



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 3, 2020 – 06:01 am BST

PDB ID : 6CFK  
Title : Crystal structure of the Thermus thermophilus 70S ribosome in complex with D-histidyl-CAM and bound to protein Y (YfiA) at 2.7Å resolution  
Authors : Tereshchenkov, A.G.; Dobosz-Bartoszek, M.; Osterman, I.A.; Marks, J.; Sergeeva, V.A.; Kasatsky, P.; Komarova, E.S.; Stavrianidi, A.N.; Rodin, I.A.; Konevega, A.L.; Sergiev, P.V.; Sumbatyan, N.V.; Mankin, A.S.; Bogdanov, A.A.; Polikanov, Y.S.  
Deposited on : 2018-02-15  
Resolution : 2.70 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

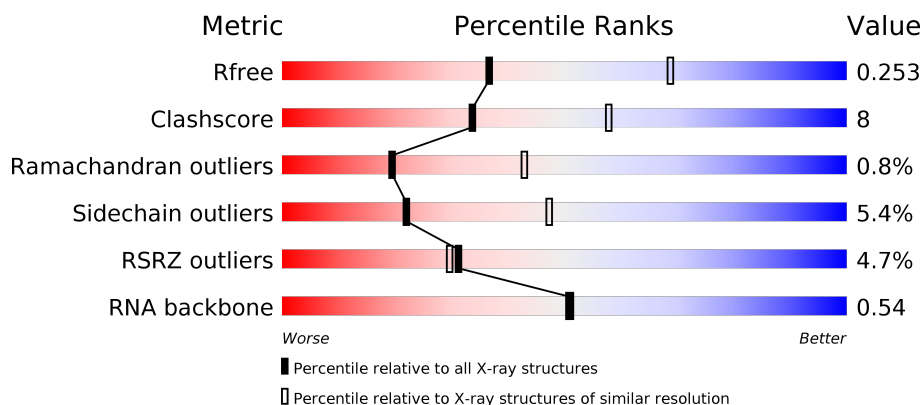
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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.







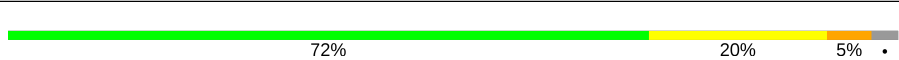
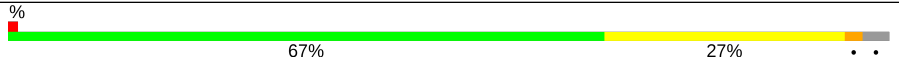
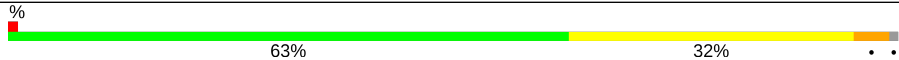
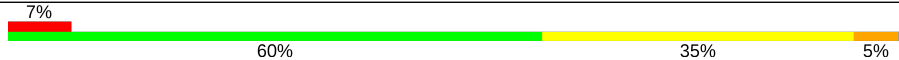
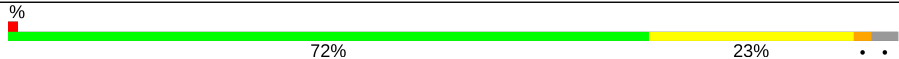
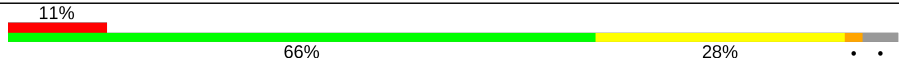
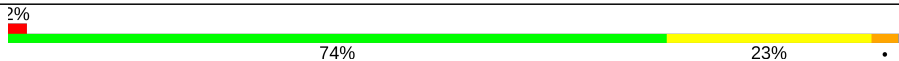
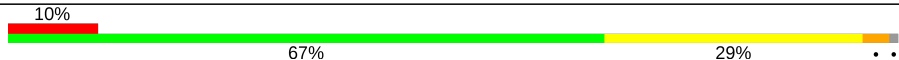
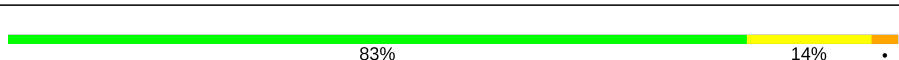
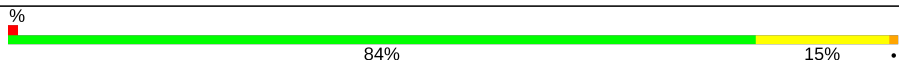


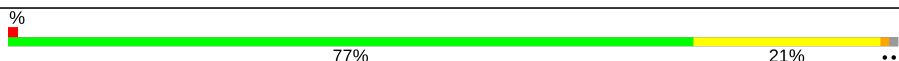
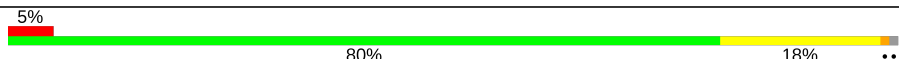
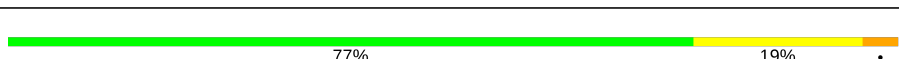

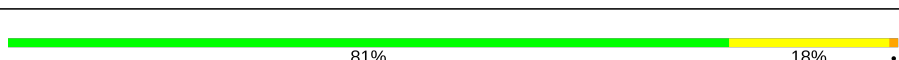
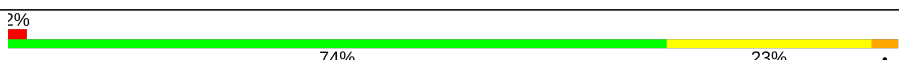
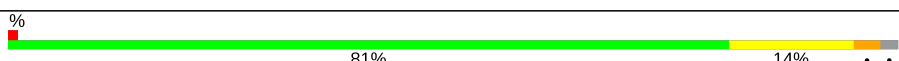
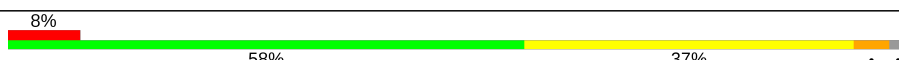
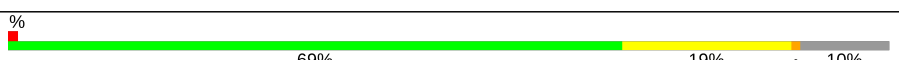
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)
RNA backbone	3102	1159 (3.00-2.40)

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	<div> <div>2%</div> <div>64% 28% 6% ..</div> </div>
1	2A	2915	<div> <div>2%</div> <div>57% 33% 8% .</div> </div>
2	1B	121	<div> <div>75% 21% ..</div> </div>
2	2B	121	<div> <div>59% 35% 6% .</div> </div>

*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	















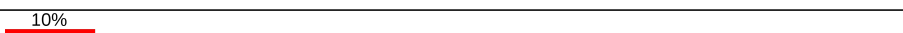
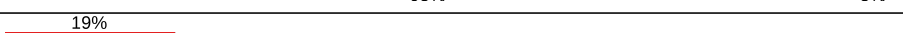
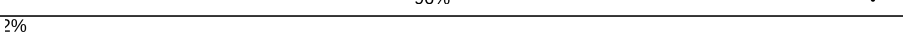


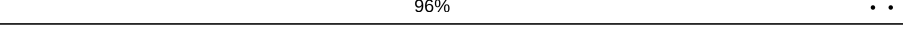
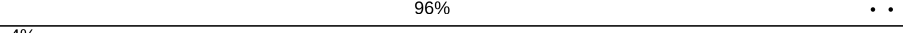
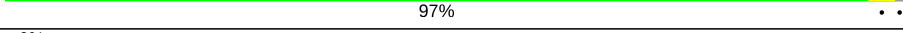
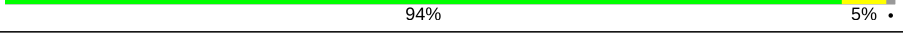
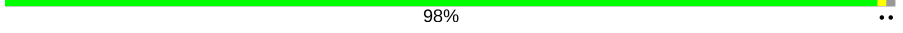
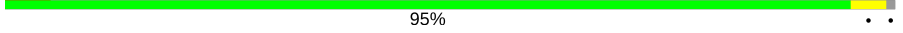
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	2T	146	% 66% 21% 10%
16	1U	118	% 80% 17% ...
16	2U	118	8% 76% 22%
17	1V	101	74% 24%
17	2V	101	3% 72% 25%
18	1W	113	% 83% 13%
18	2W	113	7% 81% 15%
19	1X	96	% 76% 20%
19	2X	96	5% 79% 18%
20	1Y	110	% 72% 23%
20	2Y	110	14% 75% 22%
21	1Z	206	% 78% 19%
21	2Z	206	4% 73% 22%
22	10	85	% 74% 15% 9%
22	20	85	14% 73% 16% 9%
23	11	98	5% 79% 17%
23	21	98	8% 72% 23%
24	12	72	% 82% 14%
24	22	72	3% 81% 15%
25	13	60	75% 18% 5%
25	23	60	23% 65% 30%
26	14	71	6% 63% 28% 6%
26	24	71	8% 44% 49%
27	15	60	67% 28%
27	25	60	3% 82% 15%

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	1y	113	
53	2y	113	

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	MG	1A	3189	-	-	-	X
54	MG	1A	3921	-	-	-	X
54	MG	1F	311	-	-	-	X
54	MG	1a	1767	-	-	-	X
54	MG	1a	1851	-	-	-	X
54	MG	2A	3146	-	-	-	X
54	MG	2A	3206	-	-	-	X

## 2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 295438 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	2872	Total	C	N	O	P	0	0	0
			61869	27540	11574	19884	2871			
1	2A	2867	Total	C	N	O	P	0	0	0
			61758	27491	11552	19850	2865			

- 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
			2572	1145	476	832	119			
2	2B	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

- 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
			2131	1346	422	360	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
			1426	916	253	253	4			
6	2G	181	Total	C	N	O	S	0	0	0
			1424	912	259	249	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	173	Total	C	N	O	S	0	0	0
			1324	842	247	234	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	1I	147	Total	C	N	O	S	0	0	0
			1094	699	191	203	1			
8	2I	146	Total	C	N	O	S	0	0	0
			1076	687	186	202	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
			1121	722	208	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
			877	553	175	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	0	0	0
			1091	680	225	185	1		
15	2T	131	Total	C	N	O	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
			775	498	141	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
			810	520	153	131	6			
20	2Y	107	Total	C	N	O	S	0	0	0
			810	519	153	132	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	1Z	203	Total	C	N	O	S	0	0	0
			1587	1011	282	292	2			
21	2Z	201	Total	C	N	O	S	0	0	0
			1557	995	274	286	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	10	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			
22	20	77	Total	C	N	O	S	0	0	0
			608	375	129	103	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
			754	475	148	130	1			
23	21	97	Total	C	N	O	S	0	0	0
			759	478	149	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
			592	368	119	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
			546	346	96	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
			536	342	98	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
			459	288	90	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	1504	Total	C	N	O	P	0	0	0
			32331	14396	5990	10441	1504			

- 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
			1842	1175	330	332	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
			1558	979	305	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
			1665	1043	329	286	7			
35	2d	208	Total	C	N	O	S	0	0	0
			1668	1047	330	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
			1133	716	214	199	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
			814	516	144	151	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
			1235	769	244	216	6			
38	2g	155	Total	C	N	O	S	0	0	0
			1229	766	241	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
			1098	694	210	192	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
			986	625	193	168			
40	2i	126	Total	C	N	O	0	0	0
			966	613	186	167			

- 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
			719	446	142	131			
41	2j	96	Total	C	N	O	0	0	0
			710	442	137	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
			834	520	156	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	116	Total	C	N	O	S	0	0	0
			914	564	189	159	2			
44	2m	114	Total	C	N	O	S	0	0	0
			895	550	186	157	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
			648	415	120	111	2			
50	2s	83	Total	C	N	O	S	0	0	0
			645	410	118	115	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
			732	449	157	124	2			
51	2t	98	Total	C	N	O	S	0	0	0
			733	451	154	126	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 protein called Ribosome-associated inhibitor A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	1y	97	Total	C	N	O	S	0	0	0
			764	478	144	139	3			
53	2y	96	Total	C	N	O	S	0	0	0
			749	468	141	137	3			

- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	2E	6	Total	Mg	0	0
			6	6		
54	17	2	Total	Mg	0	0
			2	2		
54	1T	3	Total	Mg	0	0
			3	3		
54	1N	3	Total	Mg	0	0
			3	3		
54	20	1	Total	Mg	0	0
			1	1		
54	18	1	Total	Mg	0	0
			1	1		
54	1o	1	Total	Mg	0	0
			1	1		
54	2W	2	Total	Mg	0	0
			2	2		
54	2I	1	Total	Mg	0	0
			1	1		
54	13	2	Total	Mg	0	0
			2	2		
54	1f	2	Total	Mg	0	0
			2	2		
54	1P	3	Total	Mg	0	0
			3	3		
54	2B	19	Total	Mg	0	0
			19	19		
54	2a	151	Total	Mg	0	0
			151	151		
54	1E	7	Total	Mg	0	0
			7	7		
54	1b	1	Total	Mg	0	0
			1	1		
54	2F	3	Total	Mg	0	0
			3	3		
54	2p	1	Total	Mg	0	0
			1	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	28	3	Total 3	Mg 3	0	0
54	2e	1	Total 1	Mg 1	0	0
54	1W	2	Total 2	Mg 2	0	0
54	1A	1024	Total 1024	Mg 1024	0	0
54	1t	1	Total 1	Mg 1	0	0
54	1n	1	Total 1	Mg 1	0	0
54	2P	2	Total 2	Mg 2	0	0
54	1X	2	Total 2	Mg 2	0	0
54	2q	1	Total 1	Mg 1	0	0
54	1y	4	Total 4	Mg 4	0	0
54	1S	1	Total 1	Mg 1	0	0
54	25	1	Total 1	Mg 1	0	0
54	2T	4	Total 4	Mg 4	0	0
54	1D	13	Total 13	Mg 13	0	0
54	2N	1	Total 1	Mg 1	0	0
54	1e	2	Total 2	Mg 2	0	0
54	2G	3	Total 3	Mg 3	0	0
54	2f	1	Total 1	Mg 1	0	0
54	1V	3	Total 3	Mg 3	0	0
54	2X	1	Total 1	Mg 1	0	0
54	1a	255	Total 255	Mg 255	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	2Q	2	Total 2	Mg 2	0	0
54	15	3	Total 3	Mg 3	0	0
54	2j	1	Total 1	Mg 1	0	0
54	1R	3	Total 3	Mg 3	0	0
54	1G	4	Total 4	Mg 4	0	0
54	2O	1	Total 1	Mg 1	0	0
54	11	3	Total 3	Mg 3	0	0
54	1d	6	Total 6	Mg 6	0	0
54	2r	1	Total 1	Mg 1	0	0
54	1H	2	Total 2	Mg 2	0	0
54	21	1	Total 1	Mg 1	0	0
54	1i	1	Total 1	Mg 1	0	0
54	2R	1	Total 1	Mg 1	0	0
54	1Z	1	Total 1	Mg 1	0	0
54	2D	8	Total 8	Mg 8	0	0
54	14	1	Total 1	Mg 1	0	0
54	1U	2	Total 2	Mg 2	0	0
54	1O	2	Total 2	Mg 2	0	0
54	19	2	Total 2	Mg 2	0	0
54	1l	2	Total 2	Mg 2	0	0
54	2V	1	Total 1	Mg 1	0	0

*Continued on next page...*

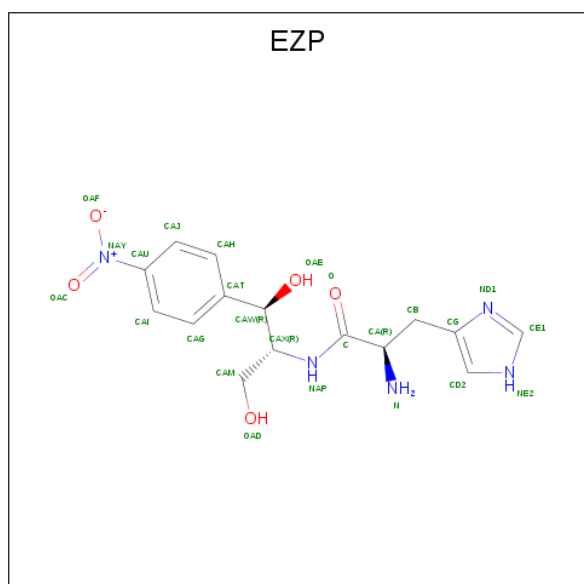
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	1F	13	Total Mg 13 13	0	0
54	10	6	Total Mg 6 6	0	0
54	1g	3	Total Mg 3 3	0	0
54	2t	1	Total Mg 1 1	0	0
54	1Q	4	Total Mg 4 4	0	0
54	2A	721	Total Mg 721 721	0	0
54	1h	2	Total Mg 2 2	0	0
54	1B	29	Total Mg 29 29	0	0

- Molecule 55 is POTASSIUM ION (three-letter code: K) (formula: K).

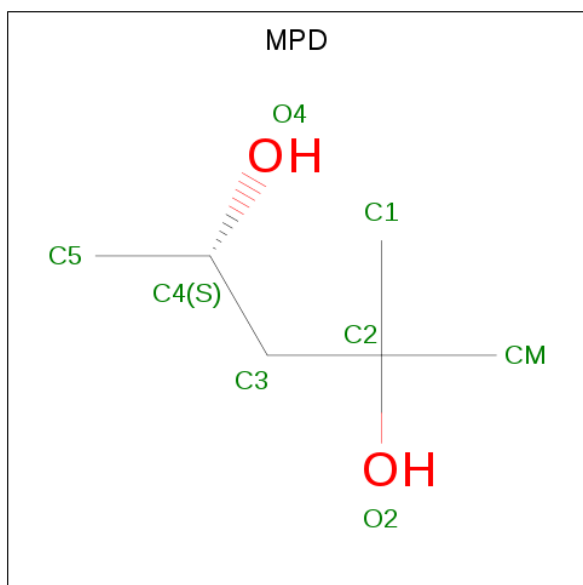
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
55	1A	1	Total K 1 1	0	0
55	2A	1	Total K 1 1	0	0

- Molecule 56 is N-[(1R,2R)-1,3-dihydroxy-1-(4-nitrophenyl)propan-2-yl]-D-histidinamide (three-letter code: EZP) (formula: C<sub>15</sub>H<sub>19</sub>N<sub>5</sub>O<sub>5</sub>).



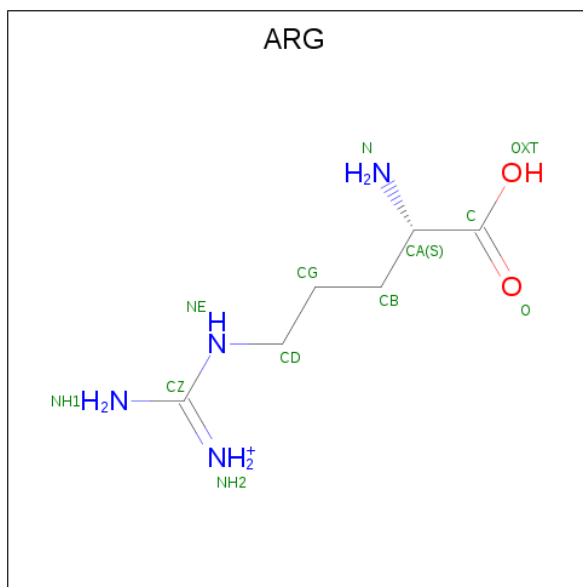
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
56	1A	1	Total	C	N	O	0	0
			25	15	5	5		
56	2A	1	Total	C	N	O	0	0
			25	15	5	5		

- Molecule 57 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
57	1A	1	Total	C	O	0	0
			8	6	2		
57	1T	1	Total	C	O	0	0
			8	6	2		
57	18	1	Total	C	O	0	0
			8	6	2		
57	1a	1	Total	C	O	0	0
			8	6	2		
57	2A	1	Total	C	O	0	0
			8	6	2		
57	2A	1	Total	C	O	0	0
			8	6	2		
57	2B	1	Total	C	O	0	0
			8	6	2		

- Molecule 58 is ARGinine (three-letter code: ARG) (formula:  $C_6H_{15}N_4O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
58	1B	1	Total	C	N	O	0	0
			12	6	4	2		
58	1F	1	Total	C	N	O	0	0
			12	6	4	2		

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

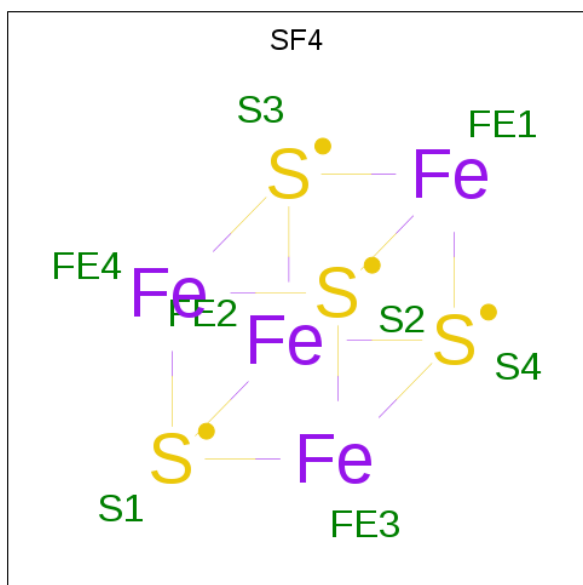
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	1Y	1	Total	Zn	0	0
			1	1		
59	14	1	Total	Zn	0	0
			1	1		
59	1n	1	Total	Zn	0	0
			1	1		
59	15	1	Total	Zn	0	0
			1	1		
59	29	1	Total	Zn	0	0
			1	1		
59	19	1	Total	Zn	0	0
			1	1		
59	26	1	Total	Zn	0	0
			1	1		
59	25	1	Total	Zn	0	0
			1	1		
59	24	1	Total	Zn	0	0
			1	1		
59	2n	1	Total	Zn	0	0
			1	1		

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	2Y	1	Total	Zn	0	0
			1	1		
59	16	1	Total	Zn	0	0
			1	1		

- Molecule 60 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



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

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1A	2980	Total	O	0	0
			2980	2980		
61	1B	105	Total	O	0	0
			105	105		
61	1D	116	Total	O	0	0
			116	116		
61	1E	76	Total	O	0	0
			76	76		
61	1F	63	Total	O	0	0
			63	63		

Continued on next page...



*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	1G	22	Total 22	O 22	0	0
61	1H	16	Total 16	O 16	0	0
61	1I	7	Total 7	O 7	0	0
61	1N	50	Total 50	O 50	0	0
61	1O	22	Total 22	O 22	0	0
61	1P	58	Total 58	O 58	0	0
61	1Q	42	Total 42	O 42	0	0
61	1R	37	Total 37	O 37	0	0
61	1S	13	Total 13	O 13	0	0
61	1T	42	Total 42	O 42	0	0
61	1U	45	Total 45	O 45	0	0
61	1V	37	Total 37	O 37	0	0
61	1W	24	Total 24	O 24	0	0
61	1X	24	Total 24	O 24	0	0
61	1Y	15	Total 15	O 15	0	0
61	1Z	14	Total 14	O 14	0	0
61	10	22	Total 22	O 22	0	0
61	11	28	Total 28	O 28	0	0
61	12	14	Total 14	O 14	0	0
61	13	22	Total 22	O 22	0	0
61	14	2	Total 2	O 2	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	15	26	Total 26	O 26	0	0
61	16	17	Total 17	O 17	0	0
61	17	14	Total 14	O 14	0	0
61	18	30	Total 30	O 30	0	0
61	19	8	Total 8	O 8	0	0
61	1a	261	Total 261	O 261	0	0
61	1b	1	Total 1	O 1	0	0
61	1d	9	Total 9	O 9	0	0
61	1e	6	Total 6	O 6	0	0
61	1f	3	Total 3	O 3	0	0
61	1h	1	Total 1	O 1	0	0
61	1i	1	Total 1	O 1	0	0
61	1j	1	Total 1	O 1	0	0
61	1k	1	Total 1	O 1	0	0
61	1l	4	Total 4	O 4	0	0
61	1n	1	Total 1	O 1	0	0
61	1o	5	Total 5	O 5	0	0
61	1p	3	Total 3	O 3	0	0
61	1y	5	Total 5	O 5	0	0
61	2A	1686	Total 1686	O 1686	0	0
61	2B	65	Total 65	O 65	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	2D	52	Total 52	O 52	0	0
61	2E	25	Total 25	O 25	0	0
61	2F	21	Total 21	O 21	0	0
61	2G	7	Total 7	O 7	0	0
61	2H	4	Total 4	O 4	0	0
61	2I	4	Total 4	O 4	0	0
61	2N	6	Total 6	O 6	0	0
61	2O	22	Total 22	O 22	0	0
61	2P	23	Total 23	O 23	0	0
61	2Q	30	Total 30	O 30	0	0
61	2R	21	Total 21	O 21	0	0
61	2S	8	Total 8	O 8	0	0
61	2T	10	Total 10	O 10	0	0
61	2U	14	Total 14	O 14	0	0
61	2V	9	Total 9	O 9	0	0
61	2W	21	Total 21	O 21	0	0
61	2X	9	Total 9	O 9	0	0
61	2Y	3	Total 3	O 3	0	0
61	2Z	15	Total 15	O 15	0	0
61	20	13	Total 13	O 13	0	0
61	21	24	Total 24	O 24	0	0

*Continued on next page...*

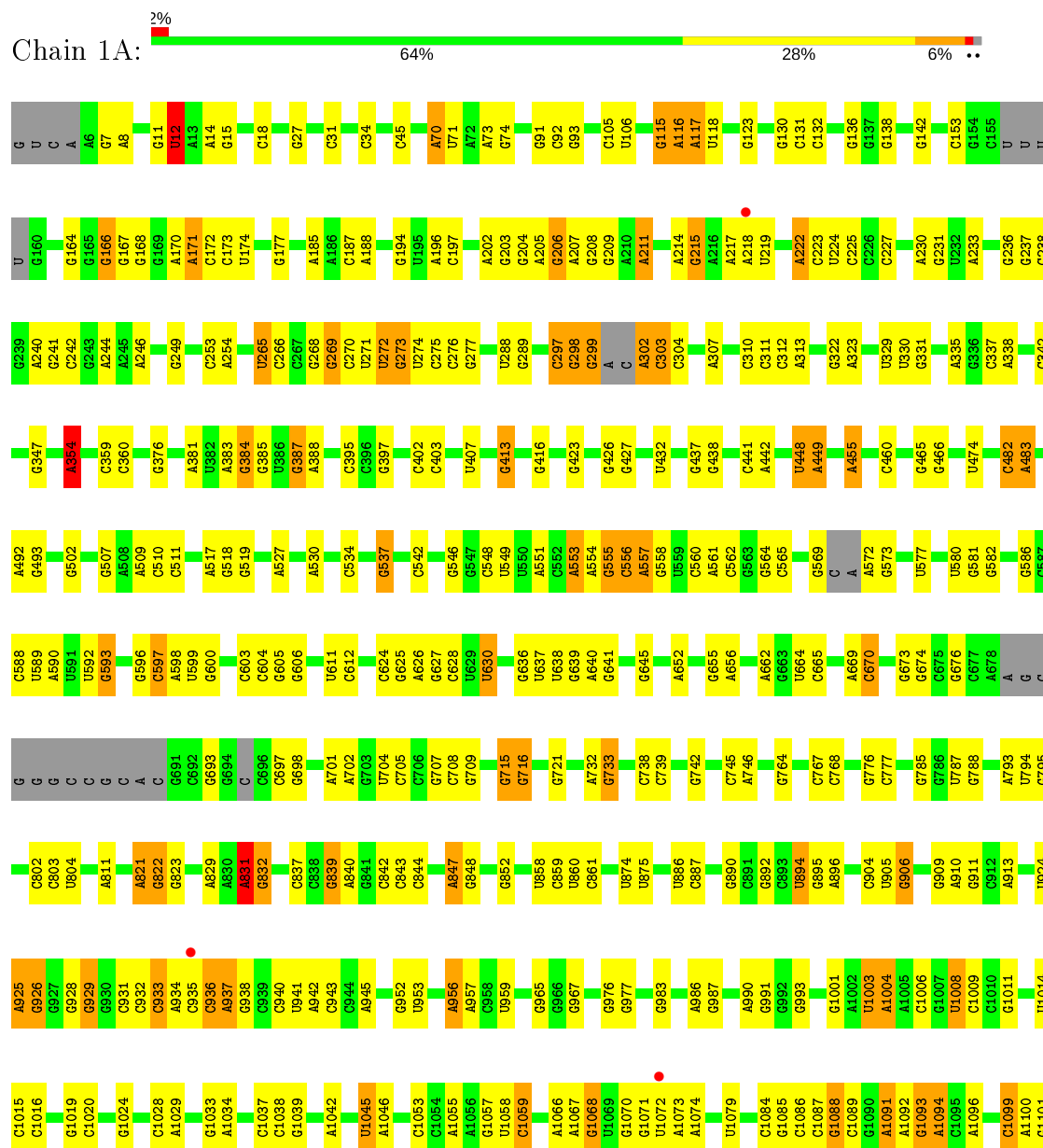
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	22	5	Total 5	O 5	0	0
61	23	3	Total 3	O 3	0	0
61	24	2	Total 2	O 2	0	0
61	25	9	Total 9	O 9	0	0
61	26	6	Total 6	O 6	0	0
61	27	7	Total 7	O 7	0	0
61	28	15	Total 15	O 15	0	0
61	29	2	Total 2	O 2	0	0
61	2a	100	Total 100	O 100	0	0
61	2d	6	Total 6	O 6	0	0
61	2e	1	Total 1	O 1	0	0
61	2f	1	Total 1	O 1	0	0
61	2j	2	Total 2	O 2	0	0
61	2l	1	Total 1	O 1	0	0
61	2m	1	Total 1	O 1	0	0
61	2o	2	Total 2	O 2	0	0
61	2p	1	Total 1	O 1	0	0
61	2q	1	Total 1	O 1	0	0
61	2r	4	Total 4	O 4	0	0
61	2y	1	Total 1	O 1	0	0

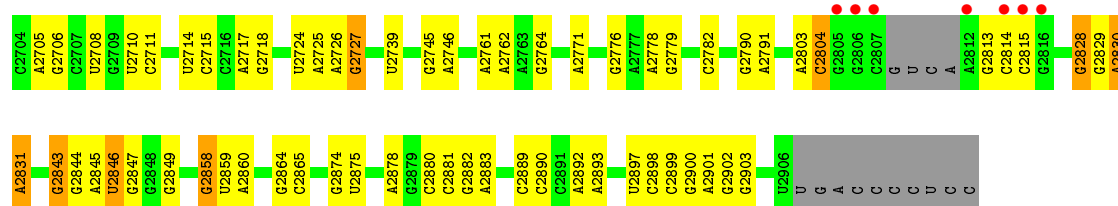
### 3 Residue-property plots

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 ( $\text{RSRZ} > 2$ ). 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.

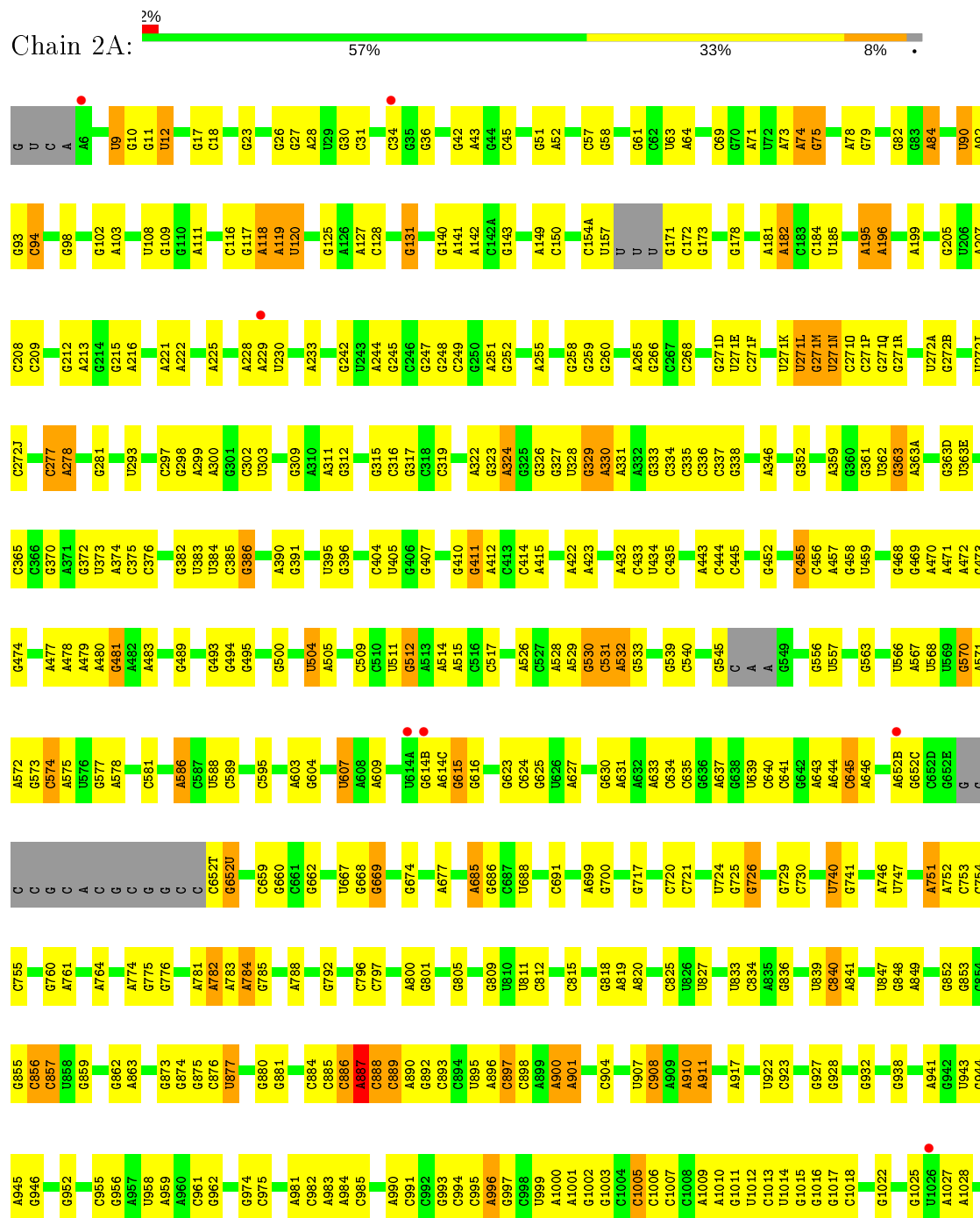
#### • Molecule 1: 23S Ribosomal RNA



U2566	C2436	G2209	U2140	A2042	A1878	C1757	G1631	C1514	A1405	G1296	A1174	G1102
U2567	A2437	C2210	A2141	C2043	U1882	G1766	A1632	C1515	A1406	G1296	A1175	A1103
A2573	A2438	U2211	U2144	U2044	U1883	A1767	A1633	A1516		A1299	U1176	G1104
G2440	G2439	G2212	G2145	G2045	G1889	U1768	C1635	A1518	G1410	G1302	C1180	U1106
G2441	G2440	G2213		U2050		U1769			G1411		G1181	U1107
A2442	G2436	G2214	A2148	G2051	U1895		G1652	G1529			G1108	
A2576	G2337	G2215	G2149	A2052	U1896		G1653		C1416	G1305	G1184	
A2577	C2338	A2220	C2150	A2053	U1899	G1777	A1654	A1532	G1417		C1185	C1109
A2578	A2444		C2151	G2054	A1899	G1787	A1655	G1533	U1418	G1310	C1186	C1110
G2580	G2341	G2227	U2152	A2055	C1901	U1793	A1656		G1428	G1311	U1187	U1111
		G2228	G2153	C2058		G1794	G1674	C1539	A1425	G1312	A1188	U1112
		A2229	U2154	G2059	A1911	G1795	U1675	A1541	G1427	G1313		A1113
		A2237	A2156	G2060				A1542	G1428	G1314	C1196	A1114
			C2158	C2065	G1921	A1804	A1679		C1429	A1315		A1115
		U2244	C2159		A1922				C1430	C1316	C1199	A1116
		U2245	C2160	G2071	G1928	U1809	G1682	C1550	G1431	A1318	A1201	G1117
		G2246	C2161	G2072		U1810	U1686	C1551	C1432		A1202	C1118
			C2162	A2073	A1935	A1811	U1687	C1552	C1433	G1327		G1120
		G2250	C2163	G2074	C1936	C1812	C1687	C1553	C1434	G1331	G1210	C1122
		G2251	C2164	C2077		C1813	A1688	A1554	G1435	G1332	U1211	A1123
		U2255	C2165	G2078	A1941	A1814	G1689	C1555	U1436	A1332	C1212	U1124
		U2256	U2166		C1942	A1815		A1556		A1333	C1216	C1125
			C2167	A2082	G1943	A1816	G1694	A1557	A1441	A1334	G1217	C1126
		G2271	C2168	G2083		A1817	G1695			C1335	U1127	
		A2279	G2169	A2084	G1951	C1821	A1699	U1566	U1452	C1336	G1218	
			C2170	C2085	G1952	A1822	G1700	G1567	C1453	C1337	U1219	
		G2272	G2171				A1701		G1462	C1338	U1220	A1130
		A2281	C2172	G2089	A1958	U1825		A1575	C1463		G1223	A1131
		G2282	C2173	U2090	A1959	C1826	G1705		G1464	C1343	C1224	G1133
		G2283	G2174	G2091	A1960	U1827		C1579	G1465		C1225	A1134
		G2289	C2175	A2093	C1964	C1828	A1711	G	U1466	U1346	G1135	
		A2290	G2176	G2092	U1965	U1829		U	A1347	A1347	U1136	
		G2291	G2178	G2094		G1830	A1715	A	G1467	A1349	C1226	
			C2179	A2104	A1974	C1831	A1716	C		G1349	A1227	G1137
		C2295	A2180		U1977	G1832	C1717		A1473	C1350	G1138	
		A2299	G2181	U2108	U1977	A1833	U1718	G1584	C1474	C1351	G1139	
		A2300	C2182	G2109		C1834	C1719	G1588	G1475	C1352	U1140	
		A2301	C2183		U1985	C1835	U1720	A1589	C1476		A1141	
		G2302		C2119		U1836	G1721	C1590	U1477	G1355	U1142	
		U2303	C2186	U2120	C1989	A1841	C1730	C1594	A1485		C1246	
		C2304	G2187	U2121		G1842	C1731	C1595	A1491	A1358	A1255	
		G2316	C2188	G2122	A1992	A1843	C1732			U1359	U1256	
		A2317	U2189	G2123	A1993	G1844	C1733	C1604	G1495	C1360	G1257	
			G2190	U2124	A1994	G1845	G1734	A1605	G1496	C1361	A1149	
			A2193	G2125		A1846			G1497	A1367	C1263	
			U2194		C2010	G1847	U1740	A1613	C1498		G1264	U1151
			A2195	C2129					C1499			G1152
			A2196	C2130	U2015	G1857	A1747	A1616		G1370	G1273	
			A2198	U2131			A1748	A1617	A1500		G1274	C1155
				G2132	C2018	A1860	G1749	U1501	G1502		G1275	A1156
					G2019		G1750	A1618			A1157	
				U2135		G1870			G1506		G1285	G1158
				A2136	A2035	G1871	U1753	U1625	A1507	G1378	U1286	
				G2138	A2036		C1754		G1508		A1287	G1162
				A2139	A2037	C1874	C1755	G1628	C1509	U1387	A1288	
								A1630			G1171	

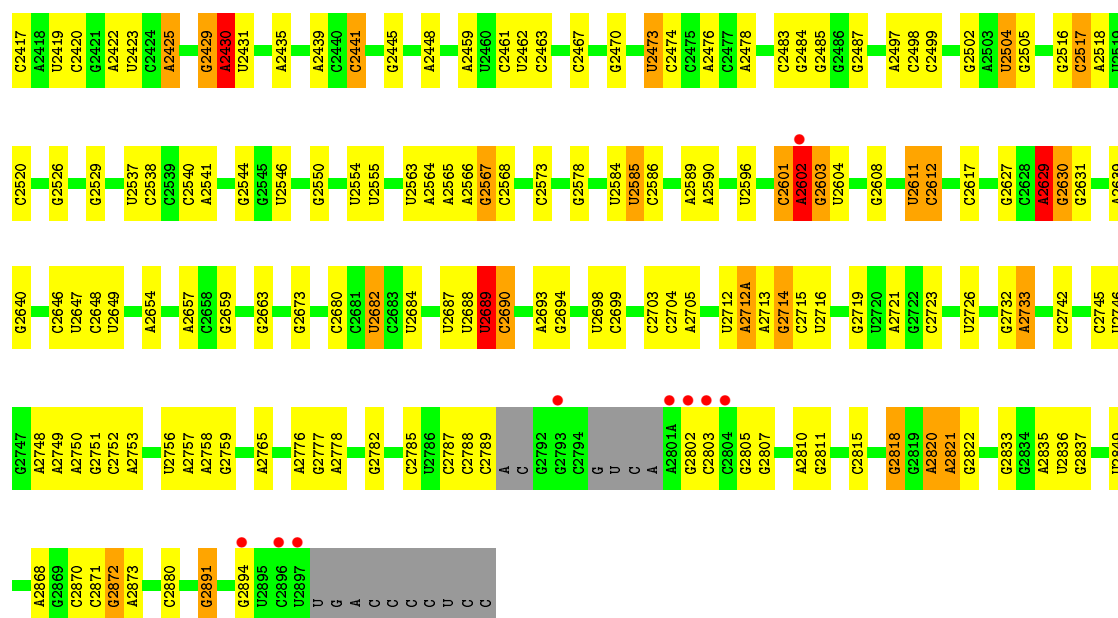


• Molecule 1: 23S Ribosomal RNA



G2321	G2322	G2323	G2324	G2325	G2326	A2327	A2328	G2329	G2332	A2333	G2334	A2335	A2336	G2343	G2344	G2347	G2350	G2354	G2355	G2356	G2357	G2358	G2364	G2365	A2366	G2375	A2376	A2377	A2378	G2379	G2383	G2384	G2385	A2388	G2389	G2390	G2391	G2397	G2400	U2401	G2402	U2406	G2410	G2414																
U2243	U2244	C2248	G2251	G2252	G2253	G2260	G2261	U2262	A2267	C2268	A2269	G2270	G2271	U2272	A2273	A2274	C2275	G2280	C2283	G2284	G2285	A2286	A2287	A2288	G2289	C2292	G2295	U2296	G2297	A2298	G2299	G2302	G2303	G2304	A2305	G2307	G2308	A2309	A2310	A2311	U2312	C2313	G2314	G2315	G2316	G2317	G2318	G2319	G2320											
G2148	G2149	G2150	G2151	G2152	G2153	G2154	G2155	G2156	A2158	G2159	G2160	C2161	G2162	G2163	G2164	G2165	G2166	U2167	G2168	A2169	A2170	A2171	U2172	A2173	C2174	G2175	A2176	C2177	G2178	U2180	G2181	G2182	G2183	G2184	G2185	G2186	G2187	G2188	U2189	G2190	G2191	G2192	A2198	G2206	G2207	A2208	G2219	A2225	G2237	G2238	G2239									
U2079	U2086	G2087	G2088	U2092	G2093	G2094	G2095	U2096	U2099	G2100	G2101	U2102	C2103	G2104	G2105	G2106	G2107	G2108	U2109	G2110	C2111	G2112	U2113	A2114	G2115	G2116	G2117	G2118	G2119	G2120	G2121	G2122	G2123	G2124	G2125	U2126	G2127	G2128	C2129	U2130	G2131	U2132	G2133	A2134	A2135	G2206	G2207	A2208	C2139	G2140	G2141	G2142	G2143	G2144	G2145	G2146	G2147			
C1947	U1817	U1818	G1826	G1827	G1828	A1829	G1830	G1831	G1832	U1835	G1839	G1842	A1847	A1848	G1858	U1864	A1876	A1877	G1878	C1881	G1882	U1889	A1890	G1899	A1900	A1901	G1902	G1906	G1910	U1911	A1912	A1913	U1914	U1915	A1916	U1917	G1921	G1929	G1930	A1937	A1938	U1939	U1946																	
C1947	U1952	A1953	G1954	U1955	U1963	U1967	U1970	A1971	A1972	U1991	G1992	U1993	G1996	G1997	A2001	G2002	A2014	A2020	C2021	U2022	G2023	A2030	A2031	G2032	A2033	G2036	G2037	G2038	G2039	G2040	C2043	A2051	G2055	G2056	A2060	G2061	A2062	G2069	G2070	U2074	U2075																			
G1031	A1032	G1033	G1034	G1035	G1036	G1037	G1038	C1041	G1044	U1045	A1046	G1047	A1048	G1052	C1053	A1054	G1055	G1056	A1057	G1058	G1059	U1060	U	G1062	G1063	G1064	U1065	U1066	A1067	G1068	A1069	A1070	G1071	G1072	A1073	G1074	G1075	G1076	A1077	U1078	C1079	C1080	U1081	U1082	U1083	A1084	A1085	A1086	G1087	A1088	G1089	U1090	G1091	G1092	G1093	U1094				
A1095	A1096	U1097	A1098	G1099	G1100	U1101	C1102	A1103	C1104	U1105	G1109	G1110	A1111	G1112	U1113	G1114	G1115	G1116	G1117	G1118	G1119	G1120	G1121	G1122	G1125	A1126	U1129	U1130	G1131	G1135	G1136	U1141	U1142	A1142A	G1153	G1154	A1155	U1165	C1166	U1167	G1168	A1169	G1170	G	A	U	G	U	A	C1178	G1179	G1180								
C1181	A1286	G1186	U1287	U1288	C1291	U1292	C1293	G1195	G1203	A1204	U1205	U1300	A1301	G1209	A1302	G1303	U1211	G1212	U1313	C1314	C1315	G1221A	U1316	G1222	G1223	G1319	C1320	A1321	U1226	G1229	G1235	G1236	A1237	G1238	G1338	U1240	A1241	U1341	A1246	A1342	U1253	A1254	U1255	G1256	C1261	G1264	A1281	G1285	G1286	A1367	G1271	A1272	U1273	A1274	U1371	U1372	A1278	A1379	G1380	G1281
A1384	G1385	C1386	A1392	A1393	U1394	U1405	U1406	G1409	G1410	C1411	A1412	G1413	G1416	C1417	U1420	G1421	G1422	A1427	C1428	G1429	C1430	U1431	G1442	A1445	C1446	G1447	G1448	A1449	G1450	C1450A	G1455	G1459	C1467	A1471	U1481	G1482	A1486	G1487	U1488	U1489	A1490	G1491	G1492	C1493																
A1494	A1495	A1496	U1497	C1498	U1503	C1504	C1505	C1506	A1508	C1509	A1509A	A1509B	G1510	U1514	G1515	U1518	G1519	G1525	G1526	G1527	A1528	G1529	G1533	U	A	C1536	G1537	G1538	G1539	U1540	G1541	A1542	C1543	C1547	C1557	A1558	G1559	A1566	A1569	C1577	U1578	A1579	A1580	G1581	C1582	A1583	C1584													
A1586	A1587	C1588	U1589	G1591	G1595	A1596	A1597	C1598	C1599	C1607	A1608	A1609	A1610	A1614	U1629	A1631A	U1639	G1640	C1644	G1647	C1648	A1654	C1657	G1658	A1664	A1665	G1666	A1668	A1669	G1674	C1675	U1680	C1686	G1687	U1688	G1696	A1700	A1701	G1702	G1703																				
G1707	C1708	U1709	C1710	U1720	G1721	A1722	U1739	G1740	G1746	G1748	A1749	G1750	C1754	A1755	G1756	A1762	G1763	G1764	C1771	G1772	A1773	U1776	U1777	U1779	A1780	G1781	G1782	A1783	A1784	A1785	A1786	A1791	G1792	C1793	U1794	C1795	U1796	C1797	U1798	G1799	C1800	G1801	A1802	A1803	G1807	A1815	G1816													
G1817	U1818	G1826	G1827	G1828	A1829	G1830	G1831	G1832	G1835	G1839	G1842	A1847	A1848	G1858	U1864	A1876	A1877	G1878	C1881	G1882	U1889	A1890	G1899	A1900	A1901	G1902	G1906	G1910	U1911	A1912	A1913	U1914	U1915	A1916	U1917	G1921	G1929	G1930	A1937	A1938	U1939	U1946																		
C1947	U1952	A1953	G1954	U1955	U1963	U1967	U1970	A1971	A1972	U1991	G1992	U1993	G1996	G1997	A2001	G2002	A2014	A2020	C2021	U2022	G2023	A2030	A2031	G2032	A2033	G2036	G2037	G2038	G2039	G2040	C2043	A2051	G2055	G2056	A2060	G2061	A2062	G2069	G2070	U2074	U2075																			
G2148	G2149	G2150	G2151	G2152	G2153	G2154	G2155	G2156	A2158	G2159	G2160	C2161	G2162	G2163	G2164	G2165	G2166	U2167	G2168	A2169	A2170	A2171	U2172	A2173	C2174	G2175	A2176	C2177	G2178	U2180	G2181	G2182	G2183	G2184	G2185	G2186	G2187	G2188	U2189	G2190	G2191	G2192	A2198	G2206	G2207	A2208	G2219	A2225	G2237	G2238	G2239									
U2079	U2086	G2087	G2088	U2092	G2093	G2094	G2095	U2096	U2099	G2100	G2101	U2102	C2103	G2104	G2105	G2106	G2107	G2108	U2109	G2110	C2111	G2112	U2113	A2114	G2115	G2116	G2117	G2118	G2119	G2120	G2121	G2122	G2123	G2124	G2125	U2126	G2127	G2128	C2129	U2130	G2131	U2132	G2133	A2134	A2135	G2206	G2207	A2208	C2139	G2140	G2141	G2142	G2143	G2144	G2145	G2146	G2147			
C1947	U1817	U1818	G1826	G1827	G1828	A1829	G1830	G1831	G1832	U1835	G1839	G1842	A1847	A1848	G1858	U1864	A1876	A1877	G1878	C1881	G1882	U1889	A1890	G1899	A1900	A1901	G1902	G1906	G1910	U1911	A1912	A1913	U1914	U1915	A1916	U1917	G1921	G1929	G1930	A1937	A1938	U1939	U1946																	
C1947	U1952	A1953	G1954	U1955	U1963	U1967	U1970	A1971	A1972	U1991	G1992	U1993	G1996	G1997	A2001	G2002	A2014	A2020	C2021	U2022	G2023	A2030	A2031	G2032	A2033	G2036	G2037	G2038	G2039	G2040	C2043	A2051	G2055	G2056	A2060	G2061	A2062	G2069	G2070	U2074	U2075																			
G2148	G2149	G2150	G2151	G2152	G2153	G2154	G2155	G2156	A2158	G2159	G2160	C2161	G2162	G2163	G2164	G2165	G2166	U2167	G2168	A2169	A2170	A2171	U2172	A2173	C2174	G2175	A2176	C2177	G2178	U2180	G2181	G2182	G2183	G2184	G2185	G2186	G2187	G2188	U2189	G2190	G2191	G2192	A2198	G2206	G2207	A2208	G2219	A2225	G2237	G2238	G2239									
U2079	U2086	G2087	G2088	U2092	G2093	G2094	G2095	U2096	U2099	G2100	G2101	U2102	C2103	G2104	G2105	G2106	G2107	G2108	U2109	G2110	C2111	G2112	U2113	A2114	G2115	G2116	G2117	G2118	G2119	G2120	G2121	G2122	G2123	G2124	G2125	U2126	G2127	G2128	C2129	U2130	G2131	U2132	G2133	A2134	A2135	G2206	G2207	A2208	C2139	G2140	G2141	G2142	G2143	G2144	G2145	G2146	G2147			
C1947	U1817	U1818	G1826	G1827	G1828	A1829	G1830	G1831	G1832	U1835	G1839	G1842	A1847	A1848	G1858	U1864	A1876	A1877	G1878	C1881	G1882	U1889	A1890	G1899	A1900	A1901	G1902	G1906	G1910	U1911	A1912	A1913	U1914	U1915	A1916	U1917	G1921	G1929	G1930	A1937	A1938	U1939	U1946																	
C1947	U1952	A1953	G1954	U1955	U1963	U1967	U1970	A1971	A1972	U1991	G1992	U1993	G1996	G1997	A2001	G2002	A2014	A2020	C2021	U2022	G2023	A2030	A2031	G2032	A2033	G2036	G2037	G2038	G2039	G2040	C2043	A2051	G2055	G2056	A2060	G2061	A2062	G2069	G2070	U2074	U2075																			
G2148	G2149	G2150	G2151	G2152	G2153	G2154	G2155	G2156	A2158	G2159	G2160	C2161	G2162	G2163	G2164	G2165	G2166	U2167	G2168	A2169	A2170	A2171	U2172	A2173	C2174	G2175	A2176	C2177	G2178	U2180	G2181	G2182	G2183	G2184	G2185	G2186	G2187	G2188	U2189	G2190	G2191	G2192	A2198	G2206	G2207	A2208	G2219	A2225	G2237	G2238	G2239									
U2079	U2086	G2087	G2088	U2092	G2093	G2094	G2095	U2096	U2099	G2100	G2101	U2102	C2103	G2104	G2105	G2106	G2107	G2108	U2109	G2110	C2111	G2112	U2113	A2114	G2115	G2116	G2117	G2118	G2119	G2120	G2121	G2122	G2123	G2124	G2125	U2126	G2127	G2128	C2129	U2130	G2131	U2132	G2133	A2134	A2135	G2206	G2207	A2208	C2139	G2140	G2141	G2142	G2143	G2144	G2145	G2146	G2147			
C1947	U1817	U1818	G1826	G1827	G1828	A1829	G1830	G1831	G1832	U1835	G1839	G1842	A1847	A1848	G1858	U1864	A1876	A1877	G1878	C1881	G1882	U1889	A1890	G1899	A1900	A1901	G1902	G1906	G1910	U1911	A1912	A1913	U1914	U1915	A1916	U1917	G1921	G1929	G1930	A1937	A1938	U1939	U1946																	
C1947	U1952	A1953	G1954	U1955	U1963	U1967	U1970	A1971	A1972	U1991	G1992	U1993	G1996	G1997	A2001	G2002	A2014	A2020	C2021	U2022	G2023	A2030	A2031	G2032	A2033	G2036	G2037	G2038	G2039	G2040	C2043	A2051	G2055	G2056	A2060	G2061	A2062	G2069	G2070	U2074	U2075																			
G2148	G2149	G2150	G2151	G2152	G2153	G2154	G2155	G2156	A2158	G2159	G2160	C2161	G2162	G2163	G2164	G2165	G2166	U2167	G2168	A2169	A2170	A2171																																						





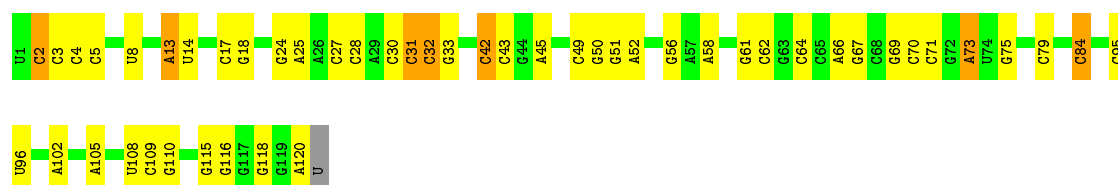
• Molecule 2: 5S Ribosomal RNA

Chain 1B: 75% 21%



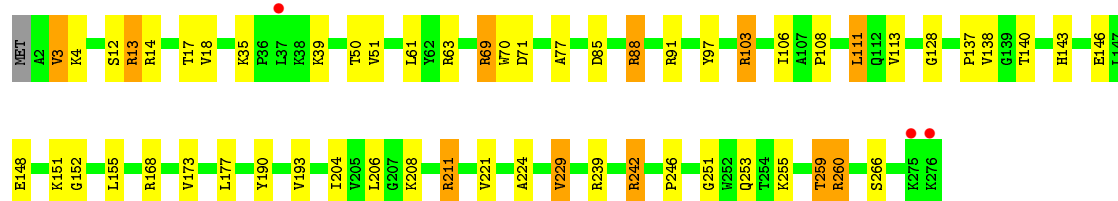
• Molecule 2: 5S Ribosomal RNA

Chain 2B: 59% 35% 6%



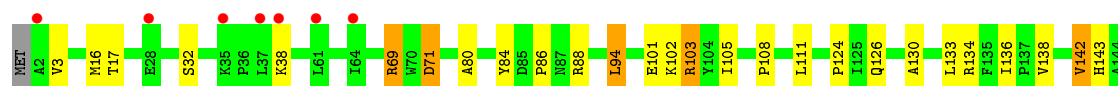
• Molecule 3: 50S ribosomal protein L2

Chain 1D: 79% 17%

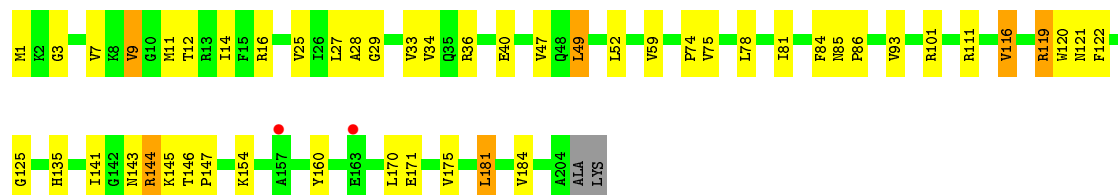
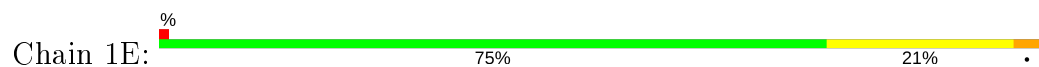


• Molecule 3: 50S ribosomal protein L2

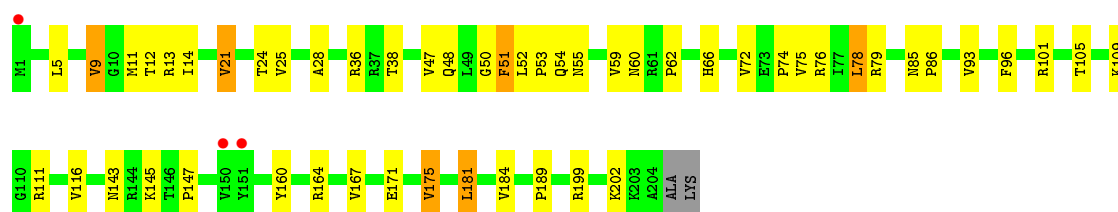
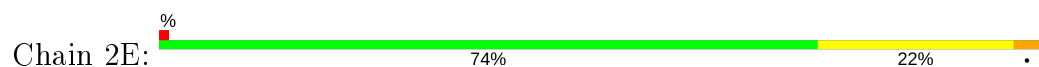
Chain 2D: 5% 82% 15%



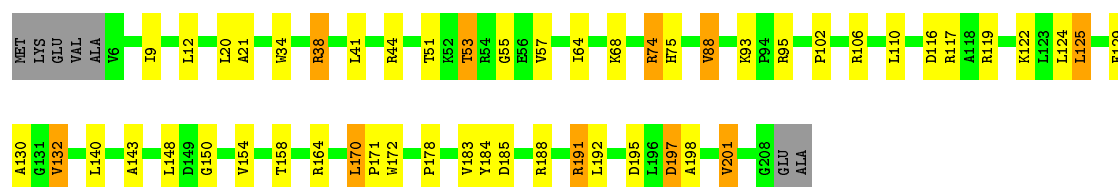
• Molecule 4: 50S ribosomal protein L3



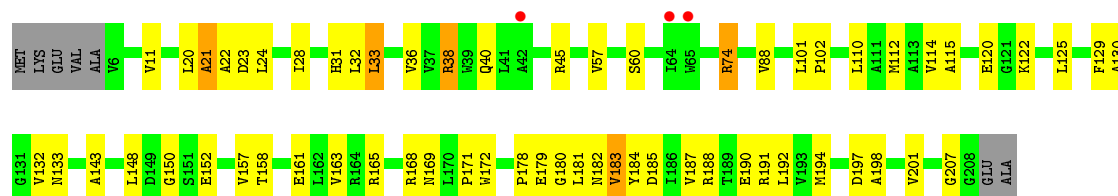
• Molecule 4: 50S ribosomal protein L3



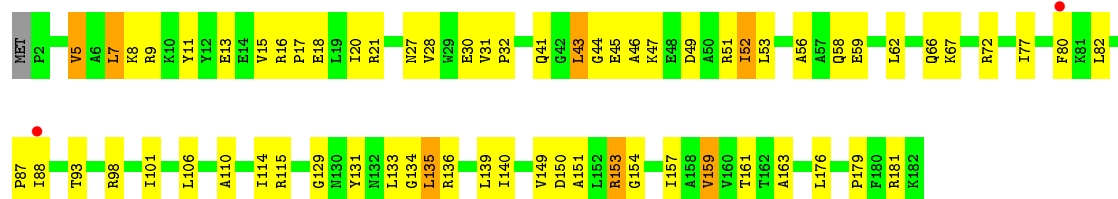
• Molecule 5: 50S ribosomal protein L4



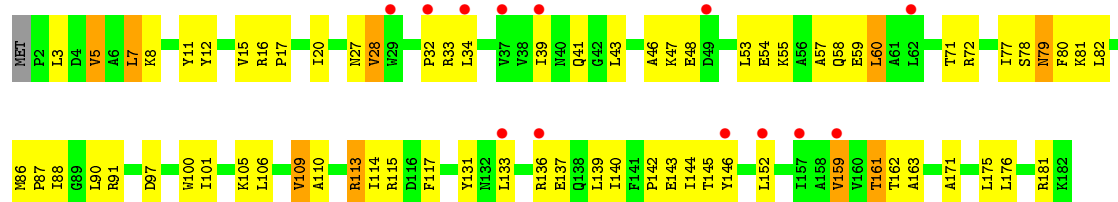
• Molecule 5: 50S ribosomal protein L4



• Molecule 6: 50S ribosomal protein L5



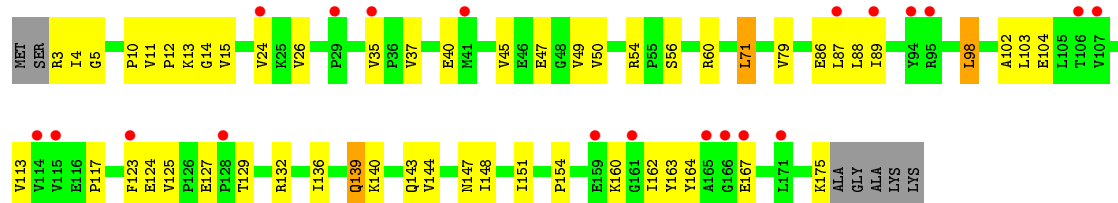
• Molecule 6: 50S ribosomal protein L5



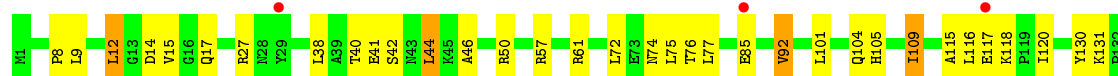
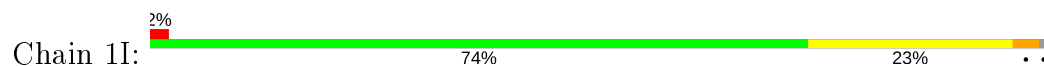
• Molecule 7: 50S ribosomal protein L6



• Molecule 7: 50S ribosomal protein L6

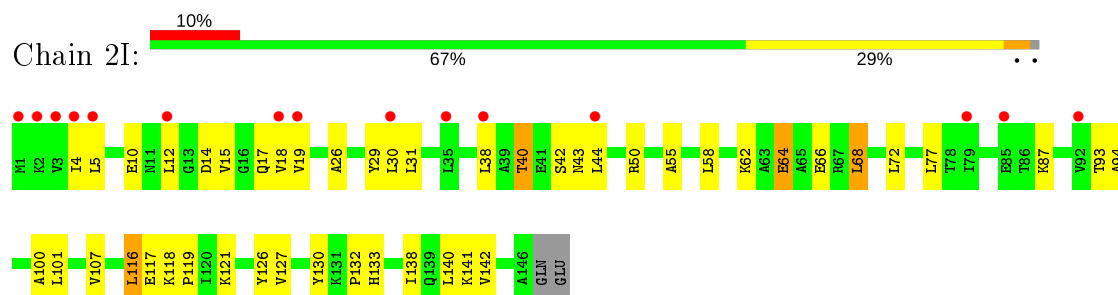


• Molecule 8: 50S ribosomal protein L9

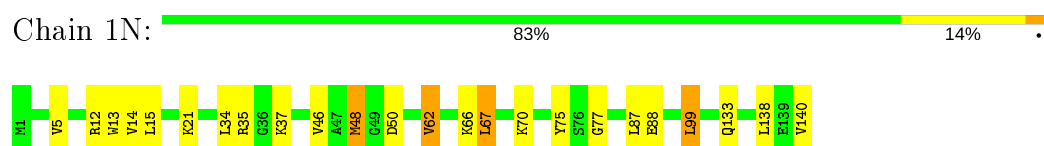




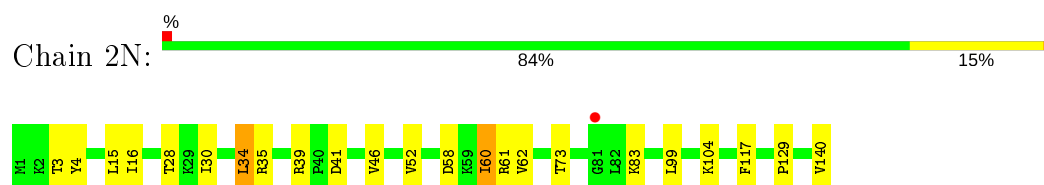
- Molecule 8: 50S ribosomal protein L9



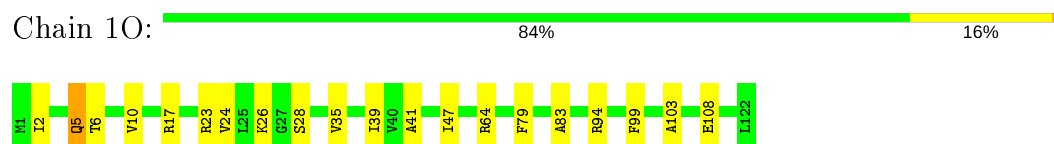
- Molecule 9: 50S ribosomal protein L13



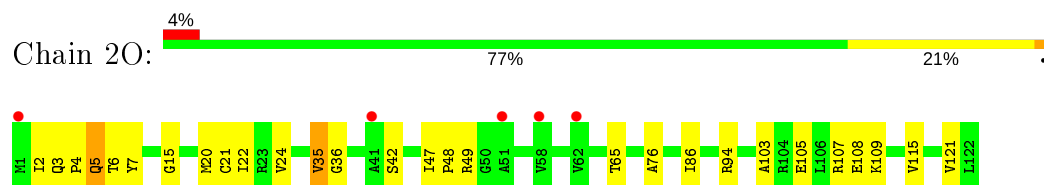
- Molecule 9: 50S ribosomal protein L13



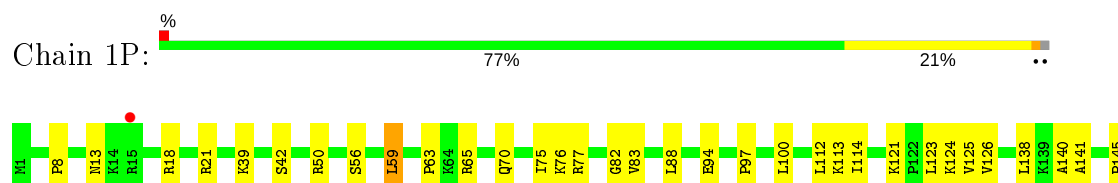
- Molecule 10: 50S ribosomal protein L14



- Molecule 10: 50S ribosomal protein L14



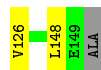
- Molecule 11: 50S ribosomal protein L15





- Molecule 11: 50S ribosomal protein L15

Chain 2P: 5% 80% 18% ..



- Molecule 12: 50S ribosomal protein L16

Chain 1Q: 77% 19% .



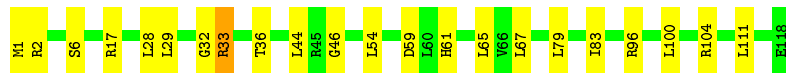
- Molecule 12: 50S ribosomal protein L16

Chain 2Q: 5% 68% 30% .



- Molecule 13: 50S ribosomal protein L17

Chain 1R: 81% 18% .



- Molecule 13: 50S ribosomal protein L17

Chain 2R: 2% 74% 23% .

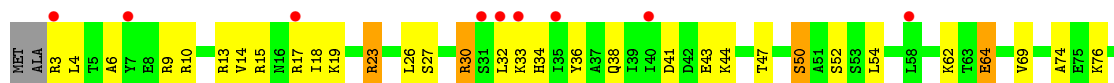


- Molecule 14: 50S ribosomal protein L18

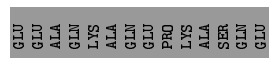
Chain 1S: 81% 14% . .



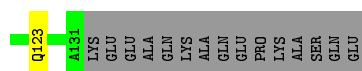
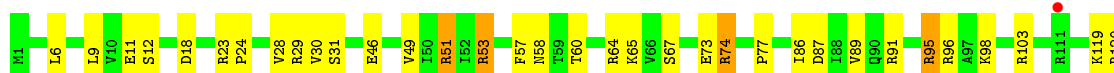
- Molecule 14: 50S ribosomal protein L18



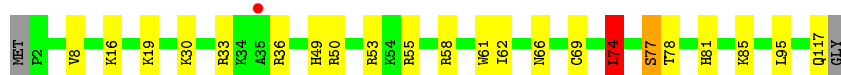
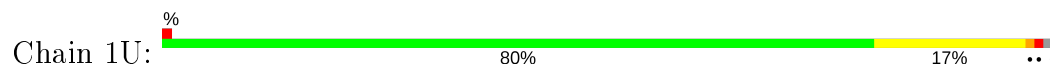
- Molecule 15: 50S ribosomal protein L19



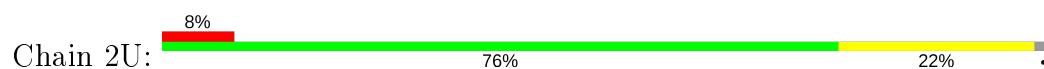
- Molecule 15: 50S ribosomal protein L19




- Molecule 16: 50S ribosomal protein L20

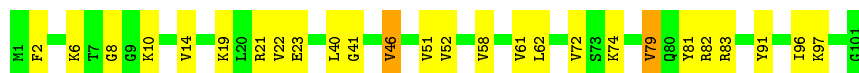


- Molecule 16: 50S ribosomal protein L20




- Molecule 17: 50S ribosomal protein L21

Chain 1V:  74% 24%




- Molecule 17: 50S ribosomal protein L21

Chain 2V:  3% 72% 25%




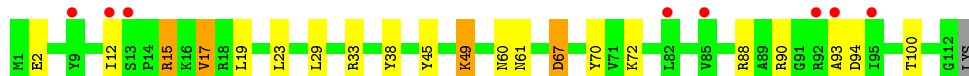
- Molecule 18: 50S ribosomal protein L22

Chain 1W:  83% 13%




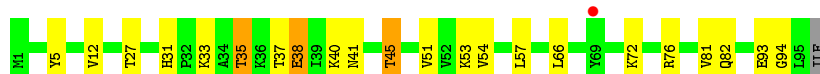
- Molecule 18: 50S ribosomal protein L22

Chain 2W:  7% 81% 15%




- Molecule 19: 50S ribosomal protein L23

Chain 1X:  76% 20%



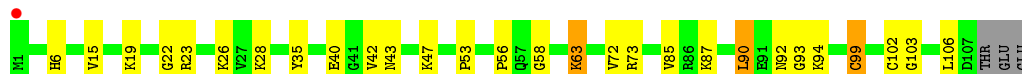
- Molecule 19: 50S ribosomal protein L23

Chain 2X:  5% 79% 18%

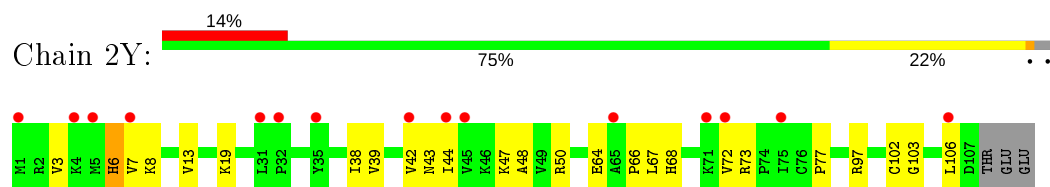


- Molecule 20: 50S ribosomal protein L24

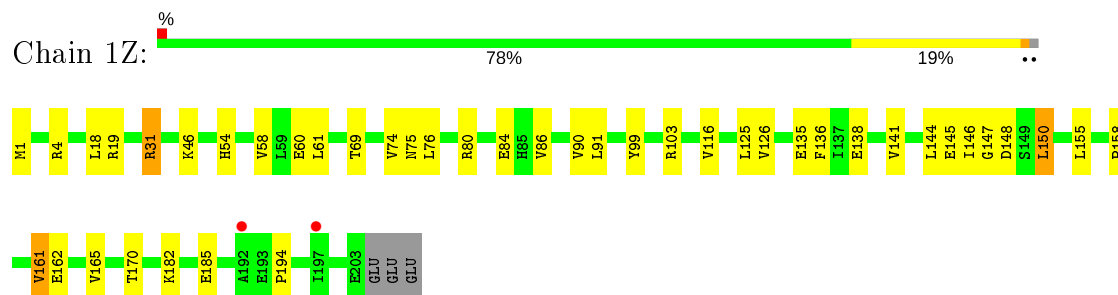
Chain 1Y:  72% 23%



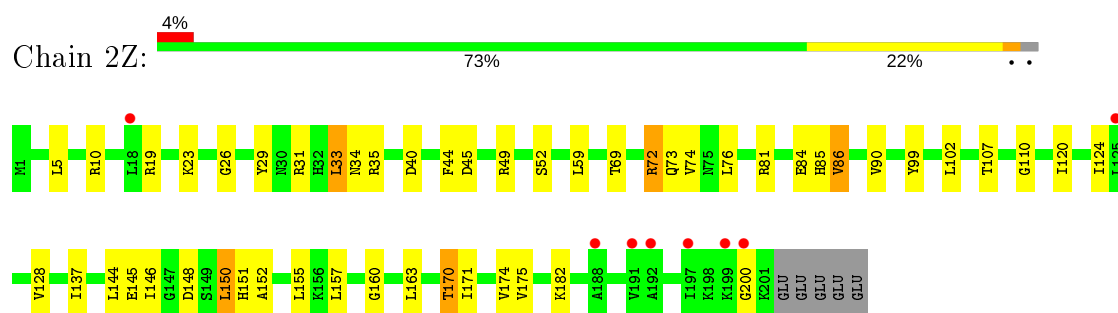
- Molecule 20: 50S ribosomal protein L24



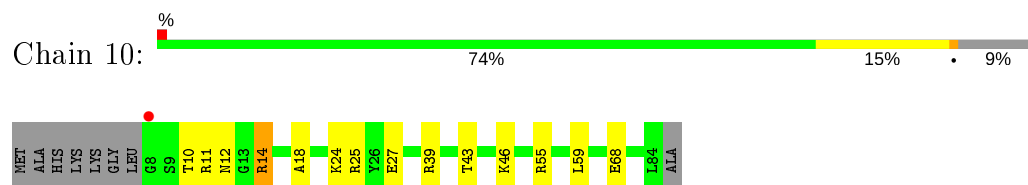
- Molecule 21: 50S ribosomal protein L25



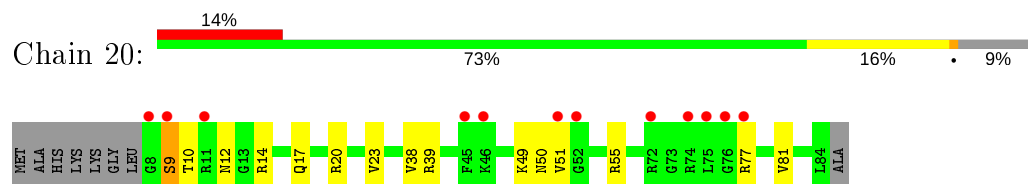
- Molecule 21: 50S ribosomal protein L25



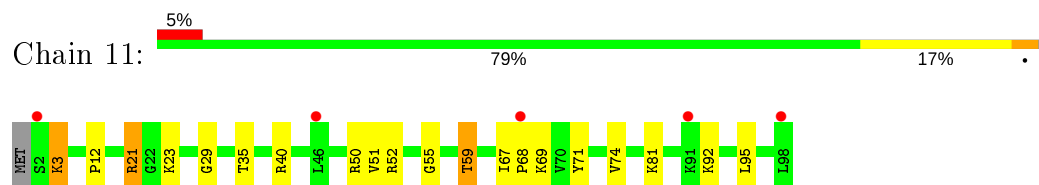
- Molecule 22: 50S ribosomal protein L27



- Molecule 22: 50S ribosomal protein L27

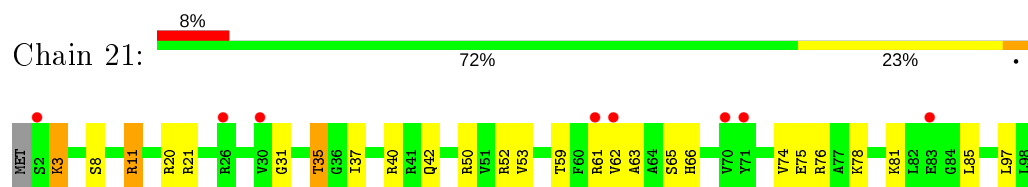


- Molecule 23: 50S ribosomal protein L28

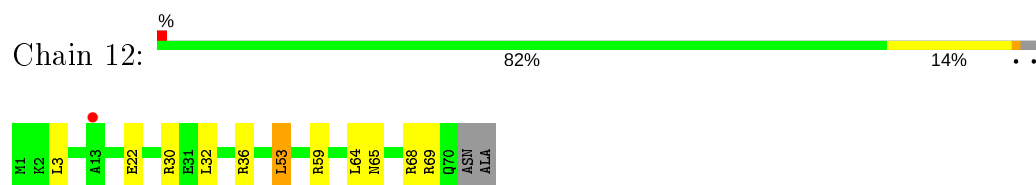




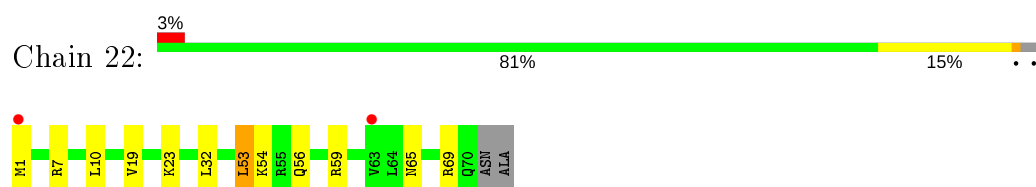
- Molecule 23: 50S ribosomal protein L28



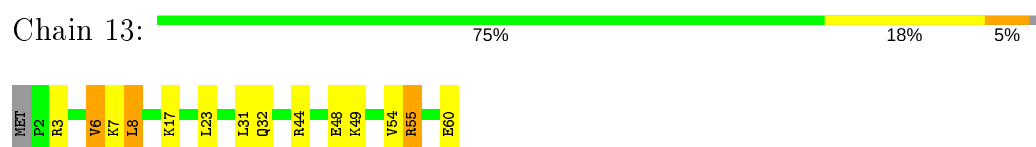
- Molecule 24: 50S ribosomal protein L29



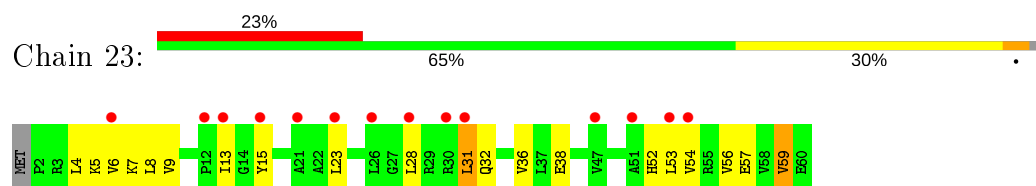
- Molecule 24: 50S ribosomal protein L29



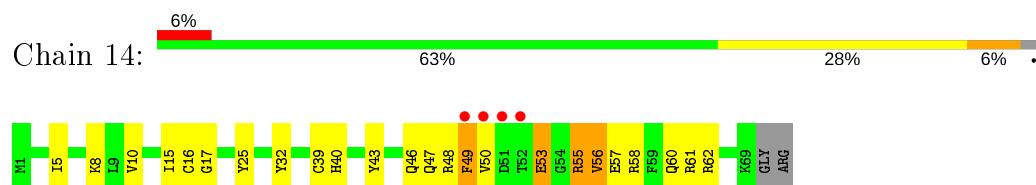
- Molecule 25: 50S ribosomal protein L30



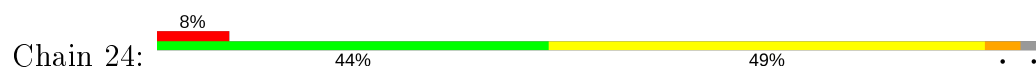
- Molecule 25: 50S ribosomal protein L30

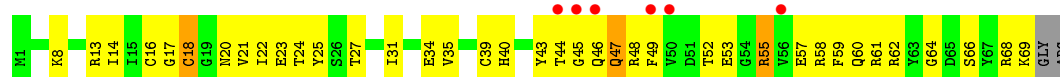


- Molecule 26: 50S ribosomal protein L31

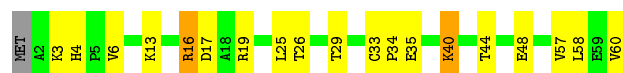


- Molecule 26: 50S ribosomal protein L31

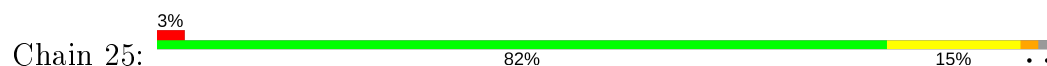




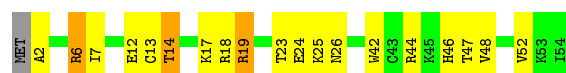
- Molecule 27: 50S ribosomal protein L32



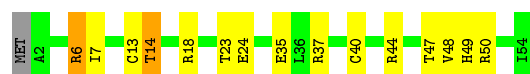
- Molecule 27: 50S ribosomal protein L32



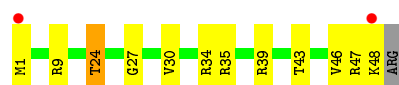
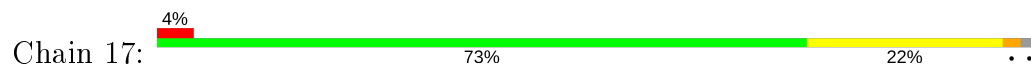
- Molecule 28: 50S ribosomal protein L33



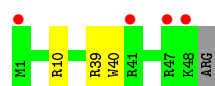
- Molecule 28: 50S ribosomal protein L33



- Molecule 29: 50S ribosomal protein L34

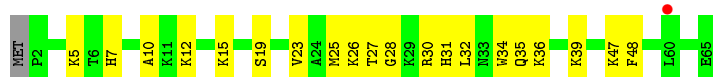


- Molecule 29: 50S ribosomal protein L34

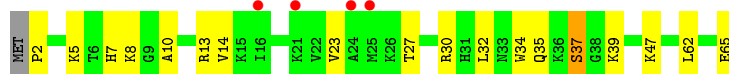


- Molecule 30: 50S ribosomal protein L35





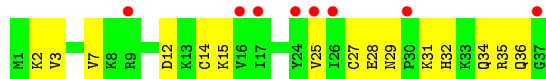
- Molecule 30: 50S ribosomal protein L35



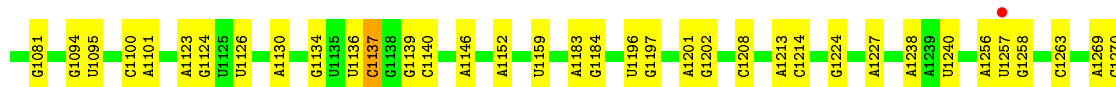
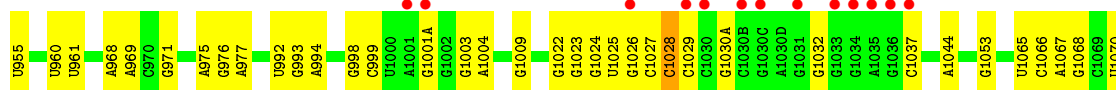
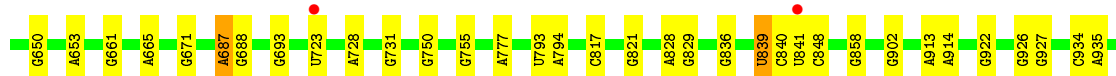
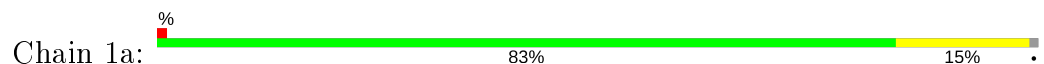
- Molecule 31: 50S ribosomal protein L36

