12	11:1P:148:LEU:HD23	2.01	0.40
14:1S:84:GLN:HA	14:1S:111:GLU:HB2	2.02	0.40
21:1Z:52:SER:OG	21:1Z:54:HIS:ND1	2.54	0.40
23:21:23:LYS:HB3	23:21:29:GLY:HA3	2.03	0.40
1:2A:1932:A:H2'	1:2A:1933:G:O4'	2.21	0.40
1:2A:608:A:H3'	1:2A:609:A:H8	2.57	0.40
1:2A:800:A:OP1	1:2A:800:A:H8	2.04	0.40
4:2E:117:MET:SD	4:2E:136:ARG:HA	2.62	0.40
5:2F:54:ARG:NH2	5:2F:77:ASP:OD1	2.54	0.40
14:2S:25:ARG:CG	14:2S:40:ILE:HB	2.51	0.40
1:1A:2046:G:O5'	27:15:19:ARG:HA	2.21	0.40
30:18:52:LYS:N	30:18:53:PRO:HD2	2.37	0.40
1:1A:1006:C:C2	1:1A:1138:G:N2	2.89	0.40
1:1A:1825:A:H2'	1:1A:1826:G:C8	2.56	0.40
1:1A:1786:A:H1'	1:1A:1938:A:N6	2.36	0.40
1:1A:2418:A:H2'	1:1A:2419:U:C6	2.56	0.40
1:1A:816:C:H2'	1:1A:817:C:C6	2.56	0.40
2:1B:78:A:C2	2:1B:100:A:C4	3.10	0.40
3:1D:65:ILE:HB	3:1D:67:PHE:CE2	2.56	0.40
5:1F:29:ASN:ND2	5:1F:32:LEU:HB2	2.36	0.40
6:1G:4:ASP:OD1	6:1G:9:ARG:HD2	2.20	0.40
9:1N:13:TRP:CE2	9:1N:133:GLN:HG2	2.56	0.40
1:1A:2470:G:P	12:1Q:56:ARG:HH21	2.44	0.40
20:1Y:68:HIS:HB3	20:1Y:71:LYS:HG3	2.03	0.40
21:1Z:54:HIS:CG	21:1Z:101:PRO:HG3	2.56	0.40
1:2A:2353:G:O2'	22:20:33:ALA:O	2.27	0.40
1:2A:1159:U:H2'	1:2A:1160:G:H8	1.86	0.40
1:2A:1196:C:H2'	1:2A:1197:G:C8	2.56	0.40
1:2A:1313:U:H2'	1:2A:1314:C:H6	4.29	0.40
1:2A:133:C:H42	1:2A:146:G:H1	1.69	0.40
1:2A:1942:5MC:HM53	1:2A:1943:U:C2	2.56	0.40
1:2A:2023:G:H2'	1:2A:2024:G:H8	1.87	0.40
1:2A:19:C:H2'	1:2A:20:C:H6	1.85	0.40
1:2A:2591:C:OP1	3:2D:239:ARG:HD2	2.22	0.40
1:2A:1637:A:H4'	1:2A:2711:A:O2'	2.22	0.40
1:2A:817:C:C2	1:2A:818:G:C8	3.09	0.40
4:2E:13:ARG:HB3	4:2E:22:PRO:HA	2.02	0.40
7:2H:18:GLU:HB3	7:2H:25:LYS:HB2	2.02	0.40
7:2H:33:LEU:HD21	7:2H:136:ILE:HG13	2.03	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:2Q:43:THR:HA	12:2Q:94:VAL:HG12	2.02	0.40
14:2S:10:ARG:HG2	14:2S:91:PRO:HA	2.03	0.40
16:2U:5:LYS:HG3	16:2U:7:GLY:H	1.86	0.40
17:2V:10:LYS:HE2	17:2V:10:LYS:HB2	1.91	0.40
1:1A:1062:G:O5'	1:1A:1070:A:O2'	2.31	0.40
1:1A:2171:A:O2'	1:1A:2172:U:H5''	2.21	0.40
1:1A:2561:A:H2'	1:1A:2562:U:O4'	2.22	0.40
1:1A:2565:A:H5''	1:1A:2566:A:OP2	2.22	0.40
1:1A:863:A:H2'	1:1A:864:G:H8	1.86	0.40
2:1B:43:C:OP1	26:14:6:HIS:NE2	2.54	0.40
3:1D:72:LYS:HD3	3:1D:97:TYR:CE1	2.57	0.40
4:1E:34:VAL:HG23	4:1E:48:GLN:HB3	2.02	0.40
26:24:28:LYS:HA	26:24:29:PRO:HD3	1.96	0.40
1:2A:1184:G:H3'	1:2A:1184:G:OP1	4.50	0.40
1:2A:1186:G:H2'	1:2A:1187:G:O4'	2.35	0.40
1:2A:1759:A:H1'	1:2A:2711:A:C2	2.57	0.40
1:2A:2638:G:P	4:2E:82:ARG:HH22	2.44	0.40
1:2A:383:U:H2'	1:2A:385:C:H5	1.85	0.40
1:2A:71:A:H5''	1:2A:73:A:C8	2.56	0.40
1:2A:729:G:O2'	1:2A:763:G:H4'	2.20	0.40
1:2A:765:G:H2'	1:2A:766:C:C6	2.55	0.40
1:2A:956:G:OP2	12:2Q:14:ARG:NH1	2.54	0.40
5:2F:178:PRO:HB2	5:2F:201:VAL:HG21	2.03	0.40
4:2E:15:PHE:CD2	15:2T:81:PRO:HD3	2.56	0.40
1:1A:1105:U:H2'	1:1A:1106:G:C8	2.55	0.40
1:1A:1186:G:H2'	1:1A:1187:G:O4'	2.21	0.40
1:1A:1427:A:H4'	1:1A:1428:C:O4'	2.22	0.40
1:1A:1778:U:H2'	1:1A:1784:A:N6	2.37	0.40
1:1A:1932:A:H2'	1:1A:1933:G:O4'	2.22	0.40
1:1A:2179:C:H2'	1:1A:2180:U:C6	2.56	0.40
1:1A:2264:C:H2'	1:1A:2265:U:O4'	2.22	0.40
1:1A:2441:C:OP2	1:1A:2586:C:O2'	2.34	0.40
1:1A:2639:A:H2'	1:1A:2640:G:O4'	2.21	0.40
2:1B:45:A:C6	2:1B:46:A:C5	3.10	0.40
6:1G:126:ASP:CG	6:1G:130:ASN:HB2	2.42	0.40
8:1I:8:PRO:HD3	8:1I:15:VAL:HB	2.04	0.40
17:1V:57:VAL:HG22	17:1V:99:ILE:HG12	2.02	0.40
30:28:58:ILE:HA	30:28:61:LEU:HD12	2.03	0.40
1:2A:1826:G:H4'	3:2D:242:ARG:HH21	1.87	0.40
1:2A:74:A:H4'	1:2A:75:G:O5'	2.22	0.40
7:2H:71:LEU:HA	7:2H:71:LEU:HD12	1.81	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:2T:8:LYS:HB3	15:2T:8:LYS:HE3	1.95	0.40
21:2Z:36:LYS:HB2	21:2Z:36:LYS:HE3	1.85	0.40
1:1A:1310:G:OP2	29:17:9:ARG:NE	2.50	0.40
1:1A:1410:G:H2'	1:1A:1411:C:C6	3.05	0.40
1:1A:194:G:C2	1:1A:202:U:H1'	2.56	0.40
1:1A:2279:G:N7	22:10:14:ARG:NH1	2.70	0.40
1:1A:476:G:N1	1:1A:479:A:OP2	2.54	0.40
1:1A:738:G:C6	1:1A:739:G:C2	3.09	0.40
5:1F:178:PRO:HB2	5:1F:201:VAL:HG21	2.04	0.40
1:1A:1665:A:H4'	10:1O:67:LYS:HB2	2.02	0.40
17:1V:43:GLU:N	17:1V:43:GLU:OE1	2.48	0.40
22:20:24:LYS:N	22:20:37:LEU:O	2.36	0.40
23:21:8:SER:HB3	23:21:66:HIS:NE2	2.37	0.40
1:2A:1019:U:OP1	1:2A:1035:U:O2'	2.32	0.40
1:2A:1372:U:H2'	1:2A:1373:A:O4'	2.21	0.40
1:2A:142(A):C:O2	19:2X:37:THR:HG21	2.21	0.40
1:2A:142:A:N3	1:2A:1408:C:H1'	2.36	0.40
1:2A:1839:G:C8	1:2A:1927:A:H1'	2.55	0.40
1:2A:2074:U:H2'	1:2A:2075:U:C6	2.57	0.40
1:2A:2572:A:N7	4:2E:145:LYS:HB2	2.37	0.40
1:2A:2623:G:H21	27:25:22:HIS:HE1	1.69	0.40
1:2A:2778:A:H4'	1:2A:2779:U:OP2	2.22	0.40
1:2A:2820:A:HO2'	1:2A:2821:A:P	2.40	0.40
1:2A:348:G:H2'	1:2A:349:G:C8	2.57	0.40
1:2A:531:C:P	1:2A:561:G:H22	2.44	0.40
1:2A:587:C:H4'	1:2A:588:U:C6	2.57	0.40
1:2A:999:U:H5''	1:2A:1154:G:O6	2.21	0.40
10:2O:101:PRO:HD3	15:2T:68:TYR:HB2	2.04	0.40
13:2R:12:ARG:O	13:2R:17:ARG:NH1	2.55	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	256 (94%)	16 (6%)	1 (0%)	34	62
3	2D	273/276 (99%)	256 (94%)	17 (6%)	0	100	100
4	1E	202/206 (98%)	188 (93%)	13 (6%)	1 (0%)	29	57
4	2E	202/206 (98%)	190 (94%)	10 (5%)	2 (1%)	15	40
5	1F	201/210 (96%)	196 (98%)	3 (2%)	2 (1%)	15	40
5	2F	201/210 (96%)	193 (96%)	7 (4%)	1 (0%)	29	57
6	1G	179/182 (98%)	166 (93%)	11 (6%)	2 (1%)	14	38
6	2G	179/182 (98%)	159 (89%)	18 (10%)	2 (1%)	14	38
7	1H	172/180 (96%)	163 (95%)	8 (5%)	1 (1%)	25	53
7	2H	172/180 (96%)	158 (92%)	11 (6%)	3 (2%)	9	27
8	1I	144/148 (97%)	130 (90%)	13 (9%)	1 (1%)	22	50
8	2I	144/148 (97%)	131 (91%)	12 (8%)	1 (1%)	22	50
9	1N	138/140 (99%)	132 (96%)	6 (4%)	0	100	100
9	2N	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
10	1O	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
10	2O	120/122 (98%)	108 (90%)	12 (10%)	0	100	100
11	1P	147/150 (98%)	143 (97%)	4 (3%)	0	100	100
11	2P	147/150 (98%)	138 (94%)	9 (6%)	0	100	100
12	1Q	139/141 (99%)	130 (94%)	9 (6%)	0	100	100
12	2Q	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
13	1R	116/118 (98%)	108 (93%)	8 (7%)	0	100	100
13	2R	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
14	1S	108/112 (96%)	102 (94%)	5 (5%)	1 (1%)	17	43
14	2S	108/112 (96%)	101 (94%)	6 (6%)	1 (1%)	17	43
15	1T	129/146 (88%)	122 (95%)	6 (5%)	1 (1%)	19	46
15	2T	129/146 (88%)	120 (93%)	9 (7%)	0	100	100
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
17	1V	99/101 (98%)	91 (92%)	7 (7%)	1 (1%)	15	40
17	2V	99/101 (98%)	92 (93%)	5 (5%)	2 (2%)	7	23
18	1W	110/113 (97%)	105 (96%)	4 (4%)	1 (1%)	17	43
18	2W	110/113 (97%)	106 (96%)	4 (4%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	1X	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
19	2X	93/96 (97%)	90 (97%)	3 (3%)	0	100	100
20	1Y	105/110 (96%)	97 (92%)	8 (8%)	0	100	100
20	2Y	105/110 (96%)	99 (94%)	5 (5%)	1 (1%)	15	40
21	1Z	148/206 (72%)	135 (91%)	12 (8%)	1 (1%)	22	50
21	2Z	156/206 (76%)	131 (84%)	22 (14%)	3 (2%)	8	24
22	10	81/85 (95%)	79 (98%)	2 (2%)	0	100	100
22	20	81/85 (95%)	75 (93%)	6 (7%)	0	100	100
23	11	95/98 (97%)	92 (97%)	2 (2%)	1 (1%)	14	38
23	21	95/98 (97%)	94 (99%)	1 (1%)	0	100	100
24	12	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
24	22	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
25	13	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
25	23	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
26	14	67/71 (94%)	48 (72%)	15 (22%)	4 (6%)	1	4
26	24	67/71 (94%)	51 (76%)	13 (19%)	3 (4%)	2	7
27	15	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
27	25	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
28	16	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
28	26	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
29	17	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
29	27	46/49 (94%)	46 (100%)	0	0	100	100
30	18	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
30	28	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
31	19	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
31	29	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
33	1b	229/256 (90%)	195 (85%)	28 (12%)	6 (3%)	5	17
33	2b	229/256 (90%)	199 (87%)	24 (10%)	6 (3%)	5	17
34	1c	204/239 (85%)	189 (93%)	14 (7%)	1 (0%)	29	57
34	2c	204/239 (85%)	185 (91%)	18 (9%)	1 (0%)	29	57
35	1d	206/209 (99%)	193 (94%)	13 (6%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	2d	206/209 (99%)	195 (95%)	10 (5%)	1 (0%)	29	57
36	1e	146/162 (90%)	129 (88%)	14 (10%)	3 (2%)	7	22
36	2e	146/162 (90%)	134 (92%)	10 (7%)	2 (1%)	11	31
37	1f	98/101 (97%)	93 (95%)	5 (5%)	0	100	100
37	2f	98/101 (97%)	90 (92%)	8 (8%)	0	100	100
38	1g	153/156 (98%)	137 (90%)	13 (8%)	3 (2%)	7	23
38	2g	153/156 (98%)	142 (93%)	8 (5%)	3 (2%)	7	23
39	1h	135/138 (98%)	131 (97%)	4 (3%)	0	100	100
39	2h	135/138 (98%)	130 (96%)	5 (4%)	0	100	100
40	1i	125/128 (98%)	111 (89%)	14 (11%)	0	100	100
40	2i	125/128 (98%)	115 (92%)	9 (7%)	1 (1%)	19	46
41	1j	95/105 (90%)	83 (87%)	8 (8%)	4 (4%)	3	8
41	2j	94/105 (90%)	81 (86%)	8 (8%)	5 (5%)	2	5
42	1k	112/129 (87%)	106 (95%)	5 (4%)	1 (1%)	17	43
42	2k	112/129 (87%)	102 (91%)	8 (7%)	2 (2%)	8	25
43	1l	119/132 (90%)	113 (95%)	6 (5%)	0	100	100
43	2l	119/132 (90%)	114 (96%)	5 (4%)	0	100	100
44	1m	121/126 (96%)	113 (93%)	7 (6%)	1 (1%)	19	46
44	2m	120/126 (95%)	107 (89%)	11 (9%)	2 (2%)	9	27
45	1n	58/61 (95%)	54 (93%)	4 (7%)	0	100	100
45	2n	58/61 (95%)	52 (90%)	6 (10%)	0	100	100
46	1o	86/89 (97%)	82 (95%)	3 (4%)	1 (1%)	13	35
46	2o	86/89 (97%)	81 (94%)	4 (5%)	1 (1%)	13	35
47	1p	80/88 (91%)	72 (90%)	8 (10%)	0	100	100
47	2p	80/88 (91%)	74 (92%)	6 (8%)	0	100	100
48	1q	97/105 (92%)	92 (95%)	4 (4%)	1 (1%)	15	40
48	2q	97/105 (92%)	92 (95%)	5 (5%)	0	100	100
49	1r	66/88 (75%)	62 (94%)	4 (6%)	0	100	100
49	2r	66/88 (75%)	66 (100%)	0	0	100	100
50	1s	81/93 (87%)	74 (91%)	6 (7%)	1 (1%)	13	35
50	2s	81/93 (87%)	73 (90%)	8 (10%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	1t	94/106 (89%)	86 (92%)	5 (5%)	3 (3%)	4	13
51	2t	94/106 (89%)	80 (85%)	7 (7%)	7 (7%)	1	2
52	1u	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
52	2u	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
All	All	11370/12128 (94%)	10568 (93%)	709 (6%)	93 (1%)	19	46

All (93) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	1H	126	PRO
26	14	55	ARG
41	1j	56	HIS
5	2F	89	VAL
26	24	55	ARG
33	2b	125	PRO
44	2m	5	ALA
51	2t	100	ILE
14	1S	94	TYR
15	1T	128	GLU
26	14	58	ARG
33	1b	17	PHE
33	1b	21	ARG
33	1b	165	VAL
50	1s	81	ARG
6	2G	47	LYS
7	2H	126	PRO
14	2S	96	GLY
17	2V	100	ARG
21	2Z	31	ARG
33	2b	128	GLU
36	2e	85	GLY
38	2g	82	GLY
41	2j	75	ILE
41	2j	79	ARG
44	2m	104	ARG
51	2t	10	LEU
51	2t	96	GLY
6	1G	47	LYS
17	1V	53	GLU
18	1W	11	ARG
21	1Z	165	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
26	14	53	GLU
36	1e	86	ALA
41	1j	75	ILE
41	1j	78	ASN
48	1q	68	ARG
51	1t	100	ILE
17	2V	24	LYS
21	2Z	142	SER
33	2b	9	GLU
36	2e	77	PRO
41	2j	55	LYS
4	1E	52	LEU
5	1F	130	ALA
23	11	3	LYS
26	14	64	GLY
33	1b	9	GLU
33	1b	20	GLU
36	1e	85	GLY
38	1g	4	ARG
4	2E	113	PHE
7	2H	12	PRO
7	2H	47	GLU
8	2I	39	ALA
20	2Y	106	LEU
33	2b	74	LYS
33	2b	124	SER
41	2j	29	ARG
41	2j	78	ASN
42	2k	54	ARG
51	2t	102	GLY
3	1D	200	ASP
6	1G	43	LEU
8	1I	11	ASN
33	1b	125	PRO
38	1g	114	ARG
41	1j	55	LYS
44	1m	67	GLU
51	1t	47	GLY
51	1t	96	GLY
21	2Z	79	ARG
26	24	47	GLN
38	2g	54	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
40	2i	56	LEU
51	2t	9	ASN
51	2t	47	GLY
51	2t	68	LYS
4	2E	52	LEU
26	24	64	GLY
33	2b	189	ASP
34	2c	66	VAL
34	1c	66	VAL
36	1e	69	VAL
38	2g	80	VAL
38	1g	80	VAL
46	2o	20	GLY
5	1F	89	VAL
42	1k	105	VAL
46	1o	20	GLY
6	2G	24	GLY
42	2k	49	GLY
35	2d	5	ILE

### 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%)	208 (97%)	7 (3%)	38	68
3	2D	215/218 (99%)	204 (95%)	11 (5%)	24	52
4	1E	164/166 (99%)	151 (92%)	13 (8%)	12	31
4	2E	164/166 (99%)	152 (93%)	12 (7%)	14	35
5	1F	160/166 (96%)	147 (92%)	13 (8%)	11	30
5	2F	159/166 (96%)	147 (92%)	12 (8%)	13	34
6	1G	143/156 (92%)	137 (96%)	6 (4%)	30	60
6	2G	143/156 (92%)	133 (93%)	10 (7%)	15	37
7	1H	144/148 (97%)	134 (93%)	10 (7%)	15	38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	2H	144/148 (97%)	140 (97%)	4 (3%)	43	73
8	1I	113/124 (91%)	103 (91%)	10 (9%)	10	26
8	2I	105/124 (85%)	99 (94%)	6 (6%)	20	47
9	1N	118/119 (99%)	110 (93%)	8 (7%)	16	38
9	2N	118/119 (99%)	109 (92%)	9 (8%)	13	33
10	1O	100/100 (100%)	95 (95%)	5 (5%)	24	53
10	2O	100/100 (100%)	99 (99%)	1 (1%)	76	91
11	1P	115/116 (99%)	108 (94%)	7 (6%)	18	43
11	2P	115/116 (99%)	108 (94%)	7 (6%)	18	43
12	1Q	111/111 (100%)	108 (97%)	3 (3%)	44	74
12	2Q	111/111 (100%)	109 (98%)	2 (2%)	59	82
13	1R	101/101 (100%)	92 (91%)	9 (9%)	9	26
13	2R	101/101 (100%)	91 (90%)	10 (10%)	8	21
14	1S	86/88 (98%)	81 (94%)	5 (6%)	20	46
14	2S	85/88 (97%)	80 (94%)	5 (6%)	19	45
15	1T	115/127 (91%)	107 (93%)	8 (7%)	15	37
15	2T	113/127 (89%)	109 (96%)	4 (4%)	36	67
16	1U	93/94 (99%)	90 (97%)	3 (3%)	39	69
16	2U	93/94 (99%)	92 (99%)	1 (1%)	73	90
17	1V	80/82 (98%)	73 (91%)	7 (9%)	10	26
17	2V	80/82 (98%)	77 (96%)	3 (4%)	33	64
18	1W	90/92 (98%)	87 (97%)	3 (3%)	38	68
18	2W	90/92 (98%)	89 (99%)	1 (1%)	73	90
19	1X	77/78 (99%)	73 (95%)	4 (5%)	23	51
19	2X	77/78 (99%)	72 (94%)	5 (6%)	17	41
20	1Y	85/91 (93%)	79 (93%)	6 (7%)	14	36
20	2Y	85/91 (93%)	80 (94%)	5 (6%)	19	45
21	1Z	135/179 (75%)	123 (91%)	12 (9%)	9	26
21	2Z	137/179 (76%)	131 (96%)	6 (4%)	28	58
22	10	65/67 (97%)	61 (94%)	4 (6%)	18	43
22	20	65/67 (97%)	61 (94%)	4 (6%)	18	43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	11	80/83 (96%)	73 (91%)	7 (9%)	10	26
23	21	80/83 (96%)	77 (96%)	3 (4%)	33	64
24	12	65/67 (97%)	65 (100%)	0	100	100
24	22	65/67 (97%)	65 (100%)	0	100	100
25	13	51/52 (98%)	49 (96%)	2 (4%)	32	63
25	23	50/52 (96%)	47 (94%)	3 (6%)	19	45
26	14	59/63 (94%)	55 (93%)	4 (7%)	16	38
26	24	53/63 (84%)	48 (91%)	5 (9%)	8	23
27	15	50/52 (96%)	46 (92%)	4 (8%)	12	31
27	25	50/52 (96%)	45 (90%)	5 (10%)	7	21
28	16	51/52 (98%)	48 (94%)	3 (6%)	19	45
28	26	50/52 (96%)	45 (90%)	5 (10%)	7	21
29	17	41/42 (98%)	37 (90%)	4 (10%)	8	21
29	27	41/42 (98%)	37 (90%)	4 (10%)	8	21
30	18	54/55 (98%)	49 (91%)	5 (9%)	9	24
30	28	54/55 (98%)	48 (89%)	6 (11%)	6	16
31	19	34/34 (100%)	33 (97%)	1 (3%)	42	72
31	29	34/34 (100%)	34 (100%)	0	100	100
33	1b	192/220 (87%)	180 (94%)	12 (6%)	18	42
33	2b	187/220 (85%)	171 (91%)	16 (9%)	10	27
34	1c	142/188 (76%)	132 (93%)	10 (7%)	15	37
34	2c	140/188 (74%)	135 (96%)	5 (4%)	35	66
35	1d	169/181 (93%)	157 (93%)	12 (7%)	14	36
35	2d	173/181 (96%)	165 (95%)	8 (5%)	27	56
36	1e	113/123 (92%)	106 (94%)	7 (6%)	18	43
36	2e	114/123 (93%)	110 (96%)	4 (4%)	36	67
37	1f	84/90 (93%)	81 (96%)	3 (4%)	35	66
37	2f	85/90 (94%)	81 (95%)	4 (5%)	26	56
38	1g	119/127 (94%)	115 (97%)	4 (3%)	37	67
38	2g	120/127 (94%)	116 (97%)	4 (3%)	38	68
39	1h	114/119 (96%)	109 (96%)	5 (4%)	28	58

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	2h	114/119 (96%)	106 (93%)	8 (7%)	15	37
40	1i	90/99 (91%)	85 (94%)	5 (6%)	21	47
40	2i	89/99 (90%)	86 (97%)	3 (3%)	37	67
41	1j	66/92 (72%)	62 (94%)	4 (6%)	18	43
41	2j	69/92 (75%)	66 (96%)	3 (4%)	29	59
42	1k	82/99 (83%)	78 (95%)	4 (5%)	25	54
42	2k	83/99 (84%)	77 (93%)	6 (7%)	14	35
43	1l	96/108 (89%)	93 (97%)	3 (3%)	40	71
43	2l	96/108 (89%)	91 (95%)	5 (5%)	23	51
44	1m	93/101 (92%)	89 (96%)	4 (4%)	29	59
44	2m	92/101 (91%)	89 (97%)	3 (3%)	38	68
45	1n	49/50 (98%)	45 (92%)	4 (8%)	11	29
45	2n	49/50 (98%)	46 (94%)	3 (6%)	18	43
46	1o	78/80 (98%)	76 (97%)	2 (3%)	46	75
46	2o	78/80 (98%)	74 (95%)	4 (5%)	24	52
47	1p	69/74 (93%)	65 (94%)	4 (6%)	20	46
47	2p	68/74 (92%)	62 (91%)	6 (9%)	10	26
48	1q	94/97 (97%)	89 (95%)	5 (5%)	22	50
48	2q	94/97 (97%)	92 (98%)	2 (2%)	53	79
49	1r	59/77 (77%)	57 (97%)	2 (3%)	37	67
49	2r	59/77 (77%)	55 (93%)	4 (7%)	16	38
50	1s	69/80 (86%)	61 (88%)	8 (12%)	5	14
50	2s	67/80 (84%)	61 (91%)	6 (9%)	9	25
51	1t	70/82 (85%)	69 (99%)	1 (1%)	67	86
51	2t	70/82 (85%)	67 (96%)	3 (4%)	29	59
52	1u	18/22 (82%)	18 (100%)	0	100	100
52	2u	18/22 (82%)	17 (94%)	1 (6%)	21	47
All	All	9303/10064 (92%)	8784 (94%)	519 (6%)	21	47

All (519) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	10	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	1D	111	LEU
3	1D	155	LEU
3	1D	193	VAL
3	1D	221	VAL
3	1D	229	VAL
3	1D	242	ARG
4	1E	2	LYS
4	1E	12	THR
4	1E	21	VAL
4	1E	24	THR
4	1E	34	VAL
4	1E	47	VAL
4	1E	81	ILE
4	1E	113	PHE
4	1E	116	VAL
4	1E	128	SER
4	1E	175	VAL
4	1E	181	LEU
4	1E	195	LEU
5	1F	33	LEU
5	1F	48	THR
5	1F	53	THR
5	1F	70	THR
5	1F	88	VAL
5	1F	93	LYS
5	1F	106	ARG
5	1F	140	LEU
5	1F	144	LYS
5	1F	149	ASP
5	1F	170	LEU
5	1F	175	THR
5	1F	192	LEU
6	1G	3	LEU
6	1G	31	VAL
6	1G	43	LEU
6	1G	82	LEU
6	1G	145	THR
6	1G	159	VAL
7	1H	7	LEU
7	1H	15	VAL
7	1H	42	ARG
7	1H	70	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
7	1H	90	LYS
7	1H	124	GLU
7	1H	125	VAL
7	1H	129	THR
7	1H	134	SER
7	1H	149	ARG
8	1I	12	LEU
8	1I	20	ASP
8	1I	38	LEU
8	1I	75	LEU
8	1I	86	THR
8	1I	92	VAL
8	1I	101	LEU
8	1I	123	LEU
8	1I	136	VAL
8	1I	140	LEU
9	1N	28	THR
9	1N	35	ARG
9	1N	46	VAL
9	1N	48	MET
9	1N	87	LEU
9	1N	99	LEU
9	1N	138	LEU
9	1N	140	VAL
10	1O	10	VAL
10	1O	75	SER
10	1O	80	ASP
10	1O	94	ARG
10	1O	98	VAL
11	1P	57	THR
11	1P	65	ARG
11	1P	70	GLN
11	1P	83	VAL
11	1P	95	VAL
11	1P	125	VAL
11	1P	147	LEU
12	1Q	8	LYS
12	1Q	75	THR
12	1Q	138	ASP
13	1R	2	ARG
13	1R	28	LEU
13	1R	29	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
13	1R	36	THR
13	1R	44	LEU
13	1R	54	LEU
13	1R	67	LEU
13	1R	96	ARG
13	1R	111	LEU
14	1S	3	ARG
14	1S	14	VAL
14	1S	21	THR
14	1S	46	VAL
14	1S	53	SER
15	1T	6	LEU
15	1T	21	GLU
15	1T	28	VAL
15	1T	49	VAL
15	1T	82	LEU
15	1T	90	GLN
15	1T	95	ARG
15	1T	96	ARG
16	1U	77	SER
16	1U	78	THR
16	1U	83	LEU
17	1V	46	VAL
17	1V	51	VAL
17	1V	52	VAL
17	1V	62	LEU
17	1V	72	VAL
17	1V	79	VAL
17	1V	82	ARG
18	1W	92	ARG
18	1W	96	ILE
18	1W	107	LEU
19	1X	27	THR
19	1X	50	LYS
19	1X	75	ASP
19	1X	80	ILE
20	1Y	1	MET
20	1Y	7	VAL
20	1Y	37	VAL
20	1Y	49	VAL
20	1Y	72	VAL
20	1Y	107	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
21	1Z	18	LEU
21	1Z	33	LEU
21	1Z	41	LEU
21	1Z	75	ASN
21	1Z	76	LEU
21	1Z	123	ASP
21	1Z	135	GLU
21	1Z	140	ASP
21	1Z	146	ILE
21	1Z	154	ASP
21	1Z	165	VAL
21	1Z	170	THR
22	10	10	THR
22	10	39	ARG
22	10	43	THR
22	10	72	ARG
23	11	11	ARG
23	11	35	THR
23	11	38	SER
23	11	40	ARG
23	11	59	THR
23	11	78	LYS
23	11	95	LEU
25	13	30	ARG
25	13	34	GLU
26	14	46	GLN
26	14	49	PHE
26	14	52	THR
26	14	58	ARG
27	15	6	VAL
27	15	16	ARG
27	15	29	THR
27	15	57	VAL
28	16	6	ARG
28	16	24	GLU
28	16	48	VAL
29	17	1	MET
29	17	39	ARG
29	17	41	ARG
29	17	43	THR
30	18	14	VAL
30	18	31	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
30	18	34	TRP
30	18	52	LYS
30	18	59	LYS
31	19	6	SER
33	1b	21	ARG
33	1b	24	TRP
33	1b	49	GLU
33	1b	67	THR
33	1b	76	GLN
33	1b	87	ARG
33	1b	94	ASN
33	1b	108	ILE
33	1b	117	GLU
33	1b	160	ASP
33	1b	170	GLU
33	1b	197	VAL
34	1c	3	ASN
34	1c	5	ILE
34	1c	15	THR
34	1c	28	GLN
34	1c	36	ASP
34	1c	49	SER
34	1c	57	ILE
34	1c	165	THR
34	1c	175	LEU
34	1c	206	GLU
35	1d	5	ILE
35	1d	26	CYS
35	1d	59	ARG
35	1d	71	SER
35	1d	76	ARG
35	1d	107	ARG
35	1d	127	THR
35	1d	135	LEU
35	1d	137	SER
35	1d	139	ARG
35	1d	155	LEU
35	1d	194	LEU
36	1e	16	THR
36	1e	31	LEU
36	1e	41	VAL
36	1e	47	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
36	1e	68	GLU
36	1e	75	THR
36	1e	83	GLU
37	1f	21	LEU
37	1f	43	LEU
37	1f	73	ASN
38	1g	20	ASP
38	1g	75	VAL
38	1g	79	ARG
38	1g	92	SER
39	1h	14	ARG
39	1h	17	THR
39	1h	85	ARG
39	1h	105	ARG
39	1h	133	LEU
40	1i	27	THR
40	1i	64	THR
40	1i	87	GLN
40	1i	108	VAL
40	1i	111	ARG
41	1j	8	LEU
41	1j	15	THR
41	1j	49	VAL
41	1j	81	THR
42	1k	16	SER
42	1k	18	ARG
42	1k	81	ASP
42	1k	120	ARG
43	1l	44	THR
43	1l	58	VAL
43	1l	117	ARG
44	1m	17	VAL
44	1m	43	THR
44	1m	86	CYS
44	1m	109	THR
45	1n	18	VAL
45	1n	22	THR
45	1n	33	VAL
45	1n	44	LEU
46	1o	39	LEU
46	1o	87	ILE
47	1p	1	MET

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
47	1p	2	VAL
47	1p	20	VAL
47	1p	67	THR
48	1q	9	VAL
48	1q	36	ILE
48	1q	53	LEU
48	1q	63	ARG
48	1q	72	ARG
49	1r	31	LEU
49	1r	54	ARG
50	1s	12	ASP
50	1s	14	HIS
50	1s	30	LEU
50	1s	33	THR
50	1s	39	THR
50	1s	41	VAL
50	1s	66	MET
50	1s	77	THR
51	1t	15	ARG
3	2D	10	THR
3	2D	15	PHE
3	2D	32	SER
3	2D	115	GLN
3	2D	138	VAL
3	2D	142	VAL
3	2D	193	VAL
3	2D	200	ASP
3	2D	229	VAL
3	2D	242	ARG
3	2D	271	ILE
4	2E	9	VAL
4	2E	12	THR
4	2E	21	VAL
4	2E	27	LEU
4	2E	38	THR
4	2E	55	ASN
4	2E	76	ARG
4	2E	113	PHE
4	2E	116	VAL
4	2E	119	ARG
4	2E	163	GLU
4	2E	195	LEU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
5	2F	12	LEU
5	2F	24	LEU
5	2F	53	THR
5	2F	57	VAL
5	2F	65	TRP
5	2F	88	VAL
5	2F	106	ARG
5	2F	125	LEU
5	2F	153	SER
5	2F	158	THR
5	2F	170	LEU
5	2F	191	ARG
6	2G	5	VAL
6	2G	43	LEU
6	2G	79	ASN
6	2G	97	ASP
6	2G	109	VAL
6	2G	130	ASN
6	2G	145	THR
6	2G	150	ASP
6	2G	161	THR
6	2G	165	THR
7	2H	67	LEU
7	2H	105	LEU
7	2H	107	VAL
7	2H	134	SER
8	2I	38	LEU
8	2I	42	SER
8	2I	123	LEU
8	2I	125	GLU
8	2I	127	VAL
8	2I	144	VAL
9	2N	28	THR
9	2N	32	THR
9	2N	34	LEU
9	2N	43	THR
9	2N	60	ILE
9	2N	73	THR
9	2N	121	LYS
9	2N	127	ASP
9	2N	139	GLU
10	2O	116	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
11	2P	42	SER
11	2P	65	ARG
11	2P	75	ILE
11	2P	95	VAL
11	2P	99	LEU
11	2P	136	GLU
11	2P	148	LEU
12	2Q	75	THR
12	2Q	139	GLU
13	2R	24	GLN
13	2R	29	LEU
13	2R	35	THR
13	2R	44	LEU
13	2R	67	LEU
13	2R	86	ARG
13	2R	89	ASP
13	2R	91	GLN
13	2R	96	ARG
13	2R	100	LEU
14	2S	4	LEU
14	2S	8	GLU
14	2S	48	LEU
14	2S	53	SER
14	2S	110	LEU
15	2T	57	PHE
15	2T	67	SER
15	2T	74	ARG
15	2T	88	ILE
16	2U	17	ILE
17	2V	7	THR
17	2V	51	VAL
17	2V	79	VAL
18	2W	49	LYS
19	2X	50	LYS
19	2X	52	VAL
19	2X	70	LEU
19	2X	75	ASP
19	2X	82	GLN
20	2Y	1	MET
20	2Y	8	LYS
20	2Y	90	LEU
20	2Y	99	CYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
20	2Y	107	ASP
21	2Z	24	LEU
21	2Z	123	ASP
21	2Z	124	ILE
21	2Z	154	ASP
21	2Z	170	THR
21	2Z	174	VAL
22	20	14	ARG
22	20	20	ARG
22	20	53	MET
22	20	67	VAL
23	21	3	LYS
23	21	11	ARG
23	21	35	THR
25	23	30	ARG
25	23	31	LEU
25	23	54	VAL
26	24	3	GLU
26	24	26	SER
26	24	37	SER
26	24	52	THR
26	24	67	TYR
27	25	6	VAL
27	25	26	THR
27	25	33	CYS
27	25	40	LYS
27	25	58	LEU
28	26	9	LEU
28	26	13	CYS
28	26	14	THR
28	26	30	THR
28	26	47	THR
29	27	4	THR
29	27	41	ARG
29	27	43	THR
29	27	46	VAL
30	28	14	VAL
30	28	30	ARG
30	28	31	HIS
30	28	32	LEU
30	28	37	SER
30	28	57	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
33	2b	7	VAL
33	2b	22	LYS
33	2b	24	TRP
33	2b	79	ASP
33	2b	94	ASN
33	2b	108	ILE
33	2b	111	ARG
33	2b	121	LEU
33	2b	124	SER
33	2b	127	ILE
33	2b	158	LEU
33	2b	164	VAL
33	2b	189	ASP
33	2b	192	SER
33	2b	209	ARG
33	2b	233	SER
34	2c	47	LEU
34	2c	115	LEU
34	2c	144	SER
34	2c	154	SER
34	2c	193	TYR
35	2d	9	CYS
35	2d	83	SER
35	2d	85	LYS
35	2d	108	LEU
35	2d	118	ARG
35	2d	119	GLN
35	2d	135	LEU
35	2d	194	LEU
36	2e	41	VAL
36	2e	87	SER
36	2e	111	GLU
36	2e	120	THR
37	2f	19	LEU
37	2f	48	LEU
37	2f	61	LEU
37	2f	83	ASP
38	2g	10	ARG
38	2g	75	VAL
38	2g	79	ARG
38	2g	104	LEU
39	2h	2	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
39	2h	3	THR
39	2h	25	ASP
39	2h	63	LEU
39	2h	83	ILE
39	2h	105	ARG
39	2h	135	CYS
39	2h	137	VAL
40	2i	65	VAL
40	2i	102	LEU
40	2i	105	ASP
41	2j	59	SER
41	2j	68	HIS
41	2j	89	ASP
42	2k	16	SER
42	2k	24	SER
42	2k	48	ILE
42	2k	109	VAL
42	2k	116	HIS
42	2k	119	CYS
43	2l	27	LEU
43	2l	55	VAL
43	2l	67	THR
43	2l	113	ARG
43	2l	122	THR
44	2m	47	ASP
44	2m	77	ASN
44	2m	103	THR
45	2n	22	THR
45	2n	33	VAL
45	2n	49	HIS
46	2o	5	LYS
46	2o	21	ASP
46	2o	39	LEU
46	2o	65	ARG
47	2p	2	VAL
47	2p	20	VAL
47	2p	21	VAL
47	2p	44	THR
47	2p	62	VAL
47	2p	67	THR
48	2q	12	SER
48	2q	19	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
49	2r	31	LEU
49	2r	37	VAL
49	2r	66	LEU
49	2r	76	LEU
50	2s	33	THR
50	2s	39	THR
50	2s	65	ASN
50	2s	66	MET
50	2s	77	THR
50	2s	83	HIS
51	2t	24	LEU
51	2t	71	THR
51	2t	99	LEU
52	2u	7	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (97) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	96	HIS
3	1D	116	GLN
3	1D	143	HIS
3	1D	201	HIS
5	1F	69	HIS
5	1F	75	HIS
5	1F	204	ASN
6	1G	27	ASN
6	1G	40	ASN
6	1G	58	GLN
6	1G	79	ASN
8	1I	139	GLN
11	1P	35	HIS
11	1P	128	HIS
13	1R	71	GLN
14	1S	38	GLN
15	1T	58	ASN
16	1U	94	ASN
18	1W	60	ASN
20	1Y	6	HIS
21	1Z	34	ASN
22	10	29	GLN
22	10	50	ASN
24	12	65	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
26	14	20	ASN
26	14	40	HIS
30	18	35	GLN
31	19	34	GLN
33	1b	40	HIS
33	1b	78	GLN
34	1c	6	HIS
34	1c	162	GLN
34	1c	176	HIS
36	1e	78	HIS
36	1e	130	ASN
37	1f	73	ASN
38	1g	28	ASN
38	1g	64	GLN
38	1g	86	GLN
38	1g	153	HIS
40	1i	3	GLN
40	1i	31	GLN
40	1i	58	HIS
40	1i	87	GLN
40	1i	117	HIS
40	1i	124	GLN
41	1j	56	HIS
44	1m	92	HIS
46	1o	51	HIS
50	1s	14	HIS
50	1s	23	ASN
50	1s	47	HIS
51	1t	42	GLN
3	2D	87	ASN
3	2D	116	GLN
8	2I	11	ASN
10	2O	5	GLN
12	2Q	123	HIS
16	2U	44	ASN
18	2W	62	HIS
19	2X	31	HIS
21	2Z	32	HIS
21	2Z	132	ASN
22	20	29	GLN
22	20	35	ASN
23	21	56	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
24	22	65	ASN
28	26	32	ASN
31	29	34	GLN
33	2b	40	HIS
33	2b	78	GLN
33	2b	212	GLN
34	2c	6	HIS
34	2c	104	GLN
35	2d	77	ASN
35	2d	116	GLN
35	2d	119	GLN
35	2d	123	HIS
35	2d	125	HIS
36	2e	20	GLN
36	2e	78	HIS
36	2e	130	ASN
37	2f	13	ASN
37	2f	32	ASN
37	2f	100	ASN
40	2i	23	ASN
40	2i	31	GLN
40	2i	38	GLN
40	2i	117	HIS
41	2j	21	GLN
41	2j	56	HIS
44	2m	62	ASN
47	2p	16	HIS
49	2r	63	GLN
50	2s	23	ASN
50	2s	69	HIS
51	2t	42	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2861/2915 (98%)	492 (17%)	23 (0%)
1	2A	2788/2915 (95%)	540 (19%)	19 (0%)
2	1B	119/121 (98%)	10 (8%)	0
2	2B	118/121 (97%)	33 (27%)	0
32	1a	1494/1521 (98%)	276 (18%)	0
32	2a	1498/1521 (98%)	319 (21%)	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
53	1v	12/27 (44%)	2 (16%)	0
53	2v	12/27 (44%)	4 (33%)	0
54	1w	68/76 (89%)	25 (36%)	0
54	1y	70/76 (92%)	25 (35%)	0
54	2w	68/76 (89%)	29 (42%)	0
54	2y	68/76 (89%)	32 (47%)	0
55	1x	75/77 (97%)	11 (14%)	0
55	2x	75/77 (97%)	15 (20%)	0
All	All	9326/9626 (96%)	1813 (19%)	42 (0%)

All (1813) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	10	G
1	1A	34	C
1	1A	45	C
1	1A	58	G
1	1A	59	U
1	1A	63	U
1	1A	71	A
1	1A	74	A
1	1A	75	G
1	1A	84	A
1	1A	92	A
1	1A	95	G
1	1A	118	A
1	1A	119	A
1	1A	120	U
1	1A	125	G
1	1A	177	G
1	1A	182	A
1	1A	184	C
1	1A	196	A
1	1A	199	A
1	1A	201	C
1	1A	205	G
1	1A	214	G
1	1A	216	A
1	1A	222	A
1	1A	225	A
1	1A	228	A
1	1A	229	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	1A	230	U
1	1A	233	A
1	1A	248	G
1	1A	269	U
1	1A	271(E)	U
1	1A	271(G)	C
1	1A	271(L)	U
1	1A	271(M)	G
1	1A	271(N)	U
1	1A	271(O)	C
1	1A	271(R)	G
1	1A	272(A)	U
1	1A	272(B)	G
1	1A	279	C
1	1A	311	A
1	1A	329	G
1	1A	330	A
1	1A	336	C
1	1A	342	G
1	1A	352	G
1	1A	363	G
1	1A	363(B)	G
1	1A	372	G
1	1A	386	G
1	1A	396	G
1	1A	404	C
1	1A	405	U
1	1A	411	G
1	1A	412	A
1	1A	418	G
1	1A	428	A
1	1A	433	C
1	1A	443	A
1	1A	444	C
1	1A	446	G
1	1A	448	U
1	1A	449	A
1	1A	457	A
1	1A	481	G
1	1A	504	U
1	1A	505	A
1	1A	509	C

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	1A	528	A
1	1A	530	G
1	1A	531	C
1	1A	532	A
1	1A	533	G
1	1A	545	G
1	1A	549	G
1	1A	555	U
1	1A	563	G
1	1A	573	G
1	1A	575	A
1	1A	594	U
1	1A	603	A
1	1A	604	G
1	1A	607	U
1	1A	614(B)	G
1	1A	615	G
1	1A	616	G
1	1A	627	A
1	1A	637	A
1	1A	645	C
1	1A	646	A
1	1A	652(A)	A
1	1A	652(E)	G
1	1A	652(T)	C
1	1A	668	G
1	1A	669	G
1	1A	686	G
1	1A	702	G
1	1A	717	G
1	1A	728	G
1	1A	730	C
1	1A	757	U
1	1A	764	A
1	1A	775	G
1	1A	776	G
1	1A	782	A
1	1A	784	A
1	1A	785	G
1	1A	789	A
1	1A	790	C
1	1A	792	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	1A	805	G
1	1A	812	C
1	1A	819	A
1	1A	825	C
1	1A	827	U
1	1A	830	G
1	1A	855	G
1	1A	859	G
1	1A	866	A
1	1A	879	G
1	1A	880	G
1	1A	883	G
1	1A	884	C
1	1A	885	C
1	1A	887	A
1	1A	888	C
1	1A	889	C
1	1A	890	A
1	1A	894	C
1	1A	895	U
1	1A	896	A
1	1A	897	C
1	1A	907	U
1	1A	910	A
1	1A	911	A
1	1A	927	G
1	1A	931	G
1	1A	932	G
1	1A	934	G
1	1A	935	C
1	1A	945	A
1	1A	946	G
1	1A	953	A
1	1A	957	A
1	1A	959	A
1	1A	961	C
1	1A	967	C
1	1A	974	G
1	1A	975	C
1	1A	975(A)	G
1	1A	983	A
1	1A	996	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	1A	1012	U
1	1A	1013	C
1	1A	1025	G
1	1A	1026	U
1	1A	1027	A
1	1A	1033	U
1	1A	1041	C
1	1A	1044	G
1	1A	1046	A
1	1A	1047	G
1	1A	1048	A
1	1A	1050	A
1	1A	1054	A
1	1A	1055	G
1	1A	1058	G
1	1A	1059	G
1	1A	1066	U
1	1A	1068	G
1	1A	1071	G
1	1A	1073	A
1	1A	1074	G
1	1A	1075	C
1	1A	1076	C
1	1A	1078	U
1	1A	1079	C
1	1A	1080	C
1	1A	1081	U
1	1A	1083	U
1	1A	1085	A
1	1A	1088	A
1	1A	1089	G
1	1A	1090	U
1	1A	1094	U
1	1A	1095	A
1	1A	1097	U
1	1A	1098	A
1	1A	1100	C
1	1A	1101	U
1	1A	1103	A
1	1A	1107	G
1	1A	1111	A
1	1A	1112	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	1A	1127	A
1	1A	1128	A
1	1A	1130	U
1	1A	1135	C
1	1A	1136	G
1	1A	1156	A
1	1A	1170	G
1	1A	1171	G
1	1A	1173	G
1	1A	1174	A
1	1A	1175	U
1	1A	1176	G
1	1A	1177	A
1	1A	1178	C
1	1A	1202	C
1	1A	1211	U
1	1A	1218	C
1	1A	1236	G
1	1A	1241	A
1	1A	1252	G
1	1A	1253	A
1	1A	1256	G
1	1A	1267	U
1	1A	1271	G
1	1A	1272	A
1	1A	1273	U
1	1A	1300	U
1	1A	1301	A
1	1A	1318	C
1	1A	1352	U
1	1A	1359	A
1	1A	1360	A
1	1A	1365	A
1	1A	1384	A
1	1A	1385	G
1	1A	1416	G
1	1A	1417	C
1	1A	1420	U
1	1A	1421	G
1	1A	1428	C
1	1A	1445	A
1	1A	1450	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	1A	1455	G
1	1A	1459	G
1	1A	1467	C
1	1A	1478	G
1	1A	1482	G
1	1A	1493	C
1	1A	1494	A
1	1A	1497	U
1	1A	1508	A
1	1A	1509	C
1	1A	1509(A)	A
1	1A	1525	G
1	1A	1542	A
1	1A	1546	C
1	1A	1554	A
1	1A	1558	A
1	1A	1559	G
1	1A	1566	A
1	1A	1569	A
1	1A	1578	U
1	1A	1580	A
1	1A	1584	C
1	1A	1586	A
1	1A	1608	A
1	1A	1609	A
1	1A	1610	A
1	1A	1612	C
1	1A	1622	G
1	1A	1646	C
1	1A	1648	C
1	1A	1651	G
1	1A	1654	A
1	1A	1658	C
1	1A	1669	A
1	1A	1674	G
1	1A	1695	G
1	1A	1700	A
1	1A	1703	G
1	1A	1746	G
1	1A	1756	G
1	1A	1762	A
1	1A	1763	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	1A	1764	G
1	1A	1773	A
1	1A	1780	A
1	1A	1781	C
1	1A	1782	C
1	1A	1786	A
1	1A	1791	A
1	1A	1800	C
1	1A	1801	G
1	1A	1811	G
1	1A	1812	A
1	1A	1816	G
1	1A	1847	A
1	1A	1848	A
1	1A	1858	G
1	1A	1861	G
1	1A	1877	A
1	1A	1878	G
1	1A	1889	A
1	1A	1898	U
1	1A	1900	A
1	1A	1906	G
1	1A	1915	5MU
1	1A	1919	A
1	1A	1921	G
1	1A	1927	A
1	1A	1929	G
1	1A	1930	G
1	1A	1938	A
1	1A	1955	U
1	1A	1963	U
1	1A	1967	C
1	1A	1970	A
1	1A	1971	A
1	1A	1972	A
1	1A	1992	G
1	1A	1993	U
1	1A	1994	C
1	1A	1997	G
1	1A	2020	A
1	1A	2023	G
1	1A	2031	A

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	1A	2032	G
1	1A	2033	A
1	1A	2043	C
1	1A	2055	C
1	1A	2056	G
1	1A	2060	A
1	1A	2061	G
1	1A	2062	A
1	1A	2069	G
1	1A	2092	U
1	1A	2096	U
1	1A	2104	G
1	1A	2113	U
1	1A	2120	G
1	1A	2126	A
1	1A	2127	G
1	1A	2131	G
1	1A	2132	U
1	1A	2133	G
1	1A	2134	A
1	1A	2135	A
1	1A	2138	C
1	1A	2140	C
1	1A	2142	C
1	1A	2143	C
1	1A	2144	U
1	1A	2146	C
1	1A	2149	G
1	1A	2150	U
1	1A	2151	G
1	1A	2155	G
1	1A	2157	G
1	1A	2158	A
1	1A	2159	G
1	1A	2160	G
1	1A	2162	G
1	1A	2164	C
1	1A	2165	G
1	1A	2166	G
1	1A	2167	U
1	1A	2171	A
1	1A	2172	U

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1A	2174	C
1	1A	2175	C
1	1A	2181	G
1	1A	2182	G
1	1A	2183	C
1	1A	2184	G
1	1A	2189	U
1	1A	2198	A
1	1A	2206	G
1	1A	2207	G
1	1A	2208	A
1	1A	2218	U
1	1A	2225	A
1	1A	2238	G
1	1A	2239	G
1	1A	2267	A
1	1A	2268	A
1	1A	2269	A
1	1A	2273	A
1	1A	2279	G
1	1A	2280	G
1	1A	2283	C
1	1A	2286	A
1	1A	2287	A
1	1A	2289	G
1	1A	2305	A
1	1A	2306	C
1	1A	2307	G
1	1A	2308	G
1	1A	2314	C
1	1A	2320	A
1	1A	2322	A
1	1A	2325	G
1	1A	2334	G
1	1A	2335	A
1	1A	2336	A
1	1A	2347	C
1	1A	2350	C
1	1A	2358	G
1	1A	2361	A
1	1A	2383	G
1	1A	2385	C

