



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 4, 2025 – 08:31 AM EST

PDB ID : 4Y4P  
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome with rRNA modifications and bound to mRNA and A-, P- and E-site tRNAs at 2.5Å resolution  
Authors : Polikanov, Y.S.; Melnikov, S.V.; Soll, D.; Steitz, T.A.  
Deposited on : 2015-02-10  
Resolution : 2.50 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 types of validation reports are described at

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

---

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

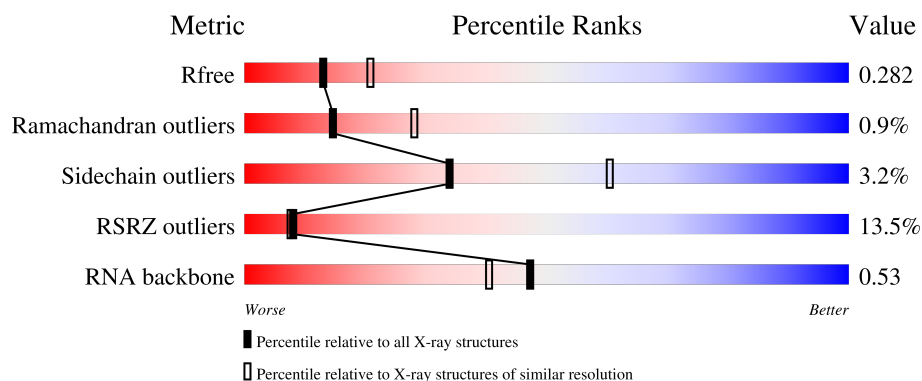
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	164625	5504 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)
RNA backbone	3690	1181 (2.80-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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>6%</div> <div>81%</div> <div>16%</div> <div>..</div> </div>
1	2A	2915	<div> <div>4%</div> <div>77%</div> <div>18%</div> <div>..</div> </div>
2	1B	121	<div> <div>%</div> <div>89%</div> <div>9%</div> <div>..</div> </div>
2	2B	121	<div> <div>12%</div> <div>68%</div> <div>31%</div> <div>..</div> </div>
3	1D	276	<div> <div>%</div> <div>97%</div> <div>.</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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	
15	2T	146	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
16	1U	118	<div> <div>2%</div> <div>97%</div> <div>..</div> </div>
16	2U	118	<div> <div>%</div> <div>97%</div> <div>..</div> </div>
17	1V	101	<div> <div>3%</div> <div>94%</div> <div>5% .</div> </div>
17	2V	101	<div> <div>5%</div> <div>94%</div> <div>5% .</div> </div>
18	1W	113	<div> <div>2%</div> <div>95%</div> <div>..</div> </div>
18	2W	113	<div> <div>2%</div> <div>95%</div> <div>..</div> </div>
19	1X	96	<div> <div>3%</div> <div>97%</div> <div>..</div> </div>
19	2X	96	<div> <div>%</div> <div>97%</div> <div>...</div> </div>
20	1Y	110	<div> <div>8%</div> <div>93%</div> <div>5% .</div> </div>
20	2Y	110	<div> <div>12%</div> <div>93%</div> <div>5% .</div> </div>
21	1Z	206	<div> <div>10%</div> <div>71%</div> <div>25%</div> </div>
21	2Z	206	<div> <div>47%</div> <div>77%</div> <div>22%</div> </div>
22	10	85	<div> <div>94%</div> <div>...</div> </div>
22	20	85	<div> <div>20%</div> <div>95%</div> <div>..</div> </div>
23	11	98	<div> <div>%</div> <div>98%</div> <div>..</div> </div>
23	21	98	<div> <div>13%</div> <div>97%</div> <div>..</div> </div>
24	12	72	<div> <div>7%</div> <div>96%</div> <div>..</div> </div>
24	22	72	<div> <div>4%</div> <div>97%</div> <div>.</div> </div>
25	13	60	<div> <div>2%</div> <div>95%</div> <div>..</div> </div>
25	23	60	<div> <div>3%</div> <div>93%</div> <div>5% .</div> </div>
26	14	71	<div> <div>31%</div> <div>87%</div> <div>10% .</div> </div>
26	24	71	<div> <div>51%</div> <div>86%</div> <div>11% .</div> </div>
27	15	60	<div> <div>2%</div> <div>93%</div> <div>5% .</div> </div>
27	25	60	<div> <div>2%</div> <div>92%</div> <div>7% .</div> </div>
28	16	54	<div> <div>2%</div> <div>94%</div> <div>..</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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	
40	2i	128	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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	
53	1v	24	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	2v	24	
54	1w	76	
54	1y	76	
54	2w	76	
54	2y	76	
55	1x	77	
55	2x	77	

## 2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 300910 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

*Continued on next page...*

*Continued from previous page...*

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

*Continued on next page...*

*Continued from previous page...*

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

*Continued on next page...*

*Continued from previous page...*

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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

- Molecule 53 is a RNA chain called mRNA.

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

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

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1A	1141	Total	Mg	0	0
			1141	1141		
56	1B	37	Total	Mg	0	0
			37	37		
56	1D	12	Total	Mg	0	0
			12	12		
56	1E	11	Total	Mg	0	0
			11	11		
56	1F	8	Total	Mg	0	0
			8	8		
56	1G	5	Total	Mg	0	0
			5	5		
56	1I	1	Total	Mg	0	0
			1	1		
56	1N	6	Total	Mg	0	0
			6	6		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1O	7	Total 7	Mg 7	0	0
56	1P	4	Total 4	Mg 4	0	0
56	1Q	6	Total 6	Mg 6	0	0
56	1R	3	Total 3	Mg 3	0	0
56	1S	3	Total 3	Mg 3	0	0
56	1T	2	Total 2	Mg 2	0	0
56	1U	8	Total 8	Mg 8	0	0
56	1V	3	Total 3	Mg 3	0	0
56	1W	5	Total 5	Mg 5	0	0
56	1X	6	Total 6	Mg 6	0	0
56	1Y	3	Total 3	Mg 3	0	0
56	1Z	3	Total 3	Mg 3	0	0
56	10	6	Total 6	Mg 6	0	0
56	11	3	Total 3	Mg 3	0	0
56	12	1	Total 1	Mg 1	0	0
56	13	3	Total 3	Mg 3	0	0
56	15	2	Total 2	Mg 2	0	0
56	16	3	Total 3	Mg 3	0	0
56	17	1	Total 1	Mg 1	0	0
56	18	3	Total 3	Mg 3	0	0
56	19	2	Total 2	Mg 2	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	1a	229	Total 229	Mg 229	0	0
56	1b	2	Total 2	Mg 2	0	0
56	1d	1	Total 1	Mg 1	0	0
56	1e	1	Total 1	Mg 1	0	0
56	1f	2	Total 2	Mg 2	0	0
56	1l	3	Total 3	Mg 3	0	0
56	1n	2	Total 2	Mg 2	0	0
56	1s	1	Total 1	Mg 1	0	0
56	1t	1	Total 1	Mg 1	0	0
56	1v	1	Total 1	Mg 1	0	0
56	1w	11	Total 11	Mg 11	0	0
56	1x	16	Total 16	Mg 16	0	0
56	1y	4	Total 4	Mg 4	0	0
56	2A	909	Total 909	Mg 909	0	0
56	2B	21	Total 21	Mg 21	0	0
56	2D	5	Total 5	Mg 5	0	0
56	2E	9	Total 9	Mg 9	0	0
56	2F	4	Total 4	Mg 4	0	0
56	2G	1	Total 1	Mg 1	0	0
56	2N	1	Total 1	Mg 1	0	0
56	2O	1	Total 1	Mg 1	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2P	1	Total 1	Mg 1	0	0
56	2Q	3	Total 3	Mg 3	0	0
56	2R	1	Total 1	Mg 1	0	0
56	2T	3	Total 3	Mg 3	0	0
56	2U	4	Total 4	Mg 4	0	0
56	2V	1	Total 1	Mg 1	0	0
56	2W	3	Total 3	Mg 3	0	0
56	2X	3	Total 3	Mg 3	0	0
56	2Y	1	Total 1	Mg 1	0	0
56	2Z	1	Total 1	Mg 1	0	0
56	20	3	Total 3	Mg 3	0	0
56	23	2	Total 2	Mg 2	0	0
56	25	4	Total 4	Mg 4	0	0
56	27	1	Total 1	Mg 1	0	0
56	28	2	Total 2	Mg 2	0	0
56	2a	244	Total 244	Mg 244	0	0
56	2d	1	Total 1	Mg 1	0	0
56	2e	1	Total 1	Mg 1	0	0
56	2f	1	Total 1	Mg 1	0	0
56	2g	1	Total 1	Mg 1	0	0
56	2i	1	Total 1	Mg 1	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	2j	2	Total 2	Mg 2	0	0
56	2l	2	Total 2	Mg 2	0	0
56	2n	1	Total 1	Mg 1	0	0
56	2q	2	Total 2	Mg 2	0	0
56	2r	2	Total 2	Mg 2	0	0
56	2t	1	Total 1	Mg 1	0	0
56	2v	2	Total 2	Mg 2	0	0
56	2w	8	Total 8	Mg 8	0	0
56	2x	5	Total 5	Mg 5	0	0
56	2y	7	Total 7	Mg 7	0	0

- Molecule 57 is POTASSIUM ION (three-letter code: K) (formula: K).

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

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

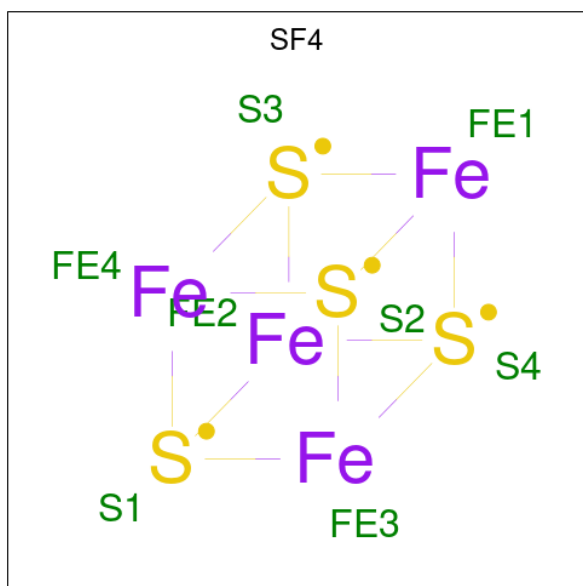
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	1Y	1	Total 1	Zn 1	0	0
58	14	1	Total 1	Zn 1	0	0
58	15	1	Total 1	Zn 1	0	0
58	16	1	Total 1	Zn 1	0	0
58	19	1	Total 1	Zn 1	0	0

*Continued on next page...*

Continued from previous page...

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

- Molecule 59 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



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

- Molecule 60 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1A	2238	Total 2238	O 2238	0	0
60	1B	68	Total 68	O 68	0	0
60	1D	28	Total 28	O 28	0	0
60	1E	28	Total 28	O 28	0	0
60	1F	13	Total 13	O 13	0	0
60	1G	7	Total 7	O 7	0	0
60	1H	2	Total 2	O 2	0	0
60	1I	3	Total 3	O 3	0	0
60	1N	7	Total 7	O 7	0	0
60	1O	8	Total 8	O 8	0	0
60	1P	23	Total 23	O 23	0	0
60	1Q	14	Total 14	O 14	0	0
60	1R	14	Total 14	O 14	0	0
60	1S	5	Total 5	O 5	0	0
60	1T	8	Total 8	O 8	0	0
60	1U	11	Total 11	O 11	0	0
60	1V	9	Total 9	O 9	0	0
60	1W	6	Total 6	O 6	0	0
60	1X	8	Total 8	O 8	0	0
60	1Y	4	Total 4	O 4	0	0
60	1Z	1	Total 1	O 1	0	0
60	10	12	Total 12	O 12	0	0

Continued on next page...



*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	11	10	Total 10	O 10	0	0
60	12	4	Total 4	O 4	0	0
60	13	6	Total 6	O 6	0	0
60	14	1	Total 1	O 1	0	0
60	15	6	Total 6	O 6	0	0
60	16	3	Total 3	O 3	0	0
60	17	9	Total 9	O 9	0	0
60	18	13	Total 13	O 13	0	0
60	1a	438	Total 438	O 438	0	0
60	1b	1	Total 1	O 1	0	0
60	1d	1	Total 1	O 1	0	0
60	1e	1	Total 1	O 1	0	0
60	1f	1	Total 1	O 1	0	0
60	1g	1	Total 1	O 1	0	0
60	1i	1	Total 1	O 1	0	0
60	1l	8	Total 8	O 8	0	0
60	1m	2	Total 2	O 2	0	0
60	1o	1	Total 1	O 1	0	0
60	1p	1	Total 1	O 1	0	0
60	1q	4	Total 4	O 4	0	0
60	1u	1	Total 1	O 1	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	1v	5	Total 5	O 5	0	0
60	1w	21	Total 21	O 21	0	0
60	1x	15	Total 15	O 15	0	0
60	1y	1	Total 1	O 1	0	0
60	2A	1389	Total 1389	O 1389	0	0
60	2B	26	Total 26	O 26	0	0
60	2D	28	Total 28	O 28	0	0
60	2E	16	Total 16	O 16	0	0
60	2F	16	Total 16	O 16	0	0
60	2H	1	Total 1	O 1	0	0
60	2I	4	Total 4	O 4	0	0
60	2N	1	Total 1	O 1	0	0
60	2P	14	Total 14	O 14	0	0
60	2Q	2	Total 2	O 2	0	0
60	2R	2	Total 2	O 2	0	0
60	2T	6	Total 6	O 6	0	0
60	2U	2	Total 2	O 2	0	0
60	2V	2	Total 2	O 2	0	0
60	2W	2	Total 2	O 2	0	0
60	2X	5	Total 5	O 5	0	0
60	2Y	1	Total 1	O 1	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2Z	2	Total 2	O 2	0	0
60	20	7	Total 7	O 7	0	0
60	21	12	Total 12	O 12	0	0
60	22	1	Total 1	O 1	0	0
60	23	1	Total 1	O 1	0	0
60	25	4	Total 4	O 4	0	0
60	26	1	Total 1	O 1	0	0
60	27	4	Total 4	O 4	0	0
60	28	6	Total 6	O 6	0	0
60	29	1	Total 1	O 1	0	0
60	2a	377	Total 377	O 377	0	0
60	2d	1	Total 1	O 1	0	0
60	2e	2	Total 2	O 2	0	0
60	2g	1	Total 1	O 1	0	0
60	2i	1	Total 1	O 1	0	0
60	2j	4	Total 4	O 4	0	0
60	2l	5	Total 5	O 5	0	0
60	2o	1	Total 1	O 1	0	0
60	2p	2	Total 2	O 2	0	0
60	2q	1	Total 1	O 1	0	0
60	2r	1	Total 1	O 1	0	0

*Continued on next page...*

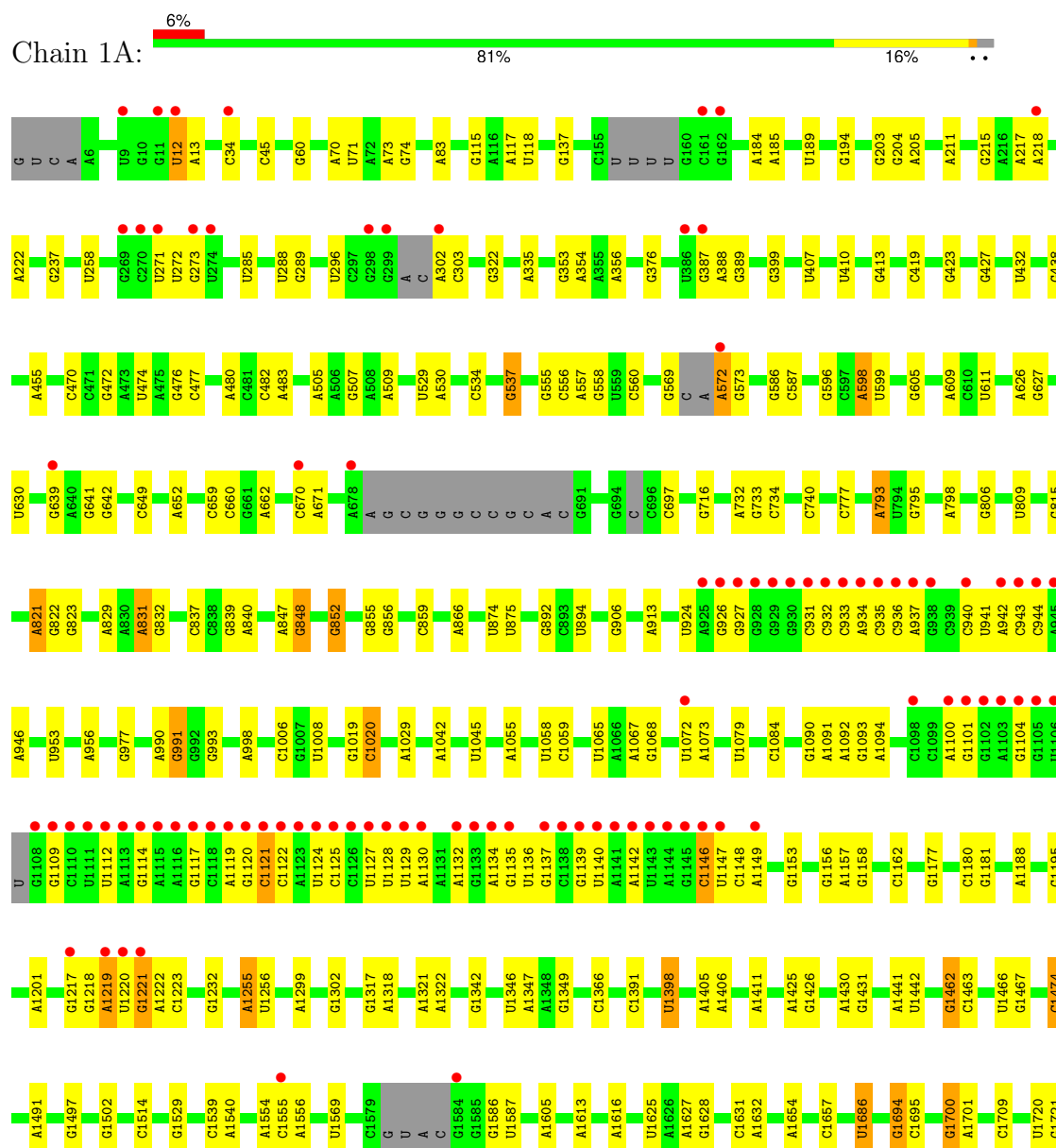
*Continued from previous page...*

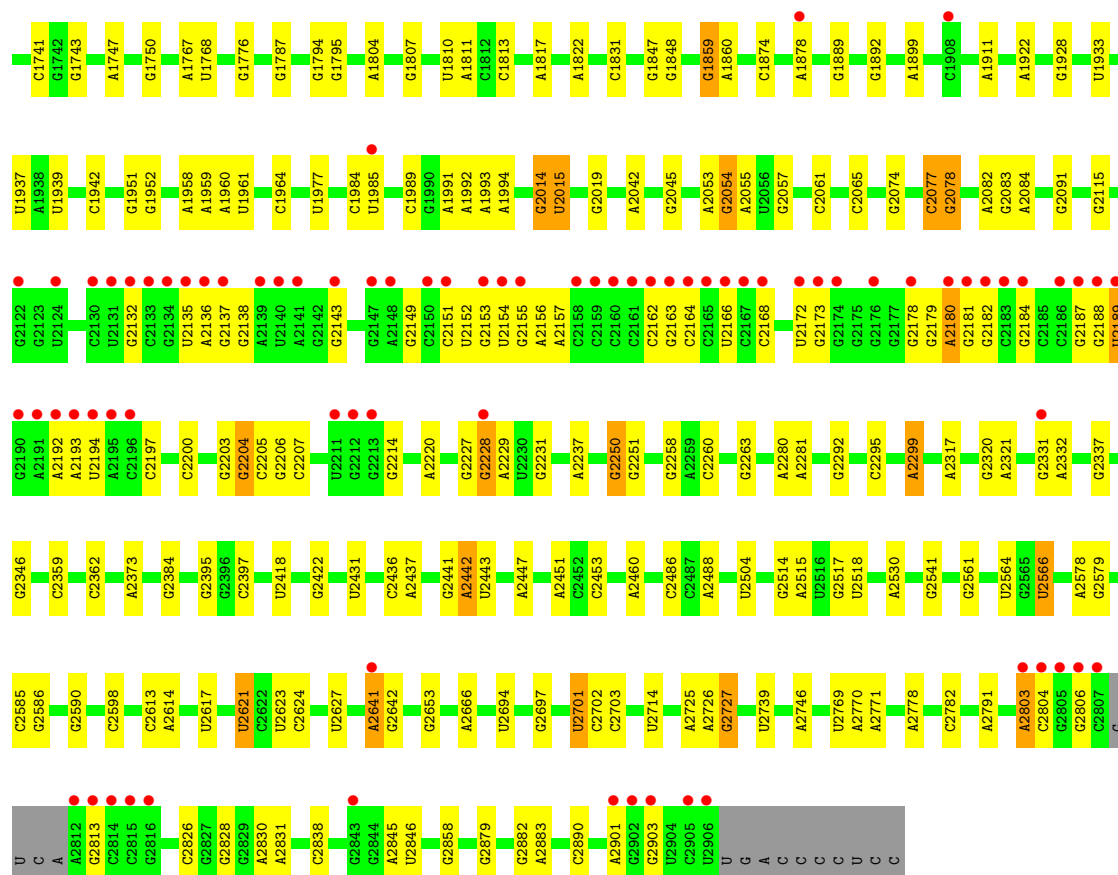
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	2t	4	Total 4	O 4	0	0
60	2u	1	Total 1	O 1	0	0
60	2v	1	Total 1	O 1	0	0
60	2w	2	Total 2	O 2	0	0
60	2x	7	Total 7	O 7	0	0
60	2y	19	Total 19	O 19	0	0

### 3 Residue-property plots [i](#)

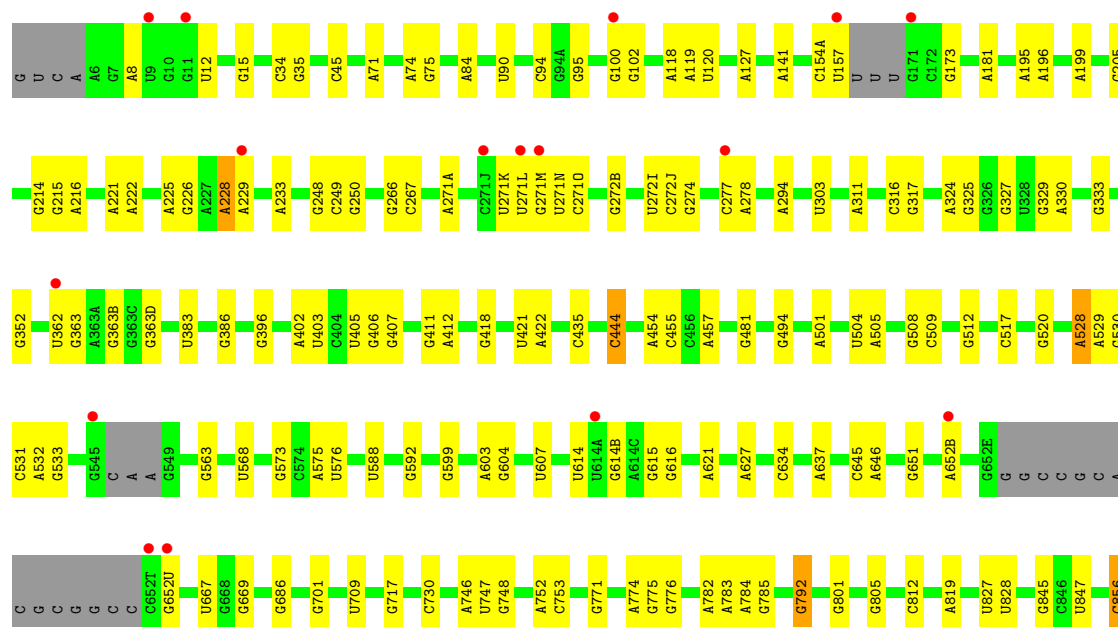
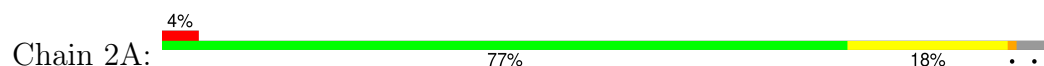
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

#### • Molecule 1: 23S Ribosomal RNA





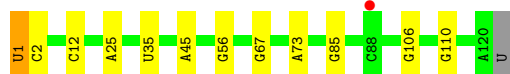
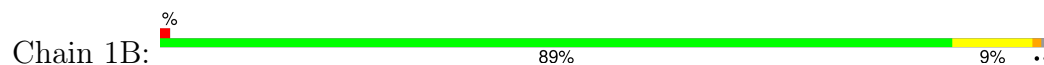
• Molecule 1: 23S Ribosomal RNA



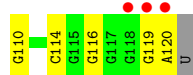
U2712	C2474	C2326	A2173	U1931	G1747A	U1514	U1352	G1170	A	C961	C857
A2712A	C2475	A2327	C2174	A1936	G1756	U1514	A1359	G1171	G	G974	U858
A2713	C2476	A2328	C2175	A1937	U1757	C1530	A1360	G	C	C975	G859
G2714	C2477	C2329	A2176	A1938	G1758	C1531	A1361	U	C	A	A866
U2726	A2478	G2334	C2177	A1939	U1759	C1532	A1365	G	U	A883	G869
A2733	G2490	A2335	C2178	C1942	A1762	U1533	A1368	A	C	A966	A870
U2739	U2491	A2336	C2185	U1955	G1764	A	G1369	C1178	U	G997	G874
G2744	U2492	G2341	U2189	U1956	U1765	C1536	G1371	C1180	U	C998	G875
G2751	G2502	A2346	G2192	C1962	G1769	U	U1372	U1188	A	U1012	A878
A2758	U2503	C2347	A2198	U1963	A1773	C1536	G1377	U1205	A	C1013	G879
A2764	G2505	C2350	G2206	C1967	A1780	C1547	G1384	G1206	G	G1017	G880
A2765	U2506	G2354	G2207	C2128	C1781	A1558	A1384	G1219	A	A1020	G881
G2766	C2512	G2354	A2208	A1970	C1782	A1569	G1385	U1210	G	A1021	G882
A2778	G2518	C2363	U2218	A1971	A1786	A1578	C1386	U1211	U	G1022	G883
C2789	C2520	A2376	A2225	G1992	A1791	U1578	C1411	C1218	C	G1025	G884
A	U2552	G2383	U2232	U1983	C1800	A1580	G1416	G1219	G	U1026	G885
C	G2553	G2384	G2235	G1997	G1801	A1586	C1417	A1220	U	U1033	G886
G2792	G2554	C2385	G2239	A2020	G1811	A1597	U1420	C1224	A	A	G887
G2793	U2555	G2403	G2240	G2023	A1812	A1597	G1421	U1237	U	C1038	G888
C2794	G2556	G2406	G2251	G2027	G1816	A1608	A1427	G1248	G	G1039	C893
U	A2566	G2410	G2275	A2031	G1828	A1609	A1435	G1250	U	C1040	C894
C	G2567	G2419	G2279	G2032	G1835	A1610	G1436	C1252	C	G1041	U895
A2801A	C2573	A2425	C2283	A2033	G1839	A1616	C1437	A1253	U	C1042	A896
G2802	G2578	A2426	A2287	C2043	A1847	U1629	A1445	G1256	A	G	G897
C2803	C2427	G2428	G2295	G2046	A1848	G1647	A1449	G1268	C	A	A898
G2805	G2429	A2430	U2296	G2055	G1857	C1648	G1450	A1271	A	A900	A899
G2807	A2434	A2435	C2297	G2056	G1877	A1654	A1460	U1273	G	A	A901
G2818	A2439	A2439	G2302	A2060	A1878	G1674	C1467	G1279	C	C	A910
A2820	C2440	C2441	G2303	G2061	G1878	A1696	A1471	A1287	G	A	A911
A2821	G2445	G2445	G2304	A2062	A1889	A1698	G1482	C1298	C	A	C912
C2824	G2448	G2448	A2305	G2069	A1900	G1697	A1490	U1300	U	G	G928
G2833	G2458	G2458	G2308	G2093	G1906	A1699	A1493	A1301	G	G	G932
U2836	G2465	G2465	A2310	U2099	U1911	A1700	C1493	G1302	U	A	A933
G2839	C2465	C2465	C2313	C2105	A1912	G1703	A1494	G1303	C	C	A941
G2872	C2465	C2465	G2318	C2106	C1914	G1721	A1495	U1313	U	U	G944
C2879	G2468	G2468	A2320	C2107	A1915	A1722	A1496	U1314	U	U	G946
C2880	A2469	A2469	G2321	U2108	A1916	U1739	U1497	G1314	A	C	A953
G2894	U2689	U2689	C2324	U2109	U1917	G1740	A1508	A1321	A	A	U958
U2895	C2690	C2690	A2171	C2110	G1929	G1746	C1509	C1345	G	G	A959
			G2325	G2112	G1930	G1747	A1509A	G1169	C	C	A960



- Molecule 2: 5S Ribosomal RNA



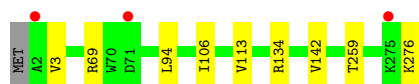
- Molecule 2: 5S Ribosomal RNA



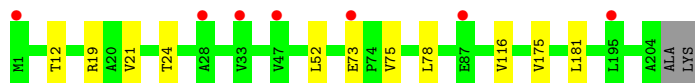
- Molecule 3: 50S ribosomal protein L2



- Molecule 3: 50S ribosomal protein L2



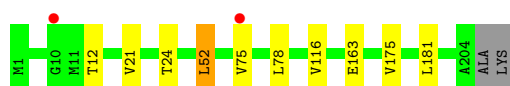
- Molecule 4: 50S ribosomal protein L3



- Molecule 4: 50S ribosomal protein L3







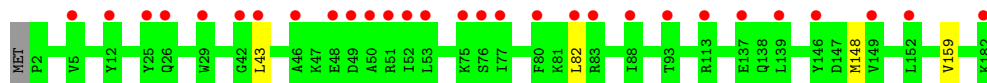
- Molecule 5: 50S ribosomal protein L4



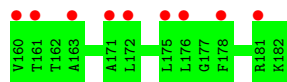
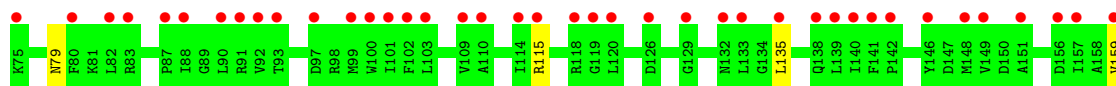
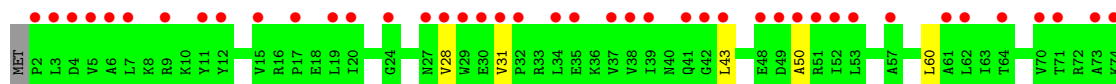
- Molecule 5: 50S ribosomal protein L4



- Molecule 6: 50S ribosomal protein L5



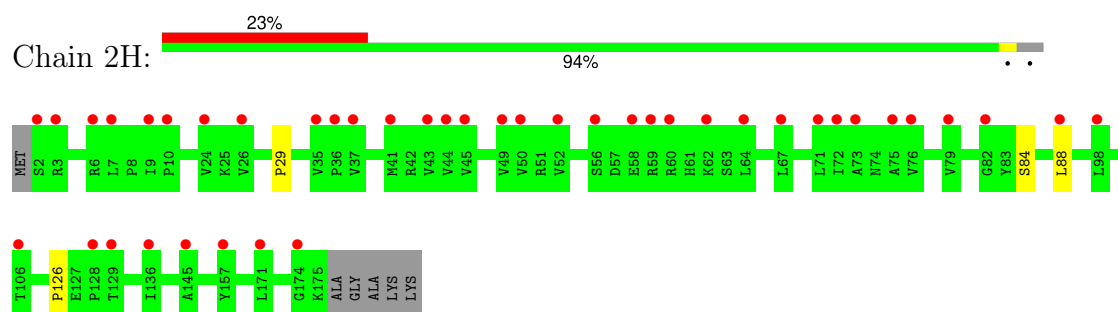
- Molecule 6: 50S ribosomal protein L5



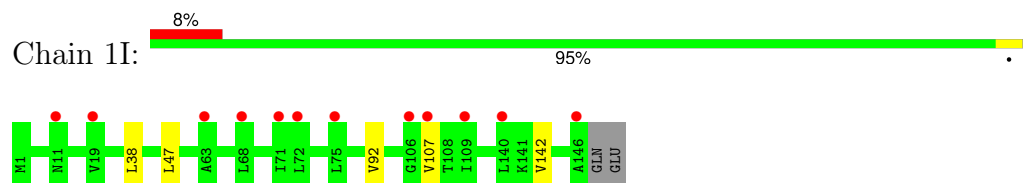
- Molecule 7: 50S ribosomal protein L6



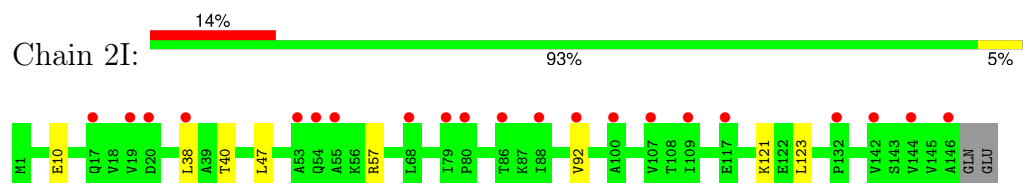
- Molecule 7: 50S ribosomal protein L6



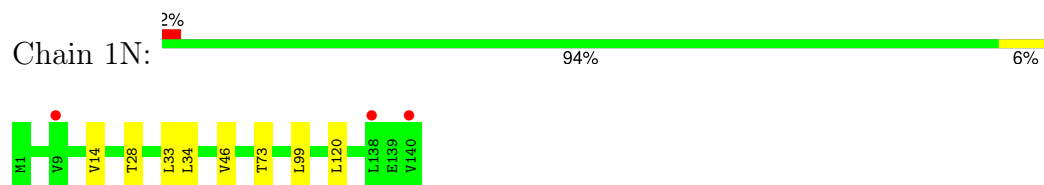
- Molecule 8: 50S ribosomal protein L9



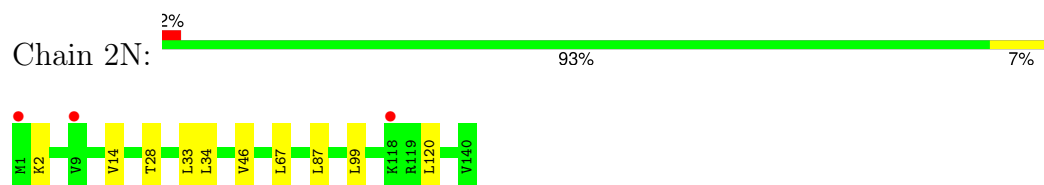
- Molecule 8: 50S ribosomal protein L9



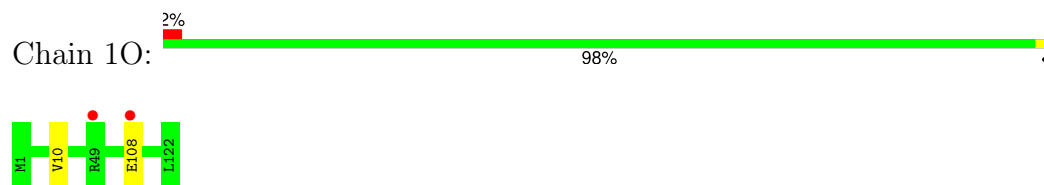
- Molecule 9: 50S ribosomal protein L13



- Molecule 9: 50S ribosomal protein L13



- Molecule 10: 50S ribosomal protein L14

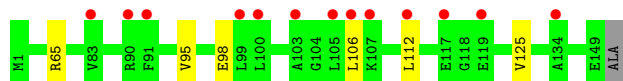


- Molecule 10: 50S ribosomal protein L14





- Molecule 11: 50S ribosomal protein L15



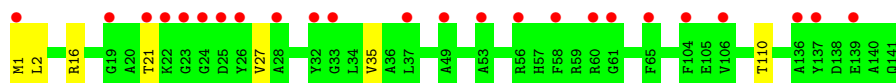
- Molecule 11: 50S ribosomal protein L15



- Molecule 12: 50S ribosomal protein L16



- Molecule 12: 50S ribosomal protein L16



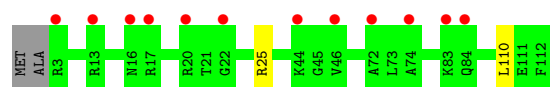
- Molecule 13: 50S ribosomal protein L17



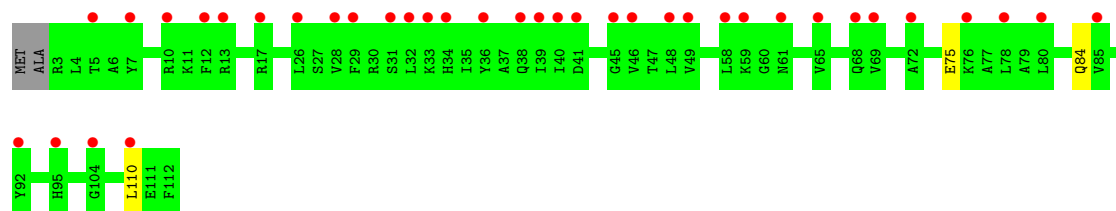
- Molecule 13: 50S ribosomal protein L17



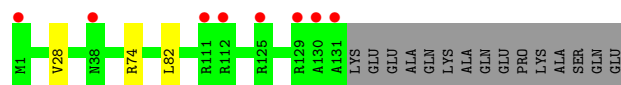
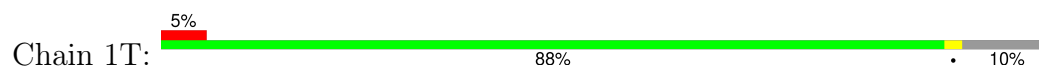
- Molecule 14: 50S ribosomal protein L18



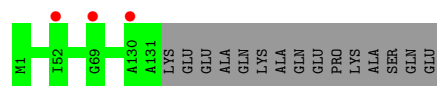
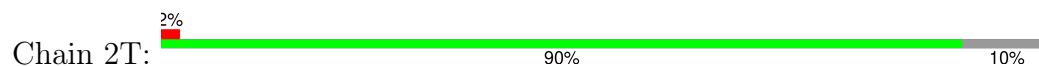
- Molecule 14: 50S ribosomal protein L18



- Molecule 15: 50S ribosomal protein L19



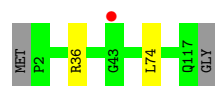
- Molecule 15: 50S ribosomal protein L19



- Molecule 16: 50S ribosomal protein L20



- Molecule 16: 50S ribosomal protein L20



- Molecule 17: 50S ribosomal protein L21





- Molecule 17: 50S ribosomal protein L21



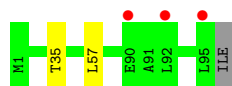
- Molecule 18: 50S ribosomal protein L22



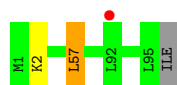
- Molecule 18: 50S ribosomal protein L22



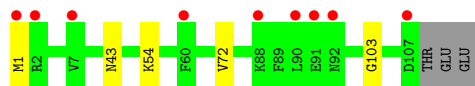
- Molecule 19: 50S ribosomal protein L23



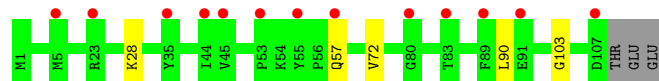
- Molecule 19: 50S ribosomal protein L23



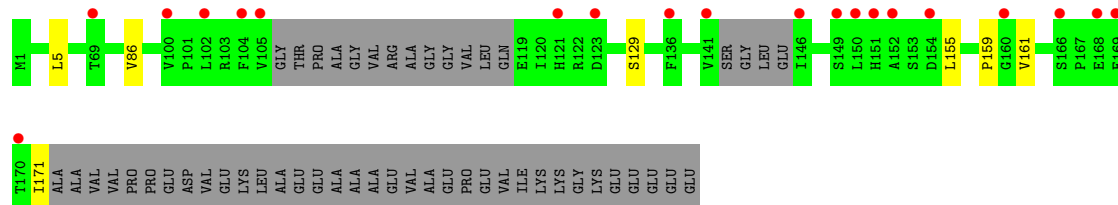
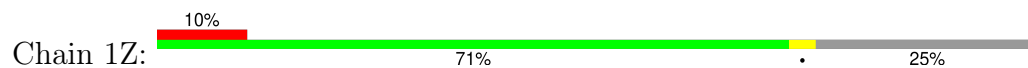
- Molecule 20: 50S ribosomal protein L24



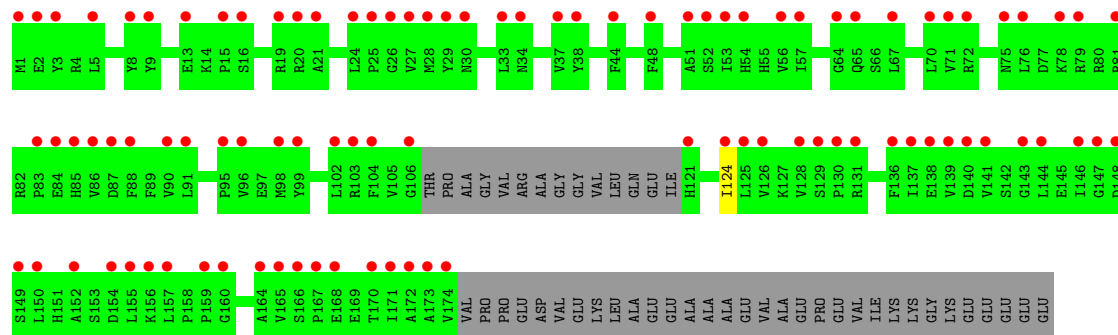
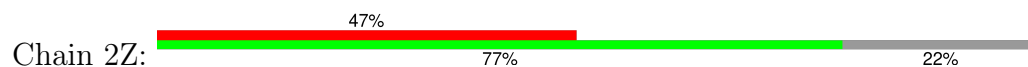
- Molecule 20: 50S ribosomal protein L24



- Molecule 21: 50S ribosomal protein L25



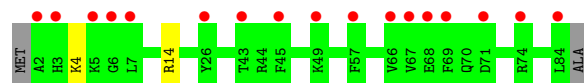
- Molecule 21: 50S ribosomal protein L25



- Molecule 22: 50S ribosomal protein L27

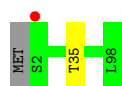


- Molecule 22: 50S ribosomal protein L27

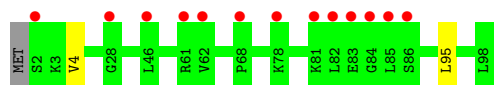


- Molecule 23: 50S ribosomal protein L28

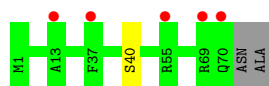




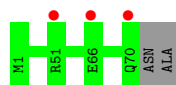
- Molecule 23: 50S ribosomal protein L28



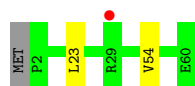
- Molecule 24: 50S ribosomal protein L29



- Molecule 24: 50S ribosomal protein L29



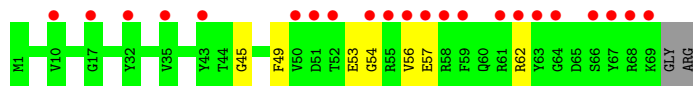
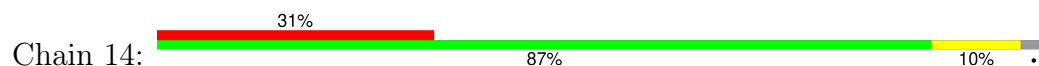
- Molecule 25: 50S ribosomal protein L30



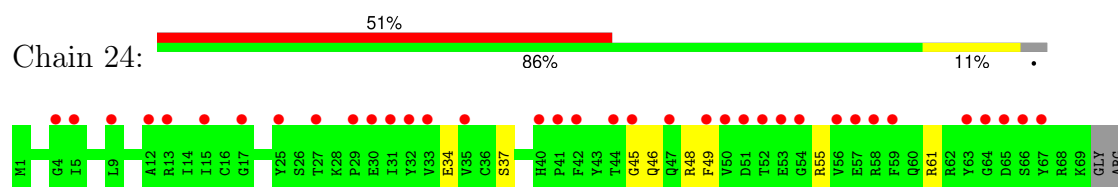
- Molecule 25: 50S ribosomal protein L30



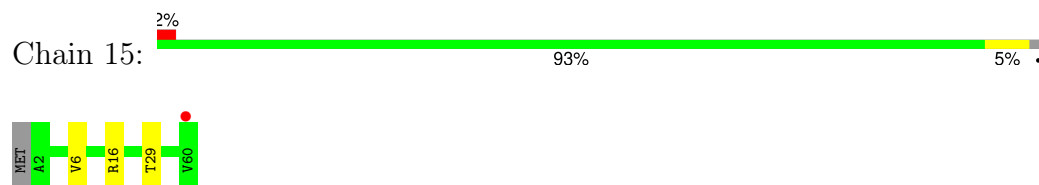
- Molecule 26: 50S ribosomal protein L31



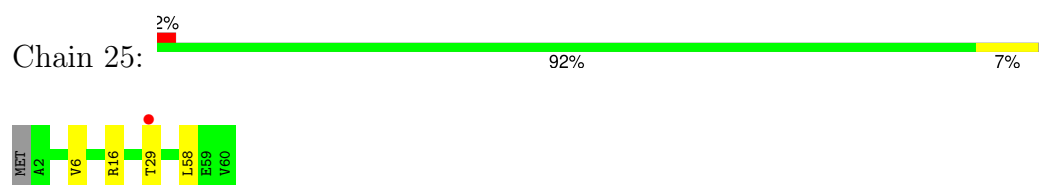
- Molecule 26: 50S ribosomal protein L31



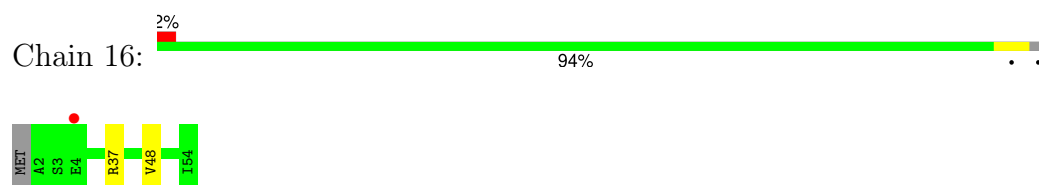
- Molecule 27: 50S ribosomal protein L32



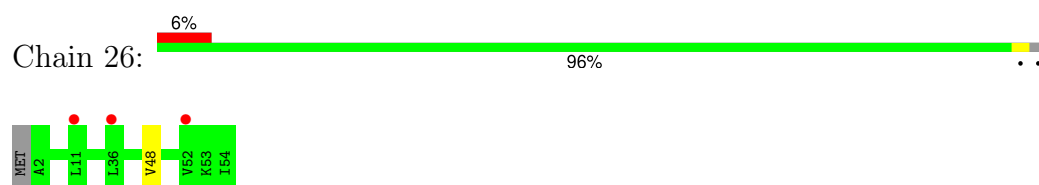
- Molecule 27: 50S ribosomal protein L32



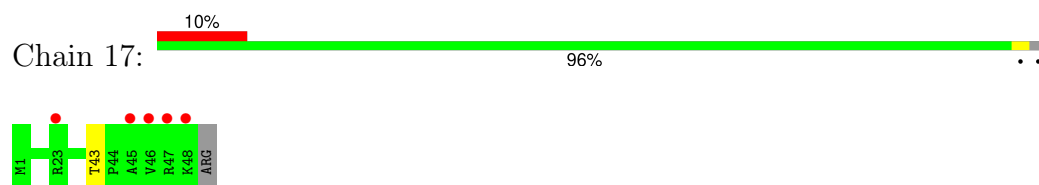
- Molecule 28: 50S ribosomal protein L33



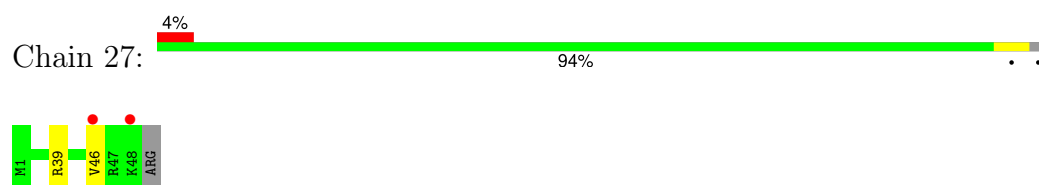
- Molecule 28: 50S ribosomal protein L33



- Molecule 29: 50S ribosomal protein L34

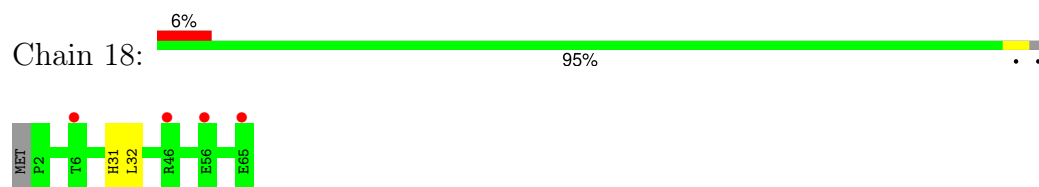


- Molecule 29: 50S ribosomal protein L34

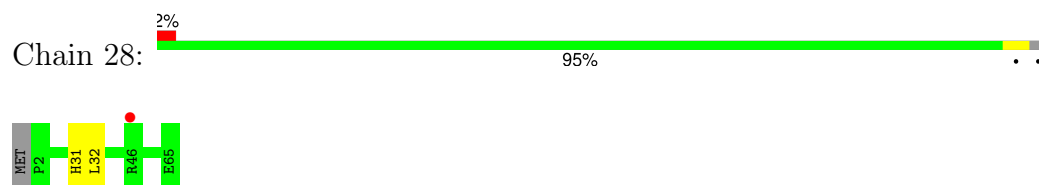




- Molecule 30: 50S ribosomal protein L35



- Molecule 30: 50S ribosomal protein L35

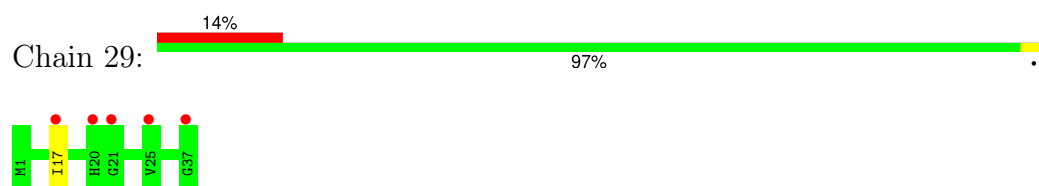


- Molecule 31: 50S ribosomal protein L36

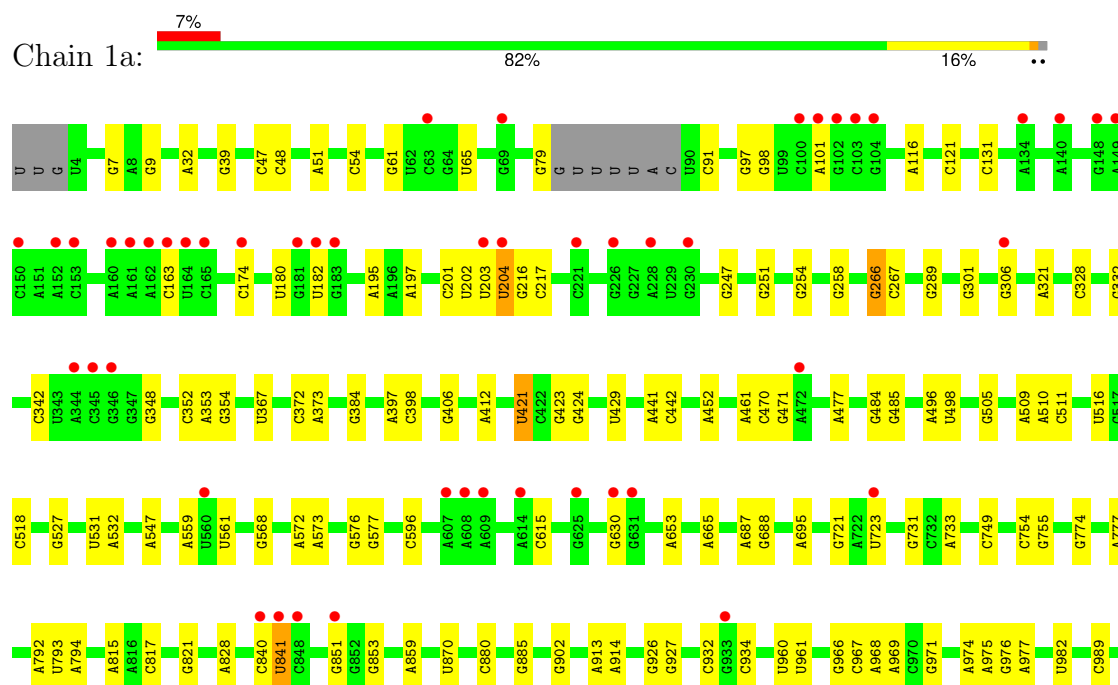


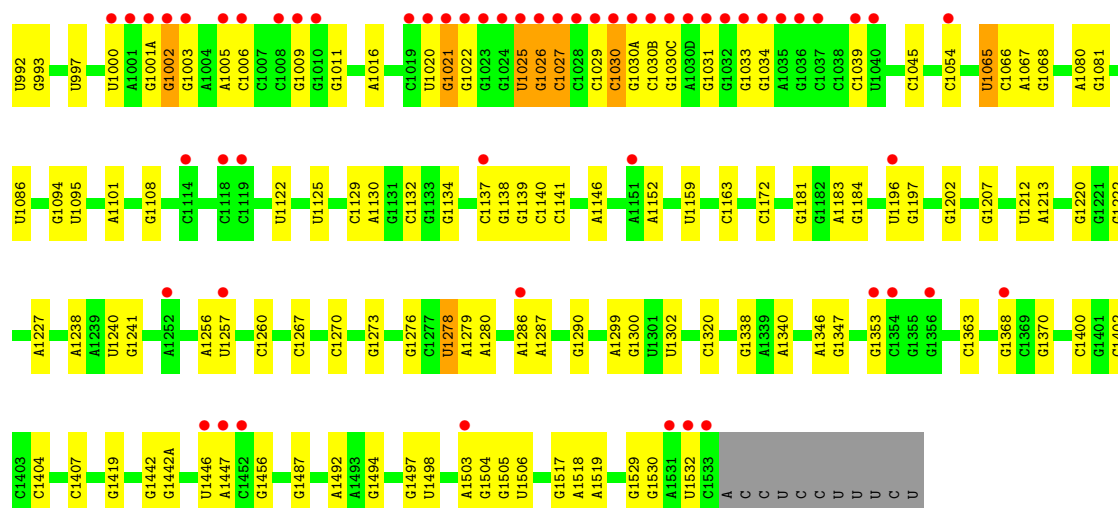
There are no outlier residues recorded for this chain.

- Molecule 31: 50S ribosomal protein L36

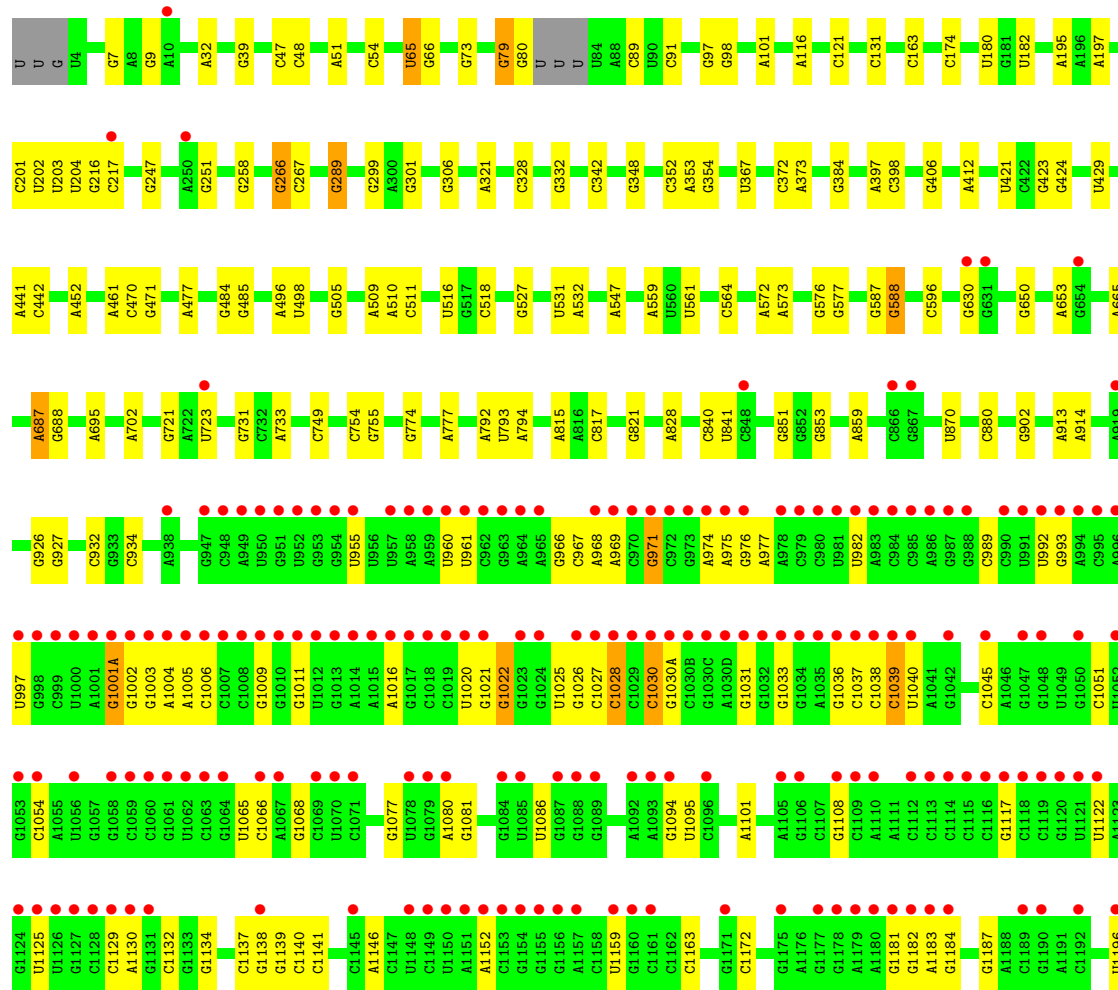
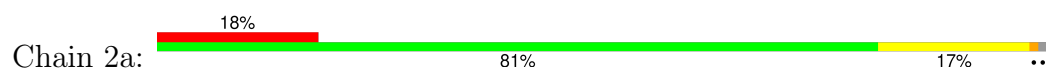


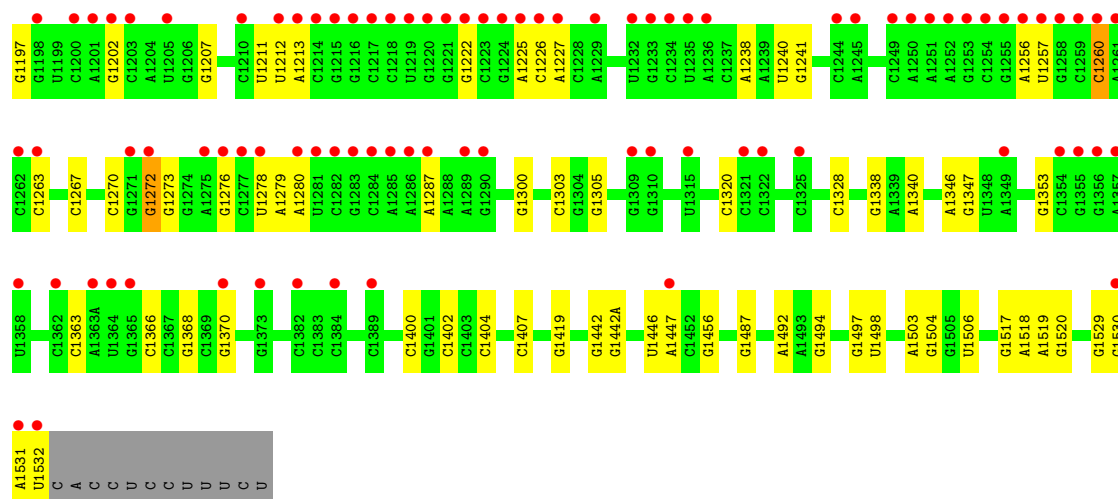
- Molecule 32: 16S Ribosomal RNA



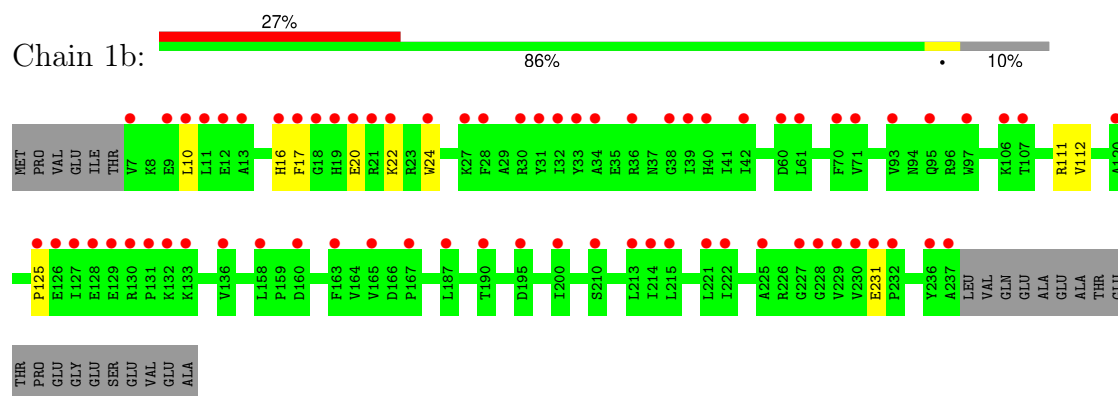


- Molecule 32: 16S Ribosomal RNA

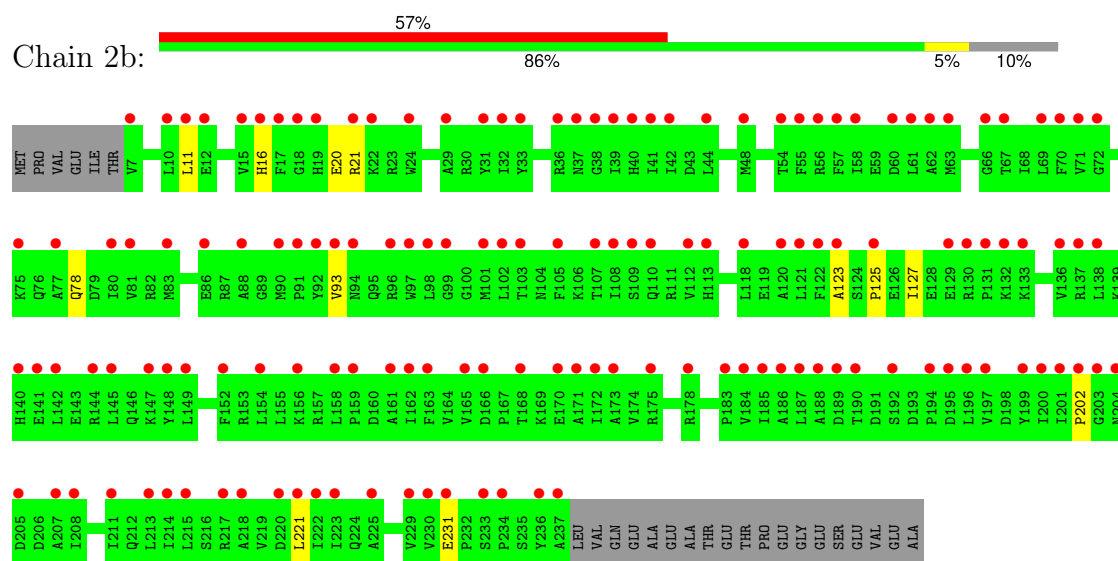




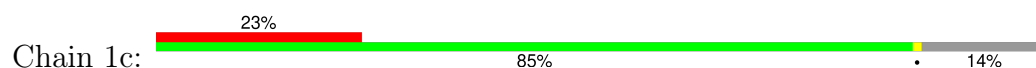
• Molecule 33: 30S ribosomal protein S2

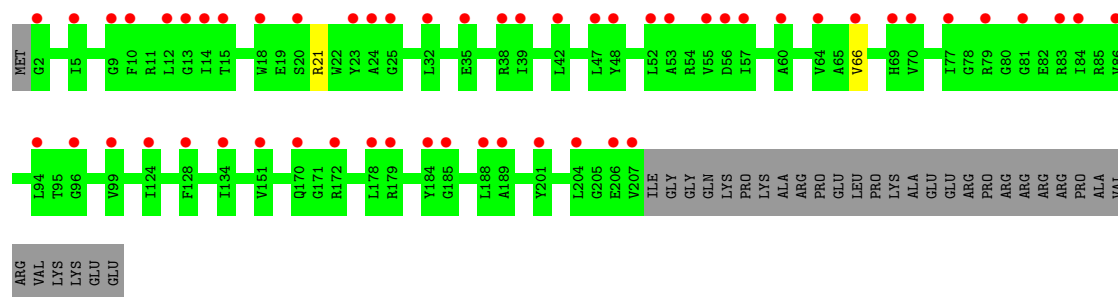


• Molecule 33: 30S ribosomal protein S2



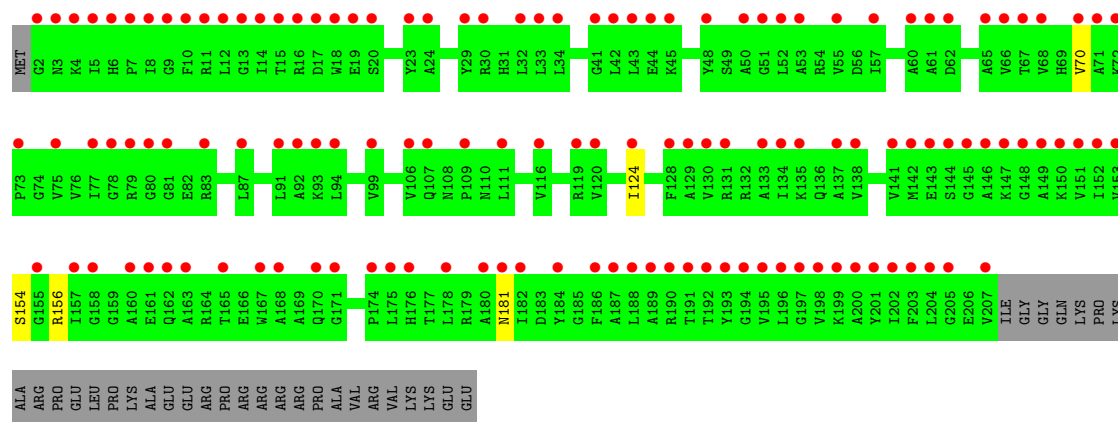
• Molecule 34: 30S ribosomal protein S3





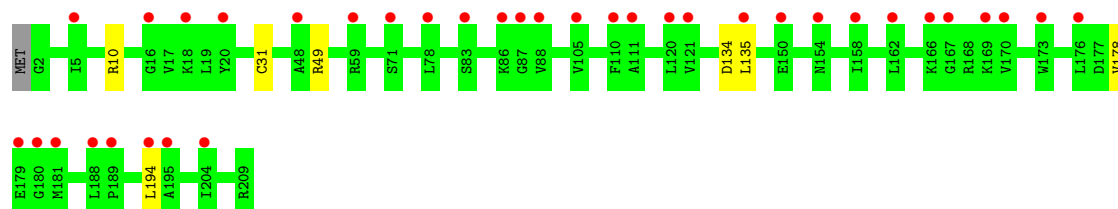
• Molecule 34: 30S ribosomal protein S3

Chain 2c: 56% 84% 14%



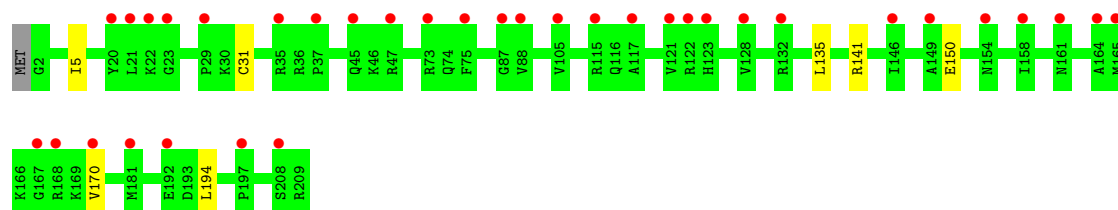
• Molecule 35: 30S ribosomal protein S4

Chain 1d: 17% 96%

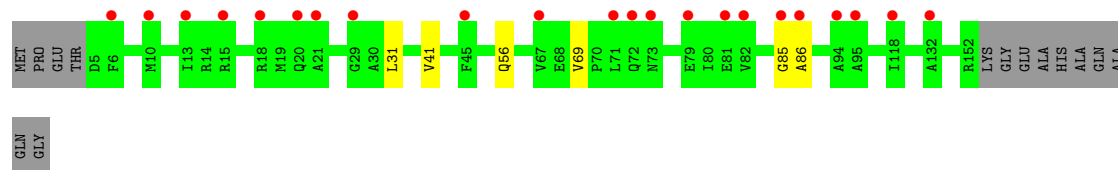
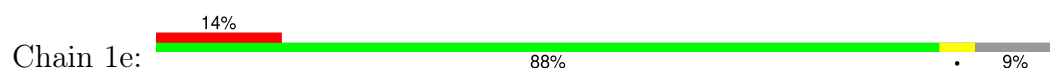


• Molecule 35: 30S ribosomal protein S4

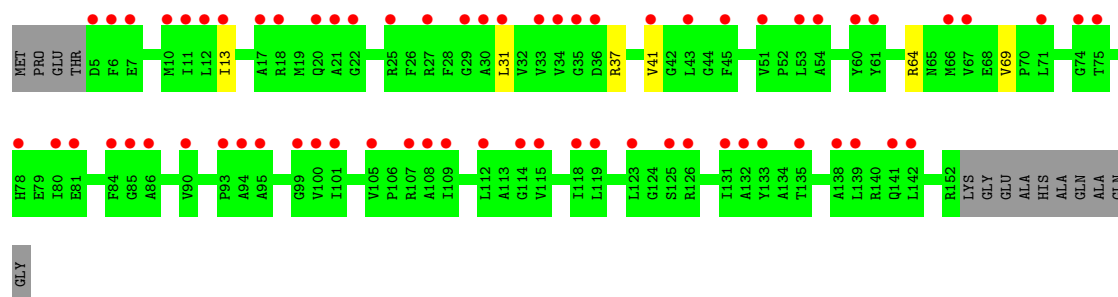
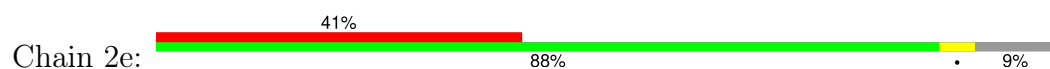
Chain 2d: 17% 96%



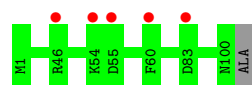
• Molecule 36: 30S ribosomal protein S5



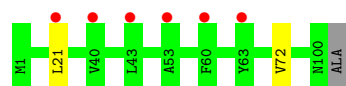
- Molecule 36: 30S ribosomal protein S5



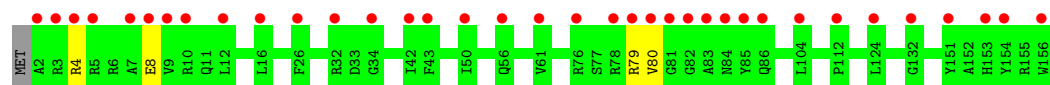
- Molecule 37: 30S ribosomal protein S6



- Molecule 37: 30S ribosomal protein S6

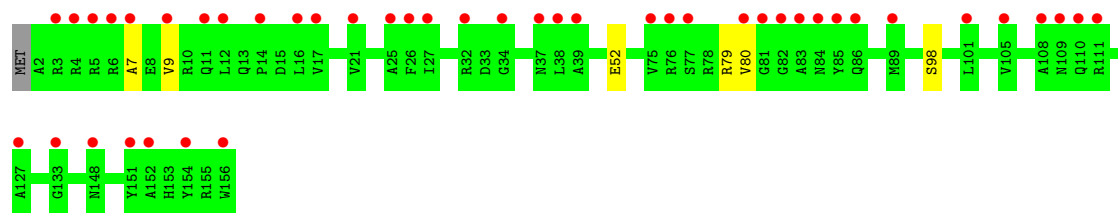


- Molecule 38: 30S ribosomal protein S7



- Molecule 38: 30S ribosomal protein S7

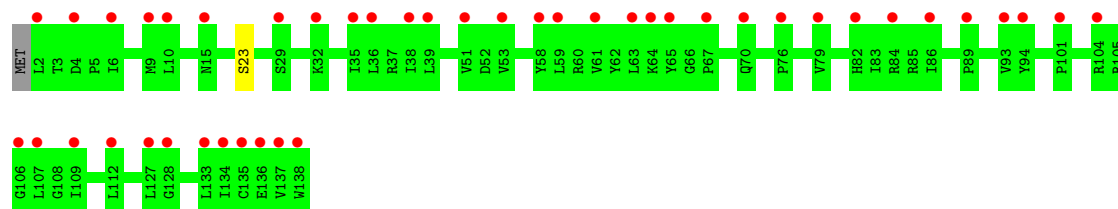




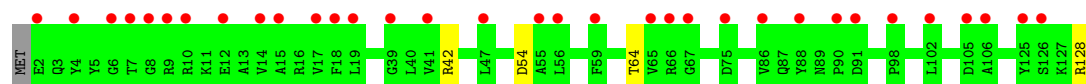
- Molecule 39: 30S ribosomal protein S8



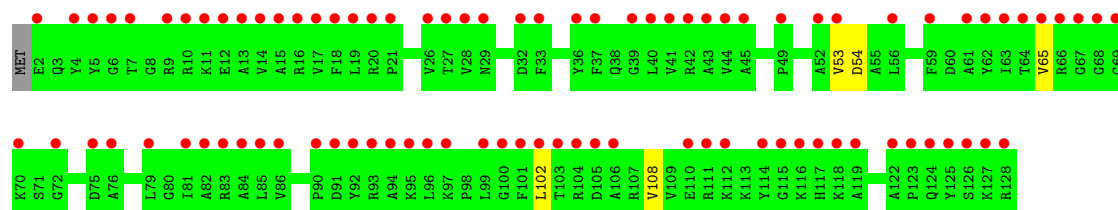
- Molecule 39: 30S ribosomal protein S8



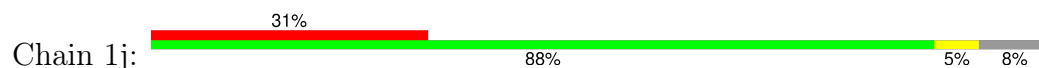
- Molecule 40: 30S ribosomal protein S9

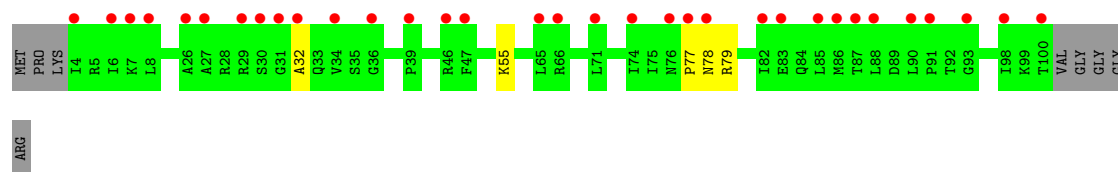


- Molecule 40: 30S ribosomal protein S9

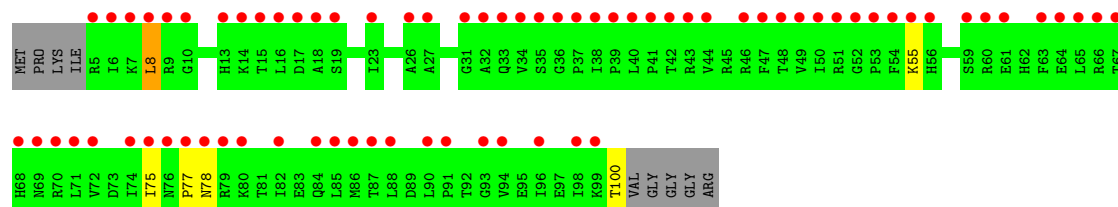
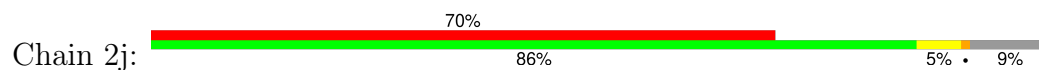