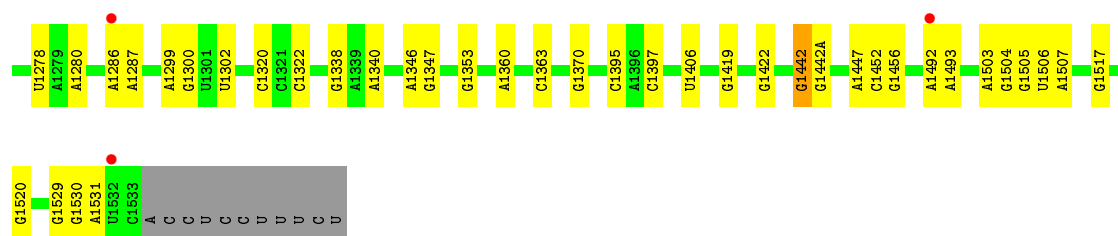


- Molecule 31: 50S ribosomal protein L36

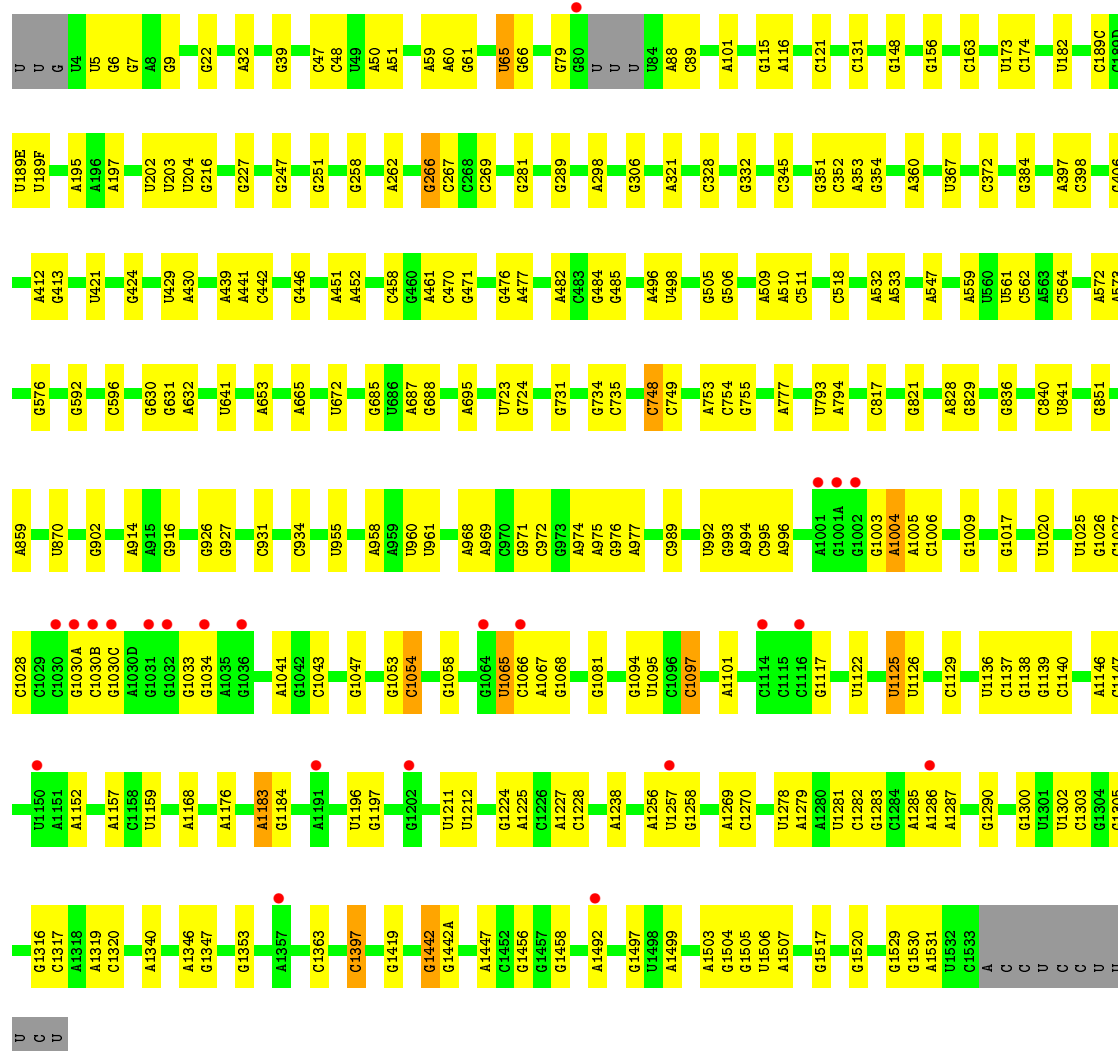
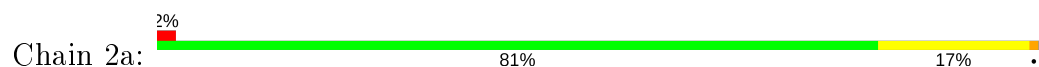


- Molecule 32: 16S Ribosomal RNA

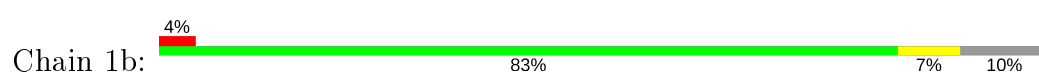




• Molecule 32: 16S Ribosomal RNA




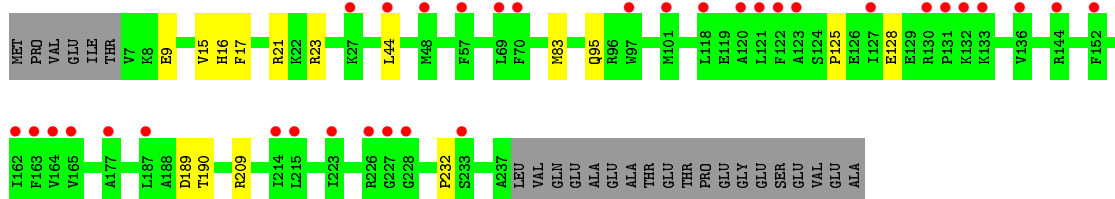
• Molecule 33: 30S ribosomal protein S2




THR  
PRO  
GLU  
GLY  
GLU  
SER  
GLU  
VAL  
GLU  
ALA

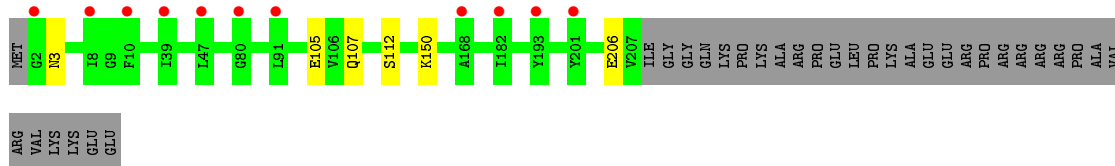
- Molecule 33: 30S ribosomal protein S2

Chain 2b: 




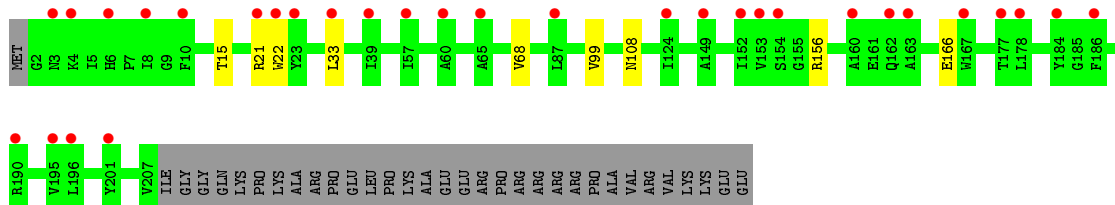
- Molecule 34: 30S ribosomal protein S3

Chain 1c: 



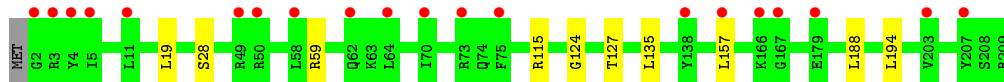
- Molecule 34: 30S ribosomal protein S3

Chain 2c: 



- Molecule 35: 30S ribosomal protein S4

Chain 1d: 



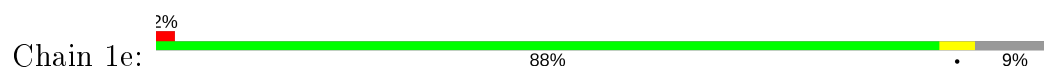
- Molecule 35: 30S ribosomal protein S4

Chain 2d: 

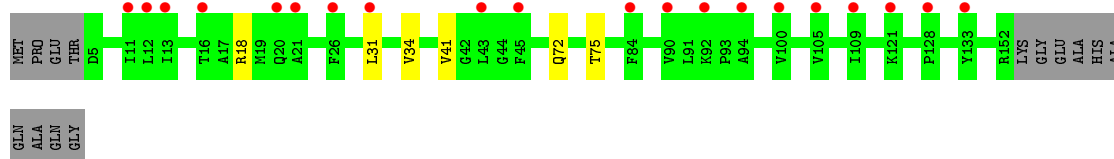
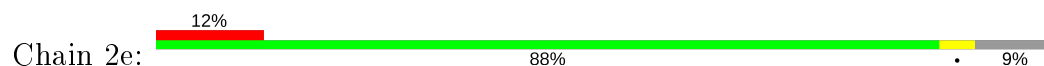




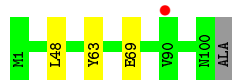
- Molecule 36: 30S ribosomal protein S5



- Molecule 36: 30S ribosomal protein S5



- Molecule 37: 30S ribosomal protein S6



- Molecule 37: 30S ribosomal protein S6



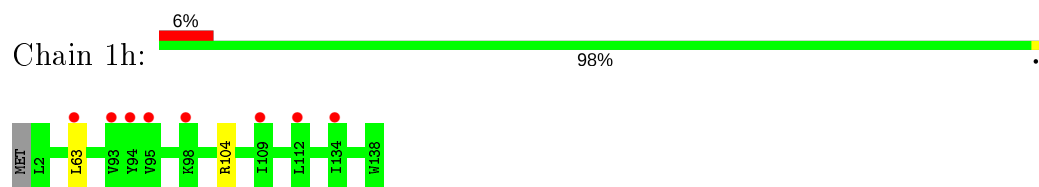
- Molecule 38: 30S ribosomal protein S7



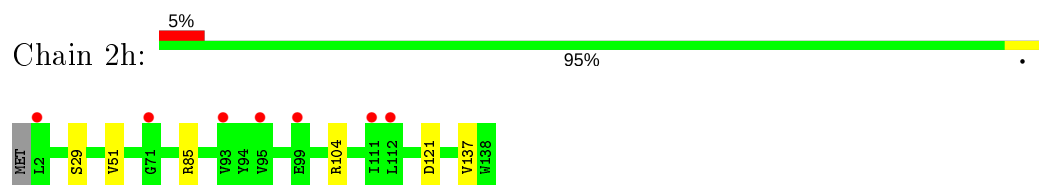
- Molecule 38: 30S ribosomal protein S7



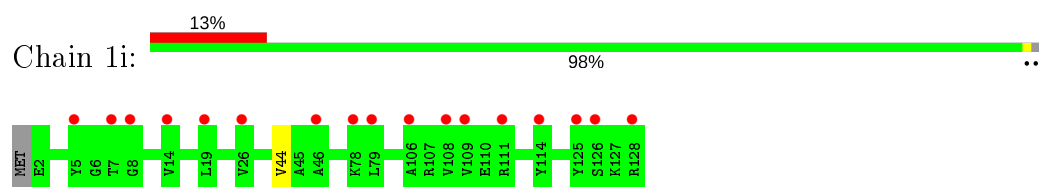
- Molecule 39: 30S ribosomal protein S8



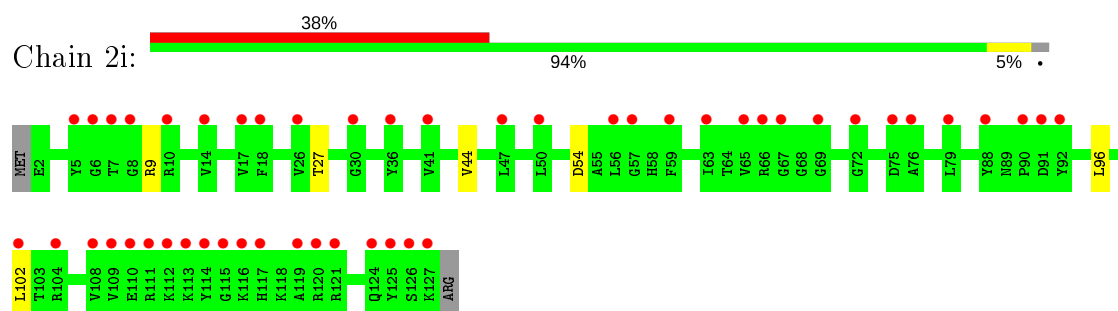
- Molecule 39: 30S ribosomal protein S8



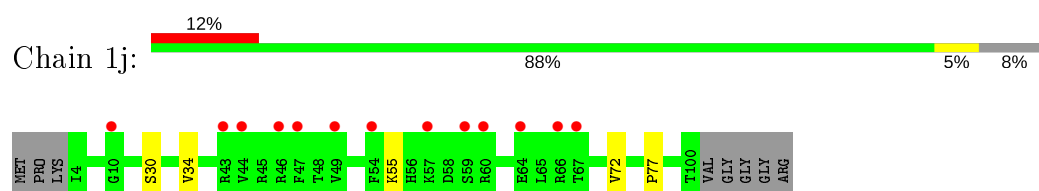
- Molecule 40: 30S ribosomal protein S9



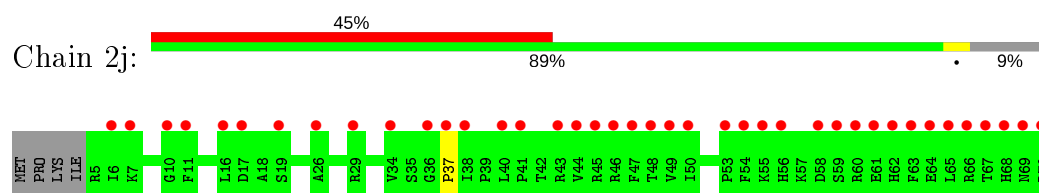
- Molecule 40: 30S ribosomal protein S9

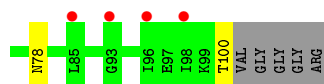


- Molecule 41: 30S ribosomal protein S10



- Molecule 41: 30S ribosomal protein S10

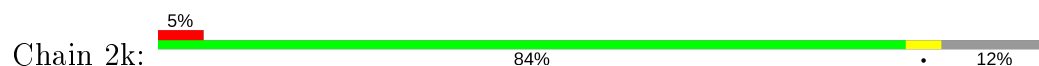




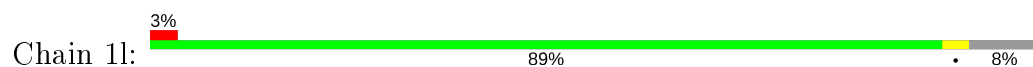
- Molecule 42: 30S ribosomal protein S11



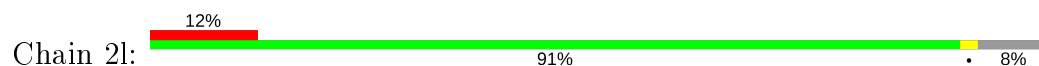
- Molecule 42: 30S ribosomal protein S11



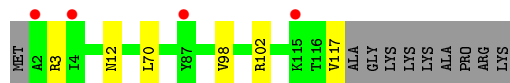
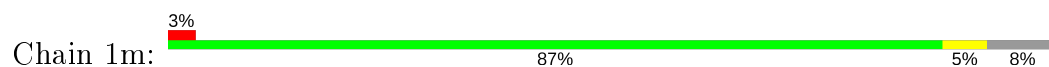
- Molecule 43: 30S ribosomal protein S12



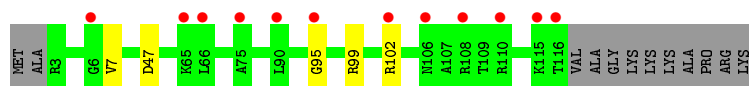
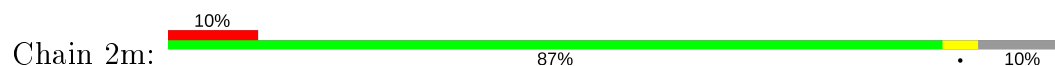
- Molecule 43: 30S ribosomal protein S12



- Molecule 44: 30S ribosomal protein S13

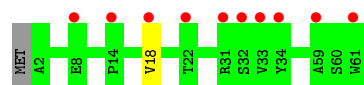


- Molecule 44: 30S ribosomal protein S13

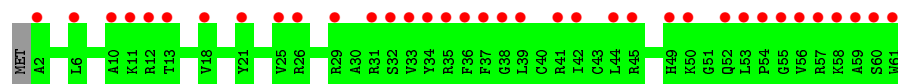


- Molecule 45: 30S ribosomal protein S14 type Z





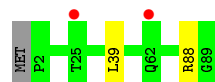
- Molecule 45: 30S ribosomal protein S14 type Z



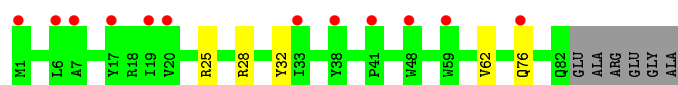
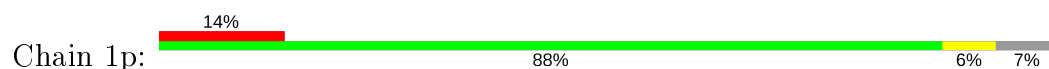
- Molecule 46: 30S ribosomal protein S15



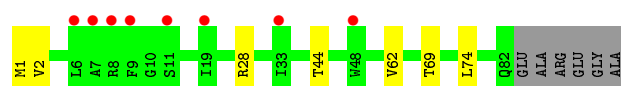
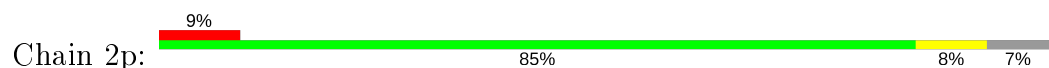
- Molecule 46: 30S ribosomal protein S15



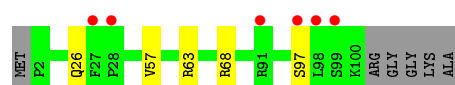
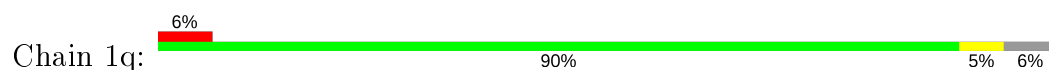
- Molecule 47: 30S ribosomal protein S16



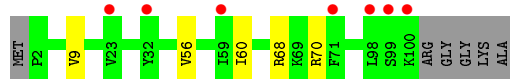
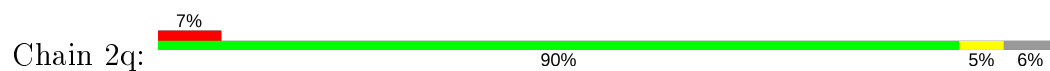
- Molecule 47: 30S ribosomal protein S16



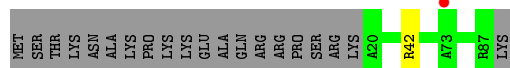
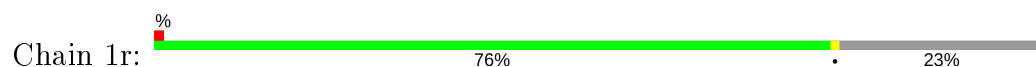
- Molecule 48: 30S ribosomal protein S17



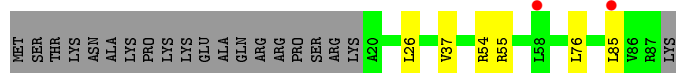
- Molecule 48: 30S ribosomal protein S17



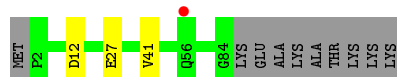
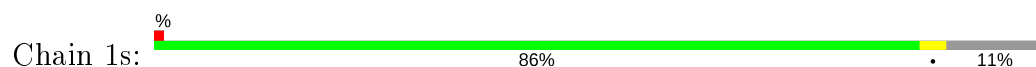
- Molecule 49: 30S ribosomal protein S18



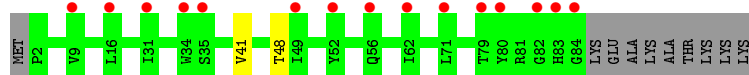
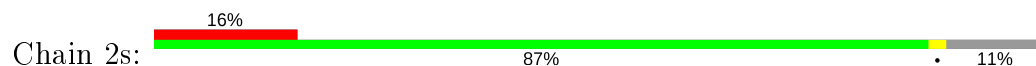
- Molecule 49: 30S ribosomal protein S18



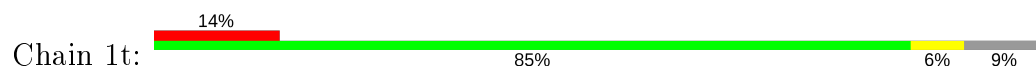
- Molecule 50: 30S ribosomal protein S19



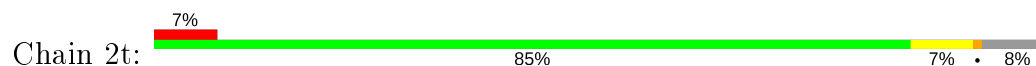
- Molecule 50: 30S ribosomal protein S19

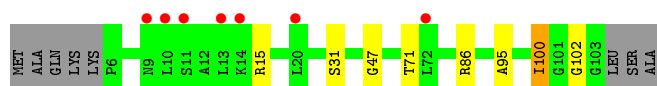


- Molecule 51: 30S ribosomal protein S20

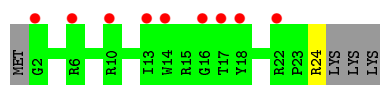
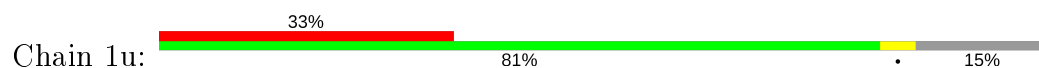


- Molecule 51: 30S ribosomal protein S20

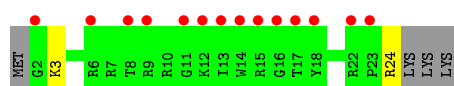
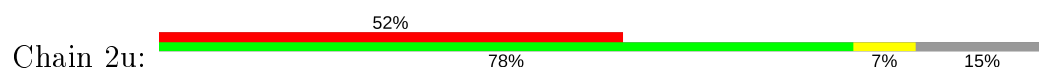




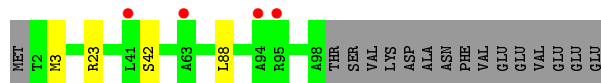
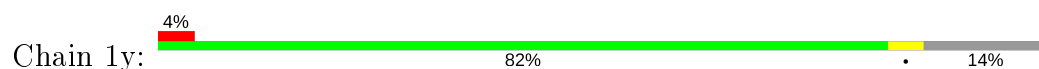
- Molecule 52: 30S ribosomal protein Thx



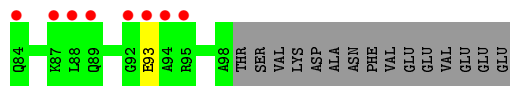
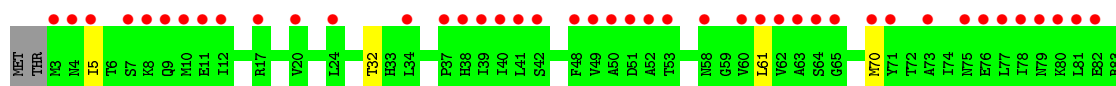
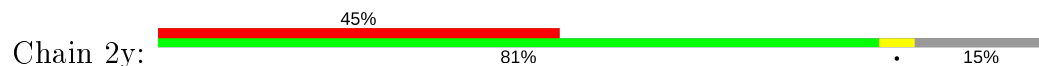
- Molecule 52: 30S ribosomal protein Thx



- Molecule 53: Ribosome-associated inhibitor A



- Molecule 53: Ribosome-associated inhibitor A



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.09Å 449.12Å 621.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	121.92 – 2.70 364.10 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.2 (121.92-2.70) 99.2 (364.10-2.70)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.24 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.8.2	Depositor
R, $R_{free}$	0.206 , 0.253 0.207 , 0.253	Depositor DCC
$R_{free}$ test set	79057 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.6	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 53.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	295438	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.62% 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, MPD, OMG, MA6, ZN, SF4, 0TD, EZP, MG, 2MA, 2MU, 2MG, 5MC, UR3, 4OC, M2G, 7MG, K, PSU

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	0.51	0/69029	0.96	51/107746 (0.0%)
1	2A	0.41	0/68901	0.90	41/107544 (0.0%)
2	1B	0.43	0/2876	0.90	1/4486 (0.0%)
2	2B	0.37	0/2878	0.87	0/4490
3	1D	0.37	0/2181	0.59	0/2940
3	2D	0.33	0/2186	0.55	0/2944
4	1E	0.37	0/1592	0.55	0/2149
4	2E	0.31	0/1592	0.53	0/2149
5	1F	0.34	0/1619	0.53	0/2193
5	2F	0.31	0/1615	0.52	0/2188
6	1G	0.30	0/1451	0.50	0/1961
6	2G	0.30	0/1449	0.47	0/1957
7	1H	0.33	0/1356	0.51	0/1834
7	2H	0.29	0/1350	0.47	0/1826
8	1I	0.30	0/1109	0.52	0/1512
8	2I	0.28	0/1091	0.49	0/1490
9	1N	0.36	0/1148	0.55	0/1547
9	2N	0.29	0/1144	0.48	0/1543
10	1O	0.36	0/943	0.56	0/1269
10	2O	0.33	0/943	0.54	0/1269
11	1P	0.34	0/1152	0.57	0/1533
11	2P	0.32	0/1152	0.54	0/1533
12	1Q	0.35	0/1143	0.52	0/1527
12	2Q	0.30	0/1143	0.49	0/1527
13	1R	0.34	0/982	0.58	0/1312
13	2R	0.31	0/982	0.55	1/1312 (0.1%)
14	1S	0.31	0/887	0.52	0/1180
14	2S	0.30	0/880	0.50	0/1172
15	1T	0.33	0/1105	0.54	0/1477
15	2T	0.30	0/1097	0.51	0/1468
16	1U	0.36	0/977	0.53	1/1301 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	2U	0.30	0/977	0.45	0/1301
17	1V	0.34	0/786	0.54	0/1053
17	2V	0.32	0/782	0.52	0/1049
18	1W	0.33	0/897	0.51	0/1205
18	2W	0.32	0/897	0.50	0/1205
19	1X	0.38	0/764	0.56	0/1025
19	2X	0.31	0/764	0.55	1/1025 (0.1%)
20	1Y	0.37	0/823	0.54	0/1099
20	2Y	0.33	0/823	0.51	0/1100
21	1Z	0.30	0/1620	0.52	0/2200
21	2Z	0.30	0/1590	0.49	0/2162
22	10	0.35	0/616	0.56	0/821
22	20	0.33	0/616	0.50	0/821
23	11	0.33	0/761	0.51	0/1013
23	21	0.32	0/766	0.50	0/1018
24	12	0.30	0/590	0.51	0/781
24	22	0.30	0/594	0.44	0/785
25	13	0.33	0/474	0.52	0/635
25	23	0.30	0/469	0.49	0/630
26	14	0.32	0/559	0.54	0/754
26	24	0.35	0/549	0.54	0/741
27	15	0.40	0/473	0.65	2/639 (0.3%)
27	25	0.33	0/469	0.53	0/635
28	16	0.33	0/460	0.56	0/613
28	26	0.32	0/456	0.49	0/608
29	17	0.38	0/426	0.58	0/561
29	27	0.31	0/426	0.50	0/561
30	18	0.36	0/525	0.56	0/691
30	28	0.31	0/525	0.52	0/691
31	19	0.37	0/310	0.53	0/407
31	29	0.31	0/310	0.52	0/407
32	1a	0.37	0/35795	0.88	18/55864 (0.0%)
32	2a	0.37	0/35890	0.89	32/56012 (0.1%)
33	1b	0.30	0/1876	0.50	0/2533
33	2b	0.33	0/1860	0.52	1/2518 (0.0%)
34	1c	0.29	0/1582	0.47	0/2137
34	2c	0.30	0/1566	0.48	0/2119
35	1d	0.30	0/1695	0.49	0/2274
35	2d	0.29	0/1698	0.46	0/2277
36	1e	0.31	0/1149	0.52	0/1548
36	2e	0.30	0/1149	0.51	0/1548
37	1f	0.32	0/827	0.51	0/1120
37	2f	0.29	0/829	0.50	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	1g	0.29	0/1254	0.44	0/1683
38	2g	0.29	0/1248	0.43	0/1676
39	1h	0.28	0/1118	0.48	0/1506
39	2h	0.28	0/1108	0.47	0/1494
40	1i	0.28	0/1005	0.50	0/1351
40	2i	0.30	0/985	0.47	0/1329
41	1j	0.30	0/732	0.49	0/993
41	2j	0.28	0/723	0.48	0/984
42	1k	0.30	0/849	0.48	0/1150
42	2k	0.30	0/848	0.54	0/1149
43	1l	0.30	0/937	0.51	0/1260
43	2l	0.29	0/937	0.53	0/1260
44	1m	0.28	0/924	0.46	0/1242
44	2m	0.30	0/905	0.49	0/1217
45	1n	0.31	0/501	0.46	0/664
45	2n	0.31	0/501	0.47	0/664
46	1o	0.28	0/739	0.48	0/985
46	2o	0.28	0/739	0.46	0/985
47	1p	0.30	0/697	0.53	0/939
47	2p	0.29	0/693	0.49	0/935
48	1q	0.30	0/836	0.51	0/1117
48	2q	0.29	0/836	0.49	0/1117
49	1r	0.28	0/560	0.48	0/746
49	2r	0.28	0/560	0.47	0/746
50	1s	0.27	0/663	0.50	0/895
50	2s	0.28	0/660	0.49	0/893
51	1t	0.27	0/734	0.45	0/969
51	2t	0.27	0/736	0.41	0/976
52	1u	0.25	0/203	0.48	0/266
52	2u	0.32	0/203	0.51	0/266
53	1y	0.29	0/776	0.47	0/1048
53	2y	0.27	0/761	0.45	0/1030
All	All	0.40	0/309937	0.82	149/463223 (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
19	1X	0	1
26	24	0	1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	#Chirality outliers	#Planarity outliers
33	1b	0	2
All	All	0	4

There are no bond length outliers.

All (149) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1003	G	N3-C4-C5	-8.97	124.12	128.60
32	2a	1003	G	C8-N9-C4	-8.85	102.86	106.40
1	1A	537	G	O4'-C1'-N9	8.36	114.89	108.20
1	1A	354	A	C2-N3-C4	-8.34	106.43	110.60
32	1a	1028	C	C2-N3-C4	7.73	123.77	119.90
1	2A	2629	A	O4'-C1'-N9	7.72	114.38	108.20
32	2a	1397	C	C2-N1-C1'	7.66	127.22	118.80
1	1A	354	A	N1-C2-N3	7.59	133.10	129.30
32	2a	1397	C	N1-C2-O2	7.47	123.38	118.90
1	1A	1121	C	N1-C2-O2	7.20	123.22	118.90
2	1B	57	A	N9-C4-C5	-7.15	102.94	105.80
32	2a	1003	G	C4-N9-C1'	7.04	135.66	126.50
1	2A	1648	C	O5'-P-OP1	-6.96	99.44	105.70
1	1A	1132	A	N1-C6-N6	-6.89	114.46	118.60
1	2A	1614	A	O5'-P-OP1	-6.77	99.61	105.70
1	2A	1992	G	P-O3'-C3'	6.73	127.78	119.70
33	2b	232	PRO	C-N-CA	6.71	138.47	121.70
32	1a	1028	C	C5-C6-N1	6.69	124.34	121.00
32	2a	266	G	P-O3'-C3'	6.64	127.67	119.70
32	2a	1225	A	C5-C6-N6	6.64	129.01	123.70
1	2A	1313	U	C2-N1-C1'	6.58	125.59	117.70
1	2A	1092	C	N1-C2-O2	6.53	122.82	118.90
1	1A	593	G	C5-C6-O6	-6.33	124.80	128.60
1	1A	2858	G	O4'-C1'-N9	6.31	113.25	108.20
1	1A	1222	A	O5'-P-OP1	-6.27	100.06	105.70
1	2A	1082	U	C2-N1-C1'	6.27	125.23	117.70
1	2A	2103	C	C2-N3-C4	6.23	123.02	119.90
1	2A	2130	U	C5-C6-N1	6.21	125.80	122.70
19	2X	57	LEU	CA-CB-CG	6.18	129.52	115.30
32	2a	1004	A	O4'-C1'-N9	6.17	113.14	108.20
1	2A	1082	U	N3-C2-O2	-6.17	117.89	122.20
1	2A	383	U	O4'-C1'-N1	6.15	113.12	108.20
32	2a	1225	A	N1-C6-N6	-6.14	114.92	118.60
1	1A	1418	U	C5-C4-O4	-6.14	122.22	125.90
32	2a	1003	G	C2-N3-C4	6.10	114.95	111.90

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1092	C	C6-N1-C2	-6.09	117.86	120.30
32	2a	1003	G	N7-C8-N9	6.07	116.13	113.10
32	1a	1442	G	N3-C4-C5	-6.05	125.58	128.60
32	1a	1137	C	C6-N1-C2	-6.04	117.88	120.30
1	1A	2058	C	O5'-P-OP1	-6.03	100.27	105.70
1	2A	1092	C	C5-C6-N1	6.03	124.02	121.00
1	1A	2605	U	N3-C4-O4	-6.01	115.19	119.40
1	1A	2331	G	O4'-C1'-N9	5.98	112.98	108.20
1	1A	1134	A	O4'-C1'-N9	5.97	112.98	108.20
1	1A	2512	U	N3-C2-O2	-5.97	118.02	122.20
32	2a	1397	C	C6-N1-C1'	-5.89	113.73	120.80
16	1U	74	LEU	CA-CB-CG	5.85	128.76	115.30
32	1a	266	G	P-O3'-C3'	5.85	126.72	119.70
32	1a	1067	A	P-O3'-C3'	5.85	126.72	119.70
1	2A	1076	C	OP1-P-O3'	5.82	118.01	105.20
1	1A	12	U	C2-N1-C1'	5.81	124.67	117.70
27	15	58	LEU	CA-CB-CG	5.80	128.65	115.30
1	1A	848	G	O5'-P-OP2	-5.80	100.48	105.70
1	1A	715	G	OP2-P-O3'	5.79	117.93	105.20
1	1A	1398	U	O5'-P-OP1	-5.76	100.51	105.70
27	15	25	LEU	C-N-CA	-5.68	107.50	121.70
1	1A	1220	U	P-O3'-C3'	5.67	126.51	119.70
32	2a	1065	U	P-O3'-C3'	5.67	126.50	119.70
1	1A	1255	A	P-O3'-C3'	5.65	126.48	119.70
1	1A	1121	C	C2-N1-C1'	5.63	124.99	118.80
1	1A	2045	G	O5'-P-OP1	-5.63	100.64	105.70
1	1A	1150	C	C5-C4-N4	5.63	124.14	120.20
1	1A	2043	C	C6-N1-C2	5.62	122.55	120.30
1	1A	2701	U	P-O3'-C3'	5.60	126.42	119.70
1	1A	1418	U	N3-C4-O4	5.60	123.32	119.40
1	2A	2108	C	C2-N3-C4	5.60	122.70	119.90
1	1A	215	G	O4'-C1'-N9	5.57	112.66	108.20
32	1a	839	U	P-O3'-C3'	5.57	126.38	119.70
1	1A	847	A	O5'-P-OP1	-5.53	100.73	105.70
1	2A	2430	A	O5'-P-OP2	-5.52	100.73	105.70
1	1A	1184	G	O5'-P-OP2	-5.52	100.73	105.70
1	1A	593	G	C4-C5-N7	5.49	113.00	110.80
1	2A	2689	U	N3-C2-O2	-5.49	118.36	122.20
1	2A	2185	C	C2-N3-C4	5.47	122.63	119.90
32	2a	1054	C	N1-C2-O2	5.47	122.18	118.90
1	2A	2287	A	O4'-C1'-N9	5.46	112.57	108.20
32	1a	115	G	P-O3'-C3'	5.45	126.24	119.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2602	A	P-O3'-C3'	5.44	126.22	119.70
1	2A	1313	U	N3-C2-O2	-5.43	118.40	122.20
1	1A	588	C	C6-N1-C2	-5.42	118.13	120.30
1	1A	1221	G	OP1-P-O3'	5.42	117.11	105.20
1	1A	1462	G	O4'-C1'-N9	5.41	112.53	108.20
1	2A	2161	C	C5-C4-N4	5.41	123.99	120.20
32	2a	754	C	C2-N1-C1'	5.41	124.75	118.80
32	2a	1097	C	C2-N1-C1'	5.41	124.75	118.80
1	2A	2218	U	N3-C2-O2	-5.39	118.43	122.20
32	2a	1097	C	N3-C2-O2	-5.39	118.13	121.90
32	2a	1125	U	N1-C2-O2	5.34	126.54	122.80
1	2A	2104	G	C4-N9-C1'	5.33	133.43	126.50
32	2a	1033	G	C5-C6-O6	5.33	131.80	128.60
1	1A	1101	G	C6-N1-C2	5.33	128.30	125.10
32	1a	1137	C	C5-C6-N1	5.32	123.66	121.00
32	1a	1028	C	C6-N1-C2	-5.31	118.17	120.30
1	2A	512	G	O4'-C1'-N9	5.31	112.45	108.20
32	2a	1003	G	N3-C4-N9	5.31	129.19	126.00
32	1a	955	U	C5-C4-O4	5.30	129.08	125.90
32	1a	922	G	C5-C6-O6	5.30	131.78	128.60
1	1A	2453	C	N3-C2-O2	-5.29	118.19	121.90
1	1A	1299	A	C5-N7-C8	5.29	106.55	103.90
32	1a	687	A	P-O3'-C3'	5.27	126.03	119.70
1	1A	892	G	O4'-C1'-N9	5.27	112.41	108.20
1	1A	1958	A	O4'-C1'-N9	5.27	112.41	108.20
1	2A	2218	U	N1-C2-O2	5.25	126.48	122.80
1	1A	1246	C	C6-N1-C2	5.25	122.40	120.30
32	2a	1058	G	C5-C6-O6	-5.25	125.45	128.60
32	2a	115	G	P-O3'-C3'	5.24	125.99	119.70
1	1A	2331	G	N3-C2-N2	-5.24	116.23	119.90
1	1A	1921	G	N3-C4-N9	5.22	129.13	126.00
32	2a	1067	A	P-O3'-C3'	5.22	125.97	119.70
1	1A	31	C	O5'-P-OP1	-5.22	101.00	105.70
32	2a	65	U	P-O3'-C3'	5.20	125.94	119.70
1	2A	1082	U	N1-C2-O2	5.20	126.44	122.80
1	2A	2473	U	C2-N1-C1'	5.18	123.91	117.70
1	2A	2689	U	P-O3'-C3'	5.18	125.91	119.70
32	2a	687	A	P-O3'-C3'	5.17	125.90	119.70
1	2A	195	A	P-O3'-C3'	5.16	125.89	119.70
1	2A	2103	C	C5-C4-N4	5.15	123.81	120.20
32	2a	1442	G	C4-N9-C1'	5.15	133.20	126.50
1	2A	1092	C	C2-N1-C1'	5.15	124.46	118.80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2108	C	N1-C2-O2	5.15	121.99	118.90
32	2a	1183	A	P-O3'-C3'	5.14	125.87	119.70
1	2A	801	G	O5'-P-OP2	-5.14	101.07	105.70
32	1a	839	U	OP1-P-O3'	5.13	116.49	105.20
32	2a	266	G	OP2-P-O3'	5.13	116.48	105.20
1	2A	570	G	C5-C6-N1	5.12	114.06	111.50
32	1a	1201	A	P-O3'-C3'	5.12	125.85	119.70
1	2A	784	A	O4'-C1'-N9	5.12	112.30	108.20
1	1A	2694	U	O5'-P-OP2	-5.12	101.10	105.70
32	2a	60	A	P-O3'-C3'	5.12	125.84	119.70
32	2a	955	U	C2-N3-C4	5.10	130.06	127.00
1	2A	1644	C	N1-C2-O2	5.09	121.96	118.90
1	1A	993	G	O5'-P-OP1	-5.09	101.12	105.70
1	2A	2154	G	C5-C6-O6	5.08	131.65	128.60
1	1A	2442	A	C2-N3-C4	5.08	113.14	110.60
32	1a	1123	A	C6-N1-C2	5.08	121.65	118.60
1	1A	894	U	C2-N1-C1'	5.08	123.79	117.70
1	2A	1313	U	N1-C2-O2	5.07	126.35	122.80
13	2R	113	LEU	CA-CB-CG	5.07	126.95	115.30
1	1A	1431	G	O4'-C1'-N9	5.07	112.25	108.20
1	1A	1011	G	N1-C6-O6	-5.06	116.87	119.90
32	1a	913	A	P-O3'-C3'	5.06	125.77	119.70
1	1A	1700	G	P-O3'-C3'	5.05	125.76	119.70
1	1A	1150	C	N3-C4-N4	-5.05	114.47	118.00
1	1A	831	A	O4'-C1'-N9	5.04	112.23	108.20
1	2A	1111	A	O4'-C1'-N9	5.03	112.23	108.20
32	2a	748	C	P-O3'-C3'	5.03	125.73	119.70
1	2A	887	A	O4'-C1'-N9	5.02	112.22	108.20
32	1a	1395	C	C2-N3-C4	5.02	122.41	119.90
32	2a	1126	U	N1-C2-O2	5.00	126.30	122.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
19	1X	93	GLU	Peptide
33	1b	127	ILE	Peptide
33	1b	231	GLU	Peptide
26	24	18	CYS	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	61869	0	31201	614	0
1	2A	61758	0	31149	755	0
2	1B	2572	0	1305	16	0
2	2B	2573	0	1306	34	0
3	1D	2131	0	2207	49	0
3	2D	2136	0	2218	34	0
4	1E	1559	0	1618	33	0
4	2E	1559	0	1618	39	0
5	1F	1584	0	1625	32	0
5	2F	1580	0	1619	42	0
6	1G	1426	0	1445	42	0
6	2G	1424	0	1441	50	0
7	1H	1330	0	1407	26	0
7	2H	1324	0	1402	39	0
8	1I	1094	0	1127	32	0
8	2I	1076	0	1094	29	0
9	1N	1121	0	1195	18	0
9	2N	1117	0	1184	14	0
10	1O	933	0	996	12	0
10	2O	933	0	996	18	0
11	1P	1135	0	1212	29	0
11	2P	1135	0	1212	21	0
12	1Q	1122	0	1179	24	0
12	2Q	1122	0	1179	27	0
13	1R	968	0	1033	12	0
13	2R	968	0	1033	18	0
14	1S	877	0	938	18	0
14	2S	870	0	923	37	0
15	1T	1091	0	1151	23	0
15	2T	1083	0	1136	25	0
16	1U	959	0	1019	16	0
16	2U	959	0	1019	22	0
17	1V	775	0	841	13	0
17	2V	771	0	830	21	0
18	1W	886	0	940	10	0
18	2W	886	0	940	13	0
19	1X	750	0	814	14	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	2X	750	0	814	9	0
20	1Y	810	0	892	21	0
20	2Y	810	0	887	20	0
21	1Z	1587	0	1598	23	0
21	2Z	1557	0	1564	36	0
22	10	608	0	622	10	0
22	20	608	0	622	12	0
23	11	754	0	823	14	0
23	21	759	0	837	20	0
24	12	588	0	643	10	0
24	22	592	0	654	8	0
25	13	469	0	518	11	0
25	23	464	0	514	16	0
26	14	546	0	522	15	0
26	24	536	0	514	29	0
27	15	459	0	476	11	0
27	25	455	0	465	9	0
28	16	453	0	473	11	0
28	26	449	0	469	10	0
29	17	418	0	467	10	0
29	27	418	0	467	3	0
30	18	517	0	582	16	0
30	28	517	0	582	12	0
31	19	307	0	335	9	0
31	29	307	0	335	10	0
32	1a	32246	0	16296	0	0
32	2a	32331	0	16339	0	0
33	1b	1842	0	1862	0	0
33	2b	1825	0	1828	0	0
34	1c	1558	0	1557	0	0
34	2c	1542	0	1517	0	0
35	1d	1665	0	1687	0	0
35	2d	1668	0	1703	0	0
36	1e	1133	0	1191	0	0
36	2e	1133	0	1191	0	0
37	1f	814	0	808	0	0
37	2f	816	0	808	0	0
38	1g	1235	0	1249	0	0
38	2g	1229	0	1238	0	0
39	1h	1098	0	1143	0	0
39	2h	1088	0	1126	0	0
40	1i	986	0	990	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	2i	966	0	953	0	0
41	1j	719	0	672	0	0
41	2j	710	0	661	0	0
42	1k	834	0	838	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	914	0	954	0	0
44	2m	895	0	920	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	648	0	658	0	0
50	2s	645	0	635	0	0
51	1t	732	0	809	0	0
51	2t	733	0	795	0	0
52	1u	199	0	208	0	0
52	2u	199	0	208	0	0
53	1y	764	0	786	0	0
53	2y	749	0	757	0	0
54	10	6	0	0	0	0
54	11	3	0	0	0	0
54	13	2	0	0	0	0
54	14	1	0	0	0	0
54	15	3	0	0	0	0
54	17	2	0	0	0	0
54	18	1	0	0	0	0
54	19	2	0	0	0	0
54	1A	1024	0	0	0	0
54	1B	29	0	0	0	0
54	1D	13	0	0	0	0
54	1E	7	0	0	0	0
54	1F	13	0	0	0	0
54	1G	4	0	0	0	0
54	1H	2	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	1N	3	0	0	0	0
54	1O	2	0	0	0	0
54	1P	3	0	0	0	0
54	1Q	4	0	0	0	0
54	1R	3	0	0	0	0
54	1S	1	0	0	0	0
54	1T	3	0	0	0	0
54	1U	2	0	0	0	0
54	1V	3	0	0	0	0
54	1W	2	0	0	0	0
54	1X	2	0	0	0	0
54	1Z	1	0	0	0	0
54	1a	255	0	0	0	0
54	1b	1	0	0	0	0
54	1d	6	0	0	0	0
54	1e	2	0	0	0	0
54	1f	2	0	0	0	0
54	1g	3	0	0	0	0
54	1h	2	0	0	0	0
54	1i	1	0	0	0	0
54	1l	2	0	0	0	0
54	1n	1	0	0	0	0
54	1o	1	0	0	0	0
54	1t	1	0	0	0	0
54	1y	4	0	0	0	0
54	20	1	0	0	0	0
54	21	1	0	0	0	0
54	25	1	0	0	0	0
54	28	3	0	0	0	0
54	2A	721	0	0	0	0
54	2B	19	0	0	0	0
54	2D	8	0	0	0	0
54	2E	6	0	0	0	0
54	2F	3	0	0	0	0
54	2G	3	0	0	0	0
54	2I	1	0	0	0	0
54	2N	1	0	0	0	0
54	2O	1	0	0	0	0
54	2P	2	0	0	0	0
54	2Q	2	0	0	0	0
54	2R	1	0	0	0	0
54	2T	4	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	2V	1	0	0	0	0
54	2W	2	0	0	0	0
54	2X	1	0	0	0	0
54	2a	151	0	0	0	0
54	2e	1	0	0	0	0
54	2f	1	0	0	0	0
54	2j	1	0	0	0	0
54	2p	1	0	0	0	0
54	2q	1	0	0	0	0
54	2r	1	0	0	0	0
54	2t	1	0	0	0	0
55	1A	1	0	0	0	0
55	2A	1	0	0	0	0
56	1A	25	0	0	0	0
56	2A	25	0	0	0	0
57	18	8	0	14	1	0
57	1A	8	0	14	0	0
57	1T	8	0	14	1	0
57	1a	8	0	14	0	0
57	2A	16	0	28	2	0
57	2B	8	0	14	0	0
58	1B	12	0	12	3	0
58	1F	12	0	12	3	0
59	14	1	0	0	0	0
59	15	1	0	0	0	0
59	16	1	0	0	0	0
59	19	1	0	0	0	0
59	1Y	1	0	0	0	0
59	1n	1	0	0	0	0
59	24	1	0	0	0	0
59	25	1	0	0	0	0
59	26	1	0	0	0	0
59	29	1	0	0	0	0
59	2Y	1	0	0	0	0
59	2n	1	0	0	0	0
60	1d	8	0	0	0	0
60	2d	8	0	0	0	0
61	10	22	0	0	0	0
61	11	28	0	0	0	0
61	12	14	0	0	2	0
61	13	22	0	0	2	0
61	14	2	0	0	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	15	26	0	0	0	0
61	16	17	0	0	1	0
61	17	14	0	0	2	0
61	18	30	0	0	0	0
61	19	8	0	0	1	0
61	1A	2980	0	0	97	0
61	1B	105	0	0	3	0
61	1D	116	0	0	6	0
61	1E	76	0	0	4	0
61	1F	63	0	0	5	0
61	1G	22	0	0	0	0
61	1H	16	0	0	0	0
61	1I	7	0	0	1	0
61	1N	50	0	0	0	0
61	1O	22	0	0	0	0
61	1P	58	0	0	4	0
61	1Q	42	0	0	3	0
61	1R	37	0	0	0	0
61	1S	13	0	0	1	0
61	1T	42	0	0	3	0
61	1U	45	0	0	4	0
61	1V	37	0	0	1	0
61	1W	24	0	0	0	0
61	1X	24	0	0	1	0
61	1Y	15	0	0	1	0
61	1Z	14	0	0	0	0
61	1a	261	0	0	0	0
61	1b	1	0	0	0	0
61	1d	9	0	0	0	0
61	1e	6	0	0	0	0
61	1f	3	0	0	0	0
61	1h	1	0	0	0	0
61	1i	1	0	0	0	0
61	1j	1	0	0	0	0
61	1k	1	0	0	0	0
61	1l	4	0	0	0	0
61	1n	1	0	0	0	0
61	1o	5	0	0	0	0
61	1p	3	0	0	0	0
61	1y	5	0	0	0	0
61	20	13	0	0	2	0
61	21	24	0	0	5	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	22	5	0	0	0	0
61	23	3	0	0	1	0
61	24	2	0	0	0	0
61	25	9	0	0	1	0
61	26	6	0	0	1	0
61	27	7	0	0	0	0
61	28	15	0	0	1	0
61	29	2	0	0	0	0
61	2A	1686	0	0	84	0
61	2B	65	0	0	6	0
61	2D	52	0	0	2	0
61	2E	25	0	0	2	0
61	2F	21	0	0	3	0
61	2G	7	0	0	0	0
61	2H	4	0	0	0	0
61	2I	4	0	0	0	0
61	2N	6	0	0	0	0
61	2O	22	0	0	0	0
61	2P	23	0	0	0	0
61	2Q	30	0	0	0	0
61	2R	21	0	0	1	0
61	2S	8	0	0	2	0
61	2T	10	0	0	0	0
61	2U	14	0	0	2	0
61	2V	9	0	0	0	0
61	2W	21	0	0	0	0
61	2X	9	0	0	0	0
61	2Y	3	0	0	0	0
61	2Z	15	0	0	3	0
61	2a	100	0	0	0	0
61	2d	6	0	0	0	0
61	2e	1	0	0	0	0
61	2f	1	0	0	0	0
61	2j	2	0	0	0	0
61	2l	1	0	0	0	0
61	2m	1	0	0	0	0
61	2o	2	0	0	0	0
61	2p	1	0	0	0	0
61	2q	1	0	0	0	0
61	2r	4	0	0	0	0
61	2y	1	0	0	0	0
All	All	295438	0	194513	2320	0

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

All (2320) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1128:U:H3	1:1A:1132:A:N6	1.36	1.23
1:1A:2159:C:N4	1:1A:2176:G:H1	1.50	1.09
1:2A:2139:C:N4	1:2A:2152:G:H1	1.56	1.01
1:1A:2331:G:H22	14:1S:3:ARG:HD3	1.23	1.01
1:1A:1128:U:O4	1:1A:1132:A:N1	1.99	0.94
1:2A:2107:C:H42	1:2A:2182:G:H1	0.99	0.92
1:2A:1041:C:H42	1:2A:1114:G:H1	1.18	0.91
29:17:24:THR:HG22	29:17:27:GLY:H	1.32	0.91
1:2A:2319:G:H22	14:2S:3:ARG:HD3	1.34	0.90
10:1O:35:VAL:HG11	10:1O:103:ALA:HB3	1.54	0.89
1:2A:2107:C:N4	1:2A:2182:G:H1	1.69	0.89
1:1A:1829:U:H5'	3:1D:259:THR:HG22	1.55	0.88
1:2A:1842:G:O2'	3:2D:253:GLN:NE2	2.08	0.87
1:2A:1011:G:H1	1:2A:1018:C:H42	18.79	0.86
1:1A:2159:C:H42	1:1A:2176:G:H1	0.87	0.86
20:1Y:92:ASN:HB2	20:1Y:94:LYS:H	1.39	0.85
1:2A:1422:G:H5''	10:2O:48:PRO:HB3	99.81	0.85
1:1A:2159:C:N3	1:1A:2176:G:N2	2.23	0.85
1:1A:1128:U:H3	1:1A:1132:A:H61	0.85	0.85
1:1A:2125:C:H42	1:1A:2208:G:H1	1.21	0.84
6:1G:161:THR:HG22	6:1G:163:ALA:H	1.39	0.84
1:2A:2099:U:H3	1:2A:2190:G:H1	1.15	0.84
1:1A:542:C:OP1	27:15:16:ARG:NH2	2.10	0.83
1:1A:2138:G:H1	1:1A:2187:G:H22	1.26	0.82
4:1E:47:VAL:HG21	4:1E:86:PRO:HD2	1.62	0.82
11:1P:100:LEU:HD12	11:1P:112:LEU:HD11	1.61	0.81
1:2A:1011:G:H1	1:2A:1018:C:N4	18.91	0.81
1:2A:1084:A:H3'	1:2A:1085:A:H4'	1.63	0.81
1:2A:2136:C:N4	1:2A:2155:G:H1	1.77	0.81
1:2A:2365:G:N7	30:28:39:LYS:NZ	2.30	0.80
4:2E:47:VAL:HG11	4:2E:86:PRO:HD2	1.63	0.79
1:2A:2602:A:H1'	1:2A:2603:G:H5''	1.62	0.79
1:1A:242:C:OP1	61:1A:4117:HOH:O	1.99	0.79
2:1B:81:G:N7	58:1B:228:ARG:NH2	2.30	0.79
1:2A:2136:C:C2	1:2A:2155:G:N2	2.51	0.79
1:2A:788:A:N6	61:2A:3845:HOH:O	2.16	0.79
3:1D:17:THR:O	3:1D:211:ARG:NH2	2.16	0.79

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:11:G:H2'	1:1A:12:U:H5''	1.65	0.79
1:2A:2748:A:H5'	7:2H:4:ILE:HD12	1.65	0.78
25:13:8:LEU:HD13	25:13:31:LEU:HD23	1.66	0.77
1:1A:1131:A:O2'	1:1A:1150:C:O2'	2.02	0.77
1:2A:2139:C:H42	1:2A:2152:G:H1	0.81	0.77
11:2P:59:LEU:HD11	30:28:10:ALA:HB2	1.66	0.77
1:2A:2805:G:H2'	1:2A:2807:G:C8	2.20	0.77
1:1A:427:G:N7	61:1A:4153:HOH:O	2.16	0.77
1:1A:2125:C:N4	1:1A:2208:G:H1	1.82	0.77
2:1B:23:G:O6	61:1B:3101:HOH:O	2.02	0.77
11:1P:59:LEU:HD11	30:18:10:ALA:HB2	1.63	0.77
29:17:34:ARG:HE	29:17:39:ARG:HG3	1.50	0.77
1:1A:1128:U:N3	1:1A:1132:A:N6	2.20	0.76
7:2H:164:TYR:HB2	7:2H:167:GLU:HB2	1.68	0.76
1:1A:1378:G:OP1	61:1A:4118:HOH:O	2.03	0.75
3:1D:242:ARG:HG3	3:1D:242:ARG:HH11	1.50	0.75
22:20:10:THR:HG22	22:20:12:ASN:H	1.50	0.75
1:2A:2379:G:OP1	14:2S:23:ARG:NH2	2.14	0.75
1:1A:787:U:OP2	61:1A:4119:HOH:O	2.05	0.74
1:2A:1057:A:N6	1:2A:1087:G:OP1	2.20	0.74
1:1A:1045:U:OP2	61:1A:4120:HOH:O	2.05	0.74
1:2A:994:C:OP1	16:2U:53:ARG:NH2	2.19	0.74
16:2U:89:GLU:HG2	17:2V:50:PRO:HB3	1.69	0.74
1:1A:2138:G:OP2	1:1A:2188:G:N2	2.20	0.74
3:1D:88:ARG:NH1	61:1D:402:HOH:O	2.20	0.74
1:2A:11:G:H2'	1:2A:12:U:H5'	1.68	0.74
4:1E:28:ALA:HB3	4:1E:93:VAL:HG12	1.69	0.74
5:1F:197:ASP:OD1	5:1F:197:ASP:N	2.19	0.74
24:22:32:LEU:HD11	24:22:54:LYS:HG3	1.69	0.74
1:2A:1360:A:OP2	9:2N:35:ARG:NH2	118.25	0.74
1:2A:751:A:H5'	18:2W:90:ARG:HA	1.70	0.74
1:2A:323:G:HO2'	1:2A:1205:U:H3	1.34	0.74
3:2D:206:LEU:HD22	3:2D:211:ARG:HG2	1.68	0.74
61:2A:3804:HOH:O	13:2R:3:HIS:NE2	2.21	0.74
1:2A:958:U:OP2	12:2Q:14:ARG:NH1	2.21	0.73
1:2A:2128:C:H42	1:2A:2160:G:H1	1.36	0.73
1:2A:2141:G:O6	1:2A:2150:U:O2	2.06	0.73
1:2A:2206:G:H3'	1:2A:2207:G:H8	1.54	0.73
1:2A:2116:G:OP1	1:2A:2117:A:N6	2.22	0.73
2:2B:49:C:OP1	61:2B:3101:HOH:O	2.05	0.73
28:16:6:ARG:NE	28:16:24:GLU:OE1	2.19	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2139:C:N3	1:2A:2152:G:N2	2.32	0.73
1:2A:143:G:H4'	19:2X:35:THR:HG21	1.71	0.73
1:2A:1798:U:H5'	3:2D:259:THR:HG22	1.70	0.72
25:13:6:VAL:HG12	25:13:54:VAL:HG11	1.71	0.72
1:2A:1782:C:OP1	61:2A:3815:HOH:O	2.07	0.72
3:2D:134:ARG:NH1	3:2D:188:GLU:OE2	2.21	0.72
1:1A:597:C:N3	4:1E:145:LYS:NZ	2.37	0.72
1:1A:2702:C:OP1	13:1R:17:ARG:NH2	2.23	0.72
1:1A:1093:G:H2'	1:1A:1156:G:H22	1.52	0.72
1:1A:493:G:OP2	29:17:34:ARG:HD3	1.88	0.72
1:1A:1436:U:O2	1:1A:1441:A:N6	2.19	0.72
21:2Z:19:ARG:NH1	21:2Z:84:GLU:O	2.22	0.72
1:1A:1815:A:OP2	61:1A:4119:HOH:O	2.07	0.72
1:1A:395:C:OP2	61:1A:4121:HOH:O	2.07	0.71
1:1A:397:G:OP2	61:1A:4123:HOH:O	2.08	0.71
5:1F:53:THR:HG22	5:1F:55:GLY:H	1.56	0.71
1:1A:715:G:N7	61:1A:4191:HOH:O	2.24	0.71
1:1A:656:A:OP1	11:1P:65:ARG:NH1	2.22	0.71
1:1A:2658:C:OP2	1:1A:2745:G:O2'	2.08	0.71
1:1A:2831:A:OP2	61:1A:4115:HOH:O	2.06	0.71
1:2A:1286:A:C8	1:2A:1287:A:H4'	8.27	0.71
1:2A:2248:C:OP2	61:2A:3817:HOH:O	2.08	0.71
9:1N:21:LYS:NZ	9:1N:140:VAL:OXT	2.24	0.71
8:1I:92:VAL:HG13	8:1I:120:ILE:HB	1.71	0.71
1:2A:1257:C:OP2	61:2A:3816:HOH:O	2.08	0.71
1:2A:2122:U:H3	1:2A:2176:A:H61	1.39	0.71
1:2A:2425:A:N7	61:2A:3882:HOH:O	2.23	0.71
1:1A:1034:A:OP1	61:1A:4122:HOH:O	2.07	0.70
1:1A:1343:C:OP1	61:1A:4124:HOH:O	2.08	0.70
19:1X:35:THR:HG22	19:1X:38:GLU:H	1.56	0.70
1:1A:449:A:OP2	61:1A:4123:HOH:O	2.08	0.70
13:2R:97:VAL:HG22	13:2R:114:VAL:HG22	1.72	0.70
21:2Z:144:LEU:HD21	21:2Z:150:LEU:HD13	1.72	0.70
4:2E:48:GLN:HE21	4:2E:78:LEU:HG	1.57	0.70
1:2A:277:C:O2'	1:2A:278:A:OP1	2.10	0.70
1:2A:2036:C:O2'	61:2A:3818:HOH:O	2.10	0.70
1:2A:2206:G:H3'	1:2A:2207:G:C8	2.26	0.70
1:2A:955:C:OP1	12:2Q:87:LYS:NZ	2.22	0.70
1:1A:2042:A:OP2	61:1A:4126:HOH:O	2.09	0.70
1:2A:2126:A:H4'	1:2A:2127:G:O5'	1.91	0.70
1:2A:1566:A:OP1	3:2D:211:ARG:NH1	2.25	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1H:21:PRO:O	7:1H:23:ARG:NH1	2.25	0.69
1:1A:2708:U:O3'	61:1A:4129:HOH:O	2.11	0.69
1:1A:2073:A:OP2	61:1A:4128:HOH:O	2.10	0.69
1:2A:2296:U:OP2	14:2S:9:ARG:NH2	2.25	0.69
3:2D:71:ASP:OD2	3:2D:103:ARG:NH2	2.23	0.69
1:2A:956:G:H5''	12:2Q:77:LYS:HD2	1.75	0.69
1:1A:788:G:OP2	61:1A:4127:HOH:O	2.10	0.69
1:2A:154(A):C:H42	1:2A:171:G:H1	1.39	0.69
1:2A:2156:G:N7	1:2A:2157:G:N2	2.41	0.69
1:2A:2483:C:N3	12:2Q:124:LYS:NZ	2.40	0.69
10:2O:35:VAL:HG11	10:2O:103:ALA:HB3	1.73	0.69
6:2G:97:ASP:HA	6:2G:100:TRP:HD1	1.56	0.69
23:11:52:ARG:NH2	23:11:55:GLY:O	2.25	0.69
1:1A:359:C:H4'	20:1Y:73:ARG:HD3	1.74	0.69
23:21:75:GLU:HA	23:21:78:LYS:HE2	1.73	0.69
1:1A:168:G:N7	61:1A:4208:HOH:O	2.27	0.68
5:2F:21:ALA:HB3	5:2F:22:ALA:HA	1.74	0.68
21:2Z:31:ARG:NH1	61:2Z:302:HOH:O	2.26	0.68
1:2A:1087:G:H1	1:2A:1102:C:H42	1.41	0.68
1:2A:1793:C:OP1	61:2A:3820:HOH:O	2.11	0.68
4:2E:11:MET:HG2	4:2E:24:THR:HG22	1.75	0.68
1:2A:2815:C:H5'	27:25:29:THR:HG21	1.75	0.68
1:1A:136:G:OP2	61:1A:4131:HOH:O	2.12	0.68
1:1A:1694:G:OP1	61:1A:4130:HOH:O	2.11	0.68
1:1A:2776:G:OP2	61:1A:4132:HOH:O	2.12	0.68
1:2A:1664:A:OP1	61:2A:3819:HOH:O	2.11	0.68
1:2A:2602:A:H1'	1:2A:2603:G:C5'	2.23	0.68
1:2A:2499:C:OP2	61:2A:3823:HOH:O	2.12	0.68
26:24:18:CYS:SG	26:24:39:CYS:HB3	2.34	0.68
8:2I:4:ILE:HG12	8:2I:18:VAL:HG22	1.75	0.68
1:1A:1679:A:N7	61:1A:4214:HOH:O	2.27	0.67
1:2A:2107:C:N3	1:2A:2182:G:N2	2.35	0.67
2:1B:82:G:OP2	61:1B:3102:HOH:O	2.12	0.67
1:2A:111:A:N3	61:2A:3903:HOH:O	2.26	0.67
1:2A:2431:U:OP1	61:2A:3821:HOH:O	2.11	0.67
1:1A:1435:G:H2'	1:1A:1436:U:C6	3.06	0.67
1:1A:1747:A:OP2	61:1A:4136:HOH:O	2.12	0.67
15:1T:39:ARG:HH12	15:1T:41:ARG:HD3	1.57	0.67
7:2H:113:VAL:HG11	7:2H:151:ILE:HD13	1.74	0.67
23:11:21:ARG:HD3	23:11:35:THR:HG21	1.74	0.67
25:23:13:ILE:O	61:23:201:HOH:O	2.12	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2G:3:LEU:O	6:2G:8:LYS:NZ	2.27	0.67
1:2A:1264:G:OP1	27:25:19:ARG:NH2	2.17	0.67
8:2I:55:ALA:HA	8:2I:58:LEU:HB3	1.77	0.67
1:1A:1039:G:OP1	16:1U:50:ARG:NH2	2.27	0.67
1:1A:1748:A:OP2	61:1A:4135:HOH:O	2.12	0.67
1:1A:2459:G:OP2	61:1A:4133:HOH:O	2.12	0.67
20:1Y:102:CYS:SG	20:1Y:103:GLY:N	2.67	0.67
1:2A:2285:C:OP2	28:26:6:ARG:NH1	2.27	0.67
1:2A:84:A:N1	1:2A:98:G:O2'	2.27	0.67
1:1A:2460:A:OP1	61:1A:4137:HOH:O	2.13	0.67
4:2E:28:ALA:HB3	4:2E:93:VAL:HG12	1.77	0.67
7:1H:97:ARG:NE	7:1H:104:GLU:OE1	2.28	0.67
1:2A:1281:G:N7	61:2A:3920:HOH:O	2.28	0.67
1:2A:2267:A:OP2	61:2A:3825:HOH:O	2.12	0.66
1:2A:2504:U:OP2	61:2A:3824:HOH:O	2.12	0.66
1:2A:526:A:OP1	61:2A:3826:HOH:O	2.13	0.66
1:1A:455:A:OP1	61:1A:4134:HOH:O	2.12	0.66
1:2A:1002:G:H2'	1:2A:1003:G:C8	3.40	0.66
1:2A:530:G:O6	61:2A:3822:HOH:O	2.12	0.66
23:11:50:ARG:HG2	23:11:59:THR:HG22	1.76	0.66
1:1A:1361:C:OP2	61:1A:4118:HOH:O	2.14	0.66
6:1G:139:LEU:HD21	6:1G:149:VAL:HG11	1.77	0.66
1:2A:1064:C:H3'	1:2A:1065:U:H5'	1.76	0.66
7:2H:3:ARG:HE	7:2H:54:ARG:HH12	1.43	0.66
19:2X:53:LYS:HB3	19:2X:82:GLN:HB3	1.78	0.66
1:1A:1871:G:N7	61:1A:4222:HOH:O	2.28	0.66
1:2A:1119:C:H2'	1:2A:1120:G:H8	2.72	0.66
1:2A:1771:C:OP1	61:2A:3829:HOH:O	2.13	0.66
1:2A:365:C:OP2	61:2A:3827:HOH:O	2.13	0.66
4:2E:199:ARG:NH1	61:2E:401:HOH:O	2.20	0.66
1:1A:1847:G:O6	3:1D:35:LYS:NZ	2.24	0.66
1:1A:272:U:OP1	8:1I:50:ARG:NH1	2.29	0.66
2:1B:6:C:H2'	2:1B:7:G:H5''	1.77	0.66
1:2A:1064:C:H3'	1:2A:1065:U:C5'	2.25	0.66
1:2A:881:G:H1	1:2A:895:U:H3	1.41	0.66
1:2A:2759:G:N2	7:2H:139:GLN:OE1	2.28	0.66
22:10:11:ARG:O	22:10:14:ARG:NH2	2.26	0.66
1:2A:999:U:OP2	61:2A:3828:HOH:O	2.13	0.66
23:11:51:VAL:HG11	23:11:74:VAL:HG21	1.76	0.66
27:25:16:ARG:NH1	27:25:17:ASP:OD1	2.29	0.66
1:2A:1110:G:H1'	1:2A:1111:A:C8	2.31	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1780:A:OP1	61:2A:3815:HOH:O	2.14	0.66
1:2A:2237:G:OP1	61:2A:3832:HOH:O	2.14	0.66
1:1A:1517:G:N3	1:1A:1941:A:O2'	112.90	0.65
1:1A:2320:G:O2'	1:1A:2322:A:N7	2.24	0.65
1:2A:1322:A:OP1	61:2A:3834:HOH:O	2.14	0.65
1:1A:273:G:H21	8:1I:50:ARG:HD3	1.61	0.65
11:1P:42:SER:O	61:1P:301:HOH:O	2.14	0.65
1:2A:131:G:OP1	61:2A:3831:HOH:O	2.14	0.65
6:2G:72:ARG:HG2	6:2G:87:PRO:HA	1.79	0.65
1:1A:1428:G:N7	61:1A:4232:HOH:O	2.29	0.65
1:1A:1529:G:H1	1:1A:1552:C:H42	1.43	0.65
3:1D:69:ARG:NH2	3:1D:128:GLY:O	2.29	0.65
5:1F:185:ASP:HA	5:1F:188:ARG:HD3	1.77	0.65
17:1V:74:LYS:HB2	17:1V:83:ARG:HB2	1.77	0.65
1:2A:1371:G:N7	61:2A:3919:HOH:O	2.28	0.65
17:1V:40:LEU:HB2	17:1V:46:VAL:HG13	1.79	0.65
1:2A:1445:A:OP1	61:2A:3833:HOH:O	2.14	0.65
1:2A:2111:C:H42	1:2A:2147:G:H22	1.44	0.65
1:2A:990:A:OP2	61:2A:3836:HOH:O	2.14	0.65
1:2A:994:C:OP2	16:2U:54:LYS:NZ	2.26	0.65
1:1A:1059:C:OP2	61:1A:4139:HOH:O	2.14	0.65
1:1A:2060:G:O6	61:1A:4125:HOH:O	2.08	0.65
14:1S:93:LYS:O	61:1S:8101:HOH:O	2.13	0.65
23:21:37:ILE:O	61:21:8101:HOH:O	2.15	0.65
1:2A:2429:G:OP1	61:2A:3809:HOH:O	2.13	0.65
6:2G:47:LYS:HG3	6:2G:48:GLU:H	1.61	0.65
31:29:2:LYS:NZ	31:29:31:LYS:O	2.30	0.65
1:1A:1199:C:OP2	61:1A:4120:HOH:O	2.15	0.65
3:1D:108:PRO:HD2	3:1D:111:LEU:HG	1.79	0.65
21:2Z:52:SER:O	61:2Z:301:HOH:O	2.13	0.65
1:1A:1717:C:OP2	61:1A:4107:HOH:O	2.15	0.65
1:1A:555:G:N1	1:1A:2045:G:OP1	2.27	0.65
4:1E:29:GLY:HA3	61:1E:3105:HOH:O	1.96	0.65
21:1Z:144:LEU:HD21	21:1Z:150:LEU:HD13	1.79	0.65
23:21:20:ARG:NH1	61:21:8103:HOH:O	2.29	0.65
1:2A:395:U:O2'	61:2A:3835:HOH:O	2.14	0.65
6:2G:113:ARG:NH1	6:2G:139:LEU:O	2.30	0.65
2:2B:115:G:N7	61:2B:3109:HOH:O	2.29	0.64
3:2D:235:GLY:O	61:2D:401:HOH:O	2.14	0.64
5:1F:12:LEU:HD13	5:1F:124:LEU:HD11	1.79	0.64
1:2A:2379:G:O2'	14:2S:17:ARG:NH1	2.31	0.64