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	1A	2400	G
1	1A	2406	U
1	1A	2410	G
1	1A	2423	U
1	1A	2424	C
1	1A	2425	A
1	1A	2429	G
1	1A	2430	A
1	1A	2435	A
1	1A	2439	A
1	1A	2441	C
1	1A	2447	G
1	1A	2448	A
1	1A	2449	U
1	1A	2468	G
1	1A	2476	A
1	1A	2487	G
1	1A	2490	G
1	1A	2502	G
1	1A	2505	G
1	1A	2506	U
1	1A	2507	C
1	1A	2518	A
1	1A	2520	C
1	1A	2529	G
1	1A	2542	A
1	1A	2554	U
1	1A	2566	A
1	1A	2567	G
1	1A	2573	C
1	1A	2574	G
1	1A	2582	G
1	1A	2601	C
1	1A	2602	A
1	1A	2609	U
1	1A	2611	U
1	1A	2612	C
1	1A	2629	A
1	1A	2630	G
1	1A	2632	A
1	1A	2654	A
1	1A	2663	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	1A	2689	U
1	1A	2691	C
1	1A	2702	U
1	1A	2703	C
1	1A	2712(A)	A
1	1A	2713	A
1	1A	2714	G
1	1A	2726	U
1	1A	2732	G
1	1A	2733	A
1	1A	2738	A
1	1A	2739	U
1	1A	2744	G
1	1A	2749	A
1	1A	2750	A
1	1A	2752	C
1	1A	2757	A
1	1A	2758	A
1	1A	2764	A
1	1A	2765	A
1	1A	2766	G
1	1A	2778	A
1	1A	2780	G
1	1A	2789	C
1	1A	2790	A
1	1A	2791	C
1	1A	2794	C
1	1A	2802	G
1	1A	2807	G
1	1A	2818	G
1	1A	2820	A
1	1A	2821	A
1	1A	2833	G
1	1A	2835	A
1	1A	2836	U
1	1A	2866	U
1	1A	2872	G
1	1A	2876	G
1	1A	2880	C
1	1A	2892	A
1	1A	2893	G
1	1A	2894	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	1A	2897	U
2	1B	2	C
2	1B	15	A
2	1B	24	G
2	1B	42	C
2	1B	52	A
2	1B	56	G
2	1B	73	A
2	1B	85	G
2	1B	106	G
2	1B	110	G
32	1a	6	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	52	G
32	1a	61	G
32	1a	79	G
32	1a	91	C
32	1a	98	G
32	1a	101	A
32	1a	116	A
32	1a	121	C
32	1a	129	U
32	1a	131	C
32	1a	145	G
32	1a	174	C
32	1a	180	U
32	1a	181	G
32	1a	185	A
32	1a	189(F)	U
32	1a	189(G)	G
32	1a	189(H)	G
32	1a	189(J)	G
32	1a	195	A
32	1a	197	A
32	1a	199	G
32	1a	201	C

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	1a	202	U
32	1a	203	U
32	1a	204	U
32	1a	216	G
32	1a	218	C
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	321	A
32	1a	328	C
32	1a	332	G
32	1a	336	C
32	1a	341	C
32	1a	342	C
32	1a	344	A
32	1a	345	C
32	1a	347	G
32	1a	349	A
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	363	A
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	384	G
32	1a	390	C
32	1a	397	A
32	1a	398	C
32	1a	406	G
32	1a	409	G
32	1a	412	A
32	1a	413	G
32	1a	421	U
32	1a	422	C
32	1a	424	G
32	1a	429	U
32	1a	435	C

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	1a	439	A
32	1a	452	A
32	1a	453	A
32	1a	461	A
32	1a	470	C
32	1a	484	G
32	1a	485	G
32	1a	496	A
32	1a	498	U
32	1a	505	G
32	1a	509	A
32	1a	510	A
32	1a	511	C
32	1a	518	C
32	1a	522	C
32	1a	525	C
32	1a	531	U
32	1a	532	A
32	1a	543	C
32	1a	545	C
32	1a	547	A
32	1a	559	A
32	1a	561	U
32	1a	564	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	628	G
32	1a	630	G
32	1a	634	C
32	1a	653	A
32	1a	665	A
32	1a	666	G
32	1a	673	G
32	1a	687	A
32	1a	688	G
32	1a	693	G
32	1a	694	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
32	1a	695	A
32	1a	702	A
32	1a	703	G
32	1a	721	G
32	1a	723	U
32	1a	724	G
32	1a	728	A
32	1a	731	G
32	1a	734	G
32	1a	747	C
32	1a	749	C
32	1a	755	G
32	1a	773	G
32	1a	774	G
32	1a	777	A
32	1a	792	A
32	1a	793	U
32	1a	794	A
32	1a	802	A
32	1a	806	C
32	1a	816	A
32	1a	817	C
32	1a	827	U
32	1a	828	A
32	1a	840	C
32	1a	841	U
32	1a	851	G
32	1a	859	A
32	1a	895	G
32	1a	902	G
32	1a	914	A
32	1a	916	G
32	1a	926	G
32	1a	927	G
32	1a	932	C
32	1a	934	C
32	1a	936	C
32	1a	939	G
32	1a	950	U
32	1a	960	U
32	1a	961	U
32	1a	967	5MC

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	992	U
32	1a	993	G
32	1a	997	U
32	1a	999	C
32	1a	1000	U
32	1a	1003	G
32	1a	1005	A
32	1a	1006	C
32	1a	1009	G
32	1a	1020	U
32	1a	1022	G
32	1a	1024	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C
32	1a	1028	C
32	1a	1030	C
32	1a	1030(A)	G
32	1a	1030(C)	G
32	1a	1031	G
32	1a	1037	C
32	1a	1040	U
32	1a	1043	C
32	1a	1044	A
32	1a	1054	C
32	1a	1065	U
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	1108	G
32	1a	1118	C

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
32	1a	1121	U
32	1a	1123	A
32	1a	1125	U
32	1a	1136	U
32	1a	1137	C
32	1a	1138	G
32	1a	1139	G
32	1a	1140	C
32	1a	1146	A
32	1a	1152	A
32	1a	1154	G
32	1a	1157	A
32	1a	1159	U
32	1a	1179	A
32	1a	1182	G
32	1a	1183	A
32	1a	1184	G
32	1a	1196	U
32	1a	1197	G
32	1a	1202	G
32	1a	1212	U
32	1a	1213	A
32	1a	1214	C
32	1a	1220	G
32	1a	1227	A
32	1a	1238	A
32	1a	1253	G
32	1a	1256	A
32	1a	1257	U
32	1a	1258	G
32	1a	1270	C
32	1a	1273	G
32	1a	1275	A
32	1a	1276	G
32	1a	1279	A
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A
32	1a	1294	G
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
32	1a	1305	G
32	1a	1319	A
32	1a	1322	C
32	1a	1338	G
32	1a	1340	A
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1363(A)	A
32	1a	1364	U
32	1a	1368	G
32	1a	1370	G
32	1a	1371	G
32	1a	1379	G
32	1a	1400	5MC
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1446	U
32	1a	1447	A
32	1a	1452	C
32	1a	1458	G
32	1a	1475	G
32	1a	1487	G
32	1a	1492	A
32	1a	1494	G
32	1a	1497	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
53	1v	24	C
54	1w	2	G
54	1w	9	A
54	1w	19	G
54	1w	24	G
54	1w	25	C

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
54	1w	29	U
54	1w	35	A
54	1w	36	C
54	1w	45	G
54	1w	46	7MG
54	1w	47	U
54	1w	48	C
54	1w	49	G
54	1w	50	G
54	1w	51	C
54	1w	56	C
54	1w	58	A
54	1w	59	U
54	1w	61	C
54	1w	62	C
54	1w	63	G
54	1w	66	A
54	1w	69	A
54	1w	70	C
54	1w	74	C
55	1x	9	G
55	1x	13	C
55	1x	18	G
55	1x	20	U
55	1x	21	A
55	1x	25	C
55	1x	47	U
55	1x	60	U
55	1x	61	C
55	1x	69	C
55	1x	76	A
54	1y	2	G
54	1y	3	G
54	1y	5	G
54	1y	6	A
54	1y	9	A
54	1y	13	C
54	1y	19	G
54	1y	20	G
54	1y	21	A
54	1y	24	G
54	1y	25	C

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
54	1y	32	C
54	1y	33	U
54	1y	35	A
54	1y	40	G
54	1y	45	G
54	1y	46	7MG
54	1y	47	U
54	1y	48	C
54	1y	54	5MU
54	1y	60	C
54	1y	61	C
54	1y	64	U
54	1y	65	C
54	1y	71	C
1	2A	10	G
1	2A	11	G
1	2A	15	G
1	2A	34	C
1	2A	35	G
1	2A	45	C
1	2A	63	U
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	79	G
1	2A	84	A
1	2A	90	U
1	2A	94	C
1	2A	100	G
1	2A	102	G
1	2A	118	A
1	2A	120	U
1	2A	123	G
1	2A	125	G
1	2A	128	C
1	2A	149	A
1	2A	154(A)	C
1	2A	157	U
1	2A	181	A
1	2A	196	A
1	2A	199	A
1	2A	205	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	2A	214	G
1	2A	215	G
1	2A	216	A
1	2A	221	A
1	2A	222	A
1	2A	225	A
1	2A	228	A
1	2A	229	A
1	2A	230	U
1	2A	232	G
1	2A	233	A
1	2A	236	C
1	2A	243	U
1	2A	248	G
1	2A	249	C
1	2A	250	G
1	2A	271(A)	A
1	2A	271(J)	C
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	271(O)	C
1	2A	272(A)	U
1	2A	272(B)	G
1	2A	272(J)	C
1	2A	277	C
1	2A	278	A
1	2A	290	G
1	2A	294	A
1	2A	300	A
1	2A	311	A
1	2A	312	G
1	2A	317	G
1	2A	324	A
1	2A	327	G
1	2A	329	G
1	2A	332	A
1	2A	352	G
1	2A	354	G
1	2A	363(B)	G
1	2A	363(C)	G
1	2A	364	C

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	2A	371	A
1	2A	372	G
1	2A	386	G
1	2A	399	G
1	2A	405	U
1	2A	407	G
1	2A	411	G
1	2A	412	A
1	2A	428	A
1	2A	434	U
1	2A	435	C
1	2A	443	A
1	2A	444	C
1	2A	446	G
1	2A	454	A
1	2A	455	C
1	2A	456	C
1	2A	457	A
1	2A	462	C
1	2A	481	G
1	2A	494	G
1	2A	499	U
1	2A	505	A
1	2A	509	C
1	2A	521	G
1	2A	527	C
1	2A	528	A
1	2A	529	A
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	551	G
1	2A	554	U
1	2A	556	G
1	2A	563	G
1	2A	568	U
1	2A	573	G
1	2A	574	C
1	2A	575	A
1	2A	586	A
1	2A	588	U
1	2A	592	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	614(A)	U
1	2A	614(B)	G
1	2A	614(C)	A
1	2A	615	G
1	2A	627	A
1	2A	634	C
1	2A	637	A
1	2A	640	C
1	2A	645	C
1	2A	646	A
1	2A	647	G
1	2A	651	G
1	2A	652(A)	A
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	652(U)	G
1	2A	653	A
1	2A	656	G
1	2A	668	G
1	2A	669	G
1	2A	684	G
1	2A	686	G
1	2A	698	C
1	2A	717	G
1	2A	726	G
1	2A	730	C
1	2A	747	U
1	2A	753	C
1	2A	771	G
1	2A	775	G
1	2A	776	G
1	2A	777	A
1	2A	779	U
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	790	C
1	2A	792	G
1	2A	793	A

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	2A	805	G
1	2A	811	U
1	2A	812	C
1	2A	819	A
1	2A	822	U
1	2A	827	U
1	2A	832	G
1	2A	848	G
1	2A	857	C
1	2A	859	G
1	2A	866	A
1	2A	869	G
1	2A	874	G
1	2A	878	A
1	2A	879	G
1	2A	880	G
1	2A	884	C
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	890	A
1	2A	892	G
1	2A	893	C
1	2A	894	C
1	2A	895	U
1	2A	896	A
1	2A	898	C
1	2A	900	A
1	2A	901	A
1	2A	910	A
1	2A	915	C
1	2A	917	A
1	2A	932	G
1	2A	938	G
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	953	A
1	2A	958	U
1	2A	959	A
1	2A	961	C

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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	1003	G
1	2A	1010	A
1	2A	1012	U
1	2A	1013	C
1	2A	1017	G
1	2A	1022	G
1	2A	1025	G
1	2A	1033	U
1	2A	1038	C
1	2A	1041	C
1	2A	1042	G
1	2A	1043	C
1	2A	1114	G
1	2A	1116	C
1	2A	1117	G
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1139	G
1	2A	1142	U
1	2A	1143	A
1	2A	1151	G
1	2A	1155	A
1	2A	1167	U
1	2A	1169	G
1	2A	1171	G
1	2A	1179	C
1	2A	1210	A
1	2A	1211	U
1	2A	1212	G
1	2A	1229	G
1	2A	1236	G
1	2A	1239	G
1	2A	1244	G
1	2A	1247	A
1	2A	1248	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	2A	1253	A
1	2A	1256	G
1	2A	1265	A
1	2A	1271	G
1	2A	1272	A
1	2A	1277	G
1	2A	1300	U
1	2A	1301	A
1	2A	1314	C
1	2A	1333	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	1416	G
1	2A	1417	C
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	1451	C
1	2A	1455	G
1	2A	1460	A
1	2A	1461	G
1	2A	1463	C
1	2A	1467	C
1	2A	1471	A
1	2A	1482	G
1	2A	1490	A
1	2A	1493	C
1	2A	1497	U
1	2A	1508	A
1	2A	1509	C

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	2A	1509(A)	A
1	2A	1531	C
1	2A	1532	C
1	2A	1533	G
1	2A	1542	A
1	2A	1548	C
1	2A	1558	A
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1584	C
1	2A	1586	A
1	2A	1603	A
1	2A	1608	A
1	2A	1610	A
1	2A	1634	A
1	2A	1648	C
1	2A	1654	A
1	2A	1664	A
1	2A	1674	G
1	2A	1688	U
1	2A	1696	G
1	2A	1700	A
1	2A	1721	G
1	2A	1722	A
1	2A	1740	G
1	2A	1746	G
1	2A	1756	G
1	2A	1758	G
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A
1	2A	1776	G
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	1808	U
1	2A	1811	G
1	2A	1812	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	2A	1816	G
1	2A	1847	A
1	2A	1848	A
1	2A	1877	A
1	2A	1878	G
1	2A	1893	C
1	2A	1895	C
1	2A	1900	A
1	2A	1906	G
1	2A	1913	A
1	2A	1914	C
1	2A	1919	A
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	1960	A
1	2A	1963	U
1	2A	1965	C
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1984	G
1	2A	1992	G
1	2A	1993	U
1	2A	1996	C
1	2A	1997	G
1	2A	2020	A
1	2A	2023	G
1	2A	2031	A
1	2A	2032	G
1	2A	2033	A
1	2A	2036	C
1	2A	2043	C
1	2A	2049	G
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	2A	2062	A
1	2A	2067	G
1	2A	2069	G
1	2A	2092	U
1	2A	2093	G
1	2A	2096	U
1	2A	2099	U
1	2A	2100	G
1	2A	2108	C
1	2A	2109	U
1	2A	2110	G
1	2A	2111	C
1	2A	2112	G
1	2A	2115	G
1	2A	2116	G
1	2A	2119	A
1	2A	2120	G
1	2A	2121	G
1	2A	2122	U
1	2A	2125	G
1	2A	2126	A
1	2A	2127	G
1	2A	2129	C
1	2A	2131	G
1	2A	2132	U
1	2A	2133	G
1	2A	2134	A
1	2A	2135	A
1	2A	2137	C
1	2A	2138	C
1	2A	2140	C
1	2A	2142	C
1	2A	2146	C
1	2A	2150	U
1	2A	2153	G
1	2A	2156	G
1	2A	2157	G
1	2A	2158	A
1	2A	2161	C
1	2A	2162	G
1	2A	2164	C
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	2169	A
1	2A	2171	A
1	2A	2172	U
1	2A	2173	A
1	2A	2178	C
1	2A	2188	C
1	2A	2189	U
1	2A	2192	G
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2218	U
1	2A	2225	A
1	2A	2238	G
1	2A	2239	G
1	2A	2249	U
1	2A	2263	C
1	2A	2275	C
1	2A	2279	G
1	2A	2283	C
1	2A	2287	A
1	2A	2302	G
1	2A	2303	G
1	2A	2305	A
1	2A	2308	G
1	2A	2309	A
1	2A	2312	U
1	2A	2317	C
1	2A	2320	A
1	2A	2322	A
1	2A	2325	G
1	2A	2329	G
1	2A	2334	G
1	2A	2336	A
1	2A	2343	C
1	2A	2346	A
1	2A	2347	C
1	2A	2350	C
1	2A	2354	G
1	2A	2358	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	2A	2361	A
1	2A	2368	C
1	2A	2376	A
1	2A	2377	A
1	2A	2383	G
1	2A	2385	C
1	2A	2388	A
1	2A	2396	G
1	2A	2403	C
1	2A	2406	U
1	2A	2422	A
1	2A	2425	A
1	2A	2427	C
1	2A	2428	G
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	2448	A
1	2A	2459	A
1	2A	2468	G
1	2A	2469	A
1	2A	2476	A
1	2A	2478	A
1	2A	2480	C
1	2A	2483	C
1	2A	2490	G
1	2A	2491	U
1	2A	2494	G
1	2A	2499	C
1	2A	2502	G
1	2A	2504	U
1	2A	2505	G
1	2A	2506	U
1	2A	2518	A
1	2A	2520	C
1	2A	2529	G
1	2A	2530	A
1	2A	2549	G
1	2A	2554	U

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	2A	2555	U
1	2A	2566	A
1	2A	2567	G
1	2A	2572	A
1	2A	2582	G
1	2A	2602	A
1	2A	2611	U
1	2A	2612	C
1	2A	2629	A
1	2A	2630	G
1	2A	2634	G
1	2A	2638	G
1	2A	2646	C
1	2A	2662	A
1	2A	2663	G
1	2A	2689	U
1	2A	2702	U
1	2A	2703	C
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2718	G
1	2A	2726	U
1	2A	2733	A
1	2A	2739	U
1	2A	2748	A
1	2A	2751	G
1	2A	2759	G
1	2A	2764	A
1	2A	2765	A
1	2A	2766	G
1	2A	2778	A
1	2A	2779	U
1	2A	2804	C
1	2A	2807	G
1	2A	2811	G
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2835	A
1	2A	2839	G
1	2A	2872	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	2A	2876	G
1	2A	2879	C
1	2A	2883	A
1	2A	2886	G
1	2A	2892	A
1	2A	2894	G
1	2A	2895	U
1	2A	2897	U
2	2B	2	C
2	2B	4	C
2	2B	5	C
2	2B	7	G
2	2B	8	U
2	2B	9	G
2	2B	12	C
2	2B	13	A
2	2B	19	G
2	2B	20	C
2	2B	29	A
2	2B	32	C
2	2B	33	G
2	2B	35	U
2	2B	38	C
2	2B	42	C
2	2B	44	G
2	2B	53	A
2	2B	56	G
2	2B	63	G
2	2B	67	G
2	2B	69	G
2	2B	73	A
2	2B	75	G
2	2B	85	G
2	2B	88	C
2	2B	94	C
2	2B	108	U
2	2B	110	G
2	2B	114	C
2	2B	116	G
2	2B	118	G
2	2B	119	G
32	2a	7	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
32	2a	8	A
32	2a	9	G
32	2a	13	U
32	2a	30	U
32	2a	32	A
32	2a	39	G
32	2a	47	C
32	2a	48	C
32	2a	51	A
32	2a	54	C
32	2a	66	G
32	2a	70	G
32	2a	73	G
32	2a	78	G
32	2a	80	G
32	2a	88	A
32	2a	89	C
32	2a	101	A
32	2a	116	A
32	2a	121	C
32	2a	131	C
32	2a	142	G
32	2a	144	G
32	2a	151	A
32	2a	159	G
32	2a	163	C
32	2a	174	C
32	2a	182	U
32	2a	195	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	249	U
32	2a	250	A
32	2a	251	G
32	2a	266	G
32	2a	267	C
32	2a	279	A
32	2a	281	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
32	2a	289	G
32	2a	299	G
32	2a	300	A
32	2a	306	G
32	2a	316	G
32	2a	318	G
32	2a	319	G
32	2a	321	A
32	2a	322	C
32	2a	328	C
32	2a	332	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	366	C
32	2a	367	U
32	2a	372	C
32	2a	373	A
32	2a	397	A
32	2a	398	C
32	2a	404	U
32	2a	406	G
32	2a	412	A
32	2a	415	A
32	2a	421	U
32	2a	423	G
32	2a	424	G
32	2a	427	U
32	2a	428	G
32	2a	429	U
32	2a	433	C
32	2a	439	A
32	2a	442	C
32	2a	443	C
32	2a	452	A
32	2a	470	C
32	2a	484	G
32	2a	485	G
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	509	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
32	2a	510	A
32	2a	511	C
32	2a	513	C
32	2a	518	C
32	2a	521	G
32	2a	527	7MG
32	2a	531	U
32	2a	532	A
32	2a	533	A
32	2a	547	A
32	2a	559	A
32	2a	561	U
32	2a	562	C
32	2a	564	C
32	2a	565	U
32	2a	566	G
32	2a	572	A
32	2a	573	A
32	2a	576	G
32	2a	577	G
32	2a	581	G
32	2a	586	C
32	2a	596	C
32	2a	630	G
32	2a	650	G
32	2a	653	A
32	2a	657	G
32	2a	665	A
32	2a	671	G
32	2a	687	A
32	2a	688	G
32	2a	694	A
32	2a	695	A
32	2a	702	A
32	2a	703	G
32	2a	705	U
32	2a	721	G
32	2a	723	U
32	2a	724	G
32	2a	729	A
32	2a	731	G
32	2a	742	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
32	2a	749	C
32	2a	755	G
32	2a	777	A
32	2a	787	A
32	2a	790	A
32	2a	793	U
32	2a	794	A
32	2a	796	C
32	2a	815	A
32	2a	817	C
32	2a	821	G
32	2a	828	A
32	2a	836	G
32	2a	838	G
32	2a	839	U
32	2a	840	C
32	2a	841	U
32	2a	853	G
32	2a	855	G
32	2a	859	A
32	2a	870	U
32	2a	872	A
32	2a	873	A
32	2a	876	G
32	2a	885	G
32	2a	899	C
32	2a	902	G
32	2a	914	A
32	2a	916	G
32	2a	927	G
32	2a	931	C
32	2a	932	C
32	2a	934	C
32	2a	935	A
32	2a	936	C
32	2a	942	G
32	2a	960	U
32	2a	961	U
32	2a	965	A
32	2a	966	M2G
32	2a	968	A
32	2a	969	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
32	2a	971	G
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	979	C
32	2a	982	U
32	2a	984	C
32	2a	989	C
32	2a	992	U
32	2a	993	G
32	2a	996	A
32	2a	997	U
32	2a	998	G
32	2a	999	C
32	2a	1001(A)	G
32	2a	1002	G
32	2a	1003	G
32	2a	1004	A
32	2a	1005	A
32	2a	1006	C
32	2a	1009	G
32	2a	1011	G
32	2a	1020	U
32	2a	1022	G
32	2a	1024	G
32	2a	1025	U
32	2a	1026	G
32	2a	1027	C
32	2a	1028	C
32	2a	1030	C
32	2a	1030(A)	G
32	2a	1030(C)	G
32	2a	1031	G
32	2a	1032	G
32	2a	1035	A
32	2a	1037	C
32	2a	1039	C
32	2a	1040	U
32	2a	1042	G
32	2a	1046	A
32	2a	1053	G

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	2a	1055	A
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1076	C
32	2a	1077	G
32	2a	1081	G
32	2a	1085	U
32	2a	1087	G
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A
32	2a	1112	C
32	2a	1117	G
32	2a	1118	C
32	2a	1122	U
32	2a	1125	U
32	2a	1129	C
32	2a	1130	A
32	2a	1134	G
32	2a	1136	U
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1140	C
32	2a	1146	A
32	2a	1152	A
32	2a	1157	A
32	2a	1159	U
32	2a	1160	G
32	2a	1172	C
32	2a	1173	G
32	2a	1175	G
32	2a	1181	G
32	2a	1182	G
32	2a	1184	G
32	2a	1196	U
32	2a	1197	G
32	2a	1201	A
32	2a	1202	G
32	2a	1204	A
32	2a	1208	C

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
32	2a	1209	C
32	2a	1210	C
32	2a	1211	U
32	2a	1213	A
32	2a	1214	C
32	2a	1215	G
32	2a	1222	G
32	2a	1223	C
32	2a	1226	C
32	2a	1228	C
32	2a	1238	A
32	2a	1240	U
32	2a	1256	A
32	2a	1257	U
32	2a	1260	C
32	2a	1261	A
32	2a	1262	C
32	2a	1270	C
32	2a	1273	G
32	2a	1275	A
32	2a	1278	U
32	2a	1279	A
32	2a	1280	A
32	2a	1287	A
32	2a	1294	G
32	2a	1299	A
32	2a	1302	U
32	2a	1303	C
32	2a	1305	G
32	2a	1306	A
32	2a	1313	U
32	2a	1320	C
32	2a	1322	C
32	2a	1323	G
32	2a	1336	C
32	2a	1338	G
32	2a	1346	A
32	2a	1347	G
32	2a	1350	A
32	2a	1358	U
32	2a	1363	C
32	2a	1363(A)	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
32	2a	1368	G
32	2a	1388	C
32	2a	1394	A
32	2a	1397	C
32	2a	1406	U
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1447	A
32	2a	1452	C
32	2a	1456	G
32	2a	1492	A
32	2a	1499	A
32	2a	1503	A
32	2a	1504	G
32	2a	1506	U
32	2a	1507	A
32	2a	1508	G
32	2a	1517	G
32	2a	1520	G
32	2a	1529	G
32	2a	1530	G
32	2a	1531	A
32	2a	1532	U
53	2v	13	A
53	2v	14	A
53	2v	19	G
53	2v	24	C
54	2w	2	G
54	2w	3	G
54	2w	5	G
54	2w	8	4SU
54	2w	9	A
54	2w	10	G
54	2w	13	C
54	2w	14	A
54	2w	19	G
54	2w	22	G
54	2w	29	U
54	2w	32	C
54	2w	47	U
54	2w	48	C

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
54	2w	49	G
54	2w	51	C
54	2w	55	PSU
54	2w	56	C
54	2w	58	A
54	2w	59	U
54	2w	60	C
54	2w	62	C
54	2w	65	C
54	2w	68	C
54	2w	69	A
54	2w	70	C
54	2w	73	A
54	2w	74	C
54	2w	75	C
55	2x	4	G
55	2x	9	G
55	2x	13	C
55	2x	19	G
55	2x	20	U
55	2x	21	A
55	2x	34	C
55	2x	47	U
55	2x	48	C
55	2x	56	C
55	2x	57	A
55	2x	61	C
55	2x	67	C
55	2x	68	C
55	2x	76	A
54	2y	2	G
54	2y	5	G
54	2y	6	A
54	2y	7	U
54	2y	8	4SU
54	2y	9	A
54	2y	13	C
54	2y	15	G
54	2y	19	G
54	2y	24	G
54	2y	26	A
54	2y	30	C

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
54	2y	31	C
54	2y	32	C
54	2y	35	A
54	2y	38	A
54	2y	40	G
54	2y	41	A
54	2y	43	G
54	2y	45	G
54	2y	49	G
54	2y	51	C
54	2y	52	G
54	2y	53	G
54	2y	55	PSU
54	2y	57	G
54	2y	58	A
54	2y	59	U
54	2y	61	C
54	2y	69	A
54	2y	70	C
54	2y	73	A

All (42) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	266	G
1	1A	271(K)	U
1	1A	278	A
1	1A	362	U
1	1A	548	A
1	1A	827	U
1	1A	895	U
1	1A	1047	G
1	1A	1065	U
1	1A	1067	A
1	1A	1174	A
1	1A	1175	U
1	1A	1176	G
1	1A	1210	A
1	1A	1420	U
1	1A	1442	G
1	1A	1508	A
1	1A	1653	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	1A	1992	G
1	1A	2134	A
1	1A	2181	G
1	1A	2183	C
1	1A	2756	U
1	2A	228	A
1	2A	266	G
1	2A	271(M)	G
1	2A	277	C
1	2A	528	A
1	2A	614(B)	G
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	1653	G
1	2A	1790	C
1	2A	1913	A
1	2A	1992	G
1	2A	2119	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
32	UR3	1a	1498	32	14,22,23	0.74	0	15,32,35	0.66	0
43	0TD	1l	92	43	4,9,10	3.14	1 (25%)	3,11,13	11.35	1 (33%)
1	PSU	2A	1911	1	17,21,22	1.51	2 (11%)	20,30,33	3.17	6 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	PSU	1A	1917	1	17,21,22	1.63	2 (11%)	20,30,33	3.07	6 (30%)
55	5MC	1x	32	55	15,22,23	1.32	1 (6%)	19,32,35	1.39	3 (15%)
1	PSU	2A	1917	1,56	17,21,22	1.56	2 (11%)	20,30,33	3.14	6 (30%)
54	6MZ	1y	37	54	18,25,26	0.99	1 (5%)	16,36,39	2.21	4 (25%)
32	UR3	2a	1498	32	14,22,23	0.80	1 (7%)	15,32,35	0.70	0
32	7MG	2a	527	32,56	22,26,27	1.75	4 (18%)	28,39,42	2.74	9 (32%)
32	5MC	1a	1404	32	15,22,23	1.28	1 (6%)	19,32,35	1.36	3 (15%)
32	PSU	2a	516	32	17,21,22	1.45	2 (11%)	20,30,33	3.08	6 (30%)
32	5MC	2a	967	32	15,22,23	1.37	1 (6%)	19,32,35	1.33	3 (15%)
54	5MU	1y	54	54	15,22,23	1.06	1 (6%)	16,32,35	1.74	2 (12%)
1	PSU	1A	1911	1	17,21,22	1.54	3 (17%)	20,30,33	3.10	6 (30%)
1	PSU	1A	2605	1,56	17,21,22	1.53	3 (17%)	20,30,33	3.15	6 (30%)
32	2MG	2a	1207	32,56	19,26,27	1.25	2 (10%)	21,38,41	2.13	6 (28%)
32	PSU	1a	516	32,56	17,21,22	1.53	3 (17%)	20,30,33	3.03	6 (30%)
1	2MU	2A	2552	1,56	14,22,24	0.90	0	14,31,36	0.85	0
32	5MC	2a	1404	32	15,22,23	1.23	1 (6%)	19,32,35	1.52	4 (21%)
32	7MG	1a	527	32	22,26,27	1.77	3 (13%)	28,39,42	2.84	9 (32%)
54	4SU	1w	8	54	14,21,22	1.33	1 (7%)	15,30,33	1.42	2 (13%)
1	PSU	2A	2605	1	17,21,22	1.54	3 (17%)	20,30,33	3.17	6 (30%)
32	4OC	2a	1402	32,56	16,23,24	0.62	0	17,32,35	1.24	1 (5%)
1	5MU	1A	1939	1	15,22,23	1.07	1 (6%)	16,32,35	1.90	2 (12%)
32	MA6	2a	1518	32	19,26,27	0.99	1 (5%)	18,38,41	1.73	6 (33%)
32	MA6	1a	1518	32	19,26,27	0.99	1 (5%)	18,38,41	1.74	6 (33%)
54	CM0	2w	34	54	16,26,27	1.09	1 (6%)	18,37,40	1.93	4 (22%)
1	2MA	2A	2503	1	17,25,26	1.36	2 (11%)	19,37,40	2.13	3 (15%)
55	PSU	2x	55	55	17,21,22	1.47	2 (11%)	20,30,33	3.12	6 (30%)
54	6MZ	2w	37	54	18,25,26	0.96	1 (5%)	16,36,39	1.72	3 (18%)
1	4OC	1A	1920	1	15,22,24	0.64	0	17,31,35	1.59	2 (11%)
32	2MG	1a	1207	32,56	19,26,27	1.28	2 (10%)	21,38,41	2.42	8 (38%)
54	PSU	1w	55	54	17,21,22	1.37	2 (11%)	20,30,33	3.34	6 (30%)
32	5MC	2a	1407	32,56	15,22,23	1.31	1 (6%)	19,32,35	1.35	3 (15%)
1	5MC	2A	1962	1,56	15,22,23	1.32	1 (6%)	19,32,35	1.36	3 (15%)
32	5MC	1a	1407	32	15,22,23	1.34	1 (6%)	19,32,35	1.34	3 (15%)
32	5MC	1a	1400	32	15,22,23	1.32	1 (6%)	19,32,35	1.39	3 (15%)
32	4OC	1a	1402	32	16,23,24	0.67	0	17,32,35	1.15	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	OMG	2A	2251	1,55,56	18,26,27	1.21	2 (11%)	20,38,41	2.09	6 (30%)
1	4OC	2A	1920	1	15,22,24	0.64	0	17,31,35	1.47	2 (11%)
54	4SU	1y	8	54	14,21,22	1.24	1 (7%)	15,30,33	1.80	3 (20%)
32	MA6	2a	1519	32	19,26,27	0.99	1 (5%)	18,38,41	1.66	5 (27%)
1	OMG	1A	2251	1,55,56	18,26,27	1.15	2 (11%)	20,38,41	2.16	6 (30%)
1	2MU	1A	2552	1,56	14,22,24	0.86	0	14,31,36	0.68	1 (7%)
55	PSU	1x	55	55	17,21,22	1.58	2 (11%)	20,30,33	3.14	6 (30%)
54	4SU	2w	8	54	14,21,22	1.30	1 (7%)	15,30,33	1.33	2 (13%)
54	7MG	1w	46	54	22,26,27	1.80	4 (18%)	28,39,42	2.75	9 (32%)
1	5MC	2A	1942	1	15,22,23	1.30	1 (6%)	19,32,35	1.32	3 (15%)
54	5MU	1w	54	54	15,22,23	1.00	1 (6%)	16,32,35	1.85	2 (12%)
1	5MU	1A	1915	1	15,22,23	1.08	1 (6%)	16,32,35	2.01	1 (6%)
54	5MU	2y	54	54	15,22,23	1.03	1 (6%)	16,32,35	1.72	2 (12%)
1	5MC	1A	1962	1,56	15,22,23	1.29	1 (6%)	19,32,35	1.34	3 (15%)
1	5MU	2A	1915	1	15,22,23	1.07	1 (6%)	16,32,35	1.85	2 (12%)
54	PSU	1y	55	54	17,21,22	1.54	3 (17%)	20,30,33	3.14	6 (30%)
54	PSU	2w	55	54	17,21,22	1.33	2 (11%)	20,30,33	3.17	6 (30%)
55	4SU	1x	8	55	14,21,22	1.40	2 (14%)	15,30,33	2.22	2 (13%)
54	PSU	2y	55	54	17,21,22	1.60	3 (17%)	20,30,33	3.16	6 (30%)
54	6MZ	2y	37	54,32	18,25,26	0.95	1 (5%)	16,36,39	2.02	4 (25%)
54	7MG	2y	46	54	22,26,27	1.79	3 (13%)	28,39,42	3.15	11 (39%)
54	CM0	1w	34	54	16,26,27	1.07	2 (12%)	18,37,40	1.92	3 (16%)
32	M2G	1a	966	32	20,27,28	1.40	3 (15%)	22,40,43	2.14	5 (22%)
54	7MG	1y	46	54	22,26,27	1.81	3 (13%)	28,39,42	2.88	9 (32%)
54	4SU	2y	8	54	14,21,22	1.34	1 (7%)	15,30,33	1.40	3 (20%)
1	5MC	1A	1942	1	15,22,23	1.31	1 (6%)	19,32,35	1.34	3 (15%)
1	2MA	1A	2503	1,56	17,25,26	1.32	2 (11%)	19,37,40	2.14	4 (21%)
55	5MU	1x	54	55	15,22,23	1.04	1 (6%)	16,32,35	2.15	1 (6%)
1	5MU	2A	1939	1,56	15,22,23	1.08	1 (6%)	16,32,35	1.77	2 (12%)
54	6MZ	1w	37	54	18,25,26	0.96	1 (5%)	16,36,39	2.04	4 (25%)
32	5MC	1a	967	32	15,22,23	1.30	1 (6%)	19,32,35	1.32	3 (15%)
54	5MU	2w	54	54	15,22,23	1.04	1 (6%)	16,32,35	2.06	2 (12%)
54	CM0	1y	34	54	16,26,27	1.13	1 (6%)	18,37,40	1.90	4 (22%)
54	7MG	2w	46	54	22,26,27	1.81	4 (18%)	28,39,42	2.57	8 (28%)
32	M2G	2a	966	32	20,27,28	1.42	3 (15%)	22,40,43	2.17	7 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	MA6	1a	1519	32	19,26,27	1.04	1 (5%)	18,38,41	1.75	6 (33%)
55	5MC	2x	32	55	15,22,23	1.35	1 (6%)	19,32,35	1.35	3 (15%)
43	0TD	2l	92	43	4,9,10	3.09	1 (25%)	3,11,13	1.94	1 (33%)
55	4SU	2x	8	55	14,21,22	1.38	2 (14%)	15,30,33	2.09	2 (13%)
54	CM0	2y	34	54	16,26,27	1.14	2 (12%)	18,37,40	1.97	3 (16%)
55	5MU	2x	54	55	15,22,23	1.10	1 (6%)	16,32,35	1.94	2 (12%)
32	5MC	2a	1400	32	15,22,23	1.41	1 (6%)	19,32,35	1.42	3 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	UR3	1a	1498	32	-	1/5/25/26	0/2/2/2
43	0TD	1l	92	43	-	2/3/12/14	-
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/5/25/26	0/2/2/2
1	PSU	2A	1917	1,56	-	0/7/25/26	0/2/2/2
54	6MZ	1y	37	54	-	0/5/27/28	0/3/3/3
32	UR3	2a	1498	32	-	1/5/25/26	0/2/2/2
32	7MG	2a	527	32,56	-	3/7/37/38	0/3/3/3
32	5MC	1a	1404	32	-	0/5/25/26	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	2/5/25/26	0/2/2/2
54	5MU	1y	54	54	-	2/5/25/26	0/2/2/2
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	2605	1,56	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32,56	-	2/5/27/28	0/3/3/3
32	PSU	1a	516	32,56	-	0/7/25/26	0/2/2/2
1	2MU	2A	2552	1,56	-	0/7/27/28	0/2/2/2
32	5MC	2a	1404	32	-	0/5/25/26	0/2/2/2
32	7MG	1a	527	32	-	1/7/37/38	0/3/3/3
54	4SU	1w	8	54	-	0/5/25/26	0/2/2/2
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
32	4OC	2a	1402	32,56	-	2/9/29/30	0/2/2/2
1	5MU	1A	1939	1	-	0/5/25/26	0/2/2/2
32	MA6	2a	1518	32	-	1/7/29/30	0/3/3/3
32	MA6	1a	1518	32	-	1/7/29/30	0/3/3/3

Continued on next page...



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	CM0	2w	34	54	-	3/8/30/31	0/2/2/2
1	2MA	2A	2503	1	-	2/3/25/26	0/3/3/3
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
54	6MZ	2w	37	54	-	2/5/27/28	0/3/3/3
1	4OC	1A	1920	1	-	0/7/27/30	0/2/2/2
32	2MG	1a	1207	32,56	-	0/5/27/28	0/3/3/3
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
32	5MC	2a	1407	32,56	-	0/5/25/26	0/2/2/2
1	5MC	2A	1962	1,56	-	2/5/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/5/25/26	0/2/2/2
32	5MC	1a	1400	32	-	2/5/25/26	0/2/2/2
32	4OC	1a	1402	32	-	4/9/29/30	0/2/2/2
1	OMG	2A	2251	1,55,56	-	0/5/27/28	0/3/3/3
1	4OC	2A	1920	1	-	0/7/27/30	0/2/2/2
54	4SU	1y	8	54	-	2/5/25/26	0/2/2/2
32	MA6	2a	1519	32	-	4/7/29/30	0/3/3/3
1	OMG	1A	2251	1,55,56	-	0/5/27/28	0/3/3/3
1	2MU	1A	2552	1,56	-	0/7/27/28	0/2/2/2
55	PSU	1x	55	55	-	0/7/25/26	0/2/2/2
54	4SU	2w	8	54	-	1/5/25/26	0/2/2/2
54	7MG	1w	46	54	-	2/7/37/38	0/3/3/3
1	5MC	2A	1942	1	-	0/5/25/26	0/2/2/2
54	5MU	1w	54	54	-	0/5/25/26	0/2/2/2
1	5MU	1A	1915	1	-	3/5/25/26	0/2/2/2
54	5MU	2y	54	54	-	3/5/25/26	0/2/2/2
1	5MC	1A	1962	1,56	-	2/5/25/26	0/2/2/2
1	5MU	2A	1915	1	-	0/5/25/26	0/2/2/2
54	PSU	1y	55	54	-	0/7/25/26	0/2/2/2
54	PSU	2w	55	54	-	0/7/25/26	0/2/2/2
55	4SU	1x	8	55	-	0/5/25/26	0/2/2/2
54	PSU	2y	55	54	-	0/7/25/26	0/2/2/2
54	6MZ	2y	37	54,32	-	1/5/27/28	0/3/3/3
54	7MG	2y	46	54	-	2/7/37/38	0/3/3/3
54	CM0	1w	34	54	-	5/8/30/31	0/2/2/2
32	M2G	1a	966	32	-	4/7/29/30	0/3/3/3
54	7MG	1y	46	54	-	5/7/37/38	0/3/3/3
54	4SU	2y	8	54	-	1/5/25/26	0/2/2/2
1	5MC	1A	1942	1	-	0/5/25/26	0/2/2/2

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MA	1A	2503	1,56	-	2/3/25/26	0/3/3/3
55	5MU	1x	54	55	-	0/5/25/26	0/2/2/2
1	5MU	2A	1939	1,56	-	2/5/25/26	0/2/2/2
54	6MZ	1w	37	54	-	0/5/27/28	0/3/3/3
32	5MC	1a	967	32	-	2/5/25/26	0/2/2/2
54	5MU	2w	54	54	-	0/5/25/26	0/2/2/2
54	CM0	1y	34	54	-	1/8/30/31	0/2/2/2
54	7MG	2w	46	54	-	2/7/37/38	0/3/3/3
32	M2G	2a	966	32	-	4/7/29/30	0/3/3/3
32	MA6	1a	1519	32	-	3/7/29/30	0/3/3/3
55	5MC	2x	32	55	-	1/5/25/26	0/2/2/2
43	0TD	2l	92	43	-	1/3/12/14	-
55	4SU	2x	8	55	-	1/5/25/26	0/2/2/2
54	CM0	2y	34	54	-	4/8/30/31	0/2/2/2
55	5MU	2x	54	55	-	0/5/25/26	0/2/2/2
32	5MC	2a	1400	32	-	3/5/25/26	0/2/2/2

All (122) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-6.03	1.69	1.84
43	2l	92	0TD	CB-SB	-5.93	1.69	1.84
54	2w	46	7MG	C6-C5	5.44	1.48	1.41
54	1y	46	7MG	C6-C5	5.04	1.48	1.41
32	2a	1400	5MC	C5-C4	5.04	1.49	1.41
32	2a	527	7MG	C6-C5	5.00	1.48	1.41
32	2a	967	5MC	C5-C4	4.91	1.49	1.41
55	2x	32	5MC	C5-C4	4.82	1.48	1.41
54	1w	46	7MG	C6-C5	4.78	1.48	1.41
55	1x	32	5MC	C5-C4	4.76	1.48	1.41
54	2y	46	7MG	C5-C4	4.72	1.48	1.39
32	1a	1407	5MC	C5-C4	4.72	1.48	1.41
1	2A	1942	5MC	C5-C4	4.70	1.48	1.41
32	1a	1400	5MC	C5-C4	4.69	1.48	1.41
1	2A	1962	5MC	C5-C4	4.69	1.48	1.41
1	1A	1942	5MC	C5-C4	4.68	1.48	1.41
32	1a	967	5MC	C5-C4	4.68	1.48	1.41
1	2A	2503	2MA	C6-C5	4.64	1.48	1.41
32	1a	527	7MG	C6-C5	4.62	1.47	1.41
32	2a	1407	5MC	C5-C4	4.62	1.48	1.41

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1y	46	7MG	C5-C4	4.60	1.48	1.39
1	1A	1962	5MC	C5-C4	4.59	1.48	1.41
55	1x	55	PSU	C5-C1'	-4.59	1.48	1.52
1	1A	1917	PSU	C5-C1'	-4.58	1.48	1.52
32	1a	1404	5MC	C5-C4	4.54	1.48	1.41
1	1A	2503	2MA	C6-C5	4.53	1.48	1.41
54	2y	55	PSU	C5-C1'	-4.49	1.48	1.52
32	1a	527	7MG	C5-C4	4.48	1.47	1.39
54	2y	8	4SU	C4-S4	-4.45	1.59	1.67
54	1y	55	PSU	C5-C1'	-4.42	1.48	1.52
32	2a	1404	5MC	C5-C4	4.38	1.48	1.41
54	1w	46	7MG	C5-C4	4.37	1.47	1.39
54	2y	46	7MG	C6-C5	4.36	1.47	1.41
32	1a	1207	2MG	C6-C5	4.33	1.48	1.41
32	2a	527	7MG	C5-C4	4.30	1.47	1.39
54	2w	46	7MG	C5-C4	4.30	1.47	1.39
1	2A	1917	PSU	C5-C1'	-4.28	1.48	1.52
32	2a	966	M2G	C6-C5	4.24	1.48	1.41
32	2a	1207	2MG	C6-C5	4.23	1.48	1.41
1	2A	2605	PSU	C5-C1'	-4.17	1.48	1.52
32	1a	966	M2G	C6-C5	4.16	1.48	1.41
54	1w	8	4SU	C4-S4	-4.13	1.59	1.67
55	1x	8	4SU	C4-S4	-4.11	1.60	1.67
1	2A	2251	OMG	C6-C5	4.10	1.48	1.41
32	1a	516	PSU	C5-C1'	-4.03	1.48	1.52
54	1y	8	4SU	C4-S4	-4.01	1.60	1.67
54	2w	8	4SU	C4-S4	-4.01	1.60	1.67
1	1A	2605	PSU	C5-C1'	-3.94	1.48	1.52
1	1A	1911	PSU	C5-C1'	-3.89	1.48	1.52
55	2x	8	4SU	C4-S4	-3.88	1.60	1.67
1	1A	2251	OMG	C6-C5	3.78	1.47	1.41
32	1a	527	7MG	C5-N7	-3.77	1.33	1.39
1	2A	1911	PSU	C5-C1'	-3.76	1.49	1.52
54	2y	46	7MG	C5-N7	-3.71	1.33	1.39
55	2x	55	PSU	C5-C1'	-3.57	1.49	1.52
54	2y	34	CM0	C4-C5	3.57	1.49	1.40
55	2x	55	PSU	C4-C5	3.57	1.49	1.41
54	2w	34	CM0	C4-C5	3.50	1.48	1.40
32	2a	516	PSU	C4-C5	3.49	1.49	1.41
54	1y	34	CM0	C4-C5	3.49	1.48	1.40
1	1A	1911	PSU	C4-C5	3.48	1.48	1.41
1	2A	1915	5MU	C4-C5	3.46	1.48	1.41

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	1911	PSU	C4-C5	3.45	1.48	1.41
32	2a	516	PSU	C5-C1'	-3.44	1.49	1.52
32	2a	966	M2G	C2-N2	3.43	1.40	1.34
32	1a	966	M2G	C2-N2	3.42	1.40	1.34
1	2A	1917	PSU	C4-C5	3.42	1.48	1.41
54	1y	46	7MG	C5-N7	-3.42	1.34	1.39
1	1A	1915	5MU	C4-C5	3.41	1.48	1.41
1	2A	1939	5MU	C4-C5	3.39	1.48	1.41
54	2w	55	PSU	C4-C5	3.39	1.48	1.41
54	1w	34	CM0	C4-C5	3.39	1.48	1.40
55	2x	54	5MU	C4-C5	3.37	1.48	1.41
54	2y	54	5MU	C4-C5	3.36	1.48	1.41
54	1w	46	7MG	C5-N7	-3.35	1.34	1.39
32	1a	516	PSU	C4-C5	3.34	1.48	1.41
54	1y	54	5MU	C4-C5	3.34	1.48	1.41
1	1A	1917	PSU	C4-C5	3.32	1.48	1.41
54	2y	55	PSU	C4-C5	3.30	1.48	1.41
1	1A	1939	5MU	C4-C5	3.30	1.48	1.41
32	2a	527	7MG	C5-N7	-3.27	1.34	1.39
1	2A	2605	PSU	C4-C5	3.27	1.48	1.41
55	1x	54	5MU	C4-C5	3.24	1.48	1.41
54	2w	46	7MG	C5-N7	-3.21	1.34	1.39
54	1w	55	PSU	C4-C5	3.21	1.48	1.41
54	2w	54	5MU	C4-C5	3.19	1.48	1.41
55	1x	55	PSU	C4-C5	3.10	1.48	1.41
54	1w	54	5MU	C4-C5	3.10	1.48	1.41
1	1A	2605	PSU	C4-C5	3.07	1.48	1.41
54	1y	55	PSU	C4-C5	3.07	1.48	1.41
55	2x	8	4SU	C2-N3	-2.95	1.32	1.38
54	1w	55	PSU	C5-C1'	-2.92	1.49	1.52
55	1x	8	4SU	C2-N3	-2.85	1.32	1.38
54	2y	37	6MZ	C5-C4	2.68	1.48	1.40
54	2w	55	PSU	C5-C1'	-2.65	1.50	1.52
54	1w	37	6MZ	C5-C4	2.62	1.47	1.40
32	2a	1519	MA6	C5-C4	2.61	1.47	1.40
54	1y	37	6MZ	C5-C4	2.59	1.47	1.40
32	2a	1518	MA6	C5-C4	2.58	1.47	1.40
54	2w	37	6MZ	C5-C4	2.56	1.47	1.40
32	2a	966	M2G	C5-C4	2.55	1.47	1.40
54	1w	46	7MG	C4-N9	-2.55	1.33	1.38
32	2a	1207	2MG	C5-C4	2.52	1.47	1.40
32	1a	1518	MA6	C5-C4	2.51	1.47	1.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1a	1519	MA6	C5-C4	2.47	1.47	1.40
1	2A	2251	OMG	C5-C4	2.46	1.47	1.40
32	1a	1207	2MG	C5-C4	2.45	1.47	1.40
32	1a	966	M2G	C5-C4	2.42	1.47	1.40
1	1A	2251	OMG	C5-C4	2.32	1.47	1.40
1	2A	2503	2MA	C5-C4	2.30	1.47	1.40
54	2w	46	7MG	C4-N9	-2.27	1.34	1.38
1	1A	2503	2MA	C5-C4	2.23	1.46	1.40
1	1A	2605	PSU	C2-N3	-2.21	1.33	1.38
32	2a	527	7MG	C4-N9	-2.18	1.34	1.38
32	2a	1498	UR3	C4-N3	2.15	1.41	1.38
32	1a	516	PSU	O4'-C1'	-2.15	1.41	1.44
54	1y	55	PSU	O4'-C1'	-2.08	1.41	1.44
1	2A	2605	PSU	C2-N3	-2.06	1.34	1.38
1	1A	1911	PSU	O4'-C1'	-2.03	1.41	1.44
54	2y	55	PSU	O4'-C1'	-2.03	1.41	1.44
54	2y	34	CM0	C2-N3	-2.01	1.34	1.38
54	1w	34	CM0	C2-N3	-2.00	1.34	1.38

All (320) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	1l	92	0TD	CSB-SB-CB	-19.61	63.27	101.85
54	2y	46	7MG	N3-C4-N9	10.11	139.90	126.91
32	1a	527	7MG	N3-C4-N9	9.64	139.29	126.91
54	1y	46	7MG	N3-C4-N9	9.51	139.12	126.91
32	2a	527	7MG	N3-C4-N9	9.05	138.54	126.91
54	1w	55	PSU	N1-C2-N3	-8.80	121.43	128.43
1	1A	2605	PSU	N1-C2-N3	-8.78	121.45	128.43
54	1w	46	7MG	N3-C4-N9	8.78	138.19	126.91
54	2w	55	PSU	N1-C2-N3	-8.77	121.45	128.43
32	2a	516	PSU	N1-C2-N3	-8.76	121.47	128.43
1	2A	2605	PSU	N1-C2-N3	-8.71	121.51	128.43
1	2A	1911	PSU	N1-C2-N3	-8.52	121.66	128.43
55	2x	55	PSU	N1-C2-N3	-8.52	121.66	128.43
1	2A	1917	PSU	N1-C2-N3	-8.29	121.84	128.43
55	1x	55	PSU	N1-C2-N3	-8.27	121.86	128.43
1	1A	1911	PSU	N1-C2-N3	-8.26	121.86	128.43
32	1a	516	PSU	N1-C2-N3	-8.23	121.89	128.43
54	1y	55	PSU	N1-C2-N3	-8.20	121.91	128.43
54	2y	55	PSU	N1-C2-N3	-8.15	121.95	128.43
55	1x	54	5MU	C4-N3-C2	8.12	122.00	115.14