- Molecule 41: 30S ribosomal protein S10

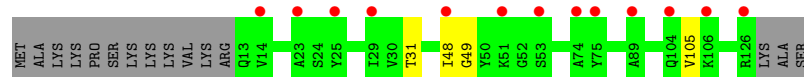
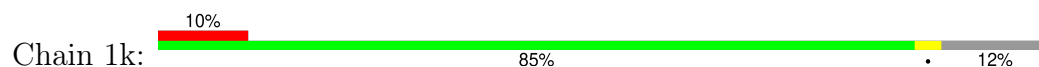




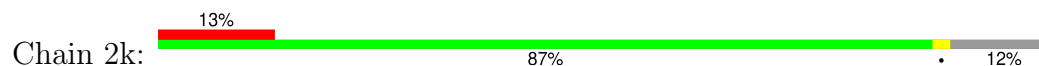
- Molecule 41: 30S ribosomal protein S10



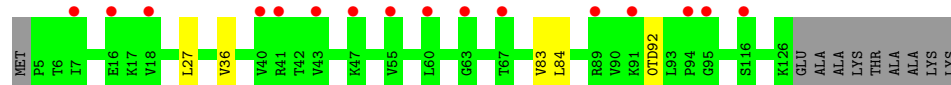
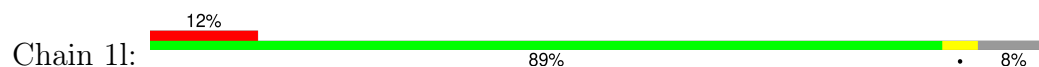
- Molecule 42: 30S ribosomal protein S11



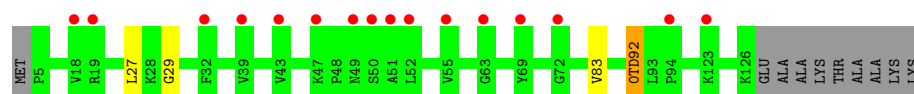
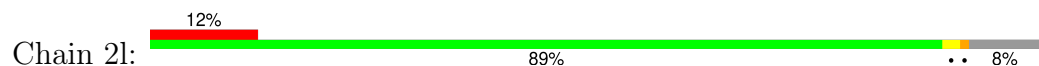
- Molecule 42: 30S ribosomal protein S11



- Molecule 43: 30S ribosomal protein S12



- Molecule 43: 30S ribosomal protein S12

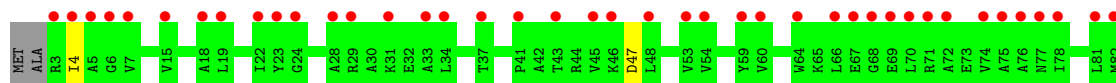


- Molecule 44: 30S ribosomal protein S13

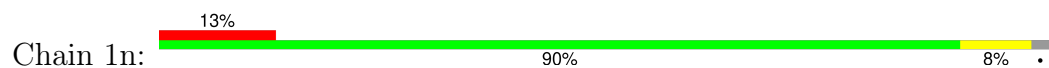




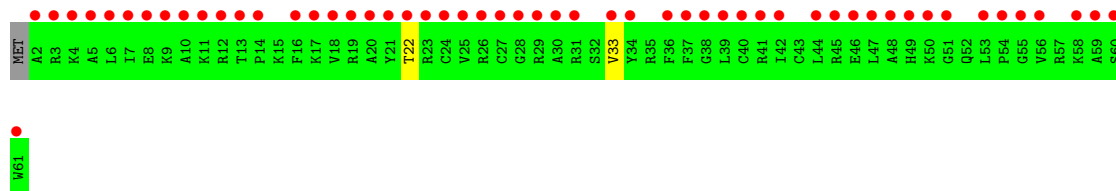
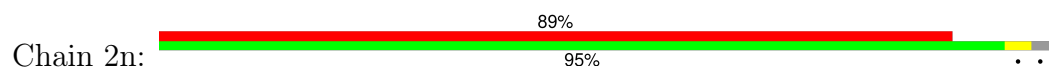
- Molecule 44: 30S ribosomal protein S13



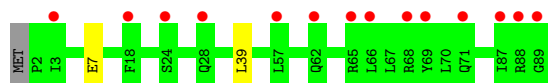
- Molecule 45: 30S ribosomal protein S14 type Z



- Molecule 45: 30S ribosomal protein S14 type Z



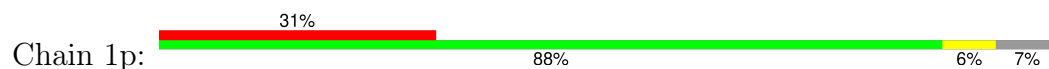
- Molecule 46: 30S ribosomal protein S15



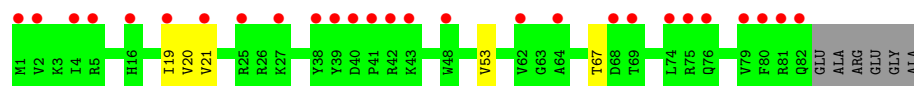
- Molecule 46: 30S ribosomal protein S15



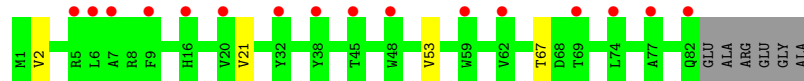
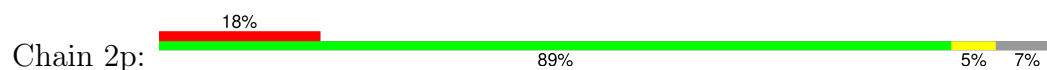
- Molecule 47: 30S ribosomal protein S16



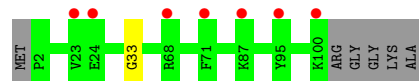




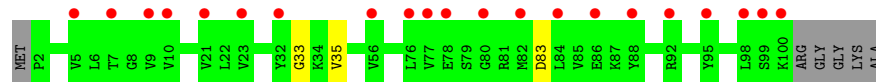
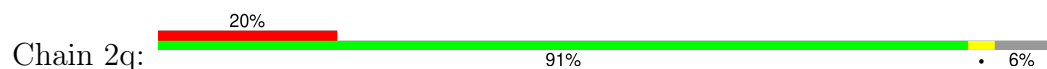
- Molecule 47: 30S ribosomal protein S16



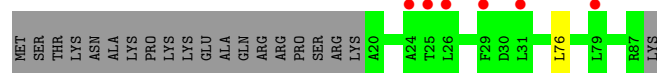
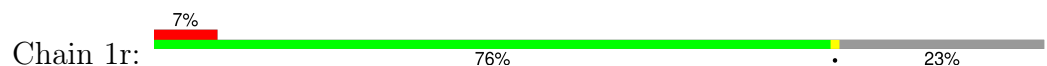
- Molecule 48: 30S ribosomal protein S17



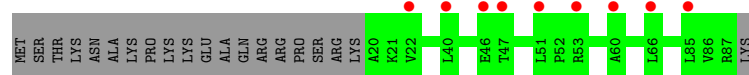
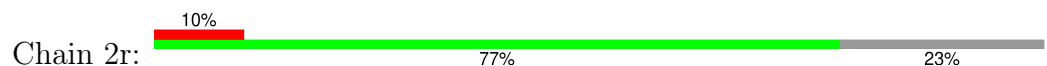
- Molecule 48: 30S ribosomal protein S17



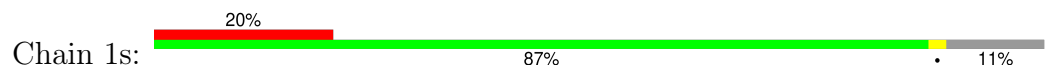
- Molecule 49: 30S ribosomal protein S18



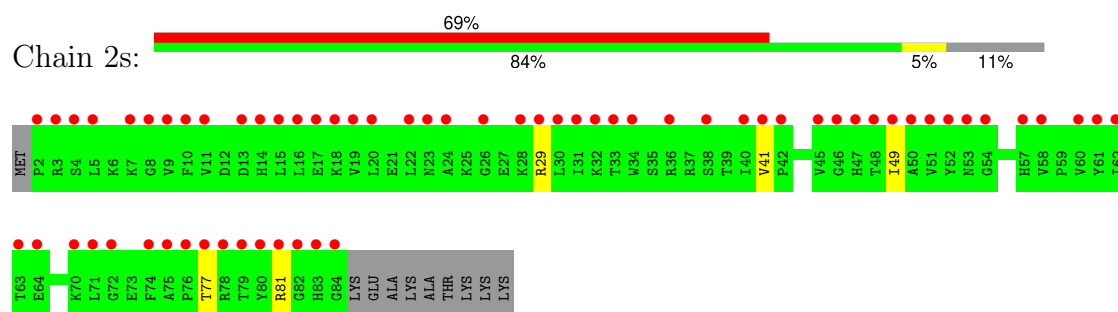
- Molecule 49: 30S ribosomal protein S18



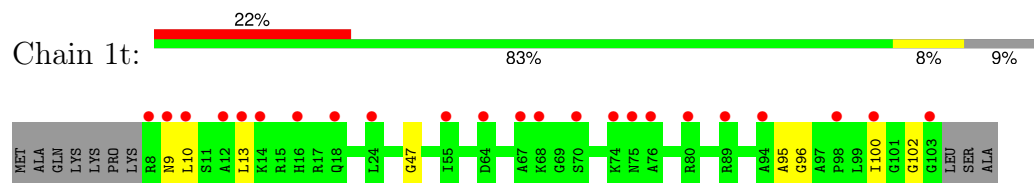
- Molecule 50: 30S ribosomal protein S19



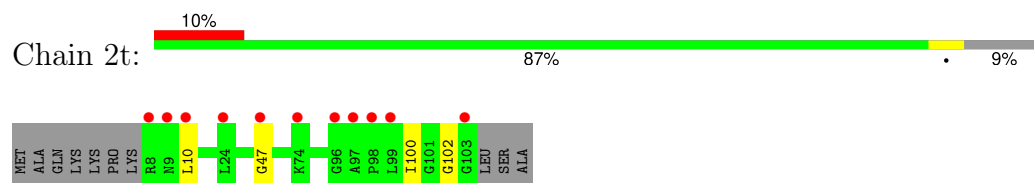
- Molecule 50: 30S ribosomal protein S19



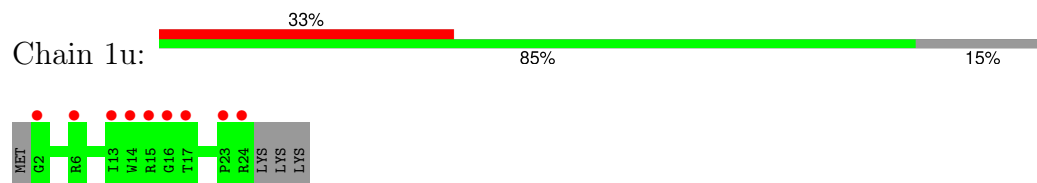
- Molecule 51: 30S ribosomal protein S20



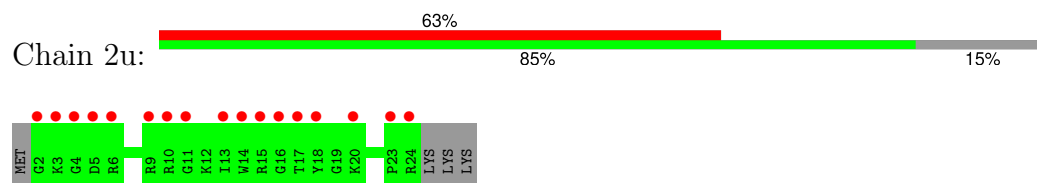
- Molecule 51: 30S ribosomal protein S20



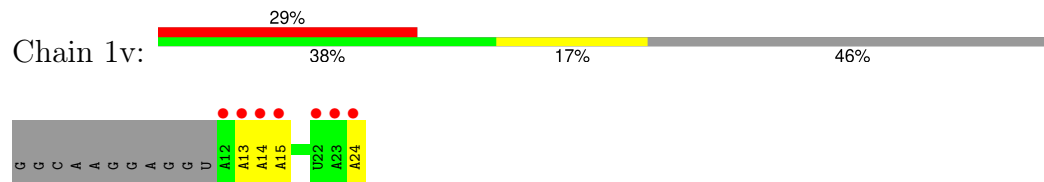
- Molecule 52: 30S ribosomal protein Thx



- Molecule 52: 30S ribosomal protein Thx

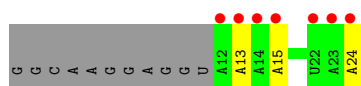


- Molecule 53: mRNA

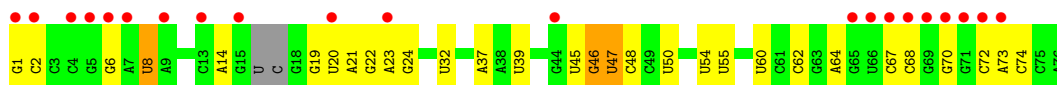


- Molecule 53: mRNA

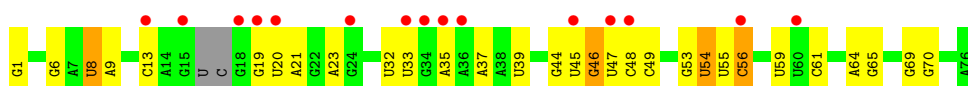




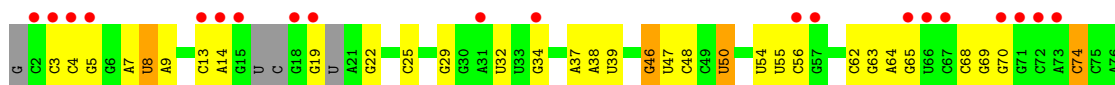
- Molecule 54: A-site and E-site tRNAs



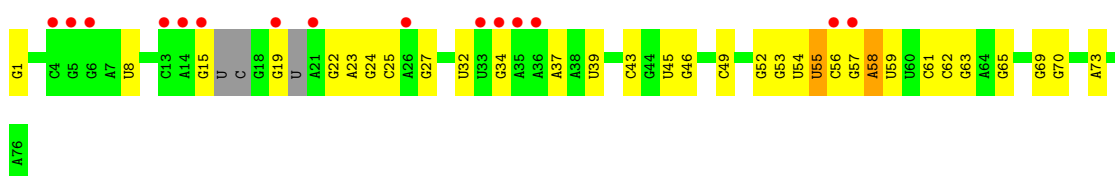
- Molecule 54: A-site and E-site tRNAs



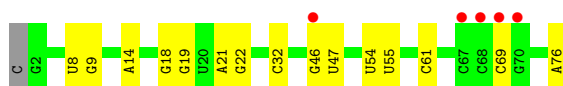
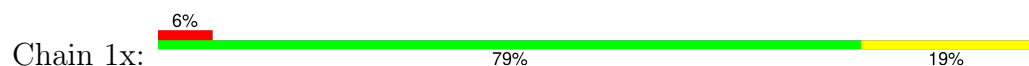
- Molecule 54: A-site and E-site tRNAs



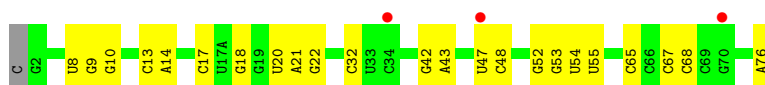
- Molecule 54: A-site and E-site tRNAs



- Molecule 55: P-site tRNA



- Molecule 55: P-site tRNA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	209.70Å 450.05Å 624.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	122.01 – 2.50 122.01 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.8 (122.01-2.50) 97.8 (122.01-2.50)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.22 (at 2.52Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.231 , 0.281 0.232 , 0.282	Depositor DCC
$R_{free}$ test set	98495 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.4	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 57.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	300910	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% 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: 4OC, ZN, 0TD, 7MG, M2G, K, UR3, 2MG, PSU, MIA, 4SU, 2MA, 2MU, OMG, 5MC, MA6, MG, 5MU, SF4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	1A	0.61	0/69009	1.05	129/107712 (0.1%)
1	2A	0.52	1/67293 (0.0%)	1.03	84/105034 (0.1%)
2	1B	0.51	1/2882 (0.0%)	0.87	0/4494
2	2B	0.59	1/2879 (0.0%)	1.01	4/4487 (0.1%)
3	1D	0.44	0/2186	0.61	0/2944
3	2D	0.38	0/2186	0.61	0/2944
4	1E	0.43	0/1592	0.61	0/2149
4	2E	0.37	0/1592	0.59	0/2149
5	1F	0.40	0/1619	0.58	0/2193
5	2F	0.37	0/1615	0.58	0/2188
6	1G	0.34	0/1448	0.54	0/1957
6	2G	0.36	0/1453	0.58	0/1963
7	1H	0.36	0/1356	0.55	0/1834
7	2H	0.33	0/1356	0.55	0/1834
8	1I	0.31	0/1112	0.55	0/1514
8	2I	0.30	0/1079	0.54	0/1475
9	1N	0.39	0/1144	0.57	0/1543
9	2N	0.36	0/1144	0.58	0/1543
10	1O	0.42	0/943	0.58	0/1269
10	2O	0.35	0/943	0.54	0/1269
11	1P	0.39	0/1152	0.60	0/1533
11	2P	0.36	0/1152	0.62	0/1533
12	1Q	0.41	0/1143	0.57	0/1527
12	2Q	0.37	0/1143	0.60	0/1527
13	1R	0.43	0/982	0.63	0/1312
13	2R	0.38	0/982	0.60	0/1312
14	1S	0.34	0/883	0.56	0/1176
14	2S	0.38	0/880	0.59	0/1172
15	1T	0.39	0/1105	0.61	1/1477 (0.1%)
15	2T	0.36	0/1097	0.59	0/1468
16	1U	0.46	0/977	0.62	0/1301

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	2U	0.39	0/977	0.60	0/1301
17	1V	0.45	0/782	0.62	0/1049
17	2V	0.35	0/782	0.59	0/1049
18	1W	0.45	0/897	0.66	0/1205
18	2W	0.39	0/897	0.58	0/1205
19	1X	0.44	0/764	0.61	0/1025
19	2X	0.40	0/764	0.63	1/1025 (0.1%)
20	1Y	0.39	0/819	0.57	0/1095
20	2Y	0.35	0/819	0.56	0/1095
21	1Z	0.35	0/1267	0.59	0/1717
21	2Z	0.31	0/1299	0.53	0/1763
22	10	0.43	0/662	0.66	1/881 (0.1%)
22	20	0.33	0/662	0.56	0/881
23	11	0.39	0/762	0.58	0/1014
23	21	0.35	0/762	0.57	0/1014
24	12	0.35	0/590	0.56	0/781
24	22	0.33	0/590	0.51	0/781
25	13	0.41	0/474	0.60	0/635
25	23	0.33	0/469	0.57	0/630
26	14	0.35	0/565	0.69	1/761 (0.1%)
26	24	0.37	0/545	0.64	0/737
27	15	0.42	0/469	0.64	0/635
27	25	0.38	0/469	0.60	1/635 (0.2%)
28	16	0.44	0/460	0.56	0/613
28	26	0.35	0/456	0.51	0/608
29	17	0.44	0/426	0.70	0/561
29	27	0.42	0/426	0.66	0/561
30	18	0.41	0/525	0.59	0/691
30	28	0.39	0/525	0.60	0/691
31	19	0.42	0/310	0.60	0/407
31	29	0.38	0/310	0.60	0/407
32	1a	0.43	0/35795	0.92	40/55864 (0.1%)
32	2a	0.45	3/35886 (0.0%)	0.98	62/56005 (0.1%)
33	1b	0.31	0/1881	0.59	0/2542
33	2b	0.34	0/1860	0.57	0/2518
34	1c	0.28	0/1572	0.49	0/2126
34	2c	0.34	0/1566	0.55	0/2119
35	1d	0.31	0/1685	0.54	0/2262
35	2d	0.31	0/1704	0.52	0/2284
36	1e	0.31	0/1145	0.55	0/1543
36	2e	0.34	0/1149	0.61	0/1548
37	1f	0.32	0/823	0.53	0/1115
37	2f	0.32	0/829	0.51	0/1123

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	1g	0.29	0/1250	0.52	0/1679
38	2g	0.31	0/1254	0.54	0/1683
39	1h	0.30	0/1108	0.54	0/1494
39	2h	0.30	0/1108	0.55	0/1494
40	1i	0.31	0/1002	0.59	0/1346
40	2i	0.32	0/997	0.56	0/1343
41	1j	0.30	0/722	0.54	0/982
41	2j	0.34	0/727	0.59	1/988 (0.1%)
42	1k	0.30	0/844	0.55	0/1145
42	2k	0.31	0/848	0.52	0/1149
43	1l	0.34	0/937	0.54	0/1260
43	2l	0.32	0/937	0.59	1/1260 (0.1%)
44	1m	0.32	0/969	0.57	0/1302
44	2m	0.31	0/961	0.57	0/1291
45	1n	0.33	0/501	0.51	0/664
45	2n	0.31	0/501	0.53	0/664
46	1o	0.30	0/739	0.49	0/985
46	2o	0.30	0/739	0.51	0/985
47	1p	0.31	0/697	0.54	0/939
47	2p	0.31	0/693	0.53	0/935
48	1q	0.33	0/836	0.55	0/1117
48	2q	0.31	0/836	0.52	0/1117
49	1r	0.32	0/560	0.53	0/746
49	2r	0.30	0/560	0.51	0/746
50	1s	0.29	0/667	0.58	0/900
50	2s	0.38	0/661	0.66	0/893
51	1t	0.28	0/730	0.53	0/965
51	2t	0.30	0/729	0.54	0/965
52	1u	0.27	0/203	0.46	0/266
52	2u	0.34	0/203	0.50	0/266
53	1v	0.46	0/310	0.93	0/480
53	2v	0.60	0/310	0.91	0/480
54	1w	0.57	1/1606 (0.1%)	1.10	3/2497 (0.1%)
54	1y	0.56	1/1606 (0.1%)	1.13	9/2497 (0.4%)
54	2w	0.53	0/1556	1.12	2/2418 (0.1%)
54	2y	0.59	1/1583 (0.1%)	1.17	4/2459 (0.2%)
55	1x	0.57	3/1725 (0.2%)	1.16	16/2689 (0.6%)
55	2x	0.49	0/1725	1.06	8/2689 (0.3%)
All	All	0.49	12/316686 (0.0%)	0.92	368/474113 (0.1%)

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
43	2l	0	1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	2y	1	G	OP3-P	-10.21	1.48	1.61
2	1B	1	U	OP3-P	-10.20	1.49	1.61
54	1y	1	G	OP3-P	-10.20	1.49	1.61
2	2B	1	U	OP3-P	-9.87	1.49	1.61
54	1w	1	G	OP3-P	-9.63	1.49	1.61
32	2a	1272	G	N1-C2	-9.38	1.30	1.37
32	2a	1272	G	C6-N1	-8.82	1.33	1.39
55	1x	14	A	N7-C5	-5.80	1.35	1.39
55	1x	22	G	N7-C5	5.47	1.42	1.39
32	2a	1263	C	N3-C4	-5.32	1.30	1.33
1	2A	2287	A	N9-C4	-5.20	1.34	1.37
55	1x	14	A	C8-N7	-5.06	1.28	1.31

All (368) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1263	C	N1-C2-O2	22.29	132.27	118.90
32	2a	1272	G	N3-C2-N2	21.80	135.16	119.90
32	2a	1272	G	C5-C6-O6	20.59	140.96	128.60
32	2a	1272	G	N1-C2-N2	-18.95	99.14	116.20
32	2a	1263	C	C2-N3-C4	15.04	127.42	119.90
1	1A	1686	U	O5'-P-OP2	-14.11	93.01	105.70
32	2a	1263	C	N3-C2-O2	-12.82	112.93	121.90
1	1A	1121	C	N1-C2-O2	12.15	126.19	118.90
32	2a	1272	G	N1-C6-O6	-12.10	112.64	119.90
32	2a	1272	G	C6-N1-C2	12.00	132.30	125.10
32	2a	1263	C	C5-C6-N1	11.97	126.99	121.00
1	1A	1132	A	N1-C6-N6	-11.68	111.59	118.60
1	1A	1109	G	C5-C6-O6	10.74	135.04	128.60
32	2a	1272	G	C5-C6-N1	-10.27	106.37	111.50
1	1A	1121	C	C2-N3-C4	10.09	124.94	119.90
55	1x	14	A	C4-C5-C6	10.08	122.04	117.00
1	1A	599	U	O5'-P-OP1	-10.05	96.65	105.70
32	2a	1263	C	C6-N1-C2	-9.80	116.38	120.30
1	1A	1020	C	N1-C2-O2	-9.76	113.04	118.90
1	1A	1807	G	O5'-P-OP2	-9.76	96.92	105.70

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	1x	14	A	C5-N7-C8	9.62	108.71	103.90
1	1A	611	U	O5'-P-OP2	-9.61	97.05	105.70
2	2B	80	U	O4'-C1'-N1	9.56	115.85	108.20
55	1x	46	G	C6-N1-C2	-9.00	119.70	125.10
32	1a	1034	G	N3-C2-N2	8.56	125.89	119.90
1	1A	2189	U	C2-N1-C1'	8.55	127.96	117.70
1	1A	1109	G	C6-N1-C2	8.53	130.22	125.10
1	1A	1398	U	O5'-P-OP1	-8.49	98.06	105.70
1	1A	537	G	O4'-C1'-N9	8.48	114.98	108.20
1	2A	2136	C	N1-C2-O2	8.47	123.98	118.90
1	2A	2473	U	C2-N1-C1'	8.45	127.84	117.70
32	2a	1001(A)	G	N3-C4-N9	8.41	131.04	126.00
1	1A	649	C	O5'-P-OP1	-8.39	98.15	105.70
32	1a	1030(B)	C	C2-N1-C1'	8.36	128.00	118.80
32	1a	1034	G	N9-C4-C5	-8.27	102.09	105.40
1	2A	1352	U	O5'-P-OP1	-8.26	98.27	105.70
54	1y	33	U	C2-N1-C1'	8.22	127.57	117.70
32	2a	1272	G	C2-N3-C4	-8.21	107.79	111.90
32	2a	1039	C	C5-C4-N4	-8.12	114.52	120.20
32	2a	79	G	C5-C6-O6	8.08	133.45	128.60
1	1A	1121	C	N3-C2-O2	-8.02	116.29	121.90
32	2a	1263	C	C4-C5-C6	-7.98	113.41	117.40
1	1A	848	G	O5'-P-OP2	-7.90	98.59	105.70
1	2A	2149	G	N3-C4-N9	7.89	130.74	126.00
32	2a	1263	C	C2-N1-C1'	7.83	127.42	118.80
32	1a	1030(B)	C	C6-N1-C2	-7.82	117.17	120.30
1	1A	798	A	O5'-P-OP1	-7.75	98.73	105.70
1	2A	2492	U	O5'-P-OP1	-7.74	98.74	105.70
19	2X	57	LEU	CA-CB-CG	7.70	133.00	115.30
32	2a	1263	C	C5-C4-N4	7.69	125.58	120.20
55	2x	14	A	C4-C5-C6	7.67	120.83	117.00
32	2a	1272	G	C4-N9-C1'	7.64	136.44	126.50
55	1x	22	G	C5-N7-C8	-7.57	100.52	104.30
32	2a	1272	G	C8-N9-C1'	-7.56	117.17	127.00
32	2a	1039	C	C2-N1-C1'	7.56	127.11	118.80
1	1A	2189	U	N1-C2-O2	7.55	128.09	122.80
1	1A	1232	G	N1-C6-O6	-7.54	115.37	119.90
1	1A	2504	U	O5'-P-OP1	-7.53	98.93	105.70
55	1x	14	A	C5-C6-N1	-7.51	113.95	117.70
55	1x	22	G	C4-C5-C6	-7.46	114.33	118.80
1	1A	2189	U	N3-C2-O2	-7.43	117.00	122.20
1	1A	2260	C	O5'-P-OP2	-7.39	99.05	105.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	254	G	O5'-P-OP1	-7.30	99.13	105.70
1	1A	821	A	C8-N9-C4	-7.29	102.88	105.80
55	2x	14	A	C5-N7-C8	7.28	107.54	103.90
54	1y	56	C	N1-C2-O2	7.24	123.24	118.90
1	2A	801	G	O5'-P-OP2	-7.23	99.19	105.70
1	1A	1045	U	O5'-P-OP2	-7.19	99.23	105.70
32	1a	1034	G	C4-C5-N7	7.18	113.67	110.80
32	1a	1030	C	N1-C2-O2	7.08	123.15	118.90
32	1a	1034	G	C6-N1-C2	7.04	129.33	125.10
1	1A	1132	A	C5-C6-N6	7.03	129.32	123.70
32	2a	754	C	C2-N1-C1'	7.03	126.53	118.80
32	1a	1027	C	N3-C2-O2	-6.99	117.00	121.90
54	1y	33	U	N1-C2-O2	6.97	127.68	122.80
1	2A	2139	C	C2-N1-C1'	6.92	126.41	118.80
1	1A	2077	C	OP1-P-O3'	6.91	120.41	105.20
32	1a	1027	C	N3-C4-C5	-6.87	119.15	121.90
32	1a	1002	G	N3-C4-N9	6.82	130.09	126.00
32	1a	1034	G	N3-C4-N9	6.80	130.08	126.00
32	1a	1034	G	C8-N9-C1'	-6.76	118.21	127.00
1	2A	512	G	O4'-C1'-N9	6.75	113.60	108.20
1	1A	1020	C	C2-N1-C1'	-6.75	111.38	118.80
1	1A	2014	G	P-O3'-C3'	6.74	127.79	119.70
1	1A	1121	C	C6-N1-C2	-6.72	117.61	120.30
32	2a	1039	C	C6-N1-C1'	-6.70	112.76	120.80
1	2A	2473	U	N1-C2-O2	6.69	127.49	122.80
1	1A	2015	U	O5'-P-OP1	-6.67	99.70	105.70
32	2a	1004	A	N7-C8-N9	6.67	117.14	113.80
32	2a	754	C	N1-C2-O2	6.65	122.89	118.90
32	1a	1002	G	C4-N9-C1'	6.64	135.14	126.50
32	2a	1263	C	N1-C2-N3	-6.64	114.55	119.20
1	1A	840	A	O5'-P-OP2	-6.64	99.72	105.70
32	1a	1025	U	N1-C2-O2	6.64	127.44	122.80
1	1A	993	G	O5'-P-OP1	-6.63	99.73	105.70
1	2A	2492	U	O5'-P-OP2	6.56	118.57	110.70
1	1A	2727	G	O5'-P-OP2	-6.56	99.80	105.70
1	1A	215	G	O4'-C1'-N9	6.52	113.42	108.20
32	1a	1027	C	C5-C4-N4	6.51	124.76	120.20
32	1a	1002	G	C8-N9-C1'	-6.50	118.55	127.00
1	2A	2136	C	N3-C2-O2	-6.48	117.36	121.90
1	2A	2149	G	C8-N9-C1'	-6.48	118.58	127.00
1	2A	2149	G	C4-N9-C1'	6.47	134.91	126.50
54	1w	47	U	C2-N1-C1'	6.47	125.46	117.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	892	G	O4'-C1'-N9	6.45	113.36	108.20
1	1A	2566	U	O5'-P-OP1	-6.41	99.93	105.70
1	1A	1128	U	N3-C4-C5	6.39	118.43	114.60
32	2a	1263	C	N3-C4-N4	-6.38	113.53	118.00
32	1a	1034	G	C4-N9-C1'	6.35	134.76	126.50
1	2A	2149	G	N9-C4-C5	-6.35	102.86	105.40
54	1y	64	A	C5-C6-N6	6.35	128.78	123.70
1	2A	1698	A	O4'-C1'-N9	6.33	113.27	108.20
1	1A	1221	G	OP1-P-O3'	6.33	119.12	105.20
1	2A	1131	G	O4'-C1'-N9	6.32	113.26	108.20
1	1A	1121	C	C5-C4-N4	6.32	124.62	120.20
1	2A	2897	U	C2-N1-C1'	6.32	125.28	117.70
32	2a	588	G	O5'-P-OP2	-6.27	100.06	105.70
1	1A	1109	G	N3-C2-N2	6.26	124.28	119.90
1	1A	2054	G	C5-N7-C8	6.22	107.41	104.30
32	2a	1037	C	C6-N1-C2	-6.21	117.81	120.30
1	1A	2694	U	O5'-P-OP2	-6.19	100.13	105.70
1	1A	806	G	C5-C6-O6	-6.19	124.89	128.60
1	2A	2473	U	N3-C2-O2	-6.17	117.88	122.20
32	1a	1030(B)	C	C5-C6-N1	6.17	124.09	121.00
1	1A	1958	A	O4'-C1'-N9	6.16	113.13	108.20
1	2A	2430	A	O4'-C1'-N9	6.16	113.13	108.20
1	1A	809	U	C5-C4-O4	-6.15	122.21	125.90
55	1x	46	G	C5-C6-N1	6.15	114.57	111.50
54	1y	64	A	N1-C6-N6	-6.14	114.92	118.60
1	1A	1859	G	O5'-P-OP2	-6.13	100.19	105.70
54	2y	58	A	OP1-P-O3'	6.12	118.66	105.20
55	1x	22	G	C8-N9-C1'	6.11	134.95	127.00
32	1a	841	U	C5-C6-N1	6.11	125.75	122.70
1	1A	2180	A	N1-C2-N3	6.10	132.35	129.30
1	1A	2641	A	P-O3'-C3'	6.10	127.02	119.70
32	2a	1001(A)	G	N9-C4-C5	-6.10	102.96	105.40
1	2A	576	U	O5'-P-OP1	-6.09	100.22	105.70
54	1w	22	G	N1-C6-O6	6.05	123.53	119.90
1	2A	2174	C	C2-N1-C1'	6.05	125.45	118.80
32	2a	1366	C	C2-N3-C4	6.03	122.92	119.90
54	2y	22	G	N1-C6-O6	6.03	123.52	119.90
55	2x	14	A	C5-C6-N1	-6.03	114.69	117.70
1	2A	614	U	N3-C2-O2	-6.03	117.98	122.20
1	1A	2803	A	C2-N3-C4	6.00	113.60	110.60
1	2A	928	G	C8-N9-C4	-5.99	104.00	106.40
1	1A	572	A	P-O3'-C3'	5.98	126.87	119.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1039	C	N1-C2-O2	5.98	122.49	118.90
32	1a	266	G	P-O3'-C3'	5.97	126.87	119.70
1	1A	2180	A	P-O3'-C3'	5.97	126.86	119.70
1	2A	1372	U	C5-C4-O4	-5.96	122.32	125.90
1	2A	1314	C	C5-C6-N1	5.96	123.98	121.00
1	2A	783	A	C2-N3-C4	5.94	113.57	110.60
1	2A	2140	C	C2-N1-C1'	5.93	125.33	118.80
32	1a	1030	C	C2-N3-C4	5.92	122.86	119.90
55	1x	22	G	N3-C4-N9	-5.92	122.45	126.00
1	1A	1109	G	N1-C6-O6	-5.91	116.36	119.90
1	1A	894	U	C2-N1-C1'	5.89	124.77	117.70
32	2a	1187	G	N3-C4-N9	-5.89	122.47	126.00
1	1A	476	G	N1-C6-O6	-5.88	116.37	119.90
1	1A	605	G	C5-C6-O6	5.88	132.13	128.60
1	1A	1020	C	C6-N1-C1'	5.87	127.84	120.80
1	2A	2363	C	C6-N1-C2	5.87	122.65	120.30
32	2a	1039	C	N3-C4-N4	5.87	122.11	118.00
32	1a	1278	U	C5-C6-N1	5.87	125.63	122.70
1	1A	852	G	N9-C4-C5	-5.87	103.05	105.40
1	2A	1313	U	C2-N1-C1'	5.86	124.73	117.70
32	1a	1030(B)	C	N1-C2-O2	5.85	122.41	118.90
1	1A	2826	C	C6-N1-C2	-5.83	117.97	120.30
1	2A	2149	G	C6-C5-N7	-5.83	126.90	130.40
54	2w	50	U	C5-C4-O4	-5.82	122.41	125.90
32	2a	1030	C	N1-C2-O2	5.82	122.39	118.90
1	1A	2627	U	O5'-P-OP1	-5.81	100.47	105.70
1	2A	2139	C	C6-N1-C1'	-5.80	113.83	120.80
1	1A	1109	G	C5-C6-N1	-5.80	108.60	111.50
1	1A	1121	C	N3-C4-C5	-5.79	119.58	121.90
15	1T	82	LEU	CA-CB-CG	-5.79	101.99	115.30
1	1A	2858	G	O4'-C1'-N9	5.78	112.83	108.20
1	1A	2431	U	N3-C4-O4	-5.77	115.36	119.40
1	2A	1993	U	O5'-P-OP1	-5.76	100.51	105.70
55	1x	14	A	C8-N9-C1'	-5.76	117.33	127.70
1	1A	1121	C	C2-N1-C1'	5.75	125.13	118.80
55	2x	20	U	N1-C2-O2	5.75	126.83	122.80
55	1x	22	G	C5-C6-N1	5.75	114.38	111.50
1	2A	944	G	C4-N9-C1'	5.75	133.97	126.50
32	2a	266	G	N3-C4-C5	-5.74	125.73	128.60
1	1A	1232	G	C5-C6-O6	5.74	132.04	128.60
1	2A	2473	U	C6-N1-C1'	-5.74	113.17	121.20
32	2a	1054	C	C2-N1-C1'	5.73	125.11	118.80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	2689	U	P-O3'-C3'	5.72	126.57	119.70
1	2A	1992	G	P-O3'-C3'	5.72	126.56	119.70
1	1A	1121	C	C5-C6-N1	5.71	123.86	121.00
55	1x	22	G	N3-C4-C5	5.71	131.45	128.60
1	2A	856	C	C6-N1-C2	-5.70	118.02	120.30
1	1A	12	U	C2-N1-C1'	5.69	124.53	117.70
54	1y	33	U	N3-C2-O2	-5.69	118.22	122.20
32	2a	1225	A	C5-C6-N6	5.69	128.25	123.70
1	1A	1720	U	C5-C6-N1	-5.66	119.87	122.70
32	1a	1034	G	C6-C5-N7	-5.66	127.00	130.40
32	2a	299	G	C5-C6-O6	-5.66	125.21	128.60
55	2x	20	U	N3-C2-O2	-5.65	118.24	122.20
1	2A	2152	G	N3-C4-N9	5.64	129.38	126.00
2	2B	30	C	C6-N1-C2	-5.64	118.05	120.30
1	1A	322	G	C5-N7-C8	5.63	107.12	104.30
55	1x	22	G	C4-N9-C1'	-5.63	119.17	126.50
1	1A	2697	G	N1-C6-O6	-5.63	116.52	119.90
1	2A	746	A	O4'-C1'-N9	5.62	112.70	108.20
43	2l	29	GLY	N-CA-C	-5.62	99.05	113.10
1	1A	472	G	N1-C6-O6	5.62	123.27	119.90
1	1A	793	A	O4'-C1'-N9	5.61	112.69	108.20
1	2A	2174	C	N1-C2-O2	5.61	122.26	118.90
55	1x	14	A	C4-N9-C1'	5.60	136.38	126.30
1	1A	1991	A	OP1-P-O3'	5.59	117.50	105.20
1	2A	933	A	O4'-C1'-N9	5.58	112.66	108.20
1	1A	2299	A	O4'-C1'-N9	5.57	112.66	108.20
1	2A	228	A	P-O3'-C3'	5.57	126.39	119.70
32	2a	1054	C	O4'-C1'-N1	5.57	112.66	108.20
2	2B	1	U	C2-N1-C1'	5.57	124.38	117.70
32	1a	754	C	C2-N1-C1'	5.56	124.92	118.80
32	2a	299	G	N1-C6-O6	5.56	123.23	119.90
1	1A	598	A	O5'-P-OP1	-5.55	100.70	105.70
1	2A	1791	A	O5'-P-OP1	-5.55	100.71	105.70
1	2A	2107	C	C2-N3-C4	5.53	122.66	119.90
1	1A	399	G	O4'-C1'-N9	5.53	112.62	108.20
54	2w	74	C	N1-C2-O2	5.53	122.22	118.90
1	2A	444	C	O5'-P-OP1	-5.50	100.75	105.70
1	1A	2078	G	O4'-C1'-N9	-5.50	103.80	108.20
1	1A	1694	G	O4'-C1'-N9	-5.49	103.81	108.20
32	2a	1028	C	C2-N3-C4	5.49	122.65	119.90
1	2A	747	U	O5'-P-OP1	-5.49	100.76	105.70
1	1A	2442	A	C2-N3-C4	5.49	113.34	110.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	1028	C	C5-C6-N1	5.48	123.74	121.00
1	1A	1342	G	O5'-P-OP2	-5.47	100.77	105.70
1	1A	1700	G	C8-N9-C4	-5.47	104.21	106.40
55	2x	17	C	C2-N1-C1'	5.46	124.81	118.80
1	1A	587	C	N1-C2-O2	-5.46	115.63	118.90
1	2A	1313	U	O4'-C1'-N1	5.46	112.56	108.20
1	1A	472	G	C5-C6-O6	-5.45	125.33	128.60
1	1A	356	A	N1-C6-N6	-5.44	115.33	118.60
1	1A	1657	C	N1-C2-O2	5.44	122.17	118.90
26	14	54	GLY	N-CA-C	5.44	126.70	113.10
1	1A	184	A	P-O3'-C3'	5.44	126.22	119.70
1	2A	1372	U	N3-C4-O4	5.43	123.20	119.40
1	2A	2712	U	O4'-C1'-N1	5.43	112.54	108.20
32	1a	1026	G	O4'-C1'-N9	5.43	112.54	108.20
55	1x	22	G	N1-C6-O6	-5.41	116.65	119.90
1	1A	795	G	O4'-C1'-N9	5.41	112.53	108.20
54	1y	56	C	C2-N3-C4	5.40	122.60	119.90
32	2a	1001(A)	G	C4-C5-N7	5.40	112.96	110.80
54	1y	33	U	C6-N1-C1'	-5.40	113.64	121.20
1	1A	732	A	C8-N9-C4	-5.39	103.64	105.80
1	1A	2613	C	C6-N1-C2	-5.38	118.15	120.30
32	1a	1021	G	O4'-C1'-N9	5.38	112.50	108.20
32	2a	754	C	N3-C2-O2	-5.38	118.14	121.90
1	1A	1462	G	O4'-C1'-N9	5.37	112.50	108.20
32	1a	1002	G	N3-C4-C5	-5.37	125.92	128.60
1	2A	2149	G	C4-C5-N7	5.37	112.95	110.80
32	2a	79	G	N1-C6-O6	-5.37	116.68	119.90
1	2A	226	G	O4'-C1'-N9	5.36	112.49	108.20
1	1A	2701	U	P-O3'-C3'	5.35	126.12	119.70
32	2a	1001(A)	G	C8-N9-C1'	-5.34	120.06	127.00
54	2y	58	A	P-O3'-C3'	5.34	126.11	119.70
32	2a	1022	G	N3-C2-N2	5.33	123.63	119.90
1	2A	792	G	O4'-C1'-N9	-5.33	103.94	108.20
32	2a	289	G	O5'-P-OP2	-5.32	100.91	105.70
1	1A	605	G	N1-C6-O6	-5.32	116.71	119.90
32	2a	1004	A	C8-N9-C4	-5.32	103.67	105.80
1	1A	2431	U	N1-C2-O2	5.31	126.52	122.80
1	2A	1314	C	C6-N1-C2	-5.31	118.18	120.30
1	1A	1177	G	O4'-C1'-N9	5.31	112.45	108.20
1	2A	1279	G	O5'-P-OP2	-5.31	100.92	105.70
1	2A	1698	A	C6-C5-N7	-5.31	128.59	132.30
1	1A	2189	U	C6-N1-C1'	-5.30	113.77	121.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	1x	46	G	C5-C6-O6	-5.30	125.42	128.60
32	1a	1065	U	P-O3'-C3'	5.30	126.06	119.70
1	1A	2697	G	C6-C5-N7	5.29	133.57	130.40
32	2a	1001(A)	G	C4-N9-C1'	5.29	133.38	126.50
1	1A	831	A	N9-C4-C5	5.29	107.92	105.80
1	1A	1874	C	N1-C2-O2	-5.29	115.73	118.90
32	1a	841	U	C6-N1-C2	-5.28	117.83	121.00
32	1a	1025	U	N3-C2-O2	-5.27	118.51	122.20
1	2A	912	C	C6-N1-C2	-5.27	118.19	120.30
32	2a	65	U	P-O3'-C3'	5.27	126.02	119.70
32	2a	1001(A)	G	N3-C4-C5	-5.26	125.97	128.60
32	1a	1030	C	N3-C2-O2	-5.26	118.22	121.90
1	2A	945	A	O4'-C1'-N9	5.26	112.41	108.20
1	1A	2074	G	N1-C6-O6	-5.26	116.75	119.90
1	1A	285	U	O4'-C1'-N1	5.26	112.40	108.20
1	2A	141	A	N7-C8-N9	5.25	116.43	113.80
32	2a	1260	C	C6-N1-C2	-5.25	118.20	120.30
1	2A	2142	C	C2-N1-C1'	5.25	124.58	118.80
1	2A	1530	C	P-O3'-C3'	5.25	126.00	119.70
1	2A	528	A	P-O3'-C3'	5.23	125.98	119.70
41	2j	8	LEU	CA-CB-CG	5.23	127.34	115.30
1	2A	646	A	O4'-C1'-N9	5.23	112.38	108.20
1	1A	2331	G	C5-N7-C8	-5.22	101.69	104.30
1	2A	383	U	O4'-C1'-N1	5.22	112.38	108.20
1	1A	2054	G	C4-C5-N7	-5.22	108.71	110.80
1	2A	2152	G	C5-C6-O6	-5.21	125.47	128.60
32	2a	754	C	C6-N1-C1'	-5.21	114.54	120.80
1	1A	1219	A	P-O3'-C3'	5.21	125.96	119.70
1	1A	2883	A	O4'-C1'-N9	5.20	112.36	108.20
1	2A	845	G	C4-N9-C1'	5.20	133.26	126.50
1	2A	528	A	OP1-P-O3'	5.20	116.64	105.20
1	1A	856	G	N1-C6-O6	-5.19	116.78	119.90
1	1A	1709	C	N3-C2-O2	-5.19	118.27	121.90
1	1A	855	G	O5'-P-OP2	-5.18	101.04	105.70
32	1a	421	U	C2-N1-C1'	5.18	123.92	117.70
32	2a	299	G	C6-C5-N7	-5.18	127.29	130.40
1	1A	815	G	C5-C6-O6	5.18	131.71	128.60
32	2a	687	A	P-O3'-C3'	5.17	125.91	119.70
1	1A	2074	G	C5-C6-O6	5.17	131.70	128.60
32	1a	1067	A	P-O3'-C3'	5.16	125.90	119.70
54	1w	60	U	N3-C2-O2	-5.16	118.59	122.20
1	2A	2427	C	O5'-P-OP1	-5.16	101.06	105.70

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2a	266	G	P-O3'-C3'	5.16	125.89	119.70
32	2a	955	U	C2-N3-C4	5.16	130.09	127.00
22	10	13	GLY	N-CA-C	5.15	125.98	113.10
1	2A	228	A	OP1-P-O3'	5.15	116.54	105.20
1	1A	734	C	C6-N1-C2	-5.14	118.24	120.30
1	1A	2258	G	C8-N9-C4	5.14	108.46	106.40
32	1a	204	U	N1-C2-O2	5.14	126.40	122.80
55	2x	17	C	C6-N1-C2	-5.14	118.24	120.30
32	1a	615	C	C6-N1-C2	-5.13	118.25	120.30
1	1A	2598	C	C6-N1-C2	-5.12	118.25	120.30
1	2A	1377	G	N1-C6-O6	-5.12	116.83	119.90
1	2A	1411	C	C2-N1-C1'	5.12	124.43	118.80
1	1A	991	G	O5'-P-OP1	-5.11	101.10	105.70
1	1A	1255	A	P-O3'-C3'	5.11	125.84	119.70
1	2A	748	G	C4-N9-C1'	-5.11	119.86	126.50
54	1y	56	C	N3-C2-O2	-5.10	118.33	121.90
2	2B	42	C	N1-C2-O2	5.10	121.96	118.90
1	1A	2204	G	N3-C4-N9	-5.09	122.94	126.00
1	1A	2701	U	C6-N1-C2	-5.09	117.94	121.00
1	1A	2228	G	C4-N9-C1'	5.09	133.12	126.50
1	2A	912	C	N1-C2-O2	5.09	121.95	118.90
1	2A	1597	A	N1-C6-N6	-5.09	115.55	118.60
54	2y	43	C	C2-N1-C1'	5.09	124.39	118.80
32	2a	971	G	C4-C5-N7	-5.08	108.77	110.80
1	2A	2512	C	N1-C2-O2	-5.08	115.85	118.90
32	1a	1034	G	N1-C2-N3	-5.07	120.86	123.90
1	1A	419	C	O5'-P-OP1	-5.07	101.14	105.70
1	1A	1810	U	O4'-C1'-N1	5.07	112.25	108.20
1	1A	815	G	N1-C6-O6	-5.06	116.86	119.90
1	2A	2046	G	C8-N9-C1'	-5.06	120.42	127.00
1	1A	740	C	N1-C2-O2	5.06	121.93	118.90
1	1A	1474	C	N3-C2-O2	-5.06	118.36	121.90
27	25	58	LEU	CA-CB-CG	5.06	126.93	115.30
32	1a	1030(B)	C	C6-N1-C1'	-5.05	114.73	120.80
1	1A	410	U	C2-N1-C1'	-5.05	111.64	117.70
1	1A	2838	C	N1-C2-O2	-5.05	115.87	118.90
1	1A	2250	G	N3-C4-N9	5.05	129.03	126.00
1	2A	2804	C	C6-N1-C2	-5.05	118.28	120.30
1	1A	2621	U	C5-C6-N1	-5.05	120.18	122.70
1	2A	1698	A	N1-C6-N6	5.04	121.63	118.60
1	2A	944	G	C8-N9-C1'	-5.04	120.45	127.00
1	2A	1298	C	O5'-P-OP2	-5.04	101.16	105.70

*Continued on next page...*



Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	12	U	C5-C6-N1	5.04	125.22	122.70
32	2a	299	G	C4-C5-N7	5.04	112.81	110.80
1	2A	928	G	N7-C8-N9	5.03	115.62	113.10
55	2x	14	A	C8-N9-C1'	-5.02	118.66	127.70
1	1A	560	C	N3-C2-O2	-5.02	118.38	121.90
32	1a	913	A	P-O3'-C3'	5.02	125.72	119.70
1	2A	1653	G	P-O3'-C3'	5.02	125.72	119.70
1	2A	2321	G	C4-N9-C1'	5.01	133.01	126.50
1	2A	2139	C	N1-C2-O2	5.01	121.91	118.90
1	2A	2167	U	N1-C2-O2	5.01	126.31	122.80
32	2a	913	A	P-O3'-C3'	5.01	125.71	119.70
1	1A	1146	C	C2-N1-C1'	5.00	124.30	118.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
43	2l	92	0TD	Mainchain

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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%)	262 (96%)	11 (4%)	0	100	100
3	2D	273/276 (99%)	260 (95%)	11 (4%)	2 (1%)	19	35
4	1E	202/206 (98%)	193 (96%)	8 (4%)	1 (0%)	25	44
4	2E	202/206 (98%)	194 (96%)	7 (4%)	1 (0%)	25	44

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	1F	201/210 (96%)	198 (98%)	2 (1%)	1 (0%)	25	44
5	2F	201/210 (96%)	197 (98%)	2 (1%)	2 (1%)	13	25
6	1G	179/182 (98%)	170 (95%)	9 (5%)	0	100	100
6	2G	179/182 (98%)	168 (94%)	10 (6%)	1 (1%)	22	39
7	1H	172/180 (96%)	164 (95%)	7 (4%)	1 (1%)	22	39
7	2H	172/180 (96%)	158 (92%)	12 (7%)	2 (1%)	11	21
8	1I	144/148 (97%)	132 (92%)	12 (8%)	0	100	100
8	2I	144/148 (97%)	128 (89%)	14 (10%)	2 (1%)	9	17
9	1N	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
9	2N	138/140 (99%)	133 (96%)	4 (3%)	1 (1%)	19	35
10	1O	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
10	2O	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
11	1P	147/150 (98%)	139 (95%)	8 (5%)	0	100	100
11	2P	147/150 (98%)	137 (93%)	10 (7%)	0	100	100
12	1Q	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
12	2Q	139/141 (99%)	131 (94%)	7 (5%)	1 (1%)	19	35
13	1R	116/118 (98%)	111 (96%)	5 (4%)	0	100	100
13	2R	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
14	1S	108/112 (96%)	106 (98%)	2 (2%)	0	100	100
14	2S	108/112 (96%)	105 (97%)	2 (2%)	1 (1%)	14	28
15	1T	129/146 (88%)	123 (95%)	6 (5%)	0	100	100
15	2T	129/146 (88%)	125 (97%)	4 (3%)	0	100	100
16	1U	114/118 (97%)	114 (100%)	0	0	100	100
16	2U	114/118 (97%)	114 (100%)	0	0	100	100
17	1V	99/101 (98%)	97 (98%)	1 (1%)	1 (1%)	13	25
17	2V	99/101 (98%)	97 (98%)	1 (1%)	1 (1%)	13	25
18	1W	110/113 (97%)	110 (100%)	0	0	100	100
18	2W	110/113 (97%)	110 (100%)	0	0	100	100
19	1X	93/96 (97%)	90 (97%)	3 (3%)	0	100	100
19	2X	93/96 (97%)	88 (95%)	4 (4%)	1 (1%)	12	23
20	1Y	105/110 (96%)	98 (93%)	5 (5%)	2 (2%)	6	12

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	2Y	105/110 (96%)	99 (94%)	4 (4%)	2 (2%)	6	12
21	1Z	148/206 (72%)	136 (92%)	11 (7%)	1 (1%)	19	35
21	2Z	156/206 (76%)	141 (90%)	15 (10%)	0	100	100
22	10	81/85 (95%)	80 (99%)	0	1 (1%)	11	21
22	20	81/85 (95%)	77 (95%)	3 (4%)	1 (1%)	11	21
23	11	95/98 (97%)	92 (97%)	3 (3%)	0	100	100
23	21	95/98 (97%)	91 (96%)	4 (4%)	0	100	100
24	12	68/72 (94%)	68 (100%)	0	0	100	100
24	22	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
25	13	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
25	23	57/60 (95%)	53 (93%)	3 (5%)	1 (2%)	7	12
26	14	67/71 (94%)	58 (87%)	4 (6%)	5 (8%)	1	1
26	24	67/71 (94%)	53 (79%)	10 (15%)	4 (6%)	1	1
27	15	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
27	25	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
28	16	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
28	26	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
29	17	46/49 (94%)	44 (96%)	2 (4%)	0	100	100
29	27	46/49 (94%)	44 (96%)	1 (2%)	1 (2%)	5	9
30	18	62/65 (95%)	62 (100%)	0	0	100	100
30	28	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
31	19	35/37 (95%)	35 (100%)	0	0	100	100
31	29	35/37 (95%)	35 (100%)	0	0	100	100
33	1b	229/256 (90%)	200 (87%)	22 (10%)	7 (3%)	3	5
33	2b	229/256 (90%)	202 (88%)	19 (8%)	8 (4%)	3	4
34	1c	204/239 (85%)	188 (92%)	15 (7%)	1 (0%)	25	44
34	2c	204/239 (85%)	187 (92%)	15 (7%)	2 (1%)	13	25
35	1d	206/209 (99%)	196 (95%)	9 (4%)	1 (0%)	25	44
35	2d	206/209 (99%)	197 (96%)	8 (4%)	1 (0%)	25	44
36	1e	146/162 (90%)	137 (94%)	6 (4%)	3 (2%)	5	10
36	2e	146/162 (90%)	139 (95%)	5 (3%)	2 (1%)	9	17

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	1f	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
37	2f	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
38	1g	153/156 (98%)	144 (94%)	6 (4%)	3 (2%)	6	11
38	2g	153/156 (98%)	143 (94%)	7 (5%)	3 (2%)	6	11
39	1h	135/138 (98%)	133 (98%)	2 (2%)	0	100	100
39	2h	135/138 (98%)	131 (97%)	4 (3%)	0	100	100
40	1i	125/128 (98%)	115 (92%)	9 (7%)	1 (1%)	16	31
40	2i	125/128 (98%)	114 (91%)	10 (8%)	1 (1%)	16	31
41	1j	95/105 (90%)	86 (90%)	4 (4%)	5 (5%)	1	1
41	2j	94/105 (90%)	85 (90%)	5 (5%)	4 (4%)	2	3
42	1k	112/129 (87%)	106 (95%)	4 (4%)	2 (2%)	7	12
42	2k	112/129 (87%)	107 (96%)	3 (3%)	2 (2%)	7	12
43	1l	119/132 (90%)	115 (97%)	4 (3%)	0	100	100
43	2l	119/132 (90%)	112 (94%)	7 (6%)	0	100	100
44	1m	121/126 (96%)	114 (94%)	7 (6%)	0	100	100
44	2m	120/126 (95%)	110 (92%)	9 (8%)	1 (1%)	16	31
45	1n	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
45	2n	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
46	1o	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
46	2o	86/89 (97%)	81 (94%)	4 (5%)	1 (1%)	11	21
47	1p	80/88 (91%)	76 (95%)	3 (4%)	1 (1%)	10	19
47	2p	80/88 (91%)	76 (95%)	3 (4%)	1 (1%)	10	19
48	1q	97/105 (92%)	93 (96%)	3 (3%)	1 (1%)	13	25
48	2q	97/105 (92%)	94 (97%)	2 (2%)	1 (1%)	13	25
49	1r	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
49	2r	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
50	1s	81/93 (87%)	75 (93%)	5 (6%)	1 (1%)	11	21
50	2s	81/93 (87%)	74 (91%)	5 (6%)	2 (2%)	4	7
51	1t	94/106 (89%)	87 (93%)	0	7 (7%)	1	1
51	2t	94/106 (89%)	86 (92%)	4 (4%)	4 (4%)	2	3
52	1u	21/27 (78%)	21 (100%)	0	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	2u	21/27 (78%)	21 (100%)	0	0	100	100
All	All	11370/12128 (94%)	10779 (95%)	488 (4%)	103 (1%)	14	28

All (103) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1F	130	ALA
7	1H	126	PRO
21	1Z	159	PRO
26	14	62	ARG
33	1b	10	LEU
38	1g	79	ARG
40	1i	54	ASP
41	1j	55	LYS
50	1s	81	ARG
51	1t	10	LEU
51	1t	100	ILE
5	2F	21	ALA
5	2F	130	ALA
7	2H	126	PRO
8	2I	10	GLU
17	2V	79	VAL
26	24	55	ARG
26	24	61	ARG
29	27	46	VAL
33	2b	16	HIS
33	2b	123	ALA
34	2c	181	ASN
38	2g	79	ARG
44	2m	4	ILE
50	2s	81	ARG
51	2t	10	LEU
17	1V	79	VAL
26	14	45	GLY
26	14	56	VAL
42	1k	49	GLY
3	2D	69	ARG
6	2G	50	ALA
8	2I	40	THR
14	2S	84	GLN
26	24	45	GLY
40	2i	54	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
51	2t	47	GLY
4	1E	52	LEU
22	10	13	GLY
33	1b	17	PHE
38	1g	80	VAL
41	1j	32	ALA
41	1j	77	PRO
41	1j	78	ASN
51	1t	47	GLY
51	1t	96	GLY
51	1t	102	GLY
4	2E	52	LEU
9	2N	2	LYS
19	2X	2	LYS
26	24	46	GLN
33	2b	125	PRO
36	2e	37	ARG
41	2j	77	PRO
48	2q	33	GLY
50	2s	29	ARG
26	14	57	GLU
33	1b	16	HIS
33	1b	20	GLU
33	1b	22	LYS
34	1c	66	VAL
35	1d	178	VAL
36	1e	86	ALA
51	1t	95	ALA
3	2D	3	VAL
20	2Y	103	GLY
33	2b	20	GLU
33	2b	78	GLN
34	2c	156	ARG
38	2g	7	ALA
38	2g	80	VAL
41	2j	78	ASN
51	2t	100	ILE
20	1Y	54	LYS
26	14	53	GLU
33	1b	231	GLU
41	1j	79	ARG
42	1k	105	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
20	2Y	57	GLN
22	20	4	LYS
33	2b	21	ARG
33	2b	231	GLU
41	2j	55	LYS
42	2k	49	GLY
46	2o	88	ARG
38	1g	4	ARG
51	1t	9	ASN
7	2H	29	PRO
36	2e	69	VAL
42	2k	105	VAL
47	2p	53	VAL
48	1q	33	GLY
25	23	59	VAL
51	2t	102	GLY
20	1Y	103	GLY
36	1e	69	VAL
36	1e	85	GLY
47	1p	53	VAL
33	2b	202	PRO
41	2j	75	ILE
12	2Q	27	VAL
35	2d	5	ILE
33	1b	125	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	215/218 (99%)	209 (97%)	6 (3%)	38	65
3	2D	215/218 (99%)	208 (97%)	7 (3%)	33	59
4	1E	164/166 (99%)	154 (94%)	10 (6%)	15	32
4	2E	164/166 (99%)	154 (94%)	10 (6%)	15	32
5	1F	160/166 (96%)	150 (94%)	10 (6%)	15	30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	2F	159/166 (96%)	150 (94%)	9 (6%)	17	35
6	1G	143/156 (92%)	139 (97%)	4 (3%)	38	65
6	2G	143/156 (92%)	135 (94%)	8 (6%)	17	36
7	1H	144/148 (97%)	141 (98%)	3 (2%)	48	74
7	2H	144/148 (97%)	142 (99%)	2 (1%)	62	83
8	1I	113/124 (91%)	108 (96%)	5 (4%)	24	47
8	2I	105/124 (85%)	99 (94%)	6 (6%)	17	35
9	1N	118/119 (99%)	110 (93%)	8 (7%)	13	27
9	2N	118/119 (99%)	109 (92%)	9 (8%)	11	22
10	1O	100/100 (100%)	98 (98%)	2 (2%)	50	75
10	2O	100/100 (100%)	99 (99%)	1 (1%)	73	88
11	1P	115/116 (99%)	109 (95%)	6 (5%)	19	39
11	2P	115/116 (99%)	112 (97%)	3 (3%)	41	68
12	1Q	111/111 (100%)	108 (97%)	3 (3%)	40	67
12	2Q	111/111 (100%)	105 (95%)	6 (5%)	18	37
13	1R	101/101 (100%)	90 (89%)	11 (11%)	5	10
13	2R	101/101 (100%)	94 (93%)	7 (7%)	13	26
14	1S	86/88 (98%)	84 (98%)	2 (2%)	45	72
14	2S	85/88 (97%)	83 (98%)	2 (2%)	44	70
15	1T	115/127 (91%)	113 (98%)	2 (2%)	56	79
15	2T	113/127 (89%)	113 (100%)	0	100	100
16	1U	93/94 (99%)	92 (99%)	1 (1%)	70	87
16	2U	93/94 (99%)	91 (98%)	2 (2%)	47	73
17	1V	80/82 (98%)	74 (92%)	6 (8%)	11	23
17	2V	80/82 (98%)	74 (92%)	6 (8%)	11	23
18	1W	90/92 (98%)	85 (94%)	5 (6%)	17	36
18	2W	90/92 (98%)	85 (94%)	5 (6%)	17	36
19	1X	77/78 (99%)	75 (97%)	2 (3%)	41	68
19	2X	77/78 (99%)	76 (99%)	1 (1%)	65	85
20	1Y	85/91 (93%)	82 (96%)	3 (4%)	31	57
20	2Y	85/91 (93%)	82 (96%)	3 (4%)	31	57

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	1Z	135/179 (75%)	129 (96%)	6 (4%)	24	47
21	2Z	137/179 (76%)	136 (99%)	1 (1%)	81	93
22	10	65/67 (97%)	63 (97%)	2 (3%)	35	62
22	20	65/67 (97%)	64 (98%)	1 (2%)	60	82
23	11	80/83 (96%)	79 (99%)	1 (1%)	65	85
23	21	80/83 (96%)	78 (98%)	2 (2%)	42	69
24	12	65/67 (97%)	64 (98%)	1 (2%)	60	82
24	22	65/67 (97%)	65 (100%)	0	100	100
25	13	51/52 (98%)	49 (96%)	2 (4%)	27	52
25	23	50/52 (96%)	48 (96%)	2 (4%)	27	51
26	14	59/63 (94%)	58 (98%)	1 (2%)	56	79
26	24	53/63 (84%)	49 (92%)	4 (8%)	11	23
27	15	50/52 (96%)	47 (94%)	3 (6%)	16	33
27	25	50/52 (96%)	47 (94%)	3 (6%)	16	33
28	16	51/52 (98%)	49 (96%)	2 (4%)	27	52
28	26	50/52 (96%)	49 (98%)	1 (2%)	50	75
29	17	41/42 (98%)	40 (98%)	1 (2%)	44	70
29	27	41/42 (98%)	40 (98%)	1 (2%)	44	70
30	18	54/55 (98%)	52 (96%)	2 (4%)	29	55
30	28	54/55 (98%)	52 (96%)	2 (4%)	29	55
31	19	34/34 (100%)	34 (100%)	0	100	100
31	29	34/34 (100%)	33 (97%)	1 (3%)	37	64
33	1b	192/220 (87%)	189 (98%)	3 (2%)	58	80
33	2b	187/220 (85%)	183 (98%)	4 (2%)	48	74
34	1c	142/188 (76%)	141 (99%)	1 (1%)	81	93
34	2c	140/188 (74%)	137 (98%)	3 (2%)	48	74
35	1d	169/181 (93%)	163 (96%)	6 (4%)	30	56
35	2d	173/181 (96%)	167 (96%)	6 (4%)	31	57
36	1e	113/123 (92%)	110 (97%)	3 (3%)	40	67
36	2e	114/123 (93%)	110 (96%)	4 (4%)	31	57
37	1f	84/90 (93%)	84 (100%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	2f	85/90 (94%)	83 (98%)	2 (2%)	44	70
38	1g	119/127 (94%)	118 (99%)	1 (1%)	79	91
38	2g	120/127 (94%)	117 (98%)	3 (2%)	42	69
39	1h	114/119 (96%)	112 (98%)	2 (2%)	54	78
39	2h	114/119 (96%)	113 (99%)	1 (1%)	75	90
40	1i	90/99 (91%)	87 (97%)	3 (3%)	33	59
40	2i	89/99 (90%)	85 (96%)	4 (4%)	23	46
41	1j	66/92 (72%)	66 (100%)	0	100	100
41	2j	69/92 (75%)	67 (97%)	2 (3%)	37	64
42	1k	82/99 (83%)	80 (98%)	2 (2%)	44	70
42	2k	83/99 (84%)	83 (100%)	0	100	100
43	1l	96/108 (89%)	92 (96%)	4 (4%)	25	49
43	2l	96/108 (89%)	94 (98%)	2 (2%)	48	74
44	1m	93/101 (92%)	92 (99%)	1 (1%)	70	87
44	2m	92/101 (91%)	91 (99%)	1 (1%)	70	87
45	1n	49/50 (98%)	44 (90%)	5 (10%)	6	12
45	2n	49/50 (98%)	47 (96%)	2 (4%)	26	50
46	1o	78/80 (98%)	76 (97%)	2 (3%)	41	68
46	2o	78/80 (98%)	77 (99%)	1 (1%)	65	85
47	1p	69/74 (93%)	65 (94%)	4 (6%)	17	34
47	2p	68/74 (92%)	65 (96%)	3 (4%)	24	47
48	1q	94/97 (97%)	94 (100%)	0	100	100
48	2q	94/97 (97%)	92 (98%)	2 (2%)	48	74
49	1r	59/77 (77%)	58 (98%)	1 (2%)	56	79
49	2r	59/77 (77%)	59 (100%)	0	100	100
50	1s	69/80 (86%)	68 (99%)	1 (1%)	62	83
50	2s	67/80 (84%)	64 (96%)	3 (4%)	23	46
51	1t	70/82 (85%)	69 (99%)	1 (1%)	62	83
51	2t	70/82 (85%)	70 (100%)	0	100	100
52	1u	18/22 (82%)	18 (100%)	0	100	100
52	2u	18/22 (82%)	18 (100%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9303/10064 (92%)	9005 (97%)	298 (3%)	34 60

All (298) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1D	3	VAL
3	1D	106	ILE
3	1D	113	VAL
3	1D	142	VAL
3	1D	229	VAL
3	1D	257	LEU
4	1E	12	THR
4	1E	19	ARG
4	1E	21	VAL
4	1E	24	THR
4	1E	73	GLU
4	1E	75	VAL
4	1E	78	LEU
4	1E	116	VAL
4	1E	175	VAL
4	1E	181	LEU
5	1F	53	THR
5	1F	57	VAL
5	1F	74	ARG
5	1F	106	ARG
5	1F	125	LEU
5	1F	132	VAL
5	1F	170	LEU
5	1F	183	VAL
5	1F	192	LEU
5	1F	201	VAL
6	1G	43	LEU
6	1G	82	LEU
6	1G	148	MET
6	1G	159	VAL
7	1H	51	ARG
7	1H	71	LEU
7	1H	129	THR
8	1I	38	LEU
8	1I	47	LEU
8	1I	92	VAL
8	1I	107	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
8	1I	142	VAL
9	1N	14	VAL
9	1N	28	THR
9	1N	33	LEU
9	1N	34	LEU
9	1N	46	VAL
9	1N	73	THR
9	1N	99	LEU
9	1N	120	LEU
10	1O	10	VAL
10	1O	108	GLU
11	1P	65	ARG
11	1P	95	VAL
11	1P	98	GLU
11	1P	106	LEU
11	1P	112	LEU
11	1P	125	VAL
12	1Q	35	VAL
12	1Q	109	VAL
12	1Q	110	THR
13	1R	6	SER
13	1R	24	GLN
13	1R	29	LEU
13	1R	36	THR
13	1R	44	LEU
13	1R	54	LEU
13	1R	65	LEU
13	1R	79	LEU
13	1R	100	LEU
13	1R	111	LEU
13	1R	114	VAL
14	1S	25	ARG
14	1S	110	LEU
15	1T	28	VAL
15	1T	74	ARG
16	1U	74	LEU
17	1V	46	VAL
17	1V	51	VAL
17	1V	52	VAL
17	1V	72	VAL
17	1V	79	VAL
17	1V	82	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
18	1W	17	VAL
18	1W	19	LEU
18	1W	23	LEU
18	1W	67	ASP
18	1W	107	LEU
19	1X	35	THR
19	1X	57	LEU
20	1Y	1	MET
20	1Y	43	ASN
20	1Y	72	VAL
21	1Z	5	LEU
21	1Z	86	VAL
21	1Z	129	SER
21	1Z	155	LEU
21	1Z	161	VAL
21	1Z	171	ILE
22	10	14	ARG
22	10	43	THR
23	11	35	THR
24	12	40	SER
25	13	23	LEU
25	13	54	VAL
26	14	49	PHE
27	15	6	VAL
27	15	16	ARG
27	15	29	THR
28	16	37	ARG
28	16	48	VAL
29	17	43	THR
30	18	31	HIS
30	18	32	LEU
33	1b	24	TRP
33	1b	111	ARG
33	1b	112	VAL
34	1c	21	ARG
35	1d	10	ARG
35	1d	31	CYS
35	1d	49	ARG
35	1d	134	ASP
35	1d	135	LEU
35	1d	194	LEU
36	1e	31	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
36	1e	41	VAL
36	1e	56	GLN
38	1g	8	GLU
39	1h	69	ARG
39	1h	112	LEU
40	1i	42	ARG
40	1i	64	THR
40	1i	128	ARG
42	1k	31	THR
42	1k	48	ILE
43	1l	27	LEU
43	1l	36	VAL
43	1l	83	VAL
43	1l	84	LEU
44	1m	102	ARG
45	1n	3	ARG
45	1n	6	LEU
45	1n	22	THR
45	1n	23	ARG
45	1n	33	VAL
46	1o	7	GLU
46	1o	39	LEU
47	1p	19	ILE
47	1p	20	VAL
47	1p	21	VAL
47	1p	67	THR
49	1r	76	LEU
50	1s	41	VAL
51	1t	13	LEU
3	2D	94	LEU
3	2D	106	ILE
3	2D	113	VAL
3	2D	134	ARG
3	2D	142	VAL
3	2D	259	THR
3	2D	276	LYS
4	2E	12	THR
4	2E	21	VAL
4	2E	24	THR
4	2E	52	LEU
4	2E	75	VAL
4	2E	78	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
4	2E	116	VAL
4	2E	163	GLU
4	2E	175	VAL
4	2E	181	LEU
5	2F	53	THR
5	2F	70	THR
5	2F	74	ARG
5	2F	106	ARG
5	2F	170	LEU
5	2F	183	VAL
5	2F	192	LEU
5	2F	197	ASP
5	2F	201	VAL
6	2G	28	VAL
6	2G	31	VAL
6	2G	43	LEU
6	2G	60	LEU
6	2G	79	ASN
6	2G	115	ARG
6	2G	135	LEU
6	2G	159	VAL
7	2H	84	SER
7	2H	88	LEU
8	2I	38	LEU
8	2I	47	LEU
8	2I	57	ARG
8	2I	92	VAL
8	2I	121	LYS
8	2I	123	LEU
9	2N	14	VAL
9	2N	28	THR
9	2N	33	LEU
9	2N	34	LEU
9	2N	46	VAL
9	2N	67	LEU
9	2N	87	LEU
9	2N	99	LEU
9	2N	120	LEU
10	2O	8	LEU
11	2P	95	VAL
11	2P	99	LEU
11	2P	106	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
12	2Q	1	MET
12	2Q	2	LEU
12	2Q	16	ARG
12	2Q	21	THR
12	2Q	35	VAL
12	2Q	110	THR
13	2R	18	LEU
13	2R	24	GLN
13	2R	29	LEU
13	2R	44	LEU
13	2R	65	LEU
13	2R	100	LEU
13	2R	111	LEU
14	2S	75	GLU
14	2S	110	LEU
16	2U	36	ARG
16	2U	74	LEU
17	2V	43	GLU
17	2V	46	VAL
17	2V	51	VAL
17	2V	72	VAL
17	2V	79	VAL
17	2V	82	ARG
18	2W	17	VAL
18	2W	19	LEU
18	2W	23	LEU
18	2W	67	ASP
18	2W	107	LEU
19	2X	57	LEU
20	2Y	28	LYS
20	2Y	72	VAL
20	2Y	90	LEU
21	2Z	124	ILE
22	20	14	ARG
23	21	4	VAL
23	21	95	LEU
25	23	30	ARG
25	23	54	VAL
26	24	34	GLU
26	24	37	SER
26	24	48	ARG
26	24	49	PHE