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1070:G:OP2	61:1A:4113:HOH:O	2.14	0.64
1:1A:2324:U:H5'	6:1G:88:ILE:HD11	1.78	0.64
58:1F:314:ARG:N	61:1F:403:HOH:O	2.31	0.64
2:2B:14:U:OP2	2:2B:70:C:O2'	2.11	0.64
1:2A:1189:A:OP2	61:2A:3840:HOH:O	2.15	0.64
1:1A:206:G:OP2	61:1A:4142:HOH:O	2.15	0.64
1:1A:2163:G:O6	1:1A:2172:U:O2	2.15	0.64
1:2A:2589:A:OP1	61:2A:3837:HOH:O	2.15	0.64
1:1A:1556:A:H2'	1:1A:1557:A:O4'	1.98	0.64
28:26:14:THR:OG1	28:26:48:VAL:O	2.16	0.64
1:2A:2805:G:H2'	1:2A:2807:G:H8	1.63	0.64
6:2G:57:ALA:HB2	6:2G:90:LEU:HD13	1.80	0.64
1:1A:407:U:OP1	61:1A:4143:HOH:O	2.15	0.64
5:1F:122:LYS:HB3	5:1F:191:ARG:HG3	1.79	0.64
1:1A:1705:C:OP1	61:1A:4141:HOH:O	2.15	0.64
8:1I:130:TYR:HB3	8:1I:138:ILE:HB	1.79	0.64
1:2A:326:G:N7	61:2A:3933:HOH:O	2.30	0.64
1:2A:2376:A:N3	14:2S:106:ARG:NH2	2.46	0.64
1:1A:1068:G:OP2	1:1A:1068:G:H8	6.91	0.63
1:2A:127:A:H5''	1:2A:128:C:C6	2.33	0.63
7:2H:98:LEU:HD22	7:2H:125:VAL:HG23	1.80	0.63
12:2Q:11:LYS:NZ	12:2Q:88:GLY:O	2.22	0.63
1:2A:2328:A:H2'	1:2A:2329:G:C8	2.33	0.63
5:1F:116:ASP:OD1	5:1F:119:ARG:NH2	2.32	0.63
5:1F:93:LYS:O	61:1F:401:HOH:O	2.15	0.63
1:2A:944:G:N1	1:2A:1338:G:OP2	84.93	0.63
1:2A:688:U:OP1	61:2A:3839:HOH:O	2.15	0.63
7:2H:143:GLN:NE2	7:2H:147:ASN:OD1	2.29	0.63
1:1A:1220:U:O2'	1:1A:1221:G:O5'	2.15	0.63
1:2A:1796:U:H2'	1:2A:1797:C:C6	2.34	0.63
1:2A:2070:G:OP2	61:2A:3838:HOH:O	2.15	0.63
1:1A:1016:C:OP2	61:1A:4149:HOH:O	2.16	0.63
23:21:50:ARG:HG2	23:21:59:THR:HG22	1.79	0.63
1:2A:2364:C:OP1	22:20:55:ARG:NH1	2.32	0.63
15:2T:30:VAL:HG22	15:2T:86:ILE:HG12	1.78	0.63
5:2F:122:LYS:NZ	5:2F:152:GLU:OE2	2.28	0.63
1:1A:354:A:H2	1:1A:1255:A:HO2'	1.47	0.63
1:1A:776:G:C6	3:1D:208:LYS:HB2	2.34	0.63
1:2A:857:C:OP2	22:20:77:ARG:NH2	2.32	0.63
1:1A:1028:C:N3	1:1A:1033:G:O6	12.93	0.62
4:1E:36:ARG:NH1	4:1E:85:ASN:OD1	2.32	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:630:G:N2	1:2A:633:A:OP2	2.27	0.62
1:2A:796:C:H2'	1:2A:797:C:C6	2.34	0.62
8:2I:126:TYR:O	8:2I:142:VAL:N	2.31	0.62
3:1D:148:GLU:HB2	3:1D:151:LYS:HD2	1.80	0.62
12:1Q:111:GLU:OE2	12:1Q:133:ARG:NH2	2.32	0.62
5:2F:129:PHE:CD2	5:2F:163:VAL:HG21	2.34	0.62
26:24:24:THR:OG1	26:24:25:TYR:N	2.31	0.62
1:2A:2753:A:N3	31:29:15:LYS:NZ	2.47	0.62
1:1A:1115:A:O2'	1:1A:1119:A:N6	2.30	0.62
1:1A:272:U:H4'	8:1I:50:ARG:HH22	1.64	0.62
26:14:61:ARG:HG3	26:14:62:ARG:H	1.64	0.62
1:1A:1057:G:OP1	16:1U:77:SER:OG	2.16	0.62
1:1A:2331:G:H22	14:1S:3:ARG:CD	2.06	0.62
14:2S:50:SER:O	14:2S:76:LYS:NZ	2.29	0.62
1:1A:1202:A:OP1	16:1U:55:ARG:NH1	2.32	0.62
1:1A:546:G:O6	61:1A:4140:HOH:O	2.15	0.62
1:1A:2331:G:N2	14:1S:3:ARG:HD3	2.06	0.62
1:1A:1273:G:OP2	16:1U:16:LYS:NZ	2.32	0.62
19:1X:54:VAL:HG22	19:1X:81:VAL:HG12	1.80	0.62
1:2A:631:A:OP1	11:2P:65:ARG:NH1	2.33	0.62
12:2Q:43:THR:N	12:2Q:46:GLN:OE1	2.28	0.62
1:1A:130:G:O6	61:1A:4144:HOH:O	2.15	0.62
8:1I:109:ILE:HG13	8:1I:130:TYR:CZ	2.34	0.62
16:1U:33:ARG:NH2	61:1U:303:HOH:O	2.31	0.62
2:2B:13:A:N1	2:2B:69:G:O2'	2.32	0.62
12:1Q:7:MET:HE1	21:1Z:194:PRO:HB2	1.82	0.62
1:2A:2312:U:H5'	6:2G:88:ILE:HD11	1.80	0.62
11:2P:126:VAL:HG12	11:2P:148:LEU:HD23	1.82	0.62
1:2A:1104:C:H2'	1:2A:1105:U:H6	1.65	0.62
7:1H:101:ARG:HG2	7:1H:117:PRO:HG2	1.81	0.62
1:2A:568:U:O2'	61:2A:3830:HOH:O	2.13	0.62
1:1A:1410:G:N7	23:11:3:LYS:HE2	2.15	0.61
1:1A:2849:G:H5'	13:1R:46:GLY:HA2	1.81	0.61
1:2A:726:G:O6	61:2A:3841:HOH:O	2.16	0.61
1:1A:2412:G:OP2	61:1A:4150:HOH:O	2.16	0.61
1:1A:2859:U:OP2	15:1T:95:ARG:NH1	2.32	0.61
1:1A:640:A:OP2	61:1A:4152:HOH:O	2.16	0.61
1:1A:655:G:OP2	30:18:15:LYS:NZ	2.28	0.61
1:1A:976:G:H5'	1:1A:1358:U:O2'	103.51	0.61
26:24:59:PHE:HA	26:24:60:GLN:C	2.19	0.61
22:10:27:GLU:HG3	22:10:68:GLU:HA	1.83	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2010:C:OP2	61:1A:4148:HOH:O	2.16	0.61
1:2A:1286:A:H8	1:2A:1287:A:H4'	8.18	0.61
1:2A:2134:A:O2'	1:2A:2159:G:N3	2.33	0.61
1:2A:302:C:H42	1:2A:315:G:H1	1.48	0.61
1:2A:2136:C:N3	1:2A:2155:G:N2	2.48	0.61
1:2A:2318:G:N2	14:2S:3:ARG:HE	1.98	0.61
6:2G:106:LEU:HA	6:2G:110:ALA:HB3	1.82	0.61
7:2H:24:VAL:HG13	7:2H:37:VAL:HG21	1.83	0.61
1:1A:2124:U:O2	1:1A:2209:G:O6	2.19	0.61
24:22:19:VAL:HG12	24:22:23:LYS:HE3	1.81	0.61
18:2W:2:GLU:OE2	18:2W:72:LYS:NZ	2.31	0.61
5:1F:195:ASP:HB2	5:1F:198:ALA:H	1.66	0.61
12:1Q:119:ARG:NH1	61:1Q:303:HOH:O	2.31	0.61
3:2D:133:LEU:HB3	3:2D:173:VAL:HG11	1.82	0.61
1:1A:1532:A:H2'	1:1A:1533:G:H8	1.65	0.61
1:1A:310:C:H2'	1:1A:311:C:C6	2.36	0.61
1:1A:676:G:OP1	30:18:19:SER:OG	2.17	0.61
21:2Z:23:LYS:HD3	21:2Z:40:ASP:HA	1.81	0.61
25:23:7:LYS:HE3	25:23:32:GLN:HE21	1.66	0.61
1:2A:1186:G:OP2	61:2A:3836:HOH:O	2.15	0.61
1:2A:2079:U:O3'	23:21:35:THR:OG1	2.19	0.61
1:2A:2099:U:O2	1:2A:2190:G:N2	2.32	0.61
6:2G:105:LYS:NZ	6:2G:143:GLU:OE2	2.27	0.61
1:2A:2659:G:H4'	7:2H:175:LYS:HD3	1.81	0.61
1:1A:1111:U:O2	1:1A:1112:U:N3	2.34	0.61
1:1A:2137:G:H2'	1:1A:2139:A:N6	2.16	0.61
1:1A:2164:C:O2	1:1A:2171:G:N1	2.33	0.61
28:16:2:ALA:N	61:16:601:HOH:O	2.33	0.60
1:1A:673:G:H2'	1:1A:674:G:C8	3.05	0.60
21:1Z:158:PRO:HG2	21:1Z:161:VAL:HG11	1.82	0.60
1:1A:2189:U:H2'	1:1A:2190:G:C8	2.36	0.60
19:1X:31:HIS:HD2	19:1X:33:LYS:H	1.49	0.60
1:2A:1783:A:OP2	61:2A:3847:HOH:O	2.17	0.60
1:2A:404:C:OP2	61:2A:3846:HOH:O	2.16	0.60
8:2I:4:ILE:HD11	8:2I:44:LEU:HD12	1.82	0.60
1:1A:1223:C:H2'	1:1A:1224:C:C6	2.36	0.60
16:1U:55:ARG:NH2	61:1U:302:HOH:O	2.29	0.60
15:2T:51:ARG:HB2	15:2T:98:LYS:HD3	1.83	0.60
16:2U:10:ARG:NH1	61:2U:302:HOH:O	2.34	0.60
1:1A:1318:A:H5''	14:1S:3:ARG:HH12	127.09	0.60
1:1A:2859:U:H4'	1:1A:2878:A:C2	2.36	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2870:C:H2'	1:2A:2871:C:O4'	2.00	0.60
1:2A:362:U:O2'	1:2A:363:G:H5'	2.00	0.60
14:2S:27:SER:HA	14:2S:88:ASP:HB3	1.82	0.60
1:1A:2465:A:OP1	61:1A:4147:HOH:O	2.15	0.60
2:1B:66:A:H61	2:1B:108:U:H2'	1.66	0.60
14:1S:27:SER:HA	14:1S:88:ASP:HB3	1.83	0.60
20:1Y:92:ASN:N	20:1Y:93:GLY:HA2	2.16	0.60
1:2A:1062:G:N7	1:2A:1070:A:H1'	2.16	0.60
1:2A:309:G:N3	1:2A:329:G:O2'	2.35	0.60
12:2Q:68:ILE:HG22	12:2Q:101:ARG:HE	1.64	0.60
1:1A:1532:A:H2'	1:1A:1533:G:C8	2.36	0.60
1:1A:2649:U:OP2	61:1A:4146:HOH:O	2.15	0.60
22:20:17:GLN:NE2	61:20:5003:HOH:O	2.34	0.60
1:2A:2001:A:H2'	1:2A:2002:G:C8	2.37	0.60
7:1H:11:VAL:HG13	7:1H:15:VAL:HG22	1.84	0.60
1:2A:1371:G:HO2'	1:2A:1372:U:H5	1.50	0.60
7:2H:98:LEU:HD13	7:2H:103:LEU:HD13	1.84	0.60
26:14:16:CYS:SG	26:14:17:GLY:N	2.74	0.60
15:1T:96:ARG:NH2	61:1T:303:HOH:O	2.33	0.60
21:1Z:69:THR:HG22	21:1Z:90:VAL:HA	1.82	0.60
1:2A:2417:C:OP1	11:2P:65:ARG:NH2	2.35	0.60
1:2A:586:A:N1	1:2A:809:G:O2'	2.29	0.60
7:2H:113:VAL:HG21	7:2H:151:ILE:HG21	1.84	0.60
1:2A:1101:U:H2'	1:2A:1102:C:H6	1.67	0.60
1:1A:1827:U:H2'	1:1A:1828:C:C6	2.36	0.60
1:1A:2348:A:H61	22:10:43:THR:HG22	1.67	0.60
12:1Q:109:VAL:HG13	12:1Q:113:GLN:HB2	1.84	0.60
5:2F:178:PRO:HB2	5:2F:201:VAL:HG21	1.83	0.60
1:1A:2164:C:N3	1:1A:2171:G:O6	2.35	0.59
1:2A:1007:C:OP1	9:2N:35:ARG:NH1	2.35	0.59
1:2A:1507:A:O2'	1:2A:1508:A:O5'	2.20	0.59
1:1A:492:A:OP1	29:17:34:ARG:NH1	2.35	0.59
1:1A:2416:C:O3'	11:1P:77:ARG:NH2	2.35	0.59
26:24:48:ARG:HD2	26:24:52:THR:HA	1.82	0.59
1:2A:1009:A:OP2	61:2A:3844:HOH:O	2.16	0.59
1:1A:1140:U:H1'	1:1A:1143:U:H5	1.66	0.59
1:1A:1218:G:O2'	1:1A:1219:A:O5'	2.19	0.59
5:1F:53:THR:CG2	5:1F:55:GLY:H	2.14	0.59
21:2Z:33:LEU:HD11	21:2Z:90:VAL:HG21	1.84	0.59
1:1A:1313:U:OP1	61:1A:4151:HOH:O	2.16	0.59
1:2A:2119:A:H61	1:2A:2168:G:H21	1.48	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2128:C:H1'	1:2A:2173:A:H2	1.67	0.59
7:2H:3:ARG:NH1	7:2H:5:GLY:H	2.00	0.59
1:2A:271(L):U:H5'	8:2I:50:ARG:HH12	1.66	0.59
1:1A:1124:U:H4'	1:1A:1125:C:H5'	1.85	0.59
1:1A:1889:G:O6	61:1A:4145:HOH:O	2.15	0.59
17:2V:52:VAL:HG23	17:2V:55:ALA:HB3	1.83	0.59
28:16:14:THR:O	28:16:17:LYS:NZ	2.34	0.59
1:1A:116:A:H61	1:1A:313:A:H1'	39.30	0.59
1:1A:2045:G:H5'	1:1A:2629:C:H4'	1.83	0.59
26:24:16:CYS:SG	26:24:17:GLY:N	2.75	0.59
1:2A:2526:G:O6	61:2A:3842:HOH:O	2.16	0.59
17:2V:40:LEU:HB2	17:2V:46:VAL:HG13	1.84	0.59
1:2A:2155:G:C2	1:2A:2156:G:H1'	2.37	0.59
1:1A:1218:G:O2'	1:1A:1219:A:O4'	2.21	0.59
1:1A:1398:U:OP1	61:1A:4154:HOH:O	2.17	0.59
1:1A:1475:G:H2'	1:1A:1476:C:C6	2.38	0.59
5:1F:41:LEU:HA	5:1F:44:ARG:HD3	1.85	0.59
1:2A:2128:C:N4	1:2A:2160:G:H1	2.00	0.59
6:2G:5:VAL:HG23	6:2G:8:LYS:HB3	1.84	0.59
1:1A:2136:A:H3'	1:1A:2137:G:C8	2.37	0.59
1:2A:2355:C:H1'	22:20:39:ARG:HH21	1.67	0.59
1:2A:1003:G:N3	1:2A:1003:G:H3'	4.35	0.59
1:2A:2327:A:H2'	1:2A:2328:A:C8	2.37	0.59
14:2S:74:ALA:HB2	14:2S:105:ALA:HA	1.85	0.59
15:2T:65:LYS:HE3	15:2T:67:SER:HB2	1.85	0.59
6:1G:66:GLN:NE2	6:1G:93:THR:O	2.36	0.59
8:1I:77:LEU:HD12	8:1I:104:GLN:HE21	1.66	0.59
1:2A:1006:C:H2'	1:2A:1007:C:C6	3.25	0.59
1:1A:1001:G:O6	61:1A:4138:HOH:O	2.13	0.58
27:25:16:ARG:HH11	27:25:16:ARG:HG2	1.68	0.58
28:26:35:GLU:OE2	28:26:50:ARG:NH1	2.36	0.58
1:2A:2104:G:N2	1:2A:2105:C:N3	2.51	0.58
1:1A:1317:G:OP2	61:1A:4130:HOH:O	2.16	0.58
1:1A:2339:A:H2'	1:1A:2340:A:C8	2.38	0.58
24:22:1:MET:SD	24:22:56:GLN:NE2	2.74	0.58
1:2A:2144:U:H5''	1:2A:2145:C:C5	2.38	0.58
8:2I:5:LEU:HD21	8:2I:12:LEU:HD22	1.85	0.58
1:1A:2442:A:H2'	1:1A:2442:A:N3	2.17	0.58
1:1A:645:G:H5'	1:1A:645:G:N3	2.18	0.58
1:2A:1065:U:H3	1:2A:1073:A:H61	1.51	0.58
5:2F:132:VAL:HG21	5:2F:163:VAL:HG22	1.86	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:16:13:CYS:SG	28:16:47:THR:HG21	2.44	0.58
1:1A:1053:C:OP1	9:1N:35:ARG:NH1	2.37	0.58
1:1A:1232:G:H5''	17:1V:81:TYR:CE1	2.37	0.58
1:1A:2703:C:OP2	61:1A:4159:HOH:O	2.17	0.58
1:2A:1068:G:H8	1:2A:1068:G:OP2	6.81	0.58
1:2A:1669:A:OP2	61:2A:3849:HOH:O	2.17	0.58
1:2A:2206:G:H5''	1:2A:2207:G:C8	2.38	0.58
10:2O:36:GLY:HA3	10:2O:109:LYS:HD2	1.85	0.58
9:1N:70:LYS:HD3	9:1N:87:LEU:HD12	1.84	0.58
1:1A:2104:A:N1	61:1A:4269:HOH:O	2.32	0.58
24:22:65:ASN:OD1	24:22:69:ARG:NH1	2.36	0.58
1:2A:1828:G:OP1	61:2A:3850:HOH:O	2.17	0.58
1:2A:2315:G:H2'	1:2A:2316:C:C6	2.39	0.58
1:2A:2596:U:OP2	61:2A:3843:HOH:O	2.16	0.58
1:2A:800:A:OP1	1:2A:800:A:H8	1.87	0.58
13:2R:29:LEU:HB3	13:2R:75:LEU:HD21	1.84	0.58
1:1A:437:G:OP1	61:1A:4157:HOH:O	2.17	0.58
4:1E:121:ASN:ND2	61:1E:3103:HOH:O	2.36	0.58
1:2A:1405:U:H2'	1:2A:1406:U:C6	2.37	0.58
3:2D:108:PRO:HB3	3:2D:143:HIS:CE1	2.39	0.58
1:1A:2156:A:O2'	1:1A:2181:G:N3	2.37	0.57
1:1A:2705:A:H2'	1:1A:2706:G:H8	1.69	0.57
1:1A:745:C:H2'	1:1A:746:A:C8	6.90	0.57
16:1U:78:THR:HG22	16:1U:117:GLN:HE22	1.68	0.57
2:2B:58:A:OP2	61:2B:3102:HOH:O	2.16	0.57
4:2E:111:ARG:HD3	4:2E:160:TYR:CE2	2.39	0.57
6:2G:137:GLU:HG2	6:2G:152:LEU:HD22	1.85	0.57
2:2B:75:G:O3'	21:2Z:10:ARG:NH2	2.37	0.57
1:1A:138:G:H1	1:1A:225:C:H42	81.89	0.57
58:1B:228:ARG:N	61:1B:3108:HOH:O	2.37	0.57
11:1P:75:ILE:O	61:1P:302:HOH:O	2.18	0.57
1:2A:1803:A:O2'	3:2D:259:THR:HG21	2.04	0.57
1:1A:1114:G:O2'	1:1A:1142:A:O2'	1.99	0.57
1:1A:664:U:H2'	1:1A:665:C:C6	2.39	0.57
1:2A:78:A:H2'	1:2A:79:G:C8	2.39	0.57
3:2D:69:ARG:NH2	3:2D:105:ILE:HD13	2.20	0.57
6:2G:7:LEU:HD23	6:2G:100:TRP:HE3	1.69	0.57
12:1Q:122:GLY:O	61:1Q:301:HOH:O	2.17	0.57
1:2A:1073:A:H2'	1:2A:1074:G:C8	2.39	0.57
1:2A:2356:C:O3'	22:20:20:ARG:HD3	2.05	0.57
1:2A:873:G:H1	1:2A:904:C:H42	1.51	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:2I:94:ALA:HB2	8:2I:116:LEU:HD22	1.84	0.57
3:1D:253:GLN:HB3	61:1D:403:HOH:O	2.03	0.57
21:2Z:157:LEU:HD11	21:2Z:163:LEU:HB2	1.86	0.57
8:1I:116:LEU:HD11	8:1I:120:ILE:HG13	1.87	0.57
1:2A:1364:G:OP2	23:21:3:LYS:HG3	2.04	0.57
1:2A:1011:G:N2	1:2A:1018:C:N3	21.27	0.57
7:2H:86:GLU:OE2	7:2H:132:ARG:NH2	2.38	0.57
1:1A:1834:A:O2'	3:1D:259:THR:HG21	2.04	0.57
21:1Z:136:PHE:HE1	21:1Z:138:GLU:HG3	1.69	0.57
1:2A:1266:G:O5'	18:2W:15:ARG:NH2	2.38	0.57
1:1A:347:G:C8	5:1F:171:PRO:HG3	2.40	0.57
8:1I:77:LEU:HB3	8:1I:142:VAL:HG22	1.85	0.57
11:1P:63:PRO:HD3	30:18:27:THR:HG22	1.87	0.57
1:2A:1014:U:H2'	1:2A:1015:G:H8	1.68	0.57
1:2A:652(T):C:H2'	1:2A:652(U):G:C8	2.40	0.57
5:2F:190:GLU:O	61:2F:3101:HOH:O	2.17	0.57
1:1A:1485:A:OP1	61:1A:4162:HOH:O	2.18	0.57
1:1A:2155:G:H3'	1:1A:2179:G:H21	1.69	0.57
1:2A:1062:G:H1	1:2A:1088:A:H8	1.52	0.57
1:2A:991:C:OP2	61:2A:3836:HOH:O	2.17	0.57
5:2F:185:ASP:HA	5:2F:188:ARG:HD3	1.87	0.57
1:1A:240:A:C5	1:1A:241:G:H1'	2.40	0.56
1:2A:2099:U:O4	1:2A:2190:G:O6	2.23	0.56
1:2A:2584:U:H2'	1:2A:2585:U:H2'	1.86	0.56
1:2A:588:U:H2'	1:2A:589:C:C6	2.39	0.56
6:2G:54:GLU:O	6:2G:58:GLN:N	2.34	0.56
7:2H:11:VAL:HG21	7:2H:50:VAL:HG23	1.87	0.56
1:1A:1398:U:OP2	61:1A:4155:HOH:O	2.17	0.56
18:1W:37:ARG:NH1	27:15:48:GLU:OE2	2.38	0.56
22:20:23:VAL:HG22	22:20:38:VAL:HG22	1.88	0.56
31:29:14:CYS:HA	31:29:27:CYS:HB2	1.86	0.56
1:2A:1031:G:H21	31:29:36:GLN:HE22	1.53	0.56
1:2A:2161:C:O2'	1:2A:2173:A:O2'	2.22	0.56
1:2A:2287:A:O2'	1:2A:2289:G:N7	2.36	0.56
15:2T:53:ARG:NH1	15:2T:53:ARG:HB3	2.21	0.56
16:2U:8:VAL:HG13	16:2U:11:ARG:HH21	1.69	0.56
17:2V:72:VAL:HG13	17:2V:85:LYS:HB3	1.87	0.56
1:1A:1809:U:H2'	1:1A:1815:A:N6	2.20	0.56
1:1A:483:A:OP2	61:1A:4161:HOH:O	2.17	0.56
1:2A:574:C:N3	4:2E:145:LYS:NZ	2.51	0.56
1:2A:2295:C:H5	14:2S:13:ARG:HH12	1.51	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1D:206:LEU:HD22	3:1D:211:ARG:HG2	1.87	0.56
1:2A:1356:G:OP1	61:2A:3848:HOH:O	2.17	0.56
1:2A:2810:A:N6	1:2A:2891:G:O2'	2.37	0.56
1:2A:995:C:O2	9:2N:3:THR:OG1	2.21	0.56
1:1A:2037:A:N3	27:15:4:HIS:HE1	2.03	0.56
1:2A:2136:C:N4	1:2A:2155:G:N1	2.51	0.56
1:2A:483:A:H5''	20:2Y:50:ARG:HD3	1.86	0.56
11:1P:82:GLY:HA2	11:1P:113:LYS:O	2.04	0.56
1:2A:572:A:OP2	17:2V:78:LYS:NZ	2.39	0.56
11:2P:63:PRO:HD3	30:28:27:THR:HG22	1.86	0.56
14:2S:93:LYS:NZ	61:2S:202:HOH:O	2.33	0.56
22:10:24:LYS:O	22:10:25:ARG:NH1	2.37	0.56
15:1T:93:ARG:NH2	61:1T:305:HOH:O	2.38	0.56
1:2A:1324:G:N7	61:2A:3963:HOH:O	2.33	0.56
1:2A:1889:A:H2'	1:2A:1890:A:C8	2.40	0.56
1:2A:2134:A:N7	1:2A:2157:G:H5'	2.20	0.56
6:1G:59:GLU:OE2	6:1G:153:ARG:NH2	2.38	0.56
1:2A:2206:G:H8	1:2A:2207:G:N7	2.04	0.56
1:2A:2602:A:H4'	1:2A:2603:G:OP1	2.05	0.56
1:2A:855:G:H2'	1:2A:856:C:C6	2.41	0.56
4:2E:143:ASN:HD22	4:2E:147:PRO:HD3	1.70	0.56
1:2A:2590:A:O3'	3:2D:239:ARG:NH2	2.39	0.56
1:2A:2689:U:OP2	1:2A:2719:G:N2	2.36	0.56
1:2A:382:G:OP2	61:2A:3851:HOH:O	2.18	0.56
4:2E:52:LEU:HB3	4:2E:53:PRO:HD2	1.87	0.56
1:1A:1476:C:H2'	1:1A:1477:U:C6	2.41	0.56
23:21:3:LYS:HB2	23:21:61:ARG:HH22	1.70	0.56
1:2A:1796:U:H2'	1:2A:1797:C:H6	1.69	0.56
1:2A:1864:U:OP1	1:2A:2410:G:O2'	2.20	0.56
1:1A:2511:C:OP1	61:1A:4137:HOH:O	2.18	0.56
5:1F:143:ALA:HB1	5:1F:148:LEU:HB2	1.88	0.56
1:2A:2131:G:OP1	1:2A:2132:U:H5'	2.06	0.56
2:2B:116:G:N7	61:2B:3112:HOH:O	2.33	0.56
5:2F:143:ALA:HB1	5:2F:148:LEU:HB2	1.88	0.56
1:1A:1129:U:H1'	1:1A:1132:A:N6	2.21	0.55
1:2A:1011:G:OP2	16:2U:66:ASN:ND2	2.37	0.55
1:2A:1187:G:H5'	17:2V:81:TYR:CE1	2.41	0.55
1:1A:831:A:H5'	1:1A:832:G:OP1	2.06	0.55
19:1X:31:HIS:CD2	19:1X:33:LYS:H	2.24	0.55
19:1X:41:ASN:O	19:1X:45:THR:HG23	2.05	0.55
1:2A:1514:U:H2'	1:2A:1515:G:H8	1.70	0.55

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1428:C:O2'	1:2A:1569:A:OP2	2.18	0.55
1:2A:2150:U:H2'	1:2A:2151:G:C8	2.41	0.55
1:2A:328:U:H4'	20:2Y:68:HIS:CD2	2.41	0.55
3:2D:224:ALA:O	61:2D:402:HOH:O	2.18	0.55
6:2G:46:ALA:HB2	6:2G:53:LEU:HD12	1.88	0.55
1:2A:1278:A:OP1	13:2R:36:THR:HG23	2.06	0.55
1:1A:1613:A:OP1	3:1D:211:ARG:NH1	2.36	0.55
8:1I:57:ARG:O	8:1I:61:ARG:HG2	2.07	0.55
30:28:13:ARG:O	61:28:8101:HOH:O	2.18	0.55
1:2A:2316:C:H2'	1:2A:2317:C:H6	1.72	0.55
1:2A:2537:U:H2'	1:2A:2538:C:C6	2.42	0.55
26:24:59:PHE:HA	26:24:61:ARG:N	2.21	0.55
1:2A:1153:C:OP2	61:2A:3828:HOH:O	2.18	0.55
1:2A:615:G:OP1	5:2F:40:GLN:HG3	2.06	0.55
7:2H:87:LEU:HD23	7:2H:164:TYR:HA	1.88	0.55
1:1A:1425:A:H4'	1:1A:1426:G:OP2	2.06	0.55
1:1A:312:C:H2'	1:1A:313:A:H8	1.71	0.55
1:2A:2122:U:H3	1:2A:2176:A:N6	2.04	0.55
1:2A:212:G:H2'	1:2A:213:A:O4'	2.07	0.55
24:12:65:ASN:O	24:12:69:ARG:HG3	2.07	0.55
1:1A:173:C:H2'	1:1A:174:U:C6	2.42	0.55
1:1A:611:U:H2'	1:1A:612:C:C6	2.42	0.55
1:2A:1041:C:N4	1:2A:1114:G:H1	1.97	0.55
1:2A:984:A:H5''	1:2A:985:C:H5	1.71	0.55
19:2X:43:VAL:HG21	19:2X:81:VAL:HG11	1.89	0.55
2:2B:28:C:OP1	14:2S:36:TYR:OH	2.23	0.55
5:2F:184:TYR:CE2	5:2F:188:ARG:HD2	2.42	0.55
1:1A:1754:G:O6	61:1A:4158:HOH:O	2.17	0.55
1:1A:2705:A:H2'	1:1A:2706:G:C8	2.42	0.55
1:1A:2121:U:H3	1:1A:2212:G:H1	1.55	0.55
1:1A:2899:C:H2'	1:1A:2900:G:O4'	2.07	0.55
22:20:9:SER:OG	22:20:10:THR:N	2.40	0.55
1:2A:1068:G:H3'	1:2A:1096:A:OP2	2.07	0.55
1:2A:2584:U:H5''	1:2A:2602:A:C2	2.42	0.55
1:2A:2849:U:O4	15:2T:23:ARG:NH2	2.39	0.55
1:1A:625:G:O2'	1:1A:702:A:N6	2.40	0.55
6:1G:16:ARG:NE	6:1G:31:VAL:HG21	2.20	0.55
25:23:9:VAL:HG12	25:23:32:GLN:HE22	1.72	0.55
31:29:25:VAL:HB	31:29:34:GLN:HB2	1.89	0.55
1:2A:2074:U:H2'	1:2A:2075:U:C6	2.41	0.55
1:2A:23:G:OP1	1:2A:504:U:N3	2.40	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1G:9:ARG:NH1	6:1G:13:GLU:OE2	2.40	0.54
6:1G:67:LYS:HD3	26:14:5:ILE:HB	1.89	0.54
1:2A:1166:C:H2'	1:2A:1167:U:C6	2.42	0.54
1:2A:271(M):G:O2'	1:2A:271(N):U:O5'	2.22	0.54
8:2I:117:GLU:HG3	8:2I:118:LYS:H	1.71	0.54
4:2E:181:LEU:HD11	15:2T:6:LEU:HD23	1.89	0.54
3:1D:4:LYS:HB3	3:1D:18:VAL:HG23	1.89	0.54
1:2A:1639:U:H2'	1:2A:1640:C:H5''	1.90	0.54
1:2A:277:C:HO2'	1:2A:278:A:P	2.27	0.54
9:1N:46:VAL:HG23	9:1N:48:MET:HG2	1.89	0.54
20:1Y:23:ARG:NH1	61:1Y:601:HOH:O	2.30	0.54
6:2G:80:PHE:O	6:2G:82:LEU:N	2.40	0.54
17:2V:95:LEU:HD22	17:2V:97:LYS:HD3	1.89	0.54
1:1A:924:U:H2'	1:1A:925:A:H5''	1.89	0.54
9:1N:13:TRP:CE2	9:1N:133:GLN:HG2	2.43	0.54
22:20:49:LYS:HG2	22:20:50:ASN:ND2	2.22	0.54
1:2A:2375:G:N1	61:2A:3961:HOH:O	2.33	0.54
1:1A:2151:C:N3	1:1A:2181:G:O6	2.40	0.54
1:1A:354:A:H2	1:1A:1255:A:O2'	1.90	0.54
1:2A:2171:A:H4'	1:2A:2172:U:OP1	2.07	0.54
1:1A:2348:A:H61	22:10:43:THR:CG2	2.20	0.54
1:1A:1099:C:N3	1:1A:1152:G:O6	2.41	0.54
16:1U:69:CYS:HB3	16:1U:74:LEU:HD12	1.90	0.54
1:2A:11:G:C2'	1:2A:12:U:H5'	2.36	0.54
11:2P:97:PRO:HD3	11:2P:126:VAL:O	2.07	0.54
14:2S:43:GLU:OE2	22:20:49:LYS:NZ	2.37	0.54
5:1F:164:ARG:HE	58:1F:314:ARG:HH12	1.55	0.54
15:1T:24:PRO:HA	15:1T:49:VAL:HG22	1.89	0.54
1:2A:2123:G:O6	1:2A:2175:C:N3	2.41	0.54
24:12:22:GLU:OE2	24:12:68:ARG:NH2	2.41	0.54
1:1A:1346:U:H4'	1:1A:1347:A:H5''	1.89	0.54
1:1A:2892:A:OP1	13:1R:96:ARG:NH1	2.38	0.54
3:1D:69:ARG:HG2	3:1D:69:ARG:HH11	1.73	0.54
1:2A:1063:G:N2	1:2A:1075:C:N3	2.56	0.54
1:2A:624:C:H2'	1:2A:625:G:H8	2.91	0.54
1:2A:876:C:H2'	1:2A:877:U:O4'	2.08	0.54
8:2I:40:THR:HG23	8:2I:43:ASN:HB2	1.90	0.54
19:2X:31:HIS:CD2	19:2X:33:LYS:H	2.26	0.54
1:1A:1110:C:N4	1:1A:1111:U:O2	2.41	0.54
1:1A:215:G:H21	1:1A:217:A:H62	1.55	0.54
1:1A:2144:U:H3	1:1A:2198:A:H61	1.56	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2389:A:H2'	1:1A:2390:A:C8	2.43	0.54
1:1A:957:A:H2'	12:1Q:9:TYR:OH	2.08	0.54
25:23:6:VAL:HG22	25:23:56:VAL:HG22	1.90	0.54
1:2A:2314:C:H2'	1:2A:2315:G:C8	2.43	0.54
1:2A:78:A:H2'	1:2A:79:G:H8	1.73	0.54
3:2D:69:ARG:HH21	3:2D:105:ILE:HD13	1.73	0.54
6:2G:101:ILE:HG22	6:2G:105:LYS:HE2	1.89	0.54
14:2S:89:ARG:NH1	61:2S:203:HOH:O	2.39	0.54
1:1A:482:C:H4'	61:1A:4543:HOH:O	2.07	0.54
8:1I:27:ARG:HD2	23:11:71:TYR:CE2	2.43	0.54
10:1O:64:ARG:HD3	10:1O:79:PHE:CD1	2.43	0.54
23:21:31:GLY:O	61:21:8102:HOH:O	2.19	0.54
1:2A:271(L):U:H5'	8:2I:50:ARG:HH22	1.73	0.54
1:2A:614(C):A:C4	5:2F:180:GLY:HA2	2.42	0.54
5:2F:40:GLN:HE22	5:2F:182:ASN:HB2	1.73	0.54
13:1R:33:ARG:NH2	27:15:57:VAL:O	2.27	0.53
1:1A:936:C:O2'	1:1A:937:A:O5'	2.26	0.53
6:1G:16:ARG:HB2	6:1G:17:PRO:HD3	1.89	0.53
9:1N:12:ARG:NH1	9:1N:50:ASP:OD2	2.40	0.53
1:2A:1316:U:H2'	1:2A:1317:A:H8	1.73	0.53
1:2A:1362:C:H2'	1:2A:1363:C:H5''	3.95	0.53
1:2A:2130:U:H2'	1:2A:2158:A:H61	1.73	0.53
1:2A:729:G:C6	3:2D:208:LYS:HB2	2.42	0.53
10:2O:115:VAL:HG13	10:2O:121:VAL:HG21	1.89	0.53
17:2V:28:GLU:O	17:2V:61:VAL:HG21	2.08	0.53
4:1E:143:ASN:HD22	4:1E:147:PRO:HD3	1.73	0.53
1:2A:1057:A:N7	1:2A:1086:A:H2'	2.23	0.53
1:2A:641:C:O2'	1:2A:2350:C:OP1	2.17	0.53
6:2G:15:VAL:HG22	6:2G:175:LEU:HB3	1.89	0.53
1:1A:2291:G:O6	22:10:14:ARG:HG3	2.08	0.53
23:11:3:LYS:O	23:11:12:PRO:HD3	2.09	0.53
1:1A:1318:A:H5''	14:1S:3:ARG:NH1	127.56	0.53
3:1D:71:ASP:HB3	3:1D:103:ARG:NH2	2.23	0.53
3:1D:85:ASP:OD2	3:1D:88:ARG:HD2	2.08	0.53
61:1A:6219:HOH:O	18:1W:92:ARG:HD2	2.08	0.53
1:2A:1001:A:OP2	61:2A:3852:HOH:O	2.19	0.53
1:2A:1188:U:H4'	17:2V:79:VAL:HG22	1.89	0.53
13:2R:56:LYS:NZ	13:2R:90:ARG:O	2.41	0.53
1:1A:2340:A:H2'	1:1A:2341:G:C8	2.43	0.53
21:1Z:144:LEU:HD11	21:1Z:150:LEU:HD22	1.90	0.53
1:2A:1246:A:OP1	5:2F:38:ARG:NH1	2.41	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1538:G:H2'	1:2A:1539:G:H8	1.73	0.53
1:2A:2140:C:H2'	1:2A:2141:G:H8	1.73	0.53
1:2A:2125:G:H22	1:2A:2172:U:H3'	1.72	0.53
1:2A:2540:C:H2'	1:2A:2541:A:O4'	2.08	0.53
1:2A:322:A:OP2	5:2F:169:ASN:HB2	2.08	0.53
18:2W:12:ILE:HD13	18:2W:17:VAL:HG13	1.90	0.53
1:1A:1071:G:C4	1:1A:1180:C:H1'	2.44	0.53
1:1A:1360:C:OP1	61:1A:4118:HOH:O	2.19	0.53
1:2A:667:U:O2	30:28:2:PRO:HD2	2.09	0.53
7:2H:127:GLU:C	7:2H:129:THR:H	2.11	0.53
8:2I:72:LEU:HD21	8:2I:107:VAL:HG11	1.90	0.53
12:2Q:34:LEU:HB2	12:2Q:118:LEU:HD22	1.89	0.53
19:2X:12:VAL:HG22	19:2X:29:TRP:CE2	2.44	0.53
30:18:28:GLY:O	30:18:36:LYS:NZ	2.37	0.53
1:1A:2814:C:H2'	1:1A:2815:C:C6	2.44	0.53
1:1A:630:U:OP1	5:1F:102:PRO:HA	2.08	0.53
1:1A:1845:G:H4'	3:1D:51:VAL:HG21	1.91	0.53
4:1E:101:ARG:CZ	4:1E:171:GLU:HB2	2.39	0.53
1:2A:1028:A:N6	1:2A:1125:G:H2'	2.24	0.53
2:2B:4:C:H2'	2:2B:5:C:C6	2.43	0.53
6:2G:145:THR:OG1	6:2G:146:TYR:N	2.40	0.53
1:1A:1046:A:N6	1:1A:1211:U:O2	28.10	0.53
1:1A:1310:G:OP1	27:15:19:ARG:NH2	2.27	0.53
1:1A:1899:A:H5'	1:1A:1900:G:OP2	2.09	0.53
1:1A:669:A:H4'	1:1A:670:C:H5	1.74	0.53
11:1P:50:ARG:HD3	30:18:7:HIS:CD2	2.44	0.53
14:1S:11:LYS:HG3	14:1S:91:PRO:HD3	1.90	0.53
1:2A:1525:G:H2'	1:2A:1526:G:C8	2.43	0.53
1:2A:2136:C:C4	1:2A:2155:G:N1	2.70	0.53
7:2H:154:PRO:HB3	7:2H:163:TYR:CZ	2.44	0.53
1:2A:11:G:N7	61:2A:3971:HOH:O	2.34	0.53
1:2A:125:G:O6	29:27:10:ARG:NH1	2.42	0.53
1:2A:1910:G:H2'	1:2A:1911:PSU:H6	1.73	0.53
1:2A:2673:G:O2'	61:2A:3853:HOH:O	2.19	0.53
1:2A:300:A:H1'	1:2A:319:C:H1'	1.90	0.53
1:2A:479:A:N3	1:2A:481:G:H5''	2.24	0.53
1:1A:636:G:O2'	1:1A:640:A:N1	2.38	0.53
11:1P:56:SER:N	61:1P:304:HOH:O	2.29	0.53
12:1Q:21:THR:HG21	12:1Q:101:ARG:N	2.23	0.53
1:2A:323:G:O2'	1:2A:1205:U:N3	2.33	0.53
1:2A:434:U:H2'	1:2A:435:C:C6	6.28	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:2Q:31:ASP:OD1	12:2Q:134:ARG:NH1	2.30	0.53
1:2A:1688:U:O2	1:2A:1700:A:H5'	2.10	0.53
9:2N:4:TYR:O	16:2U:64:ARG:NH2	2.35	0.53
1:1A:1285:G:H2'	1:1A:1286:U:O4'	2.09	0.52
10:1O:2:ILE:HD12	10:1O:6:THR:HG21	1.90	0.52
1:2A:607:U:OP1	5:2F:102:PRO:HA	2.08	0.52
6:2G:12:TYR:HA	6:2G:16:ARG:CG	2.39	0.52
1:1A:1529:G:H1	1:1A:1552:C:N4	2.07	0.52
24:12:64:LEU:HD21	24:12:68:ARG:HE	1.74	0.52
2:1B:77:U:OP1	21:1Z:19:ARG:NH2	2.42	0.52
4:1E:111:ARG:HD2	4:1E:160:TYR:CD2	2.45	0.52
7:1H:7:LEU:HD12	7:1H:8:PRO:HD2	1.91	0.52
10:1O:64:ARG:HG2	10:1O:83:ALA:HB3	1.92	0.52
1:2A:1007:C:N3	1:2A:1022:G:O6	16.78	0.52
1:2A:2319:G:N1	14:2S:3:ARG:HA	2.24	0.52
1:2A:2546:U:OP1	61:2A:3854:HOH:O	2.19	0.52
1:2A:315:G:H2'	1:2A:316:C:C6	2.45	0.52
12:2Q:58:PHE:O	12:2Q:60:ARG:N	2.42	0.52
6:1G:101:ILE:HD13	26:14:25:TYR:HB2	1.91	0.52
1:1A:2227:G:H2'	1:1A:2228:G:C2	2.44	0.52
6:1G:43:LEU:HD11	6:1G:153:ARG:HD3	1.91	0.52
7:1H:159:GLU:HG2	7:1H:169:VAL:HG11	1.91	0.52
1:2A:885:C:H2'	1:2A:886:C:H4'	1.92	0.52
8:2I:130:TYR:HB3	8:2I:138:ILE:HB	1.90	0.52
20:2Y:77:PRO:HD2	20:2Y:106:LEU:HD23	1.91	0.52
20:2Y:44:ILE:HD13	20:2Y:64:GLU:HG3	1.91	0.52
1:1A:1452:U:H2'	1:1A:1453:C:C6	2.44	0.52
6:1G:179:PRO:HG3	26:14:43:TYR:OH	2.10	0.52
2:2B:2:C:H2'	2:2B:3:C:C6	2.45	0.52
4:2E:52:LEU:O	4:2E:76:ARG:N	2.41	0.52
6:2G:15:VAL:HG21	6:2G:176:LEU:HD23	1.91	0.52
10:2O:76:ALA:O	15:2T:74:ARG:HG3	2.09	0.52
1:1A:1140:U:H1'	1:1A:1143:U:C5	2.44	0.52
1:1A:166:G:H2'	1:1A:167:G:C8	3.77	0.52
1:1A:276:C:H2'	1:1A:277:G:O4'	2.09	0.52
4:1E:40:GLU:OE1	4:1E:40:GLU:N	2.30	0.52
6:1G:41:GLN:HB3	6:1G:43:LEU:HD13	1.91	0.52
7:1H:40:GLU:CD	7:1H:60:ARG:HH12	2.12	0.52
15:1T:96:ARG:HB3	15:1T:96:ARG:HH11	1.73	0.52
16:1U:33:ARG:NH1	61:1U:306:HOH:O	2.42	0.52
23:21:40:ARG:NH2	23:21:42:GLN:HG2	2.25	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:24:48:ARG:HG3	26:24:52:THR:HG23	1.91	0.52
1:2A:1783:A:OP1	61:2A:3857:HOH:O	2.19	0.52
1:2A:1778:U:H2'	1:2A:1784:A:N6	2.25	0.52
4:2E:111:ARG:HD3	4:2E:160:TYR:CD2	2.44	0.52
4:2E:50:GLY:O	4:2E:51:PHE:HB2	2.08	0.52
15:2T:28:VAL:HG13	15:2T:86:ILE:HG23	1.92	0.52
1:1A:2658:C:H2'	1:1A:2659:U:O4'	2.10	0.52
1:1A:847:A:OP1	1:1A:847:A:H8	1.92	0.52
4:1E:119:ARG:HD2	4:1E:120:TRP:CE2	2.45	0.52
1:2A:1503:U:H2'	1:2A:1504:C:C6	2.45	0.52
2:2B:24:G:H4'	2:2B:25:A:C8	2.45	0.52
29:17:34:ARG:NE	29:17:39:ARG:HG3	2.22	0.52
1:1A:153:C:OP2	23:11:92:LYS:NZ	2.33	0.52
1:1A:196:A:H2'	1:1A:197:C:O4'	2.10	0.52
11:1P:140:ALA:O	25:23:38:GLU:HG2	2.10	0.52
1:2A:2526:G:H5'	1:2A:2742:C:O2'	2.09	0.52
2:2B:42:C:O2'	61:2B:3103:HOH:O	2.18	0.52
2:2B:33:G:H1'	2:2B:50:G:H22	1.75	0.52
5:2F:11:VAL:HG22	5:2F:125:LEU:HB2	1.92	0.52
1:1A:174:U:H4'	1:1A:207:A:H4'	1.92	0.52
1:1A:2132:G:OP1	1:1A:2140:U:N3	2.42	0.52
6:1G:18:GLU:OE2	6:1G:21:ARG:NH1	2.43	0.52
1:2A:1420:U:O2'	1:2A:1421:G:OP1	2.26	0.52
1:2A:1952:A:OP1	10:2O:42:SER:OG	2.21	0.52
1:2A:2104:G:N2	1:2A:2105:C:C2	2.78	0.52
1:2A:2102:U:O2	1:2A:2187:G:O6	2.27	0.52
1:2A:2313:C:H2'	1:2A:2314:C:C6	2.45	0.52
1:2A:2462:U:H2'	1:2A:2463:C:C6	2.45	0.52
1:2A:774:A:N3	1:2A:774:A:H2'	2.25	0.52
21:2Z:10:ARG:NH1	21:2Z:26:GLY:O	2.43	0.52
1:1A:1073:A:C2	1:1A:2500:A:H5'	2.45	0.52
1:1A:2205:C:H2'	1:1A:2206:G:H8	1.75	0.52
4:1E:47:VAL:HG12	4:1E:49:LEU:HD13	1.91	0.52
17:1V:21:ARG:HD3	17:1V:91:TYR:CD1	2.44	0.52
1:2A:1410:G:H2'	1:2A:1411:C:C6	2.55	0.52
1:2A:1667:G:O2'	1:2A:1991:U:O4	2.13	0.52
1:2A:271(R):G:OP1	23:21:76:ARG:NH1	2.43	0.52
1:2A:2445:G:OP1	5:2F:74:ARG:NH2	2.43	0.52
1:1A:1554:A:H4'	1:1A:1556:A:C5	2.45	0.51
1:2A:2286:A:H4'	1:2A:2287:A:O4'	2.10	0.51
1:2A:2023:G:H5'	1:2A:2617:C:H4'	1.92	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:659:C:H2'	1:2A:660:G:H8	1.74	0.51
5:2F:24:LEU:HD23	5:2F:115:ALA:HA	1.92	0.51
5:2F:40:GLN:NE2	5:2F:182:ASN:HB2	2.24	0.51
1:1A:207:A:N6	61:1A:4387:HOH:O	2.43	0.51
1:1A:2576:A:C2	1:1A:2659:U:H4'	2.45	0.51
1:1A:933:C:H3'	1:1A:934:A:H5''	1.92	0.51
1:2A:1748:G:H2'	1:2A:1749:A:O4'	2.10	0.51
1:2A:1794:U:H2'	1:2A:1795:C:C6	2.45	0.51
1:2A:2299:G:N1	1:2A:2318:G:N7	2.58	0.51
1:2A:2687:U:H2'	1:2A:2688:U:O4'	2.10	0.51
3:2D:124:PRO:HB2	3:2D:126:GLN:HG2	1.93	0.51
10:2O:15:GLY:O	10:2O:47:ILE:HG13	2.10	0.51
24:12:59:ARG:NH2	61:12:103:HOH:O	2.42	0.51
1:1A:1087:C:H5'	1:1A:1088:G:OP2	2.10	0.51
1:1A:2137:G:H2'	1:1A:2139:A:H61	1.75	0.51
3:1D:242:ARG:HD2	3:1D:246:PRO:HG3	1.93	0.51
3:1D:77:ALA:HB2	3:1D:97:TYR:CD1	2.46	0.51
7:1H:3:ARG:NH2	7:1H:65:HIS:HB3	2.25	0.51
7:1H:86:GLU:OE2	7:1H:132:ARG:NH2	2.44	0.51
1:2A:2400:G:H4'	28:26:18:ARG:HG2	1.92	0.51
9:2N:58:ASP:N	9:2N:58:ASP:OD1	2.43	0.51
17:2V:5:VAL:HG11	17:2V:57:VAL:HG21	1.92	0.51
31:19:15:LYS:HE2	31:19:17:ILE:HD13	1.92	0.51
1:1A:1370:G:N7	61:1A:4278:HOH:O	2.34	0.51
25:23:8:LEU:HG	25:23:31:LEU:HD22	1.91	0.51
1:2A:1445(A):C:H2'	1:2A:1446:C:H6	1.75	0.51
1:2A:2318:G:H21	14:2S:3:ARG:HE	1.57	0.51
1:2A:300:A:H2'	1:2A:334:C:H1'	1.91	0.51
2:2B:75:G:H22	21:2Z:73:GLN:NE2	2.08	0.51
3:2D:148:GLU:HB2	3:2D:151:LYS:HD2	1.92	0.51
6:2G:101:ILE:HD13	26:24:25:TYR:HB2	1.91	0.51
1:2A:2467:C:H4'	12:2Q:123:HIS:CD2	2.46	0.51
12:2Q:141:GLN:HE22	21:2Z:74:VAL:HG13	1.76	0.51
1:1A:2164:C:H2'	1:1A:2165:C:C6	2.45	0.51
3:1D:137:PRO:O	3:1D:140:THR:HG23	2.10	0.51
1:2A:1096:A:C5	1:2A:1097:U:H5	2.29	0.51
1:2A:1104:C:H2'	1:2A:1105:U:C6	2.45	0.51
1:2A:2127:G:H2'	1:2A:2128:C:O4'	2.10	0.51
1:2A:2267:A:H5''	1:2A:2268:A:H5'	1.91	0.51
1:2A:740:U:OP2	61:2A:3857:HOH:O	2.19	0.51
1:1A:1117:G:O2'	1:1A:1135:G:H2'	2.09	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1219:A:HI'	1:1A:1220:U:H5'	1.92	0.51
26:24:34:GLU:HG2	26:24:35:VAL:HG12	1.92	0.51
26:24:40:HIS:HB3	26:24:43:TYR:CD2	2.46	0.51
1:2A:2680:C:H5'	4:2E:189:PRO:HA	1.93	0.51
1:1A:959:U:OP1	61:1A:4165:HOH:O	2.19	0.51
21:1Z:1:MET:N	21:1Z:135:GLU:OE2	2.43	0.51
1:2A:1066:U:O2'	1:2A:1068:G:OP2	2.27	0.51
1:2A:1073:A:H2'	1:2A:1074:G:H8	1.76	0.51
1:2A:120:U:OP2	61:2A:3856:HOH:O	2.19	0.51
1:2A:207:A:OP2	61:2A:3855:HOH:O	2.19	0.51
1:2A:888:C:H2'	1:2A:889:C:N3	2.26	0.51
2:2B:102:A:OP2	61:2B:3104:HOH:O	2.19	0.51
27:15:16:ARG:HG3	27:15:17:ASP:N	2.25	0.51
1:1A:1305:G:N2	1:1A:1331:G:HI'	39.88	0.51
3:1D:168:ARG:N	3:1D:168:ARG:HH11	5.50	0.51
23:21:53:VAL:HG22	23:21:74:VAL:HG13	1.93	0.51
1:2A:2115:G:N3	1:2A:2115:G:H2'	2.26	0.51
8:2I:62:LYS:O	8:2I:66:GLU:HG2	2.11	0.51
1:1A:1264:G:OP2	16:1U:19:LYS:NZ	2.37	0.51
1:1A:2316:G:H22	1:1A:2324:U:H3	1.57	0.51
8:1I:130:TYR:HD2	8:1I:138:ILE:HD12	1.76	0.51
1:2A:1101:U:H2'	1:2A:1102:C:C6	2.45	0.51
1:2A:452:G:OP2	61:2A:3859:HOH:O	2.19	0.51
1:2A:668:G:H5'	1:2A:669:G:OP2	2.11	0.51
1:2A:911:A:H2'	12:2Q:9:TYR:OH	2.10	0.51
21:2Z:102:LEU:HD23	21:2Z:137:ILE:HB	1.92	0.51
1:1A:2377:G:N7	30:18:39:LYS:NZ	2.48	0.51
6:1G:16:ARG:O	6:1G:20:ILE:HG13	2.10	0.51
8:1I:46:ALA:O	8:1I:50:ARG:HG2	2.11	0.51
15:1T:51:ARG:HG3	15:1T:98:LYS:HE3	1.93	0.51
30:28:23:VAL:HG11	30:28:47:LYS:HD3	1.93	0.51
1:2A:2022:U:O2'	1:2A:2617:C:H5'	2.11	0.51
1:2A:1818:U:O2'	3:2D:154:LYS:O	2.20	0.51
3:2D:80:ALA:HB3	3:2D:94:LEU:HD23	1.91	0.51
10:2O:86:ILE:HG22	10:2O:94:ARG:HD3	1.93	0.51
14:2S:14:VAL:O	14:2S:18:ILE:HG12	2.11	0.51
1:1A:1829:U:OP1	61:1A:4164:HOH:O	2.19	0.50
7:1H:124:GLU:HG3	7:1H:132:ARG:HB3	1.94	0.50
8:1I:77:LEU:HD12	8:1I:104:GLN:NE2	2.26	0.50
11:1P:88:LEU:HD11	11:1P:114:ILE:HD12	1.93	0.50
11:1P:138:LEU:HD23	11:1P:145:PRO:HB3	1.94	0.50