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2w	46	7MG	N3-C4-N9	8.02	137.22	126.91
1	1A	1917	PSU	N1-C2-N3	-8.01	122.07	128.43
54	1w	55	PSU	C4-N3-C2	7.52	121.49	115.14
1	1A	1915	5MU	C4-N3-C2	7.52	121.49	115.14
55	1x	8	4SU	C2-N3-C4	7.52	126.05	115.15
54	2w	54	5MU	C4-N3-C2	7.45	121.43	115.14
54	2w	55	PSU	C4-N3-C2	7.06	121.11	115.14
55	2x	54	5MU	C4-N3-C2	7.02	121.07	115.14
1	2A	1911	PSU	C4-N3-C2	6.91	120.97	115.14
55	2x	8	4SU	C2-N3-C4	6.87	125.11	115.15
1	1A	1911	PSU	C4-N3-C2	6.82	120.90	115.14
32	2a	516	PSU	C4-N3-C2	6.80	120.89	115.14
1	2A	1915	5MU	C4-N3-C2	6.79	120.88	115.14
1	1A	2605	PSU	C4-N3-C2	6.70	120.80	115.14
55	2x	55	PSU	C4-N3-C2	6.69	120.79	115.14
1	2A	2503	2MA	C2-N3-C4	6.60	120.88	115.52
1	1A	1917	PSU	C4-N3-C2	6.57	120.69	115.14
54	1w	54	5MU	C4-N3-C2	6.57	120.69	115.14
32	1a	516	PSU	C4-N3-C2	6.56	120.68	115.14
1	2A	2605	PSU	C4-N3-C2	6.55	120.67	115.14
1	2A	1917	PSU	C4-N3-C2	6.55	120.67	115.14
54	2y	34	CM0	C4-N3-C2	6.50	120.63	115.14
54	2y	55	PSU	C4-N3-C2	6.47	120.61	115.14
55	1x	55	PSU	C4-N3-C2	6.43	120.57	115.14
54	2w	34	CM0	C4-N3-C2	6.35	120.50	115.14
54	1y	55	PSU	C4-N3-C2	6.29	120.46	115.14
54	1w	34	CM0	C4-N3-C2	6.29	120.46	115.14
1	1A	1939	5MU	C4-N3-C2	6.28	120.44	115.14
54	1y	54	5MU	C4-N3-C2	6.24	120.41	115.14
54	2y	46	7MG	C6-N1-C2	6.23	125.83	115.93
54	1y	37	6MZ	C2-N1-C6	6.21	121.91	116.59
54	2y	54	5MU	C4-N3-C2	6.17	120.35	115.14
1	1A	2503	2MA	C2-N3-C4	6.15	120.52	115.52
1	2A	1939	5MU	C4-N3-C2	6.02	120.23	115.14
54	1w	37	6MZ	C2-N1-C6	5.92	121.67	116.59
54	1y	34	CM0	C4-N3-C2	5.79	120.03	115.14
54	2y	37	6MZ	C2-N1-C6	5.77	121.54	116.59
32	1a	527	7MG	C5-C4-N3	-5.69	117.19	126.49
54	2y	46	7MG	C5-C4-N3	-5.60	117.35	126.49
54	1w	46	7MG	N7-C8-N9	-5.57	95.42	103.38
1	2A	1917	PSU	C5-C4-N3	-5.55	118.21	125.36
54	1w	55	PSU	C5-C4-N3	-5.53	118.24	125.36

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1911	PSU	C5-C4-N3	-5.50	118.27	125.36
1	1A	1917	PSU	C5-C4-N3	-5.48	118.30	125.36
54	2w	37	6MZ	C2-N1-C6	5.44	121.25	116.59
54	2y	55	PSU	C5-C4-N3	-5.43	118.36	125.36
32	2a	527	7MG	N7-C8-N9	-5.39	95.67	103.38
32	2a	966	M2G	C6-N1-C2	5.38	122.59	116.18
54	1y	46	7MG	C5-C4-N3	-5.36	117.75	126.49
55	1x	55	PSU	C5-C4-N3	-5.34	118.48	125.36
1	2A	1911	PSU	C5-C4-N3	-5.31	118.52	125.36
32	1a	516	PSU	C5-C4-N3	-5.30	118.53	125.36
55	2x	55	PSU	C5-C4-N3	-5.20	118.66	125.36
54	1y	46	7MG	N7-C8-N9	-5.19	95.96	103.38
32	1a	966	M2G	C6-N1-C2	5.16	122.33	116.18
54	1y	55	PSU	C5-C4-N3	-5.16	118.71	125.36
54	2w	46	7MG	N7-C8-N9	-5.16	96.00	103.38
1	1A	2251	OMG	C2-N3-C4	5.14	121.23	115.36
54	2w	46	7MG	C5-C4-N3	-5.12	118.14	126.49
32	2a	516	PSU	C5-C4-N3	-5.08	118.81	125.36
54	2w	55	PSU	C5-C4-N3	-5.06	118.84	125.36
32	2a	527	7MG	C5-C4-N3	-5.06	118.22	126.49
1	1A	2503	2MA	C5-C6-N1	-5.05	117.76	123.06
32	1a	966	M2G	C2-N3-C4	5.05	121.01	115.28
32	2a	1207	2MG	C2-N3-C4	5.04	121.00	115.28
54	1y	46	7MG	C6-N1-C2	4.93	123.76	115.93
1	2A	2503	2MA	C5-C6-N1	-4.92	117.90	123.06
54	1y	8	4SU	C2-N3-C4	4.91	122.27	115.15
1	2A	2251	OMG	C2-N3-C4	4.87	120.91	115.36
1	1A	2605	PSU	C5-C4-N3	-4.86	119.10	125.36
32	1a	527	7MG	N7-C8-N9	-4.86	96.43	103.38
1	2A	2605	PSU	C5-C4-N3	-4.86	119.11	125.36
54	1w	55	PSU	C5-C1'-C2'	-4.83	106.69	115.32
32	1a	1207	2MG	C6-N1-C2	4.83	123.83	115.18
54	1w	46	7MG	C6-N1-C2	4.77	123.51	115.93
1	1A	1920	4OC	C2-N3-C4	4.76	121.17	116.34
32	1a	1207	2MG	C2-N3-C4	4.73	120.65	115.28
32	2a	966	M2G	C2-N3-C4	4.73	120.65	115.28
32	1a	1207	2MG	C5-C6-N1	-4.72	116.98	123.43
32	1a	527	7MG	C6-C5-C4	4.72	120.26	115.20
54	1w	46	7MG	C5-C4-N3	-4.66	118.89	126.49
54	2y	46	7MG	N7-C8-N9	-4.57	96.84	103.38
1	2A	1917	PSU	C5-C6-N1	-4.53	118.88	124.44
54	1y	55	PSU	C5-C6-N1	-4.51	118.90	124.44

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	1x	55	PSU	C5-C6-N1	-4.47	118.95	124.44
1	2A	1920	4OC	C2-N3-C4	4.45	120.85	116.34
32	2a	527	7MG	C6-N1-C2	4.44	122.99	115.93
54	2y	46	7MG	C6-C5-C4	4.39	119.91	115.20
54	1w	8	4SU	C2-N3-C4	4.27	121.34	115.15
1	1A	2605	PSU	C6-N1-C2	4.25	122.36	115.36
1	2A	2605	PSU	C6-N1-C2	4.24	122.36	115.36
54	2y	55	PSU	C5-C6-N1	-4.24	119.23	124.44
1	2A	2605	PSU	C5-C6-N1	-4.23	119.25	124.44
54	1y	46	7MG	C6-C5-C4	4.22	119.72	115.20
32	2a	966	M2G	C5-C6-N1	-4.21	117.67	123.43
32	1a	516	PSU	C5-C6-N1	-4.21	119.27	124.44
55	2x	55	PSU	C6-N1-C2	4.19	122.28	115.36
1	2A	1917	PSU	C6-N1-C2	4.19	122.27	115.36
55	2x	55	PSU	C5-C6-N1	-4.19	119.29	124.44
32	2a	516	PSU	C6-N1-C2	4.15	122.21	115.36
1	1A	2605	PSU	C5-C6-N1	-4.14	119.35	124.44
1	1A	1917	PSU	C5-C6-N1	-4.12	119.37	124.44
55	1x	55	PSU	C6-N1-C2	4.12	122.16	115.36
32	1a	527	7MG	C6-N1-C2	4.11	122.46	115.93
54	2y	46	7MG	C5-C6-N1	-4.11	114.69	123.14
54	1y	37	6MZ	C9-N6-C6	-4.10	119.34	122.87
1	2A	1911	PSU	C6-N1-C2	4.08	122.10	115.36
54	1y	55	PSU	C6-N1-C2	4.08	122.08	115.36
32	1a	1207	2MG	C6-C5-C4	-4.07	116.91	120.80
54	2y	55	PSU	C6-N1-C2	4.06	122.05	115.36
32	1a	516	PSU	C6-N1-C2	4.05	122.03	115.36
54	2w	46	7MG	C6-N1-C2	4.01	122.30	115.93
54	2y	55	PSU	C5-C1'-C2'	-3.99	108.20	115.32
1	1A	1911	PSU	C6-N1-C2	3.99	121.94	115.36
54	1y	55	PSU	C5-C1'-C2'	-3.98	108.22	115.32
1	1A	1917	PSU	C6-N1-C2	3.97	121.90	115.36
1	2A	2251	OMG	C5-C6-N1	-3.97	118.01	123.43
1	1A	2251	OMG	C6-N1-C2	3.96	122.21	115.93
32	2a	1207	2MG	C5-C6-N1	-3.93	118.05	123.43
32	1a	966	M2G	C5-C6-N1	-3.92	118.07	123.43
1	2A	2251	OMG	C6-N1-C2	3.91	122.15	115.93
1	2A	1911	PSU	C5-C6-N1	-3.91	119.63	124.44
54	2w	55	PSU	C6-N1-C2	3.91	121.81	115.36
55	2x	32	5MC	C2-N3-C4	3.90	120.72	116.02
1	1A	1911	PSU	C5-C6-N1	-3.89	119.66	124.44
32	1a	966	M2G	C6-C5-C4	-3.87	117.11	120.80

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	527	7MG	C6-C5-C4	3.86	119.34	115.20
32	2a	516	PSU	C5-C6-N1	-3.80	119.77	124.44
55	2x	8	4SU	C5-C4-N3	-3.80	118.75	123.83
54	2w	46	7MG	C6-C5-C4	3.79	119.27	115.20
32	2a	967	5MC	C2-N3-C4	3.78	120.58	116.02
32	2a	1207	2MG	C6-N1-C2	3.76	121.92	115.18
32	2a	1402	4OC	CM4-N4-C4	-3.76	119.74	122.97
32	2a	1404	5MC	C2-N3-C4	3.76	120.55	116.02
54	1w	46	7MG	C6-C5-C4	3.75	119.23	115.20
32	1a	1402	4OC	CM4-N4-C4	-3.74	119.76	122.97
54	2w	8	4SU	C2-N3-C4	3.73	120.56	115.15
54	1w	46	7MG	C5-C6-N1	-3.72	115.50	123.14
55	1x	32	5MC	C2-N3-C4	3.71	120.49	116.02
1	2A	1942	5MC	C2-N3-C4	3.70	120.49	116.02
54	1y	46	7MG	C5-C6-N1	-3.70	115.54	123.14
32	1a	1404	5MC	C2-N3-C4	3.68	120.46	116.02
54	1w	55	PSU	C6-N1-C2	3.67	121.42	115.36
32	1a	967	5MC	C2-N3-C4	3.67	120.45	116.02
1	1A	2251	OMG	C5-C6-N1	-3.65	118.43	123.43
1	2A	1962	5MC	C2-N3-C4	3.65	120.43	116.02
55	1x	55	PSU	C5-C1'-C2'	-3.63	108.85	115.32
55	1x	8	4SU	C5-C4-N3	-3.62	118.98	123.83
1	2A	2605	PSU	C5-C1'-C2'	-3.62	108.87	115.32
32	2a	1407	5MC	C2-N3-C4	3.62	120.38	116.02
1	1A	1942	5MC	C2-N3-C4	3.61	120.38	116.02
32	1a	1400	5MC	C2-N3-C4	3.60	120.36	116.02
1	1A	2251	OMG	C6-C5-C4	-3.59	117.37	120.80
54	2y	8	4SU	C2-N3-C4	3.56	120.31	115.15
1	2A	1911	PSU	C5-C1'-C2'	-3.56	108.98	115.32
32	2a	1404	5MC	N4-C4-N3	3.56	122.06	117.03
32	1a	1407	5MC	C2-N3-C4	3.55	120.30	116.02
32	2a	527	7MG	C5-C6-N1	-3.55	115.85	123.14
32	2a	1207	2MG	C6-C5-C4	-3.55	117.41	120.80
32	1a	527	7MG	C5-C6-N1	-3.53	115.89	123.14
1	1A	2251	OMG	N3-C2-N1	-3.52	122.53	127.22
32	2a	966	M2G	C6-C5-C4	-3.51	117.44	120.80
32	2a	1518	MA6	C9-N6-C6	-3.51	108.90	119.51
1	1A	1962	5MC	C2-N3-C4	3.49	120.23	116.02
32	1a	1519	MA6	C4-C5-N7	-3.48	105.77	109.40
1	2A	2251	OMG	C6-C5-C4	-3.48	117.47	120.80
54	2w	55	PSU	C5-C1'-C2'	-3.48	109.11	115.32
32	1a	1519	MA6	N3-C2-N1	-3.47	123.26	128.68

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1y	8	4SU	C5-C4-N3	-3.45	119.21	123.83
54	2w	46	7MG	C5-C6-N1	-3.45	116.05	123.14
54	1w	37	6MZ	C9-N6-C6	-3.44	119.91	122.87
32	2a	1518	MA6	N3-C2-N1	-3.41	123.35	128.68
32	2a	1400	5MC	C2-N3-C4	3.41	120.13	116.02
32	2a	1519	MA6	N1-C6-N6	3.39	120.63	117.06
54	2y	46	7MG	N2-C2-N3	3.36	122.48	117.25
32	1a	1518	MA6	C9-N6-C6	-3.34	109.41	119.51
54	1y	37	6MZ	N3-C2-N1	-3.31	123.50	128.68
32	1a	1518	MA6	N3-C2-N1	-3.30	123.53	128.68
1	1A	1917	PSU	C5-C1'-C2'	-3.27	109.48	115.32
54	2w	55	PSU	C5-C6-N1	-3.27	120.42	124.44
32	2a	1519	MA6	C4-C5-N7	-3.24	106.02	109.40
54	2y	37	6MZ	C4-C5-N7	-3.22	106.04	109.40
32	1a	1207	2MG	C4-C5-N7	-3.20	106.07	109.40
32	1a	1519	MA6	C9-N6-C6	-3.14	109.99	119.51
54	2y	37	6MZ	C9-N6-C6	-3.14	120.16	122.87
54	1w	34	CM0	O5-C5-C4	3.10	118.99	115.19
1	2A	2251	OMG	N3-C2-N1	-3.09	123.09	127.22
1	1A	1939	5MU	C5-C6-N1	-3.06	118.90	122.19
54	1w	37	6MZ	N3-C2-N1	-3.04	123.92	128.68
43	2l	92	0TD	CSB-SB-CB	-3.04	95.88	101.85
32	2a	1519	MA6	C9-N6-C6	-3.02	110.36	119.51
32	1a	1207	2MG	CM2-N2-C2	-3.01	119.95	123.59
32	1a	1518	MA6	C4-C5-N7	-2.99	106.28	109.40
1	2A	2503	2MA	C4-C5-N7	-2.98	106.29	109.40
32	2a	1519	MA6	N3-C2-N1	-2.95	124.07	128.68
54	1y	34	CM0	C7-O5-C5	2.93	123.52	117.76
32	2a	1207	2MG	CM2-N2-C2	-2.92	120.06	123.59
32	1a	1518	MA6	N1-C6-N6	2.91	120.12	117.06
32	1a	1404	5MC	N4-C4-N3	2.90	121.13	117.03
32	2a	1400	5MC	C5-C6-N1	-2.89	119.08	122.19
32	2a	1518	MA6	C4-C5-N7	-2.89	106.39	109.40
1	1A	1942	5MC	N4-C4-N3	2.88	121.10	117.03
54	1w	55	PSU	C5-C6-N1	-2.86	120.92	124.44
1	2A	1939	5MU	C5-C6-N1	-2.84	119.14	122.19
54	1w	37	6MZ	C4-C5-N7	-2.81	106.47	109.40
32	2a	1207	2MG	C4-C5-N7	-2.80	106.48	109.40
54	2w	8	4SU	C5-C4-N3	-2.80	120.08	123.83
1	1A	2605	PSU	C5-C1'-C2'	-2.80	110.33	115.32
54	1y	37	6MZ	C4-C5-N7	-2.78	106.50	109.40
54	2w	46	7MG	C8-N7-C5	2.76	116.11	108.94

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1911	PSU	C5-C1'-C2'	-2.75	110.42	115.32
54	1w	8	4SU	C5-C4-N3	-2.73	120.18	123.83
54	2y	37	6MZ	N3-C2-N1	-2.73	124.41	128.68
1	1A	1920	4OC	N4-C4-N3	2.72	120.80	116.49
54	2w	37	6MZ	N3-C2-N1	-2.71	124.44	128.68
54	1y	46	7MG	C8-N7-C5	2.71	115.98	108.94
1	1A	1962	5MC	N4-C4-N3	2.70	120.86	117.03
32	2a	527	7MG	C8-N7-C5	2.70	115.96	108.94
32	1a	1400	5MC	N4-C4-N3	2.68	120.81	117.03
1	2A	1962	5MC	N4-C4-N3	2.67	120.80	117.03
54	1w	46	7MG	C8-N7-C5	2.65	115.82	108.94
54	2y	46	7MG	C5-C4-N9	-2.64	102.74	106.44
1	2A	1942	5MC	N4-C4-N3	2.62	120.73	117.03
32	1a	1407	5MC	N4-C4-N3	2.62	120.73	117.03
32	2a	1518	MA6	N1-C6-N6	2.61	119.80	117.06
32	1a	527	7MG	C8-N7-C5	2.60	115.71	108.94
54	2w	34	CM0	C5-C4-N3	-2.59	119.11	122.66
54	1y	8	4SU	C6-N1-C2	-2.59	117.09	121.20
32	2a	1407	5MC	N4-C4-N3	2.58	120.68	117.03
1	1A	2251	OMG	C4-C5-N7	-2.58	106.71	109.40
54	2y	34	CM0	O5-C5-C4	2.57	118.34	115.19
54	2w	34	CM0	O5-C5-C4	2.56	118.33	115.19
32	1a	967	5MC	N4-C4-N3	2.56	120.65	117.03
1	2A	2251	OMG	C4-C5-N7	-2.55	106.74	109.40
32	1a	1518	MA6	C10-N6-C9	-2.55	107.92	116.12
32	1a	966	M2G	C4-C5-N7	-2.54	106.75	109.40
32	2a	966	M2G	N3-C2-N2	2.53	119.75	117.18
54	1w	46	7MG	C5-C4-N9	-2.51	102.92	106.44
32	2a	1518	MA6	C10-N6-C9	-2.50	108.05	116.12
55	1x	32	5MC	N4-C4-N3	2.50	120.57	117.03
54	2y	34	CM0	C5-C4-N3	-2.49	119.24	122.66
32	1a	1207	2MG	N3-C2-N1	-2.49	122.30	126.23
54	1w	54	5MU	C5-C6-N1	-2.46	119.54	122.19
32	1a	1400	5MC	C5-C6-N1	-2.46	119.54	122.19
54	2y	46	7MG	C8-N7-C5	2.46	115.33	108.94
1	2A	1917	PSU	C5-C1'-C2'	-2.45	110.94	115.32
1	1A	2503	2MA	C4-C5-N7	-2.44	106.86	109.40
1	2A	1920	4OC	N4-C4-N3	2.41	120.30	116.49
54	2y	46	7MG	C2-N3-C4	2.39	120.50	113.89
55	2x	55	PSU	C5-C1'-C2'	-2.38	111.08	115.32
55	2x	32	5MC	N4-C4-N3	2.37	120.38	117.03
54	2y	46	7MG	N1-C2-N3	-2.37	121.70	125.42

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1y	46	7MG	C5-C4-N9	-2.37	103.12	106.44
32	2a	966	M2G	C4-C5-N7	-2.36	106.94	109.40
54	1y	34	CM0	C5-C4-N3	-2.35	119.44	122.66
1	1A	1962	5MC	C5-C6-N1	-2.32	119.70	122.19
54	2w	46	7MG	C2-N3-C4	2.31	120.28	113.89
54	1w	34	CM0	C5-C4-N3	-2.30	119.50	122.66
32	2a	527	7MG	C5-C4-N9	-2.29	103.23	106.44
32	1a	516	PSU	O4'-C1'-C2'	2.28	108.35	104.66
54	1y	46	7MG	C2-N3-C4	2.26	120.15	113.89
32	1a	1407	5MC	C5-C6-N1	-2.25	119.77	122.19
32	1a	527	7MG	C2-N3-C4	2.24	120.07	113.89
54	2w	54	5MU	C5-C6-N1	-2.23	119.79	122.19
32	2a	967	5MC	C5-C6-N1	-2.22	119.80	122.19
32	1a	1518	MA6	C10-N6-C6	-2.22	112.80	119.51
54	2y	8	4SU	C3'-C2'-C1'	2.21	104.31	100.98
54	2w	37	6MZ	C4-C5-N7	-2.21	107.09	109.40
32	2a	1400	5MC	N4-C4-N3	2.21	120.15	117.03
32	2a	1404	5MC	CM5-C5-C4	-2.20	119.50	121.72
32	2a	527	7MG	C2-N3-C4	2.18	119.92	113.89
1	2A	1915	5MU	C5-C6-N1	-2.17	119.85	122.19
1	1A	2503	2MA	C1'-N9-C4	-2.16	122.84	126.64
55	1x	32	5MC	C5-C6-N1	-2.16	119.87	122.19
55	2x	54	5MU	C5-C6-N1	-2.16	119.87	122.19
1	2A	1962	5MC	C5-C6-N1	-2.15	119.88	122.19
54	1w	46	7MG	C2-N3-C4	2.15	119.83	113.89
32	1a	1207	2MG	N2-C2-N3	2.14	119.01	116.96
32	2a	1407	5MC	C5-C6-N1	-2.13	119.89	122.19
32	1a	1404	5MC	C5-C6-N1	-2.13	119.90	122.19
32	2a	966	M2G	CM1-N2-C2	-2.12	119.27	121.29
54	2y	54	5MU	C5-C6-N1	-2.10	119.93	122.19
32	1a	527	7MG	C5-C4-N9	-2.10	103.51	106.44
54	1y	34	CM0	O5-C5-C4	2.09	117.75	115.19
32	2a	967	5MC	N4-C4-N3	2.09	119.99	117.03
54	1y	54	5MU	C5-C6-N1	-2.09	119.94	122.19
54	2y	8	4SU	C5-C4-N3	-2.08	121.04	123.83
32	1a	967	5MC	C5-C6-N1	-2.08	119.95	122.19
1	1A	1942	5MC	C5-C6-N1	-2.08	119.96	122.19
32	2a	1404	5MC	C5-C6-N1	-2.07	119.96	122.19
32	1a	1519	MA6	N1-C6-N6	2.06	119.23	117.06
32	1a	1519	MA6	C1'-N9-C4	-2.05	123.04	126.64
55	2x	32	5MC	C5-C6-N1	-2.05	119.99	122.19
32	2a	1518	MA6	C10-N6-C6	-2.04	113.32	119.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1519	MA6	C10-N6-C6	-2.04	113.33	119.51
1	1A	2552	2MU	C5-C4-N3	-2.03	118.84	123.31
32	1a	1519	MA6	C10-N6-C6	-2.02	113.40	119.51
1	2A	1942	5MC	C5-C6-N1	-2.02	120.02	122.19
32	2a	516	PSU	O4'-C1'-C2'	2.01	107.92	104.66
54	2w	34	CM0	C7-O5-C5	2.01	121.71	117.76

There are no chirality outliers.

All (94) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	1498	UR3	O4'-C1'-N1-C6
32	2a	1402	4OC	O4'-C4'-C5'-O5'
32	2a	1498	UR3	O4'-C1'-N1-C6
54	1y	54	5MU	C3'-C4'-C5'-O5'
54	1y	54	5MU	O4'-C4'-C5'-O5'
32	2a	1207	2MG	C3'-C4'-C5'-O5'
54	2w	37	6MZ	N1-C6-N6-C9
1	2A	1962	5MC	O4'-C1'-N1-C6
1	2A	1962	5MC	C2'-C1'-N1-C6
32	1a	1400	5MC	O4'-C4'-C5'-O5'
43	2l	92	0TD	CG-CB-SB-CSB
32	1a	1402	4OC	N3-C4-N4-CM4
32	1a	1402	4OC	C5-C4-N4-CM4
54	1y	8	4SU	C2'-C1'-N1-C6
54	1y	8	4SU	O4'-C1'-N1-C6
32	2a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
54	2w	8	4SU	C2'-C1'-N1-C6
54	1w	46	7MG	O4'-C4'-C5'-O5'
54	1w	46	7MG	C3'-C4'-C5'-O5'
54	2y	8	4SU	C2'-C1'-N1-C6
1	1A	1915	5MU	C2'-C1'-N1-C6
1	1A	1915	5MU	C3'-C4'-C5'-O5'
54	2y	54	5MU	C2'-C1'-N1-C6
54	2y	54	5MU	C3'-C4'-C5'-O5'
1	1A	1962	5MC	O4'-C1'-N1-C6
1	1A	1962	5MC	C2'-C1'-N1-C6
54	2y	46	7MG	C2'-C1'-N9-C8
54	1w	34	CM0	C4-C5-O5-C7
54	1y	46	7MG	C4'-C5'-O5'-P
54	1y	46	7MG	C3'-C4'-C5'-O5'

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
1	2A	1939	5MU	C2'-C1'-N1-C6
1	2A	1939	5MU	O4'-C1'-N1-C6
32	1a	967	5MC	O4'-C4'-C5'-O5'
32	1a	967	5MC	C3'-C4'-C5'-O5'
32	2a	966	M2G	N1-C2-N2-CM1
32	2a	966	M2G	N1-C2-N2-CM2
32	2a	966	M2G	N3-C2-N2-CM1
32	2a	966	M2G	N3-C2-N2-CM2
32	1a	1519	MA6	C5-C6-N6-C10
55	2x	32	5MC	C2'-C1'-N1-C6
55	2x	8	4SU	C2'-C1'-N1-C6
54	2y	34	CM0	C4-C5-O5-C7
32	2a	1400	5MC	O4'-C1'-N1-C6
32	2a	1400	5MC	C2'-C1'-N1-C6
32	2a	1402	4OC	C3'-C4'-C5'-O5'
32	2a	1207	2MG	O4'-C4'-C5'-O5'
32	1a	1400	5MC	C3'-C4'-C5'-O5'
1	1A	1915	5MU	O4'-C4'-C5'-O5'
54	2y	54	5MU	O4'-C4'-C5'-O5'
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	967	5MC	O4'-C4'-C5'-O5'
32	1a	1402	4OC	O4'-C4'-C5'-O5'
54	2y	46	7MG	C2'-C1'-N9-C4
32	2a	527	7MG	C4'-C5'-O5'-P
32	1a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	527	7MG	C3'-C4'-C5'-O5'
54	1w	34	CM0	O4'-C4'-C5'-O5'
54	1y	46	7MG	O4'-C4'-C5'-O5'
32	1a	1518	MA6	C5-C6-N6-C10
54	1w	34	CM0	C6-C5-O5-C7
54	1w	34	CM0	C8-C7-O5-C5
32	2a	527	7MG	O4'-C4'-C5'-O5'
54	2y	34	CM0	C6-C5-O5-C7
54	1y	34	CM0	C4-C5-O5-C7
54	2w	37	6MZ	C5-C6-N6-C9
54	1w	34	CM0	C3'-C4'-C5'-O5'
54	2w	34	CM0	C8-C7-O5-C5
32	1a	966	M2G	N1-C2-N2-CM2
54	1y	46	7MG	C2'-C1'-N9-C8
54	2w	46	7MG	C2'-C1'-N9-C8
54	2w	34	CM0	C4-C5-O5-C7
32	1a	966	M2G	N1-C2-N2-CM1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
32	1a	966	M2G	N3-C2-N2-CM2
54	2w	34	CM0	C6-C5-O5-C7
32	2a	967	5MC	C3'-C4'-C5'-O5'
32	1a	1402	4OC	C3'-C4'-C5'-O5'
32	2a	1518	MA6	C5-C6-N6-C10
32	2a	1519	MA6	C5-C6-N6-C10
32	1a	966	M2G	N3-C2-N2-CM1
1	2A	2503	2MA	O4'-C4'-C5'-O5'
1	2A	2503	2MA	C4'-C5'-O5'-P
1	1A	2503	2MA	C4'-C5'-O5'-P
32	2a	1519	MA6	C4'-C5'-O5'-P
32	1a	527	7MG	C4'-C5'-O5'-P
54	2y	37	6MZ	C4'-C5'-O5'-P
54	2y	34	CM0	C8-C7-O5-C5
43	1l	92	0TD	CA-CB-SB-CSB
54	1y	46	7MG	O4'-C1'-N9-C8
54	2w	46	7MG	O4'-C1'-N9-C8
32	2a	1400	5MC	O4'-C4'-C5'-O5'
43	1l	92	0TD	CG-CB-SB-CSB
1	1A	2503	2MA	O4'-C4'-C5'-O5'
54	2y	34	CM0	O4'-C4'-C5'-O5'

There are no ring outliers.

12 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2A	1917	PSU	1	0
1	2A	2552	2MU	2	0
1	2A	2605	PSU	1	0
1	1A	1939	5MU	1	0
1	2A	2503	2MA	1	0
1	2A	2251	OMG	1	0
1	2A	1920	4OC	1	0
1	1A	2251	OMG	1	0
1	1A	2552	2MU	1	0
1	2A	1942	5MC	1	0
1	2A	1915	5MU	2	0
1	1A	1942	5MC	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2761 ligands modelled in this entry, 2757 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
57	ERY	1A	4074	-	53,53,53	0.93	2 (3%)	82,82,82	1.73	23 (28%)
59	SF4	1d	302	35	0,12,12	0.00	-	-		
59	SF4	2d	302	35	0,12,12	0.00	-	-		
57	ERY	2A	3875	-	53,53,53	0.93	2 (3%)	82,82,82	1.65	16 (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
57	ERY	1A	4074	-	-	5/72/107/107	0/3/3/3
59	SF4	1d	302	35	-	-	0/6/5/5
59	SF4	2d	302	35	-	-	0/6/5/5
57	ERY	2A	3875	-	-	12/72/107/107	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	2A	3875	ERY	O2-C1	4.88	1.45	1.34
57	1A	4074	ERY	O2-C1	4.85	1.45	1.34
57	1A	4074	ERY	O2-C13	-2.12	1.42	1.46
57	2A	3875	ERY	O2-C13	-2.05	1.42	1.46

All (39) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	1A	4074	ERY	C25-C24-C23	4.73	116.78	109.97
57	1A	4074	ERY	O5-C16-C15	-4.27	106.11	112.96
57	2A	3875	ERY	C13-O2-C1	-4.04	111.00	118.18
57	2A	3875	ERY	O5-C16-C15	-4.00	106.55	112.96
57	2A	3875	ERY	O2-C1-C2	3.93	120.18	111.56
57	2A	3875	ERY	O5-C16-C17	3.91	109.61	103.81
57	2A	3875	ERY	C26-C25-C24	3.65	116.86	110.46
57	1A	4074	ERY	O7-C5-C6	3.50	110.71	106.39
57	1A	4074	ERY	O2-C1-C2	3.42	119.08	111.56
57	2A	3875	ERY	C16-C15-C14	-3.38	109.22	115.07
57	2A	3875	ERY	C25-C24-C23	3.36	114.80	109.97
57	1A	4074	ERY	C15-C16-C17	3.33	113.64	107.67
57	1A	4074	ERY	C22-C23-C24	3.26	114.52	109.19
57	1A	4074	ERY	O3-C3-C4	3.12	111.98	108.22
57	1A	4074	ERY	C26-C25-C24	3.09	115.87	110.46
57	2A	3875	ERY	C12-C11-C10	-3.09	112.55	116.43
57	1A	4074	ERY	C13-O2-C1	-3.03	112.80	118.18
57	2A	3875	ERY	C34-C10-C11	-2.95	110.71	114.38
57	1A	4074	ERY	C6-C5-C4	-2.92	109.92	114.05
57	1A	4074	ERY	O4-C18-C21	2.91	112.99	106.70
57	2A	3875	ERY	C25-C24-N1	-2.88	107.52	115.67
57	1A	4074	ERY	C22-O9-C26	-2.75	108.56	112.91
57	1A	4074	ERY	O5-C16-C17	2.72	107.84	103.81
57	2A	3875	ERY	O4-C18-C21	2.66	112.44	106.70
57	2A	3875	ERY	O7-C5-C6	2.54	109.53	106.39
57	1A	4074	ERY	C16-C17-C18	2.53	115.01	111.14
57	1A	4074	ERY	C7-C8-C9	-2.46	109.09	113.32
57	2A	3875	ERY	C20-O5-C16	2.45	122.66	117.55
57	1A	4074	ERY	C6-C7-C8	-2.43	110.19	115.38
57	1A	4074	ERY	O2-C1-O1	-2.40	119.46	123.94
57	2A	3875	ERY	C22-O9-C26	-2.39	109.12	112.91
57	1A	4074	ERY	C20-O5-C16	2.36	122.48	117.55
57	2A	3875	ERY	O2-C1-O1	-2.35	119.54	123.94
57	1A	4074	ERY	C25-C24-N1	-2.25	109.32	115.67
57	2A	3875	ERY	C22-C23-C24	2.20	112.79	109.19
57	1A	4074	ERY	C14-O4-C18	2.18	119.72	113.84
57	1A	4074	ERY	C16-C15-C14	-2.13	111.37	115.07
57	1A	4074	ERY	C2-C3-C4	-2.08	107.02	113.05
57	1A	4074	ERY	C22-O7-C5	-2.02	112.75	116.25

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	2A	3875	ERY	C9-C10-C11-C12
57	2A	3875	ERY	C34-C10-C11-C12
57	2A	3875	ERY	C15-C16-O5-C20
57	2A	3875	ERY	C17-C16-O5-C20
57	2A	3875	ERY	C19-C16-O5-C20
57	1A	4074	ERY	C15-C16-O5-C20
57	1A	4074	ERY	C17-C16-O5-C20
57	1A	4074	ERY	C19-C16-O5-C20
57	2A	3875	ERY	C25-C24-N1-C29
57	1A	4074	ERY	C25-C24-N1-C29
57	2A	3875	ERY	C34-C10-C11-O12
57	2A	3875	ERY	C9-C10-C11-O12
57	2A	3875	ERY	C33-C8-C9-O11
57	2A	3875	ERY	C32-C6-C7-C8
57	1A	4074	ERY	C30-C2-C3-C4
57	2A	3875	ERY	C34-C10-C9-C8
57	2A	3875	ERY	C7-C8-C9-O11

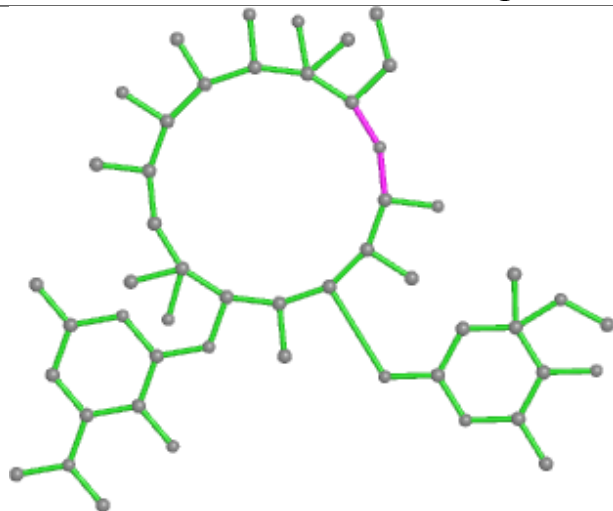
There are no ring outliers.

2 monomers are involved in 6 short contacts:

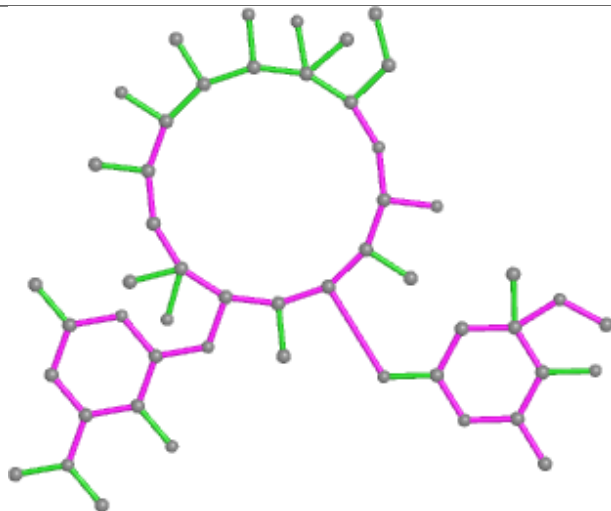
Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	1A	4074	ERY	3	0
57	2A	3875	ERY	3	0

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

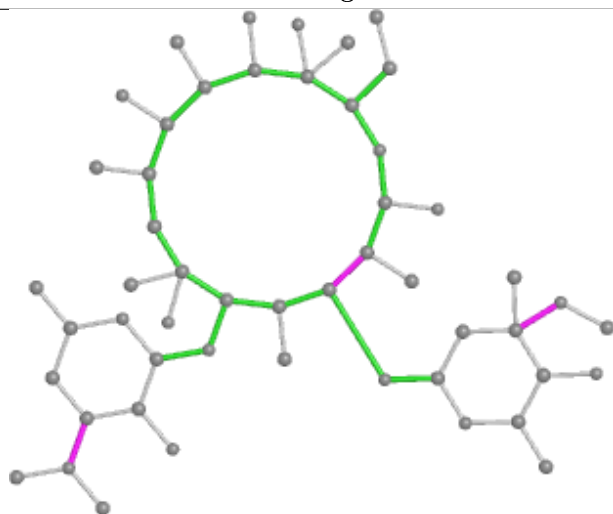
## Ligand ERY 1A 4074



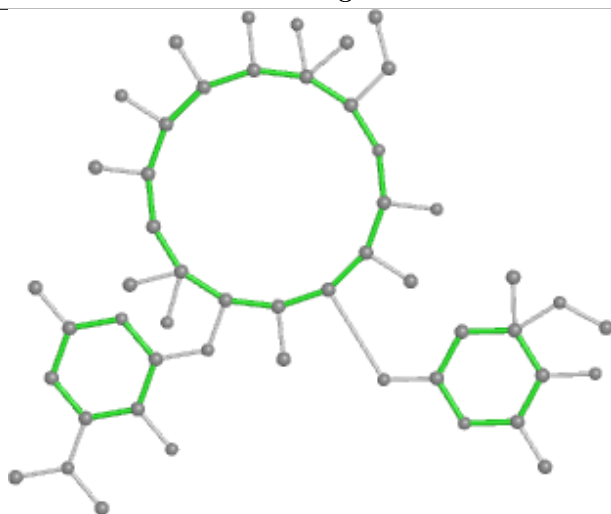
Bond lengths



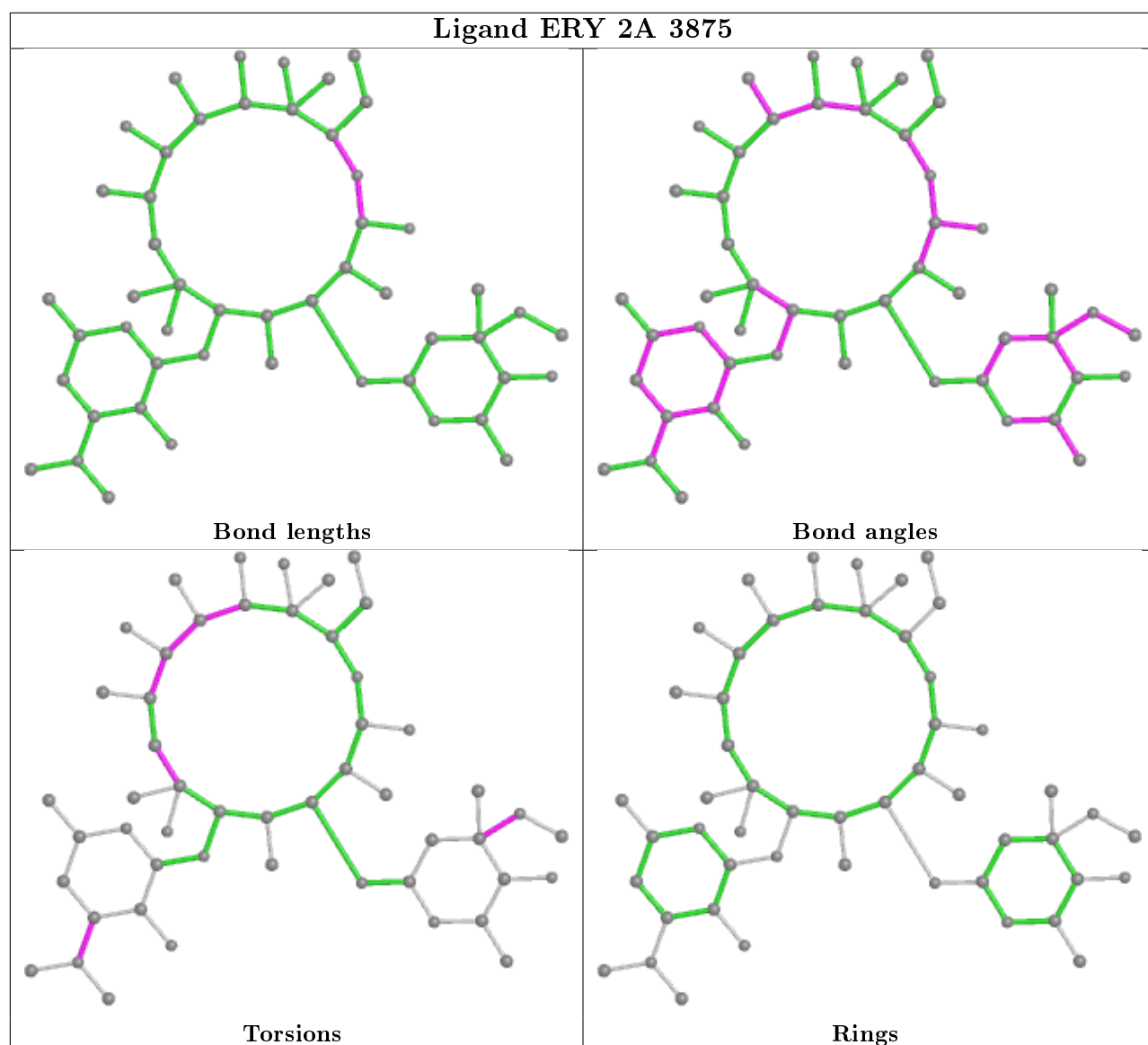
Bond angles



Torsions



Rings



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	1A	2860/2915 (98%)	0.08	12 (0%) 92 92	10, 28, 83, 100	0
1	2A	2789/2915 (95%)	0.00	9 (0%) 94 94	28, 51, 82, 99	0
2	1B	120/121 (99%)	-0.10	0 100 100	19, 42, 58, 77	0
2	2B	120/121 (99%)	-0.11	0 100 100	53, 72, 81, 86	0
3	1D	275/276 (99%)	0.03	1 (0%) 92 92	13, 30, 43, 72	0
3	2D	275/276 (99%)	0.64	15 (5%) 25 20	25, 44, 58, 68	0
4	1E	204/206 (99%)	0.08	0 100 100	11, 33, 48, 71	0
4	2E	204/206 (99%)	0.32	5 (2%) 57 54	27, 54, 65, 72	0
5	1F	203/210 (96%)	0.17	1 (0%) 91 90	13, 33, 57, 76	0
5	2F	203/210 (96%)	0.41	8 (3%) 39 34	29, 56, 70, 79	0
6	1G	181/182 (99%)	0.02	1 (0%) 89 89	32, 51, 66, 76	0
6	2G	181/182 (99%)	0.95	27 (14%) 2 1	61, 72, 79, 89	0
7	1H	174/180 (96%)	-0.13	0 100 100	27, 44, 55, 61	0
7	2H	174/180 (96%)	1.15	34 (19%) 1 1	62, 73, 81, 89	0
8	1I	146/148 (98%)	-0.10	0 100 100	39, 62, 73, 79	0
8	2I	146/148 (98%)	0.22	8 (5%) 25 20	45, 65, 77, 83	0
9	1N	140/140 (100%)	0.01	0 100 100	14, 32, 49, 60	0
9	2N	140/140 (100%)	0.74	16 (11%) 5 3	43, 58, 69, 77	0
10	1O	122/122 (100%)	0.23	0 100 100	22, 33, 51, 56	0
10	2O	122/122 (100%)	0.67	10 (8%) 11 8	36, 52, 62, 70	0
11	1P	149/150 (99%)	0.25	3 (2%) 65 62	13, 38, 59, 67	0
11	2P	149/150 (99%)	0.42	8 (5%) 25 21	34, 56, 71, 86	0
12	1Q	141/141 (100%)	0.14	1 (0%) 87 87	20, 34, 46, 70	0
12	2Q	141/141 (100%)	0.89	16 (11%) 5 3	42, 58, 68, 75	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	1R	118/118 (100%)	0.11	0 100 100	16, 26, 38, 56	0
13	2R	118/118 (100%)	0.45	5 (4%) 36 31	32, 46, 56, 66	0
14	1S	110/112 (98%)	-0.05	0 100 100	29, 41, 53, 56	0
14	2S	110/112 (98%)	0.38	4 (3%) 42 37	56, 67, 75, 78	0
15	1T	131/146 (89%)	0.09	0 100 100	26, 38, 56, 70	0
15	2T	131/146 (89%)	0.37	4 (3%) 49 44	43, 55, 68, 76	0
16	1U	116/118 (98%)	0.21	1 (0%) 84 84	13, 21, 38, 53	0
16	2U	116/118 (98%)	0.59	6 (5%) 27 22	35, 56, 65, 71	0
17	1V	101/101 (100%)	-0.01	0 100 100	16, 29, 48, 57	0
17	2V	101/101 (100%)	0.55	7 (6%) 16 12	42, 61, 71, 76	0
18	1W	112/113 (99%)	0.06	0 100 100	13, 22, 37, 61	0
18	2W	112/113 (99%)	0.57	11 (9%) 7 5	33, 43, 56, 79	0
19	1X	95/96 (98%)	-0.06	0 100 100	16, 31, 46, 64	0
19	2X	95/96 (98%)	0.81	11 (11%) 4 3	34, 53, 63, 78	0
20	1Y	107/110 (97%)	0.04	0 100 100	23, 40, 58, 71	0
20	2Y	107/110 (97%)	0.85	15 (14%) 2 2	45, 60, 74, 81	0
21	1Z	154/206 (74%)	0.31	2 (1%) 77 76	31, 53, 75, 81	0
21	2Z	160/206 (77%)	0.60	10 (6%) 20 15	60, 72, 83, 87	0
22	10	83/85 (97%)	0.40	6 (7%) 15 11	19, 29, 53, 72	0
22	20	83/85 (97%)	1.18	15 (18%) 1 1	43, 57, 68, 75	0
23	11	97/98 (98%)	0.17	2 (2%) 63 60	15, 37, 62, 70	0
23	21	97/98 (98%)	0.69	7 (7%) 15 11	37, 50, 63, 70	0
24	12	70/72 (97%)	0.14	0 100 100	25, 37, 49, 65	0
24	22	70/72 (97%)	0.30	3 (4%) 35 30	45, 60, 70, 71	0
25	13	59/60 (98%)	0.07	0 100 100	15, 27, 55, 70	0
25	23	59/60 (98%)	1.22	11 (18%) 1 1	49, 58, 68, 75	0
26	14	69/71 (97%)	-0.05	0 100 100	48, 67, 79, 85	0
26	24	69/71 (97%)	0.57	8 (11%) 4 3	69, 79, 86, 90	0
27	15	59/60 (98%)	0.06	0 100 100	11, 22, 40, 53	0
27	25	59/60 (98%)	0.27	2 (3%) 45 39	33, 43, 59, 68	0
28	16	53/54 (98%)	-0.05	0 100 100	24, 35, 49, 57	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	26	53/54 (98%)	0.63	5 (9%) 8 5	42, 53, 64, 69	0
29	17	48/49 (97%)	0.17	2 (4%) 36 31	14, 20, 43, 59	0
29	27	48/49 (97%)	1.09	6 (12%) 3 2	25, 36, 57, 75	0
30	18	64/65 (98%)	0.23	1 (1%) 72 70	20, 26, 33, 47	0
30	28	64/65 (98%)	0.85	6 (9%) 8 5	38, 49, 58, 63	0
31	19	37/37 (100%)	0.16	0 100 100	22, 32, 44, 53	0
31	29	37/37 (100%)	1.47	12 (32%) 0 0	51, 61, 71, 75	0
32	1a	1488/1521 (97%)	-0.06	4 (0%) 94 94	28, 60, 83, 97	0
32	2a	1491/1521 (98%)	0.05	16 (1%) 80 80	45, 68, 87, 97	0
33	1b	231/256 (90%)	0.31	8 (3%) 44 38	54, 69, 78, 88	0
33	2b	231/256 (90%)	1.21	53 (22%) 0 0	60, 77, 86, 92	0
34	1c	206/239 (86%)	0.93	28 (13%) 3 2	53, 65, 74, 81	0
34	2c	206/239 (86%)	1.32	61 (29%) 0 0	58, 75, 83, 100	0
35	1d	208/209 (99%)	0.27	7 (3%) 45 39	52, 64, 72, 80	0
35	2d	208/209 (99%)	0.38	6 (2%) 51 47	43, 60, 68, 79	0
36	1e	148/162 (91%)	0.42	8 (5%) 25 21	48, 58, 66, 71	0
36	2e	148/162 (91%)	0.78	14 (9%) 8 5	58, 69, 77, 83	0
37	1f	100/101 (99%)	0.04	1 (1%) 82 81	45, 59, 67, 70	0
37	2f	100/101 (99%)	-0.07	1 (1%) 82 81	53, 63, 69, 74	0
38	1g	155/156 (99%)	0.34	12 (7%) 13 10	52, 62, 72, 80	0
38	2g	155/156 (99%)	0.72	22 (14%) 2 2	58, 70, 79, 88	0
39	1h	137/138 (99%)	0.44	9 (6%) 18 14	48, 58, 67, 70	0
39	2h	137/138 (99%)	0.69	12 (8%) 10 6	55, 67, 74, 75	0
40	1i	127/128 (99%)	0.98	20 (15%) 2 1	51, 68, 78, 86	0
40	2i	127/128 (99%)	1.95	55 (43%) 0 0	60, 76, 83, 88	0
41	1j	97/105 (92%)	0.69	11 (11%) 5 3	56, 70, 79, 84	0
41	2j	96/105 (91%)	1.47	31 (32%) 0 0	65, 75, 84, 89	0
42	1k	114/129 (88%)	0.80	14 (12%) 4 2	36, 57, 67, 71	0
42	2k	114/129 (88%)	0.99	18 (15%) 2 1	50, 65, 73, 77	0
43	1l	121/132 (91%)	0.09	1 (0%) 86 85	41, 52, 63, 70	0
43	2l	121/132 (91%)	0.44	7 (5%) 23 18	49, 62, 72, 75	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	1m	123/126 (97%)	0.23	4 (3%) 46 41	49, 61, 73, 82	0
44	2m	122/126 (96%)	1.34	26 (21%) 0 0	64, 75, 84, 89	0
45	1n	60/61 (98%)	0.99	9 (15%) 2 1	52, 62, 70, 75	0
45	2n	60/61 (98%)	2.68	39 (65%) 0 0	68, 76, 82, 84	0
46	1o	88/89 (98%)	0.10	2 (2%) 60 57	42, 55, 68, 73	0
46	2o	88/89 (98%)	0.33	1 (1%) 80 80	53, 64, 74, 78	0
47	1p	82/88 (93%)	1.28	17 (20%) 1 0	50, 62, 74, 76	0
47	2p	82/88 (93%)	0.51	3 (3%) 41 36	48, 59, 66, 78	0
48	1q	99/105 (94%)	0.41	5 (5%) 28 23	42, 55, 67, 73	0
48	2q	99/105 (94%)	0.55	7 (7%) 16 12	54, 63, 72, 77	0
49	1r	68/88 (77%)	0.32	3 (4%) 34 29	47, 58, 68, 73	0
49	2r	68/88 (77%)	0.33	1 (1%) 73 72	57, 62, 72, 76	0
50	1s	83/93 (89%)	0.15	2 (2%) 59 56	52, 63, 72, 77	0
50	2s	83/93 (89%)	0.81	10 (12%) 4 3	66, 76, 83, 92	0
51	1t	96/106 (90%)	0.41	4 (4%) 36 31	45, 61, 69, 72	0
51	2t	96/106 (90%)	0.55	9 (9%) 8 5	44, 60, 74, 79	0
52	1u	23/27 (85%)	1.03	5 (21%) 0 0	57, 63, 67, 72	0
52	2u	23/27 (85%)	2.50	13 (56%) 0 0	65, 74, 78, 79	0
53	1v	13/27 (48%)	0.77	1 (7%) 13 10	40, 63, 82, 88	0
53	2v	13/27 (48%)	1.12	4 (30%) 0 0	61, 75, 87, 90	0
54	1w	67/76 (88%)	0.99	10 (14%) 2 1	54, 83, 92, 98	0
54	1y	68/76 (89%)	0.52	4 (5%) 22 17	33, 86, 92, 98	0
54	2w	67/76 (88%)	1.88	27 (40%) 0 0	65, 89, 93, 98	0
54	2y	67/76 (88%)	1.04	10 (14%) 2 1	50, 89, 94, 96	0
55	1x	72/77 (93%)	-0.02	0 100 100	36, 61, 72, 78	0
55	2x	72/77 (93%)	0.05	1 (1%) 75 74	49, 73, 82, 92	0
All	All	20879/21754 (95%)	0.30	973 (4%) 31 27	10, 56, 81, 100	0

All (973) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	2m	124	PRO	13.8
45	2n	25	VAL	9.7

Continued on next page...