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
27	25	6	VAL
27	25	16	ARG
27	25	29	THR
28	26	48	VAL
29	27	39	ARG
30	28	31	HIS
30	28	32	LEU
31	29	17	ILE
33	2b	11	LEU
33	2b	93	VAL
33	2b	127	ILE
33	2b	221	LEU
34	2c	70	VAL
34	2c	124	ILE
34	2c	154	SER
35	2d	31	CYS
35	2d	135	LEU
35	2d	141	ARG
35	2d	150	GLU
35	2d	170	VAL
35	2d	194	LEU
36	2e	13	ILE
36	2e	31	LEU
36	2e	41	VAL
36	2e	64	ARG
37	2f	21	LEU
37	2f	72	VAL
38	2g	9	VAL
38	2g	52	GLU
38	2g	98	SER
39	2h	23	SER
40	2i	53	VAL
40	2i	65	VAL
40	2i	102	LEU
40	2i	108	VAL
41	2j	8	LEU
41	2j	100	THR
43	2l	27	LEU
43	2l	83	VAL
44	2m	47	ASP
45	2n	22	THR
45	2n	33	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
46	2o	39	LEU
47	2p	2	VAL
47	2p	21	VAL
47	2p	67	THR
48	2q	35	VAL
48	2q	83	ASP
50	2s	41	VAL
50	2s	49	ILE
50	2s	77	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (95) such sidechains are listed below:

Mol	Chain	Res	Type
4	1E	48	GLN
5	1F	8	GLN
8	1I	105	HIS
13	1R	71	GLN
19	1X	31	HIS
19	1X	82	GLN
20	1Y	6	HIS
20	1Y	43	ASN
23	1I	56	GLN
24	12	9	GLN
25	13	32	GLN
34	1c	6	HIS
34	1c	162	GLN
34	1c	181	ASN
35	1d	116	GLN
35	1d	119	GLN
35	1d	123	HIS
35	1d	125	HIS
36	1e	78	HIS
37	1f	100	ASN
38	1g	28	ASN
38	1g	86	GLN
40	1i	3	GLN
40	1i	31	GLN
40	1i	34	ASN
40	1i	58	HIS
40	1i	89	ASN
40	1i	124	GLN
41	1j	56	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
42	1k	99	GLN
43	1l	99	HIS
47	1p	16	HIS
48	1q	26	GLN
50	1s	23	ASN
50	1s	69	HIS
50	1s	83	HIS
3	2D	87	ASN
4	2E	48	GLN
5	2F	69	HIS
6	2G	41	GLN
9	2N	38	HIS
10	2O	3	GLN
12	2Q	12	GLN
12	2Q	13	GLN
12	2Q	57	HIS
12	2Q	123	HIS
13	2R	13	HIS
14	2S	38	GLN
15	2T	79	HIS
16	2U	81	HIS
16	2U	117	GLN
18	2W	60	ASN
19	2X	31	HIS
19	2X	82	GLN
20	2Y	6	HIS
21	2Z	55	HIS
21	2Z	73	GLN
22	20	35	ASN
23	21	56	GLN
24	22	9	GLN
24	22	65	ASN
26	24	46	GLN
33	2b	40	HIS
33	2b	94	ASN
33	2b	140	HIS
34	2c	6	HIS
34	2c	37	GLN
34	2c	98	ASN
34	2c	104	GLN
35	2d	119	GLN
35	2d	123	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
35	2d	125	HIS
35	2d	161	ASN
36	2e	73	ASN
36	2e	78	HIS
36	2e	130	ASN
37	2f	64	GLN
37	2f	73	ASN
38	2g	28	ASN
38	2g	86	GLN
38	2g	109	ASN
39	2h	78	GLN
40	2i	3	GLN
40	2i	58	HIS
40	2i	89	ASN
40	2i	124	GLN
42	2k	22	HIS
42	2k	78	GLN
43	2l	49	ASN
43	2l	99	HIS
44	2m	12	ASN
44	2m	77	ASN
46	2o	28	GLN
50	2s	47	HIS
51	2t	75	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2861/2915 (98%)	414 (14%)	43 (1%)
1	2A	2788/2915 (95%)	510 (18%)	28 (1%)
2	1B	120/121 (99%)	11 (9%)	1 (0%)
2	2B	118/121 (97%)	35 (29%)	0
32	1a	1494/1521 (98%)	241 (16%)	0
32	2a	1498/1521 (98%)	253 (16%)	0
53	1v	12/24 (50%)	4 (33%)	0
53	2v	12/24 (50%)	3 (25%)	0
54	1w	71/76 (93%)	22 (30%)	0
54	1y	71/76 (93%)	23 (32%)	0
54	2w	68/76 (89%)	27 (39%)	0
54	2y	69/76 (90%)	23 (33%)	0
55	1x	75/77 (97%)	8 (10%)	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
55	2x	75/77 (97%)	16 (21%)	0
All	All	9332/9620 (97%)	1590 (17%)	72 (0%)

All (1590) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	13	A
1	1A	34	C
1	1A	45	C
1	1A	60	G
1	1A	70	A
1	1A	71	U
1	1A	73	A
1	1A	74	G
1	1A	83	A
1	1A	117	A
1	1A	118	U
1	1A	137	G
1	1A	185	A
1	1A	189	U
1	1A	194	G
1	1A	203	G
1	1A	204	G
1	1A	205	A
1	1A	211	A
1	1A	217	A
1	1A	218	A
1	1A	222	A
1	1A	237	G
1	1A	258	U
1	1A	271	U
1	1A	272	U
1	1A	273	G
1	1A	288	U
1	1A	289	G
1	1A	296	U
1	1A	303	C
1	1A	335	A
1	1A	353	G
1	1A	354	A
1	1A	376	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	1A	387	G
1	1A	388	A
1	1A	389	G
1	1A	407	U
1	1A	413	G
1	1A	423	G
1	1A	427	G
1	1A	432	U
1	1A	438	G
1	1A	455	A
1	1A	470	C
1	1A	474	U
1	1A	477	C
1	1A	480	A
1	1A	482	C
1	1A	483	A
1	1A	505	A
1	1A	507	G
1	1A	529	U
1	1A	530	A
1	1A	534	C
1	1A	537	G
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	598	A
1	1A	609	A
1	1A	626	A
1	1A	627	G
1	1A	630	U
1	1A	639	G
1	1A	641	G
1	1A	642	G
1	1A	652	A
1	1A	659	C
1	1A	660	C
1	1A	662	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	1A	670	C
1	1A	671	A
1	1A	697	C
1	1A	716	G
1	1A	733	G
1	1A	777	C
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	848	G
1	1A	852	G
1	1A	859	C
1	1A	866	A
1	1A	874	U
1	1A	875	U
1	1A	906	G
1	1A	913	A
1	1A	924	U
1	1A	926	G
1	1A	927	G
1	1A	931	C
1	1A	932	C
1	1A	933	C
1	1A	934	A
1	1A	935	C
1	1A	936	C
1	1A	937	A
1	1A	940	C
1	1A	941	U
1	1A	942	A
1	1A	943	C
1	1A	944	C
1	1A	946	A
1	1A	953	U
1	1A	956	A
1	1A	977	G
1	1A	990	A
1	1A	991	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	1A	998	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	1055	A
1	1A	1058	U
1	1A	1059	C
1	1A	1068	G
1	1A	1072	U
1	1A	1073	A
1	1A	1079	U
1	1A	1084	C
1	1A	1090	G
1	1A	1091	A
1	1A	1092	A
1	1A	1093	G
1	1A	1094	A
1	1A	1100	A
1	1A	1101	G
1	1A	1104	G
1	1A	1112	U
1	1A	1114	G
1	1A	1117	G
1	1A	1119	A
1	1A	1120	G
1	1A	1121	C
1	1A	1122	C
1	1A	1124	U
1	1A	1125	C
1	1A	1127	U
1	1A	1129	U
1	1A	1130	A
1	1A	1134	A
1	1A	1135	G
1	1A	1136	U
1	1A	1137	G
1	1A	1139	G
1	1A	1140	U
1	1A	1142	A

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	1A	1146	C
1	1A	1147	U
1	1A	1148	C
1	1A	1149	A
1	1A	1153	G
1	1A	1156	G
1	1A	1157	A
1	1A	1158	G
1	1A	1162	C
1	1A	1180	C
1	1A	1181	G
1	1A	1195	G
1	1A	1201	A
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	1256	U
1	1A	1299	A
1	1A	1302	G
1	1A	1317	G
1	1A	1318	A
1	1A	1322	A
1	1A	1346	U
1	1A	1347	A
1	1A	1349	G
1	1A	1366	C
1	1A	1391	C
1	1A	1398	U
1	1A	1405	A
1	1A	1406	A
1	1A	1411	A
1	1A	1426	G
1	1A	1430	A
1	1A	1431	G
1	1A	1441	A
1	1A	1442	U
1	1A	1462	G
1	1A	1463	C

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	1A	1466	U
1	1A	1467	G
1	1A	1474	C
1	1A	1491	A
1	1A	1497	G
1	1A	1502	G
1	1A	1514	C
1	1A	1529	G
1	1A	1539	C
1	1A	1540	A
1	1A	1554	A
1	1A	1555	C
1	1A	1556	A
1	1A	1569	U
1	1A	1586	G
1	1A	1587	U
1	1A	1605	A
1	1A	1613	A
1	1A	1616	A
1	1A	1625	U
1	1A	1627	A
1	1A	1628	G
1	1A	1631	C
1	1A	1632	A
1	1A	1654	A
1	1A	1686	U
1	1A	1694	G
1	1A	1695	C
1	1A	1701	A
1	1A	1721	G
1	1A	1741	C
1	1A	1743	G
1	1A	1747	A
1	1A	1750	G
1	1A	1767	A
1	1A	1768	U
1	1A	1776	G
1	1A	1787	G
1	1A	1794	G
1	1A	1795	G
1	1A	1804	A
1	1A	1811	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	1A	1813	C
1	1A	1817	A
1	1A	1822	A
1	1A	1831	C
1	1A	1847	G
1	1A	1848	G
1	1A	1859	G
1	1A	1860	A
1	1A	1878	A
1	1A	1889	G
1	1A	1892	G
1	1A	1899	A
1	1A	1911	A
1	1A	1922	A
1	1A	1928	G
1	1A	1951	G
1	1A	1952	G
1	1A	1959	A
1	1A	1960	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	2014	G
1	1A	2015	U
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	2057	G
1	1A	2061	C
1	1A	2065	C
1	1A	2077	C
1	1A	2078	G
1	1A	2082	A
1	1A	2083	G
1	1A	2084	A
1	1A	2091	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	1A	2115	G
1	1A	2132	G
1	1A	2135	U
1	1A	2136	A
1	1A	2137	G
1	1A	2138	G
1	1A	2143	G
1	1A	2149	G
1	1A	2151	C
1	1A	2152	U
1	1A	2153	G
1	1A	2154	U
1	1A	2155	G
1	1A	2156	A
1	1A	2157	A
1	1A	2162	C
1	1A	2163	G
1	1A	2164	C
1	1A	2166	U
1	1A	2168	C
1	1A	2172	U
1	1A	2173	G
1	1A	2178	G
1	1A	2179	G
1	1A	2180	A
1	1A	2181	G
1	1A	2182	G
1	1A	2184	G
1	1A	2187	G
1	1A	2188	G
1	1A	2189	U
1	1A	2193	A
1	1A	2194	U
1	1A	2197	C
1	1A	2200	C
1	1A	2203	G
1	1A	2204	G
1	1A	2206	G
1	1A	2207	C
1	1A	2214	G
1	1A	2220	A
1	1A	2227	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	1A	2228	G
1	1A	2229	A
1	1A	2231	G
1	1A	2237	A
1	1A	2250	G
1	1A	2251	G
1	1A	2280	A
1	1A	2281	A
1	1A	2292	G
1	1A	2295	C
1	1A	2299	A
1	1A	2317	A
1	1A	2320	G
1	1A	2321	A
1	1A	2332	A
1	1A	2337	G
1	1A	2346	G
1	1A	2359	C
1	1A	2362	C
1	1A	2373	A
1	1A	2384	G
1	1A	2395	G
1	1A	2397	C
1	1A	2418	U
1	1A	2422	G
1	1A	2436	C
1	1A	2437	A
1	1A	2441	G
1	1A	2442	A
1	1A	2443	U
1	1A	2447	A
1	1A	2451	A
1	1A	2453	C
1	1A	2460	A
1	1A	2486	C
1	1A	2488	A
1	1A	2514	G
1	1A	2517	G
1	1A	2518	U
1	1A	2530	A
1	1A	2541	G
1	1A	2561	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	1A	2566	U
1	1A	2578	A
1	1A	2579	G
1	1A	2585	C
1	1A	2586	G
1	1A	2590	G
1	1A	2614	A
1	1A	2621	U
1	1A	2623	U
1	1A	2624	C
1	1A	2641	A
1	1A	2642	G
1	1A	2653	G
1	1A	2666	A
1	1A	2701	U
1	1A	2702	C
1	1A	2703	C
1	1A	2714	U
1	1A	2725	A
1	1A	2726	A
1	1A	2727	G
1	1A	2739	U
1	1A	2746	A
1	1A	2770	A
1	1A	2771	A
1	1A	2778	A
1	1A	2782	C
1	1A	2791	A
1	1A	2803	A
1	1A	2804	C
1	1A	2806	G
1	1A	2813	G
1	1A	2828	G
1	1A	2830	A
1	1A	2831	A
1	1A	2845	A
1	1A	2846	U
1	1A	2879	G
1	1A	2882	G
1	1A	2890	C
1	1A	2901	A
1	1A	2903	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	1B	2	C
2	1B	12	C
2	1B	25	A
2	1B	35	U
2	1B	45	A
2	1B	56	G
2	1B	67	G
2	1B	73	A
2	1B	85	G
2	1B	106	G
2	1B	110	G
32	1a	7	G
32	1a	9	G
32	1a	32	A
32	1a	39	G
32	1a	47	C
32	1a	48	C
32	1a	51	A
32	1a	54	C
32	1a	61	G
32	1a	65	U
32	1a	79	G
32	1a	91	C
32	1a	97	G
32	1a	98	G
32	1a	101	A
32	1a	116	A
32	1a	121	C
32	1a	131	C
32	1a	163	C
32	1a	174	C
32	1a	180	U
32	1a	182	U
32	1a	195	A
32	1a	197	A
32	1a	201	C
32	1a	202	U
32	1a	203	U
32	1a	204	U
32	1a	216	G
32	1a	217	C
32	1a	247	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
32	1a	251	G
32	1a	258	G
32	1a	266	G
32	1a	267	C
32	1a	289	G
32	1a	301	G
32	1a	306	G
32	1a	321	A
32	1a	328	C
32	1a	332	G
32	1a	342	C
32	1a	348	G
32	1a	352	C
32	1a	353	A
32	1a	354	G
32	1a	367	U
32	1a	372	C
32	1a	373	A
32	1a	384	G
32	1a	397	A
32	1a	398	C
32	1a	406	G
32	1a	412	A
32	1a	421	U
32	1a	423	G
32	1a	424	G
32	1a	429	U
32	1a	441	A
32	1a	442	C
32	1a	452	A
32	1a	461	A
32	1a	470	C
32	1a	471	G
32	1a	477	A
32	1a	484	G
32	1a	485	G
32	1a	496	A
32	1a	498	U
32	1a	505	G
32	1a	509	A
32	1a	510	A
32	1a	511	C

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
32	1a	518	C
32	1a	531	U
32	1a	532	A
32	1a	547	A
32	1a	559	A
32	1a	561	U
32	1a	568	G
32	1a	572	A
32	1a	573	A
32	1a	576	G
32	1a	577	G
32	1a	596	C
32	1a	630	G
32	1a	653	A
32	1a	665	A
32	1a	687	A
32	1a	688	G
32	1a	695	A
32	1a	721	G
32	1a	723	U
32	1a	731	G
32	1a	733	A
32	1a	749	C
32	1a	755	G
32	1a	774	G
32	1a	777	A
32	1a	792	A
32	1a	793	U
32	1a	794	A
32	1a	815	A
32	1a	817	C
32	1a	821	G
32	1a	828	A
32	1a	840	C
32	1a	841	U
32	1a	851	G
32	1a	853	G
32	1a	859	A
32	1a	870	U
32	1a	880	C
32	1a	885	G
32	1a	902	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
32	1a	914	A
32	1a	926	G
32	1a	927	G
32	1a	932	C
32	1a	934	C
32	1a	960	U
32	1a	961	U
32	1a	968	A
32	1a	969	A
32	1a	971	G
32	1a	974	A
32	1a	975	A
32	1a	976	G
32	1a	977	A
32	1a	982	U
32	1a	989	C
32	1a	992	U
32	1a	993	G
32	1a	997	U
32	1a	1000	U
32	1a	1001(A)	G
32	1a	1002	G
32	1a	1003	G
32	1a	1005	A
32	1a	1006	C
32	1a	1009	G
32	1a	1011	G
32	1a	1016	A
32	1a	1020	U
32	1a	1021	G
32	1a	1022	G
32	1a	1025	U
32	1a	1026	G
32	1a	1027	C
32	1a	1029	C
32	1a	1030	C
32	1a	1030(A)	G
32	1a	1030(C)	G
32	1a	1031	G
32	1a	1033	G
32	1a	1039	C
32	1a	1045	C

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	1a	1054	C
32	1a	1065	U
32	1a	1066	C
32	1a	1068	G
32	1a	1080	A
32	1a	1081	G
32	1a	1086	U
32	1a	1094	G
32	1a	1095	U
32	1a	1101	A
32	1a	1108	G
32	1a	1122	U
32	1a	1125	U
32	1a	1129	C
32	1a	1130	A
32	1a	1132	C
32	1a	1134	G
32	1a	1137	C
32	1a	1138	G
32	1a	1139	G
32	1a	1140	C
32	1a	1141	C
32	1a	1146	A
32	1a	1152	A
32	1a	1159	U
32	1a	1163	C
32	1a	1172	C
32	1a	1181	G
32	1a	1183	A
32	1a	1184	G
32	1a	1196	U
32	1a	1197	G
32	1a	1202	G
32	1a	1212	U
32	1a	1213	A
32	1a	1220	G
32	1a	1222	G
32	1a	1227	A
32	1a	1238	A
32	1a	1240	U
32	1a	1241	G
32	1a	1256	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
32	1a	1257	U
32	1a	1260	C
32	1a	1267	C
32	1a	1270	C
32	1a	1273	G
32	1a	1276	G
32	1a	1278	U
32	1a	1279	A
32	1a	1280	A
32	1a	1286	A
32	1a	1287	A
32	1a	1290	G
32	1a	1299	A
32	1a	1300	G
32	1a	1302	U
32	1a	1320	C
32	1a	1338	G
32	1a	1340	A
32	1a	1346	A
32	1a	1347	G
32	1a	1353	G
32	1a	1363	C
32	1a	1368	G
32	1a	1370	G
32	1a	1419	G
32	1a	1442	G
32	1a	1442(A)	G
32	1a	1446	U
32	1a	1447	A
32	1a	1456	G
32	1a	1487	G
32	1a	1492	A
32	1a	1494	G
32	1a	1497	G
32	1a	1503	A
32	1a	1504	G
32	1a	1505	G
32	1a	1506	U
32	1a	1517	G
32	1a	1529	G
32	1a	1530	G
32	1a	1532	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
53	1v	13	A
53	1v	14	A
53	1v	15	A
53	1v	24	A
54	1w	2	C
54	1w	6	G
54	1w	8	4SU
54	1w	14	A
54	1w	19	G
54	1w	20	U
54	1w	21	A
54	1w	23	A
54	1w	24	G
54	1w	45	U
54	1w	46	7MG
54	1w	47	U
54	1w	48	C
54	1w	50	U
54	1w	62	C
54	1w	64	A
54	1w	67	C
54	1w	68	C
54	1w	70	G
54	1w	72	C
54	1w	73	A
54	1w	74	C
55	1x	9	G
55	1x	18	G
55	1x	19	G
55	1x	21	A
55	1x	47	U
55	1x	61	C
55	1x	69	C
55	1x	76	A
54	1y	6	G
54	1y	8	4SU
54	1y	9	A
54	1y	13	C
54	1y	19	G
54	1y	20	U
54	1y	21	A
54	1y	23	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
54	1y	35	A
54	1y	44	G
54	1y	45	U
54	1y	46	7MG
54	1y	47	U
54	1y	48	C
54	1y	49	C
54	1y	53	G
54	1y	54	5MU
54	1y	56	C
54	1y	59	U
54	1y	61	C
54	1y	65	G
54	1y	69	G
54	1y	70	G
1	2A	8	A
1	2A	12	U
1	2A	15	G
1	2A	34	C
1	2A	35	G
1	2A	45	C
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	95	G
1	2A	100	G
1	2A	102	G
1	2A	118	A
1	2A	119	A
1	2A	120	U
1	2A	127	A
1	2A	154(A)	C
1	2A	157	U
1	2A	173	G
1	2A	181	A
1	2A	196	A
1	2A	199	A
1	2A	205	G
1	2A	214	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	2A	215	G
1	2A	216	A
1	2A	221	A
1	2A	222	A
1	2A	225	A
1	2A	228	A
1	2A	229	A
1	2A	233	A
1	2A	248	G
1	2A	249	C
1	2A	250	G
1	2A	267	C
1	2A	271(A)	A
1	2A	271(K)	U
1	2A	271(L)	U
1	2A	271(M)	G
1	2A	271(N)	U
1	2A	271(O)	C
1	2A	272(B)	G
1	2A	272(I)	U
1	2A	272(J)	C
1	2A	274	G
1	2A	277	C
1	2A	278	A
1	2A	294	A
1	2A	303	U
1	2A	311	A
1	2A	316	C
1	2A	317	G
1	2A	324	A
1	2A	325	G
1	2A	327	G
1	2A	329	G
1	2A	330	A
1	2A	333	G
1	2A	352	G
1	2A	362	U
1	2A	363	G
1	2A	363(B)	G
1	2A	363(D)	G
1	2A	386	G
1	2A	396	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	2A	402	A
1	2A	403	U
1	2A	405	U
1	2A	406	G
1	2A	407	G
1	2A	411	G
1	2A	412	A
1	2A	418	G
1	2A	421	U
1	2A	422	A
1	2A	435	C
1	2A	444	C
1	2A	454	A
1	2A	455	C
1	2A	457	A
1	2A	481	G
1	2A	494	G
1	2A	501	A
1	2A	504	U
1	2A	505	A
1	2A	508	G
1	2A	509	C
1	2A	517	C
1	2A	520	G
1	2A	529	A
1	2A	530	G
1	2A	531	C
1	2A	532	A
1	2A	533	G
1	2A	563	G
1	2A	568	U
1	2A	573	G
1	2A	575	A
1	2A	588	U
1	2A	592	G
1	2A	599	G
1	2A	603	A
1	2A	604	G
1	2A	607	U
1	2A	614(B)	G
1	2A	615	G
1	2A	616	G

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	2A	621	A
1	2A	627	A
1	2A	634	C
1	2A	637	A
1	2A	645	C
1	2A	651	G
1	2A	652(B)	A
1	2A	652(U)	G
1	2A	667	U
1	2A	669	G
1	2A	686	G
1	2A	701	G
1	2A	709	U
1	2A	717	G
1	2A	730	C
1	2A	752	A
1	2A	753	C
1	2A	771	G
1	2A	775	G
1	2A	776	G
1	2A	782	A
1	2A	784	A
1	2A	785	G
1	2A	792	G
1	2A	805	G
1	2A	812	C
1	2A	819	A
1	2A	827	U
1	2A	828	U
1	2A	847	U
1	2A	857	C
1	2A	859	G
1	2A	866	A
1	2A	869	G
1	2A	870	A
1	2A	874	G
1	2A	875	G
1	2A	879	G
1	2A	880	G
1	2A	884	C
1	2A	886	C
1	2A	887	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	2A	888	C
1	2A	889	C
1	2A	890	A
1	2A	893	C
1	2A	894	C
1	2A	895	U
1	2A	896	A
1	2A	900	A
1	2A	901	A
1	2A	910	A
1	2A	915	C
1	2A	917	A
1	2A	932	G
1	2A	933	A
1	2A	941	A
1	2A	944	G
1	2A	945	A
1	2A	946	G
1	2A	953	A
1	2A	958	U
1	2A	959	A
1	2A	961	C
1	2A	974	G
1	2A	975	C
1	2A	983	A
1	2A	996	A
1	2A	997	G
1	2A	998	C
1	2A	1012	U
1	2A	1013	C
1	2A	1017	G
1	2A	1020	A
1	2A	1022	G
1	2A	1025	G
1	2A	1026	U
1	2A	1033	U
1	2A	1038	C
1	2A	1039	G
1	2A	1041	C
1	2A	1042	G
1	2A	1043	C
1	2A	1114	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	2A	1116	C
1	2A	1130	U
1	2A	1135	C
1	2A	1136	G
1	2A	1139	G
1	2A	1142	U
1	2A	1144	G
1	2A	1166	C
1	2A	1169	G
1	2A	1171	G
1	2A	1180	C
1	2A	1188	U
1	2A	1205	U
1	2A	1206	G
1	2A	1210	A
1	2A	1211	U
1	2A	1218	C
1	2A	1220	A
1	2A	1224	C
1	2A	1237	A
1	2A	1248	G
1	2A	1250	G
1	2A	1252	G
1	2A	1253	A
1	2A	1256	G
1	2A	1268	A
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	1314	C
1	2A	1321	A
1	2A	1345	C
1	2A	1352	U
1	2A	1359	A
1	2A	1360	A
1	2A	1365	A
1	2A	1368	G
1	2A	1370	C

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	2A	1384	A
1	2A	1385	G
1	2A	1386	C
1	2A	1411	C
1	2A	1416	G
1	2A	1417	C
1	2A	1420	U
1	2A	1421	G
1	2A	1427	A
1	2A	1428	C
1	2A	1435	G
1	2A	1437	C
1	2A	1445	A
1	2A	1449	A
1	2A	1450	G
1	2A	1460	A
1	2A	1467	C
1	2A	1471	A
1	2A	1482	G
1	2A	1490	A
1	2A	1493	C
1	2A	1494	A
1	2A	1495	A
1	2A	1496	A
1	2A	1497	U
1	2A	1508	A
1	2A	1509	C
1	2A	1509(A)	A
1	2A	1514	U
1	2A	1531	C
1	2A	1532	C
1	2A	1533	G
1	2A	1543	C
1	2A	1547	C
1	2A	1558	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	1608	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	2A	1609	A
1	2A	1610	A
1	2A	1616	A
1	2A	1629	U
1	2A	1647	G
1	2A	1648	C
1	2A	1654	A
1	2A	1674	G
1	2A	1696	G
1	2A	1700	A
1	2A	1703	G
1	2A	1721	G
1	2A	1722	A
1	2A	1739	U
1	2A	1740	G
1	2A	1746	G
1	2A	1747(A)	G
1	2A	1756	G
1	2A	1758	G
1	2A	1762	A
1	2A	1763	G
1	2A	1764	G
1	2A	1769	G
1	2A	1773	A
1	2A	1780	A
1	2A	1782	C
1	2A	1786	A
1	2A	1791	A
1	2A	1800	C
1	2A	1801	G
1	2A	1811	G
1	2A	1812	A
1	2A	1816	G
1	2A	1828	G
1	2A	1835	G
1	2A	1839	G
1	2A	1847	A
1	2A	1848	A
1	2A	1857	G
1	2A	1877	A
1	2A	1878	G
1	2A	1889	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	2A	1900	A
1	2A	1906	G
1	2A	1913	A
1	2A	1914	C
1	2A	1929	G
1	2A	1930	G
1	2A	1931	U
1	2A	1936	A
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	1992	G
1	2A	1993	U
1	2A	1997	G
1	2A	2020	A
1	2A	2023	G
1	2A	2027	G
1	2A	2031	A
1	2A	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	2093	G
1	2A	2099	U
1	2A	2105	C
1	2A	2108	C
1	2A	2110	G
1	2A	2111	C
1	2A	2112	G
1	2A	2116	G
1	2A	2119	A
1	2A	2120	G
1	2A	2122	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	2A	2125	G
1	2A	2126	A
1	2A	2127	G
1	2A	2129	C
1	2A	2131	G
1	2A	2132	U
1	2A	2134	A
1	2A	2135	A
1	2A	2136	C
1	2A	2137	C
1	2A	2138	C
1	2A	2140	C
1	2A	2142	C
1	2A	2146	C
1	2A	2150	U
1	2A	2151	G
1	2A	2154	G
1	2A	2155	G
1	2A	2156	G
1	2A	2157	G
1	2A	2158	A
1	2A	2161	C
1	2A	2165	G
1	2A	2166	G
1	2A	2167	U
1	2A	2168	G
1	2A	2169	A
1	2A	2172	U
1	2A	2174	C
1	2A	2178	C
1	2A	2185	C
1	2A	2189	U
1	2A	2192	G
1	2A	2198	A
1	2A	2206	G
1	2A	2207	G
1	2A	2208	A
1	2A	2218	U
1	2A	2225	A
1	2A	2232	U
1	2A	2235	G
1	2A	2239	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	2A	2275	C
1	2A	2279	G
1	2A	2283	C
1	2A	2287	A
1	2A	2302	G
1	2A	2305	A
1	2A	2308	G
1	2A	2319	G
1	2A	2320	A
1	2A	2321	G
1	2A	2324	C
1	2A	2325	G
1	2A	2327	A
1	2A	2328	A
1	2A	2329	G
1	2A	2334	G
1	2A	2336	A
1	2A	2341	G
1	2A	2346	A
1	2A	2347	C
1	2A	2350	C
1	2A	2354	G
1	2A	2376	A
1	2A	2383	G
1	2A	2385	C
1	2A	2403	C
1	2A	2406	U
1	2A	2410	G
1	2A	2419	U
1	2A	2425	A
1	2A	2426	A
1	2A	2429	G
1	2A	2430	A
1	2A	2434	A
1	2A	2435	A
1	2A	2439	A
1	2A	2441	C
1	2A	2445	G
1	2A	2448	A
1	2A	2458	G
1	2A	2465	C
1	2A	2468	G

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	2A	2469	A
1	2A	2474	C
1	2A	2476	A
1	2A	2477	C
1	2A	2478	A
1	2A	2490	G
1	2A	2491	U
1	2A	2502	G
1	2A	2505	G
1	2A	2506	U
1	2A	2518	A
1	2A	2520	C
1	2A	2525	G
1	2A	2529	G
1	2A	2554	U
1	2A	2555	U
1	2A	2566	A
1	2A	2567	G
1	2A	2573	C
1	2A	2578	G
1	2A	2602	A
1	2A	2609	U
1	2A	2611	U
1	2A	2612	C
1	2A	2629	A
1	2A	2630	G
1	2A	2634	G
1	2A	2654	A
1	2A	2663	G
1	2A	2664	G
1	2A	2689	U
1	2A	2690	C
1	2A	2712(A)	A
1	2A	2713	A
1	2A	2714	G
1	2A	2726	U
1	2A	2733	A
1	2A	2739	U
1	2A	2744	G
1	2A	2751	G
1	2A	2758	A
1	2A	2764	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	2A	2765	A
1	2A	2766	G
1	2A	2778	A
1	2A	2789	C
1	2A	2793	G
1	2A	2802	G
1	2A	2803	C
1	2A	2807	G
1	2A	2818	G
1	2A	2820	A
1	2A	2821	A
1	2A	2824	C
1	2A	2833	G
1	2A	2836	U
1	2A	2839	G
1	2A	2872	G
1	2A	2879	C
1	2A	2880	C
1	2A	2894	G
1	2A	2895	U
1	2A	2897	U
2	2B	2	C
2	2B	5	C
2	2B	8	U
2	2B	9	G
2	2B	19	G
2	2B	20	C
2	2B	25	A
2	2B	32	C
2	2B	34	U
2	2B	38	C
2	2B	42	C
2	2B	52	A
2	2B	53	A
2	2B	56	G
2	2B	57	A
2	2B	58	A
2	2B	63	G
2	2B	65	C
2	2B	66	A
2	2B	67	G
2	2B	72	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	2B	73	A
2	2B	74	U
2	2B	75	G
2	2B	85	G
2	2B	88	C
2	2B	90	A
2	2B	91	C
2	2B	106	G
2	2B	108	U
2	2B	110	G
2	2B	114	C
2	2B	116	G
2	2B	119	G
2	2B	120	A
32	2a	7	G
32	2a	9	G
32	2a	32	A
32	2a	39	G
32	2a	47	C
32	2a	48	C
32	2a	51	A
32	2a	54	C
32	2a	65	U
32	2a	66	G
32	2a	73	G
32	2a	79	G
32	2a	80	G
32	2a	89	C
32	2a	91	C
32	2a	97	G
32	2a	98	G
32	2a	101	A
32	2a	116	A
32	2a	121	C
32	2a	131	C
32	2a	163	C
32	2a	174	C
32	2a	180	U
32	2a	182	U
32	2a	195	A
32	2a	197	A
32	2a	201	C

*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	217	C
32	2a	247	G
32	2a	251	G
32	2a	258	G
32	2a	266	G
32	2a	267	C
32	2a	289	G
32	2a	301	G
32	2a	306	G
32	2a	321	A
32	2a	328	C
32	2a	332	G
32	2a	342	C
32	2a	348	G
32	2a	352	C
32	2a	353	A
32	2a	354	G
32	2a	367	U
32	2a	372	C
32	2a	373	A
32	2a	384	G
32	2a	397	A
32	2a	398	C
32	2a	406	G
32	2a	412	A
32	2a	421	U
32	2a	423	G
32	2a	424	G
32	2a	429	U
32	2a	441	A
32	2a	442	C
32	2a	452	A
32	2a	461	A
32	2a	470	C
32	2a	471	G
32	2a	477	A
32	2a	484	G
32	2a	485	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
32	2a	496	A
32	2a	498	U
32	2a	505	G
32	2a	509	A
32	2a	510	A
32	2a	511	C
32	2a	518	C
32	2a	531	U
32	2a	532	A
32	2a	547	A
32	2a	559	A
32	2a	561	U
32	2a	564	C
32	2a	572	A
32	2a	573	A
32	2a	576	G
32	2a	577	G
32	2a	587	G
32	2a	588	G
32	2a	596	C
32	2a	630	G
32	2a	650	G
32	2a	653	A
32	2a	665	A
32	2a	687	A
32	2a	688	G
32	2a	695	A
32	2a	702	A
32	2a	721	G
32	2a	723	U
32	2a	731	G
32	2a	733	A
32	2a	749	C
32	2a	755	G
32	2a	774	G
32	2a	777	A
32	2a	792	A
32	2a	793	U
32	2a	794	A
32	2a	815	A
32	2a	817	C
32	2a	821	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
32	2a	828	A
32	2a	840	C
32	2a	841	U
32	2a	851	G
32	2a	853	G
32	2a	859	A
32	2a	870	U
32	2a	880	C
32	2a	902	G
32	2a	914	A
32	2a	926	G
32	2a	927	G
32	2a	932	C
32	2a	934	C
32	2a	960	U
32	2a	961	U
32	2a	968	A
32	2a	969	A
32	2a	971	G
32	2a	974	A
32	2a	975	A
32	2a	976	G
32	2a	977	A
32	2a	982	U
32	2a	989	C
32	2a	992	U
32	2a	993	G
32	2a	997	U
32	2a	1001(A)	G
32	2a	1002	G
32	2a	1003	G
32	2a	1005	A
32	2a	1006	C
32	2a	1009	G
32	2a	1011	G
32	2a	1016	A
32	2a	1020	U
32	2a	1021	G
32	2a	1022	G
32	2a	1025	U
32	2a	1026	G
32	2a	1027	C

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
32	2a	1028	C
32	2a	1030	C
32	2a	1030(A)	G
32	2a	1031	G
32	2a	1033	G
32	2a	1036	G
32	2a	1038	C
32	2a	1039	C
32	2a	1040	U
32	2a	1045	C
32	2a	1051	C
32	2a	1065	U
32	2a	1066	C
32	2a	1068	G
32	2a	1077	G
32	2a	1080	A
32	2a	1081	G
32	2a	1086	U
32	2a	1094	G
32	2a	1095	U
32	2a	1101	A
32	2a	1108	G
32	2a	1117	G
32	2a	1122	U
32	2a	1125	U
32	2a	1129	C
32	2a	1130	A
32	2a	1132	C
32	2a	1134	G
32	2a	1137	C
32	2a	1138	G
32	2a	1139	G
32	2a	1140	C
32	2a	1141	C
32	2a	1146	A
32	2a	1152	A
32	2a	1159	U
32	2a	1163	C
32	2a	1172	C
32	2a	1181	G
32	2a	1182	G
32	2a	1183	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
32	2a	1184	G
32	2a	1196	U
32	2a	1197	G
32	2a	1202	G
32	2a	1211	U
32	2a	1212	U
32	2a	1213	A
32	2a	1222	G
32	2a	1226	C
32	2a	1227	A
32	2a	1238	A
32	2a	1240	U
32	2a	1241	G
32	2a	1256	A
32	2a	1257	U
32	2a	1260	C
32	2a	1267	C
32	2a	1270	C
32	2a	1272	G
32	2a	1273	G
32	2a	1276	G
32	2a	1278	U
32	2a	1279	A
32	2a	1280	A
32	2a	1287	A
32	2a	1300	G
32	2a	1303	C
32	2a	1305	G
32	2a	1320	C
32	2a	1328	C
32	2a	1338	G
32	2a	1340	A
32	2a	1346	A
32	2a	1347	G
32	2a	1353	G
32	2a	1363	C
32	2a	1368	G
32	2a	1370	G
32	2a	1419	G
32	2a	1442	G
32	2a	1442(A)	G
32	2a	1446	U

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
32	2a	1447	A
32	2a	1456	G
32	2a	1487	G
32	2a	1492	A
32	2a	1494	G
32	2a	1497	G
32	2a	1503	A
32	2a	1504	G
32	2a	1506	U
32	2a	1517	G
32	2a	1520	G
32	2a	1529	G
32	2a	1530	G
32	2a	1531	A
32	2a	1532	U
53	2v	13	A
53	2v	15	A
53	2v	24	A
54	2w	3	C
54	2w	4	C
54	2w	5	G
54	2w	7	A
54	2w	8	4SU
54	2w	9	A
54	2w	13	C
54	2w	14	A
54	2w	19	G
54	2w	22	G
54	2w	25	C
54	2w	29	G
54	2w	34	G
54	2w	38	A
54	2w	46	7MG
54	2w	47	U
54	2w	48	C
54	2w	50	U
54	2w	56	C
54	2w	62	C
54	2w	63	G
54	2w	64	A
54	2w	65	G
54	2w	68	C

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
54	2w	69	G
54	2w	70	G
54	2w	74	C
55	2x	9	G
55	2x	10	G
55	2x	13	C
55	2x	18	G
55	2x	21	A
55	2x	22	G
55	2x	42	G
55	2x	43	A
55	2x	47	U
55	2x	48	C
55	2x	52	G
55	2x	53	G
55	2x	65	C
55	2x	67	C
55	2x	68	C
55	2x	76	A
54	2y	15	G
54	2y	19	G
54	2y	23	A
54	2y	24	G
54	2y	25	C
54	2y	27	G
54	2y	34	G
54	2y	45	U
54	2y	49	C
54	2y	52	G
54	2y	53	G
54	2y	55	PSU
54	2y	56	C
54	2y	57	G
54	2y	58	A
54	2y	59	U
54	2y	61	C
54	2y	62	C
54	2y	63	G
54	2y	65	G
54	2y	69	G
54	2y	70	G
54	2y	73	A

All (72) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	12	U
1	1A	115	G
1	1A	185	A
1	1A	271	U
1	1A	302	A
1	1A	509	A
1	1A	572	A
1	1A	596	G
1	1A	793	A
1	1A	821	A
1	1A	847	A
1	1A	913	A
1	1A	941	U
1	1A	1019	G
1	1A	1065	U
1	1A	1067	A
1	1A	1093	G
1	1A	1119	A
1	1A	1188	A
1	1A	1201	A
1	1A	1219	A
1	1A	1220	U
1	1A	1221	G
1	1A	1255	A
1	1A	1321	A
1	1A	1347	A
1	1A	1425	A
1	1A	1466	U
1	1A	1554	A
1	1A	1654	A
1	1A	1700	G
1	1A	2014	G
1	1A	2156	A
1	1A	2180	A
1	1A	2192	A
1	1A	2203	G
1	1A	2205	C
1	1A	2418	U
1	1A	2442	A
1	1A	2451	A
1	1A	2641	A
1	1A	2701	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	1A	2769	U
2	1B	1	U
1	2A	34	C
1	2A	195	A
1	2A	196	A
1	2A	228	A
1	2A	266	G
1	2A	271(K)	U
1	2A	271(M)	G
1	2A	277	C
1	2A	528	A
1	2A	752	A
1	2A	774	A
1	2A	827	U
1	2A	856	C
1	2A	883	G
1	2A	900	A
1	2A	1210	A
1	2A	1420	U
1	2A	1442	G
1	2A	1530	C
1	2A	1608	A
1	2A	1653	G
1	2A	1913	A
1	2A	1992	G
1	2A	2119	A
1	2A	2126	A
1	2A	2406	U
1	2A	2439	A
1	2A	2689	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
32	MA6	2a	1518	32	19,26,27	1.06	2 (10%)	18,38,41	2.30	7 (38%)
54	PSU	2y	39	54	18,21,22	1.36	2 (11%)	21,30,33	1.93	3 (14%)
54	PSU	2w	55	56,54	18,21,22	1.38	2 (11%)	21,30,33	1.94	3 (14%)
1	4OC	1A	1942	1	19,22,24	0.78	0	25,31,35	0.97	1 (4%)
1	5MC	1A	1984	1,56	19,22,23	1.57	3 (15%)	26,32,35	1.23	5 (19%)
32	7MG	1a	527	32,56	23,26,27	1.46	4 (17%)	27,39,42	2.46	7 (25%)
1	PSU	2A	2605	1	18,21,22	1.25	2 (11%)	21,30,33	2.18	6 (28%)
43	0TD	2l	92	43	8,9,10	5.75	3 (37%)	6,11,13	2.22	1 (16%)
54	7MG	2w	46	54	23,26,27	1.40	3 (13%)	27,39,42	2.47	6 (22%)
54	4SU	2w	8	54	18,21,22	1.81	4 (22%)	25,30,33	2.48	5 (20%)
32	7MG	2a	527	32,56	23,26,27	1.34	4 (17%)	27,39,42	2.59	6 (22%)
55	PSU	2x	55	55	18,21,22	1.39	2 (11%)	21,30,33	1.97	4 (19%)
54	4SU	1w	8	54	18,21,22	1.82	5 (27%)	25,30,33	1.99	5 (20%)
54	MIA	1y	37	54	17,24,32	0.98	1 (5%)	16,35,47	1.37	2 (12%)
32	UR3	1a	1498	32	19,22,23	1.10	1 (5%)	26,32,35	1.83	5 (19%)
32	PSU	1a	516	32	18,21,22	1.42	3 (16%)	21,30,33	1.88	5 (23%)
1	5MU	2A	1915	1	19,22,23	1.46	5 (26%)	27,32,35	2.23	6 (22%)
1	2MU	2A	2552	1,56	19,22,24	1.31	2 (10%)	25,31,36	1.80	5 (20%)
32	5MC	1a	1404	32	19,22,23	1.62	3 (15%)	26,32,35	1.19	3 (11%)
54	5MU	2y	54	54	19,22,23	1.51	4 (21%)	27,32,35	2.12	9 (33%)
32	2MG	1a	1207	32	18,26,27	0.96	1 (5%)	16,38,41	1.11	1 (6%)
1	PSU	1A	2617	1,56	18,21,22	1.51	4 (22%)	21,30,33	2.12	4 (19%)
32	5MC	1a	1400	32	19,22,23	1.60	3 (15%)	26,32,35	1.15	2 (7%)
55	5MU	2x	54	55	19,22,23	1.39	5 (26%)	27,32,35	2.22	6 (22%)
32	PSU	2a	516	32	18,21,22	1.34	2 (11%)	21,30,33	1.90	4 (19%)
1	PSU	1A	1933	1	18,21,22	1.33	2 (11%)	21,30,33	2.07	4 (19%)
1	5MC	1A	1964	1,56	19,22,23	1.51	3 (15%)	26,32,35	1.23	2 (7%)
32	4OC	1a	1402	32	20,23,24	0.79	0	25,32,35	1.03	2 (8%)
55	4SU	1x	8	55	18,21,22	2.11	5 (27%)	25,30,33	1.64	6 (24%)
1	2MA	1A	2515	1,56	17,25,26	1.07	2 (11%)	16,37,40	1.41	3 (18%)
55	5MC	2x	32	55	19,22,23	1.56	3 (15%)	26,32,35	1.19	3 (11%)
32	5MC	1a	1407	32	19,22,23	1.66	3 (15%)	26,32,35	1.24	4 (15%)
32	2MG	2a	1207	32	18,26,27	0.91	1 (5%)	16,38,41	1.37	2 (12%)
32	MA6	1a	1519	32	19,26,27	1.14	2 (10%)	18,38,41	1.97	5 (27%)
32	5MC	2a	1404	32	19,22,23	1.70	3 (15%)	26,32,35	1.19	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
55	5MC	1x	32	55	19,22,23	1.67	3 (15%)	26,32,35	1.23	3 (11%)
54	PSU	1y	39	54	18,21,22	1.42	2 (11%)	21,30,33	1.84	4 (19%)
32	M2G	2a	966	32	20,27,28	1.32	3 (15%)	19,40,43	1.07	1 (5%)
32	MA6	1a	1518	32	19,26,27	1.06	1 (5%)	18,38,41	2.36	7 (38%)
1	2MU	1A	2564	1,56	19,22,24	1.20	2 (10%)	25,31,36	2.02	6 (24%)
54	7MG	2y	46	54	23,26,27	1.45	4 (17%)	27,39,42	2.79	6 (22%)
1	2MA	2A	2503	1,56	17,25,26	1.08	1 (5%)	16,37,40	1.47	3 (18%)
54	MIA	1w	37	54	24,31,32	2.20	3 (12%)	22,44,47	2.48	6 (27%)
54	PSU	2y	55	54	18,21,22	1.33	3 (16%)	21,30,33	1.91	5 (23%)
1	PSU	2A	1917	1	18,21,22	1.36	2 (11%)	21,30,33	1.96	3 (14%)
54	PSU	1y	55	54	18,21,22	1.33	2 (11%)	21,30,33	2.13	4 (19%)
54	7MG	1y	46	54	23,26,27	1.35	4 (17%)	27,39,42	2.61	6 (22%)
32	MA6	2a	1519	32	19,26,27	1.12	2 (10%)	18,38,41	2.25	5 (27%)
54	5MU	2w	54	54	19,22,23	1.39	4 (21%)	27,32,35	1.89	6 (22%)
32	5MC	2a	967	32	19,22,23	1.92	2 (10%)	26,32,35	1.16	4 (15%)
54	7MG	1w	46	54	23,26,27	1.48	4 (17%)	27,39,42	2.54	7 (25%)
54	PSU	1y	32	54	18,21,22	1.41	3 (16%)	21,30,33	1.89	3 (14%)
32	UR3	2a	1498	32	19,22,23	1.07	2 (10%)	26,32,35	1.81	4 (15%)
55	4SU	2x	8	55	18,21,22	2.04	6 (33%)	25,30,33	1.43	5 (20%)
55	PSU	1x	55	55,56	18,21,22	1.35	2 (11%)	21,30,33	2.01	4 (19%)
54	PSU	1w	32	56,54	18,21,22	1.35	2 (11%)	21,30,33	2.01	3 (14%)
54	PSU	2w	32	54	18,21,22	1.38	2 (11%)	21,30,33	1.99	4 (19%)
1	5MC	2A	1962	1,56	19,22,23	1.52	3 (15%)	26,32,35	1.29	3 (11%)
54	PSU	1w	39	54	18,21,22	1.37	2 (11%)	21,30,33	1.96	3 (14%)
32	5MC	2a	1400	32	19,22,23	1.68	3 (15%)	26,32,35	1.20	3 (11%)
55	5MU	1x	54	55,56	19,22,23	1.45	6 (31%)	27,32,35	1.89	6 (22%)
32	M2G	1a	966	32	20,27,28	1.44	3 (15%)	19,40,43	1.00	1 (5%)
1	PSU	2A	1911	1	18,21,22	1.42	2 (11%)	21,30,33	1.84	4 (19%)
1	5MC	2A	1942	1	19,22,23	1.50	2 (10%)	26,32,35	1.12	2 (7%)
32	5MC	1a	967	32	19,22,23	1.67	3 (15%)	26,32,35	1.15	3 (11%)
54	PSU	2y	32	54	18,21,22	1.36	2 (11%)	21,30,33	1.93	4 (19%)
54	MIA	2w	37	54	19,27,32	1.80	3 (15%)	18,39,47	1.38	4 (22%)
43	0TD	1l	92	43	8,9,10	5.73	6 (75%)	6,11,13	4.21	3 (50%)
32	4OC	2a	1402	32,56	20,23,24	0.81	0	25,32,35	1.07	1 (4%)
54	5MU	1y	54	54	19,22,23	1.55	6 (31%)	27,32,35	1.99	6 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	5MU	1A	1937	1	19,22,23	1.35	5 (26%)	27,32,35	2.18	7 (25%)
32	5MC	2a	1407	32	19,22,23	1.52	3 (15%)	26,32,35	1.21	4 (15%)
1	OMG	1A	2263	1,55,56	19,26,27	0.96	1 (5%)	21,38,41	1.05	2 (9%)
54	4SU	1y	8	54	18,21,22	1.72	4 (22%)	25,30,33	1.88	6 (24%)
54	PSU	1w	55	54	18,21,22	1.37	2 (11%)	21,30,33	1.98	3 (14%)
1	4OC	2A	1920	1	19,22,24	0.76	0	25,31,35	0.85	0
1	5MU	2A	1939	1,56	19,22,23	1.46	6 (31%)	27,32,35	2.51	6 (22%)
54	5MU	1w	54	54	19,22,23	1.47	5 (26%)	27,32,35	2.07	6 (22%)
1	5MU	1A	1961	1,56	19,22,23	1.32	4 (21%)	27,32,35	2.59	6 (22%)
54	MIA	2y	37	54	17,24,32	0.96	1 (5%)	16,35,47	1.35	2 (12%)
54	PSU	2w	39	54	18,21,22	1.35	2 (11%)	21,30,33	1.81	4 (19%)
1	OMG	2A	2251	1,55,56	19,26,27	0.90	1 (5%)	21,38,41	1.19	3 (14%)
54	4SU	2y	8	54	18,21,22	1.87	4 (22%)	25,30,33	2.25	5 (20%)
1	PSU	1A	1939	1	18,21,22	1.42	4 (22%)	21,30,33	2.12	4 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	MA6	2a	1518	32	-	0/7/29/30	0/3/3/3
54	PSU	2y	39	54	-	0/7/25/26	0/2/2/2
54	PSU	2w	55	56,54	-	0/7/25/26	0/2/2/2
1	4OC	1A	1942	1	-	1/9/27/30	0/2/2/2
1	5MC	1A	1984	1,56	-	0/7/25/26	0/2/2/2
32	7MG	1a	527	32,56	-	2/7/37/38	0/3/3/3
1	PSU	2A	2605	1	-	0/7/25/26	0/2/2/2
43	0TD	2l	92	43	-	1/7/12/14	-
54	7MG	2w	46	54	-	4/7/37/38	0/3/3/3
54	4SU	2w	8	54	-	1/7/25/26	0/2/2/2
32	7MG	2a	527	32,56	-	3/7/37/38	0/3/3/3
55	PSU	2x	55	55	-	0/7/25/26	0/2/2/2
54	4SU	1w	8	54	-	0/7/25/26	0/2/2/2
54	MIA	1y	37	54	-	0/3/25/34	0/3/3/3
32	UR3	1a	1498	32	-	0/7/25/26	0/2/2/2
32	PSU	1a	516	32	-	0/7/25/26	0/2/2/2
1	5MU	2A	1915	1	-	0/7/25/26	0/2/2/2
1	2MU	2A	2552	1,56	-	0/9/27/28	0/2/2/2

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	5MC	1a	1404	32	-	0/7/25/26	0/2/2/2
54	5MU	2y	54	54	-	2/7/25/26	0/2/2/2
32	2MG	1a	1207	32	-	0/5/27/28	0/3/3/3
1	PSU	1A	2617	1,56	-	0/7/25/26	0/2/2/2
32	5MC	1a	1400	32	-	2/7/25/26	0/2/2/2
55	5MU	2x	54	55	-	0/7/25/26	0/2/2/2
32	PSU	2a	516	32	-	0/7/25/26	0/2/2/2
1	PSU	1A	1933	1	-	0/7/25/26	0/2/2/2
1	5MC	1A	1964	1,56	-	0/7/25/26	0/2/2/2
32	4OC	1a	1402	32	-	3/9/29/30	0/2/2/2
55	4SU	1x	8	55	-	0/7/25/26	0/2/2/2
1	2MA	1A	2515	1,56	-	1/3/25/26	0/3/3/3
55	5MC	2x	32	55	-	0/7/25/26	0/2/2/2
32	5MC	1a	1407	32	-	0/7/25/26	0/2/2/2
32	2MG	2a	1207	32	-	0/5/27/28	0/3/3/3
32	MA6	1a	1519	32	-	3/7/29/30	0/3/3/3
32	5MC	2a	1404	32	-	0/7/25/26	0/2/2/2
55	5MC	1x	32	55	-	0/7/25/26	0/2/2/2
54	PSU	1y	39	54	-	0/7/25/26	0/2/2/2
32	M2G	2a	966	32	-	0/7/29/30	0/3/3/3
32	MA6	1a	1518	32	-	0/7/29/30	0/3/3/3
1	2MU	1A	2564	1,56	-	0/9/27/28	0/2/2/2
54	7MG	2y	46	54	-	3/7/37/38	0/3/3/3
1	2MA	2A	2503	1,56	-	1/3/25/26	0/3/3/3
54	MIA	1w	37	54	-	1/11/33/34	0/3/3/3
54	PSU	2y	55	54	-	2/7/25/26	0/2/2/2
1	PSU	2A	1917	1	-	0/7/25/26	0/2/2/2
54	PSU	1y	55	54	-	1/7/25/26	0/2/2/2
54	7MG	1y	46	54	-	2/7/37/38	0/3/3/3
32	MA6	2a	1519	32	-	2/7/29/30	0/3/3/3
54	5MU	2w	54	54	-	0/7/25/26	0/2/2/2
32	5MC	2a	967	32	-	0/7/25/26	0/2/2/2
54	7MG	1w	46	54	-	3/7/37/38	0/3/3/3
54	PSU	1y	32	54	-	0/7/25/26	0/2/2/2
32	UR3	2a	1498	32	-	0/7/25/26	0/2/2/2
55	4SU	2x	8	55	-	1/7/25/26	0/2/2/2
55	PSU	1x	55	55,56	-	0/7/25/26	0/2/2/2
54	PSU	1w	32	56,54	-	0/7/25/26	0/2/2/2
54	PSU	2w	32	54	-	0/7/25/26	0/2/2/2
1	5MC	2A	1962	1,56	-	0/7/25/26	0/2/2/2

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	PSU	1w	39	54	-	1/7/25/26	0/2/2/2
32	5MC	2a	1400	32	-	0/7/25/26	0/2/2/2
55	5MU	1x	54	55,56	-	0/7/25/26	0/2/2/2
32	M2G	1a	966	32	-	0/7/29/30	0/3/3/3
1	PSU	2A	1911	1	-	0/7/25/26	0/2/2/2
1	5MC	2A	1942	1	-	0/7/25/26	0/2/2/2
32	5MC	1a	967	32	-	0/7/25/26	0/2/2/2
54	PSU	2y	32	54	-	1/7/25/26	0/2/2/2
54	MIA	2w	37	54	-	2/7/29/34	0/3/3/3
43	0TD	1l	92	43	-	3/7/12/14	-
32	4OC	2a	1402	32,56	-	2/9/29/30	0/2/2/2
54	5MU	1y	54	54	-	3/7/25/26	0/2/2/2
1	5MU	1A	1937	1	-	0/7/25/26	0/2/2/2
32	5MC	2a	1407	32	-	0/7/25/26	0/2/2/2
1	OMG	1A	2263	1,55,56	-	0/5/27/28	0/3/3/3
54	4SU	1y	8	54	-	3/7/25/26	0/2/2/2
54	PSU	1w	55	54	-	0/7/25/26	0/2/2/2
1	4OC	2A	1920	1	-	0/9/27/30	0/2/2/2
1	5MU	2A	1939	1,56	-	0/7/25/26	0/2/2/2
54	5MU	1w	54	54	-	0/7/25/26	0/2/2/2
1	5MU	1A	1961	1,56	-	0/7/25/26	0/2/2/2
54	MIA	2y	37	54	-	3/3/25/34	0/3/3/3
54	PSU	2w	39	54	-	0/7/25/26	0/2/2/2
1	OMG	2A	2251	1,55,56	-	0/5/27/28	0/3/3/3
54	4SU	2y	8	54	-	0/7/25/26	0/2/2/2
1	PSU	1A	1939	1	-	0/7/25/26	0/2/2/2

All (236) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	2l	92	0TD	CB-SB	-15.10	1.67	1.82
43	1l	92	0TD	CB-SB	-15.01	1.67	1.82
32	2a	967	5MC	C5-C4	7.30	1.49	1.44
54	1w	37	MIA	C2-S10	-6.99	1.70	1.75
54	1w	37	MIA	C13-C14	6.94	1.53	1.32
54	2w	37	MIA	C2-S10	-6.20	1.70	1.75
32	2a	1400	5MC	C5-C4	6.11	1.48	1.44
32	1a	967	5MC	C5-C4	6.09	1.48	1.44
32	2a	1404	5MC	C5-C4	6.09	1.48	1.44
32	1a	1407	5MC	C5-C4	5.94	1.48	1.44
55	1x	32	5MC	C5-C4	5.87	1.48	1.44

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	1a	1400	5MC	C5-C4	5.77	1.48	1.44
32	1a	1404	5MC	C5-C4	5.73	1.48	1.44
1	1A	1984	5MC	C5-C4	5.50	1.48	1.44
1	1A	1964	5MC	C5-C4	5.42	1.48	1.44
55	2x	32	5MC	C5-C4	5.37	1.48	1.44
32	2a	1407	5MC	C5-C4	5.31	1.48	1.44
1	2A	1962	5MC	C5-C4	5.21	1.48	1.44
1	2A	1942	5MC	C5-C4	5.10	1.48	1.44
54	2y	8	4SU	C4-S4	-5.05	1.59	1.68
54	2w	8	4SU	C4-S4	-4.97	1.59	1.68
55	1x	8	4SU	C4-N3	-4.95	1.32	1.37
54	1w	8	4SU	C4-S4	-4.77	1.60	1.68
43	2l	92	0TD	CB-CA	-4.68	1.53	1.54
55	2x	8	4SU	C4-N3	-4.66	1.32	1.37
55	2x	8	4SU	C4-S4	-4.40	1.60	1.68
54	1y	8	4SU	C4-S4	-4.36	1.61	1.68
32	1a	966	M2G	C2-N3	4.26	1.36	1.30
54	1y	32	PSU	C6-C5	4.13	1.39	1.35
55	1x	8	4SU	C4-S4	-4.10	1.61	1.68
54	2w	55	PSU	C6-C5	4.09	1.39	1.35
54	1y	39	PSU	C6-C5	4.05	1.39	1.35
54	1w	55	PSU	C6-C5	4.04	1.39	1.35
55	2x	55	PSU	C6-C5	3.97	1.39	1.35
32	2a	966	M2G	C2-N3	3.96	1.36	1.30
32	1a	527	7MG	C4-N9	-3.88	1.33	1.37
54	2y	32	PSU	C6-C5	3.86	1.39	1.35
1	2A	1911	PSU	C6-C5	3.84	1.39	1.35
55	1x	8	4SU	C2-N3	-3.80	1.31	1.38
54	2y	46	7MG	C5-C4	3.75	1.49	1.37
54	2w	46	7MG	C4-N9	-3.73	1.33	1.37
32	2a	516	PSU	C6-C5	3.72	1.39	1.35
54	2w	39	PSU	C6-C5	3.72	1.39	1.35
54	1w	39	PSU	C6-C5	3.67	1.39	1.35
32	1a	516	PSU	C6-C5	3.63	1.39	1.35
54	1w	46	7MG	C4-N9	-3.61	1.33	1.37
54	2w	32	PSU	C6-C5	3.60	1.39	1.35
54	2y	39	PSU	C6-C5	3.57	1.39	1.35
1	2A	2605	PSU	C6-C5	3.57	1.39	1.35
1	2A	1917	PSU	C6-C5	3.56	1.39	1.35
54	1w	46	7MG	C5-C4	3.52	1.48	1.37
54	1y	55	PSU	C6-C5	3.52	1.39	1.35
54	1y	46	7MG	C5-C4	3.47	1.48	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	1x	55	PSU	C6-C5	3.45	1.39	1.35
54	2y	54	5MU	C2-N1	3.44	1.43	1.38
32	1a	527	7MG	C5-C4	3.40	1.48	1.37
54	2w	46	7MG	C5-C4	3.35	1.47	1.37
54	1w	32	PSU	C6-C5	3.35	1.39	1.35
54	1y	8	4SU	C4-N3	-3.32	1.34	1.37
32	2a	527	7MG	C5-C4	3.28	1.47	1.37
43	1l	92	0TD	CSB-SB	-3.27	1.73	1.79
55	1x	8	4SU	C5-C4	-3.26	1.38	1.42
55	2x	8	4SU	C5-C4	-3.16	1.38	1.42
54	1w	8	4SU	C4-N3	-3.15	1.34	1.37
1	2A	1942	5MC	C6-C5	3.14	1.39	1.34
1	1A	1939	PSU	C6-C5	3.14	1.38	1.35
1	1A	1933	PSU	C6-C5	3.13	1.38	1.35
32	2a	1404	5MC	C6-C5	3.10	1.39	1.34
32	1a	966	M2G	C2-N2	3.10	1.40	1.35
54	1y	54	5MU	C6-C5	3.09	1.39	1.34
55	2x	54	5MU	C6-C5	3.04	1.39	1.34
54	1w	54	5MU	C6-C5	3.01	1.39	1.34
54	2y	8	4SU	C4-N3	-2.96	1.34	1.37
54	2w	8	4SU	C2-N1	2.93	1.43	1.38
32	1a	967	5MC	C6-C5	2.93	1.39	1.34
55	2x	8	4SU	C2-N3	-2.92	1.32	1.38
1	1A	2617	PSU	C4-N3	-2.92	1.33	1.38
55	2x	32	5MC	C6-C5	2.92	1.39	1.34
32	1a	1404	5MC	C6-C5	2.91	1.39	1.34
54	2y	55	PSU	C6-C5	2.89	1.38	1.35
54	2w	8	4SU	C4-N3	-2.89	1.34	1.37
54	2w	54	5MU	C6-C5	2.87	1.39	1.34
32	1a	1407	5MC	C6-C5	2.87	1.39	1.34
55	1x	32	5MC	C6-C5	2.87	1.39	1.34
43	1l	92	0TD	CA-N	-2.86	1.39	1.47
54	1y	54	5MU	C2-N1	2.85	1.42	1.38
1	1A	2617	PSU	C2-N1	-2.85	1.32	1.36
1	1A	1939	PSU	C4-N3	-2.85	1.33	1.38
32	2a	527	7MG	C4-N9	-2.84	1.34	1.37
55	1x	54	5MU	C6-C5	2.84	1.39	1.34
54	1w	8	4SU	C5-C4	-2.82	1.39	1.42
1	2A	1915	5MU	C2-N1	2.82	1.42	1.38
1	2A	1939	5MU	C4-C5	2.82	1.49	1.44
1	1A	2263	OMG	C6-N1	-2.81	1.33	1.37
32	1a	1498	UR3	C2-N1	2.81	1.42	1.38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	1915	5MU	C6-C5	2.81	1.39	1.34
1	1A	1961	5MU	C6-C5	2.80	1.39	1.34
32	1a	1518	MA6	C6-C5	2.79	1.49	1.44
1	2A	1939	5MU	C6-C5	2.79	1.39	1.34
55	1x	54	5MU	C4-N3	-2.79	1.33	1.38
54	2y	8	4SU	C5-C4	-2.78	1.39	1.42
32	1a	1400	5MC	C6-C5	2.78	1.39	1.34
32	2a	967	5MC	C6-C5	2.77	1.39	1.34
1	1A	1933	PSU	C4-N3	-2.77	1.33	1.38
32	2a	1400	5MC	C6-C5	2.76	1.39	1.34
54	2w	37	MIA	C6-C5	2.75	1.49	1.44
32	2a	966	M2G	C2-N2	2.75	1.40	1.35
1	2A	1915	5MU	C4-C5	2.74	1.49	1.44
54	2y	46	7MG	C8-N9	2.73	1.47	1.45
54	2y	8	4SU	C2-N1	2.73	1.42	1.38
43	2l	92	0TD	OD2-CG	-2.69	1.22	1.30
54	1y	54	5MU	C4-N3	-2.69	1.33	1.38
54	2y	37	MIA	C2-N3	2.69	1.36	1.32
55	2x	54	5MU	C4-C5	2.69	1.49	1.44
54	1w	54	5MU	C2-N1	2.68	1.42	1.38
32	2a	1518	MA6	C6-C5	2.68	1.48	1.44
1	1A	2617	PSU	C2-N3	-2.67	1.33	1.37
32	1a	516	PSU	C4-N3	-2.67	1.33	1.38
54	2y	54	5MU	C6-C5	2.67	1.39	1.34
54	1w	54	5MU	C4-C5	2.65	1.49	1.44
43	1l	92	0TD	OD2-CG	-2.64	1.22	1.30
1	2A	1962	5MC	C6-N1	-2.64	1.33	1.38
54	1y	54	5MU	C4-C5	2.64	1.49	1.44
1	1A	2564	2MU	C4-N3	-2.61	1.34	1.38
1	2A	1939	5MU	C4-N3	-2.61	1.34	1.38
1	1A	1937	5MU	C6-C5	2.60	1.38	1.34
1	1A	1984	5MC	C6-N1	-2.60	1.33	1.38
54	1y	37	MIA	C2-N3	2.60	1.36	1.32
54	1y	39	PSU	C4-N3	-2.59	1.34	1.38
54	1w	54	5MU	C4-N3	-2.58	1.34	1.38
1	1A	1961	5MU	C4-N3	-2.56	1.34	1.38
1	2A	1962	5MC	C6-C5	2.56	1.38	1.34
54	1w	39	PSU	C4-N3	-2.56	1.34	1.38
54	2y	46	7MG	C6-N1	-2.53	1.34	1.38
32	2a	1407	5MC	C6-N1	-2.53	1.33	1.38
54	2y	39	PSU	C4-N3	-2.53	1.34	1.38
54	2w	32	PSU	C4-N3	-2.52	1.34	1.38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	2552	2MU	C4-N3	-2.51	1.34	1.38
1	2A	1911	PSU	C4-N3	-2.51	1.34	1.38
32	2a	1498	UR3	C2-N1	2.51	1.42	1.38
32	1a	1207	2MG	C6-N1	-2.50	1.34	1.37
43	1l	92	0TD	CB-CG	-2.50	1.47	1.52
55	1x	32	5MC	C6-N1	-2.50	1.33	1.38
54	2w	54	5MU	C4-C5	2.49	1.48	1.44
54	2w	46	7MG	C8-N9	2.49	1.47	1.45
1	1A	1964	5MC	C6-C5	2.49	1.38	1.34
54	2w	8	4SU	C5-C4	-2.48	1.39	1.42
54	1w	46	7MG	C8-N9	2.48	1.47	1.45
54	1w	46	7MG	C6-N1	-2.48	1.34	1.38
54	2y	54	5MU	C4-C5	2.47	1.48	1.44
54	2w	54	5MU	C2-N1	2.47	1.42	1.38
1	1A	1937	5MU	C4-N3	-2.46	1.34	1.38
54	2w	39	PSU	C4-N3	-2.46	1.34	1.38
55	2x	55	PSU	C4-N3	-2.46	1.34	1.38
55	1x	54	5MU	C4-C5	2.45	1.48	1.44
54	2y	55	PSU	C4-N3	-2.45	1.34	1.38
54	1w	32	PSU	C4-N3	-2.45	1.34	1.38
54	2y	54	5MU	C4-N3	-2.43	1.34	1.38
54	1y	8	4SU	C5-C4	-2.42	1.39	1.42
55	1x	8	4SU	O2-C2	2.42	1.27	1.23
54	1w	37	MIA	C6-C5	2.41	1.48	1.44
54	2w	55	PSU	C4-N3	-2.39	1.34	1.38
32	2a	527	7MG	C6-N1	-2.37	1.34	1.38
55	1x	55	PSU	C4-N3	-2.37	1.34	1.38
32	2a	1407	5MC	C6-C5	2.36	1.38	1.34
1	1A	1961	5MU	C6-N1	-2.36	1.34	1.38
1	2A	2552	2MU	C5-C4	2.36	1.48	1.43
43	1l	92	0TD	CB-CA	-2.36	1.54	1.54
1	2A	1915	5MU	C4-N3	-2.36	1.34	1.38
54	1y	55	PSU	C4-N3	-2.36	1.34	1.38
32	1a	527	7MG	C6-N1	-2.36	1.34	1.38
1	2A	1917	PSU	C4-N3	-2.33	1.34	1.38
32	1a	966	M2G	C6-N1	-2.32	1.34	1.37
54	1y	46	7MG	C4-N9	-2.32	1.35	1.37
54	1w	8	4SU	C2-N1	2.32	1.42	1.38
54	2y	32	PSU	C4-N3	-2.30	1.34	1.38
1	1A	2515	2MA	C2-N3	2.30	1.36	1.31
32	2a	1519	MA6	C6-C5	2.29	1.48	1.44
32	2a	1400	5MC	C6-N1	-2.29	1.34	1.38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2A	1939	5MU	C2-N3	-2.28	1.34	1.38
54	1y	46	7MG	C6-N1	-2.28	1.34	1.38
1	2A	2605	PSU	C4-N3	-2.27	1.34	1.38
54	2w	37	MIA	C6-N1	2.27	1.36	1.33
1	1A	1937	5MU	C4-C5	2.27	1.48	1.44
1	1A	1937	5MU	C2-N1	2.26	1.42	1.38
1	2A	1939	5MU	C6-N1	-2.26	1.34	1.38
1	1A	1984	5MC	C6-C5	2.26	1.38	1.34
54	1y	46	7MG	C8-N9	2.25	1.47	1.45
32	2a	527	7MG	C5-C6	2.25	1.49	1.43
32	1a	527	7MG	C8-N9	2.25	1.47	1.45
1	2A	2503	2MA	C2-N3	2.24	1.36	1.31
32	1a	1400	5MC	C6-N1	-2.22	1.34	1.38
1	1A	2564	2MU	C2-N3	-2.22	1.34	1.38
54	1y	32	PSU	C4-N3	-2.22	1.34	1.38
55	2x	54	5MU	C4-N3	-2.20	1.34	1.38
1	1A	1939	PSU	C2-N1	-2.19	1.33	1.36
1	1A	1961	5MU	C2-N3	-2.19	1.34	1.38
32	1a	967	5MC	C6-N1	-2.19	1.34	1.38
32	2a	1498	UR3	C6-C5	2.19	1.40	1.35
54	1y	54	5MU	C2-N3	-2.18	1.34	1.38
32	2a	1207	2MG	C6-N1	-2.17	1.34	1.37
32	2a	1518	MA6	C6-N1	2.17	1.35	1.32
32	2a	516	PSU	C4-N3	-2.17	1.34	1.38
54	2y	55	PSU	C2-N1	-2.16	1.33	1.36
55	1x	54	5MU	C2-N3	-2.16	1.34	1.38
1	1A	1964	5MC	C6-N1	-2.15	1.34	1.38
32	1a	516	PSU	C2-N3	-2.15	1.33	1.37
32	1a	1404	5MC	C6-N1	-2.14	1.34	1.38
1	2A	2251	OMG	C6-N1	-2.14	1.34	1.37
55	1x	54	5MU	C2-N1	2.14	1.41	1.38
54	1w	55	PSU	C4-N3	-2.13	1.34	1.38
1	2A	1939	5MU	C2-N1	2.13	1.41	1.38
1	1A	2617	PSU	C6-C5	2.12	1.37	1.35
1	1A	1937	5MU	C6-N1	-2.12	1.34	1.38
32	2a	1519	MA6	C6-N1	2.12	1.35	1.32
32	1a	1519	MA6	C6-C5	2.11	1.48	1.44
32	1a	1407	5MC	C6-N1	-2.11	1.34	1.38
1	1A	2515	2MA	C6-N6	2.10	1.36	1.27
54	2w	54	5MU	C4-N3	-2.10	1.34	1.38
55	2x	8	4SU	O2-C2	2.10	1.26	1.23
32	1a	1519	MA6	C6-N1	2.09	1.35	1.32