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1R:59:ASP:N	13:1R:59:ASP:OD1	2.41	0.50
1:2A:1412:A:H2'	1:2A:1413:G:H8	1.76	0.50
1:2A:2698:U:H2'	1:2A:2699:C:C6	2.46	0.50
1:2A:962:G:OP1	61:2A:3858:HOH:O	2.19	0.50
4:2E:202:LYS:NZ	61:2E:401:HOH:O	2.43	0.50
15:2T:60:THR:HG22	15:2T:77:PRO:HA	1.93	0.50
1:1A:1239:A:H62	1:1A:1299:A:N6	21.12	0.50
1:1A:1682:G:N2	61:1A:4403:HOH:O	2.44	0.50
1:1A:2044:U:O2'	1:1A:2629:C:H5'	2.12	0.50
4:1E:116:VAL:HG13	4:1E:122:PHE:HB2	1.92	0.50
1:2A:1707:G:H2'	1:2A:1708:C:C6	2.46	0.50
4:2E:105:THR:HG21	4:2E:164:ARG:HE	1.76	0.50
1:1A:2534:U:O2'	1:1A:2659:U:OP1	2.20	0.50
4:1E:119:ARG:HG3	4:1E:160:TYR:HB2	1.92	0.50
6:1G:77:ILE:HB	6:1G:82:LEU:HB2	1.93	0.50
8:1I:40:THR:O	8:1I:44:LEU:HB2	2.11	0.50
1:2A:1754:C:P	15:2T:96:ARG:HH12	2.35	0.50
1:2A:2314:C:H2'	1:2A:2315:G:H8	1.76	0.50
8:2I:14:ASP:O	8:2I:17:GLN:HB2	2.10	0.50
1:1A:1255:A:H5''	1:1A:1257:G:O4'	2.11	0.50
1:1A:1633:A:H2'	1:1A:1634:C:C6	2.47	0.50
1:1A:1964:5MC:OP2	1:1A:1965:U:O2'	2.24	0.50
1:1A:2204:G:H2'	1:1A:2205:C:C6	2.46	0.50
1:1A:2897:U:H2'	1:1A:2898:C:C6	2.46	0.50
1:1A:890:G:O2'	1:1A:906:G:O6	46.19	0.50
3:1D:155:LEU:HD23	3:1D:177:LEU:HD22	1.93	0.50
1:2A:577:G:O2'	1:2A:1254:A:OP1	2.26	0.50
1:2A:154(A):C:N3	1:2A:171:G:N2	2.60	0.50
1:2A:886:C:H2'	1:2A:887:A:O4'	2.12	0.50
2:2B:2:C:H2'	2:2B:3:C:H6	1.77	0.50
7:2H:104:GLU:HA	7:2H:113:VAL:O	2.12	0.50
1:2A:84:A:H5'	20:2Y:8:LYS:HB3	1.93	0.50
1:1A:2089:G:N7	61:1A:4289:HOH:O	2.35	0.50
28:26:35:GLU:HA	28:26:49:HIS:O	2.12	0.50
1:2A:2166:G:H2'	1:2A:2167:U:O4'	2.11	0.50
1:2A:245:G:O6	30:28:8:LYS:NZ	2.43	0.50
1:2A:473:G:C2	1:2A:474:G:C4	3.99	0.50
5:2F:183:VAL:O	5:2F:187:VAL:HG23	2.11	0.50
1:1A:1836:U:O2	3:1D:50:THR:HB	2.11	0.50
1:2A:1427:A:H4'	1:2A:1428:C:O5'	2.12	0.50
1:2A:154(A):C:N4	1:2A:171:G:H1	2.08	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:27:G:O2'	1:2A:28:A:OP2	2.28	0.50
1:2A:528:A:O2'	1:2A:529:A:H5'	2.11	0.50
7:2H:35:VAL:HG13	7:2H:71:LEU:HD22	1.93	0.50
17:2V:60:GLU:HB2	17:2V:97:LYS:HE2	1.94	0.50
1:2A:2327:A:O3'	21:2Z:200:GLY:HA2	2.11	0.50
1:1A:105:C:H2'	1:1A:106:U:H6	1.75	0.50
1:1A:1128:U:C4	1:1A:1132:A:N1	2.78	0.50
1:1A:821:A:HO2'	1:1A:822:G:H8	1.60	0.50
1:1A:7:G:H2'	1:1A:8:A:O4'	2.12	0.50
1:2A:1412:A:H2'	1:2A:1413:G:C8	2.46	0.50
1:2A:2129:C:N3	1:2A:2159:G:O6	2.45	0.50
1:2A:2189:U:H2'	1:2A:2190:G:C8	2.47	0.50
7:2H:10:PRO:HA	7:2H:49:VAL:HG22	1.92	0.50
11:2P:88:LEU:HD11	11:2P:114:ILE:HD12	1.92	0.50
1:1A:383:A:H2'	1:1A:384:G:O4'	2.12	0.50
5:1F:150:GLY:HA2	5:1F:172:TRP:CE3	2.46	0.50
1:2A:1005:C:O2'	9:2N:28:THR:HG21	2.11	0.50
1:2A:1075:C:H2'	1:2A:1076:C:H5'	1.92	0.50
1:2A:149:A:H2'	1:2A:150:C:C6	3.00	0.50
15:2T:95:ARG:HG2	15:2T:95:ARG:HH11	1.76	0.50
1:1A:236:G:H4'	1:1A:413:G:C5	2.47	0.49
1:2A:30:G:H2'	1:2A:31:C:C6	2.47	0.49
16:2U:6:THR:HG21	16:2U:10:ARG:HH21	1.77	0.49
1:1A:2244:U:P	23:11:40:ARG:HH12	2.36	0.49
1:1A:310:C:H2'	1:1A:311:C:H6	1.75	0.49
1:1A:331:G:H21	1:1A:354:A:H62	1.58	0.49
1:1A:715:G:H5'	1:1A:716:G:OP2	2.11	0.49
1:1A:911:G:N7	12:1Q:22:LYS:NZ	2.60	0.49
8:1I:72:LEU:C	8:1I:74:ASN:H	2.15	0.49
11:1P:121:LYS:HB3	11:1P:123:LEU:HG	1.94	0.49
1:2A:2159:G:C2	1:2A:2160:G:H1'	2.47	0.49
1:2A:1783:A:H5'	1:2A:2608:G:H4'	1.94	0.49
1:2A:258:G:H1	1:2A:268:C:H42	33.54	0.49
1:2A:900:A:H2'	1:2A:901:A:O4'	2.12	0.49
1:2A:927:G:H2'	1:2A:928:G:O4'	2.10	0.49
4:2E:59:VAL:HG21	4:2E:74:PRO:HB3	1.94	0.49
6:2G:109:VAL:HG21	26:24:14:ILE:HG21	1.93	0.49
6:2G:131:TYR:HB3	6:2G:159:VAL:HG13	1.94	0.49
8:2I:127:VAL:HA	8:2I:141:LYS:HA	1.94	0.49
12:2Q:45:GLN:OE1	12:2Q:45:GLN:N	2.44	0.49
25:13:6:VAL:CG1	25:13:54:VAL:HG11	2.42	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:17:35:ARG:NH1	61:17:201:HOH:O	2.44	0.49
1:1A:1129:U:H1'	1:1A:1132:A:H61	1.76	0.49
1:1A:1312:G:O5'	18:1W:15:ARG:NH2	2.45	0.49
4:1E:11:MET:O	4:1E:12:THR:HG23	2.12	0.49
19:1X:40:LYS:HG3	19:1X:51:VAL:HB	1.94	0.49
2:2B:3:C:H2'	2:2B:4:C:C6	2.47	0.49
8:2I:93:THR:HG22	8:2I:119:PRO:HB3	1.92	0.49
14:2S:3:ARG:NH1	14:2S:4:LEU:O	2.45	0.49
16:2U:5:LYS:HE2	61:2U:306:HOH:O	2.12	0.49
17:2V:62:LEU:HD12	17:2V:93:GLU:HG2	1.94	0.49
1:2A:299:A:N1	1:2A:322:A:O2'	2.37	0.49
13:2R:95:THR:HG22	13:2R:116:LEU:HD23	1.95	0.49
25:13:54:VAL:HG12	25:13:55:ARG:N	2.28	0.49
26:14:46:GLN:O	26:14:48:ARG:N	2.44	0.49
28:16:6:ARG:NH1	28:16:26:ASN:HB2	2.27	0.49
14:2S:64:GLU:HG2	26:24:59:PHE:CZ	85.29	0.49
31:29:12:ASP:N	31:29:12:ASP:OD1	2.46	0.49
1:2A:2260:C:OP1	61:2A:3863:HOH:O	2.20	0.49
1:2A:2787:C:H1'	4:2E:62:PRO:HG3	1.92	0.49
1:2A:746:A:H2'	1:2A:2612:C:H5''	1.93	0.49
5:2F:161:GLU:O	5:2F:165:ARG:HG3	2.13	0.49
25:13:49:LYS:O	61:13:201:HOH:O	2.20	0.49
1:1A:1549:U:H2'	1:1A:1550:C:H6	1.77	0.49
1:1A:2880:C:H2'	1:1A:2881:C:O4'	2.13	0.49
1:1A:636:G:N2	1:1A:640:A:O2'	2.45	0.49
1:1A:860:U:H2'	1:1A:861:C:C6	2.48	0.49
1:1A:967:G:O6	61:1A:4160:HOH:O	2.17	0.49
3:1D:204:ILE:O	61:1D:401:HOH:O	2.18	0.49
4:1E:47:VAL:HG23	4:1E:84:PHE:O	2.13	0.49
9:1N:75:TYR:CE2	9:1N:77:GLY:HA2	2.48	0.49
26:24:46:GLN:O	26:24:48:ARG:N	2.45	0.49
1:2A:1316:U:H2'	1:2A:1317:A:C8	2.47	0.49
1:2A:1409:C:O2	1:2A:1491:G:N2	42.43	0.49
1:2A:2243:U:H2'	1:2A:2244:U:C6	2.48	0.49
1:2A:42:G:H2'	1:2A:43:A:O4'	2.12	0.49
1:2A:922:U:H2'	1:2A:923:C:C6	2.48	0.49
24:12:36:ARG:HD3	61:12:107:HOH:O	2.12	0.49
1:1A:1219:A:H4'	1:1A:1220:U:OP1	2.12	0.49
1:1A:1222:A:H2'	1:1A:1222:A:N3	2.28	0.49
1:1A:2108:U:H2'	1:1A:2109:G:C8	2.48	0.49
9:1N:138:LEU:HB3	9:1N:140:VAL:HG13	1.94	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1E:181:LEU:HD11	15:1T:6:LEU:HD23	1.95	0.49
26:24:18:CYS:HB2	26:24:20:ASN:H	1.76	0.49
1:2A:1815:A:OP2	61:2A:3860:HOH:O	2.20	0.49
1:2A:1876:A:H2'	1:2A:1877:A:C8	2.47	0.49
1:2A:2062:A:H2'	1:2A:2062:A:N3	2.27	0.49
1:2A:2115:G:N2	1:2A:2119:A:H5'	2.27	0.49
1:2A:2704:C:H2'	1:2A:2705:A:O4'	2.13	0.49
26:14:15:ILE:HB	26:14:32:TYR:CD1	2.48	0.49
1:1A:1110:C:C4	1:1A:1120:G:N1	2.81	0.49
1:1A:465:G:H2'	1:1A:466:G:C8	2.47	0.49
1:1A:1766:G:H2'	1:1A:1769:G:O6	2.13	0.49
1:1A:211:A:H3'	1:1A:448:U:H5'	1.95	0.49
1:1A:209:G:O2'	1:1A:222:A:N3	2.39	0.49
1:1A:2575:U:H4'	10:1O:28:SER:HA	1.95	0.49
23:21:21:ARG:NH2	61:21:8105:HOH:O	2.45	0.49
1:2A:1062:G:C5	1:2A:1070:A:H1'	2.47	0.49
1:2A:1079:C:C4	1:2A:1080:C:C2	3.00	0.49
1:2A:1165:U:H2'	1:2A:1166:C:C6	2.47	0.49
1:2A:1680:U:N3	1:2A:1764:G:OP2	2.40	0.49
1:2A:2320:A:H2'	1:2A:2320:A:N3	2.27	0.49
1:2A:2689:U:H5'	1:2A:2689:U:O2	2.13	0.49
1:2A:297:C:H2'	1:2A:298:G:O4'	2.13	0.49
2:2B:75:G:H21	21:2Z:85:HIS:CE1	2.31	0.49
29:17:30:VAL:O	29:17:34:ARG:HG2	2.13	0.49
1:1A:2084:A:H2'	1:1A:2084:A:N3	2.26	0.49
20:1Y:23:ARG:HH11	20:1Y:26:LYS:HD2	12.77	0.49
1:2A:1287:A:H8	13:2R:104:ARG:HD3	1.78	0.49
28:16:23:THR:OG1	28:16:24:GLU:N	2.46	0.48
1:1A:1091:A:OP1	1:1A:1091:A:H4'	2.13	0.48
1:1A:2094:G:N2	61:1A:4429:HOH:O	2.45	0.48
1:1A:2326:C:H2'	1:1A:2327:G:C8	2.47	0.48
5:1F:38:ARG:NH2	61:1F:408:HOH:O	2.46	0.48
7:1H:40:GLU:OE2	7:1H:60:ARG:NH1	2.46	0.48
8:1I:115:ALA:HB2	8:1I:131:LYS:HE2	1.95	0.48
21:1Z:141:VAL:HB	21:1Z:144:LEU:HD12	1.95	0.48
1:2A:455:C:N3	1:2A:472:A:H2'	2.28	0.48
2:2B:84:C:OP1	25:23:15:TYR:OH	2.24	0.48
61:2A:4393:HOH:O	5:2F:74:ARG:HG3	2.12	0.48
25:13:3:ARG:NH1	25:13:60:GLU:OE2	2.45	0.48
1:1A:1817:A:H1'	1:1A:1960:A:N6	2.28	0.48
1:1A:1874:C:H5'	3:1D:253:GLN:OE1	2.13	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2157:A:H62	1:1A:2178:G:N2	2.11	0.48
1:1A:337:C:H2'	1:1A:338:A:C8	2.88	0.48
12:1Q:108:GLY:HA3	21:1Z:116:VAL:HG13	1.95	0.48
12:1Q:110:THR:HG23	12:1Q:113:GLN:OE1	2.13	0.48
31:29:27:CYS:SG	31:29:28:GLU:N	2.86	0.48
1:2A:2161:C:HO2'	1:2A:2173:A:HO2'	1.53	0.48
3:2D:101:GLU:OE2	3:2D:103:ARG:HD3	2.13	0.48
1:1A:1539:C:H5	1:1A:2227:G:HO2'	1.61	0.48
1:1A:952:G:O6	61:1A:4166:HOH:O	2.20	0.48
4:1E:59:VAL:HG21	4:1E:74:PRO:HB3	1.94	0.48
1:2A:1292:U:H2'	1:2A:1293:C:C6	2.48	0.48
1:2A:272(I):U:H3	1:2A:363(A):A:H61	1.61	0.48
4:2E:54:GLN:OE1	4:2E:55:ASN:N	2.44	0.48
12:2Q:135:ASP:OD1	12:2Q:136:ALA:N	2.45	0.48
1:1A:230:A:H5''	61:1A:6566:HOH:O	2.13	0.48
1:1A:2710:U:H2'	1:1A:2711:C:C6	2.49	0.48
1:1A:572:A:N6	17:1V:19:LYS:H	2.11	0.48
1:1A:71:U:OP1	61:1A:4163:HOH:O	2.19	0.48
15:1T:16:ARG:HG2	15:1T:18:ASP:OD1	2.14	0.48
15:1T:68:TYR:CE2	57:1T:204:MPD:H51	2.48	0.48
1:2A:1063:G:H2'	1:2A:1065:U:C6	2.48	0.48
1:2A:1292:U:H2'	1:2A:1293:C:H6	1.78	0.48
1:2A:1786:A:H1'	1:2A:1938:A:N6	2.27	0.48
8:2I:77:LEU:HD21	8:2I:100:ALA:HB3	1.93	0.48
31:19:17:ILE:HA	31:19:17:ILE:HD12	1.72	0.48
1:1A:1033:G:O2'	1:1A:1046:A:N3	2.43	0.48
1:1A:2018:C:H4'	1:1A:2019:G:OP1	2.12	0.48
1:1A:794:U:O2	1:1A:2036:A:H1'	2.13	0.48
1:1A:2164:C:C2	1:1A:2171:G:N1	2.81	0.48
1:1A:2326:C:H2'	1:1A:2327:G:H8	1.79	0.48
1:1A:572:A:H61	17:1V:19:LYS:H	1.59	0.48
1:1A:70:A:N7	19:1X:31:HIS:HE1	2.11	0.48
1:1A:91:G:H2'	1:1A:92:C:H6	1.79	0.48
2:1B:106:G:H5'	21:1Z:31:ARG:HG2	1.96	0.48
7:1H:13:LYS:HA	7:1H:14:GLY:HA2	1.60	0.48
1:2A:372:G:H8	23:21:65:SER:O	1.96	0.48
1:2A:1807:G:OP1	61:2A:3861:HOH:O	2.20	0.48
1:2A:2157:G:H5''	1:2A:2158:A:H5'	1.94	0.48
1:2A:2639:A:H2'	1:2A:2640:G:O4'	2.14	0.48
1:2A:373:U:H2'	1:2A:374:A:H8	1.78	0.48
6:2G:77:ILE:HG21	6:2G:80:PHE:CD2	2.48	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1666:G:H1'	10:2O:3:GLN:HE21	1.78	0.48
1:1A:1024:G:H2'	1:1A:1024:G:N3	2.89	0.48
15:1T:51:ARG:NH1	61:1T:306:HOH:O	2.38	0.48
16:1U:36:ARG:NH2	61:1U:307:HOH:O	2.47	0.48
31:29:29:ASN:HB3	31:29:32:HIS:ND1	2.28	0.48
1:2A:2646:C:H2'	1:2A:2647:U:O4'	2.13	0.48
1:2A:2544:G:H1'	1:2A:2646:C:H4'	1.95	0.48
1:2A:495:G:N3	18:2W:61:ASN:ND2	2.58	0.48
1:1A:1103:A:N1	1:1A:1127:U:O4	2.47	0.48
17:1V:21:ARG:HD3	17:1V:91:TYR:CE1	2.48	0.48
20:1Y:6:HIS:H	20:1Y:6:HIS:CD2	2.30	0.48
1:2A:208:C:H2'	1:2A:209:C:C6	2.48	0.48
7:2H:89:ILE:HB	7:2H:129:THR:HA	1.96	0.48
11:2P:95:VAL:CG2	11:2P:125:VAL:HG12	2.44	0.48
1:2A:1287:A:C8	13:2R:104:ARG:HD3	2.48	0.48
12:2Q:138:ASP:OD2	21:2Z:81:ARG:NH1	2.47	0.48
1:1A:1674:G:H2'	1:1A:1675:U:C6	2.49	0.48
1:1A:1814:A:H5'	1:1A:2620:G:H4'	1.96	0.48
7:1H:23:ARG:HD2	7:1H:34:GLU:OE1	2.14	0.48
26:24:48:ARG:HB3	26:24:52:THR:OG1	2.13	0.48
1:2A:1581:G:H2'	1:2A:1582:C:O4'	2.14	0.48
1:2A:251:A:C5	1:2A:252:G:H1'	2.48	0.48
8:2I:31:LEU:HD21	8:2I:38:LEU:HG	1.94	0.48
12:2Q:111:GLU:OE2	12:2Q:133:ARG:NH2	2.46	0.48
14:2S:23:ARG:HH11	14:2S:84:GLN:HB3	1.79	0.48
20:2Y:7:VAL:HG21	20:2Y:72:VAL:HG12	1.96	0.48
6:1G:114:ILE:HG12	6:1G:140:ILE:HG12	1.94	0.48
6:1G:27:ASN:HB3	6:1G:30:GLU:HG3	1.96	0.48
1:2A:1607:C:H4'	1:2A:1608:A:O5'	2.13	0.48
1:2A:2316:C:H2'	1:2A:2317:C:C6	2.48	0.48
1:2A:2391:G:O6	1:2A:2425:A:H8	1.97	0.48
1:2A:2639:A:OP2	61:2A:3864:HOH:O	2.20	0.48
6:2G:115:ARG:HD3	6:2G:136:ARG:HH22	1.78	0.48
1:1A:167:G:OP2	61:1A:4169:HOH:O	2.20	0.48
1:1A:1719:C:OP1	61:1A:4171:HOH:O	2.20	0.48
1:1A:2353:G:H2'	1:1A:2354:C:C6	2.49	0.48
1:1A:303:C:H42	1:1A:385:G:H1	1.62	0.48
26:24:13:ARG:HH12	26:24:23:GLU:HG2	1.78	0.48
1:2A:330:A:HO2'	1:2A:331:A:H8	1.61	0.48
1:2A:539:G:H2'	1:2A:540:C:C6	2.49	0.48
4:2E:36:ARG:NH1	4:2E:85:ASN:OD1	2.47	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:2Y:97:ARG:HB3	20:2Y:106:LEU:HD12	1.94	0.48
1:1A:1793:A:H2'	61:1A:6306:HOH:O	2.14	0.47
1:1A:2175:G:H2'	1:1A:2176:G:C8	2.49	0.47
1:1A:840:A:OP2	1:1A:2093:A:O2'	2.29	0.47
1:1A:1834:A:H4'	3:1D:259:THR:HG23	1.96	0.47
9:1N:62:VAL:HG11	9:1N:66:LYS:HB2	1.95	0.47
1:2A:1079:C:N4	1:2A:1080:C:N3	2.62	0.47
1:2A:1237:A:OP1	61:2A:3867:HOH:O	2.20	0.47
1:2A:1507:A:O2'	1:2A:1508:A:O4'	2.32	0.47
1:2A:1776:G:OP1	61:2A:3866:HOH:O	2.20	0.47
1:2A:2732:G:H3'	1:2A:2733:A:O4'	2.13	0.47
19:2X:65:ARG:HB3	19:2X:70:LEU:HD23	1.96	0.47
1:1A:2255:U:H2'	1:1A:2256:U:C6	2.49	0.47
1:1A:802:C:O2'	1:1A:803:C:H5'	2.14	0.47
5:1F:9:ILE:HG21	5:1F:125:LEU:HD22	1.95	0.47
1:2A:1119:C:H2'	1:2A:1120:G:C8	3.46	0.47
1:2A:1579:A:H2'	1:2A:1580:A:C8	2.48	0.47
1:2A:2657:A:O2'	7:2H:160:LYS:NZ	2.46	0.47
13:2R:44:LEU:HD22	13:2R:48:VAL:HG23	1.96	0.47
4:1E:12:THR:HG21	15:1T:11:GLU:OE2	2.14	0.47
5:1F:51:THR:HB	5:1F:88:VAL:HG11	1.96	0.47
8:1I:9:LEU:HA	8:1I:9:LEU:HD12	1.72	0.47
12:1Q:7:MET:HE3	12:1Q:7:MET:HB2	1.68	0.47
20:1Y:15:VAL:O	20:1Y:22:GLY:N	2.42	0.47
23:21:59:THR:HG23	61:21:8114:HOH:O	2.13	0.47
1:2A:1180:C:H2'	1:2A:1181:C:C6	2.50	0.47
1:2A:2125:G:N2	1:2A:2172:U:H3'	2.29	0.47
1:2A:2564:A:C2	1:2A:2647:U:H4'	2.48	0.47
5:2F:28:ILE:HG23	5:2F:112:MET:HE3	1.95	0.47
5:2F:36:VAL:O	5:2F:40:GLN:HB2	2.14	0.47
6:2G:55:LYS:O	6:2G:59:GLU:N	2.40	0.47
7:2H:45:VAL:HA	7:2H:50:VAL:HG22	1.95	0.47
1:1A:1028:C:O2	1:1A:1033:G:N1	14.85	0.47
1:1A:1053:C:OP1	9:1N:37:LYS:NZ	2.47	0.47
1:1A:1211:U:H2'	1:1A:1212:C:C6	2.50	0.47
1:1A:1217:G:H5'	61:1A:4221:HOH:O	2.14	0.47
1:1A:1766:G:H5'	1:1A:1767:A:OP2	2.15	0.47
1:1A:2804:C:H5'	1:1A:2902:G:N2	2.30	0.47
1:1A:738:C:H2'	1:1A:739:C:H6	2.11	0.47
3:1D:12:SER:HB3	3:1D:208:LYS:HB3	1.97	0.47
21:1Z:103:ARG:HD3	21:1Z:136:PHE:CD1	2.49	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1647:G:H3'	1:2A:1647:G:OP2	2.14	0.47
1:2A:662:G:O2'	1:2A:836:G:OP1	26.72	0.47
10:2O:35:VAL:HG22	10:2O:65:THR:HG23	1.96	0.47
1:1A:1273:G:H3'	1:1A:1274:G:H8	3.03	0.47
1:1A:2584:A:N7	4:1E:144:ARG:HD2	2.30	0.47
7:1H:124:GLU:OE2	7:1H:132:ARG:HD2	2.15	0.47
10:1O:39:ILE:HD12	10:1O:41:ALA:HB2	1.97	0.47
14:1S:14:VAL:O	14:1S:18:ILE:HG12	2.14	0.47
1:2A:2103:C:N4	1:2A:2104:G:O6	2.47	0.47
1:2A:422:A:N7	61:2A:3990:HOH:O	2.35	0.47
1:2A:691:C:OP1	61:2A:3862:HOH:O	2.20	0.47
1:2A:720:C:H2'	1:2A:721:C:H6	1.79	0.47
21:2Z:150:LEU:HB3	21:2Z:171:ILE:HD11	1.96	0.47
1:1A:1004:A:O2'	1:1A:1038:C:O2	54.10	0.47
6:1G:150:ASP:OD1	6:1G:151:ALA:N	2.47	0.47
1:2A:1379:A:H4'	1:2A:1380:G:OP2	2.15	0.47
1:2A:1538:G:H2'	1:2A:1539:G:C8	2.50	0.47
1:2A:271(E):U:H2'	1:2A:271(F):C:C6	2.50	0.47
6:2G:11:TYR:CZ	6:2G:16:ARG:HD3	2.49	0.47
6:2G:82:LEU:HA	6:2G:86:MET:SD	2.55	0.47
15:2T:24:PRO:HA	15:2T:49:VAL:HG23	1.96	0.47
1:2A:1155:A:H5''	16:2U:55:ARG:HD3	1.96	0.47
21:2Z:35:ARG:HA	21:2Z:35:ARG:HD2	1.54	0.47
1:1A:91:G:H2'	1:1A:92:C:C6	2.49	0.47
3:1D:69:ARG:HG2	3:1D:69:ARG:NH1	2.30	0.47
11:1P:112:LEU:HD23	11:1P:113:LYS:N	2.29	0.47
11:1P:76:LYS:NZ	61:1P:309:HOH:O	2.47	0.47
18:1W:68:ARG:HH11	18:1W:111:HIS:HA	1.80	0.47
23:21:76:ARG:HH22	23:21:97:LEU:HB3	1.79	0.47
1:2A:271(L):U:O5'	1:2A:271(L):U:H6	1.98	0.47
1:2A:578:A:H3'	61:2A:4047:HOH:O	2.15	0.47
1:1A:268:G:H5'	23:11:81:LYS:HE2	1.96	0.47
24:12:22:GLU:HG3	24:12:64:LEU:HD11	1.96	0.47
28:16:18:ARG:HD2	28:16:42:TRP:CD1	2.50	0.47
1:1A:2045:G:H4'	1:1A:2629:C:O3'	2.15	0.47
1:1A:2213:G:H5'	1:1A:2214:G:OP2	2.14	0.47
1:1A:2298:A:H4'	1:1A:2299:A:O4'	2.15	0.47
6:1G:77:ILE:HG22	6:1G:80:PHE:H	1.80	0.47
1:2A:82:G:N1	1:2A:103:A:OP2	2.42	0.47
20:2Y:13:VAL:HB	20:2Y:72:VAL:HG13	1.97	0.47
1:1A:1093:G:O2'	1:1A:1094:A:H8	1.97	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2177:G:H3'	1:1A:2178:G:C8	2.50	0.47
1:1A:297:C:H42	1:1A:387:G:H1	1.63	0.47
1:1A:638:U:H5''	58:1F:314:ARG:N	2.30	0.47
6:1G:115:ARG:H	6:1G:136:ARG:NH2	2.12	0.47
8:1I:117:GLU:HG3	8:1I:118:LYS:H	1.80	0.47
1:2A:2134:A:H5''	1:2A:2156:G:H22	1.79	0.47
1:2A:2298:A:N6	1:2A:2318:G:C8	2.82	0.47
1:1A:2053:A:C6	1:1A:2510:C:H1'	2.50	0.47
58:1B:228:ARG:HE	58:1B:228:ARG:HB3	1.64	0.47
6:1G:43:LEU:HB3	6:1G:44:GLY:H	1.58	0.47
15:1T:53:ARG:HB3	15:1T:53:ARG:CZ	2.45	0.47
19:1X:12:VAL:HG21	19:1X:27:THR:HG22	1.96	0.47
1:2A:1410:G:H2'	1:2A:1411:C:H6	1.80	0.47
1:2A:171:G:H2'	1:2A:172:C:C6	2.50	0.47
1:2A:2308:G:H5''	1:2A:2310:A:OP2	2.15	0.47
1:2A:674:G:O2'	5:2F:74:ARG:HD3	2.15	0.47
12:2Q:51:ARG:O	12:2Q:55:VAL:HG12	2.15	0.47
1:1A:2228:G:O2'	1:1A:2229:A:OP1	2.31	0.47
1:1A:2250:G:H2'	1:1A:2250:G:N3	2.29	0.47
1:1A:858:U:H2'	11:1P:21:ARG:HA	1.96	0.47
3:1D:91:ARG:N	61:1D:408:HOH:O	2.40	0.47
11:1P:94:GLU:HA	11:1P:124:LYS:O	2.15	0.47
1:2A:1010:A:OP2	61:2A:3844:HOH:O	2.20	0.47
1:2A:1489:U:HO2'	1:2A:1490:A:H8	1.58	0.47
1:2A:2273:A:H2'	1:2A:2274:A:C8	2.50	0.47
1:2A:2390:U:P	30:28:35:GLN:HE22	2.37	0.47
1:2A:271(P):C:O3'	8:2I:42:SER:OG	2.31	0.47
1:2A:840:C:H2'	1:2A:841:A:C8	2.50	0.47
11:2P:91:PHE:CE1	11:2P:99:LEU:HD21	2.49	0.47
12:2Q:73:PRO:HB3	12:2Q:93:TYR:CE1	2.49	0.47
13:2R:87:TYR:OH	13:2R:117:VAL:O	2.14	0.47
1:1A:1028:C:N3	1:1A:1033:G:C6	13.31	0.46
1:1A:1091:A:O2'	1:1A:1093:G:C4	2.67	0.46
1:1A:131:C:H2'	1:1A:132:C:C6	2.86	0.46
2:1B:66:A:N6	2:1B:108:U:H2'	2.29	0.46
6:1G:135:LEU:O	6:1G:154:GLY:HA3	2.15	0.46
27:25:15:ARG:NH1	61:25:601:HOH:O	2.33	0.46
1:2A:1503:U:H2'	1:2A:1504:C:H6	1.79	0.46
1:2A:2109:U:O2	1:2A:2181:G:N2	2.48	0.46
1:2A:51:G:H4'	1:2A:52:A:H5'	1.97	0.46
1:2A:856:C:H2'	1:2A:857:C:C6	2.50	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2S:26:LEU:HD22	14:2S:87:PHE:HD1	1.80	0.46
22:10:43:THR:OG1	22:10:46:LYS:HG2	2.13	0.46
1:1A:2169:G:H2'	1:1A:2170:G:O4'	2.15	0.46
1:1A:2164:C:N3	1:1A:2171:G:C6	2.84	0.46
1:1A:2441:G:OP1	61:1A:4109:HOH:O	2.21	0.46
1:1A:2490:A:OP2	31:19:2:LYS:NZ	2.39	0.46
1:1A:265:U:H2'	1:1A:266:C:C6	2.50	0.46
1:1A:560:C:O3'	16:1U:53:ARG:NH1	2.48	0.46
1:1A:2694:U:O2'	15:1T:58:ASN:ND2	2.48	0.46
1:2A:1817:G:OP1	3:2D:88:ARG:NH2	2.41	0.46
1:1A:1118:C:N4	1:1A:1144:A:OP2	2.49	0.46
1:1A:2186:C:H3'	1:1A:2187:G:C8	2.51	0.46
1:1A:2376:C:H2'	1:1A:2377:G:O4'	2.14	0.46
1:1A:2602:A:O3'	3:1D:239:ARG:NH2	2.48	0.46
11:2P:50:ARG:HD3	30:28:7:HIS:CD2	2.50	0.46
1:2A:1506:C:H2'	1:2A:1507:A:H5'	1.96	0.46
1:2A:2684:U:OP2	61:2A:3865:HOH:O	2.20	0.46
1:2A:2749:A:OP1	7:2H:3:ARG:NH1	2.48	0.46
1:2A:747:U:O2	1:2A:2014:A:H1'	2.15	0.46
4:2E:79:ARG:HD3	4:2E:79:ARG:HA	1.76	0.46
26:14:62:ARG:HD3	26:14:62:ARG:HA	1.57	0.46
1:1A:1104:G:O6	1:1A:1126:C:N3	2.49	0.46
1:1A:1210:G:H2'	1:1A:1211:U:C6	2.51	0.46
1:1A:1343:C:H5''	61:1A:4124:HOH:O	2.15	0.46
1:1A:1604:C:H5''	1:1A:1605:A:OP2	2.16	0.46
20:1Y:90:LEU:HB3	20:1Y:92:ASN:HD22	1.80	0.46
26:24:40:HIS:HB3	26:24:43:TYR:CE2	2.50	0.46
1:2A:1360:A:H2'	1:2A:1361:G:O4'	2.27	0.46
1:2A:2119:A:O2'	1:2A:2120:G:H5'	2.16	0.46
1:2A:2364:C:H2'	1:2A:2365:G:O4'	2.15	0.46
1:2A:2377:A:H2'	1:2A:2378:A:C8	2.50	0.46
1:2A:271(D):G:H2'	1:2A:271(E):U:C6	2.50	0.46
1:2A:644:A:H4'	1:2A:645:C:H5	1.80	0.46
8:2I:64:GLU:O	8:2I:68:LEU:HB2	2.15	0.46
18:2W:45:TYR:OH	18:2W:49:LYS:NZ	2.33	0.46
26:14:56:VAL:HG22	26:14:60:GLN:OE1	2.15	0.46
1:1A:1008:U:H2'	1:1A:1009:C:C6	2.50	0.46
1:1A:1102:G:N2	1:1A:1150:C:N3	2.64	0.46
1:1A:272:U:H4'	8:1I:50:ARG:NH2	2.28	0.46
1:1A:2762:A:OP1	7:1H:3:ARG:NH1	2.48	0.46
1:2A:2630:G:H2'	1:2A:2631:G:O4'	2.16	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2D:145:VAL:HG12	3:2D:146:GLU:O	2.16	0.46
11:2P:82:GLY:HA2	11:2P:113:LYS:O	2.15	0.46
16:2U:106:PHE:O	16:2U:110:VAL:HG23	2.15	0.46
25:13:44:ARG:O	25:13:48:GLU:HG3	2.15	0.46
1:1A:2623:U:C4	27:15:3:LYS:HG2	2.51	0.46
1:1A:1355:G:OP1	29:17:9:ARG:HG3	2.15	0.46
1:1A:1144:A:H2'	1:1A:1145:G:O4'	2.15	0.46
1:1A:1733:C:H2'	1:1A:1734:G:O4'	2.16	0.46
1:1A:1753:U:OP1	61:1A:4168:HOH:O	2.20	0.46
1:1A:986:A:H2'	1:1A:987:G:O4'	2.46	0.46
5:1F:184:TYR:CE2	5:1F:188:ARG:HD2	2.50	0.46
1:1A:2331:G:N1	14:1S:3:ARG:HA	2.30	0.46
19:1X:53:LYS:HB3	19:1X:82:GLN:HB3	1.96	0.46
20:1Y:99:CYS:HB2	20:1Y:106:LEU:HD21	1.98	0.46
1:2A:1002:G:H2'	1:2A:1003:G:O4'	2.16	0.46
1:2A:2092:U:H4'	1:2A:2093:G:O5'	2.16	0.46
1:2A:2484:G:C2	1:2A:2485:G:C8	3.03	0.46
5:2F:207:GLY:O	61:2F:3102:HOH:O	2.20	0.46
13:2R:67:LEU:HD13	13:2R:76:VAL:HG21	1.98	0.46
14:2S:10:ARG:HH21	14:2S:91:PRO:HB2	1.81	0.46
15:2T:29:ARG:NH2	15:2T:46:GLU:OE1	2.48	0.46
16:2U:11:ARG:O	16:2U:15:LYS:HG3	2.15	0.46
17:2V:43:GLU:OE1	17:2V:43:GLU:N	2.48	0.46
21:2Z:5:LEU:HB3	21:2Z:59:LEU:HD23	1.98	0.46
1:1A:1221:G:H21	1:1A:1223:C:P	2.38	0.46
1:1A:1220:U:H1'	1:1A:1221:G:OP1	2.16	0.46
1:1A:1617:A:H2'	1:1A:1618:A:C8	2.50	0.46
1:1A:2299:A:O2'	1:1A:2300:A:H3'	2.15	0.46
1:1A:238:C:O2	30:18:12:LYS:NZ	2.37	0.46
17:1V:14:VAL:HB	17:1V:96:ILE:HG13	1.98	0.46
17:1V:8:GLY:O	17:1V:10:LYS:NZ	2.43	0.46
18:1W:68:ARG:HH12	18:1W:112:GLY:H	1.64	0.46
21:1Z:19:ARG:NH1	21:1Z:84:GLU:O	2.49	0.46
1:2A:2383:G:OP2	30:28:37:SER:HB2	2.16	0.46
1:2A:1065:U:H4'	1:2A:1066:U:O5'	2.16	0.46
1:2A:514:A:N3	1:2A:581:C:O2'	2.46	0.46
3:2D:133:LEU:HD23	3:2D:136:ILE:HD12	1.97	0.46
6:2G:32:PRO:HB3	6:2G:163:ALA:HB2	1.98	0.46
1:1A:1715:A:H4'	1:1A:1716:A:O5'	2.16	0.46
1:1A:172:C:N4	1:1A:202:A:H61	2.14	0.46
4:1E:143:ASN:HD22	4:1E:147:PRO:CD	2.28	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1003:U:H5''	12:1Q:14:ARG:HD3	1.97	0.46
1:1A:926:G:O6	20:1Y:87:LYS:HE2	157.80	0.46
25:23:57:GLU:HG2	25:23:59:VAL:HG13	1.97	0.46
1:2A:1365:A:O2'	23:21:11:ARG:NH1	2.49	0.46
1:2A:2723:C:OP1	13:2R:3:HIS:ND1	2.30	0.46
1:2A:952:G:OP1	12:2Q:16:ARG:NH2	2.47	0.46
2:2B:61:G:H2'	2:2B:62:C:C6	2.51	0.46
6:2G:39:ILE:O	6:2G:91:ARG:HB2	2.16	0.46
7:2H:117:PRO:HG3	7:2H:123:PHE:CE2	2.51	0.46
1:1A:1335:C:H2'	1:1A:1336:C:C6	2.51	0.46
1:1A:2125:C:N3	1:1A:2208:G:N2	2.49	0.46
1:1A:2138:G:P	1:1A:2188:G:H21	2.38	0.46
17:1V:2:PHE:CE2	17:1V:41:GLY:HA3	2.51	0.46
21:1Z:146:ILE:HA	21:1Z:147:GLY:HA2	1.68	0.46
1:2A:1014:U:H2'	1:2A:1015:G:C8	2.48	0.46
1:2A:2321:G:O2'	1:2A:2322:A:OP1	2.27	0.46
1:2A:2782:G:OP2	61:2A:3868:HOH:O	2.21	0.46
1:2A:384:U:H2'	1:2A:385:C:H6	1.79	0.46
1:2A:834:C:O2	1:2A:852:G:N2	38.67	0.46
7:2H:98:LEU:HD12	7:2H:102:ALA:O	2.15	0.46
8:2I:77:LEU:HD13	8:2I:101:LEU:HD23	1.97	0.46
13:2R:72:ASP:OD1	61:2R:301:HOH:O	2.21	0.46
1:2A:2319:G:H1	14:2S:3:ARG:HA	1.80	0.46
1:2A:996:A:H4'	16:2U:91:ASP:OD2	2.16	0.46
30:18:23:VAL:HG13	30:18:47:LYS:HB3	1.98	0.46
1:1A:1405:A:H61	1:1A:1418:U:H3	1.63	0.46
1:1A:2136:A:H3'	1:1A:2137:G:H8	1.79	0.46
1:1A:329:U:H2'	1:1A:330:U:C6	2.51	0.46
1:1A:580:U:H2'	1:1A:581:G:O4'	2.70	0.46
1:1A:928:G:H2'	1:1A:929:G:O4'	2.16	0.46
6:1G:11:TYR:HA	6:1G:15:VAL:HB	1.98	0.46
1:2A:1491:G:N2	1:2A:1913:A:H2	104.94	0.46
1:2A:2310:A:H61	6:2G:79:ASN:HD22	1.64	0.46
1:2A:2849:U:H4'	1:2A:2868:A:C2	2.51	0.46
1:2A:69:C:O2	1:2A:73:A:O2'	2.30	0.46
16:2U:91:ASP:N	17:2V:11:GLN:OE1	2.38	0.46
1:1A:2205:C:H2'	1:1A:2206:G:C8	2.51	0.45
6:1G:131:TYR:HB3	6:1G:159:VAL:HG13	1.97	0.45
14:1S:10:ARG:O	14:1S:14:VAL:HG13	2.15	0.45
1:2A:1025:G:C4	1:2A:1135:C:H1'	2.51	0.45
1:2A:2315:G:H2'	1:2A:2316:C:H6	1.80	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2648:C:H2'	1:2A:2649:U:C6	2.51	0.45
1:2A:2712:U:H2'	1:2A:2714:G:H5''	1.98	0.45
9:2N:104:LYS:HE2	9:2N:117:PHE:CZ	2.50	0.45
13:2R:36:THR:HG22	13:2R:37:THR:H	1.81	0.45
21:2Z:110:GLY:HA3	21:2Z:174:VAL:HG11	1.97	0.45
25:13:7:LYS:HE3	25:13:32:GLN:NE2	2.30	0.45
1:1A:2050:U:H2'	1:1A:2051:G:O4'	2.15	0.45
1:1A:2245:U:H2'	1:1A:2246:G:C8	2.52	0.45
1:1A:2662:U:H2'	1:1A:2663:C:C6	2.50	0.45
1:1A:268:G:O2'	1:1A:269:G:OP2	2.30	0.45
1:1A:2701:U:H4'	1:1A:2702:C:H5'	1.97	0.45
1:1A:733:G:OP2	61:1A:4170:HOH:O	2.20	0.45
1:1A:795:G:C8	18:1W:89:ALA:HB1	2.51	0.45
6:1G:77:ILE:HG21	6:1G:80:PHE:CD2	2.52	0.45
7:1H:17:VAL:HG22	7:1H:26:VAL:HG22	1.97	0.45
7:1H:3:ARG:NH1	7:1H:5:GLY:H	2.13	0.45
12:1Q:2:LEU:HG	12:1Q:69:PHE:CE1	2.51	0.45
20:1Y:15:VAL:HG21	20:1Y:42:VAL:HG11	1.98	0.45
1:2A:1092:C:O2	1:2A:1092:C:H2'	2.17	0.45
1:2A:1366:A:H2'	1:2A:1367:A:O4'	2.16	0.45
1:2A:2261:C:H1'	1:2A:2388:A:N3	2.30	0.45
6:2G:27:ASN:OD1	6:2G:28:VAL:N	2.48	0.45
21:2Z:152:ALA:O	21:2Z:155:LEU:HB2	2.16	0.45
1:1A:1841:A:H2'	1:1A:1842:G:O4'	2.16	0.45
1:1A:965:G:N2	1:1A:2281:A:OP2	2.49	0.45
7:1H:24:VAL:HG22	7:1H:35:VAL:HB	1.98	0.45
17:1V:22:VAL:HG23	17:1V:23:GLU:O	2.15	0.45
26:24:57:GLU:HA	26:24:58:ARG:HA	1.44	0.45
30:28:62:LEU:HB3	30:28:65:GLU:HG2	1.99	0.45
1:2A:259:G:H2'	1:2A:260:G:O4'	2.47	0.45
1:2A:328:U:H4'	20:2Y:68:HIS:CG	2.51	0.45
1:2A:862:G:H2'	1:2A:863:A:O4'	2.16	0.45
6:2G:16:ARG:HH22	6:2G:28:VAL:HB	1.82	0.45
24:12:53:LEU:HD23	24:12:53:LEU:HA	1.72	0.45
30:18:23:VAL:CG1	30:18:47:LYS:HD3	2.47	0.45
1:1A:1541:A:C6	1:1A:1542:A:C6	3.04	0.45
3:1D:71:ASP:HB3	3:1D:103:ARG:HH22	1.80	0.45
3:1D:3:VAL:HG13	3:1D:17:THR:HB	1.98	0.45
6:1G:7:LEU:HA	6:1G:7:LEU:HD23	1.75	0.45
10:1O:64:ARG:NH2	10:1O:99:PHE:O	2.49	0.45
1:1A:1700:G:H3'	13:1R:2:ARG:HD3	1.98	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2830:A:P	13:1R:2:ARG:HH22	2.39	0.45
1:1A:582:G:H22	16:1U:49:HIS:CE1	2.35	0.45
16:1U:81:HIS:CE1	16:1U:85:LYS:HD2	2.51	0.45
1:2A:517:C:OP1	27:25:16:ARG:NH2	2.49	0.45
1:2A:1204:A:H61	1:2A:1240:U:H2'	1.81	0.45
1:2A:635:C:O2'	1:2A:639:U:OP1	2.23	0.45
1:2A:740:U:H2'	1:2A:741:G:C8	2.52	0.45
3:2D:102:LYS:C	3:2D:103:ARG:HG2	2.36	0.45
16:2U:9:VAL:O	16:2U:13:LYS:HG3	2.17	0.45
17:1V:6:LYS:HG2	61:1V:3118:HOH:O	2.16	0.45
1:2A:1598:C:H2'	1:2A:1599:C:H6	1.82	0.45
1:2A:2168:G:H2'	1:2A:2170:A:OP2	2.17	0.45
1:2A:2473:U:H2'	1:2A:2473:U:O2	2.17	0.45
1:2A:2872:G:C2	1:2A:2873:A:N6	2.85	0.45
57:2A:3710:MPD:HM2	61:2A:4463:HOH:O	2.15	0.45
1:2A:375:C:H2'	1:2A:376:C:C6	2.51	0.45
4:2E:52:LEU:H	4:2E:76:ARG:HB2	1.80	0.45
15:2T:64:ARG:HB2	15:2T:73:GLU:HG2	1.99	0.45
1:1A:1119:A:N3	1:1A:1119:A:H2'	2.32	0.45
1:1A:1740:U:H1'	3:1D:14:ARG:NH1	2.32	0.45
1:1A:2119:C:H2'	1:1A:2120:U:O4'	2.17	0.45
1:1A:402:C:H2'	1:1A:403:C:C6	2.52	0.45
5:1F:64:ILE:HD11	5:1F:75:HIS:HB2	1.97	0.45
19:1X:76:ARG:HG3	61:1X:201:HOH:O	2.17	0.45
21:1Z:31:ARG:H	21:1Z:31:ARG:HG3	1.46	0.45
1:2A:1110:G:H1'	1:2A:1111:A:H8	1.77	0.45
1:2A:2262:U:H4'	1:2A:2328:A:C2	2.52	0.45
1:2A:445:C:OP1	16:2U:2:PRO:HA	2.16	0.45
20:2Y:39:VAL:HB	20:2Y:42:VAL:HB	1.99	0.45
1:1A:2155:G:H3'	1:1A:2179:G:N2	2.31	0.45
1:2A:1533:G:N2	1:2A:1536:C:N3	2.64	0.45
1:2A:2497:A:H5''	61:2A:4548:HOH:O	2.16	0.45
11:2P:99:LEU:HD23	11:2P:100:LEU:HD23	1.98	0.45
1:2A:994:C:H3'	16:2U:54:LYS:HE3	1.98	0.45
1:1A:1124:U:C4	1:1A:1134:A:H5''	2.52	0.45
1:1A:1221:G:N2	1:1A:1223:C:OP1	2.40	0.45
1:1A:1405:A:N6	1:1A:1418:U:H3	2.14	0.45
1:1A:1594:C:H2'	1:1A:1595:C:H6	1.82	0.45
1:1A:1942:4OC:HM22	1:1A:1943:G:H5'	1.99	0.45
1:1A:2455:C:OP1	5:1F:68:LYS:HD3	2.17	0.45
1:1A:2699:U:H2'	1:1A:2700:U:O4'	2.16	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:1P:94:GLU:HG3	11:1P:124:LYS:HD3	1.99	0.45
1:1A:2347:A:OP2	14:1S:13:ARG:HG3	2.16	0.45
1:2A:1047:G:HO2'	1:2A:1048:A:H8	1.63	0.45
1:2A:2298:A:H2'	1:2A:2299:G:O4'	2.16	0.45
1:2A:623:G:H2'	1:2A:624:C:C6	2.52	0.45
1:2A:1224:C:O2'	17:2V:85:LYS:HA	2.17	0.45
1:1A:2190:G:C2	1:1A:2193:A:C8	3.05	0.45
4:1E:7:VAL:HG13	4:1E:27:LEU:HB3	1.99	0.45
1:2A:1098:A:H3'	1:2A:1099:G:H8	1.82	0.45
1:2A:1818:U:O4	3:2D:154:LYS:HD2	2.17	0.45
4:2E:101:ARG:NH1	4:2E:171:GLU:HB2	2.32	0.45
6:2G:11:TYR:HA	6:2G:15:VAL:HB	1.98	0.45
9:2N:60:ILE:HG13	9:2N:61:ARG:H	1.80	0.45
14:2S:85:VAL:HG11	14:2S:110:LEU:HG	1.99	0.45
20:2Y:38:ILE:HD13	20:2Y:66:PRO:HA	1.97	0.45
1:1A:1417:G:H2'	1:1A:1418:U:H5	1.82	0.45
1:1A:215:G:N2	1:1A:217:A:H62	2.15	0.45
12:1Q:21:THR:HG23	12:1Q:99:PRO:O	2.17	0.45
21:1Z:75:ASN:O	21:1Z:84:GLU:HG2	2.17	0.45
22:20:10:THR:O	61:20:5001:HOH:O	2.21	0.45
1:2A:1035:U:H2'	1:2A:1036:G:C8	2.52	0.45
1:2A:1831:G:H2'	1:2A:1832:C:C6	2.52	0.45
1:2A:471:A:H8	1:2A:471:A:O5'	2.00	0.45
1:2A:874:G:O2'	21:2Z:120:ILE:HD11	2.17	0.45
2:2B:17:C:H2'	2:2B:18:G:O4'	2.16	0.45
7:2H:140:LYS:HB2	7:2H:140:LYS:HE3	1.82	0.45
12:2Q:111:GLU:O	12:2Q:115:MET:HG2	2.17	0.45
15:2T:95:ARG:NH1	15:2T:95:ARG:HG2	2.32	0.45
23:11:69:LYS:HA	23:11:69:LYS:HD2	1.81	0.44
25:13:3:ARG:HD2	25:13:60:GLU:CD	2.37	0.44
2:1B:93:G:OP1	21:1Z:80:ARG:NH2	2.48	0.44
10:1O:64:ARG:HB2	10:1O:79:PHE:CG	2.52	0.44
1:1A:416:G:O6	11:1P:70:GLN:HB3	2.17	0.44
26:24:53:GLU:HG2	26:24:55:ARG:H	1.81	0.44
1:2A:1589:C:H2'	1:2A:1590:U:H6	1.82	0.44
1:2A:184:C:H2'	1:2A:185:U:C6	2.52	0.44
1:2A:1916:A:H2'	1:2A:1917:PSU:O4'	2.17	0.44
1:2A:2788:C:N3	1:2A:2789:C:N4	2.64	0.44
1:2A:422:A:H2'	1:2A:423:A:C8	2.53	0.44
4:2E:9:VAL:HG22	4:2E:25:VAL:HB	1.98	0.44
6:2G:15:VAL:HA	6:2G:175:LEU:HD23	1.99	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:2O:105:GLU:OE1	10:2O:105:GLU:N	2.48	0.44
1:1A:1296:G:N7	11:1P:18:ARG:NH1	2.61	0.44
1:1A:1829:U:H5'	3:1D:259:THR:CG2	2.39	0.44
1:1A:2495:C:N3	12:1Q:124:LYS:NZ	2.55	0.44
1:1A:2724:U:OP1	1:1A:2727:G:H4'	2.17	0.44
1:1A:924:U:C2'	1:1A:925:A:H5''	2.48	0.44
4:1E:125:GLY:O	61:1E:3101:HOH:O	2.21	0.44
5:1F:102:PRO:O	5:1F:106:ARG:HG3	2.17	0.44
6:1G:7:LEU:HD22	6:1G:176:LEU:HD22	1.98	0.44
6:1G:32:PRO:HB3	6:1G:163:ALA:HB2	1.98	0.44
9:1N:67:LEU:O	9:1N:88:GLU:HG3	2.17	0.44
20:1Y:47:LYS:HD2	20:1Y:63:LYS:HE3	1.98	0.44
1:2A:1514:U:H2'	1:2A:1515:G:C8	2.50	0.44
1:2A:1583:A:OP1	1:2A:1584:C:H5	2.00	0.44
1:2A:2693:A:H2'	1:2A:2694:G:H8	1.82	0.44
1:2A:335:C:H4'	20:2Y:73:ARG:HD2	1.99	0.44
1:2A:839:U:H5''	1:2A:840:C:H5	6.27	0.44
3:2D:16:MET:HG3	3:2D:206:LEU:O	2.16	0.44
5:2F:32:LEU:O	5:2F:36:VAL:HG23	2.17	0.44
1:1A:1549:U:H2'	1:1A:1550:C:C6	2.51	0.44
1:1A:208:G:OP2	61:1A:4172:HOH:O	2.21	0.44
1:1A:312:C:H2'	1:1A:313:A:C8	2.52	0.44
1:1A:843:C:H2'	1:1A:844:C:C6	2.53	0.44
3:1D:260:ARG:NH2	3:1D:266:SER:OG	2.48	0.44
6:1G:106:LEU:HA	6:1G:110:ALA:HB3	1.99	0.44
1:1A:272:U:H5'	8:1I:50:ARG:HH12	1.83	0.44
9:1N:62:VAL:CG1	9:1N:66:LYS:HB2	2.46	0.44
1:2A:1085:A:N3	1:2A:1085:A:H2'	2.33	0.44
1:2A:2114:A:C2	1:2A:2115:G:H1'	2.52	0.44
1:2A:2184:G:H2'	1:2A:2185:C:O4'	2.17	0.44
6:2G:139:LEU:HA	6:2G:144:ILE:HB	1.99	0.44
16:2U:88:ILE:HG22	16:2U:90:VAL:HG23	1.99	0.44
26:14:15:ILE:HB	26:14:32:TYR:HD1	1.81	0.44
27:15:34:PRO:HG2	27:15:35:GLU:OE1	2.17	0.44
1:1A:1338:U:H2'	1:1A:1339:C:C6	2.52	0.44
1:1A:1374:G:O2'	1:1A:1375:U:H2'	2.18	0.44
1:1A:2211:U:H2'	1:1A:2212:G:H8	1.82	0.44
1:1A:2579:G:H2'	1:1A:2580:C:C6	2.52	0.44
4:1E:9:VAL:HG22	4:1E:25:VAL:HB	1.98	0.44
6:1G:43:LEU:C	6:1G:45:GLU:H	2.21	0.44
1:2A:1038:C:O5'	1:2A:1038:C:H6	4.01	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1057:A:HO2'	1:2A:1058:G:P	2.40	0.44
1:2A:2811:G:OP1	4:2E:60:ASN:HB2	2.17	0.44
1:2A:760:G:H2'	1:2A:761:A:O4'	2.17	0.44
1:2A:782:A:H5'	1:2A:783:A:N7	2.33	0.44
4:2E:5:LEU:HD11	4:2E:79:ARG:HB2	2.00	0.44
20:2Y:102:CYS:SG	20:2Y:103:GLY:N	2.91	0.44
31:19:25:VAL:O	31:19:33:LYS:HA	2.17	0.44
1:1A:1109:G:H5''	1:1A:1111:U:H5	1.83	0.44
1:1A:2717:A:H2'	1:1A:2718:G:O4'	2.18	0.44
1:2A:1448:G:H1'	1:2A:1528:A:N1	2.32	0.44
5:2F:33:LEU:HA	5:2F:33:LEU:HD12	1.78	0.44
8:2I:26:ALA:O	8:2I:31:LEU:HB2	2.17	0.44
1:1A:231:G:C8	30:18:5:LYS:HG2	2.52	0.44
1:1A:1226:C:H4'	1:1A:1227:A:OP1	4.92	0.44
1:1A:2357:G:N3	1:1A:2393:C:H2'	2.33	0.44
61:1A:5741:HOH:O	3:1D:229:VAL:HG22	2.17	0.44
4:1E:170:LEU:HB3	4:1E:184:VAL:CG2	2.48	0.44
5:1F:140:LEU:HD11	5:1F:170:LEU:HD11	2.00	0.44
5:1F:183:VAL:HG13	61:1F:437:HOH:O	2.16	0.44
6:1G:5:VAL:CG2	6:1G:8:LYS:H	2.30	0.44
9:1N:99:LEU:HD23	9:1N:99:LEU:HA	1.76	0.44
14:1S:110:LEU:HA	14:1S:110:LEU:HD12	1.73	0.44
15:1T:37:GLY:HA2	15:1T:38:ASN:HA	1.62	0.44
1:2A:1131:G:O6	1:2A:2040:C:H1'	2.17	0.44
1:2A:1991:U:H2'	1:2A:1992:G:H5''	1.98	0.44
1:2A:2142:C:H2'	1:2A:2143:C:C6	2.53	0.44
1:2A:720:C:H2'	1:2A:721:C:C6	2.51	0.44
1:2A:443:A:N7	5:2F:45:ARG:HG2	2.33	0.44
10:2O:15:GLY:HA2	10:2O:47:ILE:HD11	1.99	0.44
15:2T:53:ARG:CZ	15:2T:53:ARG:HB3	2.46	0.44
1:1A:1110:C:OP2	1:1A:1111:U:H6	2.01	0.44
1:1A:1140:U:C2	1:1A:1142:A:H5''	2.53	0.44
1:1A:116:A:C8	1:1A:117:A:C8	3.05	0.44
1:1A:2334:A:H2'	1:1A:2335:G:O4'	2.17	0.44
1:1A:742:G:OP1	1:1A:1426:G:O2'	2.28	0.44
6:1G:58:GLN:O	6:1G:62:LEU:HG	2.17	0.44
5:1F:34:TRP:NE1	11:1P:8:PRO:HD3	2.32	0.44
6:2G:142:PRO:O	26:24:31:ILE:HD13	2.17	0.44
31:29:3:VAL:HA	31:29:35:ARG:O	2.17	0.44
1:2A:1032:A:H2	1:2A:1122:G:H22	1.65	0.44
1:2A:1495:A:H2'	1:2A:1496:A:C8	2.53	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2143:C:H2'	1:2A:2144:U:H5'	2.00	0.44
1:2A:2693:A:H2'	1:2A:2694:G:C8	2.53	0.44
1:2A:875:G:H2'	1:2A:876:C:O4'	2.17	0.44
4:2E:28:ALA:HB3	4:2E:93:VAL:CG1	2.46	0.44
8:2I:62:LYS:HG2	8:2I:133:HIS:CE1	2.53	0.44
17:2V:31:ALA:O	17:2V:61:VAL:HG22	2.17	0.44
1:1A:2137:G:N3	1:1A:2139:A:N6	2.66	0.44
1:1A:2135:U:O4	1:1A:2190:G:H4'	2.17	0.44
5:1F:129:PHE:O	5:1F:132:VAL:HG13	2.18	0.44
15:1T:108:ARG:HA	15:1T:111:ARG:NH1	2.33	0.44
1:2A:1097:U:H2'	1:2A:1098:A:O4'	2.17	0.44
1:2A:108:U:H2'	1:2A:109:G:C8	2.53	0.44
1:2A:1518:U:H2'	1:2A:1519:G:O4'	2.18	0.44
9:2N:60:ILE:HG13	9:2N:61:ARG:N	2.33	0.44
11:2P:38:GLN:HB3	11:2P:45:LEU:HD23	2.00	0.44
16:2U:8:VAL:HG13	16:2U:11:ARG:NH2	2.32	0.44
20:2Y:43:ASN:HD22	20:2Y:67:LEU:HD21	1.83	0.44
1:1A:1099:C:O2	1:1A:1152:G:N1	2.49	0.44
1:1A:2411:G:H3'	61:1A:4150:HOH:O	2.17	0.44
12:1Q:35:VAL:CG1	12:1Q:130:LYS:HB3	2.48	0.44
13:1R:79:LEU:HA	13:1R:83:ILE:HB	2.00	0.44
21:1Z:125:LEU:HB3	21:1Z:165:VAL:HG13	2.00	0.44
26:24:68:ARG:O	26:24:69:LYS:HB3	2.18	0.44
1:2A:102:G:OP1	24:22:7:ARG:NH2	2.50	0.44
1:2A:1939:5MU:OP1	1:2A:2604:U:O2'	2.36	0.44
1:2A:833:U:O2	11:2P:55:ARG:NH1	2.49	0.44
6:2G:12:TYR:HA	6:2G:16:ARG:HG3	2.00	0.44
9:2N:34:LEU:HD12	9:2N:34:LEU:HA	1.88	0.44
21:2Z:151:HIS:HA	21:2Z:170:THR:HA	1.99	0.44
21:2Z:29:TYR:HB3	21:2Z:34:ASN:HD22	1.83	0.44
1:1A:1314:A:H2'	1:1A:1315:A:O4'	2.18	0.43
1:1A:1630:A:H5'	1:1A:1631:C:OP1	2.18	0.43
1:1A:2162:C:N3	1:1A:2173:G:O6	2.51	0.43
1:1A:2371:C:H2'	1:1A:2372:A:O4'	2.18	0.43
1:1A:2874:G:OP1	15:1T:119:LYS:HD2	2.18	0.43
1:1A:387:G:H2'	1:1A:388:A:H8	1.83	0.43
5:1F:178:PRO:HB2	5:1F:201:VAL:CG2	2.48	0.43
12:1Q:58:PHE:O	12:1Q:60:ARG:N	2.50	0.43
1:2A:1016:G:C4	1:2A:1017:G:C8	3.06	0.43
1:2A:2141:G:C6	1:2A:2151:G:C6	3.06	0.43
1:2A:2323:G:H1	1:2A:2332:U:H3	1.66	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2051:A:H5'	1:2A:2578:G:O4'	2.17	0.43
1:2A:2611:U:H6	1:2A:2611:U:H5'	1.83	0.43
1:2A:2836:U:H2'	1:2A:2837:G:C8	2.53	0.43
1:2A:1772:G:O6	57:2A:3710:MPD:H32	2.18	0.43
7:2H:13:LYS:HA	7:2H:14:GLY:HA2	1.59	0.43
20:2Y:73:ARG:HG2	20:2Y:73:ARG:HH11	1.82	0.43
21:2Z:182:LYS:HD2	61:2Z:306:HOH:O	2.18	0.43
24:12:32:LEU:HD22	24:12:36:ARG:NH1	2.34	0.43
25:13:55:ARG:NH1	61:13:202:HOH:O	2.51	0.43
1:1A:1508:G:H2'	1:1A:1509:C:O4'	2.36	0.43
1:1A:1686:U:H4'	1:1A:2711:C:H4'	2.00	0.43
1:1A:2346:G:H5'	14:1S:9:ARG:HG2	1.99	0.43
1:1A:936:C:H2'	1:1A:937:A:O4'	4.43	0.43
7:1H:84:SER:HA	7:1H:133:VAL:O	2.18	0.43
17:1V:58:VAL:HG12	17:1V:97:LYS:HB2	1.99	0.43
20:1Y:92:ASN:HB2	20:1Y:94:LYS:N	2.19	0.43
1:2A:1504:C:H2'	1:2A:1505:C:C6	2.54	0.43
1:2A:244:A:C2	1:2A:255:A:C4	3.06	0.43
3:2D:84:TYR:HE2	3:2D:86:PRO:HB3	1.83	0.43
2:2B:42:C:N4	6:2G:91:ARG:HH22	2.16	0.43
9:2N:30:ILE:HG23	9:2N:52:VAL:HG11	2.00	0.43
13:2R:63:ARG:O	13:2R:67:LEU:HB2	2.18	0.43
16:2U:34:LYS:HA	16:2U:34:LYS:HD2	1.70	0.43
26:14:49:PHE:HB3	26:14:50:VAL:H	1.47	0.43
31:19:25:VAL:HB	31:19:34:GLN:HB2	1.99	0.43
1:1A:123:G:O2'	29:17:48:LYS:HE3	2.17	0.43
1:1A:1634:C:H2'	1:1A:1635:C:C6	2.52	0.43
1:1A:1815:A:H4'	1:1A:1816:A:O5'	2.18	0.43
1:1A:2071:G:H5'	61:1A:4313:HOH:O	2.17	0.43
1:1A:2533:C:C4	1:1A:2534:U:C4	3.06	0.43
1:1A:2889:C:OP2	61:1A:4173:HOH:O	2.21	0.43
1:1A:637:U:H5'	1:1A:640:A:N6	2.33	0.43
1:1A:929:G:H1	1:1A:940:C:H42	1.66	0.43
1:1A:2858:G:H3'	15:1T:95:ARG:O	2.18	0.43
26:24:8:LYS:O	26:24:27:THR:HG22	2.18	0.43
1:2A:459:U:H4'	29:27:40:TRP:CZ3	2.52	0.43
1:2A:724:U:H2'	1:2A:725:G:O4'	2.18	0.43
5:2F:132:VAL:O	5:2F:133:ASN:ND2	2.51	0.43
6:2G:161:THR:CG2	6:2G:163:ALA:H	2.31	0.43
1:1A:956:A:N1	1:1A:2289:G:H1'	2.34	0.43
1:1A:2402:U:P	30:18:35:GLN:HE22	2.42	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:465:G:H2'	1:1A:466:G:H8	1.83	0.43
1:1A:599:U:H2'	1:1A:600:G:C8	2.54	0.43
3:1D:108:PRO:HG3	3:1D:143:HIS:CE1	2.53	0.43
11:1P:141:ALA:HA	25:23:38:GLU:HG2	2.01	0.43
1:2A:1450:G:H2'	1:2A:1450(A):C:C6	2.53	0.43
1:2A:2130:U:H6	1:2A:2130:U:H3'	1.84	0.43
5:2F:101:LEU:HD12	5:2F:102:PRO:HD2	2.00	0.43
5:2F:24:LEU:HD21	5:2F:114:VAL:HG12	1.99	0.43
7:2H:11:VAL:HG23	7:2H:49:VAL:HA	2.00	0.43
9:2N:73:THR:HA	9:2N:83:LYS:O	2.19	0.43
2:2B:52:A:C6	14:2S:33:LYS:HE3	2.52	0.43
28:16:12:GLU:OE1	28:16:19:ARG:NH1	2.51	0.43
1:1A:1810:U:H2'	61:1A:4556:HOH:O	2.17	0.43
1:1A:297:C:N4	1:1A:298:G:O6	2.51	0.43
1:1A:342:C:N4	1:1A:347:G:O6	5.78	0.43
1:1A:886:U:H2'	1:1A:887:C:C6	2.53	0.43
4:1E:16:ARG:NH1	4:1E:171:GLU:OE2	2.42	0.43
5:1F:117:ARG:NH2	61:1F:411:HOH:O	2.51	0.43
9:1N:12:ARG:HG2	9:1N:14:VAL:HG23	2.01	0.43
25:23:6:VAL:HG13	25:23:54:VAL:HG13	1.99	0.43
1:2A:1045:A:H5'	1:2A:1047:G:O5'	2.17	0.43
1:2A:1359:A:H61	1:2A:1372:U:H3	1.65	0.43
1:2A:1409:C:H2'	1:2A:1410:G:C8	2.53	0.43
1:2A:1847:A:H3'	1:2A:1848:A:H5'	2.00	0.43
1:2A:1952:A:C6	1:2A:1953:A:N1	2.86	0.43
1:2A:1996:C:H4'	1:2A:1997:G:OP1	2.18	0.43
1:2A:2179:C:C4	1:2A:2180:U:C4	3.07	0.43
1:2A:93:G:H2'	1:2A:94:C:C6	2.53	0.43
6:2G:33:ARG:HH21	6:2G:162:THR:HG21	1.83	0.43
9:2N:39:ARG:NH2	9:2N:41:ASP:OD2	2.50	0.43
15:2T:9:LEU:O	15:2T:12:SER:OG	2.35	0.43
1:1A:2283:G:OP1	22:10:18:ALA:HB1	2.19	0.43
28:16:44:ARG:HG2	28:16:44:ARG:HH11	1.82	0.43
1:1A:1299:A:H5''	1:1A:1299:A:N3	6.11	0.43
1:1A:2549:U:H2'	1:1A:2550:C:C6	2.54	0.43
1:1A:704:U:H2'	1:1A:705:C:C6	2.54	0.43
8:1I:75:LEU:HD13	8:1I:105:HIS:ND1	2.34	0.43
9:1N:12:ARG:HB3	9:1N:50:ASP:OD1	2.19	0.43
21:1Z:136:PHE:CE1	21:1Z:138:GLU:HG3	2.51	0.43
1:2A:1015:G:O2'	1:2A:1016:G:H5'	2.19	0.43
1:2A:1223:G:N2	1:2A:1226:A:OP2	2.38	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1430:C:H2'	1:2A:1431:U:C6	2.53	0.43
1:2A:1504:C:H2'	1:2A:1505:C:H6	1.83	0.43
1:2A:2567:G:H2'	1:2A:2568:C:C6	2.53	0.43
1:2A:887:A:O2'	1:2A:888:C:H3'	2.18	0.43
5:2F:74:ARG:HD2	61:2F:3107:HOH:O	2.19	0.43
6:2G:15:VAL:HG13	6:2G:175:LEU:HD23	2.00	0.43
1:2A:993:G:N2	17:2V:23:GLU:OE2	2.52	0.43
18:2W:29:LEU:HD21	18:2W:33:ARG:NH2	2.33	0.43
21:2Z:99:TYR:HA	21:2Z:124:ILE:O	2.18	0.43
1:1A:217:A:H2'	1:1A:219:U:O4'	2.19	0.43
1:1A:233:A:C2	1:1A:244:A:C4	3.07	0.43
6:1G:110:ALA:HA	6:1G:140:ILE:O	2.19	0.43
6:1G:72:ARG:HG2	6:1G:87:PRO:HA	2.00	0.43
7:1H:20:ALA:HB1	7:1H:21:PRO:HD2	2.00	0.43
1:2A:2461:C:H2'	1:2A:2462:U:C6	2.54	0.43
1:2A:361:G:O2'	1:2A:362:U:H5'	2.18	0.43
4:2E:11:MET:CG	4:2E:24:THR:HG22	2.46	0.43
4:2E:36:ARG:HG2	4:2E:47:VAL:HG12	2.01	0.43
26:14:40:HIS:HB3	26:14:43:TYR:HD2	1.84	0.43
1:1A:1335:C:H2'	1:1A:1336:C:H6	1.83	0.43
1:1A:2603:C:H2'	1:1A:2604:G:C8	2.54	0.43
2:1B:96:U:H2'	2:1B:97:G:C8	2.54	0.43
24:22:53:LEU:HD23	24:22:53:LEU:HA	1.88	0.43
24:22:10:LEU:HD21	24:22:59:ARG:HD2	2.01	0.43
25:23:6:VAL:HG12	25:23:28:LEU:HD11	2.00	0.43
1:2A:1315:C:OP2	61:2A:3810:HOH:O	2.20	0.43
1:2A:1525:G:H2'	1:2A:1526:G:H8	1.83	0.43
1:2A:2037:G:H2'	1:2A:2038:G:C8	2.54	0.43
1:2A:207:A:H2'	1:2A:208:C:O4'	2.19	0.43
1:2A:2602:A:H1'	1:2A:2603:G:O5'	2.17	0.43
1:2A:478:A:N1	1:2A:500:G:H4'	2.33	0.43
1:2A:570:G:H5''	61:2A:5018:HOH:O	2.18	0.43
2:2B:43:C:C4	2:2B:45:A:C6	3.07	0.43
5:2F:179:GLU:CD	5:2F:179:GLU:H	2.22	0.43
7:2H:40:GLU:OE1	7:2H:60:ARG:NH1	2.49	0.43
27:15:40:LYS:NZ	27:15:44:THR:O	2.52	0.43
29:17:34:ARG:NH2	61:17:202:HOH:O	2.51	0.43
1:1A:1220:U:HO2'	1:1A:1221:G:P	2.39	0.43
1:1A:1557:A:H2'	1:1A:1558:G:O4'	2.19	0.43
1:1A:1566:U:H2'	1:1A:1567:G:O4'	2.19	0.43
1:1A:1825:U:H2'	1:1A:1826:C:H6	1.84	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2388:A:H2'	1:1A:2389:A:O4'	2.19	0.43
1:1A:2846:U:H2'	1:1A:2847:G:C8	2.54	0.43
1:1A:592:U:C4	1:1A:593:G:C6	3.07	0.43
6:1G:46:ALA:HB1	6:1G:51:ARG:HA	2.01	0.43
16:1U:58:ARG:HA	16:1U:61:TRP:CE3	2.54	0.43
21:1Z:182:LYS:O	21:1Z:185:GLU:HG2	2.19	0.43
1:2A:1291:C:H2'	1:2A:1292:U:C6	2.54	0.43
1:2A:140:G:N2	1:2A:1596:A:H4'	2.34	0.43
1:2A:479:A:H4'	1:2A:480:A:OP1	2.18	0.43
1:2A:848:G:H2'	1:2A:849:A:C8	2.54	0.43
5:2F:150:GLY:HA2	5:2F:172:TRP:CD2	2.54	0.43
12:2Q:39:PRO:HD3	12:2Q:99:PRO:HG3	2.00	0.43
1:1A:1109:G:H1	1:1A:1121:C:N4	2.17	0.43
1:1A:1825:U:H2'	1:1A:1826:C:C6	2.53	0.43
1:1A:187:C:H5'	1:1A:2256:U:OP1	2.19	0.43
1:1A:342:C:N3	1:1A:347:G:N1	6.93	0.43
1:1A:171:A:H2	1:1A:460:C:O2	2.01	0.43
1:1A:904:C:N4	1:1A:905:U:O4	2.52	0.43
2:1B:78:A:C2	2:1B:100:A:C4	3.07	0.43
3:1D:242:ARG:HG3	3:1D:242:ARG:NH1	2.24	0.43
12:1Q:37:LEU:HD21	12:1Q:130:LYS:HE2	1.99	0.43
12:1Q:87:LYS:HA	12:1Q:87:LYS:HD2	4.23	0.43
14:1S:11:LYS:HD3	14:1S:15:ARG:HH12	1.84	0.43
20:1Y:28:LYS:HG3	20:1Y:40:GLU:HG3	2.01	0.43
1:2A:242:G:C8	30:28:5:LYS:HG2	2.54	0.43
1:2A:634:C:H2'	1:2A:635:C:C6	2.53	0.43
1:2A:781:A:H2	1:2A:1776:G:N3	2.17	0.43
5:2F:120:GLU:HB3	5:2F:122:LYS:HG2	2.01	0.43
7:2H:12:PRO:O	7:2H:15:VAL:HG22	2.19	0.43
16:2U:34:LYS:NZ	16:2U:37:GLU:OE1	2.41	0.43
1:1A:1224:C:H2'	1:1A:1225:C:H6	1.84	0.42
1:1A:1730:C:H2'	1:1A:1731:C:C6	2.54	0.42
1:1A:2585:C:H3'	61:1A:4593:HOH:O	2.19	0.42
1:1A:441:C:H2'	1:1A:442:A:C8	2.54	0.42
1:1A:537:G:N1	61:1A:4190:HOH:O	2.24	0.42
3:1D:113:VAL:HG12	61:1D:475:HOH:O	2.19	0.42
6:1G:133:LEU:HD11	6:1G:157:ILE:HD12	2.01	0.42
20:1Y:92:ASN:HD22	20:1Y:92:ASN:H	1.67	0.42
1:2A:1540:U:H2'	1:2A:1541:G:O4'	2.19	0.42
1:2A:196:A:H2'	1:2A:196:A:N3	2.34	0.42
1:2A:2153:G:H2'	1:2A:2154:G:C8	2.54	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2218:U:O4'	23:21:52:ARG:NH2	2.52	0.42
1:2A:783:A:H2'	1:2A:783:A:N3	2.33	0.42
1:2A:897:C:H2'	1:2A:898:C:C6	2.54	0.42
1:2A:9:U:O4	1:2A:2629:A:H2	2.02	0.42
4:2E:181:LEU:HA	4:2E:181:LEU:HD12	1.71	0.42
10:2O:107:ARG:HB3	10:2O:107:ARG:HE	1.53	0.42
10:2O:4:PRO:O	10:2O:5:GLN:HB2	2.19	0.42
14:2S:15:ARG:HB3	14:2S:19:LYS:HE3	2.01	0.42
15:2T:29:ARG:HB3	15:2T:87:ASP:HB2	2.00	0.42
15:2T:73:GLU:OE2	15:2T:103:ARG:NE	2.41	0.42
17:2V:76:LYS:HB2	17:2V:81:TYR:HB3	2.01	0.42
26:14:57:GLU:HB2	26:14:58:ARG:HA	2.01	0.42
31:19:7:VAL:HG12	31:19:34:GLN:HB3	2.00	0.42
1:1A:1653:C:H4'	1:1A:1654:A:O5'	2.19	0.42
1:1A:2303:U:H2'	1:1A:2304:C:C6	2.53	0.42
1:1A:2804:C:OP2	1:1A:2804:C:H6	2.02	0.42
3:1D:71:ASP:OD2	3:1D:103:ARG:NH2	2.45	0.42
1:1A:2761:A:H5'	7:1H:4:ILE:HD12	2.01	0.42
13:1R:28:LEU:O	13:1R:32:GLY:N	2.49	0.42
26:24:45:GLY:C	26:24:47:GLN:H	2.23	0.42
1:2A:1016:G:H2'	1:2A:1017:G:O4'	2.18	0.42
1:2A:1539:G:H2'	1:2A:1540:U:H6	1.84	0.42
1:2A:1739:U:O2'	1:2A:1740:G:H8	2.02	0.42
1:2A:2128:C:H1'	1:2A:2173:A:C2	2.51	0.42
1:2A:2715:C:H2'	1:2A:2716:U:H6	1.84	0.42
1:2A:493:G:H2'	1:2A:494:G:O4'	2.18	0.42
1:2A:566:U:H2'	1:2A:567:A:O4'	2.19	0.42
2:2B:66:A:H61	2:2B:109:C:H5''	1.84	0.42
2:2B:95:C:H2'	2:2B:96:U:C6	2.54	0.42
11:2P:98:GLU:CD	11:2P:98:GLU:H	2.23	0.42
1:1A:1347:A:C8	1:1A:1349:G:C8	3.07	0.42
1:1A:2177:G:H3'	1:1A:2178:G:H8	1.84	0.42
1:1A:211:A:H5''	1:1A:448:U:OP1	2.19	0.42
2:1B:96:U:H2'	2:1B:97:G:H8	1.84	0.42
3:1D:146:GLU:HG2	3:1D:152:GLY:C	2.39	0.42
1:1A:721:G:H1'	5:1F:74:ARG:HD3	2.02	0.42
15:1T:99:LEU:O	15:1T:102:ILE:HG12	2.19	0.42
20:1Y:23:ARG:HD3	20:1Y:23:ARG:HA	1.93	0.42
20:1Y:53:PRO:O	20:1Y:56:PRO:HD3	2.19	0.42
1:2A:1069:A:H2'	1:2A:1073:A:N7	2.35	0.42
1:2A:140:G:N3	1:2A:142:A:N6	2.58	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1631(A):A:OP1	61:2A:3870:HOH:O	2.21	0.42
1:2A:2430:A:H5'	1:2A:2431:U:OP2	2.19	0.42
1:2A:2647:U:H2'	1:2A:2648:C:C6	2.54	0.42
1:2A:2776:A:H4'	1:2A:2777:G:H5''	2.00	0.42
4:2E:78:LEU:HA	4:2E:78:LEU:HD12	1.87	0.42
7:2H:124:GLU:HB2	7:2H:132:ARG:HB3	2.01	0.42
1:2A:2818:G:OP2	13:2R:42:LYS:NZ	2.52	0.42
22:10:43:THR:HG23	22:10:43:THR:O	2.20	0.42
1:1A:1115:A:H4'	1:1A:1116:A:H5''	2.01	0.42
1:1A:1144:A:H3'	1:1A:1145:G:H8	1.84	0.42
1:1A:1288:A:N3	1:1A:1352:C:O2'	95.27	0.42
1:1A:1432:C:H2'	1:1A:1433:C:C6	2.54	0.42
1:1A:1749:G:H2'	1:1A:1750:G:O4'	2.19	0.42
1:1A:2159:C:N4	1:1A:2176:G:N1	2.34	0.42
1:1A:2155:G:C2	1:1A:2179:G:H2'	2.54	0.42
1:1A:2383:G:H21	28:16:46:HIS:CE1	2.37	0.42
1:1A:502:G:H4'	1:1A:527:A:N1	2.35	0.42
8:1I:133:HIS:ND1	8:1I:134:PRO:O	2.48	0.42
1:1A:360:C:HO2'	20:1Y:35:TYR:HH	1.63	0.42
25:23:5:LYS:NZ	25:23:57:GLU:OE1	2.38	0.42
1:2A:1000:A:H62	1:2A:1154:G:H2'	1.84	0.42
1:2A:2750:A:OP1	1:2A:2750:A:H8	2.02	0.42
1:2A:566:U:H5''	11:2P:29:LYS:HE3	2.00	0.42
6:2G:114:ILE:HB	6:2G:117:PHE:HD1	1.83	0.42
1:1A:1815:A:OP1	61:1A:4176:HOH:O	2.22	0.42
1:1A:2279:A:H5''	1:1A:2280:A:H5'	2.00	0.42
1:1A:2639:G:N2	1:1A:2790:G:OP2	2.52	0.42
1:1A:299:G:O5'	1:1A:299:G:H8	2.70	0.42
1:1A:441:C:H4'	1:1A:1901:C:O2	2.19	0.42
1:1A:553:A:O2'	1:1A:554:A:H5'	2.20	0.42
1:1A:842:C:H2'	1:1A:843:C:C6	2.54	0.42
1:1A:933:C:C3'	1:1A:934:A:H5''	2.49	0.42
11:1P:97:PRO:HD3	11:1P:126:VAL:O	2.19	0.42
12:1Q:48:GLU:O	12:1Q:52:VAL:HG23	2.20	0.42
1:1A:1333:A:H8	13:1R:104:ARG:HD3	1.84	0.42
26:24:53:GLU:H	26:24:53:GLU:CD	2.22	0.42
28:26:23:THR:OG1	28:26:24:GLU:N	2.50	0.42
1:2A:1045:A:H2'	1:2A:1045:A:N3	2.34	0.42
1:2A:172:C:H2'	1:2A:173:G:H8	1.85	0.42
1:2A:1902:C:H5'	3:2D:246:PRO:HD3	2.02	0.42
1:2A:414:C:H2'	1:2A:415:A:C8	2.55	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:2H:13:LYS:HE3	7:2H:13:LYS:HB2	1.70	0.42
7:2H:154:PRO:HB3	7:2H:163:TYR:CE1	2.54	0.42
14:2S:76:LYS:HB3	14:2S:76:LYS:HE2	1.70	0.42
21:2Z:72:ARG:HD3	21:2Z:72:ARG:HA	1.86	0.42
27:15:33:CYS:HB2	27:15:40:LYS:HD3	2.01	0.42
30:18:23:VAL:HG11	30:18:47:LYS:HD3	2.00	0.42
31:19:33:LYS:HG3	61:19:604:HOH:O	2.19	0.42
1:1A:1004:A:C5	1:1A:1037:C:C2	53.89	0.42
1:1A:1113:A:H2'	1:1A:1113:A:N3	2.34	0.42
1:1A:1634:C:H2'	1:1A:1635:C:H6	1.84	0.42
1:1A:1652:G:H5''	1:1A:1653:C:OP1	2.19	0.42
1:1A:2071:G:N7	61:1A:4315:HOH:O	2.37	0.42
1:1A:217:A:OP1	11:1P:76:LYS:HE3	2.19	0.42
1:1A:767:C:H2'	1:1A:768:C:C6	2.54	0.42
1:1A:776:G:C5	3:1D:208:LYS:HB2	2.54	0.42
12:1Q:35:VAL:HG13	12:1Q:130:LYS:HB3	2.00	0.42
1:2A:1002:G:C4	1:2A:1003:G:C8	3.29	0.42
1:2A:1002:G:N3	1:2A:1003:G:H8	3.80	0.42
1:2A:1341:U:OP2	1:2A:1394:U:O2'	2.28	0.42
1:2A:1720:U:H2'	1:2A:1721:G:O4'	2.19	0.42
1:2A:1826:G:H4'	3:2D:242:ARG:CZ	2.50	0.42
1:2A:2112:G:H2'	1:2A:2113:U:C6	2.54	0.42
1:2A:643:A:C8	28:26:44:ARG:NH1	2.88	0.42
1:2A:897:C:H2'	1:2A:898:C:H6	1.85	0.42
5:2F:157:VAL:HB	5:2F:194:MET:HG2	2.01	0.42
5:2F:31:HIS:HB2	11:2P:9:ASN:OD1	2.20	0.42
1:2A:2296:U:OP2	14:2S:6:ALA:HB2	2.20	0.42
21:2Z:102:LEU:HD11	21:2Z:124:ILE:HB	2.01	0.42
26:14:8:LYS:HE3	26:14:10:VAL:HG12	2.02	0.42
1:1A:1219:A:C1'	1:1A:1220:U:H5'	2.49	0.42
1:1A:2686:G:H5''	10:1O:26:LYS:HE3	2.02	0.42
8:1I:9:LEU:HD23	8:1I:12:LEU:HD13	2.02	0.42
21:1Z:4:ARG:NE	21:1Z:60:GLU:OE2	2.43	0.42
26:24:64:GLY:C	26:24:66:SER:H	2.23	0.42
1:2A:1721:G:H8	1:2A:1741:A:H62	1.66	0.42
1:2A:390:A:H4'	1:2A:391:G:H5'	2.02	0.42
1:2A:818:G:O2'	1:2A:819:A:H5'	5.14	0.42
1:2A:981:A:H8	1:2A:982:C:C5	2.38	0.42
6:2G:171:ALA:O	6:2G:175:LEU:HB2	2.19	0.42
8:2I:12:LEU:HD23	8:2I:19:VAL:HG21	2.01	0.42
1:1A:1014:U:H2'	1:1A:1015:C:C6	2.54	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1315:A:H2'	1:1A:1316:C:C6	2.54	0.42
1:1A:2251:G:H5'	3:1D:251:GLY:HA3	2.01	0.42
1:1A:517:A:H2'	1:1A:518:G:O4'	2.19	0.42
3:1D:13:ARG:HA	3:1D:13:ARG:HD2	1.75	0.42
14:1S:58:LEU:HD23	14:1S:58:LEU:HA	1.76	0.42
1:2A:1053:C:H4'	1:2A:1054:A:OP1	2.19	0.42
1:2A:1069:A:H5'	1:2A:1096:A:H5'	2.00	0.42
1:2A:511:U:H4'	1:2A:1235:G:H4'	2.01	0.42
1:2A:1260:G:C6	1:2A:1261:C:C4	3.08	0.42
1:2A:1371:G:O2'	1:2A:1372:U:H5	2.03	0.42
1:2A:2689:U:H4'	1:2A:2690:C:H5'	2.02	0.42
1:2A:2627:G:N2	1:2A:2777:G:OP2	2.45	0.42
1:2A:531:C:H4'	1:2A:532:A:H5''	2.01	0.42
1:2A:639:U:H2'	1:2A:640:C:C6	2.55	0.42
6:2G:41:GLN:HG3	6:2G:60:LEU:HD22	2.02	0.42
12:2Q:29:PHE:HB2	12:2Q:105:GLU:OE1	2.19	0.42
17:2V:4:ILE:HD12	17:2V:39:LEU:HD22	2.01	0.42
22:10:10:THR:HG22	22:10:12:ASN:H	1.84	0.42
1:1A:1497:G:H2'	1:1A:1498:C:C6	2.55	0.42
1:1A:1495:G:O2'	1:1A:1575:A:N1	2.40	0.42
1:1A:1695:C:OP1	61:1A:4130:HOH:O	2.21	0.42
1:1A:2864:G:H2'	1:1A:2865:C:C6	2.54	0.42
1:1A:518:G:H2'	1:1A:519:G:O4'	2.20	0.42
1:1A:589:U:H2'	1:1A:590:A:O4'	2.20	0.42
1:1A:831:A:C8	1:1A:839:G:C5	3.08	0.42
7:1H:87:LEU:HD23	7:1H:164:TYR:HA	2.02	0.42
12:1Q:110:THR:OG1	12:1Q:113:GLN:HG3	2.20	0.42
25:23:52:HIS:CD2	25:23:53:LEU:HG	2.54	0.42
1:2A:1059:G:C5	1:2A:1060:U:N3	2.88	0.42
1:2A:1209:G:O2'	1:2A:1237:A:N1	2.47	0.42
1:2A:1324:G:C4	1:2A:1328:G:O6	2.72	0.42
1:2A:118:A:N3	1:2A:178:G:H1'	2.35	0.42
1:2A:2165:G:H2'	1:2A:2166:G:O4'	2.19	0.42
1:2A:271(Q):G:H2'	1:2A:271(R):G:C8	2.55	0.42
1:2A:2723:C:OP2	4:2E:109:LYS:NZ	2.49	0.42
1:2A:407:G:H5''	61:2A:3964:HOH:O	2.18	0.42
1:2A:483:A:O4'	20:2Y:48:ALA:HB1	2.19	0.42
2:2B:5:C:OP1	2:2B:61:G:O2'	2.29	0.42
7:2H:26:VAL:HG12	7:2H:79:VAL:HG21	2.02	0.42
14:2S:30:ARG:HG3	14:2S:97:ARG:CZ	2.50	0.42
17:2V:52:VAL:CG2	17:2V:55:ALA:HB3	2.48	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:2W:88:ARG:NH1	18:2W:94:ASP:OD2	2.52	0.42
21:2Z:146:ILE:HA	21:2Z:174:VAL:HG12	2.01	0.42
28:16:7:ILE:HD11	28:16:25:LYS:HE2	2.01	0.42
1:1A:1141:A:H2'	1:1A:1142:A:C8	2.55	0.42
1:1A:1701:A:OP1	13:1R:1:MET:N	2.47	0.42
1:1A:2846:U:C4	1:1A:2893:A:N6	2.87	0.42
1:1A:2875:U:OP2	15:1T:119:LYS:NZ	2.50	0.42
1:1A:510:C:H2'	1:1A:511:C:C6	2.55	0.42
1:1A:787:U:H2'	1:1A:788:G:C8	2.54	0.42
1:1A:895:G:H2'	1:1A:896:A:C8	2.55	0.42
8:1I:14:ASP:OD1	8:1I:15:VAL:N	2.53	0.42
9:1N:14:VAL:HG13	9:1N:138:LEU:HG	2.02	0.42
1:2A:1171:G:N2	1:2A:1179:C:C2	2.87	0.42
1:2A:2137:C:H2'	1:2A:2138:C:O4'	2.20	0.42
1:2A:2103:C:O2	1:2A:2187:G:N1	2.53	0.42
1:2A:2397:G:N2	1:2A:2420:C:H1'	2.35	0.42
1:2A:2712(A):A:OP2	61:2A:3872:HOH:O	2.22	0.42
1:2A:384:U:H2'	1:2A:385:C:C6	2.53	0.42
17:2V:71:LEU:HD23	17:2V:71:LEU:HA	1.86	0.42
25:13:31:LEU:HD23	25:13:31:LEU:HA	1.80	0.41
30:18:15:LYS:HB3	57:18:102:MPD:H52	2.01	0.41
11:1P:63:PRO:HG2	30:18:25:MET:HB2	2.01	0.41
1:1A:1055:A:OP2	9:1N:37:LYS:NZ	2.48	0.41
1:1A:105:C:H2'	1:1A:106:U:C6	2.54	0.41
1:1A:1096:A:C2	1:1A:2764:G:C4	3.08	0.41
1:1A:1594:C:H2'	1:1A:1595:C:C6	2.55	0.41
1:1A:2596:U:H2'	1:1A:2597:U:H2'	2.02	0.41
1:1A:548:C:H2'	1:1A:549:U:O4'	2.19	0.41
1:1A:561:A:H2'	1:1A:562:C:C6	2.55	0.41
3:1D:70:TRP:HB3	3:1D:190:TYR:CE2	2.55	0.41
1:1A:2317:A:H5''	6:1G:134:GLY:HA3	2.00	0.41
8:1I:109:ILE:HD12	8:1I:109:ILE:HA	1.77	0.41
9:1N:62:VAL:HG13	9:1N:66:LYS:HD2	2.02	0.41
18:1W:68:ARG:NH1	18:1W:112:GLY:H	2.18	0.41
1:1A:1387:U:O4'	19:1X:57:LEU:HD23	2.19	0.41
1:2A:1274:A:N3	1:2A:1297:C:H1'	2.35	0.41
1:2A:118:A:H1'	1:2A:178:G:O4'	2.20	0.41
1:2A:271(Q):G:H2'	1:2A:271(R):G:H8	1.85	0.41
1:2A:2745:C:C4	1:2A:2746:U:C4	3.08	0.41
1:2A:515:A:H1'	1:2A:581:C:H1'	2.01	0.41
4:2E:13:ARG:O	15:2T:57:PHE:HE2	2.02	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:2O:2:ILE:HD12	10:2O:6:THR:HG21	2.01	0.41
19:2X:11:PRO:HB3	19:2X:92:LEU:HD11	2.02	0.41
1:1A:2156:A:N6	1:1A:2179:G:H4'	2.35	0.41
1:1A:269:G:H2'	1:1A:270:C:C6	2.55	0.41
1:1A:542:C:OP2	27:15:13:LYS:HE3	2.19	0.41
6:1G:133:LEU:HG	6:1G:157:ILE:HB	2.00	0.41
6:1G:66:GLN:OE1	6:1G:98:ARG:NE	2.50	0.41
1:1A:2573:A:H2	10:1O:23:ARG:NH2	2.18	0.41
14:1S:15:ARG:HE	14:1S:88:ASP:CG	2.23	0.41
25:23:4:LEU:O	25:23:36:VAL:HA	2.20	0.41
25:23:8:LEU:HB2	25:23:28:LEU:HD13	2.02	0.41
1:2A:108:U:OP1	1:2A:293:U:O2'	2.38	0.41
1:2A:1527:G:H5''	1:2A:1528:A:OP1	2.20	0.41
1:2A:1899:G:N3	1:2A:1899:G:H2'	2.34	0.41
1:2A:2252:G:H2'	1:2A:2253:G:H8	1.85	0.41
3:2D:17:THR:O	3:2D:211:ARG:NH2	2.53	0.41
5:2F:152:GLU:OE1	5:2F:191:ARG:HD2	2.20	0.41
8:2I:87:LYS:HA	8:2I:87:LYS:HD2	1.86	0.41
8:2I:87:LYS:HE2	8:2I:121:LYS:HG3	2.02	0.41
14:2S:41:ASP:OD2	14:2S:44:LYS:HB2	2.20	0.41
14:2S:93:LYS:HG2	14:2S:95:HIS:HB3	2.01	0.41
21:2Z:5:LEU:O	21:2Z:59:LEU:HA	2.21	0.41
1:1A:1473:A:H4'	1:1A:1474:C:O4'	2.20	0.41
1:1A:894:U:OP2	61:1A:4175:HOH:O	2.22	0.41
1:1A:909:G:H2'	1:1A:910:A:O4'	2.20	0.41
2:1B:15:A:OP1	2:1B:108:U:O2'	2.26	0.41
1:1A:142:G:H1'	19:1X:37:THR:HG21	2.01	0.41
11:1P:141:ALA:HA	25:23:38:GLU:CG	2.50	0.41
1:2A:108:U:H2'	1:2A:109:G:H8	1.85	0.41
1:2A:17:G:C6	1:2A:18:C:N4	2.89	0.41
1:2A:2251:OMG:HM23	1:2A:2251:OMG:H1'	1.76	0.41
1:2A:2406:U:OP2	1:2A:2406:U:H2'	2.20	0.41
1:2A:2498:C:OP2	61:2A:3823:HOH:O	2.21	0.41
1:2A:57:C:H2'	1:2A:58:G:O4'	2.20	0.41
1:2A:825:C:O2	11:2P:55:ARG:NH1	2.45	0.41
2:2B:73:A:C4	2:2B:105:A:C2	3.08	0.41
5:2F:23:ASP:O	5:2F:24:LEU:HD12	2.20	0.41
2:2B:50:G:OP2	14:2S:62:LYS:HB2	2.21	0.41
23:11:50:ARG:HG2	23:11:59:THR:CG2	2.49	0.41
1:1A:1086:C:H2'	1:1A:1087:C:O4'	2.20	0.41
1:1A:131:C:H2'	1:1A:132:C:H6	2.29	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:2137:G:N2	1:1A:2141:A:N7	2.68	0.41
1:1A:564:G:H2'	1:1A:565:C:C6	2.56	0.41
2:1B:90:A:N7	2:1B:91:C:H1'	2.35	0.41
18:1W:65:LEU:HD23	18:1W:65:LEU:HA	1.76	0.41
26:24:14:ILE:O	26:24:21:VAL:HA	2.21	0.41
26:24:14:ILE:HB	26:24:22:ILE:HD13	2.02	0.41
1:2A:2344:U:H3'	28:26:37:ARG:O	2.20	0.41
1:2A:1076:C:H4'	1:2A:1077:A:OP1	2.20	0.41
1:2A:116:C:H2'	1:2A:117:G:O4'	2.21	0.41
1:2A:118:A:C8	1:2A:119:A:C8	3.08	0.41
1:2A:1429:G:H2'	1:2A:1430:C:C6	2.55	0.41
1:2A:1827:C:C2'	1:2A:1828:G:H5'	2.51	0.41
1:2A:2271:G:C5	1:2A:2272:U:C4	3.08	0.41
1:2A:2785:C:O2'	4:2E:66:HIS:ND1	2.42	0.41
2:2B:17:C:N4	2:2B:109:C:N3	2.68	0.41
3:2D:38:LYS:HD2	3:2D:38:LYS:HA	1.88	0.41
6:2G:3:LEU:HD22	26:24:25:TYR:OH	2.19	0.41
8:2I:29:TYR:HD2	8:2I:30:LEU:HD23	1.86	0.41
2:2B:31:C:N4	14:2S:32:LEU:HD22	2.35	0.41
1:2A:997:G:H5''	16:2U:92:ARG:NH1	2.35	0.41
20:2Y:19:LYS:HB3	20:2Y:19:LYS:HE2	1.79	0.41
20:2Y:6:HIS:CD2	20:2Y:7:VAL:HG23	2.55	0.41
21:2Z:76:LEU:HD12	21:2Z:76:LEU:H	1.85	0.41
31:19:4:ARG:O	31:19:36:GLN:HA	2.20	0.41
31:19:8:LYS:H	31:19:34:GLN:HE22	1.68	0.41
1:1A:1588:G:H3'	1:1A:1589:A:H2'	2.03	0.41
1:1A:1730:C:H2'	1:1A:1731:C:H6	1.85	0.41
1:1A:2073:A:H4'	4:1E:141:ILE:HG12	2.03	0.41
1:1A:2123:G:H2'	1:1A:2124:U:O4'	2.20	0.41
1:1A:227:C:C2	1:1A:249:G:C2	3.08	0.41
1:1A:605:G:H2'	1:1A:606:G:C8	2.56	0.41
2:1B:11:C:OP2	2:1B:12:C:N4	2.45	0.41
4:1E:3:GLY:HA3	4:1E:81:ILE:HD12	2.02	0.41
23:21:81:LYS:HE3	23:21:81:LYS:HB3	1.87	0.41
28:26:13:CYS:SG	28:26:47:THR:HG21	2.59	0.41
1:2A:1221(A):C:C2	1:2A:1229:G:C2	3.09	0.41
1:2A:1288:U:C2	1:2A:1327:C:O2	2.74	0.41
1:2A:1686:C:H2'	1:2A:1687:G:O4'	2.20	0.41
1:2A:2119:A:H61	1:2A:2168:G:N2	2.18	0.41
1:2A:2187:G:N7	1:2A:2188:C:C4	2.89	0.41
1:2A:1493:C:N4	1:2A:2206:G:O2'	2.53	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:2366:A:OP1	61:2A:3875:HOH:O	2.22	0.41
1:2A:2031:A:C6	1:2A:2498:C:H1'	2.55	0.41
1:2A:336:C:H2'	1:2A:337:C:C6	3.02	0.41
4:2E:14:ILE:HG13	4:2E:21:VAL:HG13	2.01	0.41
4:2E:167:VAL:CG1	4:2E:189:PRO:HD3	2.50	0.41
8:2I:14:ASP:OD1	8:2I:15:VAL:N	2.53	0.41
21:2Z:128:VAL:HG23	21:2Z:160:GLY:O	2.19	0.41
1:1A:1314:A:C2	1:1A:2035:A:C4	3.09	0.41
1:1A:2157:A:H61	1:1A:2177:G:N2	2.18	0.41
1:1A:27:G:C2	1:1A:537:G:N3	2.89	0.41
1:1A:551:A:H2'	61:1A:4675:HOH:O	2.21	0.41
1:1A:18:C:O2'	1:1A:577:U:OP1	2.35	0.41
5:1F:148:LEU:HD22	5:1F:154:VAL:HG21	2.03	0.41
15:1T:33:LYS:HG3	15:1T:34:VAL:N	2.35	0.41
1:2A:1422:G:O3'	10:2O:49:ARG:NH1	99.95	0.41
1:2A:1539:G:H2'	1:2A:1540:U:C6	2.56	0.41
1:2A:1557:C:H5''	1:2A:1558:A:OP2	2.20	0.41
4:2E:12:THR:HG21	15:2T:11:GLU:OE2	2.20	0.41
6:2G:34:LEU:HD11	6:2G:176:LEU:HD13	2.01	0.41
6:2G:55:LYS:HA	6:2G:58:GLN:HB3	2.02	0.41
14:2S:14:VAL:HG21	14:2S:90:GLY:O	2.20	0.41
1:2A:480:A:OP2	20:2Y:47:LYS:HD3	2.20	0.41
1:1A:1291:G:OP1	11:1P:13:ASN:ND2	2.36	0.41
1:1A:1516:A:H2'	1:1A:1517:G:O4'	2.21	0.41
1:1A:2703:C:O3'	1:1A:2881:C:H4'	2.19	0.41
1:1A:302:A:H2'	1:1A:303:C:C6	2.55	0.41
1:1A:556:C:H4'	1:1A:557:A:H5''	2.02	0.41
3:1D:255:LYS:O	61:1D:403:HOH:O	2.22	0.41
7:1H:149:ARG:NH1	7:1H:167:GLU:OE2	2.49	0.41
8:1I:8:PRO:HD3	8:1I:15:VAL:HB	2.01	0.41
14:1S:11:LYS:HD3	14:1S:15:ARG:NH1	2.36	0.41
18:1W:20:VAL:O	18:1W:23:LEU:HB2	2.19	0.41
1:2A:1002:G:N3	1:2A:1003:G:C8	3.73	0.41
1:2A:1203:G:C6	1:2A:1204:A:N6	2.89	0.41
1:2A:1486:A:H2'	1:2A:1487:G:H8	1.85	0.41
1:2A:2252:G:H2'	1:2A:2253:G:C8	2.55	0.41
1:2A:2601:C:H5''	1:2A:2602:A:OP2	2.21	0.41
1:2A:489:G:N7	18:2W:49:LYS:NZ	2.69	0.41
1:2A:884:C:H42	1:2A:892:G:H1	1.68	0.41
1:2A:9:U:H3	1:2A:2629:A:H2	1.67	0.41
3:2D:206:LEU:HA	3:2D:206:LEU:HD23	1.76	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:2O:7:TYR:CE1	10:2O:20:MET:HB2	2.55	0.41
12:2Q:57:HIS:NE2	12:2Q:116:GLU:HB3	2.36	0.41
1:2A:2682:U:O2'	15:2T:58:ASN:ND2	2.53	0.41
18:2W:67:ASP:N	18:2W:67:ASP:OD1	2.53	0.41
21:2Z:69:THR:HG22	21:2Z:90:VAL:HA	2.03	0.41
30:18:26:LYS:HD2	30:18:48:PHE:CD2	2.55	0.41
1:1A:166:G:H2'	1:1A:167:G:H8	3.47	0.41
1:1A:1821:C:H2'	1:1A:1822:A:C5	2.55	0.41
1:1A:2321:A:H2'	1:1A:2322:A:O4'	2.20	0.41
8:1I:105:HIS:N	8:1I:105:HIS:CD2	2.86	0.41
21:1Z:145:GLU:O	21:1Z:148:ASP:N	2.33	0.41
22:20:51:VAL:HG22	22:20:81:VAL:HG23	2.02	0.41
1:2A:1053:C:H2'	1:2A:1054:A:H8	1.84	0.41
1:2A:1056:G:H5''	1:2A:1057:A:H5'	2.03	0.41
1:2A:1065:U:H3	1:2A:1073:A:N6	2.17	0.41
1:2A:1590:U:H2'	1:2A:1591:G:C8	2.55	0.41
1:2A:1598:C:H2'	1:2A:1599:C:C6	2.56	0.41
1:2A:1915:5MU:H2'	1:2A:1916:A:O4'	2.21	0.41
1:2A:1952:A:N3	10:2O:22:ILE:HD12	2.36	0.41
1:2A:754:C:H2'	1:2A:755:C:C6	2.55	0.41
1:2A:910:A:C6	1:2A:911:A:C6	3.09	0.41
7:2H:144:VAL:O	7:2H:148:ILE:HG12	2.20	0.41
7:2H:3:ARG:HH21	7:2H:54:ARG:NH1	2.19	0.41
1:1A:1066:A:N1	1:1A:1186:U:O2'	2.40	0.41
1:1A:1074:A:H61	1:1A:1171:G:H2'	1.85	0.41
1:1A:1699:A:O2'	1:1A:1700:G:H5'	2.21	0.41
1:1A:1857:G:OP1	3:1D:224:ALA:N	2.52	0.41
1:1A:2360:U:O4	1:1A:2394:G:N1	2.54	0.41
1:1A:2843:G:O2'	1:1A:2844:G:H5'	2.20	0.41
1:1A:831:A:C6	3:1D:229:VAL:HG11	2.56	0.41
1:1A:92:C:H2'	1:1A:93:G:C8	3.45	0.41
12:1Q:137:TYR:O	12:1Q:141:GLN:HG2	2.21	0.41
19:1X:72:LYS:HE3	19:1X:72:LYS:HB3	1.91	0.41
1:2A:1027:A:C6	1:2A:1126:A:C4	3.09	0.41
1:2A:1065:U:H4'	1:2A:1066:U:C5'	2.51	0.41
1:2A:1587:A:H2'	1:2A:1588:C:C6	2.56	0.41
1:2A:2104:G:N7	1:2A:2186:G:N2	2.69	0.41
1:2A:820:A:H1'	1:2A:943:U:H1'	2.03	0.41
2:2B:70:C:H2'	2:2B:71:C:H6	1.86	0.41
4:2E:96:PHE:O	4:2E:175:VAL:HG11	2.20	0.41
18:2W:60:ASN:HD22	18:2W:60:ASN:N	2.19	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2A:1341:U:O4	19:2X:16:LYS:HE2	2.20	0.41
21:2Z:144:LEU:HD11	21:2Z:150:LEU:HD22	2.03	0.41
23:11:67:ILE:N	23:11:68:PRO:HD2	2.36	0.41
1:1A:2860:A:H2	13:1R:61:HIS:CG	2.38	0.41
4:1E:144:ARG:HB3	4:1E:145:LYS:H	1.53	0.41
7:1H:22:GLY:HA2	7:1H:37:VAL:O	2.21	0.41
1:1A:1716:A:C8	10:1O:5:GLN:HG3	2.56	0.41
16:1U:62:ILE:O	16:1U:66:ASN:HB2	2.21	0.41
1:2A:747:U:C5	27:25:4:HIS:CE1	3.09	0.41
1:2A:1091:G:N3	1:2A:1091:G:H2'	2.36	0.41
1:2A:111:A:H4'	24:22:69:ARG:NH1	2.35	0.41
1:2A:1449:A:N3	1:2A:1529:G:H1'	2.35	0.41
1:2A:1709:U:H2'	1:2A:1710:C:C6	2.56	0.41
1:2A:1881:C:H2'	1:2A:1882:C:C6	2.56	0.41
1:2A:2302:G:C2	1:2A:2303:G:C8	3.09	0.41
1:2A:2461:C:H2'	1:2A:2462:U:H6	1.85	0.41
1:2A:556:G:H2'	1:2A:557:U:C6	2.56	0.41
1:2A:64:A:O3'	19:2X:71:GLY:HA3	2.21	0.41
3:2D:69:ARG:HD2	3:2D:130:ALA:CB	2.51	0.41
1:2A:811:U:H2'	11:2P:21:ARG:HA	2.03	0.41
21:2Z:45:ASP:O	21:2Z:49:ARG:HG3	2.20	0.41
23:11:23:LYS:HB3	23:11:29:GLY:HA3	2.03	0.41
1:1A:1140:U:H2'	1:1A:1142:A:OP2	2.21	0.41
1:1A:2141:A:N6	1:1A:2193:A:N7	2.69	0.41
1:1A:2271:G:C8	1:1A:2439:C:C4	3.09	0.41
1:1A:624:C:O2	1:1A:628:C:H4'	2.21	0.41
4:1E:119:ARG:HD3	61:1E:3133:HOH:O	2.22	0.41
4:1E:146:THR:HA	4:1E:147:PRO:HA	1.86	0.41
7:1H:154:PRO:HB3	7:1H:163:TYR:CE1	2.56	0.41
4:1E:14:ILE:HB	15:1T:14:TYR:CZ	2.56	0.41
18:1W:79:GLY:HA3	18:1W:100:THR:HG22	2.03	0.41
23:21:62:VAL:HG22	23:21:63:ALA:O	2.21	0.41
61:2A:4295:HOH:O	27:25:15:ARG:HG2	2.20	0.41
1:2A:1055:G:H3'	1:2A:1056:G:H8	1.86	0.41
1:2A:1319:G:C6	1:2A:1320:C:N4	2.89	0.41
1:2A:1509(B):A:H2'	1:2A:1510:G:C8	2.56	0.41
1:2A:1498:C:O4'	1:2A:1577:C:H4'	2.21	0.41
1:2A:2086:U:H2'	1:2A:2087:G:C8	2.56	0.41
1:2A:26:G:C6	1:2A:27:G:N1	2.89	0.41
1:2A:281:G:H1'	1:2A:359:A:H61	1.85	0.41
1:2A:699:A:H2'	1:2A:700:G:O4'	2.20	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:2E:9:VAL:HG13	4:2E:25:VAL:O	2.21	0.41
1:2A:662:G:H5''	11:2P:16:ARG:HG2	2.03	0.41
1:1A:1223:C:H2'	1:1A:1224:C:H6	1.82	0.40
1:1A:223:C:H2'	1:1A:224:U:H6	1.86	0.40
1:1A:707:G:O3'	5:1F:38:ARG:NH2	2.54	0.40
1:1A:708:C:H2'	1:1A:709:G:H8	2.17	0.40
6:1G:56:ALA:O	6:1G:59:GLU:HB2	2.21	0.40
8:1I:76:THR:O	8:1I:105:HIS:HE1	2.04	0.40
61:1A:4412:HOH:O	11:1P:39:LYS:HD3	2.20	0.40
1:2A:1031:G:N2	31:29:36:GLN:HE22	2.17	0.40
1:2A:1204:A:OP1	1:2A:1204:A:H8	2.04	0.40
1:2A:1359:A:N6	1:2A:1372:U:H3	2.18	0.40
1:2A:1657:C:H2'	1:2A:1658:C:C6	2.56	0.40
15:2T:18:ASP:OD1	15:2T:18:ASP:N	2.53	0.40
24:12:3:LEU:HD23	24:12:3:LEU:HA	1.89	0.40
26:14:53:GLU:HB2	26:14:55:ARG:H	1.84	0.40
1:1A:1122:C:O2'	1:1A:1123:A:OP2	2.33	0.40
1:1A:115:G:H4'	1:1A:116:A:O5'	4.88	0.40
1:1A:2515:2MA:O2'	1:1A:2517:G:OP2	2.28	0.40
61:1A:4141:HOH:O	4:1E:135:HIS:NE2	2.37	0.40
5:1F:20:LEU:HG	5:1F:21:ALA:N	2.36	0.40
7:1H:137:ASP:HB3	7:1H:140:LYS:HB3	2.03	0.40
8:1I:14:ASP:O	8:1I:17:GLN:HB3	2.21	0.40
10:1O:17:ARG:NH1	10:1O:47:ILE:HD13	2.36	0.40
1:2A:2307:G:OP1	1:2A:2307:G:H8	2.04	0.40
1:2A:2751:G:H3'	1:2A:2752:C:C6	2.56	0.40
1:2A:2821:A:H2'	1:2A:2822:G:C8	2.57	0.40
1:2A:324:A:N6	1:2A:338:G:O2'	2.53	0.40
1:2A:363(D):G:H2'	1:2A:363(E):U:O4'	2.22	0.40
1:2A:411:G:C5	11:2P:72:PRO:HB3	2.56	0.40
1:2A:410:G:H21	1:2A:432:A:H62	42.93	0.40
1:2A:477:A:H2'	1:2A:478:A:C8	2.56	0.40
1:2A:478:A:C6	1:2A:480:A:C6	3.09	0.40
1:2A:27:G:N2	1:2A:512:G:H1'	2.36	0.40
1:2A:659:C:H2'	1:2A:660:G:C8	2.55	0.40
1:2A:685:A:H5''	61:2A:3845:HOH:O	2.21	0.40
1:2A:907:U:C2'	1:2A:908:C:H5'	2.51	0.40
7:2H:88:LEU:N	7:2H:163:TYR:O	2.52	0.40
12:2Q:75:THR:HA	12:2Q:89:ASN:O	2.20	0.40
21:2Z:44:PHE:CZ	21:2Z:86:VAL:HG11	2.57	0.40
1:1A:1217:G:H3'	1:1A:1218:G:H5'	2.03	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:27:G:N2	1:1A:537:G:H1'	2.36	0.40
1:1A:603:C:H2'	1:1A:604:C:C6	2.56	0.40
12:1Q:75:THR:HG22	61:1Q:329:HOH:O	2.21	0.40
20:1Y:19:LYS:HB3	20:1Y:19:LYS:HE2	1.90	0.40
21:1Z:54:HIS:HD2	21:1Z:99:TYR:O	2.05	0.40
23:21:8:SER:HB3	23:21:66:HIS:CD2	2.56	0.40
18:2W:38:TYR:CE1	27:25:41:PRO:HD3	2.56	0.40
28:26:37:ARG:NH1	61:26:603:HOH:O	2.53	0.40
1:2A:1442:G:H2'	1:2A:1442:G:N3	3.00	0.40
1:2A:2516:G:C2'	1:2A:2517:C:H5'	2.52	0.40
1:2A:79:G:O2'	1:2A:346:A:N3	2.44	0.40
1:2A:468:G:N7	29:27:39:ARG:NH2	2.63	0.40
1:2A:458:G:O2'	1:2A:469:G:O6	2.30	0.40
6:2G:17:PRO:HA	6:2G:20:ILE:HB	2.03	0.40
20:2Y:7:VAL:HG11	20:2Y:13:VAL:HG11	2.03	0.40
21:2Z:145:GLU:HB2	21:2Z:148:ASP:OD2	2.21	0.40
1:1A:1463:C:H2'	1:1A:1464:G:O4'	2.20	0.40
1:1A:1688:A:H2'	1:1A:1689:G:O4'	2.22	0.40
1:1A:1756:U:H2'	1:1A:1757:C:C6	2.57	0.40
1:1A:1895:U:OP1	1:1A:2422:G:O2'	2.25	0.40
1:1A:2159:C:C2	1:1A:2176:G:N2	2.84	0.40
1:1A:214:A:O2'	1:1A:246:A:H4'	2.22	0.40
1:1A:2564:2MU:H2'	1:1A:2566:U:OP2	2.20	0.40
1:1A:2828:G:O2'	1:1A:2829:G:H5'	2.22	0.40
1:1A:669:A:H4'	1:1A:670:C:C5	2.55	0.40
2:1B:24:G:N7	2:1B:56:G:H2'	2.36	0.40
8:1I:14:ASP:OD1	8:1I:15:VAL:HG12	2.21	0.40
8:1I:42:SER:HB2	61:1I:5007:HOH:O	2.21	0.40
26:24:47:GLN:O	26:24:48:ARG:HB2	2.21	0.40
1:2A:1481:U:H2'	1:2A:1482:G:C8	7.10	0.40
1:2A:182:A:H2	1:2A:433:C:O2	2.03	0.40
1:2A:1946:U:H2'	1:2A:1947:C:C6	2.56	0.40
1:2A:571:A:C8	1:2A:2030:A:N6	2.89	0.40
1:2A:2116:G:H3'	1:2A:2117:A:C8	2.57	0.40
1:2A:2238:G:N3	1:2A:2238:G:H2'	2.36	0.40
1:2A:2441:C:OP2	1:2A:2586:C:O2'	2.31	0.40
1:2A:1669:A:H5"	1:2A:2550:G:OP1	2.20	0.40
1:2A:373:U:H2'	1:2A:374:A:C8	2.55	0.40
1:2A:410:G:N3	1:2A:432:A:N6	42.04	0.40
1:2A:74:A:H4'	1:2A:75:G:O5'	2.21	0.40
3:2D:142:VAL:HG23	3:2D:193:VAL:HA	2.03	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:2G:97:ASP:HA	6:2G:100:TRP:CD1	2.46	0.40
8:2I:72:LEU:HD12	8:2I:138:ILE:HG21	2.02	0.40
12:2Q:110:THR:OG1	12:2Q:112:GLU:HG3	2.22	0.40
12:2Q:36:ALA:HB2	12:2Q:103:MET:SD	2.61	0.40
14:2S:34:HIS:O	14:2S:97:ARG:NH2	2.54	0.40
14:2S:38:GLN:HB2	14:2S:47:THR:HG23	2.04	0.40
15:2T:119:LYS:O	15:2T:123:GLN:HB2	2.21	0.40
1:2A:1614:A:C2	18:2W:93:ALA:HB2	2.56	0.40
1:1A:1464:G:OP2	15:1T:111:ARG:NH2	103.84	0.40
1:1A:1882:U:H2'	1:1A:1883:C:O4'	2.21	0.40
1:1A:2473:C:H2'	1:1A:2474:U:C6	2.57	0.40
1:1A:322:G:H5''	1:1A:323:A:OP1	2.22	0.40
1:1A:426:G:OP2	61:1A:4177:HOH:O	2.22	0.40
6:1G:129:GLY:O	6:1G:161:THR:HB	2.20	0.40
19:1X:5:TYR:CZ	24:12:30:ARG:HB2	2.56	0.40
20:1Y:56:PRO:C	20:1Y:58:GLY:H	2.24	0.40
1:2A:247:G:H4'	1:2A:386:G:C5	2.57	0.40
1:2A:2563:U:O2	1:2A:2565:A:H8	2.04	0.40
1:2A:2820:A:OP1	13:2R:2:ARG:NH2	2.55	0.40
1:2A:90:U:H1'	1:2A:92:A:C8	2.57	0.40
2:2B:32:C:C4	2:2B:33:G:N7	2.90	0.40
5:2F:110:LEU:HD11	5:2F:181:LEU:HG	2.03	0.40
5:2F:197:ASP:OD1	5:2F:198:ALA:N	2.55	0.40
7:2H:148:ILE:HG22	7:2H:162:ILE:HD13	2.03	0.40
9:2N:15:LEU:HD23	9:2N:16:ILE:N	2.37	0.40
13:2R:72:ASP:OD2	13:2R:75:LEU:HB2	2.21	0.40
2:2B:27:C:H5''	14:2S:54:LEU:HD11	2.04	0.40
15:2T:91:ARG:HD2	15:2T:120:ARG:NH1	2.37	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1D	273/276 (99%)	258 (94%)	15 (6%)	0	100	100
3	2D	273/276 (99%)	258 (94%)	15 (6%)	0	100	100
4	1E	202/206 (98%)	192 (95%)	9 (4%)	1 (0%)	29	54
4	2E	202/206 (98%)	192 (95%)	9 (4%)	1 (0%)	29	54
5	1F	201/210 (96%)	191 (95%)	9 (4%)	1 (0%)	29	54
5	2F	201/210 (96%)	191 (95%)	7 (4%)	3 (2%)	10	26
6	1G	179/182 (98%)	163 (91%)	15 (8%)	1 (1%)	25	50
6	2G	179/182 (98%)	166 (93%)	10 (6%)	3 (2%)	9	23
7	1H	172/180 (96%)	162 (94%)	9 (5%)	1 (1%)	25	50
7	2H	171/180 (95%)	152 (89%)	19 (11%)	0	100	100
8	1I	145/148 (98%)	129 (89%)	15 (10%)	1 (1%)	22	46
8	2I	144/148 (97%)	130 (90%)	12 (8%)	2 (1%)	11	28
9	1N	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
9	2N	138/140 (99%)	130 (94%)	7 (5%)	1 (1%)	22	46
10	1O	120/122 (98%)	111 (92%)	8 (7%)	1 (1%)	19	43
10	2O	120/122 (98%)	111 (92%)	8 (7%)	1 (1%)	19	43
11	1P	147/150 (98%)	138 (94%)	9 (6%)	0	100	100
11	2P	147/150 (98%)	137 (93%)	9 (6%)	1 (1%)	22	46
12	1Q	139/141 (99%)	134 (96%)	4 (3%)	1 (1%)	22	46
12	2Q	139/141 (99%)	131 (94%)	7 (5%)	1 (1%)	22	46
13	1R	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
13	2R	116/118 (98%)	109 (94%)	7 (6%)	0	100	100
14	1S	108/112 (96%)	99 (92%)	8 (7%)	1 (1%)	17	40
14	2S	108/112 (96%)	96 (89%)	12 (11%)	0	100	100
15	1T	129/146 (88%)	121 (94%)	7 (5%)	1 (1%)	19	43
15	2T	129/146 (88%)	121 (94%)	8 (6%)	0	100	100
16	1U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
16	2U	114/118 (97%)	109 (96%)	5 (4%)	0	100	100
17	1V	99/101 (98%)	97 (98%)	1 (1%)	1 (1%)	15	37
17	2V	99/101 (98%)	93 (94%)	5 (5%)	1 (1%)	15	37
18	1W	110/113 (97%)	107 (97%)	3 (3%)	0	100	100
18	2W	110/113 (97%)	107 (97%)	3 (3%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	1X	93/96 (97%)	91 (98%)	1 (1%)	1 (1%)	14	34
19	2X	93/96 (97%)	89 (96%)	3 (3%)	1 (1%)	14	34
20	1Y	105/110 (96%)	95 (90%)	10 (10%)	0	100	100
20	2Y	105/110 (96%)	98 (93%)	7 (7%)	0	100	100
21	1Z	201/206 (98%)	189 (94%)	12 (6%)	0	100	100
21	2Z	199/206 (97%)	183 (92%)	16 (8%)	0	100	100
22	10	75/85 (88%)	73 (97%)	2 (3%)	0	100	100
22	20	75/85 (88%)	72 (96%)	3 (4%)	0	100	100
23	11	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	14	34
23	21	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	14	34
24	12	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
24	22	68/72 (94%)	66 (97%)	2 (3%)	0	100	100
25	13	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
25	23	57/60 (95%)	55 (96%)	1 (2%)	1 (2%)	8	21
26	14	67/71 (94%)	52 (78%)	12 (18%)	3 (4%)	2	5
26	24	67/71 (94%)	53 (79%)	9 (13%)	5 (8%)	1	1
27	15	57/60 (95%)	57 (100%)	0	0	100	100
27	25	57/60 (95%)	55 (96%)	1 (2%)	1 (2%)	8	21
28	16	51/54 (94%)	48 (94%)	3 (6%)	0	100	100
28	26	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
29	17	46/49 (94%)	46 (100%)	0	0	100	100
29	27	46/49 (94%)	45 (98%)	1 (2%)	0	100	100
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	62 (100%)	0	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
33	1b	229/256 (90%)	200 (87%)	20 (9%)	9 (4%)	3	6
33	2b	229/256 (90%)	200 (87%)	22 (10%)	7 (3%)	4	9
34	1c	204/239 (85%)	191 (94%)	12 (6%)	1 (0%)	29	54
34	2c	204/239 (85%)	172 (84%)	29 (14%)	3 (2%)	10	26
35	1d	206/209 (99%)	192 (93%)	13 (6%)	1 (0%)	29	54