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
44	2m	102	ARG	8.8
44	2m	6	GLY	8.7
44	2m	123	ALA	8.4
33	2b	165	VAL	8.4
22	10	5	LYS	7.6
45	2n	39	LEU	7.5
12	2Q	104	PHE	7.2
44	2m	5	ALA	7.2
22	10	7	LEU	7.0
40	1i	106	ALA	6.9
52	2u	14	TRP	6.4
41	2j	58	ASP	6.2
33	2b	187	LEU	6.1
54	2w	1	G	6.1
22	20	2	ALA	6.1
34	2c	56	ASP	6.0
52	2u	2	GLY	6.0
45	2n	38	GLY	6.0
29	27	48	LYS	5.9
40	2i	17	VAL	5.9
38	2g	82	GLY	5.9
41	2j	49	VAL	5.9
40	2i	7	THR	5.8
45	2n	37	PHE	5.8
33	2b	163	PHE	5.6
22	10	6	GLY	5.5
36	2e	31	LEU	5.5
38	2g	80	VAL	5.5
33	2b	70	PHE	5.4
34	1c	200	ALA	5.4
6	2G	28	VAL	5.3
7	2H	100	GLY	5.3
29	27	47	ARG	5.2
45	2n	34	TYR	5.2
6	2G	34	LEU	5.1
45	2n	7	ILE	5.1
38	2g	79	ARG	5.1
34	2c	15	THR	5.1
34	2c	157	ILE	5.0
34	2c	184	TYR	4.9
34	2c	80	GLY	4.9
44	1m	123	ALA	4.8

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
34	1c	179	ARG	4.8
22	20	6	GLY	4.8
40	2i	110	GLU	4.7
42	2k	90	GLY	4.7
44	2m	122	LYS	4.7
36	2e	13	ILE	4.7
45	2n	42	ILE	4.7
54	2w	71	C	4.7
54	2w	72	C	4.7
34	2c	201	TYR	4.7
41	2j	63	PHE	4.7
45	2n	11	LYS	4.7
40	1i	113	LYS	4.6
6	2G	140	ILE	4.6
31	29	37	GLY	4.6
52	2u	6	ARG	4.5
32	2a	1030(B)	C	4.5
1	2A	2146	C	4.5
19	2X	92	LEU	4.5
22	20	7	LEU	4.5
45	2n	44	LEU	4.5
33	2b	81	VAL	4.5
33	2b	197	VAL	4.5
54	2w	4	U	4.5
26	24	49	PHE	4.5
34	2c	202	ILE	4.4
40	2i	19	LEU	4.4
33	2b	120	ALA	4.4
33	2b	31	TYR	4.4
40	2i	115	GLY	4.4
9	2N	10	GLU	4.4
34	2c	206	GLU	4.4
7	2H	103	LEU	4.4
34	1c	12	LEU	4.4
3	2D	217	ARG	4.4
45	2n	29	ARG	4.4
40	2i	26	VAL	4.3
34	1c	206	GLU	4.3
42	2k	50	TYR	4.3
54	2w	73	A	4.3
41	2j	55	LYS	4.3
1	1A	2145	C	4.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
41	2j	60	ARG	4.3
51	2t	24	LEU	4.3
54	2w	76	A	4.2
54	2w	56	C	4.2
33	2b	186	ALA	4.2
38	2g	85	TYR	4.2
40	2i	125	TYR	4.2
20	2Y	48	ALA	4.2
49	1r	78	LEU	4.2
33	1b	231	GLU	4.2
29	17	46	VAL	4.1
25	23	51	ALA	4.1
25	23	2	PRO	4.1
44	2m	120	LYS	4.1
41	2j	47	PHE	4.1
34	2c	199	LYS	4.1
38	1g	156	TRP	4.1
40	2i	15	ALA	4.1
54	2w	31	C	4.0
40	2i	9	ARG	4.0
50	2s	38	SER	4.0
42	2k	89	ALA	4.0
40	2i	65	VAL	4.0
7	2H	113	VAL	4.0
41	2j	50	ILE	4.0
20	2Y	57	GLN	4.0
24	22	1	MET	3.9
54	2y	36	C	3.9
34	1c	113	ALA	3.9
1	1A	2141	G	3.9
38	2g	81	GLY	3.9
44	1m	56	LEU	3.9
53	2v	24	C	3.9
8	2l	38	LEU	3.9
45	2n	10	ALA	3.9
29	27	46	VAL	3.9
40	2i	83	ARG	3.9
33	2b	97	TRP	3.9
33	2b	214	ILE	3.8
34	2c	198	VAL	3.8
36	2e	84	PHE	3.8
40	2i	18	PHE	3.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
31	29	13	LYS	3.8
9	2N	45	ASN	3.8
34	2c	167	TRP	3.8
40	2i	77	ILE	3.8
44	2m	4	ILE	3.8
54	1w	70	C	3.8
44	1m	124	PRO	3.8
41	2j	48	THR	3.8
34	2c	186	PHE	3.8
34	2c	188	LEU	3.8
39	2h	133	LEU	3.8
7	2H	102	ALA	3.7
40	2i	79	LEU	3.7
40	2i	114	TYR	3.7
40	1i	65	VAL	3.7
7	2H	72	ILE	3.7
10	2O	1	MET	3.7
41	2j	62	HIS	3.7
33	2b	101	MET	3.6
40	2i	80	GLY	3.6
21	2Z	172	ALA	3.6
34	2c	173	VAL	3.6
49	2r	85	LEU	3.6
51	1t	14	LYS	3.6
34	2c	160	ALA	3.6
23	2l	46	LEU	3.6
54	2y	33	U	3.6
44	1m	2	ALA	3.6
20	2Y	46	LYS	3.6
40	2i	5	TYR	3.6
52	2u	17	THR	3.6
25	23	60	GLU	3.6
33	2b	201	ILE	3.6
34	2c	53	ALA	3.6
14	2S	32	LEU	3.6
6	2G	142	PRO	3.6
54	1w	56	C	3.6
54	2w	3	G	3.6
34	2c	4	LYS	3.5
9	2N	1	MET	3.5
36	2e	12	LEU	3.5
47	1p	42	ARG	3.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
22	20	38	VAL	3.5
52	2u	5	ASP	3.5
40	2i	36	TYR	3.5
32	1a	1036	G	3.5
23	1l	2	SER	3.5
40	1i	42	ARG	3.5
40	2i	27	THR	3.5
45	2n	36	PHE	3.5
41	2j	91	PRO	3.5
33	2b	48	MET	3.5
33	2b	92	TYR	3.5
33	2b	215	LEU	3.5
7	2H	101	ARG	3.5
34	2c	60	ALA	3.5
34	1c	13	GLY	3.4
39	1h	2	LEU	3.4
45	2n	6	LEU	3.4
23	2l	62	VAL	3.4
33	2b	71	VAL	3.4
34	1c	39	ILE	3.4
40	2i	33	PHE	3.4
43	2l	29	GLY	3.4
44	2m	104	ARG	3.4
53	2v	12	A	3.4
41	2j	65	LEU	3.4
7	2H	115	VAL	3.4
22	20	5	LYS	3.4
40	1i	111	ARG	3.4
45	2n	53	LEU	3.4
34	2c	180	ALA	3.4
45	2n	50	LYS	3.4
33	2b	164	VAL	3.4
39	2h	83	ILE	3.4
42	2k	87	THR	3.4
52	2u	15	ARG	3.4
7	2H	56	SER	3.4
42	2k	121	PRO	3.4
44	2m	9	ILE	3.4
38	1g	84	ASN	3.4
45	2n	60	SER	3.4
44	2m	121	LYS	3.4
42	2k	25	TYR	3.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
32	2a	1220	G	3.4
47	1p	1	MET	3.4
51	2t	72	LEU	3.3
41	2j	53	PRO	3.3
3	2D	51	VAL	3.3
52	2u	22	ARG	3.3
40	1i	110	GLU	3.3
7	2H	145	ALA	3.3
34	1c	185	GLY	3.3
34	2c	205	GLY	3.3
52	1u	17	THR	3.3
38	2g	156	TRP	3.3
21	2Z	83	PRO	3.3
51	2t	9	ASN	3.3
44	2m	66	LEU	3.3
6	2G	39	ILE	3.3
47	1p	36	ILE	3.3
33	2b	200	ILE	3.3
41	2j	51	ARG	3.3
45	2n	59	ALA	3.3
33	2b	184	VAL	3.3
45	2n	8	GLU	3.3
32	2a	1202	G	3.3
34	2c	179	ARG	3.2
36	2e	11	ILE	3.2
54	2w	40	G	3.2
25	23	47	VAL	3.2
34	2c	174	PRO	3.2
45	2n	31	ARG	3.2
54	1y	20	G	3.2
55	2x	70	G	3.2
38	2g	3	ARG	3.2
9	2N	44	PRO	3.2
54	2w	2	G	3.2
34	1c	8	ILE	3.2
6	2G	159	VAL	3.2
9	2N	140	VAL	3.2
5	2F	55	GLY	3.2
33	2b	202	PRO	3.2
22	20	45	PHE	3.2
45	2n	32	SER	3.2
17	2V	94	LEU	3.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
20	2Y	44	ILE	3.2
44	2m	25	ILE	3.2
22	20	3	HIS	3.2
6	2G	12	TYR	3.2
38	2g	40	ALA	3.1
44	2m	92	HIS	3.1
38	1g	85	TYR	3.1
41	1j	8	LEU	3.1
16	1U	117	GLN	3.1
7	2H	47	GLU	3.1
9	2N	82	LEU	3.1
34	1c	10	PHE	3.1
33	2b	99	GLY	3.1
40	2i	117	HIS	3.1
50	2s	80	TYR	3.1
53	1v	24	C	3.1
33	2b	185	ILE	3.1
6	2G	115	ARG	3.1
54	2w	75	C	3.1
31	29	25	VAL	3.1
54	2w	70	C	3.1
34	1c	57	ILE	3.1
40	2i	14	VAL	3.1
44	2m	7	VAL	3.1
45	2n	61	TRP	3.1
9	2N	85	ILE	3.1
32	2a	973	G	3.1
40	1i	15	ALA	3.0
31	29	15	LYS	3.0
7	2H	123	PHE	3.0
6	2G	48	GLU	3.0
39	1h	90	GLY	3.0
41	1j	98	ILE	3.0
19	2X	83	VAL	3.0
24	22	60	LEU	3.0
39	2h	2	LEU	3.0
3	1D	276	LYS	3.0
31	29	2	LYS	3.0
33	2b	118	LEU	3.0
34	1c	33	LEU	3.0
45	2n	4	LYS	3.0
40	2i	21	PRO	3.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
23	2l	2	SER	3.0
42	1k	98	LEU	3.0
31	29	33	LYS	3.0
43	2l	64	TYR	3.0
44	2m	88	ARG	3.0
9	2N	26	LEU	3.0
12	2Q	17	LEU	3.0
47	1p	45	THR	3.0
44	2m	100	GLY	3.0
31	29	26	ILE	3.0
34	2c	14	ILE	3.0
38	1g	153	HIS	3.0
32	2a	1030(A)	G	3.0
32	2a	1034	G	3.0
22	20	75	LEU	3.0
35	1d	139	ARG	3.0
36	2e	82	VAL	3.0
11	1P	105	LEU	3.0
50	1s	71	LEU	3.0
40	2i	66	ARG	3.0
9	2N	73	THR	3.0
26	24	46	GLN	2.9
52	2u	13	ILE	2.9
12	2Q	97	VAL	2.9
36	1e	82	VAL	2.9
33	2b	16	HIS	2.9
35	1d	157	LEU	2.9
40	2i	116	LYS	2.9
40	2i	92	TYR	2.9
41	2j	61	GLU	2.9
54	2w	57	G	2.9
35	2d	49	ARG	2.9
33	2b	135	GLN	2.9
3	2D	38	LYS	2.9
17	2V	71	LEU	2.9
34	2c	155	GLY	2.9
51	1t	18	GLN	2.9
41	1j	44	VAL	2.9
41	2j	92	THR	2.9
54	2y	28	C	2.9
13	2R	10	LEU	2.9
25	23	26	LEU	2.9

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
34	2c	159	GLY	2.9
54	2y	53	G	2.9
40	2i	62	TYR	2.9
38	1g	79	ARG	2.9
12	2Q	103	MET	2.9
25	23	28	LEU	2.9
33	2b	49	GLU	2.9
36	1e	119	LEU	2.9
41	2j	85	LEU	2.9
20	2Y	65	ALA	2.9
19	2X	18	TYR	2.9
41	2j	96	ILE	2.9
22	20	76	GLY	2.9
42	1k	84	VAL	2.9
5	2F	89	VAL	2.9
23	11	98	LEU	2.9
19	2X	69	TYR	2.8
7	2H	99	VAL	2.8
38	2g	39	ALA	2.8
44	2m	70	LEU	2.8
40	2i	127	LYS	2.8
21	1Z	171	ILE	2.8
12	2Q	34	LEU	2.8
34	2c	33	LEU	2.8
11	2P	1	MET	2.8
45	2n	2	ALA	2.8
50	2s	79	THR	2.8
18	2W	103	ILE	2.8
43	2l	7	ILE	2.8
30	28	2	PRO	2.8
19	2X	89	ILE	2.8
23	21	10	LYS	2.8
32	2a	1026	G	2.8
34	1c	207	VAL	2.8
45	2n	56	VAL	2.8
41	1j	66	ARG	2.8
6	2G	137	GLU	2.8
12	2Q	1	MET	2.8
18	2W	92	ARG	2.8
34	2c	77	ILE	2.8
50	2s	82	GLY	2.8
45	1n	25	VAL	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
7	2H	124	GLU	2.8
33	2b	132	LYS	2.8
35	1d	165	MET	2.8
38	2g	73	MET	2.8
44	2m	65	LYS	2.8
34	2c	124	ILE	2.8
44	2m	97	PRO	2.8
52	2u	11	GLY	2.8
8	2I	12	LEU	2.8
29	27	1	MET	2.8
20	2Y	58	GLY	2.8
47	1p	78	GLY	2.8
28	26	54	ILE	2.8
38	2g	4	ARG	2.8
10	2O	99	PHE	2.7
22	20	69	PHE	2.7
45	2n	23	ARG	2.7
1	1A	1059	G	2.7
50	2s	12	ASP	2.7
14	2S	58	LEU	2.7
6	2G	169	ALA	2.7
40	2i	52	ALA	2.7
54	2w	74	C	2.7
32	2a	1357	A	2.7
5	2F	90	PHE	2.7
17	2V	75	PHE	2.7
41	2j	54	PHE	2.7
42	1k	21	ILE	2.7
47	2p	9	PHE	2.7
33	2b	183	PRO	2.7
40	2i	82	ALA	2.7
10	2O	65	THR	2.7
19	2X	45	THR	2.7
45	2n	15	LYS	2.7
6	2G	152	LEU	2.7
34	2c	17	ASP	2.7
34	2c	197	GLY	2.7
42	2k	119	CYS	2.7
54	1w	69	A	2.7
39	2h	10	LEU	2.7
40	1i	50	LEU	2.7
35	1d	164	ALA	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
52	1u	18	TYR	2.7
23	21	37	ILE	2.7
22	20	4	LYS	2.7
54	1w	72	C	2.7
7	2H	105	LEU	2.7
34	2c	7	PRO	2.7
41	2j	10	GLY	2.7
36	2e	105	VAL	2.7
20	2Y	93	GLY	2.7
42	2k	88	GLY	2.7
12	2Q	130	LYS	2.7
41	2j	11	PHE	2.7
34	2c	8	ILE	2.7
1	2A	1509	C	2.7
4	2E	116	VAL	2.7
31	29	5	ALA	2.7
21	2Z	150	LEU	2.7
34	2c	170	GLN	2.7
3	2D	275	LYS	2.7
35	2d	198	VAL	2.7
41	2j	52	GLY	2.7
18	2W	81	ALA	2.7
34	1c	193	TYR	2.6
36	2e	109	ILE	2.6
9	2N	23	LEU	2.6
33	2b	131	PRO	2.6
7	2H	165	ALA	2.6
54	2y	32	C	2.6
41	2j	56	HIS	2.6
34	1c	72	LYS	2.6
36	1e	88	LYS	2.6
44	2m	60	VAL	2.6
26	24	45	GLY	2.6
42	1k	28	THR	2.6
40	1i	49	PRO	2.6
36	1e	89	ILE	2.6
40	2i	126	SER	2.6
31	29	12	ASP	2.6
40	2i	111	ARG	2.6
45	2n	12	ARG	2.6
33	2b	188	ALA	2.6
15	2T	57	PHE	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	2A	2132	U	2.6
11	2P	125	VAL	2.6
36	2e	90	VAL	2.6
40	2i	109	VAL	2.6
54	2y	66	A	2.6
38	1g	83	ALA	2.6
6	2G	41	GLN	2.6
33	1b	80	ILE	2.6
22	20	21	LEU	2.6
34	2c	204	LEU	2.6
39	1h	133	LEU	2.6
40	2i	119	ALA	2.6
40	1i	7	THR	2.6
54	2y	39	G	2.6
7	2H	130	ARG	2.6
40	1i	81	ILE	2.6
46	2o	87	ILE	2.6
34	1c	47	LEU	2.6
25	23	18	ASP	2.6
38	2g	154	TYR	2.6
4	2E	114	ALA	2.6
34	2c	168	ALA	2.6
40	2i	61	ALA	2.6
40	2i	64	THR	2.6
34	2c	182	ILE	2.6
44	2m	101	GLN	2.6
54	1y	24	G	2.6
12	2Q	132	VAL	2.6
39	1h	80	ILE	2.6
39	1h	83	ILE	2.6
12	2Q	37	LEU	2.6
35	1d	135	LEU	2.6
45	2n	47	LEU	2.6
32	1a	1030(B)	C	2.6
54	2w	15	G	2.6
40	2i	16	ARG	2.6
38	2g	84	ASN	2.6
7	2H	151	ILE	2.5
10	2O	2	ILE	2.5
12	2Q	129	THR	2.5
33	1b	227	GLY	2.5
36	2e	81	GLU	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
40	2i	39	GLY	2.5
25	23	29	ARG	2.5
54	2w	32	C	2.5
40	2i	71	SER	2.5
41	1j	59	SER	2.5
40	2i	55	ALA	2.5
40	2i	106	ALA	2.5
48	1q	27	PHE	2.5
15	2T	102	ILE	2.5
30	28	16	ILE	2.5
3	2D	50	THR	2.5
9	2N	83	LYS	2.5
36	2e	98	THR	2.5
6	2G	70	VAL	2.5
19	2X	68	ARG	2.5
3	2D	56	GLY	2.5
6	2G	157	ILE	2.5
11	2P	44	GLY	2.5
51	2t	83	ARG	2.5
14	2S	34	HIS	2.5
42	1k	82	VAL	2.5
3	2D	2	ALA	2.5
34	1c	5	ILE	2.5
34	2c	5	ILE	2.5
42	1k	42	TRP	2.5
38	1g	80	VAL	2.5
42	1k	14	VAL	2.5
33	2b	129	GLU	2.5
40	1i	4	TYR	2.5
45	2n	58	LYS	2.5
3	2D	273	ARG	2.5
6	2G	138	GLN	2.5
51	2t	41	ILE	2.5
12	2Q	118	LEU	2.5
7	2H	76	VAL	2.5
34	2c	177	THR	2.5
29	27	27	GLY	2.5
34	2c	13	GLY	2.5
13	2R	51	LEU	2.5
27	25	30	LEU	2.5
16	2U	9	VAL	2.5
23	21	61	ARG	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
42	2k	31	THR	2.5
12	2Q	32	TYR	2.5
1	1A	889	C	2.5
33	1b	201	ILE	2.5
41	2j	40	LEU	2.5
6	2G	181	ARG	2.5
34	2c	58	GLU	2.5
42	2k	42	TRP	2.5
54	2w	39	G	2.5
19	2X	66	LEU	2.5
34	2c	57	ILE	2.5
40	2i	81	ILE	2.5
47	1p	39	TYR	2.5
7	2H	133	VAL	2.5
32	2a	1257	U	2.5
45	2n	45	ARG	2.5
54	1w	4	U	2.5
39	2h	3	THR	2.5
41	1j	48	THR	2.5
6	2G	62	LEU	2.5
28	26	7	ILE	2.5
40	1i	114	TYR	2.5
47	1p	60	LEU	2.5
54	2w	10	G	2.5
1	2A	2145	C	2.4
9	2N	74	ARG	2.4
34	2c	49	SER	2.4
40	2i	123	PRO	2.4
52	1u	6	ARG	2.4
26	24	42	PHE	2.4
33	2b	28	PHE	2.4
3	2D	206	LEU	2.4
31	29	17	ILE	2.4
36	1e	81	GLU	2.4
38	1g	12	LEU	2.4
42	2k	91	ARG	2.4
42	2k	126	ARG	2.4
45	2n	41	ARG	2.4
52	2u	21	TYR	2.4
7	2H	35	VAL	2.4
42	2k	114	VAL	2.4
16	2U	7	GLY	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
34	2c	2	GLY	2.4
28	26	2	ALA	2.4
38	2g	152	ALA	2.4
34	2c	131	ARG	2.4
41	2j	98	ILE	2.4
51	2t	13	LEU	2.4
33	2b	152	PHE	2.4
33	2b	130	ARG	2.4
34	1c	38	ARG	2.4
34	2c	21	ARG	2.4
40	2i	91	ASP	2.4
9	2N	69	GLN	2.4
5	2F	82	ILE	2.4
8	2I	37	VAL	2.4
21	2Z	25	PRO	2.4
34	2c	138	VAL	2.4
18	2W	13	SER	2.4
45	1n	50	LYS	2.4
1	1A	888	C	2.4
30	28	58	ILE	2.4
34	1c	178	LEU	2.4
45	2n	49	HIS	2.4
47	2p	19	ILE	2.4
49	1r	40	LEU	2.4
6	2G	182	LYS	2.4
7	2H	77	LYS	2.4
23	2l	28	GLY	2.4
41	1j	60	ARG	2.4
43	2l	55	VAL	2.4
11	1P	40	SER	2.4
47	1p	14	ASN	2.4
34	2c	152	ILE	2.4
36	1e	91	LEU	2.4
50	2s	49	ILE	2.4
34	2c	6	HIS	2.4
3	2D	52	ARG	2.4
3	2D	53	PHE	2.4
41	2j	66	ARG	2.4
35	2d	37	PRO	2.4
38	2g	151	TYR	2.4
45	1n	56	VAL	2.4
52	1u	2	GLY	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
38	1g	86	GLN	2.4
12	2Q	40	ALA	2.4
11	2P	45	LEU	2.4
32	2a	1116	C	2.4
42	2k	96	ARG	2.4
7	2H	32	GLU	2.4
11	2P	51	PHE	2.4
45	1n	8	GLU	2.4
40	2i	54	ASP	2.4
9	2N	116	LEU	2.4
21	2Z	144	LEU	2.4
41	2j	71	LEU	2.4
1	1A	1064	C	2.4
7	2H	119	GLU	2.3
33	2b	93	VAL	2.3
40	2i	6	GLY	2.3
13	2R	69	ASP	2.3
18	2W	94	ASP	2.3
41	2j	89	ASP	2.3
47	1p	27	LYS	2.3
47	1p	69	THR	2.3
54	2w	5	G	2.3
33	2b	42	ILE	2.3
7	2H	34	GLU	2.3
28	26	5	VAL	2.3
45	2n	33	VAL	2.3
26	24	32	TYR	2.3
33	2b	161	ALA	2.3
42	2k	26	ASN	2.3
43	1l	7	ILE	2.3
54	2w	19	G	2.3
54	2y	23	A	2.3
12	1Q	106	VAL	2.3
20	2Y	5	MET	2.3
15	2T	105	LEU	2.3
17	2V	25	LEU	2.3
37	1f	58	GLY	2.3
47	1p	31	LYS	2.3
54	2w	18	G	2.3
7	2H	114	VAL	2.3
20	2Y	45	VAL	2.3
43	2l	18	VAL	2.3

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
16	2U	2	PRO	2.3
47	2p	39	TYR	2.3
7	2H	46	GLU	2.3
4	2E	195	LEU	2.3
15	2T	48	ILE	2.3
50	2s	32	LYS	2.3
40	2i	3	GLN	2.3
45	2n	26	ARG	2.3
3	2D	221	VAL	2.3
7	2H	52	VAL	2.3
1	1A	2112	G	2.3
6	2G	32	PRO	2.3
43	2l	31	PRO	2.3
10	2O	7	TYR	2.3
11	1P	110	TYR	2.3
6	2G	43	LEU	2.3
30	28	29	LYS	2.3
34	2c	187	ALA	2.3
44	2m	87	TYR	2.3
12	2Q	15	GLY	2.3
19	2X	28	PHE	2.3
7	2H	43	VAL	2.3
54	1w	31	C	2.3
19	2X	1	MET	2.3
21	2Z	5	LEU	2.3
20	2Y	2	ARG	2.3
38	2g	78	ARG	2.3
40	1i	37	PHE	2.3
7	2H	80	SER	2.3
48	1q	26	GLN	2.3
50	2s	53	ASN	2.3
1	1A	2146	C	2.3
42	1k	68	ALA	2.3
51	2t	25	ARG	2.3
34	2c	158	GLY	2.3
39	2h	86	ILE	2.3
6	2G	27	ASN	2.3
24	22	2	LYS	2.3
40	2i	28	VAL	2.3
48	1q	35	VAL	2.3
33	1b	202	PRO	2.3
42	1k	65	ALA	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
33	2b	32	ILE	2.3
33	2b	33	TYR	2.3
42	1k	75	TYR	2.3
40	1i	78	LYS	2.3
29	27	36	GLN	2.3
33	2b	209	ARG	2.2
52	1u	22	ARG	2.2
17	2V	85	LYS	2.2
34	1c	196	LEU	2.2
36	2e	86	ALA	2.2
45	1n	2	ALA	2.2
45	2n	30	ALA	2.2
34	1c	182	ILE	2.2
50	2s	44	MET	2.2
25	23	6	VAL	2.2
44	2m	98	VAL	2.2
54	2w	69	A	2.2
54	2y	35	A	2.2
49	1r	87	ARG	2.2
19	2X	2	LYS	2.2
7	2H	96	ALA	2.2
36	2e	17	ALA	2.2
41	2j	8	LEU	2.2
47	1p	16	HIS	2.2
40	2i	35	GLU	2.2
31	29	19	ARG	2.2
47	1p	2	VAL	2.2
32	2a	1286	A	2.2
33	2b	37	ASN	2.2
5	2F	77	ASP	2.2
45	2n	22	THR	2.2
18	2W	86	LEU	2.2
32	2a	1224	G	2.2
40	1i	117	HIS	2.2
54	1w	3	G	2.2
10	2O	19	ILE	2.2
16	2U	17	ILE	2.2
40	2i	59	PHE	2.2
40	2i	120	ARG	2.2
47	1p	65	GLN	2.2
3	2D	5	LYS	2.2
38	2g	36	LYS	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
39	1h	93	VAL	2.2
40	2i	108	VAL	2.2
32	1a	1035	A	2.2
39	2h	123	GLU	2.2
41	1j	40	LEU	2.2
45	2n	55	GLY	2.2
5	2F	78	ILE	2.2
42	2k	125	PHE	2.2
11	2P	18	ARG	2.2
45	1n	61	TRP	2.2
52	2u	18	TYR	2.2
8	2I	92	VAL	2.2
54	2w	28	C	2.2
20	2Y	43	ASN	2.2
33	2b	94	ASN	2.2
9	2N	99	LEU	2.2
17	2V	18	LEU	2.2
34	1c	122	GLU	2.2
33	1b	194	PRO	2.2
33	2b	211	ILE	2.2
34	2c	10	PHE	2.2
42	1k	16	SER	2.2
54	2y	38	A	2.2
9	2N	78	TYR	2.2
32	1a	1027	C	2.2
34	2c	19	GLU	2.2
42	2k	52	GLY	2.2
33	2b	69	LEU	2.2
35	1d	19	LEU	2.2
47	1p	47	ASP	2.2
1	2A	229	A	2.2
45	2n	54	PRO	2.2
1	2A	2128	C	2.2
7	2H	95	ARG	2.2
32	2a	1036	G	2.2
22	10	4	LYS	2.2
41	1j	5	ARG	2.2
42	1k	17	GLY	2.2
38	2g	99	LEU	2.2
38	2g	147	ALA	2.2
39	2h	135	CYS	2.2
34	1c	15	THR	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
41	2j	19	SER	2.2
36	2e	148	VAL	2.2
48	2q	32	TYR	2.2
20	2Y	50	ARG	2.2
39	1h	91	ARG	2.2
44	2m	24	GLY	2.2
1	2A	2896	C	2.2
34	2c	37	GLN	2.2
34	2c	134	ILE	2.2
22	10	3	HIS	2.2
26	24	40	HIS	2.2
26	24	33	VAL	2.2
34	1c	153	VAL	2.2
38	1g	78	ARG	2.2
45	1n	57	ARG	2.2
53	2v	13	A	2.2
6	2G	139	LEU	2.1
35	1d	158	ILE	2.1
36	1e	11	ILE	2.1
30	18	65	GLU	2.1
47	1p	66	PRO	2.1
10	2O	121	VAL	2.1
6	2G	146	TYR	2.1
34	1c	17	ASP	2.1
34	2c	162	GLN	2.1
47	1p	59	TRP	2.1
6	2G	136	ARG	2.1
34	1c	35	GLU	2.1
39	1h	92	ARG	2.1
44	2m	69	GLU	2.1
54	1w	71	C	2.1
21	2Z	170	THR	2.1
22	10	8	GLY	2.1
27	25	29	THR	2.1
39	2h	90	GLY	2.1
48	2q	9	VAL	2.1
33	1b	31	TYR	2.1
33	2b	44	LEU	2.1
22	20	40	GLN	2.1
34	2c	71	ALA	2.1
48	1q	28	PRO	2.1
10	2O	85	VAL	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
33	2b	210	SER	2.1
40	2i	67	GLY	2.1
32	2a	1030(C)	G	2.1
33	2b	221	LEU	2.1
39	1h	10	LEU	2.1
48	1q	43	LEU	2.1
34	2c	59	ARG	2.1
51	2t	80	ARG	2.1
21	1Z	124	ILE	2.1
33	1b	214	ILE	2.1
34	2c	163	ALA	2.1
36	1e	118	ILE	2.1
54	1y	35	A	2.1
54	2w	23	A	2.1
40	1i	70	LYS	2.1
48	2q	12	SER	2.1
10	2O	8	LEU	2.1
10	2O	17	ARG	2.1
18	2W	99	ARG	2.1
22	20	41	ARG	2.1
46	1o	66	LEU	2.1
52	2u	10	ARG	2.1
42	1k	15	ALA	2.1
3	2D	210	GLY	2.1
50	2s	26	GLY	2.1
54	1w	73	A	2.1
7	2H	117	PRO	2.1
54	2w	30	C	2.1
31	29	24	TYR	2.1
21	2Z	171	ILE	2.1
25	23	25	ALA	2.1
1	1A	2133	G	2.1
29	17	48	LYS	2.1
39	2h	16	ALA	2.1
41	2j	32	ALA	2.1
13	2R	68	ARG	2.1
37	2f	6	VAL	2.1
40	2i	20	ARG	2.1
45	2n	57	ARG	2.1
54	2w	62	C	2.1
42	1k	41	THR	2.1
35	2d	164	ALA	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
39	2h	13	ILE	2.1
40	1i	77	ILE	2.1
43	2l	30	ALA	2.1
14	2S	45	GLY	2.1
51	1t	47	GLY	2.1
18	2W	8	ARG	2.1
18	2W	80	PRO	2.1
25	23	59	VAL	2.1
48	2q	19	VAL	2.1
6	1G	80	PHE	2.1
17	2V	20	LEU	2.1
35	2d	196	LEU	2.1
41	1j	63	PHE	2.1
45	1n	49	HIS	2.1
51	2t	70	SER	2.1
18	2W	35	ILE	2.1
33	2b	34	ALA	2.1
48	2q	38	ARG	2.1
52	2u	16	GLY	2.1
8	2I	21	VAL	2.1
12	2Q	96	VAL	2.1
38	1g	17	VAL	2.1
45	1n	11	LYS	2.1
38	2g	153	HIS	2.0
1	1A	1095	A	2.0
53	2v	14	A	2.0
20	2Y	61	ILE	2.0
35	2d	47	ARG	2.0
38	2g	25	ALA	2.0
39	2h	106	GLY	2.0
20	2Y	47	LYS	2.0
40	2i	70	LYS	2.0
5	2F	114	VAL	2.0
34	1c	198	VAL	2.0
34	2c	203	PHE	2.0
7	2H	111	HIS	2.0
33	2b	113	HIS	2.0
1	2A	2153	G	2.0
3	2D	250	TRP	2.0
22	20	42	GLY	2.0
30	28	10	ALA	2.0
30	28	34	TRP	2.0