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	1w	54	5MU	C2-N3	-2.08	1.34	1.38
55	2x	8	4SU	C2-N1	2.07	1.41	1.38
1	1A	1939	PSU	C2-N3	-2.07	1.34	1.37
54	2y	46	7MG	C2-N3	2.07	1.38	1.33
55	1x	54	5MU	C6-N1	-2.05	1.34	1.38
54	1w	8	4SU	C2-N3	-2.04	1.34	1.38
32	2a	1404	5MC	C6-N1	-2.02	1.34	1.38
55	2x	54	5MU	C6-N1	-2.02	1.34	1.38
55	2x	54	5MU	C2-N1	2.02	1.41	1.38
54	1y	54	5MU	C6-N1	-2.02	1.34	1.38
54	1y	32	PSU	C4-C5	2.01	1.49	1.44
1	2A	1915	5MU	C2-N3	-2.01	1.34	1.38
54	1y	8	4SU	C6-C5	2.01	1.39	1.35
32	2a	966	M2G	C6-N1	-2.00	1.34	1.37
55	2x	32	5MC	C6-N1	-2.00	1.34	1.38

All (345) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2y	46	7MG	N9-C4-N3	10.07	140.22	125.46
54	1y	46	7MG	N9-C4-N3	9.11	138.80	125.46
54	1w	37	MIA	C12-C13-C14	-8.83	111.17	127.01
54	1w	46	7MG	N9-C4-N3	8.77	138.32	125.46
32	2a	527	7MG	N9-C4-N3	8.50	137.91	125.46
32	1a	527	7MG	N9-C4-N3	8.37	137.72	125.46
54	2w	46	7MG	N9-C4-N3	7.71	136.76	125.46
54	2w	8	4SU	C4-N3-C2	-7.55	120.08	127.31
43	1l	92	0TD	CB-CA-N	-7.31	94.29	109.10
32	2a	1498	UR3	C4-N3-C2	-7.02	118.93	124.58
32	1a	1498	UR3	C4-N3-C2	-6.78	119.13	124.58
43	1l	92	0TD	CSB-SB-CB	6.71	114.44	102.36
54	1y	55	PSU	N1-C2-N3	6.64	122.17	115.17
1	1A	1939	PSU	N1-C2-N3	6.57	122.10	115.17
1	1A	1961	5MU	O4-C4-C5	-6.45	117.54	124.92
1	1A	2617	PSU	N1-C2-N3	6.42	121.94	115.17
1	1A	1961	5MU	C5-C4-N3	6.41	120.89	115.32
32	1a	1518	MA6	C2-N1-C6	6.41	123.12	116.84
54	2w	8	4SU	C5-C4-N3	6.36	120.67	114.75
55	2x	55	PSU	N1-C2-N3	6.36	121.87	115.17
54	2w	32	PSU	N1-C2-N3	6.32	121.83	115.17
1	2A	1939	5MU	C4-N3-C2	-6.19	119.23	127.34
54	2y	8	4SU	C4-N3-C2	-6.15	121.42	127.31

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1961	5MU	C4-N3-C2	-6.14	119.29	127.34
1	1A	1933	PSU	N1-C2-N3	6.14	121.64	115.17
55	1x	55	PSU	N1-C2-N3	6.12	121.62	115.17
54	1w	32	PSU	N1-C2-N3	6.12	121.62	115.17
1	2A	1917	PSU	N1-C2-N3	6.10	121.60	115.17
54	1w	39	PSU	N1-C2-N3	6.08	121.58	115.17
1	2A	2605	PSU	N1-C2-N3	6.05	121.55	115.17
54	2y	8	4SU	C5-C4-N3	6.01	120.34	114.75
32	2a	1518	MA6	C2-N1-C6	5.99	122.71	116.84
54	2y	32	PSU	N1-C2-N3	5.96	121.45	115.17
54	2y	39	PSU	N1-C2-N3	5.94	121.43	115.17
54	2w	55	PSU	N1-C2-N3	5.90	121.39	115.17
54	1y	39	PSU	N1-C2-N3	5.88	121.37	115.17
54	1y	32	PSU	N1-C2-N3	5.83	121.32	115.17
1	2A	1939	5MU	C5-C4-N3	5.82	120.38	115.32
54	1w	55	PSU	N1-C2-N3	5.78	121.27	115.17
54	2y	46	7MG	C5-C4-N3	-5.76	117.31	128.13
1	2A	1911	PSU	N1-C2-N3	5.76	121.24	115.17
32	1a	516	PSU	N1-C2-N3	5.71	121.19	115.17
32	2a	516	PSU	N1-C2-N3	5.67	121.15	115.17
32	2a	527	7MG	N9-C8-N7	-5.62	95.42	103.37
54	1w	8	4SU	C4-N3-C2	-5.55	121.99	127.31
54	1y	8	4SU	C4-N3-C2	-5.55	122.00	127.31
54	2w	39	PSU	N1-C2-N3	5.53	121.00	115.17
32	2a	1519	MA6	C2-N1-C6	5.50	122.23	116.84
55	2x	54	5MU	N3-C2-N1	5.42	121.94	114.89
54	2w	46	7MG	N9-C8-N7	-5.42	95.70	103.37
1	2A	1915	5MU	C4-N3-C2	-5.40	120.26	127.34
55	2x	54	5MU	C4-N3-C2	-5.39	120.28	127.34
54	1w	54	5MU	N3-C2-N1	5.36	121.87	114.89
54	2y	55	PSU	N1-C2-N3	5.36	120.82	115.17
1	2A	1915	5MU	C5-C4-N3	5.36	119.98	115.32
1	1A	1937	5MU	C4-N3-C2	-5.34	120.34	127.34
54	1w	8	4SU	C5-C4-N3	5.30	119.68	114.75
54	1y	46	7MG	N9-C8-N7	-5.26	95.92	103.37
1	2A	1939	5MU	C5-C6-N1	-5.25	117.61	123.31
32	2a	527	7MG	C5-C4-N3	-5.23	118.30	128.13
54	1w	46	7MG	N9-C8-N7	-5.18	96.03	103.37
1	1A	2564	2MU	N3-C2-N1	5.17	121.62	114.89
43	2l	92	0TD	CSB-SB-CB	5.14	111.61	102.36
54	1y	46	7MG	C5-C4-N3	-5.11	118.54	128.13
54	1w	54	5MU	C4-N3-C2	-5.04	120.73	127.34

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2564	2MU	C4-N3-C2	-5.04	120.36	126.61
1	2A	1939	5MU	N3-C2-N1	5.02	121.42	114.89
1	1A	1937	5MU	N3-C2-N1	5.01	121.42	114.89
32	1a	527	7MG	N9-C8-N7	-4.94	96.38	103.37
54	1y	54	5MU	N3-C2-N1	4.92	121.30	114.89
32	1a	527	7MG	C5-C4-N3	-4.90	118.92	128.13
1	2A	2605	PSU	C4-N3-C2	-4.84	119.70	126.37
1	1A	1937	5MU	C5-C4-N3	4.84	119.53	115.32
1	2A	2552	2MU	N3-C2-N1	4.82	121.17	114.89
54	2y	46	7MG	C2-N3-C4	4.81	120.58	112.30
54	1y	54	5MU	C4-N3-C2	-4.81	121.04	127.34
32	1a	1519	MA6	C2-N1-C6	4.72	121.47	116.84
54	2y	46	7MG	N9-C8-N7	-4.71	96.71	103.37
54	2w	46	7MG	C5-C4-N3	-4.70	119.30	128.13
1	1A	1961	5MU	N3-C2-N1	4.70	121.00	114.89
55	1x	54	5MU	N3-C2-N1	4.69	121.00	114.89
1	2A	1915	5MU	N3-C2-N1	4.63	120.92	114.89
1	1A	1961	5MU	C5-C6-N1	-4.61	118.30	123.31
1	2A	1939	5MU	O4-C4-C5	-4.60	119.65	124.92
54	1w	46	7MG	C5-C4-N3	-4.52	119.64	128.13
1	2A	1915	5MU	O4-C4-C5	-4.52	119.75	124.92
54	2y	8	4SU	C5-C4-S4	-4.52	119.15	124.31
1	2A	2552	2MU	C4-N3-C2	-4.51	121.02	126.61
54	2y	54	5MU	C5-C4-N3	4.50	119.23	115.32
32	2a	527	7MG	C2-N3-C4	4.49	120.04	112.30
55	1x	54	5MU	C4-N3-C2	-4.45	121.50	127.34
54	2y	54	5MU	C4-N3-C2	-4.41	121.55	127.34
1	1A	1933	PSU	C4-N3-C2	-4.39	120.32	126.37
1	1A	2617	PSU	C4-N3-C2	-4.39	120.33	126.37
1	1A	1937	5MU	O4-C4-C5	-4.39	119.90	124.92
32	2a	1519	MA6	N1-C6-N6	4.37	121.88	116.83
54	1y	46	7MG	C2-N3-C4	4.34	119.78	112.30
54	1w	54	5MU	C5-C4-N3	4.34	119.10	115.32
54	1y	8	4SU	N3-C2-N1	4.30	120.49	114.89
54	1y	54	5MU	C5-C4-N3	4.29	119.05	115.32
54	2w	54	5MU	O4-C4-C5	-4.27	120.03	124.92
55	2x	54	5MU	C5-C4-N3	4.26	119.02	115.32
55	2x	54	5MU	O4-C4-C5	-4.21	120.10	124.92
54	2y	37	MIA	N3-C2-N1	-4.19	122.98	128.67
54	2w	8	4SU	N3-C2-N1	4.19	120.35	114.89
54	1w	37	MIA	C15-C14-C13	-4.18	110.11	122.66
54	2y	54	5MU	N3-C2-N1	4.16	120.31	114.89

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2w	54	5MU	C4-N3-C2	-4.15	121.90	127.34
1	1A	1939	PSU	C4-N3-C2	-4.15	120.66	126.37
54	2w	54	5MU	N3-C2-N1	4.12	120.25	114.89
32	1a	1400	5MC	C5-C6-N1	-4.11	118.84	123.31
55	1x	8	4SU	C6-C5-C4	-4.10	116.40	119.95
54	1y	37	MIA	N3-C2-N1	-4.10	123.11	128.67
54	1w	55	PSU	O2-C2-N1	-4.07	118.59	122.79
54	2w	46	7MG	C2-N3-C4	4.06	119.29	112.30
54	2y	54	5MU	O4-C4-C5	-4.04	120.30	124.92
54	1w	32	PSU	C4-N3-C2	-4.04	120.81	126.37
54	2w	32	PSU	C4-N3-C2	-4.03	120.82	126.37
1	1A	1939	PSU	O2-C2-N1	-4.03	118.64	122.79
54	2w	8	4SU	C5-C4-S4	-4.01	119.73	124.31
54	1y	55	PSU	O2-C2-N1	-3.98	118.69	122.79
55	1x	55	PSU	C4-N3-C2	-3.95	120.93	126.37
32	2a	1518	MA6	N3-C2-N1	-3.95	123.32	128.67
32	1a	1518	MA6	N3-C2-N1	-3.94	123.32	128.67
54	2w	54	5MU	C5-C4-N3	3.94	118.75	115.32
54	1y	8	4SU	C5-C4-N3	3.94	118.41	114.75
32	2a	1519	MA6	N3-C2-N1	-3.94	123.33	128.67
54	1y	55	PSU	C4-N3-C2	-3.92	120.97	126.37
1	1A	1964	5MC	C5-C6-N1	-3.91	119.06	123.31
54	2y	55	PSU	C4-N3-C2	-3.90	120.99	126.37
32	1a	527	7MG	C2-N3-C4	3.88	118.97	112.30
55	2x	55	PSU	C4-N3-C2	-3.84	121.08	126.37
55	2x	8	4SU	C1'-N1-C2	3.84	124.49	117.59
1	2A	1915	5MU	C5-C6-N1	-3.82	119.16	123.31
54	2y	55	PSU	O2-C2-N1	-3.82	118.85	122.79
55	1x	54	5MU	C5-C4-N3	3.82	118.64	115.32
1	2A	1917	PSU	C4-N3-C2	-3.81	121.12	126.37
1	2A	2503	2MA	C4-N3-C2	-3.81	120.37	123.30
54	2y	32	PSU	C4-N3-C2	-3.81	121.13	126.37
54	2w	55	PSU	C4-N3-C2	-3.80	121.14	126.37
32	1a	967	5MC	C5-C6-N1	-3.79	119.19	123.31
1	2A	1917	PSU	O2-C2-N1	-3.79	118.88	122.79
54	2y	39	PSU	C4-N3-C2	-3.77	121.17	126.37
32	2a	516	PSU	C4-N3-C2	-3.77	121.18	126.37
54	1w	39	PSU	O2-C2-N1	-3.77	118.91	122.79
32	2a	1518	MA6	C9-N6-C6	-3.75	109.05	119.40
54	1w	32	PSU	O2-C2-N1	-3.75	118.92	122.79
54	1w	54	5MU	O4-C4-C5	-3.74	120.64	124.92
1	2A	1962	5MC	C5-C6-N1	-3.74	119.25	123.31

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	2w	39	PSU	C4-N3-C2	-3.71	121.26	126.37
1	1A	2617	PSU	O2-C2-N1	-3.70	118.97	122.79
55	1x	8	4SU	O2-C2-N1	3.69	127.60	122.80
54	1w	39	PSU	C4-N3-C2	-3.69	121.28	126.37
32	1a	516	PSU	C4-N3-C2	-3.63	121.36	126.37
32	2a	1400	5MC	C5-C6-N1	-3.63	119.37	123.31
54	1w	8	4SU	N3-C2-N1	3.62	119.60	114.89
1	1A	2564	2MU	O2-C2-N1	-3.60	118.11	122.80
54	1y	54	5MU	C5-C6-N1	-3.60	119.40	123.31
1	1A	1933	PSU	O2-C2-N1	-3.60	119.08	122.79
54	1w	55	PSU	C4-N3-C2	-3.57	121.45	126.37
54	2y	8	4SU	N3-C2-N1	3.56	119.53	114.89
55	2x	54	5MU	O2-C2-N1	-3.55	118.17	122.80
54	1y	32	PSU	C4-N3-C2	-3.54	121.49	126.37
32	1a	1404	5MC	C5-C6-N1	-3.54	119.47	123.31
54	1w	46	7MG	C2-N3-C4	3.53	118.38	112.30
32	1a	1519	MA6	N1-C6-N6	3.53	120.91	116.83
54	1w	37	MIA	C16-C14-C13	-3.50	112.16	122.66
55	1x	54	5MU	C5-C6-N1	-3.48	119.53	123.31
54	1y	54	5MU	O4-C4-C5	-3.47	120.94	124.92
32	2a	967	5MC	C5-C6-N1	-3.47	119.55	123.31
1	1A	2515	2MA	C8-N7-C5	3.46	108.44	102.55
32	1a	1519	MA6	C9-N6-C6	-3.46	109.85	119.40
54	2y	39	PSU	O2-C2-N1	-3.46	119.22	122.79
32	1a	1518	MA6	C4-C5-N7	-3.45	105.69	109.34
54	1w	8	4SU	C5-C4-S4	-3.44	120.38	124.31
54	2y	54	5MU	C1'-N1-C2	3.43	123.75	117.59
32	1a	1407	5MC	C5-C6-N1	-3.43	119.59	123.31
55	2x	54	5MU	C5-C6-N1	-3.41	119.61	123.31
1	1A	2564	2MU	C5-C4-N3	3.40	119.56	114.80
54	1y	39	PSU	C4-N3-C2	-3.39	121.70	126.37
54	1w	46	7MG	C5-C4-N9	-3.39	102.00	106.33
1	1A	2564	2MU	O4-C4-C5	-3.38	119.33	125.16
1	2A	1942	5MC	C5-C6-N1	-3.38	119.64	123.31
32	2a	516	PSU	O2-C2-N1	-3.36	119.32	122.79
1	2A	1911	PSU	C4-N3-C2	-3.36	121.75	126.37
54	1y	32	PSU	O2-C2-N1	-3.36	119.33	122.79
32	2a	1407	5MC	C5-C4-N3	-3.33	118.34	121.75
32	1a	1518	MA6	C9-N6-C6	-3.33	110.23	119.40
54	1w	54	5MU	C5-C6-N1	-3.31	119.72	123.31
1	2A	2605	PSU	O2-C2-N1	-3.31	119.38	122.79
55	1x	32	5MC	C5-C4-N3	-3.30	118.38	121.75

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1937	5MU	C5-C6-N1	-3.28	119.75	123.31
54	2w	55	PSU	O2-C2-N1	-3.27	119.42	122.79
54	2w	32	PSU	O2-C2-N1	-3.27	119.42	122.79
32	2a	1519	MA6	C9-N6-C6	-3.25	110.44	119.40
55	1x	55	PSU	O2-C2-N1	-3.24	119.45	122.79
54	2y	54	5MU	C1'-N1-C6	-3.23	115.83	121.15
55	1x	54	5MU	O4-C4-C5	-3.23	121.23	124.92
32	2a	1207	2MG	C8-N7-C5	3.22	108.03	102.55
55	2x	8	4SU	C5-C4-N3	3.22	117.74	114.75
1	2A	2552	2MU	O2-C2-N1	-3.21	118.61	122.80
54	2y	32	PSU	O2-C2-N1	-3.19	119.50	122.79
1	1A	1961	5MU	O2-C2-N1	-3.16	118.68	122.80
55	1x	32	5MC	C5-C6-N1	-3.15	119.89	123.31
1	2A	2251	OMG	C8-N7-C5	3.15	107.91	102.55
32	2a	1404	5MC	C5-C6-N1	-3.15	119.90	123.31
32	1a	1207	2MG	C8-N7-C5	3.12	107.87	102.55
55	2x	55	PSU	O2-C2-N1	-3.10	119.59	122.79
54	1w	37	MIA	C2-N1-C6	3.06	122.86	117.42
1	1A	1964	5MC	C5-C4-N3	-3.05	118.62	121.75
1	2A	1939	5MU	O2-C2-N1	-3.03	118.85	122.80
54	2w	8	4SU	C1'-N1-C2	3.03	123.04	117.59
32	2a	1518	MA6	C4-C5-N7	-3.03	106.14	109.34
55	1x	8	4SU	C1'-N1-C2	3.03	123.03	117.59
54	2y	46	7MG	C5-C4-N9	-3.03	102.46	106.33
32	1a	1519	MA6	N3-C2-N1	-3.02	124.57	128.67
1	1A	2515	2MA	C4-N3-C2	-3.00	120.99	123.30
32	1a	1404	5MC	C5-C4-N3	-3.00	118.68	121.75
32	2a	527	7MG	C5-C6-N1	2.98	116.19	110.94
1	2A	1911	PSU	O2-C2-N1	-2.98	119.72	122.79
32	2a	1404	5MC	C5-C4-N3	-2.97	118.71	121.75
32	2a	1498	UR3	C5-C4-N3	2.96	118.94	115.04
1	1A	1984	5MC	C5-C4-N3	-2.94	118.74	121.75
54	2w	37	MIA	C12-N6-C6	-2.94	120.12	122.85
54	2w	37	MIA	C4-C5-N7	-2.94	106.23	109.34
55	2x	32	5MC	C5-C4-N3	-2.92	118.76	121.75
54	1y	46	7MG	C5-C4-N9	-2.88	102.65	106.33
1	2A	2552	2MU	C5-C4-N3	2.88	118.83	114.80
1	2A	2503	2MA	C8-N7-C5	2.86	107.42	102.55
32	2a	1407	5MC	C5-C6-N1	-2.85	120.22	123.31
32	1a	1498	UR3	C5-C4-N3	2.84	118.78	115.04
32	1a	1519	MA6	C4-C5-N7	-2.83	106.34	109.34
32	2a	1498	UR3	C6-N1-C2	-2.83	119.49	121.80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2A	1942	5MC	C5-C4-N3	-2.83	118.85	121.75
32	1a	1407	5MC	C5-C4-N3	-2.83	118.86	121.75
1	1A	1937	5MU	O2-C2-N1	-2.81	119.14	122.80
32	2a	1400	5MC	C5-C4-N3	-2.81	118.88	121.75
32	1a	966	M2G	C8-N7-C5	2.78	107.29	102.55
32	1a	1498	UR3	C1'-N1-C2	2.76	121.55	117.04
54	1y	37	MIA	C4-C5-N7	-2.75	106.43	109.34
1	2A	1962	5MC	C5-C4-N3	-2.74	118.95	121.75
1	1A	1942	4OC	O2-C2-N3	-2.74	118.02	122.33
32	1a	516	PSU	O2-C2-N1	-2.73	119.97	122.79
32	2a	966	M2G	C8-N7-C5	2.73	107.20	102.55
55	2x	32	5MC	C5-C6-N1	-2.72	120.36	123.31
1	1A	2263	OMG	C8-N7-C5	2.71	107.16	102.55
54	2w	37	MIA	C2-N1-C6	2.70	122.21	117.42
54	2y	54	5MU	C5-C6-N1	-2.69	120.39	123.31
54	1y	8	4SU	C5-C4-S4	-2.68	121.25	124.31
54	2y	54	5MU	O2-C2-N3	-2.61	116.67	121.49
54	1w	37	MIA	N3-C2-N1	-2.60	122.27	127.03
1	2A	2552	2MU	O4-C4-C5	-2.59	120.69	125.16
32	1a	527	7MG	C5-C6-N1	2.59	115.50	110.94
54	2w	46	7MG	C5-C6-N1	2.58	115.49	110.94
55	1x	8	4SU	C4-N3-C2	2.58	129.79	127.31
32	2a	1518	MA6	C10-N6-C9	-2.55	107.98	116.18
1	1A	2617	PSU	C5-C6-N1	-2.55	118.61	122.14
32	2a	967	5MC	C5-C4-N3	-2.54	119.16	121.75
32	2a	1519	MA6	C4-C5-N7	-2.51	106.68	109.34
1	1A	1984	5MC	O2-C2-N3	-2.50	118.39	122.33
1	1A	1984	5MC	C5-C6-N1	-2.50	120.60	123.31
32	1a	516	PSU	C6-C5-C4	-2.50	116.49	118.17
1	2A	2605	PSU	C6-C5-C4	-2.50	116.49	118.17
32	2a	1402	4OC	C6-C5-C4	2.49	120.00	117.00
32	1a	967	5MC	C5-C4-N3	-2.47	119.22	121.75
54	1w	37	MIA	C4-C5-N7	-2.47	106.73	109.34
54	1w	46	7MG	C4-C5-N7	2.46	108.29	105.38
1	1A	2564	2MU	C2'-C1'-N1	-2.45	109.59	114.24
32	2a	1407	5MC	O2-C2-N3	-2.44	118.48	122.33
54	2w	37	MIA	N3-C2-N1	-2.44	122.57	127.03
32	1a	1404	5MC	O2-C2-N3	-2.43	118.50	122.33
32	1a	1518	MA6	C10-N6-C9	-2.43	108.38	116.18
32	1a	1402	4OC	C6-C5-C4	2.42	119.92	117.00
54	2w	54	5MU	C5-C6-N1	-2.42	120.69	123.31
54	2w	54	5MU	C5M-C5-C4	2.42	121.36	118.78

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1a	1400	5MC	C5-C4-N3	-2.42	119.28	121.75
32	1a	1498	UR3	C3U-N3-C4	2.41	121.21	117.87
55	2x	8	4SU	O2-C2-N1	2.41	125.93	122.80
1	1A	2515	2MA	C5-C6-N1	2.38	118.56	114.12
32	1a	1402	4OC	CM4-N4-C4	-2.38	117.80	122.45
32	1a	1498	UR3	C6-N1-C2	-2.35	119.88	121.80
1	2A	2503	2MA	C5-C6-N1	2.34	118.49	114.12
32	1a	527	7MG	C5-C4-N9	-2.34	103.33	106.33
1	2A	2605	PSU	O4-C4-C5	-2.33	118.21	124.01
54	2w	39	PSU	O2-C2-N1	-2.33	120.38	122.79
1	1A	2263	OMG	C5-C6-N1	2.32	118.49	114.07
54	2y	54	5MU	C5M-C5-C4	2.31	121.25	118.78
55	1x	54	5MU	O2-C2-N1	-2.31	119.79	122.80
54	1y	39	PSU	O2-C2-N1	-2.31	120.41	122.79
55	2x	32	5MC	O2-C2-N3	-2.27	118.75	122.33
32	1a	1407	5MC	O2-C2-N3	-2.27	118.75	122.33
32	2a	1404	5MC	O2-C2-N3	-2.27	118.75	122.33
54	1w	8	4SU	C1'-N1-C2	2.27	121.67	117.59
54	1y	46	7MG	C5-C6-N1	2.27	114.93	110.94
54	2y	8	4SU	C1'-N1-C2	2.24	121.62	117.59
54	1w	54	5MU	O2-C2-N1	-2.22	119.91	122.80
54	2y	37	MIA	C4-C5-N7	-2.22	106.99	109.34
32	2a	967	5MC	CM5-C5-C6	-2.22	119.85	122.85
55	1x	8	4SU	C5-C4-N3	2.21	116.80	114.75
1	1A	1984	5MC	C1'-N1-C6	-2.20	117.52	121.15
32	1a	527	7MG	O6-C6-C5	-2.19	122.23	127.62
54	1y	54	5MU	O2-C2-N3	-2.19	117.45	121.49
32	2a	967	5MC	O2-C2-N3	-2.19	118.89	122.33
1	2A	2251	OMG	O6-C6-C5	-2.18	120.01	124.32
32	1a	967	5MC	O2-C2-N3	-2.17	118.91	122.33
1	1A	1933	PSU	C5-C6-N1	-2.17	119.13	122.14
54	2w	46	7MG	O6-C6-C5	-2.17	122.30	127.62
32	1a	1518	MA6	C10-N6-C6	-2.17	113.43	119.40
1	2A	1911	PSU	C6-C5-C4	-2.14	116.73	118.17
1	1A	1937	5MU	C5M-C5-C4	2.14	121.06	118.78
32	2a	1518	MA6	C10-N6-C6	-2.13	113.52	119.40
54	2y	46	7MG	C5-C6-N1	2.13	114.69	110.94
54	1w	46	7MG	O6-C6-C5	-2.13	122.39	127.62
55	2x	8	4SU	C1'-N1-C6	-2.13	116.23	120.78
1	2A	2251	OMG	C5-C6-N1	2.13	118.13	114.07
1	2A	1962	5MC	N4-C4-N3	2.13	122.36	118.51
55	2x	55	PSU	C5-C6-N1	-2.11	119.21	122.14

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1y	8	4SU	C1'-N1-C2	2.11	121.38	117.59
54	1y	55	PSU	O4'-C1'-C2'	2.11	108.07	105.15
54	2y	55	PSU	C6-C5-C4	-2.11	116.75	118.17
54	2y	32	PSU	O4'-C1'-C2'	2.10	108.06	105.15
55	2x	8	4SU	C6-C5-C4	-2.10	118.13	119.95
54	2y	55	PSU	O4'-C1'-C2'	2.09	108.05	105.15
32	2a	1207	2MG	N1-C2-N2	2.09	118.69	116.56
55	1x	55	PSU	C5-C6-N1	-2.09	119.25	122.14
32	2a	1407	5MC	CM5-C5-C6	-2.08	120.04	122.85
1	1A	1984	5MC	CM5-C5-C6	-2.07	120.04	122.85
32	2a	516	PSU	O4'-C1'-C2'	2.07	108.02	105.15
55	1x	8	4SU	O2-C2-N3	-2.07	117.67	121.49
32	1a	1518	MA6	C1'-N9-C4	-2.06	123.01	126.64
54	2w	32	PSU	C5-C6-N1	-2.06	119.28	122.14
1	2A	1915	5MU	C5M-C5-C4	2.05	120.98	118.78
54	1y	39	PSU	O2-C2-N3	-2.05	118.22	121.86
1	2A	2605	PSU	C5-C6-N1	-2.05	119.30	122.14
32	1a	516	PSU	O4'-C1'-C2'	2.05	107.98	105.15
1	1A	1939	PSU	C5-C6-N1	-2.03	119.32	122.14
32	1a	1407	5MC	CM5-C5-C6	-2.03	120.10	122.85
43	1l	92	0TD	O-C-CA	-2.03	119.56	124.77
54	1y	8	4SU	C6-N1-C2	-2.02	118.54	121.00
54	2w	39	PSU	C5-C6-N1	-2.02	119.34	122.14
32	2a	1400	5MC	O2-C2-N3	-2.01	119.16	122.33
32	2a	1498	UR3	C3U-N3-C4	2.01	120.66	117.87
55	1x	32	5MC	O2-C2-N3	-2.01	119.16	122.33
32	2a	1518	MA6	C1'-N9-C4	-2.01	123.11	126.64
32	2a	527	7MG	C5-C4-N9	-2.00	103.77	106.33

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	1a	1519	MA6	O4'-C4'-C5'-O5'
43	1l	92	0TD	SB-CB-CG-OD2
32	2a	1402	4OC	O4'-C4'-C5'-O5'
32	2a	1519	MA6	O4'-C4'-C5'-O5'
54	1w	37	MIA	C12-C13-C14-C16
54	1y	46	7MG	C4'-C5'-O5'-P
54	1y	54	5MU	O4'-C4'-C5'-O5'
54	2y	55	PSU	C2'-C1'-C5-C6
54	2y	55	PSU	O4'-C1'-C5-C6

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
32	1a	1400	5MC	O4'-C4'-C5'-O5'
32	1a	1402	4OC	O4'-C4'-C5'-O5'
54	2y	37	MIA	C3'-C4'-C5'-O5'
54	1y	8	4SU	C3'-C4'-C5'-O5'
54	1y	8	4SU	O4'-C4'-C5'-O5'
54	2w	46	7MG	O4'-C4'-C5'-O5'
54	1y	54	5MU	C3'-C4'-C5'-O5'
32	2a	1402	4OC	C3'-C4'-C5'-O5'
32	2a	1519	MA6	C3'-C4'-C5'-O5'
54	2w	46	7MG	C3'-C4'-C5'-O5'
32	1a	527	7MG	C3'-C4'-C5'-O5'
32	1a	1519	MA6	C3'-C4'-C5'-O5'
32	1a	1400	5MC	C3'-C4'-C5'-O5'
32	2a	527	7MG	C3'-C4'-C5'-O5'
54	2y	37	MIA	O4'-C4'-C5'-O5'
54	2y	46	7MG	O4'-C1'-N9-C4
32	1a	1402	4OC	C3'-C4'-C5'-O5'
54	2y	32	PSU	O4'-C4'-C5'-O5'
54	2w	46	7MG	C2'-C1'-N9-C8
54	1w	46	7MG	C2'-C1'-N9-C8
54	2y	46	7MG	C2'-C1'-N9-C8
32	1a	527	7MG	O4'-C4'-C5'-O5'
43	1l	92	0TD	CG-CB-SB-CSB
43	2l	92	0TD	CG-CB-SB-CSB
54	2w	37	MIA	N1-C6-N6-C12
43	1l	92	0TD	SB-CB-CG-OD1
54	1w	39	PSU	O4'-C1'-C5-C4
54	1y	55	PSU	O4'-C1'-C5-C4
32	2a	527	7MG	O4'-C4'-C5'-O5'
54	1y	46	7MG	C2'-C1'-N9-C8
54	2y	46	7MG	O4'-C1'-N9-C8
32	1a	1519	MA6	C4'-C5'-O5'-P
54	1w	46	7MG	C4'-C5'-O5'-P
32	1a	1402	4OC	C3'-C2'-O2'-CM2
54	1y	8	4SU	C4'-C5'-O5'-P
54	2y	37	MIA	C4'-C5'-O5'-P
54	2y	54	5MU	C2'-C1'-N1-C6
32	2a	527	7MG	C4'-C5'-O5'-P
54	2y	54	5MU	C2'-C1'-N1-C2
54	2w	46	7MG	O4'-C1'-N9-C8
1	2A	2503	2MA	O4'-C4'-C5'-O5'
1	1A	2515	2MA	C4'-C5'-O5'-P

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
54	1w	46	7MG	O4'-C1'-N9-C8
54	2w	37	MIA	C5-C6-N6-C12
55	2x	8	4SU	C2'-C1'-N1-C2
54	1y	54	5MU	C4'-C5'-O5'-P
1	1A	1942	4OC	C2'-C1'-N1-C2
54	2w	8	4SU	C2'-C1'-N1-C2

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 2853 ligands modelled in this entry, 2851 are monoatomic - leaving 2 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	$\# Z  > 2$
59	SF4	2d	501	35	0,12,12	-	-	-		
59	SF4	1d	501	35	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	SF4	2d	501	35	-	-	0/6/5/5
59	SF4	1d	501	35	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	1A	2860/2915 (98%)	-0.03	172 (6%) 29 27	24, 43, 91, 103	0
1	2A	2789/2915 (95%)	0.06	116 (4%) 41 38	28, 48, 89, 106	0
2	1B	120/121 (99%)	0.55	1 (0%) 82 79	39, 61, 72, 90	0
2	2B	120/121 (99%)	1.34	15 (12%) 9 9	45, 68, 77, 91	0
3	1D	275/276 (99%)	0.22	4 (1%) 71 68	25, 42, 58, 80	0
3	2D	275/276 (99%)	0.21	3 (1%) 77 74	28, 45, 61, 78	0
4	1E	204/206 (99%)	0.32	7 (3%) 48 45	23, 46, 66, 80	0
4	2E	204/206 (99%)	0.30	2 (0%) 79 76	26, 50, 67, 80	0
5	1F	203/210 (96%)	0.45	5 (2%) 58 55	22, 51, 76, 91	0
5	2F	203/210 (96%)	0.56	6 (2%) 52 49	27, 56, 76, 91	0
6	1G	181/182 (99%)	1.30	29 (16%) 6 6	48, 69, 80, 92	0
6	2G	181/182 (99%)	2.05	91 (50%) 0 0	54, 73, 81, 93	0
7	1H	174/180 (96%)	1.09	12 (6%) 24 22	47, 64, 74, 83	0
7	2H	174/180 (96%)	1.51	42 (24%) 2 2	54, 70, 78, 83	0
8	1I	146/148 (98%)	1.09	12 (8%) 19 18	49, 73, 82, 85	0
8	2I	146/148 (98%)	1.23	21 (14%) 7 7	50, 73, 82, 86	0
9	1N	140/140 (100%)	0.65	3 (2%) 63 60	31, 48, 67, 77	0
9	2N	140/140 (100%)	0.60	3 (2%) 63 60	37, 53, 71, 80	0
10	1O	122/122 (100%)	-0.02	2 (1%) 70 67	23, 40, 60, 74	0
10	2O	122/122 (100%)	0.78	4 (3%) 49 46	45, 59, 72, 81	0
11	1P	149/150 (99%)	0.74	13 (8%) 17 16	24, 53, 75, 81	0
11	2P	149/150 (99%)	0.75	9 (6%) 29 27	29, 58, 76, 85	0
12	1Q	141/141 (100%)	0.55	2 (1%) 73 70	33, 51, 68, 77	0
12	2Q	141/141 (100%)	1.16	24 (17%) 5 5	37, 56, 73, 79	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%)	0.06	0 100 100	29, 40, 55, 62	0
13	2R	118/118 (100%)	0.04	0 100 100	31, 43, 58, 65	0
14	1S	110/112 (98%)	1.09	12 (10%) 12 11	49, 62, 72, 77	0
14	2S	110/112 (98%)	1.82	37 (33%) 1 1	55, 66, 75, 79	0
15	1T	131/146 (89%)	0.59	8 (6%) 28 26	38, 50, 72, 77	0
15	2T	131/146 (89%)	0.57	3 (2%) 61 58	43, 53, 74, 78	0
16	1U	116/118 (98%)	0.29	2 (1%) 69 65	26, 39, 55, 73	0
16	2U	116/118 (98%)	0.45	1 (0%) 81 78	33, 46, 61, 73	0
17	1V	101/101 (100%)	0.48	3 (2%) 52 49	28, 51, 67, 76	0
17	2V	101/101 (100%)	0.86	5 (4%) 35 32	33, 57, 70, 76	0
18	1W	112/113 (99%)	0.04	2 (1%) 67 64	26, 37, 55, 88	0
18	2W	112/113 (99%)	0.09	2 (1%) 67 64	30, 41, 57, 88	0
19	1X	95/96 (98%)	0.41	3 (3%) 50 47	30, 44, 63, 75	0
19	2X	95/96 (98%)	0.54	1 (1%) 77 74	34, 49, 65, 76	0
20	1Y	107/110 (97%)	0.94	9 (8%) 18 17	45, 57, 74, 83	0
20	2Y	107/110 (97%)	1.27	13 (12%) 10 9	48, 61, 76, 86	0
21	1Z	154/206 (74%)	0.87	20 (12%) 9 8	38, 64, 86, 96	0
21	2Z	160/206 (77%)	2.24	96 (60%) 0 0	72, 83, 93, 99	0
22	10	83/85 (97%)	0.11	0 100 100	25, 38, 59, 71	0
22	20	83/85 (97%)	1.44	17 (20%) 3 3	41, 66, 78, 82	0
23	11	97/98 (98%)	0.17	1 (1%) 79 76	23, 44, 71, 77	0
23	21	97/98 (98%)	0.93	13 (13%) 8 8	38, 58, 74, 82	0
24	12	70/72 (97%)	0.78	5 (7%) 23 22	40, 57, 66, 79	0
24	22	70/72 (97%)	0.91	3 (4%) 40 37	46, 61, 69, 78	0
25	13	59/60 (98%)	0.48	1 (1%) 69 65	29, 45, 69, 83	0
25	23	59/60 (98%)	0.68	2 (3%) 48 45	36, 51, 72, 87	0
26	14	69/71 (97%)	1.64	22 (31%) 1 1	64, 79, 89, 97	0
26	24	69/71 (97%)	2.16	36 (52%) 0 0	70, 80, 89, 97	0
27	15	59/60 (98%)	0.02	1 (1%) 69 65	25, 36, 57, 72	0
27	25	59/60 (98%)	0.02	1 (1%) 69 65	30, 40, 60, 71	0
28	16	53/54 (98%)	0.44	1 (1%) 66 63	38, 51, 64, 74	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%)	0.77	3 (5%) 30 28	42, 54, 65, 71	0
29	17	48/49 (97%)	0.02	5 (10%) 13 12	24, 31, 58, 69	0
29	27	48/49 (97%)	-0.02	2 (4%) 41 38	28, 35, 58, 70	0
30	18	64/65 (98%)	0.40	4 (6%) 27 25	33, 42, 50, 66	0
30	28	64/65 (98%)	0.60	1 (1%) 70 67	38, 46, 53, 67	0
31	19	37/37 (100%)	0.66	0 100 100	37, 50, 67, 68	0
31	29	37/37 (100%)	1.21	5 (13%) 8 7	46, 54, 71, 72	0
32	1a	1488/1521 (97%)	0.82	105 (7%) 23 22	42, 72, 92, 103	0
32	2a	1491/1521 (98%)	1.10	277 (18%) 4 4	44, 74, 93, 103	0
33	1b	231/256 (90%)	1.58	70 (30%) 1 1	69, 82, 89, 94	0
33	2b	231/256 (90%)	2.35	145 (62%) 0 0	72, 83, 89, 94	0
34	1c	206/239 (86%)	1.57	55 (26%) 2 2	67, 80, 86, 92	0
34	2c	206/239 (86%)	2.44	133 (64%) 0 0	69, 82, 88, 93	0
35	1d	208/209 (99%)	1.35	36 (17%) 5 5	56, 72, 80, 87	0
35	2d	208/209 (99%)	1.36	35 (16%) 5 5	58, 71, 80, 88	0
36	1e	148/162 (91%)	1.30	22 (14%) 7 6	56, 72, 80, 86	0
36	2e	148/162 (91%)	1.96	67 (45%) 1 1	59, 74, 83, 87	0
37	1f	100/101 (99%)	1.02	5 (5%) 35 32	50, 66, 76, 78	0
37	2f	100/101 (99%)	1.05	6 (6%) 29 27	60, 72, 80, 86	0
38	1g	155/156 (99%)	1.48	36 (23%) 2 3	62, 74, 83, 100	0
38	2g	155/156 (99%)	1.69	44 (28%) 1 1	65, 76, 84, 102	0
39	1h	137/138 (99%)	1.19	15 (10%) 12 11	60, 72, 78, 83	0
39	2h	137/138 (99%)	1.71	44 (32%) 1 1	64, 74, 80, 84	0
40	1i	127/128 (99%)	1.48	33 (25%) 2 2	51, 75, 83, 87	0
40	2i	127/128 (99%)	2.72	90 (70%) 0 0	71, 85, 91, 92	0
41	1j	97/105 (92%)	1.79	33 (34%) 1 1	59, 78, 90, 95	0
41	2j	96/105 (91%)	2.97	74 (77%) 0 0	74, 87, 94, 98	0
42	1k	114/129 (88%)	1.06	13 (11%) 11 10	52, 69, 80, 83	0
42	2k	114/129 (88%)	1.24	17 (14%) 7 6	55, 71, 81, 87	0
43	1l	121/132 (91%)	0.98	16 (13%) 8 8	53, 64, 74, 77	0
43	2l	121/132 (91%)	1.29	16 (13%) 8 8	55, 67, 75, 80	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	1m	123/126 (97%)	1.04	12 (9%) 14 13	54, 69, 78, 82	0
44	2m	122/126 (96%)	2.51	69 (56%) 0 0	73, 84, 90, 94	0
45	1n	60/61 (98%)	1.37	8 (13%) 8 8	57, 69, 78, 82	0
45	2n	60/61 (98%)	3.14	54 (90%) 0 0	78, 85, 93, 95	0
46	1o	88/89 (98%)	1.14	14 (15%) 6 6	56, 69, 78, 82	0
46	2o	88/89 (98%)	1.29	13 (14%) 7 7	57, 70, 80, 83	0
47	1p	82/88 (93%)	1.69	27 (32%) 1 1	58, 70, 80, 83	0
47	2p	82/88 (93%)	1.53	16 (19%) 4 4	59, 69, 81, 82	0
48	1q	99/105 (94%)	1.23	7 (7%) 23 22	57, 70, 79, 82	0
48	2q	99/105 (94%)	1.44	21 (21%) 3 3	60, 70, 79, 82	0
49	1r	68/88 (77%)	1.08	6 (8%) 17 16	60, 68, 79, 82	0
49	2r	68/88 (77%)	1.20	9 (13%) 8 8	60, 70, 80, 82	0
50	1s	83/93 (89%)	1.50	19 (22%) 2 3	70, 79, 86, 91	0
50	2s	83/93 (89%)	2.73	64 (77%) 0 0	74, 81, 88, 94	0
51	1t	96/106 (90%)	1.44	23 (23%) 2 2	58, 71, 80, 86	0
51	2t	96/106 (90%)	1.15	11 (11%) 11 10	59, 71, 81, 85	0
52	1u	23/27 (85%)	1.77	9 (39%) 1 1	65, 74, 78, 80	0
52	2u	23/27 (85%)	2.85	17 (73%) 0 0	68, 75, 80, 83	0
53	1v	13/24 (54%)	1.84	7 (53%) 0 0	60, 74, 92, 98	0
53	2v	13/24 (54%)	2.44	7 (53%) 0 0	65, 78, 95, 98	0
54	1w	67/76 (88%)	1.51	21 (31%) 1 1	44, 89, 97, 101	0
54	1y	67/76 (88%)	1.50	15 (22%) 3 3	37, 91, 97, 101	0
54	2w	65/76 (85%)	1.79	20 (30%) 1 1	56, 96, 101, 104	0
54	2y	66/76 (86%)	1.66	15 (22%) 3 3	51, 95, 99, 100	0
55	1x	72/77 (93%)	0.54	5 (6%) 24 22	33, 66, 84, 87	0
55	2x	72/77 (93%)	0.99	3 (4%) 41 38	52, 81, 90, 95	0
All	All	20875/21748 (95%)	0.79	2817 (13%) 8 7	22, 63, 88, 106	0

All (2817) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	2m	102	ARG	6.9
38	1g	80	VAL	6.8

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
41	2j	40	LEU	6.7
45	2n	25	VAL	6.6
45	1n	2	ALA	6.6
38	1g	82	GLY	6.5
33	2b	165	VAL	6.3
50	2s	79	THR	6.2
52	2u	11	GLY	6.1
41	2j	47	PHE	6.0
34	2c	171	GLY	6.0
7	1H	2	SER	5.9
16	1U	117	GLN	5.9
40	2i	14	VAL	5.8
41	2j	55	LYS	5.7
52	2u	14	TRP	5.7
21	2Z	139	VAL	5.6
41	2j	65	LEU	5.6
45	2n	39	LEU	5.6
21	2Z	172	ALA	5.5
44	2m	90	LEU	5.4
44	2m	6	GLY	5.4
38	1g	79	ARG	5.4
3	1D	276	LYS	5.3
40	2i	9	ARG	5.3
1	1A	1140	U	5.3
23	2l	2	SER	5.3
44	2m	123	ALA	5.3
33	2b	237	ALA	5.2
1	1A	1104	G	5.2
44	2m	100	GLY	5.2
45	2n	34	TYR	5.2
41	2j	54	PHE	5.1
34	2c	198	VAL	5.1
44	2m	124	PRO	5.1
1	1A	1110	C	5.1
45	2n	7	ILE	5.1
34	1c	2	GLY	5.1
21	2Z	173	ALA	5.0
1	1A	1141	A	5.0
53	2v	14	A	5.0
33	2b	21	ARG	5.0
1	1A	932	C	5.0
40	2i	102	LEU	5.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
6	2G	74	LYS	5.0
33	2b	214	ILE	5.0
34	2c	182	ILE	5.0
6	2G	29	TRP	5.0
41	2j	32	ALA	5.0
40	2i	126	SER	5.0
50	2s	80	TYR	5.0
1	1A	1143	U	5.0
34	2c	2	GLY	4.9
44	2m	78	ILE	4.9
6	1G	139	LEU	4.9
33	2b	161	ALA	4.9
34	2c	189	ALA	4.9
33	2b	187	LEU	4.8
45	2n	2	ALA	4.8
45	2n	5	ALA	4.8
46	1o	87	ILE	4.8
38	2g	82	GLY	4.8
41	2j	37	PRO	4.8
32	1a	1531	A	4.8
44	2m	104	ARG	4.8
44	1m	2	ALA	4.8
44	1m	122	LYS	4.8
41	2j	41	PRO	4.8
34	2c	124	ILE	4.8
44	2m	68	GLY	4.8
26	14	59	PHE	4.8
41	2j	35	SER	4.7
33	2b	200	ILE	4.7
1	1A	2814	C	4.7
40	2i	106	ALA	4.7
1	1A	2906	U	4.7
39	1h	2	LEU	4.7
34	2c	68	VAL	4.7
41	2j	85	LEU	4.6
50	2s	13	ASP	4.6
38	2g	16	LEU	4.6
33	2b	185	ILE	4.6
1	2A	883	G	4.6
34	2c	149	ALA	4.6
52	2u	6	ARG	4.6
6	2G	159	VAL	4.5

*Continued on next page...*



*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
40	2i	11	LYS	4.5
44	2m	4	ILE	4.5
33	2b	152	PHE	4.5
1	1A	1144	A	4.5
50	2s	84	GLY	4.5
34	2c	129	ALA	4.5
34	2c	33	LEU	4.5
1	1A	1112	U	4.5
1	1A	1105	G	4.5
1	1A	1103	A	4.5
1	1A	931	C	4.4
32	1a	1023	G	4.4
1	2A	896	A	4.4
41	2j	87	THR	4.4
44	2m	120	LYS	4.4
44	2m	122	LYS	4.4
33	2b	236	TYR	4.4
32	1a	344	A	4.4
54	1w	1	G	4.4
21	2Z	146	ILE	4.4
1	1A	936	C	4.4
34	2c	137	ALA	4.4
41	1j	32	ALA	4.4
44	1m	124	PRO	4.3
6	2G	28	VAL	4.3
44	2m	60	VAL	4.3
50	2s	9	VAL	4.3
45	2n	38	GLY	4.3
34	2c	8	ILE	4.3
41	2j	50	ILE	4.3
34	1c	207	VAL	4.3
1	1A	2141	A	4.3
53	1v	12	A	4.3
32	2a	1150	U	4.3
38	2g	5	ARG	4.3
40	2i	83	ARG	4.3
40	2i	39	GLY	4.3
32	1a	163	C	4.2
32	2a	1149	C	4.2
40	2i	36	TYR	4.2
45	2n	21	TYR	4.2
1	1A	1127	U	4.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
21	1Z	141	VAL	4.2
45	2n	29	ARG	4.2
50	2s	75	ALA	4.2
36	2e	22	GLY	4.2
33	2b	163	PHE	4.2
6	2G	15	VAL	4.2
9	1N	9	VAL	4.2
21	1Z	149	SER	4.2
34	2c	197	GLY	4.2
1	1A	1106	U	4.2
32	2a	1119	C	4.2
34	2c	187	ALA	4.2
44	2m	118	ALA	4.2
50	2s	54	GLY	4.2
44	2m	96	LEU	4.2
24	12	70	GLN	4.2
32	2a	1219	U	4.2
38	2g	84	ASN	4.2
41	2j	78	ASN	4.2
1	1A	933	C	4.2
40	2i	90	PRO	4.1
21	2Z	171	ILE	4.1
32	2a	1222	G	4.1
40	2i	62	TYR	4.1
45	2n	55	GLY	4.1
54	2w	3	C	4.1
41	2j	74	ILE	4.1
45	2n	3	ARG	4.1
40	2i	37	PHE	4.1
7	2H	52	VAL	4.1
21	2Z	86	VAL	4.1
26	14	56	VAL	4.1
38	2g	80	VAL	4.1
32	2a	1033	G	4.1
40	2i	124	GLN	4.1
34	2c	52	LEU	4.1
1	1A	1142	A	4.1
24	12	69	ARG	4.1
40	2i	10	ARG	4.1
54	2y	36	A	4.1
33	2b	39	ILE	4.1
40	2i	125	TYR	4.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
33	2b	61	LEU	4.1
40	2i	19	LEU	4.1
1	2A	229	A	4.1
41	2j	42	THR	4.1
45	2n	13	THR	4.1
27	15	60	VAL	4.1
45	2n	18	VAL	4.1
50	2s	24	ALA	4.1
6	2G	11	TYR	4.0
34	2c	9	GLY	4.0
38	1g	81	GLY	4.0
32	1a	1001(A)	G	4.0
33	2b	91	PRO	4.0
38	1g	8	GLU	4.0
32	2a	1030	C	4.0
40	2i	7	THR	4.0
54	1w	73	A	4.0
41	2j	49	VAL	4.0
38	2g	81	GLY	4.0
41	2j	38	ILE	4.0
1	1A	1102	G	4.0
33	2b	81	VAL	4.0
1	2A	2136	C	4.0
21	2Z	144	LEU	4.0
26	14	58	ARG	4.0
34	2c	48	TYR	4.0
42	2k	25	TYR	4.0
45	2n	40	CYS	4.0
1	1A	2163	G	4.0
1	1A	2813	G	4.0
32	1a	630	G	4.0
32	2a	1127	G	4.0
33	2b	184	VAL	4.0
6	2G	50	ALA	4.0
33	1b	228	GLY	4.0
47	2p	48	TRP	4.0
52	1u	2	GLY	4.0
22	20	84	LEU	4.0
33	2b	11	LEU	4.0
25	23	2	PRO	4.0
26	24	32	TYR	4.0
44	2m	23	TYR	4.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
33	1b	127	ILE	4.0
33	2b	230	VAL	4.0
50	2s	2	PRO	3.9
41	2j	13	HIS	3.9
32	2a	1038	C	3.9
38	2g	85	TYR	3.9
53	2v	12	A	3.9
47	1p	82	GLN	3.9
32	2a	1126	U	3.9
33	1b	120	ALA	3.9
34	2c	188	LEU	3.9
36	2e	12	LEU	3.9
50	2s	82	GLY	3.9
44	2m	67	GLU	3.9
1	2A	2155	G	3.9
32	1a	1036	G	3.9
32	2a	973	G	3.9
32	2a	1220	G	3.9
54	2w	71	G	3.9
34	1c	184	TYR	3.9
32	2a	1183	A	3.9
47	2p	82	GLN	3.9
26	24	49	PHE	3.9
40	2i	27	THR	3.9
7	2H	45	VAL	3.9
45	2n	58	LYS	3.9
38	2g	7	ALA	3.9
45	2n	6	LEU	3.9
1	1A	1145	G	3.9
32	2a	1018	C	3.9
40	2i	67	GLY	3.9
33	2b	101	MET	3.9
34	2c	5	ILE	3.9
44	2m	87	TYR	3.9
38	2g	76	ARG	3.9
6	1G	80	PHE	3.8
1	1A	2136	A	3.8
32	1a	1002	G	3.8
32	1a	1035	A	3.8
32	2a	1224	G	3.8
54	2w	73	A	3.8
1	1A	935	C	3.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
32	2a	1019	C	3.8
33	1b	229	VAL	3.8
26	24	65	ASP	3.8
39	2h	2	LEU	3.8
50	2s	71	LEU	3.8
40	2i	15	ALA	3.8
51	1t	103	GLY	3.8
33	2b	201	ILE	3.8
44	2m	106	ASN	3.8
42	2k	126	ARG	3.8
47	1p	42	ARG	3.8
50	2s	81	ARG	3.8
44	2m	105	THR	3.8
40	2i	99	LEU	3.8
44	2m	54	VAL	3.8
45	2n	53	LEU	3.8
1	1A	1114	G	3.8
1	1A	1116	A	3.8
1	1A	1146	C	3.8
32	1a	1026	G	3.8
33	2b	123	ALA	3.8
53	2v	13	A	3.8
40	2i	49	PRO	3.8
41	1j	86	MET	3.8
1	1A	1111	U	3.8
34	2c	170	GLN	3.8
40	2i	20	ARG	3.8
6	1G	146	TYR	3.8
51	1t	13	LEU	3.8
44	2m	117	VAL	3.8
40	2i	105	ASP	3.8
36	2e	81	GLU	3.8
32	1a	160	A	3.8
32	1a	1005	A	3.8
32	2a	1030(A)	G	3.8
32	2a	1034	G	3.8
32	2a	1036	G	3.8
54	2y	19	G	3.8
21	2Z	137	ILE	3.8
34	1c	39	ILE	3.8
40	2i	81	ILE	3.8
21	2Z	149	SER	3.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
40	2i	5	TYR	3.8
45	1n	34	TYR	3.8
34	2c	53	ALA	3.8
26	24	31	ILE	3.8
32	2a	994	A	3.8
1	2A	1536	C	3.8
32	1a	204	U	3.8
35	1d	194	LEU	3.7
38	1g	85	TYR	3.7
41	2j	8	LEU	3.7
34	2c	195	VAL	3.7
36	1e	10	MET	3.7
33	1b	125	PRO	3.7
15	1T	130	ALA	3.7
26	14	54	GLY	3.7
33	2b	38	GLY	3.7
33	1b	21	ARG	3.7
32	1a	1447	A	3.7
1	2A	1043	C	3.7
32	2a	1030(B)	C	3.7
32	2a	1216	G	3.7
50	2s	10	PHE	3.7
50	2s	22	LEU	3.7
33	2b	199	TYR	3.7
40	2i	61	ALA	3.7
21	1Z	146	ILE	3.7
21	1Z	150	LEU	3.7
45	2n	49	HIS	3.7
54	1w	4	C	3.7
26	14	50	VAL	3.7
33	1b	165	VAL	3.7
44	2m	98	VAL	3.7
1	1A	1221	G	3.7
15	1T	131	ALA	3.7
22	20	5	LYS	3.7
29	17	48	LYS	3.7
32	2a	1058	G	3.7
36	2e	85	GLY	3.7
36	2e	86	ALA	3.7
19	1X	95	LEU	3.7
33	2b	118	LEU	3.7
34	2c	12	LEU	3.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
32	1a	1001	A	3.7
32	2a	1251	A	3.7
53	2v	24	A	3.7
1	1A	2807	C	3.7
5	1F	131	GLY	3.7
6	2G	146	TYR	3.7
33	2b	71	VAL	3.7
35	1d	167	GLY	3.7
40	2i	41	VAL	3.7
36	2e	94	ALA	3.7
38	1g	2	ALA	3.7
33	2b	222	ILE	3.7
54	1w	65	G	3.7
38	2g	12	LEU	3.6
41	2j	88	LEU	3.6
32	1a	1257	U	3.6
41	2j	10	GLY	3.6
32	2a	1092	A	3.6
32	2a	1286	A	3.6
1	1A	1138	C	3.6
1	2A	2803	C	3.6
32	2a	980	C	3.6
32	2a	1260	C	3.6
1	1A	1133	G	3.6
1	1A	1139	G	3.6
41	2j	59	SER	3.6
21	1Z	168	GLU	3.6
7	2H	50	VAL	3.6
21	2Z	26	GLY	3.6
26	24	56	VAL	3.6
45	2n	61	TRP	3.6
32	2a	975	A	3.6
26	24	51	ASP	3.6
1	1A	2905	C	3.6
32	2a	962	C	3.6
19	2X	92	LEU	3.6
1	1A	1108	G	3.6
32	1a	1024	G	3.6
14	2S	29	PHE	3.6
34	2c	151	VAL	3.6
39	1h	93	VAL	3.6
40	2i	44	VAL	3.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
40	2i	66	ARG	3.6
21	2Z	170	THR	3.6
41	1j	34	VAL	3.6
32	2a	1281	U	3.6
51	1t	12	ALA	3.6
34	2c	157	ILE	3.6
1	1A	934	A	3.6
32	2a	983	A	3.6
34	2c	142	MET	3.6
34	2c	176	HIS	3.6
21	2Z	33	LEU	3.6
34	2c	94	LEU	3.6
1	2A	2160	G	3.6
34	2c	41	GLY	3.6
6	1G	50	ALA	3.6
6	2G	57	ALA	3.6
6	2G	12	TYR	3.6
50	1s	13	ASP	3.6
1	1A	2167	C	3.5
33	1b	129	GLU	3.5
52	2u	15	ARG	3.5
40	2i	17	VAL	3.5
40	2i	45	ALA	3.5
1	1A	2174	G	3.5
1	2A	2159	G	3.5
32	1a	1003	G	3.5
32	2a	993	G	3.5
32	2a	1017	G	3.5
50	2s	40	ILE	3.5
54	2y	34	G	3.5
1	1A	271	U	3.5
1	1A	2135	U	3.5
14	2S	58	LEU	3.5
34	2c	178	LEU	3.5
45	2n	44	LEU	3.5
50	2s	20	LEU	3.5
46	1o	88	ARG	3.5
52	2u	24	ARG	3.5
53	1v	24	A	3.5
33	2b	122	PHE	3.5
1	1A	2162	C	3.5
1	2A	2804	C	3.5

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
20	2Y	80	GLY	3.5
45	2n	28	GLY	3.5
51	2t	47	GLY	3.5
21	2Z	174	VAL	3.5
34	2c	138	VAL	3.5
21	2Z	21	ALA	3.5
44	2m	5	ALA	3.5
41	2j	23	ILE	3.5
41	2j	96	ILE	3.5
1	1A	1124	U	3.5
41	2j	71	LEU	3.5
6	2G	35	GLU	3.5
1	1A	572	A	3.5
1	1A	2195	A	3.5
5	1F	208	GLY	3.5
18	1W	112	GLY	3.5
33	2b	99	GLY	3.5
40	1i	126	SER	3.5
9	1N	140	VAL	3.5
21	2Z	27	VAL	3.5
34	2c	55	VAL	3.5
34	2c	120	VAL	3.5
36	2e	41	VAL	3.5
50	2s	41	VAL	3.5
33	2b	67	THR	3.5
35	1d	169	LYS	3.5
45	2n	20	ALA	3.5
26	14	67	TYR	3.5
33	2b	148	TYR	3.5
40	2i	4	TYR	3.5
33	1b	130	ARG	3.5
34	2c	30	ARG	3.5
1	2A	171	G	3.5
1	2A	2116	G	3.5
32	1a	1030(A)	G	3.5
6	1G	42	GLY	3.5
26	14	66	SER	3.5
38	2g	34	GLY	3.5
44	2m	112	GLY	3.5
33	2b	197	VAL	3.5
40	2i	86	VAL	3.5
41	2j	14	LYS	3.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
32	2a	1531	A	3.5
43	2l	51	ALA	3.5
1	2A	886	C	3.4
32	2a	1066	C	3.4
7	2H	64	LEU	3.4
41	2j	90	LEU	3.4
50	1s	71	LEU	3.4
42	1k	25	TYR	3.4
45	2n	23	ARG	3.4
32	1a	1025	U	3.4
1	1A	1109	G	3.4
20	2Y	57	GLN	3.4
23	2l	28	GLY	3.4
32	2a	1048	G	3.4
33	2b	136	VAL	3.4
40	2i	28	VAL	3.4
35	2d	146	ILE	3.4
40	2i	13	ALA	3.4
45	2n	30	ALA	3.4
1	1A	1100	A	3.4
1	1A	1115	A	3.4
1	2A	2119	A	3.4
1	1A	1121	C	3.4
1	1A	2186	C	3.4
32	1a	1028	C	3.4
38	1g	3	ARG	3.4
40	2i	16	ARG	3.4
26	24	59	PHE	3.4
33	1b	133	LYS	3.4
38	2g	109	ASN	3.4
34	2c	155	GLY	3.4
23	1l	2	SER	3.4
21	2Z	57	ILE	3.4
34	2c	134	ILE	3.4
34	2c	200	ALA	3.4
40	2i	82	ALA	3.4
41	1j	4	ILE	3.4
1	1A	2806	G	3.4
1	2A	2133	G	3.4
1	2A	2157	G	3.4
32	2a	1272	G	3.4
44	1m	5	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>
36	2e	31	LEU	3.4
50	2s	15	LEU	3.4
33	1b	131	PRO	3.4
3	1D	275	LYS	3.4
20	1Y	1	MET	3.4
41	2j	69	ASN	3.4
41	2j	36	GLY	3.4
14	2S	69	VAL	3.4
33	1b	230	VAL	3.4
38	2g	75	VAL	3.4
50	2s	11	VAL	3.4
33	2b	162	ILE	3.4
34	2c	77	ILE	3.4
34	2c	202	ILE	3.4
36	2e	109	ILE	3.4
36	2e	118	ILE	3.4
50	1s	40	ILE	3.4
40	1i	106	ALA	3.4
40	2i	96	LEU	3.4
41	2j	79	ARG	3.4
1	1A	2212	G	3.4
1	2A	2149	G	3.4
32	1a	1034	G	3.4
54	1y	18	G	3.4
36	2e	133	TYR	3.4
32	1a	1030(B)	C	3.4
40	2i	101	PHE	3.4
44	2m	22	ILE	3.4
14	2S	5	THR	3.3
40	1i	15	ALA	3.3
44	2m	88	ARG	3.3
44	2m	121	LYS	3.3
1	2A	882	G	3.3
1	2A	2802	G	3.3
2	2B	23	G	3.3
54	1w	70	G	3.3
1	1A	937	A	3.3
48	2q	95	TYR	3.3
50	2s	52	TYR	3.3
21	2Z	48	PHE	3.3
40	1i	59	PHE	3.3
45	2n	36	PHE	3.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
34	2c	13	GLY	3.3
35	2d	87	GLY	3.3
51	2t	9	ASN	3.3
32	2a	1263	C	3.3
1	1A	1128	U	3.3
44	2m	15	VAL	3.3
8	1I	146	ALA	3.3
21	1Z	170	THR	3.3
38	2g	3	ARG	3.3
41	2j	43	ARG	3.3
44	2m	19	LEU	3.3
41	2j	99	LYS	3.3
1	1A	2137	G	3.3
32	2a	971	G	3.3
1	1A	2803	A	3.3
1	1A	2812	A	3.3
32	2a	1035	A	3.3
41	2j	68	HIS	3.3
6	2G	160	VAL	3.3
36	2e	33	VAL	3.3
43	1l	43	VAL	3.3
32	1a	1532	U	3.3
44	2m	3	ARG	3.3
50	2s	78	ARG	3.3
33	2b	196	LEU	3.3
33	2b	218	ALA	3.3
49	2r	60	ALA	3.3
26	24	57	GLU	3.3
6	2G	80	PHE	3.3
21	2Z	121	HIS	3.3
37	2f	60	PHE	3.3
41	2j	56	HIS	3.3
50	2s	14	HIS	3.3
39	2h	106	GLY	3.3
40	2i	63	ILE	3.3
1	1A	942	A	3.3
1	2A	2135	A	3.3
32	2a	953	G	3.3
32	2a	976	G	3.3
32	2a	1030(D)	A	3.3
32	2a	1110	A	3.3
40	1i	14	VAL	3.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
41	2j	72	VAL	3.3
32	2a	1124	G	3.3
21	2Z	51	ALA	3.3
41	1j	88	LEU	3.3
33	2b	22	LYS	3.3
40	2i	103	THR	3.3
32	1a	1027	C	3.3
32	1a	1037	C	3.3
32	2a	979	C	3.3
54	1w	72	C	3.3
33	2b	86	GLU	3.3
50	2s	31	ILE	3.2
33	2b	69	LEU	3.2
43	2l	52	LEU	3.2
49	2r	66	LEU	3.2
22	20	43	THR	3.2
33	2b	207	ALA	3.2
41	1j	87	THR	3.2
44	2m	72	ALA	3.2
1	1A	2173	G	3.2
6	2G	17	PRO	3.2
32	2a	1182	G	3.2
1	1A	2164	C	3.2
1	2A	885	C	3.2
1	2A	2896	C	3.2
40	2i	18	PHE	3.2
26	24	54	GLY	3.2
31	29	37	GLY	3.2
40	2i	92	TYR	3.2
47	1p	39	TYR	3.2
34	2c	91	LEU	3.2
39	2h	36	LEU	3.2
41	2j	94	VAL	3.2
48	2q	9	VAL	3.2
20	2Y	5	MET	3.2
34	2c	71	ALA	3.2
41	2j	27	ALA	3.2
50	2s	63	THR	3.2
1	1A	218	A	3.2
1	1A	1130	A	3.2
1	1A	1134	A	3.2
1	1A	1147	U	3.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
32	1a	162	A	3.2
1	1A	1135	G	3.2
1	2A	2112	G	3.2
32	1a	1021	G	3.2
36	2e	20	GLN	3.2
32	2a	995	C	3.2
40	2i	104	ARG	3.2
52	2u	10	ARG	3.2
41	2j	80	LYS	3.2
41	2j	75	ILE	3.2
21	2Z	30	ASN	3.2
40	2i	29	ASN	3.2
6	2G	5	VAL	3.2
34	2c	153	VAL	3.2
36	2e	61	TYR	3.2
33	2b	173	ALA	3.2
34	2c	168	ALA	3.2
34	2c	109	PRO	3.2
44	2m	64	TRP	3.2
32	1a	1446	U	3.2
32	2a	1085	U	3.2
1	2A	1847	A	3.2
47	1p	76	GLN	3.2
53	2v	15	A	3.2
21	2Z	136	PHE	3.2
32	1a	1033	G	3.2
32	2a	1024	G	3.2
40	2i	91	ASP	3.2
47	1p	27	LYS	3.2
1	1A	1126	C	3.2
1	1A	2160	C	3.2
21	2Z	147	GLY	3.2
32	1a	1008	C	3.2
32	2a	1116	C	3.2
32	2a	1203	C	3.2
35	2d	167	GLY	3.2
36	2e	74	GLY	3.2
54	2w	2	C	3.2
6	2G	88	ILE	3.2
7	2H	72	ILE	3.2
39	2h	135	CYS	3.2
33	2b	10	LEU	3.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
44	2m	66	LEU	3.2
14	1S	46	VAL	3.2
44	2m	53	VAL	3.2
14	2S	92	TYR	3.2
26	24	63	TYR	3.2
36	2e	17	ALA	3.2
7	2H	2	SER	3.2
34	1c	179	ARG	3.2
38	2g	4	ARG	3.2
32	2a	1357	A	3.2
31	29	21	GLY	3.1
34	2c	205	GLY	3.1
40	2i	115	GLY	3.1
41	1j	31	GLY	3.1
6	2G	82	LEU	3.1
21	2Z	150	LEU	3.1
33	2b	145	LEU	3.1
1	1A	2165	C	3.1
1	1A	2181	G	3.1
1	2A	884	C	3.1
32	1a	102	G	3.1
32	1a	1006	C	3.1
32	2a	1064	G	3.1
32	2a	1114	C	3.1
34	2c	141	VAL	3.1
45	2n	33	VAL	3.1
33	2b	31	TYR	3.1
40	1i	2	GLU	3.1
41	2j	61	GLU	3.1
12	2Q	22	LYS	3.1
14	2S	17	ARG	3.1
33	2b	144	ARG	3.1
34	1c	79	ARG	3.1
50	2s	29	ARG	3.1
34	1c	96	GLY	3.1
34	2c	128	PHE	3.1
1	1A	2139	A	3.1
1	2A	2173	A	3.1
6	2G	53	LEU	3.1
36	2e	13	ILE	3.1
46	2o	31	LEU	3.1
52	2u	5	ASP	3.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
32	2a	974	A	3.1
54	1y	35	A	3.1
38	2g	21	VAL	3.1
51	1t	9	ASN	3.1
44	2m	97	PRO	3.1
1	1A	2805	G	3.1
1	2A	2166	G	3.1
32	2a	948	C	3.1
32	2a	1115	C	3.1
33	1b	107	THR	3.1
34	2c	201	TYR	3.1
39	2h	94	TYR	3.1
50	2s	48	THR	3.1
21	2Z	52	SER	3.1
51	2t	74	LYS	3.1
7	1H	3	ARG	3.1
33	2b	175	ARG	3.1
51	2t	8	ARG	3.1
22	20	69	PHE	3.1
8	2I	68	LEU	3.1
51	2t	103	GLY	3.1
52	1u	16	GLY	3.1
1	2A	2117	A	3.1
33	2b	131	PRO	3.1
50	2s	76	PRO	3.1
54	2y	35	A	3.1
34	2c	146	ALA	3.1
41	2j	48	THR	3.1
51	1t	14	LYS	3.1
52	2u	3	LYS	3.1
32	1a	1354	C	3.1
32	2a	1037	C	3.1
32	2a	1262	C	3.1
34	2c	190	ARG	3.1
11	1P	105	LEU	3.1
33	2b	55	PHE	3.1
34	1c	52	LEU	3.1
34	2c	80	GLY	3.1
43	1l	60	LEU	3.1
39	1h	134	ILE	3.1
52	2u	16	GLY	3.1
8	1I	19	VAL	3.1