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	2d	206/209 (99%)	189 (92%)	16 (8%)	1 (0%)	29	54
36	1e	146/162 (90%)	141 (97%)	3 (2%)	2 (1%)	11	28
36	2e	146/162 (90%)	134 (92%)	12 (8%)	0	100	100
37	1f	98/101 (97%)	93 (95%)	5 (5%)	0	100	100
37	2f	98/101 (97%)	91 (93%)	7 (7%)	0	100	100
38	1g	153/156 (98%)	145 (95%)	7 (5%)	1 (1%)	22	46
38	2g	153/156 (98%)	144 (94%)	7 (5%)	2 (1%)	12	30
39	1h	135/138 (98%)	128 (95%)	7 (5%)	0	100	100
39	2h	135/138 (98%)	127 (94%)	7 (5%)	1 (1%)	22	46
40	1i	125/128 (98%)	112 (90%)	12 (10%)	1 (1%)	19	43
40	2i	124/128 (97%)	111 (90%)	10 (8%)	3 (2%)	6	15
41	1j	95/105 (90%)	77 (81%)	15 (16%)	3 (3%)	4	9
41	2j	94/105 (90%)	80 (85%)	12 (13%)	2 (2%)	7	18
42	1k	112/129 (87%)	102 (91%)	9 (8%)	1 (1%)	17	40
42	2k	112/129 (87%)	100 (89%)	11 (10%)	1 (1%)	17	40
43	1l	119/132 (90%)	115 (97%)	4 (3%)	0	100	100
43	2l	119/132 (90%)	108 (91%)	11 (9%)	0	100	100
44	1m	114/126 (90%)	104 (91%)	8 (7%)	2 (2%)	8	21
44	2m	112/126 (89%)	98 (88%)	12 (11%)	2 (2%)	8	21
45	1n	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
45	2n	58/61 (95%)	53 (91%)	5 (9%)	0	100	100
46	1o	86/89 (97%)	82 (95%)	1 (1%)	3 (4%)	3	8
46	2o	86/89 (97%)	83 (96%)	2 (2%)	1 (1%)	13	32
47	1p	80/88 (91%)	72 (90%)	7 (9%)	1 (1%)	12	30
47	2p	80/88 (91%)	68 (85%)	11 (14%)	1 (1%)	12	30
48	1q	97/105 (92%)	92 (95%)	5 (5%)	0	100	100
48	2q	97/105 (92%)	92 (95%)	5 (5%)	0	100	100
49	1r	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
49	2r	66/88 (75%)	63 (96%)	3 (4%)	0	100	100
50	1s	81/93 (87%)	71 (88%)	8 (10%)	2 (2%)	5	14
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%)	87 (93%)	5 (5%)	2 (2%)	7	18
51	2t	96/106 (91%)	89 (93%)	3 (3%)	4 (4%)	3	5
52	1u	21/27 (78%)	21 (100%)	0	0	100	100
52	2u	21/27 (78%)	16 (76%)	4 (19%)	1 (5%)	2	4
53	1y	95/113 (84%)	90 (95%)	5 (5%)	0	100	100
53	2y	94/113 (83%)	88 (94%)	6 (6%)	0	100	100
All	All	11629/12354 (94%)	10827 (93%)	706 (6%)	96 (1%)	19	43

All (96) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
26	14	47	GLN
26	14	55	ARG
33	1b	21	ARG
4	2E	51	PHE
6	2G	78	SER
6	2G	81	LYS
8	2I	10	GLU
12	2Q	59	ARG
33	2b	17	PHE
40	2i	54	ASP
6	1G	52	ILE
12	1Q	59	ARG
14	1S	59	LYS
15	1T	127	ALA
17	1V	79	VAL
33	1b	17	PHE
33	1b	20	GLU
33	1b	126	GLU
34	1c	107	GLN
38	1g	55	GLY
41	1j	77	PRO
44	1m	3	ARG
5	2F	130	ALA
10	2O	5	GLN
17	2V	79	VAL
23	21	3	LYS
26	24	62	ARG
33	2b	95	GLN
40	2i	44	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
41	2j	78	ASN
51	2t	47	GLY
51	2t	95	ALA
4	1E	52	LEU
19	1X	94	GLY
23	11	3	LYS
26	14	39	CYS
36	1e	96	PRO
41	1j	55	LYS
46	1o	19	PRO
6	2G	43	LEU
26	24	44	THR
26	24	47	GLN
33	2b	16	HIS
52	2u	3	LYS
5	1F	130	ALA
7	1H	159	GLU
8	1I	85	GLU
10	1O	5	GLN
33	1b	37	ASN
33	1b	95	GLN
41	1j	30	SER
44	1m	12	ASN
47	1p	28	ARG
50	1s	12	ASP
50	1s	27	GLU
5	2F	21	ALA
19	2X	94	GLY
33	2b	128	GLU
38	2g	7	ALA
40	2i	96	LEU
42	2k	89	ALA
47	2p	44	THR
51	2t	100	ILE
51	2t	102	GLY
35	1d	124	GLY
36	1e	97	GLY
8	2I	132	PRO
26	24	49	PHE
27	25	35	GLU
33	2b	9	GLU
34	2c	108	ASN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
34	2c	156	ARG
38	2g	97	GLN
44	2m	95	GLY
46	2o	88	ARG
33	1b	127	ILE
33	1b	232	PRO
46	1o	84	LYS
26	24	55	ARG
33	2b	21	ARG
34	2c	99	VAL
39	2h	51	VAL
9	2N	129	PRO
5	2F	171	PRO
11	2P	122	PRO
41	2j	37	PRO
44	2m	7	VAL
25	23	59	VAL
35	2d	171	GLY
40	1i	44	VAL
42	1k	105	VAL
51	1t	47	GLY
51	1t	100	ILE
33	2b	125	PRO
46	1o	86	GLY
33	1b	125	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	214/218 (98%)	195 (91%)	19 (9%)	9	22
3	2D	215/218 (99%)	197 (92%)	18 (8%)	11	25
4	1E	164/166 (99%)	151 (92%)	13 (8%)	12	28
4	2E	164/166 (99%)	154 (94%)	10 (6%)	18	41
5	1F	160/166 (96%)	145 (91%)	15 (9%)	8	20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	2F	159/166 (96%)	148 (93%)	11 (7%)	15	35
6	1G	144/156 (92%)	132 (92%)	12 (8%)	11	25
6	2G	142/156 (91%)	129 (91%)	13 (9%)	9	21
7	1H	144/148 (97%)	138 (96%)	6 (4%)	30	58
7	2H	143/148 (97%)	137 (96%)	6 (4%)	30	58
8	1I	111/124 (90%)	104 (94%)	7 (6%)	18	40
8	2I	108/124 (87%)	103 (95%)	5 (5%)	27	54
9	1N	119/119 (100%)	112 (94%)	7 (6%)	19	43
9	2N	118/119 (99%)	112 (95%)	6 (5%)	24	50
10	1O	100/100 (100%)	96 (96%)	4 (4%)	31	60
10	2O	100/100 (100%)	96 (96%)	4 (4%)	31	60
11	1P	115/116 (99%)	112 (97%)	3 (3%)	46	75
11	2P	115/116 (99%)	110 (96%)	5 (4%)	29	57
12	1Q	111/111 (100%)	104 (94%)	7 (6%)	18	40
12	2Q	111/111 (100%)	107 (96%)	4 (4%)	35	64
13	1R	101/101 (100%)	91 (90%)	10 (10%)	8	18
13	2R	101/101 (100%)	89 (88%)	12 (12%)	5	12
14	1S	87/88 (99%)	80 (92%)	7 (8%)	12	27
14	2S	85/88 (97%)	79 (93%)	6 (7%)	14	34
15	1T	115/127 (91%)	110 (96%)	5 (4%)	29	57
15	2T	113/127 (89%)	107 (95%)	6 (5%)	22	48
16	1U	93/94 (99%)	88 (95%)	5 (5%)	22	47
16	2U	93/94 (99%)	90 (97%)	3 (3%)	39	68
17	1V	81/82 (99%)	73 (90%)	8 (10%)	8	18
17	2V	80/82 (98%)	76 (95%)	4 (5%)	24	51
18	1W	90/92 (98%)	81 (90%)	9 (10%)	7	18
18	2W	90/92 (98%)	82 (91%)	8 (9%)	9	22
19	1X	77/78 (99%)	73 (95%)	4 (5%)	23	49
19	2X	77/78 (99%)	73 (95%)	4 (5%)	23	49
20	1Y	86/91 (94%)	80 (93%)	6 (7%)	15	35
20	2Y	86/91 (94%)	84 (98%)	2 (2%)	50	78

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	1Z	169/179 (94%)	154 (91%)	15 (9%)	9	22
21	2Z	165/179 (92%)	158 (96%)	7 (4%)	30	58
22	10	61/67 (91%)	57 (93%)	4 (7%)	16	38
22	20	61/67 (91%)	59 (97%)	2 (3%)	38	67
23	11	79/83 (95%)	76 (96%)	3 (4%)	33	62
23	21	81/83 (98%)	78 (96%)	3 (4%)	34	63
24	12	65/67 (97%)	64 (98%)	1 (2%)	65	86
24	22	66/67 (98%)	65 (98%)	1 (2%)	65	86
25	13	51/52 (98%)	46 (90%)	5 (10%)	8	18
25	23	50/52 (96%)	48 (96%)	2 (4%)	31	60
26	14	58/63 (92%)	55 (95%)	3 (5%)	23	49
26	24	54/63 (86%)	54 (100%)	0	100	100
27	15	51/52 (98%)	45 (88%)	6 (12%)	5	12
27	25	50/52 (96%)	47 (94%)	3 (6%)	19	42
28	16	51/52 (98%)	46 (90%)	5 (10%)	8	18
28	26	50/52 (96%)	46 (92%)	4 (8%)	12	27
29	17	41/42 (98%)	36 (88%)	5 (12%)	5	11
29	27	41/42 (98%)	41 (100%)	0	100	100
30	18	54/55 (98%)	50 (93%)	4 (7%)	13	32
30	28	54/55 (98%)	49 (91%)	5 (9%)	9	21
31	19	34/34 (100%)	32 (94%)	2 (6%)	19	43
31	29	34/34 (100%)	33 (97%)	1 (3%)	42	71
33	1b	191/220 (87%)	183 (96%)	8 (4%)	30	58
33	2b	187/220 (85%)	180 (96%)	7 (4%)	34	63
34	1c	144/188 (77%)	139 (96%)	5 (4%)	36	65
34	2c	140/188 (74%)	134 (96%)	6 (4%)	29	57
35	1d	171/181 (94%)	162 (95%)	9 (5%)	22	48
35	2d	172/181 (95%)	166 (96%)	6 (4%)	36	65
36	1e	114/123 (93%)	110 (96%)	4 (4%)	36	65
36	2e	114/123 (93%)	108 (95%)	6 (5%)	22	48
37	1f	85/90 (94%)	82 (96%)	3 (4%)	36	65

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	2f	85/90 (94%)	82 (96%)	3 (4%)	36	65
38	1g	120/127 (94%)	117 (98%)	3 (2%)	47	76
38	2g	119/127 (94%)	113 (95%)	6 (5%)	24	51
39	1h	116/119 (98%)	114 (98%)	2 (2%)	60	84
39	2h	114/119 (96%)	109 (96%)	5 (4%)	28	56
40	1i	91/99 (92%)	91 (100%)	0	100	100
40	2i	88/99 (89%)	85 (97%)	3 (3%)	37	66
41	1j	68/92 (74%)	66 (97%)	2 (3%)	42	71
41	2j	68/92 (74%)	67 (98%)	1 (2%)	65	86
42	1k	83/99 (84%)	80 (96%)	3 (4%)	35	64
42	2k	83/99 (84%)	79 (95%)	4 (5%)	25	53
43	1l	96/108 (89%)	92 (96%)	4 (4%)	30	58
43	2l	96/108 (89%)	94 (98%)	2 (2%)	53	80
44	1m	90/101 (89%)	86 (96%)	4 (4%)	28	56
44	2m	87/101 (86%)	84 (97%)	3 (3%)	37	66
45	1n	49/50 (98%)	48 (98%)	1 (2%)	55	81
45	2n	49/50 (98%)	49 (100%)	0	100	100
46	1o	78/80 (98%)	74 (95%)	4 (5%)	24	50
46	2o	78/80 (98%)	77 (99%)	1 (1%)	69	87
47	1p	69/74 (93%)	65 (94%)	4 (6%)	20	43
47	2p	68/74 (92%)	62 (91%)	6 (9%)	10	23
48	1q	94/97 (97%)	89 (95%)	5 (5%)	22	48
48	2q	94/97 (97%)	89 (95%)	5 (5%)	22	48
49	1r	59/77 (77%)	58 (98%)	1 (2%)	60	84
49	2r	59/77 (77%)	53 (90%)	6 (10%)	7	17
50	1s	68/80 (85%)	67 (98%)	1 (2%)	65	86
50	2s	67/80 (84%)	65 (97%)	2 (3%)	41	70
51	1t	71/82 (87%)	67 (94%)	4 (6%)	21	45
51	2t	70/82 (85%)	65 (93%)	5 (7%)	14	34
52	1u	18/22 (82%)	17 (94%)	1 (6%)	21	45
52	2u	18/22 (82%)	17 (94%)	1 (6%)	21	45

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	1y	82/98 (84%)	78 (95%)	4 (5%)	25	52
53	2y	79/98 (81%)	74 (94%)	5 (6%)	18	40
All	All	9524/10260 (93%)	9014 (95%)	510 (5%)	22	47

All (510) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	3	VAL
3	1D	13	ARG
3	1D	39	LYS
3	1D	61	LEU
3	1D	63	ARG
3	1D	69	ARG
3	1D	88	ARG
3	1D	103	ARG
3	1D	106	ILE
3	1D	111	LEU
3	1D	138	VAL
3	1D	173	VAL
3	1D	193	VAL
3	1D	211	ARG
3	1D	221	VAL
3	1D	229	VAL
3	1D	242	ARG
3	1D	259	THR
3	1D	260	ARG
4	1E	1	MET
4	1E	9	VAL
4	1E	33	VAL
4	1E	34	VAL
4	1E	49	LEU
4	1E	75	VAL
4	1E	78	LEU
4	1E	116	VAL
4	1E	119	ARG
4	1E	144	ARG
4	1E	154	LYS
4	1E	175	VAL
4	1E	181	LEU
5	1F	38	ARG
5	1F	53	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
5	1F	57	VAL
5	1F	74	ARG
5	1F	88	VAL
5	1F	95	ARG
5	1F	110	LEU
5	1F	125	LEU
5	1F	132	VAL
5	1F	158	THR
5	1F	170	LEU
5	1F	191	ARG
5	1F	192	LEU
5	1F	197	ASP
5	1F	201	VAL
6	1G	5	VAL
6	1G	7	LEU
6	1G	28	VAL
6	1G	43	LEU
6	1G	47	LYS
6	1G	49	ASP
6	1G	52	ILE
6	1G	53	LEU
6	1G	135	LEU
6	1G	153	ARG
6	1G	159	VAL
6	1G	181	ARG
7	1H	15	VAL
7	1H	71	LEU
7	1H	85	LYS
7	1H	122	THR
7	1H	134	SER
7	1H	149	ARG
8	1I	12	LEU
8	1I	38	LEU
8	1I	41	GLU
8	1I	44	LEU
8	1I	92	VAL
8	1I	101	LEU
8	1I	109	ILE
9	1N	5	VAL
9	1N	15	LEU
9	1N	34	LEU
9	1N	48	MET

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
9	1N	62	VAL
9	1N	67	LEU
9	1N	99	LEU
10	1O	10	VAL
10	1O	24	VAL
10	1O	94	ARG
10	1O	108	GLU
11	1P	59	LEU
11	1P	83	VAL
11	1P	125	VAL
12	1Q	2	LEU
12	1Q	6	ARG
12	1Q	7	MET
12	1Q	60	ARG
12	1Q	81	VAL
12	1Q	109	VAL
12	1Q	133	ARG
13	1R	6	SER
13	1R	29	LEU
13	1R	33	ARG
13	1R	36	THR
13	1R	44	LEU
13	1R	54	LEU
13	1R	65	LEU
13	1R	67	LEU
13	1R	100	LEU
13	1R	111	LEU
14	1S	14	VAL
14	1S	25	ARG
14	1S	50	SER
14	1S	52	SER
14	1S	59	LYS
14	1S	85	VAL
14	1S	110	LEU
15	1T	28	VAL
15	1T	33	LYS
15	1T	89	VAL
15	1T	96	ARG
15	1T	118	ARG
16	1U	8	VAL
16	1U	30	LYS
16	1U	74	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
16	1U	77	SER
16	1U	95	LEU
17	1V	46	VAL
17	1V	51	VAL
17	1V	52	VAL
17	1V	61	VAL
17	1V	62	LEU
17	1V	72	VAL
17	1V	79	VAL
17	1V	82	ARG
18	1W	11	ARG
18	1W	15	ARG
18	1W	17	VAL
18	1W	19	LEU
18	1W	23	LEU
18	1W	95	ILE
18	1W	96	ILE
18	1W	100	THR
18	1W	107	LEU
19	1X	35	THR
19	1X	38	GLU
19	1X	45	THR
19	1X	66	LEU
20	1Y	43	ASN
20	1Y	63	LYS
20	1Y	72	VAL
20	1Y	85	VAL
20	1Y	90	LEU
20	1Y	99	CYS
21	1Z	18	LEU
21	1Z	31	ARG
21	1Z	46	LYS
21	1Z	58	VAL
21	1Z	61	LEU
21	1Z	74	VAL
21	1Z	76	LEU
21	1Z	86	VAL
21	1Z	91	LEU
21	1Z	126	VAL
21	1Z	150	LEU
21	1Z	155	LEU
21	1Z	161	VAL

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
21	1Z	162	GLU
21	1Z	170	THR
22	10	14	ARG
22	10	39	ARG
22	10	55	ARG
22	10	59	LEU
23	11	21	ARG
23	11	59	THR
23	11	95	LEU
24	12	53	LEU
25	13	6	VAL
25	13	8	LEU
25	13	17	LYS
25	13	23	LEU
25	13	55	ARG
26	14	49	PHE
26	14	53	GLU
26	14	56	VAL
27	15	6	VAL
27	15	16	ARG
27	15	26	THR
27	15	29	THR
27	15	40	LYS
27	15	60	VAL
28	16	6	ARG
28	16	14	THR
28	16	19	ARG
28	16	48	VAL
28	16	52	VAL
29	17	1	MET
29	17	24	THR
29	17	43	THR
29	17	46	VAL
29	17	47	ARG
30	18	30	ARG
30	18	31	HIS
30	18	32	LEU
30	18	34	TRP
31	19	17	ILE
31	19	35	ARG
33	1b	15	VAL
33	1b	44	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
33	1b	101	MET
33	1b	111	ARG
33	1b	130	ARG
33	1b	142	LEU
33	1b	160	ASP
33	1b	178	ARG
34	1c	3	ASN
34	1c	105	GLU
34	1c	112	SER
34	1c	150	LYS
34	1c	206	GLU
35	1d	19	LEU
35	1d	28	SER
35	1d	59	ARG
35	1d	115	ARG
35	1d	127	THR
35	1d	135	LEU
35	1d	157	LEU
35	1d	188	LEU
35	1d	194	LEU
36	1e	31	LEU
36	1e	41	VAL
36	1e	69	VAL
36	1e	91	LEU
37	1f	48	LEU
37	1f	63	TYR
37	1f	69	GLU
38	1g	75	VAL
38	1g	104	LEU
38	1g	115	ARG
39	1h	63	LEU
39	1h	104	ARG
41	1j	34	VAL
41	1j	72	VAL
42	1k	16	SER
42	1k	112	THR
42	1k	114	VAL
43	1l	27	LEU
43	1l	83	VAL
43	1l	113	ARG
43	1l	117	ARG
44	1m	70	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
44	1m	98	VAL
44	1m	102	ARG
44	1m	117	VAL
45	1n	18	VAL
46	1o	3	ILE
46	1o	24	SER
46	1o	39	LEU
46	1o	66	LEU
47	1p	25	ARG
47	1p	32	TYR
47	1p	62	VAL
47	1p	76	GLN
48	1q	26	GLN
48	1q	57	VAL
48	1q	63	ARG
48	1q	68	ARG
48	1q	97	SER
49	1r	42	ARG
50	1s	41	VAL
51	1t	11	SER
51	1t	24	LEU
51	1t	58	LYS
51	1t	84	LEU
52	1u	24	ARG
53	1y	3	MET
53	1y	23	ARG
53	1y	42	SER
53	1y	88	LEU
3	2D	3	VAL
3	2D	32	SER
3	2D	69	ARG
3	2D	71	ASP
3	2D	94	LEU
3	2D	103	ARG
3	2D	111	LEU
3	2D	138	VAL
3	2D	142	VAL
3	2D	173	VAL
3	2D	193	VAL
3	2D	211	ARG
3	2D	217	ARG
3	2D	221	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	2D	229	VAL
3	2D	237	GLU
3	2D	242	ARG
3	2D	274	ARG
4	2E	9	VAL
4	2E	21	VAL
4	2E	38	THR
4	2E	72	VAL
4	2E	75	VAL
4	2E	78	LEU
4	2E	116	VAL
4	2E	175	VAL
4	2E	181	LEU
4	2E	184	VAL
5	2F	20	LEU
5	2F	33	LEU
5	2F	38	ARG
5	2F	57	VAL
5	2F	60	SER
5	2F	74	ARG
5	2F	88	VAL
5	2F	158	THR
5	2F	168	ARG
5	2F	183	VAL
5	2F	192	LEU
6	2G	5	VAL
6	2G	7	LEU
6	2G	28	VAL
6	2G	60	LEU
6	2G	71	THR
6	2G	79	ASN
6	2G	109	VAL
6	2G	113	ARG
6	2G	133	LEU
6	2G	140	ILE
6	2G	159	VAL
6	2G	161	THR
6	2G	181	ARG
7	2H	47	GLU
7	2H	56	SER
7	2H	71	LEU
7	2H	98	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
7	2H	136	ILE
7	2H	139	GLN
8	2I	40	THR
8	2I	64	GLU
8	2I	68	LEU
8	2I	116	LEU
8	2I	140	LEU
9	2N	34	LEU
9	2N	46	VAL
9	2N	60	ILE
9	2N	62	VAL
9	2N	99	LEU
9	2N	140	VAL
10	2O	21	CYS
10	2O	24	VAL
10	2O	35	VAL
10	2O	108	GLU
11	2P	4	SER
11	2P	59	LEU
11	2P	65	ARG
11	2P	83	VAL
11	2P	112	LEU
12	2Q	55	VAL
12	2Q	109	VAL
12	2Q	110	THR
12	2Q	112	GLU
13	2R	6	SER
13	2R	17	ARG
13	2R	24	GLN
13	2R	36	THR
13	2R	44	LEU
13	2R	59	ASP
13	2R	65	LEU
13	2R	67	LEU
13	2R	75	LEU
13	2R	96	ARG
13	2R	100	LEU
13	2R	111	LEU
14	2S	23	ARG
14	2S	30	ARG
14	2S	50	SER
14	2S	52	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
14	2S	64	GLU
14	2S	69	VAL
15	2T	31	SER
15	2T	51	ARG
15	2T	53	ARG
15	2T	74	ARG
15	2T	89	VAL
15	2T	95	ARG
16	2U	31	SER
16	2U	59	ARG
16	2U	95	LEU
17	2V	18	LEU
17	2V	39	LEU
17	2V	46	VAL
17	2V	79	VAL
18	2W	15	ARG
18	2W	17	VAL
18	2W	19	LEU
18	2W	23	LEU
18	2W	49	LYS
18	2W	67	ASP
18	2W	70	TYR
18	2W	100	THR
19	2X	2	LYS
19	2X	49	VAL
19	2X	57	LEU
19	2X	81	VAL
20	2Y	3	VAL
20	2Y	6	HIS
21	2Z	33	LEU
21	2Z	72	ARG
21	2Z	86	VAL
21	2Z	107	THR
21	2Z	150	LEU
21	2Z	170	THR
21	2Z	175	VAL
22	20	9	SER
22	20	14	ARG
23	21	11	ARG
23	21	35	THR
23	21	85	LEU
24	22	53	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
25	23	23	LEU
25	23	31	LEU
27	25	6	VAL
27	25	29	THR
27	25	58	LEU
28	26	6	ARG
28	26	7	ILE
28	26	14	THR
28	26	40	CYS
30	28	14	VAL
30	28	30	ARG
30	28	32	LEU
30	28	34	TRP
30	28	37	SER
31	29	7	VAL
33	2b	15	VAL
33	2b	23	ARG
33	2b	44	LEU
33	2b	83	MET
33	2b	189	ASP
33	2b	190	THR
33	2b	209	ARG
34	2c	15	THR
34	2c	21	ARG
34	2c	22	TRP
34	2c	33	LEU
34	2c	68	VAL
34	2c	166	GLU
35	2d	8	VAL
35	2d	83	SER
35	2d	122	ARG
35	2d	135	LEU
35	2d	157	LEU
35	2d	175	SER
36	2e	18	ARG
36	2e	31	LEU
36	2e	34	VAL
36	2e	41	VAL
36	2e	72	GLN
36	2e	75	THR
37	2f	61	LEU
37	2f	63	TYR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
37	2f	72	VAL
38	2g	15	ASP
38	2g	42	ILE
38	2g	75	VAL
38	2g	77	SER
38	2g	104	LEU
38	2g	155	ARG
39	2h	29	SER
39	2h	85	ARG
39	2h	104	ARG
39	2h	121	ASP
39	2h	137	VAL
40	2i	9	ARG
40	2i	27	THR
40	2i	102	LEU
41	2j	100	THR
42	2k	32	ILE
42	2k	47	VAL
42	2k	79	SER
42	2k	116	HIS
43	2l	59	ARG
43	2l	83	VAL
44	2m	47	ASP
44	2m	99	ARG
44	2m	102	ARG
46	2o	39	LEU
47	2p	1	MET
47	2p	2	VAL
47	2p	28	ARG
47	2p	62	VAL
47	2p	69	THR
47	2p	74	LEU
48	2q	9	VAL
48	2q	56	VAL
48	2q	60	ILE
48	2q	68	ARG
48	2q	70	ARG
49	2r	26	LEU
49	2r	37	VAL
49	2r	54	ARG
49	2r	55	ARG
49	2r	76	LEU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
49	2r	85	LEU
50	2s	41	VAL
50	2s	48	THR
51	2t	15	ARG
51	2t	31	SER
51	2t	71	THR
51	2t	86	ARG
51	2t	100	ILE
52	2u	24	ARG
53	2y	5	ILE
53	2y	32	THR
53	2y	61	LEU
53	2y	70	MET
53	2y	93	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (102) such sidechains are listed below:

Mol	Chain	Res	Type
4	1E	143	ASN
5	1F	69	HIS
5	1F	203	GLN
6	1G	26	GLN
7	1H	158	HIS
8	1I	104	GLN
8	1I	105	HIS
9	1N	94	HIS
13	1R	71	GLN
15	1T	58	ASN
16	1U	81	HIS
16	1U	117	GLN
19	1X	31	HIS
20	1Y	6	HIS
20	1Y	43	ASN
20	1Y	92	ASN
21	1Z	151	HIS
25	13	32	GLN
27	15	4	HIS
31	19	34	GLN
34	1c	6	HIS
34	1c	37	GLN
34	1c	69	HIS
34	1c	102	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
34	1c	162	GLN
35	1d	45	GLN
35	1d	116	GLN
35	1d	123	HIS
35	1d	125	HIS
35	1d	129	ASN
37	1f	64	GLN
37	1f	100	ASN
38	1g	28	ASN
38	1g	51	GLN
38	1g	148	ASN
40	1i	3	GLN
40	1i	73	GLN
41	1j	21	GLN
41	1j	56	HIS
41	1j	84	GLN
42	1k	93	GLN
43	1l	99	HIS
44	1m	92	HIS
46	1o	28	GLN
47	1p	13	HIS
47	1p	16	HIS
48	1q	16	GLN
50	1s	69	HIS
50	1s	83	HIS
51	1t	18	GLN
53	1y	9	GLN
53	1y	38	HIS
3	2D	126	GLN
3	2D	253	GLN
4	2E	48	GLN
5	2F	40	GLN
5	2F	69	HIS
5	2F	133	ASN
6	2G	26	GLN
6	2G	79	ASN
8	2I	43	ASN
10	2O	3	GLN
11	2P	27	HIS
12	2Q	89	ASN
12	2Q	123	HIS
12	2Q	141	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
15	2T	58	ASN
18	2W	60	ASN
19	2X	31	HIS
21	2Z	34	ASN
21	2Z	73	GLN
25	23	32	GLN
31	29	36	GLN
33	2b	40	HIS
34	2c	3	ASN
34	2c	6	HIS
34	2c	37	GLN
34	2c	69	HIS
34	2c	104	GLN
34	2c	139	GLN
34	2c	176	HIS
35	2d	77	ASN
35	2d	116	GLN
35	2d	161	ASN
36	2e	20	GLN
36	2e	78	HIS
37	2f	100	ASN
38	2g	28	ASN
38	2g	56	GLN
40	2i	3	GLN
40	2i	38	GLN
40	2i	73	GLN
41	2j	56	HIS
41	2j	68	HIS
41	2j	69	ASN
43	2l	99	HIS
45	2n	49	HIS
46	2o	28	GLN
47	2p	16	HIS
50	2s	69	HIS
50	2s	83	HIS
53	2y	38	HIS

### 5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2862/2915 (98%)	421 (14%)	29 (1%)

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2A	2855/2915 (97%)	492 (17%)	36 (1%)
2	1B	119/121 (98%)	11 (9%)	0
2	2B	119/121 (98%)	18 (15%)	0
32	1a	1494/1521 (98%)	233 (15%)	0
32	2a	1498/1521 (98%)	261 (17%)	0
All	All	8947/9114 (98%)	1436 (16%)	65 (0%)

All (1436) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	14	A
1	1A	15	G
1	1A	34	C
1	1A	45	C
1	1A	70	A
1	1A	73	A
1	1A	74	G
1	1A	116	A
1	1A	117	A
1	1A	118	U
1	1A	164	G
1	1A	166	G
1	1A	170	A
1	1A	171	A
1	1A	177	G
1	1A	185	A
1	1A	188	A
1	1A	194	G
1	1A	203	G
1	1A	204	G
1	1A	205	A
1	1A	206	G
1	1A	211	A
1	1A	218	A
1	1A	222	A
1	1A	237	G
1	1A	253	C
1	1A	254	A
1	1A	265	U
1	1A	269	G
1	1A	271	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	1A	272	U
1	1A	273	G
1	1A	274	U
1	1A	275	C
1	1A	288	U
1	1A	289	G
1	1A	297	C
1	1A	298	G
1	1A	299	G
1	1A	303	C
1	1A	304	C
1	1A	307	A
1	1A	335	A
1	1A	354	A
1	1A	376	G
1	1A	381	A
1	1A	384	G
1	1A	387	G
1	1A	413	G
1	1A	423	G
1	1A	432	U
1	1A	438	G
1	1A	448	U
1	1A	449	A
1	1A	455	A
1	1A	474	U
1	1A	482	C
1	1A	483	A
1	1A	507	G
1	1A	530	A
1	1A	534	C
1	1A	553	A
1	1A	555	G
1	1A	556	C
1	1A	557	A
1	1A	558	G
1	1A	569	G
1	1A	573	G
1	1A	586	G
1	1A	596	G
1	1A	597	C
1	1A	598	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	1A	626	A
1	1A	627	G
1	1A	630	U
1	1A	639	G
1	1A	641	G
1	1A	652	A
1	1A	662	A
1	1A	670	C
1	1A	693	G
1	1A	697	C
1	1A	698	G
1	1A	701	A
1	1A	716	G
1	1A	733	G
1	1A	764	G
1	1A	777	C
1	1A	785	G
1	1A	804	U
1	1A	822	G
1	1A	823	G
1	1A	829	A
1	1A	831	A
1	1A	832	G
1	1A	837	C
1	1A	839	G
1	1A	852	G
1	1A	859	C
1	1A	874	U
1	1A	875	U
1	1A	906	G
1	1A	913	A
1	1A	925	A
1	1A	926	G
1	1A	929	G
1	1A	931	C
1	1A	932	C
1	1A	933	C
1	1A	935	C
1	1A	936	C
1	1A	937	A
1	1A	938	G
1	1A	942	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	1A	943	C
1	1A	945	A
1	1A	953	U
1	1A	956	A
1	1A	977	G
1	1A	983	G
1	1A	990	A
1	1A	991	G
1	1A	1003	U
1	1A	1004	A
1	1A	1006	C
1	1A	1008	U
1	1A	1019	G
1	1A	1020	C
1	1A	1029	A
1	1A	1042	A
1	1A	1045	U
1	1A	1058	U
1	1A	1059	C
1	1A	1068	G
1	1A	1072	U
1	1A	1079	U
1	1A	1084	C
1	1A	1085	G
1	1A	1088	G
1	1A	1089	C
1	1A	1091	A
1	1A	1092	A
1	1A	1093	G
1	1A	1094	A
1	1A	1099	C
1	1A	1100	A
1	1A	1106	U
1	1A	1107	U
1	1A	1108	G
1	1A	1109	G
1	1A	1111	U
1	1A	1114	G
1	1A	1116	A
1	1A	1117	G
1	1A	1119	A
1	1A	1121	C

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	1A	1123	A
1	1A	1124	U
1	1A	1125	C
1	1A	1129	U
1	1A	1133	G
1	1A	1134	A
1	1A	1136	U
1	1A	1137	G
1	1A	1142	A
1	1A	1143	U
1	1A	1155	C
1	1A	1156	G
1	1A	1158	G
1	1A	1162	C
1	1A	1174	A
1	1A	1175	A
1	1A	1176	U
1	1A	1180	C
1	1A	1181	G
1	1A	1184	G
1	1A	1196	C
1	1A	1216	G
1	1A	1217	G
1	1A	1218	G
1	1A	1219	A
1	1A	1220	U
1	1A	1221	G
1	1A	1222	A
1	1A	1223	C
1	1A	1255	A
1	1A	1256	U
1	1A	1263	C
1	1A	1275	G
1	1A	1299	A
1	1A	1302	G
1	1A	1317	G
1	1A	1318	A
1	1A	1327	G
1	1A	1346	U
1	1A	1347	A
1	1A	1351	C
1	1A	1367	A

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	1A	1398	U
1	1A	1405	A
1	1A	1406	A
1	1A	1411	A
1	1A	1416	C
1	1A	1426	G
1	1A	1430	A
1	1A	1431	G
1	1A	1441	A
1	1A	1462	G
1	1A	1463	C
1	1A	1466	U
1	1A	1467	G
1	1A	1474	C
1	1A	1491	A
1	1A	1497	G
1	1A	1500	A
1	1A	1502	G
1	1A	1506	G
1	1A	1508	G
1	1A	1514	C
1	1A	1518	A
1	1A	1529	G
1	1A	1539	C
1	1A	1552	C
1	1A	1554	A
1	1A	1555	C
1	1A	1556	A
1	1A	1589	A
1	1A	1590	C
1	1A	1605	A
1	1A	1613	A
1	1A	1616	A
1	1A	1625	U
1	1A	1628	G
1	1A	1629	C
1	1A	1631	C
1	1A	1632	A
1	1A	1654	A
1	1A	1655	A
1	1A	1656	A
1	1A	1695	C

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	1A	1701	A
1	1A	1711	A
1	1A	1721	G
1	1A	1747	A
1	1A	1748	A
1	1A	1766	G
1	1A	1767	A
1	1A	1768	U
1	1A	1777	G
1	1A	1787	G
1	1A	1794	G
1	1A	1795	G
1	1A	1804	A
1	1A	1811	A
1	1A	1813	C
1	1A	1822	A
1	1A	1831	C
1	1A	1832	G
1	1A	1843	A
1	1A	1847	G
1	1A	1860	A
1	1A	1870	G
1	1A	1878	A
1	1A	1899	A
1	1A	1900	G
1	1A	1911	A
1	1A	1922	A
1	1A	1928	G
1	1A	1935	A
1	1A	1936	C
1	1A	1951	G
1	1A	1952	G
1	1A	1959	A
1	1A	1960	A
1	1A	1974	A
1	1A	1977	U
1	1A	1985	U
1	1A	1989	C
1	1A	1992	A
1	1A	1993	A
1	1A	1994	A
1	1A	2015	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	1A	2019	G
1	1A	2042	A
1	1A	2045	G
1	1A	2053	A
1	1A	2054	G
1	1A	2055	A
1	1A	2065	C
1	1A	2077	C
1	1A	2078	G
1	1A	2082	A
1	1A	2083	G
1	1A	2085	C
1	1A	2091	G
1	1A	2121	U
1	1A	2125	C
1	1A	2129	C
1	1A	2130	C
1	1A	2138	G
1	1A	2139	A
1	1A	2141	A
1	1A	2145	G
1	1A	2148	A
1	1A	2149	G
1	1A	2153	G
1	1A	2154	U
1	1A	2155	G
1	1A	2156	A
1	1A	2157	A
1	1A	2158	C
1	1A	2161	C
1	1A	2164	C
1	1A	2167	C
1	1A	2168	C
1	1A	2170	G
1	1A	2180	A
1	1A	2181	G
1	1A	2188	G
1	1A	2195	A
1	1A	2198	A
1	1A	2207	C
1	1A	2209	G
1	1A	2213	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	1A	2214	G
1	1A	2215	G
1	1A	2220	A
1	1A	2227	G
1	1A	2228	G
1	1A	2229	A
1	1A	2237	A
1	1A	2244	U
1	1A	2250	G
1	1A	2251	G
1	1A	2280	A
1	1A	2281	A
1	1A	2290	A
1	1A	2295	C
1	1A	2299	A
1	1A	2301	G
1	1A	2317	A
1	1A	2320	G
1	1A	2332	A
1	1A	2337	G
1	1A	2338	C
1	1A	2346	G
1	1A	2359	C
1	1A	2362	C
1	1A	2395	G
1	1A	2397	C
1	1A	2417	G
1	1A	2418	U
1	1A	2421	G
1	1A	2426	G
1	1A	2434	A
1	1A	2435	U
1	1A	2437	A
1	1A	2440	G
1	1A	2441	G
1	1A	2442	A
1	1A	2443	U
1	1A	2444	A
1	1A	2447	A
1	1A	2451	A
1	1A	2453	C
1	1A	2460	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	1A	2480	G
1	1A	2481	A
1	1A	2488	A
1	1A	2510	C
1	1A	2514	G
1	1A	2516	U
1	1A	2517	G
1	1A	2530	A
1	1A	2541	G
1	1A	2547	G
1	1A	2566	U
1	1A	2567	U
1	1A	2578	A
1	1A	2579	G
1	1A	2585	C
1	1A	2597	U
1	1A	2614	A
1	1A	2615	G
1	1A	2621	U
1	1A	2623	U
1	1A	2624	C
1	1A	2641	A
1	1A	2642	G
1	1A	2666	A
1	1A	2674	A
1	1A	2701	U
1	1A	2702	C
1	1A	2714	U
1	1A	2715	C
1	1A	2725	A
1	1A	2726	A
1	1A	2727	G
1	1A	2739	U
1	1A	2746	A
1	1A	2771	A
1	1A	2778	A
1	1A	2779	G
1	1A	2782	C
1	1A	2791	A
1	1A	2803	A
1	1A	2804	C
1	1A	2813	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	1A	2828	G
1	1A	2830	A
1	1A	2831	A
1	1A	2843	G
1	1A	2845	A
1	1A	2846	U
1	1A	2882	G
1	1A	2883	A
1	1A	2890	C
1	1A	2901	A
1	1A	2903	G
2	1B	7	G
2	1B	15	A
2	1B	32	C
2	1B	45	A
2	1B	53	A
2	1B	56	G
2	1B	73	A
2	1B	84	C
2	1B	106	G
2	1B	110	G
2	1B	116	G
32	1a	5	U
32	1a	9	G
32	1a	32	A
32	1a	39	G
32	1a	48	C
32	1a	51	A
32	1a	61	G
32	1a	79	G
32	1a	101	A
32	1a	116	A
32	1a	121	C
32	1a	131	C
32	1a	156	G
32	1a	159	G
32	1a	163	C
32	1a	169	C
32	1a	173	U
32	1a	174	C
32	1a	182	U
32	1a	189(F)	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
32	1a	195	A
32	1a	197	A
32	1a	199	G
32	1a	202	U
32	1a	203	U
32	1a	204	U
32	1a	216	G
32	1a	220	G
32	1a	231	G
32	1a	247	G
32	1a	251	G
32	1a	254	G
32	1a	258	G
32	1a	266	G
32	1a	267	C
32	1a	289	G
32	1a	301	G
32	1a	306	G
32	1a	321	A
32	1a	328	C
32	1a	332	G
32	1a	348	G
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	356	A
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	384	G
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	413	G
32	1a	422	C
32	1a	423	G
32	1a	424	G
32	1a	429	U
32	1a	439	A
32	1a	442	C
32	1a	443	C
32	1a	444	C

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
32	1a	452	A
32	1a	456	C
32	1a	461	A
32	1a	470	C
32	1a	475	G
32	1a	477	A
32	1a	485	G
32	1a	496	A
32	1a	498	U
32	1a	505	G
32	1a	506	G
32	1a	509	A
32	1a	510	A
32	1a	511	C
32	1a	518	C
32	1a	521	G
32	1a	532	A
32	1a	547	A
32	1a	550	G
32	1a	559	A
32	1a	561	U
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	577	G
32	1a	607	A
32	1a	617	G
32	1a	619	U
32	1a	630	G
32	1a	631	G
32	1a	632	A
32	1a	633	G
32	1a	642	A
32	1a	650	G
32	1a	653	A
32	1a	661	G
32	1a	665	A
32	1a	671	G
32	1a	687	A
32	1a	688	G
32	1a	693	G
32	1a	723	U

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
32	1a	728	A
32	1a	731	G
32	1a	750	G
32	1a	755	G
32	1a	777	A
32	1a	793	U
32	1a	794	A
32	1a	817	C
32	1a	821	G
32	1a	828	A
32	1a	829	G
32	1a	836	G
32	1a	839	U
32	1a	840	C
32	1a	841	U
32	1a	848	C
32	1a	858	G
32	1a	902	G
32	1a	914	A
32	1a	926	G
32	1a	927	G
32	1a	934	C
32	1a	935	A
32	1a	960	U
32	1a	961	U
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	992	U
32	1a	993	G
32	1a	994	A
32	1a	998	G
32	1a	999	C
32	1a	1001(A)	G
32	1a	1003	G
32	1a	1004	A
32	1a	1009	G
32	1a	1022	G
32	1a	1023	G

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	1a	1024	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C
32	1a	1028	C
32	1a	1029	C
32	1a	1030(A)	G
32	1a	1032	G
32	1a	1037	C
32	1a	1044	A
32	1a	1053	G
32	1a	1065	U
32	1a	1066	C
32	1a	1068	G
32	1a	1070	U
32	1a	1081	G
32	1a	1094	G
32	1a	1095	U
32	1a	1100	C
32	1a	1101	A
32	1a	1124	G
32	1a	1126	U
32	1a	1130	A
32	1a	1134	G
32	1a	1136	U
32	1a	1137	C
32	1a	1139	G
32	1a	1140	C
32	1a	1146	A
32	1a	1152	A
32	1a	1159	U
32	1a	1183	A
32	1a	1184	G
32	1a	1196	U
32	1a	1197	G
32	1a	1202	G
32	1a	1208	C
32	1a	1213	A
32	1a	1214	C
32	1a	1224	G
32	1a	1227	A
32	1a	1238	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
32	1a	1240	U
32	1a	1256	A
32	1a	1257	U
32	1a	1258	G
32	1a	1263	C
32	1a	1269	A
32	1a	1270	C
32	1a	1278	U
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1320	C
32	1a	1322	C
32	1a	1338	G
32	1a	1340	A
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1360	A
32	1a	1363	C
32	1a	1370	G
32	1a	1397	C
32	1a	1406	U
32	1a	1419	G
32	1a	1422	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1447	A
32	1a	1452	C
32	1a	1456	G
32	1a	1492	A
32	1a	1493	A
32	1a	1503	A
32	1a	1504	G
32	1a	1505	G
32	1a	1506	U
32	1a	1507	A
32	1a	1517	G
32	1a	1520	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
32	1a	1529	G
32	1a	1530	G
32	1a	1531	A
1	2A	9	U
1	2A	10	G
1	2A	12	U
1	2A	34	C
1	2A	36	G
1	2A	45	C
1	2A	61	G
1	2A	63	U
1	2A	71	A
1	2A	74	A
1	2A	75	G
1	2A	84	A
1	2A	90	U
1	2A	94	C
1	2A	118	A
1	2A	119	A
1	2A	120	U
1	2A	131	G
1	2A	141	A
1	2A	157	U
1	2A	181	A
1	2A	182	A
1	2A	196	A
1	2A	199	A
1	2A	205	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	233	A
1	2A	248	G
1	2A	265	A
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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	303	U
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	330	A
1	2A	333	G
1	2A	352	G
1	2A	363	G
1	2A	370	G
1	2A	386	G
1	2A	396	G
1	2A	405	U
1	2A	411	G
1	2A	412	A
1	2A	444	C
1	2A	455	C
1	2A	456	C
1	2A	457	A
1	2A	470	A
1	2A	481	G
1	2A	504	U
1	2A	505	A
1	2A	509	C
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	545	G
1	2A	563	G
1	2A	573	G
1	2A	574	C
1	2A	575	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	2A	586	A
1	2A	595	C
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	609	A
1	2A	614(B)	G
1	2A	615	G
1	2A	616	G
1	2A	627	A
1	2A	637	A
1	2A	645	C
1	2A	646	A
1	2A	652(B)	A
1	2A	652(C)	G
1	2A	652(U)	G
1	2A	669	G
1	2A	677	A
1	2A	686	G
1	2A	717	G
1	2A	726	G
1	2A	730	C
1	2A	740	U
1	2A	751	A
1	2A	752	A
1	2A	753	C
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	792	G
1	2A	805	G
1	2A	812	C
1	2A	815	C
1	2A	827	U
1	2A	847	U
1	2A	853	G
1	2A	857	C
1	2A	859	G
1	2A	877	U
1	2A	880	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	2A	886	C
1	2A	887	A
1	2A	888	C
1	2A	889	C
1	2A	890	A
1	2A	893	C
1	2A	896	A
1	2A	897	C
1	2A	901	A
1	2A	908	C
1	2A	910	A
1	2A	911	A
1	2A	917	A
1	2A	932	G
1	2A	938	G
1	2A	941	A
1	2A	945	A
1	2A	946	G
1	2A	959	A
1	2A	961	C
1	2A	974	G
1	2A	975	C
1	2A	983	A
1	2A	996	A
1	2A	1005	C
1	2A	1012	U
1	2A	1013	C
1	2A	1033	U
1	2A	1038	C
1	2A	1041	C
1	2A	1044	G
1	2A	1045	A
1	2A	1046	A
1	2A	1047	G
1	2A	1052	C
1	2A	1054	A
1	2A	1055	G
1	2A	1058	G
1	2A	1060	U
1	2A	1064	C
1	2A	1065	U
1	2A	1066	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	2A	1067	A
1	2A	1068	G
1	2A	1069	A
1	2A	1070	A
1	2A	1071	G
1	2A	1073	A
1	2A	1074	G
1	2A	1076	C
1	2A	1077	A
1	2A	1078	U
1	2A	1079	C
1	2A	1080	C
1	2A	1082	U
1	2A	1083	U
1	2A	1084	A
1	2A	1085	A
1	2A	1086	A
1	2A	1088	A
1	2A	1090	U
1	2A	1091	G
1	2A	1092	C
1	2A	1093	G
1	2A	1094	U
1	2A	1095	A
1	2A	1096	A
1	2A	1105	U
1	2A	1109	C
1	2A	1110	G
1	2A	1111	A
1	2A	1112	G
1	2A	1116	C
1	2A	1117	G
1	2A	1129	A
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1141	U
1	2A	1142(A)	A
1	2A	1169	G
1	2A	1171	G
1	2A	1195	G
1	2A	1211	U

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	2A	1212	G
1	2A	1219	G
1	2A	1220	A
1	2A	1241	A
1	2A	1253	A
1	2A	1256	G
1	2A	1271	G
1	2A	1272	A
1	2A	1273	U
1	2A	1287	A
1	2A	1300	U
1	2A	1301	A
1	2A	1303	G
1	2A	1308	A
1	2A	1314	C
1	2A	1342	A
1	2A	1352	U
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1368	G
1	2A	1384	A
1	2A	1385	G
1	2A	1386	C
1	2A	1392	A
1	2A	1416	G
1	2A	1417	C
1	2A	1420	U
1	2A	1421	G
1	2A	1427	A
1	2A	1428	C
1	2A	1445	A
1	2A	1450	G
1	2A	1455	G
1	2A	1459	G
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1542	A
1	2A	1543	C
1	2A	1547	C
1	2A	1558	A
1	2A	1559	G
1	2A	1566	A
1	2A	1569	A
1	2A	1578	U
1	2A	1580	A
1	2A	1583	A
1	2A	1584	C
1	2A	1586	A
1	2A	1595	G
1	2A	1608	A
1	2A	1610	A
1	2A	1629	U
1	2A	1640	C
1	2A	1648	C
1	2A	1654	A
1	2A	1674	G
1	2A	1675	C
1	2A	1696	G
1	2A	1700	A
1	2A	1701	A
1	2A	1703	G
1	2A	1721	G
1	2A	1722	A
1	2A	1746	G
1	2A	1750	G
1	2A	1756	G
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1773	A
1	2A	1780	A
1	2A	1782	C
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1816	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	2A	1828	G
1	2A	1829	A
1	2A	1835	G
1	2A	1839	G
1	2A	1847	A
1	2A	1848	A
1	2A	1858	G
1	2A	1877	A
1	2A	1878	G
1	2A	1882	C
1	2A	1900	A
1	2A	1906	G
1	2A	1913	A
1	2A	1914	C
1	2A	1921	G
1	2A	1929	G
1	2A	1930	G
1	2A	1937	A
1	2A	1938	A
1	2A	1955	U
1	2A	1963	U
1	2A	1967	C
1	2A	1970	A
1	2A	1971	A
1	2A	1972	A
1	2A	1993	U
1	2A	1997	G
1	2A	2020	A
1	2A	2023	G
1	2A	2031	A
1	2A	2033	A
1	2A	2043	C
1	2A	2055	C
1	2A	2056	G
1	2A	2060	A
1	2A	2061	G
1	2A	2062	A
1	2A	2069	G
1	2A	2095	C
1	2A	2096	U
1	2A	2099	U
1	2A	2100	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	2A	2103	C
1	2A	2104	G
1	2A	2105	C
1	2A	2106	G
1	2A	2107	C
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	2117	A
1	2A	2118	U
1	2A	2119	A
1	2A	2120	G
1	2A	2123	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	2136	C
1	2A	2137	C
1	2A	2138	C
1	2A	2141	G
1	2A	2145	C
1	2A	2146	C
1	2A	2147	G
1	2A	2148	G
1	2A	2149	G
1	2A	2150	U
1	2A	2151	G
1	2A	2158	A
1	2A	2159	G
1	2A	2161	C
1	2A	2162	G
1	2A	2163	C
1	2A	2164	C
1	2A	2165	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	2A	2166	G
1	2A	2172	U
1	2A	2173	A
1	2A	2176	A
1	2A	2178	C
1	2A	2181	G
1	2A	2184	G
1	2A	2186	G
1	2A	2187	G
1	2A	2189	U
1	2A	2192	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2218	U
1	2A	2219	G
1	2A	2225	A
1	2A	2239	G
1	2A	2243	U
1	2A	2268	A
1	2A	2269	A
1	2A	2275	C
1	2A	2280	G
1	2A	2283	C
1	2A	2287	A
1	2A	2289	G
1	2A	2292	C
1	2A	2302	G
1	2A	2305	A
1	2A	2308	G
1	2A	2311	A
1	2A	2312	U
1	2A	2318	G
1	2A	2319	G
1	2A	2320	A
1	2A	2321	G
1	2A	2322	A
1	2A	2325	G
1	2A	2334	G
1	2A	2335	A
1	2A	2336	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	2A	2343	C
1	2A	2347	C
1	2A	2350	C
1	2A	2354	G
1	2A	2358	G
1	2A	2366	A
1	2A	2379	G
1	2A	2383	G
1	2A	2385	C
1	2A	2402	C
1	2A	2406	U
1	2A	2410	G
1	2A	2414	G
1	2A	2419	U
1	2A	2422	A
1	2A	2423	U
1	2A	2425	A
1	2A	2429	G
1	2A	2430	A
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2448	A
1	2A	2459	A
1	2A	2470	G
1	2A	2474	C
1	2A	2476	A
1	2A	2478	A
1	2A	2487	G
1	2A	2502	G
1	2A	2504	U
1	2A	2505	G
1	2A	2517	C
1	2A	2518	A
1	2A	2520	C
1	2A	2529	G
1	2A	2554	U
1	2A	2555	U
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2585	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	2A	2602	A
1	2A	2603	G
1	2A	2611	U
1	2A	2612	C
1	2A	2629	A
1	2A	2630	G
1	2A	2654	A
1	2A	2663	G
1	2A	2682	U
1	2A	2689	U
1	2A	2690	C
1	2A	2703	C
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2721	A
1	2A	2726	U
1	2A	2733	A
1	2A	2757	A
1	2A	2758	A
1	2A	2765	A
1	2A	2778	A
1	2A	2802	G
1	2A	2803	C
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2833	G
1	2A	2835	A
1	2A	2872	G
1	2A	2880	C
1	2A	2891	G
1	2A	2894	G
2	2B	2	C
2	2B	8	U
2	2B	13	A
2	2B	30	C
2	2B	31	C
2	2B	32	C
2	2B	42	C
2	2B	51	G
2	2B	56	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	2B	64	C
2	2B	67	G
2	2B	73	A
2	2B	79	C
2	2B	84	C
2	2B	108	U
2	2B	110	G
2	2B	118	G
2	2B	120	A
32	2a	5	U
32	2a	6	G
32	2a	7	G
32	2a	9	G
32	2a	22	G
32	2a	32	A
32	2a	39	G
32	2a	47	C
32	2a	48	C
32	2a	50	A
32	2a	51	A
32	2a	59	A
32	2a	61	G
32	2a	65	U
32	2a	66	G
32	2a	79	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	148	G
32	2a	156	G
32	2a	163	C
32	2a	173	U
32	2a	174	C
32	2a	182	U
32	2a	189(C)	C
32	2a	189(E)	U
32	2a	189(F)	U
32	2a	195	A
32	2a	197	A

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
32	2a	202	U
32	2a	203	U
32	2a	204	U
32	2a	216	G
32	2a	227	G
32	2a	247	G
32	2a	251	G
32	2a	258	G
32	2a	262	A
32	2a	266	G
32	2a	267	C
32	2a	269	C
32	2a	281	G
32	2a	289	G
32	2a	298	A
32	2a	306	G
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	345	C
32	2a	351	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	360	A
32	2a	367	U
32	2a	372	C
32	2a	384	G
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	412	A
32	2a	413	G
32	2a	421	U
32	2a	424	G
32	2a	429	U
32	2a	430	A
32	2a	439	A
32	2a	441	A
32	2a	442	C
32	2a	446	G
32	2a	451	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
32	2a	452	A
32	2a	458	C
32	2a	461	A
32	2a	470	C
32	2a	471	G
32	2a	476	G
32	2a	477	A
32	2a	482	A
32	2a	484	G
32	2a	485	G
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	506	G
32	2a	509	A
32	2a	510	A
32	2a	511	C
32	2a	518	C
32	2a	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	572	A
32	2a	573	A
32	2a	576	G
32	2a	592	G
32	2a	596	C
32	2a	630	G
32	2a	631	G
32	2a	632	A
32	2a	641	U
32	2a	653	A
32	2a	665	A
32	2a	672	U
32	2a	685	G
32	2a	688	G
32	2a	695	A
32	2a	723	U
32	2a	724	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
32	2a	731	G
32	2a	734	G
32	2a	735	C
32	2a	748	C
32	2a	749	C
32	2a	753	A
32	2a	755	G
32	2a	777	A
32	2a	793	U
32	2a	794	A
32	2a	817	C
32	2a	821	G
32	2a	828	A
32	2a	829	G
32	2a	836	G
32	2a	840	C
32	2a	841	U
32	2a	851	G
32	2a	859	A
32	2a	870	U
32	2a	902	G
32	2a	914	A
32	2a	916	G
32	2a	926	G
32	2a	927	G
32	2a	931	C
32	2a	934	C
32	2a	958	A
32	2a	960	U
32	2a	961	U
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	972	C
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	989	C
32	2a	992	U
32	2a	993	G
32	2a	994	A

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	2a	995	C
32	2a	996	A
32	2a	1004	A
32	2a	1005	A
32	2a	1006	C
32	2a	1009	G
32	2a	1017	G
32	2a	1020	U
32	2a	1025	U
32	2a	1026	G
32	2a	1027	C
32	2a	1028	C
32	2a	1030(A)	G
32	2a	1030(B)	C
32	2a	1030(C)	G
32	2a	1034	G
32	2a	1041	A
32	2a	1043	C
32	2a	1047	G
32	2a	1053	G
32	2a	1054	C
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1081	G
32	2a	1094	G
32	2a	1095	U
32	2a	1097	C
32	2a	1101	A
32	2a	1117	G
32	2a	1122	U
32	2a	1125	U
32	2a	1129	C
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	1147	C
32	2a	1152	A
32	2a	1157	A

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	2a	1159	U
32	2a	1168	A
32	2a	1176	A
32	2a	1183	A
32	2a	1184	G
32	2a	1196	U
32	2a	1197	G
32	2a	1211	U
32	2a	1212	U
32	2a	1224	G
32	2a	1227	A
32	2a	1228	C
32	2a	1238	A
32	2a	1256	A
32	2a	1257	U
32	2a	1258	G
32	2a	1269	A
32	2a	1270	C
32	2a	1278	U
32	2a	1279	A
32	2a	1281	U
32	2a	1282	C
32	2a	1283	G
32	2a	1285	A
32	2a	1286	A
32	2a	1287	A
32	2a	1290	G
32	2a	1300	G
32	2a	1302	U
32	2a	1303	C
32	2a	1305	G
32	2a	1316	G
32	2a	1317	C
32	2a	1319	A
32	2a	1320	C
32	2a	1340	A
32	2a	1346	A
32	2a	1347	G
32	2a	1353	G
32	2a	1363	C
32	2a	1397	C
32	2a	1419	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1447	A
32	2a	1456	G
32	2a	1458	G
32	2a	1492	A
32	2a	1497	G
32	2a	1499	A
32	2a	1503	A
32	2a	1504	G
32	2a	1505	G
32	2a	1506	U
32	2a	1507	A
32	2a	1517	G
32	2a	1520	G
32	2a	1529	G
32	2a	1530	G
32	2a	1531	A

All (65) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	115	G
1	1A	302	A
1	1A	509	A
1	1A	732	A
1	1A	793	A
1	1A	811	A
1	1A	821	A
1	1A	874	U
1	1A	913	A
1	1A	935	C
1	1A	941	U
1	1A	1003	U
1	1A	1019	G
1	1A	1067	A
1	1A	1093	G
1	1A	1188	A
1	1A	1201	A
1	1A	1219	A
1	1A	1220	U
1	1A	1221	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	1A	1255	A
1	1A	1654	A
1	1A	1700	G
1	1A	2250	G
1	1A	2418	U
1	1A	2434	A
1	1A	2442	A
1	1A	2614	A
1	1A	2701	U
1	2A	9	U
1	2A	195	A
1	2A	249	C
1	2A	266	G
1	2A	271(M)	G
1	2A	277	C
1	2A	685	A
1	2A	752	A
1	2A	764	A
1	2A	827	U
1	2A	840	C
1	2A	856	C
1	2A	900	A
1	2A	1053	C
1	2A	1057	A
1	2A	1065	U
1	2A	1067	A
1	2A	1073	A
1	2A	1076	C
1	2A	1210	A
1	2A	1240	U
1	2A	1420	U
1	2A	1442	G
1	2A	1491	G
1	2A	1992	G
1	2A	2126	A
1	2A	2171	A
1	2A	2172	U
1	2A	2288	A
1	2A	2317	C
1	2A	2321	G
1	2A	2406	U
1	2A	2601	C

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	2A	2602	A
1	2A	2689	U
1	2A	2756	U

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

48 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	5MC	1a	967	32	15,22,23	1.25	1 (6%)	19,32,35	1.47	3 (15%)
1	5MU	2A	1939	1	15,22,23	1.16	1 (6%)	16,32,35	1.73	2 (12%)
32	4OC	1a	1402	32	16,23,24	0.61	0	17,32,35	1.57	1 (5%)
32	5MC	1a	1404	32	15,22,23	1.37	1 (6%)	19,32,35	1.20	3 (15%)
32	MA6	1a	1518	32	19,26,27	0.96	1 (5%)	18,38,41	1.66	5 (27%)
32	M2G	2a	966	32	20,27,28	1.47	3 (15%)	22,40,43	2.11	6 (27%)
32	MA6	1a	1519	32	19,26,27	1.02	1 (5%)	18,38,41	1.54	4 (22%)
43	0TD	2l	92	43	4,9,10	3.06	1 (25%)	3,11,13	5.07	1 (33%)
32	2MG	2a	1207	32	19,26,27	1.24	2 (10%)	21,38,41	2.23	7 (33%)
1	4OC	2A	1920	1	15,22,24	0.72	0	17,31,35	1.30	2 (11%)
1	OMG	1A	2263	1,54	18,26,27	1.22	2 (11%)	20,38,41	2.21	6 (30%)
32	7MG	1a	527	32,54	22,26,27	1.77	4 (18%)	28,39,42	2.63	8 (28%)
1	4OC	1A	1942	1	15,22,24	0.66	0	17,31,35	1.43	2 (11%)
32	UR3	1a	1498	32	14,22,23	0.70	0	15,32,35	0.66	0
32	PSU	1a	516	32,54	17,21,22	1.49	3 (17%)	20,30,33	3.17	6 (30%)
32	2MG	1a	1207	32	19,26,27	1.33	2 (10%)	21,38,41	2.70	11 (52%)
32	5MC	1a	1400	32	15,22,23	1.42	1 (6%)	19,32,35	1.36	3 (15%)
1	2MU	2A	2552	1,54	14,22,24	0.95	1 (7%)	14,31,36	0.79	1 (7%)
1	5MU	2A	1915	1	15,22,23	1.04	1 (6%)	16,32,35	2.00	1 (6%)
1	2MU	1A	2564	1,54	14,22,24	0.88	1 (7%)	14,31,36	1.05	2 (14%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	PSU	1A	1939	1	17,21,22	1.43	3 (17%)	20,30,33	3.20	5 (25%)
32	M2G	1a	966	32	20,27,28	1.37	3 (15%)	22,40,43	2.20	6 (27%)
1	PSU	2A	2605	1	17,21,22	1.66	4 (23%)	20,30,33	3.23	6 (30%)
1	PSU	2A	1911	1	17,21,22	1.53	2 (11%)	20,30,33	3.04	6 (30%)
1	5MC	2A	1942	1	15,22,23	1.33	1 (6%)	19,32,35	1.37	3 (15%)
1	5MC	1A	1964	1,54	15,22,23	1.21	1 (6%)	19,32,35	1.36	3 (15%)
1	5MU	1A	1961	1,54	15,22,23	1.14	2 (13%)	16,32,35	1.88	2 (12%)
32	UR3	2a	1498	32,54	14,22,23	0.73	0	15,32,35	0.74	0
1	PSU	1A	2617	1,54	17,21,22	1.63	3 (17%)	20,30,33	3.24	6 (30%)
32	5MC	1a	1407	32	15,22,23	1.36	1 (6%)	19,32,35	1.30	2 (10%)
1	PSU	2A	1917	1	17,21,22	1.48	2 (11%)	20,30,33	3.05	5 (25%)
1	5MC	2A	1962	1,54	15,22,23	1.24	1 (6%)	19,32,35	1.33	3 (15%)
32	MA6	2a	1519	32	19,26,27	0.97	1 (5%)	18,38,41	1.84	5 (27%)
32	5MC	2a	1407	32	15,22,23	1.33	1 (6%)	19,32,35	1.38	3 (15%)
43	0TD	1l	92	43	4,9,10	3.13	1 (25%)	3,11,13	3.19	1 (33%)
1	5MC	1A	1984	1,54	15,22,23	1.30	1 (6%)	19,32,35	1.26	2 (10%)
1	5MU	1A	1937	1	15,22,23	1.06	1 (6%)	16,32,35	1.99	1 (6%)
32	7MG	2a	527	32,54	22,26,27	1.71	4 (18%)	28,39,42	2.72	8 (28%)
1	PSU	1A	1933	1	17,21,22	1.63	2 (11%)	20,30,33	3.10	7 (35%)
32	5MC	2a	1400	32	15,22,23	1.36	1 (6%)	19,32,35	1.32	3 (15%)
1	OMG	2A	2251	1,54	18,26,27	1.15	2 (11%)	20,38,41	2.21	6 (30%)
1	2MA	2A	2503	1,54	17,25,26	1.24	1 (5%)	19,37,40	2.03	3 (15%)
32	5MC	2a	967	32	15,22,23	1.55	1 (6%)	19,32,35	1.28	2 (10%)
1	2MA	1A	2515	1,54	17,25,26	1.19	1 (5%)	19,37,40	2.16	3 (15%)
32	5MC	2a	1404	32	15,22,23	1.40	1 (6%)	19,32,35	1.27	3 (15%)
32	PSU	2a	516	32,54	17,21,22	1.67	3 (17%)	20,30,33	3.13	6 (30%)
32	MA6	2a	1518	32	19,26,27	1.05	1 (5%)	18,38,41	1.67	4 (22%)
32	4OC	2a	1402	32	16,23,24	0.66	0	17,32,35	1.42	1 (5%)

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	5MC	1a	967	32	-	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	5MU	2A	1939	1	-	0/5/25/26	0/2/2/2
32	4OC	1a	1402	32	-	2/9/29/30	0/2/2/2
32	5MC	1a	1404	32	-	0/5/25/26	0/2/2/2
32	MA6	1a	1518	32	-	3/7/29/30	0/3/3/3
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
32	MA6	1a	1519	32	-	3/7/29/30	0/3/3/3
43	0TD	2l	92	43	-	1/3/12/14	-
32	2MG	2a	1207	32	-	0/5/27/28	0/3/3/3
1	4OC	2A	1920	1	-	0/7/27/30	0/2/2/2
1	OMG	1A	2263	1,54	-	1/5/27/28	0/3/3/3
32	7MG	1a	527	32,54	-	0/7/37/38	0/3/3/3
1	4OC	1A	1942	1	-	1/7/27/30	0/2/2/2
32	UR3	1a	1498	32	-	0/5/25/26	0/2/2/2
32	PSU	1a	516	32,54	-	0/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	2/5/27/28	0/3/3/3
32	5MC	1a	1400	32	-	1/5/25/26	0/2/2/2
1	2MU	2A	2552	1,54	-	0/7/27/28	0/2/2/2
1	5MU	2A	1915	1	-	0/5/25/26	0/2/2/2
1	2MU	1A	2564	1,54	-	0/7/27/28	0/2/2/2
1	PSU	1A	1939	1	-	1/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/5/25/26	0/2/2/2
1	5MC	1A	1964	1,54	-	0/5/25/26	0/2/2/2
1	5MU	1A	1961	1,54	-	0/5/25/26	0/2/2/2
32	UR3	2a	1498	32,54	-	0/5/25/26	0/2/2/2
1	PSU	1A	2617	1,54	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/5/25/26	0/2/2/2
1	PSU	2A	1917	1	-	1/7/25/26	0/2/2/2
1	5MC	2A	1962	1,54	-	2/5/25/26	0/2/2/2
32	MA6	2a	1519	32	-	4/7/29/30	0/3/3/3
32	5MC	2a	1407	32	-	0/5/25/26	0/2/2/2
43	0TD	1l	92	43	-	2/3/12/14	-
1	5MC	1A	1984	1,54	-	2/5/25/26	0/2/2/2
1	5MU	1A	1937	1	-	0/5/25/26	0/2/2/2
32	7MG	2a	527	32,54	-	0/7/37/38	0/3/3/3
1	PSU	1A	1933	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	2/5/25/26	0/2/2/2
1	OMG	2A	2251	1,54	-	0/5/27/28	0/3/3/3

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MA	2A	2503	1,54	-	1/3/25/26	0/3/3/3
32	5MC	2a	967	32	-	0/5/25/26	0/2/2/2
1	2MA	1A	2515	1,54	-	2/3/25/26	0/3/3/3
32	5MC	2a	1404	32	-	0/5/25/26	0/2/2/2
32	PSU	2a	516	32,54	-	0/7/25/26	0/2/2/2
32	MA6	2a	1518	32	-	2/7/29/30	0/3/3/3
32	4OC	2a	1402	32	-	4/9/29/30	0/2/2/2

All (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	1l	92	0TD	CB-SB	-5.97	1.69	1.84
43	2l	92	0TD	CB-SB	-5.86	1.70	1.84
32	2a	967	5MC	C5-C4	5.60	1.50	1.41
32	1a	1400	5MC	C5-C4	5.05	1.49	1.41
32	2a	1404	5MC	C5-C4	4.99	1.49	1.41
32	1a	1407	5MC	C5-C4	4.86	1.48	1.41
32	2a	527	7MG	C6-C5	4.83	1.48	1.41
32	1a	1404	5MC	C5-C4	4.82	1.48	1.41
1	2A	1942	5MC	C5-C4	4.82	1.48	1.41
32	2a	516	PSU	C5-C1'	-4.78	1.48	1.52
32	2a	1400	5MC	C5-C4	4.76	1.48	1.41
1	2A	2605	PSU	C5-C1'	-4.69	1.48	1.52
32	2a	1407	5MC	C5-C4	4.63	1.48	1.41
32	1a	527	7MG	C6-C5	4.62	1.47	1.41
1	1A	1984	5MC	C5-C4	4.62	1.48	1.41
32	1a	1207	2MG	C6-C5	4.59	1.49	1.41
1	1A	2617	PSU	C5-C1'	-4.58	1.48	1.52
1	1A	1933	PSU	C5-C1'	-4.56	1.48	1.52
32	1a	967	5MC	C5-C4	4.46	1.48	1.41
1	2A	1962	5MC	C5-C4	4.40	1.48	1.41
32	1a	527	7MG	C5-C4	4.39	1.47	1.39
32	2a	1207	2MG	C6-C5	4.23	1.48	1.41
32	2a	527	7MG	C5-C4	4.22	1.47	1.39
1	1A	1964	5MC	C5-C4	4.19	1.47	1.41
1	2A	2503	2MA	C6-C5	4.19	1.47	1.41
32	1a	966	M2G	C6-C5	4.18	1.48	1.41
32	2a	966	M2G	C6-C5	4.17	1.48	1.41
1	1A	2263	OMG	C6-C5	4.03	1.48	1.41
1	1A	2515	2MA	C6-C5	3.84	1.47	1.41
1	2A	2251	OMG	C6-C5	3.78	1.47	1.41
1	2A	1939	5MU	C4-C5	3.78	1.49	1.41

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1a	527	7MG	C5-N7	-3.76	1.33	1.39
1	2A	1911	PSU	C5-C1'	-3.75	1.49	1.52
1	2A	1917	PSU	C4-C5	3.72	1.49	1.41
32	1a	516	PSU	C5-C1'	-3.71	1.49	1.52
32	2a	966	M2G	C2-N2	3.64	1.40	1.34
1	2A	1911	PSU	C4-C5	3.50	1.49	1.41
1	2A	1917	PSU	C5-C1'	-3.46	1.49	1.52
1	1A	1933	PSU	C4-C5	3.44	1.48	1.41
1	1A	1939	PSU	C4-C5	3.41	1.48	1.41
1	1A	1961	5MU	C4-C5	3.36	1.48	1.41
32	2a	527	7MG	C5-N7	-3.35	1.34	1.39
1	2A	1915	5MU	C4-C5	3.34	1.48	1.41
32	2a	516	PSU	C4-C5	3.33	1.48	1.41
1	1A	2617	PSU	C4-C5	3.31	1.48	1.41
1	1A	1937	5MU	C4-C5	3.31	1.48	1.41
32	1a	966	M2G	C2-N2	3.29	1.40	1.34
1	1A	1939	PSU	C5-C1'	-3.25	1.49	1.52
32	1a	516	PSU	C4-C5	3.19	1.48	1.41
1	2A	2605	PSU	C4-C5	2.91	1.47	1.41
32	2a	1518	MA6	C5-C4	2.88	1.48	1.40
32	2a	966	M2G	C5-C4	2.80	1.48	1.40
32	1a	527	7MG	C4-N9	-2.78	1.33	1.38
32	2a	1207	2MG	C5-C4	2.58	1.47	1.40
32	1a	1519	MA6	C5-C4	2.54	1.47	1.40
32	1a	1518	MA6	C5-C4	2.48	1.47	1.40
32	2a	1519	MA6	C5-C4	2.44	1.47	1.40
1	2A	2605	PSU	C2-N3	-2.38	1.33	1.38
32	2a	516	PSU	O4'-C1'	-2.35	1.41	1.44
1	1A	2263	OMG	C5-C4	2.34	1.47	1.40
32	1a	966	M2G	C5-C4	2.30	1.47	1.40
32	1a	516	PSU	O4'-C1'	-2.30	1.41	1.44
1	2A	2251	OMG	C5-C4	2.27	1.46	1.40
32	1a	1207	2MG	C5-C4	2.26	1.46	1.40
1	1A	1961	5MU	C2-N3	-2.22	1.33	1.38
1	1A	2617	PSU	C2-N3	-2.21	1.33	1.38
32	2a	527	7MG	C4-N9	-2.16	1.34	1.38
1	1A	1939	PSU	O4'-C1'	-2.03	1.41	1.44
1	2A	2552	2MU	C2-N3	-2.02	1.34	1.38
1	2A	2605	PSU	O4'-C1'	-2.01	1.41	1.44
1	1A	2564	2MU	C2-N3	-2.01	1.34	1.38

All (179) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1939	PSU	N1-C2-N3	-9.34	121.00	128.43
32	1a	516	PSU	N1-C2-N3	-8.83	121.41	128.43
1	2A	2605	PSU	N1-C2-N3	-8.75	121.47	128.43
43	2l	92	0TD	CSB-SB-CB	-8.71	84.73	101.85
32	2a	527	7MG	N3-C4-N9	8.57	137.92	126.91
1	1A	2617	PSU	N1-C2-N3	-8.50	121.67	128.43
32	2a	516	PSU	N1-C2-N3	-8.36	121.79	128.43
1	2A	1917	PSU	N1-C2-N3	-8.31	121.82	128.43
32	1a	527	7MG	N3-C4-N9	8.24	137.50	126.91
1	2A	1911	PSU	N1-C2-N3	-8.08	122.00	128.43
1	1A	1933	PSU	N1-C2-N3	-7.65	122.35	128.43
1	1A	2515	2MA	C2-N3-C4	7.57	121.67	115.52
1	1A	1937	5MU	C4-N3-C2	7.34	121.34	115.14
1	2A	1915	5MU	C4-N3-C2	7.31	121.31	115.14
1	1A	1939	PSU	C4-N3-C2	7.21	121.23	115.14
32	1a	516	PSU	C4-N3-C2	7.18	121.20	115.14
1	1A	2617	PSU	C4-N3-C2	7.02	121.07	115.14
1	2A	1917	PSU	C4-N3-C2	6.65	120.76	115.14
1	2A	2605	PSU	C4-N3-C2	6.64	120.75	115.14
1	2A	1911	PSU	C4-N3-C2	6.58	120.69	115.14
32	2a	516	PSU	C4-N3-C2	6.57	120.69	115.14
1	1A	1933	PSU	C4-N3-C2	6.34	120.50	115.14
1	2A	2503	2MA	C2-N3-C4	6.28	120.63	115.52
1	1A	1961	5MU	C4-N3-C2	6.16	120.35	115.14
32	1a	1402	4OC	CM4-N4-C4	-5.83	117.96	122.97
32	2a	527	7MG	N7-C8-N9	-5.70	95.23	103.38
32	2a	516	PSU	C5-C4-N3	-5.67	118.06	125.36
1	1A	1933	PSU	C5-C4-N3	-5.65	118.08	125.36
32	1a	516	PSU	C5-C4-N3	-5.48	118.30	125.36
32	2a	966	M2G	C6-N1-C2	5.46	122.68	116.18
1	2A	1939	5MU	C4-N3-C2	5.43	119.73	115.14
1	2A	1917	PSU	C5-C4-N3	-5.39	118.41	125.36
1	1A	2617	PSU	C5-C4-N3	-5.38	118.43	125.36
43	1l	92	0TD	CSB-SB-CB	-5.38	91.28	101.85
1	1A	2263	OMG	C2-N3-C4	5.15	121.24	115.36
1	2A	1911	PSU	C5-C4-N3	-5.14	118.74	125.36
32	1a	1207	2MG	C2-N3-C4	5.13	121.10	115.28
1	2A	2251	OMG	C2-N3-C4	5.10	121.18	115.36
32	2a	527	7MG	C5-C4-N3	-5.09	118.18	126.49
32	1a	527	7MG	N7-C8-N9	-5.05	96.15	103.38
32	1a	966	M2G	C6-N1-C2	4.98	122.11	116.18
1	1A	1939	PSU	C5-C4-N3	-4.95	118.98	125.36
1	2A	2605	PSU	C5-C4-N3	-4.89	119.06	125.36

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	966	M2G	C2-N3-C4	4.78	120.71	115.28
32	1a	527	7MG	C6-N1-C2	4.75	123.48	115.93
32	1a	1207	2MG	C6-C5-C4	-4.72	116.29	120.80
32	1a	527	7MG	C5-C4-N3	-4.72	118.79	126.49
1	1A	1942	4OC	C2-N3-C4	4.66	121.07	116.34
32	2a	1207	2MG	C5-C6-N1	-4.64	117.09	123.43
32	2a	527	7MG	C6-N1-C2	4.54	123.14	115.93
32	1a	966	M2G	C2-N3-C4	4.52	120.41	115.28
1	2A	2605	PSU	C5-C6-N1	-4.47	118.94	124.44
1	1A	2617	PSU	C5-C6-N1	-4.47	118.95	124.44
1	1A	1933	PSU	C5-C1'-C2'	-4.44	107.39	115.32
32	2a	516	PSU	C5-C6-N1	-4.44	118.98	124.44
1	2A	2605	PSU	C6-N1-C2	4.33	122.50	115.36
1	2A	2503	2MA	C5-C6-N1	-4.33	118.52	123.06
1	1A	1933	PSU	C5-C6-N1	-4.31	119.14	124.44
32	2a	1402	4OC	CM4-N4-C4	-4.27	119.30	122.97
32	2a	966	M2G	C5-C6-N1	-4.26	117.60	123.43
32	1a	966	M2G	C6-C5-C4	-4.24	116.75	120.80
32	2a	1207	2MG	C6-N1-C2	4.23	122.75	115.18
32	2a	516	PSU	C6-N1-C2	4.19	122.28	115.36
1	1A	1939	PSU	C6-N1-C2	4.15	122.21	115.36
32	2a	1207	2MG	C2-N3-C4	4.14	119.98	115.28
1	1A	2617	PSU	C6-N1-C2	4.13	122.17	115.36
32	1a	516	PSU	C6-N1-C2	4.09	122.11	115.36
1	2A	2251	OMG	C6-C5-C4	-4.05	116.93	120.80
32	1a	1207	2MG	C6-N1-C2	4.04	122.42	115.18
1	2A	1917	PSU	C6-N1-C2	4.04	122.03	115.36
32	2a	1519	MA6	C4-C5-N7	-4.03	105.19	109.40
1	2A	2251	OMG	C6-N1-C2	4.02	122.32	115.93
32	1a	527	7MG	C6-C5-C4	4.02	119.51	115.20
1	2A	1920	4OC	C2-N3-C4	3.99	120.39	116.34
1	1A	1933	PSU	C6-N1-C2	3.99	121.94	115.36
1	2A	1911	PSU	C6-N1-C2	3.97	121.92	115.36
32	1a	966	M2G	C5-C6-N1	-3.96	118.01	123.43
32	1a	1207	2MG	C5-C6-N1	-3.96	118.02	123.43
1	2A	2605	PSU	C5-C1'-C2'	-3.96	108.26	115.32
32	1a	516	PSU	C5-C6-N1	-3.94	119.60	124.44
32	1a	527	7MG	C5-C6-N1	-3.92	115.08	123.14
1	1A	2263	OMG	C6-N1-C2	3.91	122.15	115.93
1	2A	1911	PSU	C5-C6-N1	-3.90	119.65	124.44
1	1A	2515	2MA	C5-C6-N1	-3.89	118.98	123.06
32	2a	527	7MG	C6-C5-C4	3.85	119.33	115.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1207	2MG	C6-C5-C4	-3.82	117.15	120.80
1	1A	2263	OMG	C5-C6-N1	-3.82	118.21	123.43
32	1a	1400	5MC	C2-N3-C4	3.79	120.59	116.02
1	2A	1917	PSU	C5-C6-N1	-3.75	119.83	124.44
1	2A	2251	OMG	N3-C2-N1	-3.73	122.25	127.22
1	1A	1964	5MC	C2-N3-C4	3.73	120.52	116.02
32	1a	1518	MA6	C9-N6-C6	-3.71	108.27	119.51
32	2a	967	5MC	C2-N3-C4	3.70	120.49	116.02
32	1a	1207	2MG	C4-C5-N7	-3.67	105.57	109.40
1	1A	1984	5MC	C2-N3-C4	3.63	120.40	116.02
1	2A	2251	OMG	C5-C6-N1	-3.63	118.47	123.43
1	1A	2263	OMG	C6-C5-C4	-3.62	117.35	120.80
32	2a	1519	MA6	C10-N6-C6	-3.60	108.61	119.51
1	2A	1942	5MC	C2-N3-C4	3.60	120.36	116.02
32	1a	1207	2MG	N2-C2-N1	3.58	120.39	116.96
32	1a	1207	2MG	CM2-N2-C2	-3.57	119.28	123.59
32	1a	967	5MC	C2-N3-C4	3.57	120.33	116.02
32	1a	1407	5MC	C2-N3-C4	3.57	120.32	116.02
32	2a	527	7MG	C5-C6-N1	-3.56	115.81	123.14
32	2a	1407	5MC	C2-N3-C4	3.55	120.30	116.02
1	1A	1939	PSU	C5-C6-N1	-3.51	120.12	124.44
32	1a	1518	MA6	C4-C5-N7	-3.51	105.74	109.40
1	1A	2617	PSU	C5-C1'-C2'	-3.48	109.12	115.32
1	2A	1939	5MU	C5-C6-N1	-3.48	118.45	122.19
1	1A	1961	5MU	C5-C6-N1	-3.45	118.47	122.19
32	1a	967	5MC	N4-C4-N3	3.42	121.86	117.03
32	2a	1207	2MG	CM2-N2-C2	-3.38	119.51	123.59
32	1a	1404	5MC	C2-N3-C4	3.36	120.08	116.02
32	2a	1518	MA6	C4-C5-N7	-3.36	105.90	109.40
1	2A	1911	PSU	C5-C1'-C2'	-3.35	109.34	115.32
1	1A	2263	OMG	C4-C5-N7	-3.33	105.93	109.40
32	2a	1518	MA6	C9-N6-C6	-3.31	109.50	119.51
1	1A	2263	OMG	N3-C2-N1	-3.27	122.86	127.22
32	2a	966	M2G	C6-C5-C4	-3.23	117.72	120.80
1	2A	1962	5MC	C2-N3-C4	3.23	119.91	116.02
32	1a	1207	2MG	C1'-N9-C4	-3.19	121.05	126.64
32	2a	1518	MA6	N3-C2-N1	-3.18	123.71	128.68
32	2a	1404	5MC	C2-N3-C4	3.17	119.85	116.02
32	2a	1519	MA6	N3-C2-N1	-3.09	123.84	128.68
32	1a	1519	MA6	C9-N6-C6	-3.09	110.15	119.51
32	1a	1518	MA6	N3-C2-N1	-3.09	123.85	128.68
32	2a	1400	5MC	C2-N3-C4	3.08	119.73	116.02

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1400	5MC	C5-C6-N1	-3.00	118.96	122.19
32	1a	1519	MA6	N3-C2-N1	-2.99	124.00	128.68
32	2a	1519	MA6	C10-N6-C9	-2.98	106.51	116.12
32	2a	527	7MG	C8-N7-C5	2.96	116.64	108.94
32	1a	1519	MA6	C4-C5-N7	-2.93	106.35	109.40
32	1a	966	M2G	C4-C5-N7	-2.92	106.35	109.40
32	1a	1519	MA6	N1-C6-N6	2.92	120.13	117.06
32	2a	1404	5MC	C5-C6-N1	-2.80	119.17	122.19
1	2A	1942	5MC	N4-C4-N3	2.79	120.98	117.03
1	2A	1962	5MC	N4-C4-N3	2.77	120.94	117.03
32	2a	1407	5MC	N4-C4-N3	2.73	120.89	117.03
1	2A	2503	2MA	C4-C5-N7	-2.71	106.57	109.40
32	2a	1518	MA6	C10-N6-C9	-2.71	107.39	116.12
32	1a	1400	5MC	C5-C6-N1	-2.71	119.28	122.19
32	2a	1207	2MG	C4-C5-N7	-2.68	106.61	109.40
32	1a	527	7MG	C8-N7-C5	2.64	115.81	108.94
32	2a	1519	MA6	C9-N6-C6	-2.64	111.53	119.51
32	2a	1207	2MG	N2-C2-N1	2.55	119.41	116.96
1	1A	2515	2MA	C4-C5-N7	-2.53	106.76	109.40
1	1A	1984	5MC	N4-C4-N3	2.52	120.59	117.03
1	2A	1962	5MC	C5-C6-N1	-2.49	119.52	122.19
1	1A	1964	5MC	C5-C6-N1	-2.46	119.55	122.19
32	2a	967	5MC	C5-C6-N1	-2.45	119.56	122.19
32	2a	1400	5MC	N4-C4-N3	2.42	120.45	117.03
1	1A	2564	2MU	C5-C4-N3	-2.39	118.06	123.31
1	1A	1964	5MC	N4-C4-N3	2.38	120.40	117.03
1	2A	1942	5MC	C5-C6-N1	-2.37	119.64	122.19
32	1a	1404	5MC	C5-C6-N1	-2.35	119.66	122.19
32	2a	516	PSU	O4'-C1'-C2'	2.34	108.45	104.66
32	1a	1407	5MC	N4-C4-N3	2.32	120.32	117.03
32	1a	1400	5MC	N4-C4-N3	2.32	120.31	117.03
32	1a	966	M2G	N1-C2-N2	2.31	119.53	117.19
1	2A	2251	OMG	C4-C5-N7	-2.29	107.01	109.40
32	1a	1207	2MG	O3'-C3'-C2'	2.29	119.24	111.82
32	2a	1407	5MC	C5-C6-N1	-2.26	119.76	122.19
32	1a	1518	MA6	C10-N6-C9	-2.23	108.94	116.12
32	2a	966	M2G	C4-C5-N7	-2.22	107.08	109.40
32	1a	1404	5MC	N4-C4-N3	2.22	120.17	117.03
32	2a	527	7MG	C2-N3-C4	2.19	119.94	113.89
32	1a	516	PSU	O4'-C1'-C2'	2.17	108.18	104.66
32	1a	1207	2MG	N3-C2-N1	-2.17	122.80	126.23
32	2a	966	M2G	N3-C2-N2	2.16	119.38	117.18

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2552	2MU	C5-C4-N3	-2.13	118.62	123.31
1	1A	1942	4OC	N4-C4-N3	2.12	119.84	116.49
32	2a	1404	5MC	N4-C4-N3	2.12	120.02	117.03
32	1a	1518	MA6	C10-N6-C6	-2.09	113.19	119.51
32	1a	527	7MG	CM7-N7-C5	2.08	132.00	124.01
1	1A	2564	2MU	C6'-O2'-C2'	-2.08	109.07	114.52
32	1a	1207	2MG	O3'-C3'-C4'	2.06	117.01	111.05
32	1a	967	5MC	C5-C6-N1	-2.06	119.97	122.19
1	1A	1933	PSU	O4'-C1'-C2'	2.05	107.98	104.66
1	2A	1920	4OC	N4-C4-N3	2.02	119.68	116.49

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	1518	MA6	C5-C6-N6-C9
32	1a	1518	MA6	C5-C6-N6-C10
32	1a	1519	MA6	O4'-C4'-C5'-O5'
32	1a	1519	MA6	C5-C6-N6-C10
43	2l	92	0TD	CG-CB-SB-CSB
1	1A	1942	4OC	C2'-C1'-N1-C6
32	1a	1207	2MG	N1-C2-N2-CM2
32	1a	1207	2MG	N3-C2-N2-CM2
1	2A	1962	5MC	O4'-C1'-N1-C6
1	2A	1962	5MC	C2'-C1'-N1-C6
32	2a	1519	MA6	C5-C6-N6-C9
43	1l	92	0TD	O-C-CA-CB
43	1l	92	0TD	CG-CB-SB-CSB
1	1A	1984	5MC	O4'-C1'-N1-C6
1	1A	1984	5MC	C2'-C1'-N1-C6
32	2a	1400	5MC	O4'-C1'-N1-C6
32	2a	1400	5MC	C2'-C1'-N1-C6
32	2a	1518	MA6	C5-C6-N6-C10
32	2a	1402	4OC	N3-C4-N4-CM4
32	2a	1402	4OC	C5-C4-N4-CM4
32	1a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	1519	MA6	O4'-C4'-C5'-O5'
32	2a	1402	4OC	O4'-C4'-C5'-O5'
32	2a	1402	4OC	C3'-C4'-C5'-O5'
32	1a	1518	MA6	N1-C6-N6-C9
32	2a	1519	MA6	C3'-C4'-C5'-O5'
32	2a	1519	MA6	C5-C6-N6-C10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
32	2a	1518	MA6	C5-C6-N6-C9
1	2A	2503	2MA	O4'-C4'-C5'-O5'
32	1a	1402	4OC	O4'-C4'-C5'-O5'
1	1A	2515	2MA	C4'-C5'-O5'-P
1	1A	2515	2MA	O4'-C4'-C5'-O5'
32	1a	1402	4OC	C3'-C2'-O2'-CM2
1	1A	1939	PSU	C2'-C1'-C5-C6
1	2A	1917	PSU	C2'-C1'-C5-C6
32	1a	1400	5MC	O4'-C4'-C5'-O5'
1	1A	2263	OMG	C4'-C5'-O5'-P

There are no ring outliers.