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
42	2k	61	ALA	2.0
46	1o	87	ILE	2.0
33	2b	228	GLY	2.0
40	1i	112	LYS	2.0
54	1y	33	U	2.0
18	2W	39	THR	2.0
41	2j	15	THR	2.0
7	2H	45	VAL	2.0
8	2I	3	VAL	2.0
20	2Y	31	LEU	2.0
28	26	10	LEU	2.0
48	2q	84	LEU	2.0
40	1i	83	ARG	2.0
5	1F	111	ALA	2.0
1	1A	1058	G	2.0
1	2A	2111	C	2.0
4	2E	115	GLY	2.0
4	2E	134	ILE	2.0
12	2Q	48	GLU	2.0
48	2q	8	GLY	2.0
5	2F	51	THR	2.0
11	2P	30	THR	2.0
50	1s	39	THR	2.0
16	2U	8	VAL	2.0
16	2U	90	VAL	2.0
21	2Z	98	MET	2.0
13	2R	20	LEU	2.0
21	2Z	70	LEU	2.0
34	2c	172	ARG	2.0
38	1g	22	LEU	2.0
41	1j	71	LEU	2.0
6	2G	77	ILE	2.0
8	2I	4	ILE	2.0
11	2P	22	GLY	2.0
34	2c	200	ALA	2.0
51	1t	12	ALA	2.0
1	1A	885	C	2.0
32	2a	1114	C	2.0
6	2G	109	VAL	2.0
26	24	56	VAL	2.0
32	2a	1035	A	2.0
54	1w	57	G	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
8	2I	35	LEU	2.0
33	2b	194	PRO	2.0
33	2b	212	GLN	2.0
34	1c	199	LYS	2.0
38	2g	109	ASN	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
54	PSU	2w	55	20/21	0.48	0.35	82,96,107,108	0
54	6MZ	2y	37	23/24	0.72	0.44	71,85,103,113	0
54	4SU	2y	8	20/21	0.75	0.19	82,92,104,109	0
54	PSU	1w	55	20/21	0.75	0.24	72,82,89,91	0
54	7MG	2y	46	24/25	0.75	0.25	75,93,100,110	0
54	4SU	1y	8	20/21	0.76	0.16	81,86,90,99	0
54	CM0	2y	34	25/26	0.77	0.39	76,88,100,116	0
54	5MU	2y	54	21/22	0.78	0.30	72,85,94,106	0
54	7MG	2w	46	24/25	0.82	0.28	79,92,98,107	0
54	7MG	1y	46	24/25	0.83	0.21	79,89,97,106	0
54	CM0	1y	34	25/26	0.83	0.32	59,84,89,100	0
54	4SU	1w	8	20/21	0.83	0.20	70,83,99,103	0
54	4SU	2w	8	20/21	0.83	0.26	89,95,100,101	0
54	5MU	1y	54	21/22	0.84	0.27	75,82,94,96	0
54	7MG	1w	46	24/25	0.84	0.19	75,83,91,102	0
54	PSU	2y	55	20/21	0.85	0.20	75,83,91,100	0
54	6MZ	1y	37	23/24	0.85	0.17	77,82,90,98	0
54	5MU	2w	54	21/22	0.86	0.20	75,83,90,98	0
1	5MU	2A	1915	21/22	0.86	0.17	62,69,78,91	0
55	4SU	2x	8	20/21	0.87	0.14	58,74,79,80	0
54	PSU	1y	55	20/21	0.88	0.23	74,82,94,99	0
54	CM0	2w	34	25/26	0.89	0.24	67,82,89,101	0
32	2MG	2a	1207	24/25	0.89	0.16	65,76,81,84	0
54	5MU	1w	54	21/22	0.89	0.22	68,74,81,86	0
54	CM0	1w	34	25/26	0.90	0.20	58,70,74,78	0
32	PSU	2a	516	20/21	0.90	0.13	60,64,69,69	0
32	M2G	2a	966	25/26	0.90	0.24	54,67,78,82	0
54	6MZ	1w	37	23/24	0.90	0.23	55,64,71,73	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
55	PSU	2x	55	20/21	0.90	0.12	70,78,86,93	0
55	4SU	1x	8	20/21	0.91	0.16	55,63,69,69	0
1	PSU	2A	1911	20/21	0.92	0.14	47,60,70,71	0
32	5MC	2a	1404	21/22	0.92	0.15	45,53,57,60	0
54	6MZ	2w	37	23/24	0.92	0.20	70,77,83,86	0
32	5MC	2a	967	21/22	0.92	0.23	54,67,73,79	0
43	0TD	1l	92	10/11	0.92	0.16	46,52,54,68	0
55	5MU	2x	54	21/22	0.92	0.15	71,78,83,85	0
43	0TD	2l	92	10/11	0.93	0.16	57,62,65,66	0
1	4OC	2A	1920	21/23	0.93	0.18	57,64,67,72	0
1	5MC	2A	1942	21/22	0.93	0.17	48,62,68,77	0
55	PSU	1x	55	20/21	0.93	0.15	54,59,74,77	0
32	MA6	2a	1518	24/25	0.93	0.21	49,60,64,66	0
32	4OC	2a	1402	22/23	0.94	0.15	48,60,64,65	0
1	5MU	1A	1915	21/22	0.94	0.15	40,51,57,58	0
32	UR3	2a	1498	21/22	0.94	0.20	42,52,58,62	0
32	7MG	2a	527	24/25	0.94	0.14	57,67,69,71	0
55	5MC	2x	32	21/22	0.94	0.21	63,69,74,76	0
32	PSU	1a	516	20/21	0.94	0.14	51,60,66,73	0
55	5MU	1x	54	21/22	0.94	0.15	48,61,64,74	0
1	PSU	2A	1917	20/21	0.94	0.15	51,60,66,71	0
32	5MC	1a	1400	21/22	0.95	0.17	41,49,54,59	0
1	PSU	1A	1911	20/21	0.95	0.16	29,39,51,52	0
32	2MG	1a	1207	24/25	0.95	0.17	48,60,66,66	0
1	PSU	1A	1917	20/21	0.95	0.15	32,52,55,56	0
32	MA6	2a	1519	24/25	0.95	0.24	41,56,60,62	0
1	5MC	2A	1962	21/22	0.95	0.15	30,47,54,66	0
32	5MC	2a	1400	21/22	0.95	0.20	61,66,68,71	0
1	5MU	2A	1939	21/22	0.96	0.19	35,41,47,47	0
1	PSU	1A	2605	20/21	0.96	0.20	14,20,26,27	0
32	5MC	1a	967	21/22	0.96	0.22	49,56,65,68	0
1	OMG	2A	2251	24/25	0.96	0.21	33,39,44,46	0
55	5MC	1x	32	21/22	0.96	0.20	47,56,62,64	0
1	PSU	2A	2605	20/21	0.96	0.16	27,34,40,43	0
32	5MC	2a	1407	21/22	0.96	0.15	45,51,54,56	0
32	5MC	1a	1404	21/22	0.96	0.18	30,34,39,40	0
32	M2G	1a	966	25/26	0.96	0.20	46,52,60,65	0
32	MA6	1a	1518	24/25	0.96	0.17	32,36,40,43	0
32	5MC	1a	1407	21/22	0.96	0.16	25,36,40,42	0
1	5MC	1A	1942	21/22	0.96	0.17	29,38,46,52	0
1	2MU	2A	2552	21/23	0.96	0.19	35,42,50,58	0
32	UR3	1a	1498	21/22	0.97	0.20	31,35,39,43	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MA6	1a	1519	24/25	0.97	0.17	34,37,47,51	0
1	2MA	2A	2503	23/24	0.97	0.20	24,31,38,40	0
1	5MC	1A	1962	21/22	0.97	0.20	26,31,35,36	0
32	4OC	1a	1402	22/23	0.97	0.16	33,40,46,55	0
1	5MU	1A	1939	21/22	0.97	0.20	21,26,32,34	0
32	7MG	1a	527	24/25	0.97	0.15	32,41,45,46	0
1	4OC	1A	1920	21/23	0.97	0.18	31,40,45,46	0
1	2MU	1A	2552	21/23	0.98	0.15	16,22,26,27	0
1	OMG	1A	2251	24/25	0.98	0.18	10,15,22,23	0
1	2MA	1A	2503	23/24	0.98	0.20	6,12,15,18	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3959	1/1	0.30	0.16	50,50,50,50	0
56	MG	2A	3670	1/1	0.35	0.22	67,67,67,67	0
56	MG	2A	3819	1/1	0.42	0.16	76,76,76,76	0
56	MG	2A	3766	1/1	0.42	0.38	80,80,80,80	0
56	MG	1A	3923	1/1	0.43	0.12	68,68,68,68	0
56	MG	2a	1777	1/1	0.43	0.11	69,69,69,69	0
56	MG	2A	3775	1/1	0.44	0.26	83,83,83,83	0
56	MG	1A	4073	1/1	0.45	0.40	66,66,66,66	0
56	MG	2A	3826	1/1	0.48	0.16	70,70,70,70	0
56	MG	2A	3786	1/1	0.49	0.25	67,67,67,67	0
56	MG	2A	3794	1/1	0.50	0.36	68,68,68,68	0
56	MG	1A	3912	1/1	0.51	0.18	60,60,60,60	0
56	MG	1A	3624	1/1	0.54	0.11	31,31,31,31	0
56	MG	2A	3219	1/1	0.58	0.21	57,57,57,57	0
56	MG	1m	201	1/1	0.60	0.20	64,64,64,64	0
56	MG	1a	3218	1/1	0.60	0.15	65,65,65,65	0
56	MG	2A	3643	1/1	0.60	0.16	71,71,71,71	0
56	MG	1A	4010	1/1	0.62	0.14	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	3469	1/1	0.62	0.35	61,61,61,61	0
56	MG	2A	3784	1/1	0.63	0.11	58,58,58,58	0
56	MG	2A	3693	1/1	0.63	0.33	55,55,55,55	0
56	MG	2A	3372	1/1	0.63	0.18	57,57,57,57	0
56	MG	2T	202	1/1	0.63	0.49	55,55,55,55	0
56	MG	26	101	1/1	0.63	0.27	54,54,54,54	0
56	MG	2A	3390	1/1	0.64	0.35	53,53,53,53	0
56	MG	1A	3971	1/1	0.64	0.18	27,27,27,27	0
56	MG	2A	3521	1/1	0.64	0.13	60,60,60,60	0
56	MG	2a	1788	1/1	0.64	0.14	70,70,70,70	0
56	MG	2A	3698	1/1	0.65	0.08	51,51,51,51	0
56	MG	2a	1749	1/1	0.65	0.18	68,68,68,68	0
56	MG	2a	1612	1/1	0.66	0.15	62,62,62,62	0
56	MG	2A	3206	1/1	0.66	0.18	48,48,48,48	0
56	MG	2A	3632	1/1	0.66	0.28	61,61,61,61	0
56	MG	2A	3477	1/1	0.66	0.35	56,56,56,56	0
56	MG	2A	3243	1/1	0.66	0.33	59,59,59,59	0
56	MG	1A	3309	1/1	0.67	0.18	35,35,35,35	0
56	MG	2a	1603	1/1	0.67	0.17	50,50,50,50	0
56	MG	2A	3115	1/1	0.67	0.14	61,61,61,61	0
56	MG	2A	3491	1/1	0.67	0.12	33,33,33,33	0
56	MG	1A	3690	1/1	0.67	0.18	21,21,21,21	0
56	MG	2B	216	1/1	0.67	0.15	61,61,61,61	0
56	MG	2A	3678	1/1	0.68	0.12	76,76,76,76	0
56	MG	1A	3706	1/1	0.68	0.18	26,26,26,26	0
56	MG	1A	3270	1/1	0.69	0.22	61,61,61,61	0
56	MG	2A	3256	1/1	0.70	0.29	58,58,58,58	0
56	MG	1d	301	1/1	0.70	0.19	56,56,56,56	0
56	MG	1A	3343	1/1	0.71	0.14	43,43,43,43	0
56	MG	2A	3656	1/1	0.71	0.38	45,45,45,45	0
56	MG	2a	1752	1/1	0.71	0.06	64,64,64,64	0
56	MG	1a	3207	1/1	0.71	0.07	46,46,46,46	0
56	MG	1A	3795	1/1	0.72	0.07	69,69,69,69	0
56	MG	2A	3787	1/1	0.72	0.15	46,46,46,46	0
56	MG	2a	1758	1/1	0.72	0.09	70,70,70,70	0
56	MG	1A	3957	1/1	0.72	0.07	57,57,57,57	0
56	MG	1F	314	1/1	0.72	0.58	45,45,45,45	0
56	MG	1a	3104	1/1	0.72	0.12	72,72,72,72	0
56	MG	2A	3597	1/1	0.72	0.12	34,34,34,34	0
56	MG	1A	3472	1/1	0.72	0.24	60,60,60,60	0
56	MG	2A	3505	1/1	0.72	0.12	36,36,36,36	0
56	MG	2A	3821	1/1	0.72	0.18	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	2a	1721	1/1	0.73	0.25	55,55,55,55	0
56	MG	2A	3789	1/1	0.73	0.20	74,74,74,74	0
56	MG	2a	1832	1/1	0.73	0.17	51,51,51,51	0
56	MG	1a	3151	1/1	0.74	0.12	62,62,62,62	0
56	MG	2a	1649	1/1	0.74	0.16	54,54,54,54	0
56	MG	2a	1710	1/1	0.74	0.14	70,70,70,70	0
56	MG	1a	3075	1/1	0.74	0.29	63,63,63,63	0
56	MG	2A	3359	1/1	0.74	0.45	57,57,57,57	0
56	MG	2A	3183	1/1	0.74	0.13	35,35,35,35	0
56	MG	2A	3864	1/1	0.74	0.37	49,49,49,49	0
56	MG	1A	3626	1/1	0.74	0.15	17,17,17,17	0
56	MG	1A	3438	1/1	0.74	0.16	51,51,51,51	0
56	MG	2A	3528	1/1	0.74	0.10	66,66,66,66	0
56	MG	2A	3285	1/1	0.75	0.26	66,66,66,66	0
56	MG	2a	1685	1/1	0.75	0.15	49,49,49,49	0
56	MG	2A	3462	1/1	0.75	0.22	41,41,41,41	0
56	MG	2A	3818	1/1	0.75	0.26	56,56,56,56	0
56	MG	2A	3058	1/1	0.75	0.14	67,67,67,67	0
56	MG	2i	201	1/1	0.75	0.17	60,60,60,60	0
56	MG	1A	3116	1/1	0.75	0.22	36,36,36,36	0
56	MG	2a	1763	1/1	0.76	0.06	70,70,70,70	0
56	MG	2a	1748	1/1	0.76	0.11	59,59,59,59	0
56	MG	2a	1706	1/1	0.76	0.13	67,67,67,67	0
56	MG	1x	106	1/1	0.76	0.15	66,66,66,66	0
56	MG	2A	3026	1/1	0.76	0.11	40,40,40,40	0
56	MG	2P	202	1/1	0.76	0.23	55,55,55,55	0
56	MG	2A	3358	1/1	0.76	0.25	51,51,51,51	0
56	MG	1A	3085	1/1	0.76	0.18	16,16,16,16	0
56	MG	1A	3539	1/1	0.76	0.19	25,25,25,25	0
56	MG	2A	3840	1/1	0.77	0.09	41,41,41,41	0
56	MG	2A	3375	1/1	0.77	0.30	59,59,59,59	0
56	MG	2A	3839	1/1	0.77	0.12	47,47,47,47	0
56	MG	1A	3981	1/1	0.77	0.31	29,29,29,29	0
56	MG	2a	1759	1/1	0.77	0.20	61,61,61,61	0
56	MG	1A	3348	1/1	0.77	0.41	33,33,33,33	0
56	MG	1A	3067	1/1	0.77	0.26	44,44,44,44	0
56	MG	2A	3480	1/1	0.77	0.09	58,58,58,58	0
56	MG	2A	3498	1/1	0.77	0.17	51,51,51,51	0
56	MG	1A	4046	1/1	0.77	0.13	43,43,43,43	0
56	MG	2A	3776	1/1	0.77	0.28	74,74,74,74	0
56	MG	2A	3741	1/1	0.77	0.12	49,49,49,49	0
56	MG	2A	3277	1/1	0.77	0.31	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	3953	1/1	0.77	0.23	12,12,12,12	0
56	MG	1A	3939	1/1	0.77	0.23	47,47,47,47	0
56	MG	2A	3222	1/1	0.78	0.20	29,29,29,29	0
56	MG	1A	3888	1/1	0.78	0.15	62,62,62,62	0
56	MG	2A	3502	1/1	0.78	0.32	53,53,53,53	0
56	MG	1a	3133	1/1	0.78	0.16	53,53,53,53	0
56	MG	2A	3396	1/1	0.78	0.15	50,50,50,50	0
56	MG	1a	3084	1/1	0.78	0.31	56,56,56,56	0
56	MG	2A	3771	1/1	0.78	0.14	50,50,50,50	0
56	MG	1A	3473	1/1	0.78	0.18	51,51,51,51	0
56	MG	2A	3569	1/1	0.78	0.10	62,62,62,62	0
56	MG	1A	3941	1/1	0.78	0.15	32,32,32,32	0
56	MG	2A	3806	1/1	0.78	0.15	50,50,50,50	0
56	MG	2A	3801	1/1	0.79	0.40	63,63,63,63	0
56	MG	2A	3812	1/1	0.79	0.16	59,59,59,59	0
56	MG	2A	3860	1/1	0.79	0.18	62,62,62,62	0
56	MG	2A	3316	1/1	0.79	0.50	48,48,48,48	0
56	MG	1A	3388	1/1	0.79	0.16	53,53,53,53	0
56	MG	2A	3428	1/1	0.79	0.15	66,66,66,66	0
56	MG	1A	4034	1/1	0.79	0.07	44,44,44,44	0
56	MG	1A	3497	1/1	0.79	0.16	33,33,33,33	0
56	MG	2A	3709	1/1	0.79	0.19	60,60,60,60	0
56	MG	1a	3167	1/1	0.79	0.07	54,54,54,54	0
56	MG	2A	3797	1/1	0.79	0.07	78,78,78,78	0
56	MG	2A	3405	1/1	0.79	0.12	50,50,50,50	0
56	MG	2A	3634	1/1	0.79	0.16	68,68,68,68	0
56	MG	2A	3774	1/1	0.79	0.59	66,66,66,66	0
56	MG	2A	3762	1/1	0.79	0.10	57,57,57,57	0
56	MG	1A	3676	1/1	0.79	0.21	28,28,28,28	0
56	MG	2A	3781	1/1	0.79	0.11	51,51,51,51	0
56	MG	2a	1698	1/1	0.80	0.14	43,43,43,43	0
56	MG	2A	3848	1/1	0.80	0.05	55,55,55,55	0
56	MG	2A	3665	1/1	0.80	0.09	48,48,48,48	0
56	MG	2A	3773	1/1	0.80	0.73	71,71,71,71	0
56	MG	2A	3750	1/1	0.80	0.15	28,28,28,28	0
56	MG	2A	3289	1/1	0.80	0.11	60,60,60,60	0
56	MG	1A	3835	1/1	0.80	0.13	22,22,22,22	0
56	MG	2a	1695	1/1	0.80	0.15	63,63,63,63	0
56	MG	2a	1720	1/1	0.80	0.21	55,55,55,55	0
56	MG	1A	3867	1/1	0.80	0.20	13,13,13,13	0
56	MG	1A	3713	1/1	0.80	0.17	22,22,22,22	0
56	MG	2a	1738	1/1	0.80	0.20	76,76,76,76	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3783	1/1	0.80	0.08	53,53,53,53	0
56	MG	1A	3364	1/1	0.80	0.22	31,31,31,31	0
56	MG	2a	1736	1/1	0.80	0.15	65,65,65,65	0
56	MG	2A	3525	1/1	0.80	0.08	33,33,33,33	0
56	MG	1A	3509	1/1	0.80	0.19	23,23,23,23	0
56	MG	1A	3827	1/1	0.80	0.36	38,38,38,38	0
56	MG	1a	3188	1/1	0.80	0.13	48,48,48,48	0
56	MG	1a	3153	1/1	0.80	0.12	27,27,27,27	0
56	MG	2a	1627	1/1	0.80	0.51	53,53,53,53	0
56	MG	2A	3779	1/1	0.81	0.09	47,47,47,47	0
56	MG	2A	3749	1/1	0.81	0.25	41,41,41,41	0
56	MG	1A	3893	1/1	0.81	0.12	48,48,48,48	0
56	MG	2A	3339	1/1	0.81	0.17	68,68,68,68	0
56	MG	2A	3853	1/1	0.81	0.12	33,33,33,33	0
56	MG	2A	3843	1/1	0.81	0.08	40,40,40,40	0
56	MG	1a	3191	1/1	0.81	0.10	42,42,42,42	0
56	MG	1A	3175	1/1	0.81	0.20	19,19,19,19	0
56	MG	2A	3745	1/1	0.81	0.26	49,49,49,49	0
56	MG	2A	3208	1/1	0.81	0.24	48,48,48,48	0
56	MG	2A	3716	1/1	0.81	0.22	56,56,56,56	0
56	MG	1A	3999	1/1	0.81	0.20	39,39,39,39	0
56	MG	2A	3842	1/1	0.81	0.18	62,62,62,62	0
56	MG	1a	3138	1/1	0.81	0.16	58,58,58,58	0
56	MG	2A	3600	1/1	0.81	0.11	69,69,69,69	0
56	MG	17	105	1/1	0.81	0.20	22,22,22,22	0
56	MG	1a	3113	1/1	0.81	0.13	41,41,41,41	0
56	MG	2A	3851	1/1	0.81	0.16	37,37,37,37	0
56	MG	2A	3701	1/1	0.81	0.11	40,40,40,40	0
56	MG	2A	3829	1/1	0.81	0.06	42,42,42,42	0
56	MG	1y	103	1/1	0.81	0.33	66,66,66,66	0
56	MG	1A	3016	1/1	0.82	0.14	26,26,26,26	0
56	MG	1A	3440	1/1	0.82	0.20	38,38,38,38	0
56	MG	2A	3799	1/1	0.82	0.47	68,68,68,68	0
56	MG	1A	4071	1/1	0.82	0.30	52,52,52,52	0
56	MG	1A	3426	1/1	0.82	0.17	28,28,28,28	0
56	MG	2A	3644	1/1	0.82	0.16	54,54,54,54	0
56	MG	1A	3292	1/1	0.82	0.14	35,35,35,35	0
56	MG	2A	3676	1/1	0.82	0.21	64,64,64,64	0
56	MG	2A	3804	1/1	0.82	0.11	60,60,60,60	0
56	MG	2R	202	1/1	0.82	0.15	46,46,46,46	0
56	MG	1a	3068	1/1	0.82	0.30	57,57,57,57	0
56	MG	1A	3708	1/1	0.82	0.10	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	2a	1795	1/1	0.82	0.17	53,53,53,53	0
56	MG	2G	201	1/1	0.82	0.09	59,59,59,59	0
56	MG	1a	3195	1/1	0.82	0.16	47,47,47,47	0
56	MG	1A	3446	1/1	0.82	0.12	43,43,43,43	0
56	MG	1a	3175	1/1	0.82	0.22	66,66,66,66	0
56	MG	1y	104	1/1	0.82	0.14	61,61,61,61	0
56	MG	1A	3288	1/1	0.82	0.25	32,32,32,32	0
56	MG	1A	3911	1/1	0.82	0.16	59,59,59,59	0
56	MG	1A	3389	1/1	0.82	0.16	39,39,39,39	0
56	MG	2A	3778	1/1	0.82	0.16	61,61,61,61	0
56	MG	2A	3499	1/1	0.82	0.12	50,50,50,50	0
56	MG	1A	3505	1/1	0.82	0.12	44,44,44,44	0
56	MG	2A	3800	1/1	0.82	0.06	47,47,47,47	0
56	MG	2A	3593	1/1	0.82	0.11	31,31,31,31	0
56	MG	2a	1769	1/1	0.82	0.08	60,60,60,60	0
56	MG	2A	3347	1/1	0.82	0.13	41,41,41,41	0
56	MG	1A	3997	1/1	0.82	0.18	57,57,57,57	0
56	MG	1P	203	1/1	0.82	0.96	27,27,27,27	0
56	MG	2A	3571	1/1	0.83	0.19	53,53,53,53	0
56	MG	1A	3353	1/1	0.83	0.40	41,41,41,41	0
56	MG	2A	3751	1/1	0.83	0.32	37,37,37,37	0
56	MG	1a	3109	1/1	0.83	0.20	40,40,40,40	0
56	MG	1a	3131	1/1	0.83	0.22	53,53,53,53	0
56	MG	1a	3080	1/1	0.83	0.17	62,62,62,62	0
56	MG	1B	201	1/1	0.83	0.18	40,40,40,40	0
56	MG	2A	3796	1/1	0.83	0.20	45,45,45,45	0
56	MG	1A	4035	1/1	0.83	0.10	39,39,39,39	0
56	MG	2a	1652	1/1	0.83	0.35	60,60,60,60	0
56	MG	1A	3966	1/1	0.83	0.17	15,15,15,15	0
56	MG	1A	3772	1/1	0.83	0.17	12,12,12,12	0
56	MG	2I	101	1/1	0.83	0.16	57,57,57,57	0
56	MG	2a	1606	1/1	0.83	0.11	59,59,59,59	0
56	MG	2A	3129	1/1	0.83	0.09	43,43,43,43	0
56	MG	2A	3618	1/1	0.83	0.20	39,39,39,39	0
56	MG	2A	3217	1/1	0.83	0.42	47,47,47,47	0
56	MG	2A	3270	1/1	0.83	0.26	50,50,50,50	0
56	MG	2A	3541	1/1	0.83	0.13	53,53,53,53	0
56	MG	1A	3704	1/1	0.83	0.09	34,34,34,34	0
56	MG	2A	3424	1/1	0.83	0.28	42,42,42,42	0
56	MG	1A	3272	1/1	0.83	0.21	24,24,24,24	0
56	MG	2A	3664	1/1	0.83	0.41	54,54,54,54	0
56	MG	1A	3915	1/1	0.83	0.10	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	2E	307	1/1	0.83	0.12	25,25,25,25	0
56	MG	1a	3193	1/1	0.83	0.07	57,57,57,57	0
56	MG	2a	1645	1/1	0.83	0.20	44,44,44,44	0
56	MG	1A	3276	1/1	0.83	0.14	38,38,38,38	0
56	MG	2A	3287	1/1	0.83	0.17	58,58,58,58	0
56	MG	1B	223	1/1	0.83	0.16	43,43,43,43	0
56	MG	2a	1674	1/1	0.83	0.46	55,55,55,55	0
56	MG	2A	3197	1/1	0.83	0.15	32,32,32,32	0
56	MG	22	101	1/1	0.83	0.12	42,42,42,42	0
56	MG	2p	101	1/1	0.83	0.14	43,43,43,43	0
56	MG	1A	3186	1/1	0.83	0.39	31,31,31,31	0
56	MG	1A	3238	1/1	0.83	0.14	27,27,27,27	0
56	MG	2y	102	1/1	0.83	0.13	51,51,51,51	0
56	MG	1x	111	1/1	0.83	0.20	49,49,49,49	0
56	MG	1A	3841	1/1	0.83	0.11	34,34,34,34	0
56	MG	2A	3795	1/1	0.83	0.27	61,61,61,61	0
56	MG	1A	3325	1/1	0.83	0.24	42,42,42,42	0
56	MG	2A	3410	1/1	0.83	0.13	48,48,48,48	0
56	MG	1A	3910	1/1	0.84	0.06	58,58,58,58	0
56	MG	1a	3031	1/1	0.84	0.14	53,53,53,53	0
56	MG	1a	3206	1/1	0.84	0.11	52,52,52,52	0
56	MG	2A	3090	1/1	0.84	0.13	59,59,59,59	0
56	MG	1A	3220	1/1	0.84	0.14	53,53,53,53	0
56	MG	1B	222	1/1	0.84	0.13	53,53,53,53	0
56	MG	1A	3836	1/1	0.84	0.19	47,47,47,47	0
56	MG	1A	3684	1/1	0.84	0.21	16,16,16,16	0
56	MG	2a	1666	1/1	0.84	0.20	50,50,50,50	0
56	MG	2a	1711	1/1	0.84	0.12	47,47,47,47	0
56	MG	1A	3490	1/1	0.84	0.13	18,18,18,18	0
56	MG	1A	3659	1/1	0.84	0.17	12,12,12,12	0
56	MG	2a	1681	1/1	0.84	0.24	51,51,51,51	0
56	MG	1A	3423	1/1	0.84	0.17	50,50,50,50	0
56	MG	2A	3566	1/1	0.84	0.17	44,44,44,44	0
56	MG	2A	3614	1/1	0.84	0.11	23,23,23,23	0
56	MG	2A	3540	1/1	0.84	0.10	28,28,28,28	0
56	MG	1a	3106	1/1	0.84	0.16	20,20,20,20	0
56	MG	19	101	1/1	0.84	0.23	43,43,43,43	0
56	MG	2D	303	1/1	0.84	0.40	61,61,61,61	0
56	MG	2A	3071	1/1	0.84	0.24	30,30,30,30	0
56	MG	1A	3200	1/1	0.84	0.21	37,37,37,37	0
56	MG	2A	3770	1/1	0.84	0.34	65,65,65,65	0
56	MG	1A	4021	1/1	0.84	0.10	32,32,32,32	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	1762	1/1	0.84	0.10	66,66,66,66	0
56	MG	1A	3179	1/1	0.84	0.35	60,60,60,60	0
56	MG	1a	3214	1/1	0.84	0.08	49,49,49,49	0
56	MG	1A	3046	1/1	0.84	0.30	44,44,44,44	0
56	MG	1A	3435	1/1	0.84	0.23	50,50,50,50	0
56	MG	1a	3202	1/1	0.84	0.14	46,46,46,46	0
56	MG	2A	3239	1/1	0.84	0.22	45,45,45,45	0
56	MG	2A	3556	1/1	0.84	0.08	44,44,44,44	0
56	MG	1A	3326	1/1	0.84	0.28	29,29,29,29	0
56	MG	1A	3728	1/1	0.84	0.15	54,54,54,54	0
56	MG	2A	3014	1/1	0.85	0.18	38,38,38,38	0
56	MG	2a	1639	1/1	0.85	0.24	60,60,60,60	0
56	MG	2A	3327	1/1	0.85	0.63	44,44,44,44	0
56	MG	1w	104	1/1	0.85	0.15	51,51,51,51	0
56	MG	1A	3640	1/1	0.85	0.17	31,31,31,31	0
56	MG	2A	3765	1/1	0.85	0.30	62,62,62,62	0
56	MG	1A	4072	1/1	0.85	0.14	52,52,52,52	0
56	MG	2A	3160	1/1	0.85	0.10	50,50,50,50	0
56	MG	2a	1665	1/1	0.85	0.10	48,48,48,48	0
56	MG	2a	1770	1/1	0.85	0.16	51,51,51,51	0
56	MG	2a	1608	1/1	0.85	0.16	55,55,55,55	0
56	MG	2A	3568	1/1	0.85	0.17	46,46,46,46	0
56	MG	2a	1754	1/1	0.85	0.11	52,52,52,52	0
56	MG	1a	3107	1/1	0.85	0.13	34,34,34,34	0
56	MG	2A	3387	1/1	0.85	0.18	72,72,72,72	0
56	MG	1a	3119	1/1	0.85	0.30	42,42,42,42	0
56	MG	2B	209	1/1	0.85	0.12	41,41,41,41	0
56	MG	2a	1664	1/1	0.85	0.16	49,49,49,49	0
56	MG	2A	3074	1/1	0.85	0.41	42,42,42,42	0
56	MG	1A	3159	1/1	0.85	0.14	23,23,23,23	0
56	MG	2A	3356	1/1	0.85	0.14	55,55,55,55	0
56	MG	1a	3194	1/1	0.85	0.09	58,58,58,58	0
56	MG	2A	3294	1/1	0.85	0.11	44,44,44,44	0
56	MG	2a	1773	1/1	0.85	0.13	71,71,71,71	0
56	MG	1a	3204	1/1	0.85	0.08	49,49,49,49	0
56	MG	1a	3066	1/1	0.85	0.16	44,44,44,44	0
56	MG	2A	3120	1/1	0.85	0.45	48,48,48,48	0
56	MG	1A	3683	1/1	0.85	0.11	28,28,28,28	0
56	MG	2E	301	1/1	0.85	0.10	45,45,45,45	0
56	MG	2a	1724	1/1	0.85	0.23	64,64,64,64	0
56	MG	1A	3074	1/1	0.85	0.16	36,36,36,36	0
56	MG	2B	208	1/1	0.85	0.34	57,57,57,57	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3446	1/1	0.85	0.12	39,39,39,39	0
56	MG	1A	3460	1/1	0.85	0.15	25,25,25,25	0
56	MG	2A	3345	1/1	0.85	0.84	61,61,61,61	0
56	MG	1A	3824	1/1	0.85	0.15	25,25,25,25	0
56	MG	2A	3104	1/1	0.85	0.15	48,48,48,48	0
56	MG	2A	3245	1/1	0.85	0.37	58,58,58,58	0
56	MG	2A	3838	1/1	0.85	0.11	61,61,61,61	0
56	MG	1A	3333	1/1	0.85	0.26	42,42,42,42	0
56	MG	2a	1653	1/1	0.85	0.18	71,71,71,71	0
56	MG	1A	3437	1/1	0.85	0.14	39,39,39,39	0
56	MG	2A	3034	1/1	0.85	0.36	37,37,37,37	0
56	MG	1A	3133	1/1	0.85	0.47	19,19,19,19	0
56	MG	2a	1784	1/1	0.85	0.13	60,60,60,60	0
56	MG	1B	216	1/1	0.85	0.15	60,60,60,60	0
56	MG	1A	3409	1/1	0.85	0.26	30,30,30,30	0
56	MG	2A	3046	1/1	0.85	0.13	59,59,59,59	0
56	MG	2a	1619	1/1	0.85	0.20	44,44,44,44	0
56	MG	2A	3021	1/1	0.85	1.13	52,52,52,52	0
56	MG	1w	105	1/1	0.85	0.16	51,51,51,51	0
56	MG	1A	3420	1/1	0.85	0.79	47,47,47,47	0
56	MG	2A	3379	1/1	0.85	0.62	49,49,49,49	0
56	MG	1a	3128	1/1	0.85	0.18	34,34,34,34	0
56	MG	1A	3595	1/1	0.85	0.34	40,40,40,40	0
56	MG	1A	3566	1/1	0.85	0.25	38,38,38,38	0
56	MG	2A	3099	1/1	0.85	0.26	51,51,51,51	0
56	MG	1A	3598	1/1	0.86	0.17	36,36,36,36	0
56	MG	2A	3708	1/1	0.86	0.33	55,55,55,55	0
56	MG	2A	3538	1/1	0.86	0.14	33,33,33,33	0
56	MG	1A	3958	1/1	0.86	0.05	63,63,63,63	0
56	MG	2A	3095	1/1	0.86	0.10	66,66,66,66	0
56	MG	2A	3154	1/1	0.86	0.13	50,50,50,50	0
56	MG	2A	3035	1/1	0.86	0.13	59,59,59,59	0
56	MG	1a	3139	1/1	0.86	0.13	58,58,58,58	0
56	MG	2A	3176	1/1	0.86	0.13	43,43,43,43	0
56	MG	2A	3397	1/1	0.86	0.10	53,53,53,53	0
56	MG	1a	3054	1/1	0.86	0.19	46,46,46,46	0
56	MG	2A	3343	1/1	0.86	0.17	60,60,60,60	0
56	MG	2a	1679	1/1	0.86	0.13	58,58,58,58	0
56	MG	1Z	302	1/1	0.86	0.24	50,50,50,50	0
56	MG	2A	3391	1/1	0.86	0.40	57,57,57,57	0
56	MG	2A	3512	1/1	0.86	0.27	36,36,36,36	0
56	MG	2a	1783	1/1	0.86	0.09	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	2i	202	1/1	0.86	0.13	42,42,42,42	0
56	MG	2A	3207	1/1	0.86	0.45	61,61,61,61	0
56	MG	2A	3743	1/1	0.86	0.47	62,62,62,62	0
56	MG	1A	3075	1/1	0.86	0.24	34,34,34,34	0
56	MG	1A	3494	1/1	0.86	0.21	35,35,35,35	0
56	MG	2a	1705	1/1	0.86	0.14	51,51,51,51	0
56	MG	2A	3551	1/1	0.86	0.08	35,35,35,35	0
56	MG	1A	3890	1/1	0.86	0.16	17,17,17,17	0
56	MG	1A	3165	1/1	0.86	0.15	23,23,23,23	0
56	MG	2A	3049	1/1	0.86	0.12	54,54,54,54	0
56	MG	1A	3926	1/1	0.86	0.10	28,28,28,28	0
56	MG	2A	3330	1/1	0.86	0.11	47,47,47,47	0
56	MG	1A	3826	1/1	0.86	0.18	29,29,29,29	0
56	MG	1A	3103	1/1	0.86	0.13	46,46,46,46	0
56	MG	1A	3993	1/1	0.86	0.12	33,33,33,33	0
56	MG	1A	3662	1/1	0.86	0.14	44,44,44,44	0
56	MG	2A	3576	1/1	0.86	0.12	40,40,40,40	0
56	MG	2A	3788	1/1	0.86	0.13	40,40,40,40	0
56	MG	2a	1807	1/1	0.86	0.14	60,60,60,60	0
58	ZN	14	102	1/1	0.86	0.10	99,99,99,99	0
56	MG	1A	3094	1/1	0.86	0.26	27,27,27,27	0
56	MG	1A	3056	1/1	0.86	0.24	40,40,40,40	0
56	MG	2A	3501	1/1	0.86	0.07	42,42,42,42	0
56	MG	2A	3608	1/1	0.86	0.09	50,50,50,50	0
56	MG	2A	3312	1/1	0.86	0.10	32,32,32,32	0
56	MG	2A	3439	1/1	0.86	0.12	43,43,43,43	0
56	MG	2a	1620	1/1	0.86	0.22	46,46,46,46	0
56	MG	2A	3640	1/1	0.86	0.14	72,72,72,72	0
56	MG	2a	1617	1/1	0.86	0.11	31,31,31,31	0
56	MG	2A	3273	1/1	0.86	0.28	40,40,40,40	0
56	MG	1a	3055	1/1	0.86	0.20	58,58,58,58	0
56	MG	1a	3215	1/1	0.86	0.09	55,55,55,55	0
56	MG	2A	3533	1/1	0.86	0.10	33,33,33,33	0
56	MG	2A	3373	1/1	0.86	0.66	52,52,52,52	0
56	MG	1A	3856	1/1	0.86	0.11	28,28,28,28	0
56	MG	1A	3129	1/1	0.86	0.10	29,29,29,29	0
56	MG	2a	1663	1/1	0.86	0.09	33,33,33,33	0
56	MG	1A	3844	1/1	0.86	0.08	29,29,29,29	0
56	MG	2A	3303	1/1	0.86	0.20	56,56,56,56	0
56	MG	2A	3558	1/1	0.86	0.25	58,58,58,58	0
56	MG	1A	3526	1/1	0.86	0.17	31,31,31,31	0
56	MG	2A	3591	1/1	0.86	0.07	62,62,62,62	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3605	1/1	0.86	0.14	35,35,35,35	0
56	MG	1A	3714	1/1	0.86	0.11	25,25,25,25	0
56	MG	1a	3177	1/1	0.86	0.11	37,37,37,37	0
56	MG	2A	3736	1/1	0.86	0.25	48,48,48,48	0
56	MG	2A	3723	1/1	0.86	0.09	60,60,60,60	0
56	MG	2A	3802	1/1	0.86	0.07	54,54,54,54	0
56	MG	2a	1648	1/1	0.86	0.13	46,46,46,46	0
56	MG	2A	3032	1/1	0.86	0.14	54,54,54,54	0
56	MG	1A	3406	1/1	0.86	0.14	35,35,35,35	0
56	MG	2A	3820	1/1	0.87	0.12	32,32,32,32	0
56	MG	1B	231	1/1	0.87	0.13	41,41,41,41	0
56	MG	1a	3095	1/1	0.87	0.19	40,40,40,40	0
56	MG	2B	214	1/1	0.87	0.09	63,63,63,63	0
56	MG	2A	3650	1/1	0.87	0.19	47,47,47,47	0
56	MG	1A	3770	1/1	0.87	0.16	46,46,46,46	0
56	MG	2A	3559	1/1	0.87	0.17	39,39,39,39	0
56	MG	2a	1722	1/1	0.87	0.19	53,53,53,53	0
56	MG	2a	1669	1/1	0.87	0.18	41,41,41,41	0
56	MG	2a	1730	1/1	0.87	0.15	52,52,52,52	0
56	MG	2v	101	1/1	0.87	0.12	51,51,51,51	0
56	MG	1A	3508	1/1	0.87	0.20	31,31,31,31	0
56	MG	2A	3822	1/1	0.87	0.24	44,44,44,44	0
56	MG	2v	102	1/1	0.87	0.31	71,71,71,71	0
56	MG	1A	3397	1/1	0.87	0.13	33,33,33,33	0
56	MG	1A	3319	1/1	0.87	0.45	41,41,41,41	0
56	MG	2A	3663	1/1	0.87	0.10	41,41,41,41	0
56	MG	2A	3308	1/1	0.87	0.12	50,50,50,50	0
56	MG	2A	3833	1/1	0.87	0.09	48,48,48,48	0
56	MG	2A	3268	1/1	0.87	0.16	57,57,57,57	0
56	MG	2A	3699	1/1	0.87	0.09	39,39,39,39	0
56	MG	1A	3139	1/1	0.87	0.32	34,34,34,34	0
56	MG	2A	3365	1/1	0.87	0.15	48,48,48,48	0
56	MG	1F	306	1/1	0.87	0.21	42,42,42,42	0
56	MG	1A	3564	1/1	0.87	0.14	28,28,28,28	0
56	MG	2A	3269	1/1	0.87	0.43	44,44,44,44	0
56	MG	1A	3710	1/1	0.87	0.16	17,17,17,17	0
56	MG	1A	3569	1/1	0.87	0.20	26,26,26,26	0
56	MG	1a	3224	1/1	0.87	0.13	40,40,40,40	0
56	MG	1A	3028	1/1	0.87	0.17	32,32,32,32	0
56	MG	2A	3484	1/1	0.87	0.27	55,55,55,55	0
56	MG	1y	101	1/1	0.87	1.09	43,43,43,43	0
56	MG	2a	1709	1/1	0.87	0.20	60,60,60,60	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	1632	1/1	0.87	0.31	62,62,62,62	0
56	MG	2a	1640	1/1	0.87	0.11	56,56,56,56	0
56	MG	2A	3265	1/1	0.87	0.60	46,46,46,46	0
56	MG	2A	3201	1/1	0.87	0.15	40,40,40,40	0
56	MG	2A	3156	1/1	0.87	0.14	46,46,46,46	0
56	MG	1a	3003	1/1	0.87	0.13	55,55,55,55	0
56	MG	2A	3825	1/1	0.87	0.15	31,31,31,31	0
56	MG	2A	3596	1/1	0.87	0.10	37,37,37,37	0
56	MG	2A	3153	1/1	0.87	0.21	47,47,47,47	0
56	MG	1A	3782	1/1	0.87	0.13	18,18,18,18	0
56	MG	2a	1737	1/1	0.87	0.10	52,52,52,52	0
56	MG	2A	3506	1/1	0.87	0.24	56,56,56,56	0
56	MG	1a	3226	1/1	0.87	0.07	63,63,63,63	0
56	MG	2A	3555	1/1	0.87	0.09	33,33,33,33	0
56	MG	1A	3877	1/1	0.87	0.14	43,43,43,43	0
56	MG	2A	3769	1/1	0.87	0.12	68,68,68,68	0
56	MG	1A	3155	1/1	0.87	0.12	29,29,29,29	0
56	MG	2A	3147	1/1	0.87	0.19	41,41,41,41	0
56	MG	2a	1610	1/1	0.87	0.23	64,64,64,64	0
56	MG	2A	3531	1/1	0.87	0.36	49,49,49,49	0
56	MG	2q	202	1/1	0.87	0.14	58,58,58,58	0
56	MG	1A	4004	1/1	0.87	0.20	45,45,45,45	0
56	MG	1A	3982	1/1	0.88	0.20	15,15,15,15	0
56	MG	1A	3976	1/1	0.88	0.13	24,24,24,24	0
56	MG	1A	3273	1/1	0.88	0.16	28,28,28,28	0
56	MG	1A	3453	1/1	0.88	0.15	54,54,54,54	0
56	MG	2a	1817	1/1	0.88	0.15	38,38,38,38	0
56	MG	1A	3889	1/1	0.88	0.11	35,35,35,35	0
56	MG	2A	3378	1/1	0.88	0.12	53,53,53,53	0
56	MG	1A	3935	1/1	0.88	0.13	34,34,34,34	0
56	MG	1A	3861	1/1	0.88	0.16	29,29,29,29	0
56	MG	1A	4070	1/1	0.88	0.17	43,43,43,43	0
56	MG	2A	3174	1/1	0.88	0.13	47,47,47,47	0
56	MG	1a	3166	1/1	0.88	0.13	53,53,53,53	0
56	MG	2A	3240	1/1	0.88	0.20	40,40,40,40	0
56	MG	1A	3631	1/1	0.88	0.17	24,24,24,24	0
56	MG	1A	3879	1/1	0.88	0.10	16,16,16,16	0
56	MG	2A	3260	1/1	0.88	0.19	37,37,37,37	0
56	MG	1a	3213	1/1	0.88	0.09	66,66,66,66	0
56	MG	2A	3667	1/1	0.88	0.11	53,53,53,53	0
56	MG	1a	3086	1/1	0.88	0.10	46,46,46,46	0
56	MG	1A	3677	1/1	0.88	0.16	18,18,18,18	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	3184	1/1	0.88	0.05	46,46,46,46	0
56	MG	1V	202	1/1	0.88	0.42	24,24,24,24	0
56	MG	1A	3145	1/1	0.88	0.41	40,40,40,40	0
56	MG	1A	3798	1/1	0.88	0.08	31,31,31,31	0
56	MG	2a	1734	1/1	0.88	0.12	63,63,63,63	0
56	MG	1V	201	1/1	0.88	0.33	17,17,17,17	0
56	MG	1A	3495	1/1	0.88	0.15	29,29,29,29	0
56	MG	2A	3858	1/1	0.88	0.23	43,43,43,43	0
56	MG	1A	3819	1/1	0.88	0.17	42,42,42,42	0
56	MG	1A	3448	1/1	0.88	0.39	30,30,30,30	0
56	MG	2A	3098	1/1	0.88	0.12	43,43,43,43	0
56	MG	2A	3227	1/1	0.88	0.26	36,36,36,36	0
56	MG	2A	3068	1/1	0.88	0.09	31,31,31,31	0
56	MG	1l	201	1/1	0.88	0.14	22,22,22,22	0
56	MG	1A	3771	1/1	0.88	0.17	30,30,30,30	0
56	MG	2Z	301	1/1	0.88	0.11	61,61,61,61	0
56	MG	1Q	205	1/1	0.88	0.41	44,44,44,44	0
56	MG	2A	3482	1/1	0.88	0.10	40,40,40,40	0
56	MG	1A	3354	1/1	0.88	0.19	29,29,29,29	0
56	MG	1B	207	1/1	0.88	0.13	29,29,29,29	0
56	MG	1A	3673	1/1	0.88	0.23	49,49,49,49	0
56	MG	10	102	1/1	0.88	0.17	38,38,38,38	0
56	MG	2A	3325	1/1	0.88	0.32	60,60,60,60	0
56	MG	2a	1655	1/1	0.88	0.10	58,58,58,58	0
56	MG	2A	3792	1/1	0.88	0.25	52,52,52,52	0
56	MG	1a	3098	1/1	0.88	0.17	38,38,38,38	0
56	MG	2A	3096	1/1	0.88	0.11	38,38,38,38	0
56	MG	2A	3768	1/1	0.88	0.37	60,60,60,60	0
56	MG	1w	101	1/1	0.88	0.11	49,49,49,49	0
56	MG	2a	1701	1/1	0.88	0.16	64,64,64,64	0
56	MG	2A	3871	1/1	0.88	0.16	34,34,34,34	0
56	MG	2a	1678	1/1	0.88	0.10	57,57,57,57	0
56	MG	2A	3478	1/1	0.88	0.17	59,59,59,59	0
56	MG	1A	3909	1/1	0.88	0.13	19,19,19,19	0
56	MG	1A	3032	1/1	0.88	0.22	44,44,44,44	0
56	MG	2A	3406	1/1	0.88	0.08	37,37,37,37	0
56	MG	1A	3863	1/1	0.88	0.11	20,20,20,20	0
56	MG	2A	3076	1/1	0.88	0.30	42,42,42,42	0
56	MG	1A	3347	1/1	0.88	0.21	9,9,9,9	0
56	MG	2A	3193	1/1	0.88	0.16	40,40,40,40	0
56	MG	2A	3019	1/1	0.88	0.07	47,47,47,47	0
56	MG	2A	3304	1/1	0.88	0.39	50,50,50,50	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3487	1/1	0.88	0.16	49,49,49,49	0
56	MG	1A	3807	1/1	0.88	0.16	40,40,40,40	0
56	MG	1A	3534	1/1	0.88	0.51	50,50,50,50	0
56	MG	2A	3218	1/1	0.88	0.12	52,52,52,52	0
56	MG	1A	3206	1/1	0.88	0.24	16,16,16,16	0
56	MG	1a	3033	1/1	0.88	0.17	52,52,52,52	0
56	MG	1A	3480	1/1	0.88	0.16	49,49,49,49	0
56	MG	2A	3290	1/1	0.88	0.17	39,39,39,39	0
56	MG	1A	3039	1/1	0.88	0.46	29,29,29,29	0
56	MG	1A	3282	1/1	0.88	0.40	22,22,22,22	0
56	MG	2A	3023	1/1	0.88	0.08	42,42,42,42	0
56	MG	1A	3787	1/1	0.88	0.13	36,36,36,36	0
56	MG	2A	3344	1/1	0.88	0.21	49,49,49,49	0
56	MG	2A	3182	1/1	0.88	0.18	40,40,40,40	0
56	MG	2A	3435	1/1	0.88	0.24	51,51,51,51	0
56	MG	25	101	1/1	0.88	0.12	33,33,33,33	0
56	MG	2A	3173	1/1	0.88	0.13	33,33,33,33	0
56	MG	1A	3107	1/1	0.88	0.19	40,40,40,40	0
56	MG	1A	3471	1/1	0.88	0.20	50,50,50,50	0
56	MG	2A	3468	1/1	0.88	0.75	45,45,45,45	0
56	MG	1A	3111	1/1	0.88	0.13	28,28,28,28	0
56	MG	1A	3946	1/1	0.88	0.12	35,35,35,35	0
56	MG	1A	3823	1/1	0.88	0.17	30,30,30,30	0
56	MG	2A	3371	1/1	0.88	0.58	43,43,43,43	0
56	MG	2A	3728	1/1	0.88	0.28	66,66,66,66	0
56	MG	1A	4014	1/1	0.88	0.15	21,21,21,21	0
56	MG	2A	3144	1/1	0.88	0.08	43,43,43,43	0
56	MG	1F	305	1/1	0.88	0.22	35,35,35,35	0
56	MG	1a	3203	1/1	0.89	0.13	32,32,32,32	0
56	MG	1A	3474	1/1	0.89	0.11	38,38,38,38	0
56	MG	1A	3244	1/1	0.89	0.13	38,38,38,38	0
56	MG	2a	1672	1/1	0.89	0.27	43,43,43,43	0
56	MG	1W	203	1/1	0.89	0.15	36,36,36,36	0
56	MG	2a	1614	1/1	0.89	0.08	53,53,53,53	0
56	MG	1A	3830	1/1	0.89	0.09	28,28,28,28	0
56	MG	2A	3180	1/1	0.89	0.31	48,48,48,48	0
56	MG	2A	3291	1/1	0.89	0.08	32,32,32,32	0
56	MG	2A	3697	1/1	0.89	0.11	53,53,53,53	0
56	MG	1A	4043	1/1	0.89	0.14	30,30,30,30	0
56	MG	1A	3514	1/1	0.89	0.14	15,15,15,15	0
56	MG	1a	3053	1/1	0.89	0.10	62,62,62,62	0
56	MG	1A	3203	1/1	0.89	0.26	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	3596	1/1	0.89	0.37	43,43,43,43	0
56	MG	1A	3044	1/1	0.89	0.37	37,37,37,37	0
56	MG	1A	3721	1/1	0.89	0.18	24,24,24,24	0
56	MG	1A	3498	1/1	0.89	0.17	57,57,57,57	0
56	MG	2A	3686	1/1	0.89	0.15	41,41,41,41	0
56	MG	2A	3340	1/1	0.89	0.11	38,38,38,38	0
56	MG	2A	3472	1/1	0.89	0.72	64,64,64,64	0
56	MG	1A	3178	1/1	0.89	0.10	45,45,45,45	0
56	MG	2A	3319	1/1	0.89	0.09	32,32,32,32	0
56	MG	2A	3199	1/1	0.89	0.14	27,27,27,27	0
56	MG	2A	3810	1/1	0.89	0.23	49,49,49,49	0
56	MG	2A	3658	1/1	0.89	0.19	61,61,61,61	0
56	MG	1A	3352	1/1	0.89	0.13	28,28,28,28	0
56	MG	1A	3314	1/1	0.89	0.12	39,39,39,39	0
56	MG	2A	3724	1/1	0.89	0.15	45,45,45,45	0
56	MG	1A	3395	1/1	0.89	0.16	32,32,32,32	0
56	MG	1A	4030	1/1	0.89	0.08	20,20,20,20	0
56	MG	1E	302	1/1	0.89	0.41	30,30,30,30	0
56	MG	1A	3392	1/1	0.89	0.22	24,24,24,24	0
56	MG	1a	3176	1/1	0.89	0.10	45,45,45,45	0
56	MG	2x	101	1/1	0.89	0.11	55,55,55,55	0
56	MG	2A	3250	1/1	0.89	0.18	46,46,46,46	0
56	MG	1a	3093	1/1	0.89	0.23	40,40,40,40	0
56	MG	1A	3425	1/1	0.89	0.16	43,43,43,43	0
56	MG	2A	3823	1/1	0.89	0.16	38,38,38,38	0
56	MG	1A	3170	1/1	0.89	0.12	30,30,30,30	0
56	MG	1A	3049	1/1	0.89	0.11	17,17,17,17	0
56	MG	2A	3445	1/1	0.89	0.68	57,57,57,57	0
56	MG	1A	3038	1/1	0.89	0.13	27,27,27,27	0
56	MG	1x	105	1/1	0.89	0.10	60,60,60,60	0
56	MG	2A	3328	1/1	0.89	0.40	51,51,51,51	0
56	MG	2a	1765	1/1	0.89	0.10	45,45,45,45	0
56	MG	1A	3653	1/1	0.89	0.12	19,19,19,19	0
56	MG	2A	3213	1/1	0.89	0.30	38,38,38,38	0
56	MG	1A	3645	1/1	0.89	0.15	19,19,19,19	0
56	MG	1A	3791	1/1	0.89	0.16	25,25,25,25	0
56	MG	2a	1779	1/1	0.89	0.09	51,51,51,51	0
58	ZN	24	501	1/1	0.89	0.07	108,108,108,108	0
56	MG	11	101	1/1	0.89	0.09	39,39,39,39	0
56	MG	1A	3887	1/1	0.89	0.10	21,21,21,21	0
56	MG	2A	3594	1/1	0.89	0.16	42,42,42,42	0
56	MG	1A	3592	1/1	0.89	0.28	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	1a	3178	1/1	0.89	0.14	45,45,45,45	0
56	MG	2Q	202	1/1	0.89	0.36	39,39,39,39	0
56	MG	1A	3949	1/1	0.89	0.13	40,40,40,40	0
56	MG	2a	1696	1/1	0.89	0.14	33,33,33,33	0
56	MG	1A	3927	1/1	0.89	0.10	54,54,54,54	0
56	MG	1x	110	1/1	0.89	0.10	43,43,43,43	0
56	MG	2A	3684	1/1	0.89	0.06	64,64,64,64	0
56	MG	1r	101	1/1	0.89	0.10	48,48,48,48	0
56	MG	1a	3105	1/1	0.89	0.14	51,51,51,51	0
56	MG	1A	3307	1/1	0.89	0.14	41,41,41,41	0
56	MG	2a	1755	1/1	0.89	0.10	40,40,40,40	0
56	MG	1B	213	1/1	0.89	0.08	57,57,57,57	0
56	MG	2A	3847	1/1	0.89	0.17	62,62,62,62	0
56	MG	2A	3305	1/1	0.89	0.11	44,44,44,44	0
56	MG	1A	3355	1/1	0.89	0.15	42,42,42,42	0
56	MG	1A	3847	1/1	0.89	0.10	38,38,38,38	0
56	MG	1A	3298	1/1	0.89	0.11	32,32,32,32	0
56	MG	1P	206	1/1	0.89	0.13	17,17,17,17	0
56	MG	2A	3192	1/1	0.89	0.15	38,38,38,38	0
56	MG	2A	3072	1/1	0.89	0.19	52,52,52,52	0
56	MG	1A	3729	1/1	0.89	0.26	39,39,39,39	0
56	MG	2A	3121	1/1	0.89	0.20	49,49,49,49	0
56	MG	1A	3970	1/1	0.89	0.12	19,19,19,19	0
56	MG	1A	3222	1/1	0.89	0.13	25,25,25,25	0
56	MG	2A	3386	1/1	0.89	0.16	41,41,41,41	0
56	MG	1A	3189	1/1	0.89	0.14	18,18,18,18	0
56	MG	1a	3085	1/1	0.89	0.10	41,41,41,41	0
56	MG	1a	3196	1/1	0.89	0.07	38,38,38,38	0
56	MG	1A	3903	1/1	0.89	0.21	18,18,18,18	0
56	MG	2a	1716	1/1	0.89	0.14	44,44,44,44	0
56	MG	1A	3664	1/1	0.89	0.17	20,20,20,20	0
56	MG	1A	3386	1/1	0.89	0.17	38,38,38,38	0
56	MG	1a	3100	1/1	0.89	0.12	42,42,42,42	0
56	MG	1A	3257	1/1	0.89	0.14	33,33,33,33	0
56	MG	2a	1719	1/1	0.89	0.10	49,49,49,49	0
56	MG	1a	3137	1/1	0.89	0.13	43,43,43,43	0
56	MG	15	101	1/1	0.89	0.28	34,34,34,34	0
56	MG	2A	3279	1/1	0.89	0.14	32,32,32,32	0
56	MG	1A	3775	1/1	0.89	0.26	10,10,10,10	0
56	MG	2a	1827	1/1	0.90	0.11	45,45,45,45	0
56	MG	2F	303	1/1	0.90	0.24	30,30,30,30	0
56	MG	2A	3275	1/1	0.90	0.24	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	1A	3559	1/1	0.90	0.20	42,42,42,42	0
56	MG	2A	3720	1/1	0.90	0.11	46,46,46,46	0
56	MG	1A	3617	1/1	0.90	0.31	18,18,18,18	0
56	MG	1A	3808	1/1	0.90	0.09	28,28,28,28	0
56	MG	1A	3384	1/1	0.90	0.14	37,37,37,37	0
56	MG	2A	3611	1/1	0.90	0.09	27,27,27,27	0
56	MG	2A	3623	1/1	0.90	0.15	44,44,44,44	0
56	MG	2A	3313	1/1	0.90	0.26	52,52,52,52	0
56	MG	2a	1731	1/1	0.90	0.14	42,42,42,42	0
56	MG	1A	3284	1/1	0.90	0.19	16,16,16,16	0
56	MG	2a	1796	1/1	0.90	0.22	48,48,48,48	0
56	MG	2A	3574	1/1	0.90	0.09	36,36,36,36	0
56	MG	2A	3426	1/1	0.90	0.15	42,42,42,42	0
56	MG	1a	3112	1/1	0.90	0.11	48,48,48,48	0
56	MG	1A	3973	1/1	0.90	0.13	37,37,37,37	0
56	MG	2A	3170	1/1	0.90	0.08	64,64,64,64	0
56	MG	2a	1707	1/1	0.90	0.20	52,52,52,52	0
56	MG	1a	3059	1/1	0.90	0.07	48,48,48,48	0
56	MG	1E	307	1/1	0.90	0.45	36,36,36,36	0
56	MG	1a	3123	1/1	0.90	0.15	53,53,53,53	0
56	MG	1A	3454	1/1	0.90	0.21	31,31,31,31	0
56	MG	2A	3230	1/1	0.90	0.26	36,36,36,36	0
56	MG	1A	3463	1/1	0.90	0.39	25,25,25,25	0
56	MG	1A	3619	1/1	0.90	0.19	25,25,25,25	0
56	MG	2A	3845	1/1	0.90	0.10	49,49,49,49	0
56	MG	1a	3162	1/1	0.90	0.07	30,30,30,30	0
56	MG	2a	1715	1/1	0.90	0.21	51,51,51,51	0
56	MG	1A	3919	1/1	0.90	0.12	38,38,38,38	0
56	MG	1A	3871	1/1	0.90	0.32	16,16,16,16	0
56	MG	2A	3733	1/1	0.90	0.68	73,73,73,73	0
56	MG	1F	304	1/1	0.90	0.26	31,31,31,31	0
56	MG	2A	3249	1/1	0.90	0.26	54,54,54,54	0
56	MG	1W	201	1/1	0.90	0.23	24,24,24,24	0
56	MG	1A	4064	1/1	0.90	0.24	36,36,36,36	0
56	MG	1A	3380	1/1	0.90	0.21	32,32,32,32	0
56	MG	1a	3143	1/1	0.90	0.08	48,48,48,48	0
56	MG	2a	1623	1/1	0.90	0.18	44,44,44,44	0
56	MG	2a	1708	1/1	0.90	0.09	54,54,54,54	0
56	MG	2A	3688	1/1	0.90	0.12	58,58,58,58	0
56	MG	2A	3543	1/1	0.90	0.09	47,47,47,47	0
56	MG	1A	4013	1/1	0.90	0.09	40,40,40,40	0
56	MG	2a	1703	1/1	0.90	0.12	69,69,69,69	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3868	1/1	0.90	0.10	30,30,30,30	0
56	MG	1A	3885	1/1	0.90	0.09	9,9,9,9	0
56	MG	2A	3355	1/1	0.90	0.19	42,42,42,42	0
56	MG	2A	3467	1/1	0.90	0.11	50,50,50,50	0
56	MG	2A	3107	1/1	0.90	0.41	44,44,44,44	0
56	MG	2a	1812	1/1	0.90	0.18	42,42,42,42	0
56	MG	1A	3788	1/1	0.90	0.12	27,27,27,27	0
56	MG	1A	3932	1/1	0.90	0.12	37,37,37,37	0
56	MG	2a	1775	1/1	0.90	0.08	49,49,49,49	0
56	MG	1y	105	1/1	0.90	0.25	53,53,53,53	0
56	MG	2A	3836	1/1	0.90	0.09	33,33,33,33	0
56	MG	2a	1616	1/1	0.90	0.16	55,55,55,55	0
56	MG	1b	301	1/1	0.90	0.10	52,52,52,52	0
56	MG	1A	3637	1/1	0.90	0.12	34,34,34,34	0
56	MG	1a	3056	1/1	0.90	0.13	45,45,45,45	0
56	MG	1A	3017	1/1	0.90	0.14	17,17,17,17	0
56	MG	1A	3313	1/1	0.90	0.14	31,31,31,31	0
56	MG	1A	3377	1/1	0.90	0.11	38,38,38,38	0
56	MG	1A	3269	1/1	0.90	0.18	22,22,22,22	0
56	MG	1a	3145	1/1	0.90	0.14	32,32,32,32	0
56	MG	2A	3451	1/1	0.90	0.10	37,37,37,37	0
56	MG	1A	3623	1/1	0.90	0.14	20,20,20,20	0
56	MG	2D	306	1/1	0.90	0.12	35,35,35,35	0
56	MG	1A	3567	1/1	0.90	0.22	37,37,37,37	0
56	MG	1A	3756	1/1	0.90	0.16	31,31,31,31	0
56	MG	1a	3174	1/1	0.90	0.06	48,48,48,48	0
56	MG	2A	3434	1/1	0.90	0.14	30,30,30,30	0
56	MG	1A	4026	1/1	0.90	0.13	24,24,24,24	0
56	MG	2A	3780	1/1	0.90	0.13	48,48,48,48	0
56	MG	1A	3033	1/1	0.90	0.10	21,21,21,21	0
56	MG	1A	3229	1/1	0.90	0.15	29,29,29,29	0
56	MG	1A	3093	1/1	0.90	0.51	32,32,32,32	0
56	MG	1A	3914	1/1	0.90	0.19	44,44,44,44	0
56	MG	2A	3496	1/1	0.90	0.12	28,28,28,28	0
56	MG	2a	1615	1/1	0.90	0.20	37,37,37,37	0
56	MG	1w	103	1/1	0.90	0.14	44,44,44,44	0
56	MG	2A	3409	1/1	0.90	0.14	41,41,41,41	0
56	MG	1a	3011	1/1	0.90	0.14	49,49,49,49	0
56	MG	2A	3807	1/1	0.90	0.14	46,46,46,46	0
56	MG	2A	3336	1/1	0.90	0.62	47,47,47,47	0
56	MG	1A	3235	1/1	0.90	0.12	47,47,47,47	0
56	MG	2B	212	1/1	0.90	0.09	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	3619	1/1	0.90	0.08	46,46,46,46	0
56	MG	1B	220	1/1	0.90	0.15	32,32,32,32	0
56	MG	1a	3186	1/1	0.90	0.08	66,66,66,66	0
56	MG	2A	3366	1/1	0.90	0.40	39,39,39,39	0
56	MG	2A	3513	1/1	0.90	0.10	32,32,32,32	0
56	MG	2A	3729	1/1	0.90	0.46	66,66,66,66	0
56	MG	2A	3306	1/1	0.90	0.09	35,35,35,35	0
56	MG	1A	4044	1/1	0.90	0.17	29,29,29,29	0
56	MG	2a	1713	1/1	0.90	0.13	59,59,59,59	0
56	MG	1A	3724	1/1	0.90	0.10	33,33,33,33	0
56	MG	10	101	1/1	0.90	0.30	32,32,32,32	0
56	MG	1A	3657	1/1	0.90	0.23	24,24,24,24	0
56	MG	26	102	1/1	0.90	0.31	58,58,58,58	0
56	MG	2A	3715	1/1	0.90	0.17	48,48,48,48	0
56	MG	1A	3279	1/1	0.90	0.17	40,40,40,40	0
56	MG	2E	305	1/1	0.90	0.10	36,36,36,36	0
56	MG	2A	3186	1/1	0.90	0.19	36,36,36,36	0
56	MG	1a	3168	1/1	0.90	0.08	47,47,47,47	0
56	MG	2a	1631	1/1	0.90	0.18	54,54,54,54	0
56	MG	2a	1776	1/1	0.90	0.12	53,53,53,53	0
56	MG	2a	1647	1/1	0.90	0.10	52,52,52,52	0
56	MG	2a	1609	1/1	0.90	0.16	50,50,50,50	0
56	MG	2A	3626	1/1	0.90	0.13	51,51,51,51	0
56	MG	1V	203	1/1	0.90	0.55	24,24,24,24	0
56	MG	1N	203	1/1	0.90	0.21	34,34,34,34	0
56	MG	2A	3746	1/1	0.90	0.10	34,34,34,34	0
56	MG	2A	3015	1/1	0.90	0.34	30,30,30,30	0
56	MG	2A	3570	1/1	0.90	0.17	56,56,56,56	0
56	MG	1A	3574	1/1	0.90	0.41	21,21,21,21	0
56	MG	1A	3980	1/1	0.90	0.08	18,18,18,18	0
56	MG	1x	107	1/1	0.90	0.12	59,59,59,59	0
56	MG	1A	3339	1/1	0.90	0.08	21,21,21,21	0
56	MG	1A	3984	1/1	0.90	0.09	60,60,60,60	0
56	MG	1A	3963	1/1	0.90	0.17	36,36,36,36	0
56	MG	1A	3225	1/1	0.90	0.15	46,46,46,46	0
56	MG	1A	3948	1/1	0.90	0.10	17,17,17,17	0
56	MG	1w	102	1/1	0.90	0.25	48,48,48,48	0
56	MG	1A	3693	1/1	0.90	0.17	5,5,5,5	0
56	MG	2A	3598	1/1	0.90	0.07	47,47,47,47	0
56	MG	2A	3668	1/1	0.90	0.10	38,38,38,38	0
56	MG	2l	203	1/1	0.90	0.12	59,59,59,59	0
56	MG	2A	3782	1/1	0.90	0.07	53,53,53,53	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3383	1/1	0.90	0.12	34,34,34,34	0
56	MG	19	103	1/1	0.90	0.09	42,42,42,42	0
56	MG	2A	3145	1/1	0.90	0.23	42,42,42,42	0
56	MG	2A	3874	1/1	0.90	0.09	53,53,53,53	0
56	MG	2A	3683	1/1	0.90	0.08	53,53,53,53	0
56	MG	2A	3368	1/1	0.90	0.15	30,30,30,30	0
56	MG	2A	3164	1/1	0.90	0.13	54,54,54,54	0
56	MG	1a	3070	1/1	0.90	0.21	47,47,47,47	0
56	MG	1A	3301	1/1	0.91	0.15	38,38,38,38	0
56	MG	2A	3338	1/1	0.91	0.09	64,64,64,64	0
56	MG	2A	3546	1/1	0.91	0.11	22,22,22,22	0
56	MG	1B	226	1/1	0.91	0.08	51,51,51,51	0
56	MG	2a	1626	1/1	0.91	0.40	56,56,56,56	0
56	MG	1A	3271	1/1	0.91	0.20	28,28,28,28	0
56	MG	2A	3108	1/1	0.91	0.16	50,50,50,50	0
56	MG	1a	3010	1/1	0.91	0.13	58,58,58,58	0
56	MG	1A	3516	1/1	0.91	0.13	26,26,26,26	0
56	MG	1A	3003	1/1	0.91	0.12	15,15,15,15	0
56	MG	2A	3353	1/1	0.91	0.28	51,51,51,51	0
56	MG	2A	3586	1/1	0.91	0.17	43,43,43,43	0
56	MG	2A	3844	1/1	0.91	0.11	58,58,58,58	0
56	MG	1a	3155	1/1	0.91	0.11	29,29,29,29	0
56	MG	1a	3142	1/1	0.91	0.10	49,49,49,49	0
56	MG	2B	201	1/1	0.91	0.10	57,57,57,57	0
56	MG	2A	3003	1/1	0.91	0.14	41,41,41,41	0
56	MG	2A	3204	1/1	0.91	0.12	39,39,39,39	0
56	MG	1A	3875	1/1	0.91	0.19	33,33,33,33	0
56	MG	1a	3081	1/1	0.91	0.14	43,43,43,43	0
56	MG	2A	3577	1/1	0.91	0.13	41,41,41,41	0
56	MG	2A	3631	1/1	0.91	0.16	41,41,41,41	0
56	MG	2A	3258	1/1	0.91	0.55	41,41,41,41	0
56	MG	2a	1802	1/1	0.91	0.14	40,40,40,40	0
56	MG	1A	3553	1/1	0.91	0.19	36,36,36,36	0
56	MG	1A	3053	1/1	0.91	0.19	45,45,45,45	0
56	MG	2A	3349	1/1	0.91	0.13	43,43,43,43	0
56	MG	1A	3502	1/1	0.91	0.23	44,44,44,44	0
56	MG	1y	102	1/1	0.91	0.17	60,60,60,60	0
56	MG	1A	3156	1/1	0.91	0.09	30,30,30,30	0
56	MG	1A	3647	1/1	0.91	0.08	27,27,27,27	0
56	MG	1A	3620	1/1	0.91	0.23	29,29,29,29	0
56	MG	1A	3810	1/1	0.91	0.07	28,28,28,28	0
56	MG	2A	3109	1/1	0.91	0.12	36,36,36,36	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1F	307	1/1	0.91	0.11	23,23,23,23	0
56	MG	1A	4065	1/1	0.91	0.18	14,14,14,14	0
56	MG	2A	3869	1/1	0.91	0.16	49,49,49,49	0
56	MG	1e	202	1/1	0.91	0.18	45,45,45,45	0
56	MG	2A	3760	1/1	0.91	0.12	35,35,35,35	0
56	MG	2A	3228	1/1	0.91	0.80	42,42,42,42	0
56	MG	2A	3567	1/1	0.91	0.08	35,35,35,35	0
56	MG	1a	3014	1/1	0.91	0.10	48,48,48,48	0
56	MG	2A	3324	1/1	0.91	0.27	45,45,45,45	0
56	MG	25	103	1/1	0.91	0.14	25,25,25,25	0
56	MG	1A	3142	1/1	0.91	0.11	44,44,44,44	0
56	MG	2A	3717	1/1	0.91	0.13	44,44,44,44	0
56	MG	1A	3334	1/1	0.91	0.11	35,35,35,35	0