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
10	2O	98	VAL	3.1
33	2b	234	PRO	3.1
20	1Y	92	ASN	3.1
34	2c	60	ALA	3.1
36	1e	86	ALA	3.1
40	2i	76	ALA	3.1
26	14	69	LYS	3.1
32	1a	152	A	3.1
32	1a	1503	A	3.1
47	1p	43	LYS	3.1
50	2s	70	LYS	3.1
6	1G	51	ARG	3.1
14	2S	36	TYR	3.1
33	2b	92	TYR	3.1
40	2i	42	ARG	3.1
52	1u	24	ARG	3.1
32	2a	1277	C	3.1
34	2c	167	TRP	3.1
1	1A	927	G	3.0
1	1A	930	G	3.0
32	1a	346	G	3.0
32	2a	1215	G	3.0
32	2a	1356	G	3.0
35	1d	176	LEU	3.0
40	2i	56	LEU	3.0
6	2G	39	ILE	3.0
34	2c	158	GLY	3.0
36	1e	85	GLY	3.0
40	2i	100	GLY	3.0
41	2j	63	PHE	3.0
50	2s	26	GLY	3.0
26	24	50	VAL	3.0
32	2a	1196	U	3.0
33	2b	112	VAL	3.0
43	2l	18	VAL	3.0
10	1O	108	GLU	3.0
45	1n	59	ALA	3.0
6	2G	161	THR	3.0
36	2e	107	ARG	3.0
1	1A	302	A	3.0
1	2A	2310	A	3.0
33	2b	192	SER	3.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
21	2Z	125	LEU	3.0
41	1j	85	LEU	3.0
32	2a	1128	C	3.0
21	2Z	53	ILE	3.0
33	2b	57	PHE	3.0
34	1c	10	PHE	3.0
41	2j	52	GLY	3.0
41	2j	82	ILE	3.0
1	1A	2187	G	3.0
1	2A	2156	G	3.0
1	2A	2793	G	3.0
32	2a	1002	G	3.0
32	2a	1221	G	3.0
36	2e	5	ASP	3.0
21	2Z	138	GLU	3.0
35	1d	150	GLU	3.0
40	2i	12	GLU	3.0
41	2j	44	VAL	3.0
51	1t	75	ASN	3.0
45	2n	41	ARG	3.0
14	1S	84	GLN	3.0
44	2m	37	THR	3.0
46	1o	69	TYR	3.0
47	2p	38	TYR	3.0
50	2s	61	TYR	3.0
32	1a	1030(D)	A	3.0
32	2a	949	A	3.0
32	2a	1151	A	3.0
5	2F	208	GLY	3.0
6	2G	102	PHE	3.0
23	21	84	GLY	3.0
34	1c	84	ILE	3.0
34	2c	148	GLY	3.0
37	1f	60	PHE	3.0
38	1g	50	ILE	3.0
45	2n	16	PHE	3.0
32	2a	866	C	3.0
52	2u	23	PRO	3.0
1	2A	545	G	3.0
32	2a	1001(A)	G	3.0
32	2a	1117	G	3.0
33	1b	237	ALA	3.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
34	2c	180	ALA	3.0
38	1g	153	HIS	3.0
41	2j	76	ASN	3.0
45	2n	59	ALA	3.0
54	2w	15	G	3.0
55	1x	70	G	3.0
6	2G	41	GLN	3.0
35	1d	181	MET	3.0
6	2G	19	LEU	3.0
6	2G	43	LEU	3.0
33	2b	121	LEU	3.0
50	2s	30	LEU	3.0
1	1A	1119	A	3.0
1	2A	2126	A	3.0
34	2c	57	ILE	3.0
41	1j	6	ILE	3.0
33	1b	106	LYS	3.0
21	2Z	167	PRO	3.0
11	1P	119	GLU	3.0
33	2b	141	GLU	3.0
47	1p	68	ASP	3.0
1	1A	943	C	3.0
7	2H	37	VAL	3.0
40	1i	10	ARG	3.0
32	2a	1129	C	3.0
12	2Q	136	ALA	3.0
14	2S	61	ASN	3.0
44	1m	123	ALA	3.0
36	2e	10	MET	3.0
47	1p	1	MET	3.0
1	1A	1072	U	3.0
1	2A	1026	U	3.0
1	1A	1101	G	3.0
32	2a	1031	G	3.0
32	2a	1190	G	3.0
32	2a	1202	G	3.0
32	2a	1255	G	3.0
40	2i	79	LEU	2.9
44	2m	70	LEU	2.9
41	2j	19	SER	2.9
6	2G	20	ILE	2.9
6	2G	24	GLY	2.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
34	2c	194	GLY	2.9
45	2n	42	ILE	2.9
1	2A	2169	A	2.9
6	2G	2	PRO	2.9
6	2G	87	PRO	2.9
17	2V	50	PRO	2.9
32	2a	1213	A	2.9
32	2a	1280	A	2.9
53	1v	13	A	2.9
23	2l	83	GLU	2.9
26	14	55	ARG	2.9
30	18	65	GLU	2.9
33	2b	93	VAL	2.9
41	2j	34	VAL	2.9
42	2k	114	VAL	2.9
26	24	47	GLN	2.9
40	2i	122	ALA	2.9
42	2k	19	ALA	2.9
32	1a	1119	C	2.9
32	2a	990	C	2.9
41	2j	15	THR	2.9
1	2A	2132	U	2.9
33	2b	154	LEU	2.9
34	2c	32	LEU	2.9
34	2c	204	LEU	2.9
39	1h	112	LEU	2.9
40	1i	102	LEU	2.9
6	1G	75	LYS	2.9
1	2A	1171	G	2.9
22	20	26	TYR	2.9
32	1a	1031	G	2.9
32	2a	1156	G	2.9
54	2w	18	G	2.9
34	2c	145	GLY	2.9
44	2m	119	GLY	2.9
7	2H	6	ARG	2.9
14	1S	3	ARG	2.9
44	2m	94	ARG	2.9
25	23	60	GLU	2.9
26	14	57	GLU	2.9
33	1b	126	GLU	2.9
47	1p	48	TRP	2.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	1A	945	A	2.9
1	1A	2180	A	2.9
32	2a	1004	A	2.9
32	2a	1016	A	2.9
34	2c	130	VAL	2.9
41	2j	86	MET	2.9
42	1k	14	VAL	2.9
50	1s	9	VAL	2.9
3	2D	2	ALA	2.9
12	2Q	28	ALA	2.9
54	2w	72	C	2.9
1	1A	1129	U	2.9
50	2s	16	LEU	2.9
33	1b	200	ILE	2.9
33	2b	172	ILE	2.9
36	2e	131	ILE	2.9
35	1d	180	GLY	2.9
43	2l	50	SER	2.9
12	2Q	104	PHE	2.9
40	2i	59	PHE	2.9
6	2G	32	PRO	2.9
6	2G	118	ARG	2.9
46	2o	19	PRO	2.9
1	2A	2154	G	2.9
47	1p	16	HIS	2.9
54	1y	19	G	2.9
21	2Z	141	VAL	2.9
33	2b	7	VAL	2.9
34	2c	18	TRP	2.9
34	2c	70	VAL	2.9
36	2e	67	VAL	2.9
32	1a	101	A	2.9
41	1j	78	ASN	2.9
52	2u	17	THR	2.9
8	2I	38	LEU	2.9
14	2S	32	LEU	2.9
33	2b	158	LEU	2.9
39	2h	127	LEU	2.9
1	1A	1122	C	2.9
1	1A	2196	C	2.9
1	2A	2137	C	2.9
1	2A	2146	C	2.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	2A	2150	U	2.9
1	2A	2297	C	2.9
2	2B	88	C	2.9
6	2G	140	ILE	2.9
32	1a	150	C	2.9
32	2a	950	U	2.9
33	2b	211	ILE	2.9
41	1j	98	ILE	2.9
52	2u	13	ILE	2.9
54	1y	48	C	2.9
54	2w	4	C	2.9
21	2Z	99	TYR	2.9
21	2Z	166	SER	2.9
34	1c	25	GLY	2.9
34	1c	185	GLY	2.9
34	2c	10	PHE	2.9
35	1d	110	PHE	2.9
38	1g	32	ARG	2.9
50	2s	4	SER	2.9
45	2n	8	GLU	2.9
38	2g	86	GLN	2.9
6	2G	92	VAL	2.9
35	1d	170	VAL	2.9
44	2m	7	VAL	2.9
1	1A	2134	G	2.9
1	1A	2816	G	2.9
21	2Z	164	ALA	2.9
36	1e	95	ALA	2.9
40	2i	84	ALA	2.9
42	2k	89	ALA	2.9
45	2n	10	ALA	2.9
49	1r	24	ALA	2.9
40	2i	64	THR	2.9
44	2m	103	THR	2.9
32	2a	965	A	2.8
32	2a	1001	A	2.8
32	2a	1250	A	2.8
44	2m	34	LEU	2.8
33	2b	32	ILE	2.8
34	1c	14	ILE	2.8
11	2P	118	GLY	2.8
12	2Q	23	GLY	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
18	2W	112	GLY	2.8
41	2j	9	ARG	2.8
26	24	29	PRO	2.8
32	2a	1040	U	2.8
32	2a	1532	U	2.8
26	24	66	SER	2.8
35	2d	37	PRO	2.8
34	1c	201	TYR	2.8
34	2c	6	HIS	2.8
38	2g	77	SER	2.8
41	2j	77	PRO	2.8
32	2a	970	C	2.8
32	2a	1029	C	2.8
32	2a	1109	C	2.8
32	2a	1112	C	2.8
51	1t	70	SER	2.8
54	1w	2	C	2.8
55	1x	69	C	2.8
7	2H	24	VAL	2.8
8	2I	92	VAL	2.8
14	2S	28	VAL	2.8
21	2Z	90	VAL	2.8
50	2s	45	VAL	2.8
22	20	71	ASP	2.8
39	2h	64	LYS	2.8
41	2j	18	ALA	2.8
1	2A	2115	G	2.8
32	1a	306	G	2.8
32	2a	1061	G	2.8
33	1b	221	LEU	2.8
46	1o	66	LEU	2.8
54	2y	5	G	2.8
32	2a	1130	A	2.8
38	2g	32	ARG	2.8
41	1j	74	ILE	2.8
41	2j	5	ARG	2.8
45	1n	57	ARG	2.8
42	2k	125	PHE	2.8
47	1p	80	PHE	2.8
47	2p	9	PHE	2.8
50	2s	83	HIS	2.8
1	1A	2194	U	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
32	2a	952	U	2.8
32	2a	992	U	2.8
36	1e	81	GLU	2.8
54	1y	47	U	2.8
1	1A	34	C	2.8
32	2a	1054	C	2.8
32	2a	1118	C	2.8
32	2a	1217	C	2.8
21	2Z	78	LYS	2.8
21	2Z	96	VAL	2.8
34	2c	4	LYS	2.8
34	2c	66	VAL	2.8
34	2c	75	VAL	2.8
34	2c	199	LYS	2.8
51	1t	74	LYS	2.8
7	2H	145	ALA	2.8
21	2Z	87	ASP	2.8
33	2b	225	ALA	2.8
36	2e	54	ALA	2.8
42	2k	23	ALA	2.8
35	2d	47	ARG	2.8
41	2j	70	ARG	2.8
1	2A	881	G	2.8
2	2B	24	G	2.8
15	2T	52	ILE	2.8
32	1a	183	G	2.8
32	2a	630	G	2.8
32	2a	1108	G	2.8
32	2a	1171	G	2.8
32	2a	1181	G	2.8
36	1e	13	ILE	2.8
54	1w	69	G	2.8
54	1w	71	G	2.8
54	2w	19	G	2.8
21	1Z	160	GLY	2.8
35	2d	23	GLY	2.8
36	2e	78	HIS	2.8
36	2e	114	GLY	2.8
2	2B	120	A	2.8
32	2a	969	A	2.8
32	2a	1014	A	2.8
32	2a	1261	A	2.8

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
33	2b	70	PHE	2.8
34	2c	186	PHE	2.8
21	2Z	16	SER	2.8
1	2A	271(L)	U	2.8
1	2A	2113	U	2.8
32	2a	1148	U	2.8
51	1t	18	GLN	2.8
54	2y	33	U	2.8
9	2N	118	LYS	2.8
40	2i	70	LYS	2.8
44	1m	27	LYS	2.8
7	2H	35	VAL	2.8
46	2o	27	VAL	2.8
32	1a	1029	C	2.8
32	2a	1214	C	2.8
32	2a	1223	C	2.8
33	2b	171	ALA	2.8
44	2m	76	ALA	2.8
54	2w	13	C	2.8
34	2c	87	LEU	2.8
36	2e	71	LEU	2.8
36	2e	123	LEU	2.8
45	2n	47	LEU	2.8
48	2q	84	LEU	2.8
33	2b	54	THR	2.8
33	2b	94	ASN	2.8
34	1c	15	THR	2.8
34	2c	3	ASN	2.8
41	1j	46	ARG	2.8
6	1G	88	ILE	2.8
8	2I	88	ILE	2.8
38	2g	27	ILE	2.8
31	29	20	HIS	2.8
21	2Z	143	GLY	2.8
36	2e	99	GLY	2.8
41	1j	77	PRO	2.8
52	2u	2	GLY	2.8
6	2G	48	GLU	2.8
12	2Q	65	PHE	2.8
33	1b	70	PHE	2.8
33	2b	17	PHE	2.8
41	1j	47	PHE	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	1A	2176	G	2.8
32	2a	1030(C)	G	2.8
1	2A	652(B)	A	2.8
32	2a	1275	A	2.8
34	2c	147	LYS	2.8
32	2a	1078	U	2.8
34	1c	48	TYR	2.8
54	1w	20	U	2.8
21	2Z	126	VAL	2.8
35	1d	105	VAL	2.8
8	2I	146	ALA	2.8
35	1d	111	ALA	2.8
11	2P	105	LEU	2.7
21	2Z	102	LEU	2.7
26	14	51	ASP	2.7
33	2b	221	LEU	2.7
1	1A	944	C	2.7
14	1S	13	ARG	2.7
32	1a	1533	C	2.7
32	2a	1189	C	2.7
32	2a	1321	C	2.7
32	2a	1322	C	2.7
40	2i	93	ARG	2.7
40	2i	128	ARG	2.7
41	2j	66	ARG	2.7
21	2Z	98	MET	2.7
45	2n	54	PRO	2.7
14	1S	22	GLY	2.7
21	2Z	84	GLU	2.7
33	1b	227	GLY	2.7
50	2s	8	GLY	2.7
50	2s	72	GLY	2.7
50	2s	18	LYS	2.7
1	1A	2155	G	2.7
1	2A	887	A	2.7
1	2A	2125	G	2.7
2	2B	25	A	2.7
2	2B	119	G	2.7
32	1a	1032	G	2.7
32	2a	1088	G	2.7
32	2a	1131	G	2.7
36	2e	90	VAL	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
38	2g	151	TYR	2.7
54	1y	15	G	2.7
1	1A	2154	U	2.7
39	2h	93	VAL	2.7
54	2w	66	U	2.7
6	2G	133	LEU	2.7
41	1j	8	LEU	2.7
50	2s	5	LEU	2.7
34	2c	62	ASP	2.7
35	2d	35	ARG	2.7
1	1A	1555	C	2.7
1	1A	2815	C	2.7
32	1a	345	C	2.7
35	2d	29	PRO	2.7
39	2h	35	ILE	2.7
54	2w	67	C	2.7
33	2b	132	LYS	2.7
45	2n	17	LYS	2.7
45	2n	50	LYS	2.7
51	2t	96	GLY	2.7
36	2e	6	PHE	2.7
45	2n	37	PHE	2.7
7	1H	113	VAL	2.7
12	2Q	106	VAL	2.7
36	2e	100	VAL	2.7
39	2h	53	VAL	2.7
39	2h	137	VAL	2.7
40	1i	4	TYR	2.7
47	1p	2	VAL	2.7
47	2p	20	VAL	2.7
48	2q	56	VAL	2.7
6	2G	61	ALA	2.7
11	1P	106	LEU	2.7
33	2b	138	LEU	2.7
34	2c	160	ALA	2.7
40	2i	43	ALA	2.7
45	2n	24	CYS	2.7
49	2r	40	LEU	2.7
50	1s	5	LEU	2.7
26	14	68	ARG	2.7
32	1a	149	A	2.7
32	1a	161	A	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
32	1a	1286	A	2.7
32	2a	1205	U	2.7
32	2a	1358	U	2.7
51	1t	8	ARG	2.7
1	1A	929	G	2.7
1	1A	2147	G	2.7
1	1A	2184	G	2.7
2	2B	118	G	2.7
21	2Z	154	ASP	2.7
32	2a	1047	G	2.7
32	2a	1120	G	2.7
54	2y	15	G	2.7
26	24	44	THR	2.7
34	2c	192	THR	2.7
6	1G	77	ILE	2.7
21	2Z	15	PRO	2.7
47	1p	19	ILE	2.7
50	2s	42	PRO	2.7
12	2Q	139	GLU	2.7
21	2Z	106	GLY	2.7
26	24	17	GLY	2.7
33	2b	97	TRP	2.7
34	2c	19	GLU	2.7
35	2d	192	GLU	2.7
44	1m	26	GLY	2.7
1	2A	888	C	2.7
26	24	42	PHE	2.7
48	2q	99	SER	2.7
50	2s	38	SER	2.7
6	2G	109	VAL	2.7
7	1H	45	VAL	2.7
7	2H	79	VAL	2.7
14	2S	49	VAL	2.7
14	2S	65	VAL	2.7
21	2Z	128	VAL	2.7
42	2k	14	VAL	2.7
6	2G	115	ARG	2.7
33	2b	142	LEU	2.7
34	1c	178	LEU	2.7
35	1d	162	LEU	2.7
35	2d	122	ARG	2.7
40	1i	19	LEU	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>
40	2i	40	LEU	2.7
36	2e	21	ALA	2.7
40	1i	55	ALA	2.7
40	2i	119	ALA	2.7
48	1q	95	TYR	2.7
50	1s	24	ALA	2.7
32	2a	1125	U	2.7
1	1A	925	A	2.7
1	2A	2114	A	2.7
26	24	40	HIS	2.7
32	2a	1152	A	2.7
47	1p	69	THR	2.7
50	1s	14	HIS	2.7
3	1D	38	LYS	2.7
34	2c	150	LYS	2.7
35	1d	154	ASN	2.7
36	1e	118	ILE	2.7
38	2g	37	ASN	2.7
39	2h	32	LYS	2.7
1	1A	2228	G	2.7
32	2a	987	G	2.7
41	2j	53	PRO	2.7
54	1y	24	G	2.7
41	2j	93	GLY	2.7
41	2j	84	GLN	2.7
1	1A	1098	C	2.7
1	2A	2139	C	2.7
1	2A	2174	C	2.7
1	2A	2313	C	2.7
2	2B	27	C	2.7
32	2a	1027	C	2.7
32	2a	1113	C	2.7
32	2a	1254	C	2.7
54	1w	13	C	2.7
6	2G	62	LEU	2.6
7	2H	7	LEU	2.6
11	1P	100	LEU	2.6
26	24	9	LEU	2.6
29	17	46	VAL	2.6
38	1g	5	ARG	2.6
38	1g	10	ARG	2.6
6	2G	163	ALA	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
38	1g	154	TYR	2.6
18	2W	111	HIS	2.6
33	2b	60	ASP	2.6
40	2i	95	LYS	2.6
50	2s	28	LYS	2.6
1	1A	1220	U	2.6
1	1A	2166	U	2.6
6	2G	52	ILE	2.6
21	2Z	130	PRO	2.6
42	2k	117	ASN	2.6
1	1A	1149	A	2.6
12	2Q	33	GLY	2.6
45	2n	51	GLY	2.6
14	2S	68	GLN	2.6
1	1A	11	G	2.6
22	20	45	PHE	2.6
32	2a	951	G	2.6
32	2a	1032	G	2.6
32	2a	1276	G	2.6
36	2e	84	PHE	2.6
46	2o	15	PHE	2.6
54	1w	6	G	2.6
21	2Z	81	ARG	2.6
42	1k	126	ARG	2.6
32	2a	985	C	2.6
33	1b	158	LEU	2.6
34	1c	32	LEU	2.6
41	1j	71	LEU	2.6
11	1P	83	VAL	2.6
33	1b	136	VAL	2.6
43	1l	18	VAL	2.6
8	2I	53	ALA	2.6
34	1c	53	ALA	2.6
33	1b	27	LYS	2.6
21	2Z	8	TYR	2.6
38	2g	154	TYR	2.6
42	1k	75	TYR	2.6
47	1p	38	TYR	2.6
21	2Z	140	ASP	2.6
33	2b	223	ILE	2.6
35	1d	189	PRO	2.6
36	2e	135	THR	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
39	2h	4	ASP	2.6
40	2i	32	ASP	2.6
33	2b	58	ILE	2.6
1	1A	2189	U	2.6
32	2a	982	U	2.6
32	2a	1121	U	2.6
33	1b	128	GLU	2.6
4	2E	10	GLY	2.6
1	1A	1113	A	2.6
1	1A	2192	A	2.6
32	2a	959	A	2.6
34	1c	128	PHE	2.6
48	1q	71	PHE	2.6
54	2y	14	A	2.6
34	1c	18	TRP	2.6
6	2G	83	ARG	2.6
15	1T	125	ARG	2.6
29	17	47	ARG	2.6
1	1A	2153	G	2.6
1	2A	2153	G	2.6
1	2A	2319	G	2.6
32	2a	963	G	2.6
32	2a	1089	G	2.6
33	1b	187	LEU	2.6
33	2b	44	LEU	2.6
47	2p	6	LEU	2.6
49	1r	79	LEU	2.6
7	2H	49	VAL	2.6
35	1d	88	VAL	2.6
40	1i	41	VAL	2.6
43	1l	40	VAL	2.6
43	2l	39	VAL	2.6
50	2s	19	VAL	2.6
40	2i	112	LYS	2.6
45	2n	4	LYS	2.6
1	1A	1908	C	2.6
6	2G	151	ALA	2.6
21	1Z	151	HIS	2.6
32	2a	1282	C	2.6
32	2a	1362	C	2.6
33	2b	29	ALA	2.6
35	2d	164	ALA	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
54	1y	13	C	2.6
26	24	25	TYR	2.6
6	2G	49	ASP	2.6
7	2H	128	PRO	2.6
36	2e	60	TYR	2.6
39	2h	67	PRO	2.6
40	2i	114	TYR	2.6
40	1i	75	ASP	2.6
40	2i	75	ASP	2.6
51	2t	98	PRO	2.6
6	2G	101	ILE	2.6
8	2I	86	THR	2.6
33	1b	190	THR	2.6
41	2j	6	ILE	2.6
50	1s	48	THR	2.6
51	1t	100	ILE	2.6
1	1A	12	U	2.6
1	2A	2118	U	2.6
32	2a	1364	U	2.6
33	2b	66	GLY	2.6
35	2d	45	GLN	2.6
33	1b	163	PHE	2.6
33	2b	105	PHE	2.6
7	2H	41	MET	2.6
15	1T	111	ARG	2.6
41	2j	46	ARG	2.6
41	2j	51	ARG	2.6
32	1a	228	A	2.6
33	1b	10	LEU	2.6
33	1b	11	LEU	2.6
33	2b	215	LEU	2.6
36	2e	142	LEU	2.6
41	1j	65	LEU	2.6
47	2p	74	LEU	2.6
29	27	48	LYS	2.6
34	2c	72	LYS	2.6
42	2k	124	LYS	2.6
48	1q	100	LYS	2.6
8	2I	144	VAL	2.6
33	2b	229	VAL	2.6
36	2e	51	VAL	2.6
44	2m	74	VAL	2.6

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
48	2q	23	VAL	2.6
50	1s	67	VAL	2.6
6	2G	110	ALA	2.6
21	2Z	152	ALA	2.6
22	20	3	HIS	2.6
29	17	45	ALA	2.6
32	2a	947	G	2.6
32	2a	1042	G	2.6
32	2a	1094	G	2.6
34	2c	163	ALA	2.6
38	2g	83	ALA	2.6
39	1h	7	ALA	2.6
54	1w	44	G	2.6
54	2w	70	G	2.6
5	2F	14	PRO	2.6
41	2j	91	PRO	2.6
1	2A	2164	C	2.6
32	1a	153	C	2.6
32	2a	1039	C	2.6
32	2a	1354	C	2.6
32	2a	1384	C	2.6
8	2I	117	GLU	2.6
21	1Z	69	THR	2.6
21	1Z	169	GLU	2.6
33	2b	12	GLU	2.6
33	2b	80	ILE	2.6
34	1c	56	ASP	2.6
35	1d	179	GLU	2.6
43	1l	7	ILE	2.6
47	1p	4	ILE	2.6
35	1d	87	GLY	2.6
36	1e	72	GLN	2.6
1	1A	2211	U	2.6
32	1a	182	U	2.6
32	1a	1040	U	2.6
54	1w	66	U	2.6
21	2Z	131	ARG	2.6
26	24	58	ARG	2.6
35	2d	115	ARG	2.6
39	2h	104	ARG	2.6
47	1p	5	ARG	2.6
6	2G	34	LEU	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
8	1I	140	LEU	2.5
11	2P	106	LEU	2.5
21	2Z	156	LYS	2.5
33	1b	132	LYS	2.5
35	1d	135	LEU	2.5
45	2n	9	LYS	2.5
48	2q	76	LEU	2.5
38	2g	156	TRP	2.5
32	2a	10	A	2.5
32	2a	1225	A	2.5
32	2a	1363(A)	A	2.5
54	1y	36	A	2.5
33	1b	7	VAL	2.5
35	2d	105	VAL	2.5
38	2g	9	VAL	2.5
50	1s	11	VAL	2.5
36	1e	94	ALA	2.5
36	2e	95	ALA	2.5
38	2g	108	ALA	2.5
44	2m	75	ALA	2.5
24	22	66	GLU	2.5
39	2h	134	ILE	2.5
44	1m	4	ILE	2.5
1	1A	926	G	2.5
1	2A	2206	G	2.5
6	2G	156	ASP	2.5
14	2S	7	TYR	2.5
32	2a	1050	G	2.5
32	2a	1253	G	2.5
34	2c	17	ASP	2.5
1	2A	2111	C	2.5
32	2a	1028	C	2.5
40	2i	69	GLY	2.5
41	1j	76	ASN	2.5
50	2s	23	ASN	2.5
50	2s	53	ASN	2.5
54	1y	56	C	2.5
7	2H	60	ARG	2.5
33	2b	63	MET	2.5
33	2b	217	ARG	2.5
35	2d	168	ARG	2.5
44	2m	82	MET	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	2A	2144	U	2.5
32	1a	560	U	2.5
6	2G	175	LEU	2.5
14	2S	26	LEU	2.5
19	1X	92	LEU	2.5
35	2d	21	LEU	2.5
46	1o	57	LEU	2.5
21	1Z	121	HIS	2.5
1	1A	2901	A	2.5
32	1a	472	A	2.5
32	1a	609	A	2.5
38	1g	7	ALA	2.5
44	2m	33	ALA	2.5
6	1G	137	GLU	2.5
21	2Z	13	GLU	2.5
22	20	68	GLU	2.5
33	1b	12	GLU	2.5
33	2b	42	ILE	2.5
51	1t	55	ILE	2.5
12	2Q	25	ASP	2.5
33	1b	95	GLN	2.5
33	2b	103	THR	2.5
33	2b	168	THR	2.5
34	2c	15	THR	2.5
41	2j	67	THR	2.5
17	2V	65	GLY	2.5
33	1b	18	GLY	2.5
36	2e	29	GLY	2.5
46	1o	89	GLY	2.5
50	1s	26	GLY	2.5
20	1Y	2	ARG	2.5
30	28	46	ARG	2.5
36	2e	126	ARG	2.5
40	2i	111	ARG	2.5
41	1j	66	ARG	2.5
47	1p	25	ARG	2.5
49	2r	53	ARG	2.5
1	2A	2751	G	2.5
6	2G	141	PHE	2.5
12	2Q	58	PHE	2.5
32	2a	1178	G	2.5
32	2a	1283	G	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
33	2b	147	LYS	2.5
54	2w	5	G	2.5
1	1A	270	C	2.5
1	1A	2133	C	2.5
1	1A	2183	C	2.5
1	2A	2794	C	2.5
2	2B	3	C	2.5
55	1x	68	C	2.5
5	2F	24	LEU	2.5
6	2G	172	LEU	2.5
34	2c	42	LEU	2.5
40	1i	56	LEU	2.5
49	1r	31	LEU	2.5
18	1W	111	HIS	2.5
6	1G	5	VAL	2.5
8	2I	142	VAL	2.5
40	1i	86	VAL	2.5
6	1G	76	SER	2.5
6	2G	73	ALA	2.5
21	2Z	129	SER	2.5
34	1c	60	ALA	2.5
34	2c	20	SER	2.5
36	2e	138	ALA	2.5
44	2m	18	ALA	2.5
47	1p	41	PRO	2.5
4	1E	73	GLU	2.5
28	16	4	GLU	2.5
34	2c	152	ILE	2.5
36	2e	7	GLU	2.5
1	2A	2158	A	2.5
32	2a	1179	A	2.5
8	2I	54	GLN	2.5
50	1s	39	THR	2.5
52	1u	17	THR	2.5
7	2H	82	GLY	2.5
33	2b	203	GLY	2.5
40	1i	66	ARG	2.5
44	2m	114	ARG	2.5
45	2n	26	ARG	2.5
33	2b	37	ASN	2.5
40	2i	116	LYS	2.5
40	2i	127	LYS	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
6	2G	139	LEU	2.5
21	2Z	76	LEU	2.5
21	2Z	91	LEU	2.5
33	1b	61	LEU	2.5
38	1g	16	LEU	2.5
48	2q	98	LEU	2.5
51	1t	24	LEU	2.5
51	2t	10	LEU	2.5
1	1A	1117	G	2.5
1	1A	2188	G	2.5
1	2A	2145	C	2.5
1	2A	2165	G	2.5
2	1B	88	C	2.5
32	1a	230	G	2.5
32	2a	1009	G	2.5
32	2a	1069	C	2.5
32	2a	1161	C	2.5
32	1a	1020	U	2.5
32	2a	1159	U	2.5
32	2a	1235	U	2.5
6	2G	149	VAL	2.5
39	2h	51	VAL	2.5
49	2r	22	VAL	2.5
12	2Q	53	ALA	2.5
21	1Z	152	ALA	2.5
34	2c	61	ALA	2.5
51	2t	97	ALA	2.5
52	1u	14	TRP	2.5
21	1Z	166	SER	2.5
35	1d	71	SER	2.5
8	2I	109	ILE	2.5
11	1P	117	GLU	2.5
17	1V	43	GLU	2.5
34	1c	5	ILE	2.5
41	1j	83	GLU	2.5
50	2s	49	ILE	2.5
14	2S	38	GLN	2.5
6	2G	91	ARG	2.5
6	2G	93	THR	2.5
6	2G	99	MET	2.5
12	2Q	56	ARG	2.5
14	1S	20	ARG	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
29	17	23	ARG	2.5
30	18	46	ARG	2.5
36	2e	27	ARG	2.5
20	1Y	107	ASP	2.5
21	2Z	64	GLY	2.5
35	1d	16	GLY	2.5
38	2g	133	GLY	2.5
45	2n	11	LYS	2.5
51	1t	68	LYS	2.5
32	2a	986	A	2.5
32	2a	1105	A	2.5
21	2Z	38	TYR	2.5
40	2i	33	PHE	2.5
43	2l	32	PHE	2.5
6	1G	53	LEU	2.4
6	1G	152	LEU	2.4
9	1N	138	LEU	2.4
21	2Z	155	LEU	2.4
36	2e	112	LEU	2.4
44	2m	48	LEU	2.4
51	1t	10	LEU	2.4
21	2Z	54	HIS	2.4
1	1A	2124	U	2.4
1	2A	897	C	2.4
2	2B	1	U	2.4
34	1c	151	VAL	2.4
38	1g	9	VAL	2.4
48	2q	10	VAL	2.4
32	1a	226	G	2.4
54	1y	20	U	2.4
39	2h	89	PRO	2.4
12	2Q	49	ALA	2.4
44	2m	28	ALA	2.4
20	2Y	44	ILE	2.4
35	2d	158	ILE	2.4
35	2d	165	MET	2.4
39	1h	70	GLN	2.4
44	2m	101	GLN	2.4
14	2S	13	ARG	2.4
38	2g	6	ARG	2.4
40	2i	97	LYS	2.4
43	2l	47	LYS	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
22	20	6	GLY	2.4
26	24	64	GLY	2.4
38	1g	34	GLY	2.4
40	1i	67	GLY	2.4
46	2o	20	GLY	2.4
14	1S	16	ASN	2.4
6	1G	25	TYR	2.4
7	1H	7	LEU	2.4
7	2H	157	TYR	2.4
14	2S	110	LEU	2.4
21	2Z	9	TYR	2.4
21	2Z	70	LEU	2.4
21	2Z	88	PHE	2.4
34	2c	193	TYR	2.4
38	1g	26	PHE	2.4
43	2l	49	ASN	2.4
33	1b	33	TYR	2.4
33	1b	213	LEU	2.4
39	2h	58	TYR	2.4
50	1s	15	LEU	2.4
54	1w	7	A	2.4
34	1c	55	VAL	2.4
34	2c	174	PRO	2.4
35	2d	88	VAL	2.4
40	2i	123	PRO	2.4
22	20	2	ALA	2.4
32	2a	1020	U	2.4
32	2a	1070	U	2.4
33	2b	170	GLU	2.4
34	2c	44	GLU	2.4
34	2c	92	ALA	2.4
38	1g	83	ALA	2.4
1	1A	940	C	2.4
14	2S	40	ILE	2.4
24	22	70	GLN	2.4
32	2a	972	C	2.4
34	1c	124	ILE	2.4
34	2c	135	LYS	2.4
36	2e	66	MET	2.4
50	2s	7	LYS	2.4
1	1A	2143	G	2.4
1	1A	2190	G	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	2A	2110	G	2.4
1	2A	2168	G	2.4
32	1a	1009	G	2.4
7	2H	106	THR	2.4
12	2Q	19	GLY	2.4
40	1i	39	GLY	2.4
40	2i	68	GLY	2.4
41	2j	31	GLY	2.4
48	2q	7	THR	2.4
49	2r	47	THR	2.4
50	2s	77	THR	2.4
6	2G	97	ASP	2.4
37	1f	55	ASP	2.4
40	1i	105	ASP	2.4
41	2j	17	ASP	2.4
6	2G	27	ASN	2.4
21	2Z	24	LEU	2.4
33	1b	28	PHE	2.4
35	1d	78	LEU	2.4
38	1g	12	LEU	2.4
38	1g	84	ASN	2.4
41	1j	90	LEU	2.4
51	2t	99	LEU	2.4
39	2h	82	HIS	2.4
1	1A	1132	A	2.4
1	1A	2641	A	2.4
1	2A	899	A	2.4
1	2A	2134	A	2.4
2	2B	58	A	2.4
32	2a	958	A	2.4
32	2a	1005	A	2.4
32	2a	1201	A	2.4
32	2a	1289	A	2.4
5	2F	6	VAL	2.4
6	2G	37	VAL	2.4
20	2Y	45	VAL	2.4
21	1Z	100	VAL	2.4
26	14	10	VAL	2.4
35	2d	121	VAL	2.4
39	2h	101	PRO	2.4
44	2m	41	PRO	2.4
44	2m	45	VAL	2.4

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
45	2n	56	VAL	2.4
4	1E	28	ALA	2.4
23	21	81	LYS	2.4
33	2b	129	GLU	2.4
33	2b	186	ALA	2.4
33	2b	188	ALA	2.4
34	2c	131	ARG	2.4
34	2c	133	ALA	2.4
40	2i	110	GLU	2.4
41	1j	29	ARG	2.4
45	1n	20	ALA	2.4
33	1b	39	ILE	2.4
35	1d	158	ILE	2.4
48	1q	68	ARG	2.4
32	1a	203	U	2.4
1	1A	2150	C	2.4
6	1G	29	TRP	2.4
32	2a	1325	C	2.4
39	2h	138	TRP	2.4
17	1V	101	GLY	2.4
33	1b	38	GLY	2.4
33	2b	107	THR	2.4
38	1g	132	GLY	2.4
40	1i	8	GLY	2.4
43	2l	63	GLY	2.4
43	2l	72	GLY	2.4
1	1A	928	G	2.4
1	2A	2308	G	2.4
3	2D	71	ASP	2.4
6	2G	120	LEU	2.4
7	2H	71	LEU	2.4
7	2H	171	LEU	2.4
10	2O	81	ASP	2.4
32	1a	1010	G	2.4
32	2a	631	G	2.4
32	2a	1355	G	2.4
34	2c	196	LEU	2.4
36	2e	36	ASP	2.4
49	2r	51	LEU	2.4
33	2b	204	ASN	2.4
38	1g	43	PHE	2.4
32	1a	140	A	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
32	2a	996	A	2.4
33	2b	159	PRO	2.4
34	2c	73	PRO	2.4
6	2G	31	VAL	2.4
20	1Y	7	VAL	2.4
21	1Z	105	VAL	2.4
33	2b	83	MET	2.4
33	2b	90	MET	2.4
34	1c	86	VAL	2.4
36	1e	67	VAL	2.4
37	1f	54	LYS	2.4
21	2Z	79	ARG	2.4
26	24	53	GLU	2.4
34	2c	119	ARG	2.4
43	1l	41	ARG	2.4
44	2m	29	ARG	2.4
47	1p	75	ARG	2.4
21	2Z	65	GLN	2.4
39	2h	70	GLN	2.4
42	1k	74	ALA	2.4
47	1p	64	ALA	2.4
1	1A	274	U	2.4
32	2a	961	U	2.4
36	2e	125	SER	2.4
6	2G	100	TRP	2.4
26	24	45	GLY	2.4
26	24	52	THR	2.4
33	1b	24	TRP	2.4
33	2b	24	TRP	2.4
36	1e	29	GLY	2.4
44	1m	49	THR	2.4
44	1m	109	THR	2.4
45	2n	22	THR	2.4
46	2o	89	GLY	2.4
48	2q	80	GLY	2.4
1	1A	2159	C	2.3
8	1I	72	LEU	2.3
32	1a	63	C	2.3
32	1a	103	C	2.3
32	2a	984	C	2.3
32	2a	1060	C	2.3
36	1e	71	LEU	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
36	2e	139	LEU	2.3
40	2i	117	HIS	2.3
55	1x	67	C	2.3
8	2I	20	ASP	2.3
10	2O	99	PHE	2.3
20	2Y	89	PHE	2.3
21	2Z	34	ASN	2.3
35	2d	154	ASN	2.3
1	1A	299	G	2.3
1	2A	1533	G	2.3
14	2S	59	LYS	2.3
44	2m	31	LYS	2.3
45	2n	14	PRO	2.3
6	2G	38	VAL	2.3
8	1I	107	VAL	2.3
9	2N	9	VAL	2.3
11	1P	90	ARG	2.3
12	2Q	60	ARG	2.3
14	2S	46	VAL	2.3
33	1b	20	GLU	2.3
33	2b	130	ARG	2.3
34	2c	207	VAL	2.3
36	2e	25	ARG	2.3
39	2h	84	ARG	2.3
40	2i	26	VAL	2.3
43	2l	19	ARG	2.3
44	2m	69	GLU	2.3
45	2n	27	CYS	2.3
45	2n	46	GLU	2.3
1	2A	2320	A	2.3
2	2B	66	A	2.3
6	1G	26	GLN	2.3
8	1I	71	ILE	2.3
14	2S	72	ALA	2.3
32	2a	1180	A	2.3
33	1b	214	ILE	2.3
33	2b	41	ILE	2.3
34	1c	134	ILE	2.3
53	1v	14	A	2.3
7	2H	56	SER	2.3
39	2h	29	SER	2.3
11	2P	93	GLY	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
12	2Q	61	GLY	2.3
14	2S	45	GLY	2.3
14	2S	104	GLY	2.3
21	2Z	160	GLY	2.3
26	14	52	THR	2.3
32	2a	1062	U	2.3
32	2a	1232	U	2.3
32	2a	1315	U	2.3
4	1E	195	LEU	2.3
6	1G	43	LEU	2.3
14	2S	95	HIS	2.3
33	2b	113	HIS	2.3
33	2b	140	HIS	2.3
34	2c	175	LEU	2.3
35	1d	120	LEU	2.3
36	2e	43	LEU	2.3
36	2e	119	LEU	2.3
51	2t	24	LEU	2.3
6	2G	4	ASP	2.3
33	2b	195	ASP	2.3
36	1e	6	PHE	2.3
38	2g	26	PHE	2.3
44	2m	77	ASN	2.3
1	2A	2789	C	2.3
32	1a	174	C	2.3
32	1a	1039	C	2.3
32	2a	1192	C	2.3
32	2a	1244	C	2.3
54	2y	13	C	2.3
35	1d	166	LYS	2.3
48	1q	87	LYS	2.3
34	2c	184	TYR	2.3
44	2m	59	TYR	2.3
15	1T	129	ARG	2.3
22	20	74	ARG	2.3
1	1A	1584	G	2.3
1	2A	271(M)	G	2.3
1	2A	2131	G	2.3
6	2G	30	GLU	2.3
32	2a	1021	G	2.3
32	2a	1023	G	2.3
32	2a	1084	G	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
32	2a	1177	G	2.3
32	2a	1530	G	2.3
54	2w	34	G	2.3
7	2H	43	VAL	2.3
8	2I	17	GLN	2.3
34	1c	99	VAL	2.3
34	1c	170	GLN	2.3
36	2e	105	VAL	2.3
46	1o	71	GLN	2.3
50	2s	51	VAL	2.3
6	2G	171	ALA	2.3
31	29	17	ILE	2.3
33	1b	34	ALA	2.3
33	1b	225	ALA	2.3
33	2b	88	ALA	2.3
34	1c	57	ILE	2.3
40	2i	52	ALA	2.3
42	1k	89	ALA	2.3
50	2s	62	ILE	2.3
1	2A	878	A	2.3
1	2A	2171	A	2.3
32	2a	250	A	2.3
32	2a	1015	A	2.3
54	2y	21	A	2.3
26	24	4	GLY	2.3
41	1j	93	GLY	2.3
42	2k	102	GLY	2.3
6	2G	64	THR	2.3
8	1I	68	LEU	2.3
14	2S	80	LEU	2.3
21	2Z	85	HIS	2.3
34	2c	34	LEU	2.3
35	1d	188	LEU	2.3
39	2h	39	LEU	2.3
47	2p	69	THR	2.3
1	1A	2172	U	2.3
32	1a	723	U	2.3
32	2a	957	U	2.3
40	1i	18	PHE	2.3
33	1b	60	ASP	2.3
39	2h	15	ASN	2.3
42	1k	106	LYS	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
43	1l	47	LYS	2.3
1	1A	1118	C	2.3
1	1A	2130	C	2.3
1	1A	2151	C	2.3
1	1A	2168	C	2.3
1	2A	2138	C	2.3
14	1S	17	ARG	2.3
21	2Z	25	PRO	2.3
34	2c	7	PRO	2.3
34	2c	16	ARG	2.3
35	2d	73	ARG	2.3
35	2d	197	PRO	2.3
36	2e	18	ARG	2.3
36	2e	93	PRO	2.3
40	1i	90	PRO	2.3
45	2n	31	ARG	2.3
26	24	30	GLU	2.3
33	1b	236	TYR	2.3
33	2b	33	TYR	2.3
54	2w	56	C	2.3
39	2h	136	GLU	2.3
49	2r	46	GLU	2.3
21	2Z	71	VAL	2.3
33	1b	93	VAL	2.3
34	1c	70	VAL	2.3
47	2p	62	VAL	2.3
36	2e	101	ILE	2.3
39	1h	86	ILE	2.3
39	2h	38	ILE	2.3
39	2h	86	ILE	2.3
46	2o	12	ILE	2.3
35	2d	117	ALA	2.3
38	2g	127	ALA	2.3
47	2p	7	ALA	2.3
1	1A	2122	G	2.3
1	1A	2132	G	2.3
32	1a	148	G	2.3
54	2w	65	G	2.3
7	2H	88	LEU	2.3
14	2S	31	SER	2.3
21	2Z	157	LEU	2.3
28	26	11	LEU	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
33	2b	109	SER	2.3
33	2b	149	LEU	2.3
34	1c	13	GLY	2.3
35	2d	208	SER	2.3
37	2f	21	LEU	2.3
39	2h	63	LEU	2.3
39	2h	112	LEU	2.3
39	2h	128	GLY	2.3
41	1j	36	GLY	2.3
49	1r	26	LEU	2.3
1	1A	1878	A	2.3
2	2B	59	A	2.3
12	2Q	21	THR	2.3
32	1a	134	A	2.3
32	1a	608	A	2.3
32	2a	964	A	2.3
32	2a	1245	A	2.3
54	2w	31	A	2.3
1	2A	362	U	2.3
1	2A	614(A)	U	2.3
53	2v	22	U	2.3
15	1T	38	ASN	2.3
35	2d	161	ASN	2.3
33	2b	96	ARG	2.3
34	2c	11	ARG	2.3
35	1d	59	ARG	2.3
38	1g	4	ARG	2.3
41	2j	60	ARG	2.3
48	2q	92	ARG	2.3
51	1t	80	ARG	2.3
33	1b	167	PRO	2.3
43	1l	16	GLU	2.3
50	2s	17	GLU	2.3
33	2b	110	GLN	2.3
34	2c	162	GLN	2.3
48	2q	32	TYR	2.3
1	2A	652(T)	C	2.3
1	2A	2175	C	2.3
8	2I	19	VAL	2.3
8	2I	107	VAL	2.3
29	27	46	VAL	2.3
32	1a	165	C	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
32	1a	840	C	2.3
32	1a	1030	C	2.3
32	2a	1200	C	2.3
33	1b	42	ILE	2.3
34	1c	64	VAL	2.3
35	1d	204	ILE	2.3
38	2g	105	VAL	2.3
39	2h	61	VAL	2.3
48	1q	23	VAL	2.3
15	2T	130	ALA	2.3
51	1t	94	ALA	2.3
6	2G	176	LEU	2.2
14	2S	48	LEU	2.2
20	1Y	90	LEU	2.2
21	2Z	5	LEU	2.2
23	2I	82	LEU	2.2
33	1b	19	HIS	2.2
34	1c	42	LEU	2.2
34	2c	111	LEU	2.2
1	1A	162	G	2.2
1	2A	2318	G	2.2
5	1F	15	SER	2.2
11	2P	76	LYS	2.2
32	1a	625	G	2.2
32	1a	1022	G	2.2
32	2a	654	G	2.2
32	2a	1271	G	2.2
32	2a	1310	G	2.2
33	2b	190	THR	2.2
34	2c	67	THR	2.2
34	2c	144	SER	2.2
35	2d	22	LYS	2.2
39	1h	3	THR	2.2
44	1m	121	LYS	2.2
14	2S	12	PHE	2.2
22	20	57	PHE	2.2
34	2c	203	PHE	2.2
39	2h	9	MET	2.2
46	1o	18	PHE	2.2
1	1A	1219	A	2.2
21	1Z	154	ASP	2.2
21	2Z	72	ARG	2.2

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
24	12	55	ARG	2.2
32	1a	1196	U	2.2
32	2a	991	U	2.2
32	2a	997	U	2.2
32	2a	1052	U	2.2
32	2a	1056	U	2.2
33	2b	189	ASP	2.2
34	1c	38	ARG	2.2
34	1c	83	ARG	2.2
38	1g	156	TRP	2.2
40	1i	9	ARG	2.2
47	1p	81	ARG	2.2
33	2b	183	PRO	2.2
41	1j	91	PRO	2.2
33	1b	9	GLU	2.2
6	2G	138	GLN	2.2
6	2G	157	ILE	2.2
21	2Z	29	TYR	2.2
26	14	35	VAL	2.2
36	1e	82	VAL	2.2
37	2f	40	VAL	2.2
39	2h	109	ILE	2.2
41	2j	98	ILE	2.2
43	2l	55	VAL	2.2
47	1p	21	VAL	2.2
7	2H	75	ALA	2.2
8	2I	100	ALA	2.2
33	1b	13	ALA	2.2
41	2j	26	ALA	2.2
47	2p	77	ALA	2.2
2	2B	5	C	2.2
54	2y	4	C	2.2
11	1P	99	LEU	2.2
3	2D	275	LYS	2.2
16	2U	43	GLY	2.2
34	1c	9	GLY	2.2
34	2c	78	GLY	2.2
36	2e	53	LEU	2.2
39	2h	107	LEU	2.2
42	2k	103	LEU	2.2
20	1Y	88	LYS	2.2
44	2m	46	LYS	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
44	2m	95	GLY	2.2
52	2u	20	LYS	2.2
6	2G	71	THR	2.2
4	1E	1	MET	2.2
21	2Z	28	MET	2.2
11	2P	91	PHE	2.2
7	2H	3	ARG	2.2
12	1Q	60	ARG	2.2
21	2Z	20	ARG	2.2
23	2I	61	ARG	2.2
26	24	13	ARG	2.2
33	2b	36	ARG	2.2
1	1A	1120	G	2.2
1	1A	1217	G	2.2
1	1A	2178	G	2.2
1	2A	652(U)	G	2.2
32	1a	104	G	2.2
32	1a	631	G	2.2
32	1a	1356	G	2.2
32	2a	867	G	2.2
32	2a	1013	G	2.2
32	2a	1154	G	2.2
32	2a	1258	G	2.2
23	2I	68	PRO	2.2
1	1A	9	U	2.2
1	1A	1123	A	2.2
1	2A	157	U	2.2
1	2A	2130	U	2.2
32	2a	938	A	2.2
11	2P	92	GLU	2.2
32	2a	1012	U	2.2
32	2a	1093	A	2.2
33	1b	232	PRO	2.2
39	2h	76	PRO	2.2
40	1i	91	ASP	2.2
35	1d	173	TRP	2.2
40	2i	21	PRO	2.2
33	2b	231	GLU	2.2
34	1c	206	GLU	2.2
41	2j	64	GLU	2.2
34	2c	107	GLN	2.2
6	1G	52	ILE	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
21	2Z	56	VAL	2.2
22	20	66	VAL	2.2
26	24	33	VAL	2.2
26	24	35	VAL	2.2
34	1c	66	VAL	2.2
34	2c	14	ILE	2.2
35	1d	5	ILE	2.2
46	2o	87	ILE	2.2
50	1s	51	VAL	2.2
20	2Y	35	TYR	2.2
33	2b	120	ALA	2.2
34	1c	189	ALA	2.2
34	2c	50	ALA	2.2
35	2d	20	TYR	2.2
37	2f	53	ALA	2.2
39	1h	62	TYR	2.2
51	1t	67	ALA	2.2
14	2S	33	LYS	2.2
33	2b	19	HIS	2.2
23	21	85	LEU	2.2
34	1c	204	LEU	2.2
39	2h	10	LEU	2.2
41	2j	16	LEU	2.2
50	2s	32	LYS	2.2
6	2G	129	GLY	2.2
33	2b	18	GLY	2.2
36	2e	35	GLY	2.2
40	2i	6	GLY	2.2
40	2i	72	GLY	2.2
45	1n	51	GLY	2.2
1	1A	161	C	2.2
1	1A	670	C	2.2
1	1A	2158	C	2.2
1	2A	277	C	2.2
32	1a	221	C	2.2
32	1a	1019	C	2.2
32	2a	999	C	2.2
5	1F	13	SER	2.2
30	18	6	THR	2.2
21	2Z	19	ARG	2.2
24	12	37	PHE	2.2
33	1b	17	PHE	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
38	1g	78	ARG	2.2
45	2n	12	ARG	2.2
46	2o	88	ARG	2.2
6	1G	49	ASP	2.2
7	1H	57	ASP	2.2
8	2I	132	PRO	2.2
37	1f	83	ASP	2.2
38	2g	14	PRO	2.2
5	2F	161	GLU	2.2
38	1g	86	GLN	2.2
1	1A	2131	U	2.2
1	1A	2331	G	2.2
1	1A	2843	G	2.2
1	2A	880	G	2.2
1	2A	1170	G	2.2
1	2A	2167	U	2.2
32	1a	164	U	2.2
32	1a	1353	G	2.2
32	2a	988	G	2.2
54	1y	33	U	2.2
32	2a	1080	A	2.2
32	2a	1285	A	2.2
32	2a	1349	A	2.2
54	2y	57	G	2.2
7	2H	44	VAL	2.2
7	2H	136	ILE	2.2
33	1b	71	VAL	2.2
34	2c	116	VAL	2.2
38	1g	61	VAL	2.2
40	1i	17	VAL	2.2
40	2i	53	VAL	2.2
47	1p	79	VAL	2.2
48	2q	5	VAL	2.2
14	2S	76	LYS	2.2
20	2Y	55	TYR	2.2
33	1b	22	LYS	2.2
33	1b	31	TYR	2.2
33	2b	75	LYS	2.2
33	2b	133	LYS	2.2
34	2c	23	TYR	2.2
34	2c	29	TYR	2.2
35	1d	20	TYR	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
35	1d	195	ALA	2.2
36	1e	132	ALA	2.2
36	2e	132	ALA	2.2
40	1i	125	TYR	2.2
43	1l	91	LYS	2.2
45	1n	5	ALA	2.2
50	2s	50	ALA	2.2
6	1G	82	LEU	2.2
34	1c	188	LEU	2.2
38	1g	124	LEU	2.2
17	1V	1	MET	2.2
26	14	17	GLY	2.2
26	14	64	GLY	2.2
6	1G	93	THR	2.2
7	1H	59	ARG	2.2
20	2Y	23	ARG	2.2
34	2c	79	ARG	2.2
34	2c	165	THR	2.2
34	2c	191	THR	2.2
36	1e	18	ARG	2.2
38	1g	76	ARG	2.2
43	1l	67	THR	2.2
43	1l	89	ARG	2.2
47	2p	45	THR	2.2
52	1u	6	ARG	2.2
1	2A	2163	C	2.2
20	1Y	60	PHE	2.2
33	2b	233	SER	2.2
32	1a	100	C	2.2
32	2a	1045	C	2.2
32	2a	1071	C	2.2
32	2a	1218	C	2.2
6	2G	142	PRO	2.2
7	2H	36	PRO	2.2
43	1l	94	PRO	2.2
6	1G	48	GLU	2.2
19	1X	90	GLU	2.2
39	1h	4	ASP	2.2
50	1s	12	ASP	2.2
1	1A	386	U	2.2
14	2S	39	ILE	2.2
26	24	15	ILE	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
21	2Z	165	VAL	2.2
32	2a	960	U	2.2
32	2a	1122	U	2.2
32	2a	1278	U	2.2
39	1h	100	ILE	2.2
39	2h	6	ILE	2.2
33	2b	156	LYS	2.2
35	2d	170	VAL	2.2
36	2e	34	VAL	2.2
39	2h	79	VAL	2.2
43	2l	43	VAL	2.2
43	2l	123	LYS	2.2
47	1p	62	VAL	2.2
48	2q	21	VAL	2.2
48	2q	77	VAL	2.2
50	2s	60	VAL	2.2
53	1v	22	U	2.2
1	1A	273	G	2.2
1	2A	900	A	2.2
1	2A	2894	G	2.2
7	2H	73	ALA	2.2
8	1I	63	ALA	2.2
14	1S	72	ALA	2.2
32	1a	181	G	2.2
32	1a	607	A	2.2
32	1a	1151	A	2.2
32	2a	1155	G	2.2
32	2a	1175	G	2.2
32	2a	1184	G	2.2
32	2a	1236	A	2.2
32	2a	1256	A	2.2
32	2a	1365	G	2.2
32	2a	1373	G	2.2
34	2c	24	ALA	2.2
36	2e	30	ALA	2.2
40	2i	94	ALA	2.2
41	1j	27	ALA	2.2
53	1v	23	A	2.2
54	1y	34	G	2.2
54	2y	6	G	2.2
6	2G	90	LEU	2.1
12	2Q	26	TYR	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
21	1Z	102	LEU	2.1
23	21	46	LEU	2.1
26	14	63	TYR	2.1
28	26	36	LEU	2.1
34	1c	12	LEU	2.1
38	2g	101	LEU	2.1
40	1i	88	TYR	2.1
8	1I	106	GLY	2.1
15	2T	69	GLY	2.1
44	2m	24	GLY	2.1
6	1G	83	ARG	2.1
6	2G	181	ARG	2.1
10	1O	49	ARG	2.1
52	1u	15	ARG	2.1
36	2e	75	THR	2.1
6	2G	178	PHE	2.1
36	1e	45	PHE	2.1
20	2Y	53	PRO	2.1
26	24	41	PRO	2.1
41	2j	39	PRO	2.1
43	2l	94	PRO	2.1
1	1A	1125	C	2.1
1	1A	2161	C	2.1
1	2A	2108	C	2.1
3	1D	71	ASP	2.1
20	2Y	107	ASP	2.1
32	1a	1137	C	2.1
32	2a	1007	C	2.1
32	2a	1008	C	2.1
32	2a	1145	C	2.1
32	2a	1153	C	2.1
32	2a	1226	C	2.1
32	2a	1234	C	2.1
32	2a	1389	C	2.1
33	1b	195	ASP	2.1
42	2k	36	ASP	2.1
46	2o	9	GLN	2.1
26	24	5	ILE	2.1
34	1c	77	ILE	2.1
40	2i	118	LYS	2.1
4	1E	47	VAL	2.1
7	2H	26	VAL	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
7	2H	76	VAL	2.1
28	26	52	VAL	2.1
34	2c	106	VAL	2.1
50	2s	34	TRP	2.1
47	2p	16	HIS	2.1
1	2A	9	U	2.1
1	2A	2897	U	2.1
5	2F	33	LEU	2.1
6	1G	46	ALA	2.1
6	2G	7	LEU	2.1
26	24	12	ALA	2.1
32	1a	1000	U	2.1
32	2a	1257	U	2.1
33	2b	62	ALA	2.1
33	2b	77	ALA	2.1
35	1d	48	ALA	2.1
38	2g	38	LEU	2.1
38	2g	39	ALA	2.1
38	2g	152	ALA	2.1
45	2n	48	ALA	2.1
55	2x	47	U	2.1
33	2b	48	MET	2.1
39	2h	133	LEU	2.1
47	1p	74	LEU	2.1
50	1s	20	LEU	2.1
50	1s	66	MET	2.1
21	2Z	3	TYR	2.1
26	14	43	TYR	2.1
32	2a	1287	A	2.1
6	1G	113	ARG	2.1
7	2H	174	GLY	2.1
40	1i	6	GLY	2.1
54	2w	14	A	2.1
11	2P	102	ARG	2.1
51	1t	89	ARG	2.1
1	1A	269	G	2.1
1	1A	1137	G	2.1
1	2A	2207	G	2.1
32	1a	69	G	2.1
32	1a	1030(C)	G	2.1
32	1a	1368	G	2.1
32	2a	1011	G	2.1