9 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2A	1939	5MU	1	0
1	1A	1942	4OC	1	0
1	2A	1915	5MU	1	0
1	1A	2564	2MU	1	0
1	2A	1911	PSU	1	0
1	1A	1964	5MC	1	0
1	2A	1917	PSU	1	0
1	2A	2251	OMG	1	0
1	1A	2515	2MA	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2389 ligands modelled in this entry, 2376 are monoatomic - leaving 13 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
60	SF4	2d	501	35	0,12,12	0.00	-	-		
57	MPD	2A	3711	-	7,7,7	0.30	0	9,10,10	0.30	0
57	MPD	1A	3988	-	7,7,7	0.27	0	9,10,10	0.28	0
56	EZP	2A	3709	-	21,26,26	3.58	3 (14%)	26,35,35	0.92	1 (3%)
57	MPD	1T	204	-	7,7,7	0.32	0	9,10,10	0.36	0
57	MPD	1a	1854	-	7,7,7	0.38	0	9,10,10	0.38	0
56	EZP	1A	3987	-	21,26,26	2.81	3 (14%)	26,35,35	1.72	4 (15%)
57	MPD	2B	3020	-	7,7,7	0.30	0	9,10,10	0.30	0
57	MPD	18	102	-	7,7,7	0.27	0	9,10,10	0.38	0
60	SF4	1d	302	35	0,12,12	0.00	-	-		
57	MPD	2A	3710	-	7,7,7	0.39	0	9,10,10	0.30	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	SF4	2d	501	35	-	-	0/6/5/5
57	MPD	2A	3711	-	-	3/5/5/5	-
57	MPD	1A	3988	-	-	2/5/5/5	-
56	EZP	2A	3709	-	-	7/24/26/26	0/2/2/2
57	MPD	1T	204	-	-	1/5/5/5	-
57	MPD	1a	1854	-	-	2/5/5/5	-
56	EZP	1A	3987	-	-	7/24/26/26	0/2/2/2
57	MPD	2B	3020	-	-	3/5/5/5	-
57	MPD	18	102	-	-	1/5/5/5	-
60	SF4	1d	302	35	-	-	0/6/5/5
57	MPD	2A	3710	-	-	0/5/5/5	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	2A	3709	EZP	OAC-NAY	13.50	1.45	1.22
56	1A	3987	EZP	OAC-NAY	9.18	1.38	1.22
56	2A	3709	EZP	CAT-CAW	-8.10	1.39	1.51
56	1A	3987	EZP	CAT-CAW	-7.46	1.40	1.51
56	1A	3987	EZP	CAU-NAY	-4.60	1.34	1.45
56	2A	3709	EZP	CAU-NAY	-4.26	1.34	1.45

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	1A	3987	EZP	CAT-CAW-CAX	4.98	120.42	111.64
56	1A	3987	EZP	CAW-CAX-NAP	4.35	118.30	110.05
56	1A	3987	EZP	CAI-CAU-NAY	2.44	121.22	119.38
56	2A	3709	EZP	CAW-CAX-NAP	2.27	114.35	110.05
56	1A	3987	EZP	CA-C-NAP	-2.26	113.01	116.15

There are no chirality outliers.

All (26) torsion outliers are listed below:

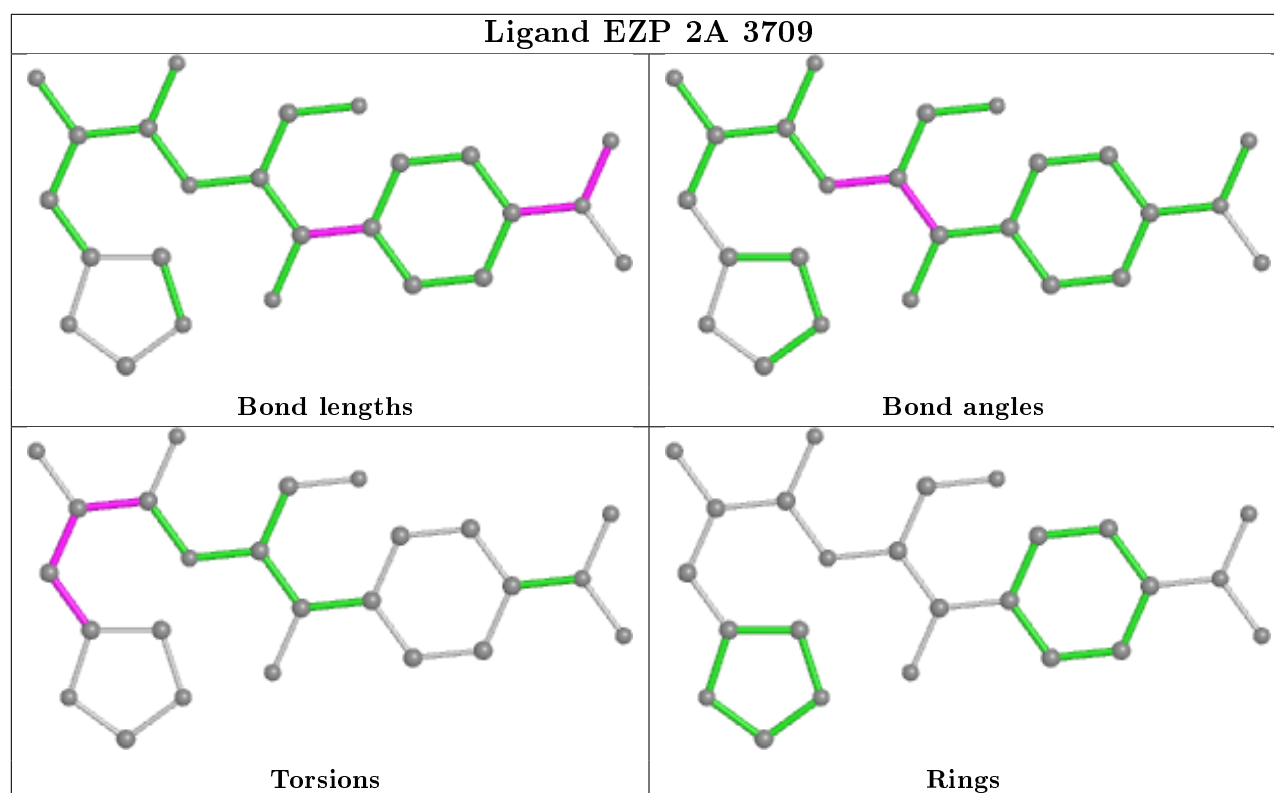
Mol	Chain	Res	Type	Atoms
56	1A	3987	EZP	NAP-C-CA-CB
56	1A	3987	EZP	O-C-CA-CB
56	1A	3987	EZP	C-CA-CB-CG
56	2A	3709	EZP	NAP-C-CA-N
56	2A	3709	EZP	NAP-C-CA-CB
56	2A	3709	EZP	O-C-CA-N
56	2A	3709	EZP	O-C-CA-CB
56	2A	3709	EZP	C-CA-CB-CG
56	2A	3709	EZP	N-CA-CB-CG
57	18	102	MPD	C2-C3-C4-C5
56	1A	3987	EZP	CAM-CAX-NAP-C
56	1A	3987	EZP	CA-CB-CG-CD2
57	1T	204	MPD	C2-C3-C4-C5
57	2B	3020	MPD	C2-C3-C4-C5
57	2A	3711	MPD	C1-C2-C3-C4
56	1A	3987	EZP	N-CA-CB-CG
57	1a	1854	MPD	CM-C2-C3-C4
57	1A	3988	MPD	O2-C2-C3-C4
57	2B	3020	MPD	O2-C2-C3-C4
57	2A	3711	MPD	C2-C3-C4-C5
57	1A	3988	MPD	C2-C3-C4-C5
57	1a	1854	MPD	C2-C3-C4-C5
56	2A	3709	EZP	CA-CB-CG-CD2
57	2A	3711	MPD	C2-C3-C4-O4
56	1A	3987	EZP	OAE-CAW-CAX-CAM
57	2B	3020	MPD	C2-C3-C4-O4

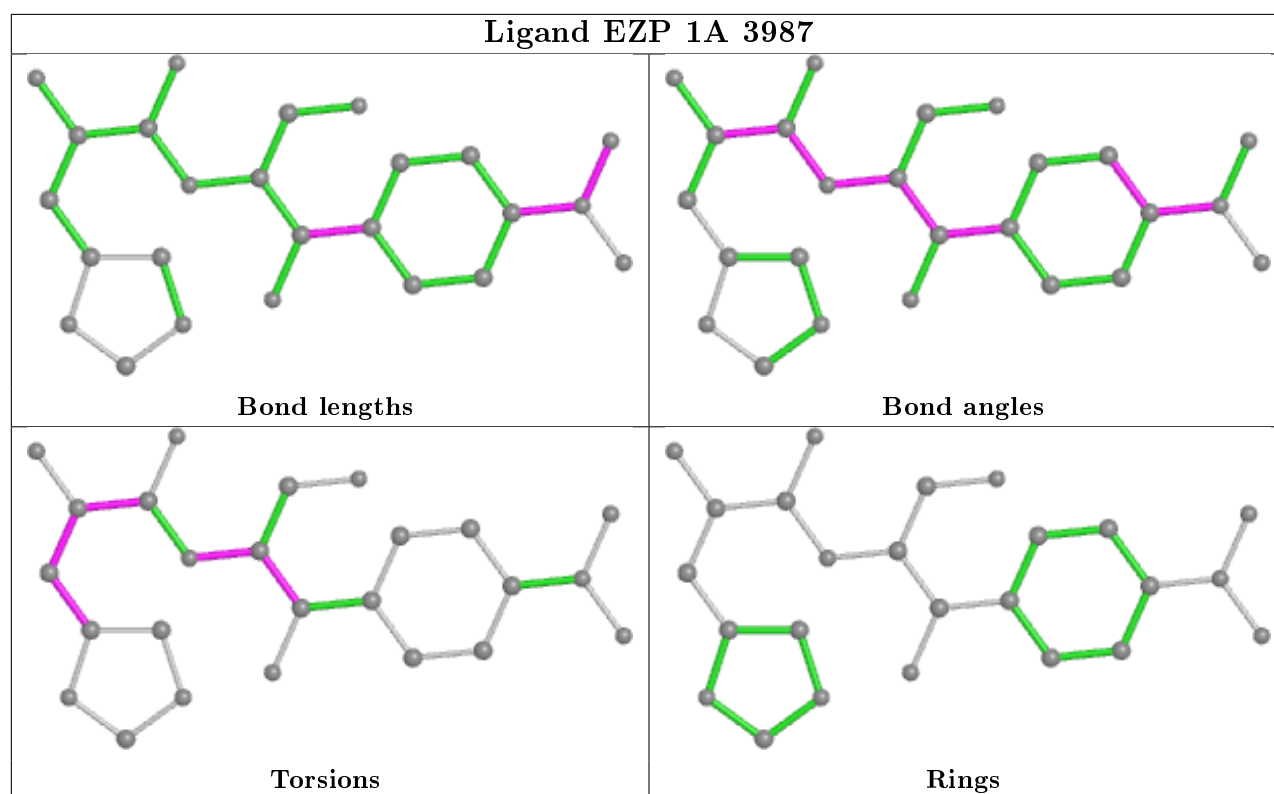
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	1T	204	MPD	1	0
57	18	102	MPD	1	0
57	2A	3710	MPD	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 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	2861/2915 (98%)	0.42	57 (1%) 65 67	15, 31, 89, 105	0
1	2A	2856/2915 (97%)	0.28	65 (2%) 60 62	27, 50, 92, 103	0
2	1B	120/121 (99%)	0.05	0 100 100	24, 44, 58, 80	0
2	2B	120/121 (99%)	-0.06	0 100 100	52, 74, 83, 90	0
3	1D	275/276 (99%)	0.60	3 (1%) 80 82	17, 32, 46, 65	0
3	2D	275/276 (99%)	0.69	13 (4%) 31 30	26, 44, 56, 76	0
4	1E	204/206 (99%)	0.51	2 (0%) 82 83	16, 34, 55, 70	0
4	2E	204/206 (99%)	0.59	3 (1%) 73 76	29, 50, 66, 79	0
5	1F	203/210 (96%)	0.37	0 100 100	16, 35, 60, 83	0
5	2F	203/210 (96%)	0.39	3 (1%) 73 76	29, 60, 72, 85	0
6	1G	181/182 (99%)	0.16	2 (1%) 80 82	39, 56, 72, 80	0
6	2G	181/182 (99%)	0.59	13 (7%) 15 13	68, 77, 85, 89	0
7	1H	174/180 (96%)	0.29	1 (0%) 89 91	32, 46, 59, 64	0
7	2H	173/180 (96%)	0.72	20 (11%) 4 3	62, 75, 82, 86	0
8	1I	147/148 (99%)	0.15	3 (2%) 65 67	34, 66, 76, 83	0
8	2I	146/148 (98%)	0.49	15 (10%) 6 5	51, 69, 81, 84	0
9	1N	140/140 (100%)	0.41	0 100 100	22, 32, 53, 67	0
9	2N	140/140 (100%)	0.41	1 (0%) 87 89	43, 57, 71, 76	0
10	1O	122/122 (100%)	0.47	0 100 100	23, 34, 50, 58	0
10	2O	122/122 (100%)	0.58	5 (4%) 37 36	38, 51, 61, 69	0
11	1P	149/150 (99%)	0.36	1 (0%) 87 89	15, 38, 58, 71	0
11	2P	149/150 (99%)	0.66	7 (4%) 31 30	32, 59, 77, 80	0
12	1Q	141/141 (100%)	0.44	0 100 100	21, 35, 46, 62	0
12	2Q	141/141 (100%)	0.66	7 (4%) 28 27	40, 57, 67, 76	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%)	0.50	0 100 100	21, 29, 44, 50	0
13	2R	118/118 (100%)	0.45	2 (1%) 70 72	31, 44, 55, 65	0
14	1S	110/112 (98%)	0.31	1 (0%) 84 85	34, 45, 56, 65	0
14	2S	110/112 (98%)	0.48	9 (8%) 11 9	59, 69, 76, 81	0
15	1T	131/146 (89%)	0.30	1 (0%) 86 87	28, 38, 62, 75	0
15	2T	131/146 (89%)	0.33	1 (0%) 86 87	41, 52, 70, 76	0
16	1U	116/118 (98%)	0.63	1 (0%) 84 85	18, 25, 39, 57	0
16	2U	116/118 (98%)	0.79	9 (7%) 13 11	33, 52, 67, 74	0
17	1V	101/101 (100%)	0.36	0 100 100	15, 35, 54, 67	0
17	2V	101/101 (100%)	0.44	3 (2%) 50 51	31, 62, 72, 77	0
18	1W	112/113 (99%)	0.46	1 (0%) 84 85	19, 27, 46, 75	0
18	2W	112/113 (99%)	0.67	8 (7%) 16 14	29, 43, 59, 84	0
19	1X	95/96 (98%)	0.44	1 (1%) 80 82	23, 32, 58, 68	0
19	2X	95/96 (98%)	0.68	5 (5%) 26 25	43, 54, 69, 74	0
20	1Y	107/110 (97%)	0.39	1 (0%) 84 85	29, 42, 62, 67	0
20	2Y	107/110 (97%)	1.10	15 (14%) 2 1	49, 63, 73, 82	0
21	1Z	203/206 (98%)	0.13	2 (0%) 82 83	35, 51, 66, 76	0
21	2Z	201/206 (97%)	0.21	8 (3%) 38 37	57, 71, 79, 88	0
22	10	77/85 (90%)	0.56	1 (1%) 77 78	24, 31, 48, 54	0
22	20	77/85 (90%)	0.99	12 (15%) 2 1	43, 57, 67, 72	0
23	11	97/98 (98%)	0.83	5 (5%) 27 25	22, 39, 61, 69	0
23	21	97/98 (98%)	0.92	8 (8%) 11 9	35, 49, 71, 73	0
24	12	70/72 (97%)	0.24	1 (1%) 75 77	29, 44, 57, 78	0
24	22	70/72 (97%)	0.40	2 (2%) 51 52	53, 64, 71, 73	0
25	13	59/60 (98%)	0.44	0 100 100	20, 30, 55, 63	0
25	23	59/60 (98%)	1.13	14 (23%) 0 0	45, 55, 69, 77	0
26	14	69/71 (97%)	0.22	4 (5%) 23 22	50, 69, 86, 90	0
26	24	69/71 (97%)	0.48	6 (8%) 10 8	70, 83, 88, 91	0
27	15	59/60 (98%)	0.53	0 100 100	17, 27, 44, 54	0
27	25	59/60 (98%)	0.38	2 (3%) 45 45	29, 44, 59, 68	0
28	16	53/54 (98%)	0.15	0 100 100	28, 36, 48, 55	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%)	0.30	0 100 100	46, 54, 63, 68	0
29	17	48/49 (97%)	0.90	2 (4%) 36 35	17, 24, 49, 58	0
29	27	48/49 (97%)	0.85	4 (8%) 11 9	28, 36, 58, 65	0
30	18	64/65 (98%)	0.64	1 (1%) 72 74	23, 28, 34, 47	0
30	28	64/65 (98%)	0.88	4 (6%) 20 19	38, 49, 56, 63	0
31	19	37/37 (100%)	0.56	1 (2%) 54 55	22, 32, 49, 53	0
31	29	37/37 (100%)	1.34	8 (21%) 0 0	50, 60, 68, 69	0
32	1a	1488/1521 (97%)	0.11	20 (1%) 77 78	32, 62, 89, 104	0
32	2a	1492/1521 (98%)	0.13	23 (1%) 73 76	42, 71, 91, 103	0
33	1b	231/256 (90%)	0.33	9 (3%) 39 38	61, 74, 83, 88	0
33	2b	231/256 (90%)	0.72	34 (14%) 2 1	66, 80, 86, 90	0
34	1c	206/239 (86%)	0.55	11 (5%) 26 25	53, 67, 77, 81	0
34	2c	206/239 (86%)	0.92	31 (15%) 2 1	70, 79, 84, 91	0
35	1d	208/209 (99%)	0.72	20 (9%) 8 6	51, 66, 75, 81	0
35	2d	208/209 (99%)	1.14	39 (18%) 1 0	55, 68, 77, 79	0
36	1e	148/162 (91%)	0.49	4 (2%) 54 55	46, 59, 69, 80	0
36	2e	148/162 (91%)	0.82	20 (13%) 3 2	57, 68, 76, 83	0
37	1f	100/101 (99%)	0.27	1 (1%) 82 83	43, 60, 70, 74	0
37	2f	100/101 (99%)	0.02	0 100 100	52, 62, 70, 76	0
38	1g	155/156 (99%)	0.31	6 (3%) 39 38	56, 65, 76, 85	0
38	2g	155/156 (99%)	0.35	10 (6%) 18 17	68, 75, 81, 87	0
39	1h	137/138 (99%)	0.63	8 (5%) 23 22	51, 62, 71, 74	0
39	2h	137/138 (99%)	0.61	7 (5%) 28 26	58, 69, 74, 82	0
40	1i	127/128 (99%)	0.71	17 (13%) 3 2	52, 73, 79, 82	0
40	2i	126/128 (98%)	1.74	49 (38%) 0 0	67, 80, 85, 87	0
41	1j	97/105 (92%)	0.50	13 (13%) 3 2	52, 72, 83, 86	0
41	2j	96/105 (91%)	2.13	47 (48%) 0 0	71, 80, 85, 87	0
42	1k	114/129 (88%)	0.22	0 100 100	39, 58, 69, 73	0
42	2k	114/129 (88%)	0.62	7 (6%) 21 20	50, 66, 75, 81	0
43	1l	121/132 (91%)	0.46	4 (3%) 46 46	42, 54, 65, 70	0
43	2l	121/132 (91%)	0.97	16 (13%) 3 2	54, 62, 69, 77	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	116/126 (92%)	0.32	4 (3%) 45 45	52, 68, 75, 79	0
44	2m	114/126 (90%)	0.82	12 (10%) 6 4	73, 80, 85, 87	0
45	1n	60/61 (98%)	1.23	10 (16%) 1 1	57, 64, 72, 79	0
45	2n	60/61 (98%)	2.71	36 (60%) 0 0	71, 79, 85, 88	0
46	1o	88/89 (98%)	0.42	0 100 100	43, 60, 71, 77	0
46	2o	88/89 (98%)	0.61	2 (2%) 60 62	54, 67, 75, 78	0
47	1p	82/88 (93%)	1.04	12 (14%) 2 1	55, 67, 77, 80	0
47	2p	82/88 (93%)	0.80	8 (9%) 7 5	55, 65, 75, 82	0
48	1q	99/105 (94%)	0.49	6 (6%) 21 20	48, 63, 72, 73	0
48	2q	99/105 (94%)	0.55	7 (7%) 16 14	53, 63, 73, 79	0
49	1r	68/88 (77%)	0.26	1 (1%) 73 76	51, 60, 73, 76	0
49	2r	68/88 (77%)	0.35	2 (2%) 51 52	59, 67, 74, 76	0
50	1s	83/93 (89%)	0.14	1 (1%) 79 80	59, 70, 76, 79	0
50	2s	83/93 (89%)	0.98	15 (18%) 1 1	70, 82, 86, 88	0
51	1t	96/106 (90%)	0.78	15 (15%) 2 1	53, 66, 76, 82	0
51	2t	98/106 (92%)	0.45	7 (7%) 16 14	53, 64, 75, 77	0
52	1u	23/27 (85%)	1.77	9 (39%) 0 0	61, 66, 69, 72	0
52	2u	23/27 (85%)	2.31	14 (60%) 0 0	73, 76, 80, 82	0
53	1y	97/113 (85%)	0.62	4 (4%) 37 36	45, 56, 67, 71	0
53	2y	96/113 (84%)	2.26	51 (53%) 0 0	60, 72, 79, 83	0
All	All	20766/21468 (96%)	0.45	976 (4%) 31 30	15, 57, 84, 105	0

All (976) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1A	1110	C	7.7
45	2n	59	ALA	7.6
1	1A	1122	C	7.4
40	2i	127	LYS	7.3
1	1A	1133	G	7.1
20	2Y	1	MET	7.0
26	24	49	PHE	7.0
1	2A	2602	A	6.7
53	2y	8	LYS	6.5
32	2a	1030(B)	C	6.3

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
45	2n	25	VAL	6.1
1	1A	1111	U	6.1
40	1i	106	ALA	6.0
1	1A	1137	G	6.0
32	2a	1030(A)	G	6.0
1	1A	1136	U	5.9
45	2n	2	ALA	5.9
42	2k	13	GLN	5.8
34	2c	8	ILE	5.8
41	2j	44	VAL	5.8
1	1A	1112	U	5.8
35	2d	146	ILE	5.8
8	2l	3	VAL	5.7
35	2d	158	ILE	5.7
41	2j	63	PHE	5.6
52	2u	6	ARG	5.6
41	2j	40	LEU	5.5
26	24	45	GLY	5.5
53	2y	40	ILE	5.5
1	1A	2614	A	5.4
41	2j	62	HIS	5.3
41	2j	48	THR	5.3
41	2j	66	ARG	5.3
53	2y	88	LEU	5.3
23	2l	2	SER	5.3
41	2j	64	GLU	5.3
41	2j	96	ILE	5.2
40	2i	109	VAL	5.2
41	2j	46	ARG	5.2
44	2m	102	ARG	5.1
53	2y	92	GLY	5.1
32	2a	1001(A)	G	5.1
52	2u	14	TRP	5.1
38	2g	7	ALA	5.1
23	1l	2	SER	5.1
52	2u	15	ARG	5.0
32	1a	1036	G	5.0
51	1t	9	ASN	5.0
40	2i	114	TYR	5.0
41	2j	6	ILE	5.0
40	2i	115	GLY	5.0
45	2n	41	ARG	5.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	2A	2153	G	4.9
40	2i	7	THR	4.9
1	1A	1126	C	4.9
41	2j	67	THR	4.9
45	2n	55	GLY	4.9
53	2y	38	HIS	4.8
41	2j	65	LEU	4.8
41	2j	45	ARG	4.8
45	2n	34	TYR	4.8
1	1A	1135	G	4.7
1	1A	2169	G	4.7
1	2A	2146	C	4.7
1	1A	1134	A	4.7
53	2y	73	ALA	4.6
41	2j	54	PHE	4.6
45	2n	44	LEU	4.6
34	2c	65	ALA	4.6
45	2n	61	TRP	4.5
45	2n	53	LEU	4.5
1	2A	2145	C	4.5
1	2A	2174	C	4.5
41	2j	47	PHE	4.5
41	2j	72	VAL	4.5
47	1p	19	ILE	4.4
1	1A	1124	U	4.4
20	2Y	5	MET	4.4
41	2j	49	VAL	4.4
1	2A	2142	C	4.4
1	2A	2802	G	4.4
34	2c	124	ILE	4.4
53	2y	78	ILE	4.4
1	2A	2140	C	4.4
34	2c	33	LEU	4.4
41	2j	38	ILE	4.4
41	2j	55	LYS	4.4
34	1c	193	TYR	4.4
45	2n	29	ARG	4.4
45	2n	31	ARG	4.4
21	2Z	191	VAL	4.3
6	2G	39	ILE	4.3
53	2y	39	ILE	4.3
1	1A	1123	A	4.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
48	2q	98	LEU	4.3
1	2A	2793	G	4.3
45	2n	35	ARG	4.2
14	2S	32	LEU	4.2
12	2Q	104	PHE	4.2
53	2y	63	ALA	4.2
50	2s	82	GLY	4.2
1	1A	1113	A	4.2
32	1a	1034	G	4.2
41	2j	59	SER	4.2
1	2A	1509	C	4.2
20	2Y	35	TYR	4.2
40	2i	66	ARG	4.2
32	2a	1257	U	4.2
1	2A	1085	A	4.2
53	2y	93	GLU	4.2
19	2X	68	ARG	4.2
53	2y	9	GLN	4.2
40	2i	111	ARG	4.2
7	2H	166	GLY	4.1
45	2n	49	HIS	4.1
7	2H	115	VAL	4.1
38	1g	16	LEU	4.1
1	2A	2155	G	4.1
40	2i	18	PHE	4.1
36	2e	12	LEU	4.1
47	2p	19	ILE	4.1
45	2n	56	VAL	4.1
1	2A	2147	G	4.1
45	2n	58	LYS	4.1
35	1d	3	ARG	4.1
1	2A	34	C	4.1
34	2c	87	LEU	4.1
45	2n	37	PHE	4.1
35	1d	2	GLY	4.1
38	2g	154	TYR	4.1
19	2X	92	LEU	4.0
36	2e	109	ILE	4.0
35	2d	184	LYS	4.0
1	2A	2897	U	4.0
53	2y	62	VAL	4.0
1	2A	2154	G	4.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
25	23	26	LEU	4.0
45	2n	39	LEU	4.0
34	2c	4	LYS	4.0
1	1A	1120	G	4.0
40	2i	5	TYR	4.0
33	2b	165	VAL	4.0
53	1y	94	ALA	4.0
33	1b	130	ARG	3.9
40	2i	79	LEU	3.9
53	2y	7	SER	3.9
1	1A	1127	U	3.9
1	1A	1148	C	3.9
32	2a	1202	G	3.9
40	2i	8	GLY	3.9
20	2Y	45	VAL	3.9
53	2y	52	ALA	3.9
53	2y	87	LYS	3.9
40	2i	56	LEU	3.9
45	2n	6	LEU	3.9
1	2A	2169	A	3.9
35	2d	120	LEU	3.9
1	1A	1149	A	3.9
45	2n	36	PHE	3.9
6	2G	136	ARG	3.8
40	1i	8	GLY	3.8
1	1A	2164	C	3.8
40	2i	110	GLU	3.8
40	2i	113	LYS	3.8
1	2A	1046	A	3.8
41	2j	69	ASN	3.8
35	2d	183	GLY	3.8
33	1b	131	PRO	3.7
41	2j	60	ARG	3.7
6	2G	157	ILE	3.7
38	2g	78	ARG	3.7
53	2y	41	LEU	3.7
35	2d	20	TYR	3.7
38	1g	156	TRP	3.7
21	2Z	197	ILE	3.7
51	2t	9	ASN	3.7
44	2m	110	ARG	3.7
45	2n	60	SER	3.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
41	2j	98	ILE	3.7
47	1p	1	MET	3.7
41	2j	68	HIS	3.7
53	2y	80	LYS	3.7
1	1A	2161	C	3.7
36	2e	13	ILE	3.7
52	2u	17	THR	3.7
1	1A	1131	A	3.7
34	2c	23	TYR	3.6
1	2A	2106	G	3.6
1	2A	652(B)	A	3.6
1	2A	1076	C	3.6
44	2m	116	THR	3.6
33	2b	70	PHE	3.6
40	2i	90	PRO	3.6
41	2j	71	LEU	3.6
53	2y	77	LEU	3.6
33	2b	233	SER	3.6
1	1A	1221	G	3.6
32	2a	1001	A	3.6
53	1y	95	ARG	3.6
33	2b	228	GLY	3.6
34	2c	6	HIS	3.6
21	2Z	192	ALA	3.5
8	2I	19	VAL	3.5
41	2j	34	VAL	3.5
52	1u	18	TYR	3.5
41	1j	44	VAL	3.5
1	1A	1132	A	3.5
1	2A	614(B)	G	3.5
12	2Q	59	ARG	3.5
1	2A	2107	C	3.5
41	2j	41	PRO	3.5
14	2S	33	LYS	3.5
40	1i	114	TYR	3.5
40	2i	125	TYR	3.5
44	1m	115	LYS	3.5
47	1p	17	TYR	3.5
53	2y	60	VAL	3.5
53	2y	12	ILE	3.5
1	2A	2138	C	3.4
35	2d	149	ALA	3.4

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
43	2l	64	TYR	3.4
44	1m	2	ALA	3.4
1	2A	2144	U	3.4
32	2a	1030	C	3.4
41	2j	70	ARG	3.4
39	1h	134	ILE	3.4
1	1A	1129	U	3.4
41	2j	29	ARG	3.4
33	1b	128	GLU	3.4
53	2y	61	LEU	3.4
38	2g	155	ARG	3.4
1	1A	1072	U	3.4
3	2D	182	LEU	3.4
14	2S	40	ILE	3.4
29	27	48	LYS	3.4
52	2u	13	ILE	3.4
33	2b	122	PHE	3.4
41	2j	43	ARG	3.4
1	2A	2139	C	3.4
32	1a	1030(B)	C	3.4
1	2A	2132	U	3.4
45	2n	12	ARG	3.4
36	2e	121	LYS	3.4
1	1A	1121	C	3.4
25	23	15	TYR	3.4
33	1b	214	ILE	3.3
47	1p	59	TRP	3.3
1	1A	2815	C	3.3
50	2s	49	ILE	3.3
7	2H	165	ALA	3.3
51	1t	18	GLN	3.3
45	1n	34	TYR	3.3
7	2H	95	ARG	3.3
36	2e	133	TYR	3.3
36	2e	94	ALA	3.3
41	2j	36	GLY	3.3
51	1t	20	LEU	3.3
32	1a	1257	U	3.3
8	2I	18	VAL	3.3
43	2l	32	PHE	3.3
31	29	37	GLY	3.3
1	2A	2162	G	3.3

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
30	28	24	ALA	3.3
32	2a	1036	G	3.3
1	2A	2896	C	3.3
48	1q	98	LEU	3.3
1	2A	2062	A	3.3
35	1d	70	ILE	3.3
20	2Y	106	LEU	3.3
32	2a	1030(C)	G	3.3
42	2k	104	GLN	3.3
1	2A	2803	C	3.2
39	1h	93	VAL	3.2
40	1i	5	TYR	3.2
53	2y	76	GLU	3.2
1	1A	2139	A	3.2
45	2n	26	ARG	3.2
32	1a	1030(C)	G	3.2
43	2l	18	VAL	3.2
36	2e	26	PHE	3.2
35	1d	138	TYR	3.2
53	2y	58	ASN	3.2
41	2j	10	GLY	3.2
35	2d	5	ILE	3.2
35	2d	157	LEU	3.2
39	2h	2	LEU	3.2
53	2y	42	SER	3.2
40	2i	63	ILE	3.2
33	2b	118	LEU	3.2
40	2i	120	ARG	3.2
37	1f	90	VAL	3.2
51	1t	72	LEU	3.2
32	1a	1286	A	3.1
1	1A	1109	G	3.1
1	1A	2806	G	3.1
32	2a	1031	G	3.1
4	2E	1	MET	3.1
22	20	8	GLY	3.1
40	2i	88	TYR	3.1
7	2H	128	PRO	3.1
53	2y	48	PHE	3.1
31	29	17	ILE	3.1
41	2j	16	LEU	3.1
41	2j	26	ALA	3.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
32	1a	1001	A	3.1
53	2y	64	SER	3.1
20	2Y	4	LYS	3.1
22	20	74	ARG	3.1
32	2a	1034	G	3.1
53	2y	20	VAL	3.1
8	2I	5	LEU	3.1
34	1c	182	ILE	3.1
41	2j	74	ILE	3.1
1	1A	2163	G	3.1
1	2A	2168	G	3.1
18	2W	92	ARG	3.1
52	1u	14	TRP	3.1
1	2A	614(A)	U	3.1
1	2A	2152	G	3.1
48	1q	27	PHE	3.1
31	29	16	VAL	3.1
40	2i	117	HIS	3.0
29	27	1	MET	3.0
1	2A	2125	G	3.0
1	2A	2179	C	3.0
45	2n	38	GLY	3.0
35	2d	8	VAL	3.0
21	2Z	18	LEU	3.0
33	2b	163	PHE	3.0
34	2c	177	THR	3.0
26	14	50	VAL	3.0
44	2m	90	LEU	3.0
53	2y	50	ALA	3.0
14	2S	35	ILE	3.0
40	2i	36	TYR	3.0
1	2A	2143	C	3.0
1	1A	218	A	3.0
1	2A	229	A	3.0
45	1n	33	VAL	3.0
33	2b	214	ILE	3.0
40	2i	6	GLY	3.0
6	2G	146	TYR	3.0
45	2n	45	ARG	3.0
1	1A	2807	C	3.0
1	2A	2124	G	3.0
1	2A	2141	G	3.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
35	2d	152	SER	3.0
34	1c	91	LEU	3.0
52	1u	2	GLY	3.0
33	2b	223	ILE	3.0
53	2y	4	ASN	3.0
50	2s	52	TYR	3.0
26	14	52	THR	3.0
33	2b	48	MET	3.0
34	2c	195	VAL	3.0
22	20	77	ARG	3.0
21	2Z	199	LYS	2.9
6	2G	152	LEU	2.9
22	20	11	ARG	2.9
1	1A	1138	C	2.9
41	1j	10	GLY	2.9
45	2n	13	THR	2.9
21	1Z	192	ALA	2.9
1	1A	1118	C	2.9
11	2P	15	ARG	2.9
51	1t	68	LYS	2.9
53	2y	94	ALA	2.9
8	2I	4	ILE	2.9
35	2d	115	ARG	2.9
34	2c	196	LEU	2.9
51	1t	13	LEU	2.9
1	1A	1125	C	2.9
20	1Y	1	MET	2.9
33	2b	101	MET	2.9
1	1A	2177	G	2.9
7	1H	2	SER	2.9
44	2m	75	ALA	2.9
40	2i	75	ASP	2.9
40	2i	126	SER	2.9
51	2t	11	SER	2.9
3	2D	276	LYS	2.9
34	2c	153	VAL	2.9
34	2c	163	ALA	2.9
38	1g	154	TYR	2.9
45	2n	10	ALA	2.9
43	2l	100	ILE	2.9
39	1h	112	LEU	2.9
29	17	1	MET	2.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
38	1g	42	ILE	2.8
41	1j	54	PHE	2.8
35	1d	58	LEU	2.8
45	2n	57	ARG	2.8
53	2y	84	GLN	2.8
3	1D	275	LYS	2.8
33	2b	132	LYS	2.8
35	1d	179	GLU	2.8
32	1a	1037	C	2.8
33	2b	131	PRO	2.8
48	2q	99	SER	2.8
43	2l	89	ARG	2.8
1	2A	2116	G	2.8
34	1c	47	LEU	2.8
7	2H	159	GLU	2.8
38	2g	8	GLU	2.8
1	1A	2814	C	2.8
44	1m	87	TYR	2.8
51	1t	14	LYS	2.8
53	2y	34	LEU	2.8
33	2b	120	ALA	2.8
51	1t	76	ALA	2.8
1	2A	1083	U	2.8
40	2i	57	GLY	2.8
1	1A	2084	A	2.8
43	1l	64	TYR	2.8
41	2j	58	ASP	2.8
3	1D	37	LEU	2.8
45	2n	42	ILE	2.8
1	1A	1128	U	2.8
1	2A	2118	U	2.8
35	2d	33	MET	2.8
1	1A	2816	G	2.8
3	2D	37	LEU	2.8
8	2I	38	LEU	2.8
53	2y	5	ILE	2.8
1	1A	1555	C	2.8
23	2l	61	ARG	2.8
35	1d	73	ARG	2.8
36	2e	21	ALA	2.7
45	2n	54	PRO	2.7
50	2s	35	SER	2.7

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
45	1n	61	TRP	2.7
3	2D	28	GLU	2.7
20	2Y	42	VAL	2.7
22	20	76	GLY	2.7
38	2g	6	ARG	2.7
43	2l	19	ARG	2.7
36	2e	90	VAL	2.7
32	2a	1002	G	2.7
23	11	98	LEU	2.7
34	2c	3	ASN	2.7
35	2d	110	PHE	2.7
36	2e	43	LEU	2.7
50	2s	71	LEU	2.7
40	1i	126	SER	2.7
32	1a	1030	C	2.7
40	1i	19	LEU	2.7
52	2u	2	GLY	2.7
33	2b	121	LEU	2.7
32	1a	1492	A	2.7
33	2b	162	ILE	2.7
35	1d	5	ILE	2.7
44	1m	4	ILE	2.7
47	1p	33	ILE	2.7
47	1p	20	VAL	2.7
53	2y	10	MET	2.7
6	2G	34	LEU	2.7
1	2A	2801(A)	A	2.7
3	2D	2	ALA	2.7
23	11	91	LYS	2.7
1	2A	2151	G	2.7
35	1d	207	TYR	2.7
40	2i	92	TYR	2.7
38	2g	34	GLY	2.6
51	1t	40	ALA	2.6
35	2d	104	VAL	2.6
35	2d	101	LEU	2.6
36	2e	92	LYS	2.6
34	2c	22	TRP	2.6
35	2d	70	ILE	2.6
48	2q	32	TYR	2.6
50	2s	34	TRP	2.6
53	2y	37	PRO	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	2D	61	LEU	2.6
35	2d	169	LYS	2.6
34	1c	10	PHE	2.6
18	2W	13	SER	2.6
34	1c	201	TYR	2.6
38	2g	9	VAL	2.6
40	2i	17	VAL	2.6
53	2y	79	ASN	2.6
7	2H	87	LEU	2.6
22	20	72	ARG	2.6
1	1A	2167	C	2.6
16	2U	46	ALA	2.6
41	2j	37	PRO	2.6
35	2d	118	ARG	2.6
50	2s	9	VAL	2.6
53	2y	3	MET	2.6
1	2A	1075	C	2.6
33	2b	123	ALA	2.6
40	2i	14	VAL	2.6
45	1n	18	VAL	2.6
35	2d	11	LEU	2.6
20	2Y	71	LYS	2.6
26	14	49	PHE	2.6
48	2q	71	PHE	2.6
10	2O	41	ALA	2.6
34	2c	160	ALA	2.6
34	2c	184	TYR	2.6
35	2d	4	TYR	2.6
22	20	46	LYS	2.6
33	2b	44	LEU	2.6
33	2b	152	PHE	2.6
34	2c	10	PHE	2.6
39	2h	99	GLU	2.6
1	1A	2138	G	2.6
43	2l	15	ARG	2.6
6	2G	32	PRO	2.6
7	2H	29	PRO	2.6
52	1u	17	THR	2.6
36	2e	20	GLN	2.6
4	2E	150	VAL	2.6
6	2G	133	LEU	2.6
53	2y	82	GLU	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
25	23	30	ARG	2.6
32	2a	1492	A	2.6
33	2b	130	ARG	2.6
43	2l	7	ILE	2.5
47	1p	76	GLN	2.5
35	2d	3	ARG	2.5
53	2y	17	ARG	2.5
23	2l	71	TYR	2.5
47	1p	6	LEU	2.5
51	2t	20	LEU	2.5
1	2A	2160	G	2.5
53	2y	75	ASN	2.5
34	1c	39	ILE	2.5
1	2A	1026	U	2.5
25	23	31	LEU	2.5
43	2l	55	VAL	2.5
47	2p	6	LEU	2.5
41	1j	67	THR	2.5
6	2G	29	TRP	2.5
29	17	48	LYS	2.5
8	2I	30	LEU	2.5
31	29	24	TYR	2.5
33	2b	215	LEU	2.5
35	1d	157	LEU	2.5
53	2y	11	GLU	2.5
34	1c	2	GLY	2.5
41	2j	50	ILE	2.5
43	2l	99	HIS	2.5
47	1p	7	ALA	2.5
50	2s	31	ILE	2.5
14	2S	58	LEU	2.5
41	1j	49	VAL	2.5
42	2k	14	VAL	2.5
43	2l	69	TYR	2.5
16	2U	40	PHE	2.5
34	1c	168	ALA	2.5
51	1t	69	GLY	2.5
35	2d	204	ILE	2.5
52	1u	13	ILE	2.5
7	2H	107	VAL	2.5
40	1i	109	VAL	2.5
40	2i	116	LYS	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	1A	2154	U	2.5
1	2A	1082	U	2.5
3	2D	38	LYS	2.5
51	2t	10	LEU	2.5
36	2e	105	VAL	2.5
39	2h	93	VAL	2.5
1	1A	935	C	2.5
1	2A	2133	G	2.5
1	1A	2597	U	2.4
43	2l	88	GLY	2.4
53	2y	89	GLN	2.4
33	2b	133	LYS	2.4
36	1e	21	ALA	2.4
43	2l	13	LYS	2.4
16	2U	17	ILE	2.4
25	23	53	LEU	2.4
53	2y	81	LEU	2.4
10	2O	58	VAL	2.4
22	20	9	SER	2.4
29	27	47	ARG	2.4
44	2m	6	GLY	2.4
47	1p	41	PRO	2.4
11	2P	32	THR	2.4
32	1a	1031	G	2.4
33	2b	164	VAL	2.4
34	2c	154	SER	2.4
40	2i	108	VAL	2.4
40	2i	121	ARG	2.4
6	1G	80	PHE	2.4
8	2l	85	GLU	2.4
33	1b	129	GLU	2.4
3	2D	35	LYS	2.4
7	2H	94	TYR	2.4
7	2H	161	GLY	2.4
41	2j	56	HIS	2.4
3	2D	64	ILE	2.4
48	1q	99	SER	2.4
1	2A	2148	G	2.4
39	2h	95	VAL	2.4
34	2c	162	GLN	2.4
32	2a	1191	A	2.4
1	2A	2175	C	2.4

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
33	1b	133	LYS	2.4
50	2s	62	ILE	2.4
38	2g	80	VAL	2.4
52	2u	16	GLY	2.4
1	2A	2159	G	2.4
7	2H	41	MET	2.4
47	1p	38	TYR	2.4
23	2l	26	ARG	2.4
35	2d	35	ARG	2.4
45	1n	14	PRO	2.4
40	1i	46	ALA	2.4
40	2i	119	ALA	2.4
41	1j	64	GLU	2.4
8	2l	35	LEU	2.4
1	2A	6	A	2.4
1	1A	2168	C	2.4
1	2A	2130	U	2.4
32	2a	1114	C	2.4
35	2d	69	GLY	2.4
40	2i	30	GLY	2.4
44	2m	95	GLY	2.4
52	1u	16	GLY	2.4
42	2k	126	ARG	2.4
52	2u	12	LYS	2.4
32	1a	1001(A)	G	2.4
34	2c	149	ALA	2.4
36	1e	134	ALA	2.4
39	2h	112	LEU	2.4
40	2i	124	GLN	2.4
43	2l	10	LEU	2.4
9	2N	81	GLY	2.4
24	22	63	VAL	2.4
35	1d	166	LYS	2.4
1	1A	1150	C	2.4
1	1A	2183	C	2.4
52	2u	18	TYR	2.4
25	23	12	PRO	2.4
45	2n	52	GLN	2.4
11	2P	6	LEU	2.4
27	25	14	ALA	2.4
35	1d	11	LEU	2.4
1	1A	2137	G	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
8	2I	92	VAL	2.4
31	29	25	VAL	2.4
35	1d	50	ARG	2.4
40	2i	104	ARG	2.4
32	1a	841	U	2.3
32	1a	1035	A	2.3
22	20	75	LEU	2.3
36	2e	31	LEU	2.3
38	2g	82	GLY	2.3
34	1c	8	ILE	2.3
40	1i	111	ARG	2.3
4	2E	151	TYR	2.3
53	2y	71	TYR	2.3
35	2d	162	LEU	2.3
32	2a	1066	C	2.3
32	2a	1357	A	2.3
40	2i	26	VAL	2.3
53	2y	49	VAL	2.3
47	2p	48	TRP	2.3
39	1h	98	LYS	2.3
44	2m	65	LYS	2.3
51	2t	14	LYS	2.3
8	2I	1	MET	2.3
20	2Y	32	PRO	2.3
32	1a	1026	G	2.3
34	2c	178	LEU	2.3
41	2j	61	GLU	2.3
41	1j	43	ARG	2.3
52	2u	11	GLY	2.3
18	2W	12	ILE	2.3
39	2h	111	ILE	2.3
7	2H	114	VAL	2.3
35	2d	105	VAL	2.3
40	1i	14	VAL	2.3
6	2G	49	ASP	2.3
16	2U	18	LEU	2.3
30	18	60	LEU	2.3
43	1l	63	GLY	2.3
50	2s	84	GLY	2.3
52	2u	9	ARG	2.3
3	2D	156	ALA	2.3
24	12	13	ALA	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
40	1i	125	TYR	2.3
35	2d	161	ASN	2.3
51	1t	75	ASN	2.3
1	2A	2157	G	2.3
32	2a	80	G	2.3
22	20	51	VAL	2.3
32	2a	1116	C	2.3
35	2d	36	ARG	2.3
35	2d	73	ARG	2.3
25	23	23	LEU	2.3
48	1q	97	SER	2.3
25	23	51	ALA	2.3
25	23	13	ILE	2.3
32	2a	1032	G	2.3
41	1j	66	ARG	2.3
52	1u	22	ARG	2.3
22	20	52	GLY	2.3
40	2i	69	GLY	2.3
47	1p	48	TRP	2.3
53	2y	65	GLY	2.3
15	1T	114	LEU	2.3
35	2d	96	LEU	2.3
49	2r	85	LEU	2.3
51	2t	72	LEU	2.3
26	24	44	THR	2.3
35	1d	4	TYR	2.3
34	2c	39	ILE	2.3
35	2d	185	PHE	2.3
39	1h	95	VAL	2.3
44	2m	108	ARG	2.3
22	10	8	GLY	2.3
33	1b	121	LEU	2.3
52	2u	23	PRO	2.3
33	2b	177	ALA	2.3
35	1d	75	PHE	2.3
40	1i	78	LYS	2.3
45	2n	11	LYS	2.3
6	2G	159	VAL	2.3
33	2b	227	GLY	2.2
19	2X	66	LEU	2.2
33	2b	69	LEU	2.2
39	1h	63	LEU	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
41	2j	85	LEU	2.2
25	23	21	ALA	2.2
1	2A	1064	C	2.2
41	1j	46	ARG	2.2
41	1j	57	LYS	2.2
50	2s	80	TYR	2.2
51	1t	83	ARG	2.2
1	2A	2173	A	2.2
17	2V	72	VAL	2.2
34	2c	152	ILE	2.2
34	2c	186	PHE	2.2
40	1i	26	VAL	2.2
26	24	46	GLN	2.2
35	2d	39	PRO	2.2
34	2c	60	ALA	2.2
34	2c	190	ARG	2.2
35	1d	49	ARG	2.2
35	2d	49	ARG	2.2
47	2p	7	ALA	2.2
33	2b	57	PHE	2.2
20	2Y	72	VAL	2.2
14	2S	31	SER	2.2
5	2F	65	TRP	2.2
8	2I	44	LEU	2.2
53	2y	24	LEU	2.2
10	2O	1	MET	2.2
33	1b	114	ARG	2.2
40	1i	128	ARG	2.2
48	1q	91	ARG	2.2
53	2y	95	ARG	2.2
20	2Y	65	ALA	2.2
40	2i	76	ALA	2.2
46	2o	25	THR	2.2
50	2s	79	THR	2.2
34	2c	201	TYR	2.2
4	1E	163	GLU	2.2
12	2Q	65	PHE	2.2
30	28	21	LYS	2.2
1	2A	2137	C	2.2
1	1A	2805	G	2.2
51	1t	73	HIS	2.2
51	2t	13	LEU	2.2

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
30	28	25	MET	2.2
49	1r	73	ALA	2.2
40	1i	7	THR	2.2
45	1n	8	GLU	2.2
17	2V	75	PHE	2.2
41	2j	11	PHE	2.2
45	2n	50	LYS	2.2
47	2p	9	PHE	2.2
19	2X	80	ILE	2.2
20	2Y	44	ILE	2.2
23	21	70	VAL	2.2
25	23	6	VAL	2.2
31	19	17	ILE	2.2
40	2i	65	VAL	2.2
29	27	41	ARG	2.2
41	2j	19	SER	2.2
20	2Y	31	LEU	2.2
50	2s	56	GLN	2.2
32	1a	1033	G	2.2
11	2P	71	VAL	2.2
20	2Y	7	VAL	2.2
33	2b	226	ARG	2.2
35	1d	203	VAL	2.2
40	1i	79	LEU	2.2
53	1y	41	LEU	2.2
23	21	83	GLU	2.2
42	2k	31	THR	2.2
53	2y	53	THR	2.2
13	2R	68	ARG	2.2
38	1g	79	ARG	2.2
26	24	56	VAL	2.2
33	2b	127	ILE	2.2
35	2d	67	ILE	2.2
1	1A	2812	A	2.2
7	2H	171	LEU	2.2
35	2d	186	LEU	2.2
43	2l	123	LYS	2.2
44	2m	115	LYS	2.2
26	14	51	ASP	2.2
41	2j	17	ASP	2.2
5	2F	42	ALA	2.2
1	2A	2109	U	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
19	1X	69	TYR	2.1
42	2k	25	TYR	2.1
48	2q	100	LYS	2.1
20	2Y	75	ILE	2.1
45	2n	33	VAL	2.1
8	2I	12	LEU	2.1
16	2U	27	LEU	2.1
36	2e	128	PRO	2.1
1	2A	2135	A	2.1
11	2P	109	GLY	2.1
40	2i	91	ASP	2.1
7	2H	106	THR	2.1
14	2S	3	ARG	2.1
47	2p	8	ARG	2.1
51	1t	67	ALA	2.1
1	2A	2804	C	2.1
12	2Q	35	VAL	2.1
31	29	26	ILE	2.1
39	1h	94	TYR	2.1
46	2o	62	GLN	2.1
48	2q	59	ILE	2.1
31	29	30	PRO	2.1
33	2b	187	LEU	2.1
45	1n	31	ARG	2.1
21	2Z	188	ALA	2.1
27	25	2	ALA	2.1
36	2e	16	THR	2.1
7	2H	167	GLU	2.1
36	2e	84	PHE	2.1
45	1n	32	SER	2.1
18	2W	95	ILE	2.1
30	28	16	ILE	2.1
36	1e	55	VAL	2.1
47	2p	33	ILE	2.1
21	2Z	200	GLY	2.1
32	2a	1150	U	2.1
40	2i	10	ARG	2.1
40	2i	67	GLY	2.1
45	1n	22	THR	2.1
52	2u	8	THR	2.1
7	2H	123	PHE	2.1
6	1G	88	ILE	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
6	2G	62	LEU	2.1
8	2I	79	ILE	2.1
14	2S	7	TYR	2.1
14	2S	17	ARG	2.1
21	2Z	125	LEU	2.1
23	2I	62	VAL	2.1
25	23	28	LEU	2.1
34	1c	80	GLY	2.1
35	2d	21	LEU	2.1
42	2k	123	LYS	2.1
53	2y	51	ASP	2.1
48	1q	28	PRO	2.1
11	2P	68	GLN	2.1
43	1l	61	THR	2.1
44	2m	106	ASN	2.1
8	2I	2	LYS	2.1
40	2i	112	LYS	2.1
43	1l	28	LYS	2.1
10	2O	62	VAL	2.1
16	2U	20	LEU	2.1
40	2i	102	LEU	2.1
41	2j	93	GLY	2.1
1	2A	2894	G	2.1
8	1I	117	GLU	2.1
18	2W	9	TYR	2.1
19	2X	89	ILE	2.1
35	1d	62	GLN	2.1
32	1a	1532	U	2.1
1	1A	2165	C	2.1
3	1D	276	LYS	2.1
17	2V	85	LYS	2.1
32	1a	1029	C	2.1
41	2j	7	LYS	2.1
11	1P	15	ARG	2.1
16	2U	31	SER	2.1
34	2c	21	ARG	2.1
36	2e	45	PHE	2.1
41	1j	60	ARG	2.1
52	1u	10	ARG	2.1
39	2h	71	GLY	2.1
8	1I	85	GLU	2.1
7	2H	24	VAL	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
26	24	50	VAL	2.1
44	2m	66	LEU	2.1
45	2n	21	TYR	2.1
32	2a	1064	G	2.1
53	1y	63	ALA	2.1
1	1A	2129	C	2.1
40	2i	72	GLY	2.1
3	2D	185	VAL	2.1
40	2i	47	LEU	2.1
35	2d	45	GLN	2.1
36	2e	11	ILE	2.1
50	2s	83	HIS	2.1
8	1l	29	TYR	2.1
43	2l	47	LYS	2.1
14	1S	13	ARG	2.1
31	29	9	ARG	2.1
52	2u	22	ARG	2.1
41	1j	59	SER	2.1
47	2p	11	SER	2.1
16	2U	43	GLY	2.1
32	1a	723	U	2.0
32	2a	1286	A	2.1
35	1d	167	GLY	2.1
41	1j	47	PHE	2.1
13	2R	18	LEU	2.0
35	1d	64	LEU	2.0
48	2q	23	VAL	2.0
50	1s	56	GLN	2.0
15	2T	111	ARG	2.0
16	1U	35	ALA	2.0
16	2U	12	ARG	2.0
45	1n	59	ALA	2.0
11	2P	30	THR	2.0
24	22	1	MET	2.0
53	2y	70	MET	2.0
36	1e	6	PHE	2.0
40	2i	50	LEU	2.0
49	2r	58	LEU	2.0
50	2s	16	LEU	2.0
1	1A	2175	G	2.0
7	2H	35	VAL	2.0
12	2Q	27	VAL	2.0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
25	23	47	VAL	2.0
32	1a	162	A	2.0
7	2H	89	ILE	2.0
33	1b	232	PRO	2.0
45	2n	18	VAL	2.0
12	2Q	5	ARG	2.0
33	2b	144	ARG	2.0
39	1h	109	ILE	2.0
12	2Q	80	GLU	2.0
4	1E	157	ALA	2.0
10	2O	51	ALA	2.0
18	2W	93	ALA	2.0
38	1g	40	ALA	2.0
33	2b	97	TRP	2.0
18	2W	82	LEU	2.0
3	2D	221	VAL	2.0
18	2W	85	VAL	2.0
23	11	68	PRO	2.0
25	23	54	VAL	2.0
36	2e	100	VAL	2.0
5	2F	64	ILE	2.0
21	1Z	197	ILE	2.0
34	2c	57	ILE	2.0
1	2A	2176	A	2.0
33	2b	27	LYS	2.0
1	2A	2123	G	2.0
3	2D	180	GLY	2.0
45	2n	32	SER	2.0
22	20	45	PHE	2.0
40	2i	59	PHE	2.0
34	2c	167	TRP	2.0
18	1W	92	ARG	2.0
23	11	46	LEU	2.0
35	2d	145	GLU	2.0
52	1u	6	ARG	2.0
6	2G	37	VAL	2.0
23	21	30	VAL	2.0
33	2b	136	VAL	2.0
40	1i	108	VAL	2.0
40	2i	41	VAL	2.0
41	2j	53	PRO	2.0
51	1t	74	LYS	2.0