56	MG	1O	202	1/1	0.91	0.12	41,41,41,41	0
56	MG	1A	3115	1/1	0.91	0.36	13,13,13,13	0
56	MG	2A	3575	1/1	0.91	0.11	43,43,43,43	0
56	MG	2A	3834	1/1	0.91	0.08	24,24,24,24	0
56	MG	1A	3697	1/1	0.91	0.18	36,36,36,36	0
56	MG	2a	1782	1/1	0.91	0.08	40,40,40,40	0
56	MG	1A	3382	1/1	0.91	0.14	36,36,36,36	0
56	MG	2A	3803	1/1	0.91	0.15	54,54,54,54	0
56	MG	1A	3194	1/1	0.91	0.35	28,28,28,28	0
56	MG	2a	1745	1/1	0.91	0.12	62,62,62,62	0
58	ZN	2Y	501	1/1	0.91	0.13	83,83,83,83	0
56	MG	2a	1677	1/1	0.91	0.10	60,60,60,60	0
56	MG	2A	3067	1/1	0.91	0.28	36,36,36,36	0
56	MG	2A	3500	1/1	0.91	0.16	53,53,53,53	0
56	MG	2a	1792	1/1	0.91	0.22	66,66,66,66	0
56	MG	1E	305	1/1	0.91	0.26	26,26,26,26	0
56	MG	1A	3335	1/1	0.91	0.17	23,23,23,23	0
56	MG	2A	3292	1/1	0.91	0.16	31,31,31,31	0
56	MG	1a	3006	1/1	0.91	0.10	29,29,29,29	0
56	MG	1a	3078	1/1	0.91	0.08	35,35,35,35	0
56	MG	1A	3052	1/1	0.91	0.14	48,48,48,48	0
56	MG	2a	1641	1/1	0.91	0.11	47,47,47,47	0
56	MG	2a	1806	1/1	0.91	0.11	63,63,63,63	0
56	MG	1A	3351	1/1	0.91	0.37	25,25,25,25	0
56	MG	1A	3933	1/1	0.91	0.20	58,58,58,58	0
56	MG	2a	1789	1/1	0.91	0.13	54,54,54,54	0
56	MG	17	103	1/1	0.91	0.25	28,28,28,28	0
56	MG	1a	3029	1/1	0.91	0.14	33,33,33,33	0
56	MG	1a	3228	1/1	0.91	0.10	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	1825	1/1	0.91	0.10	58,58,58,58	0
56	MG	2A	3385	1/1	0.91	0.15	52,52,52,52	0
56	MG	1F	301	1/1	0.91	0.49	25,25,25,25	0
56	MG	2A	3481	1/1	0.91	0.12	44,44,44,44	0
56	MG	2A	3128	1/1	0.91	0.65	44,44,44,44	0
56	MG	1A	3688	1/1	0.91	0.12	19,19,19,19	0
56	MG	1a	3074	1/1	0.91	0.09	55,55,55,55	0
56	MG	1A	3778	1/1	0.91	0.13	26,26,26,26	0
56	MG	1B	208	1/1	0.91	0.12	44,44,44,44	0
56	MG	1P	204	1/1	0.91	0.18	18,18,18,18	0
56	MG	1A	3635	1/1	0.91	0.10	26,26,26,26	0
56	MG	2a	1732	1/1	0.91	0.12	52,52,52,52	0
56	MG	2A	3341	1/1	0.91	0.08	52,52,52,52	0
56	MG	10	103	1/1	0.91	0.18	32,32,32,32	0
56	MG	2A	3430	1/1	0.91	0.25	45,45,45,45	0
56	MG	2A	3830	1/1	0.91	0.13	58,58,58,58	0
56	MG	1a	3158	1/1	0.91	0.12	51,51,51,51	0
56	MG	1A	3372	1/1	0.91	0.13	37,37,37,37	0
56	MG	1A	3609	1/1	0.91	0.40	54,54,54,54	0
56	MG	2A	3050	1/1	0.91	0.13	53,53,53,53	0
56	MG	2A	3008	1/1	0.91	0.08	49,49,49,49	0
56	MG	2A	3011	1/1	0.91	0.10	36,36,36,36	0
56	MG	1A	3800	1/1	0.91	0.11	31,31,31,31	0
56	MG	1a	3094	1/1	0.91	0.17	29,29,29,29	0
56	MG	2A	3059	1/1	0.91	0.12	34,34,34,34	0
56	MG	1A	3461	1/1	0.91	0.25	36,36,36,36	0
56	MG	1a	3041	1/1	0.91	0.10	52,52,52,52	0
56	MG	2A	3233	1/1	0.91	0.20	47,47,47,47	0
56	MG	1A	3994	1/1	0.91	0.07	50,50,50,50	0
56	MG	2A	3791	1/1	0.91	0.18	46,46,46,46	0
56	MG	1A	3413	1/1	0.91	0.14	21,21,21,21	0
56	MG	2A	3873	1/1	0.91	0.18	44,44,44,44	0
56	MG	2A	3856	1/1	0.91	0.07	45,45,45,45	0
56	MG	2Q	205	1/1	0.91	0.50	50,50,50,50	0
56	MG	20	102	1/1	0.91	0.21	68,68,68,68	0
56	MG	2A	3685	1/1	0.91	0.07	27,27,27,27	0
56	MG	1G	201	1/1	0.91	0.10	34,34,34,34	0
56	MG	2A	3136	1/1	0.91	0.09	43,43,43,43	0
56	MG	2a	1688	1/1	0.91	0.11	42,42,42,42	0
56	MG	2A	3532	1/1	0.91	0.06	31,31,31,31	0
56	MG	1A	3317	1/1	0.91	0.19	44,44,44,44	0
56	MG	1Z	301	1/1	0.91	0.22	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	3330	1/1	0.91	0.23	17,17,17,17	0
56	MG	2A	3758	1/1	0.91	0.11	47,47,47,47	0
56	MG	1B	219	1/1	0.91	0.15	53,53,53,53	0
56	MG	2A	3642	1/1	0.91	0.13	56,56,56,56	0
56	MG	2a	1741	1/1	0.91	0.12	55,55,55,55	0
56	MG	1A	3610	1/1	0.91	0.13	27,27,27,27	0
56	MG	1A	4055	1/1	0.91	0.09	41,41,41,41	0
56	MG	1a	3220	1/1	0.91	0.10	46,46,46,46	0
56	MG	2A	3298	1/1	0.91	0.15	68,68,68,68	0
56	MG	2D	307	1/1	0.91	0.10	34,34,34,34	0
56	MG	2A	3617	1/1	0.91	0.11	36,36,36,36	0
56	MG	1A	3964	1/1	0.91	0.21	63,63,63,63	0
56	MG	2a	1739	1/1	0.91	0.10	48,48,48,48	0
56	MG	1a	3071	1/1	0.91	0.14	36,36,36,36	0
56	MG	1A	3898	1/1	0.91	0.20	42,42,42,42	0
56	MG	1A	3315	1/1	0.91	0.13	42,42,42,42	0
56	MG	2a	1735	1/1	0.91	0.23	46,46,46,46	0
56	MG	1A	3095	1/1	0.91	0.11	26,26,26,26	0
56	MG	2a	1793	1/1	0.91	0.23	55,55,55,55	0
56	MG	1P	208	1/1	0.91	0.19	45,45,45,45	0
56	MG	2A	3185	1/1	0.91	0.27	41,41,41,41	0
56	MG	1A	3799	1/1	0.91	0.06	30,30,30,30	0
56	MG	1A	3295	1/1	0.91	0.14	30,30,30,30	0
56	MG	2A	3772	1/1	0.91	0.09	55,55,55,55	0
56	MG	1A	3660	1/1	0.91	0.14	60,60,60,60	0
56	MG	1a	3110	1/1	0.91	0.14	56,56,56,56	0
56	MG	2A	3131	1/1	0.91	0.10	58,58,58,58	0
56	MG	1E	301	1/1	0.91	0.17	25,25,25,25	0
56	MG	1A	3081	1/1	0.91	0.15	40,40,40,40	0
56	MG	1A	3813	1/1	0.91	0.06	24,24,24,24	0
56	MG	2A	3431	1/1	0.91	0.17	37,37,37,37	0
56	MG	1A	3573	1/1	0.91	0.10	40,40,40,40	0
56	MG	2A	3495	1/1	0.91	0.13	55,55,55,55	0
56	MG	2a	1761	1/1	0.91	0.04	68,68,68,68	0
56	MG	23	101	1/1	0.91	0.30	43,43,43,43	0
56	MG	1A	3549	1/1	0.91	0.13	21,21,21,21	0
56	MG	2A	3816	1/1	0.91	0.12	40,40,40,40	0
56	MG	2a	1808	1/1	0.91	0.21	52,52,52,52	0
56	MG	15	106	1/1	0.91	0.38	30,30,30,30	0
56	MG	1A	4056	1/1	0.91	0.12	43,43,43,43	0
56	MG	2A	3868	1/1	0.91	0.10	32,32,32,32	0
56	MG	1a	3082	1/1	0.91	0.12	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	4059	1/1	0.91	0.12	30,30,30,30	0
56	MG	1a	3024	1/1	0.91	0.25	50,50,50,50	0
56	MG	2A	3401	1/1	0.91	0.10	33,33,33,33	0
56	MG	1a	3049	1/1	0.92	0.09	47,47,47,47	0
56	MG	1A	3154	1/1	0.92	0.22	25,25,25,25	0
56	MG	2A	3016	1/1	0.92	0.12	43,43,43,43	0
56	MG	1A	3369	1/1	0.92	0.14	37,37,37,37	0
56	MG	2F	305	1/1	0.92	0.10	46,46,46,46	0
56	MG	2A	3607	1/1	0.92	0.20	32,32,32,32	0
56	MG	1A	3323	1/1	0.92	0.18	45,45,45,45	0
56	MG	2A	3022	1/1	0.92	0.23	49,49,49,49	0
56	MG	1A	3456	1/1	0.92	0.20	40,40,40,40	0
56	MG	1a	3134	1/1	0.92	0.29	45,45,45,45	0
56	MG	2A	3692	1/1	0.92	0.14	29,29,29,29	0
56	MG	2A	3194	1/1	0.92	0.16	38,38,38,38	0
56	MG	1A	3558	1/1	0.92	0.33	21,21,21,21	0
56	MG	1A	3031	1/1	0.92	0.35	20,20,20,20	0
56	MG	28	101	1/1	0.92	0.12	58,58,58,58	0
56	MG	1A	3680	1/1	0.92	0.11	18,18,18,18	0
56	MG	1A	3510	1/1	0.92	0.29	26,26,26,26	0
56	MG	1a	3126	1/1	0.92	0.14	39,39,39,39	0
56	MG	2A	3062	1/1	0.92	0.09	60,60,60,60	0
56	MG	1A	3251	1/1	0.92	0.09	32,32,32,32	0
56	MG	1A	3499	1/1	0.92	0.10	50,50,50,50	0
56	MG	2A	3606	1/1	0.92	0.15	45,45,45,45	0
56	MG	2A	3043	1/1	0.92	0.18	35,35,35,35	0
56	MG	1A	3760	1/1	0.92	0.12	14,14,14,14	0
56	MG	1F	302	1/1	0.92	0.38	22,22,22,22	0
56	MG	1A	3530	1/1	0.92	0.15	33,33,33,33	0
56	MG	1A	4052	1/1	0.92	0.21	55,55,55,55	0
56	MG	1a	3099	1/1	0.92	0.08	39,39,39,39	0
56	MG	1A	3162	1/1	0.92	0.15	18,18,18,18	0
56	MG	1A	4045	1/1	0.92	0.16	35,35,35,35	0
56	MG	2A	3342	1/1	0.92	0.18	55,55,55,55	0
56	MG	1A	3293	1/1	0.92	0.13	28,28,28,28	0
56	MG	2A	3630	1/1	0.92	0.36	37,37,37,37	0
56	MG	1A	3666	1/1	0.92	0.13	39,39,39,39	0
56	MG	1A	3318	1/1	0.92	0.15	45,45,45,45	0
56	MG	2A	3680	1/1	0.92	0.15	50,50,50,50	0
56	MG	1A	3904	1/1	0.92	0.35	19,19,19,19	0
56	MG	1A	3507	1/1	0.92	0.12	35,35,35,35	0
56	MG	1A	3152	1/1	0.92	0.09	18,18,18,18	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	2F	302	1/1	0.92	0.33	53,53,53,53	0
56	MG	2A	3731	1/1	0.92	0.21	45,45,45,45	0
56	MG	2A	3711	1/1	0.92	0.18	51,51,51,51	0
56	MG	2a	1634	1/1	0.92	0.09	50,50,50,50	0
56	MG	2A	3517	1/1	0.92	0.08	37,37,37,37	0
56	MG	2A	3318	1/1	0.92	0.27	45,45,45,45	0
56	MG	2B	218	1/1	0.92	0.12	61,61,61,61	0
56	MG	1D	306	1/1	0.92	0.10	22,22,22,22	0
56	MG	1A	3097	1/1	0.92	0.18	31,31,31,31	0
56	MG	2A	3866	1/1	0.92	0.17	37,37,37,37	0
56	MG	1A	3491	1/1	0.92	0.17	24,24,24,24	0
56	MG	1A	3897	1/1	0.92	0.12	55,55,55,55	0
56	MG	1A	3985	1/1	0.92	0.10	39,39,39,39	0
56	MG	1D	301	1/1	0.92	0.17	19,19,19,19	0
56	MG	2a	1733	1/1	0.92	0.06	66,66,66,66	0
56	MG	2A	3790	1/1	0.92	0.16	48,48,48,48	0
56	MG	2A	3808	1/1	0.92	0.10	55,55,55,55	0
56	MG	1A	3342	1/1	0.92	0.24	19,19,19,19	0
56	MG	2A	3404	1/1	0.92	0.26	44,44,44,44	0
56	MG	1A	3202	1/1	0.92	0.23	26,26,26,26	0
56	MG	1A	3102	1/1	0.92	0.16	18,18,18,18	0
56	MG	1A	3757	1/1	0.92	0.18	9,9,9,9	0
56	MG	1A	3401	1/1	0.92	0.27	38,38,38,38	0
56	MG	2A	3389	1/1	0.92	0.24	38,38,38,38	0
56	MG	1A	3715	1/1	0.92	0.09	34,34,34,34	0
56	MG	2A	3150	1/1	0.92	0.10	47,47,47,47	0
56	MG	2a	1621	1/1	0.92	0.18	65,65,65,65	0
56	MG	1A	3452	1/1	0.92	0.14	22,22,22,22	0
56	MG	1A	3122	1/1	0.92	0.30	14,14,14,14	0
56	MG	13	105	1/1	0.92	0.12	48,48,48,48	0
56	MG	2A	3629	1/1	0.92	0.14	36,36,36,36	0
56	MG	1A	3267	1/1	0.92	0.15	33,33,33,33	0
56	MG	1A	4008	1/1	0.92	0.11	37,37,37,37	0
56	MG	1A	3500	1/1	0.92	0.31	27,27,27,27	0
56	MG	1A	3193	1/1	0.92	0.16	24,24,24,24	0
56	MG	19	102	1/1	0.92	0.18	33,33,33,33	0
56	MG	1A	3300	1/1	0.92	0.12	28,28,28,28	0
56	MG	1A	3486	1/1	0.92	0.10	24,24,24,24	0
56	MG	2E	306	1/1	0.92	0.24	40,40,40,40	0
56	MG	1Q	208	1/1	0.92	0.15	15,15,15,15	0
56	MG	2Q	201	1/1	0.92	0.10	33,33,33,33	0
56	MG	1D	312	1/1	0.92	0.20	36,36,36,36	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2x	102	1/1	0.92	0.12	59,59,59,59	0
56	MG	1a	3009	1/1	0.92	0.08	48,48,48,48	0
56	MG	2A	3438	1/1	0.92	0.11	32,32,32,32	0
56	MG	2A	3416	1/1	0.92	0.14	45,45,45,45	0
56	MG	2A	3205	1/1	0.92	0.10	33,33,33,33	0
56	MG	1A	3851	1/1	0.92	0.44	36,36,36,36	0
56	MG	1a	3163	1/1	0.92	0.10	33,33,33,33	0
56	MG	1A	3362	1/1	0.92	0.15	28,28,28,28	0
56	MG	2A	3246	1/1	0.92	0.06	54,54,54,54	0
56	MG	16	101	1/1	0.92	0.23	35,35,35,35	0
56	MG	1A	3968	1/1	0.92	0.14	20,20,20,20	0
56	MG	1A	3026	1/1	0.92	0.45	17,17,17,17	0
56	MG	2A	3622	1/1	0.92	0.09	37,37,37,37	0
56	MG	1A	3529	1/1	0.92	0.41	27,27,27,27	0
56	MG	1A	3488	1/1	0.92	0.17	44,44,44,44	0
56	MG	2A	3357	1/1	0.92	0.13	43,43,43,43	0
56	MG	2A	3143	1/1	0.92	0.16	33,33,33,33	0
56	MG	1A	3922	1/1	0.92	0.07	24,24,24,24	0
56	MG	1A	3632	1/1	0.92	0.14	38,38,38,38	0
56	MG	1A	3297	1/1	0.92	0.21	28,28,28,28	0
56	MG	2A	3394	1/1	0.92	0.31	50,50,50,50	0
56	MG	2A	3105	1/1	0.92	0.15	50,50,50,50	0
56	MG	2l	201	1/1	0.92	0.12	48,48,48,48	0
56	MG	20	101	1/1	0.92	0.11	50,50,50,50	0
56	MG	1A	3185	1/1	0.92	0.10	39,39,39,39	0
56	MG	2a	1699	1/1	0.92	0.23	54,54,54,54	0
56	MG	1n	101	1/1	0.92	0.08	52,52,52,52	0
56	MG	1a	3125	1/1	0.92	0.14	35,35,35,35	0
56	MG	2A	3278	1/1	0.92	0.12	26,26,26,26	0
56	MG	2a	1650	1/1	0.92	0.37	63,63,63,63	0
56	MG	1A	3023	1/1	0.92	0.12	13,13,13,13	0
56	MG	2x	103	1/1	0.92	0.09	46,46,46,46	0
56	MG	1A	3806	1/1	0.92	0.13	16,16,16,16	0
56	MG	2A	3053	1/1	0.92	0.13	53,53,53,53	0
56	MG	1a	3223	1/1	0.92	0.08	40,40,40,40	0
56	MG	1A	3214	1/1	0.92	0.13	32,32,32,32	0
56	MG	2a	1781	1/1	0.92	0.34	41,41,41,41	0
56	MG	1A	3008	1/1	0.92	0.18	16,16,16,16	0
56	MG	1A	4012	1/1	0.92	0.24	42,42,42,42	0
56	MG	1A	3952	1/1	0.92	0.10	19,19,19,19	0
56	MG	2A	3286	1/1	0.92	0.28	46,46,46,46	0
56	MG	1A	3503	1/1	0.92	0.16	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	3541	1/1	0.92	0.14	14,14,14,14	0
56	MG	1a	3051	1/1	0.92	0.14	44,44,44,44	0
56	MG	2A	3091	1/1	0.92	0.21	36,36,36,36	0
56	MG	1a	3173	1/1	0.92	0.10	44,44,44,44	0
56	MG	1A	3360	1/1	0.92	0.30	27,27,27,27	0
56	MG	1A	3266	1/1	0.92	0.19	25,25,25,25	0
56	MG	1A	3703	1/1	0.92	0.11	38,38,38,38	0
56	MG	1A	3580	1/1	0.92	0.11	40,40,40,40	0
56	MG	2a	1799	1/1	0.92	0.21	45,45,45,45	0
56	MG	1X	102	1/1	0.92	0.13	29,29,29,29	0
56	MG	1A	3537	1/1	0.92	0.16	31,31,31,31	0
56	MG	1a	3002	1/1	0.92	0.12	42,42,42,42	0
56	MG	2A	3553	1/1	0.92	0.08	27,27,27,27	0
56	MG	2a	1712	1/1	0.92	0.14	48,48,48,48	0
56	MG	2a	1751	1/1	0.92	0.07	72,72,72,72	0
56	MG	2A	3545	1/1	0.92	0.10	32,32,32,32	0
56	MG	2A	3657	1/1	0.92	0.06	38,38,38,38	0
56	MG	1a	3222	1/1	0.92	0.09	41,41,41,41	0
56	MG	2A	3595	1/1	0.92	0.07	34,34,34,34	0
56	MG	2A	3563	1/1	0.92	0.19	50,50,50,50	0
56	MG	2a	1611	1/1	0.92	0.32	51,51,51,51	0
56	MG	1a	3047	1/1	0.92	0.17	39,39,39,39	0
56	MG	1E	306	1/1	0.92	0.24	22,22,22,22	0
56	MG	2a	1717	1/1	0.92	0.14	52,52,52,52	0
56	MG	2A	3604	1/1	0.92	0.09	33,33,33,33	0
56	MG	2A	3235	1/1	0.92	0.26	31,31,31,31	0
56	MG	1B	211	1/1	0.92	0.25	54,54,54,54	0
56	MG	1B	218	1/1	0.92	0.10	21,21,21,21	0
56	MG	1a	3038	1/1	0.92	0.11	56,56,56,56	0
56	MG	2q	203	1/1	0.92	0.12	41,41,41,41	0
56	MG	1A	3761	1/1	0.92	0.23	39,39,39,39	0
56	MG	1A	4027	1/1	0.92	0.10	48,48,48,48	0
56	MG	1A	3825	1/1	0.92	0.07	30,30,30,30	0
56	MG	1A	3797	1/1	0.92	0.07	19,19,19,19	0
56	MG	2A	3057	1/1	0.92	0.14	29,29,29,29	0
56	MG	1A	3837	1/1	0.92	0.14	27,27,27,27	0
56	MG	1A	3687	1/1	0.92	0.10	21,21,21,21	0
56	MG	1A	3236	1/1	0.92	0.14	28,28,28,28	0
56	MG	2A	3674	1/1	0.92	0.05	53,53,53,53	0
56	MG	1A	3691	1/1	0.92	0.14	16,16,16,16	0
56	MG	1Q	206	1/1	0.92	0.14	26,26,26,26	0
56	MG	1A	3884	1/1	0.92	0.11	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	1B	204	1/1	0.92	0.20	30,30,30,30	0
56	MG	2E	303	1/1	0.92	0.09	15,15,15,15	0
56	MG	1A	3470	1/1	0.92	0.12	36,36,36,36	0
56	MG	1x	104	1/1	0.92	0.11	67,67,67,67	0
56	MG	1t	201	1/1	0.92	0.09	40,40,40,40	0
56	MG	2A	3393	1/1	0.92	0.20	42,42,42,42	0
56	MG	1E	304	1/1	0.92	0.25	25,25,25,25	0
56	MG	2A	3702	1/1	0.92	0.10	29,29,29,29	0
56	MG	2A	3284	1/1	0.92	0.16	29,29,29,29	0
56	MG	2A	3223	1/1	0.92	0.13	41,41,41,41	0
56	MG	2a	1651	1/1	0.92	0.11	43,43,43,43	0
56	MG	1A	3493	1/1	0.92	0.36	55,55,55,55	0
56	MG	1A	3224	1/1	0.92	0.14	23,23,23,23	0
56	MG	1A	3117	1/1	0.92	0.75	38,38,38,38	0
56	MG	2a	1800	1/1	0.92	0.08	56,56,56,56	0
56	MG	16	104	1/1	0.93	0.20	33,33,33,33	0
56	MG	1A	3227	1/1	0.93	0.09	56,56,56,56	0
56	MG	1A	3765	1/1	0.93	0.13	33,33,33,33	0
56	MG	2A	3361	1/1	0.93	0.09	33,33,33,33	0
56	MG	2A	3101	1/1	0.93	0.14	39,39,39,39	0
56	MG	1A	3290	1/1	0.93	0.13	12,12,12,12	0
56	MG	2A	3861	1/1	0.93	0.08	33,33,33,33	0
56	MG	1a	3090	1/1	0.93	0.21	29,29,29,29	0
56	MG	1A	3698	1/1	0.93	0.13	41,41,41,41	0
56	MG	2A	3463	1/1	0.93	0.28	45,45,45,45	0
56	MG	2A	3464	1/1	0.93	0.61	41,41,41,41	0
56	MG	1B	232	1/1	0.93	0.11	35,35,35,35	0
56	MG	1A	3164	1/1	0.93	0.11	26,26,26,26	0
56	MG	2V	201	1/1	0.93	0.71	44,44,44,44	0
56	MG	2A	3583	1/1	0.93	0.08	39,39,39,39	0
56	MG	1a	3205	1/1	0.93	0.10	39,39,39,39	0
56	MG	1x	108	1/1	0.93	0.12	38,38,38,38	0
56	MG	2A	3241	1/1	0.93	0.20	38,38,38,38	0
56	MG	2A	3615	1/1	0.93	0.17	28,28,28,28	0
56	MG	2A	3510	1/1	0.93	0.17	49,49,49,49	0
56	MG	1A	3088	1/1	0.93	0.18	21,21,21,21	0
56	MG	1a	3136	1/1	0.93	0.16	44,44,44,44	0
56	MG	2A	3001	1/1	0.93	0.15	41,41,41,41	0
56	MG	2A	3764	1/1	0.93	0.20	54,54,54,54	0
56	MG	1A	3277	1/1	0.93	0.17	36,36,36,36	0
56	MG	1a	3150	1/1	0.93	0.09	43,43,43,43	0
56	MG	1a	3077	1/1	0.93	0.16	50,50,50,50	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3478	1/1	0.93	0.27	22,22,22,22	0
56	MG	1A	3496	1/1	0.93	0.13	28,28,28,28	0
56	MG	1A	3769	1/1	0.93	0.16	21,21,21,21	0
56	MG	1A	3918	1/1	0.93	0.15	27,27,27,27	0
56	MG	1A	3535	1/1	0.93	0.15	31,31,31,31	0
56	MG	2A	3456	1/1	0.93	0.23	37,37,37,37	0
56	MG	2A	3603	1/1	0.93	0.08	39,39,39,39	0
56	MG	2A	3146	1/1	0.93	0.21	29,29,29,29	0
56	MG	2X	102	1/1	0.93	0.11	45,45,45,45	0
56	MG	2A	3400	1/1	0.93	0.12	62,62,62,62	0
56	MG	2A	3537	1/1	0.93	0.13	27,27,27,27	0
56	MG	1A	3965	1/1	0.93	0.10	44,44,44,44	0
56	MG	2A	3189	1/1	0.93	0.11	46,46,46,46	0
56	MG	1P	207	1/1	0.93	0.35	29,29,29,29	0
56	MG	1a	3034	1/1	0.93	0.13	42,42,42,42	0
56	MG	1A	3733	1/1	0.93	0.17	45,45,45,45	0
56	MG	2A	3190	1/1	0.93	0.14	26,26,26,26	0
56	MG	1A	3331	1/1	0.93	0.32	42,42,42,42	0
56	MG	2A	3381	1/1	0.93	0.21	36,36,36,36	0
56	MG	1A	3527	1/1	0.93	0.20	22,22,22,22	0
56	MG	2A	3479	1/1	0.93	0.24	49,49,49,49	0
56	MG	2A	3646	1/1	0.93	0.21	34,34,34,34	0
56	MG	1a	3147	1/1	0.93	0.09	54,54,54,54	0
56	MG	1A	4032	1/1	0.93	0.08	43,43,43,43	0
56	MG	1A	3385	1/1	0.93	0.10	29,29,29,29	0
56	MG	2A	3677	1/1	0.93	0.22	36,36,36,36	0
56	MG	1a	3101	1/1	0.93	0.16	43,43,43,43	0
56	MG	2A	3504	1/1	0.93	0.18	59,59,59,59	0
56	MG	2A	3562	1/1	0.93	0.44	65,65,65,65	0
56	MG	1A	3718	1/1	0.93	0.08	22,22,22,22	0
56	MG	1A	3990	1/1	0.93	0.11	43,43,43,43	0
56	MG	1F	311	1/1	0.93	0.19	29,29,29,29	0
56	MG	1A	3130	1/1	0.93	0.08	21,21,21,21	0
56	MG	1A	3656	1/1	0.93	0.11	36,36,36,36	0
56	MG	1A	3045	1/1	0.93	0.25	41,41,41,41	0
56	MG	1A	3705	1/1	0.93	0.14	15,15,15,15	0
56	MG	1A	3764	1/1	0.93	0.11	20,20,20,20	0
56	MG	1x	112	1/1	0.93	0.12	58,58,58,58	0
56	MG	1X	104	1/1	0.93	0.12	43,43,43,43	0
56	MG	1a	3058	1/1	0.93	0.12	58,58,58,58	0
56	MG	1A	3363	1/1	0.93	0.16	34,34,34,34	0
56	MG	1A	3264	1/1	0.93	0.17	26,26,26,26	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3188	1/1	0.93	0.24	36,36,36,36	0
56	MG	27	102	1/1	0.93	0.81	51,51,51,51	0
56	MG	2E	304	1/1	0.93	0.30	57,57,57,57	0
56	MG	1A	3907	1/1	0.93	0.18	10,10,10,10	0
56	MG	2A	3581	1/1	0.93	0.12	30,30,30,30	0
56	MG	1A	4019	1/1	0.93	0.23	9,9,9,9	0
56	MG	2A	3660	1/1	0.93	0.27	56,56,56,56	0
56	MG	1A	3242	1/1	0.93	0.28	13,13,13,13	0
56	MG	1a	3149	1/1	0.93	0.07	33,33,33,33	0
56	MG	1A	3961	1/1	0.93	0.10	57,57,57,57	0
56	MG	1A	3258	1/1	0.93	0.57	39,39,39,39	0
56	MG	1A	3741	1/1	0.93	0.09	51,51,51,51	0
56	MG	1A	3492	1/1	0.93	0.09	26,26,26,26	0
56	MG	1A	3247	1/1	0.93	0.22	19,19,19,19	0
56	MG	1A	3801	1/1	0.93	0.16	46,46,46,46	0
56	MG	2A	3584	1/1	0.93	0.14	44,44,44,44	0
56	MG	1A	3862	1/1	0.93	0.09	29,29,29,29	0
56	MG	1D	309	1/1	0.93	0.14	30,30,30,30	0
56	MG	1A	3374	1/1	0.93	0.21	40,40,40,40	0
56	MG	2a	1697	1/1	0.93	0.19	55,55,55,55	0
56	MG	1A	3250	1/1	0.93	0.29	31,31,31,31	0
56	MG	2a	1602	1/1	0.93	0.33	49,49,49,49	0
56	MG	2a	1816	1/1	0.93	0.20	38,38,38,38	0
56	MG	2A	3645	1/1	0.93	0.12	38,38,38,38	0
56	MG	2A	3212	1/1	0.93	0.15	38,38,38,38	0
56	MG	2f	201	1/1	0.93	0.14	37,37,37,37	0
56	MG	2A	3579	1/1	0.93	0.14	46,46,46,46	0
56	MG	1A	3432	1/1	0.93	0.30	21,21,21,21	0
56	MG	1A	3506	1/1	0.93	0.16	43,43,43,43	0
56	MG	1A	4024	1/1	0.93	0.17	28,28,28,28	0
56	MG	1A	3090	1/1	0.93	0.62	28,28,28,28	0
56	MG	2A	3039	1/1	0.93	0.09	35,35,35,35	0
56	MG	1V	206	1/1	0.93	0.16	31,31,31,31	0
56	MG	1a	3154	1/1	0.93	0.19	34,34,34,34	0
56	MG	2A	3346	1/1	0.93	0.14	33,33,33,33	0
56	MG	2A	3740	1/1	0.93	0.22	55,55,55,55	0
56	MG	1F	303	1/1	0.93	0.55	23,23,23,23	0
56	MG	1B	228	1/1	0.93	0.10	35,35,35,35	0
56	MG	1a	3044	1/1	0.93	0.08	53,53,53,53	0
56	MG	2A	3508	1/1	0.93	0.09	43,43,43,43	0
56	MG	1A	3365	1/1	0.93	0.51	28,28,28,28	0
56	MG	2w	101	1/1	0.93	0.09	50,50,50,50	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3987	1/1	0.93	0.11	16,16,16,16	0
56	MG	2A	3148	1/1	0.93	0.33	41,41,41,41	0
56	MG	1a	3199	1/1	0.93	0.06	45,45,45,45	0
56	MG	1A	3296	1/1	0.93	0.13	16,16,16,16	0
56	MG	1a	3190	1/1	0.93	0.14	37,37,37,37	0
56	MG	2a	1637	1/1	0.93	0.23	45,45,45,45	0
56	MG	2A	3547	1/1	0.93	0.11	18,18,18,18	0
56	MG	1A	3956	1/1	0.93	0.10	50,50,50,50	0
56	MG	2a	1668	1/1	0.93	0.09	48,48,48,48	0
56	MG	1w	106	1/1	0.93	0.13	32,32,32,32	0
56	MG	2A	3123	1/1	0.93	0.07	34,34,34,34	0
56	MG	2d	301	1/1	0.93	0.08	51,51,51,51	0
56	MG	1A	3444	1/1	0.93	0.17	25,25,25,25	0
56	MG	2A	3633	1/1	0.93	0.10	41,41,41,41	0
56	MG	1A	3134	1/1	0.93	0.31	22,22,22,22	0
56	MG	1A	3943	1/1	0.93	0.09	24,24,24,24	0
56	MG	1A	3665	1/1	0.93	0.12	23,23,23,23	0
56	MG	1A	3263	1/1	0.93	0.28	24,24,24,24	0
56	MG	1a	3164	1/1	0.93	0.08	49,49,49,49	0
56	MG	1A	3294	1/1	0.93	0.18	37,37,37,37	0
56	MG	2A	3020	1/1	0.93	0.11	44,44,44,44	0
56	MG	1A	4025	1/1	0.93	0.09	42,42,42,42	0
56	MG	1A	3518	1/1	0.93	0.45	30,30,30,30	0
56	MG	1A	3750	1/1	0.93	0.13	43,43,43,43	0
56	MG	1A	3127	1/1	0.93	0.44	23,23,23,23	0
56	MG	2y	103	1/1	0.93	0.06	41,41,41,41	0
56	MG	1A	3367	1/1	0.93	0.12	18,18,18,18	0
56	MG	2A	3093	1/1	0.93	0.08	29,29,29,29	0
56	MG	1A	3018	1/1	0.93	0.14	17,17,17,17	0
56	MG	2A	3455	1/1	0.93	0.12	63,63,63,63	0
56	MG	1a	3069	1/1	0.93	0.16	54,54,54,54	0
56	MG	2A	3139	1/1	0.93	0.34	44,44,44,44	0
56	MG	2B	213	1/1	0.93	0.13	35,35,35,35	0
56	MG	1A	3084	1/1	0.93	0.08	31,31,31,31	0
56	MG	2A	3450	1/1	0.93	0.08	52,52,52,52	0
56	MG	2A	3524	1/1	0.93	0.12	31,31,31,31	0
56	MG	1a	3130	1/1	0.93	0.13	52,52,52,52	0
56	MG	1A	3148	1/1	0.93	0.40	29,29,29,29	0
56	MG	2A	3403	1/1	0.93	0.10	51,51,51,51	0
56	MG	1A	3433	1/1	0.93	0.27	22,22,22,22	0
56	MG	1A	3641	1/1	0.93	0.11	18,18,18,18	0
56	MG	2A	3841	1/1	0.93	0.08	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	2a	1768	1/1	0.93	0.14	48,48,48,48	0
56	MG	1A	3532	1/1	0.93	0.23	42,42,42,42	0
56	MG	1A	3255	1/1	0.93	0.19	20,20,20,20	0
56	MG	2A	3402	1/1	0.93	0.17	42,42,42,42	0
56	MG	1A	4023	1/1	0.93	0.09	46,46,46,46	0
56	MG	2A	3625	1/1	0.93	0.19	53,53,53,53	0
56	MG	1A	3783	1/1	0.93	0.11	17,17,17,17	0
56	MG	2A	3488	1/1	0.93	0.12	43,43,43,43	0
56	MG	1A	3368	1/1	0.93	0.10	18,18,18,18	0
56	MG	1A	3411	1/1	0.93	0.08	36,36,36,36	0
56	MG	2A	3310	1/1	0.93	0.45	24,24,24,24	0
56	MG	18	101	1/1	0.93	0.27	36,36,36,36	0
56	MG	1A	3832	1/1	0.93	0.12	35,35,35,35	0
56	MG	2a	1607	1/1	0.93	0.11	31,31,31,31	0
56	MG	2A	3689	1/1	0.93	0.14	48,48,48,48	0
56	MG	1a	3116	1/1	0.93	0.12	40,40,40,40	0
56	MG	1A	3860	1/1	0.93	0.08	25,25,25,25	0
56	MG	2B	221	1/1	0.93	0.13	56,56,56,56	0
56	MG	1R	202	1/1	0.93	0.12	23,23,23,23	0
56	MG	1A	3709	1/1	0.93	0.14	31,31,31,31	0
56	MG	2A	3549	1/1	0.93	0.27	58,58,58,58	0
56	MG	2B	211	1/1	0.93	0.13	61,61,61,61	0
56	MG	2a	1675	1/1	0.93	0.07	55,55,55,55	0
56	MG	1A	3398	1/1	0.93	0.47	33,33,33,33	0
56	MG	1A	3101	1/1	0.93	0.32	36,36,36,36	0
56	MG	1A	3696	1/1	0.93	0.16	24,24,24,24	0
56	MG	1A	3419	1/1	0.93	0.15	47,47,47,47	0
56	MG	1A	3048	1/1	0.93	0.08	27,27,27,27	0
56	MG	1A	3327	1/1	0.93	0.44	31,31,31,31	0
56	MG	1A	3177	1/1	0.93	0.19	21,21,21,21	0
56	MG	2A	3010	1/1	0.93	0.08	39,39,39,39	0
56	MG	1A	3063	1/1	0.93	0.21	26,26,26,26	0
56	MG	2A	3288	1/1	0.93	0.12	51,51,51,51	0
56	MG	1a	3189	1/1	0.93	0.11	60,60,60,60	0
56	MG	1a	3192	1/1	0.93	0.08	42,42,42,42	0
56	MG	1A	3969	1/1	0.93	0.13	13,13,13,13	0
56	MG	1a	3025	1/1	0.93	0.18	40,40,40,40	0
56	MG	1T	202	1/1	0.93	0.37	50,50,50,50	0
56	MG	2a	1774	1/1	0.93	0.18	65,65,65,65	0
56	MG	2A	3069	1/1	0.93	0.31	41,41,41,41	0
56	MG	2A	3635	1/1	0.93	0.18	59,59,59,59	0
56	MG	2a	1813	1/1	0.93	0.12	60,60,60,60	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1U	204	1/1	0.93	0.52	27,27,27,27	0
56	MG	2A	3216	1/1	0.93	0.13	39,39,39,39	0
56	MG	2A	3624	1/1	0.93	0.29	58,58,58,58	0
56	MG	2A	3511	1/1	0.93	0.21	39,39,39,39	0
56	MG	1a	3043	1/1	0.93	0.09	36,36,36,36	0
56	MG	2A	3169	1/1	0.93	0.21	35,35,35,35	0
56	MG	1A	3883	1/1	0.93	0.10	30,30,30,30	0
56	MG	1A	3991	1/1	0.93	0.15	24,24,24,24	0
56	MG	1A	3457	1/1	0.93	0.18	24,24,24,24	0
56	MG	2A	3761	1/1	0.93	0.10	42,42,42,42	0
56	MG	1A	3428	1/1	0.93	0.31	55,55,55,55	0
56	MG	2A	3835	1/1	0.93	0.07	51,51,51,51	0
56	MG	1A	3515	1/1	0.93	0.09	38,38,38,38	0
56	MG	1a	3148	1/1	0.93	0.13	46,46,46,46	0
56	MG	1a	3007	1/1	0.93	0.19	54,54,54,54	0
56	MG	1a	3135	1/1	0.93	0.21	33,33,33,33	0
56	MG	17	101	1/1	0.93	0.15	21,21,21,21	0
56	MG	2A	3088	1/1	0.93	0.07	47,47,47,47	0
56	MG	2A	3203	1/1	0.93	0.32	34,34,34,34	0
56	MG	2A	3497	1/1	0.93	0.34	72,72,72,72	0
56	MG	2A	3333	1/1	0.93	0.08	37,37,37,37	0
56	MG	1A	3237	1/1	0.93	0.13	29,29,29,29	0
56	MG	2A	3332	1/1	0.93	0.10	59,59,59,59	0
56	MG	1A	3223	1/1	0.93	0.13	29,29,29,29	0
56	MG	2a	1659	1/1	0.93	0.10	49,49,49,49	0
56	MG	2A	3202	1/1	0.93	0.16	22,22,22,22	0
56	MG	1U	208	1/1	0.93	0.34	25,25,25,25	0
56	MG	1A	3579	1/1	0.93	0.18	32,32,32,32	0
56	MG	1a	3045	1/1	0.93	0.16	48,48,48,48	0
56	MG	1a	3165	1/1	0.93	0.14	63,63,63,63	0
56	MG	1F	312	1/1	0.93	0.10	28,28,28,28	0
56	MG	2A	3086	1/1	0.93	0.11	34,34,34,34	0
56	MG	2A	3671	1/1	0.93	0.09	35,35,35,35	0
56	MG	1A	3468	1/1	0.93	0.19	25,25,25,25	0
56	MG	1A	3361	1/1	0.94	0.07	43,43,43,43	0
56	MG	2a	1742	1/1	0.94	0.09	60,60,60,60	0
56	MG	1A	3310	1/1	0.94	0.21	19,19,19,19	0
56	MG	1A	3901	1/1	0.94	0.14	32,32,32,32	0
56	MG	1A	3199	1/1	0.94	0.12	32,32,32,32	0
56	MG	2A	3309	1/1	0.94	0.26	41,41,41,41	0
56	MG	1A	3132	1/1	0.94	0.11	35,35,35,35	0
56	MG	1A	3891	1/1	0.94	0.09	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	3752	1/1	0.94	0.12	47,47,47,47	0
56	MG	2a	1683	1/1	0.94	0.14	41,41,41,41	0
56	MG	2A	3255	1/1	0.94	0.11	30,30,30,30	0
56	MG	2A	3247	1/1	0.94	0.10	32,32,32,32	0
56	MG	1A	3763	1/1	0.94	0.10	25,25,25,25	0
56	MG	1B	209	1/1	0.94	0.16	43,43,43,43	0
56	MG	2A	3756	1/1	0.94	0.47	51,51,51,51	0
56	MG	10	105	1/1	0.94	0.13	32,32,32,32	0
56	MG	2A	3655	1/1	0.94	0.30	39,39,39,39	0
56	MG	15	103	1/1	0.94	0.40	21,21,21,21	0
56	MG	1A	3654	1/1	0.94	0.07	10,10,10,10	0
56	MG	15	105	1/1	0.94	0.26	13,13,13,13	0
56	MG	2A	3264	1/1	0.94	0.38	38,38,38,38	0
56	MG	1A	3727	1/1	0.94	0.18	31,31,31,31	0
56	MG	1A	3538	1/1	0.94	0.19	20,20,20,20	0
56	MG	1x	103	1/1	0.94	0.10	57,57,57,57	0
56	MG	2A	3215	1/1	0.94	0.10	31,31,31,31	0
56	MG	1A	3306	1/1	0.94	0.11	27,27,27,27	0
56	MG	1A	3752	1/1	0.94	0.10	26,26,26,26	0
56	MG	2a	1805	1/1	0.94	0.27	54,54,54,54	0
56	MG	2A	3399	1/1	0.94	0.07	40,40,40,40	0
56	MG	1A	3588	1/1	0.94	0.10	27,27,27,27	0
56	MG	2a	1822	1/1	0.94	0.13	50,50,50,50	0
56	MG	2A	3785	1/1	0.94	0.10	70,70,70,70	0
56	MG	2A	3195	1/1	0.94	0.17	38,38,38,38	0
56	MG	1A	3719	1/1	0.94	0.09	50,50,50,50	0
56	MG	2A	3055	1/1	0.94	0.10	47,47,47,47	0
56	MG	2A	3539	1/1	0.94	0.09	56,56,56,56	0
56	MG	2a	1656	1/1	0.94	0.16	43,43,43,43	0
56	MG	2A	3659	1/1	0.94	0.18	57,57,57,57	0
56	MG	2A	3364	1/1	0.94	0.14	23,23,23,23	0
56	MG	1A	3390	1/1	0.94	0.11	25,25,25,25	0
56	MG	2A	3687	1/1	0.94	0.14	36,36,36,36	0
56	MG	2A	3599	1/1	0.94	0.08	44,44,44,44	0
56	MG	1A	3210	1/1	0.94	0.33	18,18,18,18	0
56	MG	1A	3485	1/1	0.94	0.13	43,43,43,43	0
56	MG	1A	3051	1/1	0.94	0.12	15,15,15,15	0
56	MG	1A	3781	1/1	0.94	0.14	21,21,21,21	0
56	MG	1a	3209	1/1	0.94	0.15	68,68,68,68	0
56	MG	1A	3850	1/1	0.94	0.11	23,23,23,23	0
56	MG	1A	3695	1/1	0.94	0.14	16,16,16,16	0
56	MG	1A	3421	1/1	0.94	0.09	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	1684	1/1	0.94	0.18	45,45,45,45	0
56	MG	1a	3079	1/1	0.94	0.14	48,48,48,48	0
56	MG	2A	3436	1/1	0.94	0.11	44,44,44,44	0
56	MG	2A	3085	1/1	0.94	0.22	37,37,37,37	0
56	MG	1A	3843	1/1	0.94	0.12	32,32,32,32	0
56	MG	1A	3651	1/1	0.94	0.12	8,8,8,8	0
56	MG	2A	3360	1/1	0.94	0.12	49,49,49,49	0
56	MG	2A	3163	1/1	0.94	0.16	71,71,71,71	0
56	MG	2R	201	1/1	0.94	0.12	27,27,27,27	0
56	MG	2U	203	1/1	0.94	0.43	36,36,36,36	0
56	MG	1a	3039	1/1	0.94	0.13	42,42,42,42	0
56	MG	1A	3287	1/1	0.94	0.16	28,28,28,28	0
56	MG	2g	201	1/1	0.94	0.09	57,57,57,57	0
56	MG	1A	3379	1/1	0.94	0.09	32,32,32,32	0
56	MG	2A	3276	1/1	0.94	0.28	43,43,43,43	0
56	MG	2a	1821	1/1	0.94	0.13	54,54,54,54	0
56	MG	2A	3509	1/1	0.94	0.14	19,19,19,19	0
56	MG	2a	1766	1/1	0.94	0.16	53,53,53,53	0
56	MG	2A	3165	1/1	0.94	0.08	30,30,30,30	0
56	MG	2A	3433	1/1	0.94	0.15	20,20,20,20	0
56	MG	1A	3552	1/1	0.94	0.18	23,23,23,23	0
56	MG	2Q	204	1/1	0.94	0.11	38,38,38,38	0
56	MG	2A	3044	1/1	0.94	0.11	44,44,44,44	0
56	MG	2A	3030	1/1	0.94	0.29	41,41,41,41	0
57	ERY	1A	4074	51/51	0.94	0.27	15,23,34,44	0
56	MG	2A	3158	1/1	0.94	0.09	39,39,39,39	0
56	MG	2A	3271	1/1	0.94	0.10	36,36,36,36	0
56	MG	1A	4040	1/1	0.94	0.13	12,12,12,12	0
56	MG	1A	3583	1/1	0.94	0.18	23,23,23,23	0
56	MG	2A	3314	1/1	0.94	0.16	54,54,54,54	0
56	MG	1A	3644	1/1	0.94	0.13	46,46,46,46	0
56	MG	2A	3002	1/1	0.94	0.16	35,35,35,35	0
56	MG	1A	3716	1/1	0.94	0.14	26,26,26,26	0
56	MG	1x	109	1/1	0.94	0.21	47,47,47,47	0
56	MG	2A	3094	1/1	0.94	0.13	40,40,40,40	0
56	MG	2a	1644	1/1	0.94	0.16	47,47,47,47	0
56	MG	2A	3317	1/1	0.94	0.51	47,47,47,47	0
56	MG	2A	3706	1/1	0.94	0.16	34,34,34,34	0
56	MG	2A	3125	1/1	0.94	0.43	44,44,44,44	0
56	MG	1A	3050	1/1	0.94	0.10	22,22,22,22	0
56	MG	2A	3859	1/1	0.94	0.07	60,60,60,60	0
56	MG	1A	3855	1/1	0.94	0.13	10,10,10,10	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	3170	1/1	0.94	0.07	52,52,52,52	0
56	MG	1A	3195	1/1	0.94	0.13	41,41,41,41	0
56	MG	1A	3519	1/1	0.94	0.28	20,20,20,20	0
56	MG	1A	3930	1/1	0.94	0.09	43,43,43,43	0
56	MG	1A	3921	1/1	0.94	0.14	14,14,14,14	0
56	MG	2A	3523	1/1	0.94	0.09	38,38,38,38	0
56	MG	1A	3831	1/1	0.94	0.11	22,22,22,22	0
56	MG	1a	3200	1/1	0.94	0.09	53,53,53,53	0
56	MG	1A	3092	1/1	0.94	0.22	26,26,26,26	0
56	MG	2A	3757	1/1	0.94	0.09	19,19,19,19	0
56	MG	2A	3710	1/1	0.94	0.16	51,51,51,51	0
56	MG	1A	3281	1/1	0.94	0.40	39,39,39,39	0
56	MG	1V	208	1/1	0.94	0.19	42,42,42,42	0
56	MG	1A	3622	1/1	0.94	0.10	22,22,22,22	0
56	MG	1A	3245	1/1	0.94	0.25	22,22,22,22	0
56	MG	2A	3272	1/1	0.94	0.14	35,35,35,35	0
56	MG	1A	3443	1/1	0.94	0.20	37,37,37,37	0
56	MG	1A	3570	1/1	0.94	0.18	30,30,30,30	0
56	MG	1A	3211	1/1	0.94	0.22	33,33,33,33	0
56	MG	2A	3297	1/1	0.94	0.12	27,27,27,27	0
56	MG	2A	3065	1/1	0.94	0.37	37,37,37,37	0
56	MG	2A	3653	1/1	0.94	0.20	57,57,57,57	0
56	MG	1A	3234	1/1	0.94	0.38	35,35,35,35	0
56	MG	2A	3522	1/1	0.94	0.10	51,51,51,51	0
56	MG	2A	3122	1/1	0.94	0.13	50,50,50,50	0
56	MG	1A	3663	1/1	0.94	0.20	46,46,46,46	0
56	MG	2A	3681	1/1	0.94	0.07	43,43,43,43	0
56	MG	2A	3048	1/1	0.94	0.10	48,48,48,48	0
56	MG	1A	3773	1/1	0.94	0.18	30,30,30,30	0
56	MG	1V	207	1/1	0.94	0.53	22,22,22,22	0
56	MG	2A	3529	1/1	0.94	0.10	35,35,35,35	0
56	MG	1A	3020	1/1	0.94	0.12	21,21,21,21	0
56	MG	2A	3196	1/1	0.94	0.17	33,33,33,33	0
56	MG	1A	3960	1/1	0.94	0.28	52,52,52,52	0
56	MG	2F	307	1/1	0.94	0.14	50,50,50,50	0
56	MG	1A	4048	1/1	0.94	0.11	27,27,27,27	0
56	MG	1A	3675	1/1	0.94	0.17	44,44,44,44	0
56	MG	2A	3535	1/1	0.94	0.10	55,55,55,55	0
56	MG	1A	3427	1/1	0.94	0.16	38,38,38,38	0
56	MG	1A	3483	1/1	0.94	0.28	33,33,33,33	0
56	MG	1A	3246	1/1	0.94	0.40	22,22,22,22	0
56	MG	1A	3057	1/1	0.94	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	3208	1/1	0.94	0.25	19,19,19,19	0
56	MG	1A	4009	1/1	0.94	0.11	25,25,25,25	0
56	MG	1A	3459	1/1	0.94	0.13	30,30,30,30	0
56	MG	2a	1787	1/1	0.94	0.06	59,59,59,59	0
56	MG	1W	208	1/1	0.94	0.52	36,36,36,36	0
56	MG	1U	206	1/1	0.94	0.22	25,25,25,25	0
56	MG	1a	3057	1/1	0.94	0.16	38,38,38,38	0
56	MG	2A	3422	1/1	0.94	0.21	43,43,43,43	0
56	MG	1A	3359	1/1	0.94	0.38	30,30,30,30	0
56	MG	1P	202	1/1	0.94	0.40	21,21,21,21	0
56	MG	2A	3734	1/1	0.94	0.12	20,20,20,20	0
56	MG	1a	3146	1/1	0.94	0.17	38,38,38,38	0
56	MG	2A	3013	1/1	0.94	0.40	41,41,41,41	0
56	MG	1A	3302	1/1	0.94	0.08	21,21,21,21	0
56	MG	2A	3507	1/1	0.94	0.09	29,29,29,29	0
56	MG	14	101	1/1	0.94	0.12	30,30,30,30	0
56	MG	1a	3048	1/1	0.94	0.08	54,54,54,54	0
56	MG	1A	3404	1/1	0.94	0.14	18,18,18,18	0
56	MG	1A	3942	1/1	0.94	0.06	51,51,51,51	0
56	MG	1A	3138	1/1	0.94	0.09	31,31,31,31	0
56	MG	2a	1613	1/1	0.94	0.08	50,50,50,50	0
56	MG	2A	3465	1/1	0.94	0.09	31,31,31,31	0
56	MG	2A	3282	1/1	0.94	0.64	36,36,36,36	0
56	MG	2A	3142	1/1	0.94	0.07	55,55,55,55	0
56	MG	2A	3089	1/1	0.94	0.14	35,35,35,35	0
56	MG	1A	3329	1/1	0.94	0.16	39,39,39,39	0
56	MG	1A	3015	1/1	0.94	0.18	31,31,31,31	0
56	MG	2A	3077	1/1	0.94	0.20	32,32,32,32	0
56	MG	2A	3311	1/1	0.94	0.28	34,34,34,34	0
56	MG	2a	1801	1/1	0.94	0.09	40,40,40,40	0
56	MG	12	102	1/1	0.94	0.49	28,28,28,28	0
56	MG	13	101	1/1	0.94	0.32	36,36,36,36	0
56	MG	1A	3601	1/1	0.94	0.24	43,43,43,43	0
56	MG	1A	3036	1/1	0.94	0.20	14,14,14,14	0
56	MG	1a	3050	1/1	0.94	0.09	46,46,46,46	0
56	MG	2A	3798	1/1	0.94	0.09	55,55,55,55	0
56	MG	2A	3009	1/1	0.94	0.24	45,45,45,45	0
56	MG	1a	3067	1/1	0.94	0.17	43,43,43,43	0
56	MG	1A	3996	1/1	0.94	0.15	37,37,37,37	0
56	MG	2A	3135	1/1	0.94	0.08	47,47,47,47	0
56	MG	1A	3260	1/1	0.94	0.22	27,27,27,27	0
56	MG	1A	3324	1/1	0.94	0.28	23,23,23,23	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3793	1/1	0.94	0.09	50,50,50,50	0
56	MG	2A	3362	1/1	0.94	0.12	39,39,39,39	0
56	MG	1A	3814	1/1	0.94	0.57	26,26,26,26	0
56	MG	1A	3007	1/1	0.94	0.08	16,16,16,16	0
56	MG	1A	3418	1/1	0.94	0.25	25,25,25,25	0
56	MG	2A	3612	1/1	0.94	0.11	40,40,40,40	0
56	MG	2a	1823	1/1	0.94	0.11	51,51,51,51	0
56	MG	1S	201	1/1	0.94	0.13	34,34,34,34	0
56	MG	2a	1803	1/1	0.94	0.10	55,55,55,55	0
56	MG	2A	3382	1/1	0.94	0.19	44,44,44,44	0
56	MG	1A	3174	1/1	0.94	0.14	30,30,30,30	0
56	MG	1a	3212	1/1	0.94	0.10	34,34,34,34	0
56	MG	1A	3646	1/1	0.94	0.09	28,28,28,28	0
56	MG	1a	3083	1/1	0.94	0.12	42,42,42,42	0
56	MG	2A	3814	1/1	0.94	0.15	30,30,30,30	0
56	MG	2l	205	1/1	0.94	0.07	33,33,33,33	0
56	MG	1A	3840	1/1	0.94	0.10	28,28,28,28	0
56	MG	1A	3513	1/1	0.94	0.31	23,23,23,23	0
56	MG	1A	3944	1/1	0.94	0.12	55,55,55,55	0
56	MG	10	107	1/1	0.94	0.10	34,34,34,34	0
56	MG	2a	1628	1/1	0.94	0.23	35,35,35,35	0
56	MG	1A	3407	1/1	0.94	0.11	42,42,42,42	0
56	MG	1A	3866	1/1	0.94	0.13	31,31,31,31	0
56	MG	2B	205	1/1	0.94	0.07	40,40,40,40	0
56	MG	2A	3315	1/1	0.94	0.21	45,45,45,45	0
56	MG	2a	1791	1/1	0.94	0.08	53,53,53,53	0
56	MG	2A	3300	1/1	0.94	0.15	49,49,49,49	0
56	MG	1A	3582	1/1	0.94	0.11	29,29,29,29	0
56	MG	1A	3424	1/1	0.94	0.10	50,50,50,50	0
56	MG	2a	1714	1/1	0.94	0.18	51,51,51,51	0
56	MG	2A	3133	1/1	0.94	0.14	27,27,27,27	0
56	MG	2A	3855	1/1	0.94	0.11	30,30,30,30	0
56	MG	2Q	203	1/1	0.94	0.24	44,44,44,44	0
56	MG	1A	3396	1/1	0.94	0.10	21,21,21,21	0
56	MG	2A	3721	1/1	0.94	0.06	43,43,43,43	0
56	MG	1A	3169	1/1	0.94	0.15	13,13,13,13	0
56	MG	2A	3047	1/1	0.94	0.07	49,49,49,49	0
56	MG	2A	3157	1/1	0.94	0.12	57,57,57,57	0
56	MG	1A	3006	1/1	0.94	0.12	7,7,7,7	0
56	MG	1A	3120	1/1	0.94	0.14	39,39,39,39	0
56	MG	1a	3185	1/1	0.94	0.15	64,64,64,64	0
56	MG	1A	3686	1/1	0.94	0.12	6,6,6,6	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	3588	1/1	0.94	0.05	48,48,48,48	0
56	MG	1A	3209	1/1	0.94	0.28	15,15,15,15	0
56	MG	2a	1670	1/1	0.94	0.09	40,40,40,40	0
56	MG	2A	3209	1/1	0.94	0.42	38,38,38,38	0
56	MG	1A	3305	1/1	0.94	0.16	19,19,19,19	0
56	MG	2A	3637	1/1	0.94	0.13	50,50,50,50	0
56	MG	1A	3005	1/1	0.94	0.20	30,30,30,30	0
56	MG	2A	3542	1/1	0.94	0.11	50,50,50,50	0
56	MG	1A	3876	1/1	0.94	0.17	56,56,56,56	0
56	MG	1A	3726	1/1	0.94	0.10	32,32,32,32	0
56	MG	2A	3536	1/1	0.94	0.07	42,42,42,42	0
56	MG	1A	3280	1/1	0.94	0.19	28,28,28,28	0
56	MG	1A	3043	1/1	0.94	0.17	13,13,13,13	0
56	MG	1N	201	1/1	0.94	0.43	32,32,32,32	0
56	MG	2A	3251	1/1	0.94	0.15	48,48,48,48	0
56	MG	2a	1654	1/1	0.94	0.23	50,50,50,50	0
56	MG	2a	1636	1/1	0.94	0.18	54,54,54,54	0
56	MG	2A	3392	1/1	0.94	0.24	47,47,47,47	0
56	MG	2A	3471	1/1	0.94	0.18	34,34,34,34	0
56	MG	2a	1740	1/1	0.94	0.07	60,60,60,60	0
56	MG	2A	3420	1/1	0.94	0.14	36,36,36,36	0
56	MG	1a	3061	1/1	0.94	0.51	38,38,38,38	0
56	MG	2A	3295	1/1	0.94	0.16	54,54,54,54	0
56	MG	1A	3937	1/1	0.94	0.09	58,58,58,58	0
56	MG	2A	3038	1/1	0.94	0.15	29,29,29,29	0
56	MG	1A	3681	1/1	0.94	0.15	37,37,37,37	0
56	MG	1P	201	1/1	0.94	0.35	20,20,20,20	0
56	MG	1A	3113	1/1	0.94	0.07	47,47,47,47	0
56	MG	1A	3839	1/1	0.94	0.17	29,29,29,29	0
56	MG	1A	3241	1/1	0.94	0.17	32,32,32,32	0
56	MG	1A	3231	1/1	0.94	0.16	22,22,22,22	0
56	MG	2A	3857	1/1	0.94	0.08	46,46,46,46	0
56	MG	1E	308	1/1	0.94	0.10	26,26,26,26	0
56	MG	1a	3208	1/1	0.94	0.08	34,34,34,34	0
56	MG	2A	3824	1/1	0.94	0.10	37,37,37,37	0
56	MG	1A	3815	1/1	0.94	0.13	26,26,26,26	0
56	MG	2A	3457	1/1	0.94	0.20	24,24,24,24	0
56	MG	2A	3494	1/1	0.94	0.12	42,42,42,42	0
56	MG	1A	3066	1/1	0.94	0.18	26,26,26,26	0
56	MG	1p	101	1/1	0.94	0.24	51,51,51,51	0
56	MG	1a	3114	1/1	0.94	0.16	34,34,34,34	0
56	MG	2a	1694	1/1	0.94	0.09	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	1667	1/1	0.94	0.17	27,27,27,27	0
56	MG	2A	3815	1/1	0.94	0.15	36,36,36,36	0
56	MG	16	102	1/1	0.94	0.14	23,23,23,23	0
56	MG	1A	3204	1/1	0.94	0.26	16,16,16,16	0
56	MG	1A	4039	1/1	0.94	0.11	28,28,28,28	0
56	MG	1A	3873	1/1	0.94	0.27	17,17,17,17	0
56	MG	1A	3989	1/1	0.94	0.06	29,29,29,29	0
56	MG	1A	3114	1/1	0.94	0.14	19,19,19,19	0
56	MG	2A	3602	1/1	0.94	0.26	45,45,45,45	0
56	MG	2A	3544	1/1	0.94	0.09	44,44,44,44	0
56	MG	2a	1764	1/1	0.94	0.13	46,46,46,46	0
56	MG	2a	1704	1/1	0.94	0.16	52,52,52,52	0
56	MG	1A	3655	1/1	0.94	0.16	33,33,33,33	0
56	MG	1A	3065	1/1	0.94	0.22	26,26,26,26	0
56	MG	2A	3244	1/1	0.94	0.13	39,39,39,39	0
56	MG	2A	3263	1/1	0.94	0.11	30,30,30,30	0
56	MG	2A	3041	1/1	0.94	0.61	34,34,34,34	0
56	MG	1A	3820	1/1	0.94	0.22	31,31,31,31	0
56	MG	2t	201	1/1	0.94	0.15	29,29,29,29	0
56	MG	2A	3118	1/1	0.94	0.53	67,67,67,67	0
56	MG	1A	3183	1/1	0.94	0.08	26,26,26,26	0
56	MG	2A	3033	1/1	0.94	0.24	39,39,39,39	0
56	MG	1A	3408	1/1	0.94	0.17	36,36,36,36	0
56	MG	1a	3052	1/1	0.94	0.11	40,40,40,40	0
56	MG	1S	202	1/1	0.94	0.14	51,51,51,51	0
56	MG	1A	3268	1/1	0.94	0.11	30,30,30,30	0
56	MG	2A	3703	1/1	0.94	0.08	34,34,34,34	0
56	MG	2a	1625	1/1	0.94	0.12	25,25,25,25	0
56	MG	1A	3599	1/1	0.95	0.12	25,25,25,25	0
56	MG	2A	3084	1/1	0.95	0.11	45,45,45,45	0
56	MG	1A	3451	1/1	0.95	0.17	16,16,16,16	0
56	MG	2A	3237	1/1	0.95	0.13	32,32,32,32	0
56	MG	2A	3747	1/1	0.95	0.10	45,45,45,45	0
56	MG	2A	3103	1/1	0.95	0.11	38,38,38,38	0
56	MG	1A	3602	1/1	0.95	0.29	20,20,20,20	0
56	MG	2A	3682	1/1	0.95	0.07	39,39,39,39	0
56	MG	1A	3391	1/1	0.95	0.12	32,32,32,32	0
56	MG	1W	202	1/1	0.95	0.13	18,18,18,18	0
56	MG	1a	3172	1/1	0.95	0.06	57,57,57,57	0
56	MG	1A	3226	1/1	0.95	0.28	37,37,37,37	0
56	MG	1a	3102	1/1	0.95	0.15	53,53,53,53	0
56	MG	1a	3198	1/1	0.95	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	1A	3737	1/1	0.95	0.11	14,14,14,14	0
56	MG	1A	3320	1/1	0.95	0.08	23,23,23,23	0
56	MG	2A	3018	1/1	0.95	0.24	54,54,54,54	0
56	MG	1B	225	1/1	0.95	0.11	33,33,33,33	0
56	MG	2a	1718	1/1	0.95	0.13	39,39,39,39	0
56	MG	2A	3548	1/1	0.95	0.07	32,32,32,32	0
56	MG	2A	3161	1/1	0.95	0.12	47,47,47,47	0
56	MG	2A	3178	1/1	0.95	0.09	45,45,45,45	0
56	MG	1E	310	1/1	0.95	0.14	41,41,41,41	0
56	MG	1a	3180	1/1	0.95	0.08	52,52,52,52	0
56	MG	1A	4049	1/1	0.95	0.21	35,35,35,35	0
56	MG	2U	201	1/1	0.95	0.48	38,38,38,38	0
56	MG	1A	3720	1/1	0.95	0.11	19,19,19,19	0
56	MG	1a	3035	1/1	0.95	0.09	32,32,32,32	0
56	MG	1A	3062	1/1	0.95	0.14	38,38,38,38	0
56	MG	1A	3083	1/1	0.95	0.15	42,42,42,42	0
56	MG	1A	3865	1/1	0.95	0.30	29,29,29,29	0
56	MG	1A	3143	1/1	0.95	0.12	30,30,30,30	0
56	MG	1A	3304	1/1	0.95	0.13	25,25,25,25	0
56	MG	1A	3577	1/1	0.95	0.10	16,16,16,16	0
56	MG	1A	3012	1/1	0.95	0.12	26,26,26,26	0
56	MG	1B	234	1/1	0.95	0.13	30,30,30,30	0
56	MG	2A	3331	1/1	0.95	0.12	28,28,28,28	0
56	MG	2A	3592	1/1	0.95	0.09	35,35,35,35	0
56	MG	1A	3707	1/1	0.95	0.12	4,4,4,4	0
56	MG	1A	3098	1/1	0.95	0.19	16,16,16,16	0
56	MG	1A	3233	1/1	0.95	0.18	27,27,27,27	0
56	MG	2a	1767	1/1	0.95	0.07	47,47,47,47	0
56	MG	1A	3484	1/1	0.95	0.28	34,34,34,34	0
56	MG	2A	3449	1/1	0.95	0.07	35,35,35,35	0
56	MG	1A	4054	1/1	0.95	0.16	24,24,24,24	0
56	MG	1A	3802	1/1	0.95	0.12	28,28,28,28	0
56	MG	2A	3514	1/1	0.95	0.24	48,48,48,48	0
56	MG	1A	3805	1/1	0.95	0.17	10,10,10,10	0
56	MG	1A	3219	1/1	0.95	0.34	28,28,28,28	0
56	MG	1A	3753	1/1	0.95	0.17	23,23,23,23	0
56	MG	2B	215	1/1	0.95	0.17	40,40,40,40	0
56	MG	1A	4020	1/1	0.95	0.12	36,36,36,36	0
56	MG	1a	3064	1/1	0.95	0.09	33,33,33,33	0
56	MG	1A	3874	1/1	0.95	0.11	47,47,47,47	0
56	MG	1A	3557	1/1	0.95	0.14	28,28,28,28	0
56	MG	1A	3504	1/1	0.95	0.18	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	2A	3662	1/1	0.95	0.14	55,55,55,55	0
56	MG	1A	3086	1/1	0.95	0.30	25,25,25,25	0
56	MG	1A	3678	1/1	0.95	0.09	18,18,18,18	0
56	MG	1A	3422	1/1	0.95	0.26	36,36,36,36	0
56	MG	2A	3141	1/1	0.95	0.38	47,47,47,47	0
56	MG	2A	3811	1/1	0.95	0.10	33,33,33,33	0
56	MG	2a	1624	1/1	0.95	0.24	31,31,31,31	0
56	MG	1A	3578	1/1	0.95	0.13	12,12,12,12	0
56	MG	1s	101	1/1	0.95	0.16	46,46,46,46	0
56	MG	1a	3115	1/1	0.95	0.19	19,19,19,19	0
56	MG	1A	3071	1/1	0.95	0.11	17,17,17,17	0
56	MG	1A	3252	1/1	0.95	0.15	32,32,32,32	0
56	MG	2B	203	1/1	0.95	0.06	50,50,50,50	0
56	MG	2A	3636	1/1	0.95	0.21	49,49,49,49	0
56	MG	1A	4036	1/1	0.95	0.17	10,10,10,10	0
56	MG	1A	3896	1/1	0.95	0.17	23,23,23,23	0
56	MG	1a	3132	1/1	0.95	0.08	27,27,27,27	0
56	MG	1A	3465	1/1	0.95	0.50	34,34,34,34	0
56	MG	1A	3004	1/1	0.95	0.09	39,39,39,39	0
56	MG	2a	1635	1/1	0.95	0.10	44,44,44,44	0
56	MG	1A	3816	1/1	0.95	0.10	31,31,31,31	0
56	MG	2A	3452	1/1	0.95	0.23	43,43,43,43	0
56	MG	1A	3878	1/1	0.95	0.15	12,12,12,12	0
56	MG	2E	308	1/1	0.95	0.11	38,38,38,38	0
56	MG	1A	3979	1/1	0.95	0.20	22,22,22,22	0
56	MG	1A	3674	1/1	0.95	0.10	24,24,24,24	0
56	MG	23	102	1/1	0.95	0.17	31,31,31,31	0
56	MG	2X	101	1/1	0.95	0.90	57,57,57,57	0
56	MG	1A	3079	1/1	0.95	0.15	58,58,58,58	0
56	MG	2A	3191	1/1	0.95	0.13	31,31,31,31	0
56	MG	2A	3398	1/1	0.95	0.13	40,40,40,40	0
56	MG	1A	3068	1/1	0.95	0.25	22,22,22,22	0
56	MG	1A	3479	1/1	0.95	0.18	25,25,25,25	0
56	MG	1a	3117	1/1	0.95	0.19	30,30,30,30	0
56	MG	1A	4061	1/1	0.95	0.10	58,58,58,58	0
56	MG	1A	3755	1/1	0.95	0.09	30,30,30,30	0
56	MG	2A	3587	1/1	0.95	0.07	47,47,47,47	0
56	MG	2A	3429	1/1	0.95	0.18	43,43,43,43	0
56	MG	17	104	1/1	0.95	0.14	26,26,26,26	0
56	MG	1A	3594	1/1	0.95	0.19	24,24,24,24	0
56	MG	1A	3667	1/1	0.95	0.20	44,44,44,44	0
56	MG	1a	3160	1/1	0.95	0.15	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	3732	1/1	0.95	0.06	31,31,31,31	0
56	MG	2y	101	1/1	0.95	0.07	46,46,46,46	0
56	MG	1f	201	1/1	0.95	0.16	36,36,36,36	0
56	MG	2A	3754	1/1	0.95	0.11	48,48,48,48	0
56	MG	1A	4015	1/1	0.95	0.23	41,41,41,41	0
56	MG	1N	202	1/1	0.95	0.10	27,27,27,27	0
56	MG	1A	3215	1/1	0.95	0.19	16,16,16,16	0
56	MG	1A	3905	1/1	0.95	0.12	9,9,9,9	0
56	MG	2A	3672	1/1	0.95	0.08	42,42,42,42	0
56	MG	1A	3341	1/1	0.95	0.16	16,16,16,16	0
56	MG	1x	101	1/1	0.95	0.16	22,22,22,22	0
56	MG	1A	3606	1/1	0.95	0.29	32,32,32,32	0
56	MG	1A	3700	1/1	0.95	0.16	14,14,14,14	0
56	MG	2a	1798	1/1	0.95	0.12	44,44,44,44	0
56	MG	1A	3950	1/1	0.95	0.07	42,42,42,42	0
56	MG	2A	3620	1/1	0.95	0.17	48,48,48,48	0
56	MG	2A	3117	1/1	0.95	0.07	38,38,38,38	0
56	MG	2A	3060	1/1	0.95	0.09	24,24,24,24	0
56	MG	1A	3955	1/1	0.95	0.06	23,23,23,23	0
56	MG	1A	3322	1/1	0.95	0.22	23,23,23,23	0
56	MG	2A	3078	1/1	0.95	0.07	39,39,39,39	0
56	MG	1B	229	1/1	0.95	0.08	28,28,28,28	0
56	MG	2A	3064	1/1	0.95	0.08	30,30,30,30	0
56	MG	1A	3047	1/1	0.95	0.16	6,6,6,6	0
56	MG	1x	113	1/1	0.95	0.10	42,42,42,42	0
56	MG	1A	3512	1/1	0.95	0.11	13,13,13,13	0
56	MG	2A	3299	1/1	0.95	0.07	11,11,11,11	0