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
32	2a	1087	G	2.1
32	2a	1106	G	2.1
32	2a	1160	G	2.1
7	2H	129	THR	2.1
44	2m	43	THR	2.1
21	2Z	44	PHE	2.1
21	2Z	104	PHE	2.1
50	2s	74	PHE	2.1
5	1F	14	PRO	2.1
7	2H	10	PRO	2.1
21	2Z	159	PRO	2.1
33	2b	194	PRO	2.1
35	1d	83	SER	2.1
44	2m	113	PRO	2.1
4	1E	87	GLU	2.1
20	2Y	91	GLU	2.1
21	2Z	2	GLU	2.1
33	1b	231	GLU	2.1
38	1g	56	GLN	2.1
46	2o	71	GLN	2.1
6	2G	75	LYS	2.1
7	1H	175	LYS	2.1
14	1S	44	LYS	2.1
21	1Z	123	ASP	2.1
23	2l	78	LYS	2.1
33	2b	166	ASP	2.1
34	2c	93	LYS	2.1
41	2j	7	LYS	2.1
1	2A	889	C	2.1
1	2A	2295	C	2.1
2	2B	4	C	2.1
21	2Z	124	ILE	2.1
32	1a	848	C	2.1
32	2a	1006	C	2.1
36	2e	11	ILE	2.1
41	1j	82	ILE	2.1
54	2y	56	C	2.1
33	1b	16	HIS	2.1
34	1c	69	HIS	2.1
50	2s	47	HIS	2.1
4	1E	33	VAL	2.1
4	2E	75	VAL	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
7	1H	17	VAL	2.1
34	2c	99	VAL	2.1
35	1d	121	VAL	2.1
40	1i	65	VAL	2.1
6	2G	6	ALA	2.1
7	2H	67	LEU	2.1
9	2N	1	MET	2.1
11	1P	103	ALA	2.1
17	2V	71	LEU	2.1
21	2Z	1	MET	2.1
8	2I	55	ALA	2.1
33	2b	213	LEU	2.1
34	1c	24	ALA	2.1
34	1c	47	LEU	2.1
34	2c	43	LEU	2.1
34	2c	65	ALA	2.1
36	1e	21	ALA	2.1
42	1k	23	ALA	2.1
46	2o	85	LEU	2.1
51	1t	76	ALA	2.1
7	2H	59	ARG	2.1
26	14	62	ARG	2.1
34	2c	83	ARG	2.1
38	2g	111	ARG	2.1
45	2n	45	ARG	2.1
12	2Q	24	GLY	2.1
17	2V	42	GLY	2.1
34	2c	51	GLY	2.1
50	2s	46	GLY	2.1
6	1G	12	TYR	2.1
26	14	32	TYR	2.1
26	24	67	TYR	2.1
42	2k	75	TYR	2.1
43	2l	69	TYR	2.1
1	1A	2191	A	2.1
1	2A	2176	A	2.1
32	1a	614	A	2.1
32	2a	919	A	2.1
32	2a	968	A	2.1
32	2a	1067	A	2.1
32	2a	1227	A	2.1
32	2a	1252	A	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
32	2a	1447	A	2.1
54	1w	9	A	2.1
54	2y	26	A	2.1
26	24	27	THR	2.1
50	2s	33	THR	2.1
21	1Z	104	PHE	2.1
33	2b	202	PRO	2.1
42	2k	115	PRO	2.1
1	1A	298	G	2.1
1	1A	387	G	2.1
1	1A	639	G	2.1
1	1A	938	G	2.1
1	1A	2903	G	2.1
1	2A	100	G	2.1
1	2A	1042	G	2.1
1	2A	2124	G	2.1
1	2A	2304	G	2.1
1	2A	2807	G	2.1
32	1a	851	G	2.1
32	1a	933	G	2.1
32	2a	1010	G	2.1
32	2a	1053	G	2.1
54	1w	5	G	2.1
54	1w	15	G	2.1
55	2x	70	G	2.1
34	2c	143	GLU	2.1
42	1k	104	GLN	2.1
50	1s	17	GLU	2.1
50	2s	64	GLU	2.1
22	20	49	LYS	2.1
48	2q	100	LYS	2.1
6	2G	114	ILE	2.1
8	1I	11	ASN	2.1
33	2b	220	ASP	2.1
51	1t	64	ASP	2.1
10	2O	86	ILE	2.1
33	1b	32	ILE	2.1
33	1b	40	HIS	2.1
33	1b	222	ILE	2.1
33	2b	208	ILE	2.1
35	2d	123	HIS	2.1
39	1h	6	ILE	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
39	1h	111	ILE	2.1
42	1k	29	ILE	2.1
52	1u	13	ILE	2.1
15	1T	1	MET	2.1
6	2G	103	LEU	2.1
7	2H	98	LEU	2.1
22	20	7	LEU	2.1
33	1b	215	LEU	2.1
33	2b	98	LEU	2.1
33	2b	102	LEU	2.1
38	1g	104	LEU	2.1
38	2g	17	VAL	2.1
39	2h	59	LEU	2.1
40	2i	65	VAL	2.1
40	2i	85	LEU	2.1
1	1A	2804	C	2.1
11	1P	134	ALA	2.1
14	1S	74	ALA	2.1
32	1a	1054	C	2.1
32	2a	1096	C	2.1
32	2a	1249	C	2.1
14	2S	10	ARG	2.1
21	2Z	103	ARG	2.1
24	12	13	ALA	2.1
47	2p	59	TRP	2.1
55	2x	34	C	2.1
26	14	61	ARG	2.1
33	1b	30	ARG	2.1
36	1e	15	ARG	2.1
39	1h	30	ARG	2.1
50	2s	3	ARG	2.1
1	1A	2140	U	2.1
1	2A	2109	U	2.1
32	2a	1000	U	2.1
34	1c	81	GLY	2.1
54	1y	60	U	2.1
17	2V	91	TYR	2.1
37	2f	63	TYR	2.1
42	2k	50	TYR	2.1
8	2I	80	PRO	2.1
21	2Z	95	PRO	2.1
27	25	29	THR	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
38	1g	112	PRO	2.1
46	2o	4	THR	2.1
1	1A	2148	A	2.1
1	2A	1445	A	2.1
1	2A	2801(A)	A	2.1
7	2H	58	GLU	2.1
7	2H	62	LYS	2.1
11	1P	107	LYS	2.1
14	1S	83	LYS	2.1
20	1Y	91	GLU	2.1
32	1a	1252	A	2.1
34	2c	45	LYS	2.1
34	2c	161	GLU	2.1
35	1d	18	LYS	2.1
35	1d	86	LYS	2.1
34	1c	20	SER	2.1
36	1e	20	GLN	2.1
36	1e	79	GLU	2.1
36	2e	141	GLN	2.1
38	2g	110	GLN	2.1
40	2i	2	GLU	2.1
42	1k	51	LYS	2.1
46	1o	28	GLN	2.1
53	1v	15	A	2.1
53	2v	23	A	2.1
54	1w	23	A	2.1
1	2A	11	G	2.1
1	2A	916	G	2.1
1	2A	2148	G	2.1
32	2a	954	G	2.1
32	2a	998	G	2.1
32	2a	1003	G	2.1
32	2a	1233	G	2.1
32	2a	1290	G	2.1
32	2a	1370	G	2.1
6	2G	126	ASP	2.1
8	2I	79	ILE	2.1
14	2S	41	ASP	2.1
6	2G	148	MET	2.1
21	2Z	75	ASN	2.1
33	1b	160	ASP	2.1
33	2b	16	HIS	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
33	2b	108	ILE	2.1
34	2c	181	ASN	2.1
42	1k	48	ILE	2.1
44	2m	84	ILE	2.1
46	1o	3	ILE	2.1
6	2G	70	VAL	2.0
6	2G	135	LEU	2.0
7	1H	67	LEU	2.0
12	2Q	37	LEU	2.0
21	2Z	67	LEU	2.0
23	21	62	VAL	2.0
33	2b	15	VAL	2.0
35	2d	128	VAL	2.0
37	2f	43	LEU	2.0
39	1h	118	VAL	2.0
42	2k	66	LEU	2.0
43	1l	55	VAL	2.0
44	2m	81	LEU	2.0
50	2s	58	VAL	2.0
7	1H	149	ARG	2.0
33	1b	36	ARG	2.0
34	1c	172	ARG	2.0
45	2n	19	ARG	2.0
52	2u	9	ARG	2.0
35	2d	149	ALA	2.0
36	2e	108	ALA	2.0
38	2g	25	ALA	2.0
41	1j	26	ALA	2.0
33	1b	97	TRP	2.0
1	2A	271(J)	C	2.0
6	2G	42	GLY	2.0
6	2G	119	GLY	2.0
32	2a	217	C	2.0
32	2a	848	C	2.0
32	2a	1059	C	2.0
32	2a	1210	C	2.0
32	2a	1259	C	2.0
34	2c	81	GLY	2.0
43	1l	63	GLY	2.0
43	1l	95	GLY	2.0
52	2u	4	GLY	2.0
32	1a	841	U	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
32	2a	981	U	2.0
32	2a	1212	U	2.0
12	2Q	137	TYR	2.0
21	2Z	83	PRO	2.0
33	2b	125	PRO	2.0
34	1c	23	TYR	2.0
47	2p	32	TYR	2.0
48	2q	88	TYR	2.0
49	1r	25	THR	2.0
51	1t	98	PRO	2.0
52	2u	18	TYR	2.0
21	1Z	136	PHE	2.0
40	1i	7	THR	2.0
41	1j	7	LYS	2.0
49	1r	29	PHE	2.0
16	1U	111	GLU	2.0
34	1c	35	GLU	2.0
40	1i	12	GLU	2.0
48	2q	78	GLU	2.0
23	2l	86	SER	2.0
41	1j	30	SER	2.0
1	1A	678	A	2.0
1	1A	2193	A	2.0
1	2A	1460	A	2.0
32	2a	978	A	2.0
32	2a	1157	A	2.0
32	2a	1229	A	2.0
12	2Q	1	MET	2.0
14	2S	34	HIS	2.0
36	2e	80	ILE	2.0
38	1g	42	ILE	2.0
38	2g	89	MET	2.0
48	2q	82	MET	2.0
50	2s	57	HIS	2.0
7	2H	9	ILE	2.0
8	1I	109	ILE	2.0
21	2Z	148	ASP	2.0
33	2b	205	ASP	2.0
38	2g	148	ASN	2.0
47	1p	40	ASP	2.0
6	2G	3	LEU	2.0
6	2G	9	ARG	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
7	1H	71	LEU	2.0
8	1I	75	LEU	2.0
11	1P	112	LEU	2.0
14	2S	78	LEU	2.0
6	1G	149	VAL	2.0
14	2S	85	VAL	2.0
15	1T	112	ARG	2.0
21	2Z	37	VAL	2.0
22	20	67	VAL	2.0
31	29	25	VAL	2.0
33	2b	56	ARG	2.0
33	2b	137	ARG	2.0
34	1c	94	LEU	2.0
40	1i	47	LEU	2.0
44	2m	71	ARG	2.0
46	1o	65	ARG	2.0
49	2r	85	LEU	2.0
36	2e	115	VAL	2.0
50	2s	36	ARG	2.0
1	1A	2182	G	2.0
1	1A	2213	G	2.0
1	1A	2902	G	2.0
32	2a	1026	G	2.0
32	2a	1079	G	2.0
32	2a	1138	G	2.0
32	2a	1198	G	2.0
32	2a	1309	G	2.0
54	2w	57	G	2.0
55	1x	46	G	2.0
33	2b	72	GLY	2.0
50	1s	8	GLY	2.0
45	1n	61	TRP	2.0
6	1G	182	LYS	2.0
1	1A	1985	U	2.0
32	1a	1114	C	2.0
32	1a	1118	C	2.0
32	1a	1452	C	2.0
32	2a	723	U	2.0
32	2a	955	U	2.0
32	2a	1063	C	2.0
32	2a	1284	C	2.0
32	2a	1382	C	2.0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
40	1i	98	PRO	2.0
41	1j	39	PRO	2.0
52	1u	23	PRO	2.0
54	1w	67	C	2.0
54	1w	68	C	2.0
11	1P	91	PHE	2.0
12	2Q	32	TYR	2.0
20	2Y	83	THR	2.0
35	2d	75	PHE	2.0
36	2e	45	PHE	2.0
38	1g	151	TYR	2.0
39	2h	65	TYR	2.0
41	1j	100	THR	2.0
44	1m	21	TYR	2.0
54	1y	45	U	2.0
21	2Z	168	GLU	2.0
30	18	56	GLU	2.0
38	2g	11	GLN	2.0
41	2j	33	GLN	2.0
46	1o	62	GLN	2.0
48	1q	24	GLU	2.0
48	2q	86	GLU	2.0
33	1b	210	SER	2.0
33	2b	40	HIS	2.0
35	2d	181	MET	2.0
42	1k	53	SER	2.0
43	1l	116	SER	2.0
45	2n	60	SER	2.0
46	1o	24	SER	2.0
51	1t	16	HIS	2.0
6	2G	51	ARG	2.0
6	2G	132	ASN	2.0
11	2P	90	ARG	2.0
12	1Q	6	ARG	2.0
24	22	51	ARG	2.0
25	13	29	ARG	2.0
33	2b	178	ARG	2.0
35	2d	132	ARG	2.0
36	1e	73	ASN	2.0
37	1f	46	ARG	2.0
44	2m	91	ARG	2.0
46	1o	68	ARG	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
47	2p	5	ARG	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
54	7MG	2w	46	24/25	0.51	0.16	83,96,107,134	0
54	4SU	2w	8	20/21	0.58	0.16	81,98,120,128	0
54	7MG	2y	46	24/25	0.61	0.19	68,95,99,128	0
54	PSU	2y	55	20/21	0.61	0.15	80,96,115,118	0
54	5MU	2y	54	21/22	0.63	0.17	79,93,108,123	0
54	PSU	2w	55	20/21	0.65	0.17	80,94,98,113	0
54	7MG	1w	46	24/25	0.66	0.17	76,90,101,124	0
54	7MG	1y	46	24/25	0.67	0.17	76,95,106,115	0
54	5MU	1y	54	21/22	0.68	0.15	76,87,95,116	0
54	4SU	1y	8	20/21	0.70	0.17	80,98,105,114	0
54	MIA	2y	37	22/30	0.70	0.17	72,86,94,120	0
54	PSU	1y	55	20/21	0.72	0.16	72,89,99,120	0
54	4SU	2y	8	20/21	0.74	0.16	87,94,106,113	0
32	2MG	2a	1207	24/25	0.75	0.16	74,85,90,98	0
54	PSU	2y	32	20/21	0.76	0.17	73,89,97,108	0
55	PSU	2x	55	20/21	0.80	0.14	69,84,106,107	0
54	PSU	1y	32	20/21	0.81	0.16	69,87,94,95	0
54	PSU	2y	39	20/21	0.81	0.13	78,84,100,112	0
54	4SU	1w	8	20/21	0.81	0.14	75,86,105,114	0
54	5MU	2w	54	21/22	0.82	0.15	66,85,93,101	0
55	5MU	2x	54	21/22	0.82	0.15	71,87,95,100	0
54	MIA	1y	37	22/30	0.82	0.14	76,83,93,94	0
54	PSU	1w	55	20/21	0.83	0.12	72,81,90,98	0
55	4SU	2x	8	20/21	0.83	0.15	74,85,90,96	0
1	5MU	2A	1915	21/22	0.85	0.16	64,72,79,93	0
54	PSU	2w	39	20/21	0.86	0.14	80,88,96,102	0
54	PSU	2w	32	20/21	0.87	0.13	69,85,94,103	0
32	M2G	2a	966	25/26	0.87	0.18	52,69,95,99	0
54	MIA	2w	37	25/30	0.88	0.13	70,82,91,110	0
54	PSU	1y	39	20/21	0.88	0.12	71,81,89,95	0
43	0TD	2l	92	10/11	0.89	0.14	65,68,73,79	0
55	5MC	2x	32	21/22	0.89	0.15	65,78,87,88	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	PSU	2a	516	20/21	0.90	0.10	65,72,79,83	0
32	5MC	2a	967	21/22	0.91	0.15	62,71,79,86	0
43	0TD	1l	92	10/11	0.91	0.15	61,64,70,74	0
32	5MC	2a	1400	21/22	0.91	0.16	70,74,80,93	0
54	PSU	1w	32	20/21	0.91	0.12	59,72,79,83	0
32	5MC	2a	1404	21/22	0.91	0.12	47,59,74,77	0
32	7MG	2a	527	24/25	0.91	0.12	61,70,77,88	0
55	PSU	1x	55	20/21	0.91	0.11	56,67,81,87	0
1	PSU	2A	1917	20/21	0.91	0.12	56,65,75,76	0
54	MIA	1w	37	29/30	0.92	0.14	43,62,74,78	0
32	4OC	2a	1402	22/23	0.92	0.12	45,63,71,90	0
55	5MU	1x	54	21/22	0.92	0.11	57,71,79,83	0
1	PSU	2A	1911	20/21	0.93	0.10	56,60,66,70	0
32	PSU	1a	516	20/21	0.93	0.12	63,70,78,78	0
1	5MU	1A	1937	21/22	0.93	0.12	56,67,75,82	0
54	PSU	1w	39	20/21	0.93	0.10	50,70,80,83	0
1	4OC	2A	1920	21/23	0.93	0.12	46,57,62,72	0
32	UR3	2a	1498	21/22	0.93	0.12	48,58,62,68	0
55	5MC	1x	32	21/22	0.94	0.12	44,54,67,73	0
32	2MG	1a	1207	24/25	0.94	0.09	62,72,76,80	0
54	5MU	1w	54	21/22	0.94	0.10	55,67,78,79	0
1	PSU	1A	1939	20/21	0.94	0.13	53,60,71,72	0
1	5MU	2A	1939	21/22	0.94	0.10	24,34,41,46	0
32	MA6	2a	1518	24/25	0.94	0.13	41,63,74,82	0
1	5MC	1A	1964	21/22	0.95	0.10	38,47,52,60	0
1	PSU	1A	1933	20/21	0.95	0.12	49,59,62,66	0
55	4SU	1x	8	20/21	0.95	0.10	46,60,69,73	0
1	5MC	2A	1942	21/22	0.95	0.10	45,50,58,61	0
1	5MC	2A	1962	21/22	0.95	0.10	28,43,52,59	0
32	7MG	1a	527	24/25	0.95	0.10	40,50,60,67	0
32	5MC	2a	1407	21/22	0.95	0.12	48,57,69,76	0
32	M2G	1a	966	25/26	0.95	0.10	41,55,61,77	0
32	5MC	1a	967	21/22	0.95	0.11	51,58,67,70	0
32	MA6	2a	1519	24/25	0.95	0.13	47,65,74,81	0
32	MA6	1a	1519	24/25	0.96	0.10	39,48,57,71	0
1	PSU	2A	2605	20/21	0.96	0.07	25,33,40,42	0
32	5MC	1a	1407	21/22	0.96	0.10	34,42,56,62	0
1	5MU	1A	1961	21/22	0.97	0.08	21,33,38,44	0
32	5MC	1a	1400	21/22	0.97	0.09	39,53,61,67	0
32	4OC	1a	1402	22/23	0.97	0.09	37,47,55,61	0
32	5MC	1a	1404	21/22	0.97	0.08	32,43,50,53	0
1	4OC	1A	1942	21/23	0.97	0.10	42,55,61,65	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	2MU	1A	2564	21/23	0.97	0.08	26,36,40,46	0
1	PSU	1A	2617	20/21	0.97	0.08	24,31,37,39	0
1	OMG	2A	2251	24/25	0.97	0.07	27,36,44,46	0
1	2MA	2A	2503	23/24	0.97	0.07	25,30,35,37	0
1	2MU	2A	2552	21/23	0.97	0.08	28,38,46,52	0
1	OMG	1A	2263	24/25	0.98	0.07	22,32,39,44	0
32	UR3	1a	1498	21/22	0.98	0.06	38,43,50,54	0
32	MA6	1a	1518	24/25	0.98	0.09	31,47,51,57	0
1	2MA	1A	2515	23/24	0.98	0.08	20,26,31,34	0
1	5MC	1A	1984	21/22	0.98	0.07	31,38,48,57	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3786	1/1	0.26	0.30	81,81,81,81	0
56	MG	2B	3016	1/1	0.58	0.30	81,81,81,81	0
56	MG	1A	4076	1/1	0.59	0.14	75,75,75,75	0
56	MG	1A	3671	1/1	0.63	0.23	67,67,67,67	0
56	MG	1Z	302	1/1	0.64	0.15	67,67,67,67	0
56	MG	1G	3004	1/1	0.64	0.21	92,92,92,92	0
56	MG	2a	3201	1/1	0.66	0.25	79,79,79,79	0
56	MG	1A	3468	1/1	0.68	0.19	68,68,68,68	0
56	MG	2a	3028	1/1	0.68	0.39	84,84,84,84	0
56	MG	2A	3875	1/1	0.68	0.27	76,76,76,76	0
56	MG	15	103	1/1	0.69	0.19	61,61,61,61	0
56	MG	1a	1746	1/1	0.69	0.24	84,84,84,84	0
56	MG	1B	3032	1/1	0.70	0.25	80,80,80,80	0
56	MG	2a	3210	1/1	0.70	0.18	70,70,70,70	0
56	MG	1y	3004	1/1	0.71	0.19	86,86,86,86	0
56	MG	2a	3198	1/1	0.71	0.23	83,83,83,83	0
56	MG	1A	3975	1/1	0.71	0.18	93,93,93,93	0
56	MG	1e	201	1/1	0.71	0.17	79,79,79,79	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2B	3014	1/1	0.72	0.18	77,77,77,77	0
56	MG	2A	3687	1/1	0.72	0.30	63,63,63,63	0
56	MG	1A	3894	1/1	0.73	0.21	73,73,73,73	0
56	MG	2A	3856	1/1	0.73	0.20	41,41,41,41	0
56	MG	1E	307	1/1	0.73	0.23	70,70,70,70	0
56	MG	2B	3021	1/1	0.74	0.28	75,75,75,75	0
56	MG	2a	3010	1/1	0.74	0.29	76,76,76,76	0
56	MG	1a	1773	1/1	0.74	0.13	90,90,90,90	0
56	MG	2a	3127	1/1	0.74	0.23	85,85,85,85	0
56	MG	2B	3003	1/1	0.74	0.27	74,74,74,74	0
56	MG	2A	3691	1/1	0.74	0.31	68,68,68,68	0
56	MG	2A	3686	1/1	0.74	0.24	57,57,57,57	0
56	MG	2a	3228	1/1	0.74	0.28	86,86,86,86	0
56	MG	1A	3566	1/1	0.75	0.31	72,72,72,72	0
56	MG	1a	1656	1/1	0.75	0.31	75,75,75,75	0
56	MG	1A	3466	1/1	0.75	0.16	64,64,64,64	0
56	MG	1A	3531	1/1	0.75	0.23	67,67,67,67	0
56	MG	2A	3821	1/1	0.75	0.19	79,79,79,79	0
56	MG	1B	3007	1/1	0.75	0.34	85,85,85,85	0
56	MG	1A	3994	1/1	0.76	0.19	76,76,76,76	0
56	MG	1a	1610	1/1	0.76	0.16	79,79,79,79	0
56	MG	2a	3046	1/1	0.76	0.25	64,64,64,64	0
56	MG	2A	3884	1/1	0.76	0.21	42,42,42,42	0
56	MG	2a	3131	1/1	0.76	0.31	80,80,80,80	0
56	MG	1A	4044	1/1	0.76	0.25	79,79,79,79	0
56	MG	2a	3199	1/1	0.76	0.21	72,72,72,72	0
56	MG	1A	3423	1/1	0.76	0.27	67,67,67,67	0
56	MG	1a	1750	1/1	0.76	0.32	85,85,85,85	0
56	MG	1A	3834	1/1	0.76	0.22	69,69,69,69	0
56	MG	2A	3656	1/1	0.77	0.17	77,77,77,77	0
56	MG	2a	3090	1/1	0.77	0.13	68,68,68,68	0
56	MG	1a	1776	1/1	0.77	0.13	91,91,91,91	0
56	MG	1A	3641	1/1	0.77	0.27	65,65,65,65	0
56	MG	2a	3136	1/1	0.77	0.20	73,73,73,73	0
56	MG	2a	3179	1/1	0.77	0.12	100,100,100,100	0
56	MG	2a	3192	1/1	0.77	0.23	63,63,63,63	0
56	MG	1A	3272	1/1	0.77	0.16	60,60,60,60	0
56	MG	2A	3710	1/1	0.77	0.15	63,63,63,63	0
56	MG	2A	3091	1/1	0.77	0.18	60,60,60,60	0
56	MG	2A	3536	1/1	0.77	0.14	51,51,51,51	0
56	MG	2A	3871	1/1	0.77	0.15	70,70,70,70	0
56	MG	2a	3240	1/1	0.77	0.17	63,63,63,63	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1x	102	1/1	0.78	0.28	63,63,63,63	0
56	MG	1A	3585	1/1	0.78	0.21	66,66,66,66	0
56	MG	1A	3795	1/1	0.78	0.25	51,51,51,51	0
56	MG	2A	3362	1/1	0.78	0.23	68,68,68,68	0
56	MG	2A	3712	1/1	0.78	0.16	63,63,63,63	0
56	MG	2A	3754	1/1	0.78	0.13	45,45,45,45	0
56	MG	2A	3453	1/1	0.78	0.13	45,45,45,45	0
56	MG	2A	3844	1/1	0.78	0.15	50,50,50,50	0
56	MG	1U	202	1/1	0.78	0.36	73,73,73,73	0
56	MG	1A	3912	1/1	0.78	0.19	80,80,80,80	0
56	MG	2a	3117	1/1	0.78	0.26	81,81,81,81	0
56	MG	2v	3002	1/1	0.78	0.23	77,77,77,77	0
56	MG	2y	3005	1/1	0.78	0.25	82,82,82,82	0
56	MG	1a	1738	1/1	0.79	0.14	66,66,66,66	0
56	MG	2A	3865	1/1	0.79	0.13	71,71,71,71	0
56	MG	2a	3128	1/1	0.79	0.21	87,87,87,87	0
56	MG	1A	3521	1/1	0.79	0.22	65,65,65,65	0
56	MG	1A	3319	1/1	0.79	0.26	63,63,63,63	0
56	MG	2a	3155	1/1	0.79	0.14	81,81,81,81	0
56	MG	2A	3291	1/1	0.79	0.14	56,56,56,56	0
56	MG	1A	3832	1/1	0.79	0.17	62,62,62,62	0
56	MG	2A	3374	1/1	0.79	0.24	65,65,65,65	0
56	MG	2A	3719	1/1	0.79	0.23	57,57,57,57	0
56	MG	1A	3718	1/1	0.79	0.23	67,67,67,67	0
56	MG	2a	3003	1/1	0.79	0.15	64,64,64,64	0
56	MG	2A	3773	1/1	0.79	0.18	63,63,63,63	0
56	MG	1A	3879	1/1	0.79	0.20	51,51,51,51	0
56	MG	2A	3839	1/1	0.79	0.13	45,45,45,45	0
56	MG	2A	3646	1/1	0.79	0.14	55,55,55,55	0
56	MG	1A	3555	1/1	0.80	0.31	60,60,60,60	0
56	MG	1A	3164	1/1	0.80	0.28	73,73,73,73	0
56	MG	1A	3776	1/1	0.80	0.29	75,75,75,75	0
56	MG	2A	3364	1/1	0.80	0.30	77,77,77,77	0
56	MG	2E	308	1/1	0.80	0.13	38,38,38,38	0
56	MG	2Z	8001	1/1	0.80	0.19	78,78,78,78	0
56	MG	1A	3530	1/1	0.80	0.22	63,63,63,63	0
56	MG	1B	3029	1/1	0.80	0.24	66,66,66,66	0
56	MG	1A	3073	1/1	0.80	0.30	69,69,69,69	0
56	MG	2a	3034	1/1	0.80	0.26	72,72,72,72	0
56	MG	2a	3036	1/1	0.80	0.24	83,83,83,83	0
56	MG	1A	3824	1/1	0.80	0.26	70,70,70,70	0
56	MG	2a	3229	1/1	0.80	0.33	69,69,69,69	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3880	1/1	0.80	0.13	65,65,65,65	0
56	MG	2a	3110	1/1	0.80	0.26	73,73,73,73	0
56	MG	2x	102	1/1	0.80	0.23	77,77,77,77	0
56	MG	2A	3756	1/1	0.80	0.18	42,42,42,42	0
56	MG	2E	307	1/1	0.81	0.24	54,54,54,54	0
56	MG	2A	3266	1/1	0.81	0.17	59,59,59,59	0
56	MG	2A	3855	1/1	0.81	0.13	69,69,69,69	0
56	MG	1A	3830	1/1	0.81	0.12	66,66,66,66	0
56	MG	1A	3257	1/1	0.81	0.15	68,68,68,68	0
56	MG	1A	3264	1/1	0.81	0.13	63,63,63,63	0
56	MG	1A	3694	1/1	0.81	0.18	61,61,61,61	0
56	MG	1A	3888	1/1	0.81	0.15	70,70,70,70	0
56	MG	2a	3200	1/1	0.81	0.28	76,76,76,76	0
56	MG	2A	3058	1/1	0.81	0.21	66,66,66,66	0
56	MG	2a	3204	1/1	0.81	0.25	86,86,86,86	0
56	MG	2a	3206	1/1	0.81	0.17	69,69,69,69	0
56	MG	2a	3062	1/1	0.81	0.29	70,70,70,70	0
56	MG	1A	3548	1/1	0.81	0.19	49,49,49,49	0
56	MG	2a	3104	1/1	0.81	0.25	75,75,75,75	0
56	MG	2a	3108	1/1	0.81	0.29	78,78,78,78	0
56	MG	2j	8001	1/1	0.81	0.14	75,75,75,75	0
56	MG	2A	3116	1/1	0.81	0.30	68,68,68,68	0
56	MG	2w	101	1/1	0.81	0.28	73,73,73,73	0
56	MG	2w	108	1/1	0.81	0.22	66,66,66,66	0
56	MG	2A	3822	1/1	0.81	0.17	66,66,66,66	0
56	MG	2A	3117	1/1	0.81	0.21	63,63,63,63	0
56	MG	2y	3007	1/1	0.81	0.19	68,68,68,68	0
56	MG	1A	3320	1/1	0.82	0.23	60,60,60,60	0
56	MG	1B	3020	1/1	0.82	0.27	82,82,82,82	0
56	MG	1a	1665	1/1	0.82	0.20	78,78,78,78	0
56	MG	1a	1689	1/1	0.82	0.29	73,73,73,73	0
56	MG	1A	3913	1/1	0.82	0.15	80,80,80,80	0
56	MG	1a	1744	1/1	0.82	0.23	73,73,73,73	0
56	MG	2a	3161	1/1	0.82	0.14	91,91,91,91	0
56	MG	2A	3722	1/1	0.82	0.21	58,58,58,58	0
56	MG	2A	3748	1/1	0.82	0.14	57,57,57,57	0
56	MG	1A	3962	1/1	0.82	0.15	62,62,62,62	0
56	MG	2A	3342	1/1	0.82	0.20	59,59,59,59	0
56	MG	2a	3007	1/1	0.82	0.29	71,71,71,71	0
56	MG	1A	3875	1/1	0.82	0.20	60,60,60,60	0
56	MG	2a	3013	1/1	0.82	0.34	78,78,78,78	0
56	MG	2a	3024	1/1	0.82	0.34	72,72,72,72	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1755	1/1	0.82	0.12	74,74,74,74	0
56	MG	1A	3829	1/1	0.82	0.12	59,59,59,59	0
56	MG	1A	4024	1/1	0.82	0.14	71,71,71,71	0
56	MG	2a	3037	1/1	0.82	0.17	77,77,77,77	0
56	MG	2A	3466	1/1	0.82	0.26	65,65,65,65	0
56	MG	1A	3446	1/1	0.82	0.28	61,61,61,61	0
56	MG	2A	3607	1/1	0.82	0.19	55,55,55,55	0
56	MG	2w	104	1/1	0.82	0.15	69,69,69,69	0
56	MG	2a	3103	1/1	0.82	0.25	76,76,76,76	0
56	MG	2A	3644	1/1	0.82	0.18	64,64,64,64	0
56	MG	1f	3002	1/1	0.82	0.34	80,80,80,80	0
56	MG	1A	3646	1/1	0.82	0.10	32,32,32,32	0
56	MG	1w	109	1/1	0.83	0.22	67,67,67,67	0
56	MG	1A	4072	1/1	0.83	0.18	62,62,62,62	0
56	MG	1x	103	1/1	0.83	0.15	71,71,71,71	0
56	MG	1a	1672	1/1	0.83	0.13	73,73,73,73	0
56	MG	2A	3700	1/1	0.83	0.19	65,65,65,65	0
56	MG	2A	3039	1/1	0.83	0.13	55,55,55,55	0
56	MG	2a	3040	1/1	0.83	0.16	57,57,57,57	0
56	MG	1A	3487	1/1	0.83	0.24	70,70,70,70	0
56	MG	1a	1696	1/1	0.83	0.25	71,71,71,71	0
56	MG	2a	3085	1/1	0.83	0.28	65,65,65,65	0
56	MG	1A	3734	1/1	0.83	0.10	59,59,59,59	0
56	MG	2A	3737	1/1	0.83	0.20	72,72,72,72	0
56	MG	2A	3744	1/1	0.83	0.19	55,55,55,55	0
56	MG	1Y	503	1/1	0.83	0.18	78,78,78,78	0
56	MG	2A	3126	1/1	0.83	0.23	58,58,58,58	0
56	MG	2A	3138	1/1	0.83	0.21	59,59,59,59	0
56	MG	2A	3769	1/1	0.83	0.17	62,62,62,62	0
56	MG	2A	3169	1/1	0.83	0.48	73,73,73,73	0
56	MG	2A	3808	1/1	0.83	0.15	60,60,60,60	0
56	MG	2A	3229	1/1	0.83	0.15	41,41,41,41	0
56	MG	2A	3256	1/1	0.83	0.19	53,53,53,53	0
56	MG	1B	3019	1/1	0.83	0.18	56,56,56,56	0
56	MG	2a	3166	1/1	0.83	0.13	84,84,84,84	0
56	MG	1A	3799	1/1	0.83	0.16	57,57,57,57	0
56	MG	1A	3800	1/1	0.83	0.15	65,65,65,65	0
56	MG	2A	3353	1/1	0.83	0.18	65,65,65,65	0
56	MG	1a	1612	1/1	0.83	0.15	74,74,74,74	0
56	MG	1a	1645	1/1	0.83	0.19	80,80,80,80	0
56	MG	1a	1784	1/1	0.83	0.16	74,74,74,74	0
56	MG	2A	3406	1/1	0.83	0.20	55,55,55,55	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3447	1/1	0.83	0.26	46,46,46,46	0
56	MG	2A	3893	1/1	0.83	0.16	66,66,66,66	0
56	MG	1a	1824	1/1	0.83	0.16	73,73,73,73	0
56	MG	1a	1827	1/1	0.83	0.13	58,58,58,58	0
56	MG	2A	3501	1/1	0.83	0.18	59,59,59,59	0
56	MG	1A	3316	1/1	0.83	0.23	58,58,58,58	0
56	MG	2A	3577	1/1	0.83	0.22	56,56,56,56	0
56	MG	2A	3606	1/1	0.83	0.19	61,61,61,61	0
56	MG	2w	102	1/1	0.83	0.14	62,62,62,62	0
56	MG	1a	1663	1/1	0.83	0.17	76,76,76,76	0
56	MG	1v	3001	1/1	0.83	0.33	77,77,77,77	0
56	MG	1w	101	1/1	0.83	0.17	64,64,64,64	0
56	MG	2A	3647	1/1	0.83	0.20	51,51,51,51	0
56	MG	2a	3012	1/1	0.83	0.28	71,71,71,71	0
56	MG	2a	3099	1/1	0.84	0.27	74,74,74,74	0
56	MG	1A	4026	1/1	0.84	0.14	51,51,51,51	0
56	MG	1A	3890	1/1	0.84	0.17	57,57,57,57	0
56	MG	2A	3113	1/1	0.84	0.12	52,52,52,52	0
56	MG	2A	3728	1/1	0.84	0.12	58,58,58,58	0
56	MG	2B	3010	1/1	0.84	0.17	73,73,73,73	0
56	MG	1a	1676	1/1	0.84	0.32	67,67,67,67	0
56	MG	2A	3741	1/1	0.84	0.15	61,61,61,61	0
56	MG	2B	3020	1/1	0.84	0.31	78,78,78,78	0
56	MG	1A	3774	1/1	0.84	0.13	55,55,55,55	0
56	MG	2a	3138	1/1	0.84	0.14	79,79,79,79	0
56	MG	1a	1829	1/1	0.84	0.21	73,73,73,73	0
56	MG	1A	3727	1/1	0.84	0.17	36,36,36,36	0
56	MG	2T	3001	1/1	0.84	0.17	53,53,53,53	0
56	MG	2U	202	1/1	0.84	0.14	54,54,54,54	0
56	MG	1a	1704	1/1	0.84	0.23	63,63,63,63	0
56	MG	1A	3853	1/1	0.84	0.13	52,52,52,52	0
56	MG	2A	3770	1/1	0.84	0.13	57,57,57,57	0
56	MG	1A	3871	1/1	0.84	0.24	49,49,49,49	0
56	MG	1A	3323	1/1	0.84	0.17	50,50,50,50	0
56	MG	2A	3810	1/1	0.84	0.15	51,51,51,51	0
56	MG	2A	3819	1/1	0.84	0.20	64,64,64,64	0
56	MG	1w	110	1/1	0.84	0.18	66,66,66,66	0
56	MG	1A	3794	1/1	0.84	0.20	61,61,61,61	0
56	MG	2A	3667	1/1	0.84	0.15	49,49,49,49	0
56	MG	2A	3350	1/1	0.84	0.22	61,61,61,61	0
56	MG	1A	4000	1/1	0.84	0.14	34,34,34,34	0
56	MG	2t	3001	1/1	0.84	0.18	60,60,60,60	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1x	109	1/1	0.84	0.21	82,82,82,82	0
56	MG	2a	3058	1/1	0.84	0.39	73,73,73,73	0
56	MG	2A	3699	1/1	0.84	0.11	76,76,76,76	0
56	MG	2a	3070	1/1	0.84	0.18	61,61,61,61	0
56	MG	2a	3083	1/1	0.84	0.22	72,72,72,72	0
56	MG	1a	1760	1/1	0.84	0.10	74,74,74,74	0
56	MG	1A	3757	1/1	0.84	0.17	27,27,27,27	0
56	MG	2a	3095	1/1	0.84	0.24	71,71,71,71	0
56	MG	2a	3076	1/1	0.85	0.16	73,73,73,73	0
56	MG	1A	3802	1/1	0.85	0.15	57,57,57,57	0
56	MG	2A	3625	1/1	0.85	0.21	69,69,69,69	0
56	MG	1a	1795	1/1	0.85	0.14	70,70,70,70	0
56	MG	2a	3093	1/1	0.85	0.25	64,64,64,64	0
56	MG	2A	3128	1/1	0.85	0.13	48,48,48,48	0
56	MG	1A	3823	1/1	0.85	0.21	65,65,65,65	0
56	MG	1a	1674	1/1	0.85	0.33	72,72,72,72	0
56	MG	2A	3876	1/1	0.85	0.15	66,66,66,66	0
56	MG	1A	4061	1/1	0.85	0.14	72,72,72,72	0
56	MG	1a	1688	1/1	0.85	0.26	74,74,74,74	0
56	MG	2a	3111	1/1	0.85	0.20	76,76,76,76	0
56	MG	2A	3892	1/1	0.85	0.16	78,78,78,78	0
56	MG	2a	3121	1/1	0.85	0.31	75,75,75,75	0
56	MG	2A	3259	1/1	0.85	0.26	61,61,61,61	0
56	MG	1A	3948	1/1	0.85	0.16	60,60,60,60	0
56	MG	2A	3696	1/1	0.85	0.12	58,58,58,58	0
56	MG	2A	3271	1/1	0.85	0.19	49,49,49,49	0
56	MG	1A	3332	1/1	0.85	0.30	56,56,56,56	0
56	MG	2a	3148	1/1	0.85	0.11	77,77,77,77	0
56	MG	2B	3019	1/1	0.85	0.16	76,76,76,76	0
56	MG	2A	3330	1/1	0.85	0.27	63,63,63,63	0
56	MG	2A	3341	1/1	0.85	0.19	52,52,52,52	0
56	MG	2a	3171	1/1	0.85	0.14	73,73,73,73	0
56	MG	2A	3716	1/1	0.85	0.18	55,55,55,55	0
56	MG	1B	3002	1/1	0.85	0.20	58,58,58,58	0
56	MG	1a	1718	1/1	0.85	0.24	70,70,70,70	0
56	MG	1a	1730	1/1	0.85	0.14	80,80,80,80	0
56	MG	2A	3354	1/1	0.85	0.24	68,68,68,68	0
56	MG	2A	3360	1/1	0.85	0.16	63,63,63,63	0
56	MG	1A	3343	1/1	0.85	0.27	59,59,59,59	0
56	MG	1a	1602	1/1	0.85	0.27	72,72,72,72	0
56	MG	1B	3012	1/1	0.85	0.20	55,55,55,55	0
56	MG	2a	3221	1/1	0.85	0.21	60,60,60,60	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1x	114	1/1	0.85	0.22	82,82,82,82	0
56	MG	2A	3439	1/1	0.85	0.16	60,60,60,60	0
56	MG	2a	3230	1/1	0.85	0.13	63,63,63,63	0
56	MG	2a	3233	1/1	0.85	0.16	68,68,68,68	0
56	MG	2a	3234	1/1	0.85	0.14	66,66,66,66	0
56	MG	2a	3236	1/1	0.85	0.14	75,75,75,75	0
56	MG	1y	3002	1/1	0.85	0.22	75,75,75,75	0
56	MG	1A	3630	1/1	0.85	0.12	32,32,32,32	0
56	MG	2n	502	1/1	0.85	0.11	86,86,86,86	0
56	MG	2A	3780	1/1	0.85	0.16	80,80,80,80	0
56	MG	2v	3001	1/1	0.85	0.24	69,69,69,69	0
56	MG	1a	1617	1/1	0.85	0.14	63,63,63,63	0
56	MG	1A	3708	1/1	0.85	0.19	76,76,76,76	0
56	MG	1a	1762	1/1	0.85	0.17	78,78,78,78	0
56	MG	2a	3051	1/1	0.85	0.22	69,69,69,69	0
56	MG	2A	3568	1/1	0.85	0.13	46,46,46,46	0
56	MG	1B	3024	1/1	0.85	0.10	50,50,50,50	0
56	MG	1A	3478	1/1	0.85	0.34	65,65,65,65	0
56	MG	2a	3071	1/1	0.85	0.18	75,75,75,75	0
56	MG	1A	3428	1/1	0.86	0.13	51,51,51,51	0
56	MG	2A	3101	1/1	0.86	0.25	59,59,59,59	0
56	MG	1A	3937	1/1	0.86	0.15	31,31,31,31	0
56	MG	1a	1625	1/1	0.86	0.30	63,63,63,63	0
56	MG	2a	3030	1/1	0.86	0.11	61,61,61,61	0
56	MG	1A	3440	1/1	0.86	0.18	50,50,50,50	0
56	MG	1A	3679	1/1	0.86	0.18	39,39,39,39	0
56	MG	1O	206	1/1	0.86	0.19	84,84,84,84	0
56	MG	2a	3039	1/1	0.86	0.37	73,73,73,73	0
56	MG	1w	105	1/1	0.86	0.16	87,87,87,87	0
56	MG	1A	3970	1/1	0.86	0.13	70,70,70,70	0
56	MG	1V	203	1/1	0.86	0.17	67,67,67,67	0
56	MG	2a	3053	1/1	0.86	0.29	66,66,66,66	0
56	MG	2A	3245	1/1	0.86	0.20	59,59,59,59	0
56	MG	2A	3468	1/1	0.86	0.33	59,59,59,59	0
56	MG	2a	3064	1/1	0.86	0.19	81,81,81,81	0
56	MG	2A	3481	1/1	0.86	0.20	56,56,56,56	0
56	MG	1A	3692	1/1	0.86	0.20	64,64,64,64	0
56	MG	2A	3520	1/1	0.86	0.26	65,65,65,65	0
56	MG	1A	3488	1/1	0.86	0.21	59,59,59,59	0
56	MG	2a	3232	1/1	0.86	0.18	77,77,77,77	0
56	MG	1a	1677	1/1	0.86	0.21	68,68,68,68	0
56	MG	1A	3350	1/1	0.86	0.28	59,59,59,59	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3290	1/1	0.86	0.23	50,50,50,50	0
56	MG	2A	3757	1/1	0.86	0.13	52,52,52,52	0
56	MG	1y	3001	1/1	0.86	0.12	64,64,64,64	0
56	MG	2j	8002	1/1	0.86	0.13	66,66,66,66	0
56	MG	2A	3610	1/1	0.86	0.15	67,67,67,67	0
56	MG	2A	3295	1/1	0.86	0.16	63,63,63,63	0
56	MG	1A	3357	1/1	0.86	0.16	56,56,56,56	0
56	MG	2A	3799	1/1	0.86	0.22	68,68,68,68	0
56	MG	2A	3802	1/1	0.86	0.08	56,56,56,56	0
56	MG	28	102	1/1	0.86	0.16	52,52,52,52	0
56	MG	2a	3120	1/1	0.86	0.21	72,72,72,72	0
56	MG	1a	1790	1/1	0.86	0.13	73,73,73,73	0
56	MG	1A	3245	1/1	0.86	0.21	64,64,64,64	0
56	MG	2a	3008	1/1	0.86	0.29	68,68,68,68	0
56	MG	1a	1702	1/1	0.86	0.43	73,73,73,73	0
56	MG	1A	3424	1/1	0.87	0.23	70,70,70,70	0
56	MG	1A	3863	1/1	0.87	0.23	50,50,50,50	0
56	MG	2a	3048	1/1	0.87	0.27	67,67,67,67	0
56	MG	2a	3050	1/1	0.87	0.26	61,61,61,61	0
56	MG	2A	3023	1/1	0.87	0.11	48,48,48,48	0
56	MG	1a	1660	1/1	0.87	0.15	74,74,74,74	0
56	MG	2A	3421	1/1	0.87	0.22	61,61,61,61	0
56	MG	2A	3428	1/1	0.87	0.12	52,52,52,52	0
56	MG	2a	3063	1/1	0.87	0.18	74,74,74,74	0
56	MG	2A	3437	1/1	0.87	0.14	67,67,67,67	0
56	MG	2A	3051	1/1	0.87	0.11	43,43,43,43	0
56	MG	1a	1766	1/1	0.87	0.29	76,76,76,76	0
56	MG	2A	3062	1/1	0.87	0.18	61,61,61,61	0
56	MG	2A	3459	1/1	0.87	0.18	62,62,62,62	0
56	MG	1A	3987	1/1	0.87	0.11	32,32,32,32	0
56	MG	2A	3096	1/1	0.87	0.12	59,59,59,59	0
56	MG	2A	3814	1/1	0.87	0.19	55,55,55,55	0
56	MG	1A	3541	1/1	0.87	0.16	73,73,73,73	0
56	MG	2A	3488	1/1	0.87	0.18	65,65,65,65	0
56	MG	1a	1669	1/1	0.87	0.19	73,73,73,73	0
56	MG	2A	3829	1/1	0.87	0.13	59,59,59,59	0
56	MG	2A	3505	1/1	0.87	0.16	59,59,59,59	0
56	MG	2A	3507	1/1	0.87	0.20	64,64,64,64	0
56	MG	1a	1789	1/1	0.87	0.13	72,72,72,72	0
56	MG	1A	3696	1/1	0.87	0.14	61,61,61,61	0
56	MG	1A	4012	1/1	0.87	0.12	34,34,34,34	0
56	MG	1a	1797	1/1	0.87	0.15	64,64,64,64	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3601	1/1	0.87	0.11	39,39,39,39	0
56	MG	2A	3605	1/1	0.87	0.12	51,51,51,51	0
56	MG	1A	3544	1/1	0.87	0.10	47,47,47,47	0
56	MG	2a	3135	1/1	0.87	0.15	62,62,62,62	0
56	MG	2A	3883	1/1	0.87	0.18	56,56,56,56	0
56	MG	1A	3407	1/1	0.87	0.14	65,65,65,65	0
56	MG	2A	3220	1/1	0.87	0.27	68,68,68,68	0
56	MG	2A	3614	1/1	0.87	0.12	36,36,36,36	0
56	MG	2A	3906	1/1	0.87	0.35	62,62,62,62	0
56	MG	2B	3002	1/1	0.87	0.10	49,49,49,49	0
56	MG	1A	4033	1/1	0.87	0.11	76,76,76,76	0
56	MG	2B	3006	1/1	0.87	0.16	59,59,59,59	0
56	MG	2a	3187	1/1	0.87	0.20	72,72,72,72	0
56	MG	2A	3626	1/1	0.87	0.13	53,53,53,53	0
56	MG	2A	3635	1/1	0.87	0.17	43,43,43,43	0
56	MG	1A	3667	1/1	0.87	0.12	61,61,61,61	0
56	MG	1A	3432	1/1	0.87	0.16	54,54,54,54	0
56	MG	1n	102	1/1	0.87	0.31	66,66,66,66	0
56	MG	2A	3649	1/1	0.87	0.15	69,69,69,69	0
56	MG	1A	3895	1/1	0.87	0.14	61,61,61,61	0
56	MG	19	102	1/1	0.87	0.17	51,51,51,51	0
56	MG	2a	3220	1/1	0.87	0.16	66,66,66,66	0
56	MG	1w	104	1/1	0.87	0.23	69,69,69,69	0
56	MG	2a	3224	1/1	0.87	0.20	74,74,74,74	0
56	MG	2a	3226	1/1	0.87	0.27	64,64,64,64	0
56	MG	1A	3752	1/1	0.87	0.13	41,41,41,41	0
56	MG	1a	1721	1/1	0.87	0.14	58,58,58,58	0
56	MG	2A	3307	1/1	0.87	0.23	68,68,68,68	0
56	MG	2A	3326	1/1	0.87	0.31	64,64,64,64	0
56	MG	2a	3005	1/1	0.87	0.39	75,75,75,75	0
56	MG	2a	3006	1/1	0.87	0.22	74,74,74,74	0
56	MG	1a	1603	1/1	0.87	0.11	59,59,59,59	0
56	MG	2a	3238	1/1	0.87	0.20	62,62,62,62	0
56	MG	2A	3703	1/1	0.87	0.11	47,47,47,47	0
56	MG	2A	3336	1/1	0.87	0.14	53,53,53,53	0
56	MG	2A	3711	1/1	0.87	0.20	56,56,56,56	0
56	MG	2l	202	1/1	0.87	0.10	70,70,70,70	0
56	MG	1A	3218	1/1	0.87	0.18	62,62,62,62	0
56	MG	2a	3017	1/1	0.87	0.17	66,66,66,66	0
56	MG	2a	3019	1/1	0.87	0.14	57,57,57,57	0
56	MG	1a	1743	1/1	0.87	0.17	73,73,73,73	0
56	MG	2A	3346	1/1	0.87	0.12	54,54,54,54	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3766	1/1	0.87	0.12	47,47,47,47	0
56	MG	2a	3033	1/1	0.87	0.14	63,63,63,63	0
56	MG	1x	111	1/1	0.87	0.25	66,66,66,66	0
56	MG	1A	3685	1/1	0.87	0.23	60,60,60,60	0
56	MG	2y	3002	1/1	0.87	0.17	64,64,64,64	0
56	MG	1A	3691	1/1	0.87	0.20	41,41,41,41	0
56	MG	2A	3743	1/1	0.87	0.14	75,75,75,75	0
56	MG	1A	3370	1/1	0.88	0.21	57,57,57,57	0
56	MG	2A	3333	1/1	0.88	0.14	55,55,55,55	0
56	MG	1a	1666	1/1	0.88	0.14	59,59,59,59	0
56	MG	1A	3623	1/1	0.88	0.17	59,59,59,59	0
56	MG	1w	106	1/1	0.88	0.27	74,74,74,74	0
56	MG	1A	4113	1/1	0.88	0.17	56,56,56,56	0
56	MG	2A	3733	1/1	0.88	0.14	50,50,50,50	0
56	MG	1A	3377	1/1	0.88	0.16	54,54,54,54	0
56	MG	1A	3143	1/1	0.88	0.22	55,55,55,55	0
56	MG	1A	3278	1/1	0.88	0.12	51,51,51,51	0
56	MG	1A	3783	1/1	0.88	0.14	34,34,34,34	0
56	MG	1A	3648	1/1	0.88	0.12	55,55,55,55	0
56	MG	1A	3897	1/1	0.88	0.21	62,62,62,62	0
56	MG	2a	3059	1/1	0.88	0.24	74,74,74,74	0
56	MG	1B	3028	1/1	0.88	0.09	61,61,61,61	0
56	MG	2A	3378	1/1	0.88	0.13	62,62,62,62	0
56	MG	2A	3766	1/1	0.88	0.15	52,52,52,52	0
56	MG	2a	3069	1/1	0.88	0.13	62,62,62,62	0
56	MG	1A	3504	1/1	0.88	0.13	44,44,44,44	0
56	MG	2A	3413	1/1	0.88	0.14	56,56,56,56	0
56	MG	1A	3299	1/1	0.88	0.29	61,61,61,61	0
56	MG	2A	3425	1/1	0.88	0.20	58,58,58,58	0
56	MG	2A	3795	1/1	0.88	0.13	37,37,37,37	0
56	MG	1E	302	1/1	0.88	0.28	58,58,58,58	0
56	MG	1a	1726	1/1	0.88	0.40	67,67,67,67	0
56	MG	2A	3438	1/1	0.88	0.26	68,68,68,68	0
56	MG	1A	3918	1/1	0.88	0.13	56,56,56,56	0
56	MG	2A	3812	1/1	0.88	0.10	47,47,47,47	0
56	MG	2A	3441	1/1	0.88	0.11	51,51,51,51	0
56	MG	2a	3106	1/1	0.88	0.19	62,62,62,62	0
56	MG	2A	3056	1/1	0.88	0.13	60,60,60,60	0
56	MG	1a	1735	1/1	0.88	0.20	57,57,57,57	0
56	MG	1A	3333	1/1	0.88	0.18	52,52,52,52	0
56	MG	2A	3066	1/1	0.88	0.10	41,41,41,41	0
56	MG	2A	3832	1/1	0.88	0.11	54,54,54,54	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1G	3005	1/1	0.88	0.16	66,66,66,66	0
56	MG	2A	3470	1/1	0.88	0.18	56,56,56,56	0
56	MG	2A	3854	1/1	0.88	0.11	77,77,77,77	0
56	MG	2A	3472	1/1	0.88	0.21	60,60,60,60	0
56	MG	1A	3308	1/1	0.88	0.19	51,51,51,51	0
56	MG	2A	3860	1/1	0.88	0.14	59,59,59,59	0
56	MG	2A	3100	1/1	0.88	0.12	57,57,57,57	0
56	MG	2a	3146	1/1	0.88	0.14	84,84,84,84	0
56	MG	2A	3500	1/1	0.88	0.16	55,55,55,55	0
56	MG	1R	203	1/1	0.88	0.19	47,47,47,47	0
56	MG	2A	3104	1/1	0.88	0.12	53,53,53,53	0
56	MG	2A	3506	1/1	0.88	0.18	31,31,31,31	0
56	MG	1A	3951	1/1	0.88	0.15	72,72,72,72	0
56	MG	1A	3348	1/1	0.88	0.15	62,62,62,62	0
56	MG	2a	3182	1/1	0.88	0.17	71,71,71,71	0
56	MG	1A	3542	1/1	0.88	0.29	75,75,75,75	0
56	MG	2A	3553	1/1	0.88	0.13	71,71,71,71	0
56	MG	2a	3193	1/1	0.88	0.28	73,73,73,73	0
56	MG	1A	3441	1/1	0.88	0.21	56,56,56,56	0
56	MG	2B	3001	1/1	0.88	0.21	62,62,62,62	0
56	MG	1A	3983	1/1	0.88	0.14	48,48,48,48	0
56	MG	1A	3444	1/1	0.88	0.33	63,63,63,63	0
56	MG	2B	3004	1/1	0.88	0.16	69,69,69,69	0
56	MG	2A	3604	1/1	0.88	0.26	64,64,64,64	0
56	MG	2B	3008	1/1	0.88	0.15	58,58,58,58	0
56	MG	2a	3214	1/1	0.88	0.09	91,91,91,91	0
56	MG	1A	3215	1/1	0.88	0.15	65,65,65,65	0
56	MG	2B	3011	1/1	0.88	0.25	67,67,67,67	0
56	MG	2A	3171	1/1	0.88	0.11	38,38,38,38	0
56	MG	1A	3997	1/1	0.88	0.12	39,39,39,39	0
56	MG	1A	3711	1/1	0.88	0.12	61,61,61,61	0
56	MG	2A	3239	1/1	0.88	0.14	52,52,52,52	0
56	MG	2A	3615	1/1	0.88	0.11	51,51,51,51	0
56	MG	2a	3231	1/1	0.88	0.11	68,68,68,68	0
56	MG	1A	3833	1/1	0.88	0.16	60,60,60,60	0
56	MG	1a	1613	1/1	0.88	0.11	74,74,74,74	0
56	MG	2O	8001	1/1	0.88	0.20	65,65,65,65	0
56	MG	2A	3257	1/1	0.88	0.25	65,65,65,65	0
56	MG	1A	3557	1/1	0.88	0.34	60,60,60,60	0
56	MG	1A	3836	1/1	0.88	0.20	54,54,54,54	0
56	MG	2A	3268	1/1	0.88	0.16	63,63,63,63	0
56	MG	1a	1630	1/1	0.88	0.12	60,60,60,60	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3281	1/1	0.88	0.15	63,63,63,63	0
56	MG	1a	1636	1/1	0.88	0.16	67,67,67,67	0
56	MG	2r	102	1/1	0.88	0.14	73,73,73,73	0
56	MG	2A	3685	1/1	0.88	0.10	53,53,53,53	0
56	MG	1A	3268	1/1	0.88	0.32	59,59,59,59	0
56	MG	1A	3856	1/1	0.88	0.16	47,47,47,47	0
56	MG	2A	3301	1/1	0.88	0.12	60,60,60,60	0
56	MG	2A	3304	1/1	0.88	0.17	60,60,60,60	0
56	MG	2A	3305	1/1	0.88	0.13	56,56,56,56	0
56	MG	1A	4049	1/1	0.88	0.11	55,55,55,55	0
56	MG	2a	3021	1/1	0.88	0.23	65,65,65,65	0
56	MG	2A	3322	1/1	0.88	0.16	60,60,60,60	0
56	MG	2a	3026	1/1	0.88	0.25	64,64,64,64	0
56	MG	1A	3581	1/1	0.88	0.19	58,58,58,58	0
56	MG	1A	3305	1/1	0.89	0.27	55,55,55,55	0
56	MG	1a	1623	1/1	0.89	0.14	60,60,60,60	0
56	MG	1a	1624	1/1	0.89	0.12	50,50,50,50	0
56	MG	2A	3261	1/1	0.89	0.17	59,59,59,59	0
56	MG	1A	3209	1/1	0.89	0.15	68,68,68,68	0
56	MG	2a	3014	1/1	0.89	0.18	64,64,64,64	0
56	MG	1a	1629	1/1	0.89	0.13	57,57,57,57	0
56	MG	2a	3018	1/1	0.89	0.26	65,65,65,65	0
56	MG	1A	4103	1/1	0.89	0.14	67,67,67,67	0
56	MG	1a	1633	1/1	0.89	0.15	60,60,60,60	0
56	MG	2A	3654	1/1	0.89	0.19	62,62,62,62	0
56	MG	2A	3655	1/1	0.89	0.13	65,65,65,65	0
56	MG	2A	3286	1/1	0.89	0.20	55,55,55,55	0
56	MG	1A	4104	1/1	0.89	0.09	30,30,30,30	0
56	MG	2a	3032	1/1	0.89	0.22	60,60,60,60	0
56	MG	1A	3392	1/1	0.89	0.19	56,56,56,56	0
56	MG	1A	3595	1/1	0.89	0.14	59,59,59,59	0
56	MG	1A	3901	1/1	0.89	0.22	43,43,43,43	0
56	MG	1a	1661	1/1	0.89	0.21	70,70,70,70	0
56	MG	1A	3699	1/1	0.89	0.18	64,64,64,64	0
56	MG	1A	3805	1/1	0.89	0.12	54,54,54,54	0
56	MG	2A	3309	1/1	0.89	0.12	53,53,53,53	0
56	MG	1A	3610	1/1	0.89	0.18	54,54,54,54	0
56	MG	1A	3926	1/1	0.89	0.17	53,53,53,53	0
56	MG	1B	3025	1/1	0.89	0.16	77,77,77,77	0
56	MG	2A	3332	1/1	0.89	0.14	62,62,62,62	0
56	MG	1A	3344	1/1	0.89	0.25	64,64,64,64	0
56	MG	1A	3322	1/1	0.89	0.20	59,59,59,59	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1x	104	1/1	0.89	0.23	72,72,72,72	0
56	MG	1x	108	1/1	0.89	0.19	63,63,63,63	0
56	MG	1A	3723	1/1	0.89	0.09	47,47,47,47	0
56	MG	1B	3035	1/1	0.89	0.11	59,59,59,59	0
56	MG	2A	3738	1/1	0.89	0.16	59,59,59,59	0
56	MG	2A	3740	1/1	0.89	0.13	53,53,53,53	0
56	MG	1x	113	1/1	0.89	0.18	62,62,62,62	0
56	MG	2a	3081	1/1	0.89	0.12	49,49,49,49	0
56	MG	1A	3315	1/1	0.89	0.25	61,61,61,61	0
56	MG	1x	115	1/1	0.89	0.16	75,75,75,75	0
56	MG	2A	3747	1/1	0.89	0.13	51,51,51,51	0
56	MG	1a	1691	1/1	0.89	0.26	69,69,69,69	0
56	MG	1a	1694	1/1	0.89	0.14	58,58,58,58	0
56	MG	1A	3645	1/1	0.89	0.11	37,37,37,37	0
56	MG	2A	3008	1/1	0.89	0.14	49,49,49,49	0
56	MG	2A	3765	1/1	0.89	0.13	53,53,53,53	0
56	MG	2A	3380	1/1	0.89	0.11	55,55,55,55	0
56	MG	2A	3384	1/1	0.89	0.14	62,62,62,62	0
56	MG	2A	3393	1/1	0.89	0.10	48,48,48,48	0
56	MG	2A	3397	1/1	0.89	0.16	54,54,54,54	0
56	MG	1G	3002	1/1	0.89	0.15	56,56,56,56	0
56	MG	2a	3119	1/1	0.89	0.26	71,71,71,71	0
56	MG	2A	3408	1/1	0.89	0.10	51,51,51,51	0
56	MG	2A	3410	1/1	0.89	0.19	55,55,55,55	0
56	MG	2A	3412	1/1	0.89	0.20	59,59,59,59	0
56	MG	2A	3805	1/1	0.89	0.17	77,77,77,77	0
56	MG	1A	3744	1/1	0.89	0.22	74,74,74,74	0
56	MG	1A	3745	1/1	0.89	0.14	19,19,19,19	0
56	MG	2A	3424	1/1	0.89	0.21	50,50,50,50	0
56	MG	1O	201	1/1	0.89	0.18	63,63,63,63	0
56	MG	2a	3141	1/1	0.89	0.14	94,94,94,94	0
56	MG	1A	3850	1/1	0.89	0.11	53,53,53,53	0
56	MG	2A	3429	1/1	0.89	0.09	65,65,65,65	0
56	MG	1a	1727	1/1	0.89	0.15	49,49,49,49	0
56	MG	2a	3156	1/1	0.89	0.10	69,69,69,69	0
56	MG	1A	3425	1/1	0.89	0.11	55,55,55,55	0
56	MG	2A	3080	1/1	0.89	0.15	58,58,58,58	0
56	MG	2A	3836	1/1	0.89	0.20	42,42,42,42	0
56	MG	1T	8001	1/1	0.89	0.16	63,63,63,63	0
56	MG	1A	3855	1/1	0.89	0.20	53,53,53,53	0
56	MG	2A	3450	1/1	0.89	0.24	50,50,50,50	0
56	MG	2a	3190	1/1	0.89	0.17	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
56	MG	2A	3452	1/1	0.89	0.21	42,42,42,42	0
56	MG	1A	3545	1/1	0.89	0.14	67,67,67,67	0
56	MG	1A	3649	1/1	0.89	0.10	54,54,54,54	0
56	MG	2A	3463	1/1	0.89	0.16	57,57,57,57	0
56	MG	2A	3867	1/1	0.89	0.09	64,64,64,64	0
56	MG	1A	4022	1/1	0.89	0.08	72,72,72,72	0
56	MG	1A	3866	1/1	0.89	0.18	46,46,46,46	0
56	MG	2a	3205	1/1	0.89	0.27	70,70,70,70	0
56	MG	2A	3469	1/1	0.89	0.17	55,55,55,55	0
56	MG	2a	3209	1/1	0.89	0.24	77,77,77,77	0
56	MG	1a	1751	1/1	0.89	0.16	70,70,70,70	0
56	MG	1a	1752	1/1	0.89	0.13	68,68,68,68	0
56	MG	2A	3119	1/1	0.89	0.14	47,47,47,47	0
56	MG	1A	3867	1/1	0.89	0.16	69,69,69,69	0
56	MG	1A	3484	1/1	0.89	0.13	54,54,54,54	0
56	MG	2A	3130	1/1	0.89	0.17	53,53,53,53	0
56	MG	2a	3227	1/1	0.89	0.18	59,59,59,59	0
56	MG	1A	3026	1/1	0.89	0.16	60,60,60,60	0
56	MG	2A	3147	1/1	0.89	0.18	58,58,58,58	0
56	MG	2A	3152	1/1	0.89	0.12	62,62,62,62	0
56	MG	2A	3515	1/1	0.89	0.11	55,55,55,55	0
56	MG	2A	3518	1/1	0.89	0.13	52,52,52,52	0
56	MG	2A	3153	1/1	0.89	0.18	52,52,52,52	0
56	MG	2A	3521	1/1	0.89	0.13	51,51,51,51	0
56	MG	2A	3535	1/1	0.89	0.22	59,59,59,59	0
56	MG	1a	1605	1/1	0.89	0.11	65,65,65,65	0
56	MG	2A	3540	1/1	0.89	0.10	47,47,47,47	0
56	MG	2d	502	1/1	0.89	0.17	68,68,68,68	0
56	MG	2g	8001	1/1	0.89	0.13	75,75,75,75	0
56	MG	2B	3017	1/1	0.89	0.13	65,65,65,65	0
56	MG	2A	3546	1/1	0.89	0.10	44,44,44,44	0
56	MG	2A	3549	1/1	0.89	0.16	58,58,58,58	0
56	MG	1a	1767	1/1	0.89	0.16	66,66,66,66	0
56	MG	2q	202	1/1	0.89	0.12	78,78,78,78	0
56	MG	2A	3555	1/1	0.89	0.12	43,43,43,43	0
56	MG	2A	3198	1/1	0.89	0.12	61,61,61,61	0
56	MG	2A	3206	1/1	0.89	0.20	56,56,56,56	0
56	MG	2A	3218	1/1	0.89	0.15	61,61,61,61	0
56	MG	1A	3362	1/1	0.89	0.16	54,54,54,54	0
56	MG	2W	202	1/1	0.89	0.11	58,58,58,58	0
56	MG	2A	3228	1/1	0.89	0.30	65,65,65,65	0
56	MG	20	3001	1/1	0.89	0.17	59,59,59,59	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3558	1/1	0.89	0.12	52,52,52,52	0
56	MG	1a	1779	1/1	0.89	0.12	65,65,65,65	0
56	MG	1A	4066	1/1	0.89	0.11	71,71,71,71	0
56	MG	2A	3255	1/1	0.89	0.12	59,59,59,59	0
58	ZN	24	501	1/1	0.89	0.11	128,128,128,128	0
56	MG	2A	3183	1/1	0.90	0.12	56,56,56,56	0
56	MG	2A	3186	1/1	0.90	0.17	54,54,54,54	0
56	MG	2A	3189	1/1	0.90	0.11	52,52,52,52	0
56	MG	1A	3418	1/1	0.90	0.14	54,54,54,54	0
56	MG	2A	3556	1/1	0.90	0.15	43,43,43,43	0
56	MG	2W	203	1/1	0.90	0.15	59,59,59,59	0
56	MG	1A	3525	1/1	0.90	0.22	58,58,58,58	0
56	MG	2A	3573	1/1	0.90	0.10	42,42,42,42	0
56	MG	23	101	1/1	0.90	0.17	61,61,61,61	0
56	MG	2A	3209	1/1	0.90	0.15	61,61,61,61	0
56	MG	2A	3579	1/1	0.90	0.17	60,60,60,60	0
56	MG	2A	3583	1/1	0.90	0.26	69,69,69,69	0
56	MG	11	103	1/1	0.90	0.09	65,65,65,65	0
56	MG	13	103	1/1	0.90	0.12	47,47,47,47	0
56	MG	1A	3821	1/1	0.90	0.13	47,47,47,47	0
56	MG	1a	1770	1/1	0.90	0.18	60,60,60,60	0
56	MG	16	104	1/1	0.90	0.20	53,53,53,53	0
56	MG	2A	3244	1/1	0.90	0.13	54,54,54,54	0
56	MG	18	103	1/1	0.90	0.13	72,72,72,72	0
56	MG	1A	3422	1/1	0.90	0.17	38,38,38,38	0
56	MG	2A	3619	1/1	0.90	0.14	37,37,37,37	0
56	MG	2A	3620	1/1	0.90	0.22	65,65,65,65	0
56	MG	2a	3020	1/1	0.90	0.16	71,71,71,71	0
56	MG	1a	1601	1/1	0.90	0.10	53,53,53,53	0
56	MG	1A	3342	1/1	0.90	0.14	57,57,57,57	0
56	MG	1A	4007	1/1	0.90	0.08	86,86,86,86	0
56	MG	2A	3642	1/1	0.90	0.16	47,47,47,47	0
56	MG	2a	3029	1/1	0.90	0.17	67,67,67,67	0
56	MG	1a	1794	1/1	0.90	0.12	52,52,52,52	0
56	MG	2a	3031	1/1	0.90	0.11	49,49,49,49	0
56	MG	2A	3265	1/1	0.90	0.15	59,59,59,59	0
56	MG	1A	3687	1/1	0.90	0.11	31,31,31,31	0
56	MG	1A	3053	1/1	0.90	0.13	52,52,52,52	0
56	MG	1a	1803	1/1	0.90	0.11	73,73,73,73	0
56	MG	1A	3312	1/1	0.90	0.33	59,59,59,59	0
56	MG	2a	3038	1/1	0.90	0.09	68,68,68,68	0
56	MG	1A	3082	1/1	0.90	0.19	49,49,49,49	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3664	1/1	0.90	0.11	54,54,54,54	0
56	MG	2a	3044	1/1	0.90	0.19	57,57,57,57	0
56	MG	2A	3287	1/1	0.90	0.16	55,55,55,55	0
56	MG	2A	3681	1/1	0.90	0.11	50,50,50,50	0
56	MG	1A	3188	1/1	0.90	0.12	49,49,49,49	0
56	MG	1d	502	1/1	0.90	0.29	67,67,67,67	0
56	MG	1a	1620	1/1	0.90	0.16	66,66,66,66	0
56	MG	2a	3056	1/1	0.90	0.22	63,63,63,63	0
56	MG	2a	3057	1/1	0.90	0.20	71,71,71,71	0
56	MG	1A	3698	1/1	0.90	0.12	73,73,73,73	0
56	MG	2A	3694	1/1	0.90	0.11	51,51,51,51	0
56	MG	1A	3189	1/1	0.90	0.23	43,43,43,43	0
56	MG	1A	4053	1/1	0.90	0.21	37,37,37,37	0
56	MG	1A	4060	1/1	0.90	0.09	37,37,37,37	0
56	MG	2A	3702	1/1	0.90	0.08	49,49,49,49	0
56	MG	1A	3703	1/1	0.90	0.12	56,56,56,56	0
56	MG	2A	3708	1/1	0.90	0.11	53,53,53,53	0
56	MG	2A	3313	1/1	0.90	0.27	64,64,64,64	0
56	MG	1A	3854	1/1	0.90	0.12	51,51,51,51	0
56	MG	1A	4068	1/1	0.90	0.14	48,48,48,48	0
56	MG	1w	107	1/1	0.90	0.32	67,67,67,67	0
56	MG	2a	3088	1/1	0.90	0.19	62,62,62,62	0
56	MG	2A	3717	1/1	0.90	0.11	39,39,39,39	0
56	MG	2a	3091	1/1	0.90	0.19	76,76,76,76	0
56	MG	1a	1639	1/1	0.90	0.14	62,62,62,62	0
56	MG	2a	3094	1/1	0.90	0.22	68,68,68,68	0
56	MG	1a	1640	1/1	0.90	0.14	58,58,58,58	0
56	MG	2a	3096	1/1	0.90	0.14	65,65,65,65	0
56	MG	1x	101	1/1	0.90	0.11	56,56,56,56	0
56	MG	2a	3101	1/1	0.90	0.16	56,56,56,56	0
56	MG	2A	3731	1/1	0.90	0.15	57,57,57,57	0
56	MG	2A	3340	1/1	0.90	0.13	51,51,51,51	0
56	MG	1A	3361	1/1	0.90	0.11	49,49,49,49	0
56	MG	1A	3298	1/1	0.90	0.11	43,43,43,43	0
56	MG	2A	3345	1/1	0.90	0.15	59,59,59,59	0
56	MG	1A	4084	1/1	0.90	0.10	50,50,50,50	0
56	MG	2a	3116	1/1	0.90	0.20	67,67,67,67	0
56	MG	2A	3348	1/1	0.90	0.16	48,48,48,48	0
56	MG	1x	106	1/1	0.90	0.15	63,63,63,63	0
56	MG	2A	3745	1/1	0.90	0.14	56,56,56,56	0
56	MG	1A	3445	1/1	0.90	0.34	62,62,62,62	0
56	MG	2a	3122	1/1	0.90	0.27	73,73,73,73	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	3126	1/1	0.90	0.26	69,69,69,69	0
56	MG	1A	3253	1/1	0.90	0.09	61,61,61,61	0
56	MG	1A	3724	1/1	0.90	0.14	58,58,58,58	0
56	MG	1A	4116	1/1	0.90	0.12	41,41,41,41	0
56	MG	1A	4120	1/1	0.90	0.13	44,44,44,44	0
56	MG	2A	3758	1/1	0.90	0.13	58,58,58,58	0
56	MG	2A	3764	1/1	0.90	0.13	66,66,66,66	0
56	MG	1A	3870	1/1	0.90	0.11	39,39,39,39	0
56	MG	2a	3145	1/1	0.90	0.09	76,76,76,76	0
56	MG	1A	3572	1/1	0.90	0.11	55,55,55,55	0
56	MG	1A	3732	1/1	0.90	0.21	64,64,64,64	0
56	MG	2A	3381	1/1	0.90	0.11	53,53,53,53	0
56	MG	1y	3003	1/1	0.90	0.26	71,71,71,71	0
56	MG	2A	3386	1/1	0.90	0.22	63,63,63,63	0
56	MG	2A	3783	1/1	0.90	0.16	58,58,58,58	0
56	MG	2A	3387	1/1	0.90	0.19	59,59,59,59	0
56	MG	2a	3174	1/1	0.90	0.13	69,69,69,69	0
56	MG	2a	3178	1/1	0.90	0.12	75,75,75,75	0
56	MG	2A	3798	1/1	0.90	0.14	52,52,52,52	0
56	MG	1A	3304	1/1	0.90	0.28	55,55,55,55	0
56	MG	2A	3006	1/1	0.90	0.26	56,56,56,56	0
56	MG	1a	1682	1/1	0.90	0.10	66,66,66,66	0
56	MG	1a	1683	1/1	0.90	0.14	61,61,61,61	0
56	MG	1A	3737	1/1	0.90	0.14	57,57,57,57	0
56	MG	2a	3197	1/1	0.90	0.10	69,69,69,69	0
56	MG	2A	3050	1/1	0.90	0.09	51,51,51,51	0
56	MG	1A	3378	1/1	0.90	0.13	53,53,53,53	0
56	MG	2A	3815	1/1	0.90	0.17	48,48,48,48	0
56	MG	2A	3818	1/1	0.90	0.18	66,66,66,66	0
56	MG	2A	3420	1/1	0.90	0.14	43,43,43,43	0
56	MG	2A	3053	1/1	0.90	0.15	54,54,54,54	0
56	MG	1A	3471	1/1	0.90	0.21	57,57,57,57	0
56	MG	2A	3827	1/1	0.90	0.14	58,58,58,58	0
56	MG	1A	3607	1/1	0.90	0.11	35,35,35,35	0
56	MG	2A	3426	1/1	0.90	0.18	63,63,63,63	0
56	MG	2a	3215	1/1	0.90	0.17	71,71,71,71	0
56	MG	2a	3219	1/1	0.90	0.12	65,65,65,65	0
56	MG	1A	3754	1/1	0.90	0.15	48,48,48,48	0
56	MG	2A	3064	1/1	0.90	0.10	51,51,51,51	0
56	MG	2A	3065	1/1	0.90	0.19	57,57,57,57	0
56	MG	1A	3472	1/1	0.90	0.15	56,56,56,56	0
56	MG	2A	3071	1/1	0.90	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
56	MG	1A	3905	1/1	0.90	0.14	46,46,46,46	0
56	MG	2A	3090	1/1	0.90	0.14	60,60,60,60	0
56	MG	1a	1705	1/1	0.90	0.30	63,63,63,63	0
56	MG	2A	3094	1/1	0.90	0.13	44,44,44,44	0
56	MG	1a	1709	1/1	0.90	0.14	59,59,59,59	0
56	MG	2A	3458	1/1	0.90	0.19	65,65,65,65	0
56	MG	1A	3618	1/1	0.90	0.14	56,56,56,56	0
56	MG	2a	3235	1/1	0.90	0.13	71,71,71,71	0
56	MG	1a	1720	1/1	0.90	0.21	67,67,67,67	0
56	MG	2a	3237	1/1	0.90	0.33	66,66,66,66	0
56	MG	1A	3770	1/1	0.90	0.09	74,74,74,74	0
56	MG	2A	3110	1/1	0.90	0.11	58,58,58,58	0
56	MG	2a	3242	1/1	0.90	0.18	55,55,55,55	0
56	MG	2A	3888	1/1	0.90	0.13	57,57,57,57	0
56	MG	1F	302	1/1	0.90	0.13	47,47,47,47	0
56	MG	1A	3386	1/1	0.90	0.19	54,54,54,54	0
56	MG	2A	3894	1/1	0.90	0.13	55,55,55,55	0
56	MG	1a	1729	1/1	0.90	0.27	61,61,61,61	0
56	MG	1A	3203	1/1	0.90	0.11	50,50,50,50	0
56	MG	2A	3123	1/1	0.90	0.16	56,56,56,56	0
56	MG	1a	1733	1/1	0.90	0.10	58,58,58,58	0
56	MG	1A	3406	1/1	0.90	0.17	47,47,47,47	0
56	MG	1A	3307	1/1	0.90	0.22	45,45,45,45	0
56	MG	2A	3134	1/1	0.90	0.16	72,72,72,72	0
56	MG	1A	3489	1/1	0.90	0.13	44,44,44,44	0
56	MG	1A	3955	1/1	0.90	0.11	30,30,30,30	0
56	MG	1A	3412	1/1	0.90	0.20	52,52,52,52	0
56	MG	1T	8002	1/1	0.90	0.13	58,58,58,58	0
56	MG	2A	3168	1/1	0.90	0.20	52,52,52,52	0
56	MG	1A	3512	1/1	0.90	0.11	50,50,50,50	0
56	MG	2y	3003	1/1	0.90	0.15	70,70,70,70	0
56	MG	1A	3665	1/1	0.90	0.13	60,60,60,60	0
56	MG	2A	3175	1/1	0.90	0.18	65,65,65,65	0
56	MG	2A	3544	1/1	0.90	0.11	42,42,42,42	0
56	MG	2A	3630	1/1	0.91	0.15	69,69,69,69	0
56	MG	1A	3560	1/1	0.91	0.25	55,55,55,55	0
56	MG	2A	3637	1/1	0.91	0.09	42,42,42,42	0
56	MG	2A	3308	1/1	0.91	0.11	49,49,49,49	0
56	MG	1N	201	1/1	0.91	0.36	59,59,59,59	0
56	MG	2A	3312	1/1	0.91	0.12	51,51,51,51	0
56	MG	2a	3015	1/1	0.91	0.25	62,62,62,62	0
56	MG	2a	3016	1/1	0.91	0.17	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
56	MG	2A	3001	1/1	0.91	0.15	47,47,47,47	0
56	MG	2A	3317	1/1	0.91	0.12	55,55,55,55	0
56	MG	1N	205	1/1	0.91	0.18	57,57,57,57	0
56	MG	1a	1710	1/1	0.91	0.37	77,77,77,77	0
56	MG	1a	1712	1/1	0.91	0.24	67,67,67,67	0
56	MG	2a	3022	1/1	0.91	0.13	72,72,72,72	0
56	MG	1a	1713	1/1	0.91	0.10	68,68,68,68	0
56	MG	2A	3042	1/1	0.91	0.13	42,42,42,42	0
56	MG	2A	3670	1/1	0.91	0.18	70,70,70,70	0
56	MG	2A	3335	1/1	0.91	0.15	59,59,59,59	0