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

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
1	5MU	2A	1915	21/22	0.89	0.15	76,82,88,101	0
32	5MC	2a	967	21/22	0.90	0.25	63,68,77,88	0
43	0TD	2l	92	10/11	0.92	0.28	60,65,71,95	0
1	PSU	1A	1939	20/21	0.92	0.17	62,68,77,77	0
1	PSU	2A	1917	20/21	0.92	0.13	71,78,90,90	0
32	2MG	2a	1207	24/25	0.92	0.15	76,86,91,102	0
32	M2G	2a	966	25/26	0.93	0.22	57,67,81,92	0
1	5MU	1A	1937	21/22	0.93	0.17	67,74,83,94	0
1	PSU	2A	1911	20/21	0.93	0.13	56,70,76,78	0
1	4OC	2A	1920	21/23	0.94	0.17	61,65,72,73	0
43	0TD	1l	92	10/11	0.94	0.23	50,54,59,76	0
32	PSU	2a	516	20/21	0.94	0.16	71,76,80,84	0
32	7MG	2a	527	24/25	0.95	0.18	61,67,73,74	0
1	PSU	1A	1933	20/21	0.95	0.15	55,62,65,66	0
32	PSU	1a	516	20/21	0.95	0.17	56,60,64,65	0
32	5MC	2a	1404	21/22	0.95	0.21	51,60,63,66	0
32	2MG	1a	1207	24/25	0.95	0.17	56,66,69,71	0
32	4OC	2a	1402	22/23	0.95	0.20	53,63,68,71	0
32	5MC	2a	1407	21/22	0.96	0.18	50,60,64,68	0
32	5MC	1a	967	21/22	0.96	0.19	53,58,65,71	0
32	MA6	2a	1518	24/25	0.96	0.25	51,61,66,67	0
32	7MG	1a	527	24/25	0.96	0.22	42,51,54,59	0
1	4OC	1A	1942	21/23	0.97	0.21	39,54,59,60	0
1	5MC	2A	1942	21/22	0.97	0.17	36,48,53,54	0
32	5MC	2a	1400	21/22	0.97	0.29	65,70,73,74	0
32	UR3	2a	1498	21/22	0.97	0.20	52,58,63,66	0
32	UR3	1a	1498	21/22	0.97	0.19	43,46,52,60	0
1	5MU	2A	1939	21/22	0.97	0.19	29,36,41,43	0
32	M2G	1a	966	25/26	0.97	0.18	51,53,58,61	0
1	PSU	2A	2605	20/21	0.97	0.25	29,35,39,44	0
32	4OC	1a	1402	22/23	0.98	0.18	42,47,55,56	0
32	MA6	1a	1519	24/25	0.98	0.23	37,43,46,49	0
1	5MC	1A	1984	21/22	0.98	0.21	25,33,37,45	0
32	5MC	1a	1400	21/22	0.98	0.21	40,45,49,51	0
1	2MU	2A	2552	21/23	0.98	0.22	30,36,39,41	0
1	5MC	1A	1964	21/22	0.98	0.20	26,32,38,47	0
32	5MC	1a	1404	21/22	0.98	0.20	35,44,46,49	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	OMG	2A	2251	24/25	0.98	0.23	32,36,38,39	0
1	2MA	2A	2503	23/24	0.98	0.25	24,30,35,37	0
1	PSU	1A	2617	20/21	0.98	0.20	18,22,28,28	0
1	2MA	1A	2515	23/24	0.98	0.25	16,20,24,31	0
32	5MC	1a	1407	21/22	0.98	0.19	36,45,49,56	0
32	MA6	1a	1518	24/25	0.98	0.24	34,41,46,51	0
1	5MC	2A	1962	21/22	0.98	0.19	33,43,48,58	0
32	MA6	2a	1519	24/25	0.98	0.26	51,60,64,67	0
1	OMG	1A	2263	24/25	0.99	0.23	15,21,23,26	0
1	2MU	1A	2564	21/23	0.99	0.21	20,26,28,29	0
1	5MU	1A	1961	21/22	0.99	0.20	18,24,27,32	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
54	MG	2A	3219	1/1	0.40	0.21	74,74,74,74	0
54	MG	1a	1851	1/1	0.42	0.65	94,94,94,94	0
54	MG	2A	3167	1/1	0.43	0.24	74,74,74,74	0
54	MG	2B	3007	1/1	0.47	0.27	71,71,71,71	0
54	MG	1a	1840	1/1	0.48	0.20	45,45,45,45	0
54	MG	2A	3197	1/1	0.49	0.23	73,73,73,73	0
54	MG	2A	3215	1/1	0.51	0.18	73,73,73,73	0
54	MG	1a	1828	1/1	0.54	0.18	62,62,62,62	0
54	MG	2B	3015	1/1	0.56	0.19	74,74,74,74	0
54	MG	2A	3692	1/1	0.61	0.19	63,63,63,63	0
54	MG	2A	3703	1/1	0.61	0.12	81,81,81,81	0
54	MG	2a	1684	1/1	0.62	0.13	60,60,60,60	0
54	MG	1A	3191	1/1	0.62	0.26	51,51,51,51	0
54	MG	1B	211	1/1	0.63	0.18	64,64,64,64	0
54	MG	2A	3142	1/1	0.63	0.18	68,68,68,68	0
54	MG	2a	1662	1/1	0.63	0.22	67,67,67,67	0
54	MG	1B	219	1/1	0.63	0.13	46,46,46,46	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3318	1/1	0.64	0.19	78,78,78,78	0
54	MG	2A	3338	1/1	0.65	0.19	53,53,53,53	0
54	MG	20	101	1/1	0.66	0.21	75,75,75,75	0
54	MG	1a	1830	1/1	0.66	0.21	66,66,66,66	0
54	MG	2A	3189	1/1	0.67	0.21	66,66,66,66	0
54	MG	1A	3934	1/1	0.67	0.39	50,50,50,50	0
54	MG	2A	3160	1/1	0.67	0.17	63,63,63,63	0
54	MG	1a	1766	1/1	0.68	0.28	67,67,67,67	0
54	MG	1a	1684	1/1	0.68	0.19	49,49,49,49	0
54	MG	1A	3278	1/1	0.68	0.22	38,38,38,38	0
54	MG	2a	1611	1/1	0.69	0.13	62,62,62,62	0
54	MG	1A	3327	1/1	0.69	0.19	33,33,33,33	0
54	MG	2a	1645	1/1	0.69	0.17	62,62,62,62	0
54	MG	1a	1640	1/1	0.69	0.17	59,59,59,59	0
54	MG	1a	1793	1/1	0.69	0.16	63,63,63,63	0
54	MG	1A	3982	1/1	0.69	0.08	49,49,49,49	0
54	MG	2A	3567	1/1	0.70	0.18	40,40,40,40	0
54	MG	1A	3346	1/1	0.70	0.18	48,48,48,48	0
54	MG	1a	1624	1/1	0.70	0.12	60,60,60,60	0
54	MG	2A	3173	1/1	0.70	0.20	67,67,67,67	0
54	MG	1d	307	1/1	0.70	0.14	89,89,89,89	0
54	MG	2A	3206	1/1	0.70	0.45	45,45,45,45	0
54	MG	1a	1608	1/1	0.71	0.12	63,63,63,63	0
54	MG	1B	207	1/1	0.71	0.21	41,41,41,41	0
54	MG	2A	3393	1/1	0.71	0.15	55,55,55,55	0
54	MG	1A	3986	1/1	0.71	0.34	61,61,61,61	0
54	MG	1A	3804	1/1	0.71	0.12	21,21,21,21	0
54	MG	1a	1677	1/1	0.71	0.12	64,64,64,64	0
54	MG	2I	3001	1/1	0.71	0.17	71,71,71,71	0
54	MG	2A	3635	1/1	0.71	0.10	64,64,64,64	0
54	MG	1A	3921	1/1	0.71	0.41	58,58,58,58	0
54	MG	2A	3171	1/1	0.71	0.28	58,58,58,58	0
54	MG	1A	3756	1/1	0.72	0.16	57,57,57,57	0
54	MG	1A	3422	1/1	0.72	0.13	41,41,41,41	0
54	MG	1a	1797	1/1	0.72	0.22	66,66,66,66	0
54	MG	1A	3259	1/1	0.72	0.18	62,62,62,62	0
54	MG	1A	3398	1/1	0.72	0.15	26,26,26,26	0
54	MG	1y	3002	1/1	0.73	0.25	62,62,62,62	0
54	MG	2A	3184	1/1	0.73	0.22	68,68,68,68	0
54	MG	1A	3575	1/1	0.73	0.14	65,65,65,65	0
54	MG	1A	3597	1/1	0.73	0.23	62,62,62,62	0
54	MG	2a	1673	1/1	0.73	0.15	56,56,56,56	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2I	101	1/1	0.73	0.13	67,67,67,67	0
54	MG	1a	1681	1/1	0.74	0.12	60,60,60,60	0
54	MG	2A	3198	1/1	0.74	0.22	60,60,60,60	0
54	MG	1A	3805	1/1	0.74	0.12	54,54,54,54	0
54	MG	1a	1652	1/1	0.74	0.14	61,61,61,61	0
54	MG	2A	3103	1/1	0.74	0.27	66,66,66,66	0
54	MG	1F	311	1/1	0.75	0.51	45,45,45,45	0
54	MG	1A	3957	1/1	0.75	0.32	79,79,79,79	0
54	MG	2A	3676	1/1	0.75	0.13	66,66,66,66	0
54	MG	1A	3297	1/1	0.75	0.21	37,37,37,37	0
54	MG	1A	3950	1/1	0.75	0.14	80,80,80,80	0
54	MG	2Q	3002	1/1	0.75	0.10	55,55,55,55	0
54	MG	1A	3941	1/1	0.75	0.23	68,68,68,68	0
54	MG	2A	3488	1/1	0.75	0.08	62,62,62,62	0
54	MG	1A	3894	1/1	0.76	0.38	80,80,80,80	0
54	MG	2A	3175	1/1	0.76	0.20	55,55,55,55	0
54	MG	1A	3662	1/1	0.76	0.18	62,62,62,62	0
54	MG	2a	1638	1/1	0.76	0.19	60,60,60,60	0
54	MG	2A	3685	1/1	0.76	0.13	75,75,75,75	0
54	MG	2a	1742	1/1	0.76	0.25	65,65,65,65	0
54	MG	1a	1700	1/1	0.76	0.21	65,65,65,65	0
54	MG	2a	1642	1/1	0.76	0.11	58,58,58,58	0
54	MG	1a	1752	1/1	0.76	0.17	71,71,71,71	0
54	MG	1a	1680	1/1	0.76	0.14	70,70,70,70	0
54	MG	1A	3279	1/1	0.76	0.12	61,61,61,61	0
54	MG	2A	3274	1/1	0.76	0.26	53,53,53,53	0
54	MG	1a	1834	1/1	0.76	0.29	58,58,58,58	0
54	MG	1a	1843	1/1	0.77	0.09	78,78,78,78	0
54	MG	1a	1637	1/1	0.77	0.17	67,67,67,67	0
54	MG	2B	3001	1/1	0.77	0.16	68,68,68,68	0
54	MG	1a	1606	1/1	0.77	0.14	58,58,58,58	0
54	MG	1A	3702	1/1	0.77	0.16	27,27,27,27	0
54	MG	2A	3195	1/1	0.77	0.21	54,54,54,54	0
54	MG	1a	1737	1/1	0.77	0.17	62,62,62,62	0
54	MG	2A	3098	1/1	0.77	0.19	53,53,53,53	0
54	MG	2A	3166	1/1	0.77	0.15	51,51,51,51	0
54	MG	1a	1835	1/1	0.77	0.25	67,67,67,67	0
54	MG	2B	3014	1/1	0.78	0.17	71,71,71,71	0
54	MG	2a	1630	1/1	0.78	0.12	62,62,62,62	0
54	MG	1A	3744	1/1	0.78	0.13	54,54,54,54	0
54	MG	2A	3216	1/1	0.78	0.21	54,54,54,54	0
54	MG	2W	8002	1/1	0.78	0.12	59,59,59,59	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1a	1748	1/1	0.78	0.13	57,57,57,57	0
54	MG	1A	3576	1/1	0.78	0.12	43,43,43,43	0
54	MG	1A	3783	1/1	0.78	0.13	48,48,48,48	0
54	MG	2A	3177	1/1	0.78	0.15	56,56,56,56	0
54	MG	2A	3095	1/1	0.78	0.13	58,58,58,58	0
54	MG	2a	1604	1/1	0.78	0.23	58,58,58,58	0
54	MG	2A	3673	1/1	0.78	0.17	68,68,68,68	0
54	MG	2A	3405	1/1	0.78	0.17	66,66,66,66	0
54	MG	2A	3389	1/1	0.78	0.23	47,47,47,47	0
54	MG	1A	3794	1/1	0.78	0.14	53,53,53,53	0
54	MG	2A	3332	1/1	0.78	0.14	65,65,65,65	0
54	MG	1A	3473	1/1	0.79	0.10	63,63,63,63	0
54	MG	1a	1802	1/1	0.79	0.18	62,62,62,62	0
54	MG	1A	3100	1/1	0.79	0.26	39,39,39,39	0
54	MG	1D	309	1/1	0.79	0.13	52,52,52,52	0
54	MG	2A	3226	1/1	0.79	0.23	53,53,53,53	0
54	MG	1A	3835	1/1	0.79	0.12	50,50,50,50	0
54	MG	1A	3938	1/1	0.79	0.17	64,64,64,64	0
54	MG	1A	3011	1/1	0.79	0.18	47,47,47,47	0
54	MG	2A	3149	1/1	0.79	0.12	68,68,68,68	0
58	ARG	1F	314	12/12	0.79	0.23	47,65,78,79	0
54	MG	1A	3603	1/1	0.79	0.15	60,60,60,60	0
54	MG	2a	1737	1/1	0.79	0.18	60,60,60,60	0
54	MG	1a	1674	1/1	0.79	0.13	65,65,65,65	0
54	MG	1A	3189	1/1	0.79	0.42	41,41,41,41	0
54	MG	2A	3146	1/1	0.79	0.48	52,52,52,52	0
54	MG	2a	1689	1/1	0.79	0.24	62,62,62,62	0
54	MG	1a	1668	1/1	0.79	0.25	74,74,74,74	0
54	MG	2A	3694	1/1	0.79	0.27	69,69,69,69	0
54	MG	1A	3649	1/1	0.79	0.14	58,58,58,58	0
54	MG	1a	1782	1/1	0.79	0.22	61,61,61,61	0
54	MG	2A	3385	1/1	0.79	0.13	47,47,47,47	0
54	MG	1A	3383	1/1	0.79	0.13	24,24,24,24	0
54	MG	1a	1767	1/1	0.79	0.42	58,58,58,58	0
54	MG	1A	3782	1/1	0.80	0.11	41,41,41,41	0
54	MG	2A	3621	1/1	0.80	0.14	28,28,28,28	0
54	MG	1a	1824	1/1	0.80	0.20	55,55,55,55	0
54	MG	1A	3577	1/1	0.80	0.20	26,26,26,26	0
54	MG	2B	3018	1/1	0.80	0.27	76,76,76,76	0
54	MG	1y	3001	1/1	0.80	0.38	61,61,61,61	0
54	MG	1A	3159	1/1	0.80	0.19	38,38,38,38	0
54	MG	2A	3589	1/1	0.80	0.16	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
54	MG	2A	3608	1/1	0.80	0.11	40,40,40,40	0
54	MG	2A	3386	1/1	0.80	0.14	68,68,68,68	0
54	MG	2a	1613	1/1	0.80	0.17	51,51,51,51	0
54	MG	1d	301	1/1	0.80	0.11	68,68,68,68	0
54	MG	2A	3398	1/1	0.80	0.28	55,55,55,55	0
54	MG	1a	1653	1/1	0.80	0.16	60,60,60,60	0
54	MG	2A	3304	1/1	0.80	0.10	44,44,44,44	0
54	MG	1A	3870	1/1	0.80	0.11	46,46,46,46	0
54	MG	2A	3697	1/1	0.80	0.11	53,53,53,53	0
54	MG	2A	3553	1/1	0.80	0.16	56,56,56,56	0
54	MG	1A	3594	1/1	0.80	0.17	54,54,54,54	0
54	MG	1A	3602	1/1	0.81	0.20	54,54,54,54	0
54	MG	1A	3962	1/1	0.81	0.08	55,55,55,55	0
54	MG	2A	3193	1/1	0.81	0.27	47,47,47,47	0
54	MG	1a	1754	1/1	0.81	0.23	68,68,68,68	0
54	MG	2A	3355	1/1	0.81	0.23	46,46,46,46	0
54	MG	2A	3326	1/1	0.81	0.17	61,61,61,61	0
54	MG	2X	101	1/1	0.81	0.13	59,59,59,59	0
54	MG	2a	1748	1/1	0.81	0.16	52,52,52,52	0
54	MG	1a	1720	1/1	0.81	0.13	60,60,60,60	0
54	MG	2A	3330	1/1	0.81	0.17	69,69,69,69	0
54	MG	1A	3047	1/1	0.81	0.51	38,38,38,38	0
54	MG	1A	3779	1/1	0.81	0.24	48,48,48,48	0
54	MG	1A	3858	1/1	0.81	0.14	28,28,28,28	0
54	MG	2A	3188	1/1	0.81	0.14	51,51,51,51	0
54	MG	2q	201	1/1	0.81	0.18	64,64,64,64	0
54	MG	1a	1629	1/1	0.81	0.09	45,45,45,45	0
54	MG	1R	203	1/1	0.81	0.17	34,34,34,34	0
54	MG	1A	3913	1/1	0.81	0.32	61,61,61,61	0
54	MG	2a	1605	1/1	0.81	0.13	57,57,57,57	0
54	MG	1A	3187	1/1	0.81	0.39	49,49,49,49	0
54	MG	2a	1682	1/1	0.81	0.13	60,60,60,60	0
54	MG	1A	3380	1/1	0.82	0.15	29,29,29,29	0
54	MG	2A	3165	1/1	0.82	0.28	64,64,64,64	0
54	MG	1A	3138	1/1	0.82	0.19	59,59,59,59	0
54	MG	2A	3544	1/1	0.82	0.09	56,56,56,56	0
54	MG	2A	3242	1/1	0.82	0.41	63,63,63,63	0
54	MG	10	105	1/1	0.82	0.21	59,59,59,59	0
54	MG	2a	1676	1/1	0.82	0.21	68,68,68,68	0
54	MG	2a	1648	1/1	0.82	0.11	60,60,60,60	0
54	MG	2A	3449	1/1	0.82	0.09	58,58,58,58	0
54	MG	1A	3908	1/1	0.82	0.10	52,52,52,52	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1a	1701	1/1	0.82	0.20	71,71,71,71	0
54	MG	1A	3151	1/1	0.82	0.47	40,40,40,40	0
54	MG	1a	1667	1/1	0.82	0.14	50,50,50,50	0
54	MG	1A	3789	1/1	0.82	0.22	31,31,31,31	0
54	MG	1A	3271	1/1	0.82	0.15	49,49,49,49	0
54	MG	1A	3144	1/1	0.82	0.11	51,51,51,51	0
54	MG	2a	1709	1/1	0.82	0.32	48,48,48,48	0
54	MG	2a	1615	1/1	0.82	0.12	60,60,60,60	0
54	MG	2a	1602	1/1	0.82	0.12	52,52,52,52	0
54	MG	2A	3563	1/1	0.82	0.11	60,60,60,60	0
54	MG	1A	3330	1/1	0.82	0.17	15,15,15,15	0
54	MG	2A	3229	1/1	0.82	0.66	49,49,49,49	0
54	MG	1A	3637	1/1	0.82	0.38	47,47,47,47	0
54	MG	2A	3640	1/1	0.82	0.08	52,52,52,52	0
54	MG	1A	3445	1/1	0.82	0.10	21,21,21,21	0
54	MG	2a	1747	1/1	0.82	0.10	61,61,61,61	0
54	MG	2a	1623	1/1	0.82	0.12	64,64,64,64	0
54	MG	2A	3203	1/1	0.82	0.11	51,51,51,51	0
54	MG	2a	1669	1/1	0.83	0.19	63,63,63,63	0
54	MG	1a	1813	1/1	0.83	0.10	60,60,60,60	0
54	MG	1y	3004	1/1	0.83	0.28	76,76,76,76	0
54	MG	2A	3502	1/1	0.83	0.27	64,64,64,64	0
54	MG	1A	3735	1/1	0.83	0.12	32,32,32,32	0
54	MG	1A	3479	1/1	0.83	0.18	20,20,20,20	0
54	MG	1A	3635	1/1	0.83	0.12	62,62,62,62	0
54	MG	1d	303	1/1	0.83	0.20	68,68,68,68	0
54	MG	2A	3053	1/1	0.83	0.28	47,47,47,47	0
54	MG	1A	3927	1/1	0.83	0.09	42,42,42,42	0
54	MG	2a	1678	1/1	0.83	0.10	57,57,57,57	0
54	MG	1A	3836	1/1	0.83	0.13	51,51,51,51	0
54	MG	1a	1707	1/1	0.83	0.09	58,58,58,58	0
54	MG	1A	3961	1/1	0.83	0.14	38,38,38,38	0
54	MG	2A	3116	1/1	0.83	0.16	53,53,53,53	0
54	MG	2A	3569	1/1	0.83	0.19	51,51,51,51	0
54	MG	1a	1679	1/1	0.83	0.22	60,60,60,60	0
54	MG	1a	1783	1/1	0.83	0.20	64,64,64,64	0
54	MG	2A	3520	1/1	0.83	0.18	54,54,54,54	0
54	MG	1a	1686	1/1	0.83	0.23	61,61,61,61	0
54	MG	1A	3567	1/1	0.83	0.12	62,62,62,62	0
54	MG	2A	3112	1/1	0.83	0.19	44,44,44,44	0
54	MG	2A	3251	1/1	0.83	0.15	60,60,60,60	0
54	MG	2A	3548	1/1	0.83	0.15	54,54,54,54	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3341	1/1	0.83	0.15	33,33,33,33	0
54	MG	2A	3060	1/1	0.83	0.16	48,48,48,48	0
54	MG	1A	3039	1/1	0.83	0.14	56,56,56,56	0
54	MG	1a	1662	1/1	0.83	0.19	56,56,56,56	0
54	MG	1A	3194	1/1	0.83	0.21	54,54,54,54	0
54	MG	2A	3056	1/1	0.83	0.32	46,46,46,46	0
54	MG	1A	3899	1/1	0.83	0.14	51,51,51,51	0
54	MG	1a	1604	1/1	0.83	0.13	62,62,62,62	0
54	MG	2A	3194	1/1	0.83	0.16	60,60,60,60	0
54	MG	1A	3190	1/1	0.83	0.19	45,45,45,45	0
54	MG	2A	3691	1/1	0.83	0.12	64,64,64,64	0
54	MG	2A	3472	1/1	0.83	0.17	52,52,52,52	0
54	MG	2A	3619	1/1	0.83	0.15	66,66,66,66	0
54	MG	1A	3737	1/1	0.83	0.24	53,53,53,53	0
54	MG	2p	3001	1/1	0.83	0.15	61,61,61,61	0
54	MG	1N	202	1/1	0.83	0.18	56,56,56,56	0
54	MG	1a	1749	1/1	0.83	0.13	46,46,46,46	0
54	MG	2j	8001	1/1	0.84	0.24	82,82,82,82	0
54	MG	1a	1814	1/1	0.84	0.23	52,52,52,52	0
54	MG	1A	3177	1/1	0.84	0.12	51,51,51,51	0
54	MG	2A	3508	1/1	0.84	0.22	57,57,57,57	0
54	MG	1a	1846	1/1	0.84	0.15	74,74,74,74	0
54	MG	1a	1620	1/1	0.84	0.14	43,43,43,43	0
54	MG	1A	3825	1/1	0.84	0.12	45,45,45,45	0
54	MG	1A	3903	1/1	0.84	0.22	63,63,63,63	0
54	MG	1A	3854	1/1	0.84	0.15	19,19,19,19	0
54	MG	1B	202	1/1	0.84	0.23	36,36,36,36	0
54	MG	2a	1614	1/1	0.84	0.21	74,74,74,74	0
54	MG	1a	1833	1/1	0.84	0.29	60,60,60,60	0
54	MG	2A	3214	1/1	0.84	0.10	56,56,56,56	0
54	MG	2a	1656	1/1	0.84	0.08	63,63,63,63	0
54	MG	1A	3817	1/1	0.84	0.16	65,65,65,65	0
54	MG	2A	3587	1/1	0.84	0.48	44,44,44,44	0
54	MG	1B	206	1/1	0.84	0.12	45,45,45,45	0
54	MG	2A	3072	1/1	0.84	0.17	49,49,49,49	0
54	MG	1A	3499	1/1	0.84	0.40	50,50,50,50	0
54	MG	2A	3191	1/1	0.84	0.23	57,57,57,57	0
54	MG	2A	3658	1/1	0.84	0.15	34,34,34,34	0
54	MG	2A	3335	1/1	0.84	0.19	56,56,56,56	0
54	MG	1a	1612	1/1	0.84	0.11	72,72,72,72	0
54	MG	1a	1617	1/1	0.84	0.15	58,58,58,58	0
54	MG	1A	3214	1/1	0.84	0.30	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
54	MG	1A	4023	1/1	0.84	0.49	36,36,36,36	0
54	MG	1a	1704	1/1	0.84	0.18	77,77,77,77	0
54	MG	2A	3401	1/1	0.84	0.07	54,54,54,54	0
54	MG	2A	3308	1/1	0.84	0.15	48,48,48,48	0
54	MG	2A	3014	1/1	0.84	0.15	51,51,51,51	0
54	MG	2A	3428	1/1	0.84	0.15	53,53,53,53	0
54	MG	1A	3748	1/1	0.84	0.12	68,68,68,68	0
54	MG	1A	3949	1/1	0.84	0.28	68,68,68,68	0
54	MG	1A	3951	1/1	0.84	0.13	50,50,50,50	0
54	MG	2a	1700	1/1	0.84	0.21	48,48,48,48	0
54	MG	1a	1715	1/1	0.84	0.20	58,58,58,58	0
54	MG	1a	1676	1/1	0.84	0.17	46,46,46,46	0
54	MG	1A	3373	1/1	0.84	0.15	25,25,25,25	0
54	MG	2A	3202	1/1	0.84	0.09	62,62,62,62	0
54	MG	2A	3303	1/1	0.85	0.11	40,40,40,40	0
54	MG	2A	3581	1/1	0.85	0.19	39,39,39,39	0
54	MG	2A	3096	1/1	0.85	0.12	60,60,60,60	0
54	MG	1A	3056	1/1	0.85	0.12	52,52,52,52	0
54	MG	1a	1659	1/1	0.85	0.12	64,64,64,64	0
54	MG	1A	3430	1/1	0.85	0.17	38,38,38,38	0
54	MG	2A	3447	1/1	0.85	0.14	55,55,55,55	0
54	MG	2A	3552	1/1	0.85	0.10	63,63,63,63	0
54	MG	2A	3218	1/1	0.85	0.23	57,57,57,57	0
54	MG	1a	1702	1/1	0.85	0.11	52,52,52,52	0
54	MG	2A	3667	1/1	0.85	0.14	49,49,49,49	0
54	MG	1A	3887	1/1	0.85	0.06	69,69,69,69	0
54	MG	2A	3021	1/1	0.85	0.09	47,47,47,47	0
54	MG	1a	1628	1/1	0.85	0.18	49,49,49,49	0
54	MG	1A	3303	1/1	0.85	0.12	55,55,55,55	0
54	MG	2a	1631	1/1	0.85	0.09	52,52,52,52	0
54	MG	1a	1755	1/1	0.85	0.11	68,68,68,68	0
54	MG	2A	3618	1/1	0.85	0.11	50,50,50,50	0
54	MG	1U	202	1/1	0.85	0.20	48,48,48,48	0
54	MG	1A	3798	1/1	0.85	0.18	35,35,35,35	0
54	MG	2A	3273	1/1	0.85	0.15	51,51,51,51	0
54	MG	1A	3663	1/1	0.85	0.11	43,43,43,43	0
54	MG	2A	3467	1/1	0.85	0.15	79,79,79,79	0
54	MG	2D	305	1/1	0.85	0.20	53,53,53,53	0
54	MG	2A	3476	1/1	0.85	0.10	54,54,54,54	0
54	MG	2A	3486	1/1	0.85	0.15	56,56,56,56	0
54	MG	2A	3610	1/1	0.85	0.22	51,51,51,51	0
54	MG	1A	3434	1/1	0.85	0.13	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
54	MG	2A	3314	1/1	0.85	0.13	30,30,30,30	0
54	MG	1A	3209	1/1	0.85	0.18	52,52,52,52	0
54	MG	2A	3087	1/1	0.85	0.10	52,52,52,52	0
54	MG	1A	3208	1/1	0.85	0.13	53,53,53,53	0
54	MG	2A	3036	1/1	0.85	0.17	57,57,57,57	0
54	MG	2a	1729	1/1	0.85	0.12	64,64,64,64	0
54	MG	2a	1726	1/1	0.85	0.19	62,62,62,62	0
54	MG	2A	3350	1/1	0.85	0.16	31,31,31,31	0
54	MG	1A	3173	1/1	0.85	0.17	43,43,43,43	0
54	MG	2B	3013	1/1	0.85	0.16	80,80,80,80	0
54	MG	2A	3080	1/1	0.85	0.23	57,57,57,57	0
54	MG	1t	3001	1/1	0.85	0.11	52,52,52,52	0
54	MG	1A	3563	1/1	0.85	0.25	30,30,30,30	0
54	MG	1a	1810	1/1	0.85	0.16	63,63,63,63	0
54	MG	1a	1777	1/1	0.85	0.21	61,61,61,61	0
54	MG	1A	3527	1/1	0.85	0.09	51,51,51,51	0
54	MG	1A	3379	1/1	0.85	0.13	73,73,73,73	0
54	MG	2A	3170	1/1	0.85	0.28	60,60,60,60	0
54	MG	2A	3669	1/1	0.86	0.17	59,59,59,59	0
54	MG	1A	3131	1/1	0.86	0.20	48,48,48,48	0
54	MG	1a	1775	1/1	0.86	0.15	59,59,59,59	0
54	MG	1a	1817	1/1	0.86	0.15	57,57,57,57	0
54	MG	1l	3002	1/1	0.86	0.21	72,72,72,72	0
54	MG	1A	3752	1/1	0.86	0.12	55,55,55,55	0
54	MG	1A	3730	1/1	0.86	0.16	26,26,26,26	0
54	MG	2A	3430	1/1	0.86	0.12	41,41,41,41	0
54	MG	1G	3003	1/1	0.86	0.15	57,57,57,57	0
54	MG	2A	3590	1/1	0.86	0.58	58,58,58,58	0
54	MG	2A	3399	1/1	0.86	0.15	42,42,42,42	0
54	MG	1D	310	1/1	0.86	0.22	62,62,62,62	0
54	MG	1A	3488	1/1	0.86	0.09	56,56,56,56	0
54	MG	2A	3137	1/1	0.86	0.21	52,52,52,52	0
54	MG	1A	3559	1/1	0.86	0.17	55,55,55,55	0
57	MPD	2A	3710	8/8	0.86	0.40	43,49,51,57	0
54	MG	1A	3720	1/1	0.86	0.10	52,52,52,52	0
54	MG	1a	1841	1/1	0.86	0.12	57,57,57,57	0
54	MG	2A	3262	1/1	0.86	0.13	62,62,62,62	0
54	MG	1a	1855	1/1	0.86	0.07	68,68,68,68	0
54	MG	1A	3339	1/1	0.86	0.13	48,48,48,48	0
57	MPD	2B	3020	8/8	0.86	0.26	61,66,69,79	0
54	MG	2A	3147	1/1	0.86	0.68	44,44,44,44	0
54	MG	1A	3642	1/1	0.86	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
54	MG	1A	3584	1/1	0.86	0.14	51,51,51,51	0
54	MG	17	102	1/1	0.86	0.14	40,40,40,40	0
54	MG	2A	3579	1/1	0.86	0.16	65,65,65,65	0
54	MG	2a	1607	1/1	0.86	0.19	64,64,64,64	0
54	MG	2A	3672	1/1	0.86	0.19	55,55,55,55	0
54	MG	1B	204	1/1	0.86	0.18	52,52,52,52	0
54	MG	1a	1641	1/1	0.86	0.22	54,54,54,54	0
54	MG	1a	1671	1/1	0.86	0.13	60,60,60,60	0
54	MG	1a	1776	1/1	0.86	0.12	69,69,69,69	0
54	MG	2A	3321	1/1	0.86	0.13	43,43,43,43	0
54	MG	2a	1685	1/1	0.86	0.16	52,52,52,52	0
54	MG	1A	3847	1/1	0.86	0.09	39,39,39,39	0
54	MG	1A	3233	1/1	0.86	0.38	48,48,48,48	0
54	MG	1A	3953	1/1	0.86	0.15	51,51,51,51	0
54	MG	2a	1618	1/1	0.86	0.22	66,66,66,66	0
54	MG	1A	3969	1/1	0.86	0.34	45,45,45,45	0
54	MG	1A	3799	1/1	0.86	0.17	46,46,46,46	0
54	MG	2a	1704	1/1	0.86	0.28	63,63,63,63	0
54	MG	1A	3082	1/1	0.86	0.14	55,55,55,55	0
54	MG	1A	3901	1/1	0.86	0.14	37,37,37,37	0
54	MG	2A	3521	1/1	0.86	0.19	51,51,51,51	0
54	MG	2A	3493	1/1	0.86	0.10	55,55,55,55	0
54	MG	2A	3675	1/1	0.86	0.11	73,73,73,73	0
54	MG	2A	3183	1/1	0.86	0.32	53,53,53,53	0
54	MG	2a	1663	1/1	0.86	0.12	48,48,48,48	0
54	MG	1a	1780	1/1	0.86	0.25	60,60,60,60	0
54	MG	1B	224	1/1	0.86	0.15	43,43,43,43	0
54	MG	1a	1794	1/1	0.86	0.10	67,67,67,67	0
54	MG	1A	3875	1/1	0.86	0.31	49,49,49,49	0
54	MG	2A	3126	1/1	0.86	0.22	42,42,42,42	0
54	MG	1A	3867	1/1	0.86	0.12	47,47,47,47	0
54	MG	2a	1627	1/1	0.86	0.09	61,61,61,61	0
54	MG	2a	1675	1/1	0.87	0.12	56,56,56,56	0
54	MG	2A	3448	1/1	0.87	0.07	47,47,47,47	0
54	MG	2A	3510	1/1	0.87	0.21	64,64,64,64	0
54	MG	2A	3651	1/1	0.87	0.11	58,58,58,58	0
54	MG	2A	3684	1/1	0.87	0.15	65,65,65,65	0
54	MG	2A	3368	1/1	0.87	0.15	30,30,30,30	0
54	MG	2a	1603	1/1	0.87	0.12	57,57,57,57	0
54	MG	28	8003	1/1	0.87	0.19	56,56,56,56	0
54	MG	1A	3670	1/1	0.87	0.18	25,25,25,25	0
54	MG	2A	3068	1/1	0.87	0.44	59,59,59,59	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3466	1/1	0.87	0.14	68,68,68,68	0
54	MG	1A	3937	1/1	0.87	0.15	74,74,74,74	0
54	MG	1A	3280	1/1	0.87	0.17	44,44,44,44	0
54	MG	2A	3071	1/1	0.87	0.31	46,46,46,46	0
54	MG	2A	3252	1/1	0.87	0.23	61,61,61,61	0
54	MG	2A	3477	1/1	0.87	0.34	59,59,59,59	0
54	MG	2A	3547	1/1	0.87	0.13	38,38,38,38	0
54	MG	1A	3906	1/1	0.87	0.19	55,55,55,55	0
54	MG	1A	3755	1/1	0.87	0.10	47,47,47,47	0
54	MG	1A	3120	1/1	0.87	0.17	44,44,44,44	0
54	MG	1G	3002	1/1	0.87	0.13	66,66,66,66	0
54	MG	1a	1658	1/1	0.87	0.15	46,46,46,46	0
54	MG	1A	3291	1/1	0.87	0.17	45,45,45,45	0
54	MG	2a	1694	1/1	0.87	0.20	60,60,60,60	0
54	MG	2a	1716	1/1	0.87	0.25	57,57,57,57	0
54	MG	2A	3397	1/1	0.87	0.35	55,55,55,55	0
54	MG	1a	1832	1/1	0.87	0.10	42,42,42,42	0
54	MG	1D	302	1/1	0.87	0.42	42,42,42,42	0
54	MG	1A	3182	1/1	0.87	0.15	43,43,43,43	0
54	MG	2P	202	1/1	0.87	0.24	59,59,59,59	0
54	MG	2A	3010	1/1	0.87	0.26	54,54,54,54	0
54	MG	2A	3659	1/1	0.87	0.41	49,49,49,49	0
54	MG	1A	3866	1/1	0.87	0.10	35,35,35,35	0
54	MG	1A	3031	1/1	0.87	0.25	39,39,39,39	0
54	MG	2A	3629	1/1	0.87	0.11	51,51,51,51	0
54	MG	2A	3370	1/1	0.87	0.10	70,70,70,70	0
54	MG	2A	3305	1/1	0.87	0.16	26,26,26,26	0
54	MG	1a	1773	1/1	0.87	0.24	61,61,61,61	0
54	MG	1A	3440	1/1	0.87	0.17	18,18,18,18	0
54	MG	1A	3252	1/1	0.87	0.12	52,52,52,52	0
54	MG	2a	1681	1/1	0.87	0.19	57,57,57,57	0
54	MG	2a	1683	1/1	0.87	0.18	57,57,57,57	0
54	MG	1A	3832	1/1	0.87	0.13	57,57,57,57	0
54	MG	2a	1651	1/1	0.87	0.19	58,58,58,58	0
54	MG	1A	3354	1/1	0.87	0.14	20,20,20,20	0
54	MG	28	8002	1/1	0.87	0.09	45,45,45,45	0
54	MG	1a	1633	1/1	0.87	0.16	37,37,37,37	0
54	MG	1H	8001	1/1	0.87	0.16	67,67,67,67	0
54	MG	2A	3285	1/1	0.87	0.16	65,65,65,65	0
54	MG	1E	305	1/1	0.87	0.15	50,50,50,50	0
54	MG	2A	3231	1/1	0.87	0.10	42,42,42,42	0
54	MG	1A	3943	1/1	0.87	0.20	52,52,52,52	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3078	1/1	0.87	0.08	63,63,63,63	0
54	MG	2a	1639	1/1	0.87	0.28	54,54,54,54	0
54	MG	2A	3599	1/1	0.87	0.15	45,45,45,45	0
54	MG	2a	1749	1/1	0.87	0.27	64,64,64,64	0
54	MG	2A	3148	1/1	0.87	0.74	57,57,57,57	0
54	MG	1A	3361	1/1	0.87	0.19	27,27,27,27	0
54	MG	1A	3757	1/1	0.87	0.11	48,48,48,48	0
54	MG	1A	3675	1/1	0.87	0.16	54,54,54,54	0
54	MG	1a	1649	1/1	0.87	0.43	41,41,41,41	0
54	MG	1A	4017	1/1	0.87	0.20	34,34,34,34	0
54	MG	1A	3158	1/1	0.87	0.23	41,41,41,41	0
54	MG	2A	3172	1/1	0.87	0.22	56,56,56,56	0
54	MG	1A	3043	1/1	0.87	0.25	52,52,52,52	0
54	MG	2A	3545	1/1	0.87	0.12	53,53,53,53	0
54	MG	1a	1650	1/1	0.87	0.22	62,62,62,62	0
54	MG	1a	1805	1/1	0.87	0.11	52,52,52,52	0
54	MG	2A	3421	1/1	0.87	0.11	62,62,62,62	0
54	MG	1A	3665	1/1	0.87	0.09	32,32,32,32	0
54	MG	1A	3342	1/1	0.87	0.10	48,48,48,48	0
54	MG	1A	3519	1/1	0.87	0.10	38,38,38,38	0
54	MG	1A	3095	1/1	0.87	0.19	49,49,49,49	0
54	MG	2A	3683	1/1	0.87	0.09	73,73,73,73	0
54	MG	1f	3002	1/1	0.87	0.14	53,53,53,53	0
54	MG	2A	3721	1/1	0.88	0.09	42,42,42,42	0
54	MG	1A	3550	1/1	0.88	0.19	53,53,53,53	0
54	MG	1A	3672	1/1	0.88	0.10	40,40,40,40	0
54	MG	2A	3562	1/1	0.88	0.09	63,63,63,63	0
54	MG	2A	3134	1/1	0.88	0.14	36,36,36,36	0
54	MG	1X	101	1/1	0.88	0.19	52,52,52,52	0
54	MG	1A	3324	1/1	0.88	0.20	39,39,39,39	0
54	MG	1A	3242	1/1	0.88	0.16	53,53,53,53	0
54	MG	2A	3124	1/1	0.88	0.27	54,54,54,54	0
54	MG	2a	1695	1/1	0.88	0.16	62,62,62,62	0
54	MG	2a	1641	1/1	0.88	0.25	66,66,66,66	0
54	MG	2A	3029	1/1	0.88	0.19	55,55,55,55	0
54	MG	2G	3003	1/1	0.88	0.17	79,79,79,79	0
54	MG	1a	1816	1/1	0.88	0.17	52,52,52,52	0
54	MG	2A	3423	1/1	0.88	0.13	45,45,45,45	0
54	MG	2A	3192	1/1	0.88	0.19	52,52,52,52	0
54	MG	1A	3618	1/1	0.88	0.13	42,42,42,42	0
54	MG	2a	1632	1/1	0.88	0.20	59,59,59,59	0
54	MG	1A	4010	1/1	0.88	0.74	31,31,31,31	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3106	1/1	0.88	0.22	46,46,46,46	0
54	MG	2f	3001	1/1	0.88	0.15	44,44,44,44	0
54	MG	2A	3662	1/1	0.88	0.13	56,56,56,56	0
54	MG	1A	3402	1/1	0.88	0.14	50,50,50,50	0
54	MG	1A	3055	1/1	0.88	0.12	45,45,45,45	0
54	MG	2a	1667	1/1	0.88	0.27	56,56,56,56	0
54	MG	1A	3355	1/1	0.88	0.14	33,33,33,33	0
54	MG	1P	202	1/1	0.88	0.12	66,66,66,66	0
54	MG	2A	3648	1/1	0.88	0.08	73,73,73,73	0
54	MG	1a	1842	1/1	0.88	0.11	51,51,51,51	0
54	MG	2A	3540	1/1	0.88	0.23	37,37,37,37	0
54	MG	2A	3111	1/1	0.88	0.13	66,66,66,66	0
54	MG	1a	1627	1/1	0.88	0.14	54,54,54,54	0
54	MG	1a	1791	1/1	0.88	0.08	60,60,60,60	0
54	MG	1A	3964	1/1	0.88	0.75	36,36,36,36	0
54	MG	1a	1808	1/1	0.88	0.19	74,74,74,74	0
54	MG	2A	3481	1/1	0.88	0.46	46,46,46,46	0
54	MG	1A	3619	1/1	0.88	0.42	25,25,25,25	0
54	MG	1a	1635	1/1	0.88	0.19	34,34,34,34	0
54	MG	2A	3408	1/1	0.88	0.14	54,54,54,54	0
54	MG	1A	3093	1/1	0.88	0.20	38,38,38,38	0
54	MG	2A	3412	1/1	0.88	0.18	61,61,61,61	0
54	MG	2a	1644	1/1	0.88	0.25	55,55,55,55	0
54	MG	2A	3632	1/1	0.88	0.11	49,49,49,49	0
54	MG	2a	1745	1/1	0.88	0.19	67,67,67,67	0
54	MG	1A	3935	1/1	0.88	0.09	55,55,55,55	0
54	MG	1A	3572	1/1	0.88	0.56	46,46,46,46	0
54	MG	1a	1729	1/1	0.88	0.25	60,60,60,60	0
54	MG	1a	1631	1/1	0.88	0.26	64,64,64,64	0
54	MG	1A	3332	1/1	0.88	0.14	60,60,60,60	0
54	MG	2A	3041	1/1	0.88	0.16	54,54,54,54	0
54	MG	2A	3602	1/1	0.88	0.15	46,46,46,46	0
54	MG	1A	3448	1/1	0.88	0.15	24,24,24,24	0
54	MG	1A	3274	1/1	0.88	0.13	40,40,40,40	0
54	MG	1A	3917	1/1	0.88	0.12	51,51,51,51	0
54	MG	1A	3258	1/1	0.88	0.24	32,32,32,32	0
54	MG	2A	3081	1/1	0.88	0.11	55,55,55,55	0
54	MG	2A	3695	1/1	0.88	0.15	36,36,36,36	0
54	MG	1A	3394	1/1	0.88	0.15	18,18,18,18	0
54	MG	1A	3181	1/1	0.88	0.17	57,57,57,57	0
54	MG	1F	310	1/1	0.88	0.11	42,42,42,42	0
54	MG	1a	1731	1/1	0.88	0.24	56,56,56,56	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1D	307	1/1	0.88	0.18	40,40,40,40	0
54	MG	1a	1742	1/1	0.89	0.25	62,62,62,62	0
54	MG	1A	4007	1/1	0.89	0.33	23,23,23,23	0
54	MG	1A	3404	1/1	0.89	0.19	65,65,65,65	0
54	MG	1A	3705	1/1	0.89	0.17	48,48,48,48	0
54	MG	1A	3399	1/1	0.89	0.16	33,33,33,33	0
54	MG	2A	3375	1/1	0.89	0.15	64,64,64,64	0
54	MG	1a	1743	1/1	0.89	0.11	62,62,62,62	0
54	MG	1A	3124	1/1	0.89	0.20	40,40,40,40	0
54	MG	2A	3301	1/1	0.89	0.10	56,56,56,56	0
54	MG	1G	3001	1/1	0.89	0.15	52,52,52,52	0
54	MG	2a	1601	1/1	0.89	0.17	48,48,48,48	0
54	MG	2A	3538	1/1	0.89	0.11	35,35,35,35	0
59	ZN	2Y	501	1/1	0.89	0.12	79,79,79,79	0
54	MG	1A	3500	1/1	0.89	0.17	44,44,44,44	0
54	MG	1A	3161	1/1	0.89	0.16	34,34,34,34	0
54	MG	2a	1693	1/1	0.89	0.14	55,55,55,55	0
54	MG	2D	307	1/1	0.89	0.50	43,43,43,43	0
54	MG	1A	3708	1/1	0.89	0.10	37,37,37,37	0
54	MG	2A	3450	1/1	0.89	0.11	55,55,55,55	0
54	MG	2B	3010	1/1	0.89	0.14	68,68,68,68	0
54	MG	1U	201	1/1	0.89	0.37	38,38,38,38	0
54	MG	2A	3687	1/1	0.89	0.14	64,64,64,64	0
54	MG	1A	3611	1/1	0.89	0.12	41,41,41,41	0
54	MG	1A	3690	1/1	0.89	0.14	46,46,46,46	0
54	MG	2A	3258	1/1	0.89	0.11	36,36,36,36	0
54	MG	1n	502	1/1	0.89	0.12	51,51,51,51	0
54	MG	2A	3019	1/1	0.89	0.17	56,56,56,56	0
54	MG	2A	3016	1/1	0.89	0.62	37,37,37,37	0
54	MG	1a	1781	1/1	0.89	0.19	58,58,58,58	0
54	MG	1A	3958	1/1	0.89	0.20	53,53,53,53	0
54	MG	2a	1680	1/1	0.89	0.09	58,58,58,58	0
54	MG	1A	3820	1/1	0.89	0.14	50,50,50,50	0
54	MG	2A	3524	1/1	0.89	0.21	26,26,26,26	0
54	MG	2A	3044	1/1	0.89	0.17	46,46,46,46	0
54	MG	1A	3749	1/1	0.89	0.19	36,36,36,36	0
54	MG	2D	301	1/1	0.89	0.10	56,56,56,56	0
54	MG	19	502	1/1	0.89	0.21	50,50,50,50	0
54	MG	2A	3245	1/1	0.89	0.20	60,60,60,60	0
54	MG	2A	3196	1/1	0.89	0.12	50,50,50,50	0
54	MG	2A	3055	1/1	0.89	0.14	38,38,38,38	0
54	MG	1o	3001	1/1	0.89	0.18	44,44,44,44	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3220	1/1	0.89	0.40	31,31,31,31	0
54	MG	2A	3287	1/1	0.89	0.17	42,42,42,42	0
54	MG	1A	3253	1/1	0.89	0.17	59,59,59,59	0
54	MG	2A	3205	1/1	0.89	0.18	60,60,60,60	0
54	MG	1A	3205	1/1	0.89	0.11	42,42,42,42	0
54	MG	1A	3530	1/1	0.89	0.12	44,44,44,44	0
54	MG	1A	3526	1/1	0.89	0.08	40,40,40,40	0
54	MG	1a	1619	1/1	0.89	0.13	54,54,54,54	0
54	MG	1A	3123	1/1	0.89	0.11	32,32,32,32	0
54	MG	2a	1746	1/1	0.89	0.18	60,60,60,60	0
54	MG	2A	3296	1/1	0.89	0.10	36,36,36,36	0
54	MG	1h	3002	1/1	0.89	0.15	64,64,64,64	0
54	MG	1A	3122	1/1	0.89	0.13	32,32,32,32	0
54	MG	2A	3633	1/1	0.89	0.10	43,43,43,43	0
54	MG	2A	3463	1/1	0.89	0.14	62,62,62,62	0
54	MG	1A	3030	1/1	0.89	0.09	54,54,54,54	0
54	MG	1A	3010	1/1	0.89	0.12	38,38,38,38	0
54	MG	2A	3230	1/1	0.89	0.30	55,55,55,55	0
54	MG	1A	3936	1/1	0.89	0.36	33,33,33,33	0
54	MG	1A	3679	1/1	0.89	0.29	52,52,52,52	0
54	MG	1A	3484	1/1	0.89	0.12	35,35,35,35	0
54	MG	1a	1622	1/1	0.89	0.11	51,51,51,51	0
54	MG	1A	3703	1/1	0.89	0.36	47,47,47,47	0
54	MG	2A	3348	1/1	0.89	0.19	42,42,42,42	0
54	MG	1B	229	1/1	0.89	0.11	41,41,41,41	0
54	MG	2A	3280	1/1	0.89	0.11	58,58,58,58	0
54	MG	2a	1649	1/1	0.89	0.16	49,49,49,49	0
54	MG	1a	1844	1/1	0.89	0.19	58,58,58,58	0
54	MG	1S	8001	1/1	0.89	0.12	62,62,62,62	0
54	MG	1A	3718	1/1	0.89	0.13	26,26,26,26	0
54	MG	2A	3468	1/1	0.89	0.16	61,61,61,61	0
54	MG	2A	3384	1/1	0.89	0.39	38,38,38,38	0
54	MG	1A	3654	1/1	0.89	0.48	42,42,42,42	0
54	MG	2A	3594	1/1	0.89	0.25	60,60,60,60	0
54	MG	2A	3156	1/1	0.89	0.12	41,41,41,41	0
54	MG	2A	3200	1/1	0.89	0.12	45,45,45,45	0
54	MG	1A	3241	1/1	0.89	0.15	43,43,43,43	0
54	MG	1A	3184	1/1	0.89	0.13	50,50,50,50	0
54	MG	1A	3810	1/1	0.89	0.09	37,37,37,37	0
54	MG	2e	3001	1/1	0.89	0.32	58,58,58,58	0
54	MG	2A	3593	1/1	0.89	0.07	53,53,53,53	0
54	MG	1A	3666	1/1	0.90	0.10	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
54	MG	1A	3573	1/1	0.90	0.70	52,52,52,52	0
54	MG	2a	1661	1/1	0.90	0.41	54,54,54,54	0
54	MG	1A	3301	1/1	0.90	0.20	27,27,27,27	0
54	MG	1A	3070	1/1	0.90	0.17	42,42,42,42	0
54	MG	2A	3058	1/1	0.90	0.21	51,51,51,51	0
54	MG	1A	3610	1/1	0.90	0.14	27,27,27,27	0
54	MG	1a	1778	1/1	0.90	0.15	60,60,60,60	0
54	MG	2A	3483	1/1	0.90	0.13	61,61,61,61	0
54	MG	1A	3071	1/1	0.90	0.49	29,29,29,29	0
54	MG	2A	3671	1/1	0.90	0.13	56,56,56,56	0
54	MG	2Q	3001	1/1	0.90	0.06	61,61,61,61	0
54	MG	2D	303	1/1	0.90	0.52	40,40,40,40	0
54	MG	1A	3928	1/1	0.90	0.12	27,27,27,27	0
54	MG	2A	3613	1/1	0.90	0.18	57,57,57,57	0
54	MG	1a	1673	1/1	0.90	0.35	55,55,55,55	0
54	MG	1A	3784	1/1	0.90	0.11	42,42,42,42	0
54	MG	1A	3534	1/1	0.90	0.15	60,60,60,60	0
54	MG	2A	3504	1/1	0.90	0.10	60,60,60,60	0
54	MG	1A	3781	1/1	0.90	0.07	40,40,40,40	0
54	MG	2A	3317	1/1	0.90	0.11	33,33,33,33	0
54	MG	2a	1720	1/1	0.90	0.18	50,50,50,50	0
54	MG	2a	1621	1/1	0.90	0.14	68,68,68,68	0
54	MG	1A	3696	1/1	0.90	0.16	52,52,52,52	0
54	MG	1A	3077	1/1	0.90	0.41	28,28,28,28	0
54	MG	2G	3002	1/1	0.90	0.16	65,65,65,65	0
54	MG	2B	3004	1/1	0.90	0.12	58,58,58,58	0
54	MG	2A	3457	1/1	0.90	0.13	54,54,54,54	0
54	MG	1A	3415	1/1	0.90	0.08	47,47,47,47	0
54	MG	1A	3751	1/1	0.90	0.31	55,55,55,55	0
54	MG	1A	3704	1/1	0.90	0.12	50,50,50,50	0
54	MG	1a	1806	1/1	0.90	0.20	53,53,53,53	0
54	MG	1A	3004	1/1	0.90	0.23	43,43,43,43	0
54	MG	1A	3256	1/1	0.90	0.15	51,51,51,51	0
54	MG	1A	3347	1/1	0.90	0.12	36,36,36,36	0
54	MG	2a	1672	1/1	0.90	0.13	62,62,62,62	0
54	MG	1a	1819	1/1	0.90	0.20	51,51,51,51	0
54	MG	1A	3079	1/1	0.90	0.63	30,30,30,30	0
54	MG	1a	1837	1/1	0.90	0.16	44,44,44,44	0
54	MG	1B	230	1/1	0.90	0.13	68,68,68,68	0
54	MG	1B	225	1/1	0.90	0.10	40,40,40,40	0
54	MG	2A	3065	1/1	0.90	0.41	49,49,49,49	0
54	MG	1A	3574	1/1	0.90	0.16	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
54	MG	15	102	1/1	0.90	0.27	42,42,42,42	0
54	MG	1A	3391	1/1	0.90	0.23	37,37,37,37	0
54	MG	2A	3720	1/1	0.90	0.10	44,44,44,44	0
54	MG	1A	3678	1/1	0.90	0.16	40,40,40,40	0
54	MG	1a	1818	1/1	0.90	0.16	62,62,62,62	0
54	MG	2A	3462	1/1	0.90	0.12	53,53,53,53	0
54	MG	1A	3615	1/1	0.90	0.18	50,50,50,50	0
54	MG	2A	3482	1/1	0.90	0.16	51,51,51,51	0
54	MG	2A	3182	1/1	0.90	0.16	53,53,53,53	0
54	MG	1A	3102	1/1	0.90	0.16	53,53,53,53	0
54	MG	2A	3244	1/1	0.90	1.30	44,44,44,44	0
54	MG	1A	3952	1/1	0.90	0.09	46,46,46,46	0
54	MG	1A	3713	1/1	0.90	0.31	49,49,49,49	0
54	MG	2A	3454	1/1	0.90	0.14	70,70,70,70	0
54	MG	1A	3426	1/1	0.90	0.20	14,14,14,14	0
54	MG	1d	304	1/1	0.90	0.12	56,56,56,56	0
54	MG	2A	3123	1/1	0.90	0.17	49,49,49,49	0
54	MG	2D	308	1/1	0.90	0.14	27,27,27,27	0
54	MG	2A	3406	1/1	0.90	0.14	54,54,54,54	0
54	MG	2A	3236	1/1	0.90	0.12	61,61,61,61	0
54	MG	2A	3063	1/1	0.90	0.47	58,58,58,58	0
54	MG	2A	3250	1/1	0.90	0.14	46,46,46,46	0
54	MG	2A	3143	1/1	0.90	0.08	41,41,41,41	0
54	MG	2F	301	1/1	0.90	0.16	39,39,39,39	0
54	MG	1A	3085	1/1	0.90	0.09	36,36,36,36	0
54	MG	1A	3449	1/1	0.90	0.17	17,17,17,17	0
54	MG	2A	3597	1/1	0.90	0.32	61,61,61,61	0
54	MG	1A	3283	1/1	0.90	0.15	32,32,32,32	0
54	MG	1A	3021	1/1	0.90	0.25	38,38,38,38	0
54	MG	1A	3528	1/1	0.90	0.13	43,43,43,43	0
54	MG	2A	3105	1/1	0.90	0.49	46,46,46,46	0
54	MG	11	103	1/1	0.90	0.10	42,42,42,42	0
54	MG	1a	1779	1/1	0.90	0.13	58,58,58,58	0
54	MG	2A	3555	1/1	0.90	0.14	61,61,61,61	0
54	MG	1A	3286	1/1	0.90	0.33	56,56,56,56	0
54	MG	1A	3659	1/1	0.90	0.53	52,52,52,52	0
54	MG	2A	3469	1/1	0.90	0.07	61,61,61,61	0
54	MG	2A	3109	1/1	0.90	0.49	39,39,39,39	0
54	MG	1a	1703	1/1	0.90	0.16	60,60,60,60	0
54	MG	1a	1726	1/1	0.90	0.19	62,62,62,62	0
54	MG	1A	3582	1/1	0.90	0.19	41,41,41,41	0
54	MG	1a	1718	1/1	0.90	0.10	56,56,56,56	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1B	221	1/1	0.90	0.18	34,34,34,34	0
54	MG	1A	3050	1/1	0.90	0.34	27,27,27,27	0
54	MG	1A	3558	1/1	0.90	0.10	34,34,34,34	0
54	MG	1y	3003	1/1	0.90	0.17	74,74,74,74	0
54	MG	2A	3519	1/1	0.90	0.15	54,54,54,54	0
54	MG	2A	3607	1/1	0.90	0.16	62,62,62,62	0
54	MG	1a	1697	1/1	0.90	0.13	51,51,51,51	0
54	MG	2A	3290	1/1	0.90	0.15	30,30,30,30	0
54	MG	2A	3644	1/1	0.90	0.15	48,48,48,48	0
54	MG	1A	3363	1/1	0.90	0.15	28,28,28,28	0
54	MG	2a	1608	1/1	0.90	0.14	62,62,62,62	0
54	MG	1B	217	1/1	0.90	0.37	61,61,61,61	0
54	MG	1a	1744	1/1	0.90	0.26	62,62,62,62	0
54	MG	2A	3220	1/1	0.90	0.14	58,58,58,58	0
54	MG	2A	3512	1/1	0.90	0.14	51,51,51,51	0
54	MG	1a	1845	1/1	0.90	0.16	78,78,78,78	0
54	MG	1N	203	1/1	0.90	0.09	53,53,53,53	0
54	MG	1a	1751	1/1	0.90	0.19	69,69,69,69	0
54	MG	2A	3088	1/1	0.90	0.10	56,56,56,56	0
54	MG	2A	3199	1/1	0.90	0.26	47,47,47,47	0
54	MG	1a	1626	1/1	0.90	0.22	59,59,59,59	0
54	MG	1A	3955	1/1	0.90	0.10	39,39,39,39	0
54	MG	2A	3656	1/1	0.90	0.21	48,48,48,48	0
54	MG	1d	305	1/1	0.90	0.19	56,56,56,56	0
54	MG	2A	3478	1/1	0.91	0.11	36,36,36,36	0
54	MG	1A	3296	1/1	0.91	0.14	19,19,19,19	0
54	MG	1A	3667	1/1	0.91	0.13	40,40,40,40	0
54	MG	1A	3411	1/1	0.91	0.12	46,46,46,46	0
54	MG	2A	3224	1/1	0.91	0.63	35,35,35,35	0
54	MG	1A	3532	1/1	0.91	0.17	17,17,17,17	0
54	MG	1A	3213	1/1	0.91	0.20	33,33,33,33	0
54	MG	2a	1617	1/1	0.91	0.19	43,43,43,43	0
54	MG	1F	313	1/1	0.91	0.10	31,31,31,31	0
54	MG	1A	3302	1/1	0.91	0.16	27,27,27,27	0
54	MG	1A	3548	1/1	0.91	0.15	34,34,34,34	0
54	MG	2A	3077	1/1	0.91	0.17	32,32,32,32	0
54	MG	2A	3682	1/1	0.91	0.10	51,51,51,51	0
54	MG	1a	1853	1/1	0.91	0.18	47,47,47,47	0
54	MG	1a	1772	1/1	0.91	0.19	57,57,57,57	0
54	MG	1A	3688	1/1	0.91	0.20	34,34,34,34	0
54	MG	1T	201	1/1	0.91	0.14	54,54,54,54	0
54	MG	2A	3358	1/1	0.91	0.17	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
54	MG	1I	102	1/1	0.91	0.18	47,47,47,47	0
54	MG	2A	3291	1/1	0.91	0.10	47,47,47,47	0
54	MG	2A	3179	1/1	0.91	0.08	65,65,65,65	0
54	MG	2A	3249	1/1	0.91	0.14	45,45,45,45	0
54	MG	1A	3543	1/1	0.91	0.24	44,44,44,44	0
54	MG	1a	1613	1/1	0.91	0.15	60,60,60,60	0
54	MG	2A	3043	1/1	0.91	0.11	68,68,68,68	0
54	MG	2A	3284	1/1	0.91	0.18	55,55,55,55	0
54	MG	2A	3554	1/1	0.91	0.09	49,49,49,49	0
54	MG	2A	3528	1/1	0.91	0.20	32,32,32,32	0
54	MG	2A	3666	1/1	0.91	0.17	51,51,51,51	0
54	MG	2A	3374	1/1	0.91	0.10	26,26,26,26	0
54	MG	2A	3507	1/1	0.91	0.17	54,54,54,54	0
54	MG	1A	3522	1/1	0.91	0.14	38,38,38,38	0
54	MG	1A	3857	1/1	0.91	0.12	26,26,26,26	0
54	MG	2A	3413	1/1	0.91	0.14	63,63,63,63	0
54	MG	2A	3328	1/1	0.91	0.15	56,56,56,56	0
54	MG	1A	3565	1/1	0.91	0.21	36,36,36,36	0
54	MG	1A	3721	1/1	0.91	0.19	25,25,25,25	0
54	MG	1A	3160	1/1	0.91	0.10	41,41,41,41	0
54	MG	1A	3686	1/1	0.91	0.18	32,32,32,32	0
54	MG	1a	1639	1/1	0.91	0.20	49,49,49,49	0
54	MG	1A	3251	1/1	0.91	0.29	23,23,23,23	0
54	MG	1A	3167	1/1	0.91	0.47	28,28,28,28	0
54	MG	1A	3946	1/1	0.91	0.09	44,44,44,44	0
54	MG	1A	3436	1/1	0.91	0.09	41,41,41,41	0
54	MG	2A	3660	1/1	0.91	0.17	61,61,61,61	0
54	MG	2A	3551	1/1	0.91	0.12	61,61,61,61	0
54	MG	1P	203	1/1	0.91	0.07	29,29,29,29	0
54	MG	1A	3878	1/1	0.91	0.32	57,57,57,57	0
54	MG	1A	3485	1/1	0.91	0.07	47,47,47,47	0
54	MG	1A	3929	1/1	0.91	0.14	38,38,38,38	0
54	MG	2a	1666	1/1	0.91	0.10	57,57,57,57	0
54	MG	2a	1635	1/1	0.91	0.15	71,71,71,71	0
54	MG	2A	3051	1/1	0.91	0.18	38,38,38,38	0
54	MG	1A	3092	1/1	0.91	0.20	32,32,32,32	0
54	MG	2A	3373	1/1	0.91	0.16	55,55,55,55	0
54	MG	2r	8001	1/1	0.91	0.15	65,65,65,65	0
54	MG	2A	3054	1/1	0.91	0.20	63,63,63,63	0
54	MG	1B	203	1/1	0.91	0.13	57,57,57,57	0
54	MG	1A	3460	1/1	0.91	0.18	30,30,30,30	0
54	MG	2B	3008	1/1	0.91	0.08	66,66,66,66	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3051	1/1	0.91	0.60	26,26,26,26	0
54	MG	1A	3140	1/1	0.91	0.46	29,29,29,29	0
54	MG	1a	1669	1/1	0.91	0.16	51,51,51,51	0
54	MG	1d	306	1/1	0.91	0.19	56,56,56,56	0
54	MG	1a	1625	1/1	0.91	0.16	51,51,51,51	0
54	MG	2A	3070	1/1	0.91	0.59	42,42,42,42	0
54	MG	1A	3217	1/1	0.91	0.61	30,30,30,30	0
54	MG	1A	3766	1/1	0.91	0.12	47,47,47,47	0
54	MG	1a	1657	1/1	0.91	0.13	59,59,59,59	0
54	MG	2a	1743	1/1	0.91	0.21	63,63,63,63	0
54	MG	2A	3598	1/1	0.91	0.09	53,53,53,53	0
54	MG	2A	3379	1/1	0.91	0.16	40,40,40,40	0
54	MG	1A	3321	1/1	0.91	0.14	16,16,16,16	0
54	MG	1A	4013	1/1	0.91	0.86	29,29,29,29	0
54	MG	1a	1696	1/1	0.91	0.15	70,70,70,70	0
54	MG	1a	1605	1/1	0.91	0.13	56,56,56,56	0
54	MG	2R	201	1/1	0.91	0.20	35,35,35,35	0
57	MPD	1a	1854	8/8	0.91	0.15	46,63,67,69	0
54	MG	1A	3514	1/1	0.91	0.20	47,47,47,47	0
54	MG	1a	1759	1/1	0.91	0.13	64,64,64,64	0
54	MG	1a	1618	1/1	0.91	0.29	51,51,51,51	0
54	MG	1a	1761	1/1	0.91	0.07	57,57,57,57	0
54	MG	2A	3509	1/1	0.91	0.20	60,60,60,60	0
54	MG	1A	3865	1/1	0.91	0.77	35,35,35,35	0
54	MG	1A	3508	1/1	0.91	0.14	29,29,29,29	0
54	MG	2A	3225	1/1	0.91	0.21	56,56,56,56	0
54	MG	1A	3493	1/1	0.91	0.15	56,56,56,56	0
54	MG	1A	3873	1/1	0.91	0.11	57,57,57,57	0
54	MG	1A	3223	1/1	0.91	0.45	28,28,28,28	0
54	MG	2A	3092	1/1	0.91	0.41	46,46,46,46	0
54	MG	1a	1753	1/1	0.91	0.15	66,66,66,66	0
54	MG	1a	1820	1/1	0.91	0.11	56,56,56,56	0
54	MG	1O	8001	1/1	0.91	0.12	43,43,43,43	0
54	MG	2A	3152	1/1	0.91	0.10	58,58,58,58	0
54	MG	2A	3079	1/1	0.91	0.14	47,47,47,47	0
54	MG	1A	3133	1/1	0.91	0.09	27,27,27,27	0
54	MG	25	502	1/1	0.91	0.24	59,59,59,59	0
54	MG	2A	3369	1/1	0.91	0.27	51,51,51,51	0
54	MG	2A	3005	1/1	0.91	0.27	41,41,41,41	0
54	MG	1A	3831	1/1	0.91	0.13	19,19,19,19	0
54	MG	2A	3573	1/1	0.91	0.16	19,19,19,19	0
54	MG	1A	3419	1/1	0.91	0.21	47,47,47,47	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2P	201	1/1	0.91	0.13	52,52,52,52	0
54	MG	2A	3717	1/1	0.91	0.27	61,61,61,61	0
54	MG	1A	3293	1/1	0.91	0.23	18,18,18,18	0
54	MG	1A	3891	1/1	0.91	0.14	30,30,30,30	0
54	MG	2A	3032	1/1	0.91	0.16	54,54,54,54	0
54	MG	2B	3002	1/1	0.91	0.20	71,71,71,71	0
54	MG	2a	1620	1/1	0.91	0.10	56,56,56,56	0
54	MG	2A	3157	1/1	0.91	0.18	42,42,42,42	0
54	MG	1A	3229	1/1	0.91	0.24	55,55,55,55	0
54	MG	1A	3148	1/1	0.91	0.35	30,30,30,30	0
54	MG	2A	3275	1/1	0.91	0.06	62,62,62,62	0
54	MG	1A	3786	1/1	0.91	0.16	40,40,40,40	0
54	MG	1A	3423	1/1	0.91	0.09	51,51,51,51	0
54	MG	1A	3486	1/1	0.91	0.18	21,21,21,21	0
54	MG	1a	1741	1/1	0.91	0.08	51,51,51,51	0
54	MG	1A	3183	1/1	0.91	0.15	45,45,45,45	0
54	MG	1a	1709	1/1	0.91	0.14	54,54,54,54	0
54	MG	1A	3940	1/1	0.91	0.38	67,67,67,67	0
54	MG	2A	3435	1/1	0.91	0.14	60,60,60,60	0
54	MG	1A	3260	1/1	0.91	0.09	38,38,38,38	0
54	MG	1A	3311	1/1	0.91	0.12	35,35,35,35	0
54	MG	1A	3513	1/1	0.91	0.14	53,53,53,53	0
54	MG	2A	3084	1/1	0.91	0.25	52,52,52,52	0
54	MG	2A	3059	1/1	0.91	0.28	42,42,42,42	0
57	MPD	1T	204	8/8	0.91	0.19	57,64,66,66	0
54	MG	2A	3661	1/1	0.91	0.07	47,47,47,47	0
54	MG	1A	3498	1/1	0.91	0.21	32,32,32,32	0
54	MG	1A	3944	1/1	0.91	0.10	47,47,47,47	0
54	MG	1B	210	1/1	0.91	0.14	50,50,50,50	0
54	MG	1A	3677	1/1	0.91	0.28	43,43,43,43	0
54	MG	2A	3425	1/1	0.91	0.13	68,68,68,68	0
54	MG	1A	3833	1/1	0.91	0.12	30,30,30,30	0
54	MG	2A	3075	1/1	0.91	0.68	42,42,42,42	0
54	MG	2a	1725	1/1	0.91	0.10	64,64,64,64	0
54	MG	1A	3552	1/1	0.91	0.12	45,45,45,45	0
54	MG	1A	3403	1/1	0.92	0.12	50,50,50,50	0
54	MG	2A	3614	1/1	0.92	0.17	58,58,58,58	0
54	MG	1A	3119	1/1	0.92	0.14	38,38,38,38	0
54	MG	1A	3446	1/1	0.92	0.22	20,20,20,20	0
54	MG	2a	1664	1/1	0.92	0.11	61,61,61,61	0
54	MG	2B	3019	1/1	0.92	0.09	65,65,65,65	0
54	MG	1A	3981	1/1	0.92	0.16	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
54	MG	1A	3083	1/1	0.92	0.26	40,40,40,40	0
54	MG	2A	3426	1/1	0.92	0.09	58,58,58,58	0
54	MG	1A	3655	1/1	0.92	0.36	30,30,30,30	0
54	MG	1A	3932	1/1	0.92	0.12	58,58,58,58	0
54	MG	1A	3773	1/1	0.92	0.17	64,64,64,64	0
54	MG	2a	1658	1/1	0.92	0.15	60,60,60,60	0
54	MG	2B	3012	1/1	0.92	0.13	50,50,50,50	0
54	MG	1A	3837	1/1	0.92	0.19	56,56,56,56	0
54	MG	1A	3437	1/1	0.92	0.20	41,41,41,41	0
54	MG	2A	3012	1/1	0.92	0.16	43,43,43,43	0
54	MG	1A	3310	1/1	0.92	0.12	38,38,38,38	0
54	MG	1A	3266	1/1	0.92	0.66	40,40,40,40	0
54	MG	2A	3164	1/1	0.92	0.11	69,69,69,69	0
54	MG	2A	3549	1/1	0.92	0.20	38,38,38,38	0
54	MG	1A	3818	1/1	0.92	0.17	31,31,31,31	0
54	MG	2A	3207	1/1	0.92	0.35	55,55,55,55	0
54	MG	2A	3268	1/1	0.92	0.10	29,29,29,29	0
54	MG	1A	3539	1/1	0.92	0.14	22,22,22,22	0
54	MG	1B	208	1/1	0.92	0.24	51,51,51,51	0
54	MG	1A	3538	1/1	0.92	0.11	55,55,55,55	0
54	MG	2A	3506	1/1	0.92	0.10	63,63,63,63	0
54	MG	1a	1839	1/1	0.92	0.08	59,59,59,59	0
54	MG	1A	3210	1/1	0.92	0.32	32,32,32,32	0
54	MG	1A	3061	1/1	0.92	0.10	43,43,43,43	0
54	MG	2F	303	1/1	0.92	0.70	43,43,43,43	0
54	MG	1a	1634	1/1	0.92	0.15	69,69,69,69	0
54	MG	1a	1768	1/1	0.92	0.15	69,69,69,69	0
54	MG	28	8001	1/1	0.92	0.09	46,46,46,46	0
54	MG	1A	3809	1/1	0.92	0.23	39,39,39,39	0
54	MG	1A	3132	1/1	0.92	0.12	40,40,40,40	0
54	MG	1e	3002	1/1	0.92	0.41	53,53,53,53	0
54	MG	1A	3322	1/1	0.92	0.17	21,21,21,21	0
54	MG	2A	3339	1/1	0.92	0.10	71,71,71,71	0
54	MG	1A	3765	1/1	0.92	0.10	39,39,39,39	0
54	MG	1A	3036	1/1	0.92	0.18	38,38,38,38	0
54	MG	2B	3011	1/1	0.92	0.08	65,65,65,65	0
54	MG	1A	3125	1/1	0.92	0.46	30,30,30,30	0
54	MG	1a	1821	1/1	0.92	0.18	44,44,44,44	0
54	MG	1A	3203	1/1	0.92	0.24	55,55,55,55	0
54	MG	1A	3632	1/1	0.92	0.13	63,63,63,63	0
54	MG	1A	3613	1/1	0.92	0.26	50,50,50,50	0
54	MG	2A	3674	1/1	0.92	0.14	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
54	MG	1A	3058	1/1	0.92	0.13	34,34,34,34	0
54	MG	2A	3503	1/1	0.92	0.11	54,54,54,54	0
54	MG	10	106	1/1	0.92	0.39	41,41,41,41	0
54	MG	1A	4027	1/1	0.92	0.48	37,37,37,37	0
54	MG	1A	3257	1/1	0.92	0.31	42,42,42,42	0
54	MG	1A	3163	1/1	0.92	0.25	47,47,47,47	0
54	MG	1A	3732	1/1	0.92	0.25	41,41,41,41	0
54	MG	1a	1803	1/1	0.92	0.10	64,64,64,64	0
54	MG	1a	1756	1/1	0.92	0.15	58,58,58,58	0
54	MG	1A	3651	1/1	0.92	0.30	30,30,30,30	0
54	MG	1A	3939	1/1	0.92	0.10	55,55,55,55	0
54	MG	1a	1691	1/1	0.92	0.16	56,56,56,56	0
54	MG	2A	3293	1/1	0.92	0.15	35,35,35,35	0
54	MG	2A	3657	1/1	0.92	0.17	43,43,43,43	0
54	MG	1a	1739	1/1	0.92	0.09	61,61,61,61	0
54	MG	2A	3281	1/1	0.92	0.18	59,59,59,59	0
54	MG	2A	3046	1/1	0.92	0.23	59,59,59,59	0
54	MG	2A	3136	1/1	0.92	0.16	51,51,51,51	0
54	MG	1A	3882	1/1	0.92	0.04	60,60,60,60	0
54	MG	2A	3419	1/1	0.92	0.20	59,59,59,59	0
54	MG	2A	3294	1/1	0.92	0.13	41,41,41,41	0
54	MG	1A	3797	1/1	0.92	0.33	34,34,34,34	0
54	MG	2A	3261	1/1	0.92	0.13	43,43,43,43	0
54	MG	1A	3392	1/1	0.92	0.22	23,23,23,23	0
54	MG	2a	1707	1/1	0.92	0.15	47,47,47,47	0
54	MG	1A	3413	1/1	0.92	0.29	57,57,57,57	0
54	MG	1A	3674	1/1	0.92	0.11	35,35,35,35	0
54	MG	2D	302	1/1	0.92	0.91	38,38,38,38	0
54	MG	2B	3017	1/1	0.92	0.13	80,80,80,80	0
54	MG	2A	3677	1/1	0.92	0.30	50,50,50,50	0
54	MG	1A	3147	1/1	0.92	0.20	39,39,39,39	0
54	MG	1A	3660	1/1	0.92	0.15	51,51,51,51	0
54	MG	1A	3408	1/1	0.92	0.19	50,50,50,50	0
54	MG	1A	3933	1/1	0.92	0.07	41,41,41,41	0
54	MG	1A	3900	1/1	0.92	0.19	40,40,40,40	0
54	MG	1A	3641	1/1	0.92	0.19	29,29,29,29	0
54	MG	2a	1655	1/1	0.92	0.14	63,63,63,63	0
54	MG	2A	3609	1/1	0.92	0.18	45,45,45,45	0
54	MG	1A	3605	1/1	0.92	0.15	44,44,44,44	0
54	MG	1A	3008	1/1	0.92	0.10	33,33,33,33	0
54	MG	1B	222	1/1	0.92	0.14	57,57,57,57	0
54	MG	1a	1812	1/1	0.92	0.10	59,59,59,59	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2T	3001	1/1	0.92	0.24	50,50,50,50	0
54	MG	1A	3780	1/1	0.92	0.21	45,45,45,45	0
54	MG	1h	3001	1/1	0.92	0.12	35,35,35,35	0
54	MG	2A	3211	1/1	0.92	0.48	46,46,46,46	0
54	MG	2A	3186	1/1	0.92	0.19	34,34,34,34	0
54	MG	1A	3118	1/1	0.92	0.17	49,49,49,49	0
54	MG	1a	1730	1/1	0.92	0.12	43,43,43,43	0
54	MG	1A	3549	1/1	0.92	0.14	38,38,38,38	0
54	MG	1A	3521	1/1	0.92	0.17	42,42,42,42	0
54	MG	1A	3739	1/1	0.92	0.20	51,51,51,51	0
54	MG	2a	1606	1/1	0.92	0.12	45,45,45,45	0
54	MG	1A	3212	1/1	0.92	0.57	37,37,37,37	0
54	MG	1a	1856	1/1	0.92	0.19	67,67,67,67	0
54	MG	1A	3197	1/1	0.92	0.14	41,41,41,41	0
54	MG	1A	3924	1/1	0.92	0.16	45,45,45,45	0
54	MG	2A	3047	1/1	0.92	0.14	56,56,56,56	0
54	MG	10	103	1/1	0.92	0.11	43,43,43,43	0
54	MG	1a	1788	1/1	0.92	0.18	54,54,54,54	0
54	MG	2E	302	1/1	0.92	0.39	67,67,67,67	0
54	MG	1a	1664	1/1	0.92	0.21	51,51,51,51	0
54	MG	1A	3038	1/1	0.92	0.13	40,40,40,40	0
54	MG	1A	3767	1/1	0.92	0.11	45,45,45,45	0
54	MG	1b	3001	1/1	0.92	0.18	76,76,76,76	0
54	MG	2A	3323	1/1	0.92	0.17	34,34,34,34	0
54	MG	1a	1689	1/1	0.92	0.18	55,55,55,55	0
54	MG	2a	1626	1/1	0.92	0.21	53,53,53,53	0
54	MG	2A	3108	1/1	0.92	0.19	62,62,62,62	0
54	MG	1A	3337	1/1	0.92	0.10	55,55,55,55	0
54	MG	2A	3153	1/1	0.92	0.47	42,42,42,42	0
54	MG	1A	3142	1/1	0.92	0.21	50,50,50,50	0
54	MG	2A	3453	1/1	0.92	0.31	64,64,64,64	0
54	MG	1A	3428	1/1	0.92	0.31	52,52,52,52	0
54	MG	2A	3456	1/1	0.92	0.14	31,31,31,31	0
54	MG	1A	3172	1/1	0.92	0.86	31,31,31,31	0
54	MG	2A	3139	1/1	0.92	0.10	58,58,58,58	0
54	MG	1A	3823	1/1	0.92	0.30	29,29,29,29	0
54	MG	1A	3292	1/1	0.92	0.17	56,56,56,56	0
54	MG	2A	3371	1/1	0.92	0.17	26,26,26,26	0
54	MG	19	503	1/1	0.92	0.16	50,50,50,50	0
54	MG	1A	3315	1/1	0.92	0.12	25,25,25,25	0
54	MG	2A	3132	1/1	0.92	0.14	43,43,43,43	0
54	MG	1A	3341	1/1	0.92	0.13	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
54	MG	1A	3261	1/1	0.92	0.44	36,36,36,36	0
54	MG	2A	3501	1/1	0.92	0.14	43,43,43,43	0
54	MG	1A	3281	1/1	0.92	0.23	36,36,36,36	0
54	MG	1A	3714	1/1	0.92	0.18	37,37,37,37	0
54	MG	1A	3263	1/1	0.92	0.39	25,25,25,25	0
54	MG	2A	3094	1/1	0.92	0.23	49,49,49,49	0
54	MG	2A	3265	1/1	0.92	0.11	57,57,57,57	0
54	MG	2A	3465	1/1	0.92	0.20	56,56,56,56	0
54	MG	1R	201	1/1	0.92	0.36	31,31,31,31	0
54	MG	1A	3966	1/1	0.92	0.43	36,36,36,36	0
54	MG	2A	3566	1/1	0.92	0.12	35,35,35,35	0
54	MG	1A	3116	1/1	0.92	0.23	28,28,28,28	0
54	MG	2A	3460	1/1	0.92	0.16	53,53,53,53	0
54	MG	1A	3075	1/1	0.92	0.39	32,32,32,32	0
54	MG	2A	3154	1/1	0.92	0.19	41,41,41,41	0
54	MG	2A	3283	1/1	0.92	0.07	50,50,50,50	0
54	MG	2A	3402	1/1	0.92	0.09	43,43,43,43	0
54	MG	2A	3702	1/1	0.92	0.09	46,46,46,46	0
54	MG	2a	1650	1/1	0.92	0.11	58,58,58,58	0
54	MG	2A	3151	1/1	0.92	0.21	66,66,66,66	0
54	MG	1A	3353	1/1	0.92	0.13	18,18,18,18	0
54	MG	2A	3680	1/1	0.92	0.12	50,50,50,50	0
54	MG	2A	3031	1/1	0.92	0.19	48,48,48,48	0
54	MG	1A	3608	1/1	0.92	0.18	50,50,50,50	0
54	MG	2A	3114	1/1	0.92	0.20	56,56,56,56	0
54	MG	1a	1836	1/1	0.92	0.09	62,62,62,62	0
54	MG	2A	3558	1/1	0.92	0.09	58,58,58,58	0
54	MG	1A	4005	1/1	0.92	0.31	32,32,32,32	0
54	MG	1A	3512	1/1	0.92	0.19	40,40,40,40	0
54	MG	1A	3848	1/1	0.92	0.14	48,48,48,48	0
54	MG	1B	215	1/1	0.92	0.28	61,61,61,61	0
54	MG	2A	3208	1/1	0.92	0.13	43,43,43,43	0
54	MG	2A	3235	1/1	0.92	0.15	54,54,54,54	0
54	MG	1A	3178	1/1	0.93	0.29	29,29,29,29	0
54	MG	2A	3040	1/1	0.93	0.09	58,58,58,58	0
54	MG	1E	301	1/1	0.93	0.16	35,35,35,35	0
54	MG	1A	3265	1/1	0.93	0.13	46,46,46,46	0
54	MG	2A	3432	1/1	0.93	0.16	57,57,57,57	0
54	MG	1A	3829	1/1	0.93	0.15	54,54,54,54	0
54	MG	2a	1625	1/1	0.93	0.13	67,67,67,67	0
54	MG	2A	3213	1/1	0.93	0.13	67,67,67,67	0
54	MG	1A	3282	1/1	0.93	0.36	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
54	MG	1A	4000	1/1	0.93	0.11	30,30,30,30	0
54	MG	2A	3439	1/1	0.93	0.14	64,64,64,64	0
54	MG	2A	3664	1/1	0.93	0.09	57,57,57,57	0
54	MG	2A	3586	1/1	0.93	0.12	84,84,84,84	0
54	MG	2A	3668	1/1	0.93	0.10	48,48,48,48	0
54	MG	2a	1721	1/1	0.93	0.18	76,76,76,76	0
54	MG	2a	1670	1/1	0.93	0.15	59,59,59,59	0
54	MG	1A	3884	1/1	0.93	0.09	48,48,48,48	0
54	MG	1A	3367	1/1	0.93	0.18	18,18,18,18	0
54	MG	1a	1831	1/1	0.93	0.10	54,54,54,54	0
54	MG	2A	3050	1/1	0.93	0.16	58,58,58,58	0
54	MG	2A	3647	1/1	0.93	0.17	57,57,57,57	0
54	MG	1A	3701	1/1	0.93	0.19	29,29,29,29	0
54	MG	1A	3487	1/1	0.93	0.46	51,51,51,51	0
54	MG	1A	3520	1/1	0.93	0.14	38,38,38,38	0
54	MG	1A	3320	1/1	0.93	0.10	24,24,24,24	0
54	MG	1A	4016	1/1	0.93	0.48	41,41,41,41	0
54	MG	1A	3235	1/1	0.93	0.39	39,39,39,39	0
54	MG	2A	3349	1/1	0.93	0.17	56,56,56,56	0
54	MG	1a	1660	1/1	0.93	0.18	46,46,46,46	0
54	MG	1A	3621	1/1	0.93	0.10	52,52,52,52	0
54	MG	2A	3532	1/1	0.93	0.17	52,52,52,52	0
54	MG	1A	3238	1/1	0.93	0.56	40,40,40,40	0
54	MG	2A	3017	1/1	0.93	0.67	41,41,41,41	0
54	MG	1A	3218	1/1	0.93	0.44	30,30,30,30	0
54	MG	1A	3883	1/1	0.93	0.56	47,47,47,47	0
54	MG	1a	1747	1/1	0.93	0.20	56,56,56,56	0
54	MG	1A	3995	1/1	0.93	0.20	26,26,26,26	0
54	MG	2A	3600	1/1	0.93	0.28	54,54,54,54	0
54	MG	2A	3612	1/1	0.93	0.13	40,40,40,40	0
54	MG	2A	3201	1/1	0.93	0.33	50,50,50,50	0
54	MG	2A	3388	1/1	0.93	0.11	51,51,51,51	0
54	MG	1A	3761	1/1	0.93	0.13	32,32,32,32	0
54	MG	2A	3034	1/1	0.93	0.17	42,42,42,42	0
54	MG	1A	3101	1/1	0.93	0.39	30,30,30,30	0
54	MG	1A	3872	1/1	0.93	0.16	50,50,50,50	0
54	MG	1A	3180	1/1	0.93	0.42	37,37,37,37	0
54	MG	2A	3161	1/1	0.93	0.17	46,46,46,46	0
54	MG	1A	3395	1/1	0.93	0.12	13,13,13,13	0
54	MG	1g	3001	1/1	0.93	0.29	52,52,52,52	0
54	MG	1A	3562	1/1	0.93	0.07	32,32,32,32	0
54	MG	2A	3190	1/1	0.93	0.12	47,47,47,47	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3452	1/1	0.93	0.15	21,21,21,21	0
54	MG	2A	3238	1/1	0.93	0.17	44,44,44,44	0
54	MG	1A	4022	1/1	0.93	0.15	30,30,30,30	0
54	MG	1a	1825	1/1	0.93	0.13	54,54,54,54	0
54	MG	2A	3500	1/1	0.93	0.12	51,51,51,51	0
54	MG	2A	3212	1/1	0.93	0.38	60,60,60,60	0
54	MG	1A	3864	1/1	0.93	0.08	36,36,36,36	0
54	MG	1a	1648	1/1	0.93	0.07	72,72,72,72	0
54	MG	1a	1655	1/1	0.93	0.26	57,57,57,57	0
54	MG	1A	3457	1/1	0.93	0.09	64,64,64,64	0
54	MG	1F	307	1/1	0.93	0.37	31,31,31,31	0
54	MG	2A	3444	1/1	0.93	0.24	60,60,60,60	0
54	MG	1A	3724	1/1	0.93	0.15	27,27,27,27	0
54	MG	1A	3425	1/1	0.93	0.13	35,35,35,35	0
54	MG	2A	3724	1/1	0.93	0.42	32,32,32,32	0
54	MG	1A	3300	1/1	0.93	0.14	23,23,23,23	0
54	MG	1A	3800	1/1	0.93	0.19	44,44,44,44	0
54	MG	2A	3383	1/1	0.93	0.23	64,64,64,64	0
54	MG	1A	3646	1/1	0.93	0.08	37,37,37,37	0
54	MG	1A	3579	1/1	0.93	0.20	24,24,24,24	0
54	MG	1A	3349	1/1	0.93	0.15	40,40,40,40	0
54	MG	2A	3570	1/1	0.93	0.19	44,44,44,44	0
54	MG	1a	1786	1/1	0.93	0.20	57,57,57,57	0
54	MG	1Z	8001	1/1	0.93	0.19	60,60,60,60	0
54	MG	1A	3463	1/1	0.93	0.13	19,19,19,19	0
54	MG	1A	3106	1/1	0.93	0.42	40,40,40,40	0
59	ZN	24	501	1/1	0.93	0.05	108,108,108,108	0
54	MG	2a	1637	1/1	0.93	0.19	63,63,63,63	0
54	MG	2A	3269	1/1	0.93	0.15	32,32,32,32	0
54	MG	1A	3272	1/1	0.93	0.16	38,38,38,38	0
54	MG	1A	3960	1/1	0.93	0.09	32,32,32,32	0
54	MG	1a	1692	1/1	0.93	0.21	46,46,46,46	0
54	MG	1A	3442	1/1	0.93	0.15	15,15,15,15	0
54	MG	2B	3003	1/1	0.93	0.09	74,74,74,74	0
54	MG	2a	1740	1/1	0.93	0.26	59,59,59,59	0
54	MG	1A	3700	1/1	0.93	0.08	34,34,34,34	0
54	MG	1a	1771	1/1	0.93	0.16	46,46,46,46	0
54	MG	2A	3582	1/1	0.93	0.17	47,47,47,47	0
54	MG	1A	3902	1/1	0.93	0.14	52,52,52,52	0
54	MG	1A	3861	1/1	0.93	0.17	22,22,22,22	0
54	MG	2A	3363	1/1	0.93	0.16	61,61,61,61	0
54	MG	1A	3712	1/1	0.93	0.11	52,52,52,52	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3815	1/1	0.93	0.10	33,33,33,33	0
54	MG	2a	1624	1/1	0.93	0.15	65,65,65,65	0
54	MG	1a	1666	1/1	0.93	0.55	50,50,50,50	0
54	MG	2G	3001	1/1	0.93	0.08	71,71,71,71	0
54	MG	2A	3434	1/1	0.93	0.13	26,26,26,26	0
54	MG	2A	3361	1/1	0.93	0.11	33,33,33,33	0
54	MG	2A	3479	1/1	0.93	0.14	41,41,41,41	0
54	MG	2A	3630	1/1	0.93	0.18	52,52,52,52	0
54	MG	1A	3877	1/1	0.93	0.10	57,57,57,57	0
54	MG	2a	1735	1/1	0.93	0.17	45,45,45,45	0
54	MG	1a	1738	1/1	0.93	0.30	62,62,62,62	0
54	MG	2A	3217	1/1	0.93	0.16	43,43,43,43	0
54	MG	2A	3362	1/1	0.93	0.14	34,34,34,34	0
54	MG	1A	3475	1/1	0.93	0.14	42,42,42,42	0
54	MG	1A	3826	1/1	0.93	0.19	26,26,26,26	0
54	MG	1T	203	1/1	0.93	0.14	52,52,52,52	0
54	MG	2A	3377	1/1	0.93	0.10	43,43,43,43	0
54	MG	2A	3004	1/1	0.93	0.17	44,44,44,44	0
54	MG	1A	3376	1/1	0.93	0.12	29,29,29,29	0
54	MG	1A	3881	1/1	0.93	0.21	43,43,43,43	0
54	MG	1A	3707	1/1	0.93	0.09	40,40,40,40	0
54	MG	2A	3144	1/1	0.93	0.10	54,54,54,54	0
54	MG	2a	1640	1/1	0.93	0.17	53,53,53,53	0
54	MG	1A	3841	1/1	0.93	0.15	29,29,29,29	0
54	MG	1A	3343	1/1	0.93	0.14	56,56,56,56	0
54	MG	1A	3427	1/1	0.93	0.13	37,37,37,37	0
54	MG	2a	1751	1/1	0.93	0.11	53,53,53,53	0
54	MG	1A	3175	1/1	0.93	0.56	35,35,35,35	0
54	MG	2A	3159	1/1	0.93	0.12	50,50,50,50	0
54	MG	1a	1848	1/1	0.93	0.21	53,53,53,53	0
54	MG	2A	3471	1/1	0.93	0.10	61,61,61,61	0
54	MG	2A	3459	1/1	0.93	0.11	38,38,38,38	0
54	MG	1A	3141	1/1	0.93	0.19	38,38,38,38	0
54	MG	2A	3247	1/1	0.93	0.07	50,50,50,50	0
54	MG	1a	1714	1/1	0.93	0.16	56,56,56,56	0
54	MG	2A	3039	1/1	0.93	0.13	56,56,56,56	0
54	MG	1F	302	1/1	0.93	0.13	32,32,32,32	0
54	MG	1A	3717	1/1	0.93	0.41	52,52,52,52	0
54	MG	1E	306	1/1	0.93	0.13	31,31,31,31	0
54	MG	1A	3166	1/1	0.93	0.10	32,32,32,32	0
54	MG	1A	3127	1/1	0.93	0.18	49,49,49,49	0
54	MG	2A	3436	1/1	0.93	0.14	56,56,56,56	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3001	1/1	0.93	0.17	46,46,46,46	0
54	MG	1A	3535	1/1	0.93	0.26	38,38,38,38	0
54	MG	1A	3942	1/1	0.93	0.20	73,73,73,73	0
54	MG	2A	3343	1/1	0.93	0.22	50,50,50,50	0
54	MG	1a	1665	1/1	0.93	0.13	59,59,59,59	0
54	MG	1A	3760	1/1	0.93	0.24	61,61,61,61	0
54	MG	1A	3471	1/1	0.93	0.10	31,31,31,31	0
54	MG	2A	3174	1/1	0.93	0.23	45,45,45,45	0
54	MG	1A	3305	1/1	0.93	0.12	39,39,39,39	0
54	MG	2A	3646	1/1	0.93	0.25	60,60,60,60	0
54	MG	1A	3868	1/1	0.93	0.20	23,23,23,23	0
54	MG	1A	3188	1/1	0.93	0.18	53,53,53,53	0
54	MG	2A	3624	1/1	0.93	0.11	37,37,37,37	0
54	MG	1A	3728	1/1	0.93	0.22	38,38,38,38	0
54	MG	2A	3083	1/1	0.93	0.17	49,49,49,49	0
54	MG	1A	3387	1/1	0.93	0.08	54,54,54,54	0
54	MG	1a	1651	1/1	0.93	0.25	59,59,59,59	0
54	MG	2A	3049	1/1	0.93	0.18	53,53,53,53	0
54	MG	1a	1757	1/1	0.93	0.11	77,77,77,77	0
54	MG	1A	3673	1/1	0.93	0.17	28,28,28,28	0
54	MG	2A	3048	1/1	0.93	0.20	61,61,61,61	0
54	MG	1A	3963	1/1	0.93	0.25	38,38,38,38	0
54	MG	1A	3968	1/1	0.93	0.10	11,11,11,11	0
54	MG	1a	1822	1/1	0.93	0.12	60,60,60,60	0
54	MG	1A	3570	1/1	0.93	0.25	47,47,47,47	0
54	MG	1A	3904	1/1	0.93	0.13	60,60,60,60	0
54	MG	1A	3768	1/1	0.93	0.11	54,54,54,54	0
54	MG	2A	3533	1/1	0.93	0.13	51,51,51,51	0
54	MG	1A	3156	1/1	0.93	0.11	49,49,49,49	0
54	MG	2A	3234	1/1	0.93	0.17	52,52,52,52	0
54	MG	2a	1653	1/1	0.93	0.10	53,53,53,53	0
54	MG	2A	3534	1/1	0.93	0.09	65,65,65,65	0
54	MG	2A	3381	1/1	0.93	0.13	53,53,53,53	0
54	MG	1A	3503	1/1	0.93	0.13	58,58,58,58	0
54	MG	2A	3023	1/1	0.93	0.26	55,55,55,55	0
54	MG	2B	3005	1/1	0.93	0.15	61,61,61,61	0
54	MG	2A	3113	1/1	0.93	0.27	59,59,59,59	0
54	MG	1A	3481	1/1	0.93	0.17	48,48,48,48	0
54	MG	1A	3687	1/1	0.93	0.10	44,44,44,44	0
54	MG	2A	3076	1/1	0.93	0.33	44,44,44,44	0
54	MG	1A	3174	1/1	0.93	0.34	34,34,34,34	0
57	MPD	1A	3988	8/8	0.93	0.21	48,52,54,59	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3446	1/1	0.93	0.13	30,30,30,30	0
54	MG	1A	3733	1/1	0.93	0.12	42,42,42,42	0
54	MG	1D	311	1/1	0.93	0.19	66,66,66,66	0
54	MG	2A	3022	1/1	0.93	0.10	39,39,39,39	0
54	MG	2A	3663	1/1	0.93	0.09	61,61,61,61	0
54	MG	1A	3583	1/1	0.93	0.22	20,20,20,20	0
54	MG	1A	3753	1/1	0.93	0.14	35,35,35,35	0
54	MG	1V	203	1/1	0.93	0.20	55,55,55,55	0
54	MG	1A	3417	1/1	0.93	0.16	20,20,20,20	0
54	MG	1a	1705	1/1	0.93	0.13	59,59,59,59	0
54	MG	1A	3335	1/1	0.93	0.15	22,22,22,22	0
54	MG	1A	3196	1/1	0.93	0.57	40,40,40,40	0
54	MG	1A	3954	1/1	0.93	0.09	36,36,36,36	0
57	MPD	2A	3711	8/8	0.93	0.12	48,60,64,64	0
54	MG	2a	1688	1/1	0.93	0.19	54,54,54,54	0
54	MG	2A	3131	1/1	0.93	0.83	44,44,44,44	0
54	MG	1A	3551	1/1	0.93	0.10	43,43,43,43	0
54	MG	2A	3417	1/1	0.93	0.12	37,37,37,37	0
54	MG	1B	218	1/1	0.93	0.10	50,50,50,50	0
54	MG	2A	3028	1/1	0.94	0.12	68,68,68,68	0
54	MG	1A	3599	1/1	0.94	0.24	45,45,45,45	0
54	MG	2A	3336	1/1	0.94	0.15	36,36,36,36	0
54	MG	1B	209	1/1	0.94	0.09	36,36,36,36	0
54	MG	1a	1621	1/1	0.94	0.11	46,46,46,46	0
54	MG	1A	3453	1/1	0.94	0.07	51,51,51,51	0
54	MG	2A	3626	1/1	0.94	0.06	70,70,70,70	0
54	MG	2a	1616	1/1	0.94	0.12	60,60,60,60	0
54	MG	1a	1740	1/1	0.94	0.09	59,59,59,59	0
54	MG	1a	1746	1/1	0.94	0.07	60,60,60,60	0
54	MG	1A	3983	1/1	0.94	0.30	36,36,36,36	0
54	MG	2A	3557	1/1	0.94	0.13	22,22,22,22	0
54	MG	1A	3014	1/1	0.94	0.39	44,44,44,44	0
54	MG	2A	3458	1/1	0.94	0.17	34,34,34,34	0
54	MG	1A	3590	1/1	0.94	0.10	32,32,32,32	0
54	MG	1A	3239	1/1	0.94	0.21	33,33,33,33	0
54	MG	2A	3052	1/1	0.94	0.22	40,40,40,40	0
54	MG	2a	1660	1/1	0.94	0.17	55,55,55,55	0
54	MG	1F	309	1/1	0.94	0.24	43,43,43,43	0
54	MG	1A	3876	1/1	0.94	0.12	27,27,27,27	0
54	MG	1l	3001	1/1	0.94	0.17	47,47,47,47	0
54	MG	1A	3821	1/1	0.94	0.14	26,26,26,26	0
54	MG	1A	4012	1/1	0.94	0.50	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
54	MG	1A	3057	1/1	0.94	0.25	27,27,27,27	0
54	MG	1a	1623	1/1	0.94	0.08	47,47,47,47	0
54	MG	1A	3236	1/1	0.94	0.73	38,38,38,38	0
54	MG	1A	3819	1/1	0.94	0.09	39,39,39,39	0
54	MG	2A	3115	1/1	0.94	0.15	63,63,63,63	0
54	MG	1A	3388	1/1	0.94	0.18	22,22,22,22	0
54	MG	1A	3802	1/1	0.94	0.06	47,47,47,47	0
54	MG	1A	3128	1/1	0.94	0.09	32,32,32,32	0
54	MG	2A	3180	1/1	0.94	0.35	63,63,63,63	0
54	MG	2A	3392	1/1	0.94	0.18	56,56,56,56	0
54	MG	1A	3542	1/1	0.94	0.23	31,31,31,31	0
54	MG	1a	1630	1/1	0.94	0.20	46,46,46,46	0
54	MG	1A	3139	1/1	0.94	0.23	29,29,29,29	0
54	MG	2A	3487	1/1	0.94	0.17	46,46,46,46	0
54	MG	2A	3309	1/1	0.94	0.14	25,25,25,25	0
54	MG	1A	3795	1/1	0.94	0.12	32,32,32,32	0
54	MG	1A	3680	1/1	0.94	0.21	25,25,25,25	0
54	MG	2A	3679	1/1	0.94	0.15	57,57,57,57	0
54	MG	2A	3636	1/1	0.94	0.24	47,47,47,47	0
54	MG	2A	3690	1/1	0.94	0.07	67,67,67,67	0
54	MG	1A	3108	1/1	0.94	0.45	42,42,42,42	0
54	MG	1A	3711	1/1	0.94	0.20	30,30,30,30	0
54	MG	1A	3524	1/1	0.94	0.10	46,46,46,46	0
54	MG	2A	3204	1/1	0.94	0.07	47,47,47,47	0
54	MG	1A	3035	1/1	0.94	0.13	38,38,38,38	0
54	MG	2A	3127	1/1	0.94	0.26	36,36,36,36	0
54	MG	1a	1796	1/1	0.94	0.24	50,50,50,50	0
54	MG	1A	3545	1/1	0.94	0.10	39,39,39,39	0
54	MG	2A	3431	1/1	0.94	0.07	53,53,53,53	0
54	MG	1A	3790	1/1	0.94	0.17	39,39,39,39	0
54	MG	1g	3002	1/1	0.94	0.09	60,60,60,60	0
54	MG	1A	4003	1/1	0.94	0.18	27,27,27,27	0
54	MG	1R	202	1/1	0.94	0.14	46,46,46,46	0
54	MG	2A	3297	1/1	0.94	0.17	51,51,51,51	0
54	MG	1A	3009	1/1	0.94	0.23	34,34,34,34	0
54	MG	1A	3626	1/1	0.94	0.14	51,51,51,51	0
54	MG	1a	1800	1/1	0.94	0.23	43,43,43,43	0
54	MG	1A	3974	1/1	0.94	0.14	45,45,45,45	0
54	MG	1A	3697	1/1	0.94	0.21	50,50,50,50	0
54	MG	2A	3583	1/1	0.94	0.14	42,42,42,42	0
54	MG	1A	3706	1/1	0.94	0.10	32,32,32,32	0
54	MG	2A	3706	1/1	0.94	0.21	48,48,48,48	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	4009	1/1	0.94	0.69	42,42,42,42	0
54	MG	1A	3370	1/1	0.94	0.14	21,21,21,21	0
54	MG	1A	3591	1/1	0.94	0.14	36,36,36,36	0
54	MG	1A	3469	1/1	0.94	0.09	29,29,29,29	0
54	MG	1a	1688	1/1	0.94	0.20	53,53,53,53	0
54	MG	1F	306	1/1	0.94	0.16	31,31,31,31	0
54	MG	1a	1723	1/1	0.94	0.14	50,50,50,50	0
54	MG	2A	3320	1/1	0.94	0.10	59,59,59,59	0
54	MG	1a	1727	1/1	0.94	0.20	43,43,43,43	0
54	MG	2A	3505	1/1	0.94	0.13	55,55,55,55	0
54	MG	1a	1685	1/1	0.94	0.29	40,40,40,40	0
54	MG	1a	1711	1/1	0.94	0.21	58,58,58,58	0
54	MG	1A	3121	1/1	0.94	0.10	57,57,57,57	0
54	MG	1g	3003	1/1	0.94	0.15	45,45,45,45	0
54	MG	1A	3727	1/1	0.94	0.25	22,22,22,22	0
54	MG	1A	3226	1/1	0.94	0.35	32,32,32,32	0
54	MG	1A	3850	1/1	0.94	0.17	48,48,48,48	0
54	MG	1A	3390	1/1	0.94	0.17	40,40,40,40	0
54	MG	1A	3400	1/1	0.94	0.15	35,35,35,35	0
54	MG	1A	3998	1/1	0.94	0.52	32,32,32,32	0
54	MG	1A	3506	1/1	0.94	0.12	33,33,33,33	0
54	MG	1f	3001	1/1	0.94	0.24	64,64,64,64	0
54	MG	2A	3719	1/1	0.94	0.23	48,48,48,48	0
54	MG	2A	3382	1/1	0.94	0.10	43,43,43,43	0
54	MG	2A	3575	1/1	0.94	0.21	41,41,41,41	0
54	MG	2a	1692	1/1	0.94	0.20	48,48,48,48	0
54	MG	1a	1690	1/1	0.94	0.17	45,45,45,45	0
54	MG	2A	3715	1/1	0.94	0.77	37,37,37,37	0
54	MG	1A	3643	1/1	0.94	0.30	56,56,56,56	0
54	MG	1A	3501	1/1	0.94	0.17	59,59,59,59	0
54	MG	2A	3652	1/1	0.94	0.20	44,44,44,44	0
54	MG	1a	1799	1/1	0.94	0.16	58,58,58,58	0
54	MG	1A	3067	1/1	0.94	0.10	38,38,38,38	0
54	MG	1A	3247	1/1	0.94	0.22	40,40,40,40	0
54	MG	1A	3295	1/1	0.94	0.17	19,19,19,19	0
54	MG	1A	3589	1/1	0.94	0.12	54,54,54,54	0
54	MG	1A	3647	1/1	0.94	0.12	38,38,38,38	0
54	MG	1A	3091	1/1	0.94	0.12	41,41,41,41	0
54	MG	1A	3019	1/1	0.94	0.44	33,33,33,33	0
54	MG	1A	3606	1/1	0.94	0.33	42,42,42,42	0
54	MG	1a	1675	1/1	0.94	0.12	42,42,42,42	0
54	MG	1A	3533	1/1	0.94	0.14	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
54	MG	2A	3489	1/1	0.94	0.14	69,69,69,69	0
54	MG	2A	3536	1/1	0.94	0.15	57,57,57,57	0
54	MG	1a	1601	1/1	0.94	0.09	56,56,56,56	0
54	MG	1A	3726	1/1	0.94	0.10	32,32,32,32	0
54	MG	10	101	1/1	0.94	0.07	47,47,47,47	0
54	MG	2A	3140	1/1	0.94	0.15	51,51,51,51	0
54	MG	1A	3560	1/1	0.94	0.10	40,40,40,40	0
54	MG	2a	1612	1/1	0.94	0.17	50,50,50,50	0
54	MG	1A	3250	1/1	0.94	0.38	27,27,27,27	0
54	MG	2A	3712	1/1	0.94	0.39	41,41,41,41	0
54	MG	1A	3681	1/1	0.94	0.17	38,38,38,38	0
54	MG	2a	1719	1/1	0.94	0.16	67,67,67,67	0
54	MG	1A	3859	1/1	0.94	0.14	16,16,16,16	0
54	MG	2A	3568	1/1	0.94	0.15	50,50,50,50	0
54	MG	1A	3313	1/1	0.94	0.10	46,46,46,46	0
54	MG	2A	3422	1/1	0.94	0.07	55,55,55,55	0
54	MG	2A	3525	1/1	0.94	0.18	28,28,28,28	0
54	MG	1A	3289	1/1	0.94	0.16	23,23,23,23	0
54	MG	1A	3461	1/1	0.94	0.10	45,45,45,45	0
54	MG	1A	3026	1/1	0.94	0.41	28,28,28,28	0
54	MG	1W	3001	1/1	0.94	0.22	46,46,46,46	0
54	MG	2A	3178	1/1	0.94	0.15	53,53,53,53	0
54	MG	2A	3122	1/1	0.94	0.20	66,66,66,66	0
54	MG	2a	1677	1/1	0.94	0.22	53,53,53,53	0
54	MG	1A	3980	1/1	0.94	0.25	48,48,48,48	0
54	MG	2a	1697	1/1	0.94	0.20	59,59,59,59	0
54	MG	2A	3176	1/1	0.94	0.21	42,42,42,42	0
54	MG	1A	3504	1/1	0.94	0.11	16,16,16,16	0
54	MG	2A	3315	1/1	0.94	0.17	73,73,73,73	0
54	MG	2A	3329	1/1	0.94	0.20	29,29,29,29	0
54	MG	2A	3665	1/1	0.94	0.20	56,56,56,56	0
54	MG	1A	3764	1/1	0.94	0.20	44,44,44,44	0
54	MG	1B	226	1/1	0.94	0.13	60,60,60,60	0
54	MG	1a	1852	1/1	0.94	0.18	54,54,54,54	0
54	MG	2A	3443	1/1	0.94	0.16	47,47,47,47	0
54	MG	1A	3758	1/1	0.94	0.06	42,42,42,42	0
54	MG	2A	3306	1/1	0.94	0.13	27,27,27,27	0
54	MG	2A	3367	1/1	0.94	0.12	47,47,47,47	0
54	MG	2a	1647	1/1	0.94	0.15	52,52,52,52	0
54	MG	1A	3598	1/1	0.94	0.18	51,51,51,51	0
54	MG	1a	1734	1/1	0.94	0.16	47,47,47,47	0
54	MG	2A	3654	1/1	0.94	0.10	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
54	MG	17	101	1/1	0.94	0.49	54,54,54,54	0
54	MG	1A	3483	1/1	0.94	0.17	49,49,49,49	0
54	MG	2N	8001	1/1	0.94	0.14	70,70,70,70	0
54	MG	10	102	1/1	0.94	0.14	36,36,36,36	0
54	MG	1A	3162	1/1	0.94	0.15	41,41,41,41	0
54	MG	1A	3288	1/1	0.94	0.16	16,16,16,16	0
54	MG	2A	3372	1/1	0.94	0.10	51,51,51,51	0
54	MG	2a	1715	1/1	0.94	0.17	60,60,60,60	0
54	MG	1A	3664	1/1	0.94	0.20	30,30,30,30	0
54	MG	1a	1807	1/1	0.94	0.23	67,67,67,67	0
54	MG	2A	3441	1/1	0.94	0.27	47,47,47,47	0
54	MG	2a	1659	1/1	0.94	0.24	48,48,48,48	0
54	MG	1A	3544	1/1	0.94	0.55	34,34,34,34	0
54	MG	2A	3601	1/1	0.94	0.31	57,57,57,57	0
54	MG	2A	3223	1/1	0.94	0.89	43,43,43,43	0
54	MG	1a	1789	1/1	0.94	0.15	69,69,69,69	0
54	MG	1T	202	1/1	0.94	0.09	48,48,48,48	0
54	MG	1A	3198	1/1	0.94	0.49	42,42,42,42	0
54	MG	1A	3581	1/1	0.94	0.17	53,53,53,53	0
54	MG	2A	3093	1/1	0.94	0.18	58,58,58,58	0
54	MG	1a	1687	1/1	0.94	0.22	54,54,54,54	0
54	MG	1A	3604	1/1	0.94	0.07	29,29,29,29	0
54	MG	2A	3494	1/1	0.94	0.21	50,50,50,50	0
54	MG	1a	1678	1/1	0.94	0.15	53,53,53,53	0
54	MG	2A	3639	1/1	0.94	0.12	56,56,56,56	0
54	MG	2A	3700	1/1	0.94	0.15	21,21,21,21	0
54	MG	2a	1723	1/1	0.94	0.19	45,45,45,45	0
54	MG	2A	3595	1/1	0.94	0.21	53,53,53,53	0
54	MG	2A	3239	1/1	0.94	0.14	50,50,50,50	0
54	MG	1a	1785	1/1	0.94	0.10	47,47,47,47	0
54	MG	1A	3816	1/1	0.94	0.13	35,35,35,35	0
59	ZN	2n	501	1/1	0.94	0.08	101,101,101,101	0
54	MG	1D	313	1/1	0.94	0.28	43,43,43,43	0
54	MG	2A	3120	1/1	0.94	0.15	41,41,41,41	0
54	MG	2A	3210	1/1	0.94	0.13	45,45,45,45	0
54	MG	15	104	1/1	0.94	0.15	62,62,62,62	0
54	MG	2A	3138	1/1	0.94	0.13	33,33,33,33	0
54	MG	2A	3642	1/1	0.94	0.16	57,57,57,57	0
54	MG	1A	3793	1/1	0.94	0.19	41,41,41,41	0
54	MG	1A	3496	1/1	0.94	0.14	47,47,47,47	0
54	MG	1A	3948	1/1	0.94	0.09	60,60,60,60	0
54	MG	2A	3233	1/1	0.94	0.13	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
54	MG	1a	1719	1/1	0.94	0.13	48,48,48,48	0
54	MG	1A	3634	1/1	0.94	0.13	59,59,59,59	0
54	MG	2a	1696	1/1	0.94	0.15	59,59,59,59	0
54	MG	2A	3693	1/1	0.94	0.10	50,50,50,50	0
54	MG	2A	3627	1/1	0.94	0.17	53,53,53,53	0
54	MG	2A	3606	1/1	0.94	0.07	50,50,50,50	0
54	MG	2W	8001	1/1	0.94	0.33	42,42,42,42	0
54	MG	1A	3048	1/1	0.94	0.30	33,33,33,33	0
54	MG	1A	3531	1/1	0.94	0.37	40,40,40,40	0
54	MG	1H	8002	1/1	0.94	0.11	37,37,37,37	0
54	MG	2a	1718	1/1	0.94	0.27	63,63,63,63	0
54	MG	2a	1738	1/1	0.94	0.30	52,52,52,52	0
54	MG	1A	3352	1/1	0.94	0.21	20,20,20,20	0
54	MG	2A	3723	1/1	0.94	0.58	37,37,37,37	0
54	MG	1A	3397	1/1	0.94	0.14	49,49,49,49	0
54	MG	2A	3101	1/1	0.94	0.21	50,50,50,50	0
54	MG	1A	3059	1/1	0.94	0.12	42,42,42,42	0
54	MG	2A	3475	1/1	0.94	0.18	30,30,30,30	0
54	MG	1A	3650	1/1	0.94	0.26	38,38,38,38	0
54	MG	1A	3905	1/1	0.94	0.08	53,53,53,53	0
54	MG	1A	3628	1/1	0.94	0.14	47,47,47,47	0
54	MG	1A	3691	1/1	0.94	0.18	17,17,17,17	0
56	EZP	2A	3709	25/25	0.94	0.46	38,42,50,58	0
54	MG	2A	3527	1/1	0.94	0.17	38,38,38,38	0
54	MG	2t	3001	1/1	0.94	0.11	45,45,45,45	0
54	MG	2A	3414	1/1	0.94	0.14	46,46,46,46	0
54	MG	1A	3871	1/1	0.94	0.24	50,50,50,50	0
54	MG	1A	3137	1/1	0.94	0.14	29,29,29,29	0
54	MG	2A	3429	1/1	0.94	0.12	59,59,59,59	0
54	MG	1A	3693	1/1	0.94	0.10	33,33,33,33	0
54	MG	2A	3591	1/1	0.94	0.26	51,51,51,51	0
54	MG	1N	201	1/1	0.94	0.32	35,35,35,35	0
54	MG	2A	3611	1/1	0.94	0.15	56,56,56,56	0
54	MG	1A	3112	1/1	0.94	0.48	34,34,34,34	0
54	MG	1A	3898	1/1	0.94	0.08	21,21,21,21	0
54	MG	2A	3073	1/1	0.94	0.12	45,45,45,45	0
54	MG	2A	3631	1/1	0.94	0.12	60,60,60,60	0
54	MG	1a	1698	1/1	0.94	0.12	36,36,36,36	0
54	MG	1a	1602	1/1	0.94	0.10	71,71,71,71	0
54	MG	2a	1622	1/1	0.94	0.09	56,56,56,56	0
54	MG	1A	3476	1/1	0.94	0.17	14,14,14,14	0
54	MG	1A	3669	1/1	0.94	0.16	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
54	MG	1F	312	1/1	0.94	0.19	51,51,51,51	0
54	MG	1A	3970	1/1	0.94	0.68	40,40,40,40	0
54	MG	1A	3362	1/1	0.94	0.11	36,36,36,36	0
54	MG	2A	3118	1/1	0.94	0.17	54,54,54,54	0
54	MG	2A	3163	1/1	0.94	0.28	53,53,53,53	0
54	MG	1A	3023	1/1	0.94	0.12	19,19,19,19	0
54	MG	1A	3777	1/1	0.94	0.10	19,19,19,19	0
54	MG	1A	3201	1/1	0.94	0.51	39,39,39,39	0
54	MG	1A	3976	1/1	0.94	0.07	38,38,38,38	0
54	MG	2A	3670	1/1	0.94	0.14	49,49,49,49	0
54	MG	1A	3862	1/1	0.94	0.18	33,33,33,33	0
54	MG	2A	3698	1/1	0.94	0.36	40,40,40,40	0
54	MG	2a	1731	1/1	0.94	0.14	61,61,61,61	0
54	MG	2A	3298	1/1	0.94	0.16	27,27,27,27	0
54	MG	2A	3495	1/1	0.94	0.20	45,45,45,45	0
54	MG	1A	3060	1/1	0.94	0.20	28,28,28,28	0
54	MG	10	104	1/1	0.94	0.16	51,51,51,51	0
54	MG	2a	1654	1/1	0.94	0.21	58,58,58,58	0
54	MG	1A	3240	1/1	0.94	0.22	37,37,37,37	0
54	MG	2a	1732	1/1	0.94	0.29	60,60,60,60	0
54	MG	1A	4008	1/1	0.94	0.29	28,28,28,28	0
54	MG	2A	3707	1/1	0.94	0.18	61,61,61,61	0
54	MG	2A	3649	1/1	0.94	0.23	38,38,38,38	0
54	MG	2A	3529	1/1	0.94	0.09	49,49,49,49	0
54	MG	2a	1730	1/1	0.94	0.22	49,49,49,49	0
54	MG	1D	303	1/1	0.94	0.20	44,44,44,44	0
54	MG	1A	3801	1/1	0.94	0.11	34,34,34,34	0
54	MG	1A	3811	1/1	0.94	0.22	31,31,31,31	0
54	MG	2A	3705	1/1	0.94	0.88	45,45,45,45	0
54	MG	1A	3609	1/1	0.94	0.37	41,41,41,41	0
54	MG	1A	3090	1/1	0.95	0.21	12,12,12,12	0
54	MG	1A	3421	1/1	0.95	0.12	30,30,30,30	0
54	MG	2A	3696	1/1	0.95	0.17	52,52,52,52	0
54	MG	2A	3718	1/1	0.95	0.44	44,44,44,44	0
54	MG	2A	3628	1/1	0.95	0.07	60,60,60,60	0
54	MG	1a	1750	1/1	0.95	0.13	59,59,59,59	0
54	MG	2A	3240	1/1	0.95	0.24	49,49,49,49	0
54	MG	1A	3224	1/1	0.95	0.42	36,36,36,36	0
54	MG	2A	3007	1/1	0.95	0.43	36,36,36,36	0
54	MG	1A	3546	1/1	0.95	0.09	52,52,52,52	0
54	MG	2A	3263	1/1	0.95	0.19	32,32,32,32	0
54	MG	1A	3497	1/1	0.95	0.07	46,46,46,46	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2a	1727	1/1	0.95	0.21	61,61,61,61	0
54	MG	1A	3851	1/1	0.95	0.10	41,41,41,41	0
56	EZP	1A	3987	25/25	0.95	0.39	16,28,47,60	0
54	MG	2E	306	1/1	0.95	0.51	44,44,44,44	0
54	MG	1A	3923	1/1	0.95	0.23	50,50,50,50	0
54	MG	1A	3152	1/1	0.95	0.23	31,31,31,31	0
54	MG	2a	1687	1/1	0.95	0.21	67,67,67,67	0
54	MG	1A	3505	1/1	0.95	0.12	27,27,27,27	0
54	MG	1A	3568	1/1	0.95	0.16	48,48,48,48	0
54	MG	2A	3699	1/1	0.95	0.28	61,61,61,61	0
54	MG	2A	3409	1/1	0.95	0.12	51,51,51,51	0
54	MG	1A	3578	1/1	0.95	0.20	23,23,23,23	0
54	MG	2A	3535	1/1	0.95	0.07	42,42,42,42	0
54	MG	1P	201	1/1	0.95	0.35	27,27,27,27	0
54	MG	1A	3230	1/1	0.95	0.19	46,46,46,46	0
54	MG	1A	3013	1/1	0.95	0.12	50,50,50,50	0
54	MG	1A	3916	1/1	0.95	0.09	29,29,29,29	0
54	MG	2a	1722	1/1	0.95	0.25	49,49,49,49	0
54	MG	1a	1712	1/1	0.95	0.18	51,51,51,51	0
54	MG	1A	3973	1/1	0.95	0.12	42,42,42,42	0
54	MG	1A	3762	1/1	0.95	0.15	19,19,19,19	0
54	MG	2A	3264	1/1	0.95	0.14	48,48,48,48	0
54	MG	2A	3550	1/1	0.95	0.16	31,31,31,31	0
54	MG	1A	3466	1/1	0.95	0.13	40,40,40,40	0
54	MG	2A	3074	1/1	0.95	0.41	39,39,39,39	0
54	MG	2A	3185	1/1	0.95	0.09	45,45,45,45	0
54	MG	1a	1694	1/1	0.95	0.21	32,32,32,32	0
54	MG	1a	1721	1/1	0.95	0.12	42,42,42,42	0
54	MG	2A	3484	1/1	0.95	0.36	65,65,65,65	0
54	MG	1A	3443	1/1	0.95	0.14	25,25,25,25	0
54	MG	1B	212	1/1	0.95	0.05	53,53,53,53	0
54	MG	2A	3354	1/1	0.95	0.17	49,49,49,49	0
54	MG	2A	3271	1/1	0.95	0.11	23,23,23,23	0
54	MG	2A	3480	1/1	0.95	0.68	37,37,37,37	0
54	MG	2A	3604	1/1	0.95	0.13	31,31,31,31	0
54	MG	2a	1741	1/1	0.95	0.15	55,55,55,55	0
54	MG	1A	3838	1/1	0.95	0.19	60,60,60,60	0
54	MG	2A	3440	1/1	0.95	0.10	49,49,49,49	0
54	MG	1A	3022	1/1	0.95	0.23	29,29,29,29	0
54	MG	1A	3316	1/1	0.95	0.10	38,38,38,38	0
54	MG	2A	3391	1/1	0.95	0.16	49,49,49,49	0
54	MG	2A	3513	1/1	0.95	0.21	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
54	MG	1A	3358	1/1	0.95	0.17	21,21,21,21	0
54	MG	1A	3557	1/1	0.95	0.13	35,35,35,35	0
54	MG	2A	3130	1/1	0.95	0.51	64,64,64,64	0
54	MG	1A	3441	1/1	0.95	0.20	34,34,34,34	0
54	MG	2A	3688	1/1	0.95	0.11	56,56,56,56	0
54	MG	2a	1636	1/1	0.95	0.11	69,69,69,69	0
54	MG	1A	3947	1/1	0.95	0.20	67,67,67,67	0
54	MG	1A	3372	1/1	0.95	0.08	47,47,47,47	0
54	MG	1A	3439	1/1	0.95	0.17	34,34,34,34	0
54	MG	1A	3135	1/1	0.95	0.15	29,29,29,29	0
54	MG	1A	3110	1/1	0.95	0.24	37,37,37,37	0
54	MG	1a	1656	1/1	0.95	0.20	63,63,63,63	0
54	MG	1a	1636	1/1	0.95	0.22	60,60,60,60	0
54	MG	1A	3556	1/1	0.95	0.14	39,39,39,39	0
54	MG	2A	3295	1/1	0.95	0.17	55,55,55,55	0
54	MG	1A	3844	1/1	0.95	0.12	46,46,46,46	0
54	MG	1B	227	1/1	0.95	0.08	52,52,52,52	0
54	MG	2E	305	1/1	0.95	0.24	52,52,52,52	0
54	MG	2A	3322	1/1	0.95	0.13	49,49,49,49	0
54	MG	2A	3045	1/1	0.95	0.10	40,40,40,40	0
54	MG	2A	3253	1/1	0.95	0.19	25,25,25,25	0
54	MG	2B	3009	1/1	0.95	0.08	62,62,62,62	0
54	MG	1A	3371	1/1	0.95	0.19	49,49,49,49	0
54	MG	1A	3040	1/1	0.95	0.15	26,26,26,26	0
54	MG	2A	3541	1/1	0.95	0.07	47,47,47,47	0
54	MG	2A	3531	1/1	0.95	0.11	54,54,54,54	0
54	MG	1A	3262	1/1	0.95	0.15	28,28,28,28	0
54	MG	2a	1717	1/1	0.95	0.18	60,60,60,60	0
54	MG	2a	1619	1/1	0.95	0.19	47,47,47,47	0
54	MG	2A	3655	1/1	0.95	0.16	42,42,42,42	0
54	MG	1A	3255	1/1	0.95	0.60	31,31,31,31	0
54	MG	2A	3556	1/1	0.95	0.25	35,35,35,35	0
54	MG	1A	3502	1/1	0.95	0.13	54,54,54,54	0
54	MG	2a	1657	1/1	0.95	0.11	44,44,44,44	0
54	MG	1a	1811	1/1	0.95	0.16	42,42,42,42	0
54	MG	1a	1616	1/1	0.95	0.12	60,60,60,60	0
54	MG	1A	3709	1/1	0.95	0.08	46,46,46,46	0
54	MG	2A	3543	1/1	0.95	0.27	49,49,49,49	0
54	MG	2a	1690	1/1	0.95	0.15	68,68,68,68	0
54	MG	2A	3360	1/1	0.95	0.13	48,48,48,48	0
54	MG	2A	3577	1/1	0.95	0.12	68,68,68,68	0
54	MG	1E	302	1/1	0.95	0.77	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
58	ARG	1B	228	12/12	0.95	0.26	26,40,53,54	0
54	MG	2a	1705	1/1	0.95	0.14	55,55,55,55	0
54	MG	1A	3078	1/1	0.95	0.08	47,47,47,47	0
54	MG	1A	3086	1/1	0.95	0.41	26,26,26,26	0
54	MG	1A	3682	1/1	0.95	0.09	38,38,38,38	0
54	MG	1A	3268	1/1	0.95	0.14	46,46,46,46	0
54	MG	1a	1774	1/1	0.95	0.17	53,53,53,53	0
54	MG	1A	3640	1/1	0.95	0.09	45,45,45,45	0
54	MG	1A	3451	1/1	0.95	0.16	15,15,15,15	0
54	MG	1A	3731	1/1	0.95	0.31	40,40,40,40	0
54	MG	1A	3523	1/1	0.95	0.19	48,48,48,48	0
54	MG	2A	3324	1/1	0.95	0.12	30,30,30,30	0
54	MG	2a	1706	1/1	0.95	0.11	63,63,63,63	0
54	MG	2a	1646	1/1	0.95	0.11	63,63,63,63	0
54	MG	2A	3002	1/1	0.95	0.16	53,53,53,53	0
54	MG	1A	3211	1/1	0.95	0.21	37,37,37,37	0
54	MG	2a	1703	1/1	0.95	0.15	61,61,61,61	0
54	MG	1a	1699	1/1	0.95	0.09	57,57,57,57	0
54	MG	2A	3129	1/1	0.95	0.09	52,52,52,52	0
54	MG	1a	1792	1/1	0.95	0.11	57,57,57,57	0
54	MG	1E	307	1/1	0.95	0.13	53,53,53,53	0
54	MG	2A	3302	1/1	0.95	0.12	25,25,25,25	0
54	MG	1a	1695	1/1	0.95	0.20	37,37,37,37	0
54	MG	1A	3745	1/1	0.95	0.27	60,60,60,60	0
54	MG	1A	3389	1/1	0.95	0.15	27,27,27,27	0
54	MG	2A	3438	1/1	0.95	0.11	50,50,50,50	0
54	MG	1a	1784	1/1	0.95	0.18	59,59,59,59	0
54	MG	2A	3588	1/1	0.95	0.12	48,48,48,48	0
54	MG	2a	1668	1/1	0.95	0.19	45,45,45,45	0
54	MG	1A	3914	1/1	0.95	0.17	38,38,38,38	0
54	MG	1A	3219	1/1	0.95	0.27	25,25,25,25	0
54	MG	1A	3612	1/1	0.95	0.18	22,22,22,22	0
54	MG	1A	3824	1/1	0.95	0.19	17,17,17,17	0
54	MG	2A	3104	1/1	0.95	0.10	42,42,42,42	0
54	MG	1A	3759	1/1	0.95	0.60	43,43,43,43	0
57	MPD	18	102	8/8	0.95	0.36	22,28,35,36	0
54	MG	1A	3094	1/1	0.95	0.46	29,29,29,29	0
54	MG	1A	3143	1/1	0.95	0.06	26,26,26,26	0
54	MG	1A	3368	1/1	0.95	0.19	16,16,16,16	0
54	MG	1A	3366	1/1	0.95	0.24	16,16,16,16	0
54	MG	2A	3546	1/1	0.95	0.26	41,41,41,41	0
54	MG	2A	3394	1/1	0.95	0.08	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
54	MG	2A	3292	1/1	0.95	0.23	47,47,47,47	0
54	MG	2a	1734	1/1	0.95	0.21	55,55,55,55	0
54	MG	1A	3863	1/1	0.95	0.12	12,12,12,12	0
54	MG	1A	3098	1/1	0.95	0.38	35,35,35,35	0
54	MG	2A	3310	1/1	0.95	0.15	29,29,29,29	0
54	MG	1B	216	1/1	0.95	0.14	33,33,33,33	0
54	MG	1E	303	1/1	0.95	0.08	32,32,32,32	0
54	MG	1A	3052	1/1	0.95	0.14	36,36,36,36	0
54	MG	2A	3470	1/1	0.95	0.41	43,43,43,43	0
54	MG	1A	3490	1/1	0.95	0.16	50,50,50,50	0
54	MG	1A	3333	1/1	0.95	0.13	25,25,25,25	0
54	MG	1a	1809	1/1	0.95	0.13	66,66,66,66	0
54	MG	2a	1714	1/1	0.95	0.16	48,48,48,48	0
54	MG	1A	3822	1/1	0.95	0.11	40,40,40,40	0
54	MG	1A	3830	1/1	0.95	0.14	41,41,41,41	0
54	MG	1A	3456	1/1	0.95	0.21	27,27,27,27	0
54	MG	1A	3284	1/1	0.95	0.50	32,32,32,32	0
54	MG	2A	3325	1/1	0.95	0.15	40,40,40,40	0
54	MG	1A	3689	1/1	0.95	0.09	22,22,22,22	0
54	MG	2A	3387	1/1	0.95	0.23	45,45,45,45	0
54	MG	1A	3770	1/1	0.95	0.18	27,27,27,27	0
54	MG	2A	3576	1/1	0.95	0.10	62,62,62,62	0
54	MG	1A	3592	1/1	0.95	0.18	44,44,44,44	0
54	MG	1B	223	1/1	0.95	0.07	46,46,46,46	0
54	MG	2a	1711	1/1	0.95	0.22	45,45,45,45	0
54	MG	1W	3002	1/1	0.95	0.14	39,39,39,39	0
54	MG	1a	1654	1/1	0.95	0.08	56,56,56,56	0
54	MG	1A	3002	1/1	0.95	0.11	47,47,47,47	0
54	MG	2A	3082	1/1	0.95	0.07	62,62,62,62	0
54	MG	1B	214	1/1	0.95	0.13	35,35,35,35	0
54	MG	2A	3498	1/1	0.95	0.17	30,30,30,30	0
54	MG	1A	3977	1/1	0.95	0.17	38,38,38,38	0
54	MG	1A	3169	1/1	0.95	0.62	33,33,33,33	0
54	MG	2A	3042	1/1	0.95	0.14	49,49,49,49	0
54	MG	2B	3006	1/1	0.95	0.13	57,57,57,57	0
54	MG	2A	3473	1/1	0.95	0.32	60,60,60,60	0
54	MG	2A	3681	1/1	0.95	0.12	69,69,69,69	0
54	MG	2a	1643	1/1	0.95	0.12	55,55,55,55	0
54	MG	1a	1647	1/1	0.95	0.15	52,52,52,52	0
54	MG	1A	3791	1/1	0.95	0.17	59,59,59,59	0
54	MG	1a	1736	1/1	0.95	0.18	57,57,57,57	0
54	MG	2A	3725	1/1	0.95	0.28	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
54	MG	2A	3110	1/1	0.95	0.40	40,40,40,40	0
54	MG	2A	3708	1/1	0.95	0.15	58,58,58,58	0
54	MG	1A	3926	1/1	0.95	0.07	45,45,45,45	0
54	MG	1A	3992	1/1	0.95	0.52	28,28,28,28	0
54	MG	2A	3623	1/1	0.95	0.10	43,43,43,43	0
54	MG	2A	3168	1/1	0.95	0.12	54,54,54,54	0
54	MG	1A	3566	1/1	0.95	0.20	35,35,35,35	0
54	MG	2a	1634	1/1	0.95	0.24	55,55,55,55	0
54	MG	1a	1763	1/1	0.95	0.18	64,64,64,64	0
54	MG	2A	3342	1/1	0.95	0.23	51,51,51,51	0
54	MG	2A	3025	1/1	0.95	0.12	44,44,44,44	0
54	MG	1A	3492	1/1	0.95	0.13	17,17,17,17	0
54	MG	1F	304	1/1	0.95	0.29	24,24,24,24	0
54	MG	2A	3288	1/1	0.95	0.12	49,49,49,49	0
54	MG	2A	3334	1/1	0.95	0.19	35,35,35,35	0
54	MG	2A	3380	1/1	0.95	0.26	56,56,56,56	0
54	MG	2A	3277	1/1	0.95	0.15	38,38,38,38	0
54	MG	1A	3275	1/1	0.95	0.21	29,29,29,29	0
54	MG	2A	3596	1/1	0.95	0.26	50,50,50,50	0
54	MG	1A	3812	1/1	0.95	0.44	35,35,35,35	0
54	MG	1A	3692	1/1	0.95	0.14	34,34,34,34	0
54	MG	1A	3381	1/1	0.95	0.11	40,40,40,40	0
54	MG	1A	3919	1/1	0.95	0.34	45,45,45,45	0
54	MG	1A	3444	1/1	0.95	0.14	24,24,24,24	0
54	MG	1A	3025	1/1	0.95	0.55	29,29,29,29	0
54	MG	1A	3382	1/1	0.95	0.14	19,19,19,19	0
54	MG	2a	1710	1/1	0.95	0.20	56,56,56,56	0
54	MG	1A	3840	1/1	0.95	0.12	33,33,33,33	0
54	MG	1A	3945	1/1	0.95	0.24	36,36,36,36	0
54	MG	1A	3385	1/1	0.95	0.11	51,51,51,51	0
54	MG	1A	3930	1/1	0.95	0.14	60,60,60,60	0
54	MG	2a	1736	1/1	0.95	0.20	61,61,61,61	0
54	MG	1A	4026	1/1	0.95	0.19	35,35,35,35	0
54	MG	1A	3237	1/1	0.95	0.24	28,28,28,28	0
54	MG	1A	3911	1/1	0.95	0.23	46,46,46,46	0
54	MG	1A	3517	1/1	0.95	0.18	48,48,48,48	0
54	MG	1A	3880	1/1	0.95	0.14	37,37,37,37	0
54	MG	2A	3061	1/1	0.95	0.27	51,51,51,51	0
54	MG	1O	8002	1/1	0.95	0.14	46,46,46,46	0
54	MG	2A	3416	1/1	0.95	0.17	54,54,54,54	0
54	MG	2a	1699	1/1	0.95	0.12	71,71,71,71	0
54	MG	2a	1744	1/1	0.95	0.14	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
54	MG	1A	3518	1/1	0.95	0.57	51,51,51,51	0
54	MG	2A	3097	1/1	0.95	0.10	67,67,67,67	0
54	MG	2A	3603	1/1	0.95	0.22	32,32,32,32	0
54	MG	1A	3401	1/1	0.95	0.11	45,45,45,45	0
54	MG	1A	3179	1/1	0.95	0.45	36,36,36,36	0
54	MG	1A	3454	1/1	0.95	0.13	22,22,22,22	0
54	MG	2A	3327	1/1	0.95	0.14	48,48,48,48	0
54	MG	1A	3065	1/1	0.95	0.40	26,26,26,26	0
54	MG	2A	3162	1/1	0.95	0.11	53,53,53,53	0
54	MG	2A	3411	1/1	0.95	0.07	55,55,55,55	0
54	MG	1a	1644	1/1	0.95	0.13	60,60,60,60	0
54	MG	1A	3807	1/1	0.95	0.17	40,40,40,40	0
54	MG	1A	3459	1/1	0.95	0.17	23,23,23,23	0
54	MG	2a	1739	1/1	0.95	0.10	51,51,51,51	0
54	MG	1A	3299	1/1	0.95	0.17	19,19,19,19	0
54	MG	1A	3099	1/1	0.95	0.34	30,30,30,30	0
54	MG	2A	3511	1/1	0.95	0.22	43,43,43,43	0
54	MG	2a	1629	1/1	0.96	0.21	60,60,60,60	0
54	MG	1F	301	1/1	0.96	0.75	41,41,41,41	0
54	MG	1A	3338	1/1	0.96	0.12	28,28,28,28	0
54	MG	1A	3623	1/1	0.96	0.13	32,32,32,32	0
54	MG	1A	3105	1/1	0.96	0.16	33,33,33,33	0
54	MG	1A	3462	1/1	0.96	0.11	48,48,48,48	0
54	MG	1A	3827	1/1	0.96	0.16	21,21,21,21	0
54	MG	1a	1610	1/1	0.96	0.15	44,44,44,44	0
54	MG	1F	303	1/1	0.96	0.17	35,35,35,35	0
54	MG	1A	3754	1/1	0.96	0.40	37,37,37,37	0
54	MG	1A	3396	1/1	0.96	0.13	21,21,21,21	0
54	MG	2A	3345	1/1	0.96	0.29	45,45,45,45	0
54	MG	1A	3028	1/1	0.96	0.13	30,30,30,30	0
54	MG	1A	3886	1/1	0.96	0.12	52,52,52,52	0
54	MG	2A	3282	1/1	0.96	0.17	33,33,33,33	0
54	MG	2A	3272	1/1	0.96	0.09	38,38,38,38	0
54	MG	1A	3775	1/1	0.96	0.26	34,34,34,34	0
54	MG	1A	3785	1/1	0.96	0.21	28,28,28,28	0
54	MG	1A	3467	1/1	0.96	0.07	49,49,49,49	0
54	MG	1A	3080	1/1	0.96	0.45	37,37,37,37	0
54	MG	1A	3007	1/1	0.96	0.13	26,26,26,26	0
54	MG	1A	3438	1/1	0.96	0.15	43,43,43,43	0
54	MG	1a	1787	1/1	0.96	0.25	40,40,40,40	0
54	MG	2a	1652	1/1	0.96	0.19	48,48,48,48	0
54	MG	1A	3029	1/1	0.96	0.14	12,12,12,12	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3741	1/1	0.96	0.15	48,48,48,48	0
54	MG	1G	3004	1/1	0.96	0.11	34,34,34,34	0
54	MG	1A	3698	1/1	0.96	0.20	58,58,58,58	0
54	MG	1A	3424	1/1	0.96	0.15	41,41,41,41	0
54	MG	2A	3037	1/1	0.96	0.16	56,56,56,56	0
54	MG	1A	3374	1/1	0.96	0.13	50,50,50,50	0
54	MG	1a	1732	1/1	0.96	0.08	59,59,59,59	0
54	MG	2D	306	1/1	0.96	0.16	56,56,56,56	0
54	MG	2A	3248	1/1	0.96	0.07	55,55,55,55	0
54	MG	1A	3554	1/1	0.96	0.17	40,40,40,40	0
54	MG	2A	3030	1/1	0.96	0.15	53,53,53,53	0
54	MG	1A	3722	1/1	0.96	0.22	39,39,39,39	0
54	MG	1a	1795	1/1	0.96	0.28	49,49,49,49	0
54	MG	1A	3012	1/1	0.96	0.20	17,17,17,17	0
54	MG	2a	1628	1/1	0.96	0.11	31,31,31,31	0
54	MG	1A	3072	1/1	0.96	0.49	26,26,26,26	0
54	MG	2A	3337	1/1	0.96	0.07	38,38,38,38	0
54	MG	1A	3588	1/1	0.96	0.16	23,23,23,23	0
54	MG	1A	3631	1/1	0.96	0.12	48,48,48,48	0
54	MG	15	103	1/1	0.96	0.09	41,41,41,41	0
54	MG	1A	3153	1/1	0.96	0.17	42,42,42,42	0
54	MG	1A	3993	1/1	0.96	0.26	26,26,26,26	0
54	MG	2A	3641	1/1	0.96	0.14	46,46,46,46	0
54	MG	1A	3668	1/1	0.96	0.17	63,63,63,63	0
54	MG	2A	3518	1/1	0.96	0.11	41,41,41,41	0
54	MG	1a	1735	1/1	0.96	0.12	51,51,51,51	0
54	MG	1A	3329	1/1	0.96	0.14	33,33,33,33	0
54	MG	2A	3564	1/1	0.96	0.12	57,57,57,57	0
54	MG	2A	3686	1/1	0.96	0.12	42,42,42,42	0
54	MG	1A	3808	1/1	0.96	0.23	41,41,41,41	0
54	MG	1a	1849	1/1	0.96	0.14	47,47,47,47	0
54	MG	2A	3353	1/1	0.96	0.21	62,62,62,62	0
54	MG	2A	3622	1/1	0.96	0.17	18,18,18,18	0
54	MG	1A	3328	1/1	0.96	0.11	13,13,13,13	0
54	MG	2A	3526	1/1	0.96	0.10	53,53,53,53	0
54	MG	1a	1762	1/1	0.96	0.17	56,56,56,56	0
54	MG	2A	3158	1/1	0.96	0.20	48,48,48,48	0
54	MG	1A	3571	1/1	0.96	0.41	27,27,27,27	0
54	MG	1V	201	1/1	0.96	0.14	50,50,50,50	0
54	MG	1A	3216	1/1	0.96	0.55	29,29,29,29	0
54	MG	2A	3024	1/1	0.96	0.08	35,35,35,35	0
54	MG	2a	1610	1/1	0.96	0.23	45,45,45,45	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3168	1/1	0.96	0.09	46,46,46,46	0
54	MG	1B	201	1/1	0.96	0.53	34,34,34,34	0
54	MG	1A	3617	1/1	0.96	0.15	38,38,38,38	0
54	MG	2A	3099	1/1	0.96	0.08	43,43,43,43	0
54	MG	1A	3750	1/1	0.96	0.16	27,27,27,27	0
54	MG	1A	3200	1/1	0.96	0.34	32,32,32,32	0
54	MG	1A	3088	1/1	0.96	0.25	32,32,32,32	0
54	MG	1A	3814	1/1	0.96	0.15	25,25,25,25	0
54	MG	1A	3215	1/1	0.96	0.31	35,35,35,35	0
54	MG	2A	3312	1/1	0.96	0.20	39,39,39,39	0
54	MG	1A	3429	1/1	0.96	0.15	41,41,41,41	0
54	MG	2A	3565	1/1	0.96	0.12	48,48,48,48	0
54	MG	2A	3254	1/1	0.96	0.14	51,51,51,51	0
54	MG	1A	3561	1/1	0.96	0.12	25,25,25,25	0
54	MG	1A	3972	1/1	0.96	0.36	32,32,32,32	0
54	MG	1A	3068	1/1	0.96	0.15	23,23,23,23	0
54	MG	1A	3465	1/1	0.96	0.19	33,33,33,33	0
54	MG	1B	213	1/1	0.96	0.18	38,38,38,38	0
54	MG	2A	3356	1/1	0.96	0.17	40,40,40,40	0
54	MG	1A	3377	1/1	0.96	0.20	44,44,44,44	0
54	MG	2A	3445	1/1	0.96	0.37	41,41,41,41	0
54	MG	1A	3046	1/1	0.96	0.36	39,39,39,39	0
54	MG	1A	3630	1/1	0.96	0.24	54,54,54,54	0
54	MG	2a	1750	1/1	0.96	0.08	59,59,59,59	0
54	MG	1A	3192	1/1	0.96	0.41	35,35,35,35	0
54	MG	1A	3129	1/1	0.96	0.43	26,26,26,26	0
54	MG	2A	3222	1/1	0.96	0.16	46,46,46,46	0
54	MG	1A	3405	1/1	0.96	0.14	17,17,17,17	0
54	MG	1a	1790	1/1	0.96	0.13	60,60,60,60	0
54	MG	1A	3150	1/1	0.96	0.69	28,28,28,28	0
54	MG	2a	1728	1/1	0.96	0.09	53,53,53,53	0
54	MG	2A	3561	1/1	0.96	0.06	38,38,38,38	0
54	MG	1A	3569	1/1	0.96	0.29	34,34,34,34	0
54	MG	1A	3304	1/1	0.96	0.17	26,26,26,26	0
54	MG	1A	3032	1/1	0.96	0.10	45,45,45,45	0
54	MG	2A	3089	1/1	0.96	0.10	41,41,41,41	0
54	MG	1a	1769	1/1	0.96	0.20	56,56,56,56	0
54	MG	2A	3347	1/1	0.96	0.20	56,56,56,56	0
54	MG	2A	3404	1/1	0.96	0.15	56,56,56,56	0
54	MG	1A	3991	1/1	0.96	0.58	43,43,43,43	0
54	MG	1A	3892	1/1	0.96	0.08	39,39,39,39	0
54	MG	1A	3734	1/1	0.96	0.26	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
54	MG	1A	3326	1/1	0.96	0.07	38,38,38,38	0
54	MG	1A	3369	1/1	0.96	0.17	16,16,16,16	0
54	MG	1A	3889	1/1	0.96	0.19	36,36,36,36	0
54	MG	2A	3620	1/1	0.96	0.13	48,48,48,48	0
54	MG	1a	1847	1/1	0.96	0.24	60,60,60,60	0
54	MG	2A	3232	1/1	0.96	0.12	44,44,44,44	0
54	MG	1A	3356	1/1	0.96	0.18	37,37,37,37	0
54	MG	2A	3085	1/1	0.96	0.16	35,35,35,35	0
54	MG	1A	3267	1/1	0.96	0.15	29,29,29,29	0
54	MG	2A	3433	1/1	0.96	0.14	57,57,57,57	0
54	MG	1A	3778	1/1	0.96	0.07	35,35,35,35	0
54	MG	2A	3038	1/1	0.96	0.11	46,46,46,46	0
54	MG	1A	3547	1/1	0.96	0.15	29,29,29,29	0
54	MG	2A	3490	1/1	0.96	0.17	44,44,44,44	0
54	MG	1a	1717	1/1	0.96	0.16	53,53,53,53	0
54	MG	2A	3542	1/1	0.96	0.19	45,45,45,45	0
54	MG	1A	3053	1/1	0.96	0.22	47,47,47,47	0
54	MG	1A	3318	1/1	0.96	0.17	26,26,26,26	0
54	MG	2a	1698	1/1	0.96	0.19	50,50,50,50	0
54	MG	1A	3909	1/1	0.96	0.08	35,35,35,35	0
54	MG	1A	3723	1/1	0.96	0.13	36,36,36,36	0
54	MG	1A	3716	1/1	0.96	0.15	47,47,47,47	0
54	MG	2A	3514	1/1	0.96	0.12	36,36,36,36	0
54	MG	2A	3410	1/1	0.96	0.17	47,47,47,47	0
54	MG	2A	3464	1/1	0.96	0.16	34,34,34,34	0
54	MG	1A	3699	1/1	0.96	0.13	42,42,42,42	0
54	MG	1A	3222	1/1	0.96	0.46	32,32,32,32	0
54	MG	1A	3206	1/1	0.96	0.23	18,18,18,18	0
54	MG	2a	1633	1/1	0.96	0.15	68,68,68,68	0
54	MG	1A	3719	1/1	0.96	0.11	56,56,56,56	0
54	MG	1A	3907	1/1	0.96	0.14	52,52,52,52	0
54	MG	1A	3386	1/1	0.96	0.12	19,19,19,19	0
54	MG	1A	3228	1/1	0.96	0.22	18,18,18,18	0
54	MG	1A	3742	1/1	0.96	0.14	32,32,32,32	0
54	MG	1a	1614	1/1	0.96	0.08	56,56,56,56	0
54	MG	2A	3286	1/1	0.96	0.14	47,47,47,47	0
54	MG	1A	3922	1/1	0.96	0.27	61,61,61,61	0
54	MG	1A	3307	1/1	0.96	0.17	31,31,31,31	0
54	MG	1a	1708	1/1	0.96	0.24	32,32,32,32	0
54	MG	2A	3013	1/1	0.96	0.50	33,33,33,33	0
54	MG	1A	3244	1/1	0.96	0.38	27,27,27,27	0
54	MG	2A	3359	1/1	0.96	0.14	52,52,52,52	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	2A	3319	1/1	0.96	0.16	39,39,39,39	0
54	MG	2A	3704	1/1	0.96	0.17	33,33,33,33	0
54	MG	2A	3255	1/1	0.96	0.12	24,24,24,24	0
54	MG	2A	3539	1/1	0.96	0.13	41,41,41,41	0
54	MG	1A	3276	1/1	0.96	0.25	26,26,26,26	0
54	MG	1A	3738	1/1	0.96	0.14	24,24,24,24	0
54	MG	1A	3636	1/1	0.96	0.22	17,17,17,17	0
54	MG	1A	3639	1/1	0.96	0.21	34,34,34,34	0
54	MG	2A	3187	1/1	0.96	0.13	44,44,44,44	0
54	MG	1A	3193	1/1	0.96	0.22	44,44,44,44	0
54	MG	1A	3622	1/1	0.96	0.14	51,51,51,51	0
54	MG	1A	3746	1/1	0.96	0.17	59,59,59,59	0
54	MG	1A	3729	1/1	0.96	0.18	31,31,31,31	0
54	MG	1A	3656	1/1	0.96	0.19	37,37,37,37	0
54	MG	1A	4024	1/1	0.96	0.50	30,30,30,30	0
54	MG	1a	1770	1/1	0.96	0.19	54,54,54,54	0
54	MG	1A	3049	1/1	0.96	0.38	38,38,38,38	0
54	MG	1A	3806	1/1	0.96	0.13	34,34,34,34	0
54	MG	1A	3743	1/1	0.96	0.24	62,62,62,62	0
54	MG	2A	3300	1/1	0.96	0.14	28,28,28,28	0
54	MG	2A	3716	1/1	0.96	0.45	51,51,51,51	0
54	MG	1A	3062	1/1	0.96	0.16	25,25,25,25	0
54	MG	2a	1712	1/1	0.96	0.18	37,37,37,37	0
54	MG	2a	1665	1/1	0.96	0.33	55,55,55,55	0
54	MG	1A	3204	1/1	0.96	0.52	27,27,27,27	0
54	MG	1A	3186	1/1	0.96	0.47	36,36,36,36	0
54	MG	2A	3418	1/1	0.96	0.13	54,54,54,54	0
54	MG	1A	3409	1/1	0.96	0.13	50,50,50,50	0
54	MG	1A	3334	1/1	0.96	0.14	25,25,25,25	0
54	MG	1A	3580	1/1	0.96	0.15	22,22,22,22	0
54	MG	1A	3074	1/1	0.96	0.44	45,45,45,45	0
54	MG	2A	3289	1/1	0.96	0.12	47,47,47,47	0
54	MG	1A	3468	1/1	0.96	0.16	45,45,45,45	0
54	MG	2A	3237	1/1	0.96	0.47	34,34,34,34	0
54	MG	1A	3232	1/1	0.96	0.48	31,31,31,31	0
54	MG	1a	1765	1/1	0.96	0.11	46,46,46,46	0
54	MG	2F	302	1/1	0.96	0.15	49,49,49,49	0
54	MG	1a	1725	1/1	0.96	0.15	46,46,46,46	0
54	MG	1a	1823	1/1	0.96	0.13	48,48,48,48	0
54	MG	1A	3207	1/1	0.96	0.43	39,39,39,39	0
54	MG	1A	4020	1/1	0.96	0.54	27,27,27,27	0
54	MG	13	102	1/1	0.96	0.14	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
54	MG	2A	3496	1/1	0.96	0.13	40,40,40,40	0
54	MG	1A	3885	1/1	0.96	0.20	53,53,53,53	0
54	MG	2A	3260	1/1	0.96	0.06	53,53,53,53	0
54	MG	1A	3555	1/1	0.96	0.18	39,39,39,39	0
54	MG	1A	3450	1/1	0.96	0.22	27,27,27,27	0
54	MG	2A	3451	1/1	0.96	0.16	49,49,49,49	0
54	MG	1a	1826	1/1	0.96	0.21	58,58,58,58	0
54	MG	2A	3689	1/1	0.96	0.06	59,59,59,59	0
54	MG	1A	3001	1/1	0.96	0.14	27,27,27,27	0
54	MG	1A	4021	1/1	0.96	0.52	35,35,35,35	0
54	MG	1a	1713	1/1	0.96	0.08	53,53,53,53	0
54	MG	2a	1679	1/1	0.96	0.15	53,53,53,53	0
54	MG	2A	3155	1/1	0.96	0.16	48,48,48,48	0
54	MG	1A	3644	1/1	0.96	0.08	58,58,58,58	0
54	MG	18	101	1/1	0.96	0.06	46,46,46,46	0
54	MG	1a	1611	1/1	0.96	0.18	37,37,37,37	0
54	MG	1D	312	1/1	0.96	0.13	54,54,54,54	0
54	MG	2A	3497	1/1	0.96	0.14	43,43,43,43	0
54	MG	1A	3325	1/1	0.96	0.27	53,53,53,53	0
54	MG	2A	3678	1/1	0.96	0.10	51,51,51,51	0
54	MG	1A	3494	1/1	0.96	0.14	38,38,38,38	0
54	MG	2A	3352	1/1	0.96	0.11	52,52,52,52	0
54	MG	1a	1661	1/1	0.96	0.11	49,49,49,49	0
54	MG	1A	3846	1/1	0.96	0.13	27,27,27,27	0
54	MG	1A	3629	1/1	0.96	0.08	41,41,41,41	0
54	MG	2D	304	1/1	0.96	0.48	42,42,42,42	0
54	MG	1A	3839	1/1	0.96	0.25	32,32,32,32	0
54	MG	1A	3455	1/1	0.96	0.16	10,10,10,10	0
54	MG	2A	3181	1/1	0.96	0.18	47,47,47,47	0
54	MG	1A	3990	1/1	0.96	0.23	20,20,20,20	0
54	MG	1A	3340	1/1	0.96	0.12	28,28,28,28	0
54	MG	2A	3523	1/1	0.96	0.23	49,49,49,49	0
54	MG	1A	3624	1/1	0.96	0.32	45,45,45,45	0
54	MG	1i	3001	1/1	0.96	0.14	53,53,53,53	0
54	MG	2A	3331	1/1	0.96	0.16	49,49,49,49	0
54	MG	2A	3121	1/1	0.96	0.19	53,53,53,53	0
54	MG	1A	3069	1/1	0.96	0.18	23,23,23,23	0
54	MG	2A	3400	1/1	0.96	0.24	36,36,36,36	0
54	MG	2A	3645	1/1	0.96	0.07	40,40,40,40	0
54	MG	1A	3695	1/1	0.96	0.11	49,49,49,49	0
54	MG	2A	3067	1/1	0.96	0.45	45,45,45,45	0
54	MG	1A	3472	1/1	0.97	0.14	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
54	MG	1A	4011	1/1	0.97	0.33	29,29,29,29	0
54	MG	2a	1671	1/1	0.97	0.25	47,47,47,47	0
54	MG	1A	3989	1/1	0.97	0.32	50,50,50,50	0
54	MG	2A	3018	1/1	0.97	0.13	40,40,40,40	0
54	MG	2A	3299	1/1	0.97	0.16	28,28,28,28	0
54	MG	2A	3580	1/1	0.97	0.17	36,36,36,36	0
54	MG	1a	1838	1/1	0.97	0.11	55,55,55,55	0
54	MG	1A	3918	1/1	0.97	0.16	38,38,38,38	0
54	MG	2A	3102	1/1	0.97	0.11	42,42,42,42	0
54	MG	2A	3020	1/1	0.97	0.31	57,57,57,57	0
54	MG	1A	4002	1/1	0.97	0.63	29,29,29,29	0
54	MG	2A	3714	1/1	0.97	0.88	45,45,45,45	0
54	MG	1A	3447	1/1	0.97	0.15	34,34,34,34	0
54	MG	1A	3246	1/1	0.97	0.14	58,58,58,58	0
54	MG	1A	3045	1/1	0.97	0.22	35,35,35,35	0
54	MG	1a	1683	1/1	0.97	0.13	59,59,59,59	0
54	MG	1A	3134	1/1	0.97	0.15	22,22,22,22	0
54	MG	2A	3376	1/1	0.97	0.10	47,47,47,47	0
54	MG	1A	3529	1/1	0.97	0.06	47,47,47,47	0
54	MG	1A	3245	1/1	0.97	0.11	27,27,27,27	0
54	MG	2A	3270	1/1	0.97	0.07	37,37,37,37	0
54	MG	1A	3975	1/1	0.97	0.09	39,39,39,39	0
54	MG	1A	3033	1/1	0.97	0.21	34,34,34,34	0
54	MG	2A	3616	1/1	0.97	0.08	45,45,45,45	0
54	MG	2a	1713	1/1	0.97	0.43	55,55,55,55	0
54	MG	2A	3364	1/1	0.97	0.26	58,58,58,58	0
54	MG	2A	3128	1/1	0.97	0.53	45,45,45,45	0
54	MG	2A	3522	1/1	0.97	0.15	47,47,47,47	0
54	MG	1F	305	1/1	0.97	0.49	34,34,34,34	0
54	MG	2A	3578	1/1	0.97	0.16	47,47,47,47	0
54	MG	1a	1710	1/1	0.97	0.12	63,63,63,63	0
54	MG	1A	4019	1/1	0.97	0.21	29,29,29,29	0
54	MG	1A	3308	1/1	0.97	0.20	34,34,34,34	0
54	MG	2E	303	1/1	0.97	0.09	44,44,44,44	0
54	MG	2T	3004	1/1	0.97	0.10	44,44,44,44	0
59	ZN	29	501	1/1	0.97	0.12	62,62,62,62	0
54	MG	2A	3615	1/1	0.97	0.14	35,35,35,35	0
54	MG	1A	3406	1/1	0.97	0.15	52,52,52,52	0
54	MG	1A	3515	1/1	0.97	0.29	30,30,30,30	0
54	MG	2A	3313	1/1	0.97	0.12	33,33,33,33	0
54	MG	2A	3537	1/1	0.97	0.15	42,42,42,42	0
54	MG	1A	3146	1/1	0.97	0.83	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
54	MG	2a	1691	1/1	0.97	0.17	56,56,56,56	0
54	MG	2A	3100	1/1	0.97	0.16	48,48,48,48	0
54	MG	1A	3149	1/1	0.97	0.25	21,21,21,21	0
54	MG	1A	3364	1/1	0.97	0.18	13,13,13,13	0
54	MG	1a	1672	1/1	0.97	0.27	51,51,51,51	0
54	MG	2T	3003	1/1	0.97	0.16	61,61,61,61	0
54	MG	1a	1804	1/1	0.97	0.18	59,59,59,59	0
54	MG	1A	3042	1/1	0.97	0.23	8,8,8,8	0
54	MG	1A	3145	1/1	0.97	0.50	43,43,43,43	0
54	MG	1a	1722	1/1	0.97	0.15	56,56,56,56	0
54	MG	1A	3653	1/1	0.97	0.45	41,41,41,41	0
54	MG	1A	3507	1/1	0.97	0.10	29,29,29,29	0
54	MG	2A	3638	1/1	0.97	0.09	32,32,32,32	0
54	MG	1A	3772	1/1	0.97	0.44	24,24,24,24	0
54	MG	1A	3294	1/1	0.97	0.10	46,46,46,46	0
54	MG	1A	3109	1/1	0.97	0.57	31,31,31,31	0
54	MG	2A	3701	1/1	0.97	0.17	47,47,47,47	0
54	MG	14	502	1/1	0.97	0.06	72,72,72,72	0
54	MG	1A	3087	1/1	0.97	0.53	26,26,26,26	0
54	MG	1A	3931	1/1	0.97	0.21	34,34,34,34	0
54	MG	2A	3141	1/1	0.97	0.37	39,39,39,39	0
54	MG	1F	308	1/1	0.97	0.39	29,29,29,29	0
54	MG	1a	1682	1/1	0.97	0.10	59,59,59,59	0
54	MG	1A	3107	1/1	0.97	0.26	27,27,27,27	0
54	MG	1A	3111	1/1	0.97	0.45	31,31,31,31	0
54	MG	2A	3474	1/1	0.97	0.13	50,50,50,50	0
54	MG	1a	1645	1/1	0.97	0.19	41,41,41,41	0
54	MG	2A	3390	1/1	0.97	0.13	31,31,31,31	0
54	MG	1X	102	1/1	0.97	0.16	31,31,31,31	0
54	MG	1a	1615	1/1	0.97	0.17	59,59,59,59	0
54	MG	1A	3348	1/1	0.97	0.13	41,41,41,41	0
54	MG	2A	3150	1/1	0.97	0.15	62,62,62,62	0
54	MG	1a	1603	1/1	0.97	0.15	45,45,45,45	0
54	MG	1A	3541	1/1	0.97	0.17	19,19,19,19	0
54	MG	2O	201	1/1	0.97	0.12	48,48,48,48	0
54	MG	2A	3015	1/1	0.97	0.42	43,43,43,43	0
54	MG	1A	3910	1/1	0.97	0.12	59,59,59,59	0
54	MG	1A	3254	1/1	0.97	0.36	30,30,30,30	0
54	MG	1A	3410	1/1	0.97	0.17	18,18,18,18	0
54	MG	1A	3715	1/1	0.97	0.11	19,19,19,19	0
54	MG	2A	3086	1/1	0.97	0.13	48,48,48,48	0
54	MG	1A	3912	1/1	0.97	0.21	43,43,43,43	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3509	1/1	0.97	0.14	41,41,41,41	0
54	MG	1A	3586	1/1	0.97	0.10	23,23,23,23	0
54	MG	2A	3209	1/1	0.97	0.65	43,43,43,43	0
54	MG	1A	3491	1/1	0.97	0.07	36,36,36,36	0
54	MG	1I	101	1/1	0.97	0.23	44,44,44,44	0
54	MG	1A	3607	1/1	0.97	0.14	50,50,50,50	0
54	MG	1e	3001	1/1	0.97	0.36	56,56,56,56	0
54	MG	1a	1632	1/1	0.97	0.13	35,35,35,35	0
54	MG	2A	3455	1/1	0.97	0.08	48,48,48,48	0
54	MG	1A	3600	1/1	0.97	0.21	27,27,27,27	0
54	MG	2A	3437	1/1	0.97	0.08	58,58,58,58	0
54	MG	1A	3893	1/1	0.97	0.11	50,50,50,50	0
54	MG	1A	3126	1/1	0.97	0.48	33,33,33,33	0
54	MG	2E	301	1/1	0.97	0.12	43,43,43,43	0
54	MG	1A	3027	1/1	0.97	0.26	34,34,34,34	0
54	MG	1A	3015	1/1	0.97	0.55	29,29,29,29	0
54	MG	1A	3984	1/1	0.97	0.12	37,37,37,37	0
54	MG	1a	1827	1/1	0.97	0.11	33,33,33,33	0
54	MG	2A	3634	1/1	0.97	0.15	42,42,42,42	0
54	MG	1A	3897	1/1	0.97	0.17	23,23,23,23	0
54	MG	1A	3478	1/1	0.97	0.17	16,16,16,16	0
54	MG	2A	3592	1/1	0.97	0.14	47,47,47,47	0
54	MG	1a	1643	1/1	0.97	0.10	52,52,52,52	0
54	MG	1A	3312	1/1	0.97	0.18	17,17,17,17	0
54	MG	1a	1733	1/1	0.97	0.12	55,55,55,55	0
54	MG	2A	3722	1/1	0.97	0.30	48,48,48,48	0
54	MG	1A	3357	1/1	0.97	0.13	20,20,20,20	0
54	MG	2A	3228	1/1	0.97	0.13	58,58,58,58	0
54	MG	2a	1701	1/1	0.97	0.26	42,42,42,42	0
54	MG	2A	3256	1/1	0.97	0.17	51,51,51,51	0
54	MG	1A	3855	1/1	0.97	0.18	25,25,25,25	0
54	MG	1A	3852	1/1	0.97	0.32	30,30,30,30	0
54	MG	1A	3176	1/1	0.97	0.17	49,49,49,49	0
54	MG	1A	3710	1/1	0.97	0.16	38,38,38,38	0
54	MG	2A	3571	1/1	0.97	0.20	42,42,42,42	0
54	MG	1a	1642	1/1	0.97	0.20	39,39,39,39	0
54	MG	1A	3248	1/1	0.97	0.14	31,31,31,31	0
54	MG	2A	3499	1/1	0.97	0.21	30,30,30,30	0
54	MG	1a	1829	1/1	0.97	0.18	42,42,42,42	0
54	MG	2A	3057	1/1	0.97	0.12	39,39,39,39	0
54	MG	2A	3033	1/1	0.97	0.17	46,46,46,46	0
54	MG	1a	1798	1/1	0.97	0.12	61,61,61,61	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3073	1/1	0.97	0.40	30,30,30,30	0
54	MG	1A	3979	1/1	0.97	0.28	47,47,47,47	0
54	MG	2A	3279	1/1	0.97	0.12	63,63,63,63	0
54	MG	1A	3375	1/1	0.97	0.15	16,16,16,16	0
54	MG	2a	1724	1/1	0.97	0.20	41,41,41,41	0
54	MG	1A	3113	1/1	0.97	0.15	18,18,18,18	0
54	MG	1a	1646	1/1	0.97	0.23	48,48,48,48	0
54	MG	1A	3925	1/1	0.97	0.14	49,49,49,49	0
54	MG	1A	3792	1/1	0.97	0.14	12,12,12,12	0
54	MG	2A	3221	1/1	0.97	0.40	57,57,57,57	0
54	MG	1A	3888	1/1	0.97	0.12	18,18,18,18	0
54	MG	1A	3227	1/1	0.97	0.35	25,25,25,25	0
54	MG	2a	1674	1/1	0.97	0.16	43,43,43,43	0
54	MG	1A	3414	1/1	0.97	0.14	49,49,49,49	0
54	MG	1A	3856	1/1	0.97	0.19	42,42,42,42	0
54	MG	1A	3978	1/1	0.97	0.34	26,26,26,26	0
54	MG	1A	3771	1/1	0.97	0.22	27,27,27,27	0
54	MG	2A	3008	1/1	0.97	0.10	57,57,57,57	0
54	MG	1A	3231	1/1	0.97	0.52	34,34,34,34	0
54	MG	1A	3685	1/1	0.97	0.10	42,42,42,42	0
54	MG	2A	3517	1/1	0.97	0.20	46,46,46,46	0
54	MG	1A	3041	1/1	0.97	0.12	12,12,12,12	0
54	MG	1A	3130	1/1	0.97	0.61	25,25,25,25	0
54	MG	1A	3066	1/1	0.97	0.50	30,30,30,30	0
54	MG	1E	304	1/1	0.97	0.17	16,16,16,16	0
54	MG	1A	3849	1/1	0.97	0.11	58,58,58,58	0
54	MG	2a	1702	1/1	0.97	0.13	73,73,73,73	0
54	MG	2A	3366	1/1	0.97	0.14	31,31,31,31	0
54	MG	1Q	201	1/1	0.97	0.12	38,38,38,38	0
54	MG	2A	3259	1/1	0.97	0.10	32,32,32,32	0
54	MG	1A	3997	1/1	0.97	0.25	23,23,23,23	0
54	MG	1A	3638	1/1	0.97	0.09	38,38,38,38	0
54	MG	1a	1745	1/1	0.97	0.09	47,47,47,47	0
54	MG	2B	3016	1/1	0.97	0.14	52,52,52,52	0
54	MG	1D	308	1/1	0.97	0.27	31,31,31,31	0
54	MG	2A	3307	1/1	0.97	0.19	51,51,51,51	0
54	MG	1a	1609	1/1	0.97	0.34	51,51,51,51	0
54	MG	2A	3125	1/1	0.97	0.20	38,38,38,38	0
54	MG	2A	3035	1/1	0.97	0.13	29,29,29,29	0
54	MG	2A	3011	1/1	0.97	0.13	21,21,21,21	0
54	MG	1A	3154	1/1	0.97	0.13	41,41,41,41	0
54	MG	1A	3097	1/1	0.97	0.58	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
54	MG	1A	3959	1/1	0.97	0.48	47,47,47,47	0
54	MG	1A	3658	1/1	0.97	0.10	24,24,24,24	0
54	MG	2A	3069	1/1	0.97	0.11	40,40,40,40	0
54	MG	1A	3249	1/1	0.97	0.41	34,34,34,34	0
54	MG	1Q	204	1/1	0.97	0.17	31,31,31,31	0
54	MG	1B	205	1/1	0.97	0.11	40,40,40,40	0
54	MG	2A	3427	1/1	0.97	0.10	57,57,57,57	0
54	MG	1A	3796	1/1	0.97	0.19	45,45,45,45	0
54	MG	2a	1708	1/1	0.97	0.27	52,52,52,52	0
54	MG	1A	3314	1/1	0.97	0.14	46,46,46,46	0
54	MG	1A	3813	1/1	0.97	0.13	56,56,56,56	0
54	MG	1A	3020	1/1	0.97	0.25	33,33,33,33	0
54	MG	1A	3063	1/1	0.97	0.24	32,32,32,32	0
54	MG	1A	3458	1/1	0.97	0.19	21,21,21,21	0
54	MG	1A	3018	1/1	0.97	0.41	24,24,24,24	0
54	MG	2a	1733	1/1	0.97	0.32	52,52,52,52	0
54	MG	2A	3516	1/1	0.97	0.20	19,19,19,19	0
54	MG	1A	3234	1/1	0.97	0.49	24,24,24,24	0
54	MG	1A	3587	1/1	0.97	0.15	26,26,26,26	0
54	MG	1A	3564	1/1	0.97	0.11	39,39,39,39	0
54	MG	2A	3227	1/1	0.97	0.66	38,38,38,38	0
54	MG	1A	3676	1/1	0.97	0.17	28,28,28,28	0
54	MG	2A	3395	1/1	0.97	0.12	56,56,56,56	0
54	MG	1a	1663	1/1	0.97	0.15	59,59,59,59	0
54	MG	2A	3267	1/1	0.97	0.14	52,52,52,52	0
54	MG	1A	3157	1/1	0.97	0.13	28,28,28,28	0
54	MG	2A	3351	1/1	0.97	0.17	25,25,25,25	0
54	MG	1A	3596	1/1	0.97	0.40	38,38,38,38	0
54	MG	2A	3062	1/1	0.97	0.43	35,35,35,35	0
54	MG	1a	1728	1/1	0.97	0.10	51,51,51,51	0
54	MG	2A	3574	1/1	0.97	0.15	52,52,52,52	0
54	MG	1A	3482	1/1	0.97	0.18	17,17,17,17	0
54	MG	1A	3350	1/1	0.97	0.17	29,29,29,29	0
54	MG	1A	3360	1/1	0.97	0.16	18,18,18,18	0
54	MG	2a	1686	1/1	0.97	0.09	52,52,52,52	0
54	MG	1A	4001	1/1	0.97	0.20	37,37,37,37	0
54	MG	2A	3584	1/1	0.97	0.13	46,46,46,46	0
54	MG	1A	3044	1/1	0.97	0.15	23,23,23,23	0
54	MG	1Q	202	1/1	0.97	0.14	29,29,29,29	0
54	MG	1A	3171	1/1	0.98	0.23	23,23,23,23	0
54	MG	1A	3114	1/1	0.98	0.15	22,22,22,22	0
54	MG	1A	3774	1/1	0.98	0.10	12,12,12,12	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1A	3269	1/1	0.98	0.15	12,12,12,12	0
54	MG	2A	3276	1/1	0.98	0.12	44,44,44,44	0
54	MG	1A	3115	1/1	0.98	0.17	22,22,22,22	0
54	MG	2A	3378	1/1	0.98	0.10	28,28,28,28	0
54	MG	2A	3572	1/1	0.98	0.10	21,21,21,21	0
54	MG	1A	3874	1/1	0.98	0.15	43,43,43,43	0
54	MG	1A	3195	1/1	0.98	0.33	33,33,33,33	0
54	MG	1A	3890	1/1	0.98	0.17	46,46,46,46	0
54	MG	1A	3273	1/1	0.98	0.11	30,30,30,30	0
54	MG	1A	3393	1/1	0.98	0.17	18,18,18,18	0
54	MG	1A	3351	1/1	0.98	0.14	18,18,18,18	0
54	MG	1A	3416	1/1	0.98	0.10	48,48,48,48	0
54	MG	1D	301	1/1	0.98	0.30	25,25,25,25	0
60	SF4	1d	302	8/8	0.98	0.17	48,59,66,72	0
54	MG	1A	3185	1/1	0.98	0.31	42,42,42,42	0
54	MG	1a	1607	1/1	0.98	0.11	51,51,51,51	0
54	MG	1A	4006	1/1	0.98	0.23	31,31,31,31	0
54	MG	1A	3474	1/1	0.98	0.15	44,44,44,44	0
54	MG	2A	3407	1/1	0.98	0.11	50,50,50,50	0
54	MG	1A	3412	1/1	0.98	0.16	45,45,45,45	0
54	MG	1a	1670	1/1	0.98	0.22	50,50,50,50	0
54	MG	1A	3344	1/1	0.98	0.12	21,21,21,21	0
54	MG	1A	3985	1/1	0.98	0.35	36,36,36,36	0
54	MG	1A	3860	1/1	0.98	0.31	43,43,43,43	0
54	MG	1a	1706	1/1	0.98	0.17	28,28,28,28	0
54	MG	1A	3489	1/1	0.98	0.14	21,21,21,21	0
54	MG	1A	3202	1/1	0.98	0.66	32,32,32,32	0
54	MG	1A	3585	1/1	0.98	0.11	36,36,36,36	0
54	MG	1A	3470	1/1	0.98	0.12	36,36,36,36	0
54	MG	1A	3553	1/1	0.98	0.14	18,18,18,18	0
54	MG	2A	3135	1/1	0.98	0.13	67,67,67,67	0
54	MG	1A	3306	1/1	0.98	0.13	23,23,23,23	0
54	MG	2A	3424	1/1	0.98	0.12	52,52,52,52	0
54	MG	2A	3559	1/1	0.98	0.19	32,32,32,32	0
54	MG	1A	3076	1/1	0.98	0.36	27,27,27,27	0
54	MG	1A	3776	1/1	0.98	0.13	26,26,26,26	0
54	MG	1A	3290	1/1	0.98	0.16	32,32,32,32	0
54	MG	2A	3064	1/1	0.98	0.23	21,21,21,21	0
54	MG	1A	3763	1/1	0.98	0.24	46,46,46,46	0
54	MG	1A	3433	1/1	0.98	0.12	32,32,32,32	0
60	SF4	2d	501	8/8	0.98	0.14	61,71,81,92	0
54	MG	1A	3999	1/1	0.98	0.53	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
54	MG	1A	3155	1/1	0.98	0.19	26,26,26,26	0
54	MG	1A	3495	1/1	0.98	0.14	18,18,18,18	0
54	MG	2A	3169	1/1	0.98	0.35	38,38,38,38	0
54	MG	1A	4025	1/1	0.98	0.37	30,30,30,30	0
54	MG	1A	3464	1/1	0.98	0.14	56,56,56,56	0
54	MG	2V	201	1/1	0.98	0.16	60,60,60,60	0
54	MG	1A	3317	1/1	0.98	0.10	56,56,56,56	0
54	MG	1A	3996	1/1	0.98	0.40	27,27,27,27	0
54	MG	2A	3119	1/1	0.98	0.09	64,64,64,64	0
54	MG	1A	3684	1/1	0.98	0.12	46,46,46,46	0
54	MG	1A	3652	1/1	0.98	0.29	44,44,44,44	0
54	MG	2A	3344	1/1	0.98	0.17	37,37,37,37	0
54	MG	1A	3510	1/1	0.98	0.15	34,34,34,34	0
54	MG	1Q	203	1/1	0.98	0.24	36,36,36,36	0
54	MG	1A	3345	1/1	0.98	0.22	50,50,50,50	0
54	MG	1a	1815	1/1	0.98	0.10	44,44,44,44	0
54	MG	1A	3853	1/1	0.98	0.14	15,15,15,15	0
54	MG	2A	3266	1/1	0.98	0.14	40,40,40,40	0
54	MG	1A	3037	1/1	0.98	0.16	39,39,39,39	0
54	MG	2T	3002	1/1	0.98	0.11	61,61,61,61	0
54	MG	1A	3407	1/1	0.98	0.12	38,38,38,38	0
54	MG	1A	3089	1/1	0.98	0.29	26,26,26,26	0
54	MG	2a	1609	1/1	0.98	0.17	46,46,46,46	0
54	MG	1A	3243	1/1	0.98	0.13	35,35,35,35	0
54	MG	1A	3614	1/1	0.98	0.16	17,17,17,17	0
54	MG	1A	3516	1/1	0.98	0.14	31,31,31,31	0
54	MG	1A	3920	1/1	0.98	0.15	21,21,21,21	0
54	MG	2A	3605	1/1	0.98	0.10	62,62,62,62	0
54	MG	1A	3136	1/1	0.98	0.20	24,24,24,24	0
54	MG	1a	1758	1/1	0.98	0.20	52,52,52,52	0
54	MG	2A	3340	1/1	0.98	0.19	55,55,55,55	0
54	MG	2A	3311	1/1	0.98	0.13	43,43,43,43	0
54	MG	1A	3842	1/1	0.98	0.10	42,42,42,42	0
54	MG	2A	3491	1/1	0.98	0.11	46,46,46,46	0
54	MG	2A	3066	1/1	0.98	0.16	51,51,51,51	0
54	MG	2A	3333	1/1	0.98	0.09	28,28,28,28	0
54	MG	2A	3485	1/1	0.98	0.10	45,45,45,45	0
54	MG	1A	3270	1/1	0.98	0.12	11,11,11,11	0
54	MG	1A	3747	1/1	0.98	0.19	44,44,44,44	0
54	MG	1A	3633	1/1	0.98	0.19	51,51,51,51	0
54	MG	1A	3104	1/1	0.98	0.38	23,23,23,23	0
54	MG	1A	3199	1/1	0.98	0.66	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
54	MG	1A	3648	1/1	0.98	0.21	32,32,32,32	0
54	MG	1A	3525	1/1	0.98	0.17	37,37,37,37	0
54	MG	1A	3965	1/1	0.98	0.20	10,10,10,10	0
54	MG	1A	3803	1/1	0.98	0.48	34,34,34,34	0
54	MG	1A	3277	1/1	0.98	0.35	28,28,28,28	0
54	MG	2A	3452	1/1	0.98	0.17	38,38,38,38	0
54	MG	1A	3418	1/1	0.98	0.14	22,22,22,22	0
54	MG	1A	3834	1/1	0.98	0.14	31,31,31,31	0
54	MG	2A	3625	1/1	0.98	0.12	16,16,16,16	0
54	MG	1A	3331	1/1	0.98	0.10	12,12,12,12	0
54	MG	1A	3671	1/1	0.98	0.10	15,15,15,15	0
54	MG	1A	3480	1/1	0.98	0.14	36,36,36,36	0
54	MG	1A	3540	1/1	0.98	0.14	25,25,25,25	0
54	MG	1A	3164	1/1	0.98	0.44	22,22,22,22	0
54	MG	2A	3145	1/1	0.98	0.63	44,44,44,44	0
54	MG	1A	3024	1/1	0.98	0.33	29,29,29,29	0
54	MG	1A	3725	1/1	0.98	0.08	36,36,36,36	0
54	MG	2A	3107	1/1	0.98	0.13	43,43,43,43	0
54	MG	1A	3378	1/1	0.98	0.09	20,20,20,20	0
54	MG	2A	3415	1/1	0.98	0.14	41,41,41,41	0
54	MG	1A	3005	1/1	0.98	0.17	15,15,15,15	0
54	MG	1A	3694	1/1	0.98	0.09	40,40,40,40	0
54	MG	2A	3026	1/1	0.98	0.42	41,41,41,41	0
54	MG	13	101	1/1	0.98	0.15	53,53,53,53	0
59	ZN	15	101	1/1	0.98	0.20	39,39,39,39	0
54	MG	2A	3090	1/1	0.98	0.14	19,19,19,19	0
59	ZN	14	501	1/1	0.98	0.14	80,80,80,80	0
54	MG	1A	3616	1/1	0.98	0.23	16,16,16,16	0
54	MG	2A	3006	1/1	0.98	0.54	43,43,43,43	0
54	MG	1A	3064	1/1	0.98	0.40	29,29,29,29	0
54	MG	1a	1760	1/1	0.98	0.19	52,52,52,52	0
54	MG	1A	3593	1/1	0.98	0.16	40,40,40,40	0
54	MG	2A	3530	1/1	0.98	0.13	25,25,25,25	0
54	MG	1A	3319	1/1	0.98	0.14	15,15,15,15	0
54	MG	1A	3225	1/1	0.98	0.30	32,32,32,32	0
54	MG	1A	3971	1/1	0.98	0.13	16,16,16,16	0
54	MG	2A	3278	1/1	0.98	0.10	25,25,25,25	0
54	MG	1A	3736	1/1	0.98	0.16	41,41,41,41	0
54	MG	2A	3241	1/1	0.98	0.20	47,47,47,47	0
54	MG	1A	3788	1/1	0.98	0.16	23,23,23,23	0
54	MG	2A	3357	1/1	0.98	0.15	41,41,41,41	0
54	MG	1A	3384	1/1	0.98	0.15	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
54	MG	1A	3006	1/1	0.98	0.17	17,17,17,17	0
54	MG	2A	3492	1/1	0.98	0.25	66,66,66,66	0
54	MG	2A	3643	1/1	0.98	0.17	34,34,34,34	0
54	MG	2A	3515	1/1	0.98	0.17	54,54,54,54	0
54	MG	2A	3713	1/1	0.98	0.82	40,40,40,40	0
54	MG	1a	1850	1/1	0.98	0.07	45,45,45,45	0
54	MG	1a	1764	1/1	0.98	0.10	61,61,61,61	0
54	MG	2A	3316	1/1	0.98	0.18	41,41,41,41	0
54	MG	1A	3595	1/1	0.98	0.20	16,16,16,16	0
54	MG	1A	3435	1/1	0.98	0.22	37,37,37,37	0
54	MG	1A	3165	1/1	0.98	0.35	28,28,28,28	0
54	MG	2A	3133	1/1	0.98	0.14	47,47,47,47	0
54	MG	1A	3359	1/1	0.98	0.14	15,15,15,15	0
54	MG	1A	3627	1/1	0.98	0.26	30,30,30,30	0
54	MG	1A	3285	1/1	0.98	0.29	36,36,36,36	0
54	MG	1A	3967	1/1	0.98	0.15	19,19,19,19	0
54	MG	1A	3845	1/1	0.98	0.17	37,37,37,37	0
54	MG	1A	4018	1/1	0.98	0.23	36,36,36,36	0
54	MG	1a	1724	1/1	0.98	0.18	41,41,41,41	0
54	MG	2A	3617	1/1	0.98	0.14	46,46,46,46	0
54	MG	1A	3365	1/1	0.98	0.15	13,13,13,13	0
54	MG	1a	1693	1/1	0.98	0.08	42,42,42,42	0
54	MG	1A	3537	1/1	0.98	0.18	46,46,46,46	0
54	MG	1A	3956	1/1	0.98	0.09	24,24,24,24	0
54	MG	2A	3396	1/1	0.98	0.21	29,29,29,29	0
54	MG	1a	1801	1/1	0.98	0.15	43,43,43,43	0
54	MG	1A	4015	1/1	0.98	0.38	39,39,39,39	0
54	MG	1D	305	1/1	0.98	0.26	39,39,39,39	0
54	MG	1A	3264	1/1	0.98	0.64	42,42,42,42	0
54	MG	1A	3477	1/1	0.98	0.16	16,16,16,16	0
54	MG	2A	3637	1/1	0.98	0.15	30,30,30,30	0
54	MG	1A	3096	1/1	0.98	0.33	25,25,25,25	0
54	MG	1A	3431	1/1	0.98	0.13	34,34,34,34	0
54	MG	1A	3103	1/1	0.98	0.47	25,25,25,25	0
54	MG	2A	3653	1/1	0.98	0.28	48,48,48,48	0
54	MG	1A	3536	1/1	0.98	0.19	26,26,26,26	0
54	MG	1A	3336	1/1	0.98	0.12	33,33,33,33	0
54	MG	1A	3896	1/1	0.98	0.12	22,22,22,22	0
54	MG	1A	3432	1/1	0.98	0.23	35,35,35,35	0
54	MG	1A	3915	1/1	0.99	0.11	25,25,25,25	0
59	ZN	26	501	1/1	0.99	0.18	59,59,59,59	0
54	MG	1a	1716	1/1	0.99	0.12	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
54	MG	2A	3003	1/1	0.99	0.16	37,37,37,37	0
55	K	2A	3246	1/1	0.99	0.11	30,30,30,30	0
54	MG	1A	3117	1/1	0.99	0.17	39,39,39,39	0
54	MG	1A	3740	1/1	0.99	0.18	29,29,29,29	0
54	MG	1A	3017	1/1	0.99	0.36	25,25,25,25	0
54	MG	2A	3650	1/1	0.99	0.16	36,36,36,36	0
54	MG	1A	3003	1/1	0.99	0.10	31,31,31,31	0
54	MG	1A	3601	1/1	0.99	0.14	31,31,31,31	0
54	MG	1A	3843	1/1	0.99	0.23	30,30,30,30	0
54	MG	1A	3420	1/1	0.99	0.13	50,50,50,50	0
54	MG	1A	3657	1/1	0.99	0.29	31,31,31,31	0
54	MG	1A	3309	1/1	0.99	0.10	34,34,34,34	0
54	MG	2A	3117	1/1	0.99	0.26	36,36,36,36	0
54	MG	1A	3221	1/1	0.99	0.51	24,24,24,24	0
54	MG	1A	3170	1/1	0.99	0.26	28,28,28,28	0
54	MG	1A	3683	1/1	0.99	0.14	25,25,25,25	0
54	MG	1A	3016	1/1	0.99	0.49	17,17,17,17	0
54	MG	1A	3769	1/1	0.99	0.17	19,19,19,19	0
54	MG	1A	3879	1/1	0.99	0.12	33,33,33,33	0
54	MG	1A	4014	1/1	0.99	0.40	28,28,28,28	0
54	MG	1A	3828	1/1	0.99	0.15	13,13,13,13	0
54	MG	1A	3511	1/1	0.99	0.07	32,32,32,32	0
54	MG	1A	4004	1/1	0.99	0.25	25,25,25,25	0
54	MG	1D	306	1/1	0.99	0.15	11,11,11,11	0
54	MG	1A	3620	1/1	0.99	0.06	44,44,44,44	0
54	MG	2A	3091	1/1	0.99	0.15	61,61,61,61	0
54	MG	2A	3243	1/1	0.99	0.15	18,18,18,18	0
54	MG	1A	3645	1/1	0.99	0.12	35,35,35,35	0
54	MG	2A	3257	1/1	0.99	0.18	43,43,43,43	0
54	MG	1A	3298	1/1	0.99	0.18	14,14,14,14	0
54	MG	2A	3346	1/1	0.99	0.21	52,52,52,52	0
54	MG	1A	3034	1/1	0.99	0.10	33,33,33,33	0
54	MG	2A	3461	1/1	0.99	0.10	55,55,55,55	0
54	MG	1A	3994	1/1	0.99	0.31	26,26,26,26	0
54	MG	1D	304	1/1	0.99	0.18	33,33,33,33	0
55	K	1A	3287	1/1	0.99	0.06	27,27,27,27	0
54	MG	2A	3009	1/1	0.99	0.20	30,30,30,30	0
54	MG	1A	3787	1/1	0.99	0.23	40,40,40,40	0
59	ZN	16	501	1/1	0.99	0.27	46,46,46,46	0
54	MG	2A	3365	1/1	0.99	0.23	32,32,32,32	0
54	MG	2A	3442	1/1	0.99	0.16	27,27,27,27	0
54	MG	1V	202	1/1	0.99	0.15	47,47,47,47	0