56	MG	2A	3850	1/1	0.95	0.29	44,44,44,44	0
56	MG	2D	302	1/1	0.95	0.22	39,39,39,39	0
56	MG	1B	210	1/1	0.95	0.13	39,39,39,39	0
56	MG	2F	306	1/1	0.95	0.41	40,40,40,40	0
56	MG	1a	3088	1/1	0.95	0.19	46,46,46,46	0
57	ERY	2A	3875	51/51	0.95	0.37	29,41,51,56	0
56	MG	2A	3527	1/1	0.95	0.10	44,44,44,44	0
56	MG	2A	3045	1/1	0.95	0.09	52,52,52,52	0
56	MG	2B	204	1/1	0.95	0.09	52,52,52,52	0
56	MG	1a	3103	1/1	0.95	0.13	37,37,37,37	0
56	MG	2a	1700	1/1	0.95	0.15	56,56,56,56	0
56	MG	1B	212	1/1	0.95	0.18	26,26,26,26	0
56	MG	1A	3934	1/1	0.95	0.11	29,29,29,29	0
56	MG	1B	235	1/1	0.95	0.15	40,40,40,40	0
56	MG	1A	3061	1/1	0.95	0.09	5,5,5,5	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	3299	1/1	0.95	0.12	6,6,6,6	0
56	MG	1A	3191	1/1	0.95	0.24	30,30,30,30	0
56	MG	2a	1725	1/1	0.95	0.08	43,43,43,43	0
56	MG	1A	3394	1/1	0.95	0.10	31,31,31,31	0
56	MG	1A	3925	1/1	0.95	0.08	21,21,21,21	0
56	MG	1a	3129	1/1	0.95	0.21	51,51,51,51	0
56	MG	1A	3387	1/1	0.95	0.28	40,40,40,40	0
56	MG	1W	205	1/1	0.95	0.10	15,15,15,15	0
56	MG	2A	3054	1/1	0.95	0.17	35,35,35,35	0
56	MG	1A	4058	1/1	0.95	0.11	42,42,42,42	0
56	MG	2A	3301	1/1	0.95	0.08	28,28,28,28	0
56	MG	1B	206	1/1	0.95	0.12	26,26,26,26	0
56	MG	1A	4067	1/1	0.95	0.17	31,31,31,31	0
56	MG	2A	3012	1/1	0.95	0.20	44,44,44,44	0
56	MG	1A	3358	1/1	0.95	0.46	23,23,23,23	0
56	MG	1A	3286	1/1	0.95	0.18	27,27,27,27	0
56	MG	1A	3974	1/1	0.95	0.07	41,41,41,41	0
56	MG	1A	3857	1/1	0.95	0.13	45,45,45,45	0
56	MG	1A	3540	1/1	0.95	0.11	20,20,20,20	0
56	MG	1a	3005	1/1	0.95	0.14	54,54,54,54	0
56	MG	2A	3042	1/1	0.95	0.14	40,40,40,40	0
56	MG	2F	301	1/1	0.95	0.14	34,34,34,34	0
56	MG	2a	1729	1/1	0.95	0.13	46,46,46,46	0
56	MG	1A	3311	1/1	0.95	0.38	28,28,28,28	0
56	MG	2a	1790	1/1	0.95	0.08	41,41,41,41	0
56	MG	1A	3767	1/1	0.95	0.12	19,19,19,19	0
56	MG	2A	3259	1/1	0.95	0.06	44,44,44,44	0
56	MG	1A	3524	1/1	0.95	0.08	40,40,40,40	0
56	MG	1A	3144	1/1	0.95	0.21	23,23,23,23	0
56	MG	1A	3739	1/1	0.95	0.11	21,21,21,21	0
56	MG	2A	3337	1/1	0.95	0.13	48,48,48,48	0
56	MG	1D	313	1/1	0.95	0.20	17,17,17,17	0
56	MG	2A	3110	1/1	0.95	0.35	33,33,33,33	0
56	MG	2x	105	1/1	0.95	0.06	33,33,33,33	0
56	MG	2A	3793	1/1	0.95	0.09	46,46,46,46	0
56	MG	2a	1820	1/1	0.95	0.13	52,52,52,52	0
56	MG	1a	3001	1/1	0.95	0.09	49,49,49,49	0
56	MG	2A	3252	1/1	0.95	0.07	41,41,41,41	0
56	MG	2A	3651	1/1	0.95	0.21	59,59,59,59	0
56	MG	1F	308	1/1	0.95	0.08	27,27,27,27	0
56	MG	2A	3719	1/1	0.95	0.18	29,29,29,29	0
56	MG	1A	3259	1/1	0.95	0.16	20,20,20,20	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3582	1/1	0.95	0.17	59,59,59,59	0
56	MG	1A	3658	1/1	0.95	0.11	28,28,28,28	0
56	MG	2A	3155	1/1	0.95	0.17	41,41,41,41	0
56	MG	2A	3395	1/1	0.95	0.46	43,43,43,43	0
56	MG	1A	4028	1/1	0.95	0.13	35,35,35,35	0
56	MG	1A	3611	1/1	0.95	0.19	36,36,36,36	0
58	ZN	1n	102	1/1	0.95	0.13	59,59,59,59	0
56	MG	1A	3135	1/1	0.95	0.16	27,27,27,27	0
56	MG	2A	3198	1/1	0.95	0.13	48,48,48,48	0
56	MG	1l	202	1/1	0.95	0.12	25,25,25,25	0
56	MG	2B	202	1/1	0.95	0.11	50,50,50,50	0
56	MG	1A	3166	1/1	0.95	0.33	18,18,18,18	0
56	MG	2A	3695	1/1	0.95	0.25	39,39,39,39	0
56	MG	1A	3682	1/1	0.95	0.12	37,37,37,37	0
56	MG	1A	3346	1/1	0.95	0.18	24,24,24,24	0
56	MG	2A	3214	1/1	0.95	0.16	34,34,34,34	0
56	MG	2A	3557	1/1	0.95	0.14	41,41,41,41	0
56	MG	1A	3701	1/1	0.95	0.13	38,38,38,38	0
56	MG	2a	1771	1/1	0.95	0.07	44,44,44,44	0
56	MG	2A	3735	1/1	0.95	0.15	28,28,28,28	0
56	MG	1A	3393	1/1	0.95	0.18	17,17,17,17	0
56	MG	1a	3111	1/1	0.95	0.10	37,37,37,37	0
56	MG	1A	3804	1/1	0.95	0.10	14,14,14,14	0
56	MG	2A	3565	1/1	0.95	0.09	25,25,25,25	0
56	MG	1A	3702	1/1	0.95	0.14	14,14,14,14	0
56	MG	2A	3087	1/1	0.95	0.08	60,60,60,60	0
56	MG	1A	3321	1/1	0.95	0.13	34,34,34,34	0
56	MG	1A	4042	1/1	0.95	0.10	31,31,31,31	0
56	MG	1A	3776	1/1	0.95	0.14	13,13,13,13	0
56	MG	1D	307	1/1	0.95	0.40	24,24,24,24	0
56	MG	2T	201	1/1	0.95	0.22	47,47,47,47	0
56	MG	1A	3108	1/1	0.95	0.19	24,24,24,24	0
56	MG	2A	3530	1/1	0.95	0.11	19,19,19,19	0
56	MG	2A	3027	1/1	0.95	0.12	32,32,32,32	0
56	MG	1A	3962	1/1	0.95	0.20	38,38,38,38	0
56	MG	1A	3607	1/1	0.95	0.25	31,31,31,31	0
56	MG	1A	3400	1/1	0.95	0.17	21,21,21,21	0
56	MG	1A	3118	1/1	0.95	0.14	16,16,16,16	0
56	MG	1A	3274	1/1	0.95	0.12	24,24,24,24	0
56	MG	2A	3320	1/1	0.95	0.30	47,47,47,47	0
56	MG	2A	3827	1/1	0.95	0.09	36,36,36,36	0
56	MG	1A	3308	1/1	0.95	0.26	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	2a	1819	1/1	0.95	0.16	67,67,67,67	0
56	MG	2A	3419	1/1	0.95	0.17	38,38,38,38	0
56	MG	1A	3589	1/1	0.95	0.09	36,36,36,36	0
56	MG	1A	3141	1/1	0.95	0.09	15,15,15,15	0
56	MG	2A	3159	1/1	0.95	0.05	42,42,42,42	0
56	MG	2A	3274	1/1	0.95	0.14	25,25,25,25	0
56	MG	2a	1690	1/1	0.95	0.14	53,53,53,53	0
56	MG	1a	3210	1/1	0.95	0.05	61,61,61,61	0
56	MG	2A	3242	1/1	0.95	0.10	55,55,55,55	0
56	MG	1F	310	1/1	0.95	0.31	15,15,15,15	0
56	MG	1A	4063	1/1	0.95	0.15	52,52,52,52	0
56	MG	2A	3140	1/1	0.95	0.08	45,45,45,45	0
56	MG	1A	3853	1/1	0.95	0.14	28,28,28,28	0
56	MG	1A	3521	1/1	0.95	0.35	24,24,24,24	0
56	MG	1A	3253	1/1	0.95	0.09	30,30,30,30	0
56	MG	2A	3070	1/1	0.95	0.23	27,27,27,27	0
56	MG	2a	1746	1/1	0.95	0.11	57,57,57,57	0
56	MG	1A	3291	1/1	0.95	0.10	23,23,23,23	0
56	MG	2a	1728	1/1	0.95	0.10	46,46,46,46	0
56	MG	1A	3125	1/1	0.95	0.68	25,25,25,25	0
56	MG	1A	3576	1/1	0.95	0.15	28,28,28,28	0
56	MG	10	106	1/1	0.95	0.17	37,37,37,37	0
56	MG	1A	3758	1/1	0.95	0.14	12,12,12,12	0
56	MG	2a	1780	1/1	0.95	0.09	47,47,47,47	0
56	MG	1A	3059	1/1	0.95	0.09	10,10,10,10	0
56	MG	1E	309	1/1	0.95	0.19	26,26,26,26	0
56	MG	2A	3149	1/1	0.95	0.55	50,50,50,50	0
56	MG	18	102	1/1	0.95	0.09	20,20,20,20	0
56	MG	2A	3229	1/1	0.95	0.36	31,31,31,31	0
56	MG	1a	3171	1/1	0.95	0.14	39,39,39,39	0
56	MG	2a	1622	1/1	0.95	0.06	47,47,47,47	0
56	MG	2a	1760	1/1	0.95	0.20	60,60,60,60	0
56	MG	1A	3010	1/1	0.95	0.23	21,21,21,21	0
56	MG	2A	3112	1/1	0.95	0.10	26,26,26,26	0
56	MG	1a	3073	1/1	0.95	0.10	65,65,65,65	0
56	MG	1a	3030	1/1	0.95	0.13	52,52,52,52	0
56	MG	1A	3285	1/1	0.95	0.14	24,24,24,24	0
56	MG	2a	1605	1/1	0.95	0.21	36,36,36,36	0
56	MG	1A	3336	1/1	0.95	0.31	27,27,27,27	0
56	MG	1A	3881	1/1	0.95	0.13	17,17,17,17	0
56	MG	1A	3604	1/1	0.95	0.30	18,18,18,18	0
56	MG	2A	3281	1/1	0.95	0.29	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	3177	1/1	0.95	0.09	37,37,37,37	0
56	MG	1A	3986	1/1	0.95	0.09	35,35,35,35	0
56	MG	1A	4041	1/1	0.95	0.15	43,43,43,43	0
56	MG	1A	3445	1/1	0.96	0.12	32,32,32,32	0
56	MG	1I	203	1/1	0.96	0.09	48,48,48,48	0
56	MG	2A	3025	1/1	0.96	0.14	38,38,38,38	0
56	MG	1E	303	1/1	0.96	0.24	25,25,25,25	0
56	MG	13	104	1/1	0.96	0.10	26,26,26,26	0
56	MG	2A	3609	1/1	0.96	0.20	33,33,33,33	0
56	MG	1a	3122	1/1	0.96	0.10	36,36,36,36	0
56	MG	1a	3219	1/1	0.96	0.08	61,61,61,61	0
56	MG	2A	3138	1/1	0.96	0.13	30,30,30,30	0
56	MG	1A	3417	1/1	0.96	0.10	18,18,18,18	0
56	MG	1A	3590	1/1	0.96	0.14	39,39,39,39	0
56	MG	2A	3453	1/1	0.96	0.11	33,33,33,33	0
56	MG	2A	3200	1/1	0.96	0.09	33,33,33,33	0
56	MG	1A	3261	1/1	0.96	0.27	31,31,31,31	0
56	MG	1A	3520	1/1	0.96	0.39	22,22,22,22	0
56	MG	1A	3228	1/1	0.96	0.08	50,50,50,50	0
56	MG	1A	3892	1/1	0.96	0.11	15,15,15,15	0
56	MG	1A	3197	1/1	0.96	0.12	17,17,17,17	0
56	MG	2a	1723	1/1	0.96	0.28	38,38,38,38	0
56	MG	1A	3240	1/1	0.96	0.40	29,29,29,29	0
56	MG	1A	3415	1/1	0.96	0.12	31,31,31,31	0
56	MG	2A	3031	1/1	0.96	0.08	26,26,26,26	0
56	MG	2A	3561	1/1	0.96	0.17	27,27,27,27	0
56	MG	2A	3321	1/1	0.96	0.14	20,20,20,20	0
56	MG	2A	3437	1/1	0.96	0.15	42,42,42,42	0
56	MG	1a	3229	1/1	0.96	0.17	41,41,41,41	0
56	MG	1A	3858	1/1	0.96	0.15	10,10,10,10	0
56	MG	1A	3669	1/1	0.96	0.10	19,19,19,19	0
56	MG	1A	3501	1/1	0.96	0.17	29,29,29,29	0
56	MG	1A	3128	1/1	0.96	0.26	17,17,17,17	0
56	MG	1A	3745	1/1	0.96	0.14	13,13,13,13	0
56	MG	1a	3157	1/1	0.96	0.38	49,49,49,49	0
56	MG	2A	3388	1/1	0.96	0.09	41,41,41,41	0
56	MG	2A	3443	1/1	0.96	0.12	34,34,34,34	0
56	MG	1A	3749	1/1	0.96	0.23	47,47,47,47	0
56	MG	1A	3608	1/1	0.96	0.15	36,36,36,36	0
56	MG	2A	3694	1/1	0.96	0.17	47,47,47,47	0
56	MG	1A	3205	1/1	0.96	0.11	20,20,20,20	0
56	MG	1R	201	1/1	0.96	0.08	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	2A	3124	1/1	0.96	0.25	41,41,41,41	0
56	MG	1A	4000	1/1	0.96	0.08	43,43,43,43	0
56	MG	1A	3350	1/1	0.96	0.80	33,33,33,33	0
56	MG	1A	3846	1/1	0.96	0.11	29,29,29,29	0
56	MG	1A	3786	1/1	0.96	0.13	16,16,16,16	0
56	MG	2A	3648	1/1	0.96	0.09	44,44,44,44	0
56	MG	2A	3116	1/1	0.96	0.10	61,61,61,61	0
56	MG	2A	3073	1/1	0.96	0.57	47,47,47,47	0
56	MG	2A	3162	1/1	0.96	0.14	43,43,43,43	0
56	MG	2f	202	1/1	0.96	0.13	47,47,47,47	0
56	MG	2a	1660	1/1	0.96	0.09	37,37,37,37	0
56	MG	1A	3854	1/1	0.96	0.13	42,42,42,42	0
56	MG	1a	3072	1/1	0.96	0.10	41,41,41,41	0
56	MG	2a	1629	1/1	0.96	0.17	37,37,37,37	0
56	MG	1A	3833	1/1	0.96	0.19	42,42,42,42	0
56	MG	1A	3489	1/1	0.96	0.22	17,17,17,17	0
56	MG	1a	3065	1/1	0.96	0.07	34,34,34,34	0
56	MG	2a	1815	1/1	0.96	0.12	56,56,56,56	0
56	MG	1A	3160	1/1	0.96	0.14	13,13,13,13	0
56	MG	1A	3789	1/1	0.96	0.12	21,21,21,21	0
56	MG	2A	3181	1/1	0.96	0.13	21,21,21,21	0
56	MG	1A	3517	1/1	0.96	0.53	33,33,33,33	0
56	MG	1A	4016	1/1	0.96	0.15	24,24,24,24	0
56	MG	1A	3565	1/1	0.96	0.12	11,11,11,11	0
56	MG	2A	3638	1/1	0.96	0.08	36,36,36,36	0
56	MG	2A	3712	1/1	0.96	0.12	34,34,34,34	0
56	MG	23	103	1/1	0.96	0.21	44,44,44,44	0
56	MG	1a	3037	1/1	0.96	0.14	41,41,41,41	0
56	MG	27	101	1/1	0.96	0.33	32,32,32,32	0
56	MG	1A	3722	1/1	0.96	0.10	16,16,16,16	0
56	MG	1a	3118	1/1	0.96	0.09	43,43,43,43	0
56	MG	2e	201	1/1	0.96	0.08	52,52,52,52	0
56	MG	1A	3256	1/1	0.96	0.12	26,26,26,26	0
58	ZN	29	501	1/1	0.96	0.08	66,66,66,66	0
56	MG	2P	201	1/1	0.96	0.31	40,40,40,40	0
56	MG	2a	1630	1/1	0.96	0.09	51,51,51,51	0
56	MG	2A	3515	1/1	0.96	0.09	48,48,48,48	0
56	MG	2A	3590	1/1	0.96	0.07	36,36,36,36	0
56	MG	2A	3470	1/1	0.96	0.10	33,33,33,33	0
56	MG	1A	3723	1/1	0.96	0.14	26,26,26,26	0
56	MG	1A	3467	1/1	0.96	0.13	14,14,14,14	0
56	MG	2A	3518	1/1	0.96	0.10	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	3151	1/1	0.96	0.18	23,23,23,23	0
56	MG	1U	205	1/1	0.96	0.09	28,28,28,28	0
56	MG	1a	3096	1/1	0.96	0.12	38,38,38,38	0
56	MG	2A	3334	1/1	0.96	0.13	32,32,32,32	0
56	MG	1A	4001	1/1	0.96	0.17	29,29,29,29	0
56	MG	2A	3029	1/1	0.96	0.08	32,32,32,32	0
56	MG	1A	3838	1/1	0.96	0.09	27,27,27,27	0
56	MG	1A	3533	1/1	0.96	0.17	36,36,36,36	0
56	MG	2A	3564	1/1	0.96	0.19	36,36,36,36	0
56	MG	1A	4033	1/1	0.96	0.08	34,34,34,34	0
56	MG	2A	3863	1/1	0.96	0.13	27,27,27,27	0
56	MG	1A	3593	1/1	0.96	0.14	30,30,30,30	0
56	MG	2D	304	1/1	0.96	0.09	25,25,25,25	0
56	MG	2A	3350	1/1	0.96	0.47	34,34,34,34	0
56	MG	1Q	203	1/1	0.96	0.24	20,20,20,20	0
56	MG	2A	3738	1/1	0.96	0.22	54,54,54,54	0
56	MG	2A	3307	1/1	0.96	0.05	52,52,52,52	0
56	MG	2A	3024	1/1	0.96	0.08	33,33,33,33	0
56	MG	1U	207	1/1	0.96	0.42	24,24,24,24	0
56	MG	1A	3469	1/1	0.96	0.12	27,27,27,27	0
56	MG	2A	3493	1/1	0.96	0.10	20,20,20,20	0
56	MG	1A	3629	1/1	0.96	0.10	18,18,18,18	0
56	MG	1A	3812	1/1	0.96	0.15	25,25,25,25	0
56	MG	1A	3785	1/1	0.96	0.10	14,14,14,14	0
56	MG	2A	3560	1/1	0.96	0.09	61,61,61,61	0
56	MG	1A	4050	1/1	0.96	0.15	38,38,38,38	0
56	MG	1A	3571	1/1	0.96	0.23	23,23,23,23	0
56	MG	2A	3210	1/1	0.96	0.16	23,23,23,23	0
56	MG	2a	1833	1/1	0.96	0.12	58,58,58,58	0
56	MG	1B	202	1/1	0.96	0.24	48,48,48,48	0
56	MG	1a	3040	1/1	0.96	0.10	51,51,51,51	0
56	MG	1A	4069	1/1	0.96	0.07	37,37,37,37	0
56	MG	2A	3805	1/1	0.96	0.07	41,41,41,41	0
56	MG	2a	1692	1/1	0.96	0.19	52,52,52,52	0
56	MG	1A	3025	1/1	0.96	0.31	13,13,13,13	0
56	MG	1A	3977	1/1	0.96	0.14	27,27,27,27	0
56	MG	2A	3184	1/1	0.96	0.14	32,32,32,32	0
56	MG	1A	3124	1/1	0.96	0.25	35,35,35,35	0
56	MG	1A	3099	1/1	0.96	0.11	22,22,22,22	0
56	MG	2A	3466	1/1	0.96	0.15	19,19,19,19	0
56	MG	2D	305	1/1	0.96	0.47	39,39,39,39	0
56	MG	1A	3176	1/1	0.96	0.13	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	3124	1/1	0.96	0.07	33,33,33,33	0
56	MG	2A	3870	1/1	0.96	0.22	48,48,48,48	0
56	MG	1a	3004	1/1	0.96	0.44	47,47,47,47	0
56	MG	2a	1772	1/1	0.96	0.14	50,50,50,50	0
56	MG	2a	1756	1/1	0.96	0.11	74,74,74,74	0
56	MG	1N	204	1/1	0.96	0.68	31,31,31,31	0
56	MG	15	107	1/1	0.96	0.28	33,33,33,33	0
56	MG	2a	1786	1/1	0.96	0.08	50,50,50,50	0
56	MG	2a	1743	1/1	0.96	0.14	56,56,56,56	0
56	MG	1A	3822	1/1	0.96	0.13	35,35,35,35	0
56	MG	2A	3063	1/1	0.96	0.13	35,35,35,35	0
56	MG	2A	3707	1/1	0.96	0.08	20,20,20,20	0
56	MG	1a	3216	1/1	0.96	0.07	33,33,33,33	0
56	MG	1A	3087	1/1	0.96	0.13	16,16,16,16	0
56	MG	1A	3900	1/1	0.96	0.16	34,34,34,34	0
56	MG	1T	201	1/1	0.96	0.17	35,35,35,35	0
56	MG	2A	3351	1/1	0.96	0.14	30,30,30,30	0
56	MG	1A	3366	1/1	0.96	0.22	29,29,29,29	0
56	MG	1A	3751	1/1	0.96	0.07	25,25,25,25	0
56	MG	1A	3112	1/1	0.96	0.23	22,22,22,22	0
56	MG	2A	3061	1/1	0.96	0.43	66,66,66,66	0
56	MG	1A	3642	1/1	0.96	0.15	17,17,17,17	0
56	MG	1A	3972	1/1	0.96	0.07	39,39,39,39	0
56	MG	2A	3075	1/1	0.96	0.12	38,38,38,38	0
56	MG	2A	3854	1/1	0.96	0.17	43,43,43,43	0
56	MG	1A	3042	1/1	0.96	0.21	14,14,14,14	0
56	MG	2A	3639	1/1	0.96	0.09	36,36,36,36	0
56	MG	1A	3829	1/1	0.96	0.26	18,18,18,18	0
56	MG	2A	3092	1/1	0.96	0.10	34,34,34,34	0
56	MG	2A	3005	1/1	0.96	0.11	39,39,39,39	0
56	MG	1A	3568	1/1	0.96	0.12	16,16,16,16	0
56	MG	2A	3232	1/1	0.96	0.13	46,46,46,46	0
56	MG	1A	4017	1/1	0.96	0.11	28,28,28,28	0
56	MG	1A	3945	1/1	0.96	0.11	31,31,31,31	0
56	MG	1A	3157	1/1	0.96	0.12	36,36,36,36	0
56	MG	1G	202	1/1	0.96	0.15	19,19,19,19	0
56	MG	1A	3104	1/1	0.96	0.30	21,21,21,21	0
56	MG	2A	3367	1/1	0.96	0.37	41,41,41,41	0
56	MG	2A	3621	1/1	0.96	0.14	31,31,31,31	0
56	MG	2A	3739	1/1	0.96	0.11	34,34,34,34	0
56	MG	1a	3062	1/1	0.96	0.07	56,56,56,56	0
56	MG	2A	3254	1/1	0.96	0.17	30,30,30,30	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3127	1/1	0.96	0.49	42,42,42,42	0
56	MG	2A	3627	1/1	0.96	0.29	40,40,40,40	0
56	MG	1A	3475	1/1	0.96	0.13	32,32,32,32	0
56	MG	1A	3091	1/1	0.96	0.36	17,17,17,17	0
56	MG	1X	105	1/1	0.96	0.13	20,20,20,20	0
56	MG	1B	230	1/1	0.96	0.10	38,38,38,38	0
56	MG	2A	3040	1/1	0.96	0.09	16,16,16,16	0
56	MG	2A	3231	1/1	0.96	0.11	41,41,41,41	0
56	MG	1a	3127	1/1	0.96	0.06	20,20,20,20	0
56	MG	1A	3035	1/1	0.96	0.20	20,20,20,20	0
56	MG	1A	4057	1/1	0.96	0.12	22,22,22,22	0
56	MG	1A	3163	1/1	0.96	0.14	24,24,24,24	0
56	MG	1A	4022	1/1	0.96	0.07	34,34,34,34	0
56	MG	1B	205	1/1	0.96	0.23	33,33,33,33	0
56	MG	2A	3384	1/1	0.96	0.10	34,34,34,34	0
56	MG	2A	3726	1/1	0.96	0.07	50,50,50,50	0
56	MG	2A	3004	1/1	0.96	0.11	32,32,32,32	0
56	MG	2O	8400	1/1	0.96	0.23	40,40,40,40	0
56	MG	1A	3430	1/1	0.96	0.16	48,48,48,48	0
56	MG	2A	3238	1/1	0.96	0.23	50,50,50,50	0
56	MG	2B	206	1/1	0.96	0.16	42,42,42,42	0
56	MG	1A	3192	1/1	0.96	0.25	23,23,23,23	0
58	ZN	2n	501	1/1	0.96	0.08	95,95,95,95	0
56	MG	1A	3312	1/1	0.96	0.12	22,22,22,22	0
56	MG	1a	3169	1/1	0.96	0.14	35,35,35,35	0
56	MG	1A	3938	1/1	0.96	0.23	47,47,47,47	0
56	MG	1E	314	1/1	0.96	0.40	29,29,29,29	0
56	MG	2a	1826	1/1	0.96	0.09	43,43,43,43	0
56	MG	1A	3902	1/1	0.96	0.06	36,36,36,36	0
56	MG	2A	3503	1/1	0.96	0.33	33,33,33,33	0
56	MG	1A	3442	1/1	0.96	0.26	33,33,33,33	0
56	MG	1A	3774	1/1	0.96	0.11	27,27,27,27	0
56	MG	1A	3936	1/1	0.96	0.07	35,35,35,35	0
56	MG	1A	3615	1/1	0.96	0.14	31,31,31,31	0
56	MG	1A	3848	1/1	0.96	0.05	38,38,38,38	0
56	MG	1A	3232	1/1	0.96	0.31	20,20,20,20	0
56	MG	2A	3442	1/1	0.96	0.17	39,39,39,39	0
56	MG	2A	3475	1/1	0.96	0.10	37,37,37,37	0
56	MG	1A	3531	1/1	0.96	0.23	25,25,25,25	0
56	MG	2a	1829	1/1	0.96	0.06	45,45,45,45	0
56	MG	1a	3121	1/1	0.96	0.10	42,42,42,42	0
56	MG	1A	3544	1/1	0.96	0.14	13,13,13,13	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	3725	1/1	0.96	0.25	34,34,34,34	0
56	MG	1A	3613	1/1	0.96	0.26	21,21,21,21	0
56	MG	1A	3572	1/1	0.96	0.17	36,36,36,36	0
56	MG	2A	3370	1/1	0.96	0.07	35,35,35,35	0
56	MG	1A	3416	1/1	0.96	0.08	39,39,39,39	0
56	MG	2T	203	1/1	0.96	0.20	34,34,34,34	0
56	MG	1A	3119	1/1	0.96	0.12	11,11,11,11	0
56	MG	2a	1811	1/1	0.96	0.11	50,50,50,50	0
56	MG	1A	3792	1/1	0.96	0.14	29,29,29,29	0
56	MG	2j	201	1/1	0.96	0.10	47,47,47,47	0
56	MG	2A	3846	1/1	0.96	0.26	46,46,46,46	0
56	MG	1A	3685	1/1	0.96	0.16	15,15,15,15	0
56	MG	1A	3150	1/1	0.96	0.11	20,20,20,20	0
56	MG	1A	3872	1/1	0.96	0.11	13,13,13,13	0
56	MG	2A	3413	1/1	0.96	0.11	39,39,39,39	0
56	MG	1Q	204	1/1	0.96	0.09	13,13,13,13	0
56	MG	2A	3713	1/1	0.96	0.07	34,34,34,34	0
56	MG	1A	3414	1/1	0.96	0.18	10,10,10,10	0
56	MG	1A	3168	1/1	0.96	0.11	32,32,32,32	0
56	MG	1A	3545	1/1	0.96	0.11	30,30,30,30	0
56	MG	2A	3649	1/1	0.96	0.18	28,28,28,28	0
56	MG	2a	1747	1/1	0.96	0.06	67,67,67,67	0
56	MG	1a	3032	1/1	0.96	0.07	32,32,32,32	0
56	MG	1A	3439	1/1	0.96	0.14	25,25,25,25	0
56	MG	1A	3040	1/1	0.96	0.12	20,20,20,20	0
56	MG	1D	303	1/1	0.96	0.08	25,25,25,25	0
56	MG	1a	3015	1/1	0.96	0.10	28,28,28,28	0
56	MG	2x	104	1/1	0.96	0.11	42,42,42,42	0
56	MG	2a	1657	1/1	0.96	0.12	48,48,48,48	0
56	MG	2k	201	1/1	0.96	0.12	51,51,51,51	0
56	MG	16	103	1/1	0.96	0.15	39,39,39,39	0
56	MG	1D	310	1/1	0.96	0.49	18,18,18,18	0
56	MG	2A	3137	1/1	0.96	0.14	24,24,24,24	0
56	MG	1A	3147	1/1	0.96	0.10	27,27,27,27	0
56	MG	2a	1638	1/1	0.96	0.17	39,39,39,39	0
56	MG	2A	3266	1/1	0.96	0.07	42,42,42,42	0
56	MG	1a	3018	1/1	0.96	0.21	49,49,49,49	0
56	MG	1A	3849	1/1	0.96	0.10	27,27,27,27	0
56	MG	2A	3418	1/1	0.96	0.15	21,21,21,21	0
56	MG	1W	207	1/1	0.96	0.27	4,4,4,4	0
56	MG	1A	3551	1/1	0.96	0.17	14,14,14,14	0
56	MG	1A	3880	1/1	0.96	0.12	20,20,20,20	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3037	1/1	0.96	0.10	9,9,9,9	0
56	MG	1A	3633	1/1	0.96	0.10	30,30,30,30	0
56	MG	1A	3182	1/1	0.96	0.15	22,22,22,22	0
56	MG	2A	3483	1/1	0.96	0.11	38,38,38,38	0
56	MG	1A	3717	1/1	0.96	0.14	17,17,17,17	0
56	MG	2A	3363	1/1	0.96	0.17	48,48,48,48	0
56	MG	2a	1797	1/1	0.96	0.11	37,37,37,37	0
56	MG	2A	3225	1/1	0.96	0.38	39,39,39,39	0
56	MG	2a	1757	1/1	0.96	0.05	54,54,54,54	0
56	MG	1a	3019	1/1	0.96	0.08	45,45,45,45	0
56	MG	2A	3102	1/1	0.96	0.12	44,44,44,44	0
56	MG	1A	3694	1/1	0.96	0.15	14,14,14,14	0
56	MG	2a	1809	1/1	0.96	0.07	44,44,44,44	0
56	MG	2A	3817	1/1	0.96	0.07	28,28,28,28	0
56	MG	1A	3600	1/1	0.96	0.13	44,44,44,44	0
56	MG	2A	3151	1/1	0.96	0.21	43,43,43,43	0
56	MG	1I	201	1/1	0.96	0.08	36,36,36,36	0
56	MG	1O	201	1/1	0.96	0.10	29,29,29,29	0
56	MG	2A	3578	1/1	0.96	0.30	44,44,44,44	0
56	MG	1A	3201	1/1	0.96	0.18	38,38,38,38	0
56	MG	1A	3511	1/1	0.96	0.11	21,21,21,21	0
56	MG	1A	3221	1/1	0.96	0.18	19,19,19,19	0
56	MG	1A	3920	1/1	0.96	0.10	31,31,31,31	0
56	MG	1A	3928	1/1	0.96	0.11	26,26,26,26	0
56	MG	1A	3523	1/1	0.96	0.14	36,36,36,36	0
56	MG	2a	1753	1/1	0.96	0.07	51,51,51,51	0
56	MG	1A	3692	1/1	0.96	0.12	10,10,10,10	0
56	MG	2a	1794	1/1	0.96	0.21	58,58,58,58	0
56	MG	25	102	1/1	0.96	0.44	40,40,40,40	0
56	MG	2A	3534	1/1	0.96	0.13	30,30,30,30	0
56	MG	1a	3028	1/1	0.96	0.12	48,48,48,48	0
56	MG	1A	3376	1/1	0.96	0.07	35,35,35,35	0
56	MG	1A	3603	1/1	0.96	0.29	16,16,16,16	0
56	MG	2A	3322	1/1	0.96	0.35	45,45,45,45	0
56	MG	2A	3302	1/1	0.96	0.10	22,22,22,22	0
56	MG	1A	3041	1/1	0.96	0.14	37,37,37,37	0
56	MG	2A	3111	1/1	0.96	0.08	52,52,52,52	0
56	MG	2A	3080	1/1	0.96	0.12	51,51,51,51	0
56	MG	1A	3345	1/1	0.96	0.16	19,19,19,19	0
56	MG	2a	1818	1/1	0.96	0.12	48,48,48,48	0
56	MG	2A	3700	1/1	0.96	0.10	55,55,55,55	0
56	MG	2A	3616	1/1	0.96	0.16	32,32,32,32	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	1702	1/1	0.96	0.14	40,40,40,40	0
56	MG	2N	201	1/1	0.96	0.08	32,32,32,32	0
56	MG	1Q	202	1/1	0.97	0.14	16,16,16,16	0
56	MG	2A	3187	1/1	0.97	0.12	39,39,39,39	0
56	MG	2A	3641	1/1	0.97	0.22	49,49,49,49	0
56	MG	1A	3522	1/1	0.97	0.10	21,21,21,21	0
56	MG	1A	3213	1/1	0.97	0.23	35,35,35,35	0
56	MG	2a	1824	1/1	0.97	0.18	26,26,26,26	0
56	MG	1V	205	1/1	0.97	0.24	19,19,19,19	0
56	MG	1A	3983	1/1	0.97	0.10	10,10,10,10	0
56	MG	2A	3744	1/1	0.97	0.11	29,29,29,29	0
56	MG	2a	1831	1/1	0.97	0.14	39,39,39,39	0
56	MG	1A	3988	1/1	0.97	0.16	20,20,20,20	0
56	MG	1A	3349	1/1	0.97	0.27	23,23,23,23	0
56	MG	2A	3849	1/1	0.97	0.09	30,30,30,30	0
56	MG	2A	3421	1/1	0.97	0.10	22,22,22,22	0
56	MG	1A	3870	1/1	0.97	0.29	23,23,23,23	0
56	MG	1A	3378	1/1	0.97	0.17	35,35,35,35	0
56	MG	2A	3867	1/1	0.97	0.09	46,46,46,46	0
56	MG	1A	3441	1/1	0.97	0.18	27,27,27,27	0
56	MG	2A	3552	1/1	0.97	0.07	56,56,56,56	0
56	MG	2l	202	1/1	0.97	0.39	45,45,45,45	0
56	MG	2A	3017	1/1	0.97	0.14	30,30,30,30	0
56	MG	1A	3638	1/1	0.97	0.12	30,30,30,30	0
56	MG	2A	3432	1/1	0.97	0.16	41,41,41,41	0
56	MG	1A	3383	1/1	0.97	0.11	22,22,22,22	0
56	MG	1A	3370	1/1	0.97	0.10	33,33,33,33	0
56	MG	2a	1691	1/1	0.97	0.09	44,44,44,44	0
56	MG	2a	1828	1/1	0.97	0.21	37,37,37,37	0
56	MG	1A	3100	1/1	0.97	0.21	22,22,22,22	0
56	MG	1A	3554	1/1	0.97	0.29	12,12,12,12	0
56	MG	1v	101	1/1	0.97	0.24	61,61,61,61	0
56	MG	1A	3627	1/1	0.97	0.11	27,27,27,27	0
56	MG	2A	3714	1/1	0.97	0.09	38,38,38,38	0
56	MG	1A	3748	1/1	0.97	0.09	34,34,34,34	0
56	MG	1A	3373	1/1	0.97	0.17	20,20,20,20	0
56	MG	1a	3042	1/1	0.97	0.11	37,37,37,37	0
56	MG	1A	3455	1/1	0.97	0.18	28,28,28,28	0
56	MG	2a	1673	1/1	0.97	0.11	48,48,48,48	0
56	MG	2A	3380	1/1	0.97	0.07	33,33,33,33	0
56	MG	2A	3460	1/1	0.97	0.14	48,48,48,48	0
56	MG	2A	3412	1/1	0.97	0.12	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	4066	1/1	0.97	0.15	21,21,21,21	0
56	MG	2A	3376	1/1	0.97	0.06	44,44,44,44	0
56	MG	1A	3940	1/1	0.97	0.06	49,49,49,49	0
56	MG	1A	3283	1/1	0.97	0.17	36,36,36,36	0
56	MG	1A	3105	1/1	0.97	0.19	11,11,11,11	0
56	MG	2a	1643	1/1	0.97	0.16	29,29,29,29	0
56	MG	13	103	1/1	0.97	0.30	26,26,26,26	0
56	MG	1A	3381	1/1	0.97	0.07	23,23,23,23	0
56	MG	1A	3784	1/1	0.97	0.09	28,28,28,28	0
56	MG	1A	3803	1/1	0.97	0.20	29,29,29,29	0
56	MG	2A	3261	1/1	0.97	0.09	26,26,26,26	0
56	MG	1A	3064	1/1	0.97	0.09	13,13,13,13	0
56	MG	1A	3995	1/1	0.97	0.17	32,32,32,32	0
56	MG	2A	3589	1/1	0.97	0.07	38,38,38,38	0
56	MG	1A	3029	1/1	0.97	0.12	11,11,11,11	0
56	MG	1A	3429	1/1	0.97	0.11	27,27,27,27	0
56	MG	1A	4007	1/1	0.97	0.13	36,36,36,36	0
56	MG	1a	3012	1/1	0.97	0.13	49,49,49,49	0
56	MG	2a	1604	1/1	0.97	0.10	39,39,39,39	0
56	MG	2A	3862	1/1	0.97	0.38	45,45,45,45	0
56	MG	1A	3450	1/1	0.97	0.08	20,20,20,20	0
56	MG	1A	3180	1/1	0.97	0.15	18,18,18,18	0
56	MG	1A	3060	1/1	0.97	0.20	18,18,18,18	0
56	MG	1A	3371	1/1	0.97	0.20	10,10,10,10	0
56	MG	1A	3916	1/1	0.97	0.10	40,40,40,40	0
56	MG	2A	3130	1/1	0.97	0.07	28,28,28,28	0
56	MG	1e	201	1/1	0.97	0.09	48,48,48,48	0
56	MG	1A	4051	1/1	0.97	0.08	16,16,16,16	0
56	MG	2A	3051	1/1	0.97	0.15	34,34,34,34	0
56	MG	1A	3375	1/1	0.97	0.08	37,37,37,37	0
56	MG	2A	3323	1/1	0.97	0.27	63,63,63,63	0
56	MG	2A	3132	1/1	0.97	0.14	40,40,40,40	0
56	MG	1A	3073	1/1	0.97	0.22	29,29,29,29	0
56	MG	1A	3464	1/1	0.97	0.38	25,25,25,25	0
56	MG	2a	1658	1/1	0.97	0.10	30,30,30,30	0
56	MG	2A	3722	1/1	0.97	0.28	39,39,39,39	0
56	MG	2a	1618	1/1	0.97	0.13	36,36,36,36	0
56	MG	1A	3555	1/1	0.97	0.21	23,23,23,23	0
56	MG	1E	313	1/1	0.97	0.18	10,10,10,10	0
56	MG	1A	3548	1/1	0.97	0.29	27,27,27,27	0
56	MG	1A	3616	1/1	0.97	0.16	19,19,19,19	0
56	MG	1a	3161	1/1	0.97	0.15	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	3462	1/1	0.97	0.28	38,38,38,38	0
56	MG	1A	3648	1/1	0.97	0.07	18,18,18,18	0
56	MG	2A	3459	1/1	0.97	0.18	35,35,35,35	0
56	MG	1A	3869	1/1	0.97	0.24	31,31,31,31	0
56	MG	1U	203	1/1	0.97	0.55	23,23,23,23	0
56	MG	1A	3908	1/1	0.97	0.10	23,23,23,23	0
56	MG	1A	3338	1/1	0.97	0.09	13,13,13,13	0
56	MG	2A	3006	1/1	0.97	0.11	42,42,42,42	0
56	MG	1A	4029	1/1	0.97	0.20	19,19,19,19	0
56	MG	2a	1726	1/1	0.97	0.27	32,32,32,32	0
56	MG	2A	3220	1/1	0.97	0.45	32,32,32,32	0
56	MG	1P	205	1/1	0.97	0.07	15,15,15,15	0
56	MG	1A	3173	1/1	0.97	0.12	21,21,21,21	0
56	MG	1A	3009	1/1	0.97	0.11	16,16,16,16	0
56	MG	2A	3865	1/1	0.97	0.13	28,28,28,28	0
56	MG	1A	3882	1/1	0.97	0.09	26,26,26,26	0
56	MG	1A	3230	1/1	0.97	0.08	24,24,24,24	0
56	MG	15	102	1/1	0.97	0.21	10,10,10,10	0
56	MG	1B	227	1/1	0.97	0.19	37,37,37,37	0
56	MG	1A	3001	1/1	0.97	0.15	35,35,35,35	0
56	MG	1a	3017	1/1	0.97	0.21	26,26,26,26	0
56	MG	1A	3137	1/1	0.97	0.19	35,35,35,35	0
56	MG	1Q	201	1/1	0.97	0.22	30,30,30,30	0
56	MG	2B	217	1/1	0.97	0.05	47,47,47,47	0
56	MG	2A	3554	1/1	0.97	0.08	45,45,45,45	0
56	MG	2A	3759	1/1	0.97	0.08	39,39,39,39	0
56	MG	1A	3399	1/1	0.97	0.17	16,16,16,16	0
56	MG	1A	3249	1/1	0.97	0.16	28,28,28,28	0
56	MG	1A	3089	1/1	0.97	0.25	28,28,28,28	0
56	MG	1A	3458	1/1	0.97	0.20	37,37,37,37	0
56	MG	2A	3248	1/1	0.97	0.14	47,47,47,47	0
56	MG	1a	3141	1/1	0.97	0.16	48,48,48,48	0
56	MG	1a	3087	1/1	0.97	0.09	39,39,39,39	0
56	MG	2A	3082	1/1	0.97	0.47	38,38,38,38	0
56	MG	2A	3415	1/1	0.97	0.09	34,34,34,34	0
56	MG	1A	3780	1/1	0.97	0.06	29,29,29,29	0
56	MG	1A	3030	1/1	0.97	0.22	17,17,17,17	0
56	MG	1a	3201	1/1	0.97	0.09	55,55,55,55	0
56	MG	2A	3175	1/1	0.97	0.14	28,28,28,28	0
56	MG	2A	3486	1/1	0.97	0.09	33,33,33,33	0
56	MG	1A	3217	1/1	0.97	0.28	42,42,42,42	0
56	MG	1A	3967	1/1	0.97	0.13	18,18,18,18	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	3110	1/1	0.97	0.38	24,24,24,24	0
56	MG	2A	3730	1/1	0.97	0.18	48,48,48,48	0
56	MG	1a	3089	1/1	0.97	0.06	33,33,33,33	0
56	MG	1A	3019	1/1	0.97	0.24	26,26,26,26	0
56	MG	2A	3767	1/1	0.97	0.10	43,43,43,43	0
56	MG	1E	312	1/1	0.97	0.12	26,26,26,26	0
56	MG	1A	3679	1/1	0.97	0.13	10,10,10,10	0
56	MG	1A	3563	1/1	0.97	0.22	16,16,16,16	0
56	MG	1A	3082	1/1	0.97	0.13	20,20,20,20	0
56	MG	1A	3403	1/1	0.97	0.15	20,20,20,20	0
56	MG	1a	3076	1/1	0.97	0.06	35,35,35,35	0
56	MG	1A	3586	1/1	0.97	0.23	25,25,25,25	0
56	MG	2A	3852	1/1	0.97	0.07	24,24,24,24	0
56	MG	1A	3731	1/1	0.97	0.12	27,27,27,27	0
56	MG	1A	3431	1/1	0.97	0.29	24,24,24,24	0
56	MG	1A	3357	1/1	0.97	0.12	17,17,17,17	0
56	MG	1A	3002	1/1	0.97	0.11	22,22,22,22	0
56	MG	1D	308	1/1	0.97	0.12	29,29,29,29	0
56	MG	1A	3998	1/1	0.97	0.08	26,26,26,26	0
56	MG	2A	3476	1/1	0.97	0.10	40,40,40,40	0
56	MG	1a	3182	1/1	0.97	0.09	51,51,51,51	0
56	MG	1a	3221	1/1	0.97	0.08	47,47,47,47	0
56	MG	1a	3120	1/1	0.97	0.14	42,42,42,42	0
56	MG	1A	3817	1/1	0.97	0.12	28,28,28,28	0
56	MG	1A	3743	1/1	0.97	0.11	16,16,16,16	0
56	MG	2A	3119	1/1	0.97	0.32	34,34,34,34	0
56	MG	2a	1646	1/1	0.97	0.08	51,51,51,51	0
56	MG	1A	3649	1/1	0.97	0.11	12,12,12,12	0
56	MG	1A	3547	1/1	0.97	0.21	9,9,9,9	0
56	MG	1W	204	1/1	0.97	0.21	25,25,25,25	0
56	MG	1A	3161	1/1	0.97	0.12	26,26,26,26	0
56	MG	1A	3278	1/1	0.97	0.11	16,16,16,16	0
56	MG	1A	3198	1/1	0.97	0.22	20,20,20,20	0
56	MG	1A	3906	1/1	0.97	0.14	9,9,9,9	0
56	MG	1A	3562	1/1	0.97	0.26	7,7,7,7	0
56	MG	2A	3628	1/1	0.97	0.06	33,33,33,33	0
56	MG	1A	3072	1/1	0.97	0.13	18,18,18,18	0
56	MG	2A	3097	1/1	0.97	0.09	37,37,37,37	0
56	MG	1A	3158	1/1	0.97	0.19	37,37,37,37	0
56	MG	1a	3023	1/1	0.97	0.12	17,17,17,17	0
56	MG	1a	3060	1/1	0.97	0.07	48,48,48,48	0
56	MG	1A	3634	1/1	0.97	0.18	14,14,14,14	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3661	1/1	0.97	0.17	34,34,34,34	0
56	MG	2A	3007	1/1	0.97	0.09	27,27,27,27	0
56	MG	2a	1778	1/1	0.97	0.14	54,54,54,54	0
56	MG	1A	3779	1/1	0.97	0.23	15,15,15,15	0
56	MG	1A	3894	1/1	0.97	0.17	27,27,27,27	0
56	MG	2a	1804	1/1	0.97	0.06	37,37,37,37	0
56	MG	1a	3046	1/1	0.97	0.16	19,19,19,19	0
56	MG	1W	206	1/1	0.97	0.10	20,20,20,20	0
56	MG	1A	3794	1/1	0.97	0.13	12,12,12,12	0
56	MG	1A	3481	1/1	0.97	0.10	26,26,26,26	0
56	MG	1A	3842	1/1	0.97	0.13	37,37,37,37	0
56	MG	1A	4011	1/1	0.97	0.17	34,34,34,34	0
56	MG	1A	3744	1/1	0.97	0.11	25,25,25,25	0
56	MG	2A	3679	1/1	0.97	0.19	51,51,51,51	0
56	MG	2a	1687	1/1	0.97	0.13	51,51,51,51	0
56	MG	1a	3179	1/1	0.97	0.07	47,47,47,47	0
56	MG	2a	1689	1/1	0.97	0.11	47,47,47,47	0
56	MG	2A	3126	1/1	0.97	0.12	44,44,44,44	0
56	MG	2A	3837	1/1	0.97	0.11	18,18,18,18	0
56	MG	1A	3670	1/1	0.97	0.11	20,20,20,20	0
56	MG	1A	3818	1/1	0.97	0.12	31,31,31,31	0
56	MG	1A	3536	1/1	0.97	0.16	31,31,31,31	0
56	MG	1E	311	1/1	0.97	0.16	30,30,30,30	0
56	MG	2A	3425	1/1	0.97	0.31	34,34,34,34	0
56	MG	1A	3895	1/1	0.97	0.16	30,30,30,30	0
56	MG	1A	3725	1/1	0.97	0.08	40,40,40,40	0
56	MG	2A	3666	1/1	0.97	0.10	30,30,30,30	0
56	MG	2A	3226	1/1	0.97	0.20	31,31,31,31	0
56	MG	2A	3601	1/1	0.97	0.07	42,42,42,42	0
56	MG	2A	3704	1/1	0.97	0.18	33,33,33,33	0
56	MG	2A	3326	1/1	0.97	0.23	31,31,31,31	0
56	MG	1A	3821	1/1	0.97	0.09	31,31,31,31	0
56	MG	1A	3190	1/1	0.97	0.11	17,17,17,17	0
56	MG	2A	3280	1/1	0.97	0.25	39,39,39,39	0
56	MG	1a	3156	1/1	0.97	0.11	34,34,34,34	0
56	MG	2A	3516	1/1	0.97	0.13	36,36,36,36	0
56	MG	1A	3550	1/1	0.97	0.11	4,4,4,4	0
56	MG	1a	3036	1/1	0.97	0.10	32,32,32,32	0
56	MG	2a	1662	1/1	0.97	0.13	43,43,43,43	0
56	MG	1A	3275	1/1	0.97	0.15	36,36,36,36	0
56	MG	2A	3152	1/1	0.97	0.30	42,42,42,42	0
56	MG	2A	3166	1/1	0.97	0.15	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	3525	1/1	0.97	0.08	30,30,30,30	0
56	MG	2A	3832	1/1	0.97	0.14	35,35,35,35	0
56	MG	1A	3080	1/1	0.97	0.11	17,17,17,17	0
56	MG	1D	302	1/1	0.97	0.69	35,35,35,35	0
56	MG	1A	3332	1/1	0.97	0.13	22,22,22,22	0
56	MG	1A	3405	1/1	0.97	0.08	38,38,38,38	0
56	MG	1a	3159	1/1	0.97	0.15	46,46,46,46	0
56	MG	2A	3221	1/1	0.97	0.17	51,51,51,51	0
56	MG	2A	3444	1/1	0.97	0.12	36,36,36,36	0
56	MG	2A	3179	1/1	0.97	0.06	33,33,33,33	0
56	MG	1A	3947	1/1	0.97	0.12	22,22,22,22	0
56	MG	1a	3184	1/1	0.97	0.11	49,49,49,49	0
56	MG	1a	3108	1/1	0.97	0.07	24,24,24,24	0
56	MG	1a	3187	1/1	0.97	0.16	29,29,29,29	0
56	MG	2a	1744	1/1	0.97	0.16	65,65,65,65	0
56	MG	1A	3614	1/1	0.97	0.25	35,35,35,35	0
56	MG	2A	3831	1/1	0.97	0.14	68,68,68,68	0
56	MG	1A	3076	1/1	0.97	0.12	32,32,32,32	0
56	MG	1A	3575	1/1	0.97	0.09	23,23,23,23	0
56	MG	2a	1830	1/1	0.97	0.18	38,38,38,38	0
56	MG	2A	3447	1/1	0.97	0.15	39,39,39,39	0
56	MG	2A	3573	1/1	0.97	0.10	28,28,28,28	0
56	MG	1G	203	1/1	0.97	0.12	34,34,34,34	0
56	MG	2B	220	1/1	0.97	0.16	57,57,57,57	0
56	MG	2A	3763	1/1	0.97	0.11	41,41,41,41	0
56	MG	2A	3374	1/1	0.97	0.06	50,50,50,50	0
56	MG	1A	3014	1/1	0.97	0.16	32,32,32,32	0
56	MG	1a	3097	1/1	0.97	0.20	34,34,34,34	0
56	MG	2A	3872	1/1	0.97	0.07	42,42,42,42	0
56	MG	1A	3131	1/1	0.97	0.11	16,16,16,16	0
56	MG	1A	3612	1/1	0.97	0.25	26,26,26,26	0
56	MG	2A	3296	1/1	0.97	0.08	46,46,46,46	0
56	MG	1A	3069	1/1	0.97	0.44	33,33,33,33	0
56	MG	1a	3016	1/1	0.97	0.12	43,43,43,43	0
56	MG	1A	3013	1/1	0.97	0.11	11,11,11,11	0
56	MG	1A	3239	1/1	0.97	0.20	9,9,9,9	0
56	MG	1A	3123	1/1	0.97	0.11	6,6,6,6	0
56	MG	2A	3354	1/1	0.97	0.25	41,41,41,41	0
56	MG	1A	3621	1/1	0.97	0.10	30,30,30,30	0
56	MG	1A	3218	1/1	0.97	0.12	19,19,19,19	0
56	MG	1A	3734	1/1	0.97	0.13	30,30,30,30	0
56	MG	2A	3613	1/1	0.97	0.28	58,58,58,58	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3466	1/1	0.97	0.22	23,23,23,23	0
56	MG	2A	3461	1/1	0.97	0.37	29,29,29,29	0
56	MG	2A	3234	1/1	0.97	0.49	37,37,37,37	0
56	MG	1a	3197	1/1	0.97	0.06	49,49,49,49	0
56	MG	2A	3526	1/1	0.97	0.17	42,42,42,42	0
56	MG	1A	3449	1/1	0.97	0.28	19,19,19,19	0
56	MG	1B	224	1/1	0.97	0.14	36,36,36,36	0
56	MG	1A	3790	1/1	0.97	0.14	10,10,10,10	0
56	MG	1A	3929	1/1	0.97	0.11	34,34,34,34	0
56	MG	1A	3924	1/1	0.97	0.09	9,9,9,9	0
56	MG	1A	3811	1/1	0.97	0.08	20,20,20,20	0
56	MG	2a	1750	1/1	0.97	0.10	51,51,51,51	0
56	MG	1A	3747	1/1	0.97	0.07	35,35,35,35	0
56	MG	2A	3224	1/1	0.97	0.42	45,45,45,45	0
56	MG	2A	3675	1/1	0.97	0.12	37,37,37,37	0
56	MG	2D	301	1/1	0.97	0.14	37,37,37,37	0
56	MG	1a	3144	1/1	0.97	0.14	61,61,61,61	0
56	MG	2A	3490	1/1	0.97	0.08	52,52,52,52	0
56	MG	2A	3369	1/1	0.97	0.27	53,53,53,53	0
56	MG	1A	3899	1/1	0.97	0.10	23,23,23,23	0
56	MG	1A	3011	1/1	0.97	0.07	25,25,25,25	0
56	MG	1A	3689	1/1	0.97	0.08	19,19,19,19	0
56	MG	1F	309	1/1	0.97	0.34	21,21,21,21	0
56	MG	1A	3070	1/1	0.97	0.27	23,23,23,23	0
56	MG	2a	1686	1/1	0.97	0.07	34,34,34,34	0
56	MG	1A	3768	1/1	0.97	0.12	22,22,22,22	0
56	MG	1A	3356	1/1	0.97	0.42	12,12,12,12	0
56	MG	1A	3034	1/1	0.97	0.18	15,15,15,15	0
56	MG	2B	210	1/1	0.97	0.15	72,72,72,72	0
56	MG	1A	3410	1/1	0.97	0.10	17,17,17,17	0
56	MG	1A	3917	1/1	0.97	0.17	34,34,34,34	0
56	MG	2A	3114	1/1	0.97	0.09	32,32,32,32	0
56	MG	1B	233	1/1	0.97	0.08	41,41,41,41	0
56	MG	1A	3975	1/1	0.97	0.05	25,25,25,25	0
56	MG	2A	3654	1/1	0.97	0.28	30,30,30,30	0
56	MG	2A	3171	1/1	0.97	0.12	27,27,27,27	0
56	MG	1A	3181	1/1	0.97	0.15	35,35,35,35	0
56	MG	2A	3100	1/1	0.97	0.20	41,41,41,41	0
56	MG	1X	101	1/1	0.97	0.23	28,28,28,28	0
56	MG	2a	1642	1/1	0.97	0.10	38,38,38,38	0
56	MG	1A	3243	1/1	0.97	0.22	16,16,16,16	0
56	MG	2A	3052	1/1	0.97	0.15	58,58,58,58	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	12	101	1/1	0.97	0.20	28,28,28,28	0
56	MG	1A	3978	1/1	0.97	0.14	24,24,24,24	0
56	MG	1A	3528	1/1	0.97	0.16	27,27,27,27	0
56	MG	2A	3669	1/1	0.97	0.13	31,31,31,31	0
56	MG	1a	3181	1/1	0.97	0.06	39,39,39,39	0
56	MG	13	106	1/1	0.97	0.20	15,15,15,15	0
56	MG	1a	3026	1/1	0.98	0.19	28,28,28,28	0
56	MG	1A	3078	1/1	0.98	0.22	30,30,30,30	0
56	MG	2a	1601	1/1	0.98	0.30	59,59,59,59	0
56	MG	2A	3492	1/1	0.98	0.14	37,37,37,37	0
56	MG	2A	3167	1/1	0.98	0.17	51,51,51,51	0
56	MG	1A	3054	1/1	0.98	0.13	23,23,23,23	0
56	MG	2A	3691	1/1	0.98	0.07	43,43,43,43	0
56	MG	2F	304	1/1	0.98	0.09	32,32,32,32	0
56	MG	2A	3414	1/1	0.98	0.11	38,38,38,38	0
56	MG	1A	3859	1/1	0.98	0.08	22,22,22,22	0
56	MG	1A	3712	1/1	0.98	0.10	28,28,28,28	0
56	MG	1A	3951	1/1	0.98	0.12	22,22,22,22	0
56	MG	1A	3585	1/1	0.98	0.25	25,25,25,25	0
56	MG	1A	3188	1/1	0.98	0.10	19,19,19,19	0
56	MG	2A	3377	1/1	0.98	0.12	29,29,29,29	0
56	MG	2a	1785	1/1	0.98	0.23	63,63,63,63	0
56	MG	2R	203	1/1	0.98	0.15	23,23,23,23	0
56	MG	1A	4003	1/1	0.98	0.08	18,18,18,18	0
56	MG	1a	3140	1/1	0.98	0.21	34,34,34,34	0
56	MG	2A	3454	1/1	0.98	0.12	31,31,31,31	0
56	MG	2A	3056	1/1	0.98	0.08	28,28,28,28	0
56	MG	1A	3762	1/1	0.98	0.07	37,37,37,37	0
56	MG	2A	3257	1/1	0.98	0.06	30,30,30,30	0
56	MG	1A	3216	1/1	0.98	0.15	37,37,37,37	0
56	MG	1A	3628	1/1	0.98	0.19	19,19,19,19	0
56	MG	1A	3476	1/1	0.98	0.13	26,26,26,26	0
58	ZN	16	105	1/1	0.98	0.19	31,31,31,31	0
56	MG	1A	3625	1/1	0.98	0.14	19,19,19,19	0
56	MG	1A	3487	1/1	0.98	0.19	14,14,14,14	0
56	MG	2a	1693	1/1	0.98	0.23	40,40,40,40	0
56	MG	2A	3727	1/1	0.98	0.07	33,33,33,33	0
56	MG	2a	1810	1/1	0.98	0.10	50,50,50,50	0
56	MG	2A	3352	1/1	0.98	0.18	9,9,9,9	0
56	MG	1V	204	1/1	0.98	0.32	25,25,25,25	0
56	MG	1A	3447	1/1	0.98	0.19	23,23,23,23	0
56	MG	2A	3696	1/1	0.98	0.09	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	3477	1/1	0.98	0.13	22,22,22,22	0
56	MG	2A	3673	1/1	0.98	0.12	27,27,27,27	0
56	MG	2A	3828	1/1	0.98	0.08	39,39,39,39	0
56	MG	1D	305	1/1	0.98	0.14	36,36,36,36	0
56	MG	1a	3183	1/1	0.98	0.06	49,49,49,49	0
56	MG	2A	3661	1/1	0.98	0.09	56,56,56,56	0
56	MG	1A	3587	1/1	0.98	0.26	13,13,13,13	0
56	MG	1A	3561	1/1	0.98	0.10	10,10,10,10	0
56	MG	1A	3289	1/1	0.98	0.20	25,25,25,25	0
56	MG	1A	4037	1/1	0.98	0.18	5,5,5,5	0
56	MG	2a	1727	1/1	0.98	0.20	44,44,44,44	0
56	MG	2A	3211	1/1	0.98	0.12	31,31,31,31	0
56	MG	1A	3738	1/1	0.98	0.12	46,46,46,46	0
56	MG	1A	3055	1/1	0.98	0.07	19,19,19,19	0
56	MG	2a	1676	1/1	0.98	0.09	36,36,36,36	0
56	MG	1A	3212	1/1	0.98	0.13	23,23,23,23	0
56	MG	1A	3618	1/1	0.98	0.37	16,16,16,16	0
56	MG	1A	4047	1/1	0.98	0.16	19,19,19,19	0
56	MG	2A	3652	1/1	0.98	0.20	35,35,35,35	0
56	MG	2A	3718	1/1	0.98	0.07	32,32,32,32	0
56	MG	1A	3254	1/1	0.98	0.17	10,10,10,10	0
56	MG	2A	3813	1/1	0.98	0.10	25,25,25,25	0
56	MG	1a	3225	1/1	0.98	0.12	41,41,41,41	0
56	MG	1A	3591	1/1	0.98	0.07	34,34,34,34	0
56	MG	1a	3021	1/1	0.98	0.13	47,47,47,47	0
56	MG	2A	3293	1/1	0.98	0.08	46,46,46,46	0
56	MG	2j	202	1/1	0.98	0.12	59,59,59,59	0
56	MG	1a	3092	1/1	0.98	0.21	40,40,40,40	0
56	MG	1a	3013	1/1	0.98	0.10	33,33,33,33	0
56	MG	1A	3024	1/1	0.98	0.11	9,9,9,9	0
56	MG	1A	3845	1/1	0.98	0.13	37,37,37,37	0
56	MG	1Q	207	1/1	0.98	0.10	25,25,25,25	0
56	MG	1A	3109	1/1	0.98	0.15	37,37,37,37	0
56	MG	1a	3027	1/1	0.98	0.09	49,49,49,49	0
56	MG	1B	215	1/1	0.98	0.12	29,29,29,29	0
56	MG	1A	3809	1/1	0.98	0.08	32,32,32,32	0
56	MG	2A	3585	1/1	0.98	0.12	34,34,34,34	0
56	MG	1A	3886	1/1	0.98	0.17	14,14,14,14	0
56	MG	2A	3605	1/1	0.98	0.12	33,33,33,33	0
56	MG	1D	311	1/1	0.98	0.14	16,16,16,16	0
56	MG	1A	3126	1/1	0.98	0.22	18,18,18,18	0
56	MG	2A	3474	1/1	0.98	0.34	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	3265	1/1	0.98	0.10	4,4,4,4	0
56	MG	1A	4018	1/1	0.98	0.13	10,10,10,10	0
56	MG	1A	3630	1/1	0.98	0.11	30,30,30,30	0
56	MG	1a	3091	1/1	0.98	0.20	24,24,24,24	0
56	MG	1A	3542	1/1	0.98	0.10	31,31,31,31	0
56	MG	1A	4005	1/1	0.98	0.07	28,28,28,28	0
56	MG	2A	3440	1/1	0.98	0.16	36,36,36,36	0
56	MG	1a	3008	1/1	0.98	0.10	17,17,17,17	0
56	MG	2B	207	1/1	0.98	0.08	48,48,48,48	0
56	MG	1A	3650	1/1	0.98	0.12	13,13,13,13	0
56	MG	1U	202	1/1	0.98	0.37	21,21,21,21	0
56	MG	1B	221	1/1	0.98	0.08	18,18,18,18	0
56	MG	2A	3407	1/1	0.98	0.31	47,47,47,47	0
56	MG	1A	3402	1/1	0.98	0.19	12,12,12,12	0
56	MG	2r	101	1/1	0.98	0.07	58,58,58,58	0
56	MG	2A	3408	1/1	0.98	0.13	41,41,41,41	0
56	MG	2A	3520	1/1	0.98	0.13	42,42,42,42	0
59	SF4	2d	302	8/8	0.98	0.15	45,64,68,72	0
56	MG	2q	201	1/1	0.98	0.11	55,55,55,55	0
56	MG	13	102	1/1	0.98	0.12	12,12,12,12	0
56	MG	2A	3748	1/1	0.98	0.07	34,34,34,34	0
56	MG	1A	4060	1/1	0.98	0.09	24,24,24,24	0
56	MG	1a	3063	1/1	0.98	0.12	48,48,48,48	0
56	MG	1B	217	1/1	0.98	0.14	17,17,17,17	0
56	MG	1A	3556	1/1	0.98	0.14	10,10,10,10	0
56	MG	1A	3436	1/1	0.98	0.08	29,29,29,29	0
56	MG	1A	3730	1/1	0.98	0.09	15,15,15,15	0
56	MG	1B	214	1/1	0.98	0.11	36,36,36,36	0
56	MG	1A	3746	1/1	0.98	0.09	13,13,13,13	0
56	MG	2A	3168	1/1	0.98	0.12	23,23,23,23	0
56	MG	2A	3550	1/1	0.98	0.09	37,37,37,37	0
56	MG	2a	1682	1/1	0.98	0.12	66,66,66,66	0
56	MG	2A	3028	1/1	0.98	0.10	20,20,20,20	0
56	MG	1A	3077	1/1	0.98	0.17	10,10,10,10	0
56	MG	1A	3759	1/1	0.98	0.10	36,36,36,36	0
56	MG	2A	3079	1/1	0.98	0.12	23,23,23,23	0
56	MG	1A	3597	1/1	0.98	0.11	11,11,11,11	0
56	MG	2A	3777	1/1	0.98	0.11	36,36,36,36	0
56	MG	1A	3732	1/1	0.98	0.13	10,10,10,10	0
56	MG	1A	3153	1/1	0.98	0.08	25,25,25,25	0
56	MG	1A	3140	1/1	0.98	0.28	22,22,22,22	0
56	MG	1A	3412	1/1	0.98	0.21	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	2A	3262	1/1	0.98	0.16	42,42,42,42	0
56	MG	1A	3146	1/1	0.98	0.10	26,26,26,26	0
56	MG	10	104	1/1	0.98	0.34	36,36,36,36	0
56	MG	1A	3172	1/1	0.98	0.25	24,24,24,24	0
56	MG	2a	1661	1/1	0.98	0.08	51,51,51,51	0
56	MG	1A	3852	1/1	0.98	0.17	13,13,13,13	0
56	MG	2B	219	1/1	0.98	0.09	52,52,52,52	0
56	MG	1A	3735	1/1	0.98	0.11	27,27,27,27	0
56	MG	1x	102	1/1	0.98	0.11	24,24,24,24	0
56	MG	2E	302	1/1	0.98	0.16	46,46,46,46	0
56	MG	1A	3058	1/1	0.98	0.09	26,26,26,26	0
56	MG	1A	4002	1/1	0.98	0.10	25,25,25,25	0
56	MG	1A	3796	1/1	0.98	0.16	47,47,47,47	0
56	MG	2A	3335	1/1	0.98	0.24	53,53,53,53	0
56	MG	2A	3742	1/1	0.98	0.15	40,40,40,40	0
56	MG	1A	3167	1/1	0.98	0.05	32,32,32,32	0
56	MG	2A	3755	1/1	0.98	0.10	40,40,40,40	0
56	MG	1A	3639	1/1	0.98	0.08	42,42,42,42	0
56	MG	2A	3485	1/1	0.98	0.13	40,40,40,40	0
56	MG	1A	3652	1/1	0.98	0.16	32,32,32,32	0
56	MG	2a	1633	1/1	0.98	0.16	36,36,36,36	0
56	MG	1A	4053	1/1	0.98	0.05	48,48,48,48	0
56	MG	1F	313	1/1	0.98	0.21	20,20,20,20	0
56	MG	2A	3737	1/1	0.98	0.05	21,21,21,21	0
56	MG	1A	3931	1/1	0.98	0.12	36,36,36,36	0
56	MG	1A	3581	1/1	0.98	0.21	20,20,20,20	0
56	MG	1A	3584	1/1	0.98	0.20	31,31,31,31	0
56	MG	1A	3207	1/1	0.98	0.13	22,22,22,22	0
56	MG	2A	3519	1/1	0.98	0.11	19,19,19,19	0
56	MG	1A	3337	1/1	0.98	0.12	23,23,23,23	0
56	MG	2A	3458	1/1	0.98	0.17	60,60,60,60	0
58	ZN	1Y	202	1/1	0.98	0.13	57,57,57,57	0
56	MG	1a	3022	1/1	0.98	0.09	22,22,22,22	0
56	MG	1U	201	1/1	0.98	0.22	20,20,20,20	0
56	MG	2A	3580	1/1	0.98	0.14	39,39,39,39	0
56	MG	1A	4062	1/1	0.98	0.08	21,21,21,21	0
56	MG	1A	3303	1/1	0.98	0.17	25,25,25,25	0
56	MG	1A	3328	1/1	0.98	0.15	21,21,21,21	0
56	MG	1A	3913	1/1	0.98	0.15	38,38,38,38	0
56	MG	2A	3427	1/1	0.98	0.13	23,23,23,23	0
56	MG	1D	304	1/1	0.98	0.09	18,18,18,18	0
56	MG	1a	3211	1/1	0.98	0.09	27,27,27,27	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1Y	201	1/1	0.98	0.22	39,39,39,39	0
56	MG	2A	3081	1/1	0.98	0.05	33,33,33,33	0
56	MG	15	104	1/1	0.98	0.40	25,25,25,25	0
56	MG	1a	3227	1/1	0.98	0.08	39,39,39,39	0
56	MG	2A	3423	1/1	0.98	0.08	22,22,22,22	0
56	MG	2A	3411	1/1	0.98	0.12	28,28,28,28	0
56	MG	1B	203	1/1	0.98	0.36	32,32,32,32	0
56	MG	1A	3096	1/1	0.98	0.24	20,20,20,20	0
56	MG	2A	3489	1/1	0.98	0.07	37,37,37,37	0
56	MG	1A	3992	1/1	0.98	0.11	20,20,20,20	0
56	MG	1A	3434	1/1	0.98	0.19	39,39,39,39	0
56	MG	1A	3766	1/1	0.98	0.10	22,22,22,22	0
56	MG	2A	3690	1/1	0.98	0.14	35,35,35,35	0
56	MG	1U	209	1/1	0.98	0.21	18,18,18,18	0
56	MG	2A	3134	1/1	0.98	0.15	37,37,37,37	0
56	MG	1A	3742	1/1	0.98	0.12	29,29,29,29	0
56	MG	2a	1680	1/1	0.98	0.16	44,44,44,44	0
56	MG	2A	3267	1/1	0.98	0.11	26,26,26,26	0
56	MG	1A	3740	1/1	0.98	0.07	45,45,45,45	0
56	MG	1A	3671	1/1	0.98	0.15	36,36,36,36	0
56	MG	1A	3777	1/1	0.98	0.11	9,9,9,9	0
56	MG	2A	3417	1/1	0.98	0.17	36,36,36,36	0
56	MG	2A	3753	1/1	0.98	0.07	47,47,47,47	0
56	MG	1A	3106	1/1	0.98	0.15	25,25,25,25	0
56	MG	1X	103	1/1	0.98	0.11	26,26,26,26	0
56	MG	1A	3546	1/1	0.98	0.15	21,21,21,21	0
56	MG	1a	3217	1/1	0.98	0.08	65,65,65,65	0
56	MG	2A	3172	1/1	0.98	0.06	33,33,33,33	0
56	MG	1A	3864	1/1	0.98	0.07	17,17,17,17	0
56	MG	2A	3283	1/1	0.98	0.14	32,32,32,32	0
56	MG	2A	3236	1/1	0.99	0.26	40,40,40,40	0
56	MG	1A	3699	1/1	0.99	0.12	38,38,38,38	0
56	MG	2A	3113	1/1	0.99	0.09	36,36,36,36	0
56	MG	1A	3482	1/1	0.99	0.09	12,12,12,12	0
56	MG	2A	3610	1/1	0.99	0.11	54,54,54,54	0
56	MG	1A	3560	1/1	0.99	0.13	11,11,11,11	0
58	ZN	15	108	1/1	0.99	0.19	33,33,33,33	0
56	MG	1E	315	1/1	0.99	0.05	23,23,23,23	0
56	MG	1A	3344	1/1	0.99	0.07	21,21,21,21	0
56	MG	2A	3473	1/1	0.99	0.14	46,46,46,46	0
56	MG	2A	3036	1/1	0.99	0.09	41,41,41,41	0
56	MG	1A	3736	1/1	0.99	0.14	17,17,17,17	0

*Continued on next page...*

*Continued from previous page...*

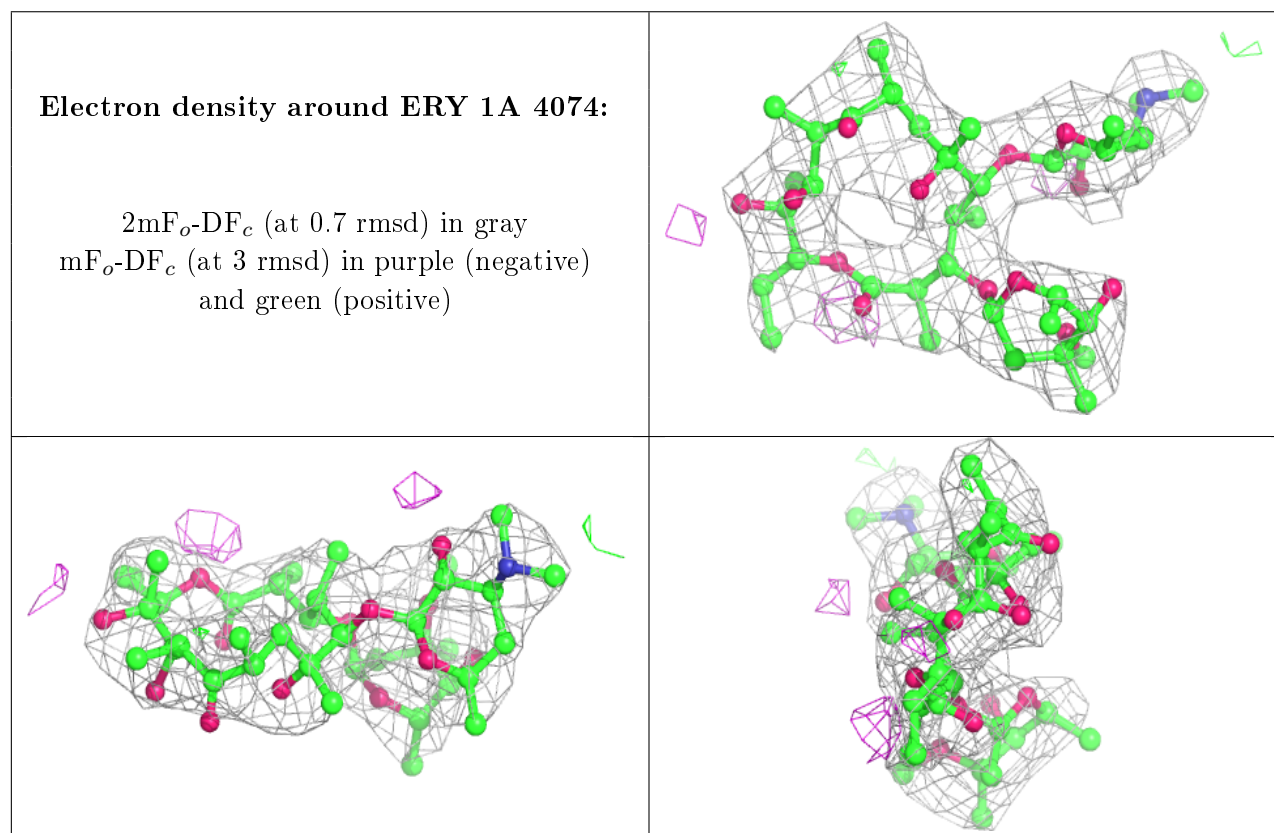
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	4006	1/1	0.99	0.07	15,15,15,15	0
56	MG	1A	3543	1/1	0.99	0.14	12,12,12,12	0
56	MG	1A	3021	1/1	0.99	0.15	16,16,16,16	0
58	ZN	26	103	1/1	0.99	0.17	55,55,55,55	0
56	MG	17	102	1/1	0.99	0.10	14,14,14,14	0
56	MG	1A	3136	1/1	0.99	0.20	19,19,19,19	0
56	MG	1A	3022	1/1	0.99	0.09	26,26,26,26	0
56	MG	2A	3253	1/1	0.99	0.31	46,46,46,46	0
56	MG	1A	3754	1/1	0.99	0.08	35,35,35,35	0
56	MG	2A	3572	1/1	0.99	0.10	34,34,34,34	0
56	MG	1A	3828	1/1	0.99	0.07	30,30,30,30	0
56	MG	2A	3448	1/1	0.99	0.18	34,34,34,34	0
56	MG	2A	3647	1/1	0.99	0.21	38,38,38,38	0
56	MG	1A	3187	1/1	0.99	0.18	19,19,19,19	0
56	MG	2A	3809	1/1	0.99	0.13	37,37,37,37	0
56	MG	1a	3020	1/1	0.99	0.06	48,48,48,48	0
59	SF4	1d	302	8/8	0.99	0.15	39,58,69,70	0
56	MG	1A	3711	1/1	0.99	0.14	10,10,10,10	0
56	MG	1A	4038	1/1	0.99	0.11	30,30,30,30	0
56	MG	2A	3037	1/1	0.99	0.12	48,48,48,48	0
56	MG	1A	3672	1/1	0.99	0.11	20,20,20,20	0
56	MG	2y	104	1/1	0.99	0.03	39,39,39,39	0
56	MG	2A	3348	1/1	0.99	0.21	26,26,26,26	0
56	MG	2W	201	1/1	0.99	0.16	40,40,40,40	0
56	MG	2l	204	1/1	0.99	0.20	49,49,49,49	0
56	MG	1A	3668	1/1	0.99	0.10	15,15,15,15	0
56	MG	2U	202	1/1	0.99	0.22	48,48,48,48	0
56	MG	1A	3027	1/1	0.99	0.08	16,16,16,16	0
56	MG	2A	3083	1/1	0.99	0.28	44,44,44,44	0
56	MG	1A	3171	1/1	0.99	0.12	10,10,10,10	0
56	MG	1A	3636	1/1	0.99	0.13	4,4,4,4	0
56	MG	1A	3340	1/1	0.99	0.10	23,23,23,23	0
58	ZN	19	104	1/1	0.99	0.14	36,36,36,36	0
56	MG	2A	3441	1/1	0.99	0.14	41,41,41,41	0
56	MG	1A	3121	1/1	0.99	0.13	12,12,12,12	0
56	MG	1A	3643	1/1	0.99	0.10	15,15,15,15	0
56	MG	1A	3834	1/1	0.99	0.12	20,20,20,20	0
56	MG	2a	1671	1/1	0.99	0.11	46,46,46,46	0
56	MG	2A	3705	1/1	0.99	0.21	41,41,41,41	0
56	MG	1A	4068	1/1	0.99	0.11	34,34,34,34	0
56	MG	1a	3152	1/1	0.99	0.09	32,32,32,32	0
56	MG	2a	1814	1/1	0.99	0.13	26,26,26,26	0

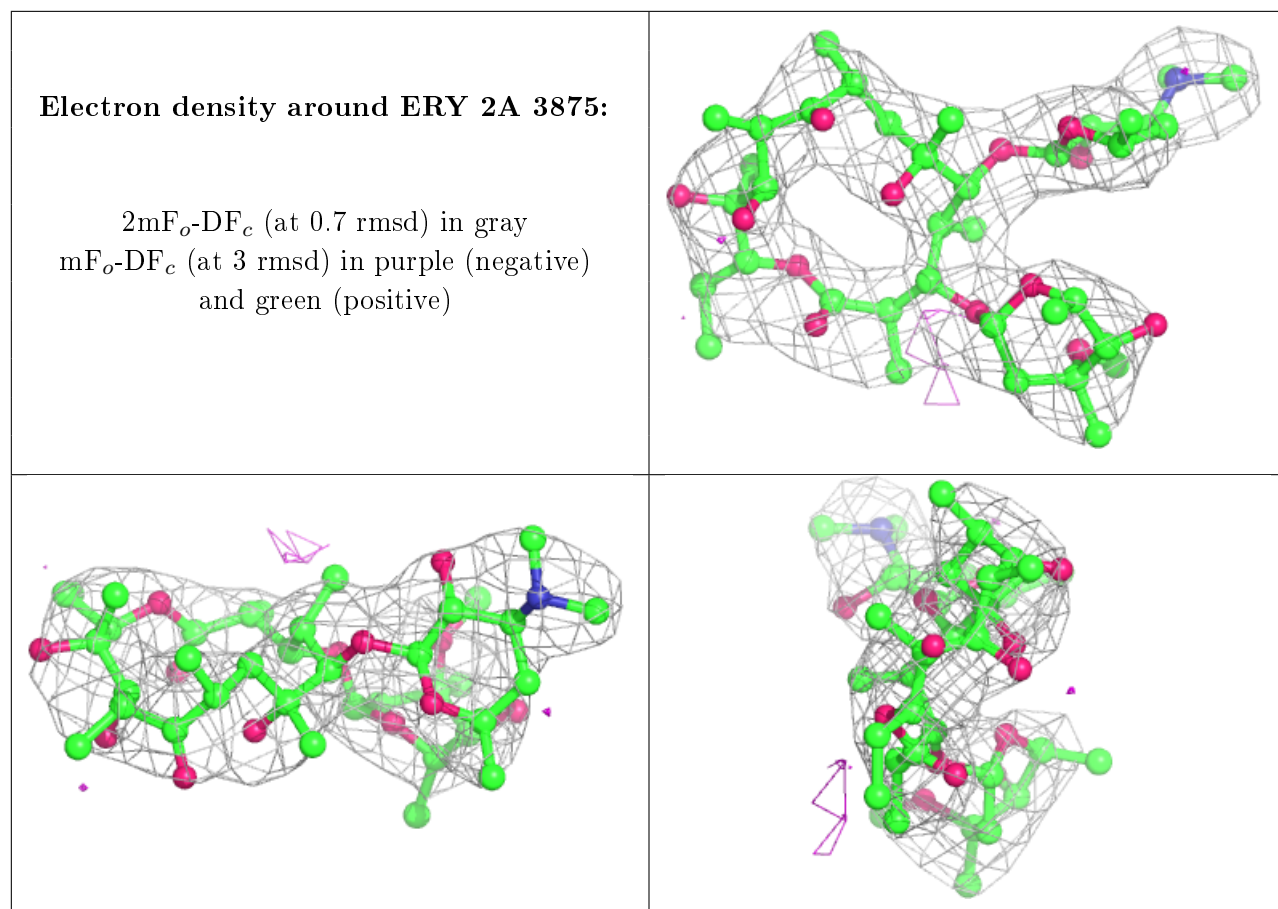
*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	4031	1/1	0.99	0.06	21,21,21,21	0
56	MG	1A	3316	1/1	0.99	0.18	20,20,20,20	0
56	MG	1A	3954	1/1	0.99	0.10	31,31,31,31	0
56	MG	1A	3248	1/1	0.99	0.10	30,30,30,30	0
58	ZN	25	104	1/1	0.99	0.17	44,44,44,44	0
56	MG	1A	3262	1/1	0.99	0.28	16,16,16,16	0
56	MG	1A	3196	1/1	0.99	0.23	23,23,23,23	0
56	MG	1Z	303	1/1	0.99	0.10	29,29,29,29	0
56	MG	1A	3149	1/1	0.99	0.23	19,19,19,19	0
56	MG	2A	3329	1/1	0.99	0.12	37,37,37,37	0
56	MG	2A	3106	1/1	0.99	0.09	35,35,35,35	0
56	MG	1U	210	1/1	0.99	0.37	15,15,15,15	0
56	MG	2A	3066	1/1	0.99	0.15	28,28,28,28	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





## 6.5 Other polymers ⓘ

There are no such residues in this entry.