56	MG	2A	3684	1/1	0.91	0.09	44,44,44,44	0
56	MG	2A	3045	1/1	0.91	0.13	58,58,58,58	0
56	MG	1A	3564	1/1	0.91	0.08	40,40,40,40	0
56	MG	1a	1719	1/1	0.91	0.29	63,63,63,63	0
56	MG	1A	3565	1/1	0.91	0.28	71,71,71,71	0
56	MG	2A	3693	1/1	0.91	0.10	35,35,35,35	0
56	MG	1O	207	1/1	0.91	0.14	65,65,65,65	0
56	MG	1a	1722	1/1	0.91	0.17	65,65,65,65	0
56	MG	2A	3698	1/1	0.91	0.09	51,51,51,51	0
56	MG	2A	3060	1/1	0.91	0.20	53,53,53,53	0
56	MG	1A	3100	1/1	0.91	0.16	60,60,60,60	0
56	MG	2A	3063	1/1	0.91	0.17	67,67,67,67	0
56	MG	1A	4001	1/1	0.91	0.09	17,17,17,17	0
56	MG	1A	4002	1/1	0.91	0.19	33,33,33,33	0
56	MG	2A	3709	1/1	0.91	0.10	33,33,33,33	0
56	MG	1A	4006	1/1	0.91	0.09	76,76,76,76	0
56	MG	2a	3054	1/1	0.91	0.16	65,65,65,65	0
56	MG	2A	3067	1/1	0.91	0.10	57,57,57,57	0
56	MG	2A	3365	1/1	0.91	0.12	56,56,56,56	0
56	MG	1A	3568	1/1	0.91	0.16	50,50,50,50	0
56	MG	1Y	502	1/1	0.91	0.20	59,59,59,59	0
56	MG	2A	3718	1/1	0.91	0.16	64,64,64,64	0
56	MG	1A	4010	1/1	0.91	0.09	26,26,26,26	0
56	MG	1A	3571	1/1	0.91	0.11	57,57,57,57	0
56	MG	2a	3067	1/1	0.91	0.38	65,65,65,65	0
56	MG	10	105	1/1	0.91	0.20	70,70,70,70	0
56	MG	1A	3848	1/1	0.91	0.10	56,56,56,56	0
56	MG	1A	3110	1/1	0.91	0.10	42,42,42,42	0
56	MG	2a	3073	1/1	0.91	0.10	66,66,66,66	0
56	MG	2a	3074	1/1	0.91	0.18	63,63,63,63	0
56	MG	1A	3851	1/1	0.91	0.17	62,62,62,62	0
56	MG	2a	3078	1/1	0.91	0.27	74,74,74,74	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3719	1/1	0.91	0.10	50,50,50,50	0
56	MG	2A	3404	1/1	0.91	0.08	53,53,53,53	0
56	MG	1A	3270	1/1	0.91	0.17	59,59,59,59	0
56	MG	2A	3742	1/1	0.91	0.11	49,49,49,49	0
56	MG	1a	1757	1/1	0.91	0.15	48,48,48,48	0
56	MG	2A	3115	1/1	0.91	0.26	51,51,51,51	0
56	MG	1A	3325	1/1	0.91	0.22	64,64,64,64	0
56	MG	1A	4052	1/1	0.91	0.10	31,31,31,31	0
56	MG	1A	3410	1/1	0.91	0.10	57,57,57,57	0
56	MG	2A	3753	1/1	0.91	0.19	45,45,45,45	0
56	MG	1A	3597	1/1	0.91	0.17	50,50,50,50	0
56	MG	1A	3598	1/1	0.91	0.15	51,51,51,51	0
56	MG	1A	4065	1/1	0.91	0.10	51,51,51,51	0
56	MG	1A	3192	1/1	0.91	0.13	52,52,52,52	0
56	MG	2A	3759	1/1	0.91	0.09	46,46,46,46	0
56	MG	1A	3124	1/1	0.91	0.21	44,44,44,44	0
56	MG	1a	1783	1/1	0.91	0.15	83,83,83,83	0
56	MG	2A	3141	1/1	0.91	0.10	51,51,51,51	0
56	MG	2a	3115	1/1	0.91	0.16	57,57,57,57	0
56	MG	1A	3614	1/1	0.91	0.08	39,39,39,39	0
56	MG	1A	4074	1/1	0.91	0.13	64,64,64,64	0
56	MG	1A	3419	1/1	0.91	0.31	60,60,60,60	0
56	MG	2A	3442	1/1	0.91	0.24	50,50,50,50	0
56	MG	2A	3155	1/1	0.91	0.09	59,59,59,59	0
56	MG	1A	3505	1/1	0.91	0.11	47,47,47,47	0
56	MG	1A	3506	1/1	0.91	0.09	42,42,42,42	0
56	MG	1a	1628	1/1	0.91	0.19	58,58,58,58	0
56	MG	2A	3801	1/1	0.91	0.10	64,64,64,64	0
56	MG	2a	3129	1/1	0.91	0.15	59,59,59,59	0
56	MG	2a	3130	1/1	0.91	0.40	72,72,72,72	0
56	MG	2A	3454	1/1	0.91	0.18	58,58,58,58	0
56	MG	2A	3455	1/1	0.91	0.27	54,54,54,54	0
56	MG	2A	3457	1/1	0.91	0.25	57,57,57,57	0
56	MG	2A	3173	1/1	0.91	0.09	51,51,51,51	0
56	MG	2A	3174	1/1	0.91	0.10	53,53,53,53	0
56	MG	2A	3461	1/1	0.91	0.27	52,52,52,52	0
56	MG	1A	3334	1/1	0.91	0.24	56,56,56,56	0
56	MG	2A	3465	1/1	0.91	0.27	55,55,55,55	0
56	MG	2a	3149	1/1	0.91	0.09	56,56,56,56	0
56	MG	2A	3177	1/1	0.91	0.22	63,63,63,63	0
56	MG	2A	3178	1/1	0.91	0.17	57,57,57,57	0
56	MG	2A	3180	1/1	0.91	0.15	51,51,51,51	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3643	1/1	0.91	0.10	34,34,34,34	0
56	MG	1A	3513	1/1	0.91	0.14	62,62,62,62	0
56	MG	2A	3474	1/1	0.91	0.14	55,55,55,55	0
56	MG	2A	3475	1/1	0.91	0.10	44,44,44,44	0
56	MG	2A	3477	1/1	0.91	0.37	56,56,56,56	0
56	MG	2A	3479	1/1	0.91	0.32	54,54,54,54	0
56	MG	1a	1828	1/1	0.91	0.14	59,59,59,59	0
56	MG	2A	3487	1/1	0.91	0.26	62,62,62,62	0
56	MG	1A	3127	1/1	0.91	0.24	51,51,51,51	0
56	MG	2A	3492	1/1	0.91	0.11	54,54,54,54	0
56	MG	2a	3194	1/1	0.91	0.16	68,68,68,68	0
56	MG	2A	3864	1/1	0.91	0.09	63,63,63,63	0
56	MG	2A	3203	1/1	0.91	0.11	46,46,46,46	0
56	MG	1A	3048	1/1	0.91	0.23	48,48,48,48	0
56	MG	2A	3503	1/1	0.91	0.11	58,58,58,58	0
56	MG	1B	3006	1/1	0.91	0.25	45,45,45,45	0
56	MG	1a	1642	1/1	0.91	0.30	67,67,67,67	0
56	MG	1l	203	1/1	0.91	0.11	63,63,63,63	0
56	MG	2A	3224	1/1	0.91	0.14	52,52,52,52	0
56	MG	2a	3208	1/1	0.91	0.16	75,75,75,75	0
56	MG	1a	1643	1/1	0.91	0.22	61,61,61,61	0
56	MG	1A	3302	1/1	0.91	0.23	56,56,56,56	0
56	MG	2A	3890	1/1	0.91	0.14	61,61,61,61	0
56	MG	1A	3908	1/1	0.91	0.28	65,65,65,65	0
56	MG	2a	3218	1/1	0.91	0.16	61,61,61,61	0
56	MG	2A	3241	1/1	0.91	0.19	56,56,56,56	0
56	MG	1B	3016	1/1	0.91	0.13	54,54,54,54	0
56	MG	1A	3787	1/1	0.91	0.11	55,55,55,55	0
56	MG	2A	3908	1/1	0.91	0.17	44,44,44,44	0
56	MG	2A	3541	1/1	0.91	0.07	30,30,30,30	0
56	MG	1A	3788	1/1	0.91	0.18	59,59,59,59	0
56	MG	1B	3021	1/1	0.91	0.12	46,46,46,46	0
56	MG	1A	3152	1/1	0.91	0.13	55,55,55,55	0
56	MG	1A	3219	1/1	0.91	0.13	37,37,37,37	0
56	MG	2B	3007	1/1	0.91	0.14	55,55,55,55	0
56	MG	1A	3231	1/1	0.91	0.22	51,51,51,51	0
56	MG	2B	3009	1/1	0.91	0.21	61,61,61,61	0
56	MG	1A	3016	1/1	0.91	0.18	51,51,51,51	0
56	MG	1A	3247	1/1	0.91	0.13	58,58,58,58	0
56	MG	1B	3033	1/1	0.91	0.13	56,56,56,56	0
56	MG	2A	3269	1/1	0.91	0.14	53,53,53,53	0
56	MG	1B	3034	1/1	0.91	0.11	58,58,58,58	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3275	1/1	0.91	0.19	58,58,58,58	0
56	MG	2A	3592	1/1	0.91	0.23	57,57,57,57	0
56	MG	2A	3599	1/1	0.91	0.09	51,51,51,51	0
56	MG	2e	3001	1/1	0.91	0.12	79,79,79,79	0
56	MG	2D	305	1/1	0.91	0.18	50,50,50,50	0
56	MG	2E	306	1/1	0.91	0.16	67,67,67,67	0
56	MG	1A	3363	1/1	0.91	0.22	60,60,60,60	0
56	MG	2A	3603	1/1	0.91	0.10	50,50,50,50	0
56	MG	2A	3284	1/1	0.91	0.16	59,59,59,59	0
56	MG	1A	3181	1/1	0.91	0.20	54,54,54,54	0
56	MG	2T	3002	1/1	0.91	0.13	58,58,58,58	0
56	MG	2T	3003	1/1	0.91	0.18	63,63,63,63	0
56	MG	1A	3822	1/1	0.91	0.10	48,48,48,48	0
56	MG	1x	112	1/1	0.91	0.18	71,71,71,71	0
56	MG	1A	3182	1/1	0.91	0.14	55,55,55,55	0
56	MG	2Y	502	1/1	0.91	0.17	54,54,54,54	0
56	MG	1F	308	1/1	0.91	0.16	53,53,53,53	0
56	MG	2w	107	1/1	0.91	0.12	75,75,75,75	0
56	MG	1A	3982	1/1	0.91	0.12	29,29,29,29	0
56	MG	2A	3303	1/1	0.91	0.11	60,60,60,60	0
56	MG	2x	104	1/1	0.91	0.20	60,60,60,60	0
56	MG	27	101	1/1	0.91	0.17	51,51,51,51	0
56	MG	1a	1701	1/1	0.91	0.24	51,51,51,51	0
56	MG	2A	3622	1/1	0.91	0.26	63,63,63,63	0
56	MG	1A	3261	1/1	0.91	0.18	55,55,55,55	0
56	MG	2A	3306	1/1	0.91	0.11	58,58,58,58	0
56	MG	1A	3293	1/1	0.92	0.20	50,50,50,50	0
56	MG	2A	3106	1/1	0.92	0.16	59,59,59,59	0
56	MG	1A	4091	1/1	0.92	0.16	49,49,49,49	0
56	MG	1A	4093	1/1	0.92	0.33	35,35,35,35	0
56	MG	2A	3478	1/1	0.92	0.11	50,50,50,50	0
56	MG	1A	3686	1/1	0.92	0.12	35,35,35,35	0
56	MG	1A	3224	1/1	0.92	0.13	50,50,50,50	0
56	MG	2A	3482	1/1	0.92	0.26	63,63,63,63	0
56	MG	2A	3484	1/1	0.92	0.13	53,53,53,53	0
56	MG	2D	301	1/1	0.92	0.11	57,57,57,57	0
56	MG	2A	3485	1/1	0.92	0.18	63,63,63,63	0
56	MG	2E	302	1/1	0.92	0.09	52,52,52,52	0
56	MG	2E	303	1/1	0.92	0.11	49,49,49,49	0
56	MG	1A	4109	1/1	0.92	0.16	49,49,49,49	0
56	MG	1a	1695	1/1	0.92	0.42	68,68,68,68	0
56	MG	1A	3689	1/1	0.92	0.12	51,51,51,51	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2F	302	1/1	0.92	0.15	53,53,53,53	0
56	MG	2G	3001	1/1	0.92	0.12	51,51,51,51	0
56	MG	2A	3493	1/1	0.92	0.19	53,53,53,53	0
56	MG	1a	1697	1/1	0.92	0.19	63,63,63,63	0
56	MG	1A	3543	1/1	0.92	0.17	73,73,73,73	0
56	MG	1A	3426	1/1	0.92	0.16	50,50,50,50	0
56	MG	1a	1703	1/1	0.92	0.31	55,55,55,55	0
56	MG	1A	4134	1/1	0.92	0.29	46,46,46,46	0
56	MG	1A	4138	1/1	0.92	0.12	43,43,43,43	0
56	MG	2A	3508	1/1	0.92	0.11	60,60,60,60	0
56	MG	1a	1707	1/1	0.92	0.37	63,63,63,63	0
56	MG	1a	1708	1/1	0.92	0.20	68,68,68,68	0
56	MG	1A	3859	1/1	0.92	0.14	44,44,44,44	0
56	MG	25	105	1/1	0.92	0.13	58,58,58,58	0
56	MG	1B	3003	1/1	0.92	0.15	56,56,56,56	0
56	MG	28	101	1/1	0.92	0.12	53,53,53,53	0
56	MG	2A	3531	1/1	0.92	0.12	51,51,51,51	0
56	MG	2A	3532	1/1	0.92	0.25	65,65,65,65	0
56	MG	2a	3004	1/1	0.92	0.21	57,57,57,57	0
56	MG	2A	3161	1/1	0.92	0.14	44,44,44,44	0
56	MG	1A	3861	1/1	0.92	0.12	33,33,33,33	0
56	MG	2A	3539	1/1	0.92	0.12	62,62,62,62	0
56	MG	1A	3169	1/1	0.92	0.22	55,55,55,55	0
56	MG	1B	3010	1/1	0.92	0.25	73,73,73,73	0
56	MG	2A	3172	1/1	0.92	0.09	47,47,47,47	0
56	MG	1A	3232	1/1	0.92	0.16	47,47,47,47	0
56	MG	1B	3014	1/1	0.92	0.09	63,63,63,63	0
56	MG	1A	3552	1/1	0.92	0.14	60,60,60,60	0
56	MG	1A	3438	1/1	0.92	0.15	50,50,50,50	0
56	MG	1a	1723	1/1	0.92	0.27	61,61,61,61	0
56	MG	2A	3560	1/1	0.92	0.13	63,63,63,63	0
56	MG	1A	3238	1/1	0.92	0.17	57,57,57,57	0
56	MG	2A	3572	1/1	0.92	0.10	44,44,44,44	0
56	MG	1A	3352	1/1	0.92	0.20	64,64,64,64	0
56	MG	1A	3878	1/1	0.92	0.12	33,33,33,33	0
56	MG	1A	3709	1/1	0.92	0.14	52,52,52,52	0
56	MG	1A	3882	1/1	0.92	0.12	36,36,36,36	0
56	MG	2A	3588	1/1	0.92	0.08	47,47,47,47	0
56	MG	2A	3590	1/1	0.92	0.14	64,64,64,64	0
56	MG	2A	3202	1/1	0.92	0.19	56,56,56,56	0
56	MG	2A	3597	1/1	0.92	0.29	61,61,61,61	0
56	MG	1A	3884	1/1	0.92	0.14	48,48,48,48	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1a	1737	1/1	0.92	0.13	66,66,66,66	0
56	MG	1B	3030	1/1	0.92	0.12	59,59,59,59	0
56	MG	2A	3213	1/1	0.92	0.11	45,45,45,45	0
56	MG	1A	3886	1/1	0.92	0.12	57,57,57,57	0
56	MG	1A	3242	1/1	0.92	0.12	43,43,43,43	0
56	MG	1A	3563	1/1	0.92	0.16	43,43,43,43	0
56	MG	2A	3227	1/1	0.92	0.23	57,57,57,57	0
56	MG	2a	3041	1/1	0.92	0.22	50,50,50,50	0
56	MG	2a	3042	1/1	0.92	0.29	58,58,58,58	0
56	MG	1A	3306	1/1	0.92	0.24	38,38,38,38	0
56	MG	2a	3045	1/1	0.92	0.13	65,65,65,65	0
56	MG	1D	305	1/1	0.92	0.10	42,42,42,42	0
56	MG	2A	3238	1/1	0.92	0.22	56,56,56,56	0
56	MG	1D	311	1/1	0.92	0.21	56,56,56,56	0
56	MG	1A	3004	1/1	0.92	0.12	34,34,34,34	0
56	MG	1E	304	1/1	0.92	0.16	55,55,55,55	0
56	MG	1A	3450	1/1	0.92	0.15	57,57,57,57	0
56	MG	2A	3246	1/1	0.92	0.10	65,65,65,65	0
56	MG	2A	3252	1/1	0.92	0.15	52,52,52,52	0
56	MG	1A	3900	1/1	0.92	0.16	44,44,44,44	0
56	MG	2A	3640	1/1	0.92	0.15	45,45,45,45	0
56	MG	1A	3458	1/1	0.92	0.17	54,54,54,54	0
56	MG	1A	3904	1/1	0.92	0.12	36,36,36,36	0
56	MG	1A	3569	1/1	0.92	0.12	54,54,54,54	0
56	MG	2a	3065	1/1	0.92	0.09	57,57,57,57	0
56	MG	1a	1771	1/1	0.92	0.11	70,70,70,70	0
56	MG	1A	3570	1/1	0.92	0.09	54,54,54,54	0
56	MG	1I	3001	1/1	0.92	0.13	70,70,70,70	0
56	MG	2A	3267	1/1	0.92	0.18	58,58,58,58	0
56	MG	1A	3465	1/1	0.92	0.15	60,60,60,60	0
56	MG	2A	3658	1/1	0.92	0.14	55,55,55,55	0
56	MG	1a	1782	1/1	0.92	0.09	79,79,79,79	0
56	MG	2A	3270	1/1	0.92	0.10	53,53,53,53	0
56	MG	1A	3743	1/1	0.92	0.16	60,60,60,60	0
56	MG	2A	3274	1/1	0.92	0.24	53,53,53,53	0
56	MG	2A	3682	1/1	0.92	0.12	70,70,70,70	0
56	MG	2a	3087	1/1	0.92	0.17	63,63,63,63	0
56	MG	1A	3112	1/1	0.92	0.14	49,49,49,49	0
56	MG	2A	3280	1/1	0.92	0.14	54,54,54,54	0
56	MG	1a	1788	1/1	0.92	0.09	69,69,69,69	0
56	MG	1A	3573	1/1	0.92	0.21	60,60,60,60	0
56	MG	1A	3936	1/1	0.92	0.10	31,31,31,31	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1Q	203	1/1	0.92	0.12	64,64,64,64	0
56	MG	2A	3288	1/1	0.92	0.08	49,49,49,49	0
56	MG	2a	3097	1/1	0.92	0.15	72,72,72,72	0
56	MG	2A	3695	1/1	0.92	0.13	38,38,38,38	0
56	MG	2a	3100	1/1	0.92	0.16	69,69,69,69	0
56	MG	1Q	205	1/1	0.92	0.12	39,39,39,39	0
56	MG	1A	3576	1/1	0.92	0.20	57,57,57,57	0
56	MG	1a	1798	1/1	0.92	0.13	56,56,56,56	0
56	MG	2a	3105	1/1	0.92	0.16	45,45,45,45	0
56	MG	1A	3947	1/1	0.92	0.09	44,44,44,44	0
56	MG	1a	1813	1/1	0.92	0.15	58,58,58,58	0
56	MG	1a	1815	1/1	0.92	0.07	64,64,64,64	0
56	MG	1a	1818	1/1	0.92	0.09	54,54,54,54	0
56	MG	2a	3114	1/1	0.92	0.10	51,51,51,51	0
56	MG	1A	3580	1/1	0.92	0.15	39,39,39,39	0
56	MG	1A	3367	1/1	0.92	0.13	57,57,57,57	0
56	MG	1U	203	1/1	0.92	0.25	42,42,42,42	0
56	MG	1A	3762	1/1	0.92	0.09	60,60,60,60	0
56	MG	2A	3310	1/1	0.92	0.23	62,62,62,62	0
56	MG	1W	201	1/1	0.92	0.24	57,57,57,57	0
56	MG	1A	3959	1/1	0.92	0.13	56,56,56,56	0
56	MG	2A	3314	1/1	0.92	0.12	47,47,47,47	0
56	MG	1A	3582	1/1	0.92	0.25	54,54,54,54	0
56	MG	2A	3321	1/1	0.92	0.19	54,54,54,54	0
56	MG	1A	3966	1/1	0.92	0.14	59,59,59,59	0
56	MG	1A	3114	1/1	0.92	0.17	57,57,57,57	0
56	MG	2A	3734	1/1	0.92	0.12	57,57,57,57	0
56	MG	2a	3132	1/1	0.92	0.25	63,63,63,63	0
56	MG	1s	101	1/1	0.92	0.15	65,65,65,65	0
56	MG	2A	3331	1/1	0.92	0.08	56,56,56,56	0
56	MG	10	106	1/1	0.92	0.10	65,65,65,65	0
56	MG	11	101	1/1	0.92	0.09	38,38,38,38	0
56	MG	1w	103	1/1	0.92	0.09	57,57,57,57	0
56	MG	1A	3256	1/1	0.92	0.09	57,57,57,57	0
56	MG	1A	3976	1/1	0.92	0.10	72,72,72,72	0
56	MG	1A	3980	1/1	0.92	0.10	74,74,74,74	0
56	MG	2a	3151	1/1	0.92	0.10	78,78,78,78	0
56	MG	2a	3152	1/1	0.92	0.09	67,67,67,67	0
56	MG	1A	3476	1/1	0.92	0.13	52,52,52,52	0
56	MG	18	102	1/1	0.92	0.17	50,50,50,50	0
56	MG	2a	3158	1/1	0.92	0.09	52,52,52,52	0
56	MG	2A	3751	1/1	0.92	0.11	61,61,61,61	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	3165	1/1	0.92	0.10	54,54,54,54	0
56	MG	1A	3779	1/1	0.92	0.12	56,56,56,56	0
56	MG	1A	3782	1/1	0.92	0.16	25,25,25,25	0
56	MG	2A	3349	1/1	0.92	0.14	58,58,58,58	0
56	MG	1A	3116	1/1	0.92	0.14	47,47,47,47	0
56	MG	1A	3995	1/1	0.92	0.10	73,73,73,73	0
56	MG	1A	3996	1/1	0.92	0.08	43,43,43,43	0
56	MG	2A	3762	1/1	0.92	0.10	52,52,52,52	0
56	MG	2A	3359	1/1	0.92	0.11	56,56,56,56	0
56	MG	1a	1604	1/1	0.92	0.14	58,58,58,58	0
56	MG	1A	3483	1/1	0.92	0.09	46,46,46,46	0
56	MG	1A	3999	1/1	0.92	0.13	55,55,55,55	0
56	MG	1A	3382	1/1	0.92	0.12	54,54,54,54	0
56	MG	2A	3771	1/1	0.92	0.12	39,39,39,39	0
56	MG	2A	3772	1/1	0.92	0.13	53,53,53,53	0
56	MG	2A	3366	1/1	0.92	0.09	54,54,54,54	0
56	MG	2A	3774	1/1	0.92	0.10	51,51,51,51	0
56	MG	2A	3367	1/1	0.92	0.23	61,61,61,61	0
56	MG	1A	3613	1/1	0.92	0.08	33,33,33,33	0
56	MG	2A	3376	1/1	0.92	0.12	58,58,58,58	0
56	MG	1A	3088	1/1	0.92	0.10	47,47,47,47	0
56	MG	1a	1618	1/1	0.92	0.09	48,48,48,48	0
56	MG	1A	4003	1/1	0.92	0.09	20,20,20,20	0
56	MG	1a	1622	1/1	0.92	0.25	62,62,62,62	0
56	MG	1A	3089	1/1	0.92	0.14	48,48,48,48	0
56	MG	1A	3395	1/1	0.92	0.13	42,42,42,42	0
56	MG	1A	3399	1/1	0.92	0.11	52,52,52,52	0
56	MG	2A	3811	1/1	0.92	0.09	47,47,47,47	0
56	MG	1A	3631	1/1	0.92	0.08	32,32,32,32	0
56	MG	2a	3222	1/1	0.92	0.14	63,63,63,63	0
56	MG	2A	3398	1/1	0.92	0.22	55,55,55,55	0
56	MG	1A	3266	1/1	0.92	0.08	52,52,52,52	0
56	MG	1A	3808	1/1	0.92	0.10	36,36,36,36	0
56	MG	2A	3018	1/1	0.92	0.14	44,44,44,44	0
56	MG	1A	3096	1/1	0.92	0.20	49,49,49,49	0
56	MG	2A	3411	1/1	0.92	0.12	53,53,53,53	0
56	MG	2A	3029	1/1	0.92	0.13	44,44,44,44	0
56	MG	2A	3035	1/1	0.92	0.08	31,31,31,31	0
56	MG	1a	1635	1/1	0.92	0.37	75,75,75,75	0
56	MG	1A	3148	1/1	0.92	0.24	48,48,48,48	0
56	MG	2A	3422	1/1	0.92	0.13	58,58,58,58	0
56	MG	1A	4036	1/1	0.92	0.09	43,43,43,43	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3328	1/1	0.92	0.16	64,64,64,64	0
56	MG	1A	4047	1/1	0.92	0.14	50,50,50,50	0
56	MG	1A	3330	1/1	0.92	0.12	50,50,50,50	0
56	MG	1A	3023	1/1	0.92	0.21	59,59,59,59	0
56	MG	2A	3434	1/1	0.92	0.12	59,59,59,59	0
56	MG	1A	3659	1/1	0.92	0.07	23,23,23,23	0
56	MG	1a	1657	1/1	0.92	0.15	57,57,57,57	0
56	MG	1A	4054	1/1	0.92	0.11	81,81,81,81	0
56	MG	1A	3831	1/1	0.92	0.29	70,70,70,70	0
56	MG	1a	1662	1/1	0.92	0.10	67,67,67,67	0
56	MG	1A	3527	1/1	0.92	0.14	40,40,40,40	0
56	MG	1A	3101	1/1	0.92	0.13	44,44,44,44	0
56	MG	1A	3285	1/1	0.92	0.18	39,39,39,39	0
56	MG	2A	3068	1/1	0.92	0.11	56,56,56,56	0
56	MG	1A	3835	1/1	0.92	0.14	59,59,59,59	0
56	MG	2A	3074	1/1	0.92	0.19	73,73,73,73	0
56	MG	2A	3077	1/1	0.92	0.09	45,45,45,45	0
56	MG	1a	1671	1/1	0.92	0.25	66,66,66,66	0
56	MG	2A	3088	1/1	0.92	0.10	49,49,49,49	0
56	MG	1A	4071	1/1	0.92	0.08	26,26,26,26	0
56	MG	2A	3910	1/1	0.92	0.18	57,57,57,57	0
56	MG	1A	3539	1/1	0.92	0.08	49,49,49,49	0
56	MG	1A	3844	1/1	0.92	0.12	54,54,54,54	0
56	MG	2y	3001	1/1	0.92	0.15	59,59,59,59	0
56	MG	1A	3682	1/1	0.92	0.12	35,35,35,35	0
56	MG	2A	3097	1/1	0.92	0.07	56,56,56,56	0
56	MG	1a	1679	1/1	0.92	0.11	73,73,73,73	0
56	MG	1a	1681	1/1	0.92	0.16	54,54,54,54	0
56	MG	2A	3471	1/1	0.92	0.23	54,54,54,54	0
56	MG	2A	3534	1/1	0.93	0.09	40,40,40,40	0
56	MG	1A	3490	1/1	0.93	0.08	50,50,50,50	0
56	MG	1a	1823	1/1	0.93	0.12	68,68,68,68	0
56	MG	1A	3722	1/1	0.93	0.14	39,39,39,39	0
56	MG	1A	3183	1/1	0.93	0.08	54,54,54,54	0
56	MG	1A	3340	1/1	0.93	0.21	58,58,58,58	0
56	MG	1A	3589	1/1	0.93	0.11	52,52,52,52	0
56	MG	1b	3001	1/1	0.93	0.07	83,83,83,83	0
56	MG	2Q	3001	1/1	0.93	0.10	50,50,50,50	0
56	MG	2A	3254	1/1	0.93	0.18	53,53,53,53	0
56	MG	2A	3552	1/1	0.93	0.12	59,59,59,59	0
56	MG	1b	3002	1/1	0.93	0.15	61,61,61,61	0
56	MG	1A	4087	1/1	0.93	0.20	54,54,54,54	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2W	201	1/1	0.93	0.14	57,57,57,57	0
56	MG	1A	3872	1/1	0.93	0.11	33,33,33,33	0
56	MG	1A	4092	1/1	0.93	0.20	37,37,37,37	0
56	MG	2A	3561	1/1	0.93	0.09	62,62,62,62	0
56	MG	1A	3729	1/1	0.93	0.11	42,42,42,42	0
56	MG	2A	3262	1/1	0.93	0.12	57,57,57,57	0
56	MG	1a	1627	1/1	0.93	0.20	55,55,55,55	0
56	MG	1A	4095	1/1	0.93	0.09	67,67,67,67	0
56	MG	1A	3592	1/1	0.93	0.12	21,21,21,21	0
56	MG	1A	3733	1/1	0.93	0.08	52,52,52,52	0
56	MG	1a	1631	1/1	0.93	0.23	54,54,54,54	0
56	MG	1A	3594	1/1	0.93	0.10	31,31,31,31	0
56	MG	1A	3420	1/1	0.93	0.20	55,55,55,55	0
56	MG	2A	3272	1/1	0.93	0.12	51,51,51,51	0
56	MG	1A	3885	1/1	0.93	0.10	37,37,37,37	0
56	MG	1a	1637	1/1	0.93	0.25	68,68,68,68	0
56	MG	2A	3278	1/1	0.93	0.11	57,57,57,57	0
56	MG	1a	1638	1/1	0.93	0.12	58,58,58,58	0
56	MG	2a	3011	1/1	0.93	0.24	64,64,64,64	0
56	MG	1A	3596	1/1	0.93	0.15	51,51,51,51	0
56	MG	2A	3282	1/1	0.93	0.15	63,63,63,63	0
56	MG	1A	4123	1/1	0.93	0.12	35,35,35,35	0
56	MG	1A	4125	1/1	0.93	0.21	54,54,54,54	0
56	MG	1A	3509	1/1	0.93	0.11	45,45,45,45	0
56	MG	1A	3185	1/1	0.93	0.12	47,47,47,47	0
56	MG	2A	3617	1/1	0.93	0.11	38,38,38,38	0
56	MG	1x	105	1/1	0.93	0.11	62,62,62,62	0
56	MG	1a	1648	1/1	0.93	0.12	59,59,59,59	0
56	MG	1x	107	1/1	0.93	0.09	61,61,61,61	0
56	MG	2A	3300	1/1	0.93	0.22	55,55,55,55	0
56	MG	1a	1651	1/1	0.93	0.13	56,56,56,56	0
56	MG	1A	3746	1/1	0.93	0.17	55,55,55,55	0
56	MG	1x	110	1/1	0.93	0.12	52,52,52,52	0
56	MG	1A	3748	1/1	0.93	0.14	25,25,25,25	0
56	MG	1A	3240	1/1	0.93	0.08	35,35,35,35	0
56	MG	1A	3753	1/1	0.93	0.14	34,34,34,34	0
56	MG	2A	3643	1/1	0.93	0.08	34,34,34,34	0
56	MG	1B	3009	1/1	0.93	0.14	43,43,43,43	0
56	MG	1A	3300	1/1	0.93	0.25	61,61,61,61	0
56	MG	1A	3756	1/1	0.93	0.09	39,39,39,39	0
56	MG	1B	3013	1/1	0.93	0.07	55,55,55,55	0
56	MG	2A	3653	1/1	0.93	0.25	58,58,58,58	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3133	1/1	0.93	0.11	44,44,44,44	0
56	MG	1A	3906	1/1	0.93	0.11	51,51,51,51	0
56	MG	1A	3907	1/1	0.93	0.15	54,54,54,54	0
56	MG	1A	3526	1/1	0.93	0.15	53,53,53,53	0
56	MG	1a	1675	1/1	0.93	0.12	60,60,60,60	0
56	MG	2A	3016	1/1	0.93	0.15	61,61,61,61	0
56	MG	2A	3017	1/1	0.93	0.21	52,52,52,52	0
56	MG	2A	3671	1/1	0.93	0.08	46,46,46,46	0
56	MG	2a	3049	1/1	0.93	0.19	55,55,55,55	0
56	MG	2A	3673	1/1	0.93	0.14	64,64,64,64	0
56	MG	2A	3674	1/1	0.93	0.15	55,55,55,55	0
56	MG	1A	3616	1/1	0.93	0.11	40,40,40,40	0
56	MG	1B	3022	1/1	0.93	0.15	60,60,60,60	0
56	MG	1A	3087	1/1	0.93	0.15	32,32,32,32	0
56	MG	1A	3190	1/1	0.93	0.15	39,39,39,39	0
56	MG	1A	3353	1/1	0.93	0.25	64,64,64,64	0
56	MG	2A	3339	1/1	0.93	0.12	51,51,51,51	0
56	MG	2a	3060	1/1	0.93	0.09	63,63,63,63	0
56	MG	2a	3061	1/1	0.93	0.18	54,54,54,54	0
56	MG	1A	3778	1/1	0.93	0.16	57,57,57,57	0
56	MG	2A	3043	1/1	0.93	0.09	53,53,53,53	0
56	MG	1a	1686	1/1	0.93	0.21	54,54,54,54	0
56	MG	2A	3343	1/1	0.93	0.10	57,57,57,57	0
56	MG	2A	3344	1/1	0.93	0.12	55,55,55,55	0
56	MG	1A	3537	1/1	0.93	0.13	49,49,49,49	0
56	MG	1A	3944	1/1	0.93	0.09	60,60,60,60	0
56	MG	1A	3637	1/1	0.93	0.11	50,50,50,50	0
56	MG	1A	3639	1/1	0.93	0.13	41,41,41,41	0
56	MG	1A	3538	1/1	0.93	0.13	54,54,54,54	0
56	MG	2a	3075	1/1	0.93	0.18	49,49,49,49	0
56	MG	2A	3705	1/1	0.93	0.12	57,57,57,57	0
56	MG	1D	302	1/1	0.93	0.20	55,55,55,55	0
56	MG	2a	3080	1/1	0.93	0.09	50,50,50,50	0
56	MG	1A	3436	1/1	0.93	0.10	45,45,45,45	0
56	MG	1D	309	1/1	0.93	0.09	46,46,46,46	0
56	MG	1A	3540	1/1	0.93	0.20	52,52,52,52	0
56	MG	1A	3251	1/1	0.93	0.09	58,58,58,58	0
56	MG	1A	3061	1/1	0.93	0.32	62,62,62,62	0
56	MG	1E	305	1/1	0.93	0.22	57,57,57,57	0
56	MG	1a	1706	1/1	0.93	0.29	60,60,60,60	0
56	MG	1A	3969	1/1	0.93	0.09	66,66,66,66	0
56	MG	2A	3720	1/1	0.93	0.08	41,41,41,41	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3372	1/1	0.93	0.18	41,41,41,41	0
56	MG	1A	3798	1/1	0.93	0.08	63,63,63,63	0
56	MG	1A	3196	1/1	0.93	0.14	59,59,59,59	0
56	MG	1A	3310	1/1	0.93	0.15	40,40,40,40	0
56	MG	1a	1711	1/1	0.93	0.18	65,65,65,65	0
56	MG	1A	3364	1/1	0.93	0.17	64,64,64,64	0
56	MG	1A	3666	1/1	0.93	0.10	34,34,34,34	0
56	MG	1A	3067	1/1	0.93	0.16	51,51,51,51	0
56	MG	2A	3095	1/1	0.93	0.08	39,39,39,39	0
56	MG	2A	3392	1/1	0.93	0.07	55,55,55,55	0
56	MG	1A	3810	1/1	0.93	0.16	45,45,45,45	0
56	MG	2a	3109	1/1	0.93	0.29	67,67,67,67	0
56	MG	2A	3394	1/1	0.93	0.18	50,50,50,50	0
56	MG	2A	3396	1/1	0.93	0.08	56,56,56,56	0
56	MG	1N	202	1/1	0.93	0.10	48,48,48,48	0
56	MG	1N	204	1/1	0.93	0.21	64,64,64,64	0
56	MG	2A	3749	1/1	0.93	0.09	48,48,48,48	0
56	MG	1A	3813	1/1	0.93	0.15	56,56,56,56	0
56	MG	2A	3752	1/1	0.93	0.19	61,61,61,61	0
56	MG	1A	3814	1/1	0.93	0.16	45,45,45,45	0
56	MG	2A	3407	1/1	0.93	0.17	61,61,61,61	0
56	MG	2A	3105	1/1	0.93	0.10	51,51,51,51	0
56	MG	2a	3124	1/1	0.93	0.21	61,61,61,61	0
56	MG	1O	202	1/1	0.93	0.14	67,67,67,67	0
56	MG	2A	3108	1/1	0.93	0.19	44,44,44,44	0
56	MG	1O	204	1/1	0.93	0.24	58,58,58,58	0
56	MG	2A	3760	1/1	0.93	0.19	58,58,58,58	0
56	MG	2A	3111	1/1	0.93	0.16	54,54,54,54	0
56	MG	2A	3419	1/1	0.93	0.11	51,51,51,51	0
56	MG	1A	3818	1/1	0.93	0.14	57,57,57,57	0
56	MG	1A	3369	1/1	0.93	0.14	57,57,57,57	0
56	MG	2A	3768	1/1	0.93	0.12	62,62,62,62	0
56	MG	2a	3137	1/1	0.93	0.08	79,79,79,79	0
56	MG	1A	3452	1/1	0.93	0.24	58,58,58,58	0
56	MG	1A	3454	1/1	0.93	0.09	59,59,59,59	0
56	MG	2a	3142	1/1	0.93	0.10	74,74,74,74	0
56	MG	1A	3206	1/1	0.93	0.16	55,55,55,55	0
56	MG	1S	3001	1/1	0.93	0.23	51,51,51,51	0
56	MG	2A	3427	1/1	0.93	0.07	45,45,45,45	0
56	MG	2A	3124	1/1	0.93	0.12	48,48,48,48	0
56	MG	2A	3777	1/1	0.93	0.10	41,41,41,41	0
56	MG	1S	3002	1/1	0.93	0.09	49,49,49,49	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	3153	1/1	0.93	0.10	74,74,74,74	0
56	MG	2A	3781	1/1	0.93	0.11	55,55,55,55	0
56	MG	2A	3430	1/1	0.93	0.08	51,51,51,51	0
56	MG	2A	3794	1/1	0.93	0.09	67,67,67,67	0
56	MG	2A	3432	1/1	0.93	0.12	60,60,60,60	0
56	MG	2A	3797	1/1	0.93	0.13	52,52,52,52	0
56	MG	1A	3827	1/1	0.93	0.16	50,50,50,50	0
56	MG	1A	3155	1/1	0.93	0.17	47,47,47,47	0
56	MG	1A	3265	1/1	0.93	0.22	63,63,63,63	0
56	MG	2a	3176	1/1	0.93	0.09	62,62,62,62	0
56	MG	1A	3094	1/1	0.93	0.15	52,52,52,52	0
56	MG	1A	3690	1/1	0.93	0.07	28,28,28,28	0
56	MG	2A	3143	1/1	0.93	0.17	56,56,56,56	0
56	MG	2A	3446	1/1	0.93	0.21	45,45,45,45	0
56	MG	1A	3267	1/1	0.93	0.10	57,57,57,57	0
56	MG	2A	3448	1/1	0.93	0.19	49,49,49,49	0
56	MG	2A	3449	1/1	0.93	0.25	47,47,47,47	0
56	MG	2A	3150	1/1	0.93	0.20	39,39,39,39	0
56	MG	2A	3816	1/1	0.93	0.16	57,57,57,57	0
56	MG	1X	105	1/1	0.93	0.08	47,47,47,47	0
56	MG	1a	1758	1/1	0.93	0.08	56,56,56,56	0
56	MG	1A	4019	1/1	0.93	0.12	42,42,42,42	0
56	MG	1a	1761	1/1	0.93	0.11	64,64,64,64	0
56	MG	2a	3202	1/1	0.93	0.15	64,64,64,64	0
56	MG	2A	3823	1/1	0.93	0.10	73,73,73,73	0
56	MG	2A	3167	1/1	0.93	0.15	52,52,52,52	0
56	MG	1A	3167	1/1	0.93	0.11	41,41,41,41	0
56	MG	1A	3567	1/1	0.93	0.12	54,54,54,54	0
56	MG	2A	3834	1/1	0.93	0.07	40,40,40,40	0
56	MG	2A	3170	1/1	0.93	0.24	54,54,54,54	0
56	MG	2a	3211	1/1	0.93	0.17	61,61,61,61	0
56	MG	2A	3462	1/1	0.93	0.23	59,59,59,59	0
56	MG	1A	3473	1/1	0.93	0.20	50,50,50,50	0
56	MG	1A	3839	1/1	0.93	0.10	66,66,66,66	0
56	MG	1A	3840	1/1	0.93	0.12	63,63,63,63	0
56	MG	1A	3095	1/1	0.93	0.12	55,55,55,55	0
56	MG	2A	3857	1/1	0.93	0.09	47,47,47,47	0
56	MG	1a	1774	1/1	0.93	0.11	60,60,60,60	0
56	MG	1a	1775	1/1	0.93	0.11	76,76,76,76	0
56	MG	12	101	1/1	0.93	0.12	60,60,60,60	0
56	MG	1a	1777	1/1	0.93	0.16	55,55,55,55	0
56	MG	1A	4046	1/1	0.93	0.07	30,30,30,30	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3326	1/1	0.93	0.15	41,41,41,41	0
56	MG	1A	3404	1/1	0.93	0.17	59,59,59,59	0
56	MG	2A	3194	1/1	0.93	0.25	67,67,67,67	0
56	MG	2A	3195	1/1	0.93	0.11	56,56,56,56	0
56	MG	2A	3197	1/1	0.93	0.28	57,57,57,57	0
56	MG	17	101	1/1	0.93	0.13	54,54,54,54	0
56	MG	1A	3002	1/1	0.93	0.11	59,59,59,59	0
56	MG	1A	3852	1/1	0.93	0.08	33,33,33,33	0
56	MG	2A	3486	1/1	0.93	0.39	55,55,55,55	0
56	MG	2A	3205	1/1	0.93	0.24	52,52,52,52	0
56	MG	2a	3239	1/1	0.93	0.11	65,65,65,65	0
56	MG	1A	3227	1/1	0.93	0.11	42,42,42,42	0
56	MG	2A	3490	1/1	0.93	0.10	61,61,61,61	0
56	MG	2A	3909	1/1	0.93	0.13	43,43,43,43	0
56	MG	1a	1793	1/1	0.93	0.10	82,82,82,82	0
56	MG	2A	3210	1/1	0.93	0.09	47,47,47,47	0
56	MG	2i	8001	1/1	0.93	0.07	51,51,51,51	0
56	MG	2A	3494	1/1	0.93	0.24	50,50,50,50	0
56	MG	1A	3710	1/1	0.93	0.18	68,68,68,68	0
56	MG	2A	3217	1/1	0.93	0.24	64,64,64,64	0
56	MG	2B	3005	1/1	0.93	0.07	53,53,53,53	0
56	MG	2q	201	1/1	0.93	0.10	76,76,76,76	0
56	MG	1A	3280	1/1	0.93	0.12	50,50,50,50	0
56	MG	2r	101	1/1	0.93	0.12	68,68,68,68	0
56	MG	2A	3219	1/1	0.93	0.11	51,51,51,51	0
56	MG	1A	3712	1/1	0.93	0.06	40,40,40,40	0
56	MG	1A	3715	1/1	0.93	0.14	54,54,54,54	0
56	MG	2A	3225	1/1	0.93	0.13	62,62,62,62	0
56	MG	2A	3226	1/1	0.93	0.09	58,58,58,58	0
56	MG	2B	3012	1/1	0.93	0.10	55,55,55,55	0
56	MG	2w	103	1/1	0.93	0.12	56,56,56,56	0
56	MG	1A	4067	1/1	0.93	0.09	56,56,56,56	0
56	MG	2B	3015	1/1	0.93	0.12	50,50,50,50	0
56	MG	1a	1606	1/1	0.93	0.12	65,65,65,65	0
56	MG	1A	3058	1/1	0.93	0.12	54,54,54,54	0
56	MG	2x	103	1/1	0.93	0.10	64,64,64,64	0
56	MG	2A	3528	1/1	0.93	0.17	57,57,57,57	0
56	MG	2A	3529	1/1	0.93	0.08	43,43,43,43	0
56	MG	2A	3530	1/1	0.93	0.12	37,37,37,37	0
56	MG	2A	3231	1/1	0.93	0.11	49,49,49,49	0
56	MG	2D	302	1/1	0.93	0.14	51,51,51,51	0
56	MG	2D	304	1/1	0.93	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
56	MG	2A	3234	1/1	0.93	0.11	52,52,52,52	0
56	MG	2A	3460	1/1	0.94	0.25	64,64,64,64	0
56	MG	2A	3891	1/1	0.94	0.12	71,71,71,71	0
56	MG	2A	3156	1/1	0.94	0.10	48,48,48,48	0
56	MG	2A	3158	1/1	0.94	0.07	41,41,41,41	0
56	MG	1A	3235	1/1	0.94	0.14	66,66,66,66	0
56	MG	2A	3899	1/1	0.94	0.13	45,45,45,45	0
56	MG	1A	3939	1/1	0.94	0.11	53,53,53,53	0
56	MG	2A	3907	1/1	0.94	0.11	57,57,57,57	0
56	MG	1E	306	1/1	0.94	0.09	31,31,31,31	0
56	MG	1A	3943	1/1	0.94	0.08	81,81,81,81	0
56	MG	1E	311	1/1	0.94	0.14	42,42,42,42	0
56	MG	1A	3759	1/1	0.94	0.11	24,24,24,24	0
56	MG	1F	306	1/1	0.94	0.12	53,53,53,53	0
56	MG	1F	307	1/1	0.94	0.10	50,50,50,50	0
56	MG	2A	3473	1/1	0.94	0.14	57,57,57,57	0
56	MG	1a	1747	1/1	0.94	0.10	49,49,49,49	0
56	MG	1A	3760	1/1	0.94	0.12	35,35,35,35	0
56	MG	1A	3236	1/1	0.94	0.24	37,37,37,37	0
56	MG	1G	3003	1/1	0.94	0.10	66,66,66,66	0
56	MG	2A	3179	1/1	0.94	0.12	59,59,59,59	0
56	MG	2A	3480	1/1	0.94	0.28	65,65,65,65	0
56	MG	1A	3117	1/1	0.94	0.24	39,39,39,39	0
56	MG	2A	3182	1/1	0.94	0.12	42,42,42,42	0
56	MG	2B	3013	1/1	0.94	0.13	61,61,61,61	0
56	MG	1a	1756	1/1	0.94	0.23	72,72,72,72	0
56	MG	1A	3954	1/1	0.94	0.09	58,58,58,58	0
56	MG	1A	3769	1/1	0.94	0.13	29,29,29,29	0
56	MG	2A	3191	1/1	0.94	0.17	50,50,50,50	0
56	MG	1a	1759	1/1	0.94	0.15	64,64,64,64	0
56	MG	1A	3380	1/1	0.94	0.18	48,48,48,48	0
56	MG	1A	3772	1/1	0.94	0.08	36,36,36,36	0
56	MG	1A	3963	1/1	0.94	0.14	60,60,60,60	0
56	MG	1A	3123	1/1	0.94	0.14	54,54,54,54	0
56	MG	2A	3498	1/1	0.94	0.08	55,55,55,55	0
56	MG	1A	3385	1/1	0.94	0.19	58,58,58,58	0
56	MG	1A	3052	1/1	0.94	0.09	56,56,56,56	0
56	MG	1A	3971	1/1	0.94	0.11	44,44,44,44	0
56	MG	1A	3973	1/1	0.94	0.07	85,85,85,85	0
56	MG	1A	3387	1/1	0.94	0.13	54,54,54,54	0
56	MG	1A	3391	1/1	0.94	0.09	41,41,41,41	0
56	MG	2F	301	1/1	0.94	0.19	58,58,58,58	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3216	1/1	0.94	0.14	56,56,56,56	0
56	MG	2A	3510	1/1	0.94	0.12	46,46,46,46	0
56	MG	1A	3979	1/1	0.94	0.11	73,73,73,73	0
56	MG	2A	3516	1/1	0.94	0.17	56,56,56,56	0
56	MG	2R	201	1/1	0.94	0.11	48,48,48,48	0
56	MG	1A	3184	1/1	0.94	0.15	62,62,62,62	0
56	MG	1A	3784	1/1	0.94	0.08	39,39,39,39	0
56	MG	1a	1781	1/1	0.94	0.08	71,71,71,71	0
56	MG	2A	3522	1/1	0.94	0.10	59,59,59,59	0
56	MG	2U	203	1/1	0.94	0.22	46,46,46,46	0
56	MG	2V	201	1/1	0.94	0.08	53,53,53,53	0
56	MG	1A	3246	1/1	0.94	0.12	58,58,58,58	0
56	MG	1S	3003	1/1	0.94	0.08	59,59,59,59	0
56	MG	1A	3626	1/1	0.94	0.09	44,44,44,44	0
56	MG	2X	102	1/1	0.94	0.10	56,56,56,56	0
56	MG	1A	3990	1/1	0.94	0.12	52,52,52,52	0
56	MG	1A	3627	1/1	0.94	0.16	62,62,62,62	0
56	MG	1A	3790	1/1	0.94	0.08	25,25,25,25	0
56	MG	1A	3491	1/1	0.94	0.13	59,59,59,59	0
56	MG	23	102	1/1	0.94	0.11	48,48,48,48	0
56	MG	25	101	1/1	0.94	0.24	55,55,55,55	0
56	MG	1A	3493	1/1	0.94	0.10	36,36,36,36	0
56	MG	2A	3235	1/1	0.94	0.16	50,50,50,50	0
56	MG	1A	3796	1/1	0.94	0.07	34,34,34,34	0
56	MG	1A	3494	1/1	0.94	0.10	39,39,39,39	0
56	MG	2a	3001	1/1	0.94	0.12	57,57,57,57	0
56	MG	1A	3495	1/1	0.94	0.10	42,42,42,42	0
56	MG	2A	3545	1/1	0.94	0.12	52,52,52,52	0
56	MG	2A	3243	1/1	0.94	0.13	52,52,52,52	0
56	MG	1A	3398	1/1	0.94	0.18	58,58,58,58	0
56	MG	1a	1804	1/1	0.94	0.08	77,77,77,77	0
56	MG	10	104	1/1	0.94	0.21	64,64,64,64	0
56	MG	2A	3247	1/1	0.94	0.12	51,51,51,51	0
56	MG	2A	3248	1/1	0.94	0.13	42,42,42,42	0
56	MG	1A	3028	1/1	0.94	0.10	34,34,34,34	0
56	MG	1A	3400	1/1	0.94	0.14	54,54,54,54	0
56	MG	1A	3402	1/1	0.94	0.18	54,54,54,54	0
56	MG	1A	3647	1/1	0.94	0.08	29,29,29,29	0
56	MG	1A	3812	1/1	0.94	0.09	45,45,45,45	0
56	MG	2A	3576	1/1	0.94	0.12	39,39,39,39	0
56	MG	13	101	1/1	0.94	0.12	55,55,55,55	0
56	MG	1A	3403	1/1	0.94	0.12	27,27,27,27	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	4021	1/1	0.94	0.19	66,66,66,66	0
56	MG	2A	3263	1/1	0.94	0.09	55,55,55,55	0
56	MG	1A	3131	1/1	0.94	0.10	72,72,72,72	0
56	MG	2A	3591	1/1	0.94	0.08	50,50,50,50	0
56	MG	1A	3652	1/1	0.94	0.08	31,31,31,31	0
56	MG	2a	3027	1/1	0.94	0.10	61,61,61,61	0
56	MG	2A	3596	1/1	0.94	0.10	47,47,47,47	0
56	MG	1A	4025	1/1	0.94	0.07	77,77,77,77	0
56	MG	1A	3658	1/1	0.94	0.12	37,37,37,37	0
56	MG	1A	4029	1/1	0.94	0.07	53,53,53,53	0
56	MG	1A	4032	1/1	0.94	0.09	68,68,68,68	0
56	MG	1A	3252	1/1	0.94	0.13	52,52,52,52	0
56	MG	1A	3660	1/1	0.94	0.17	31,31,31,31	0
56	MG	1A	4040	1/1	0.94	0.06	60,60,60,60	0
56	MG	1A	3076	1/1	0.94	0.19	53,53,53,53	0
56	MG	2A	3277	1/1	0.94	0.16	50,50,50,50	0
56	MG	1A	3825	1/1	0.94	0.11	57,57,57,57	0
56	MG	1a	1607	1/1	0.94	0.22	67,67,67,67	0
56	MG	2A	3616	1/1	0.94	0.08	46,46,46,46	0
56	MG	1A	3409	1/1	0.94	0.28	60,60,60,60	0
56	MG	1A	3254	1/1	0.94	0.16	53,53,53,53	0
56	MG	1A	4051	1/1	0.94	0.11	38,38,38,38	0
56	MG	1a	1615	1/1	0.94	0.09	67,67,67,67	0
56	MG	2a	3047	1/1	0.94	0.12	52,52,52,52	0
56	MG	2A	3623	1/1	0.94	0.11	48,48,48,48	0
56	MG	1A	3669	1/1	0.94	0.08	34,34,34,34	0
56	MG	1A	3529	1/1	0.94	0.18	43,43,43,43	0
56	MG	2A	3289	1/1	0.94	0.10	47,47,47,47	0
56	MG	2a	3052	1/1	0.94	0.12	62,62,62,62	0
56	MG	2A	3631	1/1	0.94	0.09	39,39,39,39	0
56	MG	1A	3675	1/1	0.94	0.16	32,32,32,32	0
56	MG	1A	3079	1/1	0.94	0.09	57,57,57,57	0
56	MG	2A	3638	1/1	0.94	0.13	43,43,43,43	0
56	MG	1A	3681	1/1	0.94	0.06	34,34,34,34	0
56	MG	2A	3297	1/1	0.94	0.17	51,51,51,51	0
56	MG	2A	3299	1/1	0.94	0.10	51,51,51,51	0
56	MG	1A	4062	1/1	0.94	0.06	14,14,14,14	0
56	MG	2A	3645	1/1	0.94	0.08	40,40,40,40	0
56	MG	1A	4063	1/1	0.94	0.07	57,57,57,57	0
56	MG	2A	3302	1/1	0.94	0.10	66,66,66,66	0
56	MG	1a	1626	1/1	0.94	0.15	61,61,61,61	0
56	MG	1A	3415	1/1	0.94	0.13	59,59,59,59	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	3068	1/1	0.94	0.19	72,72,72,72	0
56	MG	1A	3684	1/1	0.94	0.10	32,32,32,32	0
56	MG	1A	3417	1/1	0.94	0.13	51,51,51,51	0
56	MG	1A	3146	1/1	0.94	0.14	36,36,36,36	0
56	MG	2a	3072	1/1	0.94	0.09	53,53,53,53	0
56	MG	1A	4069	1/1	0.94	0.15	42,42,42,42	0
56	MG	2A	3659	1/1	0.94	0.08	59,59,59,59	0
56	MG	1A	4070	1/1	0.94	0.14	56,56,56,56	0
56	MG	2A	3665	1/1	0.94	0.07	52,52,52,52	0
56	MG	2a	3077	1/1	0.94	0.10	61,61,61,61	0
56	MG	1A	3260	1/1	0.94	0.09	39,39,39,39	0
56	MG	2A	3311	1/1	0.94	0.18	63,63,63,63	0
56	MG	1A	3846	1/1	0.94	0.08	53,53,53,53	0
56	MG	2A	3672	1/1	0.94	0.15	45,45,45,45	0
56	MG	1A	3194	1/1	0.94	0.22	43,43,43,43	0
56	MG	2a	3086	1/1	0.94	0.12	57,57,57,57	0
56	MG	1A	3034	1/1	0.94	0.13	45,45,45,45	0
56	MG	2A	3675	1/1	0.94	0.13	55,55,55,55	0
56	MG	2A	3676	1/1	0.94	0.12	48,48,48,48	0
56	MG	2A	3680	1/1	0.94	0.10	62,62,62,62	0
56	MG	1A	4078	1/1	0.94	0.13	41,41,41,41	0
56	MG	2A	3318	1/1	0.94	0.13	48,48,48,48	0
56	MG	2A	3683	1/1	0.94	0.11	62,62,62,62	0
56	MG	1A	4083	1/1	0.94	0.11	44,44,44,44	0
56	MG	2A	3004	1/1	0.94	0.16	48,48,48,48	0
56	MG	2A	3325	1/1	0.94	0.12	63,63,63,63	0
56	MG	1A	3197	1/1	0.94	0.09	52,52,52,52	0
56	MG	2A	3327	1/1	0.94	0.10	50,50,50,50	0
56	MG	2A	3329	1/1	0.94	0.12	56,56,56,56	0
56	MG	1A	4085	1/1	0.94	0.09	21,21,21,21	0
56	MG	2A	3010	1/1	0.94	0.15	51,51,51,51	0
56	MG	1A	3198	1/1	0.94	0.14	41,41,41,41	0
56	MG	2a	3107	1/1	0.94	0.13	57,57,57,57	0
56	MG	1a	1647	1/1	0.94	0.15	65,65,65,65	0
56	MG	2A	3334	1/1	0.94	0.29	64,64,64,64	0
56	MG	1A	3335	1/1	0.94	0.34	62,62,62,62	0
56	MG	1A	3337	1/1	0.94	0.15	48,48,48,48	0
56	MG	2A	3337	1/1	0.94	0.11	47,47,47,47	0
56	MG	2A	3704	1/1	0.94	0.07	56,56,56,56	0
56	MG	2A	3338	1/1	0.94	0.25	62,62,62,62	0
56	MG	2A	3024	1/1	0.94	0.11	49,49,49,49	0
56	MG	2a	3118	1/1	0.94	0.11	65,65,65,65	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3028	1/1	0.94	0.09	54,54,54,54	0
56	MG	1a	1652	1/1	0.94	0.21	63,63,63,63	0
56	MG	2A	3033	1/1	0.94	0.11	42,42,42,42	0
56	MG	1A	3338	1/1	0.94	0.12	49,49,49,49	0
56	MG	1A	3430	1/1	0.94	0.09	47,47,47,47	0
56	MG	2a	3125	1/1	0.94	0.09	65,65,65,65	0
56	MG	2A	3040	1/1	0.94	0.14	52,52,52,52	0
56	MG	1A	4100	1/1	0.94	0.09	47,47,47,47	0
56	MG	1A	4101	1/1	0.94	0.10	39,39,39,39	0
56	MG	1A	3857	1/1	0.94	0.15	48,48,48,48	0
56	MG	1A	3431	1/1	0.94	0.15	52,52,52,52	0
56	MG	2A	3727	1/1	0.94	0.09	51,51,51,51	0
56	MG	2A	3351	1/1	0.94	0.18	54,54,54,54	0
56	MG	2a	3134	1/1	0.94	0.21	64,64,64,64	0
56	MG	1a	1664	1/1	0.94	0.24	62,62,62,62	0
56	MG	2A	3052	1/1	0.94	0.12	58,58,58,58	0
56	MG	2A	3355	1/1	0.94	0.12	51,51,51,51	0
56	MG	2A	3736	1/1	0.94	0.20	67,67,67,67	0
56	MG	2A	3358	1/1	0.94	0.08	65,65,65,65	0
56	MG	1A	3705	1/1	0.94	0.10	42,42,42,42	0
56	MG	2A	3739	1/1	0.94	0.14	59,59,59,59	0
56	MG	1A	3150	1/1	0.94	0.16	50,50,50,50	0
56	MG	1a	1668	1/1	0.94	0.21	67,67,67,67	0
56	MG	2A	3363	1/1	0.94	0.30	65,65,65,65	0
56	MG	1A	3006	1/1	0.94	0.19	57,57,57,57	0
56	MG	1A	3437	1/1	0.94	0.09	52,52,52,52	0
56	MG	1A	3207	1/1	0.94	0.14	54,54,54,54	0
56	MG	1a	1673	1/1	0.94	0.22	67,67,67,67	0
56	MG	2A	3369	1/1	0.94	0.10	47,47,47,47	0
56	MG	2A	3370	1/1	0.94	0.15	50,50,50,50	0
56	MG	2a	3159	1/1	0.94	0.19	71,71,71,71	0
56	MG	2A	3371	1/1	0.94	0.12	48,48,48,48	0
56	MG	1A	3154	1/1	0.94	0.19	51,51,51,51	0
56	MG	1A	4131	1/1	0.94	0.13	58,58,58,58	0
56	MG	2a	3170	1/1	0.94	0.07	80,80,80,80	0
56	MG	2A	3375	1/1	0.94	0.10	52,52,52,52	0
56	MG	2a	3172	1/1	0.94	0.07	66,66,66,66	0
56	MG	1A	3062	1/1	0.94	0.29	59,59,59,59	0
56	MG	1A	4135	1/1	0.94	0.13	44,44,44,44	0
56	MG	2a	3177	1/1	0.94	0.07	67,67,67,67	0
56	MG	2A	3379	1/1	0.94	0.08	53,53,53,53	0
56	MG	1A	4137	1/1	0.94	0.07	44,44,44,44	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3072	1/1	0.94	0.09	46,46,46,46	0
56	MG	2a	3185	1/1	0.94	0.11	47,47,47,47	0
56	MG	2A	3761	1/1	0.94	0.18	46,46,46,46	0
56	MG	2A	3073	1/1	0.94	0.08	36,36,36,36	0
56	MG	1A	3874	1/1	0.94	0.12	40,40,40,40	0
56	MG	1A	3163	1/1	0.94	0.23	52,52,52,52	0
56	MG	2A	3388	1/1	0.94	0.12	56,56,56,56	0
56	MG	2a	3196	1/1	0.94	0.12	64,64,64,64	0
56	MG	2A	3767	1/1	0.94	0.09	56,56,56,56	0
56	MG	2A	3079	1/1	0.94	0.09	41,41,41,41	0
56	MG	1A	3281	1/1	0.94	0.12	50,50,50,50	0
56	MG	2A	3081	1/1	0.94	0.15	45,45,45,45	0
56	MG	2A	3082	1/1	0.94	0.10	50,50,50,50	0
56	MG	1a	1684	1/1	0.94	0.21	60,60,60,60	0
56	MG	1B	3005	1/1	0.94	0.09	55,55,55,55	0
56	MG	2A	3399	1/1	0.94	0.14	60,60,60,60	0
56	MG	2A	3402	1/1	0.94	0.12	50,50,50,50	0
56	MG	2a	3207	1/1	0.94	0.12	74,74,74,74	0
56	MG	1A	3721	1/1	0.94	0.10	57,57,57,57	0
56	MG	1A	3064	1/1	0.94	0.17	53,53,53,53	0
56	MG	2A	3782	1/1	0.94	0.06	51,51,51,51	0
56	MG	1a	1690	1/1	0.94	0.18	70,70,70,70	0
56	MG	2A	3786	1/1	0.94	0.07	48,48,48,48	0
56	MG	2A	3788	1/1	0.94	0.08	53,53,53,53	0
56	MG	2a	3216	1/1	0.94	0.19	65,65,65,65	0
56	MG	2A	3790	1/1	0.94	0.15	65,65,65,65	0
56	MG	1B	3008	1/1	0.94	0.14	57,57,57,57	0
56	MG	1A	3883	1/1	0.94	0.12	68,68,68,68	0
56	MG	2A	3796	1/1	0.94	0.09	49,49,49,49	0
56	MG	2A	3098	1/1	0.94	0.08	49,49,49,49	0
56	MG	1A	3447	1/1	0.94	0.08	46,46,46,46	0
56	MG	1B	3011	1/1	0.94	0.12	55,55,55,55	0
56	MG	2A	3414	1/1	0.94	0.16	59,59,59,59	0
56	MG	2A	3418	1/1	0.94	0.10	61,61,61,61	0
56	MG	2A	3103	1/1	0.94	0.21	42,42,42,42	0
56	MG	1A	3448	1/1	0.94	0.20	59,59,59,59	0
56	MG	2A	3809	1/1	0.94	0.09	59,59,59,59	0
56	MG	1A	3115	1/1	0.94	0.17	57,57,57,57	0
56	MG	1A	3728	1/1	0.94	0.10	26,26,26,26	0
56	MG	1A	3225	1/1	0.94	0.19	52,52,52,52	0
56	MG	1B	3017	1/1	0.94	0.20	50,50,50,50	0
56	MG	1A	3892	1/1	0.94	0.10	39,39,39,39	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3453	1/1	0.94	0.11	57,57,57,57	0
56	MG	1A	3090	1/1	0.94	0.21	54,54,54,54	0
56	MG	1A	3579	1/1	0.94	0.18	44,44,44,44	0
56	MG	1A	3735	1/1	0.94	0.12	41,41,41,41	0
56	MG	2A	3431	1/1	0.94	0.15	62,62,62,62	0
56	MG	1A	3230	1/1	0.94	0.17	60,60,60,60	0
56	MG	1A	3742	1/1	0.94	0.08	64,64,64,64	0
56	MG	2A	3436	1/1	0.94	0.11	49,49,49,49	0
56	MG	2A	3830	1/1	0.94	0.14	48,48,48,48	0
56	MG	1A	3459	1/1	0.94	0.13	47,47,47,47	0
56	MG	1A	3463	1/1	0.94	0.08	53,53,53,53	0
56	MG	2A	3127	1/1	0.94	0.08	50,50,50,50	0
56	MG	2A	3837	1/1	0.94	0.09	37,37,37,37	0
56	MG	2A	3440	1/1	0.94	0.16	43,43,43,43	0
56	MG	2A	3842	1/1	0.94	0.09	59,59,59,59	0
56	MG	2A	3843	1/1	0.94	0.13	58,58,58,58	0
56	MG	1a	1715	1/1	0.94	0.13	49,49,49,49	0
56	MG	2A	3850	1/1	0.94	0.08	59,59,59,59	0
56	MG	1a	1717	1/1	0.94	0.14	64,64,64,64	0
56	MG	2A	3444	1/1	0.94	0.17	49,49,49,49	0
56	MG	1A	3583	1/1	0.94	0.17	42,42,42,42	0
56	MG	1A	3464	1/1	0.94	0.11	45,45,45,45	0
56	MG	1A	3586	1/1	0.94	0.17	49,49,49,49	0
56	MG	1A	3301	1/1	0.94	0.10	54,54,54,54	0
56	MG	2A	3146	1/1	0.94	0.09	43,43,43,43	0
56	MG	2A	3866	1/1	0.94	0.09	42,42,42,42	0
56	MG	1A	3590	1/1	0.94	0.16	37,37,37,37	0
56	MG	2A	3148	1/1	0.94	0.14	52,52,52,52	0
56	MG	1A	3921	1/1	0.94	0.11	50,50,50,50	0
56	MG	2x	105	1/1	0.94	0.20	57,57,57,57	0
56	MG	2A	3151	1/1	0.94	0.11	40,40,40,40	0
56	MG	2A	3878	1/1	0.94	0.09	49,49,49,49	0
56	MG	2A	3456	1/1	0.94	0.28	60,60,60,60	0
56	MG	2y	3004	1/1	0.94	0.12	59,59,59,59	0
56	MG	1A	3923	1/1	0.94	0.08	47,47,47,47	0
56	MG	1A	3171	1/1	0.94	0.24	53,53,53,53	0
56	MG	1A	3180	1/1	0.94	0.11	36,36,36,36	0
58	ZN	2n	501	1/1	0.94	0.09	107,107,107,107	0
56	MG	1a	1734	1/1	0.95	0.14	67,67,67,67	0
56	MG	2A	3176	1/1	0.95	0.11	46,46,46,46	0
56	MG	1A	3949	1/1	0.95	0.10	63,63,63,63	0
56	MG	1a	1736	1/1	0.95	0.09	57,57,57,57	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3950	1/1	0.95	0.07	41,41,41,41	0
56	MG	2A	3886	1/1	0.95	0.18	45,45,45,45	0
56	MG	1A	3226	1/1	0.95	0.12	47,47,47,47	0
56	MG	2A	3889	1/1	0.95	0.10	49,49,49,49	0
56	MG	1a	1742	1/1	0.95	0.07	51,51,51,51	0
56	MG	1A	3953	1/1	0.95	0.08	46,46,46,46	0
56	MG	2A	3476	1/1	0.95	0.11	41,41,41,41	0
56	MG	2A	3185	1/1	0.95	0.08	45,45,45,45	0
56	MG	1F	301	1/1	0.95	0.11	40,40,40,40	0
56	MG	1A	3467	1/1	0.95	0.10	45,45,45,45	0
56	MG	2A	3900	1/1	0.95	0.16	44,44,44,44	0
56	MG	2A	3903	1/1	0.95	0.12	58,58,58,58	0
56	MG	2A	3190	1/1	0.95	0.09	45,45,45,45	0
56	MG	1F	303	1/1	0.95	0.12	38,38,38,38	0
56	MG	2A	3192	1/1	0.95	0.10	44,44,44,44	0
56	MG	2A	3483	1/1	0.95	0.18	55,55,55,55	0
56	MG	2A	3193	1/1	0.95	0.08	55,55,55,55	0
56	MG	1A	3166	1/1	0.95	0.20	38,38,38,38	0
56	MG	1A	3957	1/1	0.95	0.07	55,55,55,55	0
56	MG	2A	3196	1/1	0.95	0.10	56,56,56,56	0
56	MG	1A	3228	1/1	0.95	0.10	41,41,41,41	0
56	MG	1A	3600	1/1	0.95	0.07	46,46,46,46	0
56	MG	2A	3199	1/1	0.95	0.08	50,50,50,50	0
56	MG	2A	3200	1/1	0.95	0.11	42,42,42,42	0
56	MG	1A	3768	1/1	0.95	0.10	61,61,61,61	0
56	MG	2A	3495	1/1	0.95	0.07	51,51,51,51	0
56	MG	1A	3601	1/1	0.95	0.09	11,11,11,11	0
56	MG	1A	3604	1/1	0.95	0.13	65,65,65,65	0
56	MG	1A	3091	1/1	0.95	0.15	43,43,43,43	0
56	MG	1A	3383	1/1	0.95	0.10	55,55,55,55	0
56	MG	1A	3384	1/1	0.95	0.13	57,57,57,57	0
56	MG	1A	3477	1/1	0.95	0.12	48,48,48,48	0
56	MG	2A	3214	1/1	0.95	0.07	56,56,56,56	0
56	MG	1A	3119	1/1	0.95	0.11	51,51,51,51	0
56	MG	2B	3018	1/1	0.95	0.10	65,65,65,65	0
56	MG	2A	3509	1/1	0.95	0.10	38,38,38,38	0
56	MG	1N	206	1/1	0.95	0.13	42,42,42,42	0
56	MG	2A	3511	1/1	0.95	0.08	24,24,24,24	0
56	MG	1a	1769	1/1	0.95	0.08	55,55,55,55	0
56	MG	1A	3978	1/1	0.95	0.07	65,65,65,65	0
56	MG	1A	3780	1/1	0.95	0.06	21,21,21,21	0
56	MG	2A	3223	1/1	0.95	0.14	44,44,44,44	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3480	1/1	0.95	0.09	52,52,52,52	0
56	MG	1A	3120	1/1	0.95	0.09	42,42,42,42	0
56	MG	2E	304	1/1	0.95	0.17	46,46,46,46	0
56	MG	2E	305	1/1	0.95	0.10	40,40,40,40	0
56	MG	1A	3624	1/1	0.95	0.09	28,28,28,28	0
56	MG	1P	204	1/1	0.95	0.17	47,47,47,47	0
56	MG	1A	3985	1/1	0.95	0.09	23,23,23,23	0
56	MG	2E	309	1/1	0.95	0.10	60,60,60,60	0
56	MG	1a	1778	1/1	0.95	0.08	64,64,64,64	0
56	MG	1Q	204	1/1	0.95	0.08	51,51,51,51	0
56	MG	2A	3533	1/1	0.95	0.10	48,48,48,48	0
56	MG	2N	8001	1/1	0.95	0.06	47,47,47,47	0
56	MG	2A	3232	1/1	0.95	0.15	64,64,64,64	0
56	MG	1A	3625	1/1	0.95	0.08	19,19,19,19	0
56	MG	1A	3234	1/1	0.95	0.21	54,54,54,54	0
56	MG	2A	3236	1/1	0.95	0.09	53,53,53,53	0
56	MG	1A	3992	1/1	0.95	0.12	75,75,75,75	0
56	MG	1A	3993	1/1	0.95	0.10	37,37,37,37	0
56	MG	2A	3543	1/1	0.95	0.07	34,34,34,34	0
56	MG	1A	3485	1/1	0.95	0.11	48,48,48,48	0
56	MG	2A	3242	1/1	0.95	0.11	52,52,52,52	0
56	MG	1A	3486	1/1	0.95	0.07	42,42,42,42	0
56	MG	1A	3388	1/1	0.95	0.11	42,42,42,42	0
56	MG	2A	3550	1/1	0.95	0.14	44,44,44,44	0
56	MG	1A	3633	1/1	0.95	0.08	58,58,58,58	0
56	MG	2X	103	1/1	0.95	0.10	46,46,46,46	0
56	MG	1A	3636	1/1	0.95	0.09	38,38,38,38	0
56	MG	2A	3554	1/1	0.95	0.08	39,39,39,39	0
56	MG	1V	201	1/1	0.95	0.08	49,49,49,49	0
56	MG	20	3003	1/1	0.95	0.11	58,58,58,58	0
56	MG	1V	202	1/1	0.95	0.19	53,53,53,53	0
56	MG	2A	3557	1/1	0.95	0.08	45,45,45,45	0
56	MG	2A	3558	1/1	0.95	0.08	31,31,31,31	0
56	MG	25	103	1/1	0.95	0.12	52,52,52,52	0
56	MG	2A	3559	1/1	0.95	0.10	39,39,39,39	0
56	MG	2A	3249	1/1	0.95	0.10	57,57,57,57	0
56	MG	1A	3390	1/1	0.95	0.13	35,35,35,35	0
56	MG	2A	3563	1/1	0.95	0.10	49,49,49,49	0
56	MG	2A	3565	1/1	0.95	0.07	36,36,36,36	0
56	MG	1A	3093	1/1	0.95	0.17	33,33,33,33	0
56	MG	2A	3569	1/1	0.95	0.10	49,49,49,49	0
56	MG	2A	3570	1/1	0.95	0.09	53,53,53,53	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3571	1/1	0.95	0.07	35,35,35,35	0
56	MG	1W	204	1/1	0.95	0.11	40,40,40,40	0
56	MG	1a	1806	1/1	0.95	0.09	66,66,66,66	0
56	MG	2A	3574	1/1	0.95	0.08	44,44,44,44	0
56	MG	1a	1812	1/1	0.95	0.09	70,70,70,70	0
56	MG	2A	3258	1/1	0.95	0.23	58,58,58,58	0
56	MG	1A	3070	1/1	0.95	0.16	41,41,41,41	0
56	MG	2A	3580	1/1	0.95	0.13	49,49,49,49	0
56	MG	1A	3393	1/1	0.95	0.11	50,50,50,50	0
56	MG	2A	3586	1/1	0.95	0.12	53,53,53,53	0
56	MG	1A	3803	1/1	0.95	0.27	44,44,44,44	0
56	MG	1Y	504	1/1	0.95	0.19	48,48,48,48	0
56	MG	2A	3264	1/1	0.95	0.06	62,62,62,62	0
56	MG	1Z	301	1/1	0.95	0.11	56,56,56,56	0
56	MG	1a	1826	1/1	0.95	0.08	58,58,58,58	0
56	MG	1A	3039	1/1	0.95	0.09	36,36,36,36	0
56	MG	1Z	303	1/1	0.95	0.07	56,56,56,56	0
56	MG	2a	3025	1/1	0.95	0.18	57,57,57,57	0
56	MG	10	101	1/1	0.95	0.12	63,63,63,63	0
56	MG	1A	3128	1/1	0.95	0.23	41,41,41,41	0
56	MG	1A	3809	1/1	0.95	0.16	51,51,51,51	0
56	MG	1A	3129	1/1	0.95	0.18	51,51,51,51	0
56	MG	2A	3273	1/1	0.95	0.09	51,51,51,51	0
56	MG	1A	3811	1/1	0.95	0.09	45,45,45,45	0
56	MG	1A	3499	1/1	0.95	0.10	49,49,49,49	0
56	MG	2A	3611	1/1	0.95	0.11	62,62,62,62	0
56	MG	2A	3613	1/1	0.95	0.09	33,33,33,33	0
56	MG	2a	3035	1/1	0.95	0.26	63,63,63,63	0
56	MG	2A	3276	1/1	0.95	0.11	55,55,55,55	0
56	MG	1A	3501	1/1	0.95	0.12	51,51,51,51	0
56	MG	1A	3651	1/1	0.95	0.12	32,32,32,32	0
56	MG	2A	3279	1/1	0.95	0.10	53,53,53,53	0
56	MG	13	102	1/1	0.95	0.14	53,53,53,53	0
56	MG	1t	3001	1/1	0.95	0.12	58,58,58,58	0
56	MG	1A	3817	1/1	0.95	0.15	45,45,45,45	0
56	MG	2a	3043	1/1	0.95	0.10	64,64,64,64	0
56	MG	2A	3283	1/1	0.95	0.11	61,61,61,61	0
56	MG	15	102	1/1	0.95	0.08	39,39,39,39	0
56	MG	1A	3244	1/1	0.95	0.08	49,49,49,49	0
56	MG	2A	3627	1/1	0.95	0.10	50,50,50,50	0
56	MG	2A	3628	1/1	0.95	0.11	52,52,52,52	0
56	MG	2A	3629	1/1	0.95	0.08	43,43,43,43	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	16	101	1/1	0.95	0.09	45,45,45,45	0
56	MG	1A	3655	1/1	0.95	0.07	39,39,39,39	0
56	MG	1A	3318	1/1	0.95	0.07	46,46,46,46	0
56	MG	18	101	1/1	0.95	0.16	47,47,47,47	0
56	MG	1A	3130	1/1	0.95	0.11	41,41,41,41	0
56	MG	2a	3055	1/1	0.95	0.06	51,51,51,51	0
56	MG	2A	3292	1/1	0.95	0.10	54,54,54,54	0
56	MG	2A	3294	1/1	0.95	0.09	52,52,52,52	0
56	MG	1A	4037	1/1	0.95	0.10	62,62,62,62	0
56	MG	19	101	1/1	0.95	0.19	49,49,49,49	0
56	MG	1A	3507	1/1	0.95	0.21	51,51,51,51	0
56	MG	1A	4043	1/1	0.95	0.07	50,50,50,50	0
56	MG	1A	3075	1/1	0.95	0.07	28,28,28,28	0
56	MG	1A	4045	1/1	0.95	0.07	38,38,38,38	0
56	MG	2A	3651	1/1	0.95	0.15	44,44,44,44	0
56	MG	1A	3042	1/1	0.95	0.14	40,40,40,40	0
56	MG	1A	3249	1/1	0.95	0.23	56,56,56,56	0
56	MG	1A	4048	1/1	0.95	0.08	48,48,48,48	0
56	MG	1A	3514	1/1	0.95	0.12	53,53,53,53	0
56	MG	1a	1608	1/1	0.95	0.13	60,60,60,60	0
56	MG	1A	3519	1/1	0.95	0.06	49,49,49,49	0
56	MG	2A	3661	1/1	0.95	0.13	56,56,56,56	0
56	MG	2A	3662	1/1	0.95	0.10	48,48,48,48	0
56	MG	2A	3663	1/1	0.95	0.11	64,64,64,64	0
56	MG	1A	3674	1/1	0.95	0.10	39,39,39,39	0
56	MG	1A	3408	1/1	0.95	0.15	60,60,60,60	0
56	MG	1A	3676	1/1	0.95	0.12	24,24,24,24	0
56	MG	1a	1616	1/1	0.95	0.10	55,55,55,55	0
56	MG	2a	3079	1/1	0.95	0.18	59,59,59,59	0
56	MG	1A	4055	1/1	0.95	0.06	33,33,33,33	0
56	MG	1A	4056	1/1	0.95	0.06	47,47,47,47	0
56	MG	2A	3316	1/1	0.95	0.11	54,54,54,54	0
56	MG	1A	4059	1/1	0.95	0.07	21,21,21,21	0
56	MG	1A	3677	1/1	0.95	0.10	29,29,29,29	0
56	MG	2A	3320	1/1	0.95	0.22	54,54,54,54	0
56	MG	2A	3678	1/1	0.95	0.08	49,49,49,49	0
56	MG	2A	3679	1/1	0.95	0.07	41,41,41,41	0
56	MG	1A	3678	1/1	0.95	0.08	61,61,61,61	0
56	MG	1A	3838	1/1	0.95	0.16	45,45,45,45	0
56	MG	2A	3324	1/1	0.95	0.07	41,41,41,41	0
56	MG	1A	3324	1/1	0.95	0.21	55,55,55,55	0
56	MG	1A	4064	1/1	0.95	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
56	MG	1A	3250	1/1	0.95	0.11	49,49,49,49	0
56	MG	2A	3012	1/1	0.95	0.07	39,39,39,39	0
56	MG	2A	3014	1/1	0.95	0.18	43,43,43,43	0
56	MG	2A	3688	1/1	0.95	0.07	38,38,38,38	0
56	MG	2a	3102	1/1	0.95	0.20	58,58,58,58	0
56	MG	1A	3841	1/1	0.95	0.10	27,27,27,27	0
56	MG	1A	3134	1/1	0.95	0.10	54,54,54,54	0
56	MG	1A	3683	1/1	0.95	0.13	40,40,40,40	0
56	MG	1A	3528	1/1	0.95	0.07	45,45,45,45	0
56	MG	1a	1632	1/1	0.95	0.16	52,52,52,52	0
56	MG	1A	3413	1/1	0.95	0.10	36,36,36,36	0
56	MG	1A	3327	1/1	0.95	0.13	28,28,28,28	0
56	MG	2A	3030	1/1	0.95	0.09	51,51,51,51	0
56	MG	2A	3032	1/1	0.95	0.07	38,38,38,38	0
56	MG	2a	3112	1/1	0.95	0.13	54,54,54,54	0
56	MG	1A	3416	1/1	0.95	0.10	47,47,47,47	0
56	MG	2A	3034	1/1	0.95	0.08	45,45,45,45	0
56	MG	1A	4073	1/1	0.95	0.06	42,42,42,42	0
56	MG	2A	3706	1/1	0.95	0.06	47,47,47,47	0
56	MG	2A	3036	1/1	0.95	0.10	54,54,54,54	0
56	MG	2A	3038	1/1	0.95	0.08	31,31,31,31	0
56	MG	1A	3137	1/1	0.95	0.09	33,33,33,33	0
56	MG	1A	3329	1/1	0.95	0.11	43,43,43,43	0
56	MG	1A	3059	1/1	0.95	0.11	48,48,48,48	0
56	MG	2a	3123	1/1	0.95	0.13	54,54,54,54	0
56	MG	2A	3713	1/1	0.95	0.13	67,67,67,67	0
56	MG	1a	1641	1/1	0.95	0.15	58,58,58,58	0
56	MG	1A	3331	1/1	0.95	0.13	54,54,54,54	0
56	MG	1A	3421	1/1	0.95	0.09	46,46,46,46	0
56	MG	1a	1644	1/1	0.95	0.15	66,66,66,66	0
56	MG	1A	3195	1/1	0.95	0.25	40,40,40,40	0
56	MG	2A	3721	1/1	0.95	0.08	46,46,46,46	0
56	MG	1a	1646	1/1	0.95	0.08	51,51,51,51	0
56	MG	2A	3726	1/1	0.95	0.13	56,56,56,56	0
56	MG	2A	3356	1/1	0.95	0.13	55,55,55,55	0
56	MG	2A	3054	1/1	0.95	0.09	54,54,54,54	0
56	MG	2A	3730	1/1	0.95	0.09	43,43,43,43	0
56	MG	1A	3860	1/1	0.95	0.14	47,47,47,47	0
56	MG	2A	3057	1/1	0.95	0.08	46,46,46,46	0
56	MG	2a	3139	1/1	0.95	0.08	73,73,73,73	0
56	MG	2A	3361	1/1	0.95	0.12	51,51,51,51	0
56	MG	1A	4088	1/1	0.95	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
56	MG	1a	1649	1/1	0.95	0.13	45,45,45,45	0
56	MG	2A	3061	1/1	0.95	0.08	49,49,49,49	0
56	MG	1A	3697	1/1	0.95	0.11	51,51,51,51	0
56	MG	1A	3255	1/1	0.95	0.14	47,47,47,47	0
56	MG	1A	3865	1/1	0.95	0.34	43,43,43,43	0
56	MG	1A	3102	1/1	0.95	0.10	54,54,54,54	0
56	MG	1a	1659	1/1	0.95	0.22	62,62,62,62	0
56	MG	1A	3700	1/1	0.95	0.07	16,16,16,16	0
56	MG	1A	3869	1/1	0.95	0.08	56,56,56,56	0
56	MG	2A	3070	1/1	0.95	0.23	42,42,42,42	0
56	MG	1A	4102	1/1	0.95	0.12	45,45,45,45	0
56	MG	1A	3147	1/1	0.95	0.16	54,54,54,54	0
56	MG	2a	3163	1/1	0.95	0.06	72,72,72,72	0
56	MG	2a	3164	1/1	0.95	0.10	73,73,73,73	0
56	MG	2A	3750	1/1	0.95	0.13	47,47,47,47	0
56	MG	1A	3704	1/1	0.95	0.13	49,49,49,49	0
56	MG	2a	3168	1/1	0.95	0.07	78,78,78,78	0
56	MG	1A	4105	1/1	0.95	0.11	44,44,44,44	0
56	MG	1A	4108	1/1	0.95	0.21	48,48,48,48	0
56	MG	1a	1667	1/1	0.95	0.17	65,65,65,65	0
56	MG	2A	3382	1/1	0.95	0.09	50,50,50,50	0
56	MG	1A	3546	1/1	0.95	0.12	45,45,45,45	0
56	MG	1A	3706	1/1	0.95	0.11	40,40,40,40	0
56	MG	1A	3103	1/1	0.95	0.07	38,38,38,38	0
56	MG	2A	3085	1/1	0.95	0.11	44,44,44,44	0
56	MG	2A	3391	1/1	0.95	0.12	58,58,58,58	0
56	MG	2A	3086	1/1	0.95	0.10	44,44,44,44	0
56	MG	2a	3186	1/1	0.95	0.14	53,53,53,53	0
56	MG	2A	3763	1/1	0.95	0.10	52,52,52,52	0
56	MG	2a	3188	1/1	0.95	0.09	68,68,68,68	0
56	MG	2a	3189	1/1	0.95	0.11	48,48,48,48	0
56	MG	2A	3087	1/1	0.95	0.13	53,53,53,53	0
56	MG	1A	3877	1/1	0.95	0.07	39,39,39,39	0
56	MG	2A	3395	1/1	0.95	0.10	50,50,50,50	0
56	MG	1A	3427	1/1	0.95	0.10	44,44,44,44	0
56	MG	1A	4124	1/1	0.95	0.30	46,46,46,46	0
56	MG	1A	3104	1/1	0.95	0.19	40,40,40,40	0
56	MG	1A	3429	1/1	0.95	0.09	48,48,48,48	0
56	MG	1A	3151	1/1	0.95	0.14	47,47,47,47	0
56	MG	2A	3403	1/1	0.95	0.23	60,60,60,60	0
56	MG	1A	3060	1/1	0.95	0.07	45,45,45,45	0
56	MG	1a	1680	1/1	0.95	0.17	64,64,64,64	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2a	3203	1/1	0.95	0.17	62,62,62,62	0
56	MG	2A	3776	1/1	0.95	0.11	44,44,44,44	0
56	MG	2A	3099	1/1	0.95	0.11	42,42,42,42	0
56	MG	2A	3778	1/1	0.95	0.08	52,52,52,52	0
56	MG	1A	3208	1/1	0.95	0.09	55,55,55,55	0
56	MG	1A	3435	1/1	0.95	0.10	53,53,53,53	0
56	MG	1A	3153	1/1	0.95	0.11	37,37,37,37	0
56	MG	1A	3345	1/1	0.95	0.07	47,47,47,47	0
56	MG	2A	3784	1/1	0.95	0.07	47,47,47,47	0
56	MG	2a	3213	1/1	0.95	0.15	69,69,69,69	0
56	MG	1B	3004	1/1	0.95	0.19	50,50,50,50	0
56	MG	1a	1687	1/1	0.95	0.12	50,50,50,50	0
56	MG	2A	3415	1/1	0.95	0.10	50,50,50,50	0
56	MG	2A	3791	1/1	0.95	0.09	46,46,46,46	0
56	MG	2A	3792	1/1	0.95	0.15	51,51,51,51	0
56	MG	2A	3416	1/1	0.95	0.17	59,59,59,59	0
56	MG	1A	3346	1/1	0.95	0.18	48,48,48,48	0
56	MG	1A	3210	1/1	0.95	0.08	42,42,42,42	0
56	MG	2a	3223	1/1	0.95	0.24	52,52,52,52	0
56	MG	1A	3044	1/1	0.95	0.08	37,37,37,37	0
56	MG	2a	3225	1/1	0.95	0.10	57,57,57,57	0
56	MG	2A	3112	1/1	0.95	0.10	42,42,42,42	0
56	MG	1A	3351	1/1	0.95	0.20	49,49,49,49	0
56	MG	1a	1692	1/1	0.95	0.28	69,69,69,69	0
56	MG	1a	1693	1/1	0.95	0.10	58,58,58,58	0
56	MG	2A	3803	1/1	0.95	0.07	42,42,42,42	0
56	MG	1A	3899	1/1	0.95	0.11	52,52,52,52	0
56	MG	1A	3216	1/1	0.95	0.20	50,50,50,50	0
56	MG	1A	3730	1/1	0.95	0.10	43,43,43,43	0
56	MG	1A	3273	1/1	0.95	0.23	53,53,53,53	0
56	MG	1A	3354	1/1	0.95	0.15	68,68,68,68	0
56	MG	1A	3217	1/1	0.95	0.17	47,47,47,47	0
56	MG	2A	3813	1/1	0.95	0.12	48,48,48,48	0
56	MG	1A	3047	1/1	0.95	0.06	21,21,21,21	0
56	MG	1A	3001	1/1	0.95	0.10	42,42,42,42	0
56	MG	2A	3131	1/1	0.95	0.09	42,42,42,42	0
56	MG	1A	3909	1/1	0.95	0.09	40,40,40,40	0
56	MG	2a	3243	1/1	0.95	0.17	64,64,64,64	0
56	MG	1A	3741	1/1	0.95	0.10	45,45,45,45	0
56	MG	1A	3221	1/1	0.95	0.16	55,55,55,55	0
56	MG	1A	3916	1/1	0.95	0.07	53,53,53,53	0
56	MG	1B	3023	1/1	0.95	0.08	54,54,54,54	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3291	1/1	0.95	0.10	59,59,59,59	0
56	MG	2A	3828	1/1	0.95	0.09	80,80,80,80	0
56	MG	1A	3919	1/1	0.95	0.13	38,38,38,38	0
56	MG	2A	3445	1/1	0.95	0.22	55,55,55,55	0
56	MG	2A	3149	1/1	0.95	0.27	54,54,54,54	0
56	MG	1A	3920	1/1	0.95	0.09	44,44,44,44	0
56	MG	1A	3455	1/1	0.95	0.09	47,47,47,47	0
56	MG	1A	3457	1/1	0.95	0.12	59,59,59,59	0
56	MG	1B	3031	1/1	0.95	0.07	67,67,67,67	0
56	MG	1A	3005	1/1	0.95	0.11	41,41,41,41	0
56	MG	1A	3931	1/1	0.95	0.09	55,55,55,55	0
56	MG	1A	3588	1/1	0.95	0.10	46,46,46,46	0
56	MG	2A	3848	1/1	0.95	0.06	36,36,36,36	0
56	MG	2A	3159	1/1	0.95	0.19	53,53,53,53	0
56	MG	1A	3751	1/1	0.95	0.11	48,48,48,48	0
56	MG	2w	105	1/1	0.95	0.16	70,70,70,70	0
56	MG	2w	106	1/1	0.95	0.14	60,60,60,60	0
56	MG	2A	3162	1/1	0.95	0.14	53,53,53,53	0
56	MG	1A	3938	1/1	0.95	0.05	55,55,55,55	0
56	MG	1A	3294	1/1	0.95	0.16	52,52,52,52	0
56	MG	1D	307	1/1	0.95	0.12	45,45,45,45	0
56	MG	1A	3165	1/1	0.95	0.17	48,48,48,48	0
56	MG	1A	3373	1/1	0.95	0.11	52,52,52,52	0
56	MG	1A	3755	1/1	0.95	0.12	36,36,36,36	0
56	MG	2A	3464	1/1	0.95	0.25	54,54,54,54	0
56	MG	2A	3868	1/1	0.95	0.09	69,69,69,69	0
56	MG	2A	3869	1/1	0.95	0.05	56,56,56,56	0
56	MG	1a	1731	1/1	0.95	0.14	50,50,50,50	0
56	MG	2A	3872	1/1	0.95	0.07	44,44,44,44	0
57	K	1A	3584	1/1	0.95	0.09	58,58,58,58	0
56	MG	2A	3874	1/1	0.95	0.06	53,53,53,53	0
56	MG	1A	3374	1/1	0.95	0.17	55,55,55,55	0
56	MG	1B	3001	1/1	0.96	0.21	48,48,48,48	0
56	MG	2A	3608	1/1	0.96	0.05	61,61,61,61	0
56	MG	2A	3609	1/1	0.96	0.12	42,42,42,42	0
56	MG	2A	3315	1/1	0.96	0.12	54,54,54,54	0
56	MG	1A	3498	1/1	0.96	0.09	46,46,46,46	0
56	MG	2A	3612	1/1	0.96	0.08	39,39,39,39	0
56	MG	2P	201	1/1	0.96	0.06	45,45,45,45	0
56	MG	1A	3758	1/1	0.96	0.09	71,71,71,71	0
56	MG	2Q	3002	1/1	0.96	0.08	44,44,44,44	0
56	MG	1A	3222	1/1	0.96	0.13	56,56,56,56	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3917	1/1	0.96	0.06	80,80,80,80	0
56	MG	2A	3055	1/1	0.96	0.08	46,46,46,46	0
56	MG	1A	3621	1/1	0.96	0.11	48,48,48,48	0
56	MG	2A	3323	1/1	0.96	0.13	56,56,56,56	0
56	MG	1A	3622	1/1	0.96	0.07	36,36,36,36	0
56	MG	2U	204	1/1	0.96	0.14	45,45,45,45	0
56	MG	1A	3763	1/1	0.96	0.09	52,52,52,52	0
56	MG	2A	3059	1/1	0.96	0.11	46,46,46,46	0
56	MG	1A	3765	1/1	0.96	0.06	25,25,25,25	0
56	MG	2A	3328	1/1	0.96	0.13	39,39,39,39	0
56	MG	1A	3922	1/1	0.96	0.08	57,57,57,57	0
56	MG	1a	1678	1/1	0.96	0.24	63,63,63,63	0
56	MG	1A	3500	1/1	0.96	0.06	38,38,38,38	0
56	MG	1A	3019	1/1	0.96	0.15	37,37,37,37	0
56	MG	1A	3502	1/1	0.96	0.13	49,49,49,49	0
56	MG	1A	3503	1/1	0.96	0.09	32,32,32,32	0
56	MG	2A	3636	1/1	0.96	0.24	59,59,59,59	0
56	MG	1A	3049	1/1	0.96	0.11	26,26,26,26	0
56	MG	1A	3347	1/1	0.96	0.09	44,44,44,44	0
56	MG	1a	1685	1/1	0.96	0.18	51,51,51,51	0
56	MG	25	104	1/1	0.96	0.07	43,43,43,43	0
56	MG	2A	3641	1/1	0.96	0.10	57,57,57,57	0
56	MG	1A	3283	1/1	0.96	0.14	40,40,40,40	0
56	MG	1A	3777	1/1	0.96	0.11	55,55,55,55	0
56	MG	1A	3284	1/1	0.96	0.21	56,56,56,56	0
56	MG	1A	3945	1/1	0.96	0.09	41,41,41,41	0
56	MG	2a	3002	1/1	0.96	0.07	50,50,50,50	0
56	MG	2A	3076	1/1	0.96	0.11	35,35,35,35	0
56	MG	1A	3099	1/1	0.96	0.09	44,44,44,44	0
56	MG	2A	3648	1/1	0.96	0.07	51,51,51,51	0
56	MG	1A	3510	1/1	0.96	0.07	45,45,45,45	0
56	MG	1A	3638	1/1	0.96	0.07	53,53,53,53	0
56	MG	2A	3652	1/1	0.96	0.13	41,41,41,41	0
56	MG	2a	3009	1/1	0.96	0.07	60,60,60,60	0
56	MG	1A	3029	1/1	0.96	0.12	38,38,38,38	0
56	MG	1A	3292	1/1	0.96	0.09	56,56,56,56	0
56	MG	2A	3083	1/1	0.96	0.15	49,49,49,49	0
56	MG	1A	3785	1/1	0.96	0.07	47,47,47,47	0
56	MG	1A	3179	1/1	0.96	0.07	36,36,36,36	0
56	MG	2A	3352	1/1	0.96	0.11	53,53,53,53	0
56	MG	1A	3517	1/1	0.96	0.08	37,37,37,37	0
56	MG	1a	1700	1/1	0.96	0.25	50,50,50,50	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3089	1/1	0.96	0.07	46,46,46,46	0
56	MG	1A	3956	1/1	0.96	0.06	61,61,61,61	0
56	MG	1A	3518	1/1	0.96	0.12	48,48,48,48	0
56	MG	2A	3666	1/1	0.96	0.07	34,34,34,34	0
56	MG	1A	3958	1/1	0.96	0.12	44,44,44,44	0
56	MG	2A	3669	1/1	0.96	0.08	42,42,42,42	0
56	MG	1B	3037	1/1	0.96	0.06	40,40,40,40	0
56	MG	1A	3031	1/1	0.96	0.13	31,31,31,31	0
56	MG	1A	3961	1/1	0.96	0.09	38,38,38,38	0
56	MG	1A	3791	1/1	0.96	0.07	43,43,43,43	0
56	MG	1A	3792	1/1	0.96	0.07	35,35,35,35	0
56	MG	1D	310	1/1	0.96	0.14	39,39,39,39	0
56	MG	1A	3965	1/1	0.96	0.13	67,67,67,67	0
56	MG	1D	312	1/1	0.96	0.17	42,42,42,42	0
56	MG	1E	301	1/1	0.96	0.11	37,37,37,37	0
56	MG	1A	3793	1/1	0.96	0.27	37,37,37,37	0
56	MG	1a	1714	1/1	0.96	0.17	66,66,66,66	0
56	MG	1A	3968	1/1	0.96	0.06	62,62,62,62	0
56	MG	2A	3373	1/1	0.96	0.07	52,52,52,52	0
56	MG	1A	3520	1/1	0.96	0.10	41,41,41,41	0
56	MG	1A	3078	1/1	0.96	0.10	31,31,31,31	0
56	MG	1A	3522	1/1	0.96	0.07	49,49,49,49	0
56	MG	2A	3377	1/1	0.96	0.08	57,57,57,57	0
56	MG	1A	3797	1/1	0.96	0.12	53,53,53,53	0
56	MG	2A	3689	1/1	0.96	0.17	71,71,71,71	0
56	MG	2A	3690	1/1	0.96	0.13	61,61,61,61	0
56	MG	2A	3114	1/1	0.96	0.11	55,55,55,55	0
56	MG	1A	3132	1/1	0.96	0.10	40,40,40,40	0
56	MG	1A	3233	1/1	0.96	0.09	49,49,49,49	0
56	MG	1A	3977	1/1	0.96	0.10	56,56,56,56	0
56	MG	2A	3383	1/1	0.96	0.22	60,60,60,60	0
56	MG	2A	3118	1/1	0.96	0.17	50,50,50,50	0
56	MG	1F	305	1/1	0.96	0.07	48,48,48,48	0
56	MG	2A	3120	1/1	0.96	0.12	51,51,51,51	0
56	MG	2A	3122	1/1	0.96	0.07	39,39,39,39	0
56	MG	2A	3389	1/1	0.96	0.15	58,58,58,58	0
56	MG	2A	3390	1/1	0.96	0.10	57,57,57,57	0
56	MG	1A	3657	1/1	0.96	0.09	27,27,27,27	0
56	MG	1A	3433	1/1	0.96	0.15	47,47,47,47	0
56	MG	2A	3707	1/1	0.96	0.06	61,61,61,61	0
56	MG	1A	3057	1/1	0.96	0.10	54,54,54,54	0
56	MG	1A	3981	1/1	0.96	0.07	52,52,52,52	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3804	1/1	0.96	0.06	40,40,40,40	0
56	MG	1A	3366	1/1	0.96	0.07	38,38,38,38	0
56	MG	1A	3806	1/1	0.96	0.07	34,34,34,34	0
56	MG	2A	3133	1/1	0.96	0.08	49,49,49,49	0
56	MG	1A	3664	1/1	0.96	0.08	48,48,48,48	0
56	MG	2A	3401	1/1	0.96	0.14	52,52,52,52	0
56	MG	1A	3989	1/1	0.96	0.07	60,60,60,60	0
56	MG	1A	3081	1/1	0.96	0.16	34,34,34,34	0
56	MG	1A	3135	1/1	0.96	0.06	32,32,32,32	0
56	MG	1A	3533	1/1	0.96	0.09	36,36,36,36	0
56	MG	1A	3534	1/1	0.96	0.19	33,33,33,33	0
56	MG	2A	3724	1/1	0.96	0.06	57,57,57,57	0
56	MG	2A	3725	1/1	0.96	0.10	49,49,49,49	0
56	MG	1a	1745	1/1	0.96	0.11	55,55,55,55	0
56	MG	2A	3409	1/1	0.96	0.17	47,47,47,47	0
56	MG	1A	3187	1/1	0.96	0.14	47,47,47,47	0
56	MG	1A	3672	1/1	0.96	0.06	31,31,31,31	0
56	MG	1O	203	1/1	0.96	0.11	63,63,63,63	0
56	MG	1A	3815	1/1	0.96	0.22	44,44,44,44	0
56	MG	1A	3998	1/1	0.96	0.10	65,65,65,65	0
56	MG	2A	3154	1/1	0.96	0.19	48,48,48,48	0
56	MG	2a	3084	1/1	0.96	0.07	44,44,44,44	0
56	MG	1a	1753	1/1	0.96	0.09	59,59,59,59	0
56	MG	1a	1754	1/1	0.96	0.06	51,51,51,51	0
56	MG	1A	3816	1/1	0.96	0.10	49,49,49,49	0
56	MG	1A	3136	1/1	0.96	0.11	52,52,52,52	0
56	MG	2A	3160	1/1	0.96	0.18	44,44,44,44	0
56	MG	1A	3442	1/1	0.96	0.10	56,56,56,56	0
56	MG	1A	3819	1/1	0.96	0.12	48,48,48,48	0
56	MG	2A	3164	1/1	0.96	0.22	53,53,53,53	0
56	MG	1A	3443	1/1	0.96	0.09	54,54,54,54	0
56	MG	1Q	206	1/1	0.96	0.06	54,54,54,54	0
56	MG	1A	3105	1/1	0.96	0.10	40,40,40,40	0
56	MG	1A	3376	1/1	0.96	0.10	51,51,51,51	0
56	MG	1a	1764	1/1	0.96	0.05	59,59,59,59	0
56	MG	1a	1765	1/1	0.96	0.07	49,49,49,49	0
56	MG	1A	3140	1/1	0.96	0.17	43,43,43,43	0
56	MG	2A	3433	1/1	0.96	0.06	64,64,64,64	0
56	MG	1A	4011	1/1	0.96	0.06	43,43,43,43	0
56	MG	2A	3755	1/1	0.96	0.09	50,50,50,50	0
56	MG	2A	3435	1/1	0.96	0.07	49,49,49,49	0
56	MG	1a	1768	1/1	0.96	0.09	53,53,53,53	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3680	1/1	0.96	0.14	44,44,44,44	0
56	MG	1A	4016	1/1	0.96	0.07	46,46,46,46	0
56	MG	1U	201	1/1	0.96	0.11	52,52,52,52	0
56	MG	1A	4018	1/1	0.96	0.14	67,67,67,67	0
56	MG	1A	3826	1/1	0.96	0.06	42,42,42,42	0
56	MG	2A	3181	1/1	0.96	0.13	40,40,40,40	0
56	MG	2A	3443	1/1	0.96	0.23	50,50,50,50	0
56	MG	1U	208	1/1	0.96	0.09	38,38,38,38	0
56	MG	1A	4020	1/1	0.96	0.06	53,53,53,53	0
56	MG	1A	3142	1/1	0.96	0.10	23,23,23,23	0
56	MG	1A	3311	1/1	0.96	0.17	48,48,48,48	0
56	MG	2A	3187	1/1	0.96	0.11	50,50,50,50	0
56	MG	2A	3188	1/1	0.96	0.06	36,36,36,36	0
56	MG	1A	3193	1/1	0.96	0.14	34,34,34,34	0
56	MG	1A	3451	1/1	0.96	0.11	47,47,47,47	0
56	MG	1X	104	1/1	0.96	0.07	52,52,52,52	0
56	MG	1A	3107	1/1	0.96	0.15	35,35,35,35	0
56	MG	2A	3775	1/1	0.96	0.07	38,38,38,38	0
56	MG	1A	4028	1/1	0.96	0.09	69,69,69,69	0
56	MG	1a	1786	1/1	0.96	0.09	64,64,64,64	0
56	MG	1A	3553	1/1	0.96	0.26	49,49,49,49	0
56	MG	2A	3779	1/1	0.96	0.09	56,56,56,56	0
56	MG	1A	4031	1/1	0.96	0.06	54,54,54,54	0
56	MG	1A	3554	1/1	0.96	0.19	47,47,47,47	0
56	MG	1A	3144	1/1	0.96	0.09	52,52,52,52	0
56	MG	1A	3556	1/1	0.96	0.22	42,42,42,42	0
56	MG	1A	3317	1/1	0.96	0.10	47,47,47,47	0
56	MG	10	102	1/1	0.96	0.07	44,44,44,44	0
56	MG	10	103	1/1	0.96	0.08	45,45,45,45	0
56	MG	1A	3108	1/1	0.96	0.30	43,43,43,43	0
56	MG	1A	4041	1/1	0.96	0.18	36,36,36,36	0
56	MG	2A	3467	1/1	0.96	0.18	60,60,60,60	0
56	MG	2a	3144	1/1	0.96	0.11	83,83,83,83	0
56	MG	2A	3207	1/1	0.96	0.09	44,44,44,44	0
56	MG	2A	3208	1/1	0.96	0.17	57,57,57,57	0
56	MG	1A	3693	1/1	0.96	0.13	40,40,40,40	0
56	MG	1a	1811	1/1	0.96	0.08	77,77,77,77	0
56	MG	2a	3150	1/1	0.96	0.06	78,78,78,78	0
56	MG	2A	3212	1/1	0.96	0.07	52,52,52,52	0
56	MG	1A	3559	1/1	0.96	0.17	34,34,34,34	0
56	MG	1A	3842	1/1	0.96	0.11	26,26,26,26	0
56	MG	1A	3843	1/1	0.96	0.08	31,31,31,31	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3695	1/1	0.96	0.08	57,57,57,57	0
56	MG	1A	3845	1/1	0.96	0.12	38,38,38,38	0
56	MG	1A	3456	1/1	0.96	0.14	48,48,48,48	0
56	MG	1A	3847	1/1	0.96	0.08	48,48,48,48	0
56	MG	1A	3021	1/1	0.96	0.11	45,45,45,45	0
56	MG	1A	3086	1/1	0.96	0.13	50,50,50,50	0
56	MG	1A	3321	1/1	0.96	0.22	51,51,51,51	0
56	MG	1A	3202	1/1	0.96	0.07	32,32,32,32	0
56	MG	1A	3113	1/1	0.96	0.09	35,35,35,35	0
56	MG	2a	3169	1/1	0.96	0.08	51,51,51,51	0
56	MG	1A	4058	1/1	0.96	0.08	47,47,47,47	0
56	MG	1A	3038	1/1	0.96	0.08	50,50,50,50	0
56	MG	2A	3230	1/1	0.96	0.12	48,48,48,48	0
56	MG	2a	3173	1/1	0.96	0.08	62,62,62,62	0
56	MG	1A	3022	1/1	0.96	0.07	21,21,21,21	0
56	MG	1l	202	1/1	0.96	0.10	69,69,69,69	0
56	MG	1A	3396	1/1	0.96	0.07	47,47,47,47	0
56	MG	1A	3397	1/1	0.96	0.07	47,47,47,47	0
56	MG	1A	3858	1/1	0.96	0.04	30,30,30,30	0
56	MG	2a	3180	1/1	0.96	0.07	73,73,73,73	0
56	MG	2A	3237	1/1	0.96	0.10	39,39,39,39	0
56	MG	2a	3183	1/1	0.96	0.07	76,76,76,76	0
56	MG	2a	3184	1/1	0.96	0.13	54,54,54,54	0
56	MG	1A	3469	1/1	0.96	0.12	53,53,53,53	0
56	MG	1A	3040	1/1	0.96	0.07	36,36,36,36	0
56	MG	2A	3240	1/1	0.96	0.11	40,40,40,40	0
56	MG	2A	3833	1/1	0.96	0.11	55,55,55,55	0
56	MG	1A	3259	1/1	0.96	0.06	40,40,40,40	0
56	MG	2A	3504	1/1	0.96	0.05	36,36,36,36	0
56	MG	2a	3191	1/1	0.96	0.07	63,63,63,63	0
56	MG	1A	3862	1/1	0.96	0.17	43,43,43,43	0
56	MG	1A	3007	1/1	0.96	0.07	38,38,38,38	0
56	MG	1A	3474	1/1	0.96	0.23	60,60,60,60	0
56	MG	2a	3195	1/1	0.96	0.06	41,41,41,41	0
56	MG	1A	3025	1/1	0.96	0.09	41,41,41,41	0
56	MG	1A	3262	1/1	0.96	0.07	49,49,49,49	0
56	MG	1A	3720	1/1	0.96	0.07	53,53,53,53	0
56	MG	1A	3263	1/1	0.96	0.14	52,52,52,52	0
56	MG	1w	111	1/1	0.96	0.08	41,41,41,41	0
56	MG	1A	3479	1/1	0.96	0.06	38,38,38,38	0
56	MG	2A	3517	1/1	0.96	0.07	42,42,42,42	0
56	MG	2A	3253	1/1	0.96	0.07	47,47,47,47	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3858	1/1	0.96	0.08	43,43,43,43	0
56	MG	1A	3405	1/1	0.96	0.17	42,42,42,42	0
56	MG	1A	3587	1/1	0.96	0.13	38,38,38,38	0
56	MG	1A	4079	1/1	0.96	0.14	46,46,46,46	0
56	MG	2A	3527	1/1	0.96	0.06	31,31,31,31	0
56	MG	1a	1621	1/1	0.96	0.06	42,42,42,42	0
56	MG	1A	3725	1/1	0.96	0.07	52,52,52,52	0
56	MG	1A	3482	1/1	0.96	0.08	50,50,50,50	0
56	MG	2A	3260	1/1	0.96	0.11	53,53,53,53	0
56	MG	1A	3212	1/1	0.96	0.22	32,32,32,32	0
56	MG	2A	3873	1/1	0.96	0.12	40,40,40,40	0
56	MG	1A	4086	1/1	0.96	0.23	43,43,43,43	0
56	MG	1A	3213	1/1	0.96	0.09	42,42,42,42	0
56	MG	1A	3881	1/1	0.96	0.08	37,37,37,37	0
56	MG	1A	4089	1/1	0.96	0.07	36,36,36,36	0
56	MG	2A	3537	1/1	0.96	0.06	35,35,35,35	0
56	MG	2A	3881	1/1	0.96	0.07	48,48,48,48	0
56	MG	1A	4090	1/1	0.96	0.14	37,37,37,37	0
56	MG	1A	3591	1/1	0.96	0.14	52,52,52,52	0
56	MG	2A	3885	1/1	0.96	0.18	54,54,54,54	0
56	MG	1A	3158	1/1	0.96	0.11	56,56,56,56	0
56	MG	2A	3887	1/1	0.96	0.07	48,48,48,48	0
56	MG	1A	3160	1/1	0.96	0.14	41,41,41,41	0
56	MG	1A	3336	1/1	0.96	0.12	41,41,41,41	0
56	MG	1A	4097	1/1	0.96	0.07	47,47,47,47	0
56	MG	1A	3411	1/1	0.96	0.10	43,43,43,43	0
56	MG	1A	3162	1/1	0.96	0.34	44,44,44,44	0
56	MG	2A	3003	1/1	0.96	0.14	43,43,43,43	0
56	MG	1A	3889	1/1	0.96	0.14	60,60,60,60	0
56	MG	2A	3898	1/1	0.96	0.07	28,28,28,28	0
56	MG	2A	3005	1/1	0.96	0.17	48,48,48,48	0
56	MG	1A	3269	1/1	0.96	0.13	52,52,52,52	0
56	MG	2A	3902	1/1	0.96	0.15	43,43,43,43	0
56	MG	2A	3007	1/1	0.96	0.06	43,43,43,43	0
56	MG	2A	3904	1/1	0.96	0.17	41,41,41,41	0
56	MG	1A	3599	1/1	0.96	0.08	21,21,21,21	0
56	MG	1A	3339	1/1	0.96	0.14	51,51,51,51	0
56	MG	2A	3011	1/1	0.96	0.06	48,48,48,48	0
56	MG	1A	3492	1/1	0.96	0.14	52,52,52,52	0
56	MG	1A	3066	1/1	0.96	0.08	35,35,35,35	0
56	MG	1A	3898	1/1	0.96	0.10	50,50,50,50	0
56	MG	2A	3285	1/1	0.96	0.07	49,49,49,49	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3605	1/1	0.96	0.09	32,32,32,32	0
56	MG	1A	4117	1/1	0.96	0.22	39,39,39,39	0
56	MG	1A	3121	1/1	0.96	0.16	43,43,43,43	0
56	MG	1A	3750	1/1	0.96	0.09	29,29,29,29	0
56	MG	2A	3026	1/1	0.96	0.08	36,36,36,36	0
56	MG	1A	3608	1/1	0.96	0.10	51,51,51,51	0
56	MG	1a	1650	1/1	0.96	0.11	53,53,53,53	0
56	MG	2A	3293	1/1	0.96	0.08	50,50,50,50	0
56	MG	2A	3575	1/1	0.96	0.07	39,39,39,39	0
56	MG	1A	3609	1/1	0.96	0.10	50,50,50,50	0
56	MG	2A	3031	1/1	0.96	0.09	45,45,45,45	0
56	MG	2A	3578	1/1	0.96	0.07	39,39,39,39	0
56	MG	1A	4128	1/1	0.96	0.23	43,43,43,43	0
56	MG	1A	4129	1/1	0.96	0.09	42,42,42,42	0
56	MG	2A	3582	1/1	0.96	0.07	51,51,51,51	0
56	MG	1A	3017	1/1	0.96	0.12	54,54,54,54	0
56	MG	1A	4132	1/1	0.96	0.17	39,39,39,39	0
56	MG	1A	3496	1/1	0.96	0.12	38,38,38,38	0
56	MG	2x	101	1/1	0.96	0.11	42,42,42,42	0
56	MG	1A	3497	1/1	0.96	0.17	33,33,33,33	0
56	MG	1A	4136	1/1	0.96	0.08	40,40,40,40	0
56	MG	1A	3615	1/1	0.96	0.08	25,25,25,25	0
56	MG	2D	303	1/1	0.96	0.06	35,35,35,35	0
56	MG	2A	3041	1/1	0.96	0.12	49,49,49,49	0
56	MG	1A	3911	1/1	0.96	0.10	65,65,65,65	0
56	MG	2A	3598	1/1	0.96	0.09	48,48,48,48	0
56	MG	1A	4141	1/1	0.96	0.24	50,50,50,50	0
56	MG	2A	3044	1/1	0.96	0.09	48,48,48,48	0
56	MG	1A	4142	1/1	0.96	0.11	42,42,42,42	0
56	MG	2A	3046	1/1	0.96	0.07	48,48,48,48	0
56	MG	2A	3047	1/1	0.96	0.10	46,46,46,46	0
56	MG	2A	3048	1/1	0.96	0.10	41,41,41,41	0
56	MG	1A	4005	1/1	0.97	0.05	50,50,50,50	0
56	MG	2A	3692	1/1	0.97	0.10	56,56,56,56	0
56	MG	1A	3628	1/1	0.97	0.09	28,28,28,28	0
56	MG	1A	3629	1/1	0.97	0.08	32,32,32,32	0
56	MG	1A	4008	1/1	0.97	0.06	56,56,56,56	0
56	MG	1A	4009	1/1	0.97	0.09	27,27,27,27	0
56	MG	2A	3697	1/1	0.97	0.07	34,34,34,34	0
56	MG	2A	3222	1/1	0.97	0.10	38,38,38,38	0
56	MG	1D	301	1/1	0.97	0.17	46,46,46,46	0
56	MG	1A	3749	1/1	0.97	0.07	41,41,41,41	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3002	1/1	0.97	0.28	57,57,57,57	0
56	MG	1a	1670	1/1	0.97	0.09	59,59,59,59	0
56	MG	1D	304	1/1	0.97	0.13	30,30,30,30	0
56	MG	1A	3170	1/1	0.97	0.11	39,39,39,39	0
56	MG	1A	3532	1/1	0.97	0.17	36,36,36,36	0
56	MG	1A	4015	1/1	0.97	0.05	37,37,37,37	0
56	MG	1A	3864	1/1	0.97	0.14	35,35,35,35	0
56	MG	2A	3009	1/1	0.97	0.07	31,31,31,31	0
56	MG	1A	3139	1/1	0.97	0.09	48,48,48,48	0
56	MG	2A	3451	1/1	0.97	0.30	56,56,56,56	0
56	MG	1A	3634	1/1	0.97	0.09	44,44,44,44	0
56	MG	1A	3173	1/1	0.97	0.13	42,42,42,42	0
56	MG	2A	3013	1/1	0.97	0.11	44,44,44,44	0
56	MG	1A	3868	1/1	0.97	0.08	47,47,47,47	0
56	MG	2A	3015	1/1	0.97	0.11	43,43,43,43	0
56	MG	1A	3174	1/1	0.97	0.20	38,38,38,38	0
56	MG	1A	3175	1/1	0.97	0.19	40,40,40,40	0
56	MG	2a	3023	1/1	0.97	0.06	47,47,47,47	0
56	MG	1A	3389	1/1	0.97	0.11	53,53,53,53	0
56	MG	2A	3019	1/1	0.97	0.06	38,38,38,38	0
56	MG	2A	3020	1/1	0.97	0.18	49,49,49,49	0
56	MG	2A	3022	1/1	0.97	0.14	47,47,47,47	0
56	MG	1A	3640	1/1	0.97	0.10	53,53,53,53	0
56	MG	1E	308	1/1	0.97	0.14	34,34,34,34	0
56	MG	2A	3025	1/1	0.97	0.14	42,42,42,42	0
56	MG	1E	309	1/1	0.97	0.06	50,50,50,50	0
56	MG	1A	4027	1/1	0.97	0.12	50,50,50,50	0
56	MG	1A	3220	1/1	0.97	0.09	41,41,41,41	0
56	MG	1A	3642	1/1	0.97	0.07	40,40,40,40	0
56	MG	2A	3735	1/1	0.97	0.07	55,55,55,55	0
56	MG	1A	3876	1/1	0.97	0.09	49,49,49,49	0
56	MG	1A	3761	1/1	0.97	0.09	51,51,51,51	0
56	MG	1A	3460	1/1	0.97	0.11	48,48,48,48	0
56	MG	1A	4034	1/1	0.97	0.06	51,51,51,51	0
56	MG	1A	3461	1/1	0.97	0.17	44,44,44,44	0
56	MG	1G	3001	1/1	0.97	0.10	41,41,41,41	0
56	MG	1A	3880	1/1	0.97	0.12	30,30,30,30	0
56	MG	1A	3764	1/1	0.97	0.10	31,31,31,31	0
56	MG	1A	3462	1/1	0.97	0.10	32,32,32,32	0
56	MG	1a	1698	1/1	0.97	0.05	52,52,52,52	0
56	MG	2A	3746	1/1	0.97	0.05	68,68,68,68	0
56	MG	1a	1699	1/1	0.97	0.18	40,40,40,40	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	4042	1/1	0.97	0.07	46,46,46,46	0
56	MG	1A	3074	1/1	0.97	0.06	27,27,27,27	0
56	MG	1A	3767	1/1	0.97	0.07	41,41,41,41	0
56	MG	1A	3054	1/1	0.97	0.11	39,39,39,39	0
56	MG	1A	3118	1/1	0.97	0.09	38,38,38,38	0
56	MG	1A	3887	1/1	0.97	0.10	31,31,31,31	0
56	MG	1A	3010	1/1	0.97	0.14	39,39,39,39	0
56	MG	1A	3550	1/1	0.97	0.16	38,38,38,38	0
56	MG	2A	3489	1/1	0.97	0.06	41,41,41,41	0
56	MG	1A	3654	1/1	0.97	0.11	36,36,36,36	0
56	MG	1A	3775	1/1	0.97	0.11	27,27,27,27	0
56	MG	1A	3012	1/1	0.97	0.05	30,30,30,30	0
56	MG	1O	205	1/1	0.97	0.06	44,44,44,44	0
56	MG	1A	3656	1/1	0.97	0.06	46,46,46,46	0
56	MG	2A	3497	1/1	0.97	0.07	63,63,63,63	0
56	MG	1A	3271	1/1	0.97	0.10	50,50,50,50	0
56	MG	2A	3499	1/1	0.97	0.05	46,46,46,46	0
56	MG	1A	3043	1/1	0.97	0.06	39,39,39,39	0
56	MG	2a	3066	1/1	0.97	0.13	54,54,54,54	0
56	MG	1A	4057	1/1	0.97	0.06	40,40,40,40	0
56	MG	2A	3502	1/1	0.97	0.05	43,43,43,43	0
56	MG	1A	3470	1/1	0.97	0.08	47,47,47,47	0
56	MG	1A	3781	1/1	0.97	0.09	32,32,32,32	0
56	MG	1A	3080	1/1	0.97	0.14	42,42,42,42	0
56	MG	1R	202	1/1	0.97	0.12	38,38,38,38	0
56	MG	1A	3275	1/1	0.97	0.07	44,44,44,44	0
56	MG	1A	3401	1/1	0.97	0.14	35,35,35,35	0
56	MG	1A	3276	1/1	0.97	0.10	49,49,49,49	0
56	MG	1a	1725	1/1	0.97	0.27	55,55,55,55	0
56	MG	1A	3475	1/1	0.97	0.10	42,42,42,42	0
56	MG	1A	3561	1/1	0.97	0.29	48,48,48,48	0
56	MG	1a	1728	1/1	0.97	0.24	48,48,48,48	0
56	MG	1A	3670	1/1	0.97	0.07	32,32,32,32	0
56	MG	1A	3789	1/1	0.97	0.06	29,29,29,29	0
56	MG	2a	3082	1/1	0.97	0.17	54,54,54,54	0
56	MG	1A	3562	1/1	0.97	0.05	24,24,24,24	0
56	MG	2A	3296	1/1	0.97	0.11	45,45,45,45	0
56	MG	1A	3277	1/1	0.97	0.12	38,38,38,38	0
56	MG	2A	3523	1/1	0.97	0.08	27,27,27,27	0
56	MG	2A	3524	1/1	0.97	0.07	48,48,48,48	0
56	MG	2A	3526	1/1	0.97	0.04	41,41,41,41	0
56	MG	2a	3089	1/1	0.97	0.19	65,65,65,65	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3789	1/1	0.97	0.10	49,49,49,49	0
56	MG	2A	3298	1/1	0.97	0.08	41,41,41,41	0
56	MG	2a	3092	1/1	0.97	0.14	51,51,51,51	0
56	MG	1U	204	1/1	0.97	0.14	38,38,38,38	0
56	MG	2A	3078	1/1	0.97	0.09	25,25,25,25	0
56	MG	2A	3793	1/1	0.97	0.14	56,56,56,56	0
56	MG	1U	205	1/1	0.97	0.11	35,35,35,35	0
56	MG	1A	3229	1/1	0.97	0.19	33,33,33,33	0
56	MG	2a	3098	1/1	0.97	0.09	46,46,46,46	0
56	MG	1A	3149	1/1	0.97	0.11	33,33,33,33	0
56	MG	1A	3018	1/1	0.97	0.14	33,33,33,33	0
56	MG	1a	1740	1/1	0.97	0.10	35,35,35,35	0
56	MG	1A	3341	1/1	0.97	0.15	55,55,55,55	0
56	MG	2A	3800	1/1	0.97	0.05	67,67,67,67	0
56	MG	1A	3125	1/1	0.97	0.16	41,41,41,41	0
56	MG	1A	3126	1/1	0.97	0.10	41,41,41,41	0
56	MG	1X	101	1/1	0.97	0.09	40,40,40,40	0
56	MG	1X	102	1/1	0.97	0.09	46,46,46,46	0
56	MG	2A	3806	1/1	0.97	0.09	66,66,66,66	0
56	MG	1X	103	1/1	0.97	0.12	40,40,40,40	0
56	MG	2A	3542	1/1	0.97	0.04	39,39,39,39	0
56	MG	1a	1748	1/1	0.97	0.06	43,43,43,43	0
56	MG	2A	3092	1/1	0.97	0.10	43,43,43,43	0
56	MG	2a	3113	1/1	0.97	0.13	46,46,46,46	0
56	MG	1A	3191	1/1	0.97	0.18	42,42,42,42	0
56	MG	1A	3288	1/1	0.97	0.08	43,43,43,43	0
56	MG	2A	3547	1/1	0.97	0.04	37,37,37,37	0
56	MG	2A	3548	1/1	0.97	0.10	38,38,38,38	0
56	MG	1A	3045	1/1	0.97	0.08	36,36,36,36	0
56	MG	1A	3929	1/1	0.97	0.07	42,42,42,42	0
56	MG	1A	3083	1/1	0.97	0.17	44,44,44,44	0
56	MG	1A	3934	1/1	0.97	0.06	44,44,44,44	0
56	MG	1A	3574	1/1	0.97	0.23	43,43,43,43	0
56	MG	1A	3575	1/1	0.97	0.15	33,33,33,33	0
56	MG	2A	3824	1/1	0.97	0.08	78,78,78,78	0
56	MG	2A	3825	1/1	0.97	0.09	58,58,58,58	0
56	MG	2A	3826	1/1	0.97	0.15	54,54,54,54	0
56	MG	2A	3102	1/1	0.97	0.11	56,56,56,56	0
56	MG	1A	3033	1/1	0.97	0.18	36,36,36,36	0
56	MG	1A	3578	1/1	0.97	0.16	33,33,33,33	0
56	MG	1A	3940	1/1	0.97	0.05	48,48,48,48	0
56	MG	2A	3831	1/1	0.97	0.05	45,45,45,45	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3942	1/1	0.97	0.05	56,56,56,56	0
56	MG	2A	3107	1/1	0.97	0.06	46,46,46,46	0
56	MG	2A	3562	1/1	0.97	0.05	37,37,37,37	0
56	MG	1A	3807	1/1	0.97	0.07	38,38,38,38	0
56	MG	2A	3564	1/1	0.97	0.06	31,31,31,31	0
56	MG	2A	3838	1/1	0.97	0.06	47,47,47,47	0
56	MG	2A	3109	1/1	0.97	0.05	37,37,37,37	0
56	MG	2A	3840	1/1	0.97	0.12	43,43,43,43	0
56	MG	2A	3841	1/1	0.97	0.05	30,30,30,30	0
56	MG	1A	4094	1/1	0.97	0.07	37,37,37,37	0
56	MG	1A	3688	1/1	0.97	0.06	15,15,15,15	0
56	MG	1A	3349	1/1	0.97	0.12	44,44,44,44	0
56	MG	2a	3147	1/1	0.97	0.10	49,49,49,49	0
56	MG	2A	3845	1/1	0.97	0.08	42,42,42,42	0
56	MG	2A	3846	1/1	0.97	0.05	47,47,47,47	0
56	MG	1A	4099	1/1	0.97	0.09	41,41,41,41	0
56	MG	1A	3239	1/1	0.97	0.10	30,30,30,30	0
56	MG	2A	3852	1/1	0.97	0.05	49,49,49,49	0
56	MG	1A	3156	1/1	0.97	0.17	40,40,40,40	0
56	MG	2a	3154	1/1	0.97	0.11	68,68,68,68	0
56	MG	1A	3157	1/1	0.97	0.12	53,53,53,53	0
56	MG	1A	3243	1/1	0.97	0.08	53,53,53,53	0
56	MG	2a	3157	1/1	0.97	0.06	64,64,64,64	0
56	MG	1A	3024	1/1	0.97	0.09	43,43,43,43	0
56	MG	1A	3952	1/1	0.97	0.08	46,46,46,46	0
56	MG	2A	3859	1/1	0.97	0.06	53,53,53,53	0
56	MG	16	103	1/1	0.97	0.08	54,54,54,54	0
56	MG	2A	3862	1/1	0.97	0.08	71,71,71,71	0
56	MG	1A	4106	1/1	0.97	0.07	29,29,29,29	0
56	MG	1A	4107	1/1	0.97	0.10	42,42,42,42	0
56	MG	2A	3581	1/1	0.97	0.07	25,25,25,25	0
56	MG	1A	3355	1/1	0.97	0.19	47,47,47,47	0
56	MG	1A	3356	1/1	0.97	0.10	39,39,39,39	0
56	MG	1a	1780	1/1	0.97	0.07	74,74,74,74	0
56	MG	2A	3347	1/1	0.97	0.13	51,51,51,51	0
56	MG	2A	3589	1/1	0.97	0.05	45,45,45,45	0
56	MG	1A	4110	1/1	0.97	0.07	56,56,56,56	0
56	MG	2a	3175	1/1	0.97	0.06	46,46,46,46	0
56	MG	2A	3129	1/1	0.97	0.12	50,50,50,50	0
56	MG	1A	4111	1/1	0.97	0.09	34,34,34,34	0
56	MG	2A	3595	1/1	0.97	0.08	49,49,49,49	0
56	MG	2A	3877	1/1	0.97	0.15	28,28,28,28	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	4112	1/1	0.97	0.12	42,42,42,42	0
56	MG	2a	3181	1/1	0.97	0.06	69,69,69,69	0
56	MG	2A	3879	1/1	0.97	0.07	37,37,37,37	0
56	MG	2A	3132	1/1	0.97	0.14	56,56,56,56	0
56	MG	1A	3159	1/1	0.97	0.10	39,39,39,39	0
56	MG	1A	3358	1/1	0.97	0.14	33,33,33,33	0
56	MG	2A	3135	1/1	0.97	0.07	43,43,43,43	0
56	MG	2A	3602	1/1	0.97	0.07	42,42,42,42	0
56	MG	1A	3359	1/1	0.97	0.10	38,38,38,38	0
56	MG	1A	3820	1/1	0.97	0.10	41,41,41,41	0
56	MG	1A	4122	1/1	0.97	0.05	41,41,41,41	0
56	MG	2A	3144	1/1	0.97	0.16	45,45,45,45	0
56	MG	2A	3145	1/1	0.97	0.09	36,36,36,36	0
56	MG	1a	1792	1/1	0.97	0.06	59,59,59,59	0
56	MG	1A	3360	1/1	0.97	0.23	31,31,31,31	0
56	MG	1A	3960	1/1	0.97	0.08	23,23,23,23	0
56	MG	1A	3199	1/1	0.97	0.12	45,45,45,45	0
56	MG	2A	3896	1/1	0.97	0.20	39,39,39,39	0
56	MG	2A	3897	1/1	0.97	0.13	57,57,57,57	0
56	MG	1a	1609	1/1	0.97	0.16	54,54,54,54	0
56	MG	1A	4126	1/1	0.97	0.14	45,45,45,45	0
56	MG	1a	1800	1/1	0.97	0.10	70,70,70,70	0
56	MG	1A	4127	1/1	0.97	0.10	34,34,34,34	0
56	MG	1A	3593	1/1	0.97	0.10	56,56,56,56	0
56	MG	1a	1614	1/1	0.97	0.12	45,45,45,45	0
56	MG	2A	3905	1/1	0.97	0.14	38,38,38,38	0
56	MG	1A	3201	1/1	0.97	0.08	45,45,45,45	0
56	MG	1A	4130	1/1	0.97	0.06	38,38,38,38	0
56	MG	2A	3621	1/1	0.97	0.09	51,51,51,51	0
56	MG	1A	3964	1/1	0.97	0.09	45,45,45,45	0
56	MG	1a	1814	1/1	0.97	0.10	55,55,55,55	0
56	MG	1A	3248	1/1	0.97	0.16	47,47,47,47	0
56	MG	1A	4133	1/1	0.97	0.16	45,45,45,45	0
56	MG	1a	1819	1/1	0.97	0.06	48,48,48,48	0
56	MG	2A	3165	1/1	0.97	0.20	49,49,49,49	0
56	MG	2A	3166	1/1	0.97	0.12	47,47,47,47	0
56	MG	2a	3217	1/1	0.97	0.07	61,61,61,61	0
56	MG	1a	1820	1/1	0.97	0.06	57,57,57,57	0
56	MG	1a	1821	1/1	0.97	0.05	62,62,62,62	0
56	MG	2A	3633	1/1	0.97	0.12	55,55,55,55	0
56	MG	2A	3634	1/1	0.97	0.07	34,34,34,34	0
56	MG	1A	3036	1/1	0.97	0.13	31,31,31,31	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3385	1/1	0.97	0.14	52,52,52,52	0
56	MG	1A	3365	1/1	0.97	0.10	53,53,53,53	0
56	MG	1A	3161	1/1	0.97	0.17	38,38,38,38	0
56	MG	2A	3639	1/1	0.97	0.11	34,34,34,34	0
56	MG	1A	3434	1/1	0.97	0.08	48,48,48,48	0
56	MG	1A	3309	1/1	0.97	0.15	33,33,33,33	0
56	MG	1A	4140	1/1	0.97	0.06	31,31,31,31	0
56	MG	1A	3972	1/1	0.97	0.06	60,60,60,60	0
56	MG	1A	3713	1/1	0.97	0.15	62,62,62,62	0
56	MG	1A	3974	1/1	0.97	0.06	45,45,45,45	0
56	MG	1A	3368	1/1	0.97	0.19	47,47,47,47	0
56	MG	1f	3001	1/1	0.97	0.12	34,34,34,34	0
56	MG	1A	3716	1/1	0.97	0.08	28,28,28,28	0
56	MG	1A	3603	1/1	0.97	0.15	39,39,39,39	0
56	MG	1A	3051	1/1	0.97	0.06	50,50,50,50	0
56	MG	1A	3111	1/1	0.97	0.07	40,40,40,40	0
56	MG	2E	301	1/1	0.97	0.13	50,50,50,50	0
56	MG	2A	3400	1/1	0.97	0.06	56,56,56,56	0
56	MG	1n	103	1/1	0.97	0.17	48,48,48,48	0
56	MG	1A	3606	1/1	0.97	0.11	36,36,36,36	0
56	MG	2a	3244	1/1	0.97	0.07	43,43,43,43	0
56	MG	1A	3371	1/1	0.97	0.08	45,45,45,45	0
56	MG	2A	3657	1/1	0.97	0.15	39,39,39,39	0
56	MG	2f	3001	1/1	0.97	0.09	41,41,41,41	0
56	MG	1A	3515	1/1	0.97	0.09	29,29,29,29	0
56	MG	2A	3405	1/1	0.97	0.14	33,33,33,33	0
56	MG	2A	3660	1/1	0.97	0.07	45,45,45,45	0
56	MG	1A	3372	1/1	0.97	0.14	58,58,58,58	0
56	MG	2l	201	1/1	0.97	0.05	66,66,66,66	0
56	MG	1w	102	1/1	0.97	0.15	61,61,61,61	0
56	MG	2F	304	1/1	0.97	0.17	53,53,53,53	0
56	MG	1A	3013	1/1	0.97	0.18	35,35,35,35	0
56	MG	1A	3611	1/1	0.97	0.07	25,25,25,25	0
56	MG	1A	3313	1/1	0.97	0.28	49,49,49,49	0
56	MG	1A	3071	1/1	0.97	0.11	38,38,38,38	0
56	MG	1B	3015	1/1	0.97	0.09	58,58,58,58	0
56	MG	1A	3991	1/1	0.97	0.12	48,48,48,48	0
56	MG	2Q	3003	1/1	0.97	0.06	51,51,51,51	0
56	MG	1A	3092	1/1	0.97	0.07	50,50,50,50	0
56	MG	1A	3211	1/1	0.97	0.08	49,49,49,49	0
56	MG	1A	3849	1/1	0.97	0.10	44,44,44,44	0
56	MG	2A	3417	1/1	0.97	0.10	41,41,41,41	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2U	201	1/1	0.97	0.10	40,40,40,40	0
56	MG	1A	3523	1/1	0.97	0.08	44,44,44,44	0
56	MG	2A	3201	1/1	0.97	0.06	51,51,51,51	0
56	MG	1A	3620	1/1	0.97	0.12	25,25,25,25	0
56	MG	2A	3677	1/1	0.97	0.27	35,35,35,35	0
56	MG	1A	3524	1/1	0.97	0.06	47,47,47,47	0
56	MG	1A	3379	1/1	0.97	0.09	37,37,37,37	0
56	MG	2A	3423	1/1	0.97	0.07	58,58,58,58	0
56	MG	1a	1654	1/1	0.97	0.17	49,49,49,49	0
56	MG	1A	3020	1/1	0.97	0.05	25,25,25,25	0
56	MG	1B	3027	1/1	0.97	0.04	35,35,35,35	0
56	MG	1a	1658	1/1	0.97	0.13	57,57,57,57	0
56	MG	1A	3449	1/1	0.97	0.07	41,41,41,41	0
56	MG	2A	3211	1/1	0.97	0.07	43,43,43,43	0
56	MG	2y	3006	1/1	0.97	0.05	86,86,86,86	0
56	MG	1A	3381	1/1	0.97	0.07	43,43,43,43	0
56	MG	1A	3258	1/1	0.97	0.08	33,33,33,33	0
57	K	2A	3496	1/1	0.97	0.10	73,73,73,73	0
58	ZN	2Y	501	1/1	0.97	0.05	81,81,81,81	0
56	MG	1A	3138	1/1	0.97	0.25	36,36,36,36	0
56	MG	2A	3215	1/1	0.97	0.10	37,37,37,37	0
56	MG	2A	3184	1/1	0.98	0.13	48,48,48,48	0
56	MG	1A	3314	1/1	0.98	0.06	33,33,33,33	0
56	MG	1A	4098	1/1	0.98	0.08	45,45,45,45	0
56	MG	1A	3237	1/1	0.98	0.20	38,38,38,38	0
56	MG	1A	3109	1/1	0.98	0.14	35,35,35,35	0
56	MG	1A	3176	1/1	0.98	0.05	37,37,37,37	0
56	MG	2A	3882	1/1	0.98	0.07	44,44,44,44	0
56	MG	2A	3037	1/1	0.98	0.06	35,35,35,35	0
56	MG	1A	3902	1/1	0.98	0.08	33,33,33,33	0
56	MG	1A	3903	1/1	0.98	0.06	40,40,40,40	0
56	MG	1A	3178	1/1	0.98	0.10	21,21,21,21	0
56	MG	2A	3512	1/1	0.98	0.05	53,53,53,53	0
56	MG	2A	3513	1/1	0.98	0.08	34,34,34,34	0
56	MG	1A	3274	1/1	0.98	0.11	36,36,36,36	0
56	MG	1A	3241	1/1	0.98	0.07	44,44,44,44	0
56	MG	1a	1772	1/1	0.98	0.05	39,39,39,39	0
56	MG	1N	203	1/1	0.98	0.06	48,48,48,48	0
56	MG	2A	3519	1/1	0.98	0.06	33,33,33,33	0
56	MG	1A	3617	1/1	0.98	0.06	33,33,33,33	0
56	MG	2A	3357	1/1	0.98	0.05	39,39,39,39	0
56	MG	1A	3828	1/1	0.98	0.07	34,34,34,34	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3701	1/1	0.98	0.09	64,64,64,64	0
56	MG	1A	3072	1/1	0.98	0.07	19,19,19,19	0
56	MG	1A	3910	1/1	0.98	0.04	76,76,76,76	0
56	MG	2A	3901	1/1	0.98	0.12	59,59,59,59	0
56	MG	2A	3525	1/1	0.98	0.08	34,34,34,34	0
56	MG	1A	3619	1/1	0.98	0.13	31,31,31,31	0
56	MG	1A	3046	1/1	0.98	0.12	32,32,32,32	0
56	MG	2A	3204	1/1	0.98	0.14	48,48,48,48	0
56	MG	1A	3008	1/1	0.98	0.10	26,26,26,26	0
56	MG	1A	4114	1/1	0.98	0.04	34,34,34,34	0
56	MG	1A	4115	1/1	0.98	0.16	51,51,51,51	0
56	MG	1A	3915	1/1	0.98	0.05	39,39,39,39	0
56	MG	2A	3368	1/1	0.98	0.06	47,47,47,47	0
56	MG	1P	202	1/1	0.98	0.06	31,31,31,31	0
56	MG	2A	3714	1/1	0.98	0.08	39,39,39,39	0
56	MG	1a	1785	1/1	0.98	0.04	55,55,55,55	0
56	MG	1P	203	1/1	0.98	0.14	30,30,30,30	0
56	MG	1a	1787	1/1	0.98	0.05	72,72,72,72	0
56	MG	1A	3279	1/1	0.98	0.05	38,38,38,38	0
56	MG	1Q	201	1/1	0.98	0.08	36,36,36,36	0
56	MG	1A	4118	1/1	0.98	0.10	36,36,36,36	0
56	MG	1a	1791	1/1	0.98	0.05	54,54,54,54	0
56	MG	2A	3723	1/1	0.98	0.06	50,50,50,50	0
56	MG	1A	4119	1/1	0.98	0.07	34,34,34,34	0
56	MG	1A	3014	1/1	0.98	0.05	31,31,31,31	0
56	MG	1A	4013	1/1	0.98	0.05	33,33,33,33	0
56	MG	2a	3133	1/1	0.98	0.07	54,54,54,54	0
56	MG	1A	3511	1/1	0.98	0.06	45,45,45,45	0
56	MG	2A	3221	1/1	0.98	0.09	48,48,48,48	0
56	MG	2A	3729	1/1	0.98	0.06	41,41,41,41	0
56	MG	1A	3015	1/1	0.98	0.07	40,40,40,40	0
56	MG	2A	3069	1/1	0.98	0.07	40,40,40,40	0
56	MG	1A	3837	1/1	0.98	0.10	21,21,21,21	0
56	MG	2a	3140	1/1	0.98	0.04	57,57,57,57	0
56	MG	2A	3551	1/1	0.98	0.07	39,39,39,39	0
56	MG	1a	1799	1/1	0.98	0.05	49,49,49,49	0
56	MG	2a	3143	1/1	0.98	0.05	73,73,73,73	0
56	MG	1A	3282	1/1	0.98	0.06	30,30,30,30	0
56	MG	1A	3214	1/1	0.98	0.10	42,42,42,42	0
56	MG	1A	3077	1/1	0.98	0.14	35,35,35,35	0
56	MG	2A	3075	1/1	0.98	0.08	37,37,37,37	0
56	MG	1a	1805	1/1	0.98	0.05	47,47,47,47	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3516	1/1	0.98	0.15	25,25,25,25	0
56	MG	1a	1807	1/1	0.98	0.04	67,67,67,67	0
56	MG	1a	1808	1/1	0.98	0.05	53,53,53,53	0
56	MG	1a	1809	1/1	0.98	0.05	56,56,56,56	0
56	MG	1A	3927	1/1	0.98	0.04	47,47,47,47	0
56	MG	1A	3050	1/1	0.98	0.14	32,32,32,32	0
56	MG	1A	3930	1/1	0.98	0.04	30,30,30,30	0
56	MG	2A	3084	1/1	0.98	0.05	45,45,45,45	0
56	MG	2A	3566	1/1	0.98	0.09	33,33,33,33	0
56	MG	2A	3567	1/1	0.98	0.04	50,50,50,50	0
56	MG	1A	3286	1/1	0.98	0.29	49,49,49,49	0
56	MG	2F	303	1/1	0.98	0.04	48,48,48,48	0
56	MG	2a	3162	1/1	0.98	0.03	62,62,62,62	0
56	MG	1A	3933	1/1	0.98	0.05	47,47,47,47	0
56	MG	1a	1816	1/1	0.98	0.04	48,48,48,48	0
56	MG	1U	206	1/1	0.98	0.15	32,32,32,32	0
56	MG	1A	3287	1/1	0.98	0.15	30,30,30,30	0
56	MG	1A	4030	1/1	0.98	0.05	44,44,44,44	0
56	MG	1A	3771	1/1	0.98	0.08	49,49,49,49	0
56	MG	1a	1822	1/1	0.98	0.10	54,54,54,54	0
56	MG	2A	3093	1/1	0.98	0.10	54,54,54,54	0
56	MG	1A	3186	1/1	0.98	0.08	39,39,39,39	0
56	MG	2A	3250	1/1	0.98	0.07	41,41,41,41	0
56	MG	2A	3251	1/1	0.98	0.08	42,42,42,42	0
56	MG	1A	4139	1/1	0.98	0.05	35,35,35,35	0
56	MG	1A	3773	1/1	0.98	0.05	41,41,41,41	0
56	MG	1W	205	1/1	0.98	0.05	39,39,39,39	0
56	MG	1A	3289	1/1	0.98	0.07	52,52,52,52	0
56	MG	2A	3584	1/1	0.98	0.12	37,37,37,37	0
56	MG	2A	3585	1/1	0.98	0.05	43,43,43,43	0
56	MG	1A	4035	1/1	0.98	0.04	46,46,46,46	0
56	MG	2A	3587	1/1	0.98	0.05	37,37,37,37	0
56	MG	1A	3290	1/1	0.98	0.08	46,46,46,46	0
56	MG	2X	101	1/1	0.98	0.03	37,37,37,37	0
56	MG	1A	3941	1/1	0.98	0.04	46,46,46,46	0
56	MG	1A	4038	1/1	0.98	0.04	45,45,45,45	0
56	MG	1A	3701	1/1	0.98	0.08	48,48,48,48	0
56	MG	1A	3098	1/1	0.98	0.10	25,25,25,25	0
56	MG	2A	3594	1/1	0.98	0.04	38,38,38,38	0
56	MG	1A	3011	1/1	0.98	0.12	46,46,46,46	0
56	MG	1A	3063	1/1	0.98	0.08	38,38,38,38	0
56	MG	1A	3035	1/1	0.98	0.09	20,20,20,20	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3707	1/1	0.98	0.10	29,29,29,29	0
56	MG	1A	3295	1/1	0.98	0.06	48,48,48,48	0
56	MG	2A	3600	1/1	0.98	0.07	40,40,40,40	0
56	MG	1A	3296	1/1	0.98	0.08	58,58,58,58	0
56	MG	1A	3644	1/1	0.98	0.04	33,33,33,33	0
56	MG	2A	3785	1/1	0.98	0.17	45,45,45,45	0
56	MG	1A	3141	1/1	0.98	0.07	35,35,35,35	0
56	MG	2A	3787	1/1	0.98	0.05	64,64,64,64	0
56	MG	1A	4050	1/1	0.98	0.13	32,32,32,32	0
56	MG	1A	3223	1/1	0.98	0.08	32,32,32,32	0
56	MG	1A	3481	1/1	0.98	0.10	39,39,39,39	0
56	MG	1A	3714	1/1	0.98	0.07	46,46,46,46	0
56	MG	1B	3018	1/1	0.98	0.05	37,37,37,37	0
56	MG	1A	3009	1/1	0.98	0.04	24,24,24,24	0
56	MG	1A	3122	1/1	0.98	0.07	44,44,44,44	0
56	MG	1w	108	1/1	0.98	0.05	63,63,63,63	0
56	MG	2A	3121	1/1	0.98	0.13	42,42,42,42	0
56	MG	1A	3717	1/1	0.98	0.08	22,22,22,22	0
56	MG	1A	3037	1/1	0.98	0.13	40,40,40,40	0
56	MG	2a	3212	1/1	0.98	0.10	51,51,51,51	0
56	MG	1A	3535	1/1	0.98	0.20	45,45,45,45	0
56	MG	2A	3125	1/1	0.98	0.14	44,44,44,44	0
56	MG	1A	3653	1/1	0.98	0.08	27,27,27,27	0
56	MG	2A	3618	1/1	0.98	0.06	39,39,39,39	0
56	MG	1A	3536	1/1	0.98	0.16	37,37,37,37	0
56	MG	2A	3804	1/1	0.98	0.12	31,31,31,31	0
56	MG	1B	3026	1/1	0.98	0.04	42,42,42,42	0
56	MG	1A	3303	1/1	0.98	0.09	33,33,33,33	0
56	MG	2A	3807	1/1	0.98	0.07	61,61,61,61	0
56	MG	1a	1716	1/1	0.98	0.06	53,53,53,53	0
56	MG	1A	3439	1/1	0.98	0.11	40,40,40,40	0
56	MG	2A	3624	1/1	0.98	0.04	32,32,32,32	0
56	MG	1A	3145	1/1	0.98	0.15	32,32,32,32	0
56	MG	1A	3394	1/1	0.98	0.07	35,35,35,35	0
56	MG	1A	3967	1/1	0.98	0.06	65,65,65,65	0
56	MG	1A	3168	1/1	0.98	0.10	42,42,42,42	0
56	MG	2A	3136	1/1	0.98	0.12	45,45,45,45	0
56	MG	2A	3137	1/1	0.98	0.05	42,42,42,42	0
56	MG	1A	3801	1/1	0.98	0.05	28,28,28,28	0
56	MG	2A	3139	1/1	0.98	0.15	32,32,32,32	0
56	MG	2A	3140	1/1	0.98	0.14	50,50,50,50	0
56	MG	1A	3068	1/1	0.98	0.10	38,38,38,38	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	2A	3142	1/1	0.98	0.17	41,41,41,41	0
56	MG	1a	1724	1/1	0.98	0.06	36,36,36,36	0
56	MG	1A	3662	1/1	0.98	0.07	30,30,30,30	0
56	MG	1A	3663	1/1	0.98	0.05	28,28,28,28	0
56	MG	1x	116	1/1	0.98	0.05	59,59,59,59	0
56	MG	1A	3731	1/1	0.98	0.05	17,17,17,17	0
56	MG	2a	3241	1/1	0.98	0.05	41,41,41,41	0
56	MG	1A	3069	1/1	0.98	0.12	20,20,20,20	0
56	MG	1D	303	1/1	0.98	0.15	37,37,37,37	0
56	MG	1A	3106	1/1	0.98	0.07	25,25,25,25	0
56	MG	1A	3172	1/1	0.98	0.06	43,43,43,43	0
56	MG	1a	1732	1/1	0.98	0.08	48,48,48,48	0
56	MG	1A	3055	1/1	0.98	0.11	43,43,43,43	0
56	MG	1a	1611	1/1	0.98	0.06	22,22,22,22	0
56	MG	1D	308	1/1	0.98	0.06	48,48,48,48	0
56	MG	2A	3650	1/1	0.98	0.12	41,41,41,41	0
56	MG	1A	4077	1/1	0.98	0.10	11,11,11,11	0
56	MG	2A	3157	1/1	0.98	0.09	58,58,58,58	0
56	MG	1A	3736	1/1	0.98	0.09	46,46,46,46	0
56	MG	1A	3668	1/1	0.98	0.10	28,28,28,28	0
56	MG	1A	4080	1/1	0.98	0.11	23,23,23,23	0
56	MG	1a	1741	1/1	0.98	0.06	34,34,34,34	0
56	MG	1A	4082	1/1	0.98	0.11	38,38,38,38	0
56	MG	2A	3163	1/1	0.98	0.10	56,56,56,56	0
56	MG	2A	3847	1/1	0.98	0.09	42,42,42,42	0
56	MG	1A	3738	1/1	0.98	0.04	43,43,43,43	0
56	MG	2A	3849	1/1	0.98	0.10	44,44,44,44	0
56	MG	1E	303	1/1	0.98	0.08	26,26,26,26	0
56	MG	1A	3740	1/1	0.98	0.09	28,28,28,28	0
56	MG	2A	3853	1/1	0.98	0.05	50,50,50,50	0
56	MG	1A	3547	1/1	0.98	0.06	53,53,53,53	0
56	MG	1A	3056	1/1	0.98	0.10	28,28,28,28	0
56	MG	1A	3984	1/1	0.98	0.09	34,34,34,34	0
56	MG	1a	1749	1/1	0.98	0.09	45,45,45,45	0
56	MG	1A	3891	1/1	0.98	0.05	41,41,41,41	0
56	MG	1A	3986	1/1	0.98	0.08	22,22,22,22	0
56	MG	2A	3668	1/1	0.98	0.07	45,45,45,45	0
56	MG	2A	3861	1/1	0.98	0.06	36,36,36,36	0
56	MG	2A	3021	1/1	0.98	0.07	28,28,28,28	0
56	MG	2A	3863	1/1	0.98	0.06	58,58,58,58	0
56	MG	1E	310	1/1	0.98	0.03	42,42,42,42	0
56	MG	2A	3491	1/1	0.98	0.18	55,55,55,55	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	3549	1/1	0.98	0.06	38,38,38,38	0
56	MG	1A	3988	1/1	0.98	0.04	68,68,68,68	0
56	MG	1A	3893	1/1	0.98	0.12	17,17,17,17	0
56	MG	1A	3204	1/1	0.98	0.12	26,26,26,26	0
56	MG	2A	3870	1/1	0.98	0.06	33,33,33,33	0
56	MG	2A	3027	1/1	0.98	0.17	48,48,48,48	0
56	MG	1F	304	1/1	0.98	0.19	40,40,40,40	0
58	ZN	14	501	1/1	0.98	0.05	99,99,99,99	0
56	MG	1A	3673	1/1	0.98	0.09	29,29,29,29	0
56	MG	1a	1634	1/1	0.98	0.05	27,27,27,27	0
58	ZN	25	102	1/1	0.98	0.15	68,68,68,68	0
56	MG	1A	3205	1/1	0.98	0.09	42,42,42,42	0
59	SF4	1d	501	8/8	0.98	0.05	59,71,76,86	0
59	SF4	2d	501	8/8	0.98	0.05	61,71,85,99	0
56	MG	1a	1653	1/1	0.99	0.04	54,54,54,54	0
56	MG	1A	3414	1/1	0.99	0.04	39,39,39,39	0
56	MG	1l	201	1/1	0.99	0.12	43,43,43,43	0
56	MG	1a	1655	1/1	0.99	0.03	43,43,43,43	0
56	MG	1A	3914	1/1	0.99	0.08	53,53,53,53	0
56	MG	1A	4023	1/1	0.99	0.04	47,47,47,47	0
56	MG	2A	3233	1/1	0.99	0.11	32,32,32,32	0
56	MG	1A	3612	1/1	0.99	0.06	41,41,41,41	0
56	MG	1A	3632	1/1	0.99	0.03	34,34,34,34	0
56	MG	1A	3375	1/1	0.99	0.09	43,43,43,43	0
56	MG	1A	3726	1/1	0.99	0.04	48,48,48,48	0
56	MG	2A	3732	1/1	0.99	0.07	42,42,42,42	0
56	MG	2A	3514	1/1	0.99	0.04	32,32,32,32	0
56	MG	1A	3702	1/1	0.99	0.07	34,34,34,34	0
56	MG	1A	3577	1/1	0.99	0.09	27,27,27,27	0
56	MG	1A	3635	1/1	0.99	0.05	32,32,32,32	0
56	MG	1A	3065	1/1	0.99	0.13	33,33,33,33	0
56	MG	1U	207	1/1	0.99	0.13	31,31,31,31	0
56	MG	1A	3084	1/1	0.99	0.04	34,34,34,34	0
56	MG	1A	3924	1/1	0.99	0.03	50,50,50,50	0
56	MG	2A	3593	1/1	0.99	0.05	30,30,30,30	0
56	MG	1A	3925	1/1	0.99	0.04	14,14,14,14	0
56	MG	2A	3895	1/1	0.99	0.09	46,46,46,46	0
56	MG	20	3002	1/1	0.99	0.04	63,63,63,63	0
56	MG	2A	3817	1/1	0.99	0.04	56,56,56,56	0
56	MG	1A	4075	1/1	0.99	0.03	42,42,42,42	0
56	MG	1A	3085	1/1	0.99	0.11	30,30,30,30	0
56	MG	2A	3820	1/1	0.99	0.06	49,49,49,49	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1W	202	1/1	0.99	0.14	50,50,50,50	0
56	MG	1W	203	1/1	0.99	0.06	30,30,30,30	0
56	MG	1A	3896	1/1	0.99	0.12	47,47,47,47	0
56	MG	2A	3319	1/1	0.99	0.04	49,49,49,49	0
56	MG	2A	3049	1/1	0.99	0.07	23,23,23,23	0
56	MG	2a	3160	1/1	0.99	0.04	49,49,49,49	0
56	MG	1A	4121	1/1	0.99	0.09	34,34,34,34	0
56	MG	1a	1619	1/1	0.99	0.06	62,62,62,62	0
56	MG	1A	3928	1/1	0.99	0.10	31,31,31,31	0
56	MG	1A	3661	1/1	0.99	0.07	32,32,32,32	0
56	MG	1A	4039	1/1	0.99	0.02	21,21,21,21	0
56	MG	1a	1796	1/1	0.99	0.03	59,59,59,59	0
56	MG	2a	3167	1/1	0.99	0.04	69,69,69,69	0
56	MG	1A	4081	1/1	0.99	0.09	44,44,44,44	0
56	MG	1A	3032	1/1	0.99	0.18	31,31,31,31	0
56	MG	2A	3538	1/1	0.99	0.04	35,35,35,35	0
56	MG	2A	3835	1/1	0.99	0.04	43,43,43,43	0
56	MG	1a	1739	1/1	0.99	0.03	36,36,36,36	0
56	MG	1X	106	1/1	0.99	0.06	29,29,29,29	0
56	MG	1a	1801	1/1	0.99	0.04	53,53,53,53	0
56	MG	1a	1802	1/1	0.99	0.06	52,52,52,52	0
56	MG	1A	3041	1/1	0.99	0.21	38,38,38,38	0
56	MG	1A	3932	1/1	0.99	0.06	45,45,45,45	0
56	MG	1A	3177	1/1	0.99	0.15	38,38,38,38	0
56	MG	1A	4004	1/1	0.99	0.04	29,29,29,29	0
56	MG	1A	3602	1/1	0.99	0.08	25,25,25,25	0
56	MG	1A	3935	1/1	0.99	0.05	50,50,50,50	0
56	MG	1A	3551	1/1	0.99	0.16	37,37,37,37	0
56	MG	1a	1810	1/1	0.99	0.03	51,51,51,51	0
56	MG	1B	3036	1/1	0.99	0.03	36,36,36,36	0
56	MG	1A	3739	1/1	0.99	0.04	39,39,39,39	0
56	MG	1A	3297	1/1	0.99	0.14	32,32,32,32	0
56	MG	2A	3851	1/1	0.99	0.04	46,46,46,46	0
56	MG	1A	3027	1/1	0.99	0.06	33,33,33,33	0
56	MG	1A	3508	1/1	0.99	0.12	36,36,36,36	0
56	MG	1A	3097	1/1	0.99	0.04	35,35,35,35	0
56	MG	1a	1817	1/1	0.99	0.04	79,79,79,79	0
56	MG	1I	102	1/1	0.99	0.04	36,36,36,36	0
56	MG	1P	201	1/1	0.99	0.04	26,26,26,26	0
56	MG	2A	3632	1/1	0.99	0.04	41,41,41,41	0
56	MG	1A	3200	1/1	0.99	0.16	23,23,23,23	0
56	MG	1D	306	1/1	0.99	0.11	32,32,32,32	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
56	MG	1A	4096	1/1	0.99	0.05	30,30,30,30	0
56	MG	1A	4014	1/1	0.99	0.03	34,34,34,34	0
56	MG	1Q	202	1/1	0.99	0.04	46,46,46,46	0
56	MG	1a	1825	1/1	0.99	0.14	37,37,37,37	0
56	MG	1A	3030	1/1	0.99	0.05	34,34,34,34	0
56	MG	1A	3650	1/1	0.99	0.07	35,35,35,35	0
58	ZN	19	103	1/1	0.99	0.04	44,44,44,44	0
58	ZN	1n	101	1/1	0.99	0.04	71,71,71,71	0
56	MG	1a	1763	1/1	0.99	0.09	55,55,55,55	0
56	MG	1A	4017	1/1	0.99	0.05	36,36,36,36	0
56	MG	1A	3747	1/1	0.99	0.09	53,53,53,53	0
58	ZN	26	501	1/1	0.99	0.03	60,60,60,60	0
58	ZN	29	101	1/1	0.99	0.04	73,73,73,73	0
56	MG	1R	201	1/1	0.99	0.19	30,30,30,30	0
56	MG	1A	3946	1/1	0.99	0.04	49,49,49,49	0
56	MG	1A	3003	1/1	0.99	0.05	27,27,27,27	0
56	MG	1A	3873	1/1	1.00	0.07	35,35,35,35	0
58	ZN	1Y	501	1/1	1.00	0.03	60,60,60,60	0
56	MG	2A	3715	1/1	1.00	0.04	46,46,46,46	0
58	ZN	15	101	1/1	1.00	0.09	37,37,37,37	0
58	ZN	16	102	1/1	1.00	0.04	44,44,44,44	0

## 6.5 Other polymers

There are no such residues in this entry.