*Continued on next page...*

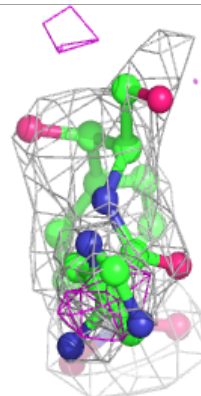
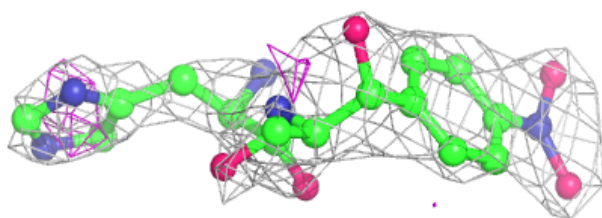
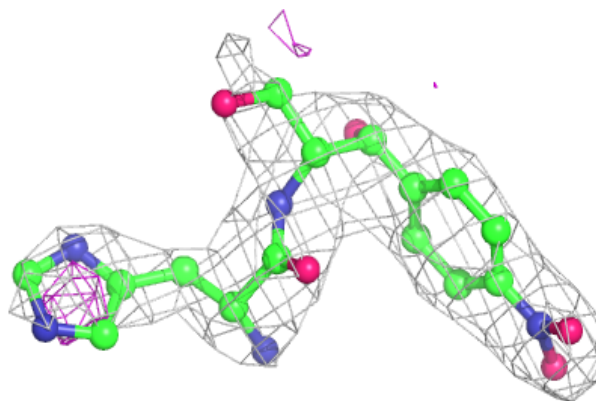
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
54	MG	1a	1638	1/1	0.99	0.16	44,44,44,44	0
54	MG	2A	3560	1/1	0.99	0.15	43,43,43,43	0
54	MG	2A	3027	1/1	0.99	0.13	30,30,30,30	0
54	MG	1A	3081	1/1	0.99	0.43	34,34,34,34	0
54	MG	1A	3323	1/1	0.99	0.14	18,18,18,18	0
54	MG	1A	3661	1/1	0.99	0.11	32,32,32,32	0
54	MG	2A	3420	1/1	0.99	0.17	28,28,28,28	0
54	MG	1A	3054	1/1	0.99	0.12	21,21,21,21	0
54	MG	1A	3895	1/1	0.99	0.11	16,16,16,16	0
54	MG	2E	304	1/1	0.99	0.13	29,29,29,29	0
54	MG	2A	3403	1/1	0.99	0.29	57,57,57,57	0
59	ZN	1n	501	1/1	0.99	0.15	60,60,60,60	0
54	MG	1B	220	1/1	0.99	0.15	20,20,20,20	0
59	ZN	19	501	1/1	0.99	0.23	39,39,39,39	0
54	MG	1A	3084	1/1	0.99	0.21	33,33,33,33	0
54	MG	1A	3869	1/1	0.99	0.14	56,56,56,56	0
54	MG	2A	3585	1/1	0.99	0.14	57,57,57,57	0
54	MG	1A	3625	1/1	0.99	0.10	35,35,35,35	0
59	ZN	1Y	501	1/1	0.99	0.20	46,46,46,46	0
59	ZN	25	501	1/1	0.99	0.22	44,44,44,44	0

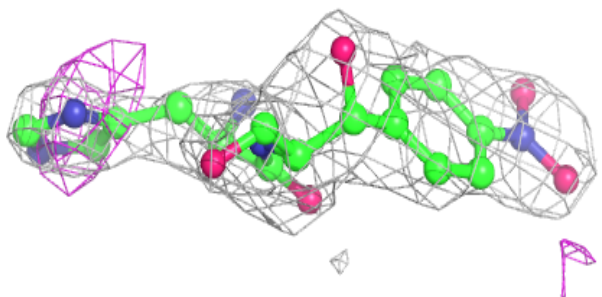
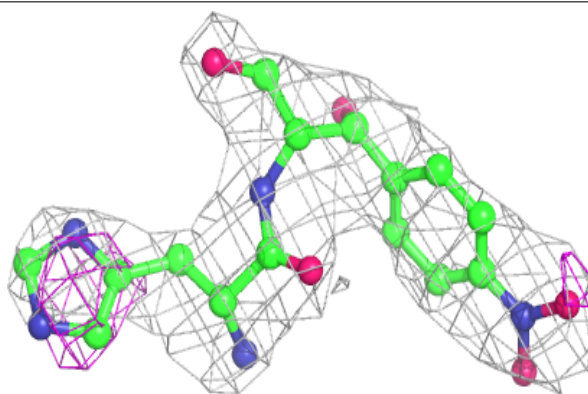
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around EZP 2A 3709:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around EZP 1A 3987:